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The space of state vectors: A hyperfinite approach

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We present a version of the formalism of Dirac based on nonstandard analysis, allowing us to deal with state vectors and operators using the resources of finite-dimensional linear algebra. The space of state vectors is a nonstandard Hilbert space with hyperfinite dimension, which includes all square-integrable functions, together with vectors representing states of definite position or momentum. Every vector is normalizable, even when its norm is infinite. Observables are represented by Hermitian operators, which are always (hyper)bounded and defined on the whole space. The connection with the standard theory is established by postulating the existence of ''hyper-observables'' and nonstandard states. Each observable in the usual sense appears as a kind of standard-scale approximation of some hyper-observable. We show that the probabilistic predictions are consistent with those of the standard theory. Consistency extends to time evolution, in the sense that if an initial nonstandard state is ''near-standard,'' then the state after a finite time shall be infinitely near the standard state obtained through the Schrödinger equation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1631394]

I. INTRODUCTION

A. Preliminaries

The essential features of the general formalism of quantum mechanics can be summarized as follows: To a quantum system a complex Hilbert space can be associated such that every physical state of the system is represented by a normalized vector and every observable is represented by a Hermitian operator on the same space. The outcome of a measurement of an observable represented by an operator A upon a state represented by a vector u is necessarily an eigenvalue of A. The probability to obtain a particular eigenvalue a is $|(u|P_a u)|^2$, where P_a is the projection operator onto the subspace spanned by the eigenvectors belonging to the eigenvalue a. Furthermore, the state of the system after the measurement is represented by a vector belonging to the same subspace. (A stronger postulate states that such vector is $P_a u/\|P_a u\|$.)

In order to completely specify the Hilbert space associated with a particular system, it suffices to postulate its Hilbert dimension, since any two Hilbert spaces with the same Hilbert dimension are necessarily isomorphic. To establish the physical meaning of concrete vectors one can proceed along the following lines: A complete set of compatible observables is chosen (see Ref. 6) and the set of all its possible outcomes is identified. A Hilbert basis is then introduced by naming its vectors after those possible outcomes. Thereafter the coordinates of any vector in that basis provide a link to physical reality, through the relation of the corresponding state to the base states. Furthermore, the basis induces a unitary isomorphism from the abstract space to a concrete space, which constitutes a representation of the abstract space: Every vector u admits a unique expression as $u=\Sigma_{i\in I} c_i u_i$, where $(u_i)_{i\in I}$ is the set of base vectors indexed on some set I and $c_i=(u_i|u)$ for every i. The indexed family $(c_i)_{i\in I}$ of coordinates is such that all values c_i are zero except at most at a countable subset of I and that $\Sigma_i|c_i|^2<+\infty$, where the sum extends over all values of $i\in I$ for which $c_i\neq 0$. The set of all families satisfying these conditions constitutes a Hilbert space (when

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the algebraic operations and inner product are defined in the obvious way) for which the mapping $u \mapsto (c_i)_{i \in I}$ is a unitary isomorphism. In this space, any observable belonging to the set that induced the representation is represented by a "multiplication operator:" If the observable has the value a_i in the state u_i, then the corresponding operator A maps $(c_i)_{i \in I}$ to $(a_i c_i)_{i \in I}$.

This general framework requires modification even in such a simple case as the one corresponding to a one-dimensional, nonrelativistic, spinless particle. In this case, the space $L^2(\mathbb{R})$ would appear as a concrete Hilbert space corresponding to the observable "position," due to the probabilistic interpretation of wave functions and the role of the operator of multiplication by the independent variable, together with the experimental fact that the position observable constitutes by itself a complete set. Thus, one is tempted to assume the existence of a Hilbert basis $(\chi_x)_{x \in \mathbb{R}}$ of vectors that would correspond to the states of definite position, in such a way that the wave function φ associated with a vector u satisfies the identity $\varphi(x) = (\chi_x | u)$, at least when φ is an element of $L^2(\mathbb{R})$ representable by a continuous function [for otherwise $\varphi(x)$ is not well-defined]. However, this is clearly impossible, since the space $L^2(\mathbb{R})$ is known to be separable. Moreover, such a family $(\chi_x)_{x \in \mathbb{R}}$ cannot be a Hilbert basis for any Hilbert space extending $L^2(\mathbb{R})$: If $u = \Sigma_{x \in \mathbb{R}} c_x \chi_x$, we would have $(\chi_x | u) = \varphi(x) = c_x$; since $c_x = 0$ except at countable values of x, this would imply that $\varphi = 0$ as an element of $L^2(\mathbb{R})$.

To overcome these difficulties while preserving as much as possible of the original formalism, Dirac assumed the existence of $(\chi_x)_{x \in \mathbb{R}}$ such that vectors could be expressed as integrals rather than sums; this was supported by the fact that wave functions yield probabilities through integral expressions, as well as by the continuous nature of the parameter x. If u is a vector associated with the wave function φ, then $u = \int_{-\infty}^{+\infty} \varphi(x) \chi_x \, dx$, and for every x_0,

$$(\chi_{x_0} | u) = \int_{-\infty}^{+\infty} \varphi(x) (\chi_{x_0} | \chi_x) \, dx = \varphi(x_0) \ . \tag{1}$$

Since the physical meaning of $(\chi_x)_{x \in \mathbb{R}}$ demands that $(\chi_{x_0} | \chi_x) = 0$ whenever $x_0 \neq x$, Dirac attributed an infinite value to $(\chi_{x_0} | \chi_{x_0})$, for otherwise one would obtain $\varphi(x_0) = 0$. Thus the "function" δ such that $\delta(x_0 - x) = (\chi_{x_0} | \chi_x)$ appears as a continuous-case counterpart of the Kronecker symbol.

It is presently understood that formulas with the δ of Dirac can be interpreted rigorously if $L^2(\mathbb{R})$ is embedded in some space of distributions in the sense of Schwartz. However, this and other similar approaches depart considerably from the original formalism, the mathematics of which is essentially basic, finite-dimensional, linear algebra. In fact, the extended space is not endowed with a *bona fide* inner product; in particular, a vector χ_x cannot be multiplied by itself—vectors with "infinite norm" certainly do not have place in a Hilbert space. Nevertheless, the "vector" χ_{x_0}, understood as the distribution $\delta(x - x_0)$ (where x is the variable and x_0 is fixed), behaves like an eigenvector of the operator of multiplication by x belonging to the eigenvalue x_0. On the other hand, even classical functions of interest may not be in $L^2(\mathbb{R})$, as it is the case with the exponentials representing eigenvectors of the momentum operator. Moreover, operators corresponding to observables are often defined on a strict subspace of the Hilbert space. The formulation of von Neumann[14] achieves mathematical rigor at the cost of renouncing the primitive simplicity: It is no longer allowed to say, in general, that the outcome of a measurement must be an eigenvalue of the operator associated to the observable. However, to determine whether an observable A has a value in an interval is to determine whether the observable $f(A)$ has value 1, where f is the characteristic function of the interval. Thus, even within this framework much of the original formalism is present.

B. Nonstandard approach

Whether or not one attributes physical meaning to a state of definite position, for example, the considerations above suggest that it would be desirable to be able to work within the original intuitive framework of Dirac, as it is usually done at an informal level. We propose a nonstandard version of the formalism of Dirac that makes it applicable rigorously, without change of form, even in cases where operators with continuous spectra arise in the standard theory. The space $\mathcal{H}$ associated with a system is now a *complex Hilbert space. (See the Appendix.) The inner product of two vectors is a *complex number, finite or infinite but always well-defined. Every non-null vector is normalizable, even when its norm is infinite. Furthermore, the space $\mathcal{H}$ has *finite dimension, and thus the features of finite-dimensional linear algebra are present, by transfer.

In order to obtain the space $\mathcal{H}$ associated with a particular system, we start from a Hilbert space $\mathcal{H}_0$ assigned to the system by the standard theory according to the formulation of von Neumann. We then define $\mathcal{H}$ as a hyperfinite subspace of the hypercomplex Hilbert space ${}^*\mathcal{H}_0$. Moreover, to each $\varphi \in \mathcal{H}_0$ we shall associate, in a canonical way, a vector $\overline{\varphi} \in \mathcal{H}$. The mapping $\varphi \mapsto \overline{\varphi}$ is linear and one-to-one, and preserves inner products up to infinitesimals. Thus, $\mathcal{H}_0$ is identifiable to a linear subspace, but not to a Hilbert subspace, of $\mathcal{H}$.

For the purpose of assigning a consistent semantics to this ''hyperfinite model,'' we may adopt the point of view that the system can be subjected (in principle) to *physical actions, some of which are associated with *experimental setups of finite or infinite (nonstandard) precision. An *action may correspond to the *measurement of an *observable, yielding *real outcomes. The system is always found in some *state, which influences the way the system responds to any *action, and in turn can be determined by a *measurement of a complete set of *observables.

The hyperfinite formalism relates to these *states and *observables in exactly the same way as the standard formalism: To each *observable β corresponds a Hermitian operator $B:\mathcal{H}\to\mathcal{H}$ such that $(u|Bu)$ is to be interpreted as the expected value of β upon *measurement on the system in the *physical state represented by the normalized vector $u \in \mathcal{H}$. (In particular, any *observable is represented by a * bounded Hermitian operator, defined on the whole space.) Moreover, if $f(\beta)$ denotes the *observable obtained by measuring β and then substituting the outcome b by $f(b)$, where f is an internal *real-valued function defined on the set of all possible outcomes of β, then the operator corresponding to $f(\beta)$ is $f(B)$, defined in the usual way by means of the spectral theorem.

The outcome of a *measurement is necessarily an eigenvalue, standard or nonstandard, of the corresponding operator, and the *state following the *measurement is represented by an eigenvector of the same operator. The *probability of a particular eigenvalue may be infinitesimal, but is always expressed in the usual way. As to the *probability of complex events, it is obtained as a *sum, since the set of possible outcomes is *finite. The integral in the formula of Dirac gives way to a *sum.

Some *states are standard, being identical to the states of the standard theory; a state represented by $\varphi \in \mathcal{H}_0$ shall be represented in the hyperfinite model by the vector $\overline{\varphi} \in \mathcal{H}$. In the same way, some *actions are standard; in particular, some *actions constitute standard measurements of observables (in the usual sense). Observables are represented in the standard theory by self-adjoint operators in $\mathcal{H}_0$, whereas *observables are represented in the hyperfinite theory by Hermitian operators on $\mathcal{H}$. An observable shall be viewed as associated with the standard experimental setups that can be used, in principle, to measure it. Hence an observable is never a special case of *observable, since the *measurement of the latter upon nonstandard *states requires nonstandard setups. Nevertheless, the relation between an observable α and an *observable β may be such that the knowledge of the probabilistic behavior of β provides all the necessary information about the probabilistic behavior of α. We shall see that this kind of relation exists for every observable: To each self-adjoint operator A in $\mathcal{H}_0$ we shall associate, in a canonical way, a Hermitian operator $\widetilde{A}$ on $\mathcal{H}$ such that a *measurement of the *observable corresponding to $\widetilde{A}$ can be viewed as a kind of generalized measurement of the observable corresponding to A.

To accept the idea that the outcome of a physical measurement can be a nonstandard number,

one must recall that the numerical outcome of a measurement is just a mathematical entity that we associate—according to some criterium previously specified—with the physical situation following the measurement. One can produce an example of nonstandard (or imaginary) measurement by choosing some standard measurement and multiplying the real-valued outcome by $1+\varepsilon$ (or by $1+i$, respectively), where ε is some infinitesimal constant. The real question would be whether the ultimate nature of a given observable (like position) is such that it is better described by a nonstandard formalism. (For the position observable, this would imply that the physical space is discrete at an infinitesimal scale of order much larger than the one associated with known quantum phenomena.) As to nonstandard probabilities, recall that a probability is just a number attributed to an event, supposed to convey information that can be confronted with experience through repetition. A probability can be an irrational number, although relative frequencies are necessarily rational numbers. Likewise, one can accept a probability that is a hyper-real number (necessarily between 0 and 1), it being understood that its standard part must be taken before submitting it to experimental verification.

Other approaches to quantum mechanics using nonstandard analysis have been developed before. We mention in particular M. O. Farrukh,[7] who replaces the usual Hilbert space by its nonstandard counterpart. In this fashion the elements of a continuous spectrum are viewed as ''almost'' eigenvalues, in the sense that for λ in that spectrum there exists a vector f such that $Af=\lambda f$ up to an infinitesimal error, where A is the nonstandard counterpart of a classical operator. The essential point of our approach is the use of a smaller, hyperfinite-dimensional, state space, which allows us to represent *all* states by eigenvectors in a strict sense. This is possible because the mathematics of hyperfinite-dimensional Hilbert spaces amounts to linear algebra.

We note also that there has been recent interest in applying hyperfinite methods to quantum physics, namely with regard to Feynman integrals and quantum field theory. See Refs. 11–13, and 18.

II. THE SPACE OF STATE VECTORS

In this section we introduce the state vector space $\mathcal{H}$ corresponding to the case $\mathcal{H}_0=L^2(\mathbb{R})$. The idea behind the construction of $\mathcal{H}$ is that a continuous square-summable function can be approximated by a piecewise-constant function with compact support, which can be obtained by dividing a large enough compact interval into subintervals of equal length and by sampling the function on each subinterval. Moreover, each such approximation lies within a finite-dimensional space. The original function appears as a kind of limit as the length of the subintervals approaches zero. The issue is how to formalize this idea, since no obvious way to define the notion of limit of a sequence of finite-dimensional Hilbert spaces is available. Nonstandard analysis provides an easy way to introduce a *finite-dimensional space including the approximations corresponding to subintervals of infinitesimal length, wherein, furthermore, vectors with infinite norm have a legitimate place. This space is, in essence, the same as the one considered by M. Kinoshita in Refs. 8, and 9, who constructs representations of the usual (standard) distributions as elements of this space of functions.

A. Definition

The construction of $\mathcal{H}$ depends on the choice of some arbitrary infinite *natural number. Henceforth, we consider that a number $w\in{}^*\mathbb{N}\setminus\mathbb{N}$ has been chosen and we denote by J_w the set $\{k\in{}^*\mathbb{N}:k\leqslant 2w^2\}$. For each $k\in J_w\cup\{0\}$ we write $x_k=-w+k/w$. The interval $[-w,w]$ is thus divided into $2w^2$ subintervals of length $1/w$. For each $k\in J_w$, let χ_k be the element of ${}^*\mathcal{H}_0$ defined by

$$\chi_k(x)=\begin{cases} w & \text{for } x_{k-1}<x\leqslant x_k,\\ 0 & \text{otherwise.}\end{cases}$$

Finally, we define $\mathcal{H}$ as the $2w^2$-dimensional subspace of ${}^*\mathcal{H}_0$ spanned by the family $(\chi_k)_{k\in J_w}$. The elements of $\mathcal{H}$ are the internal functions from ${}^*\mathbb{R}$ to ${}^*\mathbb{C}$ that are constant in each interval $(x_{k-1},x_k]$, where $k\in J_w$, and are null outside the interval $(-w,w]$. For every $k,m\in J_w$,

$$(\chi_k|\chi_m)=\int_{-\infty}^{+\infty}\overline{\chi_k(x)}\chi_m(x)\,dx=\delta_{k,m}\int_{x_{k-1}}^{x_k}w^2\,dx=w\,\delta_{k,m}\ .$$

Thus, the family $(\chi_k)_{k\in J_w}$ constitutes an orthogonal basis of $\mathcal{H}$, with $\|\chi_k\|=\sqrt{w}$ for every $k\in J_w$.

For $u\in\mathcal{H}$, let $(u_k)_{k\in J_w}$ be the family of coordinates of u in the basis $((1/w)\,\chi_k)_{k\in J_w}$:

$$u=\frac{1}{w}\sum_{k\in J_w}u_k\chi_k\,.$$

It is readily seen that

$$u_m=u(x_m)=(\chi_m|u)$$

for every $m\in J_w$. Comparison with (1) shows that the function that maps x_k to $u(x_k)$ corresponds to the wave function of the standard theory. In a similar way the vectors χ_k (with $k\in J_w$) correspond to the ill-defined vectors $|x\rangle$ (where $x\in\mathbb{R}$) of the formalism of Dirac. Observe that all points of the real line are identifiable to points of the set $\{x_k:k\in J_w\}$: To $x\in\mathbb{R}$ we associate x_k, where $k=\max\{n\in J_w:n\leqslant w(x+w)\}$. Then $x\approx x_k$, since from $x_k\leqslant x<x_{k+1}$ it follows that $0\leqslant x-x_k<x_{k+1}-x_k=1/w\approx 0$. Therefore the mapping is one-to-one, for if $x\mapsto x_k$ and $y\mapsto x_k$, then $x\approx x_k\approx y$, and $x\approx y$ implies $x=y$.

A vector $u\in\mathcal{H}$ shall be represented, in ket notation, as $|u\rangle$. We shall also write $|x_k\rangle$ instead of $|\chi_k\rangle$.

B. Representation of standard wave functions

We denote by P the projection operator of ${}^*\mathcal{H}_0$ onto $\mathcal{H}$. Let $\varphi\in{}^*\mathcal{H}_0$. Then, for each $k\in J_w$,

$$(\chi_k|P\varphi)=(\chi_k|\varphi)=\int_{-\infty}^{+\infty}\overline{\chi_k(x)}\varphi(x)\,dx=w\int_{x_{k-1}}^{x_k}\varphi\ .$$

Since $1/w$ is the length of $[x_{k-1},x_k]$, the value of $P\varphi$ on any point of $(x_{k-1},x_k]$ equals the average of φ on the same interval. We shall also write $\overline{\varphi}$ instead of $P\varphi$. Thus, $\overline{\varphi}(x_k)=w\int_{x_{k-1}}^{x_k}\varphi$ for every $k\in J_w$.

We shall see that the restriction of P to $\mathcal{H}_0$ is one-to-one, which allows us to identify the linear space $\mathcal{H}_0$ to a subspace of $\mathcal{H}$. Moreover, such identification preserves inner products up to infinitesimals. Actually, we prove a more general result: Every locally summable function can be considered as an element of $\mathcal{H}$.

Proposition 1: Let $\varphi,\psi\in L^1_{\mathrm{loc}}$. If $\overline{\varphi}(x_k)\approx\overline{\psi}(x_k)$ for all finite x_k, then $\varphi=\psi$ almost everywhere.

Proof: By linearity, it suffices to prove the case $\psi=0$. Let φ be a locally summable function such that $\overline{\varphi}(x_k)\approx 0$ for all finite x_k. We shall show that $\int_I\varphi=0$ for every bounded interval I. This implies that $\int_I\varphi=0$ for every measurable set I, whereby we conclude that $\varphi=0$ up to a set of null Lebesgue measure.

Let $a,b\in\mathbb{R}$, with $a<b$. There exist $m,n\in J_w$ such that $a\approx x_n$ and $b\approx x_m$, and x_k is finite when $n\leqslant k\leqslant m$. Let $\varepsilon\in\mathbb{R}^+$. By hypothesis, $|\overline{\varphi}(x_k)|\leqslant\varepsilon$ for all finite x_k. Thus,

$$\left|\int_{x_n}^{x_m}\varphi\right|=\left|\sum_{k=n+1}^{m}\int_{x_{k-1}}^{x_k}\varphi\right|\leqslant\sum_{k=n+1}^{m}\frac{\varepsilon}{w}\leqslant\varepsilon\frac{m-n}{w}.$$

Since ε is arbitrary and $(m-n)/w$ is finite (as the latter value is infinitely close to $b-a$), we obtain $\int_{x_n}^{x_m}\varphi\approx 0$.

On the other hand,

$$\int_a^b \varphi=\int_{x_n}^{x_m}\varphi+\int_a^{x_n}\varphi+\int_{x_m}^b \varphi.$$

The last two summands are also infinitesimal, since $\lim_{y\to x}\int_x^y\varphi=0$ implies $\int_x^y\varphi\approx 0$ for $y\approx x$. Therefore, $\int_a^b\varphi\approx 0$, whence $\int_a^b\varphi=0$. □

In the following, we shall need the lemma below, concerning a property of convergence in $L^2(\mathbb{R})$. Previously, for each $n\in\mathbb{N}$ we define $J_n=\{k\in\mathbb{N}:k\leqslant 2n^2\}$ and $x_{n,k}=-n+k/n$ for $k\in J_n\cup\{0\}$.

Lemma 1: Let $\varphi\in L^2(\mathbb{R})$, and for each $n\in\mathbb{N}$ let φ_n be the element of $L^2(\mathbb{R})$ defined by

$$\varphi_n(x)=\begin{cases} n\int_{x_{n,k-1}}^{x_{n,k}}\varphi & (if\ \ x_{n,k-1}<x\leqslant x_{n,k},\ \ with\ \ k\in J_n),\\ 0 & (otherwise).\end{cases}$$

Then, the sequence $(\varphi_n)_{n\in\mathbb{N}}$ converges in $L^2(\mathbb{R})$ to φ.

Proof: For each $n\in\mathbb{N}$, denote by P_n the projection operator that maps each φ to φ_n. Let $\varphi\in L^2(\mathbb{R})$. Given $\varepsilon\in\mathbb{R}^+$, there exists $\psi\in L^2(\mathbb{R})$ such that $\|\varphi-\psi\|<\varepsilon$ and ψ is continuous and has bounded support. We have

$$\|\varphi-P_n\varphi\|<\|\varphi-\psi\|+\|\psi-P_n\psi\|+\|P_n(\psi-\varphi)\|<2\varepsilon+\|\psi-P_n\psi\|.$$

Hence, it suffices to prove that

$$\lim_{n\to\infty}\|\psi-P_n\psi\|=0,$$

since this implies $\lim_n\|\varphi-P_n\varphi\|\leqslant 2\varepsilon$, whence $P_n\varphi\to\varphi$.

Choose $N\in\mathbb{N}$ such that $[-N,N]$ contains the support of ψ. Then $\|\psi-P_n\psi\|^2=\int_{-N}^N|\psi(t)-(P_n\psi)(t)|^2\,dt$ for every $n\in\mathbb{N}$. Let $n\geqslant N$. For each $k\in J_n$,

$$\int_{x_{n,k-1}}^{x_{n,k}}|\psi(t)-(P_n\psi)(t)|^2\,dt=\int_{x_{n,k-1}}^{x_{n,k}}|\psi(t)|^2\,dt-\frac{1}{n}|a_{k,n}|^2,$$

where $a_{k,n}=n\int_{x_{n,k-1}}^{x_{n,k}}\psi$. Hence,

$$\|\psi-P_n\psi\|^2=\sum_{k=(n-N)n+1}^{n(n+N)}\int_{x_{n,k-1}}^{x_{n,k}}|\psi(t)-(P_n\psi)(t)|^2\,dt=\int_{-N}^{N}|\psi(t)|^2\,dt-\frac{1}{n}\sum_{k=(n-N)n+1}^{n(n+N)}|a_{k,n}|^2.$$

Since ψ is continuous, $\Sigma_{k=(n-N)n+1}^{n(n+N)}|a_{k,n}|^2$ is a Riemann sum of the function $t\mapsto|\psi(t)|^2$, corresponding to the decomposition of $[-N,N]$ in subintervals of length $1/n$. Hence,

$$\lim_{n\to\infty}\frac{1}{n}\sum_{k=(n-N)n+1}^{n(n+N)}|a_{k,n}|^2=\int_{-N}^{N}|\psi(t)|^2\,dt.$$

This completes the proof. □

Lemma 2: For every $f\in L^1(\mathbb{R})$,

$$\int_{\mathbb{R}} f\approx\frac{1}{w}\sum_{k=1}^{2w^2}\overline{f}(x_k).$$

Proof: Let $f \in L^1(\mathbb{R})$. Since $\int_{\mathbb{R}} f = \lim_n \int_{-n}^{n} f$, we have $\int_{\mathbb{R}} f \approx \int_{-w}^{w} f$.
Since

$$\int_{-n}^{n} f = \sum_{k=1}^{2n^2} \int_{x_{n,k-1}}^{x_{n,k}} f$$

for all $n \in \mathbb{N}$, we obtain, by transfer,

$$\int_{-w}^{w} f = \sum_{k=1}^{2w^2} \int_{x_{k-1}}^{x_k} f = \sum_{k=1}^{2w^2} \frac{\overline{f}(x_k)}{w}.$$

□

Proposition 2: For every $\varphi, \psi \in \mathcal{H}_0$,

$$(\varphi|\psi) \approx (\overline{\varphi}|\overline{\psi}) \approx (\varphi|\overline{\psi}) \ .$$

Proof: Let $\varphi, \psi \in \mathcal{H}_0$ and let $(\varphi_n)_{n\in\mathbb{N}}$ and $(\psi_n)_{n\in\mathbb{N}}$ be the sequences associated with φ and ψ as in Lemma 1. Then $\varphi_n \to \varphi$ and $\psi_n \to \psi$ in $\mathcal{H}_0$. By the continuity of the inner product, $(\varphi_n|\psi_n) \to (\varphi|\psi)$, whence $(\varphi|\psi) \approx (\varphi_w|\psi_w)$. Therefore, $(\varphi|\psi) \approx (\overline{\varphi}|\overline{\psi})$, since $\varphi_w = \overline{\varphi}$ and $\psi_w = \overline{\psi}$.

Similarly, $(\varphi|\psi_n) \to (\varphi|\psi)$, whence $(\varphi|\psi) \approx (\varphi|\overline{\psi})$. □

Proposition 3: For every $\varphi \in \mathcal{H}_0$,

$$\varphi \approx \overline{\varphi} \ .$$

Proof: Let $\varphi \in \mathcal{H}_0$. We have

$$\|\varphi - \overline{\varphi}\|^2 = (\varphi|\varphi) - (\varphi|\overline{\varphi}) - (\overline{\varphi}|\varphi) + (\overline{\varphi}|\overline{\varphi}) \approx 0$$

by Proposition 2. □

Corollary: For every $\varphi \in \mathcal{H}_0$,

$$\|\varphi\| \approx \|\overline{\varphi}\|.$$

Proposition 4: Let $\varphi \in \mathcal{H}_0$. *If* φ *is continuous on a neighborhood of* $x \in \mathbb{R}$, *then* $\varphi(x) \approx \overline{\varphi}(x_k)$ *for* $x_k \approx x$.

Proof: For $x_k \approx x$, the interval $[x_{k-1}, x_k]$ is contained in every standard neighborhood of x. Therefore φ is continuous on $[x_{k-1}, x_k]$, whence, by the mean value theorem,

$$\overline{\varphi}(x_k) = w \int_{x_{k-1}}^{x_k} \varphi = \varphi(c) \ ,$$

where $c \in [x_{k-1}, x_k]$. Since $c \approx x$, it follows from the continuity of φ at x that $\varphi(x) \approx \varphi(c)$, and this completes the proof. □

Proposition 5: Let u, v *be vectors of* $\mathcal{H}$ *such that*

$$\langle x_k|u\rangle \approx \langle x_k|v\rangle$$

for all finite x_k. *If* $\|u - v\|$ *is finite, then*

$$\langle \overline{\varphi}|u\rangle \approx \langle \overline{\varphi}|v\rangle$$

for all $\varphi \in \mathcal{H}_0$.

Proof: Let u and v be as in the proposition. We assume without loss of generality that v is the null vector. Let $\varphi \in \mathcal{H}_0$ and let $(\varphi_n)_{n\in\mathbb{N}}$ be the sequence defined as in Lemma 1.

For every $n \in \mathbb{N}$, the estimate

$$|\langle \overline{\varphi_n}|u\rangle| \leqslant \frac{1}{w}\sum_{k=1}^{2w^2} |\overline{\overline{\varphi_n}(x_k)}\langle x_k|u\rangle| \leqslant \frac{\varepsilon}{w}\sum_{k=1}^{2w^2} |\overline{\varphi_n}(x_k)|$$

holds for all $\varepsilon \in \mathbb{R}^+$. Moreover, the value of $(1/w)\,\Sigma_{k=1}^{2w^2}|\overline{\varphi_n}(x_k)|$ is finite, by Lemma 2, since the function φ_n is summable. Therefore,

$$|\langle \overline{\varphi_n}|u\rangle| \approx 0.$$

By the principle of Cauchy (also known as Robinson's sequential lemma; see Ref. 3; see also Ref. 5), this holds for all $n \leqslant \nu$, for some $\nu \in {}^*\mathbb{N}\backslash\mathbb{N}$. Then,

$$|\langle \overline{\varphi}|u\rangle| \leqslant |\langle \overline{\varphi} - \overline{\varphi_\nu}|u\rangle| + |\langle \overline{\varphi_\nu}|u\rangle| \lesssim \|\overline{\varphi} - \overline{\varphi_\nu}\|\,\|u\|.$$

By Lemma 1, $\overline{\varphi} \approx \overline{\varphi_\nu}$, and therefore $\overline{\varphi} \approx \overline{\varphi_\nu}$, by Proposition 3. Since $\|u\|$ is finite, we conclude that $|\langle \overline{\varphi}|u\rangle| \lesssim 0$. □

Remarks:

(1) Proposition 5 extends Proposition 1, in the sense that even when $|u\rangle$ and $|v\rangle$ are not representatives of locally summable functions the hypothesis that they have the same pointwise behavior (up to infinitesimals) ensures that their relationship with the usual wave-functions is also the same (still up to infinitesimals).

(2) The thesis of Proposition 5 may not hold when $\|u-v\|$ is infinite. Consider $|u\rangle = |x_m\rangle$, where $x_m = \nu \in {}^*\mathbb{N}\backslash\mathbb{N}$, with $\nu \leqslant w^{1/4}$. Let φ be the function such that $\varphi(x) = n$ for $n - 1/n^4 \leqslant x \leqslant n$ (for every $n \in \mathbb{N}$) and $\varphi(x) = 0$ otherwise. Then $\varphi \in L^2(\mathbb{R})$ and $\langle x_k|u\rangle = 0$ for all finite x_k, but

$$\langle u|\varphi\rangle = \overline{\varphi}(x_m) = w\int_{\nu - 1/w}^{\nu} \varphi = \varphi(\nu) = \nu \neq 0.$$

III. OPERATORS

A. A position operator

Switching to the bra–ket notation, we define a "position operator" on $\mathcal{H}$ by

$$X_{\mathrm{h}} = \frac{1}{w}\sum_{k=1}^{2w^2} x_k |x_k\rangle\langle x_k|.$$

The operator X_{h} is Hermitian, since the basis $(|x_k\rangle)_{k\in J_w}$ is orthogonal and all coefficients x_k are *real. It can be shown in the usual way that $\{x_k : k \in J_w\}$ is the set of eigenvalues of X_{h} and that the eigenspace corresponding to x_k is spanned by $|x_k\rangle$. We have $\langle x_k|X_{\mathrm{h}}|u\rangle = x_k\langle x_k|u\rangle$ for all $k \in J_w$ and $u \in \mathcal{H}$. (Hence X_{h} is the restriction to $\mathcal{H}$ of the multiplicative operator in ${}^*\mathcal{H}_0$.)

The present example illustrates some of the notions introduced in Sec. I C. Assuming the usual interpretation of $\mathcal{H}_0$, the multiplicative operator X in $\mathcal{H}_0$ corresponds to the position observable α, and X_{h} corresponds to an *observable β. We shall see that α behaves as a kind of standard-scale version of β insofar as probabilities are concerned, assuming that physical states are represented by continuous wave functions.

Proposition 6: Let $f:\mathbb{R}\to\mathbb{R}$ be a bounded function, continuous except at most at a finite set of points. For every $\varphi \in \mathcal{H}_0$, if φ is continuous and belongs to the domain of $f(X)$, then

$$(\varphi|f(X)\varphi) \approx \langle \overline{\varphi}|f(X_{\mathrm{h}})|\overline{\varphi}\rangle.$$

Proof: Let $\psi(x)=f(x)\varphi(x)$ for all $x\in\mathbb{R}$. For finite x_k such that f is continuous at $\mathrm{st}(x_k)$, the function ψ is continuous on a neighborhood of x, where $x=\mathrm{st}(x_k)$. By Proposition 4, $\langle x_k|\overline{\psi}\rangle = \overline{\psi}(x_k)\approx f(x)\varphi(x)$. On the other hand, for the same x_k,

$$\langle x_k|f(X_\mathrm{h})|\overline{\varphi}\rangle = f(x_k)\overline{\varphi}(x_k)\approx f(x)\varphi(x),$$

because $f(x_k)\approx f(x)$, $\overline{\varphi}(x_k)\approx\varphi(x)$, and all these values are finite.

Let S be the set of standard points at which f is not continuous. Let $\varepsilon\in\mathbb{R}^+$, and denote by u_ε the vector of $\mathcal{H}$ such that $\langle x_k|u_\varepsilon\rangle=f(x_k)\overline{\varphi}(x_k)$ if $x_k\in\cup_{x\in S}(x-\varepsilon,x+\varepsilon)$ and such that $\langle x_k|u_\varepsilon\rangle = \overline{\psi}(x_k)$ otherwise. Hence $\langle x_k|u_\varepsilon\rangle\approx\langle x_k|f(X_\mathrm{h})|\overline{\varphi}\rangle$ for all finite x_k. Moreover, $\|u_\varepsilon-f(X_\mathrm{h})\overline{\varphi}\|$ is finite, since

$$\|u_\varepsilon-f(X_\mathrm{h})\overline{\varphi}\|\leqslant\|\overline{\psi}-f(X_\mathrm{h})\overline{\varphi}\|\leqslant\|\overline{\psi}\|+A\|\overline{\varphi}\|,$$

where A is any upper bound of $|f|$. Therefore, $\langle\overline{\varphi}|u_\varepsilon\rangle\approx\langle\overline{\varphi}|f(X_\mathrm{h})|\overline{\varphi}\rangle$, by Proposition 5.

On the other hand,

$$|u_\varepsilon-\overline{\psi}\rangle=\frac{1}{w}\sum_k\ (f(x_k)\overline{\varphi}(x_k)-\overline{\psi}(x_k))|x_k\rangle,$$

where the sum extends only over those values of k such that $x_k\in\cup_{x\in S}(x-\varepsilon,x+\varepsilon)$. Thus,

$$\langle\overline{\varphi}|u_\varepsilon-\overline{\psi}\rangle=\frac{1}{w}\sum_k\ f(x_k)|\overline{\varphi}(x_k)|^2-\frac{1}{w}\sum_k\ \overline{\overline{\varphi}(x_k)}\overline{\psi}(x_k).$$

An upper bound of the former sum is $A(1/w)\,\Sigma_k|\overline{\varphi}(x_k)|^2$, and

$$\frac{1}{w}\sum_k\ |\overline{\varphi}(x_k)|^2\approx\sum_{x\in S}\int_{x-\varepsilon}^{x+\varepsilon}|\varphi(t)|^2\,dt.$$

Similarly,

$$\frac{1}{w}\sum_k\ \overline{\overline{\varphi}(x_k)}\overline{\psi}(x_k)\approx\sum_{x\in S}\int_{x-\varepsilon}^{x+\varepsilon}\overline{\varphi(t)}\psi(t)\,dt.$$

Hence, given $\delta\in\mathbb{R}^+$, there exists $\varepsilon\in\mathbb{R}^+$ such that $|\langle\overline{\varphi}|u_\varepsilon-\overline{\psi}\rangle|<\delta$. For such ε,

$$(\varphi|f(X)\varphi)\approx\langle\overline{\varphi}|\overline{\psi}\rangle\approx\langle\overline{\varphi}|\overline{\psi}-u_\varepsilon\rangle+\langle\overline{\varphi}|u_\varepsilon\rangle\approx\langle\overline{\varphi}|\overline{\psi}-u_\varepsilon\rangle+\langle\overline{\varphi}|f(X_\mathrm{h})|\overline{\varphi}\rangle.$$

Since $|\langle\overline{\varphi}|\overline{\psi}-u_\varepsilon\rangle|<\delta$ and δ is an arbitrary element of $\mathbb{R}^+$, we conclude that $(\varphi|f(X)\varphi)\approx\langle\overline{\varphi}|f(X_\mathrm{h})|\overline{\varphi}\rangle$. □

When f is the characteristic function of a standard interval I, Proposition 6 shows that the probability $\mathrm{prob}_\varphi(\alpha\in I)$ that a measurement of α upon the state represented by φ will yield an outcome in the set I is the standard part of the *probability $^*\mathrm{prob}_{\overline{\varphi}}(\beta\in{}^*I)$ that a *measurement of β upon the same *state will yield an outcome in the interval $^*I$. In other words,

$$\mathrm{prob}_\varphi(\alpha\in I)=\mathrm{st}\,\langle\overline{\varphi}|f(X_\mathrm{h})|\overline{\varphi}\rangle.$$

Other operators can replace X_h in the statement of Proposition 6. For example, if X_h' is defined by the identity $X_\mathrm{h}'|x_k\rangle=(x_k+1/w)|x_k\rangle$, then it is easy to reproduce the proof of Proposition 6. This example shows that there is no such thing as "the position *observable," but there are several *observables that behave at standard scale like the standard position observable, at least as far as only probabilities are concerned.

B. Representation of observables

We shall associate to any self-adjoint operator A in $\mathcal{H}_0$ a Hermitian operator $\tilde{A}$ in $\mathcal{H}$. We must deal first with bounded operators. To each *bounded operator $T:{}^*\mathcal{H}_0\to{}^*\mathcal{H}_0$ we assign the operator $\overline{T}:\mathcal{H}\to\mathcal{H}$ such that

$$\overline{T}u = PTu$$

for every $u\in\mathcal{H}$. When T is self-adjoint, $\overline{T}$ is Hermitian, since $\overline{T}u = PTPu$ for all $u\in\mathcal{H}$.

*Proposition 7: Let T be a *bounded operator on ${}^*\mathcal{H}_0$ with finite norm. For every $\varphi\in\mathcal{H}_0$,*

$$\overline{T}\overline{\varphi}\approx T\overline{\varphi}\approx P(T\varphi).$$

If, moreover, $T\varphi\in\mathcal{H}_0$, then $P(T\varphi)\approx T\varphi$.

Proof: We have $\overline{\varphi}\approx\varphi$, by Proposition 3. Then $T\overline{\varphi}\approx T\varphi$, because T has finite norm. Since P also has finite norm, $\overline{T}\overline{\varphi}=P(T\overline{\varphi})\approx P(T\varphi)$. Finally, $T\varphi\approx P(T\varphi)$ when $T\varphi\in\mathcal{H}_0$, by Proposition 3. □

The conditions of Proposition 7 are satisfied, in particular, when T is a bounded operator on $\mathcal{H}_0$.

When the domain of a self-adjoint operator A is not the whole space $\mathcal{H}_0$, we cannot define $\overline{A}$ as above. However, the spectral theorem for self-adjoint operators in a Hilbert space yields the equality

$$A=\int_{-\infty}^{+\infty}\lambda\, dE_\lambda,$$

where $(E_\lambda)_{\lambda\in\mathbb{R}}$ is the spectral family associated with A. For every $n\in{}^*\mathbb{N}$, the operator

$$A_n=\int_{-n}^{+n}\lambda\, dE_\lambda$$

is a *bounded operator on ${}^*\mathcal{H}_0$. We shall define a Hermitian operator $\tilde{A}:\mathcal{H}\to\mathcal{H}$ by $\tilde{A}=\overline{A_\nu}$, where ν is an element of ${}^*\mathbb{N}\backslash\mathbb{N}$ satisfying the conditions of Proposition 8, below; these conditions ensure that an appropriate relation between the spectral families of A and $\tilde{A}$ can be obtained. When A is bounded, we have $\tilde{A}=\overline{A}$, since $A=A_\nu$ in such case.

Given a *bounded self-adjoint operator T on ${}^*\mathcal{H}_0$, we write $X(T)=\{(u|Tu):u\in{}^*\mathcal{H}_0,\ \|u\|=1\}$, and $\mu(T)=\inf X(T)$, $M(T)=\sup X(T)$. For $u\in\mathcal{H}$ we have $(u|\overline{T}u)=(u|PTu)=(Pu|Tu)=(u|Tu)$. Hence $X(\overline{T})$ is a subset of $X(T)$, and therefore $[\mu(\overline{T}),M(\overline{T})]\subset[\mu(T),M(T)]$. Hence, if f is a *real-valued function continuous on $[\mu(T),M(T)]$, both operators $f(T)$ and $f(\overline{T})$ are well-defined. Moreover, it is known that the norms thereof satisfy the conditions

$$\|f(T)\|\leqslant\sup\{|f(\lambda)|:\lambda\in[\mu(T),M(T)]\},$$

$$\|f(\overline{T})\|\leqslant\sup\{|f(\lambda)|:\lambda\in[\mu(\overline{T}),M(\overline{T})]\}.$$

Therefore, if $f(T)$ has finite norm, then $f(\overline{T})$ also has finite norm.

Proposition 8: There exists $\nu\in{}^*\mathbb{N}\backslash\mathbb{N}$ such that: For every sequence $(T_n)_{n\in\mathbb{N}}$ of bounded self-adjoint operators on $\mathcal{H}_0$ and every sequence $(f_m)_{m\in\mathbb{N}}$ of real-valued functions such that each f_m is continuous on $[\mu(T_n),M(T_n)]$ whenever $n\geqslant m$,

$$f_m(\overline{T_n})\overline{\varphi}\approx f_m(T_n)\varphi,$$

for every $\varphi\in\mathcal{H}_0$ and every $m,n\in{}^*\mathbb{N}$ such that $m\leqslant n\leqslant\nu$.

Proof: Let $(T_n)_{n\in\mathbb{N}}$, $(f_m)_{m\in\mathbb{N}}$ and φ be as in the proposition. Let $n,m\in\mathbb{N}$, with $m\leqslant n$. If u is an element of $\mathcal{H}$ such that $u\approx\varphi$, then $\overline{T_n}u=PT_nu\approx PT_n\varphi$, since the norm of PT_n is finite. By Proposition 3, $PT_n\varphi\approx T_n\varphi$, and thus $\overline{T_n}u\approx T_n\varphi$. This is readily extended to $p(\overline{T_n})u\approx p(T_n)\varphi$, where p is an arbitrary standard polynomial.

Let $\varepsilon\in\mathbb{R}^+$. Choose a standard polynomial p such that $|f_m(\lambda)-p(\lambda)|\leqslant\varepsilon$ for all λ in the interval $[\mu(T_n),M(T_n)]$. Then

$$\|f_m(T_n)\varphi-p(T_n)\varphi\|=\left\|\int_{-\infty}^{+\infty}(f_m(\lambda)-p(\lambda))\,dE_\lambda\varphi\right\|\leqslant\varepsilon\|\varphi\|,$$

where $(E_\lambda)_{\lambda\in\mathbb{R}}$ is the spectral family associated with T_n. Similarly,

$$f_m(\overline{T_n})\overline{\varphi}-p(\overline{T_n})\overline{\varphi}=\sum_i\,(f_m(\lambda_i)-p(\lambda_i))P_i\overline{\varphi},$$

where the sum extends over all eigenvalues λ_i of $\overline{T_n}$ and P_i is the projection operator onto the eigenspace corresponding to λ_i. Taking into account that every λ_i is in the interval $[\mu(T_n),M(T_n)]$, we obtain

$$\|f_m(\overline{T_n})\overline{\varphi}-p(\overline{T_n})\overline{\varphi}\|^2=\sum_i\,|f_m(\lambda_i)-p(\lambda_i)|^2\|P_i\overline{\varphi}\|^2\leqslant\varepsilon^2\|\overline{\varphi}\|^2.$$

Finally,

$$\begin{aligned}\|f_m(\overline{T_n})\overline{\varphi}-f_m(T_n)\varphi\|&\leqslant\|f_m(\overline{T_n})\overline{\varphi}-p(\overline{T_n})\overline{\varphi}\|+\|p(\overline{T_n})\overline{\varphi}-p(T_n)\varphi\|+\|p(T_n)\varphi-f_m(T_n)\varphi\|\\&\leqslant\varepsilon\|\overline{\varphi}\|+\text{infinitesimal}+\varepsilon\|\varphi\|.\end{aligned}$$

Since $\|\overline{\varphi}\|$ and $\|\varphi\|$ are finite, and ε is arbitrary, this proves that

$$f_m(\overline{T_n})\overline{\varphi}\approx f_m(T_n)\varphi.$$

Given sequences $(f_m)_{m\in\mathbb{N}}$ and $(T_n)_{n\in\mathbb{N}}$, and $j\in\mathbb{N}$, $\varphi\in\mathcal{H}_0$, write $\alpha=((f_m)_m,(T_n)_n,\varphi,j)$ and let

$$S_\alpha=\{k\in{}^*\mathbb{N}:k\geqslant j,\forall_{m,n\in{}^*\mathbb{N},m\leqslant n\leqslant k}\,\|f_m(\overline{T_n})\overline{\varphi}-f_m(T_n)\varphi\|<n^{-1}\}.$$

For $k\in\mathbb{N}$, the condition $\|f_m(\overline{T_n})\overline{\varphi}-f_m(T_n)\varphi\|<n^{-1}$ holds for $m\leqslant n\leqslant k$, since $f_m(\overline{T_n})\overline{\varphi}\approx f_m(T_n)\varphi$. Hence, any $k\in\mathbb{N}$ such that $k\geqslant j$ is an element of S_α. Moreover, the family of all sets S_α with α as above has the finite intersection property (see the Appendix)—it suffices to choose for k the greatest value of j. Therefore, by saturation,

$$\bigcap_\alpha S_\alpha\neq\varnothing,$$

and any $\nu\in\cap_\alpha S_\alpha$ satisfies the conditions of the proposition. □

Henceforth we consider that a value ν as given by Proposition 8 has been chosen. For every self-adjoint operator A we define $\widetilde{A}=\overline{A}_\nu$.

Proposition 9: Let A be a self-adjoint bounded operator on $\mathcal{H}_0$. For every real-valued function f continuous on $[\mu(A),M(A)]$,

$$f(A)\varphi\approx f(\overline{A})u$$

for all $\varphi \in \mathcal{H}_0$ and $u \in \mathcal{H}$ such that $u \approx \varphi$.

Proof: Considering the constant sequences determined by A and f, Proposition 8 yields

$$f(A)\varphi \approx f(\overline{A})\overline{\varphi}$$

for every $\varphi \in \mathcal{H}_0$. If $u \approx \varphi$, with $u \in \mathcal{H}$, then $f(\overline{A})\overline{\varphi} \approx f(\overline{A})u$, since

$$\|f(\overline{A})(\overline{\varphi} - u)\| \leqslant \|f(\overline{A})\|\,\|\overline{\varphi} - u\|$$

and the right side above is the product of a finite number by an infinitesimal. □

Proposition 10: Let A be a self-adjoint operator in $\mathcal{H}_0$. For every continuous function $f:\mathbb{R} \to \mathbb{R}$, the condition

$$f(A)\varphi \approx f(\widetilde{A})\overline{\varphi}$$

holds for every $\varphi \in \mathcal{H}_0$ belonging to the domain of $f(A)$.

Proof: Let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be the spectral family associated with A. We have

$$f(A)\varphi = \lim_n \int_{-n}^{+n} f(\lambda)\, dE_\lambda \varphi = \lim_n f(A_n)\varphi \approx f(A_\nu)\varphi.$$

By Proposition 8, making $f_n = f$ for all n,

$$f(A_\nu)\varphi \approx f(\overline{A}_\nu)\overline{\varphi}.$$

Since $\overline{A}_\nu = \widetilde{A}$, this completes the proof. □

The following proposition relates the spectral families associated with A and $\widetilde{A}$. (A related proposition, for bounded operators, is found in Ref. 4.)

Proposition 11: Let A be a self-adjoint operator in $\mathcal{H}_0$, and let $(E_\lambda)_{\lambda \in \mathbb{R}}$ and $(F_\lambda)_{\lambda \in {}^*\mathbb{R}}$ be the spectral families associated with A and $\widetilde{A}$, respectively. Let $a \in \mathbb{R}$. The conditions

$$E_a \varphi \approx F_{a+\varepsilon} u,$$

$$E_{a^-} \varphi \approx F_{a-\varepsilon} u$$

hold for every infinitesimal $\varepsilon \geqslant \nu^{-1}$ and every $\varphi \in \mathcal{H}_0$ and $u \in \mathcal{H}$ such that $u \approx \varphi$.

Proof: Let $a \in \mathbb{R}$. For $m \in {}^*\mathbb{N}$, we denote by $g_{m,a}$ the continuous function defined on ${}^*\mathbb{R}$ such that (i) $g_{m,a}(\lambda) = 1$ for $\lambda \leqslant a + (m+1)^{-1}$, (ii) $g_{m,a}(\lambda) = 0$ for $\lambda \geqslant a + m^{-1}$, and (iii) $g_{m,a}$ drops linearly from 1 to 0 in the interval $[a + (m+1)^{-1}, a + m^{-1}]$. Moreover, for $x \in {}^*\mathbb{R}$ let h_x be the function such that $h_x(\lambda) = 1$ for $\lambda \leqslant x$ and $h_x(\lambda) = 0$ for $\lambda > x$. Then

$$g_{m,a}(\lambda) \leqslant h_{a+\varepsilon}(\lambda) \leqslant g_{m-2,a}(\lambda)$$

for all m, λ, ε such that $m > 2$ and $m^{-1} \leqslant \varepsilon \leqslant (m-1)^{-1}$. For every Hermitian operator B on $\mathcal{H}$, the operational calculus yields

$$\|g_{m-2,a}(B)u - h_{a+\varepsilon}(B)u\| \leqslant \|g_{m-2,a}(B)u - g_{m,a}(B)u\|$$

for all $u \in \mathcal{H}$. Given an infinitesimal $\varepsilon \geqslant \nu^{-1}$, consider the unique $m \in {}^*\mathbb{N}$ such that $m - 1 < \varepsilon^{-1} \leqslant m$. From $\varepsilon \geqslant \nu^{-1}$ it follows that $m \leqslant \nu$. Moreover, $m^{-1} \leqslant \varepsilon < (m-1)^{-1}$. Therefore, we may particularize the inequality above with such m and ε, and $B = \overline{A}_\nu$ and with $u = \overline{\varphi}$, where $\varphi \in \mathcal{H}_0$:

$$\|g_{m-2,a}(\overline{A}_\nu)\overline{\varphi} - h_{a+\varepsilon}(\overline{A}_\nu)\overline{\varphi}\| \leqslant \|g_{m-2,a}(\overline{A}_\nu)\overline{\varphi} - g_{m,a}(\overline{A}_\nu)\overline{\varphi}\|.$$

We now show that the right side of this inequality is infinitesimal. We have $g_{m-2,a}(\overline{A}_\nu)\overline{\varphi}\approx g_{m-2,a}(A_\nu)\varphi$ and $g_{m,a}(\overline{A}_\nu)\overline{\varphi}\approx g_{m,a}(A_\nu)\varphi$, by the definition of ν. We must show that $g_{m-2,a}(A_\nu)\varphi\approx g_{m,a}(A_\nu)\varphi$: For fixed a, the sequence $(g_{n,a})_{n\in\mathbb{N}}$ is a decreasing sequence of non-negative continuous functions that converges pointwise to the function h_a. The operational calculus ensures that

$$\lim_n g_{n,a}(A)\varphi = h_a(A)\varphi$$

for every $\varphi\in\mathcal{H}_0$. Since ε is infinitesimal, m is infinite, and hence

$$g_{m-2,a}(A)\varphi\approx g_{m,a}(A)\varphi\approx h_a(A)\varphi.$$

On the other hand,

$$\begin{aligned} g_{m-2,a}(A)\varphi &= \int_{-\infty}^{a} g_{m-2,a}(\lambda)\, dE_\lambda\varphi \\ &= g_{m-2,a}(A_\nu)\varphi + \int_{-\infty}^{-\nu} dE_\lambda\varphi \\ &= g_{m-2,a}(A_\nu)\varphi + E_{-\nu}\varphi\approx g_{m-2,a}(A_\nu)\varphi. \end{aligned}$$

In a similar way, $g_{m,a}(A)\varphi\approx g_{m,a}(A_\nu)\varphi$. Thus, we have shown that $g_{m-2,a}(\overline{A}_\nu)\overline{\varphi}\approx h_{a+\varepsilon}(\overline{A}_\nu)\overline{\varphi}$. Therefore, taking into account the definition of ν,

$$h_a(A)\varphi\approx g_{m-2,a}(A)\varphi\approx g_{m-2,a}(A_\nu)\varphi\approx g_{m-2,a}(\overline{A}_\nu)\overline{\varphi}\approx h_{a+\varepsilon}(\overline{A}_\nu)\overline{\varphi}.$$

Finally, $h_a(A)\varphi = E_a\varphi$ and $h_{a+\varepsilon}(\overline{A}_\nu)\overline{\varphi} = F_{a+\varepsilon}\overline{\varphi}$; furthermore, if $u\in\mathcal{H}$ is such that $u\approx\varphi$, then $F_{a+\varepsilon}\overline{\varphi}\approx F_{a+\varepsilon}u$, since the norm of the projection operator $F_{a+\varepsilon}$ is finite.

The proof of the second condition in the thesis is similar. For $m\in{}^*\mathbb{N}$, denote by $\gamma_{m,a}$ the continuous function defined on ${}^*\mathbb{R}$ such that (i) $\gamma_{m,a}(\lambda)=1$ for $\lambda\leqslant a-m^{-1}$, (ii) $\gamma_{m,a}(\lambda)=0$ for $\lambda\geqslant a-(m+1)^{-1}$, and (iii) γ_{ma} drops linearly from 1 to 0 in the interval $[a-m^{-1}, a-(m+1)^{-1}]$. For $x\in{}^*\mathbb{R}$, denote by η_x the function such that $\eta_x(\lambda)=1$ for $\lambda<x$ and $\eta_x(\lambda)=0$ for $\lambda\geqslant x$. Proceeding as in the first part of the proof, we obtain

$$\eta_a(A)\varphi\approx\eta_{a-\varepsilon}(\overline{A}_\nu)\overline{\varphi}.$$

We have $\eta_{a-\varepsilon}(\overline{A}_\nu)\overline{\varphi} = F_{a-\varepsilon}\overline{\varphi}$; on the other hand, $\eta_a(x)=h_a(x)-\theta(x)$ for all x, where $\theta(a)=1$ and $\theta(x)=0$ for $x\neq a$. Hence, $\eta_a(A)\varphi = E_a\varphi-\theta(A)\varphi$. A straightforward computation yields $\int_{-\infty}^{+\infty}\theta(\lambda)dE_\lambda = E_{a^+}-E_{a^-}$. Therefore,

$$E_a\varphi - E_{a^+}\varphi + E_{a^-}\varphi\approx F_{a-\varepsilon}\overline{\varphi}.$$

Finally, $E_a\varphi-E_{a^+}\varphi=0$, since the function $\lambda\mapsto E_\lambda$ is necessarily continuous on the right. □

Corollary: Let A be a self-adjoint operator in $\mathcal{H}_0$, and let $(E_\lambda)_{\lambda\in\mathbb{R}}$ and $(F_\lambda)_{\lambda\in{}^*\mathbb{R}}$ be the spectral families associated with A and $\tilde{A}$, respectively. For $a\in\mathbb{R}$, if the function $\lambda\mapsto E_\lambda$ is continuous at a, then $E_a\varphi\approx F_a u$, for every $\varphi\in\mathcal{H}_0$ and every $u\in\mathcal{H}$ such that $u\approx\varphi$.

Proof: We have $E_a\varphi\approx F_{a+\varepsilon}u$ and $E_{a-}\varphi\approx F_{a-\varepsilon}u$ for $\varepsilon\approx 0$ such that $\varepsilon\geqslant\nu^{-1}$. Since $E_{a-}\varphi = E_a\varphi$, it follows that $E_a\varphi\approx F_{a+\varepsilon}u\approx F_{a-\varepsilon}u$. Since

$$\|F_{a+\varepsilon}u - F_{a-\varepsilon}u\|^2 = \|F_{a+\varepsilon}u - F_a u\|^2 + \|F_a u - F_{a-\varepsilon}u\|^2,$$

we obtain $F_{a+\varepsilon}u\approx F_a u$ and $F_a u\approx F_{a-\varepsilon}u$. □

IV. PROBABILITIES AND CONSISTENCY

A. Nonstandard and standard probabilities

A *measurement of an *observable β will yield a *real outcome, finite or infinite. By taking its standard part when the outcome is finite one obtains a standard outcome. For every bounded Borelian subset of $\mathbb{R}$, the event $\mathrm{st}\,\beta \in S$ amounts to $\beta \in \mathrm{Mon}\,S$, where

$$\mathrm{Mon}\,S = \{x \in {}^*\mathbb{R} : \exists_{y \in S}\ y \approx x\}.$$

(The restriction to bounded sets is due to the possibility that the outcome be infinite.) The question that now arises is that of how to attribute a standard probability to the event $\mathrm{st}\,\beta \in S$. Given a *probability measure P on the class $\mathrm{Bor}({}^*\mathbb{R})$ of Borelian subsets of ${}^*\mathbb{R}$, we shall define a finite σ-additive measure pr on the class $\mathrm{Bor}(\mathbb{R})$ of Borelian subsets of $\mathbb{R}$. If P is the *probability measure associated with the *measurement of an *observable β upon a given *state, then $\mathrm{pr}\,S$ can be viewed as the probability that a *measurement of β will yield a finite outcome with standard part in the Borelian set S. It may happen that $\mathrm{pr}\,\mathbb{R} < 1$, as it was to be expected since an infinite outcome of the *measurement of β does not correspond to an outcome in $\mathbb{R}$. We cannot define $\mathrm{pr}\,S$ as $\mathrm{st}\,P(\mathrm{Mon}\,S)$, since $\mathrm{Mon}\,S$ is not in general an internal set. Nevertheless, the mapping $\mathrm{st} \circ P$ can be extended as a standard probability measure P_{L} to the σ-algebra $\mathcal{A}_{\mathrm{L}}$ spanned by $\mathrm{Bor}({}^*\mathbb{R})$ (The measure P_{L} is known as a Loeb measure; see Ref. 16. Note that this construction would remain valid even if P were only *finitely* additive.) We can easily see that $\mathrm{Mon}\,S$ is in $\mathcal{A}_{\mathrm{L}}$ for every S in $\mathrm{Bor}(\mathbb{R})$: If $S = [a,b]$, with $a \leqslant b$, we have

$$\mathrm{Mon}\,S = \bigcap_{n \in \mathbb{N}} {}^*\left[a - \frac{1}{n}, b + \frac{1}{n}\right],$$

whence $\mathrm{Mon}\,S \in \mathcal{A}_{\mathrm{L}}$. Moreover, the mapping Mon is an isomorphism of σ-rings. Hence, $\mathrm{Mon}(\mathrm{Bor}(\mathbb{R}))$ is the smallest σ-ring including every Mon$S$ where S is a compact interval of $\mathbb{R}$. Therefore, $\mathrm{Mon}(\mathrm{Bor}(\mathbb{R}))$ is contained in $\mathcal{A}_{\mathrm{L}}$, since $\mathcal{A}_{\mathrm{L}}$ is a σ-ring including such sets. Thus, we define

$$\mathrm{pr}\,S = P_{\mathrm{L}}(\mathrm{Mon}\,S),$$

for every bounded S in $\mathrm{Bor}(\mathbb{R})$, and we extend pr to $\mathrm{Bor}(\mathbb{R})$ in the canonical way. Due to the properties of P_{L} and Mon, it is clear that pr is a σ-additive measure, with $\mathrm{pr}(\mathbb{R}) \leqslant 1$.

When $S = [a,b]$ with $a \leqslant b$, we have

$$\mathrm{pr}\,S = P_{\mathrm{L}}\left(\bigcap_{n \in \mathbb{N}} {}^*\left[a - \frac{1}{n}, b + \frac{1}{n}\right]\right) = \inf_{n \in \mathbb{N}} P_{\mathrm{L}}^*\left[a - \frac{1}{n}, b + \frac{1}{n}\right] = \inf_{n \in \mathbb{N}} \mathrm{st}\,P^*\left[a - \frac{1}{n}, b + \frac{1}{n}\right]. \quad (2)$$

Since a measure on $\mathrm{Bor}(\mathbb{R})$ is determined by its values on intervals, there can be no other measure satisfying (2). The considerations above are resumed in the following proposition:

*Proposition 12: Let P be a *probability measure on the Borelian subsets of* ${}^*\mathbb{R}$. *There exists a unique positive σ-additive measure* pr *on the Borelian subsets of* $\mathbb{R}$ *such that* $\mathrm{pr}[a,b]$ *is given by Eq. (2) for all* $a,b \in \mathbb{R}$ *with* $a \leqslant b$. *Furthermore,* $\mathrm{pr}\,\mathbb{R} \leqslant 1$.

In the remainder of this section, we consider that α is an observable represented by a self-adjoint operator A in $\mathcal{H}_0$ and that β is an *observable corresponding to $\tilde{A}$. We now see how β can be viewed as a kind of nonstandard ''extension'' of α.

Proposition 10 entails $\langle \overline{\varphi} | \tilde{A} | \overline{\varphi} \rangle \approx (\varphi | A\varphi)$ for every $\varphi \in \mathcal{H}_0$. Moreover, it is readily seen that if $b = \langle \overline{\varphi} | \tilde{A} | \overline{\varphi} \rangle$ and $a = (\varphi | A\varphi)$, then $\langle \overline{\varphi} | (\tilde{A} - b)^2 | \overline{\varphi} \rangle \approx (\varphi | (A-a)^2 \varphi)$. Recalling that $\|\overline{\varphi}\| \approx \|\varphi\|$, we see that on standard states the expected values and uncertainties of α and β are identical up to

infinitesimals. If $\tilde{A}|\overline{\varphi}\rangle = b|\overline{\varphi}\rangle$ with $\varphi \in \mathcal{H}_0$, $\|\varphi\| = 1$ and $b \in {}^*\mathbb{R}$, then b is finite, because $b \approx (\varphi|A\varphi)$. Setting $a = \mathrm{st}(b)$, we obtain $A\varphi \approx b\varphi \approx a\varphi$, whence $A\varphi = a\varphi$. Therefore, a standard state where β has a definite value c (necessarily finite) is also a state where α has the definite value $\mathrm{st}(c)$. (On the other hand, if α has a definite value on a standard state, then β has an ''almost definite'' value, in the sense that the uncertainty of β is infinitesimal.) Thus, α is similar in status to a function of the *observable β; however, the function $c \mapsto \mathrm{st}(c)$ is not internal, and therefore we cannot say that α is a function of β in the strict sense.

The similitude of α to a function of β extends to states on which α has a value in an interval. In fact, given $\varphi \in \mathcal{H}_0$ and $a, b \in \mathbb{R}$ with $a < b$, Proposition 11 ensures that the condition $\varphi = E_b\varphi - E_{a^-}\varphi$ is equivalent to $\overline{\varphi} \approx F_{b+\varepsilon}\overline{\varphi} - F_{a-\varepsilon}\overline{\varphi}$, where $\varepsilon \approx 0$, $\varepsilon \geqslant \nu^{-1}$ and $(E_\lambda)_{\lambda \in \mathbb{R}}$ and $(F_\lambda)_{\lambda \in {}^*\mathbb{R}}$ are the spectral families of A and $\tilde{A}$, respectively. This means that on a standard state represented by φ the observable α is in $[a,b]$ if and only if on the same state (or on a *state represented by $u \approx \varphi$, as it can be easily seen) the *observable β is ''almost'' in ${}^*(a-\varepsilon, b+\varepsilon]$—in the sense that $f(\beta)u \approx u$, where f is the characteristic function of ${}^*(a-\varepsilon, b+\varepsilon]$. In particular, if a *measurement of β ensures that β is in ${}^*(a,b]$ and if the state following the *measurement is standard, then α is in $[a,b]$, which agrees with the interpretation of α as ''standard part of β.'' However, it may happen that such a state is not standard. Suppose now that the initial state is represented by $v \in \mathcal{H}$ and that a *measurement of $f(\beta)$ is performed, with f as above. If $v \approx \psi \in \mathcal{H}_0$, then, assuming the postulate of Lüders, the state following the *measurement is represented by the vector

$$u = F_{b+\varepsilon}v - F_{a-\varepsilon}v \approx F_{b+\varepsilon}\overline{\psi} - F_{a-\varepsilon}\overline{\psi} \approx E_b\psi - E_a\psi.$$

[This presupposes that the *measurement of $f(\beta)$ involves a minimal perturbation, in that it does not constitute a *measurement of any *observable γ such that $f(\beta)$ is function of γ but γ is not function of $f(\beta)$.]

B. Consistency with the standard theory

We shall now deal with the problem of relating the probabilistic behaviors of α and β. Suppose that a *measurement of β is performed upon a standard state, yielding the outcome c. If the state following the *measurement is standard, the *measurement can be considered as a measurement of α yielding the outcome $\mathrm{st}(c)$. When such a state is not standard, it seems natural to assume that the *measurement can still be viewed as a generalized measurement of α, yielding perhaps the outcome ''infinite.'' Insofar as only probabilities are concerned, the meaning of this last statement can be made precise by saying that the probability measure associated with the measurement of α upon a standard state coincides with the measure pr associated (according to Proposition 12) with the *measurement of β upon the same state. The following proposition shows that this is indeed the case.

*Proposition 13: Let A be a self-adjoint operator in $\mathcal{H}_0$ and let $\varphi \in \mathcal{H}_0$, with $\|\varphi\| = 1$. Let P be the *probability measure associated with the operator $\tilde{A}$ and the state represented by $\overline{\varphi}$, and let* pr *be the standard measure associated with P. For all $a, b \in \mathbb{R}$ such that $a < b$,*

$$\mathrm{pr}\,(a,b] = (\varphi|f(A)\varphi),$$

where f is the characteristic function of $(a,b]$.

Proof: Let $(E_\lambda)_{\lambda \in \mathbb{R}}$ and $(F_\lambda)_{\lambda \in {}^*\mathbb{R}}$ be the spectral families associated with A and $\tilde{A}$, respectively. For some $\rho \approx 1$ dependent on φ, we have, for $a \leqslant b$ and $n \in \mathbb{N}$,

$$P^*(a - 1/n, b + 1/n] = \rho \int_{a-1/n}^{b+1/n} d(\overline{\varphi}|F_\lambda\overline{\varphi}) \approx \langle\overline{\varphi}|F_{b+1/n}|\overline{\varphi}\rangle - \langle\overline{\varphi}|F_{a-1/n}|\overline{\varphi}\rangle.$$

By overspill, this holds for some $n \in {}^*\mathbb{N}$ such that $1/n = \varepsilon \geqslant \nu^{-1}$. By Proposition 11,

$$P^*(a-\varepsilon, b+\varepsilon] \approx (\varphi|E_b\varphi) - (\varphi|E_{a^-}\varphi),$$

whence

$$\mathrm{st}\,P^*(a-\varepsilon,b+\varepsilon]=(\varphi|f(A)\varphi)+(\varphi|E_a\varphi)-(\varphi|E_{a^-}\varphi).$$

The special case $a=b$ yields the equality

$$\mathrm{st}\,P^*(a-\varepsilon,b+\varepsilon]=(\varphi|E_a\varphi)-(\varphi|E_{a^-}\varphi).$$

On the other hand, from

$$^*\left[a-\frac{1}{n+1},\,b+\frac{1}{n+1}\right]\subset{}^*\left(a-\frac{1}{n},\,b+\frac{1}{n}\right]\subset{}^*\left[a-\frac{1}{n},\,b+\frac{1}{n}\right]$$

it follows that

$$\mathrm{pr}\,[a,b]=\inf_{n\in\mathbb{N}}\mathrm{st}\,P^*\left(a-\frac{1}{n},\,b+\frac{1}{n}\right]\approx\mathrm{st}P^*(a-\varepsilon,\,b+\varepsilon],$$

where

$$\mathrm{pr}\,[a,b]=(\varphi|f(A)\varphi)+(\varphi|E_a\varphi)-(\varphi|E_{a^-}\varphi).$$

Considering once more the special case $a=b$, we obtain

$$\mathrm{pr}\,\{a\}=(\varphi|E_a\varphi)-(\varphi|E_{a^-}\varphi),$$

and from the equality

$$\mathrm{pr}\,[a,b]=\mathrm{pr}\,(a,b]+\mathrm{pr}\,\{a\}$$

it follows that $\mathrm{pr}\,(a,b]=(\varphi|f(A)\varphi)$. □

When β is *measured upon a nonstandard state it would be meaningless to ask whether the standard measure pr coincides with the probability measure associated with α. Nevertheless, when a state is represented by a vector $u\in\mathcal{H}$ such that $u\approx\varphi$, with $\varphi\in\mathcal{H}_0$, the vector φ is necessarily unique, and it is readily seen that the function pr associated with β and u coincides with the probability measure associated with α and φ.

C. Time evolution

The Schrödinger equation in the hyperfinite model assumes the same form as in the standard theory: Time appears as a continuous parameter; to each value of t corresponds a vector u_t representing the state of the system at time t; time evolution is determined by a Hermitian operator H_h, in such a way that $u_t=e^{-itH_\mathrm{h}}u_0$ for all t. We must show that the predictions of the hyperfinite model regarding time evolution are consistent with those of the standard theory. If at time $t=0$ the system is in a standard state represented by $\varphi_0\in\mathcal{H}_0$, then, according to the standard theory, at time t the system is in a standard state represented by $\varphi_t=e^{-itH}\varphi_0$, where H is a self-adjoint operator in $\mathcal{H}_0$. According to the hyperfinite model, the state is represented by $\overline{\varphi_0}$ at $t=0$ and by $u_t=e^{-itH_\mathrm{h}}\overline{\varphi_0}$ at time t. We consider that $H_\mathrm{h}=\tilde{H}$. Consistency demands that at time t the vector u_t be "equivalent" to φ_t, in the sense that all standard-scale predictions concerning probabilities and further time evolution should be the same regardless of whether the state at time t is represented by u_t or by φ_t. To ensure this it suffices that $u_t\approx\overline{\varphi_t}$: In such a case, the standard probability associated with measurements upon u_t or φ_t are the same (Proposition 13 and subsequent considerations); as to the time evolution after time t, Proposition 14 below shows that it also leads to infinitely near states, since the hypothesis is $u_0\approx\overline{\varphi_0}$ rather than $u_0=\overline{\varphi_0}$.

Proposition 14: Let H be a self-adjoint operator in $\mathcal{H}_0$ and let $u_0\in\mathcal{H}$, $\varphi_0\in\mathcal{H}_0$. If $u_0\approx\varphi_0$, then

$$u_t \approx e^{-itH}\varphi_0$$

for every finite $t \in {}^*\mathbb{R}$, *where* $u_t = e^{-it\tilde{H}}u_0$.

Proof: Set $\varphi_t = e^{-itH}\varphi_0$, $u_t = e^{-it\tilde{H}}u_0$, and $v_t = \varphi_t - u_t$, for all $t \in {}^*\mathbb{R}$. Taking into account that e^{-itH} and $e^{-it\tilde{H}}$ are unitary operators on $\mathcal{H}_0$ and $\mathcal{H}$, respectively, we obtain

$$(v_t|v_t) = (\varphi_0|\varphi_0) + (u_0|u_0) - (e^{-it\tilde{H}}u_0|e^{-itH}\varphi_0) - (e^{-itH}\varphi_0|e^{-it\tilde{H}}u_0).$$

Hence,

$$\frac{d}{dt}(v_t|v_t) = (i\tilde{H}e^{-it\tilde{H}}u_0|e^{-itH}\varphi_0) + (e^{-it\tilde{H}}u_0|iHe^{-itH}\varphi_0) + (iHe^{-itH}\varphi_0|e^{-it\tilde{H}}u_0) + (e^{-itH}\varphi_0|i\tilde{H}e^{-it\tilde{H}}u_0).$$

We have

$$(\tilde{H}e^{-it\tilde{H}}u_0|e^{-itH}\varphi_0) = (P\tilde{H}e^{-it\tilde{H}}u_0|e^{-itH}\varphi_0) = (\tilde{H}e^{-it\tilde{H}}u_0|Pe^{-itH}\varphi_0) = (e^{-it\tilde{H}}u_0|\tilde{H}Pe^{-itH}\varphi_0).$$

Moreover, $(e^{-it\tilde{H}}u_0|He^{-itH}\varphi_0) = (e^{-it\tilde{H}}u_0|PHe^{-itH}\varphi_0)$. Let $\phi = e^{-itH}\varphi_0$. It follows from Propositions 10 and 3 that $\tilde{H}\overline{\phi} \approx H\phi \approx PH\phi$. Thus $\tilde{H}Pe^{-itH}\varphi_0 \approx PHe^{-itH}\varphi_0$, whence

$$(e^{-it\tilde{H}}u_0|\tilde{H}Pe^{-itH}\varphi_0) \approx (e^{-it\tilde{H}}u_0|PHe^{-itH}\varphi_0),$$

since the norm of $e^{-it\tilde{H}}u_0$ is finite. Thus, $(d/dt)(v_t|v_t) \approx 0$ for all $t \in {}^*\mathbb{R}$, whence

$$|(v_\tau|v_\tau) - (v_0|v_0)| = \left| \int_0^\tau \frac{d}{dt}(v_t|v_t)\, dt \right| < \tau\varepsilon$$

for every $\tau \in {}^*\mathbb{R}$ and every $\varepsilon \in \mathbb{R}^+$. For finite τ, this entails $(v_\tau|v_\tau) \approx (v_0|v_0)$. By hypothesis, $(v_0|v_0) \approx 0$. Therefore, for every finite $t \in {}^*\mathbb{R}$,

$$(v_t|v_t) \approx 0,$$

$$v_t \approx 0,$$

$$\varphi_t - u_t \approx 0.$$

This completes the proof. □

It is easy to see that the proof of Proposition 14 depends on the definition of $\tilde{H}$ only through the property $\tilde{H}\overline{\phi} \approx H\phi$ (where $\phi \in \mathcal{H}_0$); thus, the statement of Proposition 14 still holds when $\tilde{H}$ is replaced by any Hermitian operator H satisfying that condition.

V. THE MULTIDIMENSIONAL CASES

Until now we have considered the simple case of $\mathcal{H}_0 = L^2(\mathbb{R})$. It is not difficult to extend the previous results to the Hilbert space associated with a system constituted by a finite number of distinguishable particles.

When $\mathcal{H}_0 = \mathbb{C}^n$, with $n \in \mathbb{N}$, we define $\mathcal{H} = {}^*\mathbb{C}^n$. Thus, we can associate with $\varphi \in \mathcal{H}_0$ the vector $\overline{\varphi} = \varphi \in \mathcal{H}$. Every normalized vector of $\mathcal{H}$ is a finite superposition of standard vectors, with finite coefficients. Moreover, every such vector is near-standard: If $u = \Sigma_{j=1}^n c_j\varphi_j$, with $\varphi_1, \ldots, \varphi_n \in \mathcal{H}_0$ and $c_1, \ldots, c_n$ finite *complex numbers, then it is readily seen that $u \approx \varphi \in \mathcal{H}_0$, where $\varphi = \Sigma_{j=1}^n \mathrm{st}(c_j)\varphi_j$. Hence, the features of $\mathcal{H}$ are essentially the same as those of $\mathcal{H}_0$.

The space $\mathcal{H}_0$ in the general case is a tensor product $\otimes_i \mathcal{H}_i$ of a finite number of Hilbert spaces; moreover, one can assume that each $\mathcal{H}_i$ is either $L^2(\mathbb{R})$ or $\mathbb{C}$. [Recall that, for example, $L^2(\mathbb{R}^2) \cong L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$.]

Denote by $\overline{\mathcal{H}_i}$ the space ${}^*\mathbb{C}$ (if $\mathcal{H}_i = \mathbb{C}$) or the space defined in Sec. II A (if $\mathcal{H}_i = L^2(\mathbb{R})$). For each i, the space $\mathcal{H}_i$ is a subspace of ${}^*\mathcal{H}_i$, and $\overline{\mathcal{H}_i}$ is also a subspace of ${}^*\mathcal{H}_i$. Hence, the tensor product $\otimes_i \overline{\mathcal{H}_i}$ is a subspace of ${}^*\mathcal{H}_0 = \otimes_i {}^*\mathcal{H}_i$, which we denote by $\mathcal{H}$. We consider henceforth the case of a tensor product of only two factors, for ease of notation.

The mapping $\varphi \mapsto \overline{\varphi}$ is defined by $\overline{\varphi} = P\varphi$, where P is the orthogonal projector of ${}^*\mathcal{H}_0$ onto $\mathcal{H}$. We can see that $P = P_1 \otimes P_2$, where each P_i is the orthogonal projector of ${}^*\mathcal{H}_i$ onto $\overline{\mathcal{H}_i}$: Let $\varphi = \varphi_1 \otimes \varphi_2$, with $\varphi_1 \in {}^*\mathcal{H}_1$ and $\varphi_2 \in {}^*\mathcal{H}_2$. Then,

$$\varphi = (\overline{\varphi_1} + \overline{\varphi_1}^{\perp}) \otimes (\overline{\varphi_2} + \overline{\varphi_2}^{\perp}) = (\overline{\varphi_1} \otimes \overline{\varphi_2}) + (\overline{\varphi_1} \otimes \overline{\varphi_2}^{\perp}) + (\overline{\varphi_1}^{\perp} \otimes \overline{\varphi_2}) + (\overline{\varphi_1}^{\perp} \otimes \overline{\varphi_2}^{\perp}).$$

Recalling the definition of inner product on a tensor product of Hilbert spaces,[15] we observe that the first term in the sum above is orthogonal to the other three terms—for example,

$$(\overline{\varphi_1} \otimes \overline{\varphi_2} | \overline{\varphi_1} \otimes \overline{\varphi_2}^{\perp}) = (\overline{\varphi_1} | \overline{\varphi_1})(\overline{\varphi_2} | \overline{\varphi_2}^{\perp}) = (\overline{\varphi_1} | \overline{\varphi_1}) \cdot 0.$$

Therefore, $P\varphi = \overline{\varphi_1} \otimes \overline{\varphi_2}$, and hence $P = P_1 \otimes P_2$.

The identity $\overline{\varphi} = \overline{\varphi_1} \otimes \overline{\varphi_2}$ entails $\overline{\varphi} \approx \varphi$, since $\overline{\varphi_1} \otimes \overline{\varphi_2}$ equals $\varphi_1 \otimes \varphi_2$ plus three infinitesimal terms, which are tensor products of infinitesimals by finite normed vectors. The relation $\overline{\varphi} \approx \varphi$ extends immediately to finite superpositions of vectors of the above form. Let now φ be a general element of $\mathcal{H}_0$. There exists a sequence $(\varphi_n)_{n \in \mathbb{N}}$ of vectors of $\mathcal{H}_0$ such that $\varphi_n \to \varphi$ and $P\varphi_n \approx \varphi_n$. Given $\varepsilon \in \mathbb{R}^+$, we have $\|\varphi - \varphi_n\| < \varepsilon$ for some $n \in \mathbb{N}$. On the other hand,

$$P\varphi - \varphi = P(\varphi - \varphi_n) + (P\varphi_n - \varphi_n) + (\varphi_n - \varphi).$$

Since $\|\varphi - \varphi_n\| < \varepsilon$, $\|P\| = 1$, and $\|P\varphi_n - \varphi_n\| \approx 0$, we obtain $\|P\varphi - \varphi\| \leqslant 3\varepsilon$, whence $P\varphi \approx \varphi$. Thus we see that Proposition 3 holds when $\mathcal{H}_0 = \mathcal{H}_1 \otimes \mathcal{H}_2$. Proposition 2 is a simple consequence thereof. Another obvious consequence is that the mapping $\varphi \mapsto \overline{\varphi}$ is one-to-one.

Given be a self-adjoint operator A on $\mathcal{H}_0 = \mathcal{H}_1 \otimes \mathcal{H}_2$, the definition of Sec. III B still makes sense: For $u \in \overline{\mathcal{H}_1} \otimes \overline{\mathcal{H}_2}$,

$$\tilde{A}u = P \int_{-\nu}^{\nu} \lambda \, dE_\lambda u.$$

Observe that the constant ν introduced in Sec. III B depends on the Hilbert space considered, but we may assume without loss of generality that ν is the same for the spaces $\mathcal{H}_0$, $\mathcal{H}_1$ and $\mathcal{H}_2$. Propositions 7–14 hold in the multidimensional case, as the proofs thereof depend on Propositions 2 and 3.

It remains to see how the operator representing an observable in a given system relates to the operator representing the same observable in a compound system (see Ref. 15): Given a self-adjoint operator A_1 in $\mathcal{H}_1$, consider the self-adjoint operator in $\mathcal{H}_1 \otimes \mathcal{H}_2$ defined by

$$B_1 = \int_{-\infty}^{+\infty} \lambda \, d(E_{1\lambda} \otimes 1),$$

where $(E_{1\lambda})_{\lambda\in\mathbb{R}}$ is the spectral family associated with A_1. (When A_1 is bounded, B_1 is simply the tensor product $A_1\otimes 1$.) We show that $\tilde{B}_1=\tilde{A}_1\otimes 1$; it suffices to prove that $\tilde{B}_1 u=(\tilde{A}_1\otimes 1)u$ for $u=u_1\otimes u_2$ with $u_1\in\overline{\mathcal{H}_1}$ and $u_2\in\overline{\mathcal{H}_2}$: Recalling the linearity and continuity properties of the tensor products of vectors and operators, we have

$$\begin{aligned}\tilde{B}_1 u &= P\int_{-\nu}^{\nu}\lambda\, d(E_{1\lambda}\otimes 1)(u_1\otimes u_2)=\int_{-\nu}^{\nu}\lambda(P_1\otimes P_2)\, d(E_{1\lambda}u_1\otimes u_2)=\int_{-\nu}^{\nu}\lambda\, d(P_1E_{1\lambda}u_1\otimes P_2u_2)\\ &=\int_{-\nu}^{\nu}\lambda\, d(P_1E_{1\lambda}u_1\otimes u_2)=\left(\int_{-\nu}^{\nu}\lambda\, d(P_1E_{1\lambda}u_1)\right)\otimes u_2=P_1\int_{-\nu}^{\nu}\lambda\, dE_{1\lambda}u_1\otimes u_2=\tilde{A}_1u_1\otimes u_2\\ &=(\tilde{A}_1\otimes 1)u.\end{aligned}$$

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APPENDIX

We work in a superstructure $\langle V(\mathbb{R}),{}^*V(\mathbb{R}),*\rangle$. Elements of $V(\mathbb{R})$ are called *standard*, and are mapped by $*$ to elements of ${}^*V(\mathbb{R})$. As usual, we omit stars when denoting the images under $*$ of standard functions or binary operations and relations. Elements of standard sets are called *internal*, and noninternal sets in $V({}^*\mathbb{R})$ are called *external*. We recall that the prefix ''hyper'' is used as a substitute for ''$*$.''

A number $x\in{}^*\mathbb{R}$ is said *finite* if there exists $m\in\mathbb{N}$ such that $|x|<m$. Each finite $x\in{}^*\mathbb{R}$ can be uniquely decomposed as $x=r+\varepsilon$, where $r\in\mathbb{R}$ and ε is infinitesimal; r is called the standard part of x and is denoted by $\mathrm{st}(x)$. If $x,y\in{}^*\mathbb{R}$ are such that $x-y$ is infinitesimal, then we say that x is infinitely close to y, and write $x\approx y$. More generally, if x and y are in a *Hilbert space we say that $x\approx y$ when $\|x-y\|\approx 0$. We write $x\lesssim y$ whenever $x<y$ or $x\approx y$.

Recall that a family of sets satisfies the finite intersection property if all finite intersections of elements of the family are nonempty. We assume the superstructure $\langle V(\mathbb{R}),{}^*V(\mathbb{R}),*\rangle$ to be saturated, i.e., given any family $\mathcal{A}$ of internal sets with cardinality less than the cardinality of $V(\mathbb{R})$, if $\mathcal{A}$ has the finite intersection property, then $\cap\mathcal{A}\neq\varnothing$.

For a survey of nonstandard analysis, see Refs. 10, 17, and 2.

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Dissipative Schrödinger–Poisson systems

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We deal with a stationary, dissipative Schrödinger–Poisson system which allows for a current flow through an open, spatially one-dimensional quantum system determined by a dissipative Schrödinger operator. This dissipative Schrödinger operator can be regarded as a pseudo-Hamiltonian of the corresponding open quantum system. The (self-adjoint) dilation of the dissipative operator serves as a quasi-Hamiltonian of the system which is used to define physical quantities such as density and current for the open quantum system. The thus defined charge density in its dependence on the electrostatic potential is the nonlinear term in Poisson's equation. We prove that the dissipative Schrödinger–Poisson system always admits a solution and all solutions are included in a ball the radius of which depends only on the data of the problem. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Schrödinger–Poisson systems describe, e.g., the nonlinear interaction between an electric field and charged carriers, electrons and holes in a semiconductor device, within this electric field (see, e.g., Refs. 28, 21, 22, and 10). In the form considered in this article a Schrödinger–Poisson system can be regarded as a nonlinear Poisson equation

$$-\nabla\cdot(\epsilon\nabla\varphi)=q(C+\mathcal{N}_+(V_+)-\mathcal{N}_-(V_-)),\quad V_\pm=V_0^\pm\pm q\varphi, \tag{1}$$

where φ denotes the electrostatic potential and $V_0^\pm$ are prescribed potentials, the band edge offsets; ϵ is the position-dependent permittivity tensor; q is the magnitude of the elementary charge; and C is a position-dependent density of fixed charges (ionized dopants). $\mathcal{N}_\pm$ are operators which associate a density of positive and negative charges (electrons and holes) to a potential which essentially is the electrostatic potential. We will regard a system confined to a bounded spatial domain Ω and (1) has to be supplemented by boundary conditions modeling the way the electrical field inside Ω is contacted to its environment (see Refs. 28 and 10).

In the framework of van Roosbroeck's system which describes the motion of electrons and holes within a semiconductor device due to drift and diffusion, the nonlinear Poisson equation (1) has been regarded with Nemytzkii operators $\mathcal{N}_\pm$ of the form

$$\mathcal{N}_\pm(V)(\mathbf{x})=c_\pm(\mathbf{x})\mathfrak{F}\left(\frac{1}{T}(q\phi_\pm(\mathbf{x})\pm V(\mathbf{x}))\right) \tag{2}$$

(see Refs. 28 and 10); Boltzmann's constant is scaled to 1. In this context we assume that the temperature T, the density of states $c_\pm$, and the electrochemical potentials $\phi_\pm$ are given functions and $\mathfrak{F}$ is a statistical distribution function, e.g., the exponential function

$$\mathfrak{F}(\zeta)=\exp(\zeta) \tag{3}$$

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or Fermi's integral to the index $\frac{1}{2}$

$$\mathfrak{F}(\zeta)=\frac{2}{\sqrt{\pi}}\int_0^\infty d\xi\,\frac{\sqrt{\xi}}{1+\exp(\xi-\zeta)},\quad \zeta\in\mathbb{R}. \tag{4}$$

With Boltzmann and Fermi–Dirac statistics, (3) and (4), respectively, (1), (2), are an operator equation in a Sobolev space which is determined by the boundary conditions imposed on the electrostatic potential. The nonlinear Poisson operator involved is strongly monotone and boundedly Lipschitz continuous, hence, the nonlinear Poisson equation has a unique solution. Obviously, this result does neither depend on the Nemytzkii structure (2) of the operators $\mathcal{N}_\pm$ nor the special functions (3), (4). If $\mathcal{N}_\pm$ are anti-monotone and boundedly Lipschitz continuous operators, then the nonlinear Poisson equation (1) has a unique solution (see, e.g., Ref. 11, Chap. III.2.1).

Statistical distribution functions like (3), (4) are based upon the assumption that the carriers of charge, electrons, and holes can move freely in all space directions. However, in nanostructured materials (quantum-wells, -wires, and -dots) this model of a three-dimensional electron-hole gas is not adequate any more. Instead the densities of charge carriers have to be directly computed by quantum mechanical expressions from the spectral representation of an appropriate Hamilton operator (see, e.g., Refs. 6, 29, 10, and 23).

Let us first consider the case of closed quantum systems situated in the bounded domain Ω for the system of positively and negatively charged carriers. These systems can be described by one-electron Hamiltonians in effective mass approximation (Ben–Daniel–Duke form) with an effective potential V:

$$H_\pm(V)\psi=-\tfrac{1}{2}\nabla\cdot(m_\pm^{-1}\nabla\psi)+V\psi, \tag{5}$$

where $\mathrm{dom}(H_\pm)$ is a Sobolev space which is determined by self-adjoint (homogeneous) boundary conditions, including mixed ones, on $\partial\Omega$. $m_\pm$ denotes the position-dependent effective mass tensor of holes and electrons, respectively; $\hbar$ is scaled to 1. In general V is a Kohn–Sham potential (see e.g., Refs. 13, 14, and 27 and the references cited there). The collective behavior of holes and electrons is described by density matrices $\varrho_\pm$. In this article we investigate stationary Schrödinger–Poisson systems, i.e., we regard density matrices which are steady states. If there are equilibrium distribution functions $f_\pm$ such that the operators

$$\varrho_\pm(V)=f_\pm(H_\pm(V))$$

are self-adjoint, non-negative, and nuclear, i.e., density matrices for all admissible potentials V, then the densities $\mathcal{N}_\pm(V)$ of positively and negatively charged carriers, respectively, are given by the Radon–Nikodým derivative of the absolutely continuous measures (with respect to the Lebesgue measure)

$$\int_\omega d\mathbf{x}\,\mathcal{N}_\pm(V)(\mathbf{x})=\mathrm{tr}(f_\pm(H_\pm(V))\chi_\omega), \tag{6}$$

respectively, where χ_ω denotes the indicator function of a set $\omega\subset\Omega$. If the functions $f_\pm$ are positive, strictly monotone, and sufficiently rapidly decreasing, then one can prove that the corresponding nonlinear Poisson equation (1) with (6) has a unique solution (see Refs. 5, 24, and 25), even for heterogeneous material compositions and mixed Dirichlet and Neumann boundary conditions for Schrödinger's operator (see Refs. 13 and 14). If the Schrödinger operators (5) include in addition to the electrostatic potential an exchange-correlation potential, then one still obtains the existence of solutions of the corresponding Schrödinger–Poisson system (see Refs. 13 and 14).

Up to this point we have supposed that the systems of positively and negatively charged carriers are in equilibrium, i.e., the corresponding quantum systems on the bounded domain occupied by the device are closed. In order to describe semiconductor devices operating far from equilibrium, we pass to open quantum systems on the bounded device domain (see also Refs. 9, 4,

and 26). In Refs. 13 and 14 we proposed non-self-adjoint boundary conditions for the Schrödinger operators (5) which are induced by a potential flow acting on the spatial boundary of the open quantum system; the spectral theory for the associated non-self-adjoint Schrödinger-type operators has been developed in Ref. 15. For these non-self-adjoint Schrödinger-type operators the notion of carrier density as sketched above is not valid anymore. However, if the boundary conditions are such that the operator becomes dissipative (see Ref. 15), then one can use the dilation theory for dissipative operators to overcome difficulties arising from the non-self-adjointness. Indeed, the dissipative Schrödinger-type operator can be regarded as a pseudo-Hamiltonian (see Ref. 7, Chap. 4.1) and its dilation, i.e., minimal self-adjoint extension, as a quasi-Hamiltonian. The quasi-Hamiltonian describes a closed quantum system containing the original open one, which is, additionally, in some sense minimal. Then steady states, carrier and current densities can be defined with respect to that larger closed system but have in fact the same meaning as above. In particular, the density matrix describes now the collective behavior of electrons and holes in the larger closed system and not only in the open system. Based upon an explicit representation of the dilation (see Ref. 16), we have established the notion of carrier and current density for this kind of non-self-adjoint Schrödinger-type operator in the spatially one-dimensional case (see Ref. 17). We prove in this article that the corresponding stationary dissipative Schrödinger–Poisson system (see Problem 4.4 for the rigorous setup of the problem), i.e., the nonlinear Poisson equation with the charged carrier densities associated with the quasi-Hamiltonian of some dissipative Schrödinger-type operators, always has a solution in the spatially one-dimensional case. However, we do not get uniqueness of solutions.

At first glance the dissipative Schrödinger–Poisson system seems to be an artificial model with little reference to applications in science. This is not so, however, as the following closer look reveals. In Ref. 1 we have investigated the widely used Schrödinger–Poisson system with quantum transmitting boundary conditions (see also Refs. 9 and 4). The quantum transmitting Schrödinger–Poisson system decomposes into dissipative Schrödinger–Poisson systems (see Ref. 1). More precisely, there is a dissipative Schrödinger–Poisson system affiliated to each energy on the continuous scale of the quantum transmitting Schrödinger–Poisson system. Thus the boundary coefficients of the Schrödinger operator depend on the energy, which leads to a family of dissipative Schrödinger-type operators labeled by the energy. The boundary conditions for Schrödinger's operator with respect to which we investigate the Schrödinger–Poisson system in this article serve as a single energy approximation of a corresponding Schrödinger–Poisson system with quantum transmitting boundary conditions (see Ref. 1).

We note that dissipative Schrödinger–Poisson systems also have been considered in a nonstationary setup (see Refs. 12 and 19). In Ref. 2 a dissipative Schrödinger-type operator has been investigated which includes additional terms modeling generation and recombination of particles.

The article is organized as follows: In Sec. II we rigorously define the Schrödinger-type operators (see also Ref. 15), briefly introduce their dilations and generalized eigenfunction expansions (see also Ref. 16), and recall the definition of the carrier density given in Ref. 17. In Sec. III we introduce, following Ref. 13, the (nonlinear) carrier density operator assigning to the potential in a Schrödinger operator the corresponding carrier density. The carrier density operator is continuous; the proof is based upon a relation between the generalized Fourier transform and the Lax–Phillips wave operator. Section IV deals with the rigorous setup of the dissipative Schrödinger–Poisson system, *a priori* estimates, and, finally, the existence of solutions.

II. NOTIONS AND DEFINITIONS

In this section we provide essential notions which are needed in the next sections to investigate the carrier density operator and to give a precise definition of the dissipative Schrödinger–Poisson system and its solution.

A. Notations

The Schrödinger–Poisson system will be regarded on the interval $\Omega=(a,b)$. By L^1 we denote the space of real-valued, Lebesgue integrable functions on the interval $[a,b]$. The space of

real-valued, Lebesgue measurable, and essentially bounded functions on $[a,b]$ will be denoted by L^∞. In order to avoid confusion we denote the space of complex-valued, square integrable functions on the interval $[a,b]$ by $\mathfrak{H}$ and write $(\cdot,\cdot)$ for the scalar product in $\mathfrak{H}$. Furthermore, we denote by $W^{1,2}$ the usual complex Sobolev space $W^{1,2}(a,b)$ and by $C[a,b]$ the space of complex-valued, continuous functions on $[a,b]$.

If $\mathcal{H}_1,\mathcal{H}_2$ are Hilbert spaces, then $\mathfrak{L}_1(\mathcal{H}_1;\mathcal{H}_2)$ denotes the space of nuclear operators from $\mathcal{H}_1$ into $\mathcal{H}_2$ and $\mathfrak{L}_2(\mathcal{H}_1;\mathcal{H}_2)$ denotes the space of Hilbert Schmidt operators, each with its canonic norm. We abbreviate $\mathfrak{L}_1(\mathcal{H};\mathcal{H})=\mathfrak{L}_1(\mathcal{H})$ and $\mathfrak{L}_2(\mathcal{H};\mathcal{H})=\mathfrak{L}_2(\mathcal{H})$. For Banach spaces X and Y, we denote by $\mathfrak{B}(X;Y)$ the space of all linear, continuous operators from X into Y. If $X=Y$, we write $\mathfrak{B}(X)$.

B. Poisson's equation

One ingredient of the Schrödinger–Poisson system is, of course, Poisson's equation which determines the electrostatic potential φ on the interval (a,b):

$$-\frac{d}{dx}\left(\epsilon(x)\frac{d}{dx}\varphi(x)\right)=q(C(x)+u^+(x)-u^-(x)),\quad x\in[a,b], \tag{7}$$

where u^+ and u^- are the densities of holes and electrons, respectively, q is the magnitude of the elementary charge, C is the doping profile of the semiconductor device, and ϵ is the dielectric permittivity. We regard the following mixed boundary conditions for Poisson's equation (7),

$$\begin{aligned}\varphi(x)&=\varphi_\Gamma(x),\quad \text{if } x\in\Gamma,\\ -\epsilon(x)\frac{d}{dx}\varphi(x)&=k(x)(\varphi(x)-\varphi_\Gamma(x)),\quad \text{if } x\in\{a,b\}\backslash\Gamma,\end{aligned} \tag{8}$$

where $\Gamma\subseteq\{a,b\}$. The function φ_Γ, defined on $[a,b]$, represents the boundary values given on Γ and the inhomogeneous boundary conditions of third kind on $\{a,b\}\backslash\Gamma$. The function $k\geqslant 0$ is defined on $\{a,b\}$. These boundary conditions describe the coupling of the semiconductor device to its environment. In particular, the Dirichlet boundary part represents Ohmic (metal) contacts of the semiconductor device (see, e.g., Refs. 28 and 10).

C. Schrödinger-type operators

The densities u^+ and u^- of holes and electrons appearing on the right-hand side of Poisson's equation (7) are determined by density matrices ϱ_+ and ϱ_- on the one hand and the spectral properties of Schrödinger-type operators H_+ and H_- on the other. Following the proposal in Ref. 13 we consider for each species (holes and electrons) a non-self-adjoint Schrödinger-type operator $H(V)$ (we drop here the index "+" and "−") on the Hilbert space $\mathfrak{H}$. It is defined by

$$\mathrm{dom}(H(V))=\left\{ g\in W^{1,2}:\ \begin{array}{l}\dfrac{1}{m}g'\in W^{1,2},\\ \dfrac{1}{2m(a)}g'(a)=-\kappa_a g(a),\\ \dfrac{1}{2m(b)}g'(b)=\kappa_b g(b)\end{array}\right\} \tag{9}$$

and

$$(H(V)g)(x)=(l(g))(x),\quad g\in\mathrm{dom}(H(V)), \tag{10}$$

where

$$(l(g))(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}g(x) + V(x)g(x) \tag{11}$$

(see Refs. 15 and 16). With respect to the coefficients in (9)–(11) we assume the function m, i.e., the effective mass, is positive and obeys $m, 1/m \in L^\infty$; the boundary coefficients κ_a, κ_b are from the upper half-plane $\mathbb{C}_+ := \{z \in \mathbb{C} : \Im(z) > 0\}$. Furthermore, it is assumed hereafter that the occurring potentials V are from L^∞. We already know the following about the operators $H(V)$.

Proposition 2.1: (See Ref. 15, Sec. 5, in particular Theorem 5.2.) The operator $H(V)$ is maximal dissipative and completely non-self-adjoint. The spectrum of $H(V)$ consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity. Since the operator $H(V)$ is completely non-self-adjoint there do not exist real eigenvalues.

In order to prove resolvent estimates for the Schrödinger-type operator $H(V)$ we regard the quadratic form associated with $H(V)$ as a perturbation of a quadratic form which is independent of the potential V and we derive relative bounds with respect to the latter. To this end we introduce the sesquilinear form $\mathfrak{h}_0$,

$$\mathfrak{h}_0[g,f] := \int_a^b dx \left\{ \frac{1}{2m(x)} g'(x)\overline{f'(x)} + g(x)\overline{f(x)} \right\}, \quad f,g \in \mathrm{dom}(\mathfrak{h}_0) = W^{1,2}$$

(see Ref. 15). The form $\mathfrak{h}_0$ is symmetric and non-negative. Since $\mathfrak{h}_0$ is closed there is a unique self-adjoint operator H_0 with the representation

$$\mathfrak{h}_0[g,f] = (H_0 g, f), \quad g \in \mathrm{dom}(H_0), \quad f \in \mathrm{dom}(\mathfrak{h}_0). \tag{12}$$

This operator H_0 can be explicitly described by (9)–(11) specifying $\kappa_a = \kappa_b = 0$ and $V \equiv 1$. Obviously, there is $H_0 \geqslant I$. In order to obtain further properties of the operators $H(V)$ we introduce certain quadratic forms in terms of which $H(V)$ can be understood as a (form) perturbation of H_0. We start with the boundary form $\mathfrak{t}_{\partial\Omega}$ defined by

$$\mathfrak{t}_{\partial\Omega}[g,f] := -\kappa_a g(a)\overline{f(a)} - \kappa_b g(b)\overline{f(b)}, \quad f,g \in \mathrm{dom}(\mathfrak{t}_{\partial\Omega}) = W^{1,2}.$$

Next we define the potential form $\mathfrak{t}_V$,

$$\mathfrak{t}_V[g,f] := \int_a^b dx\, V(x) g(x)\overline{f(x)}, \quad f,g \in \mathrm{dom}(\mathfrak{t}_V) = W^{1,2},$$

and the form sum

$$\mathfrak{t}_{\partial\Omega,V} := \mathfrak{t}_{\partial\Omega} + \mathfrak{t}_V, \quad \mathrm{dom}(\mathfrak{t}_{\partial\Omega,V}) = W^{1,2}.$$

As usual, we will denote the corresponding quadratic forms by the same symbols with a single argument. In the following we will supply relative form estimates for $\mathfrak{t}_{\partial\Omega}$, $\mathfrak{t}_V$, and $\mathfrak{t}_{\partial\Omega,V}$ with respect to $\mathfrak{h}_0$.

Proposition 2.2: (See Ref. 15, Sec. 2, in particular 2.14–18.) The quadratic form $\mathfrak{t}_{\partial\Omega,V}$ is infinitesimally small with respect to $\mathfrak{h}_0$, i.e., there is a constant c such that for each $\delta > 0$

$$|\mathfrak{t}_{\partial\Omega,V}[f]| \leqslant \delta \mathfrak{h}_0[f] + \left(\frac{c}{\delta} + \|V\|_{L^\infty} \right) \|f\|_{\mathfrak{H}}^2. \tag{13}$$

Hence, the quadratic form corresponding to the sesquilinear form $\mathfrak{h}_V$ given by

$$\mathfrak{h}_V[g,f] := \mathfrak{h}_0[g,f] + \mathfrak{t}_{\partial\Omega,V}[g,f] - (g,f) = \mathfrak{h}_0[g,f] + \mathfrak{t}_{\partial\Omega,V-1}[g,f], \quad f,g \in \mathrm{dom}(\mathfrak{h}_V) = W^{1,2},$$

is closed and sectorial. Consequently, there is a (unique) maximal sectorial operator $H(V)$ *such that the representation* $\mathfrak{h}_V[g,f]=(H(V)g,f)$ *is valid for* $g\in\mathrm{dom}(H(V))$ *and* $f\in\mathrm{dom}(\mathfrak{h}_V)$. *In particular, the thus defined operator* $H(V)$ *coincides with the operator given by (9)–(11).*

Remark 2.3: The constant c in (13) can be specified as

$$c:=\frac{(|\kappa_a|+|\kappa_b|)^2\mathfrak{g}_1^4\tilde{m}}{2},\quad \tilde{m}:=\max\{1,\|m\|_{L^\infty}\},\tag{14}$$

where $\mathfrak{g}_1$ *is the Gagliardo–Nirenberg constant, i.e.,*

$$\|\psi\|_{C[a,b]}\leqslant\mathfrak{g}_1\|\psi\|_{W^{1,2}}^{1/2}\|\psi\|_{\mathfrak{H}}^{1/2}\quad\text{for all}\quad\psi\in W^{1,2}.\tag{15}$$

Next we introduce an operator $B_\mu(V)$ in order to give a factorization of the resolvent of $H(V)$ (see Lemma 2.5). For $V\in L^\infty$ and $\mu\geqslant 0$ the sesquilinear form

$$b_\mu(V)[f,g]:=\mathfrak{t}_{\partial\Omega,V-1}[(H_0+\mu)^{-1/2}f,(H_0+\mu)^{-1/2}g],\quad f,g\in\mathrm{dom}(b_\mu(V))=\mathfrak{H},$$

defines a bounded operator $B_\mu(V)$ on $\mathfrak{H}$. For the following considerations the norm of the operator $B_\mu(V)$ is of fundamental interest.

Lemma 2.4: If $V\in L^\infty$ *and* $\mu\geqslant 0$, *then*

$$\|B_\mu(V)\|_{\mathfrak{B}(\mathfrak{H})}\leqslant\delta+\left(\frac{c}{\delta}+1+\|V\|_{L^\infty}\right)\frac{1}{1+\mu}\quad\text{for all}\quad\delta\in(0,1)\tag{16}$$

with c according to (14). In particular, if

$$\mu\geqslant 4c+2+2\|V\|_{L^\infty},\tag{17}$$

then $\|B_\mu(V)\|_{\mathfrak{B}(\mathfrak{H})}<1$ *and*

$$\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\leqslant\frac{2(\mu+1)}{\mu-1-4c-2\|V\|_{L^\infty}}.\tag{18}$$

Proof: Equation (16) follows from (13). Setting $\delta=\frac{1}{2}$ we get from (16) and (17) that $\|B_\mu(V)\|_{\mathfrak{B}(\mathfrak{H})}<1$. The last assertion follows from (16), (17) and the representation of the resolvent by Neumann's series. □

Lemma 2.5: If $V\in L^\infty$ *and* $\mu\geqslant 4c+2+2\|V\|_{L^\infty}$ *with c given by (14), then*

$$(H(V)+\mu)^{-1}=(H_0+\mu)^{-1/2}(I+B_\mu(V))^{-1}(H_0+\mu)^{-1/2}.\tag{19}$$

Proof: For any $f,g\in W^{1,2}$ and $\mu>0$ one has

$$\mathfrak{h}_V[g,f]+\mu(g,f)=((H_0+\mu)^{1/2}g,(H_0+\mu)^{1/2}f)+\mathfrak{t}_{\partial\Omega,V-1}[g,f],$$

which yields

$$\mathfrak{h}_V[g,f]+\mu(g,f)=((I+B_\mu(V))(H_0+\mu)^{1/2}g,(H_0+\mu)^{1/2}f).$$

From Lemma 2.4 we get $\|B_\mu(V)\|_{\mathfrak{B}(\mathfrak{H})}<1$. Hence, the inverse operator of $I+B_\mu(V)$ exists and is bounded. Therefore, the definition

$$R_\mu(V):=(H_0+\mu)^{-1/2}(I+B_\mu(V))^{-1}(H_0+\mu)^{-1/2}$$

is justified. Since $R_\mu(V)g\in W^{1,2}$ for all $g\in\mathfrak{H}$ we have

$$\mathfrak{h}_V[R_\mu(V)g,f]+\mu(R_\mu(V)g,f)=((H_0+\mu)^{1/2}R_\mu(V)g,(H_0+\mu)^{1/2}f+\mathfrak{t}_{\partial\Omega,V-1}[R_\mu(V)g,f],$$
$$g\in\mathfrak{H},\quad f\in W^{1,2}.$$

Consequently, we obtain

$$\mathfrak{h}_V[R_\mu(V)g,f]+\mu(R_\mu(V)g,f)=((I+B_\mu(V))^{-1}(H_0+\mu)^{-1/2}g,(H_0+\mu)^{1/2}f)$$
$$+(B_\mu(V)(I+B_\mu(V))^{-1}(H_0+\mu)^{-1/2}g,(H_0+\mu)^{1/2}f),$$

which shows that

$$\mathfrak{h}_V[R_\mu(V)g,f]+\mu(R_\mu(V)g,f)=(g,f),\quad g\in\mathfrak{H},\quad f\in W^{1,2}. \tag{20}$$

The relation (20) implies that $R_\mu(V)g\in\mathrm{dom}(H(V))$ and $(H(V)+\mu)R_\mu(V)g=g$ for any $g\in\mathfrak{H}$. Similarly, one proves that $R_\mu(V)(H(V)+\mu)g=g$ for any $g\in\mathrm{dom}(H(V))$. Hence, $(H(V)+\mu)^{-1}=R_\mu(V)$. □

D. Dilations

In the conceptual framework of quantum mechanics, physical quantities, such as the densities of electrons and holes regarded here, are derived from a Hamiltonian, i.e., a self-adjoint operator on some Hilbert space. This procedure cannot be directly applied to open quantum systems. Instead we proceed as follows: first we embed the open quantum system into an appropriate closed one and define physical quantities with respect to the closed system; finally one makes some ''projection'' onto the open (sub-)system (see Remark 2.6). This section deals with the construction of the covering closed system. In Sec. II C we have stated the spectral properties of the (completely non-self-adjoint) pseudo-Hamiltonian $H(V)$. Based upon these results we will now derive a Hamiltonian on an appropriate Hilbert space which serves as a quasi-Hamiltonian for the open quantum system under consideration. Since $H(V)$ is a maximal dissipative operator there is a larger Hilbert space $\mathfrak{K}\supseteq\mathfrak{H}$ and a self-adjoint operator $K(V)$ on $\mathfrak{K}$ such that

$$P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-z)^{-1}|\mathfrak{H}=(H(V)-z)^{-1},\quad \Im(z)>0, \tag{21}$$

where $P_{\mathfrak{H}}^{\mathfrak{K}}$ denotes the projection from $\mathfrak{K}$ onto $\mathfrak{H}$ (see Ref. 8). The operator $K(V)$ is called a self-adjoint dilation of the maximal dissipative operator $H(V)$. Obviously, from the condition (21) one gets

$$P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-z)^{-1}|\mathfrak{H}=(H(V)^*-z)^{-1},\quad \Im(z)<0.$$

If the condition

$$\operatorname*{clospan}_{z\in\mathbb{C}\setminus\mathbb{R}}(K(V)-z)^{-1}\mathfrak{H}=\mathfrak{K}$$

is satisfied, then $K(V)$ is called a minimal self-adjoint dilation of $H(V)$. Minimal self-adjoint dilations of maximal dissipative operators are determined up to an isomorphism, that means, all minimal self-adjoint dilations are unitarily equivalent.

A special feature of the spatially one-dimensional case is that the resolvent of the dilation $K(V)$ of $H(V)$ can be described by the characteristic function $\Theta_{H(V)}(z)$ of $H(V)$ (see Ref. 8). The definition of the characteristic function relies on the boundary operators $T(V)(z):\mathfrak{H}\to\mathbb{C}^2$, $z\in\mathrm{res}(H(V))$, and $T_*(V)(z):\mathfrak{H}\to\mathbb{C}^2$, $z\in\mathrm{res}(H(V)^*)$ which we will introduce now. To that end let us define the operator

$$\alpha:\mathfrak{H}\to\mathbb{C}^2,\quad \alpha f=\begin{pmatrix}\alpha_b f(b)\\ -\alpha_a f(a)\end{pmatrix},\quad f\in\mathrm{dom}(\alpha)=C[a,b],$$

where

$$\kappa_a = q_a + \frac{i}{2}\alpha_a^2 \quad \text{and} \quad \kappa_b = q_b + \frac{i}{2}\alpha_b^2, \quad q_a, q_b \in \mathbb{R}, \quad \alpha_a, \alpha_b > 0.$$

Now the boundary operators are given by

$$T(V)(z)f := \alpha(H(V) - z)^{-1}f, \quad T_*(V)(z)f := \alpha(H(V)^* - z)^{-1}f, \quad f \in \mathfrak{H}. \tag{22}$$

The characteristic function $\Theta_{H(V)}$ of the maximal dissipative operator $H(V)$ is a two-by-two matrix-valued function which satisfies the relation

$$\Theta_{H(V)}(z)T(V)(z)f = T_*(V)(z)f, \quad z \in \mathrm{res}(H(V)) \cap \mathrm{res}(H(V)^*), \quad f \in \mathfrak{H}.$$

It is a holomorphic function on $\mathrm{res}(H(V)) \cap \mathrm{res}(H(V)^*)$ and contractive on $\mathbb{C}_- \cup \mathbb{R}$, i.e.,

$$\|\Theta_{H(V)}(z)\|_{\mathfrak{B}(\mathbb{C}^2)} \leqslant 1 \quad \text{for } z \in \mathbb{C}_- \cup \mathbb{R}.$$

The characteristic function of $H(V)$ is given by

$$\Theta_{H(V)}(z) = I_{\mathbb{C}^2} - i\alpha T(V)(\overline{z})^*$$

(see Ref. 16). We now explicitly describe the resolvent of the minimal self-adjoint dilation $K(V)$ of the maximal dissipative operator $H(V)$ (see Ref. 16). The dilation space $\mathfrak{K}$ is given by

$$\mathfrak{K} = \mathcal{D}_- \oplus \mathfrak{H} \oplus \mathcal{D}_+, \tag{23}$$

where $\mathcal{D}_\pm := L^2(\mathbb{R}_\pm, \mathbb{C}^2)$. In accordance with (23) we write $\vec{f} = (f_-, f, f_+) \in \mathfrak{K}$. The resolvent of $K(V)$ is given by

$$(K(V) - z)^{-1}(f_-, f, f_+) = \begin{cases} (g_-, g, g_+) & \text{if } \Im(z) > 0, \\ (h_-, h, h_+) & \text{if } \Im(z) < 0, \end{cases} \tag{24}$$

where

$$g_-(x) = i\int_{-\infty}^{x} dy\, e^{i(x-y)z} f_-(y), \quad x \in \mathbb{R}_-,$$

$$g(x) = ((H(V) - z)^{-1}f)(x) + i\left(T_*(V)(\overline{z})^* \int_{-\infty}^{0} dy\, e^{-iyz} f_-(y)\right)(x), \quad x \in (a,b),$$

$$g_+(x) = i\int_0^x dy\, e^{i(x-y)z} f_+(y) + ie^{izx}(T(V)(z)f)(x) + i\Theta_{H(V)}(\overline{z})^* \int_{-\infty}^{0} dy\, e^{i(x-y)z} f_-(y),$$

$$x \in \mathbb{R}_+,$$

and

$$h_-(x) = -i\int_x^0 dy\, e^{i(x-y)z} f_-(y) - ie^{izx}(T_*(V)(z)f)(x) - i\Theta_{H(V)}(z)\int_0^\infty dy\, e^{i(x-y)z} f_+(y),$$

$$x \in \mathbb{R}_-,$$

$$h(x) = ((H(V)^* - z)^{-1}f)(x) - i\left(T(V)(\overline{z})^* \int_0^\infty dy\, e^{-iyz} f_+(y)\right)(x), \quad x \in (a,b),$$

$$h_+(x) = -i\int_x^\infty dy\, e^{i(x-y)z} f_+(y), \quad x \in \mathbb{R}_+ .$$

The self-adjoint operator $K(V)$ is absolutely continuous and its spectrum coincides with the real axis, i.e., $\mathrm{spec}(K(V)) = \mathbb{R}$. The multiplicity of its spectrum is two. For more details, see Ref. 16.

E. Eigenfunction expansions

We are interested in an explicit expression for the densities of electrons and holes. For a spatially one-dimensional open quantum system with a quantum transmitting boundary[9] the particle density can be expressed in terms of a density matrix, describing the collective behavior of the particles, and of certain generalized eigenfunctions of a Schrödinger operator (see Refs. 4 and 1). An analogous concept is on the agenda of this article (see Sec. II F). In pursuit of this goal we recall the properties of the generalized eigenfunctions of the quasi-Hamiltonian $K(V)$ which has been defined in Sec. II D. The generalized eigenfunctions $\vec{\psi}(V)(\cdot,\lambda,\tau)$, $\lambda \in \mathbb{R}$, $\tau = a, b$, of $K(V)$ are given by (see Ref. 16)

$$\vec{\psi}(V)(x,\lambda,\tau) := \begin{cases} \psi_-(V)(x,\lambda,\tau) := \dfrac{1}{\sqrt{2\pi}} e^{ix\lambda} e_\tau, & x \in \mathbb{R}_- , \\ \psi(V)(x,\lambda,\tau) := \dfrac{1}{\sqrt{2\pi}} ((T_*(V)(\lambda))^* e_\tau)(x), & x \in (a,b), \\ \psi_+(V)(x,\lambda,\tau) := \dfrac{1}{\sqrt{2\pi}} e^{ix\lambda} \Theta_{H(V)}(\lambda)^* e_\tau, & x \in \mathbb{R}_+ , \end{cases}$$

where the argument x has to be interpreted in the sense of (23) and

$$e_b := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e_a := \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The generalized eigenfunctions of $K(V)$ are orthogonal (see Ref. 16), and their linear span (modulo the scalar, continuous, compactly supported functions) is dense in $\mathfrak{K}$. We note that the generalized eigenfunctions $\vec{\psi}(V)(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. Using the incoming eigenfunctions one defines a transformation $\Phi(V): \mathfrak{K} \to L^2(\mathbb{R},\mathbb{C}^2)$

$$(\Phi(V)\vec{g})(\lambda) =: \hat{g}(\lambda) = \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix},$$

where

$$\hat{g}^\tau(\lambda) := \int_{\mathbb{R}_-} dx \langle g_-(x), \psi_-(V)(x,\lambda,\tau)\rangle_{\mathbb{C}^2} + \int_a^b dx\, g(x)\overline{\psi(V)(x,\lambda,\tau)} + \int_{\mathbb{R}_+} dx \langle g_+(x), \psi_+(V)(x,\lambda,\tau)\rangle_{\mathbb{C}^2},$$

and $\vec{g} = (g_-, g, g_+)$, $\tau = a, b$. $\Phi(V)$ is unitary and called the incoming Fourier transformation. The inverse incoming Fourier transformation $\Phi(V)^{-1}$ is given by

$$(\Phi(V)^{-1}\hat{g})(\cdot) = \int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}(V)(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda), \quad \hat{g} \in L^2(\mathbb{R},\mathbb{C}^2).$$

We note that

$$\Phi(V)K(V)\Phi(V)^{-1} = M,$$

where M is the multiplication operator by the independent variable λ on $L^2(\mathbb{R},\mathbb{C}^2)$, i.e.,

$$\begin{aligned}(M\hat{g})(\lambda) &:= \lambda\hat{g}(\lambda), \quad \hat{g}\in \mathrm{dom}(M), \quad \lambda\in\mathbb{R},\\ \mathrm{dom}(M) &:= \{\hat{g}\in L^2(\mathbb{R},\mathbb{C}^2): M\hat{g}\in L^2(\mathbb{R},\mathbb{C}^2)\}.\end{aligned} \tag{25}$$

The representation (25) induced by $\Phi(V)$ is called the incoming spectral representation of $K(V)$. Finally, we note that each bounded self-adjoint operator G on $\mathfrak{K}$, which commutes with $K(V)$, corresponds to a measurable function $\hat{G}\in L^\infty(\mathbb{R},\mathfrak{B}(\mathbb{C}^2))$. The multiplication operator on $L^2(\mathbb{R},\mathbb{C}^2)$ generated by $\hat{G}$, which we also denote by $\hat{G}$ and which is defined by

$$\begin{aligned}(\hat{G}\hat{g})(\lambda) &:= \hat{G}(\lambda)\hat{g}(\lambda), \quad \hat{g}\in \mathrm{dom}(\hat{G}), \quad \lambda\in\mathbb{R},\\ \mathrm{dom}(\hat{G}) &:= \{\hat{g}\in L^2(\mathbb{R},\mathbb{C}^2): \hat{G}\hat{g}\in L^2(\mathbb{R},\mathbb{C}^2)\},\end{aligned} \tag{26}$$

is unitarily equivalent to G, which means $\Phi(V)G\Phi(V)^{-1}=\hat{G}$ (see Ref. 3, 4.4.2. Proposition 18). The representation (26) is called the incoming spectral representation of G. The incoming Fourier transform $\Phi(V)$ is related to the Lax–Phillips wave operators (see Ref. 17, Remark 5.2). Since

$$e^{-itK(V)}\mathcal{D}_-\subseteq\mathcal{D}_-, \quad t\leqslant 0,$$

$$e^{-itK(V)}\mathcal{D}_+\subseteq\mathcal{D}_+, \quad t\geqslant 0,$$

as well as

$$\begin{aligned}\bigcap_{t\in\mathbb{R}} e^{-itK(V)}\mathcal{D}_- &= \bigcap_{t\in\mathbb{R}} e^{-itK(V)}\mathcal{D}_+ = \{0\},\\ \overline{\bigcup_{t\in\mathbb{R}} e^{-itK(V)}\mathcal{D}_-} &= \overline{\bigcup_{t\in\mathbb{R}} e^{-itK(V)}\mathcal{D}_+} = \mathfrak{K}\end{aligned} \tag{27}$$

the subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces with respect to $e^{-itK(V)}$ (see Ref. 3, Chap XII or Ref. 20). Further, introducing the Hilbert space $\mathfrak{K}_0$,

$$\mathfrak{K}_0 := L^2(\mathbb{R},\mathbb{C}^2)=\mathcal{D}_-\oplus\mathcal{D}_+\subseteq\mathfrak{K}=\mathcal{D}_-\oplus\mathfrak{H}\oplus\mathcal{D}_+,$$

and the self-adjoint differentiation operator K_0,

$$(K_0 f)(x) = -i\frac{d}{dx}f(x), \quad f\in\mathrm{dom}(K_0)=W^{1,2}(\mathbb{R},\mathbb{C}^2),$$

one easily verifies that $\mathcal{D}_-$ and $\mathcal{D}_+$ are incoming and outgoing subspaces with respect to e^{-itK_0}. The Lax–Phillips wave operators are defined by

$$W_\pm(K(V),K_0;J_\pm) := s-\lim_{t\to\pm\infty} e^{itK(V)}J_\pm e^{-itK_0},$$

with identification operators $J_\pm:\mathfrak{K}_0\to\mathfrak{K}$ given by

$$J_- f := (P^{\mathfrak{K}_0}_{\mathcal{D}_-}f,0,0), \quad f\in\mathfrak{K}_0,$$

$$J_+ f := (0,0,P^{\mathfrak{K}_0}_{\mathcal{D}_+}f), \quad f\in\mathfrak{K}_0,$$

where $P^{\mathfrak{K}_0}_{\mathcal{D}_-}$, $P^{\mathfrak{K}_0}_{\mathcal{D}_+}$ denote the projection from $\mathfrak{K}_0$ onto $\mathcal{D}_-$ and from $\mathfrak{K}_0$ onto $\mathcal{D}_+$, respectively. Since

$$e^{-itK(V)}|\mathcal{D}_- = e^{-itK_0}|\mathcal{D}_-, \quad t \leqslant 0,$$

$$e^{-itK(V)}|\mathcal{D}_+ = e^{-itK_0}|\mathcal{D}_+, \quad t \geqslant 0,$$

the wave operators exist. Using (27) one proves the completeness of the wave operators, i.e., $\mathrm{ran}(W_\pm(K(V),K_0;J_\pm)) = \mathfrak{K}$. For details (see Ref. 3, Chap. XII or Ref. 20). Defining the Fourier operator $\mathcal{F}: L^2(\mathbb{R},\mathbb{C}^2) \to L^2(\mathbb{R},\mathbb{C}^2)$ by

$$(\mathcal{F}f)(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx\, e^{-ix\lambda} f(x), \quad f \in L^2(\mathbb{R},\mathbb{C}^2), \quad \lambda \in \mathbb{R},$$

one gets the representation

$$\Phi(V) = \mathcal{F}W_-(K(V),K_0;J_-)^* \tag{28}$$

(see Ref. 17, Remark 5.2).

F. Carrier densities

Following Ref. 17, we now introduce the particle density and express it in terms of the generalized eigenfunctions (see Sec. II E) of the quasi-Hamiltonian associated with a dissipative open quantum system (see Sec. II D). An operator $\varrho \in \mathfrak{B}(\mathfrak{K})$ is called a density matrix if ϱ is non-negative and self-adjoint. The operator ϱ is a steady state, if ϱ commutes with $K(V)$. Thus any steady-state ϱ is unitarily equivalent to a multiplication operator $\hat{\varrho}$ on the Hilbert space $L^2(\mathbb{R},\mathbb{C}^2)$ induced by a measurable function from the space $L^\infty(\mathbb{R},\mathfrak{B}(\mathbb{C}^2))$; we denote this function by the same symbol $\hat{\varrho}$ as the multiplication operator. In the following we assume that the function $\hat{\varrho}$ is fixed, i.e., the function $\hat{\varrho}$ does not depend on the potential V. This leads to a steady state of the form

$$\varrho(V) = \Phi(V)^{-1}\hat{\varrho}\Phi(V), \tag{29}$$

which depends on V. In order to define the carrier density $u_{\hat{\varrho}}(V)$ one has to introduce the carrier density observable in terms of the generalized eigenfunctions as defined in Sec. II E:

$$D(V)(x,\lambda) := \begin{pmatrix} |\psi(V)(x,\lambda,b)|^2 & \psi(V)(x,\lambda,a)\overline{\psi(V)(x,\lambda,b)} \\ \psi(V)(x,\lambda,b)\overline{\psi(V)(x,\lambda,a)} & |\psi(V)(x,\lambda,a)|^2 \end{pmatrix}.$$

With respect to the carrier density observable $D(V)(x,\lambda)$ one defines the carrier density at $x \in [a,b]$ and at energy $\lambda \in \mathbb{R}$ by

$$u_{\hat{\varrho}}(V)(x,\lambda) := \mathrm{tr}(\hat{\varrho}(\lambda)D(V)(x,\lambda)) \geqslant 0.$$

The carrier density $u_{\hat{\varrho}}(V)$ is given by

$$u_{\hat{\varrho}}(V)(x) = \int_{\mathbb{R}} d\lambda\, u_{\hat{\varrho}}(V)(x,\lambda). \tag{30}$$

If the function $\hat{\varrho}$ satisfies the condition

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2+1}\,\|\hat{\varrho}(\lambda)\|_{\mathfrak{B}(\mathbb{C}^2)} < \infty, \tag{31}$$

then the definition (30) makes sense for a.e. $x \in [a,b]$. Moreover, in this case $u_{\hat{\varrho}}(V)$ is a *non-negative* and *integrable* function. Furthermore, $P^{\mathfrak{K}}_{\mathfrak{H}}(K(V)-i)^{-1} \in \mathfrak{L}_1(\mathfrak{K})$ and the estimate

$$\|u_{\hat{\varrho}}(V)\|_{L^1}=\mathrm{tr}(\varrho(V)P_{\mathfrak{H}}^{\mathfrak{K}})\leqslant C_{\hat{\varrho}}\|(K(V)-i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K})} \tag{32}$$

is valid (see Ref. 17). Let us introduce the operator

$$(M(h)\vec{f})(x):=(0,h(x)f(x),0),\quad \vec{f}=(f_-,f,f_+)\in\mathrm{dom}(M(h))=\mathfrak{K},$$

for functions $h\in L^\infty$. If the condition (31) is satisfied, then

$$\int_a^b dx\, u_{\hat{\varrho}}(V)(x)h(x)=\mathrm{tr}(\varrho(V)M(h)) \tag{33}$$

for any $h\in L^\infty$ (see Ref. 17).

Remark 2.6: In order to express the carrier density via the density matrix, only the action of the density matrix $\varrho(V)$ on multiplication operators on the small Hilbert space $\mathfrak{H}$ is of interest [see (33)]. This is exactly what we have addressed as "projection" onto the open quantum system in the introduction of Sec. II D.

III. THE CARRIER DENSITY OPERATOR: BOUNDEDNESS AND CONTINUITY

As in Refs. 13 and 14 we introduce the (nonlinear) carrier density operator $\mathcal{N}_{\hat{\varrho}}:L^\infty\to L^1$ defined by

$$\mathcal{N}_{\hat{\varrho}}(V):=u_{\hat{\varrho}}(V),\quad V\in\mathrm{dom}(\mathcal{N}_{\hat{\varrho}})=L^\infty, \tag{34}$$

where $u_{\hat{\varrho}}(V)$ is the carrier density defined by (30). The dissipative Schrödinger–Poisson system is essentially a nonlinear Poisson equation (1) with density operators of the form (34) for electrons and holes as nonlinearities on the right-hand side of (1). In Sec. IV we prove the existence of solutions of the dissipative Schrödinger–Poisson system by means of Schauder's fixed point theorem. To that end we need bounds of the carrier density operator and its continuity. Let us first give a bound for the carrier density operator.

Theorem 3.1: *Suppose $V\in L^\infty$. If the spectral representation $\hat{\varrho}$ of a density matrix $\varrho(V)$ [see (29)] obeys (31), then*

$$\begin{aligned}\|\mathcal{N}_{\hat{\varrho}}(V)\|_{L^1}\leqslant C_{\hat{\varrho}}(&8+4\sqrt{2}(b-a)\sqrt{\|m\|_{L^\infty}}\sqrt{8c+5+4\|V\|_{L^\infty}}\\&+8\sqrt{2}\mathfrak{g}_1(\alpha_a^2+\alpha_b^2)^{1/2}\|H_0^{-1/2}\|^{1/2}_{\mathfrak{B}(\mathfrak{H};W^{1,2})}(8c+5+4\|V\|_{L^\infty})^{1/4}),\end{aligned} \tag{35}$$

where c is defined by (14).

Proof: In view of (32) it suffices to estimate $\|(K(V)-i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K})}$. Using (24), we obtain the equation

$$(K(V)-i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\vec{f}=(0,(H(V)-i)^{-1}f,ie^{-\bullet}T(V)(i)f_+),$$

where $\vec{f}=(f_-,f,f_+)$. Thus, one can estimate

$$\|(K(V)-i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K})}\leqslant\|(H(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}+\|ie^{-\bullet}T(V)(i)\|_{\mathfrak{L}_1(\mathfrak{H};\mathcal{D}_+)}. \tag{36}$$

We estimate the first addend on the right-hand side. Let μ be a sufficiently large positive number (to be specified later). We write

$$(H(V)-i)^{-1}=(H(V)+\mu)^{-1}(1+(\mu+i)(H(V)-i)^{-1}). \tag{37}$$

Since $H(V)$ is a maximal dissipative operator one has $\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\leqslant 1$. Thus, (37) implies

$$\|(H(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}\leqslant(2+\mu)\|(H(V)+\mu)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}. \tag{38}$$

Applying the factorization formula (19) one gets

$$\|(H(V)+\mu)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}\leqslant\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}.$$

The first factor of the right-hand side can be estimated (see the Appendix)

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}\leqslant\frac{1}{1+\mu}+\sqrt{\|m\|_{L^\infty}}\frac{b-a}{\sqrt{2}}\frac{1}{\sqrt{1+\mu}}.$$

Hence,

$$\begin{aligned}\|(H(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}&\leqslant\left(\frac{2+\mu}{1+\mu}+\sqrt{\|m\|_{L^\infty}}\frac{b-a}{\sqrt{2}}\frac{2+\mu}{\sqrt{1+\mu}}\right)\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\\&\leqslant(2+\sqrt{2}\sqrt{\|m\|_{L^\infty}}(b-a)\sqrt{1+\mu})\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}.\end{aligned}$$

Setting $\mu=2(4c+2+2\|V\|_{L^\infty})$ and taking into account (18) one gets

$$\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\leqslant 4,$$

which finally implies

$$\|(H(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{H})}\leqslant 8+4\sqrt{2}(b-a)\sqrt{\|m\|_{L^\infty}}\sqrt{8c+5+4\|V\|_{L^\infty}}. \tag{39}$$

Now we are going to estimate the second term on the right-hand side of (36). Since $\|e^{-\bullet}\otimes I_{\mathbb{C}^2}\|_{\mathfrak{L}_1(\mathbb{C}^2;\mathcal{D}_+)}=\sqrt{2}$, we get, using Eq. (22), that

$$\|ie^{-\bullet}T(V)(i)\|_{\mathfrak{L}_1(\mathfrak{H};\mathcal{D}_+)}\leqslant\sqrt{2}(\alpha_a^2+\alpha_b^2)^{1/2}\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}.$$

It remains to estimate $\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}$. Taking into account (37) one obtains [analogous to (38)]

$$\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}\leqslant(2+\mu)\|(H(V)+\mu)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}.$$

As in the previous part of the proof we put $\mu=2(4c+2+2\|V\|_{L^\infty})$ and afterwards substitute $(H(V)+\mu)^{-1}$ via the factorization formula (19). This leads to the following estimate:

$$\begin{aligned}\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}&\leqslant(\mu+2)\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}\\&\quad\times\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H})}.\end{aligned}$$

By $\|(I+B_\mu(V))^{-1}\|_{\mathfrak{B}(\mathfrak{H})}\leqslant 4$ and $\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H})}\leqslant 1/\sqrt{1+\mu}$ one gets

$$\|(H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}\leqslant 4\frac{2+\mu}{\sqrt{1+\mu}}\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])}. \tag{40}$$

We estimate the last factor in this inequality by the Gagliardo–Nirenberg inequality (15). For any $\psi\in\mathfrak{H}$ one has

$$\begin{aligned}\|(H_0+\mu)^{-1/2}\psi\|_{C[a,b]} &\leqslant \mathfrak{g}_1\|(H_0+\mu)^{-1/2}\psi\|_{W^{1,2}}^{1/2}\|(H_0+\mu)^{-1/2}\psi\|_{\mathfrak{H}}^{1/2}\\ &\leqslant \mathfrak{g}_1\|H_0^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};W^{1,2})}^{1/2}\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H})}^{1/2}\|\psi\|_{\mathfrak{H}}\\ &\leqslant \mathfrak{g}_1\frac{\|H_0^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};W^{1,2})}^{1/2}}{(1+\mu)^{1/4}}\|\psi\|_{\mathfrak{H}}.\end{aligned}$$

This yields

$$\|(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])} \leqslant \mathfrak{g}_1\frac{\|H_0^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};W^{1,2})}^{1/2}}{(1+\mu)^{1/4}}.$$

Together with (40) this gives

$$\|H(V)-i)^{-1}\|_{\mathfrak{B}(\mathfrak{H};C[a,b])} \leqslant 8\,\mathfrak{g}_1\|H_0^{-1/2}\|_{\mathfrak{B}(\mathfrak{H},W^{1,2})}^{1/2}(1+\mu)^{1/4}.$$

Inserting the chosen $\mu=2(4c+2+2\|V\|_{L^\infty})$, we obtain for the second addend on the right-hand side of (36):

$$\|ie^{-\cdot}T(V)(i)\|_{\mathfrak{L}_1(\mathfrak{H};\mathcal{D}_+)} \leqslant 8\sqrt{2}\,\mathfrak{g}_1(\alpha_a^2+\alpha_b^2)^{1/2}\|H_0^{-1/2}\|_{\mathfrak{B}(\mathfrak{H};W^{1,2})}^{1/2}(8c+5+4\|V\|_{L^\infty})^{1/4}.$$

Fitting together (32), (36), (39), and the last estimate completes the proof of (35). □

Remark 3.2: One can prove that the carrier density operator takes its values not only in L^1 but in L^2. Additionally, one can prove estimates similar to (35). These facts are not needed in this article; they become, however, essential if one wants to include recombination effects of electrons and holes into the model.

Our next aim is to verify the continuity of the carrier density operator. To this end we need the continuity of the incoming Fourier transformation in dependence of the potential V.

Lemma 3.3: If V, $V_n \in L^\infty$, $n=1,2,...$, and $V_n \overset{L^\infty}{\to} V$ as $n\to\infty$, then

$$s-\lim_{n\to\infty}\Phi(V_n)=\Phi(V). \tag{41}$$

Proof: The potentials V and V_n define self-adjoint multiplication operators on the Hilbert space $\mathfrak{H}$. We denote these operators by the same symbols and extend them to the dilation space $\mathfrak{K}$ setting

$$\hat{V}=(0,V,0) \quad \text{and} \quad \hat{V}_n=(0,V_n,0), \quad n=1,2,\ldots.$$

Obviously, one has

$$K(V)=K(0)+\hat{V} \quad \text{and} \quad K(V_n)=K(0)+\hat{V}_n,$$

$n=1,2,\ldots$. Hence

$$(K(V_n)-i)^{-1}-(K(V)-i)^{-1}=(K(V_n)-i)^{-1}(\hat{V}-\hat{V}_n)(K(V)-i)^{-1},$$

$n=1,2,\ldots$. Using $(\hat{V}-\hat{V}_n)=(\hat{V}-\hat{V}_n)P_{\mathfrak{H}}^{\mathfrak{K}}$, $n=1,2,...$, we obtain the representation

$$(K(V_n)-i)^{-1}-(K(V)-i)^{-1}=(K(V_n)-i)^{-1}(\hat{V}-\hat{V}_n)P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}, \tag{42}$$

$n=1,2,\ldots$. Since $P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}$ is a nuclear operator the resolvent difference $(K(V_n)-i)^{-1}-(K(V)-i)^{-1}$ is a nuclear operator, too. By Ref. 18, Theorem X.4.12, the wave operators

$$W_-(K(V_n),K(V))=s-\lim_{t\to-\infty}e^{itK(V_n)}e^{-itK(V)}$$

as well as

$$W_-(K(V),K(V_n))=s-\lim_{t\to-\infty}e^{itK(V)}e^{-itK(V_n)},\quad n=1,2,...,$$

exist and are complete. Note that $W_-(K(V_n),K(V))^*=W_-(K(V),K(V_n))$. Using the chain rule for wave operators (Ref. 3, Theorem III.21) we find the representation

$$W_-(K(V_n),K_0;J_-)=W_-(K(V_n),K(V))W_-(K(V),K_0;J_-)$$

for $n=1,2,...$, which yields

$$W_-(K(V_n),K_0;J_-)^*=W_-(K(V),K_0;J_-)^*W_-(K(V),K(V_n)) \tag{43}$$

for $n=1,2,...$. Furthermore, from (42) one gets the estimate

$$\|(K(V_n)-i)^{-1}-(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}\leqslant\|V-V_n\|_{L^\infty}\|P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})},$$

$n=1,2,...$, which implies

$$\lim_{n\to\infty}\|(K(V_n)-i)^{-1}-(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}=0. \tag{44}$$

Therefore (see also Ref. 18, Remark X.4.17),

$$s-\lim_{n\to\infty}W_-(K(V_n),K(V))=W_-(K(V),K(V))=I_{\mathfrak{K}},$$

which yields

$$w-\lim_{n\to\infty}W_-(K(V_n),K(V))^*=w-\lim_{n\to\infty}W_-(K(V),K(V_n))=I_{\mathfrak{K}}.$$

Since $W_-(K(V),K(V_n))$, $n=1,2,...$, is a sequence of unitary operators we obtain

$$s-\lim_{n\to\infty}W_-(K(V),K(V_n))=I_{\mathfrak{K}}.$$

Finally, from (28) and (43) we get the representation

$$\Phi(V_n)=\Phi(V)W_-(K(V),K(V_n)),\quad n=1,2,....$$

Using $s-\lim_{n\to\infty}W_-(K(V),K(V_n))=I_{\mathfrak{K}}$ we complete the proof. □

Now we can verify the continuity of the carrier density operator.

Theorem 3.4: *Let* $V\in L^\infty$, $V_n\in L^\infty$, $n=1,2,...$. *If* $\hat{\varrho}$ *satisfies the condition (31) and* $V_n\overset{L^\infty}{\to}V$ *as* $n\to\infty$, *then* $u_{\hat{\varrho}}(V_n)\overset{L^1}{\to}u_{\hat{\varrho}}(V)$ *as* $n\to\infty$, *i.e.,*

$$\lim_{n\to\infty}\int_a^b dx\,|u_{\hat{\varrho}}(V_n)(x)-u_{\hat{\varrho}}(V)(x)|=0, \tag{45}$$

i.e., the carrier density operator $\mathcal{N}_{\hat{\varrho}}:L^\infty\to L^1$ *is continuous.*

Proof: By (33) we have the representation

$$\int_a^b dx(u_{\hat{\varrho}}(V_n)(x)-u_{\hat{\varrho}}(V)(x))h(x)=\mathrm{tr}((\varrho(V_n)-\varrho(V))M(h)) \tag{46}$$

for each $h \in L^\infty$ and $n=1,2,\ldots$. Since

$$\mathrm{tr}(\varrho(V)M(h)) = \mathrm{tr}(\varrho(V)(K(V)+i)(K(V)+i)^{-1}M(h)),$$

one gets

$$\begin{aligned}\mathrm{tr}((\varrho(V_n)-\varrho(V))M(h)) &= \mathrm{tr}(\varrho(V_n)(K(V_n)+i)\{(K(V_n)+i)^{-1}-(K(V)+i)^{-1}\}M(h)) \\ &\quad + \mathrm{tr}((\varrho(V_n)(K(V_n)+i)-\varrho(V)(K(V)+i))(K(V)+i)^{-1}M(h))\end{aligned} \tag{47}$$

for $n=1,2,\ldots$. By (31) we have

$$\|\varrho(V_n)(K(V_n)+i)\|_{\mathfrak{B}(\mathfrak{K})} \leqslant C_{\hat{\varrho}}$$

and therefore

$$\begin{aligned}&|\mathrm{tr}(\varrho(V_n)(K(V_n)+i)((K(V_n)+i)^{-1}-(K(V)+i)^{-1})M(h))| \\ &\quad \leqslant C_{\hat{\varrho}}\|(K(V_n)+i)^{-1}-(K(V)+i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}\end{aligned} \tag{48}$$

for $n=1,2,\ldots$. We set

$$\hat{k}(\lambda) := \hat{\varrho}(\lambda)(\lambda+i), \quad \lambda \in \mathbb{R},$$

and identify this matrix-valued function with the multiplication operator $\hat{k}$ induced by $\hat{k}$ on $L^2(\mathbb{R},\mathbb{C}^2)$. In this notation there is

$$\varrho(V_n)(K(V_n)+i) = \Phi(V_n)^{-1}\hat{k}\Phi(V_n), \quad n=1,2,\ldots,$$

$$\varrho(V)(K(V)+i) = \Phi(V)^{-1}\hat{k}\Phi(V).$$

Hence the representation

$$\varrho(V_n)(K(V_n)+i)-\varrho(V)(K(V)+i) = (\Phi(V_n)^{-1}-\Phi(V)^{-1})\hat{k}\Phi(V_n)+\Phi(V)\hat{k}(\Phi(V_n)-\Phi(V)) \tag{49}$$

is valid. From (49) we deduce the estimate

$$\begin{aligned}&|\mathrm{tr}((\varrho(V_n)(K(V_n)+i)-\varrho(V)(K(V)+i))(K(V)+i)^{-1}M(h))| \\ &\quad \leqslant C_{\hat{\varrho}}\|(\Phi(V_n)-\Phi(V))P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))}\|h\|_{L^\infty} \\ &\quad + C_{\hat{\varrho}}\|(\Phi(V_n)-\Phi(V))(K(V)+i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))}\|h\|_{L^\infty}.\end{aligned} \tag{50}$$

Taking into account (47), (48), and (50) we finally get the estimate

$$\begin{aligned}|\mathrm{tr}((\varrho(V_n)-\varrho(V))M(h))| &\leqslant C_{\hat{\varrho}}(\|(K(V_n)+i)^{-1}-(K(V)+i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})} \\ &\quad + \|(\Phi(V_n)-\Phi(V))P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))} \\ &\quad + \|(\Phi(V_n)-\Phi(V))(K(V)+i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))}\|h\|_{L^\infty}).\end{aligned}$$

Since h is arbitrary we obtain from (46) the estimate

$$\int_a^b dx\,|(u_{\hat{\varrho}}(V_n)(x)-u_{\hat{\varrho}}(V)(x))| \leqslant C_{\hat{\varrho}}(\|(K(V_n)+i)^{-1}-(K(V)+i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}$$
$$+\|(\Phi(V_n)-\Phi(V))P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))}$$
$$+\|(\Phi(V_n)-\Phi(V))(K(V)+i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathfrak{L}_1(\mathfrak{K};L^2(\mathbb{R},\mathbb{C}^2))}).$$

According to (44) the first addend on the right-hand side goes to zero as $n\to\infty$. Since $P_{\mathfrak{H}}^{\mathfrak{K}}(K(V)-i)^{-1}$ is a trace class operator, one gets by (41) that the second addend on the right-hand side tends to zero, too. Similarly one proves that the third addend tends to zero. □

IV. THE DISSIPATIVE SCHRÖDINGER–POISSON SYSTEM

In this section we first give a rigorous definition of the dissipative Schrödinger–Poisson system. The solution of the dissipative Schrödinger–Poisson system is defined as a self-consistent solution of the nonlinear Poisson equation (1) with density operators of the form (34) for electrons and holes as nonlinearities on the right-hand side of (1). We show that the existence problem of a solution can be reformulated as a fixed point problem for a certain nonlinear map. Applying Schauder's fixed point theorem we find that a solution always exists. From the technical point of view one has to ensure that this map is continuous and compact and has an invariant bounded and convex set. Let us first introduce some further notations:

Definition 4.1: We denote the real part of $W^{1,2}$ by $W_{\mathbb{R}}^{1,2}$. Let $\Gamma\subset\{a,b\}$ be the (possibly empty) Dirichlet boundary of Poisson's equation. We define

$$W_{\Gamma}^{1,2}:=W_{\mathbb{R}}^{1,2}\cap\{\psi:\psi(\Gamma)\subset\{0\}\}.$$

By $W_{\Gamma}^{-1,2}$ we denote the dual space of $W_{\Gamma}^{1,2}$ and by $\langle\cdot,\cdot\rangle_1$ the dual pairing between $W_{\Gamma}^{1,2}$ and $W_{\Gamma}^{-1,2}$. In the following we denote the embedding operator from L^1 into $W_{\Gamma}^{-1,2}$ by E_1 and its norm by ε_1. Moreover, we denote by E_∞ the dual to E_1, i.e., the embedding operator of $W_{\mathbb{R}}^{1,2}$ into L^∞ the norm of which is also ε_1.

Following Ref. 17 we deal with a dissipative Schrödinger–Poisson system constituted by two dissipative Schrödinger-type operators $H^{\pm}(V_{\pm})$:

$$H^{\pm}(V_{\pm})=-\frac{1}{2}\frac{d}{dx}\frac{1}{m_{\pm}}\frac{d}{dx}+V_{\pm},$$

one for electrons (indexed "$-$") and one for holes (indexed "$+$") and Poisson's equation (7); please note that $\hbar$ is scaled to 1. The dissipative Schrödinger-type operators are determined by the effective masses $m_{\pm}$, the boundary coefficients $\kappa_a^{\pm}$, $\kappa_b^{\pm}$ and the potentials $V_{\pm}$ which are of the form

$$V_{\pm}=V_0^{\pm}\pm q\varphi,$$

where $V_0^{\pm}$ are external potentials representing the band-edge offsets and φ is the electrostatic potential which is determined by Poisson's equation. To formulate Poisson's equation one needs the dielectric permittivity ϵ, the doping profile C, and the functions k and φ_Γ [see (8)].

Assumption 4.2: With respect to the data of the problem we assume the following:

- $(A_1^{\pm})$ *The effective masses $m_{\pm}$ are positive and obey $m_{\pm}$, $1/m_{\pm}\in L^\infty$.*
- $(A_2^{\pm})$ *The boundary coefficients $\kappa_a^{\pm}$, $\kappa_b^{\pm}$ are from the upper half-plane $\mathbb{C}_+$.*
- $(A_3^{\pm})$ *The external potentials $V_0^{\pm}$ belong to L^∞.*
- $(A_4^{\pm})$ *The matrix-valued functions $\hat{\varrho}_{\pm}\in L^\infty(\mathbb{R},\mathfrak{B}(\mathbb{C}^2))$ satisfy (31).*
- (A_5) *The doping profile C belongs to $W_{\Gamma}^{-1,2}$.*
- (A_6) *The dielectric permittivity ϵ is positive and obeys ϵ, $1/\epsilon\in L^\infty$. We set $\widetilde{\epsilon}:=\max\{1,\|1/\epsilon\|_{L^\infty}\}$.*

(A_7) *The set* Γ *is not empty, or at least one of the numbers* $k(x)\geqslant 0$, $x\in\{a,b\}\backslash\Gamma$, *is strictly positive.*

(A_8) *The function* φ_Γ *is from the space* $W^{1,2}_{\mathbb{R}}$.

To each Schrödinger operator $H^{\pm}(V_{\pm})$ corresponds a minimal self-adjoint dilation $K^{\pm}(V_{\pm})$. As in Sec. II F the functions $\hat{\varrho}_{\pm}$ define steady states $\varrho_{\pm}(V_{\pm})$, i.e., non-negative self-adjoint operators which commute with $K^{\pm}(V_{\pm})$. The carrier densities $u^{\pm}_{\hat{\varrho}_{\pm}}(V_{\pm})$ for electrons and holes are defined as in Sec. II F. Notice that the electron density $u^{-}_{\hat{\varrho}_{-}}(V_{-})$ is determined by the electron quantities m_{-}, κ^{-}_{a}, κ^{-}_{b}, and V^{-}_{0}, while the hole density $u^{+}_{\hat{\varrho}_{+}}(V_{+})$ refers to m_{+}, κ^{+}_{a}, κ^{+}_{b}, and V^{+}_{0}. The corresponding carrier density operators are denoted by $\mathcal{N}^{-}_{\hat{\varrho}_{-}}$ and $\mathcal{N}^{+}_{\hat{\varrho}_{+}}$, respectively.

A. Rigorous setup of the problem

First we give a rigorous definition of Poisson's equation and afterwards define what we call a solution of the dissipative Schrödinger–Poisson system.

Definition 4.3: The linear Poisson operator $\mathcal{P}: W^{1,2}_{\mathbb{R}}\to W^{-1,2}_{\Gamma}$ *is defined by*

$$\langle \mathcal{P}v,\varsigma\rangle_1=\int_a^b dx\,\epsilon(x)v'(x)\varsigma'(x)+\sum_{x\in\{a,b\}\backslash\Gamma}k(x)v(x)\varsigma(x),\quad v\in W^{1,2}_{\mathbb{R}},\quad \varsigma\in W^{1,2}_{\Gamma}.$$

The restriction of $\mathcal{P}$ *to the subspace* $W^{1,2}_{\Gamma}$ *will be denoted by* $\mathcal{P}_0$.

We have

$$|\langle \mathcal{P}v,\varsigma\rangle_1|\leqslant\left(\|\epsilon\|_{L^\infty}+\sum_{x\in\{a,b\}\backslash\Gamma}k(x)\varepsilon_1^2\right)\|v\|_{W^{1,2}_{\mathbb{R}}}\|\varsigma\|_{W^{1,2}_{\Gamma}}.$$

Hence $\mathcal{P}$ is continuous. Furthermore, we get

$$\|\varphi\|^2_{W^{1,2}_{\Gamma}}\leqslant(1+\gamma_k)\left(\int_a^b dx\,|\varphi'(x)|^2+\sum_{x\in\{a,b\}\backslash\Gamma}k(x)|\varphi(x)|^2\right),\forall\,\varphi\in W^{1,2}_{\Gamma},\tag{51}$$

with

$$\gamma_k:=\sup_{0\neq\psi\in W^{1,2}_{\Gamma}}\frac{\displaystyle\int_a^b dx\,\psi(x)^2}{\displaystyle\int_a^b dx\,|\psi'(x)|^2+\sum_{x\in\{a,b\}\backslash\Gamma}k(x)|\psi(x)|^2}.$$

Because the case of purely homogeneous Neumann conditions is excluded by (A_7), see Assumption 4.2, the constant γ_k is indeed finite. Thus, (51) implies

$$\|\varphi\|^2_{W^{1,2}_{\Gamma}}\leqslant\tilde{\epsilon}(1+\gamma_k)|\langle\mathcal{P}_0\varphi,\varphi\rangle_1|.$$

Therefore, we get by the Lax–Milgram lemma that the inverse of $\mathcal{P}_0$ exists and its norm does not exceed $\tilde{\epsilon}(1+\gamma_k)$. We now state what is a solution of the dissipative Schrödinger–Poisson system.

Problem 4.4: Let us assume that $u^{\pm}\in L^1$. *We say* $\varphi\in W^{1,2}_{\mathbb{R}}$ *satisfies Poisson's equation (7) if* $\varphi-\varphi_\Gamma\in W^{1,2}_{\Gamma}$ *satisfies*

$$\mathcal{P}_0(\varphi-\varphi_\Gamma)=D+qE_1u^{+}-qE_1u^{-},$$

where $D:=qC-\tilde{\varphi}_\Gamma$ *and* $\tilde{\varphi}_\Gamma$ *is the linear form* $v\mapsto\int_a^b dx\,\epsilon(x)\varphi'_\Gamma(x)v'(x)$, *on* $W^{1,2}_{\Gamma}$. *We say a triple* $(\varphi,u^{+},u^{-})\in W^{1,2}_{\mathbb{R}}\times L^1\times L^1$ *satisfies the dissipative Schrödinger–Poisson system if* φ *satisfies Poisson's equation as well as*

$$u^{+}=u^{+}_{\hat{\varrho}_{+}}(V^{+}_{0}+qE_\infty\varphi)\quad\text{and}\quad u^{-}=u^{-}_{\hat{\varrho}_{-}}(V^{-}_{0}-qE_\infty\varphi).$$

B. Existence of solutions and *a priori* estimates

We now prove that the dissipative Schrödinger–Poisson system always admits a solution and investigate these solutions. Following Ref. 13, we define a mapping the fixed points of which exactly determine the solutions of the dissipative Schrödinger–Poisson system.

By $\mathcal{J}:L^1\times L^1\to W^{1,2}_{\mathbb{R}}$ we denote the map which assigns to $(u^+,u^-)\in L^1\times L^1$ the solution of Poisson's equation. Obviously, the map $\mathcal{J}$ is continuous. Further, we define $\Psi:L^\infty\to W^{1,2}_{\mathbb{R}}$ by

$$\Psi:W\to(\mathcal{N}^+_{\hat{\varrho}_+}(V_0^+ + qW),\mathcal{N}^-_{\hat{\varrho}_-}(V_0^- - qW))\to\mathcal{J}(\mathcal{N}^+_{\hat{\varrho}_+}(V_0^+ + qW),\mathcal{N}^-_{\hat{\varrho}_-}(V_0^- - qW)).$$

Since the map $\mathcal{J}:L^1\times L^1\to W^{1,2}_{\mathbb{R}}$ is continuous and by Proposition 3.4 the maps $\mathcal{N}^\pm:L^\infty\to L^1$ are also continuous, the map $\Psi:L^\infty\to W^{1,2}_{\mathbb{R}}$ is continuous, too. With Ψ we associate the map $\Psi_\infty:L^\infty\to L^\infty$,

$$\Psi_\infty := E_\infty\Psi,$$

which is also continuous. Moreover, since E_∞ is compact, the map Ψ_∞ is also compact.

Lemma 4.5: An element $W\in L^\infty$ is a fixed point of Ψ_∞ if and only if the triple

$$(\Psi(W),u^+,u^-)=(\Psi(W),u^+_{\hat{\varrho}_+}(V_0^+ + qW),u^-_{\hat{\varrho}_-}(V_0^- - qW))$$

satisfies the dissipative Schrödinger–Poisson system.

The proof is obvious. Notice that $E_\infty\Psi(W)=\Psi_\infty(W)=W$ for any fixed point W. To prove the central results of this chapter, we also need the following technical lemma.

Lemma 4.6: Let σ_1, σ_2, σ_3 be three strictly positive numbers and let x_0 be the smallest positive root of the polynomial $p:x\mapsto x^4-\sigma_1x^2-\sigma_2x-\sigma_3$. Then for all $x>x_0$ one has $p(x)>0$. In particular, p does not admit other positive roots.

Proof: It is clear that at least one positive root x_0 exists. Then one has for $x=tx_0$ with $t>1$:

$$\begin{aligned}p(x)&=t^4x_0^4-\sigma_1t^2x_0^2-\sigma_2tx_0-\sigma_3\\&=t^4(\sigma_1x_0^2+\sigma_2x_0+\sigma_3)-\sigma_1t^2x_0^2-\sigma_2tx_0-\sigma_3\\&=\sigma_1t^2(t^2-1)x_0^2+\sigma_2t(t^3-1)x_0+\sigma_3(t^4-1)>0.\end{aligned}$$

This shows that a positive root larger than x_0 does not exist. □

Let $c_\pm$ be the constants defined by (14). We specify σ_1, σ_2, σ_3 to

$$\sigma_1 := 8\sqrt{2}q^{3/2}(b-a)\varepsilon_1^2\tilde{\epsilon}(1+\gamma_k)(C_{\hat{\varrho}_+}\sqrt{\|m_+\|}+C_{\hat{\varrho}_-}\sqrt{\|m_-\|}),\tag{52}$$

$$\sigma_2 := 16q^{5/4}\mathfrak{g}_1\varepsilon_1^2\tilde{\epsilon}(1+\gamma_k)(C_{\hat{\varrho}_+}p_+ + C_{\hat{\varrho}_-}p_-),\tag{53}$$

$$\sigma_3 := \varepsilon_1(\|\varphi_\Gamma\|_{W^{1,2}_{\mathbb{R}}}+\tilde{\epsilon}(1+\gamma_k)(\|D\|_{W^{-1,2}_\Gamma}+q\varepsilon_1(C_{\hat{\varrho}_+}r_+ + C_{\hat{\varrho}_-}r_-))),\tag{54}$$

where $C_{\hat{\varrho}_\pm}$ are according to (31), $c_\pm$ according to (14), and

$$p_\pm := ((\alpha_a^\pm)^2+(\alpha_b^\pm)^2)^{1/2}\|(H_0^\pm)^{-1/2}\|^{1/2}_{\mathfrak{B}(\mathfrak{H},W^{1,2})},\tag{55}$$

$$\begin{aligned}r_\pm :=& 8+4\sqrt{2}(b-a)\sqrt{\|m_\pm\|_{L^\infty}}\sqrt{8c_\pm+5+4\|V_0^\pm\|_{L^\infty}}\\&+8\sqrt{2}\mathfrak{g}_1((\alpha_a^\pm)^2+(\alpha_b^\pm)^2)^{1/2}\|(H_0^\pm)^{-1/2}\|^{1/2}_{\mathfrak{B}(\mathfrak{H};W^{1,2})}(8c_\pm+5+4\|V_0^\pm\|_{L^\infty})^{1/4}.\end{aligned}\tag{56}$$

Theorem 4.7: *The following statements are true:*

(1) The mapping $\Psi_\infty:L^\infty\to L^\infty$ always has a fixed point.

(2) If x_0 is the (unique) positive root of the polynomial $p:x\to x^4-\sigma_1x^2-\sigma_2x-\sigma_3$, then for any fixed point W of Ψ_∞ the inequality

$$\|W\|_{L^\infty}\leqslant x_0^4 \tag{57}$$

holds.

Proof: One has

$$\begin{aligned}\|\mathcal{J}(u^+,u^-)\|_{W^{1,2}_{\mathbb{R}}}&\leqslant\|\varphi_\Gamma\|_{W^{1,2}_{\mathbb{R}}}+\|\mathcal{P}_0^{-1}(D+qu^+-qu^-)\|_{W^{1,2}_\Gamma}\\&\leqslant\|\varphi_\Gamma\|_{W^{1,2}_{\mathbb{R}}}+\tilde{\epsilon}(1+\gamma_k)\|D+qu^+-qu^-\|_{W^{-1,2}_\Gamma}\\&\leqslant\|\varphi_\Gamma\|_{W^{1,2}_{\mathbb{R}}}+\tilde{\epsilon}(1+\gamma_k)(\|D\|_{W^{-1,2}_\Gamma}+q\varepsilon_1(\|u^+\|_{L^1}+\|u^-\|_{L^1})),\end{aligned}$$

which implies

$$\|E_\infty\mathcal{J}(u^+,u^-)\|_{L^\infty}\leqslant\varepsilon_1\|\varphi_\Gamma\|_{W^{1,2}_{\mathbb{R}}}+\varepsilon_1\tilde{\epsilon}(1+\gamma_k)(\|D\|_{W^{-1,2}_\Gamma}+q\varepsilon_1(\|u^+\|_{L^1}+\|u^-\|_{L^1})). \tag{58}$$

Since $u^\pm=\mathcal{N}^\pm_{\hat{\varrho}_\pm}(V_\pm)$ one gets from (35) the estimate

$$\begin{aligned}\|u^\pm\|_{L^1}\leqslant C_{\hat{\varrho}_\pm}&(8+4\sqrt{2}(b-a)\sqrt{\|m_\pm\|_{L^\infty}}\sqrt{8c_\pm+5+4\|V_\pm\|_{L^\infty}}\\&+8\sqrt{2}\mathfrak{g}_1((\alpha_a^\pm)^2+(\alpha_b^\pm)^2)^{1/2}\|(H_0^\pm)^{-1/2}\|^{1/2}_{\mathfrak{B}(\mathfrak{H},W^{1,2})}(8c_\pm+5+4\|V_\pm\|_{L^\infty})^{1/4}).\end{aligned}$$

By $V_\pm=V_0^\pm\pm qW$ we obtain

$$\begin{aligned}\|u^\pm\|_{L^1}\leqslant C_{\hat{\varrho}_\pm}&(8+4\sqrt{2}(b-a)\sqrt{\|m_\pm\|_{L^\infty}}\sqrt{8c_\pm+5+4\|V_0^\pm\|_{L^\infty}+4q\|W\|_{L^\infty}}\\&+8\sqrt{2}\mathfrak{g}_1((\alpha_a^\pm)^2+(\alpha_b^\pm)^2)^{1/2}\|(H_0^\pm)^{-1/2}\|^{1/2}_{\mathfrak{B}(\mathfrak{H},W^{1,2})}(8c_\pm+5+4\|V_0^\pm\|_{L^\infty}+4q\|W\|_{L^\infty})^{1/4}).\end{aligned} \tag{59}$$

Using the estimates

$$\sqrt{8c_\pm+5+4\|V_0^\pm\|_{L^\infty}+4q\|W\|_{L^\infty}}\leqslant\sqrt{8c_\pm+5+4\|V_0^\pm\|_{L^\infty}}+2\sqrt{q\|W\|_{L^\infty}}$$

and

$$(8c_\pm+5+4\|V_0^\pm\|_{L^\infty}+4q\|W\|_{L^\infty})^{1/4}\leqslant(8c_\pm+5+4\|V_0^\pm\|_{L^\infty})^{1/4}+(4q\|W\|_{L^\infty})^{1/4}$$

we get

$$\|u^\pm\|_{L^1}\leqslant\sigma_1^\pm\|W\|^{1/2}_{L^\infty}+\sigma_2^\pm\|W\|^{1/4}_{L^\infty}+\sigma_3^\pm, \tag{60}$$

with

$$\sigma_1^\pm:=8C_{\hat{\varrho}_\pm}(b-a)\sqrt{2q\|m_\pm\|_{L^\infty}},$$

$$\sigma_2^\pm:=16q^{1/4}\mathfrak{g}_1C_{\hat{\varrho}_\pm}p_\pm,$$

$$\sigma_3^\pm:=C_{\hat{\varrho}_\pm}r_\pm,$$

where $p_\pm$ and $r_\pm$ are defined by (55) and (56), respectively. Inserting (60) into (58) we obtain

$$\|E_\infty\mathcal{J}(u^+,u^-)\|_{L^\infty}\leqslant\sigma_1\|W\|^{1/2}_{L^\infty}+\sigma_2\|W\|^{1/4}_{L^\infty}+\sigma_3,$$

where σ_1, σ_2, σ_3 are the constants defined under (52)–(54). Hence we get the estimate

$$\|\Psi_\infty(W)\|_{L^\infty} \leqslant \sigma_1 \|W\|_{L^\infty}^{1/2} + \sigma_2 \|W\|_{L^\infty}^{1/4} + \sigma_3 . \tag{61}$$

If x_0 is the (unique) positive root of the polynomial $x \to x^4 - \sigma_1 x^2 - \sigma_2 x - \sigma_3$ and $\|W\|_{L^\infty} \leqslant x_0^4$, then by (61) one obtains

$$\|\Psi_\infty(W)\|_{L^\infty} \leqslant \sigma_1 (\|W\|_{L^\infty}^{1/4})^2 + \sigma_2 \|W\|_{L^\infty}^{1/4} + \sigma_3 \leqslant \sigma_1 x_0^2 + \sigma_2 x_0 + \sigma_3 = x_0^4.$$

This means, that Ψ_∞ maps the ball $\{W: \|W\|_{L^\infty} \leqslant x_0^4\}$ continuously into itself. Since Ψ_∞ is compact the image of this ball under Ψ_∞ is precompact in L^∞. Thus, by Schauder's fixed point theorem Ψ_∞ must have a fixed point. This proves the first assertion.

Assume that the second assertion is false and a fixed point W satisfying $\|W\|_{L^\infty} > x_0^4$ exists. Then (61) would give

$$(\|W\|_{L^\infty}^{1/4})^4 = \|W\|_{L^\infty} = \|\Psi_\infty(W)\|_{L^\infty} \leqslant \sigma_1 (\|W\|_{L^\infty}^{1/4})^2 + \sigma_2 \|W\|_{L^\infty}^{1/4} + \sigma_3 .$$

On account of $\|W\|_{L^\infty}^{1/4} > x_0$ this is a contradiction to Lemma 4.6. □

Now we can state our main result:

Theorem 4.8: *Under Assumption 4.2 the dissipative Schrödinger–Poisson system (see Problem 4.4) always has a solution and any solution* (φ, u^+, u^-) *of the dissipative Schrödinger–Poisson system satisfies the a priori estimates*

$$\|\varphi\|_{L^\infty} \leqslant x_0^4, \quad \|u^\pm\|_{L^1} \leqslant C_{\hat{\varrho}_\pm} \hat{r}_\pm , \tag{62}$$

where x_0 *is the unique positive root of the polynomial* $x \to x^4 - \sigma_1 x^2 - \sigma_2 x - \sigma_3$ *with coefficients given by (52)–(56) and*

$$\hat{r}_\pm := [8 + 4\sqrt{2}(b-a)\sqrt{\|m_\pm\|_{L^\infty}} \sqrt{8c_\pm + 5 + 4\|V_0^\pm\|_{L^\infty} + 4qx_0^4}$$
$$+ 8\sqrt{2}\mathfrak{g}_1((\alpha_a^\pm)^2 + (\alpha_b^\pm)^2)^{1/2} \|(H_0^\pm)^{-1/2}\|_{\mathfrak{B}(\mathfrak{H}, W^{1,2})}^{1/2} (8c_\pm + 5 + 4\|V_0^\pm\|_{L^\infty} + 4qx_0^4)^{1/4}].$$

Proof: The first assertion follows from Lemma 4.5 and Theorem 4.7. The first inequality of (62) is implied by (57), while the other estimates are obtained from (59) and the first inequality. □

V. CONCLUSION

Let us comment the results.

(i) We have shown (see Theorem 4.8) that the dissipative Schrödinger–Poisson system (see Problem 4.4) *always* has a solution, if the Assumptions 4.2 are satisfied.

(ii) The solutions (φ, u^+, u^-) of a dissipative Schrödinger–Poisson system have bounds which *only* depend on the data $m_\pm$, $\kappa_a^\pm$, $\kappa_b^\pm$, $V_0^\pm$, C, ϵ, φ_Γ, k, and the steady states $\varrho_\pm$. In particular, the bound for the electrostatic potential φ may be directly calculated from the data by Cardano's formula.

(iii) In contrast to self-adjoint Schrödinger–Poisson systems dissipative ones allow in general nontrivial currents $j_{\hat{\varrho}_\pm}^\pm$ which are independent from $x \in [a,b]$ provided the steady states $\varrho_\pm$ are determined by (29) with

$$\int_{\mathbb{R}} d\lambda \, \mathrm{tr}(\hat{\varrho}_\pm(\lambda)) < \infty$$

(see Ref. 17).

(iv) The last fact allows us to couple dissipative Schrödinger–Poisson systems to drift diffusion models acting outside the interval $[a,b]$ via a current continuity condition. In a forthcoming paper we will show how this can be done and we will prove that the coupled system has a solution.

(v) It is an open problem under which conditions the solution, guaranteed by Theorem 4.8, is unique. This situation is similar to that of the stationary Van Roosbroeck system (see Ref. 21, 3.4), or that of the Kohn-Sham equations (see Refs. 13, 14, and 27 and the references cited there).

(vi) The present article solves the dissipative Schrödinger–Poisson system in one spatial dimension; the two- and three-dimensional problems remain open.

(vii) The density matrices $\varrho_\pm$ determine the statistical properties of the quantum system. Therefore, they change from system to system.

APPENDIX: RESOLVENT ESTIMATE FOR H_0

For the operator (12) there is

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}=\sum_{l=0}^{\infty}\frac{1}{\zeta_l+1+\mu},$$

where the numbers ζ_l are the eigenvalues of the operator H_0-1. Let $\hat{H}_0$ be the self-adjoint operator (12) where m is specified to $m(x)\equiv 1$. Obviously, there is $1/\|m\|_{L^\infty}(\hat{H}_0-1)\leqslant H_0-1$. The eigenvalues of $\hat{H}_0-1$ are given by $\pi^2 l^2/(2(b-a)^2)$, $l=0,1,\ldots$. Thus the minimax principle implies

$$(1/\|m\|_{L^\infty})[\pi^2 l^2/(2(b-a)^2)]\leqslant\zeta_l, =0,1,\ldots.$$

Hence,

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}\leqslant\sum_{l=0}^{\infty}\frac{1}{(1/\|m\|_{L^\infty})[\pi^2/(2(b-a)^2)]l^2+1+\mu}.$$

For any $l\geqslant 1$ we have

$$\frac{1}{(1/\|m\|_{L^\infty})[4\pi^2/(b-a)^2]l^2+1+\mu}\leqslant\int_{l-1}^{l}\frac{ds}{(1/\|m\|_{L^\infty})[\pi^2/(2(b-a)^2)]s^2+1+\mu}.$$

Thus,

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}\leqslant\frac{1}{1+\mu}+\sum_{l=1}^{\infty}\int_{l-1}^{l}\frac{ds}{(1/\|m\|_{L^\infty})[\pi^2/(2(b-a)^2)]s^2+1+\mu},$$

which yields

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{L}_2(\mathfrak{H})}\leqslant\frac{1}{1+\mu}+\sqrt{\|m\|_{L^\infty}}\,\frac{b-a}{\sqrt{2}}\,\frac{1}{\sqrt{1+\mu}}.$$

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A polymer expansion for the quantum Heisenberg ferromagnet wave function

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A polymer expansion is given for the quantum Heisenberg ferromagnet wave function. Working on a finite lattice, one is dealing entirely with algebraic identities; there is no question of convergence. The conjecture to be pursued in further work is that effects of large polymers are small. This is relevant to the question of the utility of the expansion and its possible extension to the infinite volume. In themselves the constructions of the present paper are neat and elegant and have surprising simplicity. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1627958]

This paper assumes the fundamentals of the Heisenberg model but is basically self-contained; it arises from the work in Refs. 1 and 2, but these references need not be referred to. We intend to continue the work in the present paper, to obtain bounds on polymer contributions enabling extension to the infinite lattice.

Unpublished preprints (Refs. 1 and 2) are the previous works by the author, directly related to the current paper. Reference 1 is an experimental study of a number of approximations for certain spin expectations. Incidentally, one of the formal constructs studied below was introduced, with some properties there stated without proof, which are in the present paper. This is detailed below. We do hope that the present cluster expansion can be used to justify some of the approximations of Ref. 1; this is a line of theoretical interest for future work. In Ref. 2 there is an alternate construction of a cluster expansion to our present one. Therein there is also proof of convergence in the t small region. Our present construction is much simpler. Whether patent or latent, underlying all our work on the Heisenberg model is the hope that it eventually leads to a proof of the phase transition.

Equation (16) is the representation of the Heisenberg wave function we devote this paper towards developing. It is in the form commonly called a ''polymer expansion'' or ''cluster expansion'' in statistical mechanics nomenclature. At the end of the paper we give a brief physical discussion addressing usual interpretations of such expansions.

We work with a finite rectangular lattice, V, in d-dimensions, $\mathcal{V}$ the set of its vertices. The Hamiltonian is taken as

$$H=-\sum_{i\sim j}\ \frac{1}{2}\ (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j-1)=-\sum_{i\sim j}\ (I_{ij}-1), \tag{1}$$

where I_{ij} interchanges the spins at nearest neighbor sites i and j. The Hilbert space $\mathcal{H}$ is constructed from basis elements $\mathbf{i}_{\mathcal{S}}$, basis elements in 1–1 correspondence with subsets $\mathcal{S}$ of $\mathcal{V}$, used for their labeling. In a spin-up spin-down representation

$$\mathbf{i}_{\mathcal{S}}=\bigotimes_{i\in\mathcal{S}}\begin{pmatrix}1\\0\end{pmatrix}_i\bigotimes_{j\notin\mathcal{S}}\begin{pmatrix}0\\1\end{pmatrix}_j. \tag{2}$$

A vector $\mathbf{f}$ in $\mathcal{H}$ may be expanded as

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$$\mathbf{f}=\sum_{\mathcal{S}} f(\mathcal{S})\mathbf{i}_{\mathcal{S}}. \tag{3}$$

For two sets $\mathcal{S}$ and $\mathcal{S}'$ we write $\mathcal{S}\sim\mathcal{S}'$ if $\mathcal{S}'$ is constructed from $\mathcal{S}$ by replacing some single element of $\mathcal{S}$ by one of its nearest neighbors. That is, $\mathcal{S}\sim\mathcal{S}'$ if there is a set $\mathcal{F}$ and elements of $\mathcal{V}$, i and j, so that

$$\begin{aligned}\mathcal{S}&=\mathcal{F}\cup i,\\ \mathcal{S}'&=\mathcal{F}\cup j,\end{aligned} \tag{4}$$

where $i\sim j$ and the unions in (4) are disjoint. If we write

$$\mathbf{f}(t)=e^{-Ht}\mathbf{f}=\sum_{\mathcal{S}} f(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}, \tag{5}$$

it is easy to see that the $f(\mathcal{S},t)$ satisfy the differential equations

$$\frac{\partial}{\partial t}f(\mathcal{S},t)=\sum_{\mathcal{S}'\sim\mathcal{S}}(f(\mathcal{S}',t)-f(\mathcal{S},t)). \tag{6}$$

This is the graph heat equation, corresponding to a graph with vertices the subsets of $\mathcal{V}$, and with an edge connecting vertices $\mathcal{S}_1$ and $\mathcal{S}_2$ if and only if $\mathcal{S}_1\sim\mathcal{S}_2$. Physically, Eq. (6) is the imaginary time Schrödinger equation corresponding to the quantum Heisenberg Hamiltonian given in (1). (In Ref. 1 as in many other places the Heisenberg model has been experimentally studied by solving the coupled differential equations of (6) numerically.)

We now write $\mathcal{H}$ as direct sum

$$\mathcal{H}=\bigoplus_{n=0}^{\#(\mathcal{V})}\mathcal{H}^n, \tag{7}$$

where as indicated n ranges from 0 to $\#(\mathcal{V})$. $\mathcal{H}^n$ is spanned by the basis elements $\mathbf{i}_{\mathcal{S}}$, where $\#(\mathcal{S})=n$. $\mathcal{H}^n$ is the n spin-wave vector of the Hilbert space $\mathcal{H}$. The $\mathcal{H}^n$ are invariant subspaces of H. We write H^n for H restricted to $\mathcal{H}^n$.

We introduce operators $T^{r,s}$, where $T^{r,s}$ is a linear mapping from $\mathcal{H}^r$ to $\mathcal{H}^s$. They are defined as follows:

(1) $T^{r,r}$ is the identity on $\mathcal{H}^r$;
(2) If $s>r$,

$$T^{r,s}=0;$$

(3) If $s<r$ let $\mathbf{g}$ be in $\mathcal{H}^r$,

$$\mathbf{g}=\sum_{\mathcal{S}} g(\mathcal{S})\mathbf{i}_{\mathcal{S}}, \tag{8}$$

where $g(\mathcal{S})$ is nonzero only if $\#(\mathcal{S})=r$. Let

$$\mathbf{h}=T^{r,s}\mathbf{g}=\sum_{\mathcal{S}} h(\mathcal{S})\mathbf{i}_{\mathcal{S}}. \tag{9}$$

Then $h(\mathcal{S})=0$ unless $\#(\mathcal{S})=s$, and

$$h(\mathcal{S}) = \sum_{\mathcal{S}' \supset \mathcal{S}} g(\mathcal{S}') \quad \text{if} \quad \#(\mathcal{S}) = s. \tag{10}$$

We note that if $r > s > k$, then

$$T^{s,k} T^{r,s} = \frac{(r-k)!}{(s-k)!(r-s)!} T^{r,k}. \tag{11}$$

This is easy counting.

A nice result is that $T^{r,s}$ intertwines H^r and H^s. That is

$$T^{r,s} H^r = H^s T^{r,s}, \tag{12}$$

where both sides of (12) are viewed as mappings from $\mathcal{H}^r$ to $\mathcal{H}^s$. This is treated in Appendix A. The formalism of the mappings $T^{r,s}$ was introduced in Sec. II of Ref. 1, without proofs therein. We know of no earlier references to these operators. They may also be studied as a direct consequence of the global rotation invariance of the Heisenberg model, a viewpoint we do not pursue here. From any view, upon familiarlity the $T^{r,s}$ and their properties soon become trivial. A similar more complex parallel theory is given in Ref. 3 for random walks on the permutation group, instead of subspaces of a lattice.

We start presenting the polymer expansion for $\mathbf{f}(t)$ of Eq. (5). We assume $\mathbf{f}(t)$ is normalized so that

$$\sum_{\mathcal{S}} f(\mathcal{S}, t) = 1. \tag{13}$$

We note that if at any time this equation holds, the heat equation, Eq. (6), preserves the identity. We do not consider the possibility that the sum on the left-hand side of (13) be zero, so no such normalization is possible.

We let $\mathcal{P}$ be a partition of $\mathcal{V}$. We write $\mathcal{S}_\alpha < \mathcal{P}$ for a subset $\mathcal{S}_\alpha$ of the partition $\mathcal{P}$. One has

$$S_\alpha \cap S_\beta = \varnothing, \quad \alpha \neq \beta, \tag{14}$$

$$\bigcup_{\alpha \in I^{\mathcal{P}}} \mathcal{S}_\alpha = \mathcal{V}. \tag{15}$$

We will have (summing over all such partitions)

$$\mathbf{f}(t) = \sum_{\mathcal{P}} \bigotimes_{\mathcal{S}\alpha < \mathcal{P}} \mathbf{u}(\mathcal{S}_\alpha, t), \tag{16}$$

where

$$\mathbf{u}(\mathcal{S}_\alpha, t) = \begin{pmatrix} \phi_i(t) \\ 1 - \phi_i(t) \end{pmatrix}_i \tag{17}$$

if $\mathcal{S}_\alpha = \{i\}$.

If $\#(\mathcal{S}_\alpha) = r > 1$,

$$\mathbf{u}(\mathcal{S}_\alpha, t) = u^r(\mathcal{S}_\alpha, t) \bigotimes_{i \in \mathcal{S}\alpha} \begin{pmatrix} 1 \\ -1 \end{pmatrix}_i. \tag{18}$$

We also write

$$u(\mathcal{S},t)=u^r(\mathcal{S},t) \quad \text{if} \quad \#(\mathcal{S})=r \tag{19}$$

and, for the special case $r=1$,

$$u(\mathcal{S},t)=u^1(\mathcal{S},t)=\phi_i(t) \quad \text{if} \quad \mathcal{S}=\{i\}. \tag{20}$$

We write $\mathbf{f}(t)$ as a sum of its different spin-wave number components

$$\mathbf{f}(t)=\sum_{n=0}^{\#(\mathcal{V})} \mathbf{f}_n(t), \tag{21}$$

$$\mathbf{f}_n(t)\in\mathcal{H}^n. \tag{22}$$

We set

$$\mathbf{c}_r(t)=\sum_{n=0}^{\#(\mathcal{V})} T^{n,r}\mathbf{f}_n(t) \tag{23}$$

and

$$\mathbf{c}_r(t)=\sum_{\mathcal{S}} c^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{24}$$

(Notice that the c^r satisfy the graph heat equation, (6).) Then we find that Eq. (16) is satisfied if the $u(\mathcal{S},t)$ are chosen to satisfy:

$$c^r(\mathcal{S},t)=u^r(\mathcal{S},t)+\sum_{\mathcal{P}} \prod_{\mathcal{S}_\beta<\mathcal{P}} u(\mathcal{S}_\beta,t), \tag{25}$$

where here the $\mathcal{P}$ are all **proper** partitions of $\mathcal{S}$ and $\#(\mathcal{S})=r$. r will range from 1 to $\#(\mathcal{V})$. Equations (16) and (25) are prototype cluster-expansion/polymer-expansion equations. But the form of Eq. (18) is perhaps surprising. Appendix B treats the consistency of the formalism; that there is a unique solution for the u's from (25), and they yield Eq. (16).

We present in bold strokes the conventional ways of thinking about cluster expansions like Eq. (16). In the second term in Eq. (5) as one expands the exponent in powers of H, each I_{ij} that appears represents a ''collision'' and interchanges spins at i and j. We can neglect interchanges when both spins are the same. Then we have a picture where spins ''collide'' and change places. The evolution yields a sequence of collisions and corresponding motions of the spins. This naturally leads to a ''random-walk'' picture of spins moving and colliding. $u^r(\mathcal{S},t)$ is related to a process where the spins at the sites in $\mathcal{S}$ at time t have had a history in which they have all mutually collided, and where spins in no smaller subset of $\mathcal{S}$ has not collided with spins in the complementary portion of $\mathcal{S}$.

Reference 4 is a standard general treatment of cluster expansions, and Ref. 5 a treatment of the random walk picture sketched above. However knowledge of these detailed technical directions will not simplify our derivation above; and further, starting from Refs. 4 and 5, I think it unlikely that many researchers would find our ''simple'' result. However to get the estimates on the u^r needed for applications, these references will be useful.

The proof of convergence in the infinite volume, commonly referred to simply as ''convergence of the cluster expansion,'' depends on obtaining appropriate bounds on the u^r. Convergence in the ''small t'' region was proven in Ref. 2 for a different construction of a cluster expansion. A proof for the ''small t'' region can certainly be greatly simplified over that in Ref. 2. The author believes that the expansion converges also in the ''large t'' region, i.e., for $t>T_0$ for some T_0 (possibly even for all t). This will be difficult to prove. It seems that the proof for large t will depend on incorporating unusual probabilistic estimates, exhibiting probabilistic cancellations in

certain sums involving many terms. One may hope that the compact form of the present construction of the cluster expansion may simplify some details of a proof, still a substantial theoretical challenge.

APPENDIX A: INTERTWINING RESULT

In virtue of Eq. (11) it is enough to show $T^{r,r-1}$ intertwines. We choose to show equivalently that $T^{r,r-1}$ carries a solution of the heat equation into a solution of the heat equation. Let $f(\mathcal{S},t)$ satisfy the heat equation, and be zero unless $\#(\mathcal{S})=r$. We define

$$g(s,t)=\sum_j f(s\cup j,t),\quad \#(s)=r-1. \tag{A1}$$

We wish to show g satisfies the heat equation. Writing the heat equation for f:

$$\frac{\partial f}{\partial t}(s\cup i,t)=\sum_{\mathcal{S}'\sim(s\cup i)}(f(\mathcal{S}',t)-f(s\cup i,t)). \tag{A2}$$

We sum the two sides of (A2) over i,

$$\frac{\partial}{\partial t}g(s,t)=\sum_i\sum_{\mathcal{S}'\sim(s\cup i)}(f(\mathcal{S}',t)-f(s\cup i,t)). \tag{A3}$$

The right-hand side splits into two terms I_1 and I_2,

$$I_1=\sum_i\sum_{s'\sim s}(f(s'\cup i,t)-f(s\cup i,t)) \tag{A4}$$

and

$$I_2=\sum_i\sum_{j\sim i}(f(s\cup j,t)-f(s\cup i,t)). \tag{A5}$$

It is easy to see

$$I_1=\sum_{s'\sim s}(g(s',t)-g(s,t)) \tag{A6}$$

and just a little harder to see

$$I_2=0$$

and the result is proved.

APPENDIX B: IN THREE PARTS

We divide the demonstration of consistency into three parts:

(i) We first note that Eq. (25) has a unique solution for the u^r (these are the unknowns). One solves inductively over r, the rth equation uniquely determining u^r.

(ii) Once the u's are determined from Eq. (25), we substitute them in the right-hand side of Eq. (16) which we call $\mathbf{X}(t)$, so Eq. (16) becomes

$$\mathbf{f}(t)=\mathbf{X}(t). \tag{B1}$$

(Of course we do not know whether (B1) is true, that is what we are trying to show.) We decompose $\mathbf{X}(t)$,

$$\mathbf{X}(t)=\sum_{n=0}^{\#(\mathcal{V})}\mathbf{X}_n(t), \tag{B2}$$

$$\mathbf{X}_n(t)\in\mathcal{H}^n, \tag{B3}$$

and define

$$\mathbf{d}_r(t)=\sum_{n=0}^{\#(\mathcal{V})}T^{n,r}\mathbf{X}_n(t), \tag{B4}$$

$$\mathbf{d}_r(t)=\sum_{\mathcal{S}}d^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{B5}$$

The result we seek to now show is the following: If $d^r(\mathcal{S},t)=c^r(\mathcal{S},t)$ all $\mathcal{S},r$, then $\mathbf{f}(t)=\mathbf{X}(t)$.

This we also show by induction over r, but in the opposite direction, from $r=\#(\mathcal{V})$ down to $r=0$. At the step $r=r$ we clearly get

$$\mathbf{f}_r(t)=\mathbf{X}_r(t). \tag{B6}$$

(One only needs $T^{r,r}=I$, and $T^{r,s}=0$ if $s>r$.)

(iii) We are left with the task of showing

$$d^r(\mathcal{S},t)=c^r(\mathcal{S},t). \tag{B7}$$

We first do a preliminary investigation.

Let

$$\mathbf{h}(t)=\sum h(\mathcal{S},t)\mathbf{i}_{\mathcal{S}} \tag{B8}$$

$$=\sum_{n=0}^{\#(\mathcal{V})}\mathbf{h}_n(t), \tag{B9}$$

$$\mathbf{h}_n(t)\in\mathcal{H}^n \tag{B10}$$

and define

$$\mathbf{g}_r(t)=\sum_n T^{n,r}\mathbf{h}_n(t) \tag{B11}$$

$$=\sum_{\mathcal{S}}g^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{B12}$$

We then find the following expression for $g^r(\mathcal{S},t)$:

$$g^r(\mathcal{S},t)=\sum_{\substack{\mathcal{S}'\\ \mathcal{S}'\cap\mathcal{S}=\phi}}h(\mathcal{S}\cup\mathcal{S}',t), \tag{B13}$$

where $\#(\mathcal{S})=r$.

Now when we compute $d^r(\mathcal{S},t)$ using expression (B13) with X replacing h ($\mathbf{X}(t)=\Sigma_{\mathcal{S}}X(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}$), the only terms in the expression for $\mathbf{X}(t)$ from (16) which will contribute are of the form

$$\left(\mathbf{u}^r(\mathcal{S},t)+\sum_{\mathcal{P}}\bigotimes_{\mathcal{S}_\beta<\mathcal{P}}\mathbf{u}(\mathcal{S}_\beta,t)\right)\bigotimes_{i\notin\mathcal{S}}\begin{pmatrix}\phi_i(t)\\ 1-\phi_i(t)\end{pmatrix}_i \tag{B14}$$

using the notation from Eq. (25). That is because the sum over $\mathcal{S}'$ in (B13) may be written as an iterated sum, summing for each vertex not in $\mathcal{S}$, whether the vertex is in $\mathcal{S}'$ or not. This amounts to summing over spin-up and spin-down at that vertex. At vertex k this sum applied to the term in the tensor product

$$\begin{pmatrix} \phi_k(t) \\ 1-\phi_k(t) \end{pmatrix}_k$$

yields 1, and applied to

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix}_k$$

yields 0. We get from the terms in $\mathbf{X}(t)$ in (B14) that

$$d^r(\mathcal{S},t)=c^r(\mathcal{S},t). \tag{B15}$$

Q.E.D.

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On the Pauli operator for the Aharonov–Bohm effect with two solenoids

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We consider a spin-1/2 charged particle in the plane under the influence of two idealized Aharonov–Bohm fluxes. We show that the Pauli operator as a differential operator is defined by appropriate boundary conditions at the two vortices. Further we explicitly construct a basis in the deficiency subspaces of the symmetric operator obtained by restricting the domain to functions with supports separated from the vortices. This construction makes it possible to apply the Krein's formula to the Pauli operator. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629395]

I. INTRODUCTION

The goal of the present paper is to provide a more detailed analysis of the Pauli operator describing a spin-1/2 charged particle under the influence of two Aharonov–Bohm (AB) fluxes.[1] We consider the idealized setup when the magnetic fluxes are concentrated along two parallel lines so that the problem effectively reduces to a two-dimensional quantum system living in a perpendicular plane. In what follows we call the intersection points of the fluxes with the plane vortices.

To define the Pauli Hamiltonian with singular fluxes we use the Aharonov–Casher decomposition.[2] It makes it possible to introduce the two diagonal components of the Pauli operator corresponding to spin up and down as the unique self-adjoint operators associated to appropriate quadratic forms. Since the magnetic field vanishes outside of the vortices the two components of the Pauli Hamiltonian as well as the spinless AB Hamiltonian are self-adjoint extensions of the same symmetric operator. In the case of one AB flux all the self-adjoint extensions are known to be defined by appropriate boundary conditions at the vortex.[3,4] Thus our first goal was to distinguish the boundary conditions defining the two components of the Pauli Hamiltonian.

The second goal was to construct a basis in the deficiency subspaces in the two-vortex case. In this case as well the two diagonal components of the Pauli Hamiltonian and the spinless Hamiltonian are self-adjoint extensions of a common symmetric operator. We show that the deficiency indices of this symmetric operator are (4,4). The construction is based on the observation that the coefficients $\psi(x)$ standing at singular terms in the asymptotic expansion in the variable x_0 at a vortex of the Green function $\mathcal{G}_z(x,x_0)$ belong to the deficiency subspace with spectral parameter z. Here we make use of the explicit knowledge of the spinless two-vortex Green function $\mathcal{G}_z(x,x_0)$.[5]

The next and final goal which naturally follows is a construction of the two-vortex Green function for the Pauli Hamiltonian with the aid of the Krein's formula. Even this problem is solved explicitly. Surprisingly many features can be again derived from the asymptotic analysis near a vortex.

The paper is organized as follows. In Sec. II we summarize some basic facts and formulas concerning the spinless AB Hamiltonian with one and two vortices. In Sec. III we introduce the Pauli operator with one and two AB fluxes and derive the boundary conditions at a vortex defining

the spin up and down components of the Pauli Hamiltonian. In Sec. IV we provide a basic asymptotic analysis near a vortex of functions from the deficiency subspaces as well as that of the spinless Green function. In Sec. V we construct a basis in the deficiency subspaces. Section VI is devoted to the application of the Krein's formula to our problem.

II. PRELIMINARIES. THE AB HAMILTONIAN FOR A SPINLESS PARTICLE

The AB Hamiltonian with one vortex and describing a spinless particle, H_0, was introduced in Ref. 1 and studied in a long series of papers by many authors. For example, one can consult Ref. 6 for some mathematical details. It acts in $L^2(\mathbb{R}^2, \mathrm{d}^2x)$ and is nothing but the self-adjoint operator associated to the closure of the positive quadratic form

$$\int_{\mathbb{R}^2}\left(\left|\left(\partial_{x_1}-i\frac{\alpha x_2}{|x|^2}\right)\varphi\right|^2+\left|\left(\partial_{x_2}+i\frac{\alpha x_1}{|x|^2}\right)\varphi\right|^2\right)\mathrm{d}^2x\,, \tag{1}$$

defined on the space of test functions $\mathcal{D}(\mathbb{R}^2\backslash\{0\})$. In other words, H_0 is the Friedrichs extension of the corresponding symmetric operator with the domain $\mathcal{D}(\mathbb{R}^2\backslash\{0\})$. Owing to the gauge equivalence we can assume that $\alpha\in(0,1)$.

We shall use the polar coordinates (r,θ) with the angle $\theta\in(-\pi,\pi)$. This implies a cut along the negative x_1 half-axis. Sometimes it is convenient to apply the unitary operator

$$(U_\alpha\varphi)(r,\theta)=e^{i\alpha\theta}\varphi(r,\theta)$$

and work with the unitarily equivalent operator

$$H=U_\alpha H_0 U_\alpha^{-1}\,.$$

In particular this unitary transformation is useful when constructing the Green function. This means that

$$\mathrm{Dom}(H)=U_\alpha(\mathrm{Dom}(H_0))\,.$$

Formally, as a differential operator,

$$H=-\Delta\,.$$

The domain of H is determined by the boundary conditions at the cut, namely,

$$\psi(r,\pi)=e^{2\pi i\alpha}\psi(r,-\pi),\quad \partial_r\psi(r,\pi)=e^{2\pi i\alpha}\partial_r\psi(r,-\pi)\,. \tag{2}$$

In addition, one should take care about boundary conditions at the vortex. As analyzed in Refs. 3 and 4, the domain of H_0 is characterized by the boundary condition $\varphi(0)=0$. Since $\psi(r,\theta)=\exp(i\alpha\theta)\varphi(r,\theta)$ the same is true for $\mathrm{Dom}(H)$, namely the boundary condition at the vortex reads $\psi(0)=0$.

The generalized eigenfunctions of H,

$$\left\{\frac{1}{\sqrt{2\pi}}J_{|n+\alpha|}(k\,r)\,e^{i(n+\alpha)\theta}\right\}_{k>0,\,n\in\mathbb{Z}},$$

form a complete normalized set,

$$\int_0^\infty J_\nu(k\,x)\,J_\nu(k\,y)\,k\,\mathrm{d}k=\frac{1}{x}\,\delta(x-y)\,.$$

This makes it possible to write down the Green function and the propagator as integrals,

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=\frac{1}{2\pi}\sum_{n\in\mathbb{Z}} e^{i(n+\alpha)(\theta-\theta_0)}\int_0^\infty \frac{J_{|n+\alpha|}(k\,r)\,J_{|n+\alpha|}(k\,r_0)}{k^2-z}\,k\,\mathrm{d}k \tag{3}$$

and

$$\mathcal{K}_t(r,\theta;r_0,\theta_0)=\frac{1}{2\pi}\sum_{n\in\mathbb{Z}} e^{i(n+\alpha)(\theta-\theta_0)}\int_0^\infty e^{-i\,k^2 t}J_{|n+\alpha|}(k\,r)\,J_{|n+\alpha|}(k\,r_0)\,k\,\mathrm{d}k\,. \tag{4}$$

They are related by the Laplace transform,

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=\int_0^\infty e^{z\,t}\,\mathcal{K}_{-i\,t}(r,\theta;r_0,\theta_0)\,\mathrm{d}t\,.$$

Starting from (4) one can derive the following formula for the propagator:[5]

$$\mathcal{K}_t(r,\theta;r_0,\theta_0)=\left\{\begin{array}{c}1\\ e^{2\pi i\alpha}\\ e^{-2\pi i\alpha}\end{array}\right\}\frac{1}{4\pi i\,t}\exp\left(-\frac{1}{4i\,t}|x-x_0|^2\right)-\frac{\sin(\pi\alpha)}{\pi}\int_{-\infty}^{\infty}\frac{1}{4\pi i\,t}$$
$$\times\exp\left(-\frac{1}{4i\,t}R(s)^2\right)\frac{e^{-\alpha s+i\alpha(\theta-\theta_0)}}{1+e^{-s+i(\theta-\theta_0)}}\,\mathrm{d}s\,, \tag{5}$$

where

$$|x-x_0|^2=r^2+r_0^2-2r\,r_0\cos(\theta-\theta_0),\quad R(s)^2=r^2+r_0^2+2r\,r_0\cosh(s),$$

and the phase factor in front of the first term depends on whether

$$\theta-\theta_0\in(-\pi,\pi),\ (\pi,2\pi)\ \text{ or }\ (-2\pi,-\pi).$$

The Laplace transformation results in a formula for the Green function,

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=\left\{\begin{array}{c}1\\ e^{2\pi i\alpha}\\ e^{-2\pi i\alpha}\end{array}\right\}\frac{1}{2\pi}K_0(\sqrt{-z}|x-x_0|)$$
$$-\frac{\sin(\pi\alpha)}{\pi}\int_{-\infty}^{\infty}\frac{1}{2\pi}K_0(\sqrt{-z}\,R(s))\frac{e^{-\alpha s+i\alpha(\theta-\theta_0)}}{1+e^{-s+i(\theta-\theta_0)}}\,\mathrm{d}s\,. \tag{6}$$

The second term on the RHS of (6) can be given still another form with the aid of the identity

$$\int_{-\infty}^{\infty}K_{i\tau}(a)\,K_{-i\tau}(b)\,\frac{e^{\phi\,\tau}}{\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau\quad=\int_{-\infty}^{\infty}K_0(\sqrt{a^2+b^2+2\,a\,b\cosh(u)}\,)\,\frac{e^{-\alpha(u-i\,\phi)}}{1+e^{-u+i\,\phi}}\,\mathrm{d}u$$

for $a>0$, $b>0$, $0<\alpha<1$, and $|\phi|<\pi$. This way we get

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=\frac{1}{2\pi}K_0(\sqrt{-z}|x-x_0|)$$
$$-\frac{\sin(\pi\alpha)}{2\pi^2}\int_{-\infty}^{\infty}K_{i\tau}(\sqrt{-z}\,r)\,K_{-i\tau}(\sqrt{-z}\,r_0)\,\frac{e^{(\theta-\theta_0)\,\tau}}{\sin(\pi(\alpha+i\,\tau))}\,\mathrm{d}\tau \tag{7a}$$

for $\theta-\theta_0\in(-\pi,\pi)$,

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=e^{2\pi i\alpha}\left(\frac{1}{2\pi}K_0(\sqrt{-z}|x-x_0|)\right.$$
$$\left.-\frac{\sin(\pi\alpha)}{2\pi^2}\int_{-\infty}^{\infty}K_{i\tau}(\sqrt{-z}\,r)\,K_{-i\tau}(\sqrt{-z}\,r_0)\frac{e^{(\theta-\theta_0-2\pi)\tau}}{\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau\right) \qquad (7b)$$

for $\theta-\theta_0\in(\pi,2\pi)$, and

$$\mathcal{G}_z(r,\theta;r_0,\theta_0)=e^{-2\pi i\alpha}\left(\frac{1}{2\pi}K_0(\sqrt{-z}|x-x_0|)\right.$$
$$\left.-\frac{\sin(\pi\alpha)}{2\pi^2}\int_{-\infty}^{\infty}K_{i\tau}(\sqrt{-z}\,r)\,K_{-i\tau}(\sqrt{-z}\,r_0)\frac{e^{(\theta-\theta_0+2\pi)\tau}}{\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau\right) \qquad (7c)$$

for $\theta-\theta_0\in(-2\pi,-\pi)$.

Despite this threefold description depending on the value of $\theta-\theta_0$ the Green function should be continuous, even real analytic, in its domain of definition if $x\neq x_0$. Checking the limits from the right and left for $\theta-\theta_0=\pm\pi$ one finds that the continuity is guaranteed by the identity

$$\int_{-\infty}^{\infty}K_{i\tau}(a)\,K_{-i\tau}(b)\,\mathrm{d}\tau=\pi K_0(a+b)\quad\text{for } a>0,\ b>0.$$

Let us add a remark on deficiency subspaces. First we recall a general and easy to verify fact. Let A be a self-adjoint extension of a symmetric operator X. Denote by $\mathcal{N}(z)=\mathrm{Ker}(X^*-z)$ the deficiency subspaces, $\mathrm{Im}\,z\neq0$. Then it holds

$$f\in\mathcal{N}(w)\Rightarrow f+(z-w)(A-z)^{-1}f\in\mathcal{N}(z)\,.$$

This can be illustrated on our problem. We choose H [the one-vortex AB Hamiltonian defined by the boundary conditions (2)] for A, and X is a restriction of H obtained by requiring the supports of functions from the domain of X to be separated from the singular point (the origin). The deficiency indices are known to be (2,2). For a basis in $\mathcal{N}(z)$ we can choose the vectors

$$\psi_{-1,z}(r,\theta)=K_{1-\alpha}(\sqrt{-z}\,r)e^{i(\alpha-1)\theta},\quad \psi_{0,z}(r,\theta)=K_{\alpha}(\sqrt{-z}\,r)e^{i\alpha\theta}. \qquad (8)$$

Here $z\in\mathbb{C}\backslash\mathbb{R}_+$, $\mathrm{Re}\,\sqrt{-z}>0$. As shown in Ref. 3 it holds true that

$$\int_0^{\infty}\left(\int_{-\pi}^{\pi}\mathcal{G}_z(r,\theta;r_0,\theta_0)\,\psi_{0,w}(r_0,\theta_0)\,\mathrm{d}\theta_0\right)r_0\,\mathrm{d}r_0$$
$$=\frac{1}{z-w}e^{i\alpha\theta}\left(\left(\frac{\sqrt{-z}}{\sqrt{-w}}\right)^{\alpha}K_{\alpha}(\sqrt{-z}\,r)-K_{\alpha}(\sqrt{-w}\,r)\right),$$

hence

$$\psi_{0,w}+(z-w)(H-z)^{-1}\psi_{0,w}=\left(\frac{\sqrt{-z}}{\sqrt{-w}}\right)^{\alpha}\psi_{0,z}\,. \qquad (9)$$

Similarly,

$$\psi_{-1,w}+(z-w)(H-z)^{-1}\psi_{-1,w}=\left(\frac{\sqrt{-z}}{\sqrt{-w}}\right)^{1-\alpha}\psi_{-1,z}\,. \qquad (10)$$

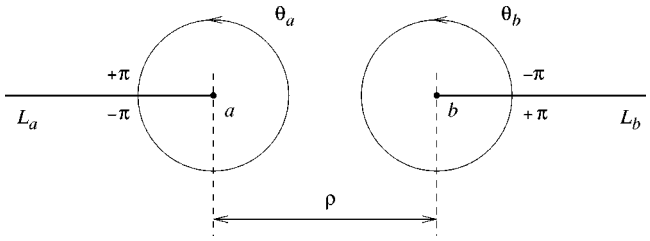

FIG. 1. Geometrical arrangement. Choice of the cuts L_a, L_b and choice of the angle variables θ_a, θ_b.

Let us now focus on the case of two vortices but still considering a spineless particle. The vortices are supposed to be located in the points $a=(0,0)$ and $b=(\rho,0)$, $\rho>0$. Let (r_a,θ_a) be the polar coordinates centered at the point a and (r_b,θ_b) be the polar coordinates centered at the point b. The two-vortex AB Hamiltonian H_0 is the unique self-adjoint operator associated to the quadratic form

$$\int_{\mathbb{R}^2}(|(-i\,\partial_{x_1}-A_1)\varphi|^2+|(-i\,\partial_{x_2}-A_2)\varphi|)^2\,\mathrm{d}^2x\,, \tag{11a}$$

where

$$A=-\alpha\,\mathrm{d}\theta_a-\beta\,\mathrm{d}\theta_b\,. \tag{11b}$$

Again, owing to the gauge equivalence, we can assume that $\alpha,\beta\in(0,1)$.

Also in this case one can pass to a unitarily equivalent formulation. The plane is cut along two half-lines,

$$L_a=(-\infty,0)\times\{0\}\quad\text{and}\quad L_b=(\rho,+\infty)\times\{0\}.$$

The values $\theta_a=\pm\pi$ correspond to the two sides of the cut L_a and similarly for θ_b and L_b. The geometrical arrangement is sketched in Fig. 1. The unitarily equivalent Hamiltonian H is formally equal to $-\Delta$ and is determined by the boundary conditions along the cut,

$$\begin{aligned}&\psi(r_a,\theta_a=\pi)=e^{2\pi i\alpha}\psi(r_a,\theta_a=-\pi),\quad \partial_{r_a}\psi(r_a,\theta_a=\pi)=e^{2\pi i\alpha}\partial_{r_a}\psi(r_a,\theta_a=-\pi)\,,\\&\psi(r_b,\theta_b=\pi)=e^{2\pi i\beta}\psi(r_b,\theta_b=-\pi),\quad \partial_{r_b}\psi(r_b,\theta_b=\pi)=e^{2\pi i\beta}\partial_{r_b}\psi(r_b,\theta_b=-\pi)\,.\end{aligned} \tag{12}$$

In addition, one should impose a boundary condition at the vortex, namely, $\psi(a)=\psi(b)=0$.

A formula for the Green function of the Hamiltonian H is known also in the case of two vortices.[5] For a couple of points $x,x_0\in\mathbb{R}^2\backslash(L_a\cup L_b)$ we set

$$\zeta_a=1\quad\text{or}\quad\zeta_a=e^{2\pi i\alpha}\quad\text{or}\quad\zeta_a=e^{-2\pi i\alpha}$$

depending on whether the segment $\overline{x_0x}$ does not intersect L_a, or $\overline{x_0x}$ intersects L_a and x_0 lies in the lower half-plane, or $\overline{x_0x}$ intersects L_a and x_0 lies in the upper half-plane. Analogously,

$$\zeta_b=1\quad\text{or}\quad\zeta_b=e^{2\pi i\beta}\quad\text{or}\quad\zeta_b=e^{-2\pi i\beta}$$

depending on whether the segment $\overline{x_0x}$ does not intersect L_b, or $\overline{x_0x}$ intersects L_b and x_0 lies in the upper half-plane, or $\overline{x_0x}$ intersects L_b and x_0 lies in the lower half-plane. Furthermore, let us set

$$\zeta_a=e^{i\alpha\eta_a},\quad \zeta_b=e^{i\beta\eta_b},\ \text{where}\quad \eta_a,\eta_b\in\{0,2\pi,-2\pi\}.$$

Remark: Notice that if $\zeta_a \neq 1$ then necessarily $\zeta_b = 1$ and vice versa.

The formula for the Green function reads

$$\begin{aligned}
\mathcal{G}_z(x,x_0) = {} & \zeta_a\zeta_b \frac{1}{2\pi} K_0(\sqrt{-z}|x-x_0|) \\
& - \zeta_a \frac{\sin(\pi\alpha)}{2\pi^2} \int_{-\infty}^{\infty} K_{i\tau}(\sqrt{-z}\, r_a)\, K_{-i\tau}(\sqrt{-z}\, r_{0a}) \frac{e^{(\theta_a-\theta_{0a}-\eta_a)\tau}}{\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau \\
& - \zeta_b \frac{\sin(\pi\beta)}{2\pi^2} \int_{-\infty}^{\infty} K_{i\tau}(\sqrt{-z}\, r_b)\, K_{-i\tau}(\sqrt{-z}\, r_{0b}) \frac{e^{(\theta_b-\theta_{0b}-\eta_b)\tau}}{\sin(\pi(\beta+i\tau))}\,\mathrm{d}\tau + \frac{1}{2\pi} \\
& \times \sum_{\gamma,\, n\geqslant 2} (-1)^n \int_{\mathbb{R}^n} K_{i\tau_n}(\sqrt{-z}\, r) K_{i(\tau_{n-1}-\tau_n)}(\sqrt{-z}\,\rho) \\
& \times \cdots \times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho) K_{-i\tau_1}(\sqrt{-z}\, r_0) \frac{\sin(\pi\sigma_n)\exp(\theta\tau_n)}{\pi\sin(\pi(\sigma_n+i\tau_n))} \\
& \times \frac{\sin(\pi\sigma_{n-1})}{\pi\sin(\pi(\sigma_{n-1}+i\tau_{n-1}))} \times \cdots \times \frac{\sin(\pi\sigma_2)}{\pi\sin(\pi(\sigma_2+i\tau_2))} \frac{\sin(\pi\sigma_1)\exp(-\theta_0\tau_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^n\tau\,.
\end{aligned} \tag{13}$$

Here the sum $\Sigma_{\gamma,\, n\geqslant 2}$ runs over all finite alternating sequences of length at least two, $\gamma = (c_n, c_{n-1}, \ldots, c_1)$, such that for all j, $c_j \in \{a,b\}$ and $c_j \neq c_{j+1}$, and $\sigma_j = \alpha$ (respectively, β) depending on whether $c_j = a$ (respectively, b). In addition, (r,θ) are the polar coordinates of the point x with respect to the center c_n, (r_0,θ_0) are the polar coordinates of the point x_0 with respect to the center c_1 (the dependence on γ is not indicated explicitly).

III. THE PAULI HAMILTONIAN WITH AB FLUXES

According to the Aharonov–Casher ansatz[2] the two diagonal components of the Pauli Hamiltonian with the third component of spin equal to $\pm 1/2$ can be factorized,

$$H^{\pm} = (p-A)^2 \mp B = P_{\pm}^{*} P_{\pm}\,,$$

where

$$P_{\pm} = (p_1 - A_1) \pm i\,(p_2 - A_2).$$

Using the complex coordinate $z = x_1 + i\,x_2$ one can rewrite the Pauli Hamiltonian as follows:

$$H^{+} = 4(-i\,\partial_z - A_z)(-i\,\partial_{\bar z} - A_{\bar z}),$$

$$H^{-} = 4(-i\,\partial_{\bar z} - A_{\bar z})(-i\,\partial_z - A_z).$$

We start our discussion from considering the situation with one vortex. Then

$$A = \frac{\alpha}{r^2}(x_2\,\mathrm{d}x_1 - x_1\,\mathrm{d}x_2) = -\alpha\;\mathrm{d}\theta = \frac{i\,\alpha}{2} e^{-2i\,\theta}\,\mathrm{d}e^{2i\,\theta} = \frac{i\,\alpha}{2}\frac{\bar z}{z}\,\mathrm{d}\frac{z}{\bar z} = \frac{i\,\alpha}{2}\left(\frac{\mathrm{d}z}{z} - \frac{\mathrm{d}\bar z}{\bar z}\right).$$

Hence

$$A_z = \frac{i\,\alpha}{2z}, \quad A_{\bar z} = -\frac{i\,\alpha}{2\bar z},$$

and we can write

$$H^+ = -4\left(\partial_z + \frac{\alpha}{2z}\right)\left(\partial_{\bar z} - \frac{\alpha}{2\bar z}\right), \quad H^- = -4\left(\partial_{\bar z} - \frac{\alpha}{2\bar z}\right)\left(\partial_z + \frac{\alpha}{2z}\right).$$

In fact, these are formal expressions. More precisely, the operators are defined as the unique self-adjoint operators associated, respectively, to the positive quadratic forms

$$\mathfrak{q}_+(\varphi) = 4\int_{\mathbb{R}^2}\left|\left(\partial_{\bar z} - \frac{\alpha}{2\bar z}\right)\varphi\right|^2 \mathrm{d}^2x, \quad \mathfrak{q}_-(\varphi) = 4\int_{\mathbb{R}^2}\left|\left(\partial_z + \frac{\alpha}{2z}\right)\varphi\right|^2 \mathrm{d}^2x, \tag{14}$$

with their natural maximal domains of definition.

Since the magnetic field vanishes on $\mathbb{R}^2\backslash\{0\}$ the operators $H^\pm$ coincide with the spinless AB Hamiltonian H_0 on the domain $\mathcal{D}(\mathbb{R}^2\backslash\{0\})$ ($\mathcal{D}$ is the space of test functions). This means that all three operators H^+, H^-, and H_0 are self-adjoint extensions of the same symmetric operator $\widetilde{X}$. From Refs. 3 and 4 it is known that all self-adjoint extensions can be described by appropriate boundary conditions at the origin. The method used to derive the boundary conditions was inspired by the description of point interactions in the plane given in Ref. 7. Let us also note that analogous boundary conditions have been derived in Ref. 8 for the model with additional homogeneous magnetic field. The Dirac operator has been discussed, for instance, in Ref. 9.

To describe the boundary conditions one introduces four functionals,

$$\Phi_1^{-1}(\varphi) = \lim_{r\downarrow 0} r^{1-\alpha}\frac{1}{2\pi}\int_0^{2\pi}\varphi(r,\theta)\, e^{i\theta}\,\mathrm{d}\theta,$$

$$\Phi_2^{-1}(\varphi) = \lim_{r\downarrow 0} r^{-1+\alpha}\left(\frac{1}{2\pi}\int_0^{2\pi}\varphi(r,\theta)\, e^{i\theta}\,\mathrm{d}\theta - r^{-1+\alpha}\Phi_1^{-1}(\varphi)\right),$$

$$\Phi_1^{0}(\varphi) = \lim_{r\downarrow 0} r^{\alpha}\frac{1}{2\pi}\int_0^{2\pi}\varphi(r,\theta)\,\mathrm{d}\theta,$$

$$\Phi_2^{0}(\varphi) = \lim_{r\downarrow 0} r^{-\alpha}\left(\frac{1}{2\pi}\int_0^{2\pi}\varphi(r,\theta)\,\mathrm{d}\theta - r^{-\alpha}\Phi_1^{0}(\varphi)\right).$$

Each boundary condition is determined by a couple of matrices $A_1, A_2 \in \mathrm{Mat}(2,\mathbb{C})$ fulfilling [the symbol (A_1, A_2) designates a 2×4 matrix]

$$\mathrm{rank}\,(A_1, A_2) = 2, \quad A_1 D^{-1} A_2^* = A_2 D^{-1} A_1^*,$$

where

$$D = \begin{pmatrix} 1-\alpha & 0 \\ 0 & \alpha \end{pmatrix}.$$

The boundary condition takes the form

$$A_1\begin{pmatrix} \Phi_1^{-1}(\varphi) \\ \Phi_1^{0}(\varphi) \end{pmatrix} + A_2\begin{pmatrix} \Phi_2^{-1}(\varphi) \\ \Phi_2^{0}(\varphi) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Two couples of matrices, $\{A_1, A_2\}$ and $\{A_1', A_2'\}$, determine the same boundary condition if and only if there exists a regular matrix $G \in \mathrm{GL}(2,\mathbb{C})$ such that $(A_1', A_2') = G(A_1, A_2)$.

For example, the domain of the spinless AB Hamiltonian H_0 is determined by the boundary conditions at the vortex $\Phi_1^{-1}(\varphi) = \Phi_1^{0}(\varphi) = 0$ and so by the couple of matrices

$$A_1=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad A_2=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}.$$

We wish to derive the boundary conditions for the Hamiltonians H^+ and H^-. According to the well-known construction, the operator A associated to a semibounded quadratic form $\mathfrak{q}$ is determined by the condition

$$\forall f\in\mathrm{Dom}(A)\subset\mathrm{Dom}(\mathfrak{q}),\quad \forall\varphi\in\mathrm{Dom}(\mathfrak{q}),\quad \langle\varphi,Af\rangle=\mathfrak{q}(\varphi,f)\,.$$

This is to say that $f\in\mathrm{Dom}(\mathfrak{q})$ belongs to $\mathrm{Dom}(A)$ if and only if there exists $g\in\mathcal{H}$ such that the equality $\langle\varphi,g\rangle=\mathfrak{q}(\varphi,f)$ holds true for all $\varphi\in\mathrm{Dom}(\mathfrak{q})$. In that case g is unique and $Af=g$. We are going to apply this prescription to the quadratic forms (14). This amounts to integration by parts.

More precisely, the Green formula implies that

$$\int_{\mathbb{R}^2}(\partial_z f)g\,\mathrm{d}^2x=-\int_{\mathbb{R}^2}f(\partial_z g)\,\mathrm{d}^2x-\lim_{a\downarrow 0}\frac{a}{2}\int_0^{2\pi}(fg)(a\cos(\theta),a\sin(\theta))\,e^{-i\theta}\,\mathrm{d}\theta\,.$$

Thus one finds that $f\in\mathrm{Dom}(\tilde{X}^*)$ belongs to $\mathrm{Dom}(H^+)$ if and only if for all $\varphi\in\mathrm{Dom}(\mathfrak{q}_+)$,

$$\lim_{a\downarrow 0}a\int_0^{2\pi}\left(\overline{\varphi}\left(\partial_{\overline{z}}-\frac{\alpha}{2\overline{z}}\right)f\right)(a\cos(\theta),a\sin(\theta))\,e^{-i\theta}\,\mathrm{d}\theta=0,$$

or, when expressing $(z,\overline{z})$ in the polar coordinates,

$$\lim_{a\downarrow 0}\int_0^{2\pi}(\overline{\varphi}(r\,\partial_r+i\,\partial_\theta-\alpha)f)(a\cos(\theta),a\sin(\theta))\,\mathrm{d}\theta=0.$$

Any $f\in\mathrm{Dom}(\tilde{X}^*)$ asymptotically behaves like

$$f=(\Phi_1^{-1}(f)\,r^{-1+\alpha}+\Phi_2^{-1}(f)\,r^{1-\alpha})e^{-i\theta}+(\Phi_1^0(f)\,r^{-\alpha}+\Phi_2^0(f)\,r^{\alpha})+\text{regular part}.$$

Hence

$$(r\,\partial_r+i\,\partial_\theta-\alpha)f\sim 2(1-\alpha)\Phi_2^{-1}(f)\,r^{1-\alpha}e^{-i\theta}-2\alpha\,\Phi_1^0(f)\,r^{-\alpha}+\cdots.$$

Notice that

$$(r\,\partial_r+i\,\partial_\theta-\alpha)r^{-1+\alpha}e^{-i\theta}=(r\,\partial_r+i\,\partial_\theta-\alpha)r^{\alpha}=0$$

and so any function of the form $r^{-1+\alpha}\eta(r)e^{-i\theta}$ or $r^{\alpha}\eta(r)$, with $\eta\in C^\infty(\mathbb{R}_+)$, $\eta(r)\equiv 1$ in a neighborhood of 0 and $\eta(r)\equiv 0$ in a neighborhood of $+\infty$, belongs to $\mathrm{Dom}(\mathfrak{q}_+)$. Therefore a sufficient and necessary condition for f to belong to $\mathrm{Dom}(H^+)$ is

$$\Phi_2^{-1}(f)=\Phi_1^0(f)=0. \tag{15}$$

The corresponding couple of matrices can be chosen as

$$A_1=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad A_2=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}.$$

The other component of the Pauli Hamiltonian, H^-, can be treated similarly. One finds that $f\in\mathrm{Dom}(\tilde{X}^*)$ belongs to $\mathrm{Dom}(H^-)$ if and only if for all $\varphi\in\mathrm{Dom}(\mathfrak{q}_-)$,

$$\lim_{a\downarrow 0}\int_0^{2\pi}(\overline{\varphi}(r\,\partial_r - i\,\partial_\theta+\alpha)f)(a\cos(\theta),a\sin(\theta))\,\mathrm{d}\theta=0,$$

which turns out to be equivalent to

$$\Phi_1^{-1}(f)=\Phi_2^0(f)=0. \tag{16}$$

The corresponding couple of matrices can be chosen as

$$A_1=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix},\quad A_2=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

The generalization to the case of several vortices is quite straightforward. One simply imposes the above derived boundary conditions at each vortex. Let us consider the case of two vortices. For the sake of simplicity we assume that the vortices are $a=(0,0)$ and $b=(1,0)$. The Pauli Hamiltonian formally reads

$$H^+=-4\left(\partial_z+\frac{1}{2}\left(\frac{\alpha}{z}+\frac{\beta}{z-1}\right)\right)\left(\partial_{\bar z}-\frac{1}{2}\left(\frac{\alpha}{\bar z}+\frac{\beta}{\bar z-1}\right)\right),$$

$$H^-=-4\left(\partial_{\bar z}-\frac{1}{2}\left(\frac{\alpha}{\bar z}+\frac{\beta}{\bar z-1}\right)\right)\left(\partial_z+\frac{1}{2}\left(\frac{\alpha}{z}+\frac{\beta}{z-1}\right)\right).$$

We still assume that $0<\alpha,\beta<1$ (in virtue of the gauge equivalence).

The Pauli Hamiltonian with two vortices is known to have zero modes.[10] They can be computed with the aid of the Aharonov–Casher ansatz since it effectively enables to reduce the second order differential equation to a first order one. Explicit solutions are even known in some essentially more complicated situations (see, for example, Ref. 11). Just for the sake of illustration let us verify that the zero modes actually satisfy the above derived boundary conditions (15) or (16).

If $\alpha+\beta<1$ then the function

$$\varphi(z)=\frac{|z|^\alpha|z-1|^\beta}{z(z-1)}$$

is L^2 integrable and solves

$$\left(\partial_{\bar z}-\frac{1}{2}\left(\frac{\alpha}{\bar z}+\frac{\beta}{\bar z-1}\right)\right)\varphi=0.$$

So it is a zero mode of H^+. It is elementary to compute its asymptotic behavior for $r_a\to 0$,

$$\varphi=r_a^{-1+\alpha}e^{-i\,\theta_a}+\left(1-\frac{\beta}{2}\right)r_a^\alpha-\frac{\beta}{2}r_a^\alpha e^{-2\,i\,\theta_a}+O(r_a^{1+\alpha}).$$

Hence φ obeys (15). The boundary condition at the vortex b is analogous.

Similarly, if $\alpha+\beta>1$ then

$$\varphi(z)=\frac{1}{|z|^\alpha|z-1|^\beta}$$

is a zero mode of H^- and

$$\varphi=-\frac{\beta}{2}r_a^{1-\alpha}e^{-i\,\theta_a}+r_a^{-\alpha}-\frac{\beta}{2}r_a^{1-\alpha}e^{i\,\theta_a}+O(r_a^{2-\alpha}).$$

Hence φ obeys (16).

IV. ASYMPTOTIC BEHAVIOR NEAR A VORTEX

Our first task in this section is the asymptotic analysis of functions from a deficiency subspace. To simplify the discussion we shall use the symbol $O(r^\gamma)$ in a sense somewhat weaker than it is common. The equality $f(r,\theta)=O(r^\gamma)$ for $r\downarrow 0$ will mean that $f(r,\theta)=\Sigma_{n\in\mathbb{Z}} f_n(r)e^{in\theta}$ and for all n it holds $f_n(r)=O(r^\gamma)$.

Lemma 1: Assume that $R>0$, $z\in\mathbb{C}\backslash\mathbb{R}_+$, $0<\alpha<1$ *and* $\varphi\in L^2(B(0,R),\mathrm{d}^2x)$ *satisfies in the weak sense the differential equation*

$$(Y-z)\varphi=0$$

on $B(0,R)\backslash\{0\}$ (*the disk centered at* 0 *with the radius equal to* R) *where* [*using the polar coordinates* (r,θ)]

$$Y=-e^{-i\alpha\theta}\Delta\, e^{i\alpha\theta}=-(\partial_{x_1}+i\alpha\,\partial_{x_1}\theta)^2-(\partial_{x_2}+i\alpha\,\partial_{x_2}\theta)^2=-\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial}{\partial\theta}+i\alpha\right)^2\right).$$

Then there exist constants c_0, d_0, c_{-1}, d_{-1}, *such that*

$$\varphi(r,\theta)=c_0r^{-\alpha}+d_0r^{\alpha}+(c_{-1}r^{-1+\alpha}+d_{-1}r^{1-\alpha})e^{-i\theta}+O(r^\gamma)\quad\text{for } r\downarrow 0\,, \tag{17}$$

where $\gamma=\min\{2-\alpha,1+\alpha\}$.

Proof: For all $n\in\mathbb{Z}$, $\eta\in\mathcal{D}((0,R))$ (the space of test functions) it holds true that

$$0=\langle(Y-\overline{z})\,\eta(r)\,e^{in\theta},\varphi\rangle=-\left\langle\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\overline{z}-\frac{(n+\alpha)^2}{r^2}\right)\eta(r)\,e^{in\theta},\varphi\right\rangle.$$

Hence

$$\varphi(r,\theta)=\sum_{n=-\infty}^{\infty} f_n(r)\,e^{in\theta},$$

where

$$\forall n\in\mathbb{Z},\ \left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+z-\frac{(n+\alpha)^2}{r^2}\right)f_n(r)=0\quad\text{on}\quad(0,R)$$

in the weak sense. This implies that the generalized derivative $\partial_r(r\,\partial_r f_n(r))$ belongs to $L^1_{\mathrm{loc}}((0,R))$ and consequently $f_n\in AC^2((\varepsilon,R))$ for all $0<\varepsilon<R$. Therefore necessarily $f_n(r)$ is a linear combination of the modified Bessel functions,

$$f_n(r)=a_n K_{n+\alpha}(\sqrt{-z}\,r)+b_n I_{|n+\alpha|}(\sqrt{-z}\,r).$$

Let us recall the asymptotic behavior of the Bessel functions. If $0<\nu$ and $\nu\notin\mathbb{N}$ then

$$I_\nu(r)=\frac{1}{\Gamma(\nu+1)}\left(\frac{r}{2}\right)^\nu+O(r^{\nu+2})$$

and

$$K_\nu(r)=\frac{\Gamma(\nu)}{2}\left(\frac{r}{2}\right)^{-\nu}(1+O(r^2))-\frac{\Gamma(1-\nu)}{2\nu}\left(\frac{r}{2}\right)^{\nu}(1+O(r^2)).$$

This implies that $f_n\in L^2((0,R),r\,\mathrm{d}r)$ if and only if either $a_n=0$ or $n\in\{0,-1\}$. This is to say that a_n can be nonzero only for $n=0,-1$. So if $n\neq 0,-1$ then $f_n(r)=O(r^{|n+\alpha|})$. This proves the lemma. □

Let H be the two-vortex spinless AB Hamiltonian defined by boundary conditions (12). The symbol X below stands for the symmetric operator obtained by restricting the domain of H so that functions from $\mathrm{Dom}\,X$ vanish in some neighborhood of the vortices. The deficiency subspaces are denoted by $\mathcal{N}(z)=\mathrm{Ker}(X^*-z)$.

Corollary 2: If $z\in\mathbb{C}\backslash\mathbb{R}_+$ and $\psi\in\mathcal{N}(z)$ then there exist constants $c_{a,0}$, $c_{a,-1}$, $c_{b,0}$, $c_{b,-1}$, such that

$$\psi(x)=c_{a,0}\,r_a^{-\alpha}\,e^{i\,\alpha\,\theta_a}+c_{a,-1}\,r_a^{-1+\alpha}\,e^{i(\alpha-1)\theta_a}+o(1)\quad\text{for } r_a\downarrow 0 \tag{18}$$

and

$$\psi(x)=c_{b,0}\,r_b^{-\beta}\,e^{i\,\beta\,\theta_b}+c_{b,-1}\,r_b^{-1+\beta}\,e^{i(\beta-1)\theta_b}+o(1)\quad\text{for } r_b\downarrow 0. \tag{19}$$

Proof: The property $\psi\in\mathcal{N}(z)$ means that $\psi\in L^2(B(0,R),\mathrm{d}^2x)$, $(-\Delta-z)\psi=0$ on $\mathbb{R}^2\backslash(L_a\cup L_b)$ in the weak sense and ψ satisfies the boundary conditions (12) on $L_a\cup L_b$. Then the function $\exp(-i\,\alpha\,\theta_a)\psi$ obeys the assumptions of Lemma 1 and relation (17) implies (18). Relation (19) can be shown similarly. □

Corollary 3: Assume that $z\in\mathbb{C}\backslash\mathbb{R}_+$, $\psi\in\mathcal{N}(z)$ and $\psi(a)=\psi(b)=0$. Then $\psi\in\mathrm{Dom}(H)$ and hence $\psi=0$.

Proof: We use once more the fact that $\exp(-i\,\alpha\,\theta_a)\psi$ obeys the assumptions of Lemma 1 and hence

$$\exp(-i\,\alpha\,\theta_a)\psi(x)=c_0 r_a^{-\alpha}+d_0 r_a^{\alpha}+(c_{-1}r_a^{-1+\alpha}+d_{-1}r_a^{1-\alpha})e^{-i\,\theta_a}+O(r_a^{\gamma})\quad\text{for } r_a\downarrow 0\,.$$

Since $\psi(a)=0$ it holds $c_{-1}=c_0=0$. Let U be the unitary operator on $L^2(\mathbb{R}^2,\mathrm{d}^2x)$ acting via multiplication by the phase factor $\exp(i\alpha\theta_a+i\beta\theta_b)$. Then $\varphi=\exp(-i\alpha\theta_a-i\beta\theta_b)\psi$ belongs to $\mathrm{Ker}(\tilde{X}^*-z)$ where $\tilde{X}=U^{-1}XU$. The function $\theta_b(x)$ is real analytic in a neighborhood of a and

$$\theta_b(x)=\sin(\theta_a)\,\frac{r_a}{\rho}+O(r_a^2)\quad\text{for } r_a\downarrow 0\,.$$

A straightforward computation gives the asymptotic behavior of φ and one finds that

$$\Phi_1^{-1}(\varphi)=c_{-1},\quad \Phi_2^{-1}(\varphi)=d_{-1}+\frac{\beta c_0}{2\rho},\quad \Phi_1^{0}(\varphi)=c_0,\quad \Phi_2^{0}(\varphi)=d_0-\frac{\beta c_{-1}}{2\rho}.$$

So one finds that the boundary condition $\Phi_1^{-1}(\varphi)=\Phi_1^0(\varphi)=0$ is satisfied at the vortex a. Analogously, the same boundary condition is fulfilled at the vortex b. As recalled in Sec. III, these boundary conditions determine the domain of H_0. Hence $\varphi\in\mathrm{Dom}(H_0)$ and $\psi\in\mathrm{Dom}(H)$. But H is positive, $z\notin\mathbb{R}_+$, and therefore $\mathrm{Dom}(H)\cap\mathcal{N}(z)=\{0\}$. This shows that $\psi=0$. □

Further we are interested in the asymptotic behavior near a vortex of the Green functions (7) and (13). It is easy to see that in the spinless case the Green function vanishes in each vortex. For example, in the case of two vortices it holds true that $\mathcal{G}_z(a,x_0)=0$. This can be derived from (13) with the aid of the relation

$$K_{i\tau}(r)\to\pi\,\delta(\tau)\quad\text{for } r\downarrow 0 \tag{20}$$

and some simple combinatorics. It is also obvious that

$$K_0(\sqrt{-z}|x-x_0|)=K_0(\sqrt{-z}\,r_{0a})+O(r_a)\quad\text{for } r_a\downarrow 0$$

(here $r_{0a}=|a-x_0|$) and

$$K_{i\nu}(\sqrt{-z}\,r_b)=K_{i\nu}(\sqrt{-z}\,\rho)+O(r_a)\quad\text{for } r_a\downarrow 0.$$

To get additional information we shall need an asymptotic formula for the integral

$$\int_{-\infty}^{\infty} K_{i\tau}(\sqrt{-z}\, r_a)\, K_{i(\nu-\tau)}(\sqrt{-z}\,\rho)\, \frac{\sin(\pi\alpha)\exp(\theta_a\tau)}{\pi\sin(\pi(\alpha+i\tau))}\, \mathrm{d}\tau\,. \tag{21}$$

Such an asymptotic analysis can be carried on with the aid of the following lemma.

Lemma 4: Suppose that $r>0$, $|\theta|<\pi$ *and* $0<\alpha<1$. *Then*

$$\int_{-\infty}^{\infty} e^{-r\cosh(s)} \frac{e^{-\alpha(u-s-i\theta)}}{1+e^{-u+s+i\theta}}\,\mathrm{d}s = \frac{\pi}{\sin(\pi\alpha)} - \frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{r}{2}\right)^{1-\alpha} e^{(1-\alpha)(u-i\theta)} - \frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{r}{2}\right)^{\alpha} e^{-\alpha(u-i\theta)} + Z(r,u)\,, \tag{22a}$$

where

$$\forall r\in(0,1), \quad \forall u\in\mathbb{R}, \quad |Z(r,u)|\leqslant Kr\cosh(u) \tag{22b}$$

and K *depends on* θ *and* α *but does not depend on* r *and* u.

Proof: The LHS of (22a) equals

$$\int_{u}^{\infty} e^{-r\cosh(s)} \frac{e^{-(1-\alpha)(s-u+i\theta)}}{1+e^{-s+u-i\theta}}\,\mathrm{d}s + \int_{-u}^{\infty} e^{-r\cosh(s)} \frac{e^{-\alpha(s+u-i\theta)}}{1+e^{-s-u+i\theta}}\,\mathrm{d}s\,. \tag{23}$$

Therefore it suffices to study integrals of the form

$$\int_{u}^{\infty} e^{-r\cosh(s)} \frac{e^{-\gamma(s-u+i\theta)}}{1+e^{-s+u-i\theta}}\,\mathrm{d}s = e^{\gamma(u-i\theta)} \int_{u}^{\infty} e^{-r\cosh(s)-\gamma s}\,\mathrm{d}s - \int_{u}^{\infty} e^{-r\cosh(s)} \frac{e^{-(\gamma+1)(s-u+i\theta)}}{1+e^{-s+u-i\theta}}\,\mathrm{d}s \tag{24}$$

for $0<\gamma<1$. The second integral on the RHS of (24) can be treated easily and one finds that

$$\int_{u}^{\infty} e^{-r\cosh(s)} \frac{e^{-(\gamma+1)(s-u+i\theta)}}{1+e^{-s+u-i\theta}}\,\mathrm{d}s = \frac{e^{-i\gamma\theta}}{\gamma} - \int_{0}^{\infty} \frac{e^{-\gamma(s+i\theta)}}{1+e^{-s-i\theta}}\,\mathrm{d}s + Z_1(r,u)\,,$$

where $Z_1(r,u)$ satisfies estimate (22b). To treat the first integral on the RHS of (24) we note that

$$e^{-r\cosh(s)} = \exp\left(-\frac{r}{2}e^{s}\right) \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{r}{2}\right)^{k} e^{-ks}$$

and therefore

$$\int_{0}^{\infty} e^{-r\cosh(s)-\gamma s}\,\mathrm{d}s = \sum_{k=0}^{\infty} \frac{1}{k!}\, 2^{-\gamma-k} r^{\gamma+k}\, \Gamma\left(-\gamma-k, \frac{r}{2}\right)\left(-\frac{r}{2}\right)^{k} = -\frac{\Gamma(1-\gamma)}{\gamma}\left(\frac{r}{2}\right)^{\gamma} + \frac{1}{\gamma} + \frac{\gamma}{1-\gamma^2}\, r + O(r^2)\,.$$

Furthermore,

$$\int_{u}^{0} e^{-r\cosh(s)-\gamma s}\,\mathrm{d}s = \frac{e^{-\gamma u}-1}{\gamma} + Z_2(r,u)\,,$$

where $Z_2(r,u)$ satisfies estimate (22b). Thus we have derived that

$$\int_u^\infty e^{-r\cosh(s)}\frac{e^{-\gamma(s-u+i\theta)}}{1+e^{-s+u-i\theta}}\,\mathrm{d}s=-\frac{\Gamma(1-\gamma)}{\gamma}\left(\frac{r}{2}\right)^{\gamma}e^{\gamma(u-i\theta)}+\int_0^\infty\frac{e^{-\gamma(s+i\theta)}}{1+e^{-s-i\theta}}\,\mathrm{d}s+Z_3(r,u)\,, \tag{25}$$

where $Z_3(r,u)$ satisfies estimate (22b). To conclude the proof it suffices to apply (25) to both integrals in (23) and to take into account that

$$\int_0^\infty\frac{e^{-(1-\alpha)(s+i\theta)}}{1+e^{-s-i\theta}}\,\mathrm{d}s+\int_0^\infty\frac{e^{-\alpha(s-i\theta)}}{1+e^{-s+i\theta}}\,\mathrm{d}s=\int_{-\infty}^\infty\frac{e^{-\alpha(s-i\theta)}}{1+e^{-s+i\theta}}\,\mathrm{d}s=\frac{\pi}{\sin(\pi\alpha)}$$

for $|\theta|<\pi$. □

Corollary 5: Under the same assumptions as in Lemma 4 it holds true that

$$\begin{aligned}&\int_{-\infty}^\infty K_{i\tau}(\sqrt{-z}\,r)\,K_{i(\nu-\tau)}(\sqrt{-z}\,\rho)\,\frac{\sin(\pi\alpha)\exp(\theta\tau)}{\pi\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau\\&\quad=K_{i\nu}(\sqrt{-z}\,\rho)-\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{\sqrt{-z}\,r}{2}\right)^{1-\alpha}e^{i(\alpha-1)\theta}K_{i\nu-1+\alpha}(\sqrt{-z}\,\rho)\\&\quad\quad-\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{\sqrt{-z}\,r}{2}\right)^{\alpha}e^{i\alpha\theta}K_{i\nu+\alpha}(\sqrt{-z}\,\rho)+O(r)\end{aligned} \tag{26}$$

for $r\downarrow 0$.

Proof: Using

$$K_{i\tau}(a)=\frac{1}{2}\int_{-\infty}^\infty e^{is\tau-a\cosh(s)}\,\mathrm{d}s\quad\text{for}\quad a>0,\ \ \tau\in\mathbb{R}, \tag{27}$$

and applying the equality

$$\int_{-\infty}^\infty e^{i\tau(u-s)}\frac{\exp(\theta\tau)}{\sin(\pi(\alpha+i\tau))}\,\mathrm{d}\tau=2\,\frac{e^{-\alpha(u-s-i\theta)}}{1+e^{-u+s+i\theta}}$$

we find that (21) equals

$$\frac{\sin(\pi\alpha)}{2\pi}\int_{-\infty}^\infty e^{-\sqrt{-z}\,\rho\cosh(u)-i\nu u}\left(\int_{-\infty}^\infty e^{-\sqrt{-z}\,r\cosh(s)}\frac{e^{-\alpha(u-s-i\theta)}}{1+e^{-u+s+i\theta}}\,\mathrm{d}s\right)\mathrm{d}u\,.$$

Now it suffices to apply (22) to the inner bracket and then to use the integral form (27) in the reversed sense. □

First let us apply (26) to the case of one vortex. In fact, the following observation about the asymptotic expansion of the Green function (7) near the vortex will be crucial for the subsequent analysis. We get either the asymptotic expansion of $\mathcal{G}_z(r,\theta;r_0,\theta_0)$ for $r\downarrow 0$, or, since in general it holds true that

$$\overline{\mathcal{G}_z(r,\theta;r_0,\theta_0)}=\mathcal{G}_z(r_0,\theta_0;r,\theta), \tag{28}$$

the expansion for $r_0\downarrow 0$ as well, namely,

$$\begin{aligned}\mathcal{G}_z(r,\theta;r_0,\theta_0)=&\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{\sqrt{-z}\,r_0}{2}\right)^{1-\alpha}K_{-1+\alpha}(\sqrt{-z}r)\,e^{i(\alpha-1)(\theta-\theta_0)}\\&+\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{\sqrt{-z}\,r_0}{2}\right)^{\alpha}K_{\alpha}(\sqrt{-z}r)\,e^{i\alpha(\theta-\theta_0)}+O(r_0)\,.\end{aligned} \tag{29}$$

One observes that the coefficients standing at $r_0^{1-\alpha}e^{-i(\alpha-1)\theta_0}$ and $r_0^{\alpha}e^{-i\alpha\theta_0}$ are, respectively, proportional to

$$K_{-1+\alpha}(\sqrt{-z}\,r)\,e^{i(\alpha-1)\theta} \quad \text{and} \quad K_{\alpha}(\sqrt{-z}\,r)\,e^{i\alpha\theta}.$$

But these functions are nothing but the basis functions in the corresponding deficiency subspace, see (8).

Next we shall consider the case of two vortices. Applying (26) to (13) we get

$$\begin{aligned}\mathcal{G}_z(x,x_0)=&\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{1-\alpha}e^{i(\alpha-1)\theta_a}\mathcal{L}_{\alpha-1}(x_0)\\&+\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{\alpha}e^{i\alpha\theta_a}\,\mathcal{L}_{\alpha}(x_0)+O(r_a)\end{aligned}\tag{30a}$$

for $r_a\downarrow 0$ where

$$\begin{aligned}\mathcal{L}_{\nu}(x_0)=&K_{\nu}(\sqrt{-z}\,r_{0a})\,e^{-i\nu\theta_{0a}}+\sum_{\gamma,\,n\geqslant 2,\,c_n=a}(-1)^{n-1}\int_{\mathbb{R}^{n-1}}K_{i\tau_{n-1}+\nu}(\sqrt{-z}\,\rho)\\&\times K_{i(\tau_{n-2}-\tau_{n-1})}(\sqrt{-z}\,\rho)\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1}(\sqrt{-z}\,r_0)\\&\times\frac{\sin(\pi\sigma_{n-1})}{\pi\sin(\pi(\sigma_{n-1}+i\tau_{n-1}))}\times\cdots\times\frac{\sin(\pi\sigma_2)}{\pi\sin(\pi(\sigma_2+i\tau_2))}\,\frac{\sin(\pi\sigma_1)\exp(-\theta_0\tau_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{n-1}\tau\end{aligned}\tag{30b}$$

[and, again, (r_0,θ_0) are the polar coordinates of the point x_0 with respect to the center c_1]. The convergence of the series in (30b) will be discussed later in Sec. V.

V. DEFICIENCY SUBSPACES FOR THE CASE OF TWO VORTICES

In this section we are going to construct a basis in the deficiency subspaces in the two-vortex case. So H designates the two-vortex spinless AB Hamiltonian described by the boundary conditions (12), X is the symmetric operator obtained by restricting the domain of H as described in Sec. IV and $\mathcal{N}(z)=\mathrm{Ker}(X^*-z)$ is a deficiency subspace.

Asymptotic expansion (29) for the one vortex case suggests that also in the two vortex case one may extract from the Green function a basis in the deficiency subspace. From (30) and (28) one derives immediately a candidate for such a basis. It is formed by the functions

$$\psi_{u,\nu,z}(x)=\sum_{n=0}^{\infty}S_n(u,\nu,z;x)\,,\tag{31a}$$

where

$$S_0(u,\nu,z;x)=K_{\nu}(\sqrt{-z}\,r_u)\,e^{i\nu\theta_u},\tag{31b}$$

$$\begin{aligned}S_n(u,\nu,z;x)=&(-1)^n\int_{\mathbb{R}^n}K_{i\tau_n}(\sqrt{-z}\,r_n)\times K_{i(\tau_{n-1}-\tau_n)}(\sqrt{-z}\rho)\\&\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\rho)\\&\times\frac{\sin(\pi\sigma_n)\exp(\theta_n\tau_n)}{\pi\sin(\pi(\sigma_n+i\tau_n))}\,\frac{\sin(\pi\sigma_{n-1})}{\pi\sin(\pi(\sigma_{n-1}+i\tau_{n-1}))}\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^n\tau\end{aligned}\tag{31c}$$

for $n \geqslant 1$, the indices are restricted to the range

$$u \in \{a,b\}, \quad \nu \in \{\omega-1,\omega\} \text{ where } \omega=\alpha \text{ if } u=a, \text{ and } \omega=\beta \text{ if } u=b, \tag{31d}$$

and to each $n \in \mathbb{N}$ one relates the unique alternating sequence $(c_n, c_{n-1}, \ldots, c_1)$, $c_j \in \{a,b\}$ and $c_j \neq c_{j+1}$, such that $c_1 \neq u$. Correspondingly, $\sigma_j=\alpha$ if $c_j=a$ and $\sigma_j=\beta$ if $c_j=b$. As usual, $(r_n,\theta_n)=(r_{c_n},\theta_{c_n})$ are the polar coordinates with respect to the center c_n, (r_c,θ_c) are the polar coordinates centered at the point c.

Let us show that the series (31a) actually converges. In the Hilbert space $L^2(\mathbb{R}, \mathrm{d}\tau)$ we introduce the vectors

$$\mathfrak{f}_{u,z}(x;\tau)=K_{i\tau}(\sqrt{-z}\, r_u)\exp(\theta_u \tau)\frac{\sin(\pi\sigma)}{\pi \sin(\pi(\sigma+i\tau))}, \qquad \mathfrak{g}_{\nu,z}(\tau)=K_{-i\tau-\nu}(\sqrt{-z}\,\rho),$$

and the operators $\mathfrak{K}_z$ and $\mathfrak{D}_u$ with the generalized kernels

$$\mathfrak{K}_z(\mu,\omega)=K_{i(\omega-\mu)}(\sqrt{-z}\rho), \qquad \mathfrak{D}_u(\mu,\omega)=\frac{\sin(\pi\sigma)}{\pi\sin(\pi(\sigma+i\mu))}\,\delta(\mu-\omega),$$

where

$$u \in \{a,b\}, \qquad \sigma=\alpha \text{ if } u=a, \text{ and } \sigma=\beta \text{ if } u=b.$$

For $u \in \{a,b\}$ let v be the complementary vortex, i.e., $\{u,v\}=\{a,b\}$. For the sake of brevity we shall use the matrixlike notation in the following paragraph. Thus the transposition will in fact indicate an integration, i.e., $\mathfrak{f}^T\mathfrak{g}=\int_{\mathbb{R}}\mathfrak{f}(\tau)\,\mathfrak{g}(\tau)\,\mathrm{d}\tau$.

We can rewrite the summands in Eq. (31a) using this notation (here $n \geqslant 1$),

$$S_{2n-1}(u,\nu,z;x)=-\mathfrak{f}_{v,z}(x)^T(\mathfrak{K}_z\mathfrak{D}_u\mathfrak{K}_z\mathfrak{D}_v)^{n-1}\mathfrak{g}_{\nu,z},$$

$$S_{2n}(u,\nu,z;x)=\mathfrak{f}_{u,z}(x)^T\mathfrak{K}_z\mathfrak{D}_v(\mathfrak{K}_z\mathfrak{D}_u\mathfrak{K}_z\mathfrak{D}_v)^{n-1}\mathfrak{g}_{\nu,z}.$$

These formulas make it possible to estimate the summands. Note that $\mathfrak{K}_z$ acts as a convolution operator and so it is diagonalized by the Fourier transform. Since

$$\int_{-\infty}^{\infty} e^{i x \tau}K_{i\tau}(a)\,\mathrm{d}\tau=\pi\, e^{-a\cosh(x)},$$

we get

$$\|\mathfrak{K}_z\|=\pi\, e^{-\mathrm{Re}(\sqrt{-z})\rho}.$$

The operator $\mathfrak{D}_u$ is already diagonal. Therefore

$$\|\mathfrak{D}_u\|=\sup_{\mu\in\mathbb{R}}\left|\frac{\sin(\pi\sigma)}{\pi\sin(\pi(\sigma+i\mu))}\right|=\frac{1}{\pi}.$$

Jointly this implies that

$$|S_{2n-1}(u,\nu,z;x)| \leqslant \|\mathfrak{f}_{v,z}(x)\|\|\mathfrak{g}_{\nu,z}\|\, e^{-(2n-2)\,\mathrm{Re}(\sqrt{-z})\,\rho},$$

$$|S_{2n}(u,\nu,z;x)| \leqslant \|\mathfrak{f}_{u,z}(x)\|\|\mathfrak{g}_{\nu,z}\|\, e^{-(2n-1)\,\mathrm{Re}(\sqrt{-z})\,\rho}.$$

The estimates show that the series (31a) converges absolutely at least as fast as a geometric series. Even one can rewrite the formula for $\psi_{u,\nu,z}(x)$ in a compact form, namely,

$$\psi_{u,\nu,z}(x)=K_\nu(\sqrt{-z}\,r_u)e^{i\nu\theta_u}+(\mathfrak{f}_{u,z}(x)^T\mathfrak{K}_z\mathfrak{D}_v-\mathfrak{f}_{v,z}(x)^T)(\mathbb{I}-\mathfrak{K}_z\mathfrak{D}_u\mathfrak{K}_z\mathfrak{D}_v)^{-1}\mathfrak{g}_{\nu,z}. \tag{32}$$

Here the inverse operator $(\mathbb{I}-\mathfrak{K}_z\mathfrak{D}_u\mathfrak{K}_z\mathfrak{D}_v)^{-1}$ exists with the norm estimated from above by $(1-\exp(-2\,\mathrm{Re}(\sqrt{-z})\,\rho))^{-1}$.

Altogether we get four functions: $\psi_{a,\alpha-1,z}$, $\psi_{a,\alpha,z}$, $\psi_{b,\beta-1,z}$, and $\psi_{b,\beta,z}$. Our goal is to show that they actually form a basis in the deficiency subspace. Obviously

$$(\Delta+z)\psi_{u,\nu,z}=0$$

since

$$(\Delta+z)K_\nu(\sqrt{-z}\,r)e^{\pm i\nu\theta}=0 \quad \text{on } \mathbb{R}^2\backslash\{0\}$$

for all $\nu\in\mathbb{C}$, $z\in\mathbb{C}\backslash\mathbb{R}_+$, and therefore all the summands satisfy the equation $(\Delta+z)S_n(u,\nu,z)=0$ in the domain $\mathbb{R}^2\backslash(L_a\cup L_b)$.

Let us verify that $\psi_{u,\nu,z}$ obeys the boundary conditions (12). For the sake of definiteness we shall consider the function $\psi_{a,\nu,z}$, $\nu\in\{\alpha-1,\alpha\}$. First we shall show that

$$e^{-i\alpha\pi}\psi_{a,\nu,z}|_{\theta_a=\pi}-e^{i\alpha\pi}\psi_{a,\nu,z}|_{\theta_a=-\pi}=0. \tag{33}$$

If $n=2m-1$ is odd then $c_n=b$. Moreover, if $\theta_a=\pm\pi$ then $\theta_b=0$ and $r_b=r_a+\rho$. Hence

$$\begin{aligned}
&e^{-i\alpha\pi}S_{2m-1}(a,\nu,z)|_{\theta_a=\pi}-e^{i\alpha\pi}S_{2m-1}(a,\nu,z)|_{\theta_a=-\pi}\\
&\quad=\int_{\mathbb{R}^{2m-1}}K_{i\tau_{2m-1}}(\sqrt{-z}(r_a+\rho))\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)\\
&\qquad\times\frac{2\,i\sin(\pi\alpha)\sin(\pi\sigma_{2m-1})}{\pi\sin(\pi(\sigma_{2m-1}+i\tau_{2m-1}))}\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m-1}\tau.
\end{aligned}$$

If $n=2m$, $m\geqslant 1$, is even then $c_n=a$ and

$$e^{-i\alpha\pi}\exp(\pi\tau_n)-e^{i\alpha\pi}\exp(-\pi\tau_n)=-2\,i\sin(\pi(\sigma_n+i\tau_n))$$

hence

$$\begin{aligned}
&e^{-i\alpha\pi}S_{2m}(a,\nu,z)|_{\theta_a=\pi}-e^{i\alpha\pi}S_{2m}(a,\nu,z)|_{\theta_a=-\pi}\\
&\quad=-\int_{\mathbb{R}^{2m}}K_{i\tau_{2m}}(\sqrt{-z}\,r_a)K_{i(\tau_{2m-1}-\tau_{2m})}(\sqrt{-z}\,\rho)\times\cdots\times K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)\\
&\qquad\times\frac{2i\sin(\pi\alpha)}{\pi}\,\frac{\sin(\pi\sigma_{2m-1})}{\pi\sin(\pi(\sigma_{2m-1}+i\tau_{2m-1}))}\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m}\tau.
\end{aligned}$$

The integration in τ_{2m} can be carried on with the aid of the identity

$$\int_{-\infty}^{\infty}K_{i\tau}(a)\,K_{i(\nu-\tau)}(b)\,\mathrm{d}\tau=\pi\,K_{i\nu}(a+b) \quad \text{for } a>0,\ b>0. \tag{34}$$

This way we get the equality

$$\begin{aligned}
&e^{-i\alpha\pi}S_{2m}(a,\nu,z)|_{\theta_a=\pi}-e^{i\alpha\pi}S_{2m}(a,\nu,z)|_{\theta_a=-\pi}\\
&\quad=-(e^{-i\alpha\pi}S_{2m-1}(a,\nu,z)|_{\theta_a=\pi}-e^{i\alpha\pi}S_{2m-1}(a,\nu,z)|_{\theta_a=-\pi})
\end{aligned}$$

valid for all $m \geqslant 1$. Obviously,

$$e^{-i\alpha\pi} S_0(a,\nu,z)\big|_{\theta_a=\pi} - e^{i\alpha\pi} S_0(a,\nu,z)\big|_{\theta_a=-\pi} = 0.$$

The last two equalities imply (33).

Similarly one can show that

$$e^{-i\beta\pi} \psi_{a,\nu,z}\big|_{\theta_b=\pi} - e^{i\beta\pi} \psi_{a,\nu,z}\big|_{\theta_b=-\pi} = 0. \tag{35}$$

Equality (34) again turns out to be useful but this time when treating the odd summands. With its aid the dimension of the integration domain is reduced by 1 and one obtains the equality

$$\begin{aligned} &e^{-i\beta\pi} S_{2m-1}(a,\nu,z)\big|_{\theta_b=\pi} - e^{i\beta\pi} S_{2m-1}(a,\nu,z)\big|_{\theta_b=-\pi} \\ &\quad = -\left(e^{-i\beta\pi} S_{2m-2}(a,\nu,z)\big|_{\theta_b=\pi} - e^{i\beta\pi} S_{2m-2}(a,\nu,z)\big|_{\theta_b=-\pi}\right) \end{aligned}$$

valid for all $m \geqslant 1$. This shows (35).

Finally we note that the remaining two boundary conditions,

$$e^{-i\alpha\pi} \frac{\partial \psi_{a,\nu,z}}{\partial r_a}\bigg|_{\theta_a=\pi} - e^{i\alpha\pi} \frac{\partial \psi_{a,\nu,z}}{\partial r_a}\bigg|_{\theta_a=-\pi} = 0,$$

$$e^{-i\beta\pi} \frac{\partial \psi_{a,\nu,z}}{\partial r_b}\bigg|_{\theta_b=\pi} - e^{i\beta\pi} \frac{\partial \psi_{a,\nu,z}}{\partial r_b}\bigg|_{\theta_b=-\pi} = 0,$$

can be verified in exactly the same way.

Next we wish to examine the asymptotic behavior of the functions $\psi_{u,\nu,z}$ near the singular points a and b. We shall again focus on the functions $\psi_{a,\nu,z}$, the functions $\psi_{b,\nu,z}$ can be treated similarly. First notice that

$$\psi_{a,\nu,z}(b) = 0. \tag{36}$$

Actually, for the even summands in (31a) the limit $x \to b$ just means setting $r_a = \rho$. To treat the odd summands one applies the limit procedure (20) for $r_b \to 0$ and finds that

$$S_{2m-1}(a,\nu,z;b) = -S_{2m-2}(a,\nu,z;b) \quad \text{for all } m \geqslant 1.$$

This shows (36).

Let us make this result more precise. The even summands in (31a) simply satisfy

$$S_{2m}(a,\nu,z;x) = S_{2m}(a,\nu,z;b) + O(r_b) \quad \text{for } x \to b.$$

Asymptotic behavior of the odd summands can be obtained with the aid of relation (26). We get [here $S_{2m-1}(a,\nu,z;b) = -S_{2m-2}(a,\nu,z;b)$]

$$\begin{aligned} S_{2m-1}(a,\nu,z;x) = S_{2m-1}(a,\nu,z;b) &+ \frac{\sin(\pi\beta)}{\pi} \frac{\Gamma(\beta)}{1-\beta} \left(\frac{\sqrt{-z}\, r_b}{2}\right)^{1-\beta} e^{i(\beta-1)\theta_b} \\ &\times \int_{\mathbb{R}^{2m-2}} K_{i\tau_{2m-2}-1+\beta}(\sqrt{-z}\rho) \times \cdots \times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho) K_{-i\tau_1-\nu}(\sqrt{-z}\rho) \\ &\times \frac{\sin(\pi\sigma_{2m-2})}{\pi \sin(\pi(\sigma_{2m-2}+i\tau_{2m-2}))} \times \cdots \times \frac{\sin(\pi\sigma_1)}{\pi \sin(\pi(\sigma_1+i\tau_1))}\, \mathrm{d}^{2m-2}\tau \end{aligned}$$

$$+\frac{\sin(\pi\beta)}{\pi}\frac{\Gamma(1-\beta)}{\beta}\left(\frac{\sqrt{-z}\,r_b}{2}\right)^{\beta}e^{i\beta\theta_b}\int_{\mathbb{R}^{2m-2}}K_{i\tau_{2m-2}+\beta}(\sqrt{-z}\,\rho)$$

$$\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\rho)\,\frac{\sin(\pi\sigma_{2m-2})}{\pi\sin(\pi(\sigma_{2m-2}+i\tau_{2m-2}))}$$

$$\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m-2}\tau+O(r_b)$$

for $x\to b$. Jointly this means that

$$\psi_{a,\nu,z}(x)=\sum_{\mu\in\{\beta-1,\,\beta\}}\frac{\sin(\pi|\mu|)}{\pi}\,\frac{\Gamma(1-|\mu|)}{|\mu|}\left(\frac{\sqrt{-z}\,r_b}{2}\right)^{|\mu|}e^{i\mu\theta_b}\mathcal{S}_{\mu,\nu}(\alpha,\beta;z)+O(r_b)\quad(37)$$

for $x\to b$ where

$$\mathcal{S}_{\omega,\nu}(\alpha,\beta;z)=K_{\omega-\nu}(\sqrt{-z}\rho)+\sum_{m=1}^{\infty}\int_{\mathbb{R}^{2m}}K_{i\tau_{2m}+\omega}(\sqrt{-z}\,\rho)\,K_{i(\tau_{2m-1}-\tau_{2m})}(\sqrt{-z}\,\rho)$$

$$\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)\,\frac{\sin(\pi\sigma_{2m})}{\pi\sin(\pi(\sigma_{2m}+i\tau_{2m}))}$$

$$\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m}\tau\qquad(38)$$

with $(\sigma_{2m},\ldots,\sigma_2,\sigma_1)=(\alpha,\ldots,\alpha,\beta)$.

The function $\psi_{a,\nu,z}$ has a singularity at the point a. Nevertheless it holds true that

$$\sum_{n=1}^{\infty}S_n(a,\nu,z;a)=0.\qquad(39)$$

The verification is similar to that of equality (36). This time it holds true that

$$S_{2m}(a,\nu,z;a)=-S_{2m-1}(a,\nu,z;a)\quad\text{for all } m\geqslant 1.$$

This shows (39). A more precise result can be derived as follows. Note that

$$S_{2m-1}(a,\nu,z;x)=S_{2m-1}(a,\nu,z;a)+O(r_a)\quad\text{for } x\to a.$$

Asymptotic behavior of the even summands can be obtained with the aid of relation (26). We get

$$S_{2m}(a,\nu,z;x)=S_{2m}(a,\nu,z;a)-\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{1-\alpha}e^{i(\alpha-1)\theta_a}$$

$$\times\int_{\mathbb{R}^{2m-1}}K_{i\tau_{2m-1}-1+\alpha}(\sqrt{-z}\,\rho)\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)$$

$$\times\frac{\sin(\pi\sigma_{2m-1})}{\pi\sin(\pi(\sigma_{2m-1}+i\tau_{2m-1}))}\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m-1}\tau$$

$$-\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{\alpha}e^{i\alpha\theta_a}\int_{\mathbb{R}^{2m-1}}K_{i\tau_{2m-1}+\alpha}(\sqrt{-z}\,\rho)$$

$$\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)\,\frac{\sin(\pi\sigma_{2m-1})}{\pi\sin(\pi(\sigma_{2m-1}+i\tau_{2m-1}))}$$

$$\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m-1}\tau+O(r_a)$$

for $x\to a$. The asymptotic behavior of the Macdonald function is given by the formula[12]

$$\begin{aligned}K_\nu(x)&=\frac{\pi}{2\sin(\nu\pi)}\left(\frac{2^\nu}{\Gamma(1-\nu)}x^{-\nu}-\frac{2^{-\nu}}{\Gamma(1+\nu)}x^\nu\right)+O(x^{-\nu+2})\\&=\frac{\Gamma(\nu)}{2}\left(\frac{x}{2}\right)^{-\nu}-\frac{\Gamma(1-\nu)}{2\nu}\left(\frac{x}{2}\right)^{\nu}+O(x^{-\nu+2})\quad\text{for } 0<\nu<1.\end{aligned}$$

Finally we arrive at the expansion

$$\begin{aligned}\psi_{a,\nu,z}(x)=&\frac{\Gamma(|\nu|)}{2}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{-|\nu|}e^{i\nu\theta_a}\\&-\sum_{\mu\in\{\alpha-1,\alpha\}}\frac{\sin(\pi|\mu|)}{\pi}\,\frac{\Gamma(1-|\mu|)}{|\mu|}\left(\frac{\sqrt{-z}\,r_a}{2}\right)^{|\mu|}e^{i\mu\theta_a}\mathcal{T}_{\mu,\nu}(\alpha,\beta;z)+O(r_a)\end{aligned}\tag{40}$$

for $x\to a$ where

$$\begin{aligned}\mathcal{T}_{\omega,\nu}(\alpha,\beta;z)=&\frac{\pi}{2\sin(\pi\alpha)}\,\delta_{\omega\nu}+\sum_{m=1}^{\infty}\int_{\mathbb{R}^{2m-1}}K_{i\tau_{2m-1}+\omega}(\sqrt{-z}\,\rho)\,K_{i(\tau_{2m-2}-\tau_{2m-1})}(\sqrt{-z}\,\rho)\\&\times\cdots\times K_{i(\tau_1-\tau_2)}(\sqrt{-z}\,\rho)K_{-i\tau_1-\nu}(\sqrt{-z}\,\rho)\,\frac{\sin(\pi\sigma_{2m-1})}{\pi\sin(\pi(\sigma_{2m-1}+i\tau_{2m-1}))}\\&\times\cdots\times\frac{\sin(\pi\sigma_1)}{\pi\sin(\pi(\sigma_1+i\tau_1))}\,\mathrm{d}^{2m-1}\tau\end{aligned}\tag{41}$$

with $(\sigma_{2m-1},\ldots,\sigma_2,\sigma_1)=(\beta,\ldots,\alpha,\beta)$.

Remark: As a consequence one can show that

$$\sum_{n=1}^{\infty}S_n(u,\nu,z;x)=\sum_{n=1}^{\infty}S_n(u,-\nu,z;x).\tag{42}$$

Actually, a short inspection of the above derivation shows that the functions

$$\tilde{\psi}_{u,\nu,z}(x)=\sum_{n=0}^{\infty}S_n(u,-\nu,z;x)$$

also satisfy the boundary conditions (12) and solve the equation $(\Delta+z)\tilde{\psi}_{u,\nu,z}=0$. Therefore the function

$$f(x)=\sum_{n=1}^{\infty}S_n(u,\nu,z;x)-\sum_{n=1}^{\infty}S_n(u,-\nu,z;x)$$

satisfies the boundary conditions (12) as well and solves $(\Delta+z)f=0$. In addition, $f(a)=f(b)=0$. Consequently, $f\in\mathrm{Dom}(H)$ and $(H-z)f=0$. Necessarily $f=0$.

Lemma 6: $\dim\mathcal{N}(z)\leqslant 4$.

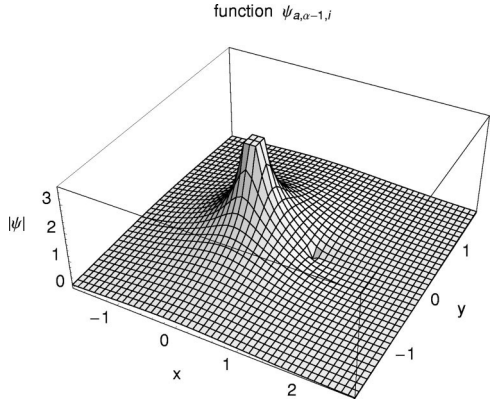

FIG. 2. Function $\psi_{a,\alpha-1,i}$ from the deficiency subspace for the values of parameters $\alpha=1/3$, $\beta=2/3$, $\rho=1$.

Proof: In virtue of Corollary 2, for any five-tuple of functions from $\mathcal{N}(z)$ there exists a nontrivial linear combination of these functions vanishing both at a and b. By Corollary 3, such a linear combination equals 0. □

Proposition 7: $\dim\mathcal{N}(z)=4$.

Proof: Owing to Lemma 6 it suffices to show that $\dim\mathcal{N}(z)\geqslant 4$. But in relation (31) we have constructed four functions $\psi_{a,\alpha-1,z}$, $\psi_{a,\alpha,z}$, $\psi_{b,\beta-1,z}$ and $\psi_{b,\beta,z}$ from the deficiency subspace $\mathcal{N}(z)$. The asymptotic expansions (37) and (40) show that these functions are actually linearly independent. □

We conclude that the functions $\{\psi_{a,\alpha-1,z},\psi_{a,\alpha,z},\psi_{b,\beta-1,z},\psi_{b,\beta,z}\}$ form a basis in $\mathcal{N}(z)$.

Remark: Formula (32) is well suited for numerical computations. To give the reader an idea about the behavior of $\psi_{u,\nu,z}$ we have plotted $|\psi_{a,\alpha-1,i}|$ in Fig. 2 and $|\psi_{b,\beta,i}|$ in Fig. 3, with $\alpha=1/3$, $\beta=2/3$ and $\rho=1$. Note that the former function vanishes in the vortex b while the latter one vanishes in the vortex a.

VI. THE KREIN'S FORMULA

We would like to emphasize once more that we are using two unitarily equivalent formulations. The operators $H^{\pm}$, H_0 are, respectively, associated to the quadratic forms (14) and (11). Let U be the unitary operator in $L^2(\mathbb{R}^2, \mathrm{d}^2x)$ acting as $U\varphi=\exp(i\alpha\theta_a+i\beta\theta_b)\varphi$. The Green function (13) corresponds to the operator $H=UH_0U^{-1}$ defined by the boundary conditions on the cut (12).

Set

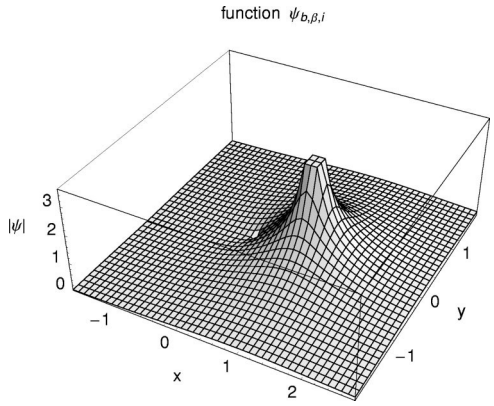

FIG. 3. Function $\psi_{b,\beta,i}$ from the deficiency subspace for the values of parameters $\alpha=1/3$, $\beta=2/3$, $\rho=1$.

$$f_{u,\nu,z}=(\sqrt{-z})^{|\nu|}\psi_{u,\nu,z}\,. \tag{43}$$

Let us enumerate the basis $\{f_{a,\alpha-1,z},f_{a,\alpha,z},f_{b,\beta-1,z},f_{b,\beta,z}\}$ in $\mathcal{N}(z)$ as $\{f_z^1,f_z^2,f_z^3,f_z^4\}$ (in this order). Set $\tilde{f}_z^j=U^{-1}f_z^j$, $R_z=(H_0-z)^{-1}$, $R_z^{\pm}=(H^{\pm}-z)^{-1}$. According to the Krein's formula

$$R_z^{\pm}-R_z=\sum_{j,\,k}\,(M_z^{\pm})^{j,k}\tilde{f}_z^j\langle\tilde{f}_{\bar{z}}^k,\cdot\,\rangle \tag{44}$$

or, in terms of Green functions,

$$\mathcal{G}_z^{\pm}(x,x_0)=\mathcal{G}_z(x,x_0)+\sum_{j,\,k}\,(M_z^{\pm})^{j,k}\,f_z^j(x)\,\overline{f_{\bar{z}}^k(x_0)}\,, \tag{45}$$

where $M_z^{\pm}$ is a holomorphic matrix-valued function defined on $\mathbb{C}\backslash\mathbb{R}$.

An operator-valued function $R_z^{\pm}$ constructed this way will be the resolvent of a self-adjoint operator if and only if it satisfies (Ref. 13, Chap. 5.2)

$$\forall z\in\mathbb{C}\backslash\mathbb{R},\quad (R_z^{\pm})^*=R_{\bar{z}}^{\pm} \tag{46}$$

and (the Hilbert identity)

$$\forall z,w\in\mathbb{C}\backslash\mathbb{R},\quad R_z^{\pm}-R_w^{\pm}=(z-w)R_z^{\pm}R_w^{\pm} \tag{47}$$

[it follows from (44) that $\mathrm{Ker}\,R_z^{\pm}=\{0\}$ for all $z\in\mathbb{C}\backslash\mathbb{R}$]. Let us analyze conditions (46) and (47). It is straightforward to see that (46) is satisfied if and only if

$$M_z^*=M_{\bar{z}}. \tag{48}$$

In equality (52) below we shall show that

$$\forall z,w\in\mathbb{C}\backslash\mathbb{R},\,\forall j,\quad \tilde{f}_w^j+(z-w)R_z\tilde{f}_w^j=\tilde{f}_z^j\,.$$

With the aid of this identity it is just an easy computation to show that (47) is equivalent to the condition

$$\forall z,w\in\mathbb{C}\backslash\mathbb{R},\quad M_z-M_w=(z-w)\,M_zP(\bar{z},w)\,M_w\,, \tag{49}$$

where $P(z,w)$ is the 4×4 matrix of scalar products,

$$P(z,w)^{j,k}=\langle f_z^j,f_w^k\rangle.$$

Equality (49) was presented in Ref. 14 and was applied to problems similar to ours, for example, in Refs. 15 and 3.

According to formula (30) and definition (31) of $\psi_{u,\nu,z}(x)$ we have

$$\begin{aligned}\mathcal{G}_z(x,x_0)=&\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(\alpha)}{1-\alpha}\left(\frac{\sqrt{-z}\,r_{0a}}{2}\right)^{1-\alpha}e^{-i(\alpha-1)\theta_{0a}}\psi_{a,\alpha-1,z}(x)\\&+\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(1-\alpha)}{\alpha}\left(\frac{\sqrt{-z}\,r_{0a}}{2}\right)^{\alpha}e^{-i\,\alpha\,\theta_{0a}}\,\psi_{a,\alpha,z}(x)+O(r_{0a})\end{aligned} \tag{50}$$

for $r_{0a}\downarrow0$. Using this asymptotic behavior and the Hilbert identity written in terms of Green functions,

$$(z-w)\int_{\mathbb{R}^2}\mathcal{G}_z(x,y)\,\mathcal{G}_w(y,x_0)\,\mathrm{d}^2y=\mathcal{G}_z(x,x_0)-\mathcal{G}_w(x,x_0)\,,$$

we obtain an equality valid for $u=a$, namely,

$$(z-w)(\sqrt{-w})^{|\nu|}\int_{\mathbb{R}^2}\mathcal{G}_z(x,y)\,\psi_{u,\nu,w}(y)\,\mathrm{d}^2y=(\sqrt{-z})^{|\nu|}\psi_{u,\nu,z}(x)-(\sqrt{-w})^{|\nu|}\psi_{u,\nu,w}(x)\,. \quad (51)$$

This means that

$$\psi_{u,\nu,w}+(z-w)(H-z)^{-1}\psi_{u,\nu,w}=\left(\frac{\sqrt{-z}}{\sqrt{-w}}\right)^{|\nu|}\psi_{u,\nu,z}$$

for $\nu\in\{\alpha-1,\alpha\}$ and $u=a$. The same argument naturally applies also to the vortex $u=b$. Using notation (43) we find that

$$f_{u,\nu,w}+(z-w)(H-z)^{-1}f_{u,\nu,w}=f_{u,\nu,z} \quad (52)$$

holds true for all $w,z\in\mathbb{C}\backslash\mathbb{R}$.

We wish to compute the 4×4 matrix of scalar products $P(z,w)$. Using (28) and applying the asymptotic behavior (50) once more, this time to equality (51), we find that the integral

$$\int_{\mathbb{R}^2}\overline{\psi_{v,\mu,z}(y)}\,\psi_{u,\nu,w}(y)\,\mathrm{d}^2y$$

equals the coefficient standing at

$$\frac{\sin(\pi|\mu|)}{2\pi^2}\,\frac{\Gamma(1-|\mu|)}{|\mu|}\left(\frac{r_v}{2}\right)^{|\mu|}e^{i\,\mu\,\theta_v}$$

when taking the asymptotic expansion of the expression

$$\frac{1}{\overline{z}-w}\left(\frac{1}{(\sqrt{-w})^{|\nu|}}\,\psi_{u,\nu,\overline{z}}(x)-\frac{1}{(\sqrt{-\overline{z}})^{|\nu|}}\,\psi_{u,\nu,w}(x)\right)$$

for $x\to v$, i.e., $r_v\downarrow0$. In virtue of (40) and (37) we get

$$\int_{\mathbb{R}^2}\overline{\psi_{a,\mu,z}(y)}\,\psi_{a,\nu,w}(y)\,\mathrm{d}^2y=-2\pi\frac{1}{\overline{z}-w}\left(\left(\frac{\sqrt{-\overline{z}}}{\sqrt{-w}}\right)^{|\nu|}\mathcal{T}_{\mu,\nu}(\alpha,\beta;\overline{z})-\left(\frac{\sqrt{-w}}{\sqrt{-\overline{z}}}\right)^{|\mu|}\mathcal{T}_{\mu,\nu}(\alpha,\beta;w)\right)$$

and

$$\int_{\mathbb{R}^2}\overline{\psi_{a,\mu,z}(y)}\,\psi_{b,\nu,w}(y)\,\mathrm{d}^2y=2\pi\frac{1}{\overline{z}-w}\left(\left(\frac{\sqrt{-\overline{z}}}{\sqrt{-w}}\right)^{|\nu|}\mathcal{S}_{\nu,\mu}(\alpha,\beta;\overline{z})-\left(\frac{\sqrt{-w}}{\sqrt{-\overline{z}}}\right)^{|\mu|}\mathcal{S}_{\nu,\mu}(\alpha,\beta;w)\right).$$

In particular,

$$\int_{\mathbb{R}^2}|\psi_{a,\nu,z}(x)|^2\,\mathrm{d}^2x=-\frac{2\pi}{\mathrm{Im}(z)}\,\mathrm{Im}\left(\left(\frac{\sqrt{-z}}{\sqrt{-\overline{z}}}\right)^{|\nu|}\mathcal{T}_{\nu,\nu}(\alpha,\beta;z)\right).$$

This means that, when passing to functions $\{f^j_z\}$ instead of $\{\psi_{u,\nu,z}\}$,

$$
\begin{aligned}
&(\overline{z}-w)\,P(z,w)\\
&\quad=-2\pi\begin{pmatrix}
(\sqrt{-\overline{z}})^{2-2\alpha}\mathcal{T}_{\alpha-1,\alpha-1}(\alpha,\beta;\overline{z}) & \sqrt{-\overline{z}}\,\mathcal{T}_{\alpha,\alpha-1}(\alpha,\beta;\overline{z})\\
\sqrt{-\overline{z}}\,\mathcal{T}_{\alpha-1,\alpha}(\alpha,\beta;\overline{z}) & (\sqrt{-\overline{z}})^{2\alpha}\mathcal{T}_{\alpha,\alpha}(\alpha,\beta;\overline{z})\\
-(\sqrt{-\overline{z}})^{2-\alpha-\beta}\mathcal{S}_{\alpha-1,\beta-1}(\beta,\alpha;\overline{z}) & -(\sqrt{-\overline{z}})^{1+\alpha-\beta}\mathcal{S}_{\alpha,\beta-1}(\beta,\alpha;\overline{z})\\
-(\sqrt{-\overline{z}})^{1-\alpha+\beta}\mathcal{S}_{\alpha-1,\beta}(\beta,\alpha;\overline{z}) & -(\sqrt{-\overline{z}})^{\alpha+\beta}\mathcal{S}_{\alpha,\beta}(\beta,\alpha;\overline{z})
\end{pmatrix}\\
&\qquad\begin{pmatrix}
-(\sqrt{-\overline{z}})^{2-\alpha-\beta}\mathcal{S}_{\beta-1,\alpha-1}(\alpha,\beta;\overline{z}) & -(\sqrt{-\overline{z}})^{1-\alpha+\beta}\mathcal{S}_{\beta,\alpha-1}(\alpha,\beta;\overline{z})\\
-(\sqrt{-\overline{z}})^{1+\alpha-\beta}\mathcal{S}_{\beta-1,\alpha}(\alpha,\beta;\overline{z}) & -(\sqrt{-\overline{z}})^{\alpha+\beta}\mathcal{S}_{\beta,\alpha}(\alpha,\beta;\overline{z})\\
(\sqrt{-\overline{z}})^{2-2\beta}\mathcal{T}_{\beta-1,\beta-1}(\beta,\alpha;\overline{z}) & \sqrt{-\overline{z}}\,\mathcal{T}_{\beta,\beta-1}(\beta,\alpha;\overline{z})\\
\sqrt{-\overline{z}}\,\mathcal{T}_{\beta-1,\beta}(\beta,\alpha;\overline{z}) & (\sqrt{-\overline{z}})^{2\beta}\mathcal{T}_{\beta,\beta}(\beta,\alpha;\overline{z})
\end{pmatrix}\\
&\qquad-(\overline{z}\leftrightarrow w)\,. \qquad (53)
\end{aligned}
$$

The Green functions $\mathcal{G}_z^{\pm}(x,x_0)$ should satisfy the corresponding boundary conditions in each variable x, x_0. Let us first consider the case of H^+. Recall that the boundary conditions which determine the domain of H^+ are $\Phi_2^{-1}=\Phi_1^0=0$ [see (15)]. Let us check the asymptotic behavior of $\mathcal{G}_z^{\pm}(x,x_0)$ for $x_0\to a$. Asymptotic behavior of $\mathcal{G}_z(x,x_0)$ is given in (50) and asymptotic behavior of $f_z^j(x_0)$ follows from (40) and (37) jointly with definition (43). The condition $\Phi_1^0=0$ means that the coefficient standing at $(r_{0a}/2)^{-\alpha}\exp(-i\alpha\theta_{0a})$ vanishes. This term occurs only in the asymptotic expansion of $f_z^2(x_0)$ and so

$$\sum_j\,(M_z^+)^{j,2}\,f_z^j(x)=0\,.$$

The set of functions $\{f_z^j\}$ is linearly independent and thus we get a condition on the matrix M_z^+: $(M_z^+)^{j,2}=0$ for all j. Considering the limit $x_0\to b$ one similarly derives the condition $(M_z^+)^{j,4}=0$. In view of (48) one obtains more, namely,

$$(M_z^+)^{j,k}=0\quad\text{whenever } j=2,4\ \text{ or } k=2,4. \qquad (54)$$

Let us denote by $M_z^{+,\mathrm{red}}$ the reduced 2×2 matrix obtained by omitting the vanishing rows and columns, i.e.,

$$M_z^{+,\mathrm{red}}=\begin{pmatrix}(M_z^+)^{1,1} & (M_z^+)^{1,3}\\ (M_z^+)^{3,1} & (M_z^+)^{3,3}\end{pmatrix}.$$

The condition $\Phi_2^{-1}=0$ for $x_0\to a$ means that the coefficient standing at $(r_{0a}/2)^{1-\alpha}\times\exp(-i(\alpha-1)\theta_{0a})$ vanishes. Using (54) we get

$$
\begin{aligned}
&\frac{\sin(\pi\alpha)}{2\pi^2}\,\frac{\Gamma(\alpha)}{1-\alpha}f_z^1(x)+\sum_j\,f_z^j(x)\Bigg(-(M_z^+)^{j,1}\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(\alpha)}{1-\alpha}(\sqrt{-z})^{2(1-\alpha)}\,\mathcal{T}_{\alpha-1,\alpha-1}(\alpha,\beta;z)\\
&\quad+(M_z^+)^{j,3}\frac{\sin(\pi\alpha)}{\pi}\,\frac{\Gamma(\alpha)}{1-\alpha}(\sqrt{-z})^{2-\alpha-\beta}\,\mathcal{S}_{\alpha-1,\beta-1}(\beta,\alpha;z)\Bigg)=0.
\end{aligned}
$$

This is equivalent to the couple of equations

$$
\begin{aligned}
&\frac{1}{2\pi}-(M_z^+)^{1,1}(\sqrt{-z})^{2(1-\alpha)}\,\mathcal{T}_{\alpha-1,\alpha-1}(\alpha,\beta;z)+(M_z^+)^{1,3}(\sqrt{-z})^{2-\alpha-\beta}\,\mathcal{S}_{\alpha-1,\beta-1}(\beta,\alpha;z)=0,\\
&-(M_z^+)^{3,1}(\sqrt{-z})^{2(1-\alpha)}\,\mathcal{T}_{\alpha-1,\alpha-1}(\alpha,\beta;z)+(M_z^+)^{3,3}(\sqrt{-z})^{2-\alpha-\beta}\,\mathcal{S}_{\alpha-1,\beta-1}(\beta,\alpha;z)=0.
\end{aligned}
$$

Analogously, another two equations are obtained when considering the limit $x_0 \to b$, namely,

$$\frac{1}{2\pi} - (M_z^+)^{3,3}(\sqrt{-z})^{2(1-\beta)}\mathcal{T}_{\beta-1,\beta-1}(\beta,\alpha;z) + (M_z^+)^{3,1}(\sqrt{-z})^{2-\alpha-\beta}\mathcal{S}_{\beta-1,\alpha-1}(\alpha,\beta;z) = 0,$$

$$-(M_z^+)^{1,3}(\sqrt{-z})^{2(1-\beta)}\mathcal{T}_{\beta-1,\beta-1}(\beta,\alpha;z) + (M_z^+)^{1,1}(\sqrt{-z})^{2-\alpha-\beta}\mathcal{S}_{\beta-1,\alpha-1}(\alpha,\beta;z) = 0.$$

The four equations can be jointly rewritten in the matrix form,

$$M_z^{+,\mathrm{red}} = \frac{1}{2\pi}\begin{pmatrix} (\sqrt{-z})^{2-2\alpha}\mathcal{T}_{\alpha-1,\alpha-1}(\alpha,\beta;z) & -(\sqrt{-z})^{2-\alpha-\beta}\mathcal{S}_{\beta-1,\alpha-1}(\alpha,\beta;z) \\ -(\sqrt{-z})^{2-\alpha-\beta}\mathcal{S}_{\alpha-1,\beta-1}(\beta,\alpha;z) & (\sqrt{-z})^{2-2\beta}\mathcal{T}_{\beta-1,\beta-1}(\beta,\alpha;z) \end{pmatrix}^{-1}. \tag{55}$$

It is straightforward to verify that the derived matrix M_z^+ actually obeys conditions (48) and (49). The former one follows from the equalities

$$\overline{\mathcal{T}_{\mu,\nu}(\alpha,\beta;z)} = \mathcal{T}_{\mu,\nu}(\alpha,\beta;\overline{z}), \quad \overline{\mathcal{S}_{\mu,\nu}(\alpha,\beta;z)} = \mathcal{S}_{\mu,\nu}(\alpha,\beta;\overline{z})$$

and

$$\mathcal{T}_{\mu,\nu}(\alpha,\beta;z) = \mathcal{T}_{\nu,\mu}(\alpha,\beta;z), \quad \mathcal{S}_{\mu,\nu}(\alpha,\beta;z) = \mathcal{S}_{\nu,\mu}(\beta,\alpha;z).$$

The latter one follows from the form of $P(z,w)$ given in (53). In fact, (53) and (55) jointly imply

$$(\overline{z}-w)\,P(z,w)^{\mathrm{red}} = (M_w^{+,\mathrm{red}})^{-1} - (M_z^{\pm,\mathrm{red}})^{-1}.$$

The other component of the Pauli operator, H^-, can be treated similarly. The boundary conditions read $\Phi_1^{-1} = \Phi_2^0 = 0$ [see (16)]. The condition $\Phi_1^{-1} = 0$ for $x_0 \to a$ means that the coefficient standing at $(r_{0a}/2)^{-1+\alpha}\exp(-i(\alpha-1)\theta_{0a})$ vanishes. Hence

$$\sum_j (M_z^-)^{j,1} f_z^j(x) = 0\,,$$

or equivalently, $(M_z^-)^{j,1} = 0$. Similarly for $x_0 \to 0$ we derive that $(M_z^-)^{j,3} = 0$, hence

$$(M_z^-)^{j,k} = 0 \quad \text{whenever } j = 1,3 \text{ or } k = 1,3. \tag{56}$$

Set

$$M_z^{-,\mathrm{red}} = \begin{pmatrix} (M_z^-)^{2,2} & (M_z^-)^{2,4} \\ (M_z^-)^{4,2} & (M_z^-)^{4,4} \end{pmatrix}.$$

The condition $\Phi_2^0 = 0$ for $x_0 \to a$ means that the coefficient standing at $(r_{0a}/2)^{\alpha}\exp(-i\alpha\theta_{0a})$ vanishes. Using (56) we get

$$\frac{\sin(\pi\alpha)}{2\pi^2}\frac{\Gamma(1-\alpha)}{\alpha} f_z^2(x) + \sum_j f_z^j(x)\Bigg(-(M_z^+)^{j,2}\frac{\sin(\pi\alpha)}{\pi}\frac{\Gamma(1-\alpha)}{\alpha}(\sqrt{-z})^{2\alpha}\mathcal{T}_{\alpha,\alpha}(\alpha,\beta;z)$$

$$+ (M_z^+)^{j,4}\frac{\sin(\pi\alpha)}{\pi}\frac{\Gamma(1-\alpha)}{\alpha}(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\alpha,\beta}(\beta,\alpha;z)\Bigg) = 0.$$

This is equivalent to the couple of equations

$$\frac{1}{2\pi} - (M_z^-)^{2,2}(\sqrt{-z})^{2\alpha}\mathcal{T}_{\alpha,\alpha}(\alpha,\beta;z) + (M_z^-)^{2,4}(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\alpha,\beta}(\beta,\alpha;z) = 0,$$

$$-(M_z^-)^{4,2}(\sqrt{-z})^{2\alpha}\mathcal{T}_{\alpha,\alpha}(\alpha,\beta;z)+(M_z^-)^{4,4}(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\alpha,\beta}(\beta,\alpha;z)=0.$$

For $x_0\to b$ one derives other two equations,

$$\frac{1}{2\pi}-(M_z^-)^{4,4}(\sqrt{-z})^{2\beta}\mathcal{T}_{\beta,\beta}(\beta,\alpha;z)+(M_z^-)^{4,2}(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\beta,\alpha}(\alpha,\beta;z)=0,$$

$$-(M_z^-)^{2,4}(\sqrt{-z})^{2\beta}\mathcal{T}_{\beta,\beta}(\beta,\alpha;z)+(M_z^-)^{2,2}(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\beta,\alpha}(\alpha,\beta;z)=0.$$

Jointly the four equations mean that

$$M_z^{-,\mathrm{red}}=\frac{1}{2\pi}\begin{pmatrix}(\sqrt{-z})^{2\alpha}\mathcal{T}_{\alpha,\alpha}(\alpha,\beta;z) & -(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\beta,\alpha}(\alpha,\beta;z)\\ -(\sqrt{-z})^{\alpha+\beta}\mathcal{S}_{\alpha,\beta}(\beta,\alpha;z) & (\sqrt{-z})^{2\beta}\mathcal{T}_{\beta,\beta}(\beta,\alpha;z)\end{pmatrix}^{-1}. \tag{57}$$

Let us note that the inverted matrices on the right-hand side of (55) and (57) are actually well defined. This is because the matrices in question depend on z analytically in the domain $\mathbb{C}\backslash\mathbb{R}_+$ and tend exponentially fast to invertible diagonal matrices for $\mathrm{Re}\,\sqrt{-z}\to+\infty$ as one can easily deduce from the discussion of the formula (32) related to the convergence of the series (31a) and from the form of matrix entries (38) and (41).

VII. CONCLUDING REMARKS

Having a formula for the Green function $\mathcal{G}_z^{\pm}(x,x_0)$ it would be, of course, desirable to use it for a more detailed analysis of the Pauli operator, first of all for its spectral analysis. This aim would assume, however, a more detailed analysis of the functions $\mathcal{S}_{\omega,\nu}(\alpha,\beta;z)$ and $\mathcal{T}_{\omega,\nu}(\alpha,\beta;z)$. In particular, it would be important to know what happens in the limit $\mathrm{Re}\,\sqrt{-z}\to 0$, i.e., when z approaches $\lambda\in\mathbb{R}_+$ from the upper or lower half-plane. Recall that both $\mathcal{S}_{\omega,\nu}(\alpha,\beta;z)$ and $\mathcal{T}_{\omega,\nu}(\alpha,\beta;z)$ are expressed as infinite series whose convergence is guaranteed for $\mathrm{Re}\,\sqrt{-z}>0$. Our first attempts in this direction suggest that such an analysis might be rather complex and should be considered as an independent problem in its own right.

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Nonadiabatic holonomy operators in classical and quantum completely integrable systems

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Given a completely integrable system, we associate to any connection on a fiber bundle in invariant tori over a parameter manifold the classical and quantum holonomy operator (generalized Berry's phase factor), without any adiabatic approximation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1627957]

I. INTRODUCTION

At present, holonomy operators in quantum systems attract special attention in connection with quantum computation (see, e.g., Refs. 1–3). They exemplify the non-Abelian generalization of Berry's geometric phase by means of driving a finite level degenerate eigenstate of a Hamiltonian over a parameter manifold. The key point is that a geometric phase depends only on the geometry of a path executed and, therefore, provides a possibility to perform quantum gate operations in an intrinsically fault-tolerant way. The problem lies in separation of a geometric phase factor from the total evolution operator without using an adiabatic assumption. First, holonomy quantum computation implies exact cyclic evolution, but exact adiabatic cyclic evolution almost never exists. Second, an adiabatic condition requires that the evolution time must be long enough.

A nonadiabatic Abelian phase was discovered by Aharonov and Anandan who considered a loop in a projective Hilbert space instead of a parameter space.[4] Non-Abelian generalization of the Aharonov–Anandan phase has been studied under rather particular assumption.[5] Moreover, a non-Abelian Aharonov–Anandan phase fails to be separated from the dynamic one in general. Recently, several schemes using the Aharonov–Anandan phase were proposed for nonadiabatic geometric gates.[6–8]

In a general setting, let us consider a linear (not necessarily finite-dimensional) dynamical system $\partial_t\psi=\hat{S}\psi$ whose linear (time-dependent) dynamic operator $\hat{S}$ falls into the sum

$$\hat{S}=\hat{S}_0+\Delta=\hat{S}_0+\Delta_\alpha\partial_t\xi^\alpha, \tag{1}$$

where $\xi(t)$ is a function of time taking its values in a finite-dimensional smooth real parameter manifold Σ coordinated by (σ^α). Let us assume that (i) the operators $\hat{S}_0(t)$ and $\Delta(t')$ commute for all instants t and t', and (ii) the operator Δ depends on time only through $\xi(t)$. Then the evolution operator $U(t)$ can be represented by the product of time-ordered exponentials

$$U(t)=U_0(t)\circ U_1(t)=T\exp\left[\int_0^t\hat{S}_0dt'\right]\circ T\exp\left[\int_0^t\Delta dt'\right], \tag{2}$$

where the second one is brought into the ordered exponential

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$$U_1(t)=T\exp\left[\int_0^t \Delta_\alpha(\xi(t'))\partial_t\xi^\alpha(t')dt'\right]=T\exp\left[\int_{\xi[0,t]}\Delta_\alpha(\sigma)d\sigma^\alpha\right] \tag{3}$$

along the curve $\xi[0,t]$ in the parameter manifold Σ. It is a nonadiabatic geometric factor depending only on the trajectory of the parameter function ξ. Accordingly, Δ is a holonomy operator. The geometric factor (3) is well defined if $\Delta_\alpha d\sigma^\alpha$ is an Ehresmann connection on a fiber bundle over a parameter manifold Σ. Then this factor is a displacement operator along an arbitrary curve $\xi[0,t]\subset\Sigma$.

A problem is that the above mentioned commutativity condition (i) is very restrictive. Moreover, it need not be preserved under time-dependent transformations.

For instance, let us consider a Hamiltonian system of dynamic variables (q,p). Written with respect to the initial data coordinates (q_0,p_0), its Hamiltonian $\mathcal{H}(q_0,p_0)$ vanishes. Given these coordinates (q_0,p_0), let one introduce a perturbed Hamiltonian $\mathcal{H}_\xi(q_0,p_0,\xi(t))$ which depends on parameter functions $\xi(t)$ and generates a holonomy operator Δ (1). Then the evolution operator of the perturbed Hamiltonian system reduces to the geometric factor (3). Relative to the original variables (q,p), a Hamiltonian of this perturbed Hamiltonian system is

$$\mathcal{H}'=\mathcal{H}(q,p,t)+\mathcal{H}_\xi(q_0(t,q,p),p_0(t,q,p),\xi(t)).$$

However, the corresponding evolution operator does not fall into the product (2) because a Hamiltonian $\mathcal{H}$ is not a function under time-dependent transformations and, consequently, the Poisson bracket $\{\mathcal{H},\mathcal{H}_\xi\}$ with respect to original variables (q,p) need not vanish.

Nevertheless, basing on this example, we can essentially extend the class of dynamical systems admitting a nonadiabatic geometric phase. We aim to describe dynamical systems where the commutativity condition (i) is not satisfied, but a part of dynamic variables is driven only by a holonomy operator. These are completely integrable Hamiltonian systems.

Let us consider a completely integrable Hamiltonian system (henceforth CIS) of m degrees of freedom around its invariant tori T^m. We show that, being constant under an internal evolution, its action variables are driven only by a perturbation holonomy operator Δ which can be associated to an arbitrary connection on a fiber bundle

$$\Sigma\times T^m\to\Sigma. \tag{4}$$

This holonomy operator is defined with respect to the initial data action-angle coordinates without any adiabatic approximation. Then we return to the original action-angle coordinates. The key point is that both classical evolution of action variables and mean values of quantum action operators relative to original action-angle coordinates are determined in full by the dynamics of initial data action and angle variables.

The plan of the paper is as follows. Section II addresses classical time-dependent CIS. The key point is that any time-dependent CIS of m degrees of freedom is extended to an autonomous CIS of $m+1$ degrees of freedom[9–11] and, as a consequence, can be provided with action-angle variables around a regular instantly compact invariant manifold.[10,11]

In Sec. III, we introduce the holonomy operator in a classical CIS by use of the fact that a generic Hamiltonian of a mechanical system with time-dependent parameters contains a term which is linear both in momenta and the temporal derivative of a parameter function.[12,13] This term comes from a connection on the configuration space of the system fibered over a parameter manifold.

Section IV is devoted to geometric quantization of a CIS with respect to the angle polarization. This polarization leads to the Schrödinger representation of action variables in the separable Hilbert space of smooth complex functions on T^m.[10,14] We show that this quantization both with respect to the original action-angle variables and the initial data action-angle variables is equivalent.

In Sec. V, the classical holonomy operator of Sec. III is quantized with respect to the initial data action-angle variables.

The symbols $\rfloor$ and $\lfloor$ below stand for the left and right interior products of multivector fields and exterior forms, respectively.

Let us recall that, given a fiber bundle $Y\to X$ coordinated by (x^λ,y^i), a connection K on $Y\to X$ is defined by a tangent-valued form

$$K=dx^\lambda\otimes(\partial_\lambda+k^i_\lambda\partial_i)$$

on Y.[15] A connection on a fiber bundle $Y\to X$ is said to be an Ehresmann connection if, given an arbitrary smooth curve $\xi([0,1])\subset X$, there exists its horizontal lift through any point of Y over $\xi(0)$.

Let X be a real axis $\mathbb{R}$ provided with the Cartesian coordinate t possessing transition functions $t'=t+\text{const}$. A connection K on a fiber bundle $Y\to\mathbb{R}$ is uniquely represented by a vector field K on Y such that $K\rfloor dt=1$.[12] This is the case of time-dependent mechanics.

II. CLASSICAL TIME-DEPENDENT CIS

Recall that the configuration space of time-dependent mechanics is a fiber bundle $Q\to\mathbb{R}$ over the time axis $\mathbb{R}$. Let it be equipped with the bundle coordinates (t,q^k), $k=1,\ldots,m$. The corresponding phase space is the vertical cotangent bundle V^*Q of $Q\to\mathbb{R}$ endowed with the induced coordinates (t,q^k,p_k) relative to the holonomic coframes $\{dq^k\}$.[12,16] The cotangent bundle T^*Q of $Q\to\mathbb{R}$ plays a role of the homogeneous phase space of time-dependent mechanics. It is equipped with the induced coordinates (t,q^k,p,p_k) relative to the holonomic coframes $\{dt,dq^k\}$. With respect to these coordinates, the canonical symplectic form and the corresponding Poisson bracket on T^*Q read

$$\Omega=dp\wedge dt+dp_k\wedge dq^k,$$

$$\{f,f'\}_T=\partial_p f\partial_t f'-\partial_t f\partial_p f'+\partial^k f\partial_k f'-\partial_k f\partial^k f',\quad f,f'\in C^\infty(T^*Q).$$

There is the one-dimensional trivial affine bundle

$$\zeta: T^*Q\to V^*Q. \tag{5}$$

As a consequence, the phase space V^*Q of time-dependent mechanics is provided with the canonical Poisson structure

$$\{f,f'\}_V=\partial^k f\partial_k f'-\partial_k f\partial^k f',\quad f,f'\in C^\infty(V^*Q), \tag{6}$$

given by the relations

$$\zeta^*\{f,f'\}_V=\{\zeta^*f,\zeta^*f'\}_T,\quad f,f'\in C^\infty(V^*Q).$$

The corresponding Poisson bivector on V^*Q reads $w_V=\partial_k\wedge\partial^k$.

A Hamiltonian of time-dependent mechanics is defined as a global section

$$h: V^*Q\to T^*Q,\quad p\circ h=-\mathcal{H}(t,q^j,p_j), \tag{7}$$

of the affine bundle ζ (5).[12,16] Given the pull-back form $h^*\Omega$, the relations $\gamma_H\rfloor dt=1$, $\gamma_H\rfloor h^*\Omega=0$ define a unique Hamilton vector field

$$\gamma_H=\partial_t+\partial^k\mathcal{H}\partial_k-\partial_k\mathcal{H}\partial^k \tag{8}$$

on V^*Q and the corresponding Hamilton equations

$$\dot q^k=\partial^k\mathcal{H},\quad \dot p_k=-\partial_k\mathcal{H}. \tag{9}$$

Note that, given a connection $\Gamma=\partial_t+\Gamma_t^i\partial_i$ on $Q\to\mathbb{R}$, any Hamiltonian $\mathcal{H}$ (7) admits the decomposition $\mathcal{H}=p_i\Gamma_t^i+\widetilde{\mathcal{H}}$ where $\widetilde{\mathcal{H}}$ is a function on V^*Q.

An integral of motion of the Hamilton equations (9) is a smooth real function F on V^*Q whose Lie derivative

$$\mathbf{L}_{\gamma_H}F=\gamma_H\rfloor dF=\partial_t F+\{\mathcal{H},F\}_V$$

along the Hamilton vector field γ_H (8) vanishes. A time-dependent Hamiltonian system of m degrees of freedom is a CIS if there exist m independent integrals of motion $\{F_k\}$ in involution with respect to the Poisson bracket $\{,\}_V$ (6). Their Hamiltonian vector fields

$$\vartheta_i=-w_V\rfloor dF_i=\partial^k F_i\partial_k-\partial_k F_i\partial^k$$

and the Hamilton vector field γ_H (8) generate a smooth regular distribution on the phase space V^*Q and the corresponding foliation of V^*Q in invariant manifolds.

One can associate to any time-dependent CIS on V^*Q an autonomous CIS on the homogeneous phase space T^*Q as follows.

Given a Hamiltonian h (7), let us consider an autonomous Hamiltonian system on the symplectic manifold (T^*Q,Ω) with the Hamiltonian

$$\mathbf{H}=\partial_t\rfloor(\Xi-\zeta^*h^*\Xi)=p+\mathcal{H}.$$

Its Hamiltonian vector field

$$\gamma_T=\partial_t-\partial_t\mathcal{H}\partial_p+\partial^k\mathcal{H}\partial_k-\partial_k\mathcal{H}\partial^k \tag{10}$$

is projected onto the Hamilton vector field γ_H (8) on V^*Q so that

$$\zeta^*(\mathbf{L}_{\gamma_H}f)=\{\mathbf{H},\zeta^*f\}_T,\quad f\in C^\infty(V^*Q).$$

An immediate consequence of this relation is the following.

(i) Given a time-dependent CIS $(H;F_k)$ on V^*Q, the Hamiltonian system $\{\mathbf{H},\zeta^*F_k\}$ on T^*Q is a CIS.

(ii) If $M\subset V^*Q$ is an invariant manifold of the time-dependent CIS $\{H;F_k\}$, then $h(M)\subset T^*Q$ is an invariant manifold of the homogeneous CIS $(\mathbf{H},\zeta^*F_k)$.

Hereafter, let the Hamilton vector field γ_H (8) be complete, i.e., the Hamilton equations (9) admit a unique global solution (a trajectory of γ_H) through every point of the phase space V^*Q. The trajectories of γ_H define a trivial bundle $V^*Q\to V_0^*Q$ over the fiber V_0^*Q of $V^*Q\to\mathbb{R}$ at $t=0$. Then any invariant manifold M of $\{H;F_k\}$ is also a trivial bundle $M=\mathbb{R}\times M_0$ over $M_0=M\cap V_0^*Q$.

If M_0 is compact, one can introduce action-angle coordinates around an invariant manifold M by use of the action-angle coordinates around the invariant manifold $h(M)$ of the corresponding autonomous CIS on T^*Q.[10] Namely, $h(M)$ has an open neighborhood which is a trivial bundle

$$U'=V'\times\mathbb{R}\times T^m\to V'\times\mathbb{R}\to V' \tag{11}$$

over a domain $V'\subset\mathbb{R}^{m+1}$ with respect to the action-angle coordinates (I_0,I_i,t,ϕ^i). Herewith, the following holds. (i) $I_0=\mathbf{H}$. (ii) The integrals of motion ζ^*F_k depend only on the action coordinates I_i. (iii) The symplectic form Ω on U' reads

$$\Omega=dI_0\wedge dt+dI_i\wedge d\phi^i.$$

The symplectic annulus U' (11) inherits the fibration structure (5) over the toroidal domain

$$U=V\times\mathbb{R}\times T^m, \quad V\subset\mathbb{R}^m. \tag{12}$$

Coordinated by (I_i,t,ϕ^i) and provided with the Poisson structure (6), the toroidal domain (12) is a phase space of the time-dependent CIS $(H;F_i)$ around its instantly compact invariant manifold M. Since $\mathbf{H}=I_0$, the Hamilton vector field (10) is $\gamma_T=\partial_t$, and so is its projection γ_H (8) onto U. Hence, the above-mentioned action-angle coordinates (I_i,t,ϕ^i) are the initial data coordinates.

These action-angle coordinates are by no means unique. Let $\mathcal{H}$ be an arbitrary smooth function on $\mathbb{R}^m$. Then the canonical transformation

$$I_0'=I_0-\mathcal{H}(I_j), \quad I_i'=I_i, \quad t'=t, \quad \varphi^i=\phi^i+t\partial^i\mathcal{H}(I_j) \tag{13}$$

gives new action-angle coordinates corresponding to a different trivialization of U' (11) [and U (12)]. Accordingly, the Hamilton vector field γ_H takes the form (8), and the Hamilton equations (9) read

$$\dot\varphi^k=\partial^k\mathcal{H}, \quad \dot I_k=0.$$

These are the Hamilton equations of an autonomous CIS with a time-independent Hamiltonian $\mathcal{H}$ on the toroidal domain U (12).

III. CLASSICAL HOLONOMY OPERATORS

The phase space of a Hamiltonian system with time-dependent parameters is a composite fiber bundle $\Pi\to\Sigma\times\mathbb{R}\to\mathbb{R}$, where $\Pi\to\Sigma\times\mathbb{R}$ is a symplectic bundle and $\Sigma\times\mathbb{R}\to\mathbb{R}$ is a parameter bundle whose sections are parameter functions.[12,13,17,18] In the case under consideration, all bundles are trivial and their trivializations hold fixed. Namely, the phase space is the product

$$\Pi=\Sigma\times U=\Sigma\times(V\times\mathbb{R}\times T^m)\to\Sigma\times\mathbb{R}\to\mathbb{R},$$

equipped with the coordinates $(\sigma^\alpha,I_k,t,\phi^k)$. Let us suppose for a time that parameters are also dynamic variables. The phase space of this system is the fiber bundle

$$\Pi'=T^*\Sigma\times U\to\Sigma\times\mathbb{R}\times T^m$$

coordinated by $(\sigma^\alpha,\sigma_\alpha,I_k,t,\phi^k)$. A generic Hamiltonian of such a system is

$$\mathcal{H}_\Sigma=\sigma_\alpha\Sigma_t^\alpha+I_k(\Lambda_t^k+\Lambda_\alpha^k\Sigma_t^\alpha)+\widetilde{\mathcal{H}}(\sigma^\beta,I_j,t,\phi^j), \tag{14}$$

where

$$\partial_t+\Sigma_t^\alpha\partial_\alpha+(\Lambda_t^k+\Lambda_\alpha^k\Sigma_t^\alpha)\partial_k$$

is a composite connection on the fiber bundle $\Sigma\times\mathbb{R}\times T^m\to\mathbb{R}$ generated by a connection $\partial_t+\Sigma_t^\alpha\partial_\alpha$ on the parameter bundle $\Sigma\times\mathbb{R}\to\mathbb{R}$ and a connection

$$\Lambda=dt\otimes(\partial_t+\Lambda_t^k\partial_k)+d\sigma^\alpha\otimes(\partial_\alpha+\Lambda_\alpha^k\partial_k) \tag{15}$$

on $\Sigma\times\mathbb{R}\times T^m\to\Sigma\times\mathbb{R}$.[12,13,18] Then a Hamiltonian system with a fixed parameter function $\sigma^\alpha=\xi^\alpha(t)$ is characterized by the Hamiltonian

$$\mathcal{H}_\xi=I_k[\Lambda_t^k(t,\phi^j)+\Lambda_\alpha^k(\xi^\beta,t,\phi^j)\partial_t\xi^\alpha]+\widetilde{\mathcal{H}}(\xi^\beta,I_j,t,\phi^j) \tag{16}$$

on the pull-back bundle $U=\xi^*\Pi$ (12).

Let (I_k, t, ϕ^k) be the initial data action-angle coordinates of a time-dependent CIS. Its Hamiltonian $\mathcal{H}$ with respect to these coordinates vanishes. Therefore, we can introduce a desired holonomy operator by the appropriate choice of the connection Λ (15). Let us put $\Lambda^k_t = 0$ and assume that coefficients Λ^k_α are independent of time, i.e., the part

$$\Lambda_\Sigma = d\sigma^\alpha \otimes (\partial_\alpha + \Lambda^k_\alpha \partial_k) \tag{17}$$

of the connection Λ (15) is a connection on the fiber bundle (4). Then the Hamiltonian of a perturbed CIS reads

$$\mathcal{H}_\xi = I_k \Lambda^k_\alpha(\xi^\beta, \phi^j)\partial_t \xi^\alpha. \tag{18}$$

Its Hamilton vector field (8) is

$$\gamma_H = \partial_t + \Lambda^i_\alpha \partial_t \xi^\alpha \partial_i - I_k \partial_i \Lambda^k_\alpha \partial_t \xi^\alpha \partial^i. \tag{19}$$

It leads to the Hamilton equations

$$\partial_t \phi^i = \Lambda^i_\alpha(\xi(t), \phi^l)\partial_t \xi^\alpha, \tag{20}$$

$$\partial_t I_i = -I_k \partial_i \Lambda^k_\alpha(\xi(t), \phi^l)\partial_t \xi^\alpha. \tag{21}$$

Note that

$$V^*\Lambda_\Sigma = d\sigma^\alpha \otimes (\partial_\alpha + \Lambda^i_\alpha \partial_i - I_k \partial_i \Lambda^k_\alpha \partial^i) \tag{22}$$

is the lift of the connection Λ_Σ (17) onto the fiber bundle $\Sigma \times (V \times T^m) \to \Sigma$, seen as a subbundle of the vertical cotangent bundle $V^*(\Sigma \times T^m) = \Sigma \times T^*T^m$ of the fiber bundle (4). It follows that any solution $I_i(t)$, $\phi^i(t)$ of the Hamilton equations (20) and (21) [i.e., an integral curve of the Hamilton vector field (19)] is a horizontal lift of the curve $\xi(t) \subset \Sigma$ with respect to the connection $V^*\Lambda_\Sigma$ (22), i.e., $I_i(t) = I_i(\xi(t))$, $\phi^i(t) = \phi^i(\xi(t))$. Thus, the right-hand side of the Hamilton equations (20) and (21) is the holonomy operator

$$\Delta = (\Lambda^i_\alpha \partial_t \xi^\alpha, -I_k \partial_i \Lambda^k_\alpha \partial_t \xi^\alpha) \tag{23}$$

[cf. (1) where $\hat{S}_0 = 0$]. It is not a linear operator, but the substitution of a solution $\phi(\xi(t))$ of the equation (20) into the Hamilton equation (21) results in a linear holonomy operator on the action variables I_i.

Let us show that the holonomy operator (23) is well defined. Since any vector field ϑ on $\mathbb{R} \times T^m$ such that $\vartheta \rfloor dt = 1$ is complete, the Hamilton equation (20) has solutions for any parameter function $\xi(t)$. It follows that any connection Λ_Σ (17) on the fiber bundle (4) is an Ehresmann connection, and so is its lift (22). Therefore, any curve $\xi([0,1]) \subset \Sigma$ can play the role of the parameter function in the holonomy operator Δ (23).

Now, let us return to the original action-angle coordinates (I_k, t, φ^k) by means of the canonical transformation (13). Relative to these coordinates, the perturbed Hamiltonian reads

$$\mathcal{H}' = I_k \Lambda^k_\alpha(\xi(t), \varphi^i - t\partial^i \mathcal{H}(I_j))\partial_t \xi^\alpha(t) + \mathcal{H}(I_j),$$

and the Hamilton equations (20) and (21) take the form

$$\partial_t \varphi^i = \partial^i \mathcal{H}(I_j) + \Lambda^i_\alpha(\xi(t), \varphi^l - t\partial^l \mathcal{H}(I_j))\partial_t \xi^\alpha(t) - tI_k \partial^i \partial^s \mathcal{H}(I_j)\partial_s \Lambda^k_\alpha(\xi(t), \varphi^l - t\partial^l \mathcal{H}(I_j))\partial_t \xi^\alpha(t),$$

$$\partial_t I_i = -I_k \partial_i \Lambda^k_\alpha(\xi(t), \varphi^l - t\partial^l \mathcal{H}(I_j))\partial_t \xi^\alpha(t).$$

Their solution is $I_i(\xi(t))$, $\varphi^i(t)=\phi^i(\xi(t))+t\partial^i\mathcal{H}(I_j(\xi(t)))$ where $I_i(\xi(t))$, $\phi^i(\xi(t))$ is a solution of the Hamilton equations (20) and (21). It is readily observed that the action variables I_k are driven only by the holonomy operator, while the angle variables φ^i have a nongeometric summand.

Let us emphasize that, in the construction of the holonomy operator (23), we did not impose any restriction on the connection Λ_Σ (17). Therefore, any connection on the fiber bundle (4) generates a holonomy operator in a CIS. However, a glance at the expression (23) shows that this operator becomes zero on action variables if all coefficients Λ^k_λ of the connection Λ_Σ (17) are constant, i.e., Λ_Σ is a principal connection on the fiber bundle (4) seen as a principal bundle with the structure group T^m.

IV. QUANTUM CIS

There are different approaches to quantization of CISs.[19] Their geometric quantization was studied at first with respect to the polarization spanned by Hamiltonian vector fields of integrals of motion.[20] For example, the well-known Simms quantization of the harmonic oscillator is of this type. In this approach, the problem is that the associated quantum algebra includes affine functions of angle coordinates which are ill defined. As a consequence, elements of the carrier space of this quantization fail to be smooth, but are tempered distributions. In recent works,[10,14] we have developed a different variant of geometric quantization of CISs by use of the angle polarization spanned by almost-Hamiltonian vector fields ∂^k of angle variables. This quantization is equivalent to geometric quantization of the cotangent bundle T^*T^m of a torus T^m with respect to the vertical polarization. The result is as follows.

Given an autonomous CIS on a symplectic annulus

$$P=V\times T^m, \quad \Omega_P=dI_i\wedge d\varphi^i$$

equipped with the action-angle coordinates (I_i,φ^i), its quantum algebra $\mathcal{A}$ with respect to the above mentioned angle polarization consists of affine functions

$$f=a^k(\varphi^j)I_k+b(\varphi^j)$$

of action coordinates I_k. They are represented by self-adjoint unbounded operators

$$\hat{f}=-ia^k\partial_k-\frac{i}{2}\partial_k a^k-a^k\lambda_k+b \tag{24}$$

in the separable pre-Hilbert space of complex half-forms on T^m. If coordinate transformations of T^m are only translations, this space can be identified with the pre-Hilbert space $\mathbb{C}^\infty(T^m)$ of smooth complex functions on T^m. Different tuples of real numbers $(\lambda_1,\ldots,\lambda_m)$ and $(\lambda'_1,\ldots,\lambda'_m)$ specify inequivalent representations (24), unless $\lambda_k-\lambda'_k\in\mathbb{Z}$ for all $k=1,\ldots,m$. These numbers come from the de Rham cohomology group $H^1(T^m)=\mathbb{R}^m$.

In particular, the action operators (24) read $\hat{I}_k=-i\partial_k-\lambda_k$. They are bounded. By virtue of the multidimensional Fourier theorem, an orthonormal basis for $\mathbb{C}^\infty(T^m)$ consists of functions

$$\psi_{(n_r)}(\varphi)=\exp[in_r\varphi^r], \quad (n_r)=(n_1,\ldots,n_m)\in\mathbb{Z}^m. \tag{25}$$

With respect to this basis, the action operators are brought into countable diagonal matrices

$$\hat{I}_k\psi_{(n_r)}=(n_k-\lambda_k)\psi_{(n_r)}, \tag{26}$$

while functions $a^k(\varphi)$ are decomposed in Fourier series of the functions $\psi_{(n_r)}$, which act on $\mathbb{C}^\infty(T^m)$ by the law

$$\hat{\psi}_{(n_r)}\psi_{(n'_r)}=\psi_{(n_r+n'_r)}. \tag{27}$$

It should be emphasized that $\hat{a}^k\hat{I}_k\neq\widehat{a^kI_k}\neq\widehat{I_ka^k}$.

If a Hamiltonian $\mathcal{H}(I_k)$ of an autonomous CIS is an analytic function on $\mathbb{R}^m$, it is uniquely quantized as a Hermitian element $\hat{\mathcal{H}}(I_k)=\mathcal{H}(\hat{I}_k)$ of the enveloping algebra of $\mathcal{A}$. It is a bounded self-adjoint operator with the countable spectrum

$$\hat{\mathcal{H}}(I_k)\psi_{(n_r)}=E_{(n_r)}\psi_{(n_r)}, \quad E_{(n_r)}=\mathcal{H}(n_k-\lambda_k), \quad n_k\in(n_r). \tag{28}$$

In order to quantize a time-dependent CIS on the Poisson toroidal domain $(U,\{,\}_V)$ (12) equipped with action-angle coordinates (I_i,t,φ^i), one may follow the instantwise geometric quantization of time-dependent mechanics.[21] As a result, we can simply replace functions on T^m with those on $\mathbb{R}\times T^m$.[10] Namely, the corresponding quantum algebra $\mathcal{A}\subset C^\infty(U)$ consists of affine functions

$$f=a^k(t,\varphi^j)I_k+b(t,\varphi^j) \tag{29}$$

of action coordinates I_k represented by the operators (24) in the space

$$E=\mathbb{C}^\infty(\mathbb{R}\times T^m) \tag{30}$$

of smooth complex functions $\psi(t,\varphi)$ on $\mathbb{R}\times T^m$. This space is provided with the structure of the pre-Hilbert $\mathbb{C}^\infty(\mathbb{R})$-module with respect to the nondegenerate $\mathbb{C}^\infty(\mathbb{R})$-bilinear form

$$\langle\psi|\psi'\rangle=\left(\frac{1}{2\pi}\right)^m\int_{T^m}\psi\overline{\psi'}\,d^m\varphi, \quad \psi,\psi'\in\mathbb{C}^\infty(\mathbb{R}\times T^m).$$

Its basis consists of the pull-back onto $\mathbb{R}\times T^m$ of the functions $\psi_{(n_r)}$ in (25).

This quantization of a time-dependent CIS is extended to the associated homogeneous CIS on the symplectic annulus (U',Ω) in (11) by means of the operator $\hat{I}_0=-i\partial_t$ in the pre-Hilbert module E in (30). Accordingly, the homogeneous Hamiltonian $\mathbf{H}$ is quantized as $\hat{\mathbf{H}}=-i\partial_t+\hat{\mathcal{H}}$. The corresponding Schrödinger equation is

$$\hat{\mathbf{H}}\psi=-i\partial_t\psi+\hat{\mathcal{H}}\psi=0, \quad \psi\in E. \tag{31}$$

For instance, the quantum Hamiltonian of the original autonomous CIS is

$$\hat{\mathbf{H}}=-i\partial_t+\mathcal{H}(\hat{I}_j).$$

Its spectrum $\hat{\mathbf{H}}\psi_{(n_r)}=E_{(n_r)}\psi_{(n_r)}$ relative to the basis $\{\psi_{(n_r)}\}$ for E in (30) coincides with that of the autonomous Hamiltonian (28). The Schrödinger equation (31) reads

$$\hat{\mathbf{H}}\psi=-i\partial_t\psi+\mathcal{H}(-i\partial_k-\lambda_k)\psi=0, \quad \psi\in E.$$

Its solutions are the Fourier series

$$\psi=\sum_{(n_r)}B_{(n_r)}\exp[-itE_{(n_r)}]\psi_{(n_r)}, \quad B_{(n_r)}\in\mathbb{C}.$$

Now, let us quantize this CIS with respect to the initial data action-angle coordinates (I_i,ϕ^i). Its quantum algebra $\mathcal{A}_0\subset C^\infty(U)$ consists of affine functions

$$f=a^k(t,\phi^j)I_k+b(t,\phi^j). \tag{32}$$

The canonical transformation (13) provides an isomorphism between Poisson algebras $\mathcal{A}$ and $\mathcal{A}_0$. Functions f in (32) are represented by the operators $\hat{f}$ in (24) in the pre-Hilbert module E_0 of smooth complex functions $\Psi(t,\phi)$ on $\mathbb{R}\times T^m$. Given its basis $\Psi_{(n_r)}(\phi)=\exp[in_r\phi^r]$, the operators $\hat{I}_k$ and $\hat{\psi}_{(n_r)}$ take the form (26) and (27), respectively. The Hamiltonian of a quantum CIS with respect to the initial data variables is $\hat{\mathbf{H}}_0=-i\partial_t$. Then one easily obtains the isometric isomorphism

$$R(\psi_{(n_r)})=\exp[itE_{(n_r)}]\Psi_{(n_r)}, \quad \langle R(\psi)|R(\psi')\rangle=\langle\psi|\psi'\rangle, \tag{33}$$

between the pre-Hilbert modules E and E_0 which provides the equivalence

$$\hat{I}_i=R^{-1}\hat{I}_iR, \quad \hat{\psi}_{(n_r)}=R^{-1}\hat{\Psi}_{(n_r)}R, \quad \hat{\mathbf{H}}=R^{-1}\hat{\mathbf{H}}_0R \tag{34}$$

of the quantizations of a CIS with respect to the original and initial data action-angle variables.

V. QUANTUM HOLONOMY OPERATORS

In view of the isomorphism (34), let us first construct a holonomy operator for a quantum CIS $(\mathcal{A}_0,\hat{\mathbf{H}}_0)$ with respect to the initial data action-angle coordinates. Let us consider the perturbed homogeneous Hamiltonian

$$\mathbf{H}_\xi=\mathbf{H}_0+\mathbf{H}_1=I_0+\partial_t\xi^\alpha(t)\Lambda^k_\alpha(\xi(t),\phi^j)I_k$$

of the classical perturbed system (18). Its perturbation term $\mathbf{H}_1$ is of the form (29) and, therefore, is quantized by the operator

$$\hat{\mathbf{H}}_1=-i\partial_t\xi^\alpha\hat{\Delta}_\alpha=-i\partial_t\xi^\alpha[\Lambda^k_\alpha\partial_k+\tfrac{1}{2}\partial_k(\Lambda^k_\alpha)-i\lambda_k\Lambda^k_\alpha].$$

The quantum Hamiltonian $\hat{\mathbf{H}}_\xi=\hat{\mathbf{H}}_0+\hat{\mathbf{H}}_1$ defines the Schrödinger equation

$$\partial_t\Psi+\partial_t\xi^\alpha[\Lambda^k_\alpha\partial_k+\tfrac{1}{2}\partial_k(\Lambda^k_\alpha)-i\lambda_k\Lambda^k_\alpha]\Psi=0. \tag{35}$$

If a solution exists, it can be written by means of the evolution operator which reduces to the geometric factor U_1 in (3). The latter can be viewed as a displacement operator along the curve $\xi[0,1]\subset\Sigma$ with respect to the connection

$$\hat{\Lambda}_\Sigma=d\sigma^\alpha(\partial_\alpha+\hat{\Delta}_\alpha) \tag{36}$$

in the $\mathbb{C}^\infty(\Sigma)$-module $\mathbb{C}^\infty(\Sigma\times T^m)$ of smooth complex functions on $\Sigma\times T^m$.[13,15,18,22] Let us study the existence of this displacement operator.

Given a connection Λ_Σ in (17), let $\Phi^i(t,\phi)$ denote the flow of the complete vector field $\partial_t+\Lambda^i_\alpha(\xi,\phi)\partial_t\xi^\alpha\partial_i$ on $\mathbb{R}\times T^m$. It is a solution of the Hamilton equation (20) with the initial data ϕ. We need the inverse flow $(\Phi^{-1})^i(t,\phi)$ which obeys the equation

$$\partial_t(\Phi^{-1})^i(t,\phi)=-\partial_t\xi^\alpha\Lambda^i_\alpha(\xi,(\Phi^{-1})^i(t,\phi))=-\partial_t\xi^\alpha\Lambda^k_\alpha(\xi,\phi)\partial_k(\Phi^{-1})^i(t,\phi).$$

Let Ψ_0 be an arbitrary complex half-form Ψ_0 on T^m possessing identical transition functions, and let the same symbol stand for its pull-back onto $\mathbb{R}\times T^m$. Given its pull-back

$$(\Phi^{-1})^*\Psi_0=\det\left(\frac{\partial(\Phi^{-1})^i}{\partial\phi^k}\right)^{1/2}\Psi_0(\Phi^{-1}(t,\phi)), \tag{37}$$

it is readily observed that

$$\Psi = (\Phi^{-1})^* \Psi_0 \exp[i\lambda_k \phi^k]$$

obeys the Schrödinger equation (35) with the initial data Ψ_0. This function is well defined only if all the numbers λ_k equal 0 or $\pm\frac{1}{2}$. Note that, if some numbers λ_k are equal to $\pm\frac{1}{2}$, then $\Psi_0 \exp[i\lambda_k \phi^k]$ is a half-density on T^m whose transition functions equal ± 1, i.e., it is a section of a nontrivial metalinear bundle over T^m.

We thus observe that if λ_k equals 0 or $\pm\frac{1}{2}$, then the displacement operator always exists and $\Delta = i\mathbf{H}_1$ is a holonomy operator. A glance at the action law (27) shows that this operator is infinite-dimensional.

For instance, let Λ_Σ in (17) be the above mentioned principal connection, i.e., $\Lambda^k_\alpha = \text{const}$. Then the Schrödinger equation (35) where $\lambda_k = 0$ takes the form

$$\partial_t \Psi(t, \phi^j) + \partial_t \xi^\alpha(t) \Lambda^k_\alpha \partial_k \Psi(t, \phi^j) = 0.$$

Its solution (37) is

$$\Psi(t, \phi^j) = \Psi_0(\phi^j - (\xi^\alpha(t) - \xi^\alpha(0))\Lambda^j_\alpha).$$

The corresponding evolution operator reduces to Berry's phase multiplier

$$U_1 \Psi_{(n_r)} = \exp[-in_j(\xi^\alpha(t) - \xi^\alpha(0))\Lambda^j_\alpha)]\Psi_{(n_r)}, \quad n_j \in (n_r).$$

It keeps the eigenvectors of the action operators $\hat{I}_i$.

In order to return to the original action-angle variables, one can employ the morphism R in (33). The corresponding Hamiltonian reads $\mathbf{H}' = R^{-1}\mathbf{H}_\xi R$. The key point is that, due to the relation (34), the action operators $\hat{I}_i$ have the same mean values

$$\langle I_k \psi | \psi \rangle = \langle I_k \Psi | \Psi \rangle, \quad \Psi = R(\psi),$$

with respect both to the original and the initial data action-angle variables. Therefore, these mean values are defined only by the holonomy operator.

VI. CONCLUSIONS

We have shown that any CIS around its compact invariant manifold admits a perturbation dependent on parameters by means of a holonomy operator associated to a connection on the fiber bundle (4).

Since action variables are driven only by a holonomy operator, one can use this operator in order to perform a dynamic transition between classical solutions or quantum states of an unperturbed CIS by an appropriate choice of a parameter function ξ. The key point is that this transition can take an arbitrary short time because we are entirely free with time parametrization of ξ and can choose it quickly changing, in contrast with slowly varying parameter functions in adiabatic models. For instance, one can choose ξ a step function; then its time derivative is a δ-function of time. This fact makes nonadiabatic holonomy operators in CISs promising for several applications, including classical and quantum scattering in integrable Hamiltonian systems,[23] quantum control operators,[24,25] and the above mentioned quantum computation. It also looks attractive that quantum holonomy operators in CISs are essentially infinite-dimensional, whereas both the existent quantum control theory and the theory of quantum information and computation[26] involve only finite-dimensional operators.

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Weak coherent state path integrals

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Weak coherent states share many properties of the usual coherent states, but do not admit a resolution of unity expressed in terms of a local integral. They arise, e.g., in the case that a group acts on an inadmissible fiducial vector. Motivated by the recent Affine Quantum Gravity Program, the present article studies the path integral representation of the affine weak coherent state matrix elements of the unitary time-evolution operator. Since weak coherent states do not admit a resolution of unity, it is clear that the standard way of constructing a path integral, by time slicing, is predestined to fail. Instead a well-defined path integral with Wiener measure, based on a continuous-time regularization, is used to approach this problem. The dynamics is rigorously established for linear Hamiltonians, and the difficulties presented by more general Hamiltonians are addressed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1627959]

I. INTRODUCTION

Unlike the standard phase space path integrals constructed by the time slicing method, the path integral with Wiener measure invented by Klauder, Daubechies, and others uses a continuous-time regularization factor.[1–5] This path integral is $\int \exp\{-i\int[qdp+dG(p,q)+h(p,q)dt]\}\, d\mu_W^\nu$, where G is an arbitrary C^1 function and h is the classical Hamiltonian in a sense which will be explained later. The pinned Wiener measure $d\mu_W^\nu$ is defined with the help of the heat kernel $\int d\mu_W^\nu := [\exp\{\nu T\Delta_{\mathrm{LB}}\}](p'',q'',q',p')$. Thus, by way of the Laplace–Beltrami operator Δ_{LB}, a metric is introduced. The formal phase space path integral $\mathcal{N}_\nu \int \exp\{-i\int[q\dot{p}+\dot{G}(p,q)+h(p,q)]dt\}\exp\{-(1/2\nu)\int(d\sigma^2/dt^2)dt\}\mathcal{D}p\mathcal{D}q$ can be given meaning by equating it to the above Wiener measure path integral. Here, $\mathcal{N}_\nu$ is a formal normalization constant, and $d\sigma^2$ is the metric mentioned above. The variables p and q in the well-defined Wiener measure path integral are stochastic variables describing Brownian Bridges. The integral $\int qdp$ has to be interpreted as a stochastic integral. The rule adopted here is the Stratonovich midpoint rule $\int qdp := \lim \Sigma \frac{1}{2}(q_{l+1}+q_l)(p_{l+1}-p_l)$, which guarantees that the ordinary rules of calculus still apply. It was shown, first for the case of a flat and spherical phase space metric,[1] then for a hyperbolic metric,[2] that the limit of diverging diffusion constant ν exists for a wide set of quantum Hamiltonians $\mathcal{H}$, including at least all Hamiltonians polynomial in the basic quantum kinematical operators. The limit is equal to the coherent state matrix element $\langle p''q''|\exp\{-iT\mathcal{H}\}|p'q'\rangle$ of the unitary time-evolution operator and the specific metric determines the coherent states in question: The flat metric is inevitably connected with the coherent states of the Heisenberg–Weyl group (and in the canonical, Cartesian form, it is connected to the canonical coherent states), the spherical metric is associated with the coherent states of the SU(2) group, and the hyperbolic metric leads to the coherent states of the affine group. And with each group comes a set of quantum kinematical operators. Thus, one can say that in these three cases the choice of geometry augmenting the classical phase space manifold determines the quantum kinematical operators uniquely! Furthermore, the classical Hamiltonian that goes with the quantum Hamiltonian $\mathcal{H}$ is given by the lower symbol (other authors call this symbol the upper symbol, since it is involved in an upper bound in the Berezin–Lieb inequalities)

h, implicitly defined by the relation $\mathcal{H}=\int h(p,q)|pq\rangle\langle pq|d\mu(p,q)$. Here, $d\mu(p,q)$ is the left-invariant group measure of the group which defines the coherent states. This measure is normalized such that $h(p,q)\equiv 1$ leads to $\mathcal{H}=\mathbb{1}$, and, thus, provides the usual resolution of unity. Since the Stratonovich rule is used, and since the coherent states merely change labels under canonical (coordinate) transformations, apart from possible phase factors, the path integral $\langle p''q''|\times\exp\{-iT\mathcal{H}\}|p'q'\rangle=\lim_{\nu\to\infty}\int\exp\{-i\int[qdp+dG(p,q)+h(p,q)dt]\}\,d\mu_W^\nu$ is covariant under canonical (coordinate) transformations and the quantization is fully geometric in nature.[3,4] The foregoing has been extended to arbitrary geometries of the phase space.[6]

In an attempt to quantize gravity,[7,8] Klauder was led to consider affine rather than canonical commutation relations for the field operators (the spatial part of the metric and its partner field). In the simplest case of constant fields, the problem reduces to a toy model of just one degree of freedom, namely, the affine coherent states. To be more precise, it includes the affine coherent states, which fulfill a fiducial vector admissibility condition,[2,5,9] but also those states which violate it. These latter states do not resolve unity anymore and, therefore, are called weak coherent states. The Affine Quantum Gravity Program has provided the motivation to raise the question of the existence of path integrals for these weak coherent states.

It is clear that a path integral cannot be constructed with weak coherent states in the standard way, since the resolution of unity is the key to the time-slicing approximation. However, the extension of the well-defined path integral with Wiener measure introduced above to the situation of weak coherent states could still be possible, and this is the goal of the present article. Two different methods to extend the Wiener measure path integral will be introduced: the first is based on the spectral decomposition of certain operators and will therefore be called the ''spectral approach.'' Unfortunately, it is limited to one very special case. The second uses an extra regularization parameter and is consequently called the ''regularizing approach.'' In both cases, the path integral for zero Hamiltonian is studied first, while the dynamics is introduced as a second step.

II. WEAK COHERENT STATE PATH INTEGRALS

A. General definitions

Coherent states are defined by two properties:[10]

(1) *Continuity:* The states $|l\rangle$ are a strongly continuous vector-valued function of the label l.
(2) *Resolution of unity:* There exists a positive measure δl on the label space $\mathfrak{L}$ such that the identity operator $\mathbb{1}$ on $\mathfrak{H}$ can, upon integration over $\mathfrak{L}$, be represented as

$$\mathbb{1}=\int|l\rangle\langle l|\,\delta l.$$

A more general class of states can be obtained by relaxing the second property:
(2′) *Completeness:* The family of vectors $(|l\rangle)$ is total, i.e., the closed linear span of $(|l\rangle)$ is the whole Hilbert space $\mathfrak{H}$.

States which share properties (1) and (2′) have been named Klauder states.[11] They are the disjoint union of the coherent states in the sense above and the weak coherent states, which do not possess a resolution of unity.

B. Affine weak coherent states

The affine group $(M_+,\circ)$ is the set $M_+:=\mathbb{R}^+\times\mathbb{R}$ with the group law $(q,p)\circ(q',p')=(qq',p+q^{-1}p')$ and has two nontrivial, inequivalent, irreducible, unitary representations[2] $U_\pm(p,q)=e^{\pm ipQ}e^{-i\ln qD}$, where the generators $Q>0$ and D obey the affine commutation relation $[Q,D]=iQ$. The uncertainty product of the irreducible, self-adjoint operators Q and D is $\Delta Q\Delta D\geqslant\frac{1}{2}\langle Q\rangle$. Setting $\langle Q\rangle=1$ leads to a one-parameter family of minimum uncertainty states given in x-representation by[5] $\eta_\beta(x)=N_\beta x^{\beta-1/2}e^{-\beta x}$ with normalization $N_\beta=(2\beta)^\beta\Gamma^{-1/2}(2\beta)$. The affine coherent states are defined as $|pq\rangle:=U_+(p,q)|\eta_\beta\rangle$. The group acts on admissible

fiducial vectors, which fulfill[2,5,9] $\langle Q^{-1}\rangle = \int_0^\infty x^{-1} |\eta_\beta(x)|^2 dx < \infty$. Namely, these are the states with $\beta > 1/2$. Weak coherent states, on the other hand, are generated by the same group action on fiducial vectors with $0 < \beta \leqslant 1/2$. For the whole parameter range $0 < \beta$, the overlap reads

$$\langle pq|rs\rangle = (qs)^{-\beta} 2^{2\beta} [(q^{-1}+s^{-1}) + i\beta^{-1}(p-r)]^{-2\beta}.$$

The construction of the affine coherent state path integral with Wiener measure[2] is based on a linear complex polarization condition. For the minimum uncertainty fiducial vectors, $(Q - 1 + i\beta^{-1}D)|\eta_\beta\rangle = 0$ holds. Hence, all functions $\psi(p,q) := \langle pq|\psi\rangle$ are annihilated by the operator $B = -iq^{-1}\partial_p + 1 + \beta^{-1} q \partial_q$. The same is true for the second-order differential operator

$$A := \tfrac{1}{2}\beta B^\dagger B = \tfrac{1}{2}\{-\beta^{-1}\partial_q q^2 \partial_q - \beta q^{-2}\partial_p^2 - 1 + \beta - 2i\beta q^{-1}\partial_p\}$$

which is a non-negative, self-adjoint operator with spectrum

$$\mathrm{spec}(A) = \{(\beta - \tfrac{1}{2})^2 - (\beta - \tfrac{1}{2} - n)^2; n \in \mathbb{N}, n < \beta - \tfrac{1}{2}\} \cup [(\beta - \tfrac{1}{2})^2, \infty).$$

For $\beta > 1/2$, the operator A has a discrete eigenvalue 0 and it follows, for $T > 0$, that $\lim_{\nu\to\infty}[e^{-\nu TA}]\delta(p-p')\delta(q-q')|_{p=p'',q=q''} = [P_0](p'',q'';p',q')$, where the expression on the right-hand side is the kernel of the projection operator onto the ground state. But this kernel is also given by $(2\pi)^{-1}(1 - (1/2\beta))\langle p''q''|p'q'\rangle$. This is the key part of the construction, since the rest follows by the Feynman–Kac–Stratonovich representation of the kernel of $e^{-\nu TA}$, which is $\mathcal{N}_\nu \int e^{-i\int q\dot{p}dt - (1/2\nu)\int[\beta^{-1}q^2\dot{p}^2 + \beta q^{-2}\dot{q}^2]dt}\mathcal{D}p\mathcal{D}q$. As stated in the Introduction, this formal expression makes sense as a Wiener measure path integral, and so finally

$$\langle p''q''|p'q'\rangle = \lim_{\nu\to\infty} 2\pi\left(1 - \frac{1}{2\beta}\right)^{-1} e^{\nu T/2} \int e^{-i\int q\, dp}\, d\mu_W^\nu(p,q),$$

which is a well-defined expression. (The path integral for a nonzero Hamiltonian is constructed in much the same way. The only difference is that νA must be replaced by an operator involving the Hamiltonian h, namely $\nu A + ih$.)

For $0 < \beta \leqslant 1/2$, i.e., in the weak coherent state case, the operator A has only a continuous spectrum, and the limit of diverging diffusion constant of the operator $e^{-\nu TA}$ is zero. Thus, the whole construction outlined above breaks down. To prevent this collapse to a trivial result, two different approaches will be discussed.

C. Spectral approach

The idea in this approach is to determine a ν-dependent rescaling factor, such that the limit of diverging diffusion constant will be nontrivial. This was proposed by Klauder.[5]

1. The general case

Let X be a non-negative self-adjoint operator on a certain Hilbert space and assume zero is in its continuous, but not in its discrete, spectrum. The operator X generates a semigroup $e^{-\nu TX}$, which has a spectral representation $e^{-\nu XT} = \int_0^\infty e^{-\nu\lambda T} d\mathbb{E}(\lambda)$ or $\langle x''|e^{-\nu TX}|x'\rangle = \int_0^\infty e^{-\nu\lambda T} d\langle x''|\mathbb{E}(\lambda)|x'\rangle$.

Since only well-behaved potentials will eventually be of interest, the reasonable assumption is made that the measure $d\langle x''|\mathbb{E}(\lambda)|x'\rangle$ has an absolutely continuous, but no singularly continuous part. Then the spectral family can be written as a (weighted) integral over one-dimensional projection operators $\mathbb{E}(\lambda) = \int_{-\infty}^{\lambda} |E\rangle\langle E|\rho(E)dE$. [For a singularly continuous measure this would not be possible: $\mu_{\mathrm{sc}}(x) = \int_{-\infty}^{x} d\mu_{\mathrm{sc}}(y) \neq \int_{-\infty}^{x} (d\mu_{\mathrm{sc}}/dy)dy = 0$ since $d\mu_{\mathrm{sc}}/dy = 0$ almost everywhere.] If the generalized eigenstates $|E\rangle$ are δ-orthonormalized, then $\rho(E) = 1$.

The matrix element of $e^{-\nu TX}$ can then be written as

$$\langle x''|e^{-\nu TX}|x'\rangle = \int_0^\infty e^{-\nu\lambda T}\psi_\lambda(x'')\psi_\lambda^*(x')\rho(\lambda)d\lambda \tag{1}$$

and the ψ_λ are continuous in λ. Moreover, ρ—being part of the measure—is at least right-continuous. For δ-orthonormalized wave functions, $\rho(\lambda)\equiv 1$.

The goal is to find the rescaling factor which saves Eq. (1) from becoming trivial in the limit of diverging diffusion constant ν. Since, for very large ν, the factor $e^{-\nu T\lambda}$ suppresses everything but the values for very small λ, the behavior of $f_{x',x''}(\lambda) := \psi_\lambda(x'')\psi_\lambda^*(x')\rho(\lambda)$ near $\lambda = 0$ is all that matters. To give an example, assume that $f_{x',x''}(\lambda) \propto \lambda^a$ for small λ. Now, the proper rescaling factor can be determined, and in the example it is

$$\int_0^\infty d\lambda\, \lambda^a e^{-\nu\lambda T} = \frac{\Gamma(a+1)}{(\nu T)^{a+1}}. \tag{2}$$

After rescaling with the inverse one gets $[(\nu T)^{a+1}/\Gamma(a+1)]\,\lambda^a e^{-\nu\lambda T} \overset{\nu\to\infty}{\longrightarrow} \delta(\lambda)$ which represents a δ-function weight on $\lambda = 0$.

The rescaling factor can be computed self-consistently, and the general formula reads

$$\frac{\int_0^\infty e^{-\nu\lambda T}\psi_\lambda(x'')\psi_\lambda^*(x')\rho(\lambda)d\lambda}{\int_0^\infty e^{-\nu\lambda T}\psi_\lambda(0)\psi_\lambda^*(0)\rho(\lambda)d\lambda} \overset{\nu\to\infty}{\rightharpoonup} \frac{\psi_0(x'')\psi_0^*(x')}{\psi_0(0)\psi_0^*(0)}. \tag{3}$$

The numerator of the last expression, $\psi_0(x'')\psi_0^*(x')$, is the kernel of the desired projection operator onto the ground state, and we have assumed that the denominator is nonzero. The convergence is in a distributional sense (denoted by the symbol $\rightharpoonup$). If the functional form of $\psi_0(x'')\psi_0^*(x')$ is known to be continuous, then the convergence is pointwise.

Observe, in the example with $f_{x',x''}(\lambda) = \lambda^a$, one must have $a > -1$, or else the rescaling factor would be identically zero (since the integral would be infinity). But, since the rescaling factor can be determined self-consistently, i.e., by the denominator of Eq. (3), which always exists, there is no hidden ''trap'' to look out for. Moreover, the evaluation of the denominator need not necessarily be at the point $x'' = x' = 0$. It could be at any point $x'' = x' = b$, $b \in \mathbb{R}$, or even $b = \pm\infty$, as long as the function $\psi_\lambda(x)$ is not 0 at b. Whatever gives the easiest result is the preferred choice. And the arbitrariness of this choice is not critical: Assume K to be the reproducing kernel of some reproducing kernel Hilbert space, and let a be a positive constant. Then, aK is just as good a reproducing kernel, since the same class of functions arises, only the inner product has to be redefined.

2. The affine case

The foregoing is now applied to the case of the affine weak coherent states. Unfortunately, A matches the required properties, namely that 0 be in the continuous spectrum, only in the case $\beta = 1/2$! This is true in spite of the fact that $A\langle pq|\psi\rangle = 0$ (for arbitrary $|\psi\rangle$), since an equation $A\psi = \alpha\psi$ need not necessarily imply $\alpha \in \mathrm{spec}(A)$. In fact, the $\psi(p,q) = \langle pq|\psi\rangle$ are not generalized eigenvectors except in the case $\beta = 1/2$.[11] Consequently, the isolating procedure can only be performed for $\beta = 1/2$, and the general theory above ensures the existence of the weak coherent state path integral.

For the case at hand a connection between the operator A and the one-dimensional Morse operator H_{Morse} exists[2] and makes the explicit functional form of the generalized eigenfunctions available. With the aid of these, the rescaling factor can be computed explicitly.

The problem to find the eigenfunctions of the operator A is first reduced to a problem on $L^2(\mathbb{R}^+)$ and then to a problem on $L^2(\mathbb{R})$, leading to the Morse operator,

$$
\begin{aligned}
A\langle U(p,q)\phi|\psi\rangle &= \langle A^* U(p,q)\phi|\psi\rangle \\
&= \tfrac{1}{2}\langle[-\beta^{-1}\partial_q q^2\partial_q - \beta q^{-2}\partial_p^2 - 2i\beta q^{-1}\partial_p + \beta - 1]e^{ipQ}e^{-i\ln qD}\phi|\psi\rangle \\
&= \tfrac{1}{2}\beta^{-1}\langle e^{ipQ}e^{-i\ln qD}\{D^2 + iD + \beta^2 Q^2 - 2\beta^2 Q + \beta^2 - \beta\}(Q^{1/2}\phi')|\psi\rangle \\
&= \tfrac{1}{2}\beta^{-1}\langle e^{ipQ}e^{-i\ln qD}Q^{1/2}\{D^2 + \beta^2 Q^2 - 2\beta^2 Q + (\beta - 1/2)^2\}\phi'|\psi\rangle, \qquad (4)
\end{aligned}
$$

where $\phi = Q^{1/2}\phi'$.

Under the unitary transformation

$$
(\tilde{U}\psi)(x) = e^{x/2}\psi(e^x), \qquad (5)
$$

the operator in braces in the last line of Eq. (4) (called H in Ref. 2) is transformed to the Morse operator,

$$
H_{\text{Morse}} = -\frac{d^2}{dx^2} + \beta^2(e^{2x} - 2e^x) + \left(\beta - \frac{1}{2}\right)^2. \qquad (6)
$$

The eigenfunctions of the Morse operator can be found in Ref. 12, and, for $\beta = 1/2$, they are given in momentum representation (and δ-orthonormalized) by

$$
\psi_\lambda(x) = \left(\frac{\lambda \sinh(2\pi\lambda)}{\pi^2}\right)^{1/2}\Gamma(i\lambda)e^{-x/2}W_{1/2,i\lambda}(e^x), \qquad (7)
$$

where W is a Whittaker function. With a mass $m = 1/2$, one has the relation $E = \lambda^2$ for energy and momentum, and the δ-orthonormalized eigenfunctions in energy representation are

$$
\psi_E(x) = \left(\frac{\sinh(2\pi\sqrt{E})}{2\pi^2}\right)^{1/2}\Gamma(i\sqrt{E})e^{-x/2}W_{1/2,i\sqrt{E}}(e^x). \qquad (8)
$$

Since the Whittaker function $W_{1/2,0}(z) = e^{-z/2}z^{1/2}$, the x-dependence of $\psi_{E=0}(x)$ is $e^{-e^x/2}$. Thus, the rescaling factor can best be determined with the choice $x'' = x' = b = -\infty$ where this function is equal to one. For small E, the function $f_{-\infty,-\infty}(E) = \psi_E(-\infty)\psi_E^*(-\infty)\rho(E) \approx \pi^{-1}E^{-1/2}$ because $\sinh(2\pi\sqrt{E}) \approx 2\pi\sqrt{E}$, $|\Gamma(i\sqrt{E})|^2 \approx 1/E$. Inserting this E-dependence into the general formula ($\rho(E) = 1$ because of δ-orthonormalization), one finds the inverse rescaling factor

$$
\int_0^\infty e^{-\nu TE} f_{-\infty,-\infty}(E)\,dE = (\pi\nu T)^{-1/2}. \qquad (9)
$$

Because of the connection between the ''Morse''-level and the original problem [Eqs. (4) and (5)], this is already the proper rescaling factor for the original problem as well.

The sought-for weak coherent state path integral for $\beta = 1/2$ and vanishing Hamiltonian is thus

$$
\langle p''q''|p'q'\rangle = \lim_{\nu\to\infty} K_\nu \int e^{-i\int q\,dp}\,d\mu_W^\nu \qquad (10)
$$

with rescaling factor $K_\nu = (\pi\nu T)^{1/2}$.

D. Introducing dynamics

Since the only case in which the spectral approach worked was $\beta = 1/2$, this value is assumed throughout the remainder of this subsection. Dynamics are introduced by the quantum Hamiltonian $\mathcal{H}$, which is a function of the basic kinematical operators Q and D. The goal is to represent the propagator $\langle p''q''|\exp\{-iT\mathcal{H}\}|p'q'\rangle$ as a (weak coherent state) path integral. The expression

$$\langle p''q''|e^{-iT\mathcal{H}}|p'q'\rangle = \lim_{\nu\to\infty} K_\nu \mathcal{N}_\nu \int e^{-i\int[q\dot{p}+h_w(p,q)]dt} e^{-(1/2\nu)\int[\beta^{-1}q^2\dot{p}^2+\beta q^{-2}\dot{q}^2]dt} \mathcal{D}p\mathcal{D}q$$

$$= \lim_{\nu\to\infty} K_\nu \int e^{-i\int[q\,dp+h_w(p,q)dt]}\, d\mu_W^\nu \tag{11}$$

was proposed[5] as the path integral for a class of Hamiltonians which contains at least all Hamiltonians polynomial in Q and D. The new symbol $h_w(p,q)$, interpreted as the classical Hamiltonian associated with the quantum Hamiltonian, is implicitly given by

$$\langle p''q''|\mathcal{H}|p'q'\rangle = \lim_{\nu\to\infty} K_\nu \int e^{-i\int q\,dp}\left[T^{-1}\int h_w(p,q)dt\right] d\mu_W^\nu \tag{12}$$

and will be called the weak symbol.

The whole conjecture is based on the observation that, for a linear Hamiltonian $RQ+SD$, the propagator can be reduced to a mere overlap:[5,11]

$$\langle p''q''|e^{-i(RQ+SD)T}|p'q'\rangle = \langle p''e^{ST}+R/S\cdot(e^{ST}-1), q''e^{-ST}|p'q'\rangle. \tag{13}$$

Consequently, the problem is already solved for a linear Hamiltonian, and what remains is to determine the weak symbol associated with $\mathcal{H}=RQ+SD$. According to Eq. (10) the path integral for this Hamiltonian is

$$\lim_{\nu\to\infty} K_\nu \int_{p',q'}^{p''e^{ST}+R/S\cdot(e^{ST}-1), q''e^{-ST}} e^{-i\int q\,dp}\, d\mu_W^\nu. \tag{14}$$

Since this is a well-defined functional integral, one can change integration variables

$$p(t)\to p(t)e^{St}+R/S(e^{St}-1),$$

$$q(t)\to q(t)e^{-St},$$

and obtain $\exp\{-i\int(qe^{-St}d[pe^{St}+R/S(e^{St}-1)]\}=\exp\{-i\int[q\,dp+(Rq+Spq)dt]\}$ as the new integrand. The new measure is [$(\cdots)^{\cdot}$ means the time derivative of the expression in parentheses]

$$d\tilde{\mu}_W^\nu = \mathcal{N}_\nu \exp\left\{-\frac{1}{2\nu}\int\left[\beta^{-1}(qe^{-St})^2\left(pe^{St}+\frac{R}{S}(e^{St}-1)\right)^{\cdot 2}+\beta(qe^{-St})^{-2}(qe^{-St})^{\cdot 2}\right]dt\right\}$$
$$\times\mathcal{D}\left[pe^{St}+\frac{R}{S}(e^{St}-1)\right]\mathcal{D}(qe^{-St}).$$

But, since the measure is actually

$$\mathcal{D}\left[pe^{St}+\frac{R}{S}(e^{St}-1)\right] = \lim_{\epsilon\to 0}\prod_{k=1}^{N} d\left[p(t)e^{St}|_{t=k\epsilon}+\frac{R}{S}(e^{St}-1)|_{t=k\epsilon}\right]$$

$$= \lim_{\epsilon\to 0}\prod_{k=1}^{N}\left[dp(t)e^{St}|_{t=k\epsilon}+(pSe^{St}+\mathrm{Re}^{St})dt|_{t=k\epsilon}\right]$$

$$= \lim_{\epsilon\to 0}\prod_{k=1}^{N}\left[dp_k e^{Sk\epsilon}+(p_k Se^{Sk\epsilon}+\mathrm{Re}^{Sk\epsilon})\epsilon\right] = \lim_{\epsilon\to 0}\prod_{k=1}^{N} dp_k e^{Sk\epsilon} = \mathcal{D}p\prod_t e^{St},$$

and analogous $\mathcal{D}(qe^{-St})=\mathcal{D}q\Pi_t e^{-St}$, the new measure can be expressed in terms of the old one as

$$d\tilde{\mu}_W^\nu = e^{-(1/2\nu)\int[\beta^{-1}q^2((Sp+R)^2+2(Sp+R)\dot{p})+\beta q^{-2}(S^2q^2-2Sq\dot{q})]dt}\, d\mu_W^\nu$$
$$= e^{-(1/2\nu)\int[\beta^{-1}q^2((Sp+R)^2dt+2(Sp+R)dp)+\beta q^{-2}(S^2q^2dt-2Sqdq)]}\, d\mu_W^\nu.$$

The first equality is again formal and gains meaning by the second line, where the stochastic integrals are understood in the Stratonovich sense, as usual. The change of variables has introduced additional terms in the exponent of the formal expression, which are at most linear in $\dot{p}$ or $\dot{q}$, respectively. These terms are not critical since, in the limit of diverging diffusion constant ν, they will vanish. This means that the total change of the measure disappears in the limit. Thus, one can write the path integral with the old measure $d\mu_W^\nu$ instead of with the new $d\tilde{\mu}_W^\nu$:

$$\langle p''q''|e^{-i(RQ+SD)T}|p'q'\rangle = \lim_{\nu\to\infty} K_\nu \int_{p',q'}^{p'',q''} e^{-i\int[q\,dp+(Rq+Spq)dt]}\, d\mu_W^\nu. \tag{15}$$

Now, the weak symbol can be read off:

$$h_w(p,q)=Rq+Spq. \tag{16}$$

The generalization to other Hamiltonians is based on the linearity, completeness, and irreducibility of the basic operators Q and D by virtue of which $\lim_{J\to\infty}\Sigma_{j=1}^J \alpha_j e^{-i(R_jQ+S_jD)}$ weakly converges to any (bounded) operator such as $e^{-i\mathcal{H}T}$. Thus,

$$\langle p''q''|e^{-i\mathcal{H}T}|p'q'\rangle = \lim_{J\to\infty}\langle p''q''|\sum_{j=1}^J \alpha_j e^{-i(R_jQ+S_jD)}|p'q'\rangle$$
$$= \lim_{J\to\infty}\lim_{\nu\to\infty} K_\nu \int e^{-i\int q\,dp}\left[\sum_{j=1}^J \alpha_j e^{-i\int(R_jq+S_jpq)dt}\right] d\mu_W^\nu \tag{17}$$

and the question, on which the next steps depend, is: Can the two limits be interchanged? In spite of some effort this question is not yet answered. Assuming that they can, however, one obtains

$$\langle p''q''|e^{-i\mathcal{H}T}|p'q'\rangle = \lim_{\nu\to\infty} K_\nu \int e^{-i\int q\,dp}\left[\lim_{J\to\infty}\sum_{j=1}^J \alpha_j e^{-i\int(R_jq+S_jpq)dt}\right] d\mu_W^\nu. \tag{18}$$

The expression $[\lim_{J\to\infty}\Sigma_{j=1}^J \alpha_j e^{-i\int(R_jq+S_jpq)dt}]=:F[\int qdt,\int pqdt]$ is, unfortunately, not of the form $e^{-i\int h_w(p,q)dt}$ for a general, local Hamiltonian h_w, e.g., $e^{-i\int q^2dt}$ with Hamiltonian q^2. To produce local Hamiltonians, one would need distributions $R(t)$ and $S(t)$ instead of the constants R and S. Then, taking, e.g., $R(t)=\delta(t-\tau)$, one gets a local expression $q(\tau)$ and, by forming functions thereof, local Hamiltonians. This was proposed in Ref. 5. However, the construction of distributions from piecewise constant functions would require yet another limiting process, and, again, the interchangeability of the limits is questionable.

In the case of a linear Hamiltonian, the weak symbol was shown to be $h_w(p,q)=Rq+Spq$. This is exactly what one would expect since the connection of the basic operators Q and D to classical variables is, according to the weak correspondence principle, q and pq, respectively. But, the correspondence for a more general Hamiltonian is not immediately clear and remains to be determined.

E. Regularizing approach

The idea for this second approach is the introduction of an additional regularization factor which will reintroduce a discrete ground state with eigenvalue zero. Then, the construction of the path integral moves along the same lines as in the coherent state case ($\beta>1/2$). The limit to remove the regularization is taken as the last step.

For large q, the overlap $\langle pq|p'q'\rangle$ is proportional to $q^{-\beta}$. Because $0<\beta\leqslant 1/2$, a regularization factor which is effective at infinity is required to produce Hilbert space vectors again. Since, for $0<\beta\leqslant 1/4$, $\int_{-\infty}^{\infty}(c^2+p^2)^{-2\beta}dp=\infty$ (where c is a constant), one must in this case regularize in p, too. For $1<4\beta<2$ this is not required. A regularization in p will make a regularization in q (for small q) necessary as well.[11]

Case 1/4<β⩽1/2: Let

$$\langle pq|rs\rangle_\varepsilon := N_\varepsilon \langle pq|rs\rangle e^{-(q+s)\varepsilon} \tag{19}$$

be a normalized vector in $L^2(M_+)$ with normalization constant N_ε. The extra factor $e^{-(q+s)\varepsilon}$ goes to one in the limit $\varepsilon\to 0$. For arbitrary $x\in\mathbb{R}$, $y\in\mathbb{R}^+$, the overlap $\langle xy|xy\rangle_\varepsilon$ equals $N_\varepsilon e^{-2y\varepsilon}$. Hence, one can write $\langle pq|rs\rangle=\lim_{\varepsilon\to 0}\langle xy|xy\rangle_\varepsilon^{-1}\langle pq|rs\rangle_\varepsilon$ in a self-consistent way without explicitly referring to the normalization constant. The following notation is used:

$$\langle xy|xy\rangle_\varepsilon =: c_{\beta,\varepsilon}\,.$$

The new operator B_ε, which annihilates the modified kernel, is derived by exploiting analyticity: $[(q^{-1}+s^{-1})+i\beta^{-1}(p-r)]^{-2\beta}=:Y$ is analytic, so $\partial_{(q^{-1}-i\beta^{-1}p)}Y=\frac{1}{2}(-q^2\partial_q+i\beta\partial_p)Y=0$. Write Y as $e^{(q+s)\varepsilon}(qs)^\beta\langle pq|rs\rangle_\varepsilon$, and move $e^{q\varepsilon}(qs)^\beta$ to the left of this operator. Then, $e^{q\varepsilon}(qs)^\beta$ can be canceled since the expression is everywhere nonzero. The result is the new operator

$$B_\varepsilon=(\beta^{-1}q\partial_q+\beta^{-1}q\varepsilon+1-iq^{-1}\partial_p)$$

for which $B_\varepsilon\langle pq|rs\rangle_\varepsilon=0$. Define $A_\varepsilon:=\frac{1}{2}\beta B_\varepsilon^\dagger B_\varepsilon$, then

$$\begin{aligned}A_\varepsilon&=\tfrac{1}{2}\beta(-iq^{-1}\partial_p+1-\beta^{-1}\partial_q q+\beta^{-1}q\varepsilon)(-iq^{-1}\partial_p+1+\beta^{-1}q\partial_q+\beta^{-1}q\varepsilon)\\&=\tfrac{1}{2}\{\beta[-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon]^2-\beta^{-1}\partial_q q^2\partial_q-1-2\beta^{-1}q\varepsilon\}.\end{aligned} \tag{20}$$

A_ε can be shown to be essentially self-adjoint since the deficiency index equation $[(A_\varepsilon^\dagger\pm i)\psi](p,q)=0$ has no solution.[11] In a slight abuse of notation the closure of this operator will be denoted by A_ε as well. It is a self-adjoint, non-negative operator with zero in its discrete spectrum.

The Feynman–Kac–Stratonovich representation of the kernel of the operator $e^{-\nu TA_\varepsilon}$ is (see Appendix for the derivation)

$$e^{-\nu A_\varepsilon T}\delta(p-p')\,\delta(q-q')|_{p=p'',q=q''}=e^{\nu T/2}\int e^{-i\int(q+\beta^{-1}q^2\varepsilon)dp+\nu\int\beta^{-1}q\varepsilon dt}\,d\mu_W^\nu$$

and it follows that

$$\langle p''q''|p'q'\rangle=\lim_{\varepsilon\to 0}c_{\beta,\varepsilon}^{-1}\langle p''q''|p'q'\rangle_\varepsilon=\lim_{\varepsilon\to 0}\lim_{\nu\to\infty}c_{\beta,\varepsilon}^{-1}e^{\nu T/2}\int e^{-i\int(q+\beta^{-1}q^2\varepsilon)dp+\nu\int\beta^{-1}q\varepsilon dt}\,d\mu_W^\nu. \tag{21}$$

The stochastic processes involved are still Brownian bridges, and, when the stochastic integrals are interpreted in the Stratonovich sense, canonical (coordinate) transformations can be made in the same way as before. Thus, the geometric nature of the quantization is preserved.

Case $0<\beta\leqslant 1/4$: For a parameter $\beta\leqslant 1/4$, a regularization for large q is not enough. It turns out that an additional p-regularization will even make a regularization for small q necessary (otherwise the overlap would be square integrable, but not in the domain of A_ε).

In the present case, let

$$\langle pq|rs\rangle_\varepsilon := N_\varepsilon \langle pq|rs\rangle e^{-(q+s)\varepsilon-(q^{-1}+s^{-1})\varepsilon-(p^2+r^2)\varepsilon}, \tag{22}$$

where $\langle pq|rs\rangle=(qs)^{-\beta}2^{2\beta}[(q^{-1}+s^{-1})+i\beta^{-1}(p-r)]^{-2\beta}$ is the (weak coherent state) overlap which is analytic in the complex variable $z:=q^{-1}+i\beta^{-1}p$, apart from the factor $(qs)^{-\beta}$. One can write the analytic part (previously called Y) as $e^{(q+s)\varepsilon+(q^{-1}+s^{-1})\varepsilon+(p^2+q^2)\varepsilon}(qs)^{\beta}\langle pq|rs\rangle_\varepsilon$, and let the differential operator $\partial_{q^{-1}-i\beta^{-1}p}=\frac{1}{2}(-q^2\partial_q+i\beta\partial_p)$ act on this expression. Using $\partial_{z^*}f=0$ (valid for an analytic function), this results in the new operator

$$B_\varepsilon=\beta^{-1}q\partial_q+1+\beta^{-1}q\varepsilon+\beta^{-1}q^{-1}\varepsilon-2ipq^{-1}\varepsilon-iq^{-1}\partial_p$$

for which $B_\varepsilon\langle pq|rs\rangle_\varepsilon=0$. As before, define $A_\varepsilon:=\frac{1}{2}\beta B_\varepsilon^\dagger B_\varepsilon$, then

$$\begin{aligned}A_\varepsilon=\tfrac{1}{2}\{&\beta(-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon\beta^{-1}q^{-1}\varepsilon)^2-2\beta q^{-2}\varepsilon+4ip\partial_q\varepsilon\\&+4\beta p^2q^{-2}\varepsilon^2-\beta^{-1}\partial_q q^2\partial_q-1-2\beta^{-1}q\varepsilon\}.\end{aligned} \tag{23}$$

Instead of trying to solve the deficiency index equation for the "new" A_ε, one can avoid the question about self-adjointness altogether.

Assume A_ε is not self-adjoint. The (sesquilinear) form $s_\varepsilon(x,y):=\langle x|A_\varepsilon y\rangle$ generated by A_ε is closable since A_ε is symmetric and bounded below.[13] There is a bijection between the set of all (densely defined) closed, below-bounded forms and the set of all self-adjoint, below-bounded operators. Let $\overline{s_\varepsilon}$ be the closure of the form generated by A_ε and $A_{\overline{s_\varepsilon}}$ be the self-adjoint operator associated with $\overline{s_\varepsilon}$. Then, $A_{\overline{s_\varepsilon}}$ preserves the lower bound and is called the Friedrichs' extension of the operator A_ε. [It is the unique extension fulfilling $D(A_{\overline{s_\varepsilon}})\subset D(\overline{s_\varepsilon})$.[13]]

In a slight abuse of notation $A_{\overline{s_\varepsilon}}$ will be written as A_ε. So from now on, A_ε denotes the Friedrichs' extension (which is trivial in the case that A_ε is already self-adjoint). Then it is clear that A_ε is non-negative.

The Feynman–Kac–Stratonovich representation of the kernel of the operator $\exp\{-\nu TA_\varepsilon\}$ is derived in much the same way as before (see Appendix)

$$e^{\nu T/2}e^{-i\beta^{-1}\varepsilon(p''-p')}\int e^{-i\int[(q+\beta^{-1}q^2\varepsilon)\,dp-2\beta pq^{-2}\varepsilon\,dq]+\nu\int[\beta q^{-2}\varepsilon+\beta^{-1}q\varepsilon]dt}\,d\mu_W^\nu.$$

Partial integration, i.e., $2\beta\varepsilon\int pq^{-2}dq=-2\beta\varepsilon\int pd(q^{-1})=-2\beta\varepsilon pq^{-1}\big|_{(p',q')}^{(p'',q'')}+2\beta\varepsilon\int q^{-1}dp$, leads to

$$e^{\nu T/2}e^{-i\beta^{-1}\varepsilon(p''-p')-2i\beta\varepsilon(p''q''^{-1}-p'q'^{-1})}\int e^{-i\int(q+\beta^{-1}q^2\varepsilon-2\beta q^{-1}\varepsilon)dp+\nu\int[\beta q^{-2}\varepsilon+\beta^{-1}q\varepsilon]dt}\,d\mu_W^\nu. \tag{24}$$

The phase factors in Eq. (24) are ν-independent, so they come outside of the ν-limit, where the ε-limit renders them unity. Finally, one gets

$$\begin{aligned}\langle p''q''|p'q'\rangle&=\lim_{\varepsilon\to 0}\lim_{\nu\to\infty}c_{\beta,\varepsilon}^{-1}\langle p''q''|p'q'\rangle_\varepsilon\\&:=\lim_{\varepsilon\to 0}\lim_{\nu\to\infty}c_{\beta,\varepsilon}^{-1}e^{\nu T/2}\int e^{-i\int(q+\beta^{-1}q^2\varepsilon-2\beta q^{-1}\varepsilon)dp+\nu\int[\beta q^{-2}\varepsilon+\beta^{-1}q\varepsilon]dt}\,d\mu_W^\nu.\end{aligned} \tag{25}$$

This is the path integral representation for $0<\beta\leqslant 1/4$.

F. Introducing dynamics

Dynamics is introduced in the same way as for the spectral approach. For a linear Hamiltonian $\mathcal{H}=RQ+SD$, the problem is already solved as it reduces to an overlap with modified ending points. What remains to do is to write down the path integral. This is straightforward since everything stated previously concerning the measure, etc., remains valid and the formula for $1/4<\beta\leqslant 1/2$ is

$$\begin{aligned}\langle p''q''|e^{-i(RQ+SD)T}|p'q'\rangle &= \left\langle p''e^{ST}+\frac{R}{S}(e^{ST}-1), q''e^{-ST}\middle| p'q'\right\rangle \\ &= \lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p''e^{ST}+(R/S)(e^{ST}-1),q''e^{-ST}} \\ &\quad\times\exp\left\{-i\int (q+\beta^{-1}q^2\varepsilon)dp+\nu\int \beta^{-1}q\varepsilon dt\right\} d\mu_W^\nu, \\ &= \lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p'',q''} \exp\left\{-i\int (qe^{-St}+\beta^{-1}q^2e^{-2St}\varepsilon)\right. \\ &\quad\left.\times d\left[pe^{St}+\frac{R}{S}(e^{St}-1)\right]+\nu\int \beta^{-1}qe^{-St}\varepsilon dt\right\} d\mu_W^\nu \\ &= \lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p'',q''} \exp\left\{-i\left[\int (q+\beta^{-1}q^2e^{-St}\varepsilon)dp\right.\right. \\ &\quad\left.+\int (q+\beta^{-1}q^2e^{-St}\varepsilon)(Sp+R)dt\right] \\ &\quad\left.+\nu\int \beta^{-1}qe^{-St}\varepsilon dt\right\} d\mu_W^\nu. \end{aligned} \tag{26}$$

Introducing the new variable $q_\varepsilon := q+\beta^{-1}q^2e^{-St}\varepsilon$, and the new measure $d\mu_W^{\nu,\varepsilon} := \exp\{\nu\int\beta^{-1}qe^{-St}\varepsilon dt\}\, d\mu_W^\nu$, the complexity of the final expression can be hidden. The new measure is equivalent to the old Wiener measure because the factor $\exp\{\nu\int\beta^{-1}qe^{-St}\varepsilon dt\}$ serves as a Radon–Nykodym derivative. Then, the formula resembles the path integral for coherent states and reads

$$\lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p'',q''} e^{-i[\int q_\varepsilon dp+(Spq_\varepsilon+Rq_\varepsilon)dt]}\, d\mu_W^{\nu,\varepsilon}. \tag{27}$$

The ε-modified Hamiltonian is given by the weak modified symbol $h_{w,\varepsilon} := Rq_\varepsilon+Spq_\varepsilon$.

The same procedure for $0<\beta\leqslant 1/4$ leads to

$$\begin{aligned}\langle p''q''|e^{-i(RQ+SD)T}|p'q'\rangle &= \lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p'',q''} \exp\left\{-i\left[\int (q+\beta^{-1}q^2e^{-St}\varepsilon\right.\right. \\ &\quad\left.-2\beta q^{-1}e^{2St}\varepsilon)dp+\int (q+\beta^{-1}q^2e^{-St}\varepsilon-2\beta q^{-1}e^{2St}\varepsilon)(Sp+R)dt\right] \\ &\quad\left.+\nu\int (\beta^{-1}qe^{-St}\varepsilon+\beta q^{-2}e^{2St}\varepsilon)dt\right\} d\mu_W^\nu \\ &= \lim_{\varepsilon\to 0}\lim_{\nu\to\infty} c_{\beta,\varepsilon}^{-1} e^{\nu T/2}\int_{p',q'}^{p'',q''} \exp\left\{-i\left[\int \tilde{q}_\varepsilon dp+\int (Sp\tilde{q}_\varepsilon\right.\right. \\ &\quad\left.\left.+R\tilde{q}_\varepsilon)dt\right]\right\} d\tilde{\mu}_W^{\nu,\varepsilon}. \end{aligned} \tag{28}$$

Here, the variable $\tilde{q}_\varepsilon := (q+\beta^{-1}q^2e^{-St}\varepsilon - 2\beta q^{-1}e^{2St}\varepsilon)$ and the Radon–Nykodym measure $d\tilde{\mu}_W^{\nu,\varepsilon} := \exp\{\nu\int(\beta^{-1}qe^{-St}\varepsilon+\beta q^{-2}e^{2St}\varepsilon)dt\}\, d\mu_W^\nu$ were used. The weak modified symbol is now $h_{w,\varepsilon} = R\tilde{q}_\varepsilon + Sp\tilde{q}_\varepsilon$.

The problem of how this can be extended to, say, all polynomial Hamiltonians was already discussed in the spectral approach. Here, on the other hand, there could be a second possibility to proceed. With the discrete ground state artifically reintroduced, it seems possible to construct the path integral in essentially the same way as for zero Hamiltonian. The operator νA_ε has to be replaced by $\nu A_\varepsilon + ih_{w,\varepsilon}$, and the conditions required for the construction will imply restrictions for the functions $h_{w,\varepsilon}$ (see Ref. 2 for a guideline to the proof). Observe, that this weak modified symbol does not necessarily have to be the same as the one mentioned in the previous parts of the subsection.

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APPENDIX: FEYNMAN–KAC–STRATONOVICH REPRESENTATION OF THE OPERATOR A_ε

The case $1/4 < \beta \leqslant 1/2$

The Feynman–Kac–Stratonovich representation of the kernel of the operator $\exp\{-\nu TA_\varepsilon\}$ is derived in the following way:

$$
\begin{aligned}
&\exp\{-\nu TA_\varepsilon\}\delta(p-p')\delta(q-q')\big|_{p=p'',q=q''} \\
&\quad = \exp\{-\tfrac{1}{2}\nu T[\beta(-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon)^2-\beta^{-1}\partial_q q^2\partial_q-1-2\beta^{-1}q\varepsilon]\} \\
&\qquad \times \int e^{ix(p-p')-ik(q-q')}\frac{dxdk}{(2\pi)^2}\bigg|_{p=p'',q=q''} \\
&\quad = e^{\nu T/2}\lim_{N\to\infty}[\exp\{-\tfrac{1}{2}\nu\delta[\beta(-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon)^2-2\beta^{-1}q\varepsilon]\} \\
&\qquad \times \exp\{-\tfrac{1}{2}\nu\delta(-\beta^{-1}\partial_q q^2\partial_q)\}]^N \int e^{ix(p-p')-ik(q-q')}\frac{dxdk}{(2\pi)^2}\bigg|_{p=p'',q=q''} \\
&\quad = \lim_{N\to\infty} e^{\nu T/2}\int \exp\Big\{i\sum x_{l+1/2}(p_{l+1}-p_l)-ik_{l+1/2}(q_{l+1}-q_l)\Big\} \\
&\qquad \times \exp\Big\{-\frac{1}{2}\nu\delta\sum[\beta(q_l^{-1}x_{l+1/2}+1+\beta^{-1}q_l\varepsilon)^2-2\beta^{-1}q_l\varepsilon]\Big\} \\
&\qquad \times \exp\Big\{-\frac{1}{2}\nu\delta\sum\beta^{-1}k_{l+1/2}^2q_l^2\Big\}\prod_{l=0}^{N}\frac{dk_{l+1/2}dx_{l+1/2}}{(2\pi)^2}\prod_{l=1}^{N}dp_ldq_l \\
&\quad =: e^{\nu T/2}\mathcal{N}\int \exp\Big\{i\int(x\dot{p}-k\dot{q})dt\Big\} \\
&\qquad \times \exp\Big\{-\frac{1}{2}\nu\int\{\beta(q^{-1}x+1+\beta^{-1}q\varepsilon)^2-2\beta^{-1}q\varepsilon+\beta^{-1}k^2q^2\}dt\Big\}\mathcal{D}x\mathcal{D}k\mathcal{D}p\mathcal{D}q \\
&\quad = e^{\nu T/2}\mathcal{N}\int \exp\Big\{i\int[(x-q-\beta^{-1}q^2\varepsilon)\dot{p}-k\dot{q}]\Big\}
\end{aligned}
$$

$$\times\exp\left\{-\frac{1}{2}\nu\int(\beta q^{-2}x^2-2\beta^{-1}q\varepsilon+\beta^{-1}k^2q^2)dt\right\}\mathcal{D}x\mathcal{D}k\mathcal{D}p\mathcal{D}q$$

$$=e^{\nu T/2}\mathcal{N}\int\exp\left\{-i\int(q+\beta^{-1}q^2\varepsilon)\dot{p}dt\right\}\exp\left\{\frac{1}{2}\nu\int 2\beta^{-1}q\varepsilon dt\right\}$$

$$\times\exp\left\{-\frac{1}{2\nu}\int[\beta^{-1}q^2\dot{p}^2+\beta q^{-2}\dot{q}^2]dt\right\}\mathcal{D}p\mathcal{D}q$$

with $N=T/\delta$. The Lie–Trotter product formula was used to go from the second to the third equality. The indices $l+1/2$ and l serve to emphasize that the temporal lattice points must not coincide for x,p or q,k, respectively. (This would violate the Heisenberg uncertainty principle.) For the endpoints, the definitions $p_0:=p'$, $p_{N+1}:=p''$, $q_0:=q'$ and $q_{N+1}:=q''$ were made. Note that $\exp\{-\frac{1}{2}\nu\delta(-\beta^{-1}\partial_q q^2\partial_q)\}\exp\{-ik(q-q')\}\approx\exp\{-\frac{1}{2}\nu\delta\beta^{-1}k^2q^2\}\exp\{-ik(q-q')\}$ only to first order in δ, but that is good enough for the path integral. In the second to last line, x was substituted by $x-q-\beta^{-1}q^2\varepsilon$, and the x- and p-integrations were carried out.

The case $0<\beta\leqslant 1/4$

The Feynman–Kac–Stratonovich representation of the kernel of the operator $\exp\{-\nu TA_\varepsilon\}$ is derived in much the same way as before, and, with the same conventions for notation, it reads

$$\exp\{-\nu TA_\varepsilon\}\delta(p-p')\delta(q-q')\big|_{p=p'',q=q''}$$

$$=\exp\{-\nu T/2[\beta(-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon+\beta^{-1}q^{-1}\varepsilon)^2-2\beta q^{-2}\varepsilon+4ip\partial_q\varepsilon+4\beta p^2q^{-2}\varepsilon^2$$

$$-\beta^{-1}\partial_q q^2\partial_q-1-2\beta^{-1}q\varepsilon]\}\int\exp\{ix(p-p')-ik(q-q')\}\frac{dxdk}{(2\pi)^2}\bigg|_{p=p'',q=q''}$$

$$=e^{\nu T/2}\lim_{N\to\infty}[\exp\{-\nu\delta/2[\beta(-iq^{-1}\partial_p+1+\beta^{-1}q\varepsilon+\beta^{-1}q^{-1}\varepsilon)^2-2\beta q^{-2}\varepsilon-2\beta^{-1}q\varepsilon]\}$$

$$\times\exp\{-\nu\delta/2(-\beta^{-1}\partial_q q^2\partial_q)\}\exp\{-\nu\delta/2\cdot 4ip\partial_q\varepsilon\}\exp\{-\nu\delta/2\cdot 4\beta p^2q^{-2}\varepsilon^2\}]^N$$

$$\times\int\exp\{ix(p-p')-ik(q-q')\}\frac{dxdk}{(2\pi)^2}\bigg|_{p=p'',q=q''}$$

$$=\lim_{N\to\infty}e^{\nu T/2}\int\exp\left\{i\sum x_{l+1/2}(p_{l+1}-p_l)-ik_{l+1/2}(q_{l+1}-q_l)\right\}$$

$$\times\exp\left\{-\nu\delta/2\sum[\beta(q_l^{-1}x_{l+1/2}+1+\beta^{-1}q_l\varepsilon+\beta^{-1}q_l^{-1}\varepsilon)^2-2\beta q_l^{-2}\varepsilon-2\beta^{-1}q_l\varepsilon]\right\}$$

$$\times\exp\left\{-\nu\delta/2\sum\beta^{-1}k_{l+1/2}^2q_l^2\right\}\exp\left\{-\nu\delta/2\sum 4ip_l(-ik_{l+1/2})\varepsilon\right\}$$

$$\times\exp\left\{-\nu\delta/2\sum 4\beta p_l^2q_l^{-2}\varepsilon^2\right\}\prod_{l=0}^{N}\frac{dk_{l+1/2}dx_{l+1/2}}{(2\pi)^2}\prod_{l=1}^{N}dp_ldq_l$$

$$=:e^{\nu T/2}\mathcal{N}\int\exp\left\{i\int(x\dot{p}-k\dot{q})dt\right\}$$

$$\times\exp\left\{-\nu/2\int\{\beta(q^{-1}x+1+\beta^{-1}q\varepsilon+\beta^{-1}q^{-1}\varepsilon)^2-2\beta q^{-2}\varepsilon\right.$$

$$\left.-2\beta^{-1}q\varepsilon+\beta^{-1}k^2q^2+4pk\varepsilon+4\beta p^2q^{-2}\varepsilon^2\}dt\right\}\mathcal{D}x\mathcal{D}k\mathcal{D}p\mathcal{D}q$$

$$
\begin{aligned}
&= e^{\nu T/2}\mathcal{N}\int \exp\left\{ i\int [(x-q-\beta^{-1}q^2\varepsilon-\beta^{-1}\varepsilon)\dot{p}-k\dot{q}]dt\right\}\\
&\quad\times\exp\left\{-\nu/2\int (\beta q^{-2}x^2-2\beta q^{-2}\varepsilon-2\beta^{-1}q\varepsilon+\beta^{-1}k^2q^2+4pk\varepsilon\right.\\
&\quad\left.+4\beta p^2q^{-2}\varepsilon^2)dt\right\}\mathcal{D}x\mathcal{D}k\mathcal{D}p\mathcal{D}q\\
&= e^{\nu T/2}\mathcal{N}\int \exp\left\{-i\int (q+\beta^{-1}\varepsilon+\beta^{-1}q^2\varepsilon)\dot{p}dt+i\int 2\beta pq^{-2}\varepsilon\dot{q}dt\right\}\\
&\quad\times\exp\left\{\nu/2\int (2\beta^{-1}q\varepsilon+2\beta q^{-2}\varepsilon)dt\right\}\\
&\quad\times\exp\left\{-1/(2\nu)\int [\beta^{-1}q^2\dot{p}^2+\beta q^{-2}\dot{q}^2]dt\right\}\mathcal{D}p\mathcal{D}q.
\end{aligned}
$$

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Expansions about free-fermion models

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A simple technique for expanding the free energy of general six-vertex models about free-fermion points is introduced. This technique is used to verify a Coulomb gas prediction about the behavior of the leading singularity in the free energy of the staggered F-model at zero staggered field. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1626270]

I. DEFINITION OF THE STAGGERED F-MODEL

The staggered F-model is a special case of the six-vertex model. The six-vertex model can be defined as follows: place arrows on the edges of a square lattice so that there are two arrows pointing into each vertex. Six types of vertices can arise (hence the name of the model). These vertices are shown in Fig. 1. By giving each vertex type an (position-dependent) energy the model is defined. These models were first introduced to study (anti-)ferroelectric systems. Later it was shown that six-vertex models can be mapped to solid-on-solid models.[4] Only a few of these models can be solved exactly. These include the free-fermion models[5,14] and models that can be solved using the Bethe ansatz.[3,8–10,2] To define the staggered F-model, we divide the lattice into two sublattices A and B, such that the nearest neighbor of an A vertex is a B vertex. The vertex energies are chosen as indicated in Fig. 1. When the staggered field (s) vanishes the model reduces to the F-model, which has been solved by Lieb.[9] At zero staggered field the model is critical. In this case the groundstate is twofold degenerate consisting of vertices of type 5 on sublattice A and vertices of type 6 on sublattice B, or vice versa. For $\beta\epsilon>0$ a nonzero staggered field lifts this degeneracy, and forces the model into an ordered state.[13]

II. COULOMB GAS RESULTS

By assuming that the F-model renormalizes to the Gaussian model, it is possible to find the behavior of the staggered F-model in infinitesimal staggered fields.[11] It is found that the leading singularity in the free energy is

$$F_s(\beta\epsilon,\beta s)\approx(\beta s)^{2/(2-\pi/4j(\beta\epsilon))}, \tag{1}$$

where

$$j(\beta\epsilon)=\tfrac{1}{2}\arccos(1-\tfrac{1}{2}\exp(2\beta\epsilon)). \tag{2}$$

At the point $\beta\epsilon=\frac{1}{2}\ln(2-\sqrt{2})\approx-0.2674$ the exponent becomes infinite. Below this point a finite staggered field is necessary to force the model to an ordered state. In this case the transition to the ordered state happens via a Kosterlitz–Thouless (KT) transition. The existence of a line of KT transitions intersecting the point ($\beta\epsilon=\frac{1}{2}\ln(2-\sqrt{2})$, $\beta s=0$) has been verified by combining the results of transfer matrix studies with scaling arguments.[11]

In this article we will verify (1) by expanding around Baxter's exact solution on the line $\beta\epsilon=\frac{1}{2}\ln 2$.

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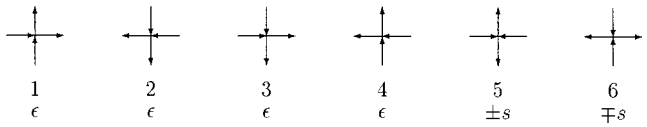

FIG. 1. The six vertices and their energies. The upper and lower signs respectively correspond to sublattices A and B.

III. BAXTER'S SOLUTION OF THE STAGGERED F-MODEL

Baxter has solved the staggered F-model at $\beta\epsilon=\frac{1}{2}\ln(2)$.[1] Later it was found that this solution could be generalized to other models if a certain condition involving the vertex weights is met. This condition is called the free-fermion condition because for eight-vertex models satisfying this condition the problem leads to a problem of noninteracting fermions in the S-matrix formulation. Let w_i be the vertex weight for a vertex of type i (see Fig. 1). Then the free-fermion condition for six-vertex models is

$$w_1w_2+w_3w_4-w_5w_6=0. \tag{3}$$

The weights w_i may be chosen inhomogeneous. We now proceed by presenting Baxter's solution of the staggered F-model.

Divide the lattice into two sublattices A and B. Choose the vertex energies as indicated in Fig. 1. Consider the ground state in which all A vertices are vertices of type 6, and all B vertices are of type 5. Any state can now be represented by drawing lines on the lattice where the arrows point oppositely to the ground state configuration. In terms of these lines the six vertices are represented by vertices with either no lines, two lines at right angles, or four lines. The energies of these vertices are respectively $-s$, ϵ and s. The next step is to replace the original lattice by a decorated lattice by replacing each original vertex by a "city" of four internally connected points (see Fig. 2).

The lines on the original lattice are regarded as dimers on the external edges of the decorated lattice. For any configuration on the original lattice, it is possible to place dimers on the internal edges of the decorated lattice, so that the lattice becomes completely covered. Now associate to each dimer a weight as indicated in Fig. 2. Demanding that the closed-packed dimer problem formulated on the decorated lattice is equivalent to our original problem yields

$$C=\exp(-\tfrac{1}{2}\beta s), \tag{4}$$

$$u=\tfrac{1}{2}\sqrt{2}\exp(\tfrac{1}{2}\beta s), \tag{5}$$

$$\beta\epsilon=\tfrac{1}{2}\ln(2). \tag{6}$$

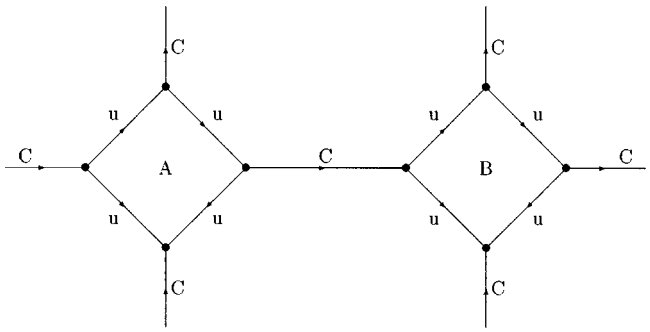

FIG. 2. The "cities" on the decorated lattice. A and B refer to the two sublattices. The meaning of the orientations on the edges is explained in the text.

To solve the close-packed dimer problem, we use the Pfaffian method.[6,7,12] This method expresses the partition function Z for a closed packed dimer model on an N by M planar lattice:

$$Z^2 = \det R. \tag{7}$$

Here R is an $N\times M$ by $N\times M$ antisymmetric matrix, defined as follows. Enumerate all the $N\times M$ vertices on the decorated lattice. If vertex i is not connected to vertex j via an edge, $R_{i,j}=0$, else $R_{i,j}=\pm$ fugacity of dimer at edge connecting i to j. The way the signs have to be chosen is explained in Ref. 7 These signs define an orientation of the edges. Positive $R_{i,j}$ is indicated by an arrow pointing from i to j.

To set up a perturbation theory about $\beta\epsilon=\frac{1}{2}\ln(2)$, we also need the inverse of R. Both the determinant and the inverse of R are easily calculated by performing a similarity transformation (see Ref. 1 for details). The determinant yields the following expression for the reduced free energy per vertex (i.e., the free energy times $-\beta$), denoted as F_{Baxter}, for an infinite by infinite lattice:

$$F_{\text{Baxter}} = \lim_{N,M\to\infty}\frac{1}{2NM}\ln\det R = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\ln[2\cosh(2\beta s)+2\cos(\theta_1)\cos(\theta_2)]d\theta_1 d\theta_2. \tag{8}$$

IV. PERTURBATION THEORY

We now proceed with the derivation of a perturbation theory about the free-fermion line of a six-vertex model. The Hamiltonian of a general six-vertex model can be defined as follows. One assigns an energy $e(p,i)$ to a vertex in state p (see Fig. 1) and position i. The configuration of the lattice can be specified by a function c which maps a position of a vertex to a number, 1,...,6, which is to be interpreted as the state of the vertex at that position. The reduced Hamiltonian (H) is defined to be the functional that assigns to each state c its energy times $-\beta$. We can thus write

$$H(c) = -\beta\sum_i e(c(i),i). \tag{9}$$

For H a Hamiltonian of a general six-vertex model and H_0 a Hamiltonian of a free-fermion model, a perturbation V can be defined so that we have

$$H = H_0 + V. \tag{10}$$

The partition function Z can be written as

$$Z = \sum_c \exp(H_0(c)+V(c)) = Z_0\langle\exp(V)\rangle. \tag{11}$$

Here Z_0 is the partition function of the free-fermion model. The reduced free energy can be expressed as

$$F = F_0 + \ln\langle\exp(V)\rangle = F_0 + \langle V\rangle + \tfrac{1}{2}\langle(V-\langle V\rangle)^2\rangle + \cdots. \tag{12}$$

Here F_0 is the reduced free energy of the free-fermion model. Now write $V=\Sigma_i V_i$ with $V_i(c(i))$ a perturbation of the vertex energy times $-\beta$ at position i. Equation (12) can be rewritten as

$$F = F_0 + \sum_i \langle V_i\rangle + \frac{1}{2}\sum_{ij}[\langle V_i V_j\rangle - \langle V_i\rangle\langle V_j\rangle] + \cdots. \tag{13}$$

To compute a free-fermion average $\langle V_{i_1}V_{i_2}\cdots V_{i_n}\rangle$, we can proceed as follows: Introduce a constraint in the free-fermion model by requiring the vertices at the positions $i_1\cdots i_n$ to be in the states $x_1\cdots x_n$. The partition function of this model is denoted by $Z_{i_1\cdots i_n}(x_1\cdots x_n)$. We can then write

$$\langle V_{i_1}V_{i_2}\cdots V_{i_n}\rangle=\sum_{x_1\cdots x_n}\frac{Z_{i_1\cdots i_n}(x_1\cdots x_n)V(x_1)\cdots V(x_n)}{Z_0}. \tag{14}$$

It now remains to calculate $Z_{i_1\cdots i_n}(x_1\cdots x_n)$. It is convenient to reformulate this problem as follows: Denote the state of an arrow located at the edge j by s_j. Put $s_j=1$ if the arrow points oppositely to the ground state configuration and $s_j=0$ otherwise. Define a constrained free-fermion model by requiring the arrow at the edge j_r to be in state s_{j_r} for $1\leqslant r\leqslant m$. We then want to evaluate the partition function of this model, which we denote as $Z^{\mathrm{cons}}(s_{j_1}\cdots s_{j_m})$. The idea is to perturb the weights of the dimers on the edges j_r infinitesimally. We redefine the weight of the dimer on the edge j_r by multiplying it by $(1+\epsilon_r)$. The partition function of the redefined free-fermion model $(Z(\epsilon_1\cdots\epsilon_m))$ can be written in terms of the constrained partition functions as

$$\begin{aligned}Z(\epsilon_1\cdots\epsilon_m)&=\sum_{\{s\}}Z^{\mathrm{cons}}(s_{j_1}\cdots s_{j_m})\prod_{k=1}^{m}(1+s_{j_k}\epsilon_k)\\&=Z_0+\sum_k Z^{\mathrm{cons}}(s_{j_k}=1)\epsilon_k+\sum_{k<l}Z^{\mathrm{cons}}(s_{j_k}=1,s_{j_l}=1)\epsilon_k\epsilon_l+\cdots.\end{aligned} \tag{15}$$

$Z(\epsilon_1\cdots\epsilon_m)$ can be calculated using (7), by making the necessary changes to R. We can write

$$R=R_0+\sum_{k=1}^{m}\epsilon_k R_{(k)}. \tag{16}$$

Here R_0 is the original unperturbed matrix; $R_{(k)}$ is defined as follows:

$$R_{(k),ij}=R_{0,ij}$$

if i and j are connected by j_k, and

$$R_{(k),ij}=0$$

if i and j are not connected by j_k.

Note that the $R_{(k)}$ have only two nonzero matrix elements. Inserting (16) in (7) and expanding gives

$$\begin{aligned}Z(\epsilon_1\cdots\epsilon_m)&=\sqrt{\det R}\\&=\sqrt{\det R_0}\exp\left(\frac{1}{2}\mathrm{Tr}\ln\left[1+\sum_k\epsilon_k R_0^{-1}R_{(k)}\right]\right)\\&=\sqrt{\det R_0}\left[1+\frac{1}{2}\sum_k\epsilon_k\mathrm{Tr}(R_0^{-1}R_{(k)})+\frac{1}{4}\sum_{k,l}\epsilon_k\epsilon_l\left[\frac{1}{2}\mathrm{Tr}(R_0^{-1}R_{(k)})\mathrm{Tr}(R_0^{-1}R_{(l)})\right.\right.\\&\quad\left.\left.-\mathrm{Tr}(R_0^{-1}R_{(k)}R_0^{-1}R_{(l)})\right]+\cdots\right].\end{aligned} \tag{17}$$

Using (17) and (15) we can directly read off the constrained partition functions if all the constrained arrows point oppositely to the ground state configuration. To calculate a general con-

strained partition function one can apply the principle of inclusion and exclusion, e.g., consider the evaluation of $Z(s_1,s_2,s_3,s_4,s_5)$, with $s_1=s_2=1$ and $s_3=s_4=s_5=0$. Put $t_3=t_4=t_5=1$. According to the principle of incusion and exclusion, we can write

$$Z(s_1,s_2,s_3,s_4,s_5)=Z(s_1,s_2)-[Z(s_1,s_2,t_3)+Z(s_1,s_2,t_4)+Z(s_1,s_2,t_5)]+Z(s_1,s_2,t_3,t_4)+Z(s_1,s_2,t_3,t_5)+Z(s_1,s_2,t_4,t_5)-Z(s_1,s_2,t_3,t_4,t_5). \tag{18}$$

V. FIRST ORDER COMPUTATION FOR THE STAGGERED F-MODEL

For the staggered F-model the expansion can be simplified. The vertex in the ground state at a particular point will be referred to as an a-vertex. A b-vertex is obtained by reversing the arrows of an a-vertex. An a-vertex (b-vertex) is thus of type 5 or 6 and has an energy of $-s$ (s). The constrained partition function corresponding to the model with one vertex constrained to be an a-vertex (b-vertex) is denoted as Z_a (Z_b). Note that under the transformation $s\rightarrow -s$ the role of vertices a and b are interchanged. We thus have

$$Z_a(\beta s)=Z_b(-\beta s). \tag{19}$$

If we put $\beta\epsilon=\frac{1}{2}\ln(2)+U$, we have, according to (13) and (14), to first order in U

$$F=F_0-\frac{Z_0-Z_a-Z_b}{Z_0}U+O(U^2). \tag{20}$$

Here F is the reduced free energy per vertex of the staggered F-model, and $F_0=F_{\text{Baxter}}$ in (8). To calculate Z_b we only have to constrain two opposing arrows of one vertex to point oppositely to an a-vertex. Using the formalism of the previous section, we have obtained

$$\frac{Z_b}{Z_0}=\frac{1}{64\pi^4}\left[\int_0^{2\pi}\int_0^{2\pi}d\theta_1 d\theta_2\frac{\exp(-2\beta s)+\cos(\theta_1)\cos(\theta_2)}{\cosh(2\beta s)+\cos(\theta_1)\cos(\theta_2)}\right]^2. \tag{21}$$

Using this, the first order expansion of the free energy can be written as

$$F=F_0+\frac{1}{2}\left[\left(\frac{\partial F_0}{\partial\beta s}\right)^2-1\right]U+\cdots. \tag{22}$$

VI. SINGULAR BEHAVIOR IN THE VICINITY OF THE FREE-FERMION LINE

We will now verify the Coulomb gas result (see Sec. II):

$$F_s\sim(\beta s)^{2/(2-\pi/4j(\beta\epsilon))} \tag{23}$$

where

$$j(\beta\epsilon)=\tfrac{1}{2}\arccos(1-\tfrac{1}{2}\exp(2\beta\epsilon)), \tag{24}$$

to first order about the free-fermion line. Putting

$$\beta\epsilon=\tfrac{1}{2}\ln(2)+U, \tag{25}$$

and expanding in powers of U yields

$$F_s = A(U)(\beta s)^2\left[-\frac{8}{\pi}(U+O(U^2))\ln(\beta s) + \frac{32}{\pi^2}(U^2+O(U^3))\ln^2|\beta s| + \cdots \right], \tag{26}$$

where the amplitude $A(U)$ is a meromorphic function. If we compare this with the nonanalytical behavior at $U=0$ [see (A11) in the Appendix], we find

$$A(U) = \frac{1}{4U} + O(1). \tag{27}$$

It then follows that the amplitude of the term $(\beta s)^2\ln^2|\beta s|$ is $(8/\pi^2)(U+O(U^2))$. It is now a simple matter to verify this using (22) and (A11). From (A11) and (22) it follows that the order U contribution to the singular part of the reduced free energy, $F_{1,s}(\beta s)$, can be written as

$$F_{1,s}(\beta s) = [B_1(\beta s)\ln|\beta s| + B_2(\beta s)\ln^2|\beta s|]U \tag{28}$$

with B_1 and B_2 regular functions of βs. Inserting (A11) in (22) gives

$$B_2(\beta s) = \frac{8}{\pi^2}\left[(\beta s)^2 - \frac{2}{3}(\beta s)^4 + \frac{79}{90}(\beta s)^6 + \cdots \right]. \tag{29}$$

We have thus verified (24) to first order in U.

VII. CONCLUSIONS AND OUTLOOK

We have presented a simple technique for expanding the free energy of six-vertex models about free-fermion points. Applying this technique to the staggered F-model has enabled us to verify a Coulomb gas prediction about the singular part of the free energy of this model. It would be interesting to perform such computations to higher order in the free-fermion expansion. It is possible that such an undertaking might lead to proofs of certain Coulomb gas results.

APPENDIX: SINGULAR PART OF THE FREE ENERGY

In this appendix we calculate the singular part of the free energy of the staggered F-model at $\beta s = 0$ on the free-fermion line. Expanding the logarithm in (8) yields

$$\begin{aligned} F_{\text{Baxter}}(\beta s) &= -\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\theta_1 d\theta_2 \sum_{n=1}^{\infty} \frac{\cos^n(\theta_1)\cos^n(\theta_2)}{n\cosh^n(2\beta s)} \\ &= -\frac{1}{2}\sum_{n=1}^{\infty} \frac{1}{2n\cosh^{2n}(2\beta s)}\left[\frac{(2n)!}{4^n n!^2}\right]^2. \end{aligned} \tag{A1}$$

Using the asymptotic expansion

$$n! = n^n \exp(-n)\sqrt{2\pi n}\exp\left(\sum_{k=1}^{\infty} \frac{B_{2k}}{2k(2k-1)}\frac{1}{n^{2k-1}} \right), \tag{A2}$$

where the B_r are the Bernoulli numbers, we find

$$F_{\text{Baxter}}(\beta s) = -\frac{1}{4\pi}\sum_{n=1}^{\infty} \frac{1}{n^2\cosh^{2n}(2\beta s)}\left[1 - \frac{1}{4n} + \frac{1}{32n^2} + \frac{1}{128n^3} + \cdots \right]. \tag{A3}$$

We can find the nonanalytical part of the function $\Sigma_{n=1}^{\infty} 1/n^p \cosh^{2n}(2\beta s)$ as follows: Put $t = \ln(\cosh^2(2\beta s))$. We then have to find the nonanalytical part of the function $U_p(t)$ with

$$U_p(t)=\sum_{n=1}^{\infty}\frac{\exp(-nt)}{n^p} \tag{A4}$$

at $t=0$ for $p\geqslant 2$. From (A4) it follows that

$$\frac{dU_{p+1}}{dt}=-U_p. \tag{A5}$$

We denote the nonanalytical part of U_p by $\tilde{U}_p$. It then follows from (A5) that

$$\frac{d\tilde{U}_{p+1}}{dt}=-\tilde{U}_p. \tag{A6}$$

For $p=1$ the sum in (A4) is easily evaluated:

$$U_1(t)=-\ln(1-\exp(-t)), \tag{A7}$$

and we see that $\tilde{U}_1(t)$ is given by

$$\tilde{U}_1(t)=-\ln(t). \tag{A8}$$

From (A8) and (A6) it then follows that

$$\tilde{U}_p(t)=(-1)^p\frac{t^{p-1}}{(p-1)!}\ln(t). \tag{A9}$$

Inserting this in (A3) gives

$$F_s(\beta s)=-\frac{1}{4\pi}\left(t+\frac{t^2}{8}+\frac{t^3}{192}-\frac{t^4}{3072}+\cdots\right)\ln(t), \tag{A10}$$

where $F_s(\beta s)$ is the singular part of the free energy and $t=2\ln(\cosh(2\beta s))$. Expanding (A10) in powers of βs gives

$$F_s(\beta s)=-\frac{2}{\pi}\left[(\beta s)^2-\frac{1}{6}(\beta s)^4+\frac{23}{180}(\beta s)^6-\frac{593}{5040}(\beta s)^8+\cdots\right]\ln|\beta s|. \tag{A11}$$

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Quantum study of the spin inversion

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Spin motion is studied by means of the direct use of the Schrödinger equation. The solution is found in terms of Lommel's polynomials. An expression of the tunneling splitting is obtained, in good agreement with the results coming from other calculations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1630704]

I. INTRODUCTION

In quantum mechanics the direct solution of a problem by means of the Schrödinger equation can be often applied in a lot of different physical situations. For instance, the results concerning the double harmonic oscillator can be suitably used in the study of transitions in a general two-state system;[1] the wave functions of a particle in a constant force field are useful when, dealing with the Wentzel–Kramers–Brillouin (WKB) method, a turning point is crossed;[2] and so on. On the ground of these considerations, we think it advisable to present here the study of a kind of spin motion using directly the Schrödinger equation. An entire spin S in a static magnetic field is considered, performing transitions between neighboring states. The solution turns out to be expressed in terms of Lommel's polynomials, and an application to a practical case is discussed.

II. MOTION EQUATION FOR THE SPIN

The Hamiltonian has the form: $H=H_0+V$, where H_0 is a static Hamiltonian (e.g., a magnetic field) and V is the term responsible for the transitions between spin states.

Starting from the discrete set of the N $(N=2S+1)$ spin eigenstates $|n\rangle$ of H_0 with energies E_n, we can write the wave function as

$$\psi(t)=\sum_{n=1}^{N} a_n(t)|n\rangle\exp(-iE_nt/\hbar). \tag{1}$$

From the Schrödinger equation, the coefficients $a_n(t)$ result:

$$i\hbar\dot{a}_n(t)=\sum_{l=1}^{N} a_l(t)V_{nl}\exp(i\omega_{nl}t), \tag{2}$$

with $V_{nl}=\langle n|V|l\rangle$ and $\omega_{nl}=(E_n-E_l)/\hbar$. Some simplifications are in order. First, we can assume that V connects only neighboring states, and does not have diagonal elements; moreover, $|\omega_{n,n\pm1}|=\omega$, independent of n, and $V^*_{n,n+1}=V_{n,n-1}=k$. Consequently, system (2) becomes

$$i\hbar\dot{a}_n(t)-k^*a_{n+1}(t)e^{-i\omega t}-ka_{n-1}(t)e^{i\omega t}=0, \tag{3}$$

with the obvious boundary conditions

$$i\hbar\dot{a}_1(t)-k^*a_2(t)e^{-i\omega t}=0, \tag{4a}$$

$$i\hbar\dot{a}_N(t)-ka_{N-1}(t)e^{i\omega t}=0. \tag{4b}$$

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The initial conditions of interest are

$$a_1(0)=1, \tag{5a}$$

$$a_n(0)=0, \quad n=2,3,\ldots N, \tag{5b}$$

which correspond to the spin up (or down).

The substitution

$$b_n(t)=a_n(t)\mathrm{e}^{-in\omega t}, \tag{6}$$

leads to

$$i\hbar[\dot{b}_n(t)+in\omega b_n(t)]-k^*b_{n+1}(t)-kb_{n-1}(t)=0, \tag{7}$$

and to the following boundary and initial conditions, respectively,

$$i\hbar[\dot{b}_1(t)+i\omega b_1(t)]-k^*b_2(t)=0, \tag{8a}$$

$$i\hbar[\dot{b}_m(t)+im\omega b_m(t)]-kb_{m-1}(t)=0 \tag{8b}$$

$$b_1(0)=1, \tag{9a}$$

$$b_n(0)=0, \quad n=2,3,\ldots,m. \tag{9b}$$

After the Laplace transform $[b_n(p)=\int_0^\infty \mathrm{d}t b_n(t)\exp(-pt)]$, introducing the further simplification $k=k^*>0$ and with the following substitutions:

$$\rho=\hbar\omega/k, \quad \tau=\omega^{-1}, \tag{10}$$

we obtain the recursive equation

$$b_{n+1}(p)=\rho(i\tau p-n)b_n(p)-b_{n-1}(p), \tag{11}$$

where conditions (8) and (9) become

$$\rho(i\tau p-1)b_1(p)-b_2(p)=i\rho\tau, \tag{12a}$$

$$\rho(i\tau p-N)b_N(p)-b_{N-1}(p)=0. \tag{12b}$$

At this point, let us recall that the Bessel functions[3] $\mathcal{Z}_\nu(z)$ (with $\mathcal{Z}=J,Y$) satisfy a recurrence relation similar to (11). In the original definition, ν and z are independent quantities, but this does not prevent $\nu=\nu(z)$, provided that derivatives with respect to z are not performed. In particular, if $\nu=\nu(z)$, these functions are not the solution to Bessel's differential equation, and all the properties obtained using this fact are lost. By rewriting this recurrence relation as

$$\mathcal{Z}_{\nu+1}(z)=\frac{2\nu}{z}\mathcal{Z}_\nu(z)-\mathcal{Z}_{\nu-1}(z), \tag{13}$$

it has the form (11) by making the following identification

$$b_n(p)=\mathcal{Z}_{i\tau p-n}(2/\rho), \tag{14}$$

where

$$z=2/\rho, \quad \nu(z)=i\tau p-n. \tag{15}$$

So, with the substitution

$$J_\nu(z)=J_{i\tau p-n}(2/\rho)=J(p,n), \tag{16a}$$

$$Y_\nu(z)=Y_{i\tau p-n}(2/\rho)=Y(p,n), \tag{16b}$$

the general solution of (11) can be written as

$$b_n(p)=A(p)J(p,n)+B(p)Y(p,n), \tag{17}$$

where A and B are found by using (12). By applying the relation (13) and introducing the quantity

$$\Delta(p,N)=J(p,0)Y(p,N+1)-Y(p,0)J(p,N+1), \tag{18}$$

we obtain

$$b_n(p)=i\rho\tau[J(p,n)Y(p,N+1)-Y(p,n)J(p,N+1)]\Delta^{-1}(p,N)=\frac{i\hbar}{k}B_n(p). \tag{19}$$

This expression can be simplified. It is obvious that the recurrence formula (13) may be used to express $\mathcal{Z}_{\mu+n}$ linearly in terms of $\mathcal{Z}_\mu$ and $\mathcal{Z}_{\mu-1}$; the coefficients in this linear relation are polynomials in $1/z$, known as Lommel's polynomials[3] and indicated as $R_{n,\mu}(z)$. In our case $(-\mu=i\tau p)$

$$\mathcal{Z}_{-\mu-n}(z)=(-1)^n[\mathcal{Z}_{-\mu}(z)R_{n,\mu}(z)+\mathcal{Z}_{-\mu+1}(z)R_{n-1,\mu+1}(z)]. \tag{20}$$

By introducing (20) into (19), it follows that

$$B_n(p,z)=(-1)^n\frac{R_{n,\mu}(z)R_{N,\mu+1}(z)-R_{n-1,\mu+1}(z)R_{N+1,\mu}(z)}{R_{0,\mu}(z)R_{N,\mu+1}(z)-R_{-1,\mu+1}(z)R_{N+1,\mu}(z)}. \tag{21}$$

By taking into account the relations[3]

$$R_{0,\mu}=1, \quad R_{-1,\mu}=0 \tag{22}$$

and

$$R_{n,\mu}(z)R_{N,\mu+1}(z)-R_{n-1,\mu+1}(z)R_{N+1,\mu}(z)=R_{N-n,\mu+n+1}(z), \tag{23}$$

this noteworthy result is obtained

$$B_n(p,z)=(-1)^n\frac{R_{N-n,\mu+n+1}(z)}{R_{N,\mu+1}(z)}. \tag{24}$$

If $n=N$, corresponding to the spin inversion, we have

$$B_N(p,z)=(-1)^N[R_{N,\mu+1}(z)]^{-1}. \tag{25}$$

From the explicit expression of Lommel's polynomials [see (27)], it is easy to see that $R_{N,\mu+1}$ is a polynomial of degree N in p, which has exactly N complex zeros p_s.

Heaviside's expansion theorem[4] gives, therefore,

$$b_n(t)=\frac{i\hbar}{k}(-1)^n\sum_{s=1}^{N}\left[\frac{R_{N-n,-ip/\omega+n+1}\big|_{p=p_s}}{R'_{N,-ip/\omega+1}\big|_{p=p_s}}\right]e^{p_s t}, \tag{26}$$

where, obviously, the $'$ denotes the derivative with respect to p.

It is now interesting to study the behavior of $b_n(p)$ when $\omega\to 0$ (remember that $\mu=-ip/\omega$, $z=2k/\hbar\omega$). By using the explicit expression of Lommel's polynomials to express $R_{N-n,\mu+n+1}(z)$,[3]

$$R_{N-n,\mu+n+1}(z)=\sum_{l=0}^{\leqslant (N-n)/2}\frac{(-1)^l(N-n-l)!\Gamma(\mu+N-l+1)}{l!(N-n-2l)!\Gamma(\mu+n+l+1)}\left(\frac{1}{2}z\right)^{-N+n+2l}, \tag{27}$$

and by observing that

$$\frac{\Gamma(\mu+N-l+1)}{\Gamma(\mu+n+l+1)}\left(\frac{1}{2}z\right)^{-N+n+2l}=\left(-\frac{i\hbar}{k}p\right)^{N-n-2l}\left[1+\frac{i\omega}{p}(N-l)\right]\times\left[1+\frac{i\omega}{p}(N-l-1)\right]\cdots\left[1+\frac{i\omega}{p}(N+l+1)\right], \tag{28}$$

in the limit $\omega\to 0$ we finally obtain

$$R_{N-n,-ip/\omega+n+1}\big|_{\omega\to 0}=\sum_{l=0}^{\leqslant (N-n)/2}\frac{(-1)^l(N-n-l)!}{l!(N-n-2l)!}\left(-\frac{i\hbar}{k}p\right)^{N-n-2l}. \tag{29}$$

This finite sum is simply the Chebyshev polynomial of the second kind $U_{N-n}(\xi)$, $\xi=-i\hbar p/2k$.[4] By posing $\xi=\cos\theta$

$$R_{N-n,-ip/\omega+n+1}\big|_{\omega\to 0}=U_{N-n}(\cos\theta)=\frac{\sin(N-n+1)\theta}{\sin\theta}, \tag{30}$$

so that (19) can be written

$$b_n(p)\big|_{\omega\to 0}=\frac{i\hbar}{k}(-1)^n\frac{\sin(N-n+1)\theta}{\sin(N+1)\theta}. \tag{31}$$

Since the distinct zeros of the denominator are

$$p_s=\frac{2ik}{\hbar}\cos\frac{s\pi}{N+1},\quad s=0,1,\ldots N, \tag{32}$$

Heaviside's expansion applied to (31) gives, in the limit $\omega\to 0$ and after straightforward calculation

$$b_n(t)=-2\frac{(-1)^n}{N+1}\sum_{s=1}^{N}\sin\frac{s\pi}{N+1}\sin\frac{ns\pi}{N+1}\exp\left(\frac{2ik}{\hbar}t\cos\frac{s\pi}{N+1}\right). \tag{33}$$

This result can be obtained in a simple way by using the difference Eqs. (11) and (12) directly with $\omega=0$, which can now be solved using the standard method.

Although p_s's cannot be explicitly calculated for $\omega\neq 0$, an expression for small values of ω can be found. By approximating the square brackets in (28) with exponentials and performing the sum in the exponent, it follows that

$$\frac{\Gamma(\mu+N-l+1)}{\Gamma(\mu+n+l+1)}\left(\frac{1}{2}z\right)^{-N+n+2l}\approx\left[-\frac{i\hbar}{k}p\exp\left(\frac{i\omega(N+n+1)}{2p}\right)\right]^{N-n-2l}. \tag{34}$$

Thus, (27) becomes

$$R_{N-n,-ip/\omega+n+1} \approx \sum_{l=0}^{\leqslant (N-n)/2} \frac{(-1)^l (N-n-l)!}{l!(N-n-2l)!} \left[-\frac{i\hbar}{k} p \exp\left(\frac{i\omega(N+n+1)}{2p} \right) \right]^{N-n-2l}. \quad (35)$$

Proceeding as before, we pose

$$\xi = -\frac{i\hbar}{k} p \exp\left(\frac{i\omega(N+n+1)}{2p} \right) = \cos\theta,$$

giving (to the first order in ω)

$$p_s \approx i\left[\alpha \cos\frac{s\pi}{N+1} - \frac{\omega}{2}(N+1) \right], \quad (36)$$

where $\alpha = 2k/\hbar$. By performing the same standard calculation as before to obtain the Laplace transform of (31), in spite of the more complicated relation connecting p and θ, it turns out that the p-derivative of $\sin(N+1)\theta$ retains its old form. Therefore, the coefficient b_n is again given by (33) within a phase factor only; thus, if ω is not too large, it is nearly insensitive to its variation.

III. CALCULATION OF THE INVERSION TIME

The first maximum $t = \overline{t}$ of b_n as a function of time indicates when the system, in the state $|1\rangle$ for $t = 0$, first "goes" into the state $|n\rangle$. A study of the function (33) is, therefore, in order. It is easy to show that, for large values of N, the sum can be written as an integral, provided that $n \ll N$ and $\alpha t \ll N$:

$$b_n(t) \simeq (-1)^n \frac{1}{\pi} \int_0^\pi d\xi [\cos(n+1)\xi - \cos(n-1)\xi] e^{i\alpha t \cos\xi} \quad (37)$$

and

$$b_n(t) \simeq (i)^{-n+1} \frac{2n}{\alpha t} J_n(\alpha t) \quad (38)$$

is obtained as a final form, where J_n is the Bessel function of the first kind, of order n.[4] The first maximum of $b_n(t)$ obviously corresponds to the first zero of $d/dt[J_n(\alpha t)/\alpha t]$. Thus, by indicating $\alpha t \equiv \tau$, we must solve the following equation:

$$\frac{dJ_n(\tau)}{d\tau} - \frac{J_n(\tau)}{\tau} = 0. \quad (39)$$

Since the first zero of $dJ_n(\alpha t)/dt$ is found to be a good first approximation of the solution $\overline{\tau}$ of (39), this solution can be found by using a Taylor expansion. A straightforward calculation leads to the result

$$\overline{\tau} \simeq n + 0.8n^{1/3} - 0.55n^{-1/3}. \quad (40)$$

This solution was obtained from the "continuous" form (38) of $b_n(t)$, but it also works very well for the true form (33) when $n = N$, $\alpha t \leqslant N$.

The result that $\overline{\tau} \sim n$ can be found in a more intuitive way by observing that $b_n(t)$ has the form of a standing wave given by the sum of a progressive wave packet and a regressive one. By retaining only the progressive component for $t > 0$ and performing the standard analysis,[5] $b_n(t)$ takes the form

$$b_n(t) \propto \int_{-\pi/2}^{\pi/2} d\xi A(\xi) e^{i(n-\alpha t)\xi}, \tag{41}$$

that is, the maximum of the packet travels with the group velocity $v_g = \alpha$; "position" n is reached at the time $\bar{t} = n/\alpha$.

We could approach the same result directly by using the sum (33). A constructive interference is obtained only in the neighborhood of the values of s where the phase is stationary, and a short calculation immediately gives the leading term of (40).

IV. AN EXAMPLE: Fe8 CLUSTER

We were interested in applying the result expressed in Eq. (40) ($\bar{\tau} \sim n$) to a cluster with 8 Fe^{+3}.[6] We deal with spin dynamics only at very low temperatures, where the tunnel effect consists essentially (or, better, exclusively) of coherent jumps between the two spin states of the ground doublet (which, for this cluster, corresponds to $S = 10$).

The main terms of the spin Hamiltonian for the ground state are

$$H_s = DS_z^2 + \frac{\varepsilon}{2}(S_+^2 + S_-^2) + H_{h.o.}, \tag{42}$$

where $H_{h.o.}$ indicates fourth-order terms in the spin components. See Ref. 6 for further details. In this case, by diagonalizing H_s in the space of the ground spin state $|10,M\rangle$, we have six quasi-degenerate lowest doublets from $M = \pm 10$ to $M = \pm 5$, corresponding merely to the axial term of H_s, and a strong mixing of the nine highest singlets with $\langle M \rangle = 0$, due to the transverse term of H_s.

In order to evaluate the quantum tunneling frequencies ω_M (i.e., for a given M, the frequencies of the coherent $M \leftrightarrow -M$ jumps) as functions of M and $\varepsilon/|D|$, it is useful to apply the Brillouin–Wigner perturbation theory. As shown in Ref. 6, the following expression for ω_M is obtained:

$$\omega_M = F(M)\left(\frac{\varepsilon}{2|D|}\right)^M \frac{|D|}{\hbar}, \tag{43}$$

where $F(M)$ is independent of ε and $|D|$, and is calculated by means of the perturbation theory (for the inversion $-10 \leftrightarrow 10$ $F(M) \simeq 1.09 \times 10^5$).

The frequency ω_M can be calculated also by means of the theory explained in the previous section, since the two states corresponding to the spin inversion ($M = \pm 10$) are quasi-degenerate and it is possible to pass from one to another only by means of the matrix element between neighboring states. On the other hand, we have seen that the coefficient b_n shows only little dependence on the energy differences. Therefore, by comparing (43) with the relation (40):

$$\Delta_{M,-M} = \hbar \omega_M = \frac{2\pi\hbar}{\bar{t}} \simeq \frac{4\pi k}{2M+1}, \tag{44}$$

where $k \equiv V_{M,M-1} = \varepsilon$, we finally obtain

$$\frac{\varepsilon}{D} = \left[4\pi\left(\frac{2^M}{2M+1}\right)\frac{1}{F(M)}\right]^{1/M-1}. \tag{45}$$

In our case, the inversion $-10 \leftrightarrow 10$ takes place by means of six jumps ($M = 6$) between the quasi-degenerate doublets with $M = \pm 10, \pm 8, \pm 6$ and the mixing of the highest singlets with

$\langle M\rangle = 0$ by running across the path: $10 \leftrightarrow 8 \leftrightarrow 6 \leftrightarrow \langle M\rangle = 0 \leftrightarrow -6 \leftrightarrow -8 \leftrightarrow -10$. In solving Eq. (45) with $M = 6$ and $F(M) \simeq 1.09 \times 10^5$, we obtain $\varepsilon/D \sim 0.25$, which can be considered to be in good agreement with the experimental result of 0.16.

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Wigner distributions and quantum mechanics on Lie groups: The case of the regular representation

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We consider the problem of setting up the Wigner distribution for states of a quantum system whose configuration space is a Lie group. The basic properties of Wigner distributions in the familiar Cartesian case are systematically generalized to accommodate new features which arise when the configuration space changes from n-dimensional Euclidean space $\mathcal{R}^n$ to a Lie group G. The notion of canonical momentum is carefully analyzed, and the meanings of marginal probability distributions and their recovery from the Wigner distribution are clarified. For the case of compact G an explicit definition of the Wigner distribution is proposed, possessing all the required properties. Geodesic curves in G which help introduce a notion of the midpoint of two group elements play a central role in the construction. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1631393]

I. INTRODUCTION

The method of Wigner distributions[1] as a description of states of quantum mechanical systems appeared in 1932, quite early in the history of quantum mechanics. For systems whose kinematics is based upon a set of Heisenberg canonical commutation relations, it gives a way of describing both pure and mixed states in a classical phase space setting, at the level of density operators. Thus it must be sharply distinguished in mathematical structure from the Hilbert space state vector or wave function description of states, which highlights the superposition principle of quantum mechanics. In the Wigner distribution language, this principle is not obvious or manifest, but is somewhat hidden in the formalism. On the other hand, the formation of convex classical statistical mixtures of general states to generate new states becomes much more obvious. Somewhat later it was appreciated that the Wigner distribution way of describing quantum mechanical states is dual to, or is naturally accompanied by, the Weyl ordering rule[2]—a convention by which one can set up a one-to-one correspondence between operators in quantum theory (in the case of the Heisenberg commutation relations) and c-number dynamical phase space variables for the comparison classical system. Thus expectation values for general quantum dynamical variables in general quantum states can be faithfully expressed in the full operator-state vector language, or equally well in

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a completely c-number classical phase space language. In this general scheme, the group $\mathrm{Sp}(2n,R)$ of linear canonical transformations for n Cartesian degrees of freedom, and the related two-fold covering group $\mathrm{Mp}(2n)$, play prominent roles.[3]

An important property of the Wigner distribution for a general quantum state is that while it is a real function on the classical phase space, it is not always pointwise non-negative. Therefore it is usually called a quasi probability distribution, and cannot be interpreted as a phase space probability density in the sense of classical statistical mechanics. However, the Wigner distribution does have the attractive property that the marginal distributions, obtained by integrating away either the momentum or the position variables, do reproduce the correct non-negative position space and momentum space probability distributions respectively as specified by quantum mechanics. This recovery or reproducibility of correct marginal distributions is of course maintained even after unitary action by any $\mathrm{Mp}(2n)$ element.

There have been several attempts[4–15] over the years to generalize the method of Wigner distributions to handle quantum mechanical situations where the basic kinematics is defined, not by Heisenberg-type canonical commutation relations, but by some Lie group which acts as the covariance group of the system of interest. (As will become clear in the sequel, the traditional case is also governed by a group, namely the Abelian group $\mathcal{R}^n$ of translations in n-dimensional Euclidean space.) A commonly studied group is SU(2), in the context of spin systems as well as two-level atoms. One of the important early efforts at providing a general group theoretical setting for the Wigner distribution is due to Stratonovich.[16] In this context we should also mention the comprehensive monograph of Dubin *et al.*[17] It seems to us, however, that in most of these attempts the requirement that certain marginal probability distributions be recovered in a natural way from the Wigner distribution corresponding to a general quantum state, which as mentioned above is an important feature of the usual Cartesian case, is not discussed in a satisfactory manner; in some of these works this important aspect is not considered at all.

The aim of the present paper is to develop from first principles the basic features of quantum kinematics for a system whose configuration space is a general non-Abelian Lie group G rather than a Cartesian space $\mathcal{R}^n$, and then set up a corresponding Wigner distribution formalism which respects the requirement that natural marginal probability distributions are reproduced in a simple manner. This involves several extensions or modifications of the familiar formalism in the Cartesian case. The role of Schrödinger wave functions is of course now played by complex square integrable functions on G, and after normalization each such wave function determines a probability distribution over G. The meaning and definition of canonical momentum variables, and determination of the momentum space probability distribution for a given state, are however nontrivial questions in which the many structural features associated with G play important roles. In particular for a non-Abelian G canonical momenta in quantum theory become noncommuting operators, leading to deep changes in the meaning of momentum eigenstates, momentum eigenvalues and momentum space, etc. It is here that the unitary representation theory of G plays an important role. We show that all these features can be properly taken into account, and a fully satisfactory Wigner distribution can be set up as a function of carefully chosen arguments. This turns out to have simple transformation properties under G action and also to reproduce the marginal position and momentum space probability distributions properly.

It needs to be emphasised that our interest in developing a Wigner distribution formalism for systems whose configuration space is a non-Abelian group is not purely academic. In fact, there are many familiar systems which fall in this category. A general rigid body which has the group SO(3) as its configuration space is a case in point. Another well studied example in this category is the relativistic spherical top[18] whose configuration space is the noncompact group SO(3,1).

The material of this paper is arranged as follows. In Sec. II we recall the main definitions and properties of Wigner distributions in the Cartesian situation. We emphasize several familiar features in this case: the possibility of use of the classical phase space as the domain of definition of Wigner distributions; the roles of the groups $\mathrm{Sp}(2n,R)$ and $\mathrm{Mp}(2n)$; the reality but in general loss of pointwise positivity of Wigner distributions; and the recovery of the coordinate space and momentum space probability distributions for a given state by integrating over half the arguments

of the Wigner distribution. Section III describes briefly the properties of Wigner distributions in the angle-angular momentum case.[19] This brings out some new features, namely, loss of the classical phase space as the domain of definition of Wigner distributions, and absence of replacements for the groups $\mathrm{Sp}(2n,R)$ and $\mathrm{Mp}(2n)$, which indicate the type of changes we should expect in the case of a general Lie group. Section IV analyzes in some detail the classical phase space that goes with a non-Abelian Lie group G as configuration space. Both global intrinsic and local coordinate based descriptions are given, and the associated classical Poisson bracket relations are developed and described in several ways. In particular a careful analysis of the concept of classical canonical momenta in this case is provided. The transition to quantum mechanics, based on Schrödinger wave functions over G, is then outlined. It is emphasised that a naive generalization of the usual canonical Heisenberg commutation relations is not possible, and all the concepts of position operators, momentum operators and their commutation relations have to be treated with care. A brief Sec. V indicates the kinds of new features we may expect to appear, based on the results and discussions of Sec. III and IV. In Sec. VI we pose the main problem of defining Wigner distributions in a suitable way, with suitable choice of arguments, subject to the main requirements already mentioned above: reasonable transformation laws under G action, recovery of marginal probability distributions, and capturing the full information contained in a general pure or mixed quantum state. We propose a solution to this problem, possessing all the desired properties. We find that our solution uses in an essential and interesting manner the concept and properties of geodesics in G leading to the notion of a midpoint of two group elements, a key ingredient in our construction. For definiteness we confine ourselves to the case of compact G. Section VII shows how the known results of Secs. II and III, for Cartesian quantum mechanics and for the angle angular-momentum pair, are easily recovered from the general case. They correspond actually to the choices $G=\mathcal{R}^n$ and $G=\mathrm{SO}(2)$, which are both Abelian and, respectively, noncompact and compact. The case of $G=\mathrm{SU}(2)$ is then briefly considered, giving adequate background details so that the structure of the Wigner distribution can be easily appreciated. Some of the important differences compared to the Cartesian case, as well as to earlier approaches, are mentioned. Section VIII contains some concluding remarks. We have included two appendices. Appendix A recollects basic results from the theory of the regular representation of G in the compact case, based essentially on the Peter–Weyl theorem. In addition certain useful operator structures are set up, which help us understand better the construction of Wigner distributions in Sec. VI. Appendix B discusses the question of completeness of the information content in the Wigner distribution set up in Sec. VI, and generalizations of the Weyl exponential operators to the non-Abelian Lie group case.

II. THE WIGNER DISTRIBUTION IN THE CARTESIAN CASE

It is useful to recall briefly the usual definition and the basic properties of the Wigner distribution in the case of Cartesian quantum mechanics, and to highlight those important features which are likely to need generalization when we later take up the treatment of quantum mechanics on a general Lie group.

We consider a quantum system whose kinematics is based on $2n$ Hermitian irreducible Cartesian position and momentum operators $\hat{q}_r,\hat{p}_r, r=1,2,\ldots,n$, obeying the standard Heisenberg commutation relations

$$[\hat{q}_r,\hat{p}_s]=i\hbar\,\delta_{rs}, \quad [\hat{q}_r,\hat{q}_s]=[\hat{p}_r,\hat{p}_s]=0, \quad r,s=1,2,\ldots,n. \tag{2.1}$$

It is useful to express these relations more compactly by defining a $2n$-dimensional column vector with Hermitian operator entries,

$$\hat{\xi}=(\hat{\xi}_a)=(\hat{q}_1\ldots\hat{q}_n \quad \hat{p}_1\ldots\hat{p}_n)^T, \quad a=1,2,\ldots,2n, \tag{2.2}$$

and a real antisymmetric nondegenerate $2n$ dimensional symplectic metric matrix β as

$$\beta=\begin{pmatrix} 0_{n\times n} & 1_{n\times n} \\ -1_{n\times n} & 0_{n\times n} \end{pmatrix}. \tag{2.3}$$

Then Eq. (2.1) can be written as

$$[\hat{\xi}_a,\hat{\xi}_b]=i\hbar\beta_{ab}. \tag{2.4}$$

These commutation relations and the Hermiticity properties are preserved when we subject the operators $\hat{\xi}_a$ to a real linear transformation by any matrix of the symplectic group $\mathrm{Sp}(2n,R)$:

$$\mathrm{Sp}(2n,R)=\{S=2n\times 2n \quad \text{real matrix} \quad |S\beta S^T=\beta\}, \tag{2.5a}$$

$$S \in \mathrm{Sp}(2n,R): \quad \hat{\xi}_a\to\hat{\xi}'_a=S_{ab}\hat{\xi}_b,$$

$$[\hat{\xi}'_a,\hat{\xi}'_b]=i\hbar\beta_{ab}. \tag{2.5b}$$

On account of the Stone–von Neumann theorem, such linear transformations must be unitarily induced; i.e., for each $S \in \mathrm{Sp}(2n,R)$, there exists a unitary operator $\overline{\mathrm{U}}(S)$, determined up to a phase, such that

$$\hat{\xi}'_a=S_{ab}\hat{\xi}_b=\overline{\mathrm{U}}(S)^{-1}\hat{\xi}_a\overline{\mathrm{U}}(S). \tag{2.6}$$

These unitary operators give a unitary representation of $\mathrm{Sp}(2n,R)$ up to phases which cannot be totally eliminated, but can at best be reduced to a sign ambiguity:

$$S',S \in \mathrm{Sp}(2n,R):\overline{\mathrm{U}}(S')\overline{\mathrm{U}}(S)=\pm\overline{\mathrm{U}}(S'S). \tag{2.7}$$

This situation may be expressed by the statement that one is actually dealing here with a true representation of the group $\mathrm{Mp}(2n)$ which is a double cover of $\mathrm{Sp}(2n,R)$. These objects will be seen to play important roles in the theory of Wigner distributions in the present case.

Vectors in the Hilbert space $\mathcal{H}$ on which the $\hat{\xi}_a$ are irreducibly represented may be described by their Schrödinger wave functions in the usual manner,

$$|\psi\rangle\in\mathcal{H}:\psi(\underline{q})=\langle\underline{q}|\psi\rangle,$$

$$\langle\underline{q}'|\underline{q}\rangle=\delta^{(n)}(\underline{q}'-\underline{q}), \tag{2.8}$$

$$\langle\psi|\psi\rangle=\|\psi\|^2=\int_{\mathcal{R}^n}\mathrm{d}^n q\,|\psi(\underline{q})|^2.$$

The (ideal) kets $|\underline{q}\rangle$ are simultaneous eigenvectors of the n commuting position operators $\hat{q}_r, r=1,\ldots,n$. Alternatively we may describe them by their momentum space wave functions $\tilde{\psi}(\underline{p})$ by taking the overlap with simultaneous eigenvectors of the commuting momentum operators $\hat{p}_r, r=1,\ldots,n$:

$$\tilde{\psi}(\underline{p})=\langle\underline{p}|\psi\rangle=\int_{\mathcal{R}^n}\frac{\mathrm{d}^n q}{(2\pi\hbar)^{n/2}}\psi(\underline{q})\exp(-i\ \underline{p}\cdot\underline{q}/\hbar),$$

$$\langle\underline{q}|\underline{p}\rangle=(2\pi\hbar)^{-n/2}\exp(i\ \underline{q}\cdot\underline{p}/\hbar), \tag{2.9}$$

$$\langle\psi|\psi\rangle=\int_{\mathcal{R}^n}\mathrm{d}^n p\,|\tilde{\psi}(\underline{p})|^2.$$

Given a pure state $|\psi\rangle$ of the above quantum system, the corresponding Wigner distribution is a function $W(\underline{q},\underline{p})$ of $2n$ classical real variables, i.e., a function on $\mathcal{R}^{2n}$. In analogy with Eq. (2.2) we assemble the arguments $q_1\cdots q_n \;\; p_1\cdots p_n$ into a real $2n$-component column vector $\xi=(\xi_a)=(q_1\cdots q_n \;\; p_1\cdots p_n)^T$, and then $W(\xi)$ is defined by a partial Fourier transformation:

$$W(\xi)=(2\pi\hbar)^{-n}\int_{\mathcal{R}^n}\mathrm{d}^n q'\;\psi(\underline{q}-\tfrac{1}{2}\underline{q}')\,\psi(\underline{q}+\tfrac{1}{2}\underline{q}')^*\exp(i\;\;\underline{p}\cdot\underline{q}'/\hbar). \tag{2.10}$$

Here the dependence of $W(\xi)$ on ψ is left implicit. For a general mixed state we define $W(\xi)$ through the configuration space matrix elements of the density operator $\hat{\rho}$,

$$W(\xi)=(2\pi\hbar)^{-n}\int_{\mathcal{R}^n}\mathrm{d}^n q'\langle\underline{q}-\tfrac{1}{2}\underline{q}'|\hat{\rho}|\underline{q}+\tfrac{1}{2}\underline{q}'\rangle\exp(i\;\;\underline{p}\cdot\underline{q}'/\hbar), \tag{2.11}$$

once again leaving the dependence on $\hat{\rho}$ implicit. It is clear by construction that $W(\xi)$ is a real phase space function. The recovery of the proper non-negative marginal probability distributions is demonstrated by

$$\begin{aligned}\int_{\mathcal{R}^n}\mathrm{d}^n p\;W(\xi)&=|\psi(\underline{q})|^2,\\ \int_{\mathcal{R}^n}\mathrm{d}^n q\;W(\xi)&=|\tilde{\psi}(\underline{p})|^2.\end{aligned} \tag{2.12}$$

On the other hand, if $W(\xi)$ and $W'(\xi)$ correspond, respectively, to $\hat{\rho}$ and $\hat{\rho}'$, it is easily shown that

$$\mathrm{Tr}(\hat{\rho}'\hat{\rho})=(2\pi\hbar)^{-n}\int_{\mathcal{R}^{2n}}\mathrm{d}^{2n}\xi\;W'(\xi)W(\xi)\geqslant 0. \tag{2.13}$$

But since it is easy to construct cases where the trace on the left-hand side actually vanishes, we can expect that in general $W(\xi)$ becomes negative in some regions of $\mathcal{R}^{2n}$. Indeed, the simplest explicit example showing this is the expression for the Wigner function for the first excited state of the harmonic oscillator in one dimension. Taking $n=1$ and setting $\hbar=1$ for simplicity, we have

$$\psi(q)=\frac{\sqrt{2}}{\pi^{1/4}}q\;\;e^{-q^2/2}\rightarrow W(\xi)=\frac{2}{\pi}\left(q^2+p^2-\frac{1}{2}\right)\;\;e^{-q^2-p^2}. \tag{2.14}$$

In this context it is interesting to recall the following two results (again in one dimension) as indicative of the characteristic features of Wigner distributions.

(i) *Hudson:*[20] For a pure state $\psi(q)$ the Wigner function is pointwise non-negative if and only if $\psi(q)$ [and hence $W(\xi)$ as well] is a (complex) Gaussian.

(ii) *Folland-Sitaram:*[21] If $W(\xi)$ has compact support in $\mathcal{R}^2$, it must vanish identically.

Under the unitary action of $\mathrm{Mp}(2n)$ on $\hat{\rho}$, $W(\xi)$ experiences a simple point transformation

$$\hat{\rho}'=\overline{\mathrm{U}}(S)\hat{\rho}\overline{\mathrm{U}}(S)^{-1}\Leftrightarrow W'(\xi)=W(S^{-1}\xi),\;S\in\mathrm{Sp}(2n,R). \tag{2.15}$$

Thus we have covariance under the group $\mathrm{Sp}(2n,R)$ which is the maximal linear homogeneous group mixing q's and p's. This combined with the results of Eq. (2.12) shows that we recover the correct marginal probability distributions by integrating over half the variables in $W(\xi)$ even after action by any $\mathrm{Sp}(2n,R)$ transformation.

The sense in which the definitions (2.10) and (2.11) of the Wigner distribution are dual to the Weyl ordering rule is as follows. The latter rule associates with each elementary classical exponential a corresponding elementary operator exponential,

$$\exp(i\ \underline{\lambda}\cdot\underline{q}-i\ \underline{\mu}\cdot\underline{p})\rightarrow\exp(i\ \underline{\lambda}\cdot\underline{\hat{q}}-i\ \underline{\mu}\cdot\underline{\hat{p}}), \tag{2.16}$$

where $\underline{\lambda}$ and $\underline{\mu}$ are arbitrary real vectors in $\mathcal{R}^n$; and this is then extended by linearity and Fourier transformation to general classical functions, say

$$f(\underline{q},\underline{p})\equiv f(\xi)\rightarrow\hat{F}. \tag{2.17}$$

Then the dual relationship is expressed by the equality of two ways of computing quantum expectation values,

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}\exp(i\ \underline{\lambda}\cdot\underline{\hat{q}}-i\ \underline{\mu}\cdot\underline{\hat{p}}))&=(2\pi\hbar)^{-n}\int_{\mathcal{R}^{2n}}\mathrm{d}^{2n}\xi\,W(\xi)\exp(i\ \underline{\lambda}\cdot\underline{q}-i\ \underline{\mu}\cdot\underline{p}),\\ \mathrm{Tr}(\hat{\rho}\hat{F})&=(2\pi\hbar)^{-n}\int_{\mathcal{R}^{2n}}\mathrm{d}^{2n}\xi W(\xi)f(\xi).\end{aligned} \tag{2.18}$$

The definition (2.10) gives $W(\xi)$ for a given pure state $\psi(\underline{q})$. By polarization we can obtain a sesquilinear expression: for any two pure states ψ, φ we can set up a (generally complex) Wigner distribution

$$W_{\psi,\varphi}(\xi)=(2\pi\hbar)^{-n}\int_{\mathcal{R}^n}\mathrm{d}^n q'\ \psi(\underline{q}-\tfrac{1}{2}\underline{q}')\varphi(\underline{q}+\tfrac{1}{2}\underline{q}')^*\exp(i\ \underline{p}\cdot\underline{q}'/\hbar), \tag{2.19}$$

linear in ψ and antilinear in φ. Under complex conjugation we have

$$W_{\psi,\varphi}(\xi)^*=W_{\varphi,\psi}(\xi), \tag{2.20}$$

and both the formula (2.13) and the $\mathrm{Mp}(2n)$ covariance law (2.15) can be easily extended for such objects. For some purposes such expressions may be useful, but we do not make much use of them.

While all of the foregoing is quite familiar, it is useful to make the following additional remarks. It is characteristic of the Heisenberg commutation relations (2.1) that even after quantization, i.e., within quantum mechanics, the possible (sets of simultaneous) eigenvalues of the (commuting) momenta $\hat{p}_r$ by themselves do not suffer any quantization. Thus a general set of eigenvalues $p_r, r=1,\ldots,n$ for $\hat{p}_r$ determines a general point in $\mathcal{R}^n$, just as the eigenvalues q_r of the position operators $\hat{q}_r$ do. It is ultimately this that allows us to describe quantum states for such systems via Wigner distributions over the classical phase space $T^*\mathcal{R}^n\simeq\mathcal{R}^{2n}$, a general point $(\underline{q},\underline{p})$ of which is made up of (nonsimultaneous) eigenvalue sets $\underline{q},\underline{p}$ for the (noncommuting) operator sets $\hat{q}_r,\hat{p}_r$. The appearance and use of the classical phase space here is not as a result of taking the classical or semiclassical limit of the quantum theory, but is a way of expressing the exact content of the quantum theory in a fully c-number language. The role and relevance of the groups $\mathrm{Sp}(2n,R),\mathrm{Mp}(2n)$ in Cartesian quantum mechanics can really be traced back to these facts; it makes sense to form canonical linear combinations of Cartesian $\hat{q}$'s and $\hat{p}$'s. The importance of these remarks is seen from a comparison with the case of an angle-angular momentum pair,[19] and the proper way to set up Wigner distributions in that case. We recall this briefly in the next section, emphasizing the differences compared to the Cartesian situation.

III. THE WIGNER DISTRIBUTION IN THE ANGLE-ANGULAR MOMENTUM CASE

For a classical angle variable $\theta\in(-\pi,\pi)$, the configuration space Q is the circle S^1; so at the classical level the phase space or cotangent bundle is the cylinder $T^*S^1\simeq S^1\times\mathcal{R}$. This contains, in addition to the coordinate θ, a generalized momentum, p_θ say, which can be any real number: $p_\theta\in\mathcal{R}$. Now in the quantum situation we have an angle operator $\hat{\theta}$ with eigenvalues $\theta\in(-\pi,\pi)$, and a conjugate angular momentum operator $\hat{M}$ whose eigenvalues are quantized and

are $m=0,\pm 1,\pm 2,...$, i.e., $m\in\mathcal{Z}$ and *not* $m\in\mathcal{R}$. It is unnatural in this case to write down a commutation relation between $\hat{\theta}$ and $\hat{M}$; rather their mutual relationship is best expressed through these eigenvalue and eigenvector statements,

$$\hat{\theta}|\theta\rangle=\theta|\theta\rangle,\quad \theta\in(-\pi,\pi),$$

$$\langle\theta'|\theta\rangle=\delta(\theta'-\theta), \tag{3.1a}$$

$$\hat{M}|m\rangle=m\hbar|m\rangle,\quad m\in\mathcal{Z},$$

$$\langle m'|m\rangle=\delta_{m'm}, \tag{3.1b}$$

$$\langle\theta|m\rangle=(2\pi)^{-1/2}\exp(im\theta), \tag{3.1c}$$

$$\int_{-\pi}^{\pi}\mathrm{d}\theta|\theta\rangle\langle\theta|=\sum_{m\in\mathcal{Z}}|m\rangle\langle m|=1. \tag{3.1d}$$

The Hilbert space $\mathcal{H}$ relevant here is $L^2(-\pi,\pi)\simeq\ell^2$. Now we define the bounded unitary exponentials (Weyl exponentials)

$$U(n)=\exp(in\hat{\theta}),\quad n\in\mathcal{Z},$$
$$V(\tau)=\exp(-i\tau\hat{M}),\quad \tau\in(-\pi,\pi). \tag{3.2}$$

[We do not need to define the more general $U(\sigma),V(\tau)$ for $\sigma,\tau\in\mathcal{R}$.] In contrast to the Cartesian case where both $\hat{q}$ and $\hat{p}$ are unbounded, here only $\hat{M}$ is unbounded. Then, for a given pure state $|\psi\rangle\in\ \mathcal{H}$ with wave function $\psi(\theta)=\langle\theta|\psi\rangle$, the Wigner distribution is a real function $W(\theta,m)$ of an angle θ and an integer m defined as follows:

$$W(\theta,m)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\tau\,\psi(\theta+\tau/2)\psi(\theta-\tau/2)^*\ \ e^{-im\tau}, \tag{3.3}$$

the arguments of ψ and ψ^* always being in the range $(-\pi,\pi)$ via shifts of amounts $\pm 2\pi$. We note that the pair (θ,m) is not a point in the classical phase space T^*S^1, just because the ''momentum'' eigenvalue m is quantized. The definition (3.3) reproduces the marginals correctly,

$$\int_{-\pi}^{\pi}\mathrm{d}\theta\,W(\theta,m)=|\langle m|\psi\rangle|^2,$$
$$\sum_{m\in\mathcal{Z}}W(\theta,m)=|\langle\theta|\psi\rangle|^2. \tag{3.4}$$

There is an accompanying dual Weyl operator correspondence as well: it takes elementary classical exponentials on $S^1\times\mathcal{Z}$ into specific products of the U's and V's of Eq. (3.2):

$$\exp(in\theta-i\tau m)\to U(n)V(\tau)e^{-in\tau/2}=V(\tau)U(n)e^{in\tau/2},$$
$$n\in\mathcal{Z},\quad \tau\in(-\pi,\pi), \tag{3.5a}$$

$$\langle\psi|U(n)V(\tau)e^{-in\tau/2}|\psi\rangle=\int_{-\pi}^{\pi}\mathrm{d}\theta\sum_{m\in\mathcal{Z}}W(\theta,m)e^{i(n\theta-\tau m)}. \tag{3.5b}$$

[The operator exponentials in (3.5a) cannot be combined into single exponentials.] It is the case that the operators $U(n)V(\tau)e^{-in\tau/2}$ for all $n\in\mathcal{Z}$ and $\tau\in(-\pi,\pi)$ do form a complete (trace orthonormal) basis for all operators on $\mathcal{H}$; and what the Weyl rule here does is to place any operator $\hat{F}$ on $\mathcal{H}$ in correspondence with a classical function $f(\theta,m)$ on $S^1\times\mathcal{Z}$, not on $T^*S^1\simeq S^1\times\mathcal{R}$.

One appreciates that here a certain amount of quantization is already incorporated into the classical phase space structure, before the Wigner distribution can be defined in a reasonable way. There is also no room for the groups $\mathrm{Sp}(2,R)$ and $\mathrm{Mp}(2)$. These characteristic differences compared to the Cartesian case will get magnified in the case of a general Lie group.

The replacements for Eqs. (2.11) and (2.13) of the Cartesian case turn out to be as follows:

$$W(\theta,m)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\tau\langle\theta+\tau/2|\hat{\rho}|\theta-\tau/2\rangle e^{-im\tau},$$
$$\mathrm{Tr}(\hat{\rho}'\hat{\rho})=\sum_{m\in\mathcal{Z}}\int_{-\pi}^{\pi}\mathrm{d}\theta\,W'(\theta,m)W(\theta,m). \tag{3.6}$$

Thus from the latter we can see again that in general $W(\theta,m)$, though real, can become negative for some arguments.

In concluding this section, we mention one interesting case which has no Cartesian analogue. Since $\hat{M}$ has a discrete spectrum, its eigenvectors are normalizable, and in that case we find

$$|\psi\rangle=|m_0\rangle:W(\theta,m)=\frac{1}{2\pi}\delta_{m,m_0}. \tag{3.7}$$

Clearly both of Eqs. (3.4) are satisfied.

IV. CLASSICAL AND QUANTUM MECHANICS ON PHASE SPACE OF A LIE GROUP

As a preliminary step towards setting up the Wigner distribution formalism for quantum systems with kinematics based on a general Lie group, we first briefly recall the important features of the corresponding classical situation.[22]

Let G be a connected Lie group of dimension n, and let us regard it as the configuration space Q of a classical dynamical system. Then the generalized coordinate for the system is a variable element $g\in G$. The corresponding phase space T^*Q is the cotangent bundle T^*G. We can describe T^*G in intrinsic purely geometric terms, which has the advantage of being globally well defined. However from the point of view of facilitating practical calculations in any particular case, and so as to avoid being too cryptic, it is also useful to develop local coordinate based descriptions of T^*G. We outline the former first, and then turn to the latter.

Intrinsic descriptions of T^*G: As is well known, every Lie group is a parallelizable differentiable manifold. Therefore, if we denote the Lie algebra of G by $\underline{G}$, and the dual to $\underline{G}$ by $\underline{G}^*$, it turns out that T^*G is essentially the Cartesian product $G\times\underline{G}^*$. This equivalence can be established in two equally good ways, neither of which is preferred. For definiteness we identify $\underline{G}$ and $\underline{G}^*$ as the tangent and cotangent spaces to G at the identity e,

$$\underline{G}=T_eG,\quad \underline{G}^*=T_e^*G. \tag{4.1}$$

The Lie group G automatically brings with it the set of left translations L_g and the set of right translations R_g. These are mutually commuting realizations of G by mappings of G onto itself. Their definitions and main properties are

$$L_g:g'\in G\to gg'\in G,$$

$$L_{g_1}\circ L_{g_2}=L_{g_1g_2};$$

$$R_g: g'\in G\to g'g^{-1}\in G, \tag{4.2}$$

$$R_{g_1}\circ R_{g_2}=R_{g_1g_2};$$

$$L_{g_1}\circ R_{g_2}=R_{g_2}\circ L_{g_1}.$$

The corresponding tangent maps and pull backs act as nonsingular linear transformations on the tangent and cotangent spaces respectively at general points of G, according to the following scheme:

$$(L_g)_*: T_{g'}G\to T_{gg'}G,$$
$$(R_g)_*: T_{g'}G\to T_{g'g^{-1}}G, \tag{4.3a}$$

$$L_g^*: T_{g'}^*G\to T_{g^{-1}g'}^*G,$$
$$R_g^*: T_{g'}^*G\to T_{g'g}^*G. \tag{4.3b}$$

Now introduce dual bases $\{e_r\},\{e^r\}, r=1,2,\ldots,n$ for T_eG, T_e^*G,

$$\underline{G}=T_eG=\mathrm{Sp}\{e_r\},\quad \underline{G}^*=T_e^*G=\mathrm{Sp}\{e^r\},$$
$$\langle e^r,e_s\rangle=\delta_s^r,\quad r,s=1,2,\ldots,n. \tag{4.4}$$

By applying the tangent maps to $\{e_r\}$ at e, we obtain two sets of bases at each T_gG, in fact two bases for general vector fields on G,

$$X_r(g)=(R_{g^{-1}})_*(e_r),$$

$$\tilde{X}_r(g)=(L_g)_*(-e_r), \tag{4.5}$$

$$T_gG=\mathrm{Sp}\{X_r(g)\}=\mathrm{Sp}\{\tilde{X}_r(g)\}.$$

[The negative sign in the second line is to secure common commutation relations in Eq. (4.6) below.] The vector fields $\{X_r\}$ are right invariant and are the generators of the left translations L_g, while the vector fields $\{\tilde{X}_r\}$ are left invariant and generate the right translations R_g. Each set obeys the commutation relations (commutators among vector fields!) characterizing the Lie algebra $\underline{G}$ of G and involving structure constants f_{rs}^t,

$$[X_r,X_s]=f_{rs}{}^tX_t,$$

$$[\tilde{X}_r,\tilde{X}_s]=f_{rs}{}^t\tilde{X}_t, \tag{4.6}$$

$$[X_r,\tilde{X}_s]=0.$$

We naturally have two dual bases for the cotangent spaces T_g^*G:

$$T_g^*G=\mathrm{Sp}\{\theta^r(g)\}=\mathrm{Sp}\{\tilde{\theta}^r(g)\},$$

$$\langle\theta^r(g),X_s(g)\rangle=\langle\tilde{\theta}^r(g),\tilde{X}_s(g)\rangle=\delta_s^r,$$

$$\theta^r(g)=R_g^*(e^r),$$

$$\tilde{\theta}^r(g)=L_{g^{-1}}^*(-e^r). \tag{4.7}$$

In terms of these forms, the commutation relations (4.6) appear as the Maurer–Cartan relations:

$$\begin{aligned} &\mathrm{d}\theta^r+\tfrac{1}{2}f_{st}{}^r\theta^s\wedge\theta^t=0,\\ &\mathrm{d}\tilde{\theta}^r+\tfrac{1}{2}f_{st}{}^r\tilde{\theta}^s\wedge\tilde{\theta}^t=0. \end{aligned} \tag{4.8}$$

At each $g \in G$ the two sets of objects are related by the $n\times n$ matrices $\mathcal{D}(g)=(\mathcal{D}_s^r(g))$ of the adjoint representation of G (superscript=row, subscript=column index):

$$\begin{aligned} \tilde{X}_r(g)&=-\mathcal{D}_r^s(g)X_s(g),\\ \theta^r(g)&=-\mathcal{D}_s^r(g)\tilde{\theta}^s(g). \end{aligned} \tag{4.9}$$

The important point is that all these maps, objects and relationships are globally well defined.

With this geometric preparation, we can easily see in two ways why the phase space T^*G is essentially the product $G\times\underline{G}^*$. A general point in T^*G is a pair (g,ω) where $g\in G$ and $\omega \in T_g^*G$. But we can expand ω in either of the two bases $\{\theta^r(g)\},\{\tilde{\theta}^r(g)\}$ for T_g^*G, and use the expansion coefficients to synthesize elements in $T_e^*G=\underline{G}^*$,

$$\omega=\omega_r\theta^r(g)=R_g^*(\omega_r e^r)\in T_g^*G\Leftrightarrow\omega_0=\omega_r e^r\in\underline{G}^*, \tag{4.10a}$$

$$\omega=-\tilde{\omega}_r\tilde{\theta}^r(g)=L_{g^{-1}}^*(\tilde{\omega}_r e^r)\in T_g^*G\Leftrightarrow\tilde{\omega}_0=\tilde{\omega}_r e^r\in\underline{G}^*. \tag{4.10b}$$

Each of these ways of setting up correspondences gives a globally well-defined method of identifying T^*G with $G\times\underline{G}^*$. For given $\omega\in T_g^*G$, ω_0 and $\tilde{\omega}_0$ are related by the coadjoint representation of G, since

$$\tilde{\omega}_r=\mathcal{D}_r^s(g)\omega_s. \tag{4.11}$$

The above development displays the structure of the classical phase space T^*G in an intrinsic and globally well-defined manner; in particular it brings out the fact that as a bundle over the base G, T^*G is trivial. (In contrast, for example, T^*S^2 is nontrivial). Now, as stated earlier, we link up to local coordinate based descriptions more suited to practical computations and statements of Poisson bracket relations.

Local coordinate descriptions of T^*G: In general the elements of a Lie group G cannot be described with the help of coordinates in a globally smooth manner. In particular this is so if G is compact. One has to work with charts or locally defined coordinates, with well-defined transition rules in overlaps, etc. For simplicity we will work within a single chart over some open neighborhood of the identity; the setting up of a suitable notation to handle a collection of charts is in principle quite straightforward but is omitted.

Let the element $g\in G$ be labeled by n real independent continuous coordinates $q^r, r=1,2,\ldots,n$; as a convention we set $q^r=0$ at e. These q's are numerical generalized coordinates; especially in case G is compact, each of them is expected to be an angle type variable. To the set of coordinates q^r corresponds the element $g(q)\in G$. We identify the basis elements e_r, e^r for T_eG and T_e^*G, Eq. (4.4), as

$$e_r=\left(\frac{\partial}{\partial q^r}\right)_0, \quad e^r=(\mathrm{d}q^r)_0. \tag{4.12}$$

For practical convenience it is often useful to work with some faithful matrix representation of G. This has nothing to do with quantization per se, but is just a convenient way of handling G less abstractly than otherwise. In this sense let $A(q)$ be some faithful matrix representation of G; we identify its generator matrices and commutation relations by

$$\begin{aligned} A(\delta q) &\simeq 1 - i\,\delta q^r T_r, \\ [T_r, T_s] &= i f_{rs}{}^t T_t. \end{aligned} \tag{4.13}$$

The product of two elements $A(q'), A(q)$ is written as

$$A(q')A(q) = A(f(q';q)), \tag{4.14}$$

where the n functions $f^r(q';q)$ of $2n$ real arguments each express the composition law in G. Certain important auxiliary functions play an important role; their definitions and some properties are summarized here,

$$\begin{aligned} \eta_s^r(q) &= \left(\frac{\partial f^r}{\partial q'^s}(q';q) \right)_{q'=0}, \\ \tilde{\eta}_s^r(q) &= \left(\frac{\partial f^r}{\partial q'^s}(q;q') \right)_{q'=0}, \end{aligned} \tag{4.15a}$$

$$\begin{aligned} (\xi_s^r(q)) &= (\eta_s^r(q))^{-1}, \\ (\tilde{\xi}_s^r(q)) &= (\tilde{\eta}_s^r(q))^{-1}, \end{aligned} \tag{4.15b}$$

$$\begin{aligned} f(\delta q; q) &\simeq q + \eta(q)\,\delta q, \\ f(q; \delta q) &\simeq q + \tilde{\eta}(q)\,\delta q, \end{aligned} \tag{4.15c}$$

$$\begin{aligned} \eta_s^r(q) \frac{\partial A(q)}{\partial q^r} &= -i T_s A(q), \\ \tilde{\eta}_s^r(q) \frac{\partial A(q)}{\partial q^r} &= -i A(q) T_s. \end{aligned} \tag{4.15d}$$

[For matrix operations here, superscripts (subscripts) are row (column) indices.] The vector fields and one forms in Eqs. (4.5) and (4.7) have the following local expressions:

$$\begin{aligned} X_r &= \eta_r^s(q) \frac{\partial}{\partial q^s}, \quad \tilde{X}_r = -\tilde{\eta}_r^s(q) \frac{\partial}{\partial q^s}, \\ \theta^r &= \xi_s^r(q)\,\mathrm{d}q^s, \quad \tilde{\theta}^r = -\tilde{\xi}_s^r(q)\,\mathrm{d}q^s, \end{aligned} \tag{4.16}$$

and the adjoint representation matrices $\mathcal{D}(g)$ are given by the product

$$\mathcal{D}(g(q)) = \xi(q)\,\tilde{\eta}(q). \tag{4.17}$$

In the sense of classical canonical mechanics when we go to T^*G we have (local) canonically conjugate momentum variables $p_r, r = 1,2,\ldots,n$; and the basic classical Poisson bracket (PB) relations are

$$\{q^r, p_s\} = \delta_s^r, \quad \{q^r, q^s\} = \{p_r, p_s\} = 0. \tag{4.18}$$

As for the ranges of these variables, while the structure of G determines the nature of the q^r, it is generally assumed that each p_r ranges independently over the entire real line $\mathcal{R}$. In other words, $T^*_g G \simeq \mathcal{R}^n$ at each $g \in G$.

While both the coordinates q^r and the momenta p_r have so far a local character, it is possible to replace the latter by certain q-dependent linear combinations which are then globally well defined. They express the structure of the phase space T^*G in a much more natural way. We get a clue to their definitions by noticing, upon combining the PB relations

$$\{A(q), p_r\} = \frac{\partial A(q)}{\partial q^r} \tag{4.19}$$

with Eq. (4.15d), that

$$\begin{aligned} \{A(q), \eta^r_s(q) p_r\} &= -iT_s A(q), \\ \{A(q), -\tilde{\eta}^r_s(q) p_r\} &= iA(q) T_s . \end{aligned} \tag{4.20}$$

These relations lead us to define generalized canonical momentum like variables $J_r, \tilde{J}_r$ as follows:

$$J_r = \eta^s_r(q) p_s , \quad \tilde{J}_r = -\tilde{\eta}^s_r(q) p_s . \tag{4.21}$$

The connection between the two sets is

$$\tilde{J}_r = -\mathcal{D}^s_r(g(q)) J_s , \tag{4.22}$$

and, consistent with Eqs. (4.13) and (4.15d), their PB relations are

$$\begin{aligned} \{J_r, J_s\} &= f_{rs}{}^t J_t , \\ \{\tilde{J}_r, \tilde{J}_s\} &= f_{rs}{}^t \tilde{J}_t , \\ \{J_r, \tilde{J}_s\} &= 0. \end{aligned} \tag{4.23}$$

The complete coordinate-based description of the basic PB relations obtaining on T^*G can now be given in many equally good ways, and we list all of them (allowing for some repetition):

$$\{q^r, q^s\} = 0, \tag{4.24a}$$

$$\begin{aligned} \{q^r, J_s\} &= \eta^r_s(q), \\ \{q^r, \tilde{J}_s\} &= -\tilde{\eta}^r_s(q), \\ \{A(q), J_r\} &= -iT_r A(q), \\ \{A(q), \tilde{J}_r\} &= iA(q) T_r , \end{aligned} \tag{4.24b}$$

$$\begin{aligned} \{J_r, J_s\} &= f_{rs}{}^t J_t , \\ \{J_r, \tilde{J}_s\} &= 0, \\ \{\tilde{J}_r, \tilde{J}_s\} &= f_{rs}{}^t \tilde{J}_t . \end{aligned} \tag{4.24c}$$

It is thus best to view the set of J_r (or $\tilde{J}_r$) as the covariant momentum canonically conjugate to the group element $g \in G$ as a generalized coordinate.

At this point, in the present framework, we recognize that the Lie group underlying the kinematic structure of Cartesian quantum mechanics for n degrees of freedom, expressed by the Heisenberg commutation relations (2.1) and (2.3), is the Abelian translation group $G=\mathcal{R}^n$ in n real dimensions. In this case, the coordinates $q^r, r=1,2,\ldots,n$ denoting an element of $\mathcal{R}^n$ are globally well defined, and $T^*G=T^*\mathcal{R}^n\simeq\mathcal{R}^{2n}$, corresponding to the Cartesian phase space q's and p's. Due to the group being Abelian, the structure constants vanish; the $n\times n$ matrices $\eta(q),\xi(q),\tilde{\eta}(q),\tilde{\xi}(q)$ of Eq. (4.15a) and (4.15b) all reduce to the identity matrix; the momenta J_r and $\tilde{J}_r$ essentially coincide as $J_r=-\tilde{J}_r=p_r$; and the PB relations (4.24) reduce to the familiar classical forms for which the Heisenberg relations (2.1) are the quantized version. We have no difficulty in principle in postulating quantum kinematics through these commutation relations.

However the angle-angular momentum case briefly described in Sec. III corresponds to the group $G=\mathrm{U}(1)\simeq\mathrm{SO}(2)$ which is of course also Abelian. But one immediately sees new features emerging. For instance, the angle variable θ is not a globally well-defined coordinate over G. It is also not very satisfactory, due to operator domain problems, to postulate simple minded Heisenberg-type commutation relations between $\hat{\theta}$ and its canonical conjugate $\hat{M}$ in the quantum case. This is over and above the fact that now $\hat{M}$ is quantized. Thus in the $G=\mathrm{SO}(2)$ case, it is better to base the treatment on the set of relations for operators, eigenvalues, and eigenvectors collected in Eqs. (3.1).

Turning to a general Lie group G where the classical PB structure on T^*G is conveyed by any of the forms given in Eqs. (4.24), it should be evident that we should not base the quantum kinematics on a naive set of commutation relations for operator forms of the group coordinates q^r and the momenta $J_r,\tilde{J}_r$. Rather, while the latter can be satisfactorily handled (and this just involves the representation theory of G), the treatment of the abstract group element g as a coordinate operator after quantization has to be handled somewhat differently.

Quantum kinematics for the Lie group case: We now motivate the forms of the replacements for the Heisenberg canonical commutation relations (2.1) and (2.4) when we consider a quantum system whose configuration space Q is a Lie group G. Just as we identified $G=\mathcal{R}^n$ for n-dimensional Cartesian quantum mechanics, where we know that the Schrödinger wave functions are complex valued square integrable functions on $\mathcal{R}^n$, we should now expect that the Schrödinger wave functions should be complex valued square integrable (in a suitable sense) functions on G. The question now is: with what algebraic operator relations do we replace the earlier canonical $\hat{q}-\hat{p}$ commutation relations?

If we try to avoid the use of (local) coordinates for group elements, in the interests of being as intrinsic as possible, we might be tempted to imagine the following: upon quantization, the classical generalized coordinate $g\in G$ is replaced by an ''operator $\hat{g}$'' for which the possible ''eigenvalues'' are the classical abstract group elements. However this seems excessively formal. A more reasonable strategy would be to first set up a classical commutative algebra $\mathcal{A}$, say, of all smooth, i.e., $\mathcal{C}^\infty$, real valued functions $f(g)$ on G,

$$\begin{gathered} g \in G\to f(g) \in \mathcal{R}: f \in \mathcal{A}, \\ f_1,f_2 \in \mathcal{A}\Rightarrow c_1f_1+c_2f_2, f_1f_2 \in \mathcal{A}. \end{gathered} \tag{4.25}$$

Here the c's are real numbers, and the above choice of functions $f\in\mathcal{A}$ captures the differentiable manifold structure of G. The left and right translations L_g,R_g of Eq. (4.2) now act on $\mathcal{A}$ as follows:

$$\begin{gathered} \text{Left action,} \quad g'\in G: f(g)\to f(g'^{-1}g), \\ \text{Right action,} \quad g'\in G: f(g)\to f(gg'). \end{gathered} \tag{4.26}$$

Upon quantization we ask for an Abelian operator algebra $\hat{\mathcal{A}}$, say, consisting of Hermitian operators such that in a natural way we ensure

$$f \in \mathcal{A} \to \hat{f} \in \hat{\mathcal{A}},$$

$$f_1, f_2 \in \mathcal{A} \Rightarrow c_1 f_1 + c_2 f_2 \to c_1 \hat{f}_1 + c_2 \hat{f}_2, \tag{4.27}$$

$$f_1 f_2 \to \hat{f}_1 \hat{f}_2 .$$

This is the replacement for the $\hat{q}-\hat{q}$ part of the canonical relations (2.1), and is the quantized version of the PB relations $\{q^r, q^s\} = 0$ in Eq. (4.24a), in a globally well-defined form.

Turning to the quantization of the remaining PB relations in Eqs. (4.24b) and (4.24c), we can work either with finite group elements or with infinitesimal generators. In the former, we ask for unitary operator families $V(g), \tilde{V}(g)$ realizing the left and right translation groups on G, and producing on $\hat{\mathcal{A}}$ the effects implied by Eq. (4.26),

$$f(g) \in \mathcal{A} \to \hat{f} \in \hat{\mathcal{A}} \Rightarrow$$

$$f(g'^{-1} g) \to V(g') \hat{f} V(g')^{-1}, \tag{4.28a}$$

$$f(gg') \to \tilde{V}(g') \hat{f} \tilde{V}(g')^{-1}, \quad g' \in G,$$

$$V(g_1) V(g_2) = V(g_1 g_2),$$

$$\tilde{V}(g_1) \tilde{V}(g_2) = \tilde{V}(g_1 g_2), \tag{4.28b}$$

$$V(g_1) \tilde{V}(g_2) = \tilde{V}(g_2) V(g_1). \tag{4.28c}$$

The operator relations (4.28a) are the quantized and finite forms of the PB relations in (4.24b) involving $\{q^r$ or $A(q)$, J_s or $\tilde{J}_s\}$; while the operator relations (4.28b) and (4.28c) are the integrated forms of the result of quantizing the PB relations (4.24c) keeping track of course of the global connectivity properties of G. The latter can also be expressed at the generator level. If the generators of $V(g), \tilde{V}(g)$ are $\hat{J}_r, \hat{\tilde{J}}_r$, respectively, we require them to be Hermitian and to obey

$$[\hat{J}_r, \hat{J}_s] = i f_{rs}{}^t \hat{J}_t,$$

$$[\hat{\tilde{J}}_r, \hat{\tilde{J}}_s] = i f_{rs}{}^t \hat{\tilde{J}}_t,$$

$$[\hat{J}_r, \hat{\tilde{J}}_s] = 0, \tag{4.29}$$

$$\hat{\tilde{J}}_r = -\mathcal{D}_r^s(g) \hat{J}_s .$$

In comparison to the canonical commutation relations (2.1), we see that Eq. (4.28a) correspond to the $\hat{q}-\hat{p}$ part, and Eqs. (4.28b), (4.28c), and (4.29) correspond to the $\hat{p}-\hat{p}$ part, respectively. Thus the complete set of algebraic relations expressing quantum kinematics for quantum mechanics on a Lie group as configuration space are Eqs. (4.27), (4.28a)–(4.28c), (4.29). These have to be realized irreducibly on a suitable Hilbert space.

A clarifying remark may be made at this point. If we were looking only for a unitary representation (UR) or unitary irreducible representation (UIR) of G, the only commutation relations to be satisfied would be those among the Hermitian generators, $\hat{J}_r$ say, of such a UR or UIR. But these comprise only a part—the $\hat{p}-\hat{p}$ part—of the complete set of algebraic relations developed above; and do not include the operators in $\hat{\mathcal{A}}$ which represent smooth functions on G and which capture the notion of position operator in this case. Conversely, a single UIR of G on some Hilbert space, over which the $\hat{J}_r$ act irreducibly, is here the analogue of a single simultaneous (ideal)

eigenvector of all the (commuting) momenta $\hat{p}_r$. The latter is always one dimensional because $\mathcal{R}^n$ is Abelian—there is just one (ideal) eigenvector $|\underline{p}\rangle$ of the $\hat{p}_r$ for given eigenvalues p_r. With a general non-Abelian Lie group G, the analogue of a ''momentum eigenstate'' is a (finite or infinite dimensional) UIR of G.

A natural representation of all the algebraic relations imposed above is via the regular representation of G. We will hereafter always assume that there is a unique (up to a factor) left and right translation invariant volume element $\mathrm{d}g$ on G, the Haar measure, which in the compact case will be normalized so that G has total volume unity,

$$f \in \mathcal{A}: \int_G \mathrm{d}g\, f(g) = \int_G \mathrm{d}g\, f(g'^{-1}g) = \int_G \mathrm{d}g\, f(gg'),$$
$$\int_G \mathrm{d}g = 1 \quad \text{if} \quad G \quad \text{compact.} \tag{4.30}$$

In local coordinates q^r for G, apart from a normalization factor, this volume element involves the determinants of the matrices $\xi(q)$, $\tilde{\xi}(q)$ defined in (4.15b),

$$\mathrm{d}g = \det(\xi(q))\mathrm{d}^n q = \det(\tilde{\xi}(q))\mathrm{d}^n q. \tag{4.31}$$

Then the Hilbert space $\mathcal{H} = L^2(G)$ is defined, in the ''Schrödinger representation,'' as

$$\mathcal{H} = \left\{ \psi(g) \in \mathcal{C} | \|\psi\|^2 = \int_G \mathrm{d}g\, |\psi(g)|^2 < \infty \right\}. \tag{4.32}$$

On this space the required operators $\hat{f} \in \hat{\mathcal{A}}, V(g'), \tilde{V}(g')$ are easily defined,

$$f(g) \in \mathcal{A} \to \hat{f} \in \hat{\mathcal{A}}: \quad (\hat{f}\psi)(g) = f(g)\psi(g),$$
$$(V(g')\psi)(g) = \psi(g'^{-1}g), \tag{4.33}$$
$$(\tilde{V}(g')\psi)(g) = \psi(gg').$$

This is indeed an irreducible representation of the complete algebraic system as is shown in Appendix A.

In local coordinates if we write $\psi(g)$ as $\psi(q)$, the generators $\hat{J}_r, \hat{\tilde{J}}_r$ are immediately obtained as

$$\hat{J}_r = -i\eta_r^s(q)\frac{\partial}{\partial q^s},$$
$$\hat{\tilde{J}}_r = i\tilde{\eta}_r^s(q)\frac{\partial}{\partial q^s}, \tag{4.34}$$
$$V(\delta q) \simeq 1 - i\delta q^r \hat{J}_r, \quad \tilde{V}(\delta q) \simeq 1 - i\delta q^r \hat{\tilde{J}}_r.$$

Thus these generators are essentially the vector fields $X_r, \tilde{X}_r$ defined earlier in Eqs. (4.5) and (4.16), but now interpreted as Hermitian operators on $L^2(G)$.

It is for the elements $|\psi\rangle$ in the Hilbert space $\mathcal{H}$ of Eq. (4.32) that we wish to set up a Wigner distribution formalism with natural properties.

V. NEW FEATURES TO BE ACCOMMODATED

For Cartesian quantum mechanics we have the well-known Stone–von Neumann theorem which states that up to unitary equivalence there is only one irreducible representation of Hermitian operators $\hat{q}_r, \hat{p}_r$ obeying the Heisenberg relations (2.1). This irreducible representation is of course describable in many ways—position representation with $\hat{q}_r$ diagonal; momentum representation with $\hat{p}_r$ diagonal; Fock basis; coherent states, etc. When $\mathcal{R}^n$ here is replaced by a general Lie group G, we have already appreciated that the basic building block for the quantum theory is *not* a UIR of G, but an irreducible representation of the entire algebraic system consisting of $\hat{\mathcal{A}}, V(\cdot)$ and $\tilde{V}(\cdot)$. A single UIR of G is too small to support the action of a group element as a generalized coordinate. To achieve this many UIR's of G have to be put together in a careful manner.

As for UIR's of G, we recall several familiar facts. If G is compact, every UIR is finite dimensional. If G is noncompact simple, then every nontrivial UIR is infinite dimensional; every finite-dimensional representation is nonunitary; and in addition there are infinite dimensional nonunitary representations.

We will for the most part and for definiteness consider the case of a compact simple Lie group G. A natural irreducible representation of the entire algebraic structure we are interested in is given, as we have seen, by the regular representation. The main features and auxiliary operators associated with it, and some notations, are given in Appendix A.

In passing we mention the fact that while for compact G every UIR is seen in the regular representation, in the noncompact case there are UIR's (the exceptional series) not contained in the regular representation.

One last general comment is important before proceeding. As we have seen in general the momenta of our problem are noncommuting operators. This is a genuine new feature absent in Cartesian quantum mechanics, and it has significant consequences. We have seen hints of this in the angle-angular momentum case in Sec. III, even though there was only one momentum $\hat{M}$ involved. For general G, the momenta $\hat{J}_r, \hat{\tilde{J}}_r$ cannot all be simultaneously diagonal and their spectra undergo quantization. Therefore the space of arguments of the Wigner distribution has to be carefully chosen; it is definitely not a function on the classical phase space T^*G in general. By the same token, there are in general no analogues to the groups $\mathrm{Sp}(2n,R), \mathrm{Mp}(2n)$ which are so important in the Cartesian case.

VI. THE WIGNER DISTRIBUTION IN THE REGULAR REPRESENTATION

Let $|\psi\rangle \in \mathcal{H} = L^2(G)$ be a normalized state vector. The corresponding ''position space'' probability density is a probability distribution on the group G given by [cf. Eq. (A5)],

$$|\psi(g)|^2 = |\langle g|\psi\rangle|^2. \tag{6.1}$$

The complementary ''momentum space'' probability distribution is (assuming G to be compact) a discrete set of probabilities indexed by the quantum numbers JMN and given by [cf. Eq. (A14)]

$$|\psi_{JMN}|^2 = |\langle JMN|\psi\rangle|^2. \tag{6.2}$$

The common normalization states that

$$\|\psi\|^2 = \int_G \mathrm{d}g\, |\psi(g)|^2 = \sum_{JMN} |\psi_{JMN}|^2 = 1. \tag{6.3}$$

At first glance we might suppose that, given $|\psi\rangle$, the corresponding Wigner distribution $W(\cdots)$ should be a real function with g and JMN (coordinates and quantized momenta) as arguments, bilinear in ψ (more precisely involving one ψ factor and one ψ^* factor), such that integration over g yields $|\psi_{JMN}|^2$ while summation over JMN yields $|\psi(g)|^2$. This would be a natural way in

which the marginals (6.1) and (6.2) are reproduced. However, we should also require covariance under both (left and right) actions by G on ψ: the choice of the arguments in $W(\cdots)$ should allow for a natural linear transformation law under each of the changes $\psi(g)\to\psi(g_1^{-1}g)$ and $\psi(g)\to\psi(gg_2)$ in ψ. Now the momentum space amplitudes ψ_{JMN} of ψ transform linearly as follows [cf. Eq. (A14)]:

$$
\begin{aligned}
&|\psi'\rangle = V(g_1)|\psi\rangle, \quad \psi'(g) = \psi(g_1^{-1}g),\\
&\psi'_{JMN} = \sum_{M'} \mathcal{D}^J_{MM'}(g_1)^* \psi_{JM'N},\\
&|\psi''\rangle = \tilde{V}(g_2)|\psi\rangle, \quad \psi''(g) = \psi(gg_2),\\
&\psi''_{JMN} = \sum_{N'} \mathcal{D}^J_{N'N}(g_2^{-1})^* \psi_{JMN'}.
\end{aligned}
\tag{6.4}
$$

Thus in each case there is a linear mixing of the components ψ_{JMN} for fixed J at the ψ level. Remembering that $W(\cdots)$ should involve the bilinear expressions $\psi\psi^*$, a little reflection shows that it would be too narrow to imagine that the Wigner distribution should be some real function $W(g;JMN)$: there would be too few momentum space arguments to support the changes (6.4) in ψ in a reasonable manner.

There is another way in which this situation could be described. As we have already pointed out in Sec. V, an essential new feature is that now the analogue of the single momentum eigenket $|\underline{p}\rangle$ in Cartesian quantum mechanics is a multidimensional object, an entire UIR of G; actually in the regular representation even more since both $\hat{J}$'s and $\hat{\tilde{J}}$'s have to be represented. In this sense, with a general Lie group G different from $\mathcal{R}^n$, there is a genuine asymmetry between positions and momenta. While the analogue of position eigenstate remains one dimensional, $|\underline{q}\rangle$ being replaced by $|g\rangle$, the momentum operators constitute the noncommutative algebra of $\hat{J}$'s and $\hat{\tilde{J}}$'s, leading to the quantum numbers JMN where only J remains fixed. (Incidentally the first part of this statement is not in conflict with the fact that G itself may be non-Abelian. In local coordinates q^r for G, the ideal ket $|g\rangle$ may be written as $|\underline{q}\rangle$, and all the q's are simultaneously diagonal.) Out of all the momentum operators, a complete commuting set consists of the (shared) Casimir operators formed out of the $\hat{J}$'s, and separately out of the $\hat{\tilde{J}}$'s, accounting for J in the set JMN; a maximal commuting subset of the $\hat{J}$'s, supplying some of the labels in M; a similar maximal commuting subset of the $\hat{\tilde{J}}$'s supplying the analogous labels in N; and further nonlinear mutually commuting expressions in $\hat{J}$'s (respectively, $\hat{\tilde{J}}$'s) to account for the remaining labels in M (respectively, N). The main point is that in the process of obtaining the marginal distribution (6.2) upon integrating the Wigner distribution with respect to its argument g, we should expect at first to get something like a density matrix within the Jth subspace of momentum labels, and then upon going to the diagonal elements recover the probabilities $|\psi_{JMN}|^2$. The transformation laws (6.4) can already be written in a matrix form (at the level of ψ, not of the density matrix) thus,

$$
\psi^{(J)} = (\psi_{JMN}) : |\psi\rangle \to V(g_1)\tilde{V}(g_2)|\psi\rangle \Rightarrow \psi^{(J)} \to \mathcal{D}^J(g_1)^* \psi^{(J)} \mathcal{D}^J(g_2^{-1})^*. \tag{6.5}
$$

Since the individual probabilities $|\psi_{JMN}|^2$ do not transform linearly among themselves under such G actions, but do bring in off-diagonal quantities, the structure of the Wigner distribution will inevitably reflect this fact.

Based on these considerations we now list the basic desired properties for the Wigner distribution $W(\cdots)$ associated with a given normalized $|\psi\rangle \in \mathcal{H}$ (for simplicity the dependence of the former on the latter is left implicit) initially as

$$\psi(g)\in\mathcal{H}\rightarrow W(g;JMN\quad M'N'),$$
$$W(g;JMN\quad M'N')^*=W(g;JM'N'\quad MN), \tag{6.6a}$$

$$\int_G \mathrm{d}g\, W(g;JMN\quad MN)=|\psi_{JMN}|^2, \tag{6.6b}$$
$$\sum_{JMN} W(g;JMN\quad MN)=|\psi(g)|^2,$$

$$\psi'(g)=\psi(g_1^{-1}g)\rightarrow W'(g;JMN\quad M'N')$$
$$=\sum_{M_1M_1'}\mathcal{D}^J_{MM_1}(g_1)D^J_{M'M_1'}(g_1)^*W(g_1^{-1}g;JM_1N\quad M_1'N'), \tag{6.6c}$$

$$\psi''(g)=\psi(gg_2)\rightarrow W''(g;JMN\quad M'N')$$
$$=\sum_{N_1N_1'} W(gg_2;JMN_1M'N_1')\mathcal{D}^J_{N_1N}(g_2^{-1})\mathcal{D}^J_{N_1'N'}(g_2^{-1})^*. \tag{6.6d}$$

One can see that the covariance conditions (6.6c) and (6.6d) are compatible with the transformation laws (6.4) for ψ_{JMN} and the requirement (6.6b) for reproduction of the marginals. Actually one has little option but to extend the requirement in the first of Eq. (6.6b) to read

$$\int_G \mathrm{d}g\, W(g;JMN\quad M'N')=\psi^*_{JMN}\quad\psi_{JM'N'}. \tag{6.7}$$

Upon then setting $M'=M,N'=N$ here one recovers the true probabilities $|\psi_{JMN}|^2$. To all of the above we add a natural condition that W be of the general structure $\psi\psi^*$.

We now propose the following form for the Wigner distribution:

$$W(g;JMNM'N')=N_J\int_G \mathrm{d}g'\int_G \mathrm{d}g''\,\delta(g^{-1}s(g',g''))\mathcal{D}^J_{MN}(g')\psi(g')^*\mathcal{D}^J_{M'N'}(g'')^*\psi(g''). \tag{6.8}$$

This involves a group element $s(g',g'')\in G$ depending on two arguments also drawn from G, which must have suitable covariance and other properties. The set of conditions (6.6a)–(6.6d), and (6.7) now translates into a set of requirements on this function $s:G\times G\rightarrow G$ which are

$$g',g''\in G\rightarrow s(g',g'')\in G,$$
$$s(g',g'')=s(g'',g'),$$
$$s(g',g')=g', \tag{6.9}$$
$$s(g_1g'g_2^{-1},g_1g''g_2^{-1})=g_1s(g',g'')g_2^{-1}.$$

Any choice of a function $s(g',g'')$ obeying these conditions leads to an acceptable definition of a Wigner distribution for quantum mechanics on a (compact) Lie group G.

The second and third lines of Eq. (6.9) suggest that we view $s(g',g'')$ as a kind of symmetric square root of the product of two (generally noncommuting) group elements $g',g''\in G$. The covariance conditions in the last line help us simplify the problem to the choice of a suitable function $s_0(g')$ of a single argument drawn from G, obeying conditions that ensure (6.9),

$$
\begin{aligned}
s(e,g)&=s_0(g),\\
s(g',g'')&=g's_0(g'^{-1}g''),\\
s_0(e)&=e,\\
s_0(g^{-1})&=g^{-1}s_0(g),\\
s_0(g'gg'^{-1})&=g's_0(g)g'^{-1}.
\end{aligned}
\tag{6.10}
$$

It is a consequence of these conditions on $s_0(g)$ that

$$
s_0(g)g=gs_0(g). \tag{6.11}
$$

We now present a solution to the above problem in the case of a compact simple Lie group G. Any such group carries a unique Riemannian metric defined in terms of the structure constants, and possessing left and right translation invariances. We shall content ourselves with a local coordinate description and use the notations of Eqs. (4.12)–(4.17). Admitting the over use of the letter g, at the identity the metric tensor has components

$$
g_{rs}(0)=-f_{ru}{}^{v}f_{sv}{}^{u}, \tag{6.12}
$$

the negative sign ensuring that the matrix $(g_{rs}(0))$ is positive definite. This tensor is checked to be invariant under the action by the adjoint representation

$$
\mathcal{D}^{u}_{r}(g)\mathcal{D}^{v}_{s}(g)g_{uv}(0)=g_{rs}(0). \tag{6.13}
$$

At a general point $g(q)\in G$ we obtain $g_{rs}(q)$ by shifting $g_{rs}(0)$ as a tensor to $g(q)$ using either left or right translation; on account of (6.13) the two results are the same and we find

$$
g_{rs}(q)=\xi^{u}{}_{r}(q)\xi^{v}{}_{s}(q)g_{uv}(0)=\tilde{\xi}^{u}{}_{r}(q)\tilde{\xi}^{v}{}_{s}(q)g_{uv}(0). \tag{6.14}
$$

Geodesics in G are curves of minimum length with respect to the above Riemannian metric. As is well known, both left and right translations, L_g and R_g, applied pointwise map geodesics onto geodesics. Thus if $g(q(\sigma))\in G$ is a solution to the variational problem

$$
\delta\int_{\sigma_1}^{\sigma_2}\mathrm{d}\sigma\left(g_{rs}(q(\sigma))\frac{\mathrm{d}q^{r}(\sigma)}{\mathrm{d}\sigma}\frac{\mathrm{d}q^{s}(\sigma)}{\mathrm{d}\sigma}\right)^{1/2}=0, \tag{6.15}
$$

where we assume an affine parametrization is chosen so that

$$
g_{rs}(q(\sigma))\frac{\mathrm{d}q^{r}(\sigma)}{\mathrm{d}\sigma}\frac{\mathrm{d}q^{s}(\sigma)}{\mathrm{d}\sigma}=\text{const}, \tag{6.16}
$$

then both $L_{g_1}g(q(\sigma))$ and $R_{g_2}g(q(\sigma))$ are solutions to the same variational problem.

We now use geodesics in G to construct the function $s_0(g)$. It is a fact that for almost all $g\in G$ (i.e., except for a set of measure zero), there is a unique geodesic [minimizing the functional appearing in Eq. (6.15)] running from the identity e to g. We assume the affine parametrization is normalized so that the geodesic passes through e at $\sigma=0$ and through g at $\sigma=1$,

$$
g\in G: g(q(0))=e,\quad g(q(1))=g. \tag{6.17}
$$

We then take $s_0(g)$ to be the half-way point reached at $\sigma=1/2$,

$$
s_0(g)=g(q(1/2)). \tag{6.18}
$$

It is a matter of easy verification that all the conditions (6.10) are indeed obeyed: one has to exploit the natural covariance and other properties of general geodesics. With this we have solved the problem of defining Wigner distributions for quantum mechanics on a (compact) Lie group, possessing all the properties listed in Eqs. (6.6a)–(6.6d), and (6.7). The fact that $s_0(g)$ is defined everywhere except possibly on a set of vanishing measure causes no problems in carrying out integrations over G, or in recovering the marginals.

It may be pointed out that for a general pair of elements $g',g'' \in G$ (except in cases amounting to a set of vanishing measure) there is a unique geodesic running from g' to g'', normalized so that the affine parameter has values $\sigma=0$ and $\sigma=1$ at start and at finish. This geodesic is the result of applying $L_{g'}$ to the geodesic from e to $g'^{-1}g''$, or equally well of applying $R_{g'^{-1}}$ to the one from e to $g''g'^{-1}$. In either view, $s(g',g'')$ is the midpoint of this geodesic, reached at $\sigma=1/2$. Moreover, geodesics passing through the identity e are one-parameter subgroups in G. If we define $s_0(g)$ in Eq. (6.18) to be the square root of the element g, we can write the general quantity $s(g',g'')$ in these suggestive ways,

$$s(g',g'')=g'(g'^{-1}g'')^{1/2}=g''(g''^{-1}g')^{1/2}=(g''g'^{-1})^{1/2}g'=(g'g''^{-1})^{1/2}g''. \tag{6.19}$$

The definition (6.8) of the Wigner distribution associated with a pure state $\psi(g)$ generalizes to a mixed state with density operator $\hat{\rho}$,

$$W(g;JMN\ \ M'N')=N_J\int_G dg'\int_G dg''\,\delta(g^{-1}s(g',g''))\langle g''|\hat{\rho}|g'\rangle \mathcal{D}^J_{MN}(g')\ \ \mathcal{D}^J_{M'N'}(g'')^*,$$

$$\int dg\, W(g;JMN\ \ M'N')=\langle JM'N'|\hat{\rho}|JMN\rangle, \tag{6.20}$$

$$\sum_{JMN} W(g;JMN\ \ MN)=\langle g|\hat{\rho}|g\rangle.$$

We now verify that $W(g;JMN\ \ M'N')$ is a faithful representation of $\hat{\rho}$ in the sense that it contains complete information concerning $\hat{\rho}$. This will be shown by developing analogues to the previous Eqs. (2.13) and (3.6); in fact we will find two separate analogues.

The Wigner distribution in Eq. (6.20) transforms according to Eqs. (6.6c) and (6.6d) under independent left and right translations. By setting $N=N'$ and then summing over N, we obtain, using (A9), a slightly simpler function, $\tilde{W}$ say, corresponding to the density operator $\hat{\rho}$,

$$\tilde{W}(g;JMM')=\sum_N W(g;JMN\ \ M'N)$$

$$=N_J\int_G dg'\int_G dg''\,\delta(g^{-1}s(g',g''))\langle g''|\hat{\rho}|g'\rangle \mathcal{D}^J_{MM'}(g'g''^{-1})\ \ . \tag{6.21}$$

This auxiliary function is invariant under right translations except for a change of argument $g \to gg_2$, while under left translations it transforms in a manner similar to Eq. (6.6d). Now consider two density operators $\hat{\rho}_1$ and $\hat{\rho}_2$, with associated functions $\tilde{W}_1$ and $\tilde{W}_2$. It can then be shown that we can obtain $\mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2)$ from $\tilde{W}_1$ and $\tilde{W}_2$ by summing over all the arguments,

$$\sum_{JMM'} N_J^{-1}\int dg\, \tilde{W}_1(g;JMM')\tilde{W}_2(g;JM'M)=\mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2). \tag{6.22}$$

The proof is presented in Appendix B. Since any density operator $\hat{\rho}_1$ is fully determined by the traces of its products with all other density operators $\hat{\rho}_2$, we can see that even the simpler function $\tilde{W}(g;JMM')$ fully characterizes $\hat{\rho}$.

Obviously another analogue to Eqs. (2.13) and (3.6) can be obtained by interchanging the roles of left and right translations in the above. If in place of (6.21) we define

$$\tilde{\tilde{W}}(g;JNN')=\sum_M W(g;JMN\ \ MN')$$
$$=N_J\int_G dg'\int_G dg''\,\delta(g^{-1}s(g',g''))\langle g''|\hat{\rho}|g'\rangle\mathcal{D}^J_{N'N}(g''^{-1}g'), \tag{6.23}$$

then for two density operators $\hat{\rho}_1$, $\hat{\rho}_2$ we have

$$\sum_{JNN'} N_J^{-1}\int dg\ \tilde{\tilde{W}}_1(g;JNN')\tilde{\tilde{W}}_2(g;JN'N)=\mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2). \tag{6.24}$$

The conclusion we can draw, in interesting contrast to the Cartesian and Abelian cases, is this. In order to be able to recover the marginal probability distributions $\langle g|\hat{\rho}|g\rangle$, $\langle JMN|\hat{\rho}|JMN\rangle$ in natural ways and also to have simple transformation behaviors under both left and right translations on G, we need to define the Wigner distribution as in Eqs. (6.8) and (6.20) with independent arguments $g\ J\ M\ N\ M'\ N'$. However, this object captures information contained in $\hat{\rho}$ in an over complete manner, since $\hat{\rho}$ is in fact completely determined in principle already by $\tilde{W}(g;JMM')$ [or $\tilde{\tilde{W}}(g;JNN')$]. All this is traceable to the fact that for non-Abelian G, the UIR's are in general multidimensional, so the concept of momentum eigenstate is also a multidimensional set of vectors.

VII. RECOVERY OF THE CARTESIAN AND ANGLE-ANGULAR MOMENTUM CASES, AND THE SU(2) CASE

We now indicate briefly how the known earlier results of Secs. II and III can be immediately recovered from the definitions of the preceding section. The expression (6.8) for the Wigner distribution $W(g;\ JMNM'N')$ uses the function $s(g',g'')$ depending symmetrically on the group elements g',g'', and is itself a group element obeying the conditions in (6.9). For the case of a compact simple Lie group G with nontrivial Cartan–Killing metric and associated geodesics, we have found a solution for $s(g',g'')$ in terms of the mid point rule. If however G is Abelian we can directly give an elementary solution for $s(g',g'')$ not using the geodesic construction at all.

For Cartesian quantum mechanics we have $G=\mathcal{R}^n$, which is Abelian. Consequently each UIR of G is one-dimensional and corresponds to a definite numerical momentum vector

$$\underline{q}\in G\rightarrow e^{i\underline{q}\cdot\underline{p}/\hbar},\underline{p}\in\mathcal{R}^n. \tag{7.1}$$

We can regard the continuous vector $\underline{p}\in\mathcal{R}^n$ (actually dual to G, the space of characters) as the analogue of the label J of the preceding section, and as each UIR is one dimensional there is no need and no room for the labels $M\ N\ M'\ N'$. If we present the usual definition (2.11) in the form

$$W(\underline{q},\underline{p})=(2\pi\hbar)^{-n}\int_{\mathcal{R}^n}d^nq'\int_{\mathcal{R}^n}d^nq''\,\delta^{(n)}(\underline{q}-\underline{s}(\underline{q}',\underline{q}''))\langle\underline{q}''|\hat{\rho}|\underline{q}'\rangle$$
$$\times\exp(i\underline{q}'\cdot\underline{p}/\hbar)\exp(-i\underline{q}''\cdot\underline{p}/\hbar),$$
$$\underline{s}(\underline{q}',\underline{q}'')=\tfrac{1}{2}(\underline{q}'+\underline{q}''), \tag{7.2}$$

we see that all the conditions (6.9) are indeed obeyed and this familiar case is seen to be a special case of our general construction.

The key point is that our construction of the Wigner distribution only depends on finding the group element $s(g',g'')$. We may use the geodesic construction if it is available, but can use any other method if a metric on G and geodesics are not available.

Turning to the compact case $G=\mathrm{SO}(2)$, this is again Abelian, so each UIR is one dimensional,

$$\theta\in G\to e^{im\theta},\quad m=0,\pm1,\pm2,\ldots. \tag{7.3}$$

We can now write the Wigner distribution (3.6) as

$$W(\theta,m)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\theta'\int_{-\pi}^{\pi}\mathrm{d}\theta''\,\delta(\theta-s(\theta',\theta''))\langle\theta''|\hat{\rho}|\theta'\rangle\exp(im\theta')\exp(-im\theta'')\quad,$$

$$s(\theta',\theta'')=\tfrac{1}{2}(\theta'+\theta'')\mod 2\pi, \tag{7.4}$$

and again see that it falls into our general pattern.

Finally we present briefly the structure and some significant features of Wigner functions in the case $G=\mathrm{SU}(2)$, in a sense the simplest yet archetypal compact non-Abelian Lie group. Here the method of geodesics is essential for the construction. We recall very rapidly the basic definitions and notations concerning SU(2), emphasizing the four-dimensional geometric aspects available in this case

The defining representation of SU(2) is via 2×2 unitary unimodular matrices, which leads immediately to the identification of the group manifold with S^3, the real unit sphere in four-dimensional Euclidean space $\mathcal{R}^4$. We shall exploit this way of picturing SU(2). We denote group elements in the abstract by $a,b,a',b',\ldots$, these symbols also standing for points on S^3:

$$\begin{gathered}a=(a_\mu)\in S^3,\quad \mu=0,1,2,3,\\ a_\mu a_\mu=a_0^2+\underline{a}\cdot\underline{a}=1.\end{gathered} \tag{7.5}$$

The spatial part (a_1,a_2,a_3) of (a_μ) is denoted by $\underline{a}$. Inverses and products of group elements are denoted by a^{-1},ab, respectively. (The group element ab is to be carefully distinguished from the four vector inner product $a\cdot b$ which is a real number.) Then in the defining representation the matrix corresponding to $a\in\mathrm{SU}(2)$ is

$$\begin{gathered}u(a)=a_0\cdot I-i\ \ \underline{a}\cdot\underline{\sigma}=\begin{pmatrix}\lambda & \mu\\ -\mu^* & \lambda^*\end{pmatrix},\\ \lambda=a_0-ia_3,\quad \mu=-(a_2+ia_1).\end{gathered} \tag{7.6}$$

Here $\underline{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are the Pauli matrices. The inverse arises by reversing the sign of $\underline{a}$,

$$u(a)^{-1}=u(a^{-1})=u(a_0,-\underline{a})=a_0\cdot I+i\underline{a}\cdot\underline{\sigma}. \tag{7.7}$$

The group multiplication law is subsumed in the description of left and right translations, each of which is realized by elements of SO(4):

$$u(a)u(b)=u(ab)=u(L(a)b),$$

$$L(a)=\begin{pmatrix}a_0 & -a_1 & -a_2 & -a_3\\ a_1 & a_0 & -a_3 & a_2\\ a_2 & a_3 & a_0 & -a_1\\ a_3 & -a_2 & a_1 & a_0\end{pmatrix}\in\mathrm{SO}(4), \tag{7.8a}$$

$$u(b)u(a^{-1})=u(ba^{-1})=u(R(a)b),$$

$$R(a)=\begin{pmatrix} a_0 & a_1 & a_2 & a_3 \\ -a_1 & a_0 & -a_3 & a_2 \\ -a_2 & a_3 & a_0 & -a_1 \\ -a_3 & -a_2 & a_1 & a_0 \end{pmatrix} \in \mathrm{SO}(4); \tag{7.8b}$$

$$L(a)L(b)=L(ab), \quad R(a)R(b)=R(ab),$$

$$L(a)R(b)=R(b)L(a). \tag{7.8c}$$

Each of these mutually commuting sets $\{L(a)\},\{R(a)\}$ faithfully represents SU(2) via SO(4) matrices. The only common elements correspond to $a=(\pm 1,\underline{0})$ leading to the two matrices $Z_2=\{\pm I\}$ within SO(4). This leads to the familiar statement

$$\mathrm{SO}(4)=\mathrm{SU}(2)\times\mathrm{SU}(2)/Z_2. \tag{7.9}$$

We mention these details since the general covariance requirements in Eqs. (6.6c) and (6.6d) require them.

The relation to the Euler angles parametrization is given by

$$u(a)=e^{-(i/2)\,\alpha\sigma_3}e^{-(i/2)\,\beta\sigma_2}e^{-(i/2)\,\gamma\sigma_3},$$

$$a_0-ia_3=\cos\beta/2\;\; e^{-i(\alpha+\gamma)/2},$$

$$a_2+ia_1=\sin\beta/2\;\; e^{i(\gamma-\alpha)/2}, \tag{7.10}$$

$$0\leqslant\alpha\leqslant 2\pi, \quad 0\leqslant\beta\leqslant\pi, \quad 0\leqslant\gamma\leqslant 4\pi.$$

We can regard α, β, γ as angular coordinates over S^3, though because of the occurrence of half angles they are not quite the natural generalization of spherical polar angles from S^2 to S^3. The invariant line element $(\mathrm{d}s)^2$ on S^3, the invariant normalized volume element $\mathrm{d}a$ on SU(2), and the element of solid angle $\mathrm{d}\Omega(a)$ on S^3 can all be easily worked out,

$$\begin{aligned}(\mathrm{d}s)^2=\mathrm{d}a_\mu\,\mathrm{d}a_\mu&=|\mathrm{d}(a_0-ia_3)|^2+|\mathrm{d}(a_2+ia_1)|^2\\&=\tfrac{1}{4}((\mathrm{d}\alpha)^2+(\mathrm{d}\beta)^2+(\mathrm{d}\gamma)^2+2\cos\beta\;\;\mathrm{d}\alpha\;\;\mathrm{d}\gamma),\end{aligned} \tag{7.11a}$$

$$\mathrm{d}a=\frac{1}{2\pi^2}\mathrm{d}\Omega(a)=\frac{1}{16\pi^2}\mathrm{d}\alpha\sin\beta\,\mathrm{d}\beta\,\mathrm{d}\gamma. \tag{7.11b}$$

It is clear that the above line element on S^3 is the one induced from the Euclidean line element in $\mathcal{R}^4$, hence the corresponding geodesics are great circle arcs. Such arcs are carried into one another by both left and right SU(2) translations—the SO(4) invariance of $(\mathrm{d}s)^2$ along with Eq. (7.9) make this obvious. Therefore, if a,b are any two points of S^3 [any two elements of SU(2)] which are not diagonally opposite one another $[u(a)\neq -u(b)]$, the (shorter) geodesic connecting them is the affinely parametrized curve

$$a(\theta)=a\cos\theta+(b-a\;\;a\cdot b)\sin\theta/\sqrt{1-(a\cdot b)^2},$$

$$0\leqslant\theta\leqslant\theta_0=\cos^{-1}(a\cdot b)\in[0,\pi). \tag{7.12}$$

Along this geodesic we have $(\mathrm{d}s)^2=(\mathrm{d}\theta)^2$, and the midpoint is given by

$$a\left(\frac{\theta_0}{2}\right)=(a+b)/\sqrt{2(1+a\cdot b)} \tag{7.13}$$

which is geometrically obvious.

The Dirac delta function accompanying the volume element da on SU(2) may be written as $\delta(a,b)$ involving two group elements, or in a more compact form as $\delta(a^{-1}b)$. Its properties are summarized by

$$\int_{\mathrm{SU}(2)} \mathrm{d}b\ \delta(a,b)\quad f(b)\equiv \int_{S^3}\frac{\mathrm{d}\Omega(b)}{2\pi^2}\,\delta(a,b)\quad f(b)=f(a),$$

i.e.,

$$\int_{S^3}\ \mathrm{d}\Omega(b)\quad \delta(a,b)\quad f(b)=2\pi^2 f(a) \tag{7.14}$$

for suitable test functions $f(b)$. We can equally well regard $\delta(a,b)$ as a delta function on SU(2) or on S^3. In terms of Euler angles we have

$$\begin{gathered} a\to(\alpha,\beta,\gamma),\quad b\to(\alpha',\beta',\gamma'),\\ \delta(a,b)=16\pi^2\delta(\alpha'-\alpha)\,\delta(\beta'-\beta)\,\delta(\gamma'-\gamma)/\sin\beta. \end{gathered} \tag{7.15}$$

The last item in this resume concerns the matrices $D^j_{mm'}(a)$ representing SU(2) elements in the various UIR's. The ranges of the UIR label j and magnetic quantum numbers m,m' are, as usual, $j=0,1/2,1,3/2,\ldots,\ \ m,m'=j,j-1,\ldots,-j$. Then with canonical basis vectors $|jm\rangle$ in the jth UIR and Hermitian generators J_1,J_2,J_3 we have from the quantum theory of angular momentum,[23]

$$D^j_{mm'}(a)=\langle jm|e^{-i\alpha J_3}e^{-i\beta J_2}e^{-i\gamma J_3}|jm'\rangle=e^{-im\alpha-im'\gamma}d^j_{mm'}(\beta),$$

$$\begin{aligned} d^j_{mm'}(\beta)&=\langle jm|e^{-i\beta J_2}|jm'\rangle\\ &=\sqrt{\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}}\left(\sin\frac{\beta}{2}\right)^{m'-m}\left(\cos\frac{\beta}{2}\right)^{m'+m}P^{(m'-m,m'+m)}_{j-m'}(\cos\beta), \end{aligned} \tag{7.16}$$

where the P's are the Jacobi polynomials. The orthogonality and completeness properties of these D-functions are

$$\begin{gathered} \int_{\mathrm{SU}(2)}\mathrm{d}a\ D^j_{mm'}(a)^*D^{j'}_{m''m'''}(a)=(2j+1)^{-1}\quad \delta_{jj'}\delta_{mm''}\delta_{m'm'''},\\ \sum_{j=0,1/2,1,\ldots}\ \sum_{m,m'=-j}^{j}(2j+1)D^j_{mm'}(a)\quad D^j_{mm'}(b)^*=\delta(a,b)=\delta(a^{-1}b). \end{gathered} \tag{7.17}$$

With these details in place we can proceed to the definition of the Wigner distribution. The Hilbert space of Schrödinger wave functions is

$$\mathcal{H}=L^2(\mathrm{SU}(2))=\left\{\psi(a)\in C\,\middle|\, a\in\mathrm{SU}(2),\|\psi\|^2=\int_{\mathrm{SU}(2)}\ \mathrm{d}a\ \ |\psi(a)|^2<\infty\right\}. \tag{7.18}$$

Given $\psi\in\mathcal{H}$, the corresponding Wigner distribution is obtained by specializing Eqs. (6.8), (6.10), and (6.18) to this case and using Eq. (7.13) above,

$$W(a;jmn\ \ m'n') = \frac{(2j+1)}{4\pi^4}\int_{S^3} d\Omega(a')\int_{S^3} d\Omega(a'')\ \ \delta\left(a, \frac{a'+a''}{\sqrt{2(1+a'\cdot a'')}}\right)$$
$$\times D^j_{mn}(a')\psi(a')^*\ \ D^j_{m'n'}(a'')^*\ \ \psi(a''). \tag{7.19}$$

The occurrence of the midpoint of the geodesic from a' to a'' within the delta function is to be noted. We see immediately that the marginals are properly reproduced,

$$\int da\ W(a;jmn\ \ m'n') = \psi_{jm'n'}\psi^*_{jmn},$$

$$\psi_{jmn} = \frac{\sqrt{2j+1}}{2\pi^2}\int d\Omega(a)\ \ D^j_{mn}(a)^*\ \ \psi(a), \tag{7.20a}$$

$$\sum_{jmn} W(a;jmn\ \ mn) = |\psi(a)|^2. \tag{7.20b}$$

Since the integrations involved in Eq. (7.19) are nontrivial, we limit ourselves to pointing out some qualitative features of the SU(2) Wigner distribution (7.19) which distinguish it from the Cartesian case as well as from earlier treatments of this problem.

(a) The appearance of all the arguments $a\ \ jmn\ \ m'n'$ in the Wigner distribution is essential to be able to satisfy the covariance laws (6.6c) and (6.6d) under independent left and right SU(2) translations, and to reproduce the configuration space and momentum space marginal probability distributions as in Eq. (7.20). In this respect the situation is markedly different from earlier approaches to the SU(2) Wigner distribution problem,[4] where attention was limited to states within some fixed (finite dimensional) UIR of SU(2) and the density matrix was expanded in the complete set of unit tensor operators within that UIR.

(b) If we consider as an idealized limit the case of $\psi(a)$ becoming a position eigenstate, the Wigner distribution simplifies as follows:

$$\psi(a) \to \delta(a, a^{(0)}),$$
$$W(a;jmn\ \ m'n') = \frac{(2j+1)}{4\pi^4}\delta(a,a^{(0)})\ \ D^j_{mn}(a^{(0)})\ \ D^j_{m'n'}(a^{(0)})^*. \tag{7.21}$$

This retains a dependence on the momentum variables $jmn\ \ m'n'$. This is in contrast to the (one-dimensional) Cartesian case where from Eq. (2.10) we find

$$\psi(q) \to \delta(q-q_0), \quad W(q,p) = \frac{1}{h}\delta(q-q_0), \tag{7.22}$$

showing no p dependence.

(c) Similarly if we consider $\psi(a)$ to be a (normalized) linear combination of $D^{j_0}_{m_0 n_0}(a)$ over $m_0\ \ n_0$ for some fixed j_0, the Wigner distribution has a nontrivial dependence on all its arguments, and *in particular is generally nonvanishing for* $j \neq j_0$. In the Cartesian case, in contrast, we have, similar to Eq. (7.22),

$$\psi(q) \to \frac{1}{h^{1/2}} e^{ip_0 q}, \quad W(q,p) = \frac{1}{h}\delta(p-p_0), \tag{7.23}$$

concentrated at $p = p_0$ and independent of q.

All these features can be attributed to the non-Abelian nature of SU(2).

VIII. CONCLUDING REMARKS

We have discussed the problem of setting up Wigner distributions for the states of a quantum system whose configuration space is a general non-Abelian Lie group G, and have given a complete solution for the case that G is compact. Many new features compared to the familiar Abelian case where $G=\mathcal{R}^n$ have appeared. For emphasis we repeat some of them here: while the classical phase space T^*G associated to G already brings in interesting structural aspects, in the quantum case the Wigner distribution is not a function defined on the classical T^*G. Instead it is a function of a classical unquantized group element $g\in G$ playing the role of coordinate variable, and quantized momenta consisting of labels $J\ M\ NM'\ N'$ associated with all the UIR's of G. The analogues of the familiar Heisenberg canonical commutation relations are now much more intricate, and the ideas of momentum eigenstates and momentum eigenvalues have to be understood with some care. While the distribution $W(g;\ JMN\ M'N')$ associated with a given $\hat{\rho}$ transforms nicely under left and right group actions, and reproduces the marginal probability distributions satisfactorily, it describes $\hat{\rho}$ in an over complete manner.

The points of view of the present work suggest that we also consider quantum systems whose covariance group is a given Lie group G, even if G is not the configuration space. These arise naturally if the configuration space is a coset space G/H, where H is some Lie subgroup of G. In that case there is only one (say left) action of G on G/H, rather than two independent mutually commuting actions. Action by G remains significant, and we would like to set up Wigner distributions for wave functions belonging to $L^2(G/H)$. Such UR's of G are typically much smaller than the regular representation.

Going beyond coset space representations, we have yet other physically interesting cases typified for example by the Schwinger oscillator representation of SU(2). Similar constructions are easily made for SU(3), etc.[24] These are not representations on spaces $L^2(G/H)$ for any choice of H; yet because of their use in various physical problems it is worthwhile to be able to set up Wigner distributions for them too.

We intend to examine some of these problems elsewhere.

APPENDIX A: THE REGULAR REPRESENTATION AND ASSOCIATED STRUCTURES

We assemble here some familiar facts concerning the regular representation of a compact Lie group, to settle notations and as preparation for setting up further operator structures. We know that the Lie group G under consideration possesses a left and right translation and inversion invariant volume element, $\mathrm{d}g$ say, so that the integral of a (complex valued) function $f(g)$ over G has the properties

$$\int_G \mathrm{d}g\, f(g)=\int_G \mathrm{d}g\quad (f(g^{-1})\quad \text{or}\quad f(g'g)\quad \text{or}\quad f(gg')), \tag{A1}$$

where g' is any fixed element in G. For the compact case we normalize $\mathrm{d}g$ so that

$$\int_G \mathrm{d}g=1. \tag{A2}$$

With such a measure the carrier space for the unitary regular representation of G is the Hilbert space $\mathcal{H}=L^2(G)$ defined as in Eq. (4.32),

$$\mathcal{H}=\left\{\psi(g)\in\mathcal{C}\,\middle|\,\|\psi\|^2=\int_G \mathrm{d}g\,|\psi(g)|^2<\infty\right\}. \tag{A3}$$

A Dirac delta function can be defined with suitable invariance properties,

$$\int_G \mathrm{d}g\, f(g) \quad \delta(g) = \int_G \mathrm{d}g\, f(g) \quad \delta(g^{-1}) = f(e),$$
$$\int_G \mathrm{d}g\, f(g) \quad \delta(gg'^{-1} \quad \text{or} \quad g^{-1}g' \quad \text{or} \quad g'^{-1}g \quad \text{or} \quad g'g^{-1}) = f(g'). \tag{A4}$$

We can introduce a convenient set of ideal basis vectors for $\mathcal{H}$ such that the wave function $\psi(g)$ is the overlap of $|\psi\rangle$ with one of these,

$$\psi(g) = \langle g|\psi\rangle,$$
$$\langle g'|g\rangle = \delta(g'g^{-1}),$$
$$\int_G \mathrm{d}g|g\rangle\langle g| = 1 \text{ on } \mathcal{H}. \tag{A5}$$

The group G can be unitarily represented on $\mathcal{H}$ in two mutually commuting ways, by left or by right translations. We denote the corresponding operators by $V(g), \tilde{V}(g)$ and define them by

$$V(g')|g\rangle = |g'g\rangle,$$
$$\tilde{V}(g')|g\rangle = |gg'^{-1}\rangle. \tag{A6}$$

Both of them are unitary and obey the composition and commutation relations

$$V(g_2)V(g_1) = V(g_2g_1),$$
$$\tilde{V}(g_2)\tilde{V}(g_1) = \tilde{V}(g_2g_1), \tag{A7}$$
$$V(g_1)\tilde{V}(g_2) = \tilde{V}(g_2)V(g_1).$$

On wave functions the effects are as given in Eq. (4.33),

$$(V(g')\psi)(g) = \psi(g'^{-1}g),$$
$$(\tilde{V}(g')\psi)(g) = \psi(gg'). \tag{A8}$$

These are infinite dimensional reducible UR's of G; and in the compact case, according to the Peter–Weyl theorem, each of them contains every UIR of G as often as its dimension. Motivated by the notations in the case of SU(2), we shall use symbols $J, J', J_1, J_2, \ldots$ to label the various UIR's of G (some of which may not be faithful); so in fact J stands for several independent discrete or quantized labels, as many as the rank of G. Within the Jth UIR, in some chosen orthonormal basis, we label rows and columns by indices $M, N, M'N', \ldots$. Once again each of these stands for a collection of discrete labels: for instance the eigenvalues of as many commuting generators as the rank of G, plus further eigenvalues of chosen commuting nonlinear polynomials in the generators. In the Jth UIR, we write $\mathcal{D}^J_{MN}(g)$ for the unitary representation matrices. These obey composition, orthogonality and completeness relations:

$$\sum_{M'} \mathcal{D}^J_{MM'}(g')\mathcal{D}^J_{M'N}(g) = \mathcal{D}^J_{MN}(g'g), \tag{A9}$$

$$\int_G \mathrm{d}g\, \mathcal{D}^{J'}_{M'N'}(g)^* \mathcal{D}^J_{MN}(g) = \delta_{J'J}\delta_{M'M}\delta_{N'N}/N_J, \tag{A10}$$

$$\sum_{JMN} N_J \mathcal{D}^J_{MN}(g)\mathcal{D}^J_{MN}(g')^* = \delta(g^{-1}g'). \tag{A11}$$

Here N_J is the dimension of the Jth UIR. With the help of these matrices we can introduce another orthonormal basis for $\mathcal{H}$ which explicitly accomplishes the simultaneous reduction of both UR's $V(\cdot), \tilde{V}(\cdot)$ into irreducibles. These basis vectors and their main properties are

$$\begin{gathered} |JMN\rangle = N_J^{1/2} \int_G \mathrm{d}g\, \mathcal{D}^J_{MN}(g)|g\rangle, \\ \langle g|JMN\rangle = N_J^{1/2}\mathcal{D}^J_{MN}(g), \\ \langle J'M'N'|JMN\rangle = \delta_{J'J}\delta_{M'M}\delta_{N'N}, \\ \sum_{JMN} |JMN\rangle\langle JMN| = 1 \ \text{ on } \ \mathcal{H}. \end{gathered} \tag{A12}$$

Under action by $V(\cdot), \tilde{V}(\cdot)$ they transform among themselves conserving J,

$$\begin{aligned} V(g)|JMN\rangle &= \sum_{M'} \mathcal{D}^J_{MM'}(g^{-1})|JM'N\rangle, \\ \tilde{V}(g)|JMN\rangle &= \sum_{N'} \mathcal{D}^J_{N'N}(g)|JMN'\rangle. \end{aligned} \tag{A13}$$

Therefore in $|JMN\rangle$ the index N counts the multiplicity of occurrence of the Jth UIR in the reduction of $V(\cdot)$, and the index M performs a similar function in the reduction of $\tilde{V}(\cdot)$. A general $|\psi\rangle$ can be expanded in either basis and we have

$$\begin{gathered} |\psi\rangle = \int_G \mathrm{d}g\ \psi(g)|g\rangle = \sum_{JMN} \psi_{JMN}|JMN\rangle, \\ \psi_{JMN} = \langle JMN|\psi\rangle = N_J^{1/2}\int_G \mathrm{d}g\, \mathcal{D}^J_{MN}(g)^*\psi(g), \\ \|\psi\|^2 = \int_G \mathrm{d}g\ \ |\psi(g)|^2 = \sum_{JMN} |\psi_{JMN}|^2. \end{gathered} \tag{A14}$$

Towards getting projections onto individual vectors $|JMN\rangle$ we set up the Fourier components of $V(\cdot)$ and $\tilde{V}(\cdot)$ as follows:

$$\begin{aligned} P_{JMN} &= N_J \int_G \mathrm{d}g\, \mathcal{D}^J_{MN}(g)V(g), \\ \tilde{P}_{JMN} &= N_J \int_G \mathrm{d}g\, \mathcal{D}^J_{MN}(g^{-1})\tilde{V}(g). \end{aligned} \tag{A15}$$

With respect to Hermitian conjugation the indices get interchanged,

$$P^\dagger_{JMN} = P_{JNM}, \quad \tilde{P}^\dagger_{JMN} = \tilde{P}_{JNM}, \tag{A16}$$

and their composition and multiplication laws are

$$P_{J'M'N'}P_{JMN}=\delta_{J'J}\delta_{N'M}P_{JM'N},$$

$$\tilde{P}_{J'M'N'}\tilde{P}_{JMN}=\delta_{J'J}\delta_{M'N}\tilde{P}_{JMN'}, \tag{A17}$$

$$P_{JMN}\tilde{P}_{J'M'N'}=\tilde{P}_{J'M'N'}P_{JMN}.$$

Their actions on the two complementary bases for $\mathcal{H}$ are immediate,

$$P_{J'M'N'}|JMN\rangle=\delta_{J'J}\delta_{N'M}|JM'N\rangle,$$

$$\tilde{P}_{J'M'N'}|JMN\rangle=\delta_{J'J}\delta_{M'N}|JMN'\rangle,$$

$$P_{JMN}|g\rangle=N_J^{1/2}\sum_{N'}\mathcal{D}^J_{N'N}(g^{-1})|JMN'\rangle, \tag{A18}$$

$$\tilde{P}_{JMN}|g\rangle=N_J^{1/2}\sum_{M'}\mathcal{D}^J_{MM'}(g^{-1})|JM'N\rangle.$$

Therefore the projections onto $|JMN\rangle$ are

$$|JMN\rangle\langle JMN|=P_{JMM}\tilde{P}_{JNN}, \tag{A19}$$

and we have the completeness identities

$$\sum_M P_{JMM}=\sum_M \tilde{P}_{JMM},$$

$$\sum_{JM} P_{JMM}=\sum_{JM}\tilde{P}_{JMM}=1 \text{ on } \mathcal{H}. \tag{A20}$$

Now we proceed to a construction of certain operators directly relevant to the Wigner distribution problem. Here we will be guided by analogy to what is done for the (one degree of freedom) $\hat{q}-\hat{p}$ pair and the $\hat{\theta}-\hat{M}$ pair, as recounted in Secs. II and III. In these cases we know that the unitary Weyl exponentials $U(\sigma)=\exp(i\sigma\hat{q})$, $V(\tau)=\exp(-i\tau\hat{p})$ and $U(n)=\exp(in\hat{\theta})$, $V(\tau)=\exp(-i\tau\hat{M})$ play important roles. It is seen that it is natural here to regard $\sigma(n)$ as a typical eigenvalue of $\hat{p}(\hat{M})$ and τ[in $\mathcal{R}$ or in $(-\pi,\pi)$] as a typical eigenvalue of $\hat{q}(\hat{\theta})$. Now the operator $V(\tau)$ has been generalized in the Lie group situation to the *two* families $V(g),\tilde{V}(g)$. These are indeed exponentials of the "momentum operators:" if the group element g is expressed as the exponential of an element in $\underline{G}$, then $V(g)$ and $\tilde{V}(g)$ are corresponding exponentials in their generators (4.34) obeying (4.29):

$$g=\exp(\tau^r\ e_r):V(g)=\exp(-i\ \tau^r\hat{J}_r),$$

$$\tilde{V}(g)=\exp(-i\ \tau^r\hat{\tilde{J}}_r). \tag{A21}$$

With τ^r as coordinates for g, these are precisely exponentials in momenta. To generalize $U(\sigma),U(n)$ we recall on the other hand that now a typical "momentum eigenvalue" is the collection of quantum numbers JMN associated with a subspace of $\mathcal{H}$ supporting a UIR of the $\hat{J}_r,\hat{\tilde{J}}_r$. This suggests that the generalization of $U(\sigma),U(n)$ must be an operator diagonal in the "coordinate" or $|g\rangle$ basis, and labeled by JMN: it must be a function of the coordinates alone. Based on this reasoning, we define operators U_{JMN} by

$$U_{JMN}|g\rangle = \mathcal{D}^J_{MN}(g)|g\rangle,$$
$$\langle g|U_{JMN} = \mathcal{D}^J_{MN}(g)\langle g|. \tag{A22}$$

Their adjoints are also diagonal in this basis,

$$U^\dagger_{JMN}|g\rangle = \mathcal{D}^J_{MN}(g)^*|g\rangle,$$
$$\langle g|U^\dagger_{JMN} = \mathcal{D}^J_{MN}(g)^*\langle g|, \tag{A23}$$

and unitarity is expressed in a matrix sense,

$$\sum_M U^\dagger_{JMN}U_{JMN'} = \sum_M U^\dagger_{JNM}U_{JN'M} = \delta_{N'N}\cdot 1 \quad \text{on} \quad \mathcal{H}. \tag{A24}$$

Being simultaneously diagonal, the commutators vanish,

$$[U_{JMN}, U_{J'M'N'}] = [U_{JMN}, U^\dagger_{J'M'N'}] = 0. \tag{A25}$$

Completeness of the $\mathcal{D}$-functions $\mathcal{D}^J_{MN}(g)$ as expressed in Eq. (A11) now means that the operators $\{U_{JMN}\}$ form a (linear) basis for the commutative algebra $\hat{\mathcal{A}}$. In fact the map (4.27) from the classical algebra $\mathcal{A}$ to the quantized $\hat{\mathcal{A}}$ can be made explicit,

$$f \in \mathcal{A}: f(g) = \sum_{JMN} f_{JMN}\mathcal{D}^J_{MN}(g) \rightarrow$$
$$\hat{f} = \sum_{JMN} f_{JMN}U_{JMN} \in \hat{\mathcal{A}}. \tag{A26}$$

The relations connecting $\{U_{JMN}\}$ to $V(\cdot), \tilde{V}(\cdot)$ are easily worked out,

$$V(g)U_{JMN}V(g)^{-1} = \sum_{M'} \mathcal{D}^J_{MM'}(g^{-1})U_{JM'N},$$
$$\tilde{V}(g)U_{JMN}\tilde{V}(g)^{-1} = \sum_{N'} \mathcal{D}^J_{N'N}(g)U_{JMN'}. \tag{A27}$$

What remains are expressions for the product of two U's, and the action of a U on $|JMN\rangle$. For both these, the Clebsch–Gordan coefficients for G have to be brought in.

Let the reduction of the direct product of the Jth and J'th UIR's of G contain various UIR's J'' with various multiplicities. This means that we have a family of Clebsch–Gordan coefficients carrying three sets of $J-M$ labels and in addition a multiplicity index λ, say; and they obey two sets of unitarity conditions,

$$\sum_{M,M'} C^{JJ'J''\lambda *}_{MM'M''}C^{JJ'J'''\lambda'}_{MM'M'''} = \delta_{J''J'''}\delta_{\lambda\lambda'}\delta_{M''M'''},$$
$$\sum_{J''\lambda M''} C^{JJ'J''\lambda *}_{MM'M''}C^{JJ'J''\lambda}_{NN'M''} = \delta_{MN}\delta_{M'N'}. \tag{A28}$$

Using these coefficients the product of two $\mathcal{D}$-functions decomposes into a sum

$$\mathcal{D}^{J}_{MN}(g)\mathcal{D}^{J'}_{M'N'}(g)=\sum_{J''\lambda M''N''} C^{JJ'J''\lambda *}_{MM'M''}C^{JJ'J''\lambda}_{NN'N''}\mathcal{D}^{J''}_{M''N''}(g). \tag{A29}$$

In all these relations the multiplicity index λ accompanying the ''final'' UIR J'' runs over as many values as the number of times J'' occurs in the product of J and J'; and at each stage we have manifest unitary invariance under changes in the choice of λ's. Combining Eq. (A29) in turn with Eqs. (A12) and (A22) we immediately get the results for the products of two U_{JMN}'s and the action of a U_{JMN} on a state $|J'M'N'\rangle$,

$$U_{JMN}U_{J'M'N'}=\sum_{J''\lambda M''N''} C^{JJ'J''\lambda *}_{MM'M''}C^{JJ'J''\lambda}_{NN'N''}U_{J''M''N''},$$

$$U_{JMN}|J'M'N'\rangle=\sum_{J''\lambda M''N''} \sqrt{\frac{N_{J'}}{N_{J''}}}C^{JJ'J''\lambda *}_{MM'M''}C^{JJ'J''\lambda}_{NN'N''}|J''M''N''\rangle. \tag{A30}$$

The unitary invariance with respect to λ is manifest.

Thus we have expressions (A6) and (A22) for the actions of $U,\ldots,V(\cdot),\tilde{V}(\cdot)$ on $|g\rangle$, and expressions (A30) and (A13) for their actions on $|JMN\rangle$.

Last we consider the question of setting up in a natural way a complete trace orthonormal set of operators on $\mathcal{H}=L^2(G)$, involving the U's, V's, and $\tilde{V}$'s in a ''symmetrical'' manner. In the Cartesian case the phase space displacement operators

$$e^{i(\sigma\hat{q}-\tau\hat{p})}=e^{i\sigma\hat{q}}e^{-i\tau\hat{p}}e^{-i\sigma\tau/2}=e^{-i\tau\hat{p}}e^{i\sigma\hat{q}}e^{i\sigma\tau/2} \tag{A31}$$

give us such a system, and they are basic to the Weyl correspondence. Already in the $\hat{\theta}-\hat{M}$ case we know from Eqs. (3.5a) and (3.5b) that we have to work with the operators

$$e^{in\hat{\theta}}e^{-i\tau\hat{M}}e^{-in\tau/2}=e^{-i\tau\hat{M}}e^{in\hat{\theta}}e^{in\tau/2}, \tag{A32}$$

which are again complete and trace orthonormal, but we can no longer write these as single exponentials. In the case of general G, this latter trend continues. Generalizing from the known examples, we now define a family of operators labeled by $g\in G$ together with JMN, as follows:

$$\hat{\mathcal{D}}(g;JMN)=V(g)U_{JMN}=\sum_{M'}\mathcal{D}^{J}_{MM'}(g^{-1})U_{JM'N}V(g). \tag{A33}$$

It is easy to show trace orthogonality, using Eqs. (A6) and (A22),

$$\begin{aligned}\mathrm{Tr}(\hat{\mathcal{D}}(g';J'M'N')^{\dagger}\hat{\mathcal{D}}(g;JMN))&=\int_G dg''\langle g''|U^{\dagger}_{J'M'N'}V(g')^{-1}V(g)U_{JMN}|g''\rangle\\&=\int_G dg''\,\mathcal{D}^{J'}_{M'N'}(g'')^{*}\mathcal{D}^{J}_{MN}(g'')\langle g''|V(g'^{-1}g)|g''\rangle\\&=\delta(g'^{-1}g)\,\delta_{J'J}\delta_{M'M}\delta_{N'N}/N_J.\end{aligned} \tag{A34}$$

As for completeness we begin with

$$\hat{\mathcal{D}}(g;JMN)|g'\rangle=\mathcal{D}^{J}_{MN}(g')|gg'\rangle, \tag{A35}$$

multiply both sides by $N_J\mathcal{D}^{J}_{MN}(g'')^{*}$, sum on JMN and use Eq. (A11) to get

$$\sum_{JMN} N_J \mathcal{D}^J_{MN}(g'')^* \hat{\mathcal{D}}(g;JMN)|g'\rangle = \delta(g''^{-1}g')|gg'\rangle = |gg''\rangle\langle g''|g'\rangle. \tag{A36}$$

Peeling off $|g'\rangle$ and then replacing gg'' by g' we get

$$|g'\rangle\langle g''| = \sum_{JMN} N_J \mathcal{D}^J_{MN}(g'')^* \hat{\mathcal{D}}(g'g''^{-1};JMN). \tag{A37}$$

This shows, albeit in a somewhat formal manner, that any operator on $\mathcal{H}$ can be linearly expanded in the set $\hat{\mathcal{D}}(g;JMN)$. If in Eq. (A33) we use $\tilde{V}(\cdot)$ in place of $V(\cdot)$ we get the alternative results,

$$\hat{\tilde{\mathcal{D}}}(g;JMN) = \tilde{V}(g)U_{JMN} = \sum_{N'} \mathcal{D}^J_{N'N}(g)U_{JMN'}\tilde{V}(g), \tag{A38}$$

$$\mathrm{Tr}(\hat{\tilde{\mathcal{D}}}(g';J'M'N')^\dagger \hat{\tilde{\mathcal{D}}}(g;JMN)) = \delta(g'^{-1}g) \quad \delta_{J'J}\delta_{M'M}\delta_{N'N}/N_J, \tag{A39}$$

$$|g'\rangle\langle g''| = \sum_{JMN} N_J \mathcal{D}^J_{MN}(g'')^* \hat{\tilde{\mathcal{D}}}(g''g'^{-1};JMN). \tag{A40}$$

One can ask whether similar completeness statements can be developed for outer products of vectors of the form $|JMN\rangle\langle J'M'N'|$. This is indeed possible, but the expressions are somewhat unwieldy and involve the Clebsch–Gordan coefficients explicity, so we omit them.

The results (A38)–(A40) prove that the representation of $\hat{\mathcal{A}}, V(\cdot)$ and $\tilde{V}(\cdot)$ on $\mathcal{H}=L^2(G)$ is irreducible, since any operator on $\mathcal{H}$ is expressible as a linear combination of the operators $\hat{\mathcal{D}}(g;JMN)$ [or $\hat{\tilde{\mathcal{D}}}(g;JMN)$].

APPENDIX B

Here we briefly outline the proofs for Eqs. (6.22) and (6.24) and also derive some useful relations similar in form to those known in the Cartesian and angle-angular momentum cases.

To prove (6.22), consider its left-hand side (LHS):

$$\sum_{JMM'} N_J^{-1} \int \mathrm{d}g \tilde{W}_1(g;JMM')\tilde{W}_2(g;JM'M). \tag{B1}$$

On substituting for $\tilde{W}$ using (6.21) and carrying out the summation over JMM' using (A11), this expression becomes

$$\int \mathrm{d}g \int \mathrm{d}g'_1 \int \mathrm{d}g''_1 \int \mathrm{d}g'_2 \int \mathrm{d}g''_2 \langle g''_1|\hat{\rho}_1|g'_1\rangle \times \langle g''_2|\hat{\rho}_2|g'_2\rangle \delta(g^{-1}s(g'_1,g''_1)) \quad \delta(g^{-1}s(g'_2,g''_2)) \quad \delta(g''_1 g'^{-1}_1 g''_2 g'^{-1}_2). \tag{B2}$$

Using the fact that $\delta(gg') = \delta(g'g)$, the third delta function in the integrand can be written as $\delta(g'^{-1}_1 g''_2 g'^{-1}_2 g''_1)$ or as $\delta((g''^{-1}_2 g'_1)^{-1} g'^{-1}_2 g''_1)$ which in turn implies that the integral vanishes unless $g''_1 = g'_2 \cdot h; g'_1 = g''_2 \cdot h$, $h \in G$. This, together with the other two delta functions implies that $h=e$. The three delta functions above are therefore equivalent to $\delta(g^{-1}s(g'_1,g''_1))\ \delta(g'^{-1}_1 g''_2)\ \delta(g''^{-1}_1 g'_2)$. On carrying out the integrals in (B2) with the help of these delta functions one obtains the right-hand side (RHS) of (6.22).

A similar line of argument can be used to establish the relation (6.24). Next we show that, in analogy with the Cartesian and angle-angular momentum cases, the Wigner distribution in (6.20) corresponding to a density operator $\hat{\rho}$ can be written in the following compact form:

$$W(g;JMN\ \ M'N')=\mathrm{Tr}[\hat{\rho}\hat{W}(g;JMNM'N')], \tag{B3}$$

where the Wigner operator $\hat{W}(g;JMNM'N')$ can be expressed in terms of operators related to $\hat{\mathcal{D}}(g;JMN)$ as follows:

$$\hat{W}(g;JMNM'N')=N_J\hat{\mathcal{D}}_1(g;JMN)\ \ \Delta\ \ \hat{\mathcal{D}}_1^{\dagger}(g;JM'N'). \tag{B4}$$

Here

$$\hat{\mathcal{D}}_1(g;JMN)=U_{JMN}V(g) \tag{B5}$$

$$=\sum_{M'}\ \mathcal{D}^J_{MM'}(g)\hat{\mathcal{D}}(g;JM'N), \tag{B6}$$

$$\Delta=\int \mathrm{d}g\sum_{JMN}\ N_J\mathcal{D}^J_{MN}(e)^*\hat{\mathcal{D}}_0(g;JMN), \tag{B7}$$

$$\hat{\mathcal{D}}_0(g;JMN)=\sum_{M'}\ \mathcal{D}^J_{MM'}(s_0(g))\hat{\mathcal{D}}(g;JM'N) \tag{B8}$$

$$=\sum_{M'}\ \mathcal{D}^J_{MM'}(s_0(g^{-1}))\hat{\mathcal{D}}_1(g;JM'N). \tag{B9}$$

Note that the operator $\hat{\mathcal{D}}_0(g;JMN)$ introduced here can be regarded as the analogue of $e^{ip\hat{q}-iq\hat{p}}$ $\equiv e^{-iq\hat{p}}e^{ip\hat{q}}e^{ipq/2}$ or of $e^{-i\tau\hat{M}}e^{in\hat{\theta}}e^{in\tau/2}$ in the angle-angular momentum case.

To show (B3), we note that the RHS of (B3) can be written as

$$\mathrm{Tr}[\hat{\rho}\hat{W}(g;JMNM'N')]=\int \mathrm{d}g_1\int \mathrm{d}g_2\langle g_2|\hat{\rho}|g_1\rangle\langle g_1|\hat{W}(g;JMNM'N')|g_2\rangle. \tag{B10}$$

Now

$$\langle g_1|\hat{W}(g;JMNM'N')|g_2\rangle=N_J\int \mathrm{d}g_3\int \mathrm{d}g_4\langle g_1|\hat{\mathcal{D}}_1(g;JMN)|g_3\rangle\langle g_3|\Delta|g_4\rangle$$
$$\times\langle g_4|\hat{\mathcal{D}}_1(g;JMN)|g_2\rangle, \tag{B11}$$

and from the definitions (B5)–(B9) of the operators that occur here it can easily be shown that

$$\langle g_1|\hat{\mathcal{D}}_1(g;JMN)|g_2\rangle=\mathcal{D}^J_{MN}(g_1)\,\delta(g_1(gg_2)^{-1}), \tag{B12}$$

$$\langle g_1|\hat{\mathcal{D}}_0(g;JMN)|g_2\rangle=\mathcal{D}^J_{MN}(s(g_1,g_2))\,\delta(g_1(gg_2)^{-1}), \tag{B13}$$

$$\langle g_1|\Delta|g_2\rangle=\int \mathrm{d}g\sum_{JMN}\ N_J\mathcal{D}^J_{MN}(e)^*\langle g_1|\hat{\mathcal{D}}_0(g;JMN)|g_2\rangle$$

$$=\int \mathrm{d}g\sum_{JMN}\ N_J\mathcal{D}^J_{MN}(e)^*\mathcal{D}^J_{MN}(s(g_1,g_2))\,\delta(g_1(gg_2)^{-1})$$

$$=\delta(s(g_1,g_2)). \tag{B14}$$

Using these in (B11) one obtains

$$\langle g_1|\hat{W}(g;JMN,M'N')|g_2\rangle = N_J \delta(g^{-1}s(g_1,g_2))\mathcal{D}^J_{MN}(g_1)\mathcal{D}^J_{M'N'}(g_2)^*, \tag{B15}$$

which when substituted in (B10) yields (B3).

On setting $N=N'$ $(M=M')$ in (B3) and summing over N (M) we obtain the following formulas for the simpler Wigner distributions in terms of simpler Wigner operators:

$$\tilde{W}(g;JMM') = \mathrm{Tr}[\hat{\rho} \quad \hat{\tilde{W}}(g;JMM'), \tag{B16}$$

$$\tilde{\tilde{W}}(g;JNN') = \mathrm{Tr}[\rho \quad \hat{\tilde{W}}(g;JNN')], \tag{B17}$$

where

$$\hat{\tilde{W}}(g;JMM') = \sum_N \hat{W}(g;JMNM'N), \tag{B18}$$

$$\hat{\tilde{W}}(g;JNN') = \sum_M \hat{W}(g;JMNMN'). \tag{B19}$$

The relations (B16) and (B17) can be inverted with the help of (6.22) and (6.24), respectively, to obtain

$$\hat{\rho} = \int \mathrm{d}g \sum_{JMM'} \frac{1}{N_J} \tilde{W}(g;JMM')\hat{\tilde{W}}(g;JM'M), \tag{B20}$$

$$\hat{\rho} = \int \mathrm{d}g \sum_{JNN'} \frac{1}{N_J} \tilde{\tilde{W}}(g;JNN')\hat{\tilde{\tilde{W}}}(g;JN'N). \tag{B21}$$

This can be seen as follows. Setting $\hat{\rho}_1 \equiv \hat{\rho}$ and $\hat{\rho}_2 = |g_2\rangle\langle g_1|$ in (6.22) and using (B16) for the second Wigner distribution one obtains

$$\langle g_1|\hat{\rho}|g_2\rangle = \int \mathrm{d}g \sum_{JMM'} \frac{1}{N_J} \tilde{W}(g;JMM')\langle g_1|\hat{\tilde{W}}(g;JM'M)|g_2\rangle, \tag{B22}$$

which on peeling off $\langle g_1|$ and $|g_2\rangle$ gives (B20). Equation (B21) can be derived in a similar fashion.

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Lattice approximations and continuum limits of ϕ_2^4-quantum fields

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Lattice ϕ_2^4-quantum field models with different lattice cutoffs in the free and interacting parts are constructed and their continuum limits are studied. A comparision with previously constructed continuum limits is given, in the spirit of a discussion on how limit models depend on chosen regularizations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1626807]

I. INTRODUCTION

The usual (continuum) ϕ_d^4-quantum field theory[1,2] is heuristically described by the following probability measure:

$$N_{\lambda_1,\lambda_2,\lambda_3}^{-1}\prod_{x\in R^d} d\phi(x)\exp\left(-\int_{R^d}(\lambda_1|\nabla\phi(x)|^2+\lambda_2\phi^2(x)+\lambda_3\phi^4(x))dx\right), \tag{1.1}$$

where $N_{\lambda_1,\lambda_2,\lambda_3}$ is the normalization constant, λ_1, λ_2, and λ_3 are real strictly positive coupling constants, and ϕ is the real-valued field. There have been many approaches to the problem of giving a meaning to the above heuristic measure for $d=2$ and $d=3$ (see Refs. 3–15 and references therein). The lattice approximation is an important tool in constructing and studying the continuum ϕ_d^4 field, Let us set $aZ^d=\{ax: x\in Z^d\}$, $a>0$. Heuristically, the quantities $\int|\nabla\phi(x)|^2dx$, $\int\phi^2(x)dx$, and $\int\phi^4(x)dx$ can be approximated, respectively, by $a^{d-2}\Sigma_{|x-y|=a;x,y\in aZ^d}(\phi_x-\phi_y)^2$, $a^d\Sigma_{x\in aZ^d}\phi_x^2$, and $a^d\Sigma_{x\in aZ^d}\phi_x^4$, as a tends to zero. Thus heuristically (1.1) can be approximated by the following heuristic probability measure:

$$N_a^{-1}\prod_{x\in aZ^d} d\phi_x \times\exp\left(2\lambda_1 a^{d-2}\sum_{|x-y|=a;x,y\in aZ^d}\phi_x\phi_y-(\lambda_2 a^d+4d\lambda_1 a^{d-2})\sum_{x\in aZ^d}\phi_x^2-\lambda_3 a^d\sum_{x\in aZ^d}\phi_x^4\right), \tag{1.2}$$

*Deceased.

where N_a is the normalization constant. (1.2) is still just a heuristic expression, because of the sums over the infinite set aZ^d, but it is indeed not hard to give a rigorous sense to (1.2) (see Refs. 3, 5, 11, and 12 and references therein). By using a natural embedding of aZ^d in R^d, the so obtained probability measure μ_a can be realized on the distribution space $\mathcal{S}'(R^d)$.[11] We call this the lattice ϕ_2^4-field measure. From μ_a by deriving suitable bounds on its moments and choosing subsequences if necessary one gets limit measures for $d=1,2,3$, by weak convergence (in the sense of moments of probability measures). These are then the continuum ϕ_d^4-field measures, realized as probability measures on $\mathcal{S}'(R^d)$, $d=1,2,3$. For suitable choices of λ_1, λ_2, and λ_3 one has indeeed even weak convergence of μ_a to a unique probability measure μ, as $a\downarrow 0$ (Refs. 5, 11, and 13) for a "simplicial approximation approach" to the continuum limit.

In this paper we consider a new lattice approximation to (1.1). For this we choose a "new cutoff" $a'=a'(a)>0$ satisfying $\lim_{a\to 0^+} a'(a)=0$. For convenience we assume $a'\geqslant a>0$ so that $a'Z^d\subset aZ^d$. Heuristically, the quantity $\int \phi^4(x)dx$ can also be approximated by $a'^d\Sigma_{x\in a'Z^d}\phi_x^4$ as a tends to zero. Thus the heuristic measure (1.1) can also be approximated by the following heuristic probability measure:

$$N_{a,a'}^{-1}\prod_{x\in aZ^d} d\phi_x \times\exp\left(2\lambda_1 a^{d-2}\sum_{|x-y|=a;x,y\in aZ^d}\phi_x\phi_y-(\lambda_2 a^d+4d\lambda_1 a^{d-2})\sum_{x\in aZ^d}\phi_x^2-\lambda_3 a'^d\sum_{x\in a'Z^d}\phi_x^4\right), \tag{1.3}$$

where $N_{a,a'}$ is the normalization constant. We denote the latter heuristic probability measure by $\nu_{a,a'}$ and call it, for simplicity, "the new lattice ϕ_2^4-fields model." This measure can be thought as describing a lattice ϕ^4-field theory with different lattice cutoffs in the free and interacting parts. Similarly as for (1.2) one can give a rigorous sense to (1.3). The basic question discussed in this paper is to what extent the continuuum limit depends on the chosen regularization a,a'. Since $a'\geqslant a$, the interaction part appears only on a subset $a'Z^d$ of the lattice points aZ^d. It is however also present in the normalization term $N_{a,a'}$, so that we can expect that the procedure of choosing $a'\neq a$ might enhance the singular behavior of moments at coinciding points, with respect to the case $a'=a$. It is natural to think that the continuum limit, without additional counterterms, only exists for a suitable dependence of a' on a. In fact we will prove in Theorem 2.1 that if $\limsup_{a\to 0^+} a'|\log a|^{5/4}<+\infty$ and the coupling λ is weak, then the continuum limit of the lattice ϕ_2^4 given by (1.3) exists and the probability measure associated to the distribution-valued field satisfies all the Osterwalder–Schrader axioms of the Euclidean quantum field, except possibily the rotation invariance. For such a result we follow the approach in Ref. 5. First we will construct an action in the finite volume Λ as a finite-difference approximation to the continuum action. Then we will define a renormalized total action in bounded lattice regions $L=aZ^d\cap\Lambda$ and $L'=a'Z^d\cap\Lambda$ with Dirichlet boundary conditions. The bare mass m will be expressed in terms of counterterms depending on both a and a', as a perturbation of the mass m_0, corresponding to the mass for the free lattice field model. By the second Griffiths inequality we will extend this action to the whole lattices aZ^d and $a'Z^d$. By the Schwinger–Dyson field equation we will express the interacting 2-points function, i.e., the interacting propagator, in terms of the interacting 4-point function, and by skeleton inequalities we will estimate the latter 4-point function from above and from below by the 2-point function, so that we will get upper and lower bounds for the 2-point function in terms of itself. Since we will prove that the 2-point function is continuous with respect to λ, and hence for a weak coupling it is close to the free propagator, we will get a uniform estimate with respect to the variables a and a' of the 2-point function. Further we will estimate the $2n$-point function from above and from below by the 2-point function, and hence by the free propagator. Therefore we will prove that its limit is nontrivial and that the distribution associated with the continuum field is uniquely determined by its moments.

In the Appendix the proof of the existence of the continuum limit is extended from the case of the above condition $\limsup_{a\to 0^+} a'|\log a|^{5/4}<+\infty$ to the one where $\limsup_{a\to 0^+} a'|\log a|^{7/6}<+\infty$. For this proof general skeleton inequalities are used. It is also remarked that our method might be further extended so that we might prove the existence of the continuum limit under the more general condition $\limsup_{a\to 0^+} a'|\log a|^{1+\epsilon}<+\infty$, with $\epsilon>0$ (in this case new counterterms are required which might modify the continuum limit).

Another basic result of the paper is stated in Theorem 2.2. It says roughly that in the presence of a space cutoff and under the assumption that $a'|\log a|^2$ stays bounded (a situation where no new counterterm is needed, as compared to the usual lattice model) the new constructed continuum ϕ_2^4 model coincides with the old one. This result also implies that for models with space cutoff in the interaction performing first the infinite volume limit $\Lambda\uparrow R^2$ and then the continuum limit leads to the same result as taking the limits in the opposite order. The proof uses the properties of Wick powers and estimates on the n-point functions of the relevant measures, in order to prove that they have the same asymptotic behavior (such measures being uniquely determined by their moments), one gets the result. We also discuss the question whether in general $\nu_{a,a'}$ and $\nu_{a,a}$ might have the same limit points. We give motivations for this not to be the case in general (this is in analogy with the situation in the discrete Edward model in two dimensions[16]).

The paper is organized as follows. In Sec. II we will give a rigorous definition of the new lattice ϕ_2^4-field model given by the measure $\nu_{a,a'}$. We also state the main results of this paper. In Sec. III we will first state some skeleton inequalities for the new lattice ϕ_2^4-field model and then derive some estimates of the corresponding two point functions. In Sec. IV we will use the Schwinger–Dyson field equation and some skeleton inequalities to derive uniform bounds on two point functions. In Sec. V we will first derive some bounds on the $2n$-point functions and then construct the new ϕ_2^4 fields by approximating from the corresponding $2n$-point functions associated with the new lattice ϕ_2^4-field measure $\nu_{a,a'}$. In Secs. VI and VII we will prove that $\{\nu_{a,a'}\}$ is weakly convergent to the *original* continuum ϕ_2^4 field [described heuristically by (1.1), constructed, e.g., in Refs. 2, 8, and 11] if $\limsup_{a\to 0^+} a'|\log a|^2<\infty$. In Sec. VIII we will discuss some properties of the continuum ϕ_2^4 field in the case where $\lim_{a\to 0^+} a'|\log a|^2=\infty$ and propose some open problems which further illustrate the interest to study the new lattice approximation of ϕ_2^4 fields given in the present paper. In the Appendix we will derive a correlation inequality up to the third order in the coupling constant λ and apply it to prove the convergence of scaled moment functions for an interaction with a suitable mass counterterms to the moment functions of a limit probability measure, in the case where $\lim_{a\to 0^+} a'|\log a|^{7/6}<\infty$.

II. MODELS AND MAIN RESULTS

To construct our new ϕ_2^4-field models, we first construct ϕ_2^4 models in a bounded lattice region, with different lattice cutoffs a and a' in the free, respectively, interacting parts. We then use the strategy of Ref. 5, applying the second Griffiths inequality[11,17] to take the "infinite-volume" limit, and then pass to the continuum limit as the lattice spacings a,a' go to zero. We note, however, that in many previous references, the continuum limit of the lattice ϕ_2^4 fields was taken before performing the infinite-volume limit.[8,11] In case λ_3 is small, we show that under some assumptions on the terms $a,a'\to 0$ the continuum ϕ_2^4 fields constructed by the above two approaches coincide. For convenience we will call the continuum ϕ_2^4 field, obtained by one of the above approaches, the original continuum ϕ_2^4 field (in the infinite-volume case, i.e., without a spatial cutoff). We remark that the approach given in Ref. 5 is also suitable for the construction of the continuum ϕ_2^4 field with spatial cutoffs.

Let Λ be a given regular bounded region in R^2 (for its definition, the reader is refered to Ref. 11, p. 267) and set

$$L=aZ^2\cap\Lambda\subset R^2,\quad L'=a'Z^2\cap\Lambda\subset R^2,$$

where $a'=a'(a)$ is assumed to satisfy the assumptions given in Sec. I, so that in particular $L'\subset L$. Let $g\geqslant 0$ be a given function in R^2 which is bounded and Borel measurable. Define an action in the finite volume $L\subset Z^2$ with Dirichlet boundary condition

$$S_{\Lambda,D}(\phi)=\frac{1}{2}\sum_{\langle xy\rangle;x,y\in L}(\phi_x-\phi_y)^2+\frac{1}{2}m^2a^2\sum_{x\in L}\phi_x^2+\frac{\lambda}{4}a'^2\sum_{x\in L'}g(x)\phi_x^4, \tag{2.1}$$

where $\langle xy\rangle$ represents the set $\{(x,y):\ |x-y|=a;\ x,y\in aZ^2\}$. Then the probability measure

$$Z_{\Lambda,D}^{-1}\prod_{x\in L}e^{-S_{\Lambda,D}(\phi)}d\phi_x \tag{2.2}$$

is well defined, where $Z_{\Lambda,D}$ is the normalization constant. Heuristically, the lattice action $S_{\Lambda,D}(\phi)$ is a finite-difference approximation to the continuum action,

$$S_{\Lambda,C}(\phi)=\int_\Lambda\left\{\frac{1}{2}[\nabla\phi(x)]^2+\frac{1}{2}m^2\phi(x)^2+\frac{\lambda}{4}g(x)\phi(x)^4\right\}dx,$$

and the probability measure (2.2) can be thought of as a finite-difference approximation to a measure on continuum fields which is heuristically given by

$$Z_{\Lambda,C}^{-1}e^{-S_{\Lambda,C}(\phi)}\prod_{x\in\Lambda}d\phi(x).$$

Let G_a be the probability measure for the free lattice field model of mass m_0 on aZ^2 [i.e., $\lambda=0$, $m^2=m_0^2$ and $L=aZ^2$ in (2.1) and (2.2)] and let $\langle\cdot\rangle_{G_a}$ denote the expectation with respect to G_a. Let

$$C^{(a)}(x-y)=\langle\phi_x\phi_y\rangle_{G_a}.$$

G_a is thus the (lattice) Gaussian measure with mean zero and covariance $C^{(a)}$. It is easy to show that[8,11]

$$C^{(a)}(x-y)=(2\pi)^{-2}\int_{[-\pi/a,\pi/a]^2}\left[m_0^2+2a^{-2}\sum_{j=1}^{2}(1-\cos ak_j)\right]^{-1}e^{ik(x-y)}dk_1dk_2,$$

where $k=(k_1,k_2)$. Let

$$G_{a,L}=N_{a,L}^{-1}\exp\left(-\frac{1}{2}\sum_{\langle xy\rangle;x,y\in L}(\phi_x-\phi_y)^2-\frac{1}{2}m_0^2a^2\sum_{x\in L}\phi_x^2\right)\prod_{x\in L}d\phi_x,$$

where $N_{a,L}$ is the normalization constant. Let

$$C_L^{(a)}(x,y)=\langle\phi_x\phi_y\rangle_{G_{a,L}}.$$

By Ref. 11, Chap. VIII, we know that

$$C^{(a)}(x-y)=\lim_{L\to aZ^2}C_L^{(a)}(x,y).$$

One can also check that $C^{(a)}(x-y)$ is bounded by $c|\log|x-y||$ for $a\leqslant|x-y|\leqslant 1$, and $C^{(a)}(0)$ behaves like $c|\log a|$ for some constant $c\in(0,\infty)$, as a tends to zero.[18] We now introduce the counterterms which are necessary to define rigorously (1.1). Let $\delta m_1^2=-3\lambda C^{(a)}(0)$ and set

$$\delta m_2^2 = \begin{cases} 6\lambda^2 a'^2 C^{(a)}(0)^3, & \limsup_{a\to 0^+} a'|\log a|^{3/2} \in (0,\infty], \\ 0, & \text{otherwise.} \end{cases}$$

It is clear that $\limsup_{a\to 0^+} \delta m_2^2 = +\infty$ if $\limsup_{a\to 0^+} a'|\log a|^{3/2} = +\infty$. We define the normalized action S_L in the bounded region L with Dirichlet boundary condition by setting

$$S_L(\phi) = \frac{1}{2} \sum_{\langle xy\rangle; x,y\in L} (\phi_x - \phi_y)^2 + \frac{1}{2} m_0^2 a^2 \sum_{x\in L} \phi_x^2 + \frac{1}{2} \delta m_1^2 a'^2 \sum_{x\in L'} g(x)\phi_x^2 + \frac{1}{2} \delta m_2^2 a'^2 \sum_{x\in L'} g(x)^2 \phi_x^2 + \frac{\lambda}{4} a'^2 \sum_{x\in L'} g(x)\phi_x^4 .$$

The expectation $\langle\cdot\rangle_L$ is defined, for any real measurable function F on R for which the right-hand side (RHS) is finite, by

$$\langle F\rangle_L = Z_L^{-1} \int \prod_{x\in L} e^{-S_L(\phi)} F(\phi)\, d\phi_x ,$$

where Z_L^{-1} is the normalization constant. If we set

$$V_{L'} = \frac{\lambda}{4} \int_{L'}' g(x)\phi_x^4 dx + \frac{1}{2} \delta m_1^2 \int_{L'}' g(x)\phi_x^2 dx + \frac{1}{2} \delta m_2^2 \int_{L'}' g(x)^2 \phi_x^2 dx,$$

then we have

$$\langle F\rangle_L = \frac{\langle F e^{-V_{L'}}\rangle_{G_{a,L}}}{\langle e^{-V_{L'}}\rangle_{G_{a,L}}}.$$

If $F(\phi)$ is a polynomial in $\{\phi_x,\ x\in L\}$ with positive coefficients and $\tilde{L}\subset aZ^2$ is a lattice containing L, then we know by the second Griffiths inequality[11,17] that

$$\langle F\rangle_L \leqslant \langle F\rangle_{\tilde{L}} .$$

Moreover, $\langle F\rangle_L$ is bounded uniformly in $L\subset aZ^2$. Thus we can define the limit

$$\langle F\rangle^{(a)} = \lim_{L\to aZ^2} \langle F\rangle_L .$$

For convenience we let the integral $\int_L dx$ denote the lattice sum on L with weight a^2 and the integral $\int_{L'}' dx$ denote the lattice sum on L' with weight a'^2. For short we denote $\int_{aZ^2} dx$ and $\int_{a'Z^2} dx$, respectively, by $\int dx$ and $\int' dx$, and write shortly V for $V_{a'Z^2}$. The expectation $\langle F\rangle := \langle F e^{-V}\rangle_{G_a} / \langle e^{-V}\rangle_{G_a}$ is then equal to $\langle F\rangle^{(a)}$. The $2n$-point function $S(x_1,\ldots,x_{2n}) := S^{(a,a')}(x_1,\ldots,x_{2n})$ is defined by

$$S^{(a,a')}(x_1,\ldots,x_{2n}) = \frac{\langle \phi_{x_1}\cdots\phi_{x_{2n}} e^{-V}\rangle_{G_a}}{\langle e^{-V}\rangle_{G_a}}. \tag{2.3}$$

We will call $S^{(a,a')}(x_1,\ldots,x_{2n})$ the $2n$-point function corresponding to (the spatial cutoff) g.

As in Ref. 5, (5.6), one can derive the following field equation for the 2-point function:

$$S(x,y)=C^{(a)}(x-y)-\delta m_1^2\int' dz g(z)C^{(a)}(x-z)S(z,y)$$
$$-\delta m_2^2\int' dz g(z)^2 C^{(a)}(x-z)S(z,y)-\lambda\int' dz C^{(a)}(x-z)g(z)\langle\phi_z^3\phi_y\rangle. \quad (2.4)$$

We remark that in the case of infinite volume [i.e., $g(x)=1,\forall x\in R^2$] we have $S(x,y)=S(0,y-x)$, and so in this case $S(x,y)$ can be denoted by $S(x-y)$.

Before stating the main theorems, let us first recall some basic results about the original ϕ_2^4 field $\nu_{\lambda,g}$ with spatial cutoff g. For simplicity we shall also denote $\nu_{\lambda,g}$ shortly by ν_λ. Let $g\in C_0(R^2)$ be a given function and μ_0 be the Gaussian measure, "free field measure," on $\mathcal{S}'(R^2)$ with covariance

$$\langle\phi(f_1)\phi(f_2)\rangle_{\mu_0}=\langle f_1,(-\Delta+m_0^2)^{-1}f_2\rangle.$$

Let :: denote the Wick power with respect to μ_0 and set $U(g)=\int_{R^2}g(x):\phi(x)^4:dx$ (for its definition, the reader is referred to Ref. 11). Then the original ϕ_2^4 field $\nu_{\lambda,g}$ with spatial cutoff $g\geqslant 0$ is given by

$$d\nu_{\lambda,g}=\left(\int \exp(-\lambda U(g))d\mu_0\right)^{-1}\exp(-\lambda U(g))d\mu_0.$$

This is a well-defined probability measure on $\mathcal{S}'(R^2)$ absolutely continuous with respect to μ_0 (Refs. 11 and 19).

The main results in this paper are as follows.

Theorem 2.1: Let $g\geqslant 0$ be a given bounded continuous function. Then there exists $\lambda_0>0$ so that for all $\lambda\leqslant\lambda_0$ there are sequences $\{a_n\}_{n\geqslant 1}$, $\{a_n'\}_{n\geqslant 1}$ with $\lim_{n\to\infty}a_n=0$ and $\lim_{n\to\infty}a_n'|\log a_n|^{5/4}<\infty$, and $\{g_n\}_{n\geqslant 1}\subset C_0(R^2)$ with $\lim_{n\to\infty}g_n(x)=g(x)$, $x\in R^2$, such that for any given $f_1,\ldots,f_{2m}\in\mathcal{S}(R^2)$ and $m\geqslant 1$ the following limit exists:

$$S(f_1,\ldots,f_{2m})=:\lim_{n\to\infty}\sum_{x_1,\ldots,x_{2m}\in a_nZ^2}S^{(a_n,a_n')}(x_1,\ldots,x_{2m})\prod_{i=1}^{2m}a_n^2f_i(x_i),$$

where $S^{(a_n,a_n')}(x_1,\ldots,x_{2m})$ is the $2m$-point function corresponding to the function g_n, defined by (2.3). Moreover, there is a probability measure $\mu_{\lambda,g}$ on $\mathcal{S}'(R^2)$ satisfying

$$\int_{\mathcal{S}'(R^2)}\phi(f_1)\cdots\phi(f_{2m})\mu_{\lambda,g}(d\phi)=S(f_1,\ldots,f_{2m}),\quad f_1,\ldots,f_{2m}\in\mathcal{S}(R^2),\ m\geqslant 1.$$

Remark: If $g(x)=1$, $\forall x\in R^2$, then $\mu_{\lambda,g}$ given in the above theorem is a continuum ϕ_2^4-quantum field in the infinite-volume case (i.e., without a spatial cutoff). If $g(\geqslant 0)\in C_0(R^2)$, then $\mu_{\lambda,g}$ given in the above theorem is a continuum ϕ_2^4-quantum field with spatial cutoff g. For simplicity we shall also denote $\mu_{\lambda,g}$ shortly by μ_λ.

If $\limsup_{a\to 0^+}a'|\log a|^{1+\epsilon}<\infty$ for some $\epsilon\in(0,1/4)$, then with an analogous procedure it should be possible to define new counterterms and prove the existence of the continuum limit of the new lattice ϕ_2^4 fields (by subsequences) with these new counterterms. In the Appendix we will discuss the case $\lim_{a\to 0^+}a'|\log a|^{7/6}<\infty$.

Remark: Our construction of a continuum limit for a lattice model yields models satisfying all Euclidean axioms,[20–23] except possibly for the axiom of rotation invariance (this is a problem common to all constructions of Euclidean quantum field models starting from lattices). In case the limit can be identified with some models constructed in other ways, the rotation invariant can be verified; see below.

The next theorem tells us that the continuum ϕ_2^4 field $\mu_{\lambda,g}$ in many cases coincides with the original ϕ_2^4 field $\nu_{\lambda,g}$.

Theorem 2.2: Assume that $g \in C_0^1(R^2)$ is non-negative, $\int_{R^2} g_x^2 dx$ is strictly positive, and $\lambda > 0$ is sufficient small. If $\lim_{n\to\infty} a_n' |\log a_n|^2 = A \in [0,\infty)$, then the measure $\mu_{\lambda,g}$ given in Theorem 2.1 coincides with the original ϕ_2^4 field measure $\nu_{\lambda,g}$.

Remark: The measure $\mu_{\lambda,g}$ in the case where $\lim_{a\to 0^+} a' |\log a|^2 = +\infty$ constructed in Theorem 1.1 is believed to be different from the measure $\nu_{\lambda,g}$ for $\lambda > 0$ [see the discussions (iii) and (v) given in Sec. VIII below]. The proof of Theorem 2.2 for $A = 0$ is much easier than the one for $A > 0$. We will prove Theorem 2.2 for $A = 0$ and $A > 0$ in Secs. VI and VII, respectively.

III. SKELETON INEQUALITIES

In this section we first give some correlation inequalities and then use these inequalities to derive some estimates of the 2-point function $S(x-y)$. In Sec. VII below we will give a more precise correlation inequality for the four point function. As in Refs. 14 and 24–26 we consider a model of one-component classical spins on a finite lattice Λ whose partition function is defined by

$$Z = \int e^{(\phi, J\phi)/2} \prod_{j\in\Lambda} g(j)(\phi_j^2) d\phi_j,$$

where $J = (J_{ij})$ is a symmetric matrix, i.e., $J_{ij} = J_{ji}$, $i,j \in \Lambda$, $\phi_j \in R$, $(\phi, J\phi) = \Sigma_{i,j\in\Lambda} J_{ij}\phi_i\phi_j$. We only consider the ferromagnetic case $J_{ij} \geqslant 0$, $\forall i,j$, and set

$$g(j)(\phi^2) = \exp\left(-\frac{\lambda_j}{4!}\phi^4 - \frac{B_j}{2}\phi^2 \right),$$

for some constants $\lambda_j \in R_+$, $B_j > 0$.

Let

$$\langle \phi_{x_1} \cdots \phi_{x_n} \rangle = Z^{-1} \int \phi_{x_1} \cdots \phi_{x_n} e^{(\phi, J\phi)/2} \prod_j g(j)(\phi_j^2) d\phi_j,$$

$x_i \in \Lambda$, $i = 1, \ldots, n$ (from now on we indicate sums and products over Λ simply by Σ_j, respectively, Π_j).

Set

$$U_4(x_1,x_2,x_3,x_4) = \langle \phi_{x_1}\phi_{x_2}\phi_{x_3}\phi_{x_4} \rangle - \langle \phi_{x_1}\phi_{x_2} \rangle \langle \phi_{x_3}\phi_{x_4} \rangle - \langle \phi_{x_1}\phi_{x_3} \rangle \langle \phi_{x_2}\phi_{x_4} \rangle - \langle \phi_{x_1}\phi_{x_4} \rangle \times \langle \phi_{x_2}\phi_{x_3} \rangle.$$

For the special case where the constants λ_j and B_j are independent of the site j, Brydges *et al.*[24] already derived some inequalities for $U_4(x_1,x_2,x_3,x_4)$ in terms of the 2-point functions. The proof of these skeleton inequalities is based on the random walk representation of the correlation functions.[3,26–28] As remarked in Ref. 24, p. 123, the arguments given in Ref. 24 are still suitable for the general cases where λ_j and B_j depend on the site j. Also instead of U_4 one can consider U_n for general n, but for simplicity we will only give the inequalities for U_4. In fact we can use the arguments given in Ref. 24 to derive the following correlation inequalities:

$$U_4(x_1,x_2,x_3,x_4) \leqslant 0, \tag{3.1}$$

$$U_4(x_1,x_2,x_3,x_4) \geqslant -\sum_z \lambda_z \langle \phi_{x_1}\phi_z \rangle \langle \phi_{x_2}\phi_z \rangle \langle \phi_{x_3}\phi_z \rangle \langle \phi_{x_4}\phi_z \rangle, \tag{3.2}$$

$$U_4(x_1,x_2,x_3,x_4)\leqslant -\sum_z \lambda_z\langle\phi_{x_1}\phi_z\rangle\langle\phi_{x_2}\phi_z\rangle\langle\phi_{x_3}\phi_z\rangle\langle\phi_{x_4}\phi_z\rangle+\frac{1}{2}\sum_{j,k}\lambda_j\lambda_k\langle\phi_{x_1}\phi_j\rangle\langle\phi_{x_2}\phi_j\rangle$$
$$\times\langle\phi_j\phi_k\rangle^2\langle\phi_{x_3}\phi_k\rangle\langle\phi_{x_4}\phi_k\rangle+\frac{1}{2}\sum_{j,k}\lambda_j\lambda_k\langle\phi_{x_1}\phi_j\rangle\langle\phi_{x_3}\phi_j\rangle\langle\phi_j\phi_k\rangle^2\langle\phi_{x_2}\phi_k\rangle$$
$$\times\langle\phi_{x_4}\phi_k\rangle+\frac{1}{2}\sum_{j,k}\lambda_j\lambda_k\langle\phi_{x_1}\phi_j\rangle\langle\phi_{x_4}\phi_j\rangle\langle\phi_j\phi_k\rangle^2\langle\phi_{x_2}\phi_k\rangle\langle\phi_{x_3}\phi_k\rangle. \quad (3.3)$$

The inequality (3.1), which is usually called the Lebowitz inequality, was first obtained by Lebowitz.[29] A further correlation inequality up to the third order will be given in the Appendix. The inequalities (3.1), (3.2), and (3.3) hold first for the finite lattice Λ. However, as in Sec. II we can use DLR equations and Griffiths' first and second inequalities to show that (3.1), (3.2), and (3.3) also hold with Λ replaced by aZ^2, for any $a>0$. In particular, (3.1), (3.2), and (3.3) can be used to discuss the models introduced in Sec. II. For this purpose we set

$$\lambda_j=\begin{cases}0, & j\in aZ^2\backslash a'Z^2,\\ 6\lambda g(j), & j\in a'Z^2,\end{cases}$$

where $g\geqslant 0$ is a given bounded Borel measurable function. By (3.1), (3.2), and (3.3) we can get the following estimates of $S(x,y)$, $x,y\in L$, from Eq. (2.4):

$$S(x,y)\geqslant C(x-y)-\delta m_1^2\int' dzC(x-z)g(z)S(z,y)$$
$$-\delta m_2^2\int' dzg(z)^2C(x-z)S(z,y)-3\lambda\int' dzC(x-z)g(z)\langle\phi_z^2\rangle\langle\phi_z\phi_y\rangle, \quad (3.4)$$

$$S(x,y)\leqslant C(x-y)-\delta m_1^2\int' dzC(x-z)g(z)S(z,y)-\delta m_2^2\int' dzg(z)^2C(x-z)S(z,y)$$
$$-3\lambda\int' dzC(x-z)g(z)\langle\phi_z^2\rangle\langle\phi_z\phi_y\rangle$$
$$+6\lambda^2\int' dzC(x-z)g(z)\int' dz_1g(z_1)\langle\phi_z\phi_{z_1}\rangle^3\langle\phi_{z_1}\phi_y\rangle, \quad (3.5)$$

$$S(x,y)\geqslant C(x-y)-\delta m_1^2\int' dzC(x-z)g(z)S(z,y)-\delta m_2^2\int' dzg_z^2C(x-z)S(z,y)$$
$$-3\lambda\int' dzC(x-z)g(z)\langle\phi_z^2\rangle\langle\phi_z\phi_y\rangle+6\lambda^2\int' dzC(x-z)g(z)\int' dz_1g(z_1)$$
$$\times\langle\phi_z\phi_{z_1}\rangle^3\langle\phi_{z_1}\phi_y\rangle,-54\lambda^3\int' dzC(x-z)g(z)\int' dz_1\int' dz_2g(z_1)g(z_2)$$
$$\times\langle\phi_z\phi_{z_1}\rangle^2\langle\phi_{z_1}\phi_{z_2}\rangle^2\langle\phi_z\phi_{z_2}\rangle\langle\phi_{z_2}\phi_y\rangle, \quad (3.6)$$

where $S(x,y)$ was defined in Sec. II and $C(x-y)=C^{(a)}(x-y)$.

Some Gaussian inequalities[19] will also be useful in the present paper. By means of the random walk representation,[19] Th. 7, and Ref. 24 one can also derive the following relation:

$$S(x_1,\ldots,x_{2n}) \leqslant \sum_{i=2}^{2n} S(x_1,x_i)S(x_2,\ldots,x_{i-1},x_{i+1},\ldots,x_{2n}), \tag{3.7}$$

for any $x_i \in L$, $i=1,\ldots,2n$.

IV. RECURSIVE ESTIMATES FOR THE 2-POINT FUNCTION

Without loss of generality, in this section we assume that the bare mass m_0 is equal to 1. In fact, if $m_0 \neq 1$ [but $m_0 \in (0,\infty)$] and if some statements given before Proposition 4.2 are changed accordingly, then the discussions given in this section are still suitable for the case of general m_0. For convenience, in this section we assume that g is a given function from aZ^2 to R such that

$$0 \leqslant g(x) \leqslant 1, \quad \forall x \in aZ^2.$$

As in Ref. 5 we introduce the notation

$$|||f||| = \|f\|_1 + \|f\|_\infty = a^2 \sum_{x \in aZ^2} |f(x)| + \sup_{x \in aZ^2} |f(x)|.$$

We also introduce the exponentially weighted L^p norms

$$\|f\|_{p,\alpha} = \left(\int_{R^2} |\cosh(\alpha x_1) f(x)|^p dx \right)^{1/p}, \quad |||f|||_\alpha = \|f\|_{1,\alpha} + \|f\|_{\infty,\alpha},$$

where $x=(x_1,x_2)$. Let

$$E^{(a,a')}(x,y) = S^{(a,a')}(x,y) - C^{(a)}(x-y),$$

where $S^{(a,a')}(x,y)$ and $C^{(a)}(x-y)$ were defined in Sec. II. We will only consider the case where both conditions

$$\limsup_{a \to 0^+} a' |\log a|^{5/4} < \infty, \quad \liminf_{a \to 0^+} a' |\log a|^{3/2} = \infty$$

are satisfied. The discussion for the other relevant case (i.e., where $\limsup_{a\to 0^+} a'|\log a|^{3/2} = 0$) is easier [the case where $\limsup_{a\to 0^+} a'|\log a|^{3/2} \in (0,\infty)$ is trivial].

In this section we denote $C^{(a)}(x-y)$ and $S^{(a,a')}(x,y)$, respectively, by $C(x-y)$ and $S(x,y)$. One of the main results in this section is as follows.

Proposition 4.1: Assume $\limsup_{a\to 0^+} a'|\log a|^{5/4} < \infty$. Then there exist polynomials P_i, Q_i, $1 \leqslant i \leqslant 3$, with positive coefficients, independent of a, except for the constant term of Q_2, such that

$$\sup_x |||E_x^{(a,a')}||| \leqslant \sum_{i=1}^{3} \lambda^i P_i(\sup_x |||E_x^{(a,a')}|||), \tag{4.1}$$

$$\sup_x \left\| E_x^{(a,a')} - 6\lambda^2 \int dz C(x-z) g(z) \int dz_1 g(z_1) C(z-z_1)^3 C(z_1-y) \right\|$$

$$\leqslant \sum_{i=1}^{3} \lambda^i Q_i(\sup_x |||E_x^{(a,a')}|||), \tag{4.2}$$

for all $a,a' \in (0,1)$, where $E_x^{(a,a')}(y)=E^{(a,a')}(x,y)$. Moreover, the polynomials P_1 and Q_1 have zero constant term, and Q_2 has a constant term which goes to zero as $a\to 0^+$.

Proof: For short we denote $E^{(a,a')}$ and $E_x^{(a,a')}$, respectively, by E and E_x. Let $C_x*S(y)=\int' dz C_x(z)S(z,y)$, where $C_x(y)=C(x-y)$. It is easy to show by Young's inequality that

$$\|C_x*E\|_1 \leqslant \int' dz C_x(z) \sup_z \|E_z\|_1 \leqslant O(1)\sup_z \|E_z\|_1, \quad \|C_x*E\|_\infty \leqslant O(1)\sup_z \|E_z\|_\infty,$$

which implies that

$$|||C_x*S||| \leqslant |||C_x*C||| + |||C_x*E||| \leqslant O(1)(1+\sup_z |||E_z|||).$$

By (3.5) and (3.6) we know that the term of order λ in the expression $S(x,y)-C(x-y)$ can be bounded by

$$\sup_x \|E_x\|_\infty \cdot |||C_x*S||| \leqslant O(1)\sup_x |||E_x||| \cdot (1+\sup_x |||E_x|||).$$

To consider the term of order λ^2 in the expression $S(x,y)-C(x-y)$, we set

$$f_1(x,y)=6\lambda^2 a'^2 \int' dz C(x-z)g(z)^2 \langle \phi_z \phi_y \rangle \langle \phi_z^2 \rangle^3,$$

$$f_2(x,y)=6\lambda^2 a'^2 \int' dz C(x-z)g(z) \sum_{z_1 \in a'Z^2 \setminus \{z\}} g(z_1)\langle \phi_z \phi_{z_1} \rangle^3 \langle \phi_{z_1} \phi_y \rangle.$$

From the assumption $\limsup_{a\to 0^+} a'|\log a|^{5/4}<\infty$ we can see that $\limsup_{a\to 0^+} a' C^{(a)}(0)=0$ and so $\{a'C^{(a)}(0)\}$ is bounded for all $a\in(0,1)$. For any fixed $x \in aZ^2$, by Young's and Hölder's inequalities we have

$$\begin{aligned}
&\left\| f_1(x,\cdot) - \delta m_2^2 \int' dz C(x-z)g(z)^2 \langle \phi_z \phi_\cdot \rangle \right\| \\
&\quad \leqslant \sup_z \| \delta m_2^2 - 6\lambda^2 a'^2 \langle \phi_z^2 \rangle^3 \|_\infty \cdot |||C_x*S||| \\
&\quad \leqslant 6\lambda^2 \sup_z \|E_z\|_\infty a'^2 [C^2(0)+C(0)\langle \phi_z^2 \rangle + \langle \phi_z^2 \rangle^2] \cdot |||C_x*S||| \\
&\quad \leqslant O(1)\lambda^2 \sup_z [a'^2 C^2(0) + a'^2 \|E_z\|_\infty^2] \|E_z\|_\infty (1+\sup_z |||E_z|||) \\
&\quad \leqslant c\lambda^2 \sup_{z\in aZ^2} |||E_z||| (1+\sup_{z\in aZ^2} |||E_z|||^3),
\end{aligned} \tag{4.3}$$

where the constant $c\in(0,\infty)$ is independent of $x\in aZ^2$. It is clear that this constant c can be chosen to satisfy $\lim_{a\to 0^+} c=0$.

Let $f_{2,x}(y)=f_2(x,y)$. Since $\limsup_{a\to 0^+} a'|\log a|^{5/4}<\infty$ and $C(x-y)$ behaves like $c|\log|x-y||$ as $|x-y|$ goes to zero, we can easily show that

$$\begin{aligned}
\sup_{x\in aZ^2} |||f_{2,x}||| &\leqslant 6\lambda^2 \sup_{x\in aZ^2} \left\| \int' dz C(x-z) a'^2 \sum_{z_1 \in a'Z^2 \setminus \{z\}} S(z,z_1)^3 S(z_1,y) \right\| \\
&\leqslant O(1)\lambda^2 (1+\sup_{z\in aZ^2} |||E_z|||^4).
\end{aligned}$$

Finally we consider the term of order λ^3 on the right-hand side of (3.6). We denote this term by $f_{3,x}(y)$. We remark that $f_{3,x}$ is the summation of the function $C(x-z)g(z)g(z_1)g(z_2)\times\langle\phi_z\phi_{z_1}\rangle^2\langle\phi_{z_1}\phi_{z_2}\rangle^2\langle\phi_z\phi_{z_2}\rangle\langle\phi_{z_2}\phi_y\rangle$ on the set $\{(z,z_1,z_2)\colon z,z_1,z_2\in a'Z^2\}$. Then this summation can be decomposed as

$$\sum_{z=z_1=z_2\in a'Z^2}+\sum_{z=z_1,z_2\neq z}+\sum_{z=z_2,z_1\neq z}+\sum_{z_1=z_2\neq z}+\sum_{z_2\neq z_1,z_2\neq z,z_1\neq z}.$$

Using this expression we get

$$\begin{aligned}\|f_{3,x}\|_\infty\leqslant 54\lambda^3&\left\|\int' dzC(x-z)a'^4\langle\phi_z^2\rangle^5\langle\phi_z\phi_y\rangle\right\|_\infty\\&+54\lambda^3\left\|\int' dzC(x-z)a'^2\langle\phi_z^2\rangle^2\sum_{z_2\neq z}\langle\phi_z\phi_{z_2}\rangle^3\langle\phi_{z_2}\phi_y\rangle\right\|_\infty\\&+54\lambda^3\left\|\int' dzC(x-z)a'^2\langle\phi_z^2\rangle\sum_{z_1\neq z}\langle\phi_z\phi_{z_1}\rangle^4\langle\phi_z\phi_y\rangle\right\|_\infty\\&+54\lambda^3\left\|\int' dzC(x-z)a'^2\sum_{z_2\neq z}\langle\phi_{z_2}^2\rangle^2\langle\phi_z\phi_{z_2}\rangle^3\langle\phi_{z_2}\phi_y\rangle\right\|_\infty\\&+54\lambda^3\left\|\int' dzC(x-z)\sum_{z_1\neq z,z_2\neq z,z_1\neq z_2}\langle\phi_z\phi_{z_1}\rangle^2\langle\phi_{z_1}\phi_{z_2}\rangle^2\langle\phi_z\phi_{z_2}\rangle\langle\phi_{z_2}\phi_y\rangle\right\|_\infty.\end{aligned}$$

Using the assumption $\limsup_{a\to 0^+}a'|\log a|^{5/4}<\infty$ and the above estimate we show that

$$\sup_{x\in aZ^2}\|f_{3,x}\|_\infty\leqslant O(1)(1+\sup_{x\in aZ^2}\|E_x\|_\infty^6).$$

By a similar argument as above we obtain

$$\sup_{x\in aZ^2}\|f_{3,x}\|_1\leqslant O(1)(1+\sup_{x\in aZ^2}\|E_x\|_1^6).$$

Therefore,

$$\sup_{x\in aZ^2}|\|f_{3,x}\||\leqslant O(1)(1+\sup_{x\in aZ^2}|\|E_x\||^6),$$

which proves (4.1).

If $\limsup_{a\to 0^+}a'|\log a|^{5/4}<\infty$, then we see that there exists $\epsilon(a)\in(0,\infty)$ with $\lim_{a\to 0^+}\epsilon(a)=0$ such that

$$\left|\left\|\int' dzC(x-z)g(z)a'^2\sum_{z_1\in a'Z^2\setminus\{z\}}g(z_1)C(z-z_1)^3C(z_1-y)-\int dzC(x-z)g(z)\int dz_1g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\leqslant\epsilon(a).$$

Using this estimate we derive the inequality

$$\begin{aligned}
&\left\|\left\| \int' dzC(x-z)g(z)a'^2 \sum_{z_1\in a'Z^2\setminus\{z\}} g(z_1)\langle\phi_z\phi_{z_1}\rangle^3\langle\phi_{z_1}\phi_y\rangle \right.\right.\\
&\qquad \left.\left. - \int dzC(x-z)g(z)\int dz_1 g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\\
&\leqslant \left\|\left\| \int' dzC(x-z)g(z)a'^2 \sum_{z_1\in a'Z^2\setminus\{;z\}} g(z_1)\langle\phi_z\phi_{z_1}\rangle^3\langle\phi_{z_1}\phi_y\rangle \right.\right.\\
&\qquad \left.\left. - \int' dzC(x-z)g(z)a'^2 \sum_{z_1\in a'Z^2\setminus\{z\}} g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\\
&\qquad + \left\|\left\| \int' dzC(x-z)g(z)a'^2 \sum_{z_1\in a'Z^2\setminus\{z\}} g(z_1)C(z-z_1)^3C(z_1-y) \right.\right.\\
&\qquad \left.\left. - \int dzC(x-z)g(z)\int dz_1 g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\\
&\leqslant \epsilon(a) + C\lambda(1+\sup_{x\in aZ^2}|||E_x|||^4).
\end{aligned}$$

Thus, by (4.3) we know that

$$\begin{aligned}
&\left\|\left\| f_1(x,y)+f_2(x,y)-6\lambda^2\int dzC(x-z)g(z)\int dz_1 g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\\
&\qquad \leqslant [\epsilon(a)+C\sup_{x\in aZ^2}|||E_x|||(1+\sup_{x\in aZ^2}|||E_x|||^3)]\lambda^2 + C\lambda^3(1+\sup_{x\in aZ^2}|||E_x|||^4), \qquad (4.4)
\end{aligned}$$

where the constant $C\in(0,\infty)$ is independent of $x\in aZ^2$. On the other hand, using the assumption $\limsup_{a\to 0^+} a'|\log a|^{5/4}<\infty$ we prove that

$$|||f_{3,x}|||\leqslant C\lambda^3(1+\sup_{x\in aZ^2}|||E_x|||^6).$$

Combining this with (4.4) we can get the desired result (4.2). The proof of Proposition 4.1 is then complete. ■

To state the next result, we let $m_0^{(a)}>0$ be the unique solution of

$$1+2a^{-2}(1-\cosh(am_0^{(a)}))=0.$$

By a Paley–Wiener theorem,[30] $C^{(a)}(x)$ decays roughly as $\exp(-m_0^{(a)}|x_1|)$ in the x_1 direction. One can show that $m_0^{(a)}<m_0=1$ for $a\in(0,1)$ and $\lim_{a\to 0^+} m_0^{(a)}=m_0=1$.

The other result in this section is as follows.

Proposition 4.2: Let $\delta\in(0,1)$ be given. There are polynomials P_i, Q_i for $1\leqslant i\leqslant 3$ with positive coefficients, independent of a, except for the constant term of Q_2, such that

$$\begin{aligned}
\sup_x|||E_x^{(a,a')}|||_\alpha &\leqslant \sum_{i=1}^3 \lambda^i P_i(\sup_x|||E_x^{(a,a')}|||_\alpha)\\
&\quad \times \sup_x\left\|\left\| E_x^{(a,a')} - 6\lambda^2\int dzC(x-z)g(z)\int dz_1 g(z_1)C(z-z_1)^3C(z_1-y)\right\|\right|\\
&\leqslant \sum_{i=1}^3 \lambda^i Q_i(\sup_x|||E_x^{(a,a')}|||_\alpha) \qquad (4.5)
\end{aligned}$$

for all $a,a' \in (0,1)$ and $\alpha \in (0,(1-\delta)m_0^{(a)})$, where the polynomials P_1 and Q_1 have zero constant term, and Q_2 has a constant term which goes to zero as $a \to 0^+$.

Some technical points in the proof of Proposition 4.2 were mentioned in the proof of Ref. 5, Theorem 7.2. The detailed proof of Proposition 4.2 is quite similar to that of above Proposition 4.1, hence it is omitted.

V. CONTINUUM LIMIT

In this section we always assume $\limsup_{a\to 0^+} a'|\log a|^{5/4} < \infty$. The main aim of this section is to complete the proof of Theorem 2.1. Let us first introduce a notation. In Sec. II we already introduced the counterterms δm_1^2 and δm_2^2, and defined a quantity $V_{L'}$ by means of δm_1^2 and δm_2^2. By means of this $V_{L'}$ we defined in Sec. II a lattice field on aZ^2 whose covariance function (i.e., 2-point function) is $S^{(a,a')}(x,y)$. Now we replace δm_1^2 and δm_2^2, respectively, by the real-valued variables ϵ_1 and ϵ_2. We can then construct a corresponding lattice field on aZ^2 and we shall denote the covariance function of this new lattice field by $S^{(\lambda,\epsilon_1,\epsilon_2)}(x,y)$.

We will first use Propositions 4.1 and 4.2 to derive some estimates on $S^{(a,a')}(x,y)$. To this end, as in Ref. 5 we need to prove the continuity of $S^{(a,a')}(x,y)$ with respect to $\lambda > 0$. Since δm_1^2 and δm_2^2 are continuous with respect to $\lambda > 0$, it suffices to prove the continuity of $S^{(\lambda,\epsilon_1,\epsilon_2)}(x,y)$ with respect to $(\lambda,\epsilon_1,\epsilon_2)$. Let

$$\mathcal{B} = \{(\lambda,\epsilon_1,\epsilon_2):\ \lambda > 0, \epsilon_1,\epsilon_2 \in R\} \cup \{(\lambda,\epsilon_1,\epsilon_2):\ \lambda = 0, \epsilon_1,\epsilon_2 > 0\}.$$

We first state two lemmas.

Lemma 5.1: Let the lattice spacing $a \in (0,1)$ and the function $g(\geqslant 0) \in C_0(R^2)$ be given. Then the following statements are true.

(i) The set

$$\mathcal{B}_0 = \{(\lambda,\epsilon_1,\epsilon_2) \in \mathcal{B}:\ \sup_{x\in aZ^2} \|S^{(\lambda,\epsilon_1,\epsilon_2)}(x,\cdot)\|_1 < \infty\}$$

is a nonempty, connected, and open subset of $\mathcal{B}$.

(ii) The map $(\lambda,\epsilon_1,\epsilon_2) \to \sup_{x\in aZ^2} \|S^{(\lambda,\epsilon_1,\epsilon_2)}(x,\cdot)\|_1$ is continuous from $\mathcal{B}$ to $[0,+\infty]$, and also continuous from $\mathcal{B}_0$ to $[0,\infty)$.

Since we already assumed in Lemma 5.1 that the function $g \geqslant 0$ has a compact support (i.e., that we are in the finite-volume case), this lemma can easily be proven (see the proof of Ref. 5, Proposition 5.1). For the infinite-volume case, the corresponding result was proven in Ref. 26, Proposition 5.1. In that case, the 2-point function $S^{(\lambda,\epsilon_1,\epsilon_2)}(x,y)$ only depends on $x-y$ (since it is translation invariant).

Similarly, we have the following result.

Lemma 5.2: Let the lattice spacing $a \in (0,1)$ and the function $g(\geqslant 0) \in C_0(R^2)$ be given. Then, for each $\alpha \geqslant 0$, the following statements are true.

(i) The set

$$\mathcal{B}_\alpha = \{(\lambda,\epsilon_1,\epsilon_2) \in \mathcal{B}:\ \sup_{x\in aZ^2} \|S^{(\lambda,\epsilon_1,\epsilon_2)}(x,\cdot)\|_{1,\alpha} < \infty\}$$

is a nonempty, connected and open subset of $\mathcal{B}$.

(ii) The map $(\lambda,\epsilon_1,\epsilon_2) \to \sup_{x\in aZ^2} \|S^{(\lambda,\epsilon_1,\epsilon_2)}(x,\cdot)\|_{1,\alpha}$ is continuous from $\mathcal{B}$ to $[0,\infty]$ and also continuous from $\mathcal{B}_\alpha$ to $[0,\infty)$.

Some technical points in the proof of Lemma 5.2 were already mentioned in the proof of Ref. 5, Proposition 7.1, so we will also omit the proof of Lemma 5.2.

For short, in this section we shall denote $C^{(a)}(x-y)$ and $S^{(a,a')}(x,y)$, respectively, by $C(x-y)$ and $S(x,y)$.

By Lemma 5.1 and Lemma 5.2 we know that $\sup_{x\in aZ^2}|||E_x|||$ and $\sup_{x\in aZ^2}|||E_x|||_\alpha$ are continuous with respect to $\lambda>0$ if $a\in(0,1)$ and $g(\geqslant 0)\in C_0(R^2)$ are fixed. Using these continuity properties together with Proposition 4.1 and Proposition 4.2 we can easily prove the following results (for their proofs, the reader is referred, respectively, to the proofs of Ref. 5, Theorem 6.1 and Theorem 7.2).

Proposition 5.3: There exist universal constants $\lambda_0>0$, $c_1,c_2\in(0,\infty)$ such that, for $0\leqslant\lambda\leqslant\lambda_0$,

$$\sup_{x\in aZ^2}|||S(x,\cdot)-C(x-\cdot)|||\leqslant c_1\lambda^2,$$

$$\sup_{x\in aZ^2}\left|\left|\left|S(x,\cdot)-C(x-\cdot)-6\lambda^2\int dzC(x-z)g(z)\int dz_1g(z_1)C(z-z_1)^3C(z_1-\cdot)\right|\right|\right|\leqslant c_2\lambda^3+\epsilon(a)\lambda^2,$$

where $\epsilon(a)>0$ satisfies $\lim_{a\to 0^+}\epsilon(a)=0$, and $g\in C_0(R^2)$ satisfies $0\leqslant g\leqslant 1$.

Proposition 5.4: Let $\delta\in(0,1)$ be given. There exist universal constants $\lambda_0>0$, $c_1,c_2\in(0,\infty)$ such that, for $0\leqslant\lambda\leqslant\lambda_0$ and $\alpha\in(0,(1-\delta)m_0^{(a)}]$,

$$\sup_{x\in aZ^2}|||S(x,\cdot)-C(x-\cdot)|||_\alpha\leqslant c_1\lambda^2,$$

$$\sup_{x\in aZ^2}\left|\left|\left|S(x,\cdot)-C(x-\cdot)-6\lambda^2\int dzC(x-z)g(z)\int dz_1g(z_1)C(z-z_1)^3C(z_1-\cdot)\right|\right|\right|_\alpha\leqslant c_2\lambda^3+\epsilon(a)\lambda^2,$$

where $\epsilon(a)>0$ satisfies $\lim_{a\to 0^+}\epsilon(a)=0$, and $g\in C_0(R^2)$ satisfies $0\leqslant g\leqslant 1$.

Remark: We remark that the polynomials P_i,Q_i for $1\leqslant i\leqslant 3$ given in Proposition 4.1 and Proposition 4.2 do not depend on the choice of g with $g\in C_0(R^2)$ and $0\leqslant g\leqslant 1$. Hence, the constants λ_0, c_1, and c_2 given in Proposition 5.3 and Proposition 5.4 do not depend on the choice of g, if $g\in C_0(R^2)$ and $0\leqslant g\leqslant 1$.

Having these propositions, we can now prove Theorem 2.1.

Proof of Theorem 2.1: By Proposition 5.4 we know that for $\alpha<m_0=1$ there are $c(\alpha)<\infty$ and $\lambda_\alpha>0$ such that

$$\sup_{x\in aZ^2}|||S(x,\cdot)-C(x-\cdot)|||_\alpha\leqslant c(\alpha)\lambda,\qquad 0\leqslant\lambda\leqslant\lambda_\alpha,$$

if $g\in C_0(R^2)$ and $0\leqslant g\leqslant 1$, where $S(x,y)$ is the 2-point function corresponding to the function g, which was defined in Sec. II. Thus, $S(x,y)$ behaves like $C(x-y)$ for $|x-y|\to 0$. By the Gaussian inequality (3.7) we know that (for S defined in Sec. II, with the given g)

$$S(x_1,\ldots,x_{2m})\leqslant\sum_{\pi\in Q_{2m}}\prod_{i=1}^{m}S(x_{\pi(2i-1)},x_{\pi(2i)}),$$

with Q_{2m} the set of all pair partitions of $\{1,2,\ldots,2m\}$. By the bound

$$|S(x,y)|\leqslant K\ C(y-x)$$

for some constant $K\in(0,\infty)$ and for all x,y, we have thus

$$S(x_1,\ldots,x_{2m})\leqslant\sum_{\pi\in Q_{2m}}\prod_{i=1}^{m}K^m\ C(x_{\pi(2i)}-x_{\pi(2i-1)}).$$

By applying the inequality for the function $C(y-x)$, cited in Sec. II, we obtain

$$C(y-x)\leqslant c\ |\log|y-x||,$$

where c is a positive constant. Finally we get

$$S(x_1,\ldots,x_{2m})\leqslant \sum_{\pi\in Q_{2m}}\prod_{i=1}^{m} C\ \ K^m\ \ |\log|x_{\pi(2i)}-x_{\pi(2i-1)}||. \tag{5.1}$$

For any given continuous function g with $0\leqslant g\leqslant 1$, we can find a series $\{g_n\}_{n\geqslant 1}\subset C_0(R^2)$ with $0\leqslant g_n\leqslant 1$ such that g_n increases to g as n increases to ∞. By Eq. (5.1) we can find sequences $\{a_n\}_{n\geqslant 1}$, $\{a_n'\}_{n\geqslant 1}$ with $\lim_{n\to\infty} a_n'|\log a_n|^{5/4}<\infty$ and $\{g_{k_n}\}_{n\geqslant 1}$ with $\lim_{n\to\infty} g_{k_n}(x)=g(x)$, such that the limit

$$\lim_{n\to\infty}\sum_{x_1,\ldots,x_{2m}\in a_nZ^2} S^{(a_n,a_n')}(x_1,\ldots,x_{2m})\prod_{i=1}^{2m} a_n^2 f_i(x_i) \tag{5.2}$$

exists for all $f_1,\ldots,f_{2m}\in\mathcal{S}(R^2)$ and $m\geqslant 1$, where $S^{(a_n,a_n')}(x_1,\ldots,x_{2m})$ is the $2m$-point function corresponding to the function g_{k_n} (of compact supports). We denote the limit (5.2) by $S(f_1,\ldots,f_{2m})$. On the other hand, by the second Griffiths inequality one gets that [see Ref. 5, (8.3)]

$$S^{(a,a')}(x_1,\ldots,x_{2m})\geqslant \frac{1}{(2m-1)!!}\sum_{\pi\in Q_{2m}}\prod_{i=1}^{m} S^{(a,a')}(x_{\pi(2i-1)},x_{\pi(2i)}).$$

This fact tells us that the continuum limits for $S^{(a,a')}(x_1,\ldots,x_{2m})$ are not identically zero. Thus, by (5.1) and Ref. 31, Theorem 1.1, we know that there is a probability measure uniquely determined by its moments μ_λ on $\mathcal{S}'(R^2)$ such that

$$\int_{\mathcal{S}'(R^2)}\phi(f_1)\cdots\phi(f_{2m})\mu_\lambda(d\phi)=S(f_1,\ldots,f_{2m}),\quad f_1,\ldots,f_{2m}\in\mathcal{S}(R^2),\ \ m\geqslant 1.$$

This then completes the proof of Theorem 2.1. ■

VI. PROOF OF THEOREM 2.2 FOR $A=0$

Let us first introduce some notations. As in Ref. 31, let (,) and $\|\ \|$ denote the inner product and the norm in $L^2(R^2)$, respectively, and H_n be the Hermite polynomial of order n. For $n\geqslant 0$, the Hermite function of order n is given by

$$h_n(x)=c_nH_n(x)\exp\left(-\frac{x^2}{2}\right),\quad x\in R,$$

where c_n is a constant for which $\|h_n\|=1$. Then $\{h_n\}_{n\geqslant 0}$ is an orthonomal base in $L^2(R^2)$. For $\beta=(\beta_1,\beta_2)$ with $\beta_1,\beta_2\geqslant 0$, the function $h_\beta\colon R^2\to R$ is defined by

$$h_\beta(x_1,x_2)=h_{\beta_1}(x_1)h_{\beta_2}(x_2).$$

Then $\{h_\beta,\ \beta\geqslant 0\}$ is an orthonormal base in $L^2(R^2)$. The m-norm $\|\cdot\|_m$ in $\mathcal{S}(R^2)$ is defined by

$$\|f\|_m^2=\sum_\beta\ (f,h_\beta)^2(2(\beta_1+\beta_2)+2)^m,\quad f\in\mathcal{S}(R^2),\ \ m\geqslant 0,$$

with $\beta=(\beta_1,\beta_2)$. Let $\Phi_m=\{f\in\mathcal{S}(R^2):\ \|f\|_m<\infty\}$. The $(-m)$-norm $\|\cdot\|_{-m}$ in $\mathcal{S}'(R^2)$ is defined by

$$\|\phi\|_{-m}^2=\sum_{\beta}\ \phi^2(h_\beta)(2(\beta_1+\beta_2)+2)^{-m},\quad \phi\in\mathcal{S}'(R^2).$$

One checks easily that

$$\|\phi\|_{-m}=\sup\{|\phi(f)|:\ f\in\mathcal{S}(R^2),\ \|f\|_m\leqslant 1\}.$$

Let Φ_m' denote the dual space of Φ_m.

In this section we let $g\geqslant 0$ be a given function in $C_0^1(R^2)$ such that $\int_{R^2}|g(x)|dx>0$. The main aim of this section is to complete the proof of Theorem 2.2 in the case where $A=0$. In other words, we will prove that μ_λ for small $\lambda>0$ is equal to the original continuum ϕ_2^4 field ν_λ if $\lim_{a\to 0^+}a'|\log a|^2=0$. For this purpose we first prove a weak convergence (see Lemma 6.1 below).

As in Sec. II, we let μ_0 be the Gaussian measure on $\mathcal{S}'(R^2)$ with the covariance $C=(-\Delta+m_0^2)^{-1}$. We define the function $f_{x,a}(\cdot)$ whose Fourier transform is

$$\hat{f}_{x,a}(k)=\begin{cases}(2\pi)^{-1}e^{-ikx}\mu_a(k)^{-1}\mu(k), & \text{if } |k_i|\leqslant\pi/a,\\ 0, & \text{otherwise,}\end{cases}$$

where $\mu^{-1}(k)=(|k|^2+m_0^2)^{-1}$ and $\mu_a^{-1}(k)=(m_0^2+2a^{-2}\Sigma_{j=1}^2(1-\cos(ak_j)))^{-1}$. It is easy to check that (see Ref. 11, Sec. VIII.1)

$$\langle\phi(f_{x,a})\phi(f_{y,a})\rangle_{\mu_0}=\langle\phi_x\phi_y\rangle_{G_a}.$$

Thus we can realize the Gaussian field ϕ_x on aZ^2 by $\phi_x=\phi(f_{x,a})$, which is well defined on $\mathcal{S}'(R^2)$.

For $\lambda>0$ we set

$$d\mu_{a,a',\lambda}=N_{a,a',\lambda}^{-1}\exp\left(-\frac{\lambda}{4}\int'g(x):\phi_x^4:dx\right)dG_a,$$

where $N_{a,a',\lambda}$ is the normalization constant such that $\mu_{a,a',\lambda}$ is a probability measure. The lattice field $\mu_{a,a',\lambda}$ on aZ^2 can be thought of as a field on $\mathcal{S}'(R^2)$:

$$d\mu_{a,a',\lambda}=N_{a,a',\lambda}^{-1}\exp\left(-\frac{\lambda}{4}\int'g(x):\phi^4(f_{x,a}):dx\right)d\mu_0.$$

It is easy to show that

$$S^{(a,a')}(x_1,\ldots,x_{2n})=\langle\phi(f_{x_1,a})\cdots\phi(f_{x_{2n},a})\rangle_{\mu_{a,a',\lambda}}.$$

Assume that $\lambda>0$ is sufficient small. By Theorem 2.1 we know that there are subsequences $\{a_n\}$ and $\{a_n'\}$ with $\lim_{n\to\infty}a_n'|\log a_n|^{5/4}<\infty$ [here we already assumed $g\in C_0^1(R^2)$] such that

$$S_n(q_1,\ldots,q_{2m}):=a^{4m}\sum_{x_1,\ldots,x_{2m}\in aZ^2}q_1(x_1)\cdots q_{2m}(x_{2m})S^{(a_n,a_n')}(x_1,\ldots,x_{2m})$$

is convergent as $n\to\infty$, where $q_1,\ldots,q_{2m}\in\mathcal{S}(R^2)$ for $m\geqslant 1$. It is clear that $\mu_{a_n,a_n',\lambda}$ can be thought of as a probability measure on $\mathcal{S}'(R^2)$.

The correlation function $\langle \phi(q_1)\cdots\phi(q_{2m})\rangle_{\mu_{a_n,a_n',\lambda}}$ is well defined, but it is not equal to $S_n(q_1,\ldots,q_{2m})$. Let us first prove a lemma.

Lemma 6.1: Assume $\lim_{n\to\infty} a_n'|\log a_n|^{5/4}<\infty$. For sufficiently small $\lambda>0$, $\{\mu_{a_n,a_n',\lambda}\}$ is weakly convergent to μ_λ as $n\to\infty$.

Proof: From the proof of Theorem 2.1 we see that

$$\lim_{n\to\infty} S_n(q_1,\ldots,q_{2m})=\langle \phi(q_1)\cdots\phi(q_{2m})\rangle_{\mu_\lambda}.$$

Thus it suffices to prove that $S_n(q_1,\ldots,q_{2m})$ and $\langle \phi(q_1)\cdots\phi(q_{2m})\rangle_{\mu_{a_n,a_n',\lambda}}$ have the same asymptotic behavior.

By Ref. 11, Theorem VIII.5 (a), p. 263, we know that

$$\langle(\phi(q_i)-\phi_a(q_i))^2\rangle_{\mu_0}\leqslant ca^2$$

for some constant $c\in(0,\infty)$, where $\phi_a(q_i)=a^2\Sigma_{x\in aZ^2}q_i(x)\phi(f_{x,a})$. Using the hypercontractivity (see Ref. 11, Theorem I.22, p. 38) we show that

$$\langle|\phi(q_i)-\phi_a(q_i)|^p\rangle_{\mu_0}^{1/p}\leqslant(p-1)^{1/2}\langle(\phi(q_i)-\phi_a(q_i))^2\rangle_{\mu_0}^{1/2}\leqslant c(p-1)^{1/2}a \tag{6.1}$$

for some constant $c\in(0,\infty)$. It is easy to show that

$$S_n(q_1,\ldots,q_{2m})=\langle \phi_a(q_1)\cdots\phi_a(q_{2m})\rangle_{\mu_{a_n,a_n',\lambda}}.$$

By the Hölder inequality we have

$$\begin{aligned}&|S_n(q_1,\ldots,q_{2m})-\langle \phi(q_1)\cdots\phi(q_{2m})\rangle_{\mu_{a_n,a_n',\lambda}}|\\&\quad\leqslant N_{a_n,a_n',\lambda}^{-1}\left\langle \exp\left(-\frac{p}{p-1}\frac{\lambda}{4}\int' g(x):\phi^4(f_{x,a_n}):dx\right)\right\rangle_{\mu_0}^{1-1/p}\\&\qquad\times\langle|\phi_a(q_1)\cdots\phi_a(q_{2m})-\phi(q_1)\cdots\phi(q_{2m})|^p\rangle_{\mu_0}^{1/p}.\end{aligned}\tag{6.2}$$

We now choose $p=a^{-1/2m}$. It is not difficult to show that there exists a constant $M<\infty$ such that $-\int' g(x):\phi^4(f_{x,a_n}):dx\leqslant M|\log a|^2$. Thus

$$\begin{aligned}\left\langle \exp\left(-\frac{p}{p-1}\frac{\lambda}{4}\int' g(x):\phi^4(f_{x,a_n}):dx\right)\right\rangle_{\mu_0}^{1-1/p}&\leqslant c\left\langle \exp\left(-\frac{\lambda}{4}\int' g(x):\phi^4(f_{x,a_n}):dx\right)\right\rangle_{\mu_0}\\&=cN_{a_n,a_n',\lambda}.\end{aligned}$$

Therefore, the left-hand side of (6.2) is less than

$$c\langle|\phi_a(q_1)\cdots\phi_a(q_{2m})-\phi(q_1)\cdots\phi(q_{2m})|^p\rangle_{\mu_0}^{1-1/p},$$

which by (6.1) goes to zero as $a\to0^+$. This then proves that $\langle \phi(q_1)\cdots\phi(q_{2m})\rangle_{\mu_{a_n,a_n',\lambda}}$ and $S_n(q_1,\ldots,q_{2m})$ have the same asymptotic behavior for $a\to0^+$. By Proposition 5.3 we know that for any given $f\in\mathcal{S}(R^2)$ there are constants $c,c'\in(0,\infty)$ such that

$$\int_{\mathcal{S}'(R^2)} |\phi(f)|\mu_\lambda(d\phi) \leqslant \limsup_{n\to\infty} a_n^4 \sum_{x_1,x_2\in a_n Z^2} f(x_1)f(x_2)S^{(a_n,a_n')}(x_1,x_2)$$

$$\leqslant c \limsup_{n\to\infty} a_n^4 \sum_{x_1,x_2\in a_n Z^2} f(x_1)f(x_2)C^{(a_n)}(x_2-x_1) \leqslant c'. \tag{6.3}$$

Using this we show following, e.g., Ref. 31, Proposition 3.7, that there are $n_0 \geqslant 1$ and $c\in(0,\infty)$ such that, for all $f\in\mathcal{S}(R^2)$,

$$\left| \int |\phi(f)|^p \mu_\lambda(d\phi) \right|^{1/p} \leqslant c\|f\|_{n_0},$$

and there exists $n_1 > n_0$ such that

$$\mu_\lambda(\Phi'_{n_1}) = 1.$$

By (6.3) and Ref. 31, Theorem 2.1, we then know that $\mu_{a_n,a_n',\lambda}$ is weakly convergent to μ_λ for sufficiently small $\lambda>0$, where μ_λ was constructed in Theorem 2.1. ■

We now prove that μ_λ coincides with ν_λ if $\lim_{a\to 0^+} a'|\log a|^2 = 0$. For this purpose we first prove a lemma.

Lemma 6.2: If $\lim_{a\to 0^+} a'|\log a|^2 < \infty$, then there are constants $C, \lambda_1 \in (0,\infty)$ such that

$$\left\langle \exp\left(-\lambda/4 \int' dx g(x) {:}\phi_x^4{:} \right) \right\rangle_{G_a} \leqslant C, \quad \forall a\in(0,1), \lambda\in[0,\lambda_1), \tag{6.4}$$

where $\int' dx$ was defined in Sec. II.

Proof: Let

$$\xi_1 = \int' dx g(x) {:}\phi_x^4{:}, \quad \xi_2 = \int dx g(x) {:}\phi_x^4{:},$$

where $\int dx$ was also defined in Sec. II. For $s\in[0,1]$ and $\lambda>0$, we define a new probability measure $G(s,\lambda)$ by

$$\langle\cdot\rangle_{G(s,\lambda)} = \frac{\left\langle \cdot \exp\left(-\frac{s\lambda}{4}\xi_1 - \frac{(1-s)\lambda}{4}\xi_2 \right) \right\rangle_{G_a}}{\left\langle \exp\left(-\frac{s\lambda}{4}\xi_1 - \frac{(1-s)\lambda}{4}\xi_2 \right) \right\rangle_{G_a}}.$$

As in the proof of Proposition 5.3 we can easily show that there is a constant $\lambda_2>0$ such that

$$|\langle\phi_x\phi_y\rangle_{G(s,\lambda)} - C^{(a)}(x,y)| \leqslant O(1)\lambda, \quad \lambda\in[0,\lambda_2),$$

for any $x,y\in aZ^2$ and $s\in[0,1]$. By the skeleton inequalities given in Sec. III [see, e.g., (3.1) and (3.2)], we know that

$$\langle\phi_x^4\rangle_{G(s,\lambda)} \leqslant 3\langle\phi_x^2\rangle^2_{G(s,\lambda)},$$

$$\langle\phi_x^4\rangle_{G(s,\lambda)} \geqslant 3\langle\phi_x^2\rangle^2_{G(s,\lambda)} - 6s\lambda \int dj g(j) \langle\phi_x\phi_j\rangle^4_{G(s,\lambda)} - 6(1-s)\lambda \int' dj g(j) \langle\phi_x\phi_j\rangle^4_{G(s,\lambda)}. \tag{6.5}$$

We remark that

$$:\phi_x^4:=\phi_x^4-6\langle\phi_x^2\rangle_{G_a}\phi_x^2+3\langle\phi_x^2\rangle_{G_a}^2.$$

Hence, there are constants $c_1,c_2,c_3\in(0,\infty)$ such that

$$\begin{aligned}\langle:\phi_x^4:\rangle_{G(s,\lambda)}&\leqslant 3\langle\phi_x^2\rangle_{G(s,\lambda)}^2-6\langle\phi_x^2\rangle_{G_a}\langle\phi_x^2\rangle_{G(s,\lambda)}+3\langle\phi_x^2\rangle_{G_a}^2\\&\leqslant 3(\langle\phi_x^2\rangle_{G(s,\lambda)}-C^{(a)}(x,x))^2\\&\leqslant c_1\lambda^2,\quad s\in[0,1],\end{aligned}$$

$$\begin{aligned}\langle:\phi_x^4:\rangle_{G(s,\lambda)}&\geqslant 3(\langle\phi_x^2\rangle_{G(s,\lambda)}-C^{(a)}(x,x))^2-O(1)\lambda\int djg(j)C^{(a)}(x,j)^4\\&\quad-O(1)\lambda\int' djg(j)C^{(a)}(x,j)^4\geqslant c_2\lambda^2-c_3\lambda,\qquad s\in[0,1],\end{aligned}$$

if $\lambda\in[0,\lambda_2)$. It follows that there is a constant $c_4\in(0,\infty)$ such that

$$\left|\left\langle\int' dxg(x):\phi_x^4:-\int dxg(x):\phi_x^4:\right\rangle_{G(s,\lambda)}\right|\leqslant c_4\lambda,\quad\forall s\in[0,1],\lambda\in[0,\lambda_2).$$

Therefore, if $\lambda\in[0,\lambda_2)$,

$$\begin{aligned}\left|\left\langle\exp\left(-\frac{\lambda}{4}\xi_1\right)\right\rangle_{G_a}-\left\langle\exp\left(-\frac{\lambda}{4}\xi_2\right)\right\rangle_{G_a}\right|&=\frac{\lambda}{4}\left|\int_0^1(\xi_2-\xi_1)\exp\left(-\frac{s\lambda}{4}\xi_1-\frac{(1-s)\lambda}{4}\xi_2\right)ds\right|\\&\leqslant\frac{c_4\lambda^2}{4}\int_0^1\left\langle\exp\left(\frac{s\lambda}{4}\xi_1-\frac{(1-s)\lambda}{4}\xi_2\right)\right\rangle_{G_a}ds\\&\leqslant\frac{c_4\lambda^2}{4}\left\langle\exp\left(-\frac{\lambda}{4}\xi_1\right)\right\rangle_{G_a}\left\langle\exp\left(-\frac{\lambda}{4}\xi_2\right)\right\rangle_{G_a}\\&\quad\text{(by Hölder's inequality).}\end{aligned}\tag{6.6}$$

On the other hand, it follows from Ref. 11, Theorem VIII.5, p. 263, that there is a constant $c_5\in(0,\infty)$ such that

$$\left\langle\exp\left(-\frac{\lambda}{4}\xi_2\right)\right\rangle_{G_a}\leqslant c_5,\quad\forall\lambda\in[0,\lambda_2).\tag{6.7}$$

Thus, by (6.5) we can easily show that (6.4) is true. The proof of Lemma 6.2 is then complete.■

If $\lim_{a\to0^+}a'|\log a|^2=0$, by (7.1) below we can easily show that there is a constant $c_6\in(0,\infty)$ such that

$$\left\langle\left(\int' dxg(x):\phi^4(f_{x,a}):-\int dxg(x):\phi^4(f_{x,a}):\right)^2\right\rangle_{\mu_0}=\langle(\xi_1-\xi_2)^2\rangle_{G_a}\leqslant c_6(a'^2|\log a|^4+a')\tag{6.8}$$

goes to zero as $a\to0^+$. Thus, by (6.4) and (6.6) we know that $\mu_{a,a',\lambda}$ and $\mu_{a,a,\lambda}$ have the same asymptotic behavior as $a\to0^+$, if $\lim_{a\to0^+}a'|\log a|^2=0$, which proves Theorem 2.2 for $A=0$.■

Remark: We guess that the left-hand side of (6.4) is also bounded on $a\in(0,1)$ if $\limsup_{a\to0^+}a'|\log a|^2<\infty$. This assertion can probably be proven by using the approach exploited in Ref. 6 or 9, where a continuum ϕ_3^4 field was constructed.

VII. PROOF OF THEOREM 2.2 FOR $A>0$

Let us first recall some properties of Wick powers (see Ref. 11, Sec. I.1). If ϕ_x is a Gaussian random variable (under the Gaussian measure G), then

$$:\exp(t\phi_x):=\exp(t\phi_x-\tfrac{1}{2}t^2\langle\phi_x^2\rangle_G),$$

which implies

$$\prod_{i=1}^{n}:\exp(t_i\phi_{x_i}):=\exp\left(\sum_{i=1}^{n}t_i\phi_{x_i}\right)\exp\left(-\frac{1}{2}\sum_{i=1}^{n}t_i^2\langle\phi_{x_i}^2\rangle_G\right)$$
$$=:\exp\left(\sum_{i=1}^{n}t_i\phi_{x_i}\right):\exp\left(\sum_{1\leqslant i<j\leqslant n}t_it_j\langle\phi_{x_i}\phi_{x_j}\rangle_G\right).$$

We remark that $\exp(\Sigma_{1\leqslant i<j\leqslant n}t_it_j\langle\phi_{x_i}\phi_{x_j}\rangle_G)$ is not random and

$$\left\langle:\exp\left(\sum_{i=1}^{n}t_i\phi_{x_i}\right):\right\rangle_G=1.$$

Therefore,

$$\left\langle\prod_{i=1}^{n}:\exp(t_i\phi_{x_i}):\right\rangle_G=\exp\left(\sum_{1\leqslant i<j\leqslant n}t_it_j\langle\phi_{x_i}\phi_{x_j}\rangle_G\right).\tag{7.1}$$

In this section we also let $g\geqslant 0$ be a given function in $C_0^1(R^2)$ such that $\int_{R^2}|g(x)|dx>0$. We always assume in this section that $\lim_{a\to 0^+}a'|\log a|^2\in(0,\infty)$. The main aim of this section is to prove Theorem 2.2 for $A>0$. Many combinatorial results will be used in the following discussions.

We set

$$\xi_1=\int'dxg(x):\phi_x^4:=\int'dxg(x):\phi^4(f_{x,a}):,$$

$$\xi_2=\int dxg(x):\phi_x^4:=\int dxg(x):\phi^4(f_{x,a}):.$$

Let

$$\sigma=4!\int_{R^2}g(x)^2dx\lim_{a\to 0^+}a'^2C^{(a)}(0)^4,$$

where $C^{(a)}(x-y)$ was defined in Sec. II. Let η be a random variable with the normal distribution $N(0,\sigma)$ and P be a probability measure under which η is independent of $U(g)$ and $\{\phi(f),\ f\in\mathcal{S}(R^2)\}$, where $U(g)$ was defined in Sec. II.

The following proposition will play a key role in the proof of Theorem 2.2 for $A>0$.

Proposition 7.1: (i) For any $x\in R$ we have

$$\lim_{a\to 0^+}G_a(\xi_1\leqslant x)=P(U(g)+\eta\leqslant x).$$

(ii) Assume that $\lambda>0$ is sufficient small. For any $f_1,\ldots,f_m\in\mathcal{S}(R^2)$ we have

$$\lim_{a\to 0^+}\langle \phi(f_1)\cdots\phi(f_m)e^{(-\lambda/4)\,\xi_1}\rangle_{\mu_0}=\langle \phi(f_1)\cdots\phi(f_m)e^{(-\lambda/4)[U(g)+\eta]}\rangle_P,$$

where $\langle\cdot\rangle_P$ denotes the expectation with respect to P.

It is easy to show that

$$\lim_{a\to 0^+} a^{2m}\sum_{x_1,\ldots,x_{2m}\in aZ^2} f_1(x_1)\cdots f_m(x_m)\langle \phi_{x_1}\cdots\phi_{x_m}\xi_2^k\rangle_{G_a}=\langle \phi(f_1)\cdots\phi(f_m)U(g)^k\rangle_{\mu_0}.$$

Therefore

$$\lim_{a\to 0^+}\langle(\xi_2+\eta)^k\rangle_P=\sum_{i=0}^{k}\binom{i}{k}\langle U(g)^i\rangle_P\langle\eta^{k-i}\rangle_P,$$

$$\lim_{a\to 0^+} a^{2m}\sum_{x_1,\ldots,x_m\in aZ^2} f_1(x_1)\cdots f_m(x_m)\langle \phi(f_{x_1,a})\cdots\phi(f_{x_m,a})(\xi_2+\eta)^k\rangle_P$$
$$=\langle \phi(f_1)\cdots\phi(f_m)(U(g)+\eta)^k\rangle_P,$$

where $\binom{i}{k}=[k(k-1)\cdots(k-i+1)]/i!$. Thus, by Lemma 6.2 we can see that Proposition 7.1 is a consequence of the following relations:

$$\lim_{a\to 0^+}(\langle\xi_1^k\rangle_{G_a}-\langle(\xi_2+\eta)^k\rangle_P)=0, \tag{7.2}$$

$$\lim_{a\to 0^+}(\langle \phi_{x_1}\cdots\phi_{x_m}\xi_1^k\rangle_{G_a}-\langle \phi_{x_1}\cdots\phi_{x_m}(\xi_2+\eta)^k\rangle_P)=0 \tag{7.3}$$

for all $k\geqslant 0$, where $x_1,\ldots,x_m\in aZ^2$ with $\#\{x_1,\ldots,x_m\}=m$. We prove only (7.2) in detail; (7.3) can be proven by a similar argument.

To prove (7.2) we need to compute the quantity $\langle\xi_1^k\rangle_{G_a}$. We remark that

$$\langle\xi_1^k\rangle_{G_a}=a'^{2k}\sum_{x_1,\ldots,x_k\in a'Z^2} g(x_1)\cdots g(x_k)\langle:\phi_{x_1}^4:\cdots:\phi_{x_k}^4:\rangle_{G_a}.$$

Thus, it suffices to compute $\langle:\phi_{x_1}^4:\cdots:\phi_{x_k}^4:\rangle_{G_a}$. For this purpose we now compare the terms with the coefficient $\Pi_{i=1}^k t_i^4$ on both sides of (7.1). In general, the term with the coefficient $\Pi_{i=1}^k t_i^4$ on the right-hand side of (7.1) can be expressed as a sum of some quantities of the following form

$$q_{a,a'}(x_1,\ldots,x_k):=\mathcal{C}_k\prod_{j=2}^{k}\langle \phi_{x_1}\phi_{x_j}\rangle_{G_a}^{l_{1,j}}\prod_{j=3}^{k}\langle \phi_{x_2}\phi_{x_j}\rangle_{G_a}^{l_{2,j}}\cdots\prod_{j=k-1}^{k}\langle \phi_{x_{k-2}}\phi_{x_j}\rangle_{G_a}^{l_{k-2,j}}\langle \phi_{x_{k-1}}\phi_{x_k}\rangle_{G_a}^{l_{k-1,k}},$$

where $\mathcal{C}_k$ is just the coefficient, $l_{i,j}\in\{0,1,2,3,4\}$, $\Sigma_{j=2}^k l_{1,j}=4$, and

$$\sum_{j=1}^{i-1} l_{j,i}+\sum_{j=i+1}^{k} l_{i,j}=4,\quad i=2,\ldots,k-1.$$

We remark that there is a one-to-one correspondence between the quantity $q_{a,a'}$ and the set of $l_{i,j}$. For convenience we will use the set of $l_{i,j}$ to represent the quantity $q_{a,a'}$.

Let

$$Q_{a,a'}(x_1,\ldots,x_k)=\sum_{l_{i,j}<4} q_{a,a'}(x_1,\ldots,x_k),$$

where the sum is taken over all $l_{i,j}$ with $l_{i,j}\in\{0,1,2,3\}$. If there is no such $l_{i,j}$, then we set $Q_{a,a'}(x_1,\ldots,x_k)=0$. Let

$$Q_k=\lim_{a\to 0^+} a^{2k}\sum_{x_1,\ldots,x_k\in aZ^2} g(x_1)\cdots g(x_k)Q_{a,a}(x_1,\ldots,x_k).$$

It is easy to prove that the latter limit indeed exists and is equal to

$$\lim_{a\to 0^+} a'^{2k}\sum_{x_1,\ldots,x_k\in a'Z^2} g(x_1)\cdots g(x_k)Q_{a,a'}(x_1,\ldots,x_k).$$

Let us first prove a lemma.

Lemma 7.2: For any $k\geqslant 2$ we have

$$\lim_{a\to 0^+}\langle\xi_2^k\rangle_{G_a}=\langle U(g)^k\rangle_{\mu_0}=\sum_{m=0}^{[k/2]}\binom{2m}{k}(2m-1)!!\langle U(g)^2\rangle_{\mu_0}^m Q_{k-2m},$$

where $(2m-1)!!=(2m-1)\cdots 3\times 1$.

Proof: The first equality is easy to prove. We only prove the second equality. As explained before, we use the set $\{l_{i,j}\}$ to represent the quantity $q_{a,a'}(x_1,\ldots,x_k)$. Let $m=\#\{(i,j):\ l_{i,j}=4\}$ and

$$F_m(a,a')=\sum_{\#\{(i,j):l_{i,j}=4\}=m} a'^{2k}\sum_{x_1,\ldots,x_k\in a'Z^2} g(x_1)\cdots g(x_k)q_{a,a'}(x_1,\ldots,x_k).$$

Then, $\langle\xi_2^k\rangle_{G_a}$ is equal to

$$a^{2k}\sum_{x_1,\ldots,x_k\in aZ^2} g(x_1)\cdots g(x_k)\langle:\phi_{x_1}^4:\cdots:\phi_{x_k}^4:\rangle_{G_a}=\sum_{m=0}^{[k/2]}F_m(a,a).$$

We already know that

$$\lim_{a\to 0^+}F_0(a,a)=\lim_{a\to 0^+}a^{2k}\sum_{x_1,\ldots,x_k\in aZ^2} g(x_1)\cdots g(x_k)Q_{a,a}(x_1,\ldots,x_k)=Q_k.$$

We now consider $F_m(a,a)$ for $m\in[1,[k/2]]$. For $m\in[1,[k/2]]$ we can choose a subset $\{i_1,i_2,\ldots,i_{2m-1},i_{2m}\}$ from the set $\{1,2,\ldots,k\}$ such that $l_{s,t}=4$, if $s<t\in\{i_1,\ldots,i_{2m}\}$. It is clear that there are $\binom{2m}{k}$ choices of such subsets. For such a fixed subset $\{i_1,i_2,\ldots,i_{2m-1},i_{2m}\}$ we can construct m pairs $(j_1,j_2),\ldots,(j_{2m-1},j_{2m})$ with $\{j_1,\ldots,j_{2m}\}=\{i_1,\ldots,i_{2m}\}$. It is clear that there are $(2m-1)!!$ choices of such pairs. Moreover, by (7.1) we easily prove that

$$\begin{aligned}&\lim_{a\to 0^+}a^4\sum_{x_1,x_2\in aZ^2} g(x_1)g(x_2)\langle:\phi_{x_1}^4::\phi_{x_2}^4:\rangle_{G_a}\\&\quad=\lim_{a\to 0^+}4!a^4\sum_{x_1,x_2\in aZ^2} g(x_1)g(x_2)\langle\phi_{x_1}\phi_{x_2}\rangle_{G_a}^4\\&\quad=\langle U(g)^2\rangle_{\mu_0}.\end{aligned}$$

From the above discussions we see that $\lim_{a\to 0^+}\langle\xi_2^k\rangle_{G_a}$ is equal to

$$\lim_{a\to 0^+}\sum_{m=0}^{[k/2]}\binom{2m}{k}\sum_{l_{j_1,j_2}=\cdots=l_{j_{2m-1},j_{2m}}=4} a^{4m}(4!)^m \sum_{x_{j_1},\ldots,x_{j_{2m}}\in aZ^2} g(x_{j_1})\cdots g(x_{j_{2m}})\langle \phi_{x_{j_1}}\phi_{x_{j_2}}\rangle_{G_a}^4\cdots$$

$$\times\langle \phi_{x_{j_{2m-1}}}\phi_{x_{j_{2m}}}\rangle_{G_a}^4 a^{2k-4m}\sum_{x_{t_1},\ldots,x_{t_{k-2m}}\in aZ^2} g(x_{t_1})\cdots g(x_{t_{k-2m}})Q_{a,a}(x_{t_1},\ldots,x_{t_{k-2m}})$$

$$=\sum_{m=0}^{[k/2]}\binom{2m}{k}(2m-1)!!\langle U(g)^2\rangle_{\mu_0}^m Q_{k-2m},$$

where $\{t_1,\ldots,t_{k-2m}\}=\{1,2,\ldots,k\}\backslash\{j_1,j_2,\ldots,j_{2m}\}$. This then completes the proof of Lemma 7.2.■

We now turn to the proof of (7.2). It is clear that (7.2) holds for $k=0$ and 1. Let us first prove (7.2) for $k=2$. By (7.1) we know that $\langle :\phi_x^4::\phi_y^4:\rangle_{G_a}=4!C^{(a)}(x-y)^4$. Hence

$$\langle \xi_1^2\rangle_{G_a}=a'^4\sum_{x,y\in a'Z^2} g(x)g(y)\langle :\phi_x^4::\phi_y^4:\rangle_{G_a}$$

$$=4!a'^4\sum_{x,y\in a'Z^2} g(x)g(y)C^{(a)}(x-y)^4$$

$$=4!a'^2C^{(a)}(0)^4a'^2\sum_{x\in a'Z^2} g(x)^2+4!a'^4\sum_{x,y\in a'Z^2,x\neq y} g(x)g(y)C^{(a)}(x-y)^4.$$

Since $\lim_{a\to 0^+} a'|\log a|^2\in(0,\infty)$, it is easy to show that

$$\lim_{a\to 0^+} 4!a'^4\sum_{x,y\in a'Z^2,x\neq y} g(x)g(y)C^{(a)}(x-y)^4$$

$$=\lim_{a\to 0^+} 4!a^4\sum_{x,y\in aZ^2} g(x)g(y)C^{(a)}(x-y)^4$$

$$=\langle U(g)^2\rangle_{\mu_0}.$$

In other words, we have

$$\lim_{a\to 0^+}\left(4!a'^4\sum_{x,y\in a'Z^2,x\neq y} g(x)g(y)C^{(a)}(x-y)^4-\langle \xi_2^2\rangle_{G_a}\right)=0.$$

Moreover,

$$\lim_{a\to 0^+} 4!a'^2C^{(a)}(0)^4a'^2\sum_{x\in a'Z^2} g(x)^2=\langle \eta^2\rangle_P=\sigma.$$

Therefore,

$$\lim_{a\to 0^+}(\langle \xi_1^2\rangle_{G_a}-\langle \eta^2\rangle_P-\langle \xi_2^2\rangle_{G_a})=0,$$

which implies (7.2) for $k=2$, since $\langle(\eta+\xi_2)^2\rangle_P=\langle \eta^2\rangle_P+\langle \xi_2^2\rangle_{G_a}$.

We now prove (7.2) for the general case. From the proof of Lemma 7.2 we see that

$$\langle \xi_1^k \rangle_{G_a} = \sum_{m=0}^{[k/2]} F_m(a,a')$$

$$= \sum_{m=0}^{[k/2]} \binom{2m}{k} \sum_{l_{j_1,j_2}=\cdots=l_{j_{2m-1},j_{2m}}=4} a'^{4m} (4!)^m \sum_{x_{j_1},\ldots,x_{j_{2m}} \in a'Z^2} g(x_{j_1}) \cdots g(x_{j_{2m}})$$

$$\times \langle \phi_{x_{j_1}} \phi_{x_{j_2}} \rangle_{G_a}^4 \cdots \langle \phi_{x_{j_{2m-1}}} \phi_{x_{j_{2m}}} \rangle_{G_a}^4 a'^{2k-4m}$$

$$\times \sum_{x_{t_1},\ldots,x_{t_{k-2m}} \in a'Z^2} g(x_{t_1}) \cdots g(x_{t_{k-2m}}) Q_{a,a'}(x_{t_1},\ldots,x_{t_{k-2m}}).$$

From the proof of (7.2) for $k=2$ we also see that

$$\lim_{a \to 0^+} 4! a'^4 \sum_{x_{j_{2i-1}}, x_{j_{2i}} \in a'Z^2} g(x_{j_{2i-1}}) g(x_{j_{2i}}) \langle \phi_{x_{j_{2i-1}}} \phi_{x_{j_{2i}}} \rangle_{G_a}^4 = \langle \eta^2 \rangle_P + \langle U(g)^2 \rangle_{\mu_0}.$$

Using this we easily show that

$$\lim_{a \to 0^+} (4!)^m a'^{4m} \sum_{x_{j_1},\ldots,x_{j_{2m}} \in a'Z^2} g(x_{j_1}) \cdots g(x_{j_{2m}}) \langle \phi_{x_{j_1}} \phi_{x_{j_2}} \rangle_{G_a}^4 \cdots \langle \phi_{x_{j_{2m-1}}} \phi_{x_{j_{2m}}} \rangle_{G_a}^4$$

$$= \sum_{l=0}^{m} \binom{l}{m} \langle \eta^2 \rangle_P^l \langle U(g)^2 \rangle_{\mu_0}^{m-l}.$$

It is clear that

$$\lim_{a \to 0^+} a'^{2k-4m} \sum_{x_{t_1}\ldots,x_{t_{k-2m}} \in a'Z^2} g(x_{t_1}) \cdots g(x_{t_{k-2m}}) Q_{a,a'}(x_{t_1},\ldots,x_{t_{k-2m}}) = Q_{k-2m}.$$

It follows, inserting this result in above expression for $\langle \xi_1^k \rangle_{G_a}$,

$$\lim_{a \to 0^+} \langle \xi_1^k \rangle_{G_a} = \sum_{m=0}^{[k/2]} \binom{2m}{k} (2m-1)!! \sum_{l=0}^{m} \binom{l}{m} \langle \eta^2 \rangle_P^l \langle U(g)^2 \rangle_{\mu_0}^{m-l} Q_{k-2m}. \tag{7.4}$$

By computation we know that the right-hand side of (7.4) is equal to

$$\sum_{l=0}^{[k/2]} \sum_{m=l}^{[k/2]} \binom{l}{m} \binom{2m}{k} (2m-1)!! \langle \eta^2 \rangle_P^l \langle U(g)^2 \rangle_{\mu_0}^{m-l} Q_{k-2m}$$

$$= \sum_{l=0}^{[k/2]} \binom{2l}{k} (2l-1)!! \langle \eta^2 \rangle_P^l \sum_{m=l}^{[k/2]} \frac{(k-2l)\cdots(k-2m+1)}{2^{m-l}(m-l)!} \langle U(g)^2 \rangle_{\mu_0}^{m-l} Q_{k-2m}$$

$$= \sum_{l=0}^{[k/2]} \binom{2l}{k} (2l-1)!! \langle \eta^2 \rangle_P^l \sum_{m=0}^{[(k-2l)/2]} \binom{2m}{k-2l} (2m-1)!! \langle U(g)^2 \rangle_{\mu_0}^{m} Q_{k-2l-2m},$$

which is equal by Lemma 7.2 to

$$\sum_{l=0}^{[k/2]} \binom{2l}{k} (2l-1)!! \langle \eta^2 \rangle_P^l \langle U(g)^{k-2l} \rangle_{\mu_0} = \langle [\eta + U(g)]^k \rangle_P.$$

This then completes the proof of (7.2), since $\lim_{a\to 0^+}\langle(\eta+\xi_2)^k\rangle_P=\langle[\eta+U(g)]^k\rangle_P$. Thus we also have completed the proof of Proposition 7.1. ■

Proof of Theorem 2.2 for A>0: By Lemma 6.1 and Lemma 6.2 we easily show that if $\lambda>0$ is sufficient small,

$$\lim_{a\to 0^+}\left\langle \exp\left(-\frac{\lambda}{4}\xi_1\right)\right\rangle_{G_a}=\left\langle \exp\left(-\frac{\lambda}{4}[U(g)+\eta]\right)\right\rangle_P$$

$$=\left\langle \exp\left(-\frac{\lambda}{4}U(g)\right)\right\rangle_{\mu_0}\left\langle \exp\left(-\frac{\lambda}{4}\eta\right)\right\rangle_P,$$

$$\lim_{a\to 0^+}\left\langle \phi(f_1)\cdots\phi(f_m)\exp\left(-\frac{\lambda}{4}\xi_1\right)\right\rangle_{G_a}=\left\langle \phi(f_1)\cdots\phi(f_m)\exp\left(-\frac{\lambda}{4}[U(g)+\eta]\right)\right\rangle_P$$

$$=\left\langle \phi(f_1)\cdots\phi(f_m)\exp\left(-\frac{\lambda}{4}U(g)\right)\right\rangle_{\mu_0}\left\langle \exp\left(-\frac{\lambda}{4}\eta\right)\right\rangle_P.$$

Therefore, if $\lambda>0$ is sufficiently small, we have

$$\lim_{a\to 0^+}\langle\phi(f_1)\cdots\phi(f_m)\rangle_{\mu_{a,a',\lambda}}=\langle\phi(f_1)\cdots\phi(f_m)\rangle_{\nu_{\lambda,g}}.$$

Since the original continuum ϕ_2^4-quantum field measure $\nu_{\lambda,g}$ is uniquely determined by its moment functions,[31] we have actually proved $\mu_{\lambda.g}=\nu_{\lambda,g}$, if $\lambda>0$ is sufficient small. This ends the proof of Theorem 2.2 for $A>0$. ■

VIII. SOME REMARKS AND OPEN PROBLEMS

In this section we give some remarks on the new lattice approximation of the continuum ϕ_2^4-quantum field. In the following we always assume that $g\in C_0^1(R^2)$ is given such that, $g\geqslant 0$, $\int_{R^2}g(x)dx>0$.

(i) *Coincidence with the original field.* Assume $\lim_{a\to 0^+}a'|\log a|^2<\infty$. In this case, we believe that $\mu_{\lambda,g}$ as given in Theorem 2.1 is well defined also for *all* $\lambda\geqslant 0$ (without the restriction $0\leqslant\lambda\leqslant\lambda_0$). If one could prove this, then from the proof of Theorem 2.2 we would have that the measure $\mu_{\lambda,g}$ with $\lambda\in[0,\infty)$ also coincides with the original ϕ_2^4-field measure with cutoff g, $\nu_{\lambda,g}$, for all λ,g. Unfortunately, we are not yet able to prove the former assertion on $\mu_{\lambda,g}$. The main difficulty is that we are not able to prove the boundedness of the sequence $\{\langle e^{-\lambda V_{a_n'Z^2}}\rangle_{G_{a_n}}\}_{n\geqslant 1}$ for all $\lambda\geqslant 0$ (we have only a control for $0\leqslant\lambda\leqslant\lambda_0$).

(ii) *A general existence result.* In Theorem 2.1 we already constructed a continuum ϕ_2^4-quantum field $\mu_{\lambda,g}$ if $\lim_{a\to 0^+}a'|\log a|^{5/4}<\infty$. From the discussion given in the Appendix we can see that we can also construct a continuum ϕ_2^4-quantum field $\mu_{\lambda,g}$ if $\lim_{a\to 0^+}a'|\log a|^{7/6}<\infty$. In general, if there is $\epsilon\in(0,\frac{1}{4})$ such that $\lim_{a\to 0^+}a'|\log a|^{1+\epsilon}<\infty$, then with similar techniques it should be possible to show that we could use the general skeleton inequalities given in Ref. 25 to define lattice ϕ_2^4 fields with new counterterms and then construct a (nontrivial) continuum ϕ_2^4-quantum field $\mu_{\lambda,g}$ by approximation from these lattice ϕ_2^4 fields with the new counterterms. Since the main idea for constructing the new continuum ϕ_2^4 field has been already explained in the proof of Theorem 2.1, we are not going to state and prove the general existence theorem.

(iii) *Singularity with respect to the Gaussian measure.* Consider the case

$$\lim_{a\to 0^+}a'|\log a|^2=\infty \qquad \lim_{a\to 0^+}a'|\log a|^{1+\epsilon}<\infty$$

for some $\epsilon \in (0,\frac{1}{4})$. The original ϕ_2^4-field measure with spatial cutoff g (i.e., the measure $\nu_{\lambda,g}$ given before Theorem 2.1) is absolutely continuous with respect to the Gaussian measure μ_0. It is easy to show that $\langle (\int' dx g(x):\phi_x^4:)^2 \rangle_{G_a}$ goes to infinity as $a \to 0^+$, if $\lim_{a\to 0^+} a'|\log a|^2 = \infty$. In another paper[18] we have proved that $\int' dx g(x):\phi_x^4:$ satisfies the central limit theorem as $a \to 0^+$, if $\lim_{a\to 0^+} a'|\log a|^2 = \infty$. In other words, we proved in Ref. 18 that there is a constant $c \in (0,\infty)$ such that

$$\lim_{a\to 0^+} G_a\left(c(a'|\log a|^2)^{-1} \int' dx g(x):\phi_x^4: \leqslant y \right) = (2\pi)^{-1/2} \int_{-\infty}^{y} e^{-|z|^2/2} dz, \quad \forall y \in R.$$

Using this fact one might try to prove that there are Borel measurable sets D_n, $n \geqslant 1$ such that

$$\lim_{n\to\infty} \mu_0(D_n) = 0, \qquad \liminf_{n\to\infty} \mu_{\lambda,g}(D_n) > 0.$$

It then would follow that the new measure $\mu_{\lambda,g}$ (constructed for $\lambda > 0$ sufficiently small) is not absolutely continuous with respect to the Gaussian measure μ_0 if $\lim_{a\to 0^+} a'|\log a|^2 = \infty$ and $\lim_{a\to 0^+} a'|\log a|^{1+\epsilon} < \infty$.

(iv) *Quasi-invariance*. Assume $\lim_{a\to 0^+} a'|\log a|^2 = \infty$ and $\lim_{a\to 0^+} a'|\log a|^{3/2} < \infty$. In this case, we believe that the new measure $\mu_{\lambda,g}$ is k quasi-invariant for a linear subset of k in $\mathcal{S}(R^2)$ (for the definition of k quasi-invariance the reader is referred to Ref. 11, 32–34, or 35; the corresponding property in the standard ϕ_2^4 model was discussed, e.g., in Refs. 35–37). In this case it should be possible to use the approach by Dirichlet forms,[35,36] as a tool, to study the stochastic quantization of the field measure $\mu_{\lambda,g}$ (similarly as it was done in Refs. 35 and 36 for the original ϕ_2^4-field measure and in Ref. 38 for the three-dimensional polymer measure).

(v) *No quasi-invariance*. Assume $\lim_{a\to 0^+} a'|\log a|^{3/2} = \infty$ and $\lim_{a\to 0^+} a'|\log a|^{1+\epsilon} < \infty$ for some $\epsilon \in (0,1/2)$. In this case we believe that $\mu_{\lambda,g}$ with small $\lambda > 0$ is not quasi-invariant for any $k \in \mathcal{S}(R^2)$. We remark that the original continuum ϕ_2^4 field is k quasi-invariant for some $k \in \mathcal{S}(R^2)$.[11,32] Thus in particular $\mu_{\lambda,g}$ would be different from the original ϕ_2^4 field measure $\nu_{\lambda,g}$. The original continuum ϕ_3^4-field measure with spatial cutoff is believed to be not k quasi-invariant and also singular with respect to the Gaussian measure μ_0 on $\mathcal{S}'(R^3)$ (cf. Ref. 39 for partial results). In this sense, the new field $\mu_{\lambda,g}$ in the present case might behave like the original ϕ_3^4-field measure.

(vi) *No Borel summability*. Assume as in (v) $\lim_{a\to 0^+} a'|\log a|^{3/2} = \infty$ and $\lim_{a\to 0^+} a'|\log a|^{1+\epsilon} < \infty$ for some $\epsilon \in (0,1/2)$. If the conjecture we made in (v) holds, we have that $\mu_{\lambda,g}$ is different from $\nu_{\lambda,g}$. In this case we expect that the expansion in powers of λ of the n-point functions of $\mu_{\lambda,g}$ is not Borel summable (whereas it is for those of the standard $\nu_{\lambda,g}$ (Ref. 40).

(vii) *Triviality*. Assume $\lim_{a\to 0^+} a'|\log a| < \infty$ and $\lim_{a\to 0^+} a'|\log a|^2 = \infty$. In this case, we believe that any lattice ϕ_2^4-field model measure with or without counterterms is weakly convergent to a Gaussian field measure (if the limit exists). This conjecture is based on an intersection (restricted to the subset $m_n Z^2$, with $m_n \in N$) property of independent random walks in Z^2. Let $\{X_n\}$ and $\{Y_n\}$ be two independent simple random walks in Z^2 with probability measure P'. Assume that $X_0 = x_n$, $Y_0 = y_n$ and $|x_n - y_n| \geqslant O(1)n^{1/2}$. Then we can easily prove that $\lim_{n\to\infty} P'$ (there are $k \geqslant 1$ and $l \geqslant 1$ such that $X_k = Y_l \in m_n Z^2) = 0$, if $\lim_{n\to\infty} m_n^2 n^{-1} (\log n)^2 = \infty$ (cf. Ref. 41, Theorem 1.3 and Lemma 4.5). It seems possible to prove the above conjecture by using the approach given in Ref. 1 or 42, where the lattice ϕ_d^4 fields for $d \geqslant 5$ with the same cutoff in the free and interacting parts were proved to be weakly convergent to the Gaussian field (if the limit exists).

(viii) *Convergence without subsequences*. Following Ref. 5, one can show that all Osterwalder–Schrader axioms, except perhaps for rotation invariance, are satisfied for the new ϕ_2^4 fields in the infinite-volume limit defined by Theorem 2.1. The continuum ϕ_2^4 and ϕ_3^4 fields are also constructed in Ref. 5 as subsequence limits of some lattice field theories. It is believed that

these fields given in Ref. 5 are also continuum limits of the corresponding lattice theories without involving subsequences. In Ref. 5, Sec. 9, Eq. (2), a way was suggested to prove that the above assertion is correct. According to this suggestion one has to formulate the ϕ_d^4 fields on two different lattices (with different lattice meshes a_1, a_1' and a_2, a_2', respectively) as a field on one lattice and then try to interpolate between the two fields in two stages [i.e., try to estimate the differences given by Ref. 5, Eq. (9.4)]. From Theorem 2.1 given above, however, we can see that each difference given in Ref. 5, Eq. (9.4), is not always convergent to zero as $a_i, i=1,2$, go to zero, although the summation of the two differences given in Ref. 5, Eq. (9.4), is believed to be convergent to zero. to It would also be very interesting to prove the existence of the continuum limit of $\nu_{a,a'}$ as $a, a' \to 0^+$ without involving subsequences.

Finally, we remark that one can also use the approach given in Ref. 5 to discuss the new convergent lattice approximation for the ϕ_3^4-quantum field.

Note added. A first version of this paper was prepared in 1995. Due to the untimely departure of Xian Yin Zhou, the revised version had to be completed by the two first named authors, without the essential precious help of Xian Yin. These authors deeply mourn the departure of their friend, whose work and inspiration were at the basis of the whole present paper.

Note added in proof. An earlier version of the present paper, with the title ''A new convergent lattice approximation for the ϕ_2^4-quantum field'' has appeared in ''Collection Papers of Zhou Xianyin,'' Beijing Normal University, Press, Beijing (Vol. II, pp. 778–810), 2002.

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APPENDIX

In this appendix, we give an estimate of U_4 (see Sec. III) up to the third order in the coupling constant λ. As in Ref. 24, Sec. 3, we write U_4 with the help of a function $F(x_1,x_2|x_3,x_4)$ in the form

$$U_4(x_1,x_2,x_3,x_4)=F(x_1,x_2|x_3,x_4)+F(x_1,x_3|x_2,x_4)+F(x_1,x_4|x_2,x_3).$$

Let

$$I_{k_1,k_2,k_3}(x_1,x_2)=\sum_{i_1,i_2,i_3}\langle\phi_{x_1}\phi_{k_{i_1}}\rangle\langle\phi_{k_{i_1}}\phi_{k_{i_2}}\rangle\langle\phi_{k_{i_2}}\phi_{k_{i_3}}\rangle\langle\phi_{k_{i_3}}\phi_{x_2}\rangle,$$

where the sum is taken over all the permutations (i_1,i_2,i_3) of the set $\{1,2,3\}$. Using the random walk representation we can show that there is $I(x_1,x_2|x_3,x_4)$ such that

$$F(x_1,x_2|x_3,x_4)\geqslant\lambda c_1(\vec{x})+\lambda^2 c_2(\vec{x})+\lambda^3 c_3(\vec{x})+\lambda^5 I(x_1,x_2|x_3,x_4),$$

with $\vec{x}=(x_1,x_2,x_3,x_4)$, $I(x_1,x_2|x_3,x_4)$ does not depend on λ, and

$$c_1(\vec{x}) \equiv -6 \int' djg(j) \langle \phi_{x_1} \phi_j \rangle \langle \phi_{x_2} \phi_j \rangle \langle \phi_{x_3} \phi_j \rangle \langle \phi_{x_4} \phi_j \rangle,$$

$$\begin{aligned} c_2(\vec{x}) \equiv & 18 \int' djg(j) \int' dkg(k) \langle \phi_{x_1} \phi_j \rangle \langle \phi_{x_2} \phi_j \rangle \langle \phi_{x_3} \phi_k \rangle \langle \phi_{x_4} \phi_k \rangle \langle \phi_j \phi_k \rangle^2 \\ & + 18 \int' djg(j) \int' dkg(k) \langle \phi_{x_3} \phi_j \rangle \langle \phi_{x_4} \phi_k \rangle \langle \phi_j \phi_k \rangle^2 (\langle \phi_{x_1} \phi_j \rangle \langle \phi_k \phi_{x_2} \rangle \\ & + \langle \phi_{x_1} \phi_k \rangle \langle \phi_j \phi_{x_2} \rangle), \end{aligned}$$

$$\begin{aligned} c_3(\vec{x}) \equiv & -8 \int' djg(j) \langle \phi_{x_3} \phi_j \rangle \langle \phi_{x_4} \phi_j \rangle \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_1} \phi_{k_1} \rangle \langle \phi_{k_1} \phi_{k_2} \rangle^2 \langle \phi_{k_2} \phi_j \rangle \\ & \times \langle \phi_j \phi_{k_1} \rangle \langle \phi_{k_1} \phi_{x_2} \rangle - 12 \int' djg(j) \langle \phi_{x_3} \phi_j \rangle \langle \phi_{x_4} \phi_j \rangle \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_1} \phi_{k_1} \rangle \\ & \times \langle \phi_{k_1} \phi_j \rangle \langle \phi_j \phi_{k_2} \rangle \langle \phi_{k_1} \phi_{k_2} \rangle^2 \langle \phi_{k_2} \phi_{x_2} \rangle - 8 \int' djg(j) \langle \phi_{x_3} \phi_j \rangle \\ & \times \langle \phi_{x_4} \phi_j \rangle \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_j \phi_{k_1} \rangle \langle \phi_{x_2} \phi_{k_2} \rangle \langle \phi_{k_1} \phi_{k_2} \rangle^2 (\langle \phi_{x_1} \phi_{k_1} \rangle^2 \langle \phi_{k_2} \phi_j \rangle \\ & + \langle \phi_{x_1} \phi_{k_2} \rangle \langle \phi_{k_1} \phi_j \rangle) - 12 \int' djg(j) \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_1} \phi_{k_1} \rangle \langle \phi_{k_1} \phi_j \rangle^2 \langle \phi_{k_1} \phi_{x_2} \rangle \\ & \times \langle \phi_{x_3} \phi_{k_2} \rangle \langle \phi_{x_4} \phi_{k_2} \rangle \langle \phi_j \phi_{k_2} \rangle^2 - 8 \int' djg(j) \int' dkg(k) \langle \phi_{x_3} \phi_j \rangle \langle \phi_{x_4} \phi_k \rangle \langle \phi_j \phi_k \rangle \\ & \times \Big[\langle \phi_k \phi_{x_2} \rangle \int' dlg(l) \langle \phi_{x_1} \phi_l \rangle \langle \phi_k \phi_l \rangle \langle \phi_j \phi_l \rangle^2 + \langle \phi_j \phi_{x_2} \rangle \int' dl \;\; g(l) (\langle \phi_{x_1} \phi_l \rangle \langle \phi_j \phi_l \rangle \\ & \times \langle \phi_k \phi_l \rangle^2) + \int' dlg(l) \langle \phi_k \phi_l \rangle \langle \phi_l \phi_{x_2} \rangle \langle \phi_l \phi_j \rangle (\langle \phi_{x_1} \phi_l \rangle \langle \phi_j \phi_k \rangle + \langle \phi_{x_1} \phi_j \rangle \langle \phi_l \phi_k \rangle) \\ & + \int' dlg(l) \langle \phi_j \phi_l \rangle \langle \phi_l \phi_{x_2} \rangle \langle \phi_l \phi_k \rangle (\langle \phi_{x_1} \phi_l \rangle \langle \phi_j \phi_k \rangle + \langle \phi_{x_1} \phi_k \rangle \langle \phi_l \phi_j \rangle) \Big] - 36 \int' djg(j) \\ & \times \langle \phi_{x_1} \phi_j \rangle \langle \phi_j \phi_{x_2} \rangle \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_3} \phi_{k_1} \rangle \langle \phi_j \phi_{k_1} \rangle \\ & \times \langle \phi_{k_1} \phi_{k_2} \rangle^2 \langle \phi_{x_4} \phi_{k_2} \rangle^2 \langle \phi_{x_4} \phi_{k_2} \rangle \langle \phi_j \phi_{k_2} \rangle - 18 \int' djg(j) \langle \phi_{x_1} \phi_j \rangle \\ & \times \langle \phi_j \phi_{x_2} \rangle \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_3} \phi_{k_1} \rangle \langle \phi_{x_4} \phi_{k_1} \rangle \langle \phi_{k_1} \phi_{k_2} \rangle^2 \langle \phi_j \phi_{k_2} \rangle^2 \\ & - \frac{8}{3} \int' djg(j) \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_3} \phi_{k_1} \rangle \langle \phi_j \phi_{k_1} \rangle \langle \phi_{x_4} \phi_{k_2} \rangle \langle \phi_j \phi_{k_2} \rangle \\ & \times I_{j,k_1,k_2}(x_1, x_2) - 6 \int' djg(j) \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_4} \phi_{k_1} \rangle \langle \phi_j \phi_{k_1} \rangle^2 \langle \phi_{x_3} \phi_{k_2} \rangle \\ & \times \langle \phi_{k_1} \phi_{k_2} \rangle \langle \phi_j \phi_{k_2} \rangle (\langle \phi_{k_2} \phi_{x_2} \rangle \langle \phi_{x_1} \phi_j \rangle + \langle \phi_j \phi_{x_2} \rangle \langle \phi_{x_1} \phi_{k_2} \rangle) \\ & - 6 \int' djg(j) \int' dk_1 g(k_1) \int' dk_2 g(k_2) \langle \phi_{x_3} \phi_{k_1} \rangle \langle \phi_j \phi_{k_1} \rangle^2 \langle \phi_{x_4} \phi_{k_2} \rangle \langle \phi_{k_1} \phi_{k_2} \rangle \langle \phi_j \phi_{k_2} \rangle \end{aligned}$$

$$\times(\langle\phi_{k_2}\phi_{x_2}\rangle\langle\phi_{x_1}\phi_j\rangle+\langle\phi_j\phi_{x_2}\rangle\langle\phi_{x_1}\phi_{k_2}\rangle)-12\int' djg(j)\int' dk_1 g(k_1)\int' dk_2 g(k_2)$$

$$\times\langle\phi_{x_3}\phi_{k_1}\rangle\langle\phi_{x_4}\phi_{k_1}\rangle\langle\phi_j\phi_{k_1}\rangle\langle\phi_j\phi_{k_2}\rangle^2\langle\phi_{k_1}\phi_{k_2}\rangle(\langle\phi_{k_2}\phi_{x_2}\rangle\langle\phi_{x_1}\phi_j\rangle+\langle\phi_j\phi_{x_2}\rangle\langle\phi_{x_1}\phi_{k_2}\rangle)$$

$$-36\int' djg(j)\int' dk_1 g(k_1)\int' dk_2 g(k_2)\langle\phi_{x_4}\phi_j\rangle\langle\phi_{x_3}\phi_{k_2}\rangle\langle\phi_j\phi_{k_2}\rangle\langle\phi_{k_1}\phi_{k_2}\rangle^2\langle\phi_j\phi_{k_1}\rangle$$

$$\times(\langle\phi_{k_1}\phi_{x_2}\rangle\langle\phi_{x_1}\phi_j\rangle+\langle\phi_j\phi_{x_2}\rangle\langle\phi_{x_1}\phi_{k_1}\rangle)-36\int' djg(j)\int' dk_1 g(k_1)\int' dk_2 g(k_2)$$

$$\times\langle\phi_{x_3}\phi_j\rangle\langle\phi_{x_4}\phi_{k_2}\rangle\langle\phi_j\phi_{k_2}\rangle\langle\phi_{k_1}\phi_{k_2}\rangle^2\times\langle\phi_j\phi_{k_1}\rangle(\langle\phi_{k_1}\phi_{x_2}\rangle\langle\phi_{x_1}\phi_j\rangle+\langle\phi_j\phi_{x_2}\rangle$$

$$\times\langle\phi_{x_1}\phi_{k_1}\rangle)-24\int' djg(j)\int' dk_1 g(k_1)\int' dk_2 g(k_2)\langle\phi_{x_3}\phi_j\rangle\langle\phi_{x_4}\phi_{k_1}\rangle\langle\phi_j\phi_{k_2}\rangle$$

$$\times\langle\phi_{k_1}\phi_{k_2}\rangle I_{j,k_1,k_2}(x_1,x_2)-24\int' djg(j)\int' dk_1 g(k_1)\int' dk_2 g(k_2)\langle\phi_{x_4}\phi_j\rangle\langle\phi_{x_3}\phi_{k_1}\rangle$$

$$\times\langle\phi_j\phi_{k_2}\rangle\langle\phi_{k_1}\phi_{k_2}\rangle I_{j,k_1,k_2}(x_1,x_2). \tag{A1}$$

Define

$$\delta m_2^3=-54\lambda^3 a'^4 C^{(a)}(0)^5$$

and

$$\overline{V}=\frac{\lambda}{4}\int' g(x)\phi_x^4 dx+\frac{1}{2}\delta m_1^2\int' g(x)\phi_x^2 dx+\frac{1}{2}\delta m_2^2\int' g(x)^2\phi_x^2 dx+\frac{1}{2}\delta m_3^2\int' g(x)^3\phi_x^2 dx,$$

$$\overline{S}^{(a,a')}(x_1,\ldots,x_{2n})=\frac{\langle\phi_{x_1}\cdots\phi_{x_{2n}}e^{-\overline{V}}\rangle_{G_a}}{\langle e^{-\overline{V}}\rangle_{G_a}}.$$

Then, proceeding as in the proof of Theorem 2.1 we can use (A1) to prove that there are sequences $\{a_n\}$, $\{a_n'\}$ with $\lim_{n\to\infty}a_n=0$ and $\lim_{n\to\infty}a_n'|\log a_n|^{7/6}<\infty$, and $\{g_n\}\subset C_0(R^2)$ with $\lim_{n\to\infty}g_n(x)=g(x)$, such that for any given $f_1,\ldots,f_{2m}\in\mathcal{S}(R^2)$ and $m\geqslant 1$ the following limit exists:

$$\overline{S}(f_1,\ldots,f_{2m})=:\lim_{n\to\infty}\sum_{x_1,\ldots,x_{2m}\in a_nZ^2}\overline{S}^{(a_n,a_n')}(x_1,\ldots,x_{2m})\prod_{i=1}^{2m}a_n^2 f_i(x_i).$$

Moreover, there is a probability measure $\overline{\mu}_{\lambda,g}$ on $\mathcal{S}'(R^2)$ satisfying

$$\int_{\mathcal{S}'(R^2)}\phi(f_1)\cdots\phi(f_{2m})\overline{\mu}_{\lambda,g}(d\phi)=\overline{S}(f_1,\ldots,f_{2m}),\qquad f_1,\ldots,f_{2m}\in\mathcal{S}(R^2),\ \ m\geqslant 1.$$

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Effective Lagrangians for scalar fields and finite size effects in field theory

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We first discuss the approach of effective field theory in a d-dimensional Euclidean space. We consider a model with two interacting scalar fields ($\mathcal{L}_{\rm int}(\varphi_1,\varphi_2) = (\lambda_2/2)(\varphi_1\varphi_2)^2$) with masses m_1 and m_2. Assuming $m_2 \gg m_1$ we show that there is a decoupling in the effective theory describing the dynamic of the light mass field. Furthermore, we consider the presence of two parallel hyperplanes which break translational symmetry, with a natural cutoff satisfying $m_2 \gg \Lambda > m_1$. Then imposing Dirichlet and also Neumann boundary conditions, we study the perturbative renormalization of the effective theory ($\lambda\varphi^4$) in a region bounded by the two parallel hyperplanes in the one-loop approximation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629138]

I. INTRODUCTION

The quantum field theory of a self-interacting scalar field has long served as a laboratory for developing methods of analysis that can be applied to theories of more direct physical interest. In this paper we consider a theory with a light mass field $\varphi_1(x)$, and a heavy mass field $\varphi_2(x)$ with masses m_1 and m_2, respectively. Our purpose is to investigate first the effective theory associated with these two interacting scalar fields defined in a d-dimensional Euclidean space. After the construction of an effective theory for the light field, we show that, in some limit, there is a decoupling between the light and heavy mass fields as stated by the Appelquist–Carazzone theorem.[1] Additionally, we impose boundary conditions on the resulting theory in order to study finite-size effects and the renormalization program in systems where translational symmetry is broken. The interest in the study of quantum fields in the presence of boundaries appears after the problem investigated by Casimir more than 50 years ago.[2] Complete reviews of this effect can be found in Refs. 3–5.

In 1948, Casimir showed that neutral perfectly conducting parallel plates in vacuum attract each other. The effect can be interpreted as follows: the presence of metallic plates changes the vacuum fluctuations of a quantized electromagnetic field. Consequently, the zero-point energy of the electromagnetic field becomes a measurable quantity. In the absence of any classical background, the renormalized vacuum expectation value of the Hamiltonian operator can be correctly defined by the Wick-ordered product. The main support for this procedure comes from the proof that for a relativistic field theory, the vacuum expectation value of the stress-energy tensor should vanish. This fact is necessary to ensure that the realization of the Poincaré generators in terms of the fields of the theory satisfy the correct commutation relations.[6] On the other hand, where external fields or macroscopic structures are present in the domain where the field is defined, more elaborated methods must be used to find the renormalized vacuum energy of the quantized field to

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avoid undesirable divergences. A cutoff regularization that identifies the divergent contributions to the vacuum energy, or any regularization procedure, followed by a renormalization, is mandatory. The fundamental idea of the Casimir renormalization procedure is the following: although the zero-point energy of a system with infinite degrees of freedom is formally divergent, the difference between the zero-point energies of two different physical configurations, in some situations, can be shown to be finite.

In quantum electrodynamics there is a standard argument used to support the implementation of a regularization procedure followed by renormalization. Both procedures are necessary to obtain the renormalized vacuum expectation value of the stress-energy tensor associated with the Maxwell field in the presence of boundaries. At high frequencies no real material is a perfect conductor and a wavelength cutoff corresponding to the finite plasma frequency must be included in the model. High energy modes are insensitive to the boundaries and only the low energy modes are affected by them. Consequently, in the study of quantum electrodynamics in the presence of conducting boundaries, starting from the generating functional for the n-point correlation functions, one may integrate out all the Fourier modes associated with the Dirac field and obtain an effective theory for the Maxwell field.

We are investigating a theory describing two massive interacting scalar fields in a d-dimensional Euclidean space. Assuming different mass scales, we are obtaining the effective action for the light mass field. One could, theoretically, envision a theory with two massive fields with different mass scales on which the mass of the heavy field is much smaller than the natural cutoff of the boundary, Λ. In this paper we are not interested in discussing this situation.

It is important to keep in mind that in order to construct an effective action that gives a good description of the physics of the light mass field in the presence of the boundaries, the Fourier modes associated with both fields with wavelength smaller than Λ^{-1} must be integrated out (note that we are always assuming a sharp cutoff). Since dealing with functional integrals with cutoffs in general models is quite complicated, we will limit ourselves to a heavy mass field without a self-interacting term in the action. We are studying finite size effects for the light mass field in three steps. First, we integrate over the modes of the heavy mass field, obtaining an effective action for the light mass field. Second, we are taking the limit in which the decoupling theorem is valid ($m_2 \to \infty$), with regard to the effective action as the fundamental action and we are assuming boundary conditions over the remaining light field. Finally, combining different analytic regularization procedures, followed by a renormalization, one is able to eliminate the usual bulk and also the additional surface divergences that appear in the theory. The final result of our procedure is that we have the effect of the compactification of one dimension, breaking the translational invariance of the original theory. In this situation we have an effective field theory of the light mass field, with finite size effects. Due to our choice (two-parallel hyperplates), the region outside the boundaries is the union of two simply connected domains. The renormalization of the interacting field theory in such a region must be carried out along the same lines as for the interior region. For simplicity we are considering only the interior region.

There are many papers in the literature discussing quantum field theory in the presence of boundaries or of macroscopic structures. The radiative corrections to the renormalized energy density associated with the Maxwell field, in the presence of perfectly conducting plates, assuming no boundary conditions for the Dirac field, was performed by Bordag *et al.*[7] Temperature corrections for this model were analyzed by Robaschik *et al.*[8] Bordag *et al.*[9] also studied the leading radiative correction to the renormalized energy, assuming that the parallel plates are represented by delta function potentials. Using the approach of effective field theory, the radiative correction to the Casimir effect integrating out the fermionic degrees of freedom was examined by Kong and Ravndal and Ravndal and Thomassen.[10] A different approach was used by Falomir *et al.*[11] These authors used a sharp cutoff to study scalar fields in the presence of a spherical shell. They assume that the boundary is transparent to the heavy modes while for the soft modes they assumed Dirichlet boundary conditions. Actor[12] studied two interacting scalar fields in the presence of macroscopic boundaries assuming that only one of the fields satisfies classical boundary conditions. Using the generalized zeta function method[13] the one-loop effective action was presented.

More recently, Melnikov[14] investigated the low-energy effective action in a model with two scalar fields and also in quantum electrodynamics. Our treatment is very similar to that of Melnikov's in the study of the low-energy effective action for a theory with two interacting scalar fields.

It is important to point out that the combination of effective field theory and finite size effects can produce unexpected new phenomena. A well-known example of this situation is the Scharnhorst effect.[15] Studying quantum electrodynamics between perfectly conducting plates, Scharnhorst concluded that the speed of light normal to the plates exceeds light speed in vacuum. Nevertheless, parallel to the plates, light travels as in unbounded space, i.e., with its vacuum speed. Further calculations by Barton[16] and also by Barton and Scharnhorst[17] confirmed the original result. The Scharnhorst effect is a consequence of the use of the Euler–Heisenberg Lagrangian density[18,19] in the presence of the plates. The central feature of this effective Lagrangian is a derivative expansion of the photon effective action obtained by integrating out the fermionic field in the Maxwell–Dirac action. For an interesting discussion concerning the velocity of propagation of signals in different effective field theory models, see Ref. 20.

Finite size effects that do not break translational invariance in quantum field theory also have been extensively studied in the literature.[21,22] For translationally invariant systems, we can change from coordinate space to momentum space representation. The latter is a more convenient framework to analyze the divergences of the n-point Schwinger functions, on which translational invariance is realized through conservation conditions. For systems where the translational invariance has been partially broken (so there is still translational invariance along certain directions) a more convenient representation for the n-point Schwinger functions is a mixed momentum-coordinate representation. Important references discussing the renormalization program in the presence of boundaries are the Symanzik[23] and also Diehl and Dietrich[24] papers.

In this paper we are studying the one-loop renormalization program in the presence of surfaces where a self-interacting scalar field satisfies boundary conditions. We are interested in investigating a very simple model where we can construct an effective field theory for the light mass field on which the decoupling theorem holds. Furthermore, we consider a self-interacting field theory in the presence of boundaries. We will consider a Casimir-type configuration where one of the coordinates, z, lies in the interval $[0,L]$ imposing Dirichlet–Dirichlet boundary conditions. For the sake of completeness we will also study the Neumann–Neumann boundary conditions.

The organization of the paper is as follows: in Sec. II we introduce a simple model of two Euclidean interacting scalar fields. By integrating out the heavy mass field in the functional integral, we are able to build the effective action for the light mass field. In Sec. III we discuss a scalar field theory with finite size effects assuming boundary conditions over hypersurfaces. We thus build the two-point and four-point functions, both for Dirichlet–Dirichlet and Neumann–Neumann boundary conditions. In Sec. IV we discuss the surface divergences of the one-loop two-point and also four-point function. In Sec. V we discuss the global approach, used to define the Casimir energy associated with a field in the presence of boundaries with well defined geometric shapes. Finally, Sec. VI contains our conclusions. In this paper we are using $\hbar = c = 1$.

II. THE EUCLIDEAN FUNCTIONAL INTEGRAL AND THE EFFECTIVE ACTION

The goal of this section is to study a very simple model of two interacting scalar fields defined in a d-dimensional Euclidean space. After the construction of an effective action,[25–28] the decoupling theorem holds. This can be done imposing the infinite mass limit for the heavy field. For this purpose we start from a model with two different mass scales. We consider two real interacting massive scalar fields $\varphi_1(x)$ and $\varphi_2(x)$ with masses m_1 and m_2, respectively, and regard field $\varphi_2(x)$ as the heavy field $(m_2 \gg m_1)$. For this theory, we will rederive the Euclidean version for the Appelquist–Carazzone theorem. For a particular self-interacting $\varphi_1(x)$ part, in the limit $m_2 \to \infty$, there is a decoupling in the effective theory. The only effects of the heavy field $\varphi_2(x)$ are a modification of the value of the renormalized mass and the coupling constant of the light field $\varphi_1(x)$.

The Schwinger functional (the generating functional of the n-point Schwinger functions) associated with two massive real fields in a d-dimensional Euclidean space given by

$$Z[j_1,j_2]=\mathcal{N}\int [d\varphi_1][d\varphi_2]\, e^{-S[\varphi_1,\varphi_2]+(\text{source terms})}, \tag{1}$$

where $[d\varphi_1][d\varphi_2]=\Pi_{x\in R^d} d\varphi_1(x)d\varphi_2(x)$ is an appropriate measure, $S[\varphi_1,\varphi_2]$ is the classical action associated with the Euclidean fields, and in the generating functional, $\mathcal{N}$ is a normalization. As usual, the n-point Schwinger functions of the theory can be obtained by functional differentiation with respect to the external sources $j_1(x)$ and $j_2(x)$. Since in this section our interest is in constructing the effective theory for the light field, the introduction of the external sources in the functional integral is not important for our discussion. We consider the theory described by the following Lagrangian density with two real scalar fields

$$\mathcal{L}(\varphi_1,\varphi_2)=\mathcal{L}_0(\varphi_1,\varphi_2)+\mathcal{L}_{int}(\varphi_1,\varphi_2), \tag{2}$$

where the free part of the Lagrangian density is given by

$$\mathcal{L}_0(\varphi_1,\varphi_2)=\tfrac{1}{2}(\partial_\mu\varphi_1)^2+\tfrac{1}{2}m_1^2\varphi_1^2+\tfrac{1}{2}(\partial_\mu\varphi_2)^2+\tfrac{1}{2}m_2^2\varphi_2^2, \tag{3}$$

and the interacting part is given by

$$\mathcal{L}_{\text{int}}(\varphi_1,\varphi_2)=V(\varphi_1)+\frac{\lambda_2}{2}(\varphi_1\varphi_2)^2. \tag{4}$$

Note that the precise form of $V(\varphi_1)$ is not important for the construction of the effective action. As we will see later in this section, the form of the $V(\varphi_1)$ is important to implement the Appelquist–Carazzone decoupling theorem.

The action of the model is given by

$$S[\varphi_1,\varphi_2]=\int d^dx\, \mathcal{L}(\varphi_1(x),\varphi_2(x)), \tag{5}$$

and using Eq. (3) and Eq. (4) can be conveniently split up as

$$S[\varphi_1,\varphi_2]=S[\varphi_1(x)]+S_{\varphi_2}[\varphi_1(x),\varphi_2(x)], \tag{6}$$

$S[\varphi_1(x)]$ being the $\varphi_2(x)$-independent part of it. In order to obtain a derivative expansion of the effective action $\Gamma_{\text{eff}}[\varphi_1]$, we have to assume $m_2\gg m_1$. The operators $(-\Delta+m_1^2)^{-1}$ and $(-\Delta+m_2^2)^{-1}$ must be used to define the free two-point Schwinger functions of the fields $\varphi_1(x)$ and $\varphi_2(x)$. As usual, Δ is the Laplacian operator in $\mathcal{R}^d$. The free two-point Schwinger functions of both fields can be represented by

$$G(x-y;m_i)=\langle x|(-\Delta+m_i^2)^{-1}|y\rangle,\ i=1,2 \tag{7}$$

and they satisfy

$$(-\Delta+m_i^2)G(x-y;m_i)=\delta^d(x-y). \tag{8}$$

To obtain an effective action for the light mass field of the theory, we integrate out the heavy field $\varphi_2(x)$ in the functional integral. The effective action of the light mass field $\Gamma_{\text{eff}}[\varphi_1]$ is defined by

$$e^{-\Gamma_{\text{eff}}[\varphi_1]}=\int [d\varphi_2]\, e^{-S[\varphi_1,\varphi_2]}. \tag{9}$$

Using Eq. (6) it is possible to write Eq. (9) as

$$e^{-\Gamma_{\text{eff}}[\varphi_1]} = e^{-S[\varphi_1]} \int [d\varphi_2]\, e^{-S_{\varphi_2}[\varphi_1,\varphi_2]}. \tag{10}$$

The first step in our calculation is straightforward, since $S_{\varphi_2}[\varphi_1,\varphi_2]$ is given by

$$S_{\varphi_2}[\varphi_1,\varphi_2] = \int d^dx \left(\varphi_2(-\Delta + m_2^2)\varphi_2 + \frac{\lambda_2}{2}(\varphi_1\varphi_2)^2 \right). \tag{11}$$

Using Eq. (11) the functional integral appearing in Eq. (10) can be performed by means of Gaussian integrations, yielding

$$e^{-\Gamma_{\text{eff}}[\varphi_1]} = e^{-S[\varphi_1]} (\det O)^{-(1/2)}, \tag{12}$$

where we have

$$O(x,y;m_2) = \langle x|O|y\rangle = (-\Delta_x + m_2^2 + \lambda_2\varphi_1^2(x))\,\delta^d(x-y). \tag{13}$$

Consequently, the effective action for the light mass field $\varphi_1(x)$ is given by

$$\Gamma_{\text{eff}}[\varphi_1] = S[\varphi_1] + \tfrac{1}{2}\operatorname{tr}\ln O. \tag{14}$$

Dropping a term that contributes trivially to the effective action $\Gamma_{\text{eff}}[\varphi_1]$, we get

$$\Gamma_{\text{eff}}[\varphi_1] = S[\varphi_1] + \tfrac{1}{2}\operatorname{tr}\ln(1 + \lambda_2(-\Delta_x + m_2^2)^{-1}\varphi_1^2). \tag{15}$$

There are many ways to evaluate the Fredholm determinant, defined by the above equation. Using a series expansion, it is possible to rewrite Eq. (15) as

$$\Gamma_{\text{eff}}[\varphi_1] = S[\varphi_1] - \frac{1}{2}\sum_{k=1}^{\infty} \frac{(-1)^k}{k} \operatorname{tr}(\lambda_2(-\Delta_x + m_2^2)^{-1}\varphi_1^2)^k, \tag{16}$$

or, in a more compact notation,

$$\Gamma_{\text{eff}}[\varphi_1] = S[\varphi_1] + \sum_{k=1}^{\infty} \Gamma^{(k)}[\varphi_1], \tag{17}$$

where each term of the series $\Gamma^{(k)}[\varphi_1]$ is given by Eq. (16). Let us study the first nontrivial contribution of this series, namely, the term $k=1$ which corresponds to a one-loop diagram. It is explicitly given by

$$\Gamma^{(1)}[\varphi_1] = \frac{\lambda_2}{2} \int d^dx\, G(x-x;m_2)\, \varphi_1^2(x). \tag{18}$$

Using the Fourier representation of the two-point Schwinger function associated with the heavy mass field $\varphi_2(x)$, and defining a new coupling constant $\sigma = \lambda_2\mu^{4-d}$, where μ is the usual dimensional parameter that appears in the dimensional regularization procedure, we readily obtain

$$\Gamma^{(1)}[\varphi_1] = \frac{\sigma}{2(2\sqrt{\pi})^d} \Gamma\left(1 - \frac{d}{2}\right) (m_2)^{d-2} \int d^dx \quad \varphi_1^2(x). \tag{19}$$

Now, the Gamma function $\Gamma(z)$ is a meromorphic function of the complex variable z with simple poles at the points $z=0,-1,-2,\ldots$. In the neighborhood of any of its poles $z=-n$, for $n=0,1,2,\ldots$, $\Gamma(z)$ has a representation given by

$$\Gamma(z)=\frac{(-1)^n}{n!}\frac{1}{(z+n)}+\Omega(z+n), \tag{20}$$

where $\Omega(z+n)$ stands for the regular part of the analytic extension of $\Gamma(z)$. Note that for odd dimensions $\Gamma^{(1)}[\varphi_1]$ is completely regular while in even dimensions ($d=2\ell$ $\ell=1,2,\ldots$) there are singularities in the dimensional regularized quantity. By using the standard dimensional regularization prescription $d=2\ell-\epsilon$ and since Eq. (19) is quadratic in the field $\varphi_1(x)$, the divergence can be absorbed in the renormalized mass of the $\varphi_1(x)$ field. Consequently, we define the renormalized mass for the light field as

$$m_{1R}^2=m_1^2-\frac{\sigma m_2^{d-2}}{(4\pi)^{d/2}}\left[\frac{(-1)^{(d/2)-1}}{\left(\frac{d}{2}-1\right)!}\frac{2}{\epsilon}+\Omega\left(\frac{\epsilon}{2}\right)\right]. \tag{21}$$

Note that for odd-dimensional cases there are no poles. We have thus shown that at the one-loop approximation, the first correction to the effective action given by $\Gamma^{(1)}[\varphi]$ that we obtain integrating out the heavy mass field $\varphi_2(x)$ is just a modification of the value of the renormalized mass associated with the light field.

We will now show that the second correction to the effective action given by $\Gamma^{(2)}[\varphi_1]$ only modifies the value of the coupling constant of the field $\varphi_1(x)$. To this end, let us study the second term of the series in Eq. (17). It corresponds to a one-loop diagram and is actually given by

$$\Gamma^{(2)}[\varphi_1]=-\frac{\sigma^2}{4}\int d^dx\int d^dy\, G(y-x;m_2)G(x-y;m_2)\varphi_1^2(x)\varphi_1^2(y), \tag{22}$$

which, upon substitution of the free two-point Schwinger function associated with the $\varphi_2(x)$ heavy field and the introduction of $I(p^2,m_2^2)$ as

$$I(p^2,m_2^2)=\frac{1}{(2\pi)^d}\int d^dq\,\frac{m_2^{4-d}}{(q^2+m_2^2)((p+q)^2+m_2^2)}, \tag{23}$$

can be written as

$$\Gamma^{(2)}[\varphi_1]=-\frac{\sigma^2}{4(2\pi)^d}\int d^dx\int d^dy\,\varphi_1^2(x)\varphi_1^2(y)\int d^dp\,e^{-ip(y-x)}m_2^{d-4}I(p^2,m_2^2). \tag{24}$$

In the regularization and renormalization procedure we have to eliminate the poles and their residues adding counterterms in the Lagrangian density. To this end, let us study the quantity $I(p^2,m_2^2)$. Using the Feynman parametrization,[29] it is possible to write $I(p^2,m_2^2)$ as

$$I(p^2,m_2^2)=N_d\left(-\frac{1}{\epsilon}+O(\epsilon)\right)\left(1-\frac{d}{2}\right)\int_0^1 dt\left(\frac{p^2}{m_2^2}t(1-t)+1\right)^{(d/2)-2}, \tag{25}$$

where N_d is the area of the sphere $S_{d-1}/(2\pi)^d$. The expression given by Eq. (25) contains a power of a binomial. In a d-dimensional Euclidean space, when d is even, the power is an integer and the use of Newton's binomial theorem gives us a direct way of evaluating $I(p^2,m_2^2)$. When d is odd, the expansion of $(1+(p^2/m_2^2)\,t(1-t))^{(d/2)-2}$ yields an infinite power series. Since we are using dimensional regularization we have an infinite power series. Note that the generalization of

the binomial series is valid for any complex exponent p. In other words, we have an everywhere convergent power series in p, hence a continuous function on p in the complex plane.[30] If we define

$$C_r^0=1, \quad C_r^1=\frac{r}{1!}, \quad C_r^2=\frac{r(r-1)}{2!}, \cdots \tag{26}$$

until

$$C_r^k=\frac{r(r-1)\cdots(r-k+1)}{k!}, \tag{27}$$

where $r=(d/2)-2$, it is possible to write $I(p^2,m_2^2)$ as

$$I(p^2,m_2^2)=\left(1-\frac{d}{2}\right)N_d\left(-\frac{1}{\epsilon}+O(\epsilon)\right)\sum_{k=0}^{\infty} C_{(d/2)-2}^k \frac{p^{2k}}{m_2^{2k}}\int_0^1 dt(t(1-t))^k. \tag{28}$$

Let us use Euler's integral of first kind $B(\alpha,\beta)$ given by[31]

$$B(\alpha,\beta)=\int_0^1 dx\, x^{\alpha-1}(1-x)^{\beta-1}=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}, \ \mathrm{Re}\,\alpha>0, \mathrm{Re}\,\beta>0. \tag{29}$$

Substituting Eq. (28) and Eq. (29) in Eq. (24), we find that the second term of the series that represents the effective action, $\Gamma^{(2)}[\varphi_1]$, can be written as

$$\Gamma^{(2)}[\varphi_1]=-\frac{\sigma^2}{4(2\pi)^d}\int d^dx \int d^dy\, \varphi_1^2(x)\varphi_1^2(y)\int d^dp\ e^{-ip(y-x)}m_2^{d-4}\left(1-\frac{d}{2}\right)$$
$$\times N_d\left(-\frac{1}{\epsilon}+O(\epsilon)\right)\sum_{k=0}^{\infty} C_{(d/2)-2}^k \frac{p^{2k}}{m_2^{2k}}B(k+1,k+1). \tag{30}$$

If we choose the self-interacting part of the field $\varphi_1(x)$ to be $\lambda_1\varphi_1^4(x)$, it is possible to define the renormalized coupling constant λ_R subtracting the polar part. Consequently, the effective action for the $\varphi_1(x)$ field is given by

$$\Gamma_{\mathrm{eff}}[\varphi_1]=\frac{1}{2}\int d^dx\ \ \varphi_1(x)(-\Delta+m_1^2)\varphi_1(x)+\lambda_R\int d^dx\ \ \varphi_1^4(x)+\frac{\sigma^2}{4!(4\pi)^2m_2^2}$$
$$\times\int d^dx\ \ \varphi_1^2(x)(-\Delta+m_1^2)\varphi_1^2(x)+O\left(\frac{\Delta}{m_2^2}\right)^2. \tag{31}$$

Note that the terms $k=3,4,...$ are not divergent (in a four-dimensional theory) and although they contribute to the effective action, in the limit $m_2\to\infty$, the heavy mass field $\varphi_2(x)$ decouples from the light mass field $\varphi_1(x)$. The effect of the heavy mass field appears only modifying the values of the renormalized mass m_{1R} and the coupling constant λ_R. We showed that the Euclidean version of the Appelquist–Carazzone decoupling theorem works in this specific model. Another well known example where the decoupling theorem can be used is in quantum electrodynamics, where for energies much lower than the electron mass it is possible to construct a derivative expansion of the Maxwell field effective action integrating out the Dirac field. This is an expected result, since we known that the Appelquist–Carazzone theorem is valid for renormalizable theories without spontaneous symmmetry breaking or chiral fermions. The above discussion justifies the approach used by some authors that have been using the Euler–Heisenberg Lagrangian density to investigate the radiative correction to the Casimir effect,[10] although these radiative corrections

are of no phenomenological significance as pointed out by Melnikov.[14] For a careful discussion of effective Lagrangians in quantum electrodynamics and finite temperature field theory, see Refs. 32 and 33, respectively.

In the next section we will study the massive $(\lambda\varphi^4)_d$ theory in the presence of two parallel hyperplanes. Consequently, going back to the Schwinger functional, we are assuming that the functional integral must be taken over the space of the functions that vanish on the boundaries. One way to implement this is to introduce delta functions in the functional integral. This is equivalent to evaluate the functional integral over a space of functions that satisfy the boundary conditions. This is the procedure that we are adopting. It is clear that this procedure will introduce additional surface divergences that can be eliminated by surface counterterms. In the end, we have the effective model for the light mass field that satisfies boundary conditions over some surfaces.

III. FINITE SIZE EFFECTS AND THE TWO AND FOUR-POINT SCHWINGER FUNCTIONS IN THE ONE-LOOP APPROXIMATION

In the last section, we studied a very simple model of two massive scalar fields where the decoupling theorem holds after the construction of an effective theory of the light mass field. We have shown that in our model of two massive interacting scalar fields, the heavy modes associated with the $\varphi_2(x)$ field completely decouple from the light ones associated with the light mass field $\varphi_1(x)$ in the limit $m_2\to\infty$. In the case of a $\lambda_1\varphi_1^4(x)$ self-interacting part, the only effect of the heavy mass field is a modification of the mass m_1 and of the coupling constant of the light mass field. We are reducing the problem in this manner since we are able to concentrate in such a one field theory, i.e., we will consider a $\lambda_1\varphi^4(x)$ self-interacting model. We will consider that the field $\varphi(x)$ depends on $d-1$ unbounded coordinates that we call $\mathbf{r}$, and one bounded coordinate which we will refer to as z that will be assumed to lie in the interval $[0,L]$. If we exclude the possibility of periodic or antiperiodic boundary conditions, this choice obviously breaks the full translational invariance because we have to assume boundary conditions on the hyperplanes $z=0$ and $z=L$.

To write the full renormalized action for the theory with boundaries we need two regulators: the first one is the usual ϵ that is introduced in the dimensional regularization procedure and the second one, that we call η, represents the distance to a boundary. According to this the full renormalized action must be given by[24]

$$S(\varphi)=\int_0^L dz\int d^{d-1}r\left(\frac{A(\epsilon)}{2}(\partial_\mu\varphi)^2+\frac{B(\epsilon)}{2}\varphi^2+\frac{C(\epsilon)}{4!}\varphi^4\right)+\int d^{d-1}r(c_1(\eta)\varphi^2(\mathbf{r},0)$$

$$+c_2(\eta)\varphi^2(\mathbf{r},L))+\int d^{d-1}r(c_3(\eta)\varphi^4(\mathbf{r},0)+c_4(\eta)\varphi^4(\mathbf{r},L)), \tag{32}$$

where $A(\epsilon)$, $B(\epsilon)$, and $C(\epsilon)$ are the usual coefficients for the bulk counterterms and the coefficients $c_i(\eta)$ $i=1,...,4$, which depend on the boundary conditions for the field, are the coefficients for the surface counterterms. As usual all of these coefficients must be calculated order by order in perturbation theory. We are considering two different possibilities for the boundary conditions, namely Dirichlet–Dirichlet (DD) and Neumann–Neumann (NN) boundary conditions. These boundary conditions are given, respectively, by

$$\varphi(\mathbf{r},z)\big|_{z=0}=\varphi(\mathbf{r},z)\big|_{z=L}=0, \tag{33}$$

and

$$\frac{\partial}{\partial z}\varphi(\mathbf{r},z)\bigg|_{z=0}=\frac{\partial}{\partial z}\varphi(\mathbf{r},z)\bigg|_{z=L}=0. \tag{34}$$

The system we are interested in is invariant only under translations along the direction parallel to the plates. This implies that what is conserved is not the full momentum but the $(d-1)$ dimen-

sional parallel momentum **p**. For such conditions, a more convenient representation of the n-point Schwinger functions is a mixed $(\mathbf{p},z)$ representation. A Euclidean scalar field $\varphi(x)$ satisfying certain homogeneous boundary conditions on $z=0$ and L can be expanded in Fourier series as

$$\varphi(\mathbf{r},z)=\frac{1}{(2\pi)^{(d-1)/2}}\sum_n u_n(z)\int d^{d-1}p\ \phi_n(\mathbf{p})\,e^{i\mathbf{p}.\mathbf{r}}, \tag{35}$$

where **p** is the continuum parallel momentum, and $u_n(z)$ stands for the eigenfunctions of the operator $-(d^2/dz^2)$,

$$-\frac{d}{dz^2}u_n(z)=k_n^2u_n(z), \tag{36}$$

where $k_n=n\pi/L$, $n=1,2,...$ for DD b.c., and $n=0,1,2,...$ for NN boundary conditions, respectively. The main difference between the boundary conditions is the presence of the zero mode. The free two-point Schwinger function of the theory $G_0^{(2)}(\mathbf{r},z,\mathbf{r}',z')$ can be expressed as

$$G_0^{(2)}(\mathbf{r},z,\mathbf{r}',z')=\frac{1}{(2\pi)^{d-1}}\sum_n u_n(z)u_n^*(z')\int d^{d-1}p\,\frac{e^{i\mathbf{p}.(\mathbf{r}-\mathbf{r}')}}{(\mathbf{p}+k_n^2+m^2)}. \tag{37}$$

Note that we have changed the notation in this section as follows: $m_1\to m$ and also $G(x,x';m_1)\to G_0(x,x')$. It is useful to define also $\boldsymbol{\rho}=\mathbf{r}-\mathbf{r}'$. When considering DD boundary conditions, one finds that the free two-point Schwinger function is explicitly given by

$$G_0^{(2)}(\boldsymbol{\rho},z,z')=\frac{2}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi z}{L}\right)\sin\left(\frac{n\pi z'}{L}\right)I_n(L,m,d,\boldsymbol{\rho}), \tag{38}$$

where

$$I_n(L,m,d,\boldsymbol{\rho})=\frac{1}{(2\pi)^{d-1}}\int d^{d-1}p\,\frac{e^{i\mathbf{p}.\boldsymbol{\rho}}}{\left(\mathbf{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right)}. \tag{39}$$

It is clear that the family of $I_n(L,m,d,\boldsymbol{\rho})$ functions can be thought of as the free propagators of a tower of massive scalar fields in $(d-1)$ dimensions, the effective mass of each mode being given by $M_n^2=m^2+(n\pi/L)^2$. This is to be expected since our theory has been formulated in a compactified space. From an even simpler point of view, $I_n(L,m,d,\boldsymbol{\rho})$ is nothing but the Fourier transform of a "spherically" $(\mathrm{SO}(d-1))$ symmetric function of the parallel momentum **p**.

We begin the study of the interacting theory by building the one-loop correction $(G_1^{(2)}(\lambda_1,x,x'))$ to the bare two-point Schwinger function $G_0^{(2)}(x,x')$, for both the DD and NN boundary conditions. Using the Feynman rules we have

$$G_1^{(2)}(\lambda_1,\mathbf{r}_1,z_1,\mathbf{r}_2,z_2)=\frac{\lambda_1}{2}\int d^{d-1}r\int_0^L dz\ G_0^{(2)}(\mathbf{r}_1-\mathbf{r},z_1,z)G_0^{(2)}(\mathbf{0},z)G_0^{(2)}(\mathbf{r}-\mathbf{r}_2,z,z_2). \tag{40}$$

Here we point out that even though the functions $G_0^{(2)}(\mathbf{r}_1-\mathbf{r}_2,z_1,z_2)$ and $G_0^{(2)}(\mathbf{r}_2-\mathbf{r}_3,z_2,z_3)$ are singular at coincident points $(\mathbf{r}_1=\mathbf{r}_2,\ z_1=z_2)$ and $(\mathbf{r}_2=\mathbf{r}_3,\ z_2=z_3)$, the singularities are integrable for points outside the plates. Using the notation $G_0^{(2)}(\mathbf{0},z)=T_{\mathrm{DD}}(L,m,d,z)$, a straightforward substitution yields the order λ_1 correction to the bare two-point Schwinger function in the one-loop approximation for the case of Dirichlet boundary conditions:

$$G_1^{(2)}(\lambda_1,\mathbf{r}_1-\mathbf{r}_2,z_1,z_2)=\frac{2\lambda_1}{(2\pi)^{d-1}L^2}\int_0^L dz\sum_{n,n'=1}^{\infty}\sin\left(\frac{n\pi z_1}{L}\right)\sin\left(\frac{n\pi z}{L}\right)\sin\left(\frac{n'\pi z}{L}\right)\sin\left(\frac{n'\pi z_2}{L}\right)$$
$$\times\int d^{d-1}p\,\frac{e^{i\mathbf{p}(\mathbf{r}_1-\mathbf{r}_2)}}{\left(\mathbf{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right)\left(\mathbf{p}^2+\left(\frac{n'\pi}{L}\right)^2+m^2\right)}T_{\mathrm{DD}}(L,m,d,z). \tag{41}$$

Note that since we use dimensional regularization techniques, we have introduced a dimensional parameter μ, defining a dimensionless coupling constant $\lambda=\lambda_1\mu^{4-d}$. The expression for the amputated one-loop two-point function $T_{\mathrm{DD}}(L,m,d,z)$ is given by

$$T_{\mathrm{DD}}(L,m,d,z)=\frac{2}{(2\pi)^{d-1}L}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi z}{L}\right)\int d^{d-1}p\,\frac{1}{\left(\mathbf{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right)}. \tag{42}$$

In the case of Neumann–Neumann boundary conditions the expression for the amputated one-loop two-point function can also be found following the same procedure, and it is given by

$$T_{\mathrm{NN}}(L,m,d,z)=\frac{1}{(2\pi)^{d-1}L}\int d^{d-1}k\,\frac{1}{(\mathbf{k}^2+m^2)}$$
$$+\frac{2}{(2\pi)^{d-1}L}\sum_{n=1}^{\infty}\cos^2\left(\frac{n\pi z}{L}\right)\int d^{d-1}p\,\frac{1}{\left(\mathbf{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right)}. \tag{43}$$

Both $T_{\mathrm{DD}}(L,m,d,z)$ and $T_{\mathrm{NN}}(L,m,d,z)$ diverge in their continuum momenta integrals and also in the discrete mode summation. Using the Feynman rules, $G_2^{(4)}(\lambda,x_1,x_2,x_3,x_4)$, i.e., the $O(\lambda^2)$ correction to the bare one-loop four-point Schwinger function, is given by

$$G_2^{(4)}(\lambda,\mathbf{r}_1,z_1,\mathbf{r}_2,z_2,\mathbf{r}_3,z_3,\mathbf{r}_4,z_4)=\frac{\lambda^2}{2}\int d^{d-1}r\int d^{d-1}r'\int_0^L dz\int_0^L dz'\;\; G_0^{(2)}(\mathbf{r}_1-\mathbf{r},z_1,z)$$
$$\times G_0^{(2)}(\mathbf{r}_2-\mathbf{r},z_2,z)(G_0^{(2)}(\mathbf{r}-\mathbf{r}',z,z'))^2$$
$$\times G_0^{(2)}(\mathbf{r}'-\mathbf{r}_3,z',z_3)G_0^{(2)}(\mathbf{r}'-\mathbf{r}_4,z',z_4). \tag{44}$$

Again, all G_0's are singular at coincident points, but the singularities are integrable for points outside the plates, except for $G_0^{(2)}(\mathbf{r}-\mathbf{r}',z,z')$.

In the next section we will begin the renormalization program for the massless one-loop two-point Schwinger functions for the case of Dirichlet–Dirichlet boundary condition. The two-point Schwinger function for the case of Dirichlet–Dirichlet boundary conditions is IR finite for $m=0$. The study of the complementary set of boundary conditions, namely, NN boundary conditions, can be performed along the same lines. When the field satisfies NN boundary conditions, infrared divergences appear and such divergences come from the zero mode contribution. For the case of NN we must have a finite Euclidean volume to regularize the theory in the infrared. Another possible solution to the problem of the infrared divergences in the case of Neumann–Neumann boundary condition is to perform a resummation of the daisy diagrams.[34–37] This procedure is standard in the study of scalar models where the translational invariance is maintained, as for example finite temperature field theory. For systems where the translational invariance is broken, the problem of how to carry out the resummation program still remains open.

IV. THE REGULARIZED ONE-LOOP TWO AND FOUR-POINT SCHWINGER FUNCTIONS

In this section we would like to discuss how to implement the one-loop renormalization program in finite size systems where flat surfaces break the translational invariance. Thus, the aim of this section is first to analyze the structure of the divergences associated with the one-loop two and four-point functions for the case of Dirichlet–Dirichlet boundary conditions.

The amputated one-loop two-point Schwinger function $T_{\mathrm{DD}}(L,m,d,z)$ can be decomposed in a translational invariant part and another one that breaks the translational invariance. Indeed, using algebraic identities as in Refs. 31 and 38, one gets

$$T_{\mathrm{DD}}(L,m,d,z)=f_1(L,m,d)-f_2(L,m,d,z), \tag{45}$$

where the functions $f_1(L,m,d)$ and $f_2(L,m,d,z)$ are given, respectively, by

$$f_1(L,m,d)=\frac{1}{2(2\pi)^{d-1}L}\sum_{n=-\infty}^{\infty}\int d^{d-1}p\,\frac{1}{\left(\mathbf{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right)} \tag{46}$$

and

$$f_2(L,m,d,z)=\frac{1}{2(2\pi)^{d-1}}\int d^{d-1}p\,\frac{1}{\sqrt{\mathbf{p}^2+m^2}}\,\frac{\cosh((L-2z)\sqrt{\mathbf{p}^2+m^2})}{\sinh(L\sqrt{\mathbf{p}^2+m^2})}. \tag{47}$$

The amputated one-loop two-point Schwinger function for the Neumann–Neumann boundary conditions, $T_{\mathrm{NN}}(L,m,d,z)$, can be similarly split up as

$$T_{\mathrm{NN}}(L,m,d,z)=f_1(L,m,d)+f_2(L,m,d,z). \tag{48}$$

The above decompositions of $T_{\mathrm{DD}}(L,m,d,z)$ and $T_{\mathrm{NN}}(L,m,d,z)$ have the same functional form. Some divergences come purely from the bulk, while others depend on the distance to the boundaries. Indeed, since $f_1(L,m,d)$ does not depend on z, it contains only bulk divergences. These divergences occur not only in the discrete sums but also in the momentum integrations. After the identification: $\beta\equiv 2L$, the term $f_1(L,m,d)$ is formally proportional to the amputated one-loop two-point function of the theory assuming that the system is in thermal equilibrium with a reservoir at temperature β^{-1}. To deal with the divergences of $f_1(L,m,d)$, or equivalently, the one-loop two-point Schwinger functions at finite temperature we have to do frequency sums and $(d-1)$ dimensional integrals for the continuum momenta. One way to perform the integrals with Matsubara sums is to analytically extend away from the discrete complex energies down to real axis with the replacement of the energy sums by contour integrals.[39,40] Another way is to use dimensional regularization and afterwards to analytically extend the modified Epstein zeta function which appears after dimensional regularization. Direct use of dimensional regularization identities and the analytic extension of the modified Epstein zeta function in the sum given by Eq. (46) which defines $f_1(L,m,d)$, gives us a polar part (size independent) plus a size-dependent analytic correction. The mass counterterm (the principal part of the Laurent series of the analytic regularized quantity) generated by $f_1(L,m,d)$ is size independent, in the same way that the finite temperature field theory has no temperature dependent counterterm. Observe that the nontranslational invariant part of the amputated one-loop two-point Schwinger function expressed by $T_{\mathrm{DD}}(L,m,d,z)$ and $T_{\mathrm{NN}}(L,m,d,z)$ has the same z dependence in modulus but with opposite signs.

We have shown that the $T_{\mathrm{DD}}(L,m,d,z)$ and $T_{\mathrm{NN}}(L,m,d,z)$ can be split into two functions $f_1(L,m,d)$ and $f_2(L,m,d,z)$ and since as we have just discussed the behavior of $f_1(L,m,d)$, we can now turn our attention to the study of the divergences contained in $f_2(L,m,d,z)$. We begin by an angular integration ($d^{d-1}p=p^{d-2}dp\,d\Omega_{d-1}$ and $\int d\Omega_d=[2\pi^{(d/2)}]/[\Gamma d/2]$) that leads to an alternative expression for the nontranslational invariant part $f_2(L,m,d,z)$, namely,

$$f_2(L,m,d,z)=\frac{1}{2}h(d)\int_0^\infty dp\,\frac{p^{d-2}}{\sqrt{p^2+m^2}}\,\frac{\cosh((L-2z)\sqrt{p^2+m^2})}{\sinh(L\sqrt{p^2+m^2})}. \tag{49}$$

Using the change of variables $s=\sqrt{p^2+m^2}$ in the above expression yields the following formula for $f_2(L,m,d,z)$:

$$f_2(L,m,d,z)=\frac{1}{2}h(d)\int_m^\infty ds(s^2-m^2)^{(d-3)/2}\cosh((L-2z)s)(\sinh Ls)^{-1}, \tag{50}$$

where $h(d)$ is an analytic function of d given by

$$h(d)=\frac{1}{2(2\sqrt{\pi})^{d-1}}\,\frac{1}{\Gamma\left(\frac{d-1}{2}\right)}.$$

We now start studying the massless case following Fosco and Svaiter.[41] In fact, we are particularly interested in examining the limits ($z\to 0^+$ and $z\to L^-$) which obviously contain the information about the effects of the boundaries. In order to fulfill this goal we introduce two new variables $x=Ls$ and $q=zs$, in terms of which we can write $f_2(L,m,d,z)|_{m=0}$ as

$$f_2(L,m,d,z)|_{m=0}=\frac{h(d)}{2L^{d-2}}\int_0^\infty dx\,x^{d-3}(\coth x-1)\cosh\left(\frac{2zx}{L}\right)+\frac{h(d)}{2z^{d-2}}\int_0^\infty dq\,q^{d-3}e^{-2q}. \tag{51}$$

The second term of Eq. (51) gives us the well known result that for a massless scalar field in $d=4$ the one-loop vacuum fluctuations diverge as $1/z^2$ if we approach the boundary at $z=0$.[42] The other term of Eq. (51) should behave as $1/(L-z)^{d-2}$. To see this let us investigate the behavior of the first integral of $f_2(L,m,d,z)|_{m=0}$ near the boundary at $z=L$. In order to do this, we make use of two formulas involving the definition for the Gamma function, and also another well known integral representation for the product of the Gamma function times the Hurwitz zeta function given by

$$\int_0^\infty dx\,x^{\mu-1}e^{-\beta x}(\coth x-1)=2^{1-\mu}\Gamma(\mu)\zeta\left(\mu,\frac{\beta}{2}+1\right)\quad \mathrm{Re}(\beta)>0,\ \mathrm{Re}(\mu)>1, \tag{52}$$

where $\zeta(z,a)$ is the Hurwitz zeta function defined by[31]

$$\zeta(z,a)=\sum_{n=0}^{\infty}\frac{1}{(n+a)^z},\quad \mathrm{Re}(z)>1,\quad a\neq 0,-1,-2,\ldots. \tag{53}$$

From the definition of the Gamma function and using Eq. (52) in Eq. (51) we may write the following closed expression:

$$f_2(L,m,d,z)|_{m=0}=\frac{h(d)}{2L^{d-2}}\left[2^{2-d}\Gamma(d-2)\left(\zeta\left(d-2,\frac{z}{L}+1\right)+\zeta\left(d-2,-\frac{z}{L}+1\right)\right)\right]$$
$$+\frac{1}{(2z)^{d-2}}h(d)\Gamma(d-2). \tag{54}$$

From this last expression and using the definition of the Hurwitz zeta function given by Eq. (53) it is evident that the regularized $f_2(L,m,d,z)|_{m=0}$ has two poles of order $(d-2)$, one at $z=0$ and another at $z=L$.

To study the massive case, from the expression given by Eq. (50) it is possible to write $f_2(L,m,d,z)$ in a more convenient way by

$$f_2(L,m,d,z)=f_{21}(L,m,d,z)+f_{22}(L,m,d,z), \tag{55}$$

where $f_{21}(L,m,d,z)$ and $f_{22}(L,m,d,z)$ are

$$f_{21}(L,m,d,z)=\frac{1}{2}h(d)\int_m^\infty ds(s^2-m^2)^{(d-3)/2}e^{-2zs}, \tag{56}$$

and

$$f_{22}(L,m,d,z)=\frac{1}{2}h(d)\int_m^\infty ds(s^2-m^2)^{(d-3)/2}(\coth Ls-1)\cosh 2zs. \tag{57}$$

Using an integral representation of the Bessel function of third kind (Macdonald's function) it is possible to find the following closed expression for $f_{12}(L,m,d,z)$:

$$f_{21}(L,m,d,z)=\frac{1}{2}\frac{1}{(2\sqrt{\pi})^{d-1}}\left(\frac{m}{z}\right)^{(d-2)/2}K_{(d-2)/2}(2mz). \tag{58}$$

For small z and finite m we have the asymptotic formula $K_\nu(z)\approx 2^{\nu-1}\Gamma(\nu)z^{-\nu}$, which means that for $z\to 0^+$, the function $f_{21}(L,m,d,z)$ diverges as $1/z^{d-2}$. To calculate $f_{22}(L,m,d,z)$ we will use the same method that we used in Sec. II. Making use of the generalized binomial formula,

$$\left(1-\frac{m^2}{s^2}\right)^{(d-3)/2}=\sum_{k=0}^{\infty}(-1)^k C^k_{(d-3)/2}\left(\frac{m}{s}\right)^{2k}, \tag{59}$$

and introducing a new variable $u=Ls$, we obtain

$$f_{22}(L,m,d,z)=\frac{h(d)}{2L^{d-2}}\sum_{k=0}^{\infty}(-1)^k C^k_{(d-3)/2}(Lm)^{2k}\int_{Lm}^\infty du\,u^{d-3-2k}(\coth u-1)\cosh\left(\frac{2zu}{L}\right). \tag{60}$$

Our next step is to show that this result can be expressed in terms of the Hurwitz zeta function. Let split $f_{22}(L,m,z,d)$ as a sum of two terms

$$f_{22}(L,m,d,z)=f^<_{22}(L,m,z,d)+f^>_{22}(L,m,z,d), \tag{61}$$

where

$$f^<_{22}(L,m,z,d)=-\frac{1}{4L^{d-2}}\sum_{k=0}^{k<(d-3)/2}C^{(1)}(d,k)(Lm)^{2k}\int_{Lm}^\infty du\,u^{d-3-2k}(\coth u-1)\cosh\left(\frac{2uz}{L}\right), \tag{62}$$

and

$$f^>_{22}(L,m,z,d)=-\frac{1}{4L^{d-2}}\sum_{k\geqslant (d-3)/2}^{\infty}C^{(1)}(d,k)(Lm)^{2k}\int_{Lm}^\infty du\,u^{d-3-2k}(\coth u-1)\cosh\left(\frac{2uz}{L}\right). \tag{63}$$

Here we have introduced $C^{(1)}(d,k)=(-1)^k C^k_{(d-3)/2}h(d)$ and also $C^{(2)}(d,k)\equiv[\Gamma(d-2-2k)/2^{d-3-2k}]\,C^{(1)}(d,k)$. Thus it is possible to write Eq. (62) in the following way:

$$f_{22}^{<}(L,m,z,d)=-\frac{1}{4L^{d-2}}\sum_{k=0}^{k<(d-3)/2}C^{(2)}(d,k)(Lm)^{2k}\left(\zeta\left(d-2-2k,-\frac{z}{L}+1\right)+\zeta\left(d-2-2k,\frac{z}{L}+1\right)\right)+\frac{1}{4L^{d-2}}\sum_{k=0}^{k<(d-3)/2}C^{(1)}(d,k)(Lm)^{2k}\times\int_0^{Lm}du\,u^{d-3-2k}(\coth u-1)\cosh\left(\frac{2uz}{L}\right),\tag{64}$$

where the singularities of $f_{22}^{<}(L,m,z,d)$ appear at $z\to L$. Turning our attention to $f_{22}^{>}(L,m,z,d)$, it is clear that in the expression above we see that the surface divergences are the same as we studied before in the massless case.

We now turn our attention back to the four-point Schwinger function in the one-loop approximation. Introducing new variables as $u_{\pm}\equiv z\pm z'$, the two-point Schwinger function in the tree-level can be split into

$$G_0^{(2)}(\boldsymbol{\rho},z,z')=G_{+}^{(2)}(\boldsymbol{\rho},u_{+})+G_{-}^{(2)}(\boldsymbol{\rho},u_{-}),\tag{65}$$

where making use of the definition of $I_n(L,m,d,\boldsymbol{\rho})$ given by Eq. (39) we have

$$G_{\pm}^{(2)}(\boldsymbol{\rho},u_{\pm})=\mp\frac{1}{L}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi u_{\pm}}{L}\right)I_n(L,m,d,\boldsymbol{\rho}).\tag{66}$$

Before we continue, let us present an explicit formula of the free two-point Schwinger function in terms of Bessel functions. Defining an analytic function $g(d)$ by

$$g(d)=\frac{1}{\sqrt{\pi}(2\pi)^{(d-1)/2}}\frac{\Gamma\left(\frac{d-2}{2}\right)}{\Gamma\left(\frac{d-3}{2}\right)},\tag{67}$$

it is possible to show that we can write $G_{\pm}^{(2)}(\rho,u_{\pm})$ as

$$G_{\pm}^{(2)}(\rho,u_{\pm})=\mp\frac{g(d)}{\rho^{(d-3)/2}L}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi u_{\pm}}{L}\right)\left(\left(\frac{n\pi}{L}\right)^2+m^2\right)^{(d-3)/4}K_{(d-3)/2}\left(\rho\left(m^2+\left(\frac{n\pi}{L}\right)^2\right)^{1/2}\right).\tag{68}$$

Using Eq. (65) and the above formula we obtain the explicit expression for the two-point Schwinger function in a generic d-dimensional Euclidean space confined between two flat parallel hyperplanes where we assume Dirichlet–Dirichlet boundary conditions. It is hard to use the above expressions for $G_{\pm}^{(2)}(\rho,u_{\pm})$ to investigate the analytic structure of the four-point function given by Eq. (44) $G_2^{(4)}(\lambda,\mathbf{r}_1,z_1,\mathbf{r}_2,z_2,\mathbf{r}_3,z_3,\mathbf{r}_4,z_4)$, for both the bulk and near the boundaries. Nevertheless from Eqs. (38) and (39) it is clear that the divergences of the four-point function in the one-loop approximation appear at coincident points and, therefore, the singular behavior is encoded in the polar part of $M(\lambda,L,m,d)$ given by

$$M(\lambda,L,m,d)=\lambda^2\int d^{d-1}r\int d^{d-1}r'\int_0^L dz\int_0^L dz'F(\mathbf{r},\mathbf{r}',z,z')(G_0^{(2)}(\mathbf{r}-\mathbf{r}',z,z'))^2,\tag{69}$$

where $F(\mathbf{r},\mathbf{r}',z,z')$ is a regular function. Exactly as in the one-loop two point function, the above equation has two kinds of singularities: those coming from the bulk and those arising from the

behavior near the surface. As before, the behavior in the bulk is that of thermal field theory. Consequently we will only discuss the singularities that arise from the boundaries. This can be done by studying the polar part of $\tilde{M}(\lambda,L,m,d)$ given by

$$\tilde{M}(\lambda,L,m,d)=\frac{\lambda^2}{2}\int_0^L dz\int_0^L dz'\,\mathcal{F}(z,z')(G_0^{(2)}(\mathbf{0},z,z'))^2, \tag{70}$$

where $\mathcal{F}(z,z')$ is a regular function. Now, we recall that the form of $G_{\pm}^{(2)}(\rho,u_{\pm})|_{\rho=0}$ is given by

$$G_{\pm}^{(2)}(\rho,u_{\pm})|_{\rho=0}=\mp\frac{1}{(2\pi)^{d-1}L}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi u_{\pm}}{L}\right)\int d^{d-1}p\,\frac{1}{\left(\mathbf{p}^2+m^2+\left(\frac{n\pi}{L}\right)^2\right)}, \tag{71}$$

from which one can show that the free correlation function is given by

$$G_0^{(2)}(\rho,z,z')|_{\rho=0}=f_2\left(L,m,d,\frac{u_-}{2}\right)-f_2\left(L,m,d,\frac{u_+}{2}\right). \tag{72}$$

For the sake of simplicity we will discuss only the massless case, since the singularities of the massive case have the same structure as the massless one. The function $f_2(L,m,d,u_+/2)$ is nonsingular in the bulk, i.e., in the interior of the interval $[0,L]$, while $f_2(L,m,d,u_-/2)$ has a singularity along the line $z=z'$. Indeed, closer inspection shows that for $0\leqslant z,z'\leqslant L$ the only singularities are those at $u_+=0$, $u_+=2L$ and also $u_-=0$. The former two are genuinely boundary singularities (the two conditions imply $z,z'\to 0$ or $z,z'\to L$), while the one coming from $z=z'$ in the whole domain is just the standard bulk singularity. One finds that the counterterms for $\tilde{M}$ are given by

$$-\text{pole}\int_0^L dz\int_0^L dz'\left[\frac{C_1}{(z+z')^{d-2}}+\frac{C_2}{(2L-z-z')^{d-2}}+\frac{C_3}{(z-z')^{d-2}}+\cdots\right]^2, \tag{73}$$

where $C_i, i=1,...,3$ are regular functions that do not depend on z nor on z'. From this discussion it is clear that in order to render the field theory finite, we must introduce surface terms in the action. This is a general statement. For any fields that satisfy boundary condition that breaks the translational invariance, in addition to the usual bulk counterterms, it is sufficient to introduce surface counterterms in the action to render the theory finite.

V. BOUNDARY EFFECTS AND RENORMALIZATION

In the last section we presented the one-loop renormalization of the $\lambda\varphi^4$ model, and also considered that the field $\varphi(x)$ depends on $d-1$ unbounded coordinates that we call $\mathbf{r}$ and one bounded coordinate defined in the interval $[0,L]$. The boundary conditions on the hyperplanes $z=0$ and $z=L$ are the usual Dirichlet–Dirichlet and also Neumann–Neumann boundary conditions.

In this section we would like to discuss briefly the global approach, used to define the Casimir energy associated with any field in the presence of surfaces with well defined geometric shape. For a updated discussion of the problem, see Ref. 43. The crucial conceptual question is the meaning of the renormalized vacuum energy associated with any field in the presence of any macroscopic structure that divides the space into the internal and the external region. It is important to keep separate different situations. In the case of the parallel plates, the region outside the plates is the union of two simply connected domains and both have the same geometry of the internal region. In this situation the Casimir renormalization procedure is well defined and the renormalized vacuum energy is unambiguously defined. In the case of the spherical or a cylindrical shell, the contribution of the exterior modes are not cancelled out in the Casimir renormalization procedure.

It is not difficult to understand the origin of the problem, which has been extensively discussed in the literature. If we are assuming perfectly reflecting boundaries, by the Weyl theorem we know that the asymptoptic distribution of eigenvalues of some elliptic differential operator is related with the geometric invariants associated with the surface where the field satisfy some boundary condition.[44,45] Consequently, in the regularized energy, we have divergent terms proportional to the volume, area, etc. In the Casimir definition of the renormalized vacuum energy, it is not possible to cancel the area contribution for a generic surface. The generalization of the Weyl's expansion can be done investigating the trace of the heat kernel on a specified manifold with boundary. We conclude that the assumption of perfect conducting static boundaries with a generic shape introduces new problems to define the renormalized vacuum energy of a quantum system in the presence of these macroscopic objects.[46–49] If someone insists in the assumption of perfect conducting boundaries there are different ways to solve the problem of infinite energy associated with the field in the presence of this configuration. One is to introduce counterterms concentrated on the boundaries, as discussed by the authors that use the generalized zeta function method.[50] A different approach is to smooth out the plate surface by a classical potential.[51,52] It is clear that the introduction of a classical potential $V(x)$ does not solve the problem of surface counterterms since in this situation we have to renormalize the potential. A very simple situation is the case of a background field where to compute the effective action we have to evaluate the following Fredholm determinant, where we are assuming that the positive potential is a large quantity

$$D(V)=\det(-\Delta+m^2+V(x))(-\Delta+m^2)^{-1}. \tag{74}$$

For sufficient regular but large $V(x)$, it is possible to show that for $d=4$ a counterterm quadratic in V is required in order to eliminate the divergences of the model.[53] Thus the introduction of a classical potential $V(x)$, in trying to improve the unphysical boundary condition, does not solve the problem of surface counterterms since in this situation we have to renormalize the potential. Instead of smoothing plate surfaces, an alternative approach to avoid surface divergences, discussed by Kennedy *et al.*,[50] is to treat the boundary as a quantum mechanical object. This approach was developed recently by Ford and Svaiter[54] to produce finite values for the renormalized $\langle\varphi^2(x)\rangle$ and other quantities that diverge as one approaches the classical boundary. We would like to stress that there will not be any surface divergences in a more exact treatment; however, one can still make the case that surface counterterms are a useful phenomenological approach for dealing with the apparent surface divergences without going into the complexity of the more exact approach.

VI. CONCLUSIONS

In this paper we discussed the approach of effective theory to perform calculations in field theory in the presence of macroscopic structures. We first assumed the theory of two interacting massive scalar fields $\varphi_1(x)$ and $\varphi_2(x)$ with masses m_1 and m_2 satisfying the condition $m_2 \gg m_1$. Integrating out the modes of the field $\varphi_2(x)$ we obtained an effective action for the $\varphi_1(x)$ field. In the limit $m_2\to\infty$ the field $\varphi_2(x)$ decouples from $\varphi_1(x)$, the only effect of $\varphi_2(x)$ being modifying both the value of the renormalized mass m_1 and the coupling constant of the light field φ_1. Thus we considered the $(\lambda/4!)\,\varphi_1^4$ model on a d-dimensional Euclidean space, where all but one of the coordinates are unbounded. Translation invariance along the bounded coordinate, z, which lies in the interval $[0,L]$, is broken because of the boundary conditions (BC's) chosen for the hyperplanes $z=0$ and $z=L$. Two different possibilities for these BC's boundary conditions are considered: DD and NN, where D denotes Dirichlet and N denotes Neumann. The renormalization procedure up to one-loop order was implemented. The main result of our investigations is that in the presence of boundaries where the field satisfies some boundary condition, the augmented action with surface counterterms can deal with the surface divergences that appear in the one-loop Feynman diagrams.

There are several directions for future research in field theory in the presence of surfaces, out of which we would like to emphasize two. The first one is to implement the renormalization

program beyond the one-loop approximation, where overlapping divergences emerge. The second one is related to the infrared divergences. As we discussed, one way to deal with the infrared divergences in the case of Neumann–Neumann boundary condition is to perform a resummation of the daisy diagrams. Although this procedure is standard in the study of scalar models at finite temperature, for systems where translational invariance is broken, the resummation program is still an open problem. Both subjects are under investigation by the authors.

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Free field dynamics in the generalized AdS (super)space

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Pure gauge representation for general vacuum background fields (Cartan forms) in the generalized AdS superspace identified with $\mathrm{OSp}(L,M)$ is found. This allows us to formulate dynamics of free massless fields in the generalized AdS space–time and to find their (generalized) conformal and higher spin field transformation laws. Generic solution of the field equations is also constructed explicitly. The results are obtained with the aid of the star product realization of ortosymplectic superalgebras. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1633022]

I. INTRODUCTION

In the recent papers[1,2] it was shown that infinite multiplets of massless higher spins in $4d$ flat Minkowski space–time admit description in terms of 10-dimensional space–time $\mathcal{M}_4$ with real symmetric bispinor matrix coordinates $X^{\alpha\beta}=X^{\beta\alpha}$ $(\alpha,\beta=1,\ldots,4)$. A single scalar field $c(X)$ in $\mathcal{M}_4$ describes massless fields of all integer spins in $4d$ Minkowski space–time upon imposing field equations found in Ref. 1. Half-integer spin massless fields are described analogously by a spinor field $c_\alpha(X)$. That massless fields of all spins have to admit some formulation in $\mathcal{M}_4$ was argued by Fronsdal in the pioneering paper[3] where it was also stressed that such infinite sets of massless fields have to form representations of the extension of the $4d$ conformal group su(2,2) to $\mathrm{sp}(8|R)$. Then in Ref. 4 it was found that world-line particle models based on sp(8) give rise to massless higher spin excitations of all spins. The explicit realization of the sp(8) symmetry by local transformations was given in Ref. 1 as well as the generalization of the proposed sp(8) covariant dynamical equations to $\mathcal{M}_M$ with arbitrary even M.

Properties of the $\mathrm{Sp}(2M)$ invariant space–time $\mathcal{M}_M$ were analyzed in Ref. 2. It was shown that the classical solutions of the field equations define a causal structure and give rise to correct quantization in a positive definite Hilbert space. Usual d-dimensional Minkowski space–time appears as a subspace of the generalized space–time. The analysis of Refs. 1 and 2 was performed for the case of flat space–time although the formalism as a whole works in any (generalized) conformally flat background. In particular it is interesting to extend this analysis to the generalized anti-de Sitter space–time which was argued in Ref. 1 to be the group manifold $\mathrm{Sp}(M)$ (M is even) having $\mathrm{Sp}(M)\times\mathrm{Sp}(M)\subset\mathrm{Sp}(2M)$ as the group of motions realized by left and right group actions on itself. Since the analysis of $\mathrm{Sp}(2M)$ invariant higher spin systems is most naturally performed in terms of star product algebras, for its extension to the generalized AdS space–time it is necessary to built star-product realizations of left invariant Cartan forms (i.e., flat connections) on $\mathrm{Sp}(M)$. This is the primary goal of this paper. Obtained results will allow us to present explicit formulas for symmetries and solutions of the massless field equations in the generalized AdS space–time. The analogous construction will also be given for the supersymmetric case associated with $\mathrm{OSp}(L,M)$.

Let us note that since the star-product formalism we apply leads to compact expressions for $\mathrm{OSp}(L,M)$ Cartan superforms, apart from the higher spin problem, the results obtained in this paper may have applications to other problems where left-invariant forms of $\mathrm{OSp}(L,M)$ appear. For example, in Ref. 5 it was shown how $\mathrm{OSp}(1,M)$ Cartan forms can be used to construct

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twistorlike actions for superparticles and possible applications to superbranes were discussed while in Ref. 6 a toy model of M theory based on osp(1,64) was suggested.

A. Generalized conformal symmetry

The generators L_{mn}, P_m, K_m, D of the conformal algebra o(d,2) satisfy the following commutation relations:

$$\begin{gathered}[L_{ab}, L_{cd}] = \eta_{ac} L_{bd} - \eta_{bc} L_{ad} + \eta_{ad} L_{cb} - \eta_{bd} L_{ca}, \\ [L_{ab}, P_c] = \eta_{ac} P_b - \eta_{bc} P_a, \quad [L_{ab}, K_c] = \eta_{ac} K_b - \eta_{bc} K_a, \\ [L_{ab}, D] = [P_a, P_b] = [K_a, K_b] = 0, \\ [P_a, K_b] = 2(\eta_{ab} D + L_{ab}), \quad [P_a, D] = P_a, \quad [K_a, D] = -K_a,\end{gathered} \tag{1.1}$$

$m,n = 0,\ldots,d-1$, $\eta_{mn} = \mathrm{diag}(1,-1,\ldots,-1)$. The conformal algebra can be realized by the vector fields

$$\begin{gathered}L_{ab} = \eta_{ac} x^c \frac{\partial}{\partial x^b} - \eta_{bc} x^c \frac{\partial}{\partial x^a}, \\ P_a = \frac{\partial}{\partial x^a}, \quad D = x^a \frac{\partial}{\partial x^a}, \\ K_a = 2\,\eta_{ac} x^c x^b \frac{\partial}{\partial x^b} - \eta_{bc} x^b x^c \frac{\partial}{\partial x^a}.\end{gathered} \tag{1.2}$$

The Poincare subalgebra is spanned by L_{mn} and P_m. K_m and D are the generators of special conformal transformations and dilatations, respectively. To embed the AdS_d algebra o($d-1$,2) into the d-dimensional conformal algebra o(d,2) one identifies the AdS_d translations with the mixture of translations and special conformal transformations in the conformal algebra

$$P^a_{\mathrm{AdS}_d} = P^a - \lambda^2 K^a. \tag{1.3}$$

The generators $P^a_{\mathrm{AdS}_d}$ and L_{ab} form the AdS_d subalgebra o($d-1$,2)$\subset$o(d,2). This embedding breaks down the manifest o(1,1) dilatation covariance because it mixes the operators P^a and K^a, which have different dimensions. λ is the dimensionful Wigner–Inönu contraction parameter to be identified with the inverse AdS_d radius.

The sp($2M$) algebra admits analogous description in terms of the generators $L_\alpha{}^\beta, P_{\alpha\beta}, K^{\alpha\beta}$, and D, where indices $\alpha,\beta,\ldots$ range from 1 to M and $L_\alpha{}^\beta$ is traceless. The commutation relations are

$$[K^{\alpha\beta}, K^{\gamma\delta}] = 0, \quad [P_{\alpha\beta}, P_{\gamma\delta}] = 0, \tag{1.4}$$

$$[D, P_{\alpha\beta}] = -P_{\alpha\beta}, \quad [D, K^{\alpha\beta}] = K^{\alpha\beta}, \quad [D, L_\alpha{}^\beta] = 0, \tag{1.5}$$

$$[L_\alpha{}^\beta, P_{\gamma\delta}] = -\delta_\gamma{}^\beta P_{\alpha\delta} - \delta_\delta{}^\beta P_{\alpha\gamma} + \frac{2}{M}\delta_\alpha{}^\beta P_{\gamma\delta}, \tag{1.6}$$

$$[L_\alpha{}^\beta, K^{\gamma\delta}] = \delta_\alpha{}^\gamma K^{\beta\delta} + \delta_\alpha{}^\delta K^{\beta\gamma} - \frac{2}{M}\delta_\alpha{}^\beta K^{\gamma\delta}, \tag{1.7}$$

$$[P_{\alpha\beta},K^{\gamma\delta}]=L_\alpha{}^\delta\delta_\beta{}^\gamma+L_\beta{}^\delta\delta_\alpha{}^\gamma+L_\alpha{}^\gamma\delta_\beta{}^\delta+L_\beta{}^\gamma\delta_\alpha{}^\delta+\frac{4}{M}D(\delta_\alpha{}^\delta\delta_\beta{}^\gamma+\delta_\beta{}^\delta\delta_\alpha{}^\gamma)\,, \tag{1.8}$$

$$[L_\alpha{}^\beta,L_\gamma{}^\delta]=\delta_\alpha{}^\delta L_\gamma{}^\beta-\delta_\gamma{}^\beta L_\alpha{}^\delta\,. \tag{1.9}$$

Note that the generalized Lorentz subalgebra generated by $L_\alpha{}^\beta$ is sl_M. Analogously to the usual conformal algebra, generalized translations generated by $P_{\alpha\beta}$ form Abelian subalgebra of $\mathrm{sp}(2M)$. Generalized special conformal transformations generate a dual Abelian subalgebra. Let us note that as shown in Ref. 2 $\mathrm{sp}(2M)$ contains conformal algebra $\mathrm{o}(d,2)$ which acts in the usual d-dimensional Minkowski space as subalgebra. In the higher spin field-theoretical models, which contain infinite towers of fields, $\mathrm{o}(d,2)$ acts individualy on every massless field while the generators in $\mathrm{sp}(2M)/\mathrm{o}(d,2)$ mix different massless fields. We therefore will call $\mathrm{sp}(2M)$ as generalized conformal algebra.

The commutation relations (1.4)–(1.9) can be realized by the vector fields

$$P_{\alpha\beta}=\frac{\partial}{\partial X^{\alpha\beta}}\,,\quad K^{\alpha\beta}=4X^{\alpha\gamma}X^{\beta\eta}\frac{\partial}{\partial X^{\gamma\eta}}\,, \tag{1.10}$$

$$L_\alpha{}^\beta=2X^{\beta\gamma}\frac{\partial}{\partial X^{\alpha\gamma}}-\frac{2}{M}\delta_\alpha{}^\beta X^{\beta\gamma}\frac{\partial}{\partial X^{\beta\gamma}}\,,\quad D=X^{\beta\gamma}\frac{\partial}{\partial X^{\beta\gamma}}\,, \tag{1.11}$$

where $X^{\alpha\beta}=X^{\beta\alpha}$ are coordinates of $\mathcal{M}_M$.

The simplest way to see that the commutation relations (1.4)–(1.9) are indeed of $\mathrm{sp}(2M)$ is to use its oscillator realization.[7] Actually, let $\hat a_\alpha$ and $\hat b^\alpha$ be oscillators with the commutation relations

$$[\hat a_\alpha,\hat b^\beta]=\delta_\alpha{}^\beta\,,\quad [\hat a_\alpha,\hat a_\beta]=0\,,\quad [\hat b^\alpha,\hat b^\beta]=0\,. \tag{1.12}$$

The generators of $\mathrm{sp}(2M)$ are spanned by the bilinears

$$\hat T_\alpha{}^\beta=\tfrac{1}{2}\{\hat a_\alpha,\hat b^\beta\}\,,\quad \hat P_{\alpha\beta}=\hat a_\alpha\hat a_\beta\,,\quad \hat K^{\alpha\beta}=\hat b^\alpha\hat b^\beta\,. \tag{1.13}$$

Instead of working in terms of operators it is convenient to use the star-product operation in the algebra of polynomials of commuting variables a_α and b^α,

$$(f\star g)(a,b)=\frac{1}{\pi^{2M}}\int f(a+u,b+t)g(a+s,b+v)e^{2(s_\alpha t^\alpha-u_\alpha v^\alpha)}\,\mathrm{d}^Mu\,\mathrm{d}^Mt\,\mathrm{d}^Ms\,\mathrm{d}^Mv\,. \tag{1.14}$$

The star-product defined this way, often called Moyal product, describes the product of symmetrized (i.e., Weyl ordered) polynomials of oscillators in terms of symbols of operators. The integral is normalized in such a way that

$$\frac{1}{\pi^{2M}}\int e^{2(s_\alpha t^\alpha-u_\alpha v^\alpha)}\,\mathrm{d}^Mu\,\mathrm{d}^Mt\,\mathrm{d}^Ms\,\mathrm{d}^Mv=1\,, \tag{1.15}$$

so that 1 is the unit element of the algebra. Equation (1.14) defines the associative algebra with the defining relations

$$[a_\alpha,b^\beta]_\star=\delta_\alpha{}^\beta\,,\quad [a_\alpha,a_\beta]_\star=0\,,\quad [b^\alpha,b^\beta]_\star=0 \tag{1.16}$$

($[a,b]_\star=a\star b-b\star a$). The star-product realization of the generators of $\mathrm{sp}(2M)$ is

$$T_\alpha{}^\beta=a_\alpha b^\beta\,,\quad P_{\alpha\beta}=a_\alpha a_\beta\,,\quad K^{\alpha\beta}=b^\alpha b^\beta\,, \tag{1.17}$$

where the gl(M) generator $T_\alpha{}^\beta$ decomposes into the sl(M) "Lorentz" and o(1,1) "dilatation" generators

$$L_\alpha{}^\beta = a_\alpha b^\beta - \frac{1}{M}\delta_\alpha{}^\beta a_\gamma b^\gamma, \quad D = \tfrac{1}{2} a_\alpha b^\alpha . \tag{1.18}$$

The bilinears of oscillators fulfil the commutation relations (1.4)–(1.9).

The embedding of the generalized AdS subalgebra into the conformal algebra sp($2M$) is achieved by identification of the (generalized) AdS translations with the mixture of translations and special conformal transformations $P^{\mathrm{AdS}}_{\alpha\beta} = P_{\alpha\beta} + \lambda^2 \eta_{\alpha\beta\gamma\delta} K^{\gamma\delta}$ with some bilinear form $\eta_{\alpha\beta\gamma\delta}$. (Note that keeping the same number of translation generators we keep dimension of the generalized space–time intact.) As argued in Ref. 1, $\eta_{\alpha\beta\gamma\delta}$ has to have the factorized form: $\eta_{\alpha\beta\gamma\delta} = V_{\alpha\gamma} V_{\beta\delta}$, where $V_{\alpha\beta}$ is some nondegenerate antisymmetric form (thus requiring M to be even). In what follows the form $V_{\alpha\beta}$ will be used to raise and lower indices according to the rule

$$A_\alpha = V_{\beta\alpha} A^\beta, \quad A^\alpha = V^{\alpha\beta} A_\beta, \quad V_{\alpha\beta} V^{\alpha\gamma} = \delta_\beta{}^\gamma . \tag{1.19}$$

Thus, the generalized AdS translations have the form

$$P^{\mathrm{AdS}}_{\alpha\beta} = P_{\alpha\beta} + \lambda^2 V_{\alpha\gamma} V_{\beta\delta} K^{\gamma\delta} = P_{\alpha\beta} + \lambda^2 K_{\alpha\beta} . \tag{1.20}$$

The commutation relations of $P^{\mathrm{AdS}}_{\alpha\beta}$ have the form

$$[P^{\mathrm{AdS}}_{\alpha\beta}, P^{\mathrm{AdS}}_{\gamma\delta}] = 2\lambda^2 (V_{\beta\gamma} L^{\mathrm{AdS}}_{\alpha\delta} + V_{\beta\delta} L^{\mathrm{AdS}}_{\alpha\gamma} + V_{\alpha\gamma} L^{\mathrm{AdS}}_{\beta\delta} + V_{\alpha\delta} L^{\mathrm{AdS}}_{\beta\gamma}) , \tag{1.21}$$

where $L^{\mathrm{AdS}}_{\alpha\beta} = L^{\mathrm{AdS}}_{\beta\alpha}$ are generators of the sp(M) subalgebra of gl_M which leaves invariant the symplectic form $V_{\alpha\beta}$. The full generalized AdS subalgebra is $\mathrm{sp}(M) \oplus \mathrm{sp}(M) \subset \mathrm{sp}(2M)$. Its Lorentz subalgebra $\mathrm{sp}^l(M)$ identifies with the diagonal sp(M) while AdS translations span $\mathrm{sp}(M) \oplus \mathrm{sp}(M)/\mathrm{sp}^l(M)$. Note that the generalized dS algebra obtained from (1.20) by virtue of the sign change $\lambda^2 \to -\lambda^2$ is $\mathrm{Sp}(M,C)^R$.

B. Fock space and Sp($2M$) covariant equations

The sp($2M$) invariant equations of all massless fields in three and four dimensions are naturally described[8,1] in terms of sections of the Fock fiber bundle over $\mathcal{M}_M$. In other words, consider functions on $\mathcal{M}_M$ taking values in the Fock module F,

$$|\Phi(b|X)\rangle = C(b|X) \star |0\rangle\langle 0| , \tag{1.22}$$

where $C(b|X)$ is some "generating function,"

$$C(b|X) = \sum_{m=0}^{\infty} \frac{1}{m!} c_{\beta_1 \cdots \beta_m}(X) b^{\beta_1} \cdots b^{\beta_m}, \tag{1.23}$$

and $|0\rangle\langle 0|$ is the Fock vacuum defined by the relations

$$a_\alpha \star |0\rangle\langle 0| = 0 , \quad |0\rangle\langle 0| \star b^\alpha = 0 . \tag{1.24}$$

$|0\rangle\langle 0|$ can be realized as an element of the star-product algebra

$$|0\rangle\langle 0| = e^{-2 a_\alpha b^\alpha} . \tag{1.25}$$

Note that the Fock vacuum is the space–time constant projector

$$d|0\rangle\langle 0| = 0 , \quad |0\rangle\langle 0| \star |0\rangle\langle 0| = |0\rangle\langle 0| , \tag{1.26}$$

where d is de Rahm differential

$$d=\mathrm{d}X^{\alpha\beta}\frac{\partial}{\partial X^{\alpha\beta}},\quad d^2=0. \tag{1.27}$$

As shown in Ref. 1 the relevant flat space $\mathrm{Sp}(2M)$ covariant equation can be formulated in the form

$$d|\Phi(b|X)\rangle - w_0\star|\Phi(b|X)\rangle=0\,, \tag{1.28}$$

where

$$w_0=\tfrac{1}{2}\mathrm{d}X^{\alpha\beta}a_\alpha a_\beta\,. \tag{1.29}$$

That the equation (1.28) does indeed describe all conformal field equations in $d=3$ and $d=4$ was shown in Refs. 8 and 1 for the cases of $M=2$ and $M=4$, respectively. In this paper we will consider the general case of any even M. It is worth to mention that the cases of $M=8$, $M=16$, and $M=32$ were argued in Ref. 2 to correspond to conformal systems in $d=6$, $d=10$, and $d=11$, respectively.

The Fock fiber bundle realization of the higher spin equations guarantees generalized conformal symmetry of the system along with its infinite-dimensional higher spin extension. Actually, let w_0 be some one-form, taking values in the higher spin algebra identified with the star product algebra (i.e., the algebra of regular functions of oscillators acting on the Fock module F)

$$w_0(X)=\sum_{m,n=0}^{\infty}\frac{1}{m!n!}w_{0\,\beta_1\cdots\beta_m}{}^{\alpha_1\cdots\alpha_n}(X)a_{\alpha_1}\cdots a_{\alpha_n}b^{\beta_1}\cdots b^{\beta_m}\,, \tag{1.30}$$

which satisfies the zero-curvature condition

$$\mathrm{d}w_0=w_0\star\wedge w_0\,. \tag{1.31}$$

The equations (1.28), (1.31) are invariant under the gauge transformations

$$\delta w_0=\mathrm{d}\epsilon-[w_0,\epsilon]_\star\,, \tag{1.32}$$

$$\delta|\Phi(b|X)\rangle=\epsilon\star|\Phi(b|X)\rangle\,, \tag{1.33}$$

where $\epsilon(a,b|X)$ is an arbitrary infinitesimal gauge parameter. Any fixed vacuum solution w_0 of the equation (1.31) breaks the local higher spin symmetry to its stability subalgebra with the infinitesimal parameters $\epsilon_0(a,b|X)$ satisfying the equation

$$\mathrm{d}\epsilon_0-[w_0,\epsilon_0]_\star=0. \tag{1.34}$$

Consistency of this equation is guaranteed by (1.31). As a result, (1.34) admits locally a pure gauge solution

$$w_0(X)=-g^{-1}(X)\star\mathrm{d}g(X)\,, \tag{1.35}$$

where $g(a,b|X)$ is some invertible element of the star-product algebra. The global symmetry parameters satisfying (1.34) then have the form

$$\epsilon_0(X)=g^{-1}(X)\star\xi\star g(X)\,, \tag{1.36}$$

where an arbitrary X-independent element $\xi=\xi(a,b)$ of the star-product algebra describes parameters of the global higher spin symmetry which acts on the solutions of the equation (1.28) (for any given w_0). In particular, the $\mathrm{sp}(2M)$ subalgebra spanned by bilinears of oscillators is thus shown to be a symmetry of the equation (1.28). (See Ref. 9.)

Analogously one solves the equation (1.28) in the form

$$|\Phi(b|X)\rangle = g^{-1}\star|\Phi(b|X_0)\rangle\,, \tag{1.37}$$

where $|\Phi(b|X_0)\rangle$ plays a role of initial data. The meaning of this formula is that the Fock module $|\Phi(b|X_0)\rangle$ parametrizes all combinations of the derivatives of the dynamical fields at $X=X_0$ which are allowed to be nonzero by the field equations. The formula (1.37) plays a role of the covariantized Taylor expansion reconstructing generic solution in terms of its derivatives at $X=X_0$. Note that the Fock module F is not unitary because it decomposes into an infinite sum of finite-dimensional (tensor) representations of the generalized noncompact Lorentz algebra $\mathrm{sl}_M(\mathbf{R})$. Nevertheless, the fact that initial data of the problem are formulated in terms of the Fock module F is closely related to the fact (see, e.g., Refs. 3 and 4) that the collection of unitary massless representations corresponding to this dynamical system in $d=4$ is described by the unitary Fock module U known as singleton representation of sp(8). (It is also well known that unitary representations of the $4d$ conformal algebra associated with massless fields admit Fock realization in terms of appropriate oscillators.[10]) As shown in Refs. 8 and 1, the modules U and F are related by some Bogolyubov transform.

The formulas (1.35), (1.37) will play the key role in our analysis. They allow one to solve the equations of motion explicitly provided that the gauge function $g(X)$ is found that corresponds to a chosen zero-curvature connection w_0. This program for the flat connection (1.29) was accomplished in Ref. 1. In this paper we will find a family of such gauge functions $g(X)$ that all nonvanishing components of w_0 take values in the AdS subalgebra $\mathrm{osp}(L|M)\oplus\mathrm{osp}(L|M)$ of $\mathrm{osp}(2L|2M)$.

II. Sp(M) AND STAR PRODUCT

As argued in Ref. 1, the generalized AdS space is identified with $\mathrm{Sp}(M)$. Let us note that the generalized conformal group $\mathrm{Sp}(2M)$ does not act globally on $\mathrm{Sp}(M)$ analogously to the usual conformal group acting in the Minkowski space–time by Möbius transformations which have singularities. Recall that usual Minkowski space–time is the big cell of the compactified Minkowski space. Analogously, the generalized Minkowski space–time is the big cell in the compactified generalized space–time $\mathcal{M}_M$. The universal covering space of $\mathrm{Sp}(M)$ can be thought of as a sort of deformation of the generalized Minkowski space–time being the big cell of $\mathcal{M}_M$.

The group $\mathrm{Sp}(M)$ is realized by the $M\times M$ matrices $U_\alpha{}^\beta$ satisfying

$$U_\alpha{}^\beta U_\gamma{}^\delta V^{\alpha\gamma} = V^{\beta\delta}\,, \tag{2.1}$$

where $V^{\alpha\beta}$ is some nondegenerate antisymmetric form $V^{\alpha\beta}=-V^{\beta\alpha}$ (M is even). The manifold $\mathrm{Sp}(M)$ is $[M(M+1)/2]$ dimensional. It can be described by local coordinates $X^{\alpha\beta}=X^{\beta\alpha}$. The simplest parametrization is

$$U_\alpha{}^\beta = (\exp(\lambda X))_\alpha{}^\beta, \tag{2.2}$$

where λ is inverse "radius" of $\mathrm{Sp}(M)$ introduced to compensate the space dimensionality of $X^{\alpha\beta}$. Note that a particular value of $\lambda\neq 0$ is irrelevant unless there are some other dimensional parameters in the theory (e.g., the gravitational constant). The exponential in (2.2) is matrix exponential of

$$X_\alpha{}^\beta = V_{\gamma\alpha}X^{\gamma\beta}\,. \tag{2.3}$$

It is elementary to see that the parametrization (2.2) solves the group equation (2.1). The exponential parametrization (2.2) provides the universal covering space[11] of $\mathrm{Sp}(M)$ [metaplectic group $\mathrm{Mp}(M)$] topologically equivalent to $R^{[M(M+1)/2]}$, the big cell of $\mathcal{M}_M$.

$\mathrm{Sp}(M)$ is invariant under the action of $\mathrm{Sp}(M)\times\mathrm{Sp}(M)$ generated by left and right actions of $\mathrm{Sp}(M)$ on itself. Using the oscillator realization of $\mathrm{sp}(M)\oplus\mathrm{sp}(M)\subset\mathrm{sp}(2M)$ we can set

$$w_0(X)=\omega_{\alpha\beta}(X)a^\alpha b^\beta+h_{\alpha\beta}(X)(a^\alpha a^\beta+\lambda^2 b^\alpha b^\beta)\,, \tag{2.4}$$

where the "Lorentz connection" $\omega_{\alpha\beta}(X)$ and the "frame" $h_{\alpha\beta}(X)$ have the form

$$\omega_{\alpha\beta}=-\tfrac{1}{2}(\mathrm{d}(U^{-1})_\alpha{}^\gamma U_{\gamma\beta}+\mathrm{d}U_\alpha{}^\gamma(U^{-1})_{\gamma\beta})\,, \tag{2.5}$$

$$h_{\alpha\beta}=\frac{1}{4\lambda}(\mathrm{d}U_\alpha{}^\gamma(U^{-1})_{\gamma\beta}-\mathrm{d}(U^{-1})_\alpha{}^\gamma U_{\gamma\beta})\,, \tag{2.6}$$

which guarantees that w_0 satisfies (1.31). In the exponential parametrization (2.2) one gets

$$\omega^{\alpha\beta}=\frac{\lambda}{2}\mathrm{d}X_{\mu\nu}\left(\int_0^1\exp(\lambda Xt)^{\mu\beta}\exp(\lambda Xt)^{\nu\alpha}\,\mathrm{d}t-\int_{-1}^0\exp(\lambda Xt)^{\mu\beta}\exp(\lambda Xt)^{\nu\alpha}\,\mathrm{d}t\right), \tag{2.7}$$

$$h^{\alpha\beta}=\frac{1}{4}\mathrm{d}X_{\mu\nu}\int_{-1}^1\exp(\lambda Xt)^{\mu\beta}\exp(\lambda Xt)^{\nu\alpha}\,\mathrm{d}t\,, \tag{2.8}$$

where we used the identity $\delta e^A=\int_0^1 e^{At}\delta A e^{A(1-t)}\,\mathrm{d}t$ valid for an arbitrary matrix A. As expected, in the flat limit $\lambda\to 0$ one recovers (1.29).

Let us now present the star-product pure gauge form (1.35) of the connection (2.4)–(2.6). The final result is

$$g=\frac{1}{\det\left\|\mathrm{ch}\dfrac{\lambda X}{2}\right\|}\exp\left(-\frac{1}{\lambda}\left(\mathrm{th}\frac{\lambda X}{2}\right)^{\alpha\beta}(a_\alpha a_\beta+\lambda^2 b_\alpha b_\beta)\right), \tag{2.9}$$

$$g^{-1}=\frac{1}{\det\left\|\mathrm{ch}\dfrac{\lambda X}{2}\right\|}\exp\left(\frac{1}{\lambda}\left(\mathrm{th}\frac{\lambda X}{2}\right)^{\alpha\beta}(a_\alpha a_\beta+\lambda^2 b_\alpha b_\beta)\right). \tag{2.10}$$

This formula is derived as follows. Let $\mathrm{sp}(M)$ be realized in terms of bilinears of oscillators α_α satisfying the commutation relations

$$[\alpha_\alpha,\alpha_\beta]_*=2V_{\alpha\beta}\,, \tag{2.11}$$

with the star product,

$$(f*g)(\alpha)=\frac{1}{\pi^M}\int f(\alpha+u)g(\alpha+v)e^{-u_\alpha v^\alpha}\,\mathrm{d}^M u\,\mathrm{d}^M v\,. \tag{2.12}$$

Consider star-product algebra elements g_1 and g_2 of the form

$$g_1=r_1 e^{1/2\,f_1^{\alpha\beta}\alpha_\alpha\alpha_\beta},\quad g_2=r_2 e^{1/2\,f_2^{\alpha\beta}\alpha_\alpha\alpha_\beta} \tag{2.13}$$

with some α-independent r_1, r_2, $f_1^{\alpha\beta}$, and $f_2^{\alpha\beta}$. Elementary evaluation of the Gaussian integrals shows that

$$g_{1,2}=g_1*g_2=r_{1,2}e^{1/2(f_1\circ f_2)^{\alpha\beta}\alpha_\alpha\alpha_\beta}\,, \tag{2.14}$$

where

$$r_{1,2}=\frac{r_1 r_2}{\sqrt{\det\|f_1 f_2+1\|}} \tag{2.15}$$

and

$$f_1\circ f_2=\frac{1}{1+f_2 f_1}(1+f_2)-\frac{1}{1+f_1 f_2}(1-f_1) \tag{2.16}$$

[with the usual matrix multiplication on the right-hand side, $AB\to A_\alpha{}^\gamma B_\gamma{}^\beta$, $(1/A)\,B \to (A^{-1})_\alpha{}^\gamma B_\gamma{}^\beta$]. Let us look for a map

$$g(U)=r(U)e^{1/2\, f^{\alpha\beta}(U)\alpha_\alpha\alpha_\beta} \tag{2.17}$$

of $\mathrm{Sp}(M)$ into the star-product algebra, such that

$$g(U_1)*g(U_2)=g(U_1U_2)=r(U_1U_2)e^{1/2\, f^{\alpha\beta}(U_1U_2)\alpha_\alpha\alpha_\beta}. \tag{2.18}$$

Equivalently, one can use the inverse map $U(f)$ requiring

$$U(f_1)U(f_2)=U(f_1\circ f_2). \tag{2.19}$$

As shown in the Appendix, the multiplication law (2.16) requires

$$U^{\alpha\beta}(f)=\left(\frac{1+f}{1-f}\right)^{\alpha\beta}. \tag{2.20}$$

The inverse formula is analogous

$$f^{\alpha\beta}(U)=\left(\frac{U-1}{1+U}\right)^{\alpha\beta}. \tag{2.21}$$

The normalization factor is

$$r(U)=\frac{2^{M/2}}{\sqrt{\det\|U+1\|}}. \tag{2.22}$$

To derive (2.9) it remains to use (2.2) and to observe that the two $\mathrm{sp}(M)$ subalgebras of $\mathrm{sp}(2M)$ are generated by the two mutually commuting sets of oscillators

$$\alpha^\pm_\alpha=\frac{a_\alpha}{\sqrt{\lambda}}\pm\sqrt{\lambda}V_{\beta\alpha}b^\beta=\frac{1}{\sqrt{\lambda}}(a_\alpha\pm\lambda b_\alpha), \tag{2.23}$$

satisfying the commutation relations

$$[\alpha^\pm_\alpha,\alpha^\pm_\beta]_*=\pm 2V_{\alpha\beta}. \tag{2.24}$$

The map (2.20) has a number of interesting properties. In particular,

$$U^{-1}(f)=U(-f), \tag{2.25}$$

$$U(f)=-U^{-1}(-f^{-1}). \tag{2.26}$$

The property (2.25) is a consequence of the elementary fact (see, e.g., Ref. 12) that the star product (2.12) admits an antiautomorphism $\rho(g(\alpha))=g(i\alpha)$, i.e., $\rho(g_1)*\rho(g_2)=\rho(g_2*g_1)$. From (2.17) it follows that $\rho(U(f))=U(-f)$. The natural group antiautomorphism is $\rho(U)=U^{-1}$. The formula (2.25) identifies the antiautomorphism ρ in the star-product algebra with that of the group $\mathrm{Sp}(M)$.

The formula (2.26) is more interesting. It does not have a global interpretation within $\mathrm{Sp}(M)$ being singular at degenerate $f^{\alpha\beta}$ (in particular for $f^{\alpha\beta}=0$ and, therefore, $U=I$). However, these maps are expected to have global meaning in $\mathcal{M}_M$ where one can define inversion by analogy with the flat case considered in Ref. 2,

$$I(f)=-f^{-1}, \quad I(U)=-U^{-1}. \tag{2.27}$$

The formula (2.26) implies that these two definitions are consistent with each other. Note that inversion defined this way maps unit element of $\mathrm{Sp}(M)$ to the central element $-I$ which does not belong to the connected component of unity $\mathrm{PSp}(M)\subset\mathrm{Sp}(M)$.

III. ARBITRARY COORDINATES

The gauge function (2.9) corresponds to the exponential realization of $\mathrm{Sp}(M)$, thus yielding global coordinates which cover the metaplectic group $\mathrm{Mp}(M)$. Our formalism allows one to write down explicit form of vacuum gauge connections (Cartan forms) in arbitrary coordinates, however. Indeed, let us consider a gauge function of the form

$$\begin{aligned} g&=\sqrt{\det\|1-\lambda^2 f^2(X)\|}\,\exp(-f(X)^{\alpha\beta}(a_\alpha a_\beta+\lambda^2 b_\alpha b_\beta))\,,\\ g^{-1}&=\sqrt{\det\|1-\lambda^2 f^2(X)\|}\,\exp(f(X)^{\alpha\beta}(a_\alpha a_\beta+\lambda^2 b_\alpha b_\beta))\,, \end{aligned} \tag{3.1}$$

where $f^{\alpha\beta}(X)=f^{\beta\alpha}(X)$ is an arbitrary function of matrix coordinates $X^{\alpha\beta}$. The zero-curvature connection (1.35) can be written in the form

$$w_0=-g(-f)\star\left(\mathrm{d}X^{\alpha\beta}\frac{\partial f_1^{\gamma\lambda}}{\partial X^{\alpha\beta}}\frac{\partial}{\partial f_1^{\gamma\lambda}}g(f_1)\right)\Bigg|_{f_1=f}. \tag{3.2}$$

Direct computation leads to the expressions for the ''Lorentz connection'' and ''frame''

$$h^{\alpha\beta}=\mathrm{d}X^{\rho\sigma}\left(\frac{1}{1-\lambda^2 f^2}\right)^{\alpha\gamma}\left(\frac{\partial f_\gamma{}^\lambda}{\partial X^{\rho\sigma}}-\lambda^2 f_\gamma{}^\mu\frac{\partial f_\mu{}^\nu}{\partial X^{\rho\sigma}}f_\nu{}^\lambda\right)\left(\frac{1}{1-\lambda^2 f^2}\right)_\lambda^\beta, \tag{3.3}$$

$$\omega^{\alpha\beta}=2\lambda^2\,\mathrm{d}X^{\rho\sigma}\left(\frac{1}{1-\lambda^2 f^2}\right)^{\alpha\gamma}\left(\frac{\partial f_\gamma{}^\mu}{\partial X^{\rho\sigma}}f_\mu{}^\lambda-f_\gamma{}^\mu\frac{\partial f_\mu{}^\lambda}{\partial X^{\rho\sigma}}\right)\left(\frac{1}{1-\lambda^2 f^2}\right)_\lambda^\beta. \tag{3.4}$$

Note that from these formulas it follows that

$$\omega^{\alpha\beta}=2h^{\alpha\gamma}f_\gamma{}^\beta-2\,f^{\alpha\gamma}h_\gamma{}^\beta+\lambda^2 f^{\alpha\gamma}\omega_\gamma{}^\lambda f_\lambda{}^\beta. \tag{3.5}$$

An arbitrary function $f^{\alpha\beta}(X)$ parametrizes various coordinate choices in $\mathrm{Sp}(M)$. A relationship with the coordinates of the exponential parametrization obviously is

$$f(\tilde{X})=\frac{1}{\lambda}\mathrm{th}\frac{\lambda X}{2}, \tag{3.6}$$

which implies locally

$$\mathrm{sh}\frac{\lambda X}{2}=\frac{\lambda f(\widetilde{X})}{\sqrt{1-\lambda^2 f^2(\widetilde{X})}},\quad \mathrm{ch}\frac{\lambda X}{2}=\frac{1}{\sqrt{1-\lambda^2 f^2(\widetilde{X})}}. \tag{3.7}$$

The formulas (3.3) and (3.4) thus provide a representation for Cartan forms in arbitrary coordinates associated with one or another function $f^{\alpha\beta}(X)$. Consider now a few particular examples. Let $f^{\alpha\beta}(X)$ be of the form

$$f^{\alpha\beta}(X)=\phi(\det\|X\|)X^{\alpha\beta}. \tag{3.8}$$

The corresponding connections are

$$h^{\alpha\beta}=\phi\cdot\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)^{\alpha\gamma}(\mathrm{d}X_\gamma{}^\lambda-\lambda^2\phi^2X_\gamma{}^\mu\,\mathrm{d}X_\mu{}^\nu X_\nu{}^\lambda)\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_\lambda^\beta$$
$$+\widetilde{\phi}\cdot\mathrm{d}X^{\rho\sigma}(X^{-1})_{\rho\sigma}\left(\frac{X}{1-\lambda^2\phi^2X^2}\right)^{\alpha\beta}, \tag{3.9}$$

$$\omega^{\alpha\beta}=2\lambda^2\phi^2\cdot\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)^{\alpha\gamma}(\mathrm{d}X_\gamma{}^\mu X_\mu{}^\lambda-X_\gamma{}^\mu\,\mathrm{d}X_\mu{}^\lambda)\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_\lambda^\beta, \tag{3.10}$$

where

$$\widetilde{\phi}=\frac{\partial\phi}{\partial\ln\det\|X\|}. \tag{3.11}$$

Another useful example results from

$$f^{\pm}_{\alpha\beta}(X)=\left(\frac{X}{1\mp\sqrt{1-\lambda^2X^2}}\right)_{\alpha\beta}. \tag{3.12}$$

The corresponding gauge function is

$$g^{\pm}=\det\left\|\frac{1+\lambda X\pm\sqrt{1-\lambda^2X^2}}{\lambda X}\right\|\exp\left(-\left(\frac{X}{1\mp\sqrt{1-\lambda^2X^2}}\right)^{\alpha\beta}(a_\alpha a_\beta+\lambda^2b_\alpha b_\beta)\right). \tag{3.13}$$

In these ''stereographic'' coordinates the ''frame'' gets the following simple form:

$$h^{\alpha\beta}=\frac{1}{2}\left(\frac{1}{\sqrt{1-\lambda^2X^2}}\right)^{\alpha\gamma}\mathrm{d}X_\gamma{}^\lambda\left(\frac{1}{\sqrt{1-\lambda^2X^2}}\right)_\lambda^\beta. \tag{3.14}$$

Let us now compare this formula with those obtained in Refs. 8 and 9 to describe massless fields in $\mathrm{AdS}_3(M=2)$ and $\mathrm{AdS}_4(M=4)$.

Let us first consider the case $M=2$. Using, for example, g^+, from (3.13) one obtains

$$g=\frac{2\sqrt{z}}{1+\sqrt{z}}\exp\left(-\frac{1}{1+\sqrt{z}}x^{\alpha\beta}(a_\alpha a_\beta+\lambda^2b_\alpha b_\beta)\right), \tag{3.15}$$

$$g^{-1}=\frac{2\sqrt{z}}{1+\sqrt{z}}\exp\left(\frac{1}{1+\sqrt{z}}x^{\alpha\beta}(a_\alpha a_\beta+\lambda^2b_\alpha b_\beta)\right), \tag{3.16}$$

where $z=1+\frac{1}{2}\lambda^2x_{\alpha\beta}x^{\alpha\beta}$. The ''frame'' and the ''Lorentz connection'' are

$$h_{\alpha\beta}=\frac{1}{2z}\mathrm{d}x_{\alpha\beta}\,,\quad \omega_{\alpha\beta}=\frac{1}{2z}(\mathrm{d}x_{\alpha}{}^{\gamma}x_{\gamma\beta}+\mathrm{d}x_{\beta}{}^{\gamma}x_{\gamma\alpha}). \tag{3.17}$$

To derive this result, which reproduces that of Ref. 8, we used a simple fact that, when $M=2$, any antisymmetric matrix is proportional to $V_{\alpha\beta}$ and, therefore, any polynomial of matrix coordinates $P(x)^{\alpha\beta}$ decomposes into a combination of its symmetric part $P_S(x_{\mu\nu}x^{\mu\nu})x^{\alpha\beta}$ and antisymmetric part $P_A(x_{\mu\nu}x^{\mu\nu})V^{\alpha\beta}$. From (3.17) it follows that the metric tensor is

$$g_{mn}=\tfrac{1}{2}h_{\alpha\beta,n}h^{\alpha\beta}{}_{,m}=\frac{1}{4}\,\frac{\eta_{mn}}{(1+\lambda^2x_kx^k)^2}\,, \tag{3.18}$$

where

$$x_n=\sigma_n{}^{\alpha\beta}x_{\alpha\beta}\,,\quad x_{\alpha\beta}=\tfrac{1}{2}\sigma_{\alpha\beta}{}^{n}x_n\,, \tag{3.19}$$

and $\sigma_n{}^{\alpha\beta}$ is a set of basis symmetric real matrices normalized to satisfy

$$\sigma_n{}^{\alpha\beta}\sigma_{m\alpha\beta}=2\,\eta_{mn}\,, \tag{3.20}$$

where η_{mn} is the flat Minkowski metric.

To consider the $4d$ case we embed AdS_4 space–time into $\mathcal{M}_4$ as follows:

$$X^{\alpha\beta}=\begin{pmatrix}\mathbf{0} & x^{\bar\alpha\dot\beta}\\ x^{\beta\bar\alpha} & \mathbf{0}\end{pmatrix}, \tag{3.21}$$

where $\bar\alpha,\bar\beta=1,2$, $\dot\alpha,\dot\beta=3,4$, and $x^{\bar\alpha\dot\beta}$ are local AdS_4 coordinates which can be expressed via the vector coordinates x^n $(n=0,\ldots,3)$ with the aid of Pauli matrices $\sigma_n{}^{\bar\alpha\dot\beta}=(I,\sigma_1{}^{\bar\alpha\dot\beta},\ldots,\sigma_3{}^{\bar\alpha\dot\beta})$ as

$$x^n=\sigma^n{}_{\bar\alpha\beta}x^{\bar\alpha\dot\beta}\,,\quad x^{\bar\alpha\dot\beta}=\tfrac{1}{2}x_n\sigma^{n\bar\alpha\dot\beta}\,,\quad \sigma_{n\,\dot\alpha\bar\beta}\sigma_m{}^{\bar\alpha\dot\beta}=2\,\eta_{mn}\,. \tag{3.22}$$

The gauge function and gravitational fields resulting from (3.13) and (3.14) are

$$g=\left(\frac{2\sqrt{z}}{1+\sqrt{z}}\right)^2\exp\left(-\frac{1}{1+\sqrt{z}}x^{\bar\alpha\dot\beta}(a_{\bar\alpha}a_{\dot\beta}+\lambda^2b_{\bar\alpha}b_{\dot\beta})\right), \tag{3.23}$$

$$h_{\bar\alpha\dot\beta}=\frac{1}{2z}\mathrm{d}x_{\bar\alpha\dot\beta}, \tag{3.24}$$

$$\omega_{\bar\alpha\bar\beta}=\frac{1}{2z}(\mathrm{d}x_{\bar\alpha}{}^{\dot\gamma}x_{\bar\beta\dot\gamma}+\mathrm{d}x_{\bar\beta}{}^{\dot\gamma}x_{\bar\alpha\dot\gamma})\,,\quad \bar\omega_{\dot\alpha\dot\beta}=\frac{1}{2z}(\mathrm{d}x^{\bar\gamma}{}_{\dot\alpha}x_{\bar\gamma\dot\beta}+\mathrm{d}x^{\bar\gamma}{}_{\dot\beta}x_{\bar\gamma\dot\alpha}), \tag{3.25}$$

where $z=1+\frac{1}{2}\lambda^2x_{\bar\alpha\dot\beta}x^{\bar\alpha\dot\beta}=1+\lambda^2x_nx^n$. These AdS_4 gravitational fields coincide with those found in Ref. 9.

IV. SYMMETRIES

Having fixed some vacuum solution w_0 of (1.31), the local higher spin symmetry is broken down to the global one with the parameter $\epsilon_0(a,b|X)$ satisfying (1.34). Once the vacuum solution w_0 is fixed in the pure gauge form (1.35) with some gauge function g, it is easy to find the gauge parameter $\epsilon_0(a,b|X)$ of the leftover global symmetry. Indeed let the generating parameter $\xi(a,b;\mu,\eta)$ in (1.36) be of the form

$$\xi=\xi_0\exp(a_\alpha\mu^\alpha-b^\alpha\eta_\alpha)\,, \tag{4.1}$$

where ξ_0 is an infinitesimal constant while μ^α and η_α are constant parameters. An arbitrary symmetry with star-product polynomial parameters can be obtained via differentiation of ξ with respect to μ^α and η_α. Substitution of (2.9) into (1.36) gives

$$\epsilon_0(a,b;\mu,\eta|X)=g^{-1}\star\xi\star g=\xi_0\exp(a_\alpha\hat{\mu}^\alpha-b^\alpha\hat{\eta}_\alpha)\,, \tag{4.2}$$

where

$$\hat{\mu}^\alpha=\mathrm{ch}(\lambda X)^{\alpha\beta}\mu_\beta-\frac{\mathrm{sh}(\lambda X)^{\alpha\beta}}{\lambda}\eta_\beta\,,\quad \hat{\eta}^\alpha=\mathrm{ch}(\lambda X)^{\alpha\beta}\eta_\beta-\lambda\cdot\mathrm{sh}(\lambda X)^{\alpha\beta}\mu_\beta\,. \tag{4.3}$$

According to (3.7), in the arbitrary coordinates associated with the function $f^{\alpha\beta}(X)$ of Sec. III, we have

$$\hat{\mu}_\alpha=\left(\frac{1+\lambda^2f^2(X)}{1-\lambda^2f^2(X)}\right)_\alpha^{\ \beta}\mu_\beta-\left(\frac{2\,f(X)}{1-\lambda^2f^2(X)}\right)_\alpha^{\ \beta}\eta_\beta\,, \tag{4.4}$$

$$\hat{\eta}_\alpha=\left(\frac{1+\lambda^2f^2(X)}{1-\lambda^2f^2(X)}\right)_\alpha^{\ \beta}\eta_\beta-\lambda^2\left(\frac{2\,f(X)}{1-\lambda^2f^2(X)}\right)_\alpha^{\ \beta}\mu_\beta\,. \tag{4.5}$$

The global symmetry transformation of the higher spin generating function

$$\delta|\Phi(b|X)\rangle\equiv\epsilon_0\star|\Phi(b|X)\rangle=\xi_0\exp(-\hat{\eta}_\alpha b^\alpha+\tfrac{1}{2}\hat{\eta}^\alpha\hat{\mu}_\alpha)\cdot C(b+\hat{\mu}|X)\star|0\rangle\langle 0| \tag{4.6}$$

implies

$$\delta C(b|X)=\xi_0C(b+\hat{\mu}|X)\exp(\tfrac{1}{2}\hat{\eta}^\alpha\hat{\mu}_\alpha-b^\alpha\hat{\eta}_\alpha)\,. \tag{4.7}$$

The dynamical fields are associated with the scalar $c(X)=C(0|X)$ and vector $c_\alpha(X)=(\partial/\partial b^\alpha)\,C(b|X)|_{b=0}$ in the expansion (1.23). [All other fields in $C(b|X)$ are expressed via derivatives of the dynamical fields.[1]] Their transformation laws are

$$\delta c(X)=\xi_0C(\hat{\mu}|X)\exp(\tfrac{1}{2}\hat{\eta}^\alpha\hat{\mu}_\alpha)\,, \tag{4.8}$$

$$\delta c_\alpha(X)=\xi_0\left(\frac{\partial}{\partial b^\alpha}C(b+\hat{\mu}|X)\bigg|_{b=0}-\hat{\eta}_\alpha C(\hat{\mu}|X)\right)\exp\left(\frac{1}{2}\,\hat{\eta}^\alpha\hat{\mu}_\alpha\right)\,. \tag{4.9}$$

Differentiating over the parameters μ^α and η_α and setting them then equal to zero one obtains explicit expressions for the higher spin symmetry transformations associated with any symmetry parameters $\epsilon_0(a,b|X)$ polynomial in the oscillators a and b. In particular, the transformation law with the parameters bilinear in the oscillators reproduces the $\mathrm{Sp}(2M)$ generalized conformal transformations in the generalized AdS space–time $\mathrm{Sp}(M)$.

V. LIGHTLIKE SOLUTIONS

Once the gauge function g is known one solves the system of free field equation (1.28) for all massless fields via (1.37). Let us consider basis lightlike solutions generated by the initial data of the form

$$C(b|0)=C_0\exp(\kappa_\alpha b^\alpha)\,, \tag{5.1}$$

where C_0 is an arbitrary constant and κ^α is some space–time constant spinor. According to (1.22) the Fock representation of the initial data has the form

$$|\Phi(b|0)\rangle = C_0 \exp(\kappa_\alpha b^\alpha) \star |0\rangle\langle 0|. \tag{5.2}$$

So the dynamical problem is solved by

$$|\Phi(b|X)\rangle = g^{-1}(X) \star |\Phi(b|0)\rangle = \frac{C_0}{\det\left\| \mathrm{ch}\dfrac{\lambda X}{2}\right\|} e^{(1/\lambda)[\mathrm{th}\,(\lambda X/2)]^{\alpha\beta}(a_\alpha a_\beta + \lambda^2 b_\alpha b_\beta)} \star e^{\kappa_\alpha b^\alpha} \star e^{-2a_\alpha b^\alpha}. \tag{5.3}$$

Elementary evaluation of Gaussian integrals gives the following result:

$$C(b|X) = \frac{C_0}{\sqrt{\det\|\mathrm{ch}\,\lambda X\|}} \exp(t^{\alpha\beta}(\lambda^2 b_\alpha b_\beta + \kappa_\alpha \kappa_\beta) + p_\beta{}^\alpha \kappa_\alpha b^\beta), \tag{5.4}$$

where we use notations

$$t_\alpha{}^\beta = \left(\frac{\mathrm{th}(\lambda X)}{2\lambda}\right)_\alpha^\beta, \quad p_\alpha{}^\beta = (\mathrm{ch}^{-1}(\lambda X))_\alpha{}^\beta, \tag{5.5}$$

equivalent by virtue of (3.7) to

$$t_\alpha{}^\beta = \left(\frac{f(X)}{1+\lambda^2 f^2(X)}\right)_\alpha^\beta, \quad p_\alpha{}^\beta = \left(\frac{1-\lambda^2 f^2(X)}{1+\lambda^2 f^2(X)}\right)_\alpha^\beta. \tag{5.6}$$

Let us stress that, according to Refs. 1 and 2, for the particular case of $M=4$ the obtained expressions describe solutions of massless equations for all spins in AdS_4, constructed in Ref. 9. Using (3.23), these solutions take the form

$$C(b|x) = z \exp\left(\frac{x^{\dot\alpha\dot\beta}}{2}(\kappa_{\dot\alpha}\kappa_{\dot\beta} + \lambda^2 b_{\dot\alpha} b_{\dot\beta}) + \sqrt{z}\kappa_\alpha b^\alpha\right). \tag{5.7}$$

For the case of $M=2$ we get solutions of the AdS_3 massless equations discussed in Ref. 8 of the form

$$C(b|x) = \sqrt{z} \exp\left(\frac{x^{\alpha\beta}}{2}(\kappa_\alpha \kappa_\beta + \lambda^2 b_\alpha b_\beta) + \sqrt{z}\kappa_\alpha b^\alpha\right). \tag{5.8}$$

Here we make use of the gauge function (3.15).

For the dynamical fields we obtain

$$c(X) = C_0 \sqrt{\det\left\|\frac{1-\lambda^2 f^2(X)}{1+\lambda^2 f^2(X)}\right\|} \exp(t^{\alpha\beta}\kappa_\alpha\kappa_\beta), \tag{5.9}$$

$$c_\alpha(X) = C_0 \sqrt{\det\left\|\frac{1-\lambda^2 f^2(X)}{1+\lambda^2 f^2(X)}\right\|} p_\alpha{}^\beta \kappa_\beta \exp(t^{\alpha\beta}\kappa_\alpha\kappa_\beta). \tag{5.10}$$

Substitution of ϵ_0 into (1.33) gives the global higher spin symmetry transformation of the solution (5.3),

$$\delta C(b|X)=C_0\xi_0\sqrt{\det\left\|\frac{1-\lambda^2 f^2(X)}{1+\lambda^2 f^2(X)}\right\|}$$
$$\times\exp\left(t^{\alpha\beta}\lambda^2(b_\alpha+\hat\mu_\alpha)(b_\beta+\hat\mu_\beta)+t^{\alpha\beta}\kappa_\alpha\kappa_\beta+p_\beta{}^\alpha\kappa_\alpha(b^\beta+\hat\mu^\beta)-\hat\eta_\alpha\left(b^\alpha+\frac{1}{2}\hat\mu^\alpha\right)\right). \tag{5.11}$$

The flat limit $\lambda\to 0$ gives

$$\delta C(b|X)=C_0\xi_0\exp(\tfrac{1}{2}X^{\alpha\beta}(\kappa_\alpha\kappa_\beta-2\kappa_\alpha\eta_\beta+\eta_\alpha\eta_\beta)+b^\alpha(\kappa_\alpha-\eta_\alpha)+\kappa_\alpha\mu^\alpha+\tfrac{1}{2}\mu_\alpha\eta^\alpha). \tag{5.12}$$

For the dynamical fields we get the plane wave solutions

$$c^{\text{plane}}(X)=C_0 e^{1/2\,X_{\alpha\beta}\kappa^\alpha\kappa^\beta},\quad c^{\text{plane}}_\alpha(X)=C_0\kappa_\alpha e^{1/2\,X_{\alpha\beta}\kappa^\alpha\kappa^\beta}, \tag{5.13}$$

with the twistorial "wave vector" $K_{\alpha\beta}=\frac{1}{2}\kappa_\alpha\kappa_\beta$.

The solution deformed to the AdS case is not strictly speaking plane wave. However it is "conformally plane wave" in the sense that it has still leftover generalized conformal invariances identified with such global symmetry transformations that

$$\delta_{\epsilon_0}|\Phi(b|X)\rangle=0\,. \tag{5.14}$$

It is easy to see using (4.2) that this condition is solved by any parameter of the form

$$\xi=f(a,b)\star(\rho^\alpha a_\alpha)\,, \tag{5.15}$$

where ρ is an arbitrary parameter such that $\rho^\alpha\kappa_\alpha=0$ and $f(a,b)$ is an arbitrary function. Indeed, according to (1.37),

$$\delta_{\epsilon_0}|\Phi(b|X)\rangle=g^{-1}\star\xi\star C(b|0)\star|0\rangle\langle 0|=g^{-1}\star f\star(\rho^\alpha a_\alpha)\star e^{\kappa_\alpha b^\alpha}\star|0\rangle\langle 0|=0\,. \tag{5.16}$$

VI. SUPEREXTENSION

The star-product formalism we use admits a straightforward generalization to the supersymmetric case associated with $\mathrm{OSp}(L|2M)$ where L is an arbitrary integer. To describe $\mathrm{osp}(L|2M)$ superalgebra let us introduce the Clifford elements ψ_i $(i=1,\dots,L)$ satisfying the anticommutation relations

$$\{\psi_i,\psi_j\}_*=\eta_{ij}\,, \tag{6.1}$$

where $\eta_{ij}=\eta_{ji}$ is some nondegenerate symmetric form. The Clifford star product in (6.1) is defined (see, e.g., Ref. 12) according to

$$(f*g)(\psi)=\frac{1}{2^L}\int f(\psi+\phi)g(\psi+\chi)e^{-2\chi^i\phi_i}\,\mathrm{d}^L\phi\,\mathrm{d}^L\chi\,, \tag{6.2}$$

where χ_i and ϕ_i are anticommuting variables. The supercharges

$$Q_{i\alpha}=a_\alpha\psi_i\,,\quad S_i^\alpha=b^\alpha\psi_i\,, \tag{6.3}$$

satisfy

$$\{Q_{i\alpha},Q_{i\beta}\}_*=\eta_{ij}P_{\alpha\beta}\,,\quad \{S_i^\alpha,S_j^\beta\}_*=\eta_{ij}K^{\alpha\beta}\,. \tag{6.4}$$

Let the Grassmann odd coordinates $\theta^{i\alpha}$ be associated with the Q-supergenerators. It is convenient to require the differential $d\theta^{i\alpha}$ to anticommute to $dX^{\alpha\beta}$ and $\theta^{i\alpha}$.

It is easy to see[1] that the gauge function

$$g = e^{-X^{\alpha\beta} a_\alpha a_\beta - \theta^{i\alpha} a_\alpha \psi_i} \tag{6.5}$$

reproduces the flat superspace vacuum one-form

$$w_0 = (\mathrm{d}X^{\alpha\beta} + \tfrac{1}{2}\mathrm{d}\theta^{i\alpha}\,\theta_i^{\beta}) P_{\alpha\beta} + \mathrm{d}\theta^{i\alpha} Q_{i\alpha}\,. \tag{6.6}$$

The left Fock module $|\Phi(b,\psi^+|X,\theta)\rangle$ satisfies the osp$(L|2M)$ supersymmetric equation

$$(d - w_0) \star |\Phi(b,\psi^+|X,\theta)\rangle = 0\,, \tag{6.7}$$

where the supersymmetric Fock vacuum $|0\rangle\langle 0|$ in addition to (1.26) is annihilated by the $\frac{1}{2}L$ (in case of even L) or $\frac{1}{2}(L-1)$ (in case of odd L) annihilation Clifford elements ψ^- and, when L is odd, it is an eigenvector of the central element $\Psi^L = \psi_1, \ldots, \psi_L$,

$$\Psi^L \star |0\rangle\langle 0| = \pm |0\rangle\langle 0|\,.$$

Let us now consider free field dynamics in the generalized AdS superspace. The corresponding supersymmetry algebra is osp$(L,M) \oplus$ osp(L,M) while the superspace is osp(L,M). To describe background fields (i.e., Cartan forms) in such a space we follow the same procedure as for Sp(M).

The OSp$(L|M)$ supergroup is realized by $(M+L)\times(M+L)$ matrices $U_A{}^B$, where $A = (\alpha, i)(\alpha = 1, \ldots, M,\ i = 1, \ldots, L)$, satisfying the group condition

$$U_A{}^B U_C{}^D \Omega^{AC} = \Omega^{BD}\,, \tag{6.8}$$

where $\Omega^{AB} = -(-1)^{\pi_A \pi_B} \Omega^{BA}$ and

$$\pi_A = \begin{cases} 1\,, & A = i, \\ 0\,, & A = \alpha. \end{cases}$$

It can be described by the local supercoordinates $X^{AB} = (-1)^{\pi_A \pi_B} X^{BA}$ with the aid of the exponential parametrization

$$U_A{}^B = \exp(\lambda X)_A{}^B\,. \tag{6.9}$$

Let us introduce the superoscillators a_A, b^A satisfying the (anti)commutation relations

$$a_A \star b^B - (-1)^{\pi_A \pi_B} b^B \star a_A = \delta_A{}^B\,, \tag{6.10}$$

with respect to the star product,

$$(f \star g)(a,b|X) = \frac{1}{2^{2L}\pi^M} \int f(a+u, b+t) g(a+s, b+v) e^{2(t^A s_A - v^A u_A)}\, \mathrm{d}u\, \mathrm{d}t\, \mathrm{d}s\, \mathrm{d}v\,, \tag{6.11}$$

where the statistics of the integration variables is defined according to

$$u_A u_B = (-1)^{\pi_A \pi_B} u_B u_A\,.$$

The integration measure is chosen so that 1 is the unit element of the star-product algebra (6.11).

Using the oscillator realization of osp$(L|M) \oplus$ osp$(L|M) \subset$ osp$(2L|2M)$ we can set

$$w_0 = \omega^{AB} a_B b_A + h^{AB} (a_B a_A + \lambda^2 b_B b_A)\,. \tag{6.12}$$

The analysis analogous to that of Sec. II shows that the gauge function

$$g=\sqrt{s\ \det\|1-\lambda^2 f^2(X)\|}\ \exp(-f^{AB}(X)(a_B a_A+\lambda^2 b_B b_A)) \tag{6.13}$$

provides the ''Lorentz connection'' ω_{AB} and the ''frame'' h_{AB} of the form

$$\omega_{AB}=\tfrac{1}{2}(\mathrm{d}U_A{}^C(U^{-1})_{CB}+\mathrm{d}(U^{-1})_A{}^C U_{CB})\,, \tag{6.14}$$

$$h_{AB}=\frac{1}{4\lambda}(\mathrm{d}U_A{}^C(U^{-1})_{CB}-\mathrm{d}(U^{-1})_A{}^C U_{CB})\,, \tag{6.15}$$

where

$$U_A{}^B=\left(\frac{1+\lambda f(X)}{1-\lambda f(X)}\right)_A^B. \tag{6.16}$$

The relationship between h_{AB} and ω_{AB} is analogous to (3.5),

$$\omega_{AB}=2h_A{}^C f_{CB}-2\,f_A{}^C h_{CB}+\lambda^2 f_A{}^C\omega_C{}^D f_{DB}\,. \tag{6.17}$$

Here is the list of the gauge functions and corresponding Cartan forms in different coordinates.

(1) The exponential parametrization (6.9),

$$g=\frac{1}{s\ \det\left\|\mathrm{ch}\dfrac{\lambda X}{2}\right\|}\exp\left(-\left(\mathrm{th}\frac{\lambda X}{2}\right)^{AB}(a_B a_A+\lambda^2 b_B b_A)\right), \tag{6.18}$$

$$\omega_{AB}=\frac{\lambda}{2}\left(\int_0^1 \exp(\lambda X t)_A{}^C\,\mathrm{d}X_C{}^D\exp(\lambda X t)_{DB}\,\mathrm{d}t-\int_{-1}^0 \exp(\lambda X t)_A{}^C\,\mathrm{d}X_C{}^D\exp(\lambda X t)_{DB}\,\mathrm{d}t\right), \tag{6.19}$$

$$h_{AB}=\frac{1}{4}\int_{-1}^1 \exp(\lambda X t)_A{}^C\,\mathrm{d}X_C{}^D\exp(\lambda X t)_{DB}\,\mathrm{d}t. \tag{6.20}$$

(2) $f^{AB}=\phi(s\ \det\|X\|)X^{AB}$,

$$g=\sqrt{s\ \det\|1-\lambda^2\phi^2\cdot X^2\|}\ \exp(-\phi X^{AB}(a_B a_A+\lambda^2 b_B b_A))\,, \tag{6.21}$$

$$\begin{aligned}h_{AB}=&\,\phi\cdot\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_A^C(\mathrm{d}X_C{}^D-\lambda^2\phi^2X_C{}^M\,\mathrm{d}X_M{}^N X_N{}^D)\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_{DB}\\&-\tilde{\phi}\cdot\left(\frac{X}{1-\lambda^2\phi^2X^2}\right)_{AB}(X^{-1})_M{}^N\,\mathrm{d}X_N{}^M\,,\end{aligned}$$

$$\omega_{AB}=2\lambda^2\phi^2\cdot\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_A^C(\mathrm{d}X_C{}^M X_M{}^D-X_C{}^M\,\mathrm{d}X_M{}^D)\left(\frac{1}{1-\lambda^2\phi^2X^2}\right)_{DB}, \tag{6.22}$$

where

$$\tilde{\phi}=\frac{\partial\phi}{\partial\ln s\ \det\|X\|}\,. \tag{6.23}$$

(3) The ''stereographic'' coordinates $f^{AB}(X)=(X/(1\mp\sqrt{1-\lambda^2X^2}))^{AB}$,

$$g^{\pm}=\sqrt{s\,\det\|1-\lambda^2 f^2(X)\|}\,\exp\left(-\left(\frac{X}{1\mp\sqrt{1-\lambda^2X^2}}\right)^{AB}(a_Ba_A+\lambda^2b_Bb_A)\right), \tag{6.24}$$

$$h_{AB}=\frac{1}{2}\left(\frac{1}{\sqrt{1-\lambda^2X^2}}\right)_A^C \mathrm{d}X_C{}^D\left(\frac{1}{\sqrt{1-\lambda^2X^2}}\right)_{DB}. \tag{6.25}$$

In the supersymmetric case, the global higher spin symmetry transformation law for the generating function $C(b|X)$ with respect to infinitesimal parameter,

$$\xi=\xi_0\exp(\mu^Aa_A-b^A\eta_A)$$

is analogous to (4.7),

$$\delta C(b|X)=C(b+\hat{\mu}|X)\exp(-(b^A+\tfrac{1}{2}\hat{\mu}^A)\,\hat{\eta}_A), \tag{6.26}$$

where

$$\hat{\mu}^A=\mathrm{ch}(\lambda X)^{AB}\mu_B-\frac{\mathrm{sh}(\lambda X)^{AB}}{\lambda}\eta_B,\quad \hat{\eta}^A=\mathrm{ch}(\lambda X)^{AB}\eta_B-\lambda\cdot\mathrm{sh}(\lambda X)^{AB}\mu_B. \tag{6.27}$$

It is straightforward to extend the rest of the analysis to the dynamics in the generalized superspace. Also, having found left invariant forms it is elementary to write down world-line particle actions (see, e.g., Refs. 4, 5, and 1 for more details and references). The form of the world-line particle Lagrangian suggested in Ref. 1 is

$$L=\dot{X}^{AB}w_{0AB}(a,b|X)+a_A\dot{b}^A, \tag{6.28}$$

where $\mathrm{d}X^{AB}w_{0AB}(a,b|X)=w_0(a,b|X)$ is the vacuum one-form satisfying the zero-curvature equation (1.31) and dot denotes the derivative with respect to the world-line parameter. Applying the Stokes theorem and using (1.31) the particle action (6.28) can be rewritten in the string form as an integral over a two-dimensional surface bounded by a particle trajectory and parametrized by σ^l,

$$S=\int_{\Sigma^2}\left(w_0(a,b|X)\star\wedge w_0(a,b|X)+\mathrm{d}a_A\wedge\mathrm{d}b^A+\left(\mathrm{d}a_A\frac{\partial}{\partial a_A}+\mathrm{d}b^A\frac{\partial}{\partial b^A}\right)\wedge w_0(a,b|X)\right), \tag{6.29}$$

where the pullback is defined as usual

$$w_0(a,b|X)=\mathrm{d}\sigma^l\frac{\partial X^{AB}}{\partial\sigma^l}w_{0AB}(a,b|X),\quad \mathrm{d}a_A=\mathrm{d}\sigma^l\frac{\partial a_A}{\partial\sigma^l},\quad \mathrm{d}b^A=\mathrm{d}\sigma^l\frac{\partial b^A}{\partial\sigma^l}. \tag{6.30}$$

The problem of calculating Cartan superforms in $\mathrm{osp}(1|2M)$ superspace was considered in Ref. 5 where a particular parametrization was found with bosonic Cartan forms being at most bilinear in fermionic coordinates. Note that the star-product algebra formalism simplifies some of the computational problems being reduced to evaluation of elementary Gaussian integrals. (See Ref. 13.)

VII. CONCLUSIONS

It is demonstrated how the star-product algebra formalism can be applied to the calculation of the vacuum of fields of the generalized AdS space associated with $\mathrm{sp}(M)\oplus\mathrm{sp}(M)$ subalgebra of the recently proposed in Ref. 2 generalized conformal symmetry $\mathrm{Sp}(2M)$. The method is universal working equally well for the supersymmetric case of $\mathrm{OSp}(L,M)$ with any M and L. The formalism of star-product algebra is shown to be very efficient for solving free field equations in

nontrivial (generalized conformally flat) geometries in $\mathcal{M}_M$ and calculating Cartan forms in arbitrary coordinates. Hopefully it may have applications to formulations of world-line (super)particle dynamics as well as (super)string actions in M theory backgrounds.

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APPENDIX

Let us prove that the formula

$$g(U)=\frac{2^{M/2}}{\sqrt{\det\|U+1\|}}\exp\left(\frac{1}{2}\left(\frac{U-1}{U+1}\right)^{\alpha\beta}\alpha_\alpha\alpha_\beta\right) \tag{A1}$$

respects the group multiplication law of $\mathrm{Sp}(M)$, i.e., that the formula (2.20) solves the equation (2.19). Let us look for $U(f)$ in the form

$$U(f)=\sum_{n=0}^{\infty} a_n f^n, \tag{A2}$$

where a_n are some coefficients. Hence $U(f_1)U(f_2)=\Sigma_{m,n=0}^{\infty}a_m a_n f_1^m f_2^n$. Since this expression contains all f_1 on the left-hand side, and f_2 on the right-hand, we have to find such a function $U(f)$ that $U(f_1\circ f_2)$ contains f_1 and f_2 in the correct order. We have

$$U(f_1\circ f_2)=\sum_{m=0}^{\infty} a_m\left\{\sum_{n=0}^{\infty} a_n(-1)^n((f_1f_2)^n(1+f_1)-(f_2f_1)^n(1+f_2))\right\}^m. \tag{A3}$$

All terms of wrong order must vanish. The analysis of a few first terms of $U(f_1\circ f_2)$ gives a hint that the coefficients are $a_n=\{a_0,a,a,a,\dots\}$, i.e.,

$$U(f)=a_0-a+\frac{a}{1-f}. \tag{A4}$$

The substitution of $U(f)$ into the equation $U^2(f)=U(f\circ f)$ fixes $a_0=1,a=2$ so that

$$U(f)=\frac{1+f}{1-f}. \tag{A5}$$

To prove that the obtained solution satisfies the equation (2.19) one has to check the identity

$$(1+f_1\circ f_2)\frac{1-f_2}{1+f_2}=(1-f_1\circ f_2)\frac{1+f_1}{1-f_1} \tag{A6}$$

equivalent to the relation

$$\begin{aligned}&\left\{1+\sum_{n=0}^{\infty}(-1)^n((f_2f_1)^n(1+f_2)-(f_1f_2)^n(1-f_1))\right\}\left(1+2\sum_{m=1}^{\infty}(-1)^m f_2^m\right)\\&\quad=\left\{1-\sum_{n=0}^{\infty}(-1)^n((f_2f_1)^n(1+f_2)-(f_1f_2)^n(1-f_1))\right\}\left(1+2\sum_{m=1}^{\infty}f_1^m\right),\end{aligned} \tag{A7}$$

which is elementary to check.

The normalization factor solves the equation

$$\frac{r(U_1)r(U_2)}{\sqrt{\det\|f_1 f_2+1\|}}=r(U_1U_2)\,, \tag{A8}$$

which is obviously true after the substitution (2.20),

$$\frac{2^{M/2}}{\sqrt{\det\|U_1+1\|}}\cdot\frac{2^{M/2}}{\sqrt{\det\|U_2+1\|}}\cdot\frac{1}{\sqrt{\det\left\|\dfrac{U_1-1}{U_1+1}\,\dfrac{U_2-1}{U_2+1}+1\right\|}}=\frac{2^{M/2}}{\sqrt{\det\|U_1U_2+1\|}}\,. \tag{A9}$$

This completes the proof of Eq. (2.20). The proof for the supersymmetric case is analogous.

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String theory extensions of Einstein–Maxwell fields: The stationary case

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We present a new approach for generating solutions in heterotic string theory compactified down to three dimensions on a torus with $d+n>2$, where d and n stand for the number of compactified space–time dimensions and Abelian gauge fields, respectively. It is shown that in the case when $d=2k+1$, and n is arbitrary, one can apply a solution-generating procedure which consists of mapping seed solutions of the stationary Einstein theory with k Maxwell fields to the heterotic string realm by using pure field redefinitions. A novel feature of this method is that it is precisely the electromagnetic sector of the stationary electrovacuum that mainly gives rise to a nontrivial multidimensional metric. This approach leads to classes of solutions which are invariant with respect to the total group of three-dimensional charging symmetries of the heterotic string theory, i.e., to all *finite* transformations which generate charged solutions from neutral ones and preserve the asymptotics of the starting field configurations. As an application of the presented approach we generate a particular extension of the stationary Einstein–multi-Maxwell theory obtained on the basis of the Kerr–multi-Newman–NUT special class of solutions and establish the conditions under which the resulting multi-dimensional metric of the heterotic string theory is asymptotically flat. [DOI: 10.1063/1.1631080]

I. INTRODUCTION

Symmetry based approaches used for the construction of solutions in the framework of effective field (low-energy) limits of string theories play an important role.[1–3] In this article we develop a new approach which allows one to extend the solution space of the stationary Einstein–multi-Maxwell (EmM) theory to the realm of heterotic string theory compactified down to three spatial dimensions on a torus. Namely, we show that a new charging symmetry invariant subspace of solutions of heterotic string theories (with $d=2k+1$ toroidally compactified space–time dimensions and arbitrary number n of original Abelian vector fields) can be generated from the solution spectrum of the stationary Einstein theory with k Maxwell fields by making use of pure field redefinitions. In particular, for the critical cases of heterotic ($d=7$) and bosonic ($d=23$) string theories one must start from the EmM theory with $k=3$ and $k=11$ Maxwell fields, respectively. Thus, the nontrivial multidimensional gravitational sector (the metric) of the heterotic string theory is mainly generated from the electromagnetic sector of the stationary EmM theory, an interesting fact that establishes a relationship between gravity and matter fields.

The toroidal compactification of heterotic string theory with arbitrary values of d and n was performed in Refs. 4 and 5, whereas the special case when the resulting theory is three-dimensional was originally studied in Refs. 6 and 7. There, the corresponding symmetric space model was identified and an explicit representation in terms of a null-curvature matrix was given (see Ref. 8 for such models and their classification). In this article we exploit the general formal-

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ism developed in Refs. 9–11 as a natural matrix generalization of the stationary Einstein–Maxwell (EM) theory written down in terms of potentials which are closely related to the Ernst ones (see Refs. 12–14). In the framework of this formalism, the subgroup of charging symmetry transformations (all finite transformations which generate charged solutions from neutral ones and preserve the asymptotic characteristics of the seed field configurations[15]) acts as a linear and homogeneous map; this fact allows one to work with the solution spectrum of the theory in a transparently charging symmetry invariant form. In particular, all the results of this article are automatically invariant with respect to the action of the total three-dimensional subgroup of charging symmetries $\mathrm{SO}(2,d-1)\times\mathrm{SO}(2,d-1+n)$ of the heterotic string theory compactified on a torus.[10]

In this article we continue our investigation on string theory extensions of EM fields. In a previous work[16] we have studied two theories with $d+n=2$; here we deal with theories with $d+n>2$. Such a split of the effective theories which arise upon toroidal compactification with arbitrary parameters d and n, in the framework of the low-energy limit of heterotic string theory, follows from the study of the general Israel–Wilson–Perjés (IWP) class of solutions of this theory performed in Ref. 11. The new formalism allows one to construct, in particular, a continuous generalization of the extremal IWP families of solutions in the corresponding string theories to the field of nonextremal ones. In Ref. 16 it was shown that the *static* EM theory plays the role of starting system for two theories with $d+n=2$; in this article we show that for the theories with $d+n>2$ such starting systems can be related to the *stationary* EmM theory and illustrate the developed general approach by considering an extension of the Kerr–multi-Newman–NUT solution to the realm of heterotic string theory.

II. NEW FORMALISM FOR 3D HETEROTIC STRING THEORY

In this section we review the necessary elements of the new formalism developed in Ref. 11 for the D-dimensional $(D=d+3)$ heterotic string theory with n Abelian gauge fields.

We start with the action for the bosonic sector of the low-energy heterotic string theory at tree level:[1,2]

$$\mathcal{S}_D=\int d^DX|\det G_{MN}|^{1/2}e^{-\Phi}\left(R_D+\Phi_{,M}\Phi^{,M}-\frac{1}{12}H_{MNK}H^{MNK}-\frac{1}{4}F^I_{MN}F^{I\,MN}\right), \tag{2.1}$$

where $H_{MNK}=\partial_M B_{NK}-\frac{1}{2}A^I_M F^I_{NK}+\text{cyclic}\{M,N,K\}$ and $F^I_{MN}=\partial_M A^I_N-\partial_N A^I_M$ $(M=1,\ldots,D)$. Here X^M is the Mth coordinate of the physical space–time of signature $(-,+,\ldots,+)$, G_{MN} is the metric, whereas Φ, B_{MN} and A^I_M $(I=1,\ldots,n)$ are the dilaton, Kalb-Ramond and Abelian gauge fields, respectively. In order to determine the resulting theory after the toroidal compactification on T^d down to three dimensions, let us set $D=d+3$, $X^m=(Y^m,x^\mu)$ with the extra-dimensional coordinates $Y^M=X^m$ $(m=1,\ldots,d)$ and the dynamical ones $x^\mu=X^{d+\mu}$ $(\mu=1,2,3)$. In Ref. 11 it was shown that, after the toroidal compactification of the first d dimensions Y^m, the resulting theory can be expressed in terms of the pair of field variables $(\mathcal{Z},h_{\mu\nu})$ which describes three-dimensional gravity, with metric $h_{\mu\nu}=h_{\mu\nu}(x^\lambda)$, coupled to a matter sector parametrized by the $(d+1)\times(d+1+n)$-matrix field variable $\mathcal{Z}=\mathcal{Z}(x^\lambda)$; its effective dynamics is given by the action

$$\mathcal{S}_3=\int d^3x h^{1/2}(-R_3+L_3), \tag{2.2}$$

where $R_3=R_3(h_{\mu\nu})$ is the curvature scalar for the line element $ds_3^2=h_{\mu\nu}dx^\mu dx^\nu$ and the matter sector of the theory reads

$$L_3=\mathrm{Tr}\,[\nabla\mathcal{Z}(\Xi-\mathcal{Z}^T\Sigma\mathcal{Z})^{-1}\nabla\mathcal{Z}^T(\Sigma-\mathcal{Z}\Xi\mathcal{Z}^T)^{-1}], \tag{2.3}$$

where $\Sigma=\mathrm{diag}(-1,-1;1,\ldots,1)$ is a $(d+1)\times(d+1)$-matrix and $\Xi=\mathrm{diag}(-1,-1;1,\ldots,1)$ is a $(d+1+n)\times(d+1+n)$-matrix.

This σ-model representation of the theory is the most compact one because of the dimensions of the matrix variable $\mathcal{Z}$. In order to come back to the original field components of the heterotic string theory from this σ-model description, it is convenient to introduce three doublets of potentials $(\mathcal{M}_\alpha,\vec{\Omega}_\alpha)$ $(\alpha=1,2,3)$ which are constructed on the basis of the field variables $(\mathcal{Z}, h_{\mu\nu})$ according to the following equations:

$$\mathcal{M}_1=\mathcal{H}^{-1},\quad \nabla\times\vec{\Omega}_1=\vec{J},$$

$$\mathcal{M}_2=\mathcal{H}^{-1}\mathcal{Z},\quad \nabla\times\vec{\Omega}_2=\mathcal{H}^{-1}\nabla\mathcal{Z}-\vec{J}\mathcal{Z}, \tag{2.4}$$

$$\mathcal{M}_3=\mathcal{Z}^T\mathcal{H}^{-1}\mathcal{Z},\quad \nabla\times\vec{\Omega}_3=\nabla\mathcal{Z}^T\mathcal{H}^{-1}\mathcal{Z}-\mathcal{Z}^T\mathcal{H}^{-1}\nabla\mathcal{Z}+\mathcal{Z}^T\vec{J}\mathcal{Z},$$

where $\mathcal{H}=\Sigma-\mathcal{Z}\Xi\mathcal{Z}^T$ and $\vec{J}=\mathcal{H}^{-1}(\mathcal{Z}\Xi\nabla\mathcal{Z}^T-\nabla\mathcal{Z}\Xi\mathcal{Z}^T)\mathcal{H}^{-1}$. In Eq. (2.4) the scalars $\mathcal{M}_\alpha$ are off-shell defined magnitudes, whereas the vectors $\vec{\Omega}_\alpha$ are defined on-shell. The scalar and vector potentials that conform each doublet have the same matrix dimensionality; let us represent them in the following block form:

$$\begin{pmatrix} 1\times1 & 1\times d\\ d\times1 & d\times d\end{pmatrix},\quad \begin{pmatrix} 1\times1 & 1\times d & 1\times n\\ d\times1 & d\times d & d\times n\end{pmatrix},\quad \begin{pmatrix} 1\times1 & 1\times d & 1\times n\\ d\times1 & d\times d & d\times n\\ n\times1 & n\times d & n\times n\end{pmatrix}, \tag{2.5}$$

for $\alpha=1,2,3$, respectively, where, for example, the ''13'' block components of the potentials $\mathcal{M}_2$ and $\vec{\Omega}_2$ are $1\times n$ matrices, the ''32'' block components of the potentials $\mathcal{M}_3$ and $\vec{\Omega}_3$ are $n\times d$ matrices, etc. Afterwards let us define the set of magnitudes which are directly involved in the solution-generating procedure that will be exposed in Sec. III; these include the following scalar matrix fields,

$$S_\alpha=U_\alpha+S_0^{-1}W_1^TW_\alpha, \tag{2.6}$$

where

$$\begin{aligned}
S_0&=-\mathcal{M}_{1,11}+2\mathcal{M}_{2,11}-\mathcal{M}_{3,11},\\
U_1&=G_0\mathcal{M}_{1,22}G_0+G_0\mathcal{M}_{2,22}+(\mathcal{M}_{2,22})^TG_0+\mathcal{M}_{3,22},\\
U_2&=G_0\mathcal{M}_{1,22}-G_0\mathcal{M}_{2,22}G_0+(\mathcal{M}_{2,22})^T-\mathcal{M}_{3,22}G_0,\\
U_3&=\sqrt{2}(G_0\mathcal{M}_{2,23}+\mathcal{M}_{3,23}),\\
W_1&=-\mathcal{M}_{1,12}G_0-\mathcal{M}_{2,12}+(\mathcal{M}_{2,21})^TG_0+\mathcal{M}_{3,12},\\
W_2&=\mathcal{M}_{1,12}-\mathcal{M}_{2,12}G_0+(\mathcal{M}_{2,21})^T-\mathcal{M}_{3,12}G_0,\\
W_3&=\sqrt{2}(\mathcal{M}_{2,13}+\mathcal{M}_{3,13}),
\end{aligned} \tag{2.7}$$

where $G_0=\mathrm{diag}(-1;1,\ldots,1)$ is a $d\times d$-matrix, and the matrix vector fields

$$\begin{aligned}
\vec{V}_1&=[-\vec{\Omega}_{1,12}G_0+\vec{\Omega}_{2,12}+(\vec{\Omega}_{2,21})^TG_0+\vec{\Omega}_{3,12}]^T,\\
\vec{V}_2&=[-\vec{\Omega}_{1,12}-\vec{\Omega}_{2,12}G_0+(\vec{\Omega}_{2,21})^T-\vec{\Omega}_{3,12}G_0]^T,
\end{aligned} \tag{2.8}$$

$$\vec{V}_3=\sqrt{2}(\vec{\Omega}_{2,13}+\vec{\Omega}_{3,13})^T.$$

In the language of these matrix variables the heterotic string theory fields read

$$ds_D^2=ds_{d+3}^2=(dY+V_{1\mu}dx^\mu)^T S_1^{-1}(dY+V_{1\nu}dx^\nu)+S_0 ds_3^2,$$

$$e^\Phi=|S_0\det S_1|^{1/2},$$

$$B_{mk}=\tfrac{1}{2}(S_1^{-1}S_2-S_2^T S_1^{-1})_{mk},$$

$$B_{m\,d+\nu}=\{V_{2\nu}+\tfrac{1}{2}(S_1^{-1}S_2-S_2^T S_1^{-1})V_{1\nu}-S_1^{-1}S_3 V_{3\nu}\}_m, \tag{2.9}$$

$$B_{d+\mu\,d+\nu}=\tfrac{1}{2}[V_{1\mu}^T(S_1^{-1}S_2-S_2^T S_1^{-1})V_{1\nu}+V_{1\mu}^T V_{2\nu}-V_{1\nu}^T V_{2\mu}],$$

$$A_m^I=(S_1^{-1}S_3)_{mI},$$

$$A_{d+\mu}^I=(-V_{3\mu}+S_3^T S_1^{-1}V_{1\mu})_I.$$

From Eq. (2.9) it follows that, apart from the magnitudes S_0, S_α and $\vec{V}_\alpha$, we also must compute $\det S_1$ and S_1^{-1} in order to obtain explicit expressions for the field components of the heterotic string theory (2.1). Therefore, after some algebraic calculations it can be proved that

$$\begin{aligned}\det S_1&=(1+S_0 W_1 U_1^{-1}W_1^T)\det U_1,\\ S_1^{-1}&=U_1^{-1}-\frac{S_0^{-1}U_1^{-1}W_1^T W_1 U_1^{-1}}{1+S_0^{-1}W_1 U_1^{-1}W_1^T}.\end{aligned} \tag{2.10}$$

Finally, let us point out that the magnitudes S_0, U_α, W_α and $\vec{V}_\alpha$ can be used to explicitly write down any solution of the theory under consideration. As it was indicated above, these magnitudes are directly involved in the solution-generating technique that will be developed in the next section, and in Sec. IV we shall calculate them in order to obtain a concrete extension of the stationary EmM theory to the realm of the low-energy heterotic string theory.

At the end of this section let us notice that the transformation

$$\mathcal{Z}\to\mathcal{C}_1\mathcal{Z}\mathcal{C}_2, \tag{2.11}$$

where $\mathcal{C}_1$ and $\mathcal{C}_2$ obey the orthogonal group conditions

$$\mathcal{C}_1^T\Sigma\mathcal{C}_1=\Sigma \quad \text{and} \quad \mathcal{C}_2^T\Xi\mathcal{C}_2=\Xi, \tag{2.12}$$

is a transparent symmetry of the Lagrangian (2.3) since it remains invariant under such a transformation. In Refs. 10 and 11 it was shown that this symmetry transformation coincides with the total group of three-dimensional charging symmetries $\mathrm{SO}(2,d-1)\times\mathrm{SO}(2,d-1+n)$. As it was mentioned before, the above reviewed formalism, based on the use of the matrix potential $\mathcal{Z}$, constitutes a *sigma*-model representation of the theory (2.3) with the lowest possible matrix dimension and is, in fact, a $\mathrm{O}(d+1,d+n+1)/\mathrm{O}[(d+1)\times(d+n+1)]$ symmetric space model of dimension $(d+1)(d+n+1)$ according to the classification of (Ref. 8). From Eq. (2.11) it also follows that the general transformation of the charging symmetry subgroup of the theory acts as a linear and homogeneous map, a fact that was just discussed in the Introduction. Since this symmetry subgroup preserves the asymptotic properties of the seed solutions when one applies a solution-generating procedure, this formalism is especially convenient for the study of asymptotically flat solutions of heterotic string theory toroidally compactified down to three dimensions because all the results can be obtained in a transparent charging symmetry invariant form.

III. STRING THEORIES FROM STATIONARY EINSTEIN–MULTI-MAXWELL SYSTEM

In this section we show how to map solutions of the stationary Einstein theory with k Maxwell fields into solutions to the three-dimensional heterotic string theory with $d=2k+1$ toroidally compactified space–time dimensions and arbitrary number n of Abelian gauge fields.

First of all, let us formulate the main idea of our approach; it is related to the heterotic string/Einstein–Maxwell theory correspondence and the explicit form of the IWP class of solutions in both of these theories.[11] In order to achieve this aim, let us represent the stationary EM theory in a very similar form to the three-dimensional effective field theory of the heterotic string represented by Eq. (2.3). Namely, it is well known that the effective three-dimensional Lagrangian of the stationary EM theory reads

$$L_3=L_{EM}=\frac{1}{2f^2}|\nabla E-\overline{F}\nabla F|^2-\frac{1}{f}|\nabla F|^2, \tag{3.1}$$

where $f=\frac{1}{2}(E+\overline{E}-|F|^2)$, and E and F are the conventional Ernst potentials. Let us introduce the 1×2 matrix potential

$$z=(z_1\ z_2) \tag{3.2}$$

with

$$z_1=\frac{1-E}{1+E},\quad z_2=\frac{\sqrt{2}F}{1+E}. \tag{3.3}$$

Then

$$L_{EM}=2\,\frac{\nabla z(\sigma_3-z^\dagger z)^{-1}\nabla z^\dagger}{1-z\sigma_3 z^\dagger}, \tag{3.4}$$

where $\sigma_3=\mathrm{diag}(1\ -1)$. By comparing Eqs. (2.3) and (3.4) it follows that the correspondence

$$\mathcal{Z}\leftrightarrow z,\quad \Xi\leftrightarrow\sigma_3,\quad \Sigma\leftrightarrow 1, \tag{3.5}$$

together with the interchange of operations $T\leftrightarrow\dagger$, relates three-dimensional heterotic string and stationary EM theories; the factor "2" in (3.4) can be understood as a consequence of the exact matrix representation of complex magnitudes (see below and Ref. 11 as well for details). It turns out that the IWP class of solutions of the EM theory[17] can be rewritten in terms of the z-potential as $z=\lambda q$, where $\lambda=\lambda(x^\mu)$ is a complex harmonic function ($\nabla^2\lambda=0$), q is a 1×2-matrix constant parameter and when the parameter $\kappa=q\sigma_3 q^\dagger$ vanishes; in this case, the corresponding three-dimensional metric $h_{\mu\nu}$ is flat. It is clear that, in view of the correspondence (3.5), the IWP class of solutions of the heterotic string theory arises in the framework of the ansatz

$$\mathcal{Z}=\Lambda\mathcal{Q}, \tag{3.6}$$

where $\Lambda=\Lambda(x^\mu)$ is a real harmonic $(d+1\times 2)$-matrix function and $\mathcal{Q}$ is a constant $(2\times d+n+1)$-matrix parameter. In Ref. 11 it was shown that this fact actually takes place if the parameter

$$\kappa=\mathcal{Q}\Xi\,\mathcal{Q}^T \tag{3.7}$$

vanishes and the three-metric $h_{\mu\nu}$ is flat again, in complete accordance with the correspondence (3.5). There, it also was shown that the restriction $\kappa=0$ completely fixes the dimensionality of the matrices Λ and $\mathcal{Q}$: for two theories with $d+n=2$, such matrices have dimensions $(d+1)\times 1$ and 1×3, respectively, whereas for the theories with $d+n>2$ the dimensions are $(d+1)\times 2$ and $2\times(d+n+1)$, respectively, as it was pointed out above.

A crucial point in our approach consists of removing the $\kappa=0$ restriction in order to consider the generalization of the IWP class of solutions of heterotic string theory to the subspace of the nonextremal solutions. This means that we shall preserve the form of the ansatz (3.6) and the dimensions of the matrices Λ and $\mathcal{Q}$, but we shall allow arbitrary values of the parameter κ defined by Eq. (3.7). Such a procedure can be applied in a very natural way in the framework of the stationary EM theory, where it defines, for instance, a continuous extension of the extremal Kerr–multi-Newman–NUT solution to the corresponding nonextremal one.[14] Such an extension is really interesting from the point of view of physical applications since the example given above concerns black hole physics in EM theory.[18] In view of the correspondence (3.5) the same motivation for the study of the ansatz (3.6) with $\kappa\neq 0$ must be valid for the low-energy heterotic string theory; thus, the study of such an ansatz is also interesting since it is related to black hole physics in the framework of string theory.[3,19]

In this article we consider string theories with $d+n>2$, when κ is a symmetric 2×2-matrix. By straightforwardly substituting the ansatz (3.6) into the equations of motion derived from Eqs. (2.2) and (2.3), one obtains

$$\begin{aligned}&\nabla^2\Lambda+2\nabla\Lambda\kappa\Lambda^T(\Sigma-\Lambda\kappa\Lambda^T)^{-1}\nabla\Lambda=0,\\ &R_{3\ \mu\nu}=Tr[\Lambda_{,(\mu}\kappa(1-\Lambda^T\Sigma\Lambda\kappa)^{-1}\Lambda^T_{,\nu)}(\Sigma-\Lambda\kappa\Lambda^T)^{-1}].\end{aligned}\tag{3.8}$$

It is obvious that in the case $\kappa=0$ we recover the extremal case studied in Ref. 11, whereas for $\kappa\neq 0$ we have the above mentioned continuous extension of the formalism to the nonextremal case. Below we study the situation when κ is nonzero and, moreover, nondegenerate matrix with signature $\tilde{\Sigma}=\mathrm{diag}(-1,-1)$. The reason for considering such a particularization of the ansatz (3.6) is that, in this case, the effective system defined by Eqs. (3.8) corresponds to some new heterotic string theory by itself. Actually, Eqs. (3.8) are the equations of motion for the action (2.2) with the matter Lagrangian (2.3) replaced by

$$\tilde{\mathcal{L}}_3=Tr[\nabla\Lambda\kappa(1-\Lambda^T\Sigma\Lambda\kappa)^{-1}\nabla\Lambda^T(\Sigma-\Lambda\kappa\Lambda^T)^{-1}].\tag{3.9}$$

Then, as an algebraic fact it follows that there exists a nondegenerate matrix K such that

$$\kappa=K\tilde{\Sigma}K^T.\tag{3.10}$$

Let us introduce the new matrix potential

$$\tilde{\mathcal{Z}}=K^T\Lambda^T\tag{3.11}$$

and set $\tilde{\Xi}=\Sigma$. We claim that it is possible to rewrite the effective Lagrangian $\tilde{\mathcal{L}}_3$ (3.9) in terms of $\tilde{\mathcal{Z}}$, $\tilde{\Sigma}$ and $\tilde{\Xi}$; the resulting Lagrangian exactly coincides with the relation (2.3) up to the tilde. Thus, the effective system (3.9) is nothing else than the heterotic string theory with $\tilde{d}=1$ compactified dimensions and $\tilde{n}=d-1$ Abelian gauge fields. From Eqs. (3.6) and (3.11) it follows that

$$\mathcal{Z}=\tilde{\mathcal{Z}}^TT,\tag{3.12}$$

where $T=K^{-1}\mathcal{Q}$. Equation (3.12) maps the space of solutions of the theory in terms of $\tilde{\mathcal{Z}}$ into that of the theory in terms of the potential $\mathcal{Z}$, so that the matrix T plays the role of a symmetry operator. Let us now calculate the general explicit form of such symmetry operator using Eqs. (3.6) and (3.10). Without loss of generality (see Ref. 11 for details), the matrix $\mathcal{Q}$ can be parametrized in the form

$$\mathcal{Q}=\begin{pmatrix}1 & 0 & n_1^T\\ 0 & 1 & n_2^T\end{pmatrix},\tag{3.13}$$

where n_a $(a=1,2)$ are two $(d+n-1)\times 1$ columns. Thus, the extremal case corresponds to the restriction $n_a^T n_b=\delta_{ab}$, i.e., it is realized by the unit orthogonal columns n_a. Our generalization of the extremal ansatz corresponds, in this geometric language, to the case of columns with arbitrary length and arbitrary angle between them, which is compatible with the signature $\tilde{\Sigma}$ of the matrix κ.

Now we are able to compute the matrix κ and to determine the quantity K using, for example, the orthogonalization procedure of the theory of quadratic forms. A special solution reads

$$K=\begin{pmatrix} \sqrt{1-n_1^T n_1} & 0 \\ -\dfrac{n_1^T n_2}{\sqrt{1-n_1^T n_1}} & \sqrt{\dfrac{1-n_1^T n_1-n_2^T n_2+(n_1^T n_1)(n_2^T n_2)-(n_1^T n_2)^2}{1-n_1^T n_1}} \end{pmatrix}. \tag{3.14}$$

In order to obtain a general solution K to the quadratic equation (3.10) one must generalize the special solution (3.14) through the map $K\to K\mathcal{C}$ where $\mathcal{C}^T\tilde{\Sigma}\mathcal{C}=\tilde{\Sigma}$, i.e., $\mathcal{C}\in O(2)$. However, this map is effectively equivalent to the transformation $\tilde{\mathcal{Z}}\to(\mathcal{C}^T)^{-1}\tilde{\mathcal{Z}}$ as it follows from Eq. (3.12). It is clear that $(\mathcal{C}^T)^{-1}$ is nothing more than an alternative notation for the "left" matrix $\mathcal{C}_1$ of the charging symmetry transformation (2.11), thus, it can be omitted when considering charging symmetry invariant classes of solutions represented by $\tilde{\mathcal{Z}}$. Thus, without loss of generality one can take $\mathcal{Q}$ and K in the form given by Eqs. (3.13) and (3.14) when constructing a symmetry operator according to Eq. (3.12). It is worth noticing that the definition of K is consistent with the assumed signature of κ.

Now let us consider a special situation with $d=2k+1$, when the potential $\tilde{\mathcal{Z}}$ can be split into $k+1$ different 2×2-matrix blocks:

$$\tilde{\mathcal{Z}}=(\tilde{\mathcal{Z}}_1,\ \tilde{\mathcal{Z}}_2,\ \ldots,\ \tilde{\mathcal{Z}}_{k+1}). \tag{3.15}$$

Let us consider a consistent ansatz with

$$\tilde{\mathcal{Z}}_{\mathcal{P}}=\begin{pmatrix} z'_{\mathcal{P}} & -z''_{\mathcal{P}} \\ z''_{\mathcal{P}} & z'_{\mathcal{P}} \end{pmatrix}, \tag{3.16}$$

where $\mathcal{P}=1,2,\ldots,k+1$. Let us introduce $k+1$ complex functions $z_{\mathcal{P}}=z'_{\mathcal{P}}+iz''_{\mathcal{P}}$. Our statement is that the heterotic string theory field equations corresponding to the special subsystem (3.15) and (3.16) can be derived from the effective Lagrangian

$$L_3=L_{EmM}=2\,\frac{\nabla\tilde{z}(\tilde{\sigma}_3-\tilde{z}^{\dagger}\tilde{z})^{-1}\nabla\tilde{z}^{\dagger}}{1-\tilde{z}\tilde{\sigma}_3\tilde{z}^{\dagger}}, \tag{3.17}$$

where $\tilde{z}=(\tilde{z}_1,\tilde{z}_2,\ \ldots,\ \tilde{z}_{k+1})$ and $\tilde{\sigma}_3=\mathrm{diag}(1,-1,-1,\ldots,-1)$. It is clear that in the case $k=1$ one recovers Eq. (3.4), i.e., one deals with the stationary EM theory. It is natural to suppose that in the case of arbitrary k one obtains the stationary Einstein theory with k Maxwell fields. In order to verify this statement it is convenient to introduce new variables [compare to Eq. (3.3)]

$$E=\frac{1-\tilde{z}_1}{1+\tilde{z}_1},\quad F_p=\frac{\sqrt{2}\tilde{z}_{p+1}}{1+\tilde{z}_1}, \tag{3.18}$$

where $p=1,2,\ldots,k$. In terms of these variables the effective Lagrangian adopts the form

$$L_{EmM}=\frac{1}{2f^2}|\nabla E-\overline{F}_p\nabla F_p|^2-\frac{1}{f}|\nabla F_p|^2, \tag{3.19}$$

where $f=\frac{1}{2}(E+\overline{E}-F_p\overline{F}_p)$, thus, the potentials E and F_p can be interpreted as the conventional Ernst potentials of the classical four-dimensional Einstein theory with k Maxwell fields in the stationary case.

The theory (3.17) can be studied in a form which is very close to that of the heterotic string theory (see Sec. II) by using the correspondence (3.5) modified to the case of k Maxwell fields, i.e., by making the following replacement:

$$z\to\tilde{z},\quad \sigma_3\to\tilde{\sigma}_3 \tag{3.20}$$

[see Eqs. (3.4) and (3.7)]. Namely, it is convenient to introduce the doublets $(\tilde{m}_\alpha,\tilde{\vec{\omega}}_\alpha)$ with

$$\tilde{m}_1=\tilde{h}^{-1},\quad \nabla\times\tilde{\vec{\omega}}_1=\tilde{\vec{j}},$$

$$\tilde{m}_2=\tilde{h}^{-1}\tilde{z},\quad \nabla\times\tilde{\vec{\omega}}_2=\tilde{h}^{-1}\nabla\tilde{z}-\tilde{\vec{j}}\tilde{z}, \tag{3.21}$$

$$\tilde{m}_3=\tilde{h}^{-1}\tilde{z}^\dagger\tilde{z},\quad \nabla\times\tilde{\vec{\omega}}_3=\tilde{h}^{-1}(\nabla\tilde{z}^\dagger\tilde{z}-\tilde{z}^\dagger\nabla\tilde{z})+\tilde{\vec{j}}\tilde{z}^\dagger\tilde{z},$$

where $\tilde{h}=-(1-\tilde{z}\tilde{\sigma}_3\tilde{z}^\dagger)$ and $\tilde{\vec{j}}=-\tilde{h}^{-2}(\tilde{z}\tilde{\sigma}_3\nabla\tilde{z}^\dagger-\nabla\tilde{z}\tilde{\sigma}_3\tilde{z}^\dagger)$ [compare with Eq. (2.4)]. It is clear that the doublet $(\tilde{m}_1,\tilde{\vec{\omega}}_1)$ consists of complex functions, whereas the doublets $(\tilde{m}_2,\tilde{\vec{\omega}}_2)$ and $(\tilde{m}_3,\tilde{\vec{\omega}}_3)$ consist of $1\times(k+1)$– and $(k+1)\times(k+1)$-matrices, respectively. From Eqs. (3.15) and (3.16) we extract a rule for reconstructing the heterotic string theory described by the potential $\tilde{\mathcal{Z}}$ of dimension $2\times[2(k+1)]$. Further, from Eqs. (3.12)–(3.14) one obtains the explicit form of the symmetry map $\tilde{\mathcal{Z}}\to\mathcal{Z}$. It is interesting that this map is nonholomorphic due to the transposition of $\tilde{\mathcal{Z}}$ in Eq. (3.12), which is equivalent to the Hermitian conjugation of $\tilde{z}$ in view of the correspondence (3.20) discussed above.

Thus, a symmetry transformation that maps the space of solutions of the stationary Einstein theory with k Maxwell fields into the corresponding subspace of solutions of the heterotic string with $d=2k+1$ toroidally compactified dimensions and n arbitrary Abelian gauge fields is established by the following procedure:

(i) First of all, one must calculate in explicit form three doublets of potentials $(\tilde{m}_\alpha,\tilde{\vec{\omega}}_\alpha)$ for the stationary EmM theory.

(ii) After that one must rewrite them in the form $(\tilde{M}_\alpha,\tilde{\vec{\Omega}}_\alpha)$ using the exact matrix representation of complex magnitudes. [Equations (3.15) and (3.16) give, in fact, an example of such a representation of the complex potential $\tilde{z}$ in terms of the real potential $\tilde{\mathcal{Z}}$.]

(iii) The next step consists of calculating the matrix potentials $(\mathcal{M}_\alpha,\vec{\Omega}_\alpha)$ for the heterotic string theory which is an image of the EmM system according to the map (3.12).

(iv) Afterwards, one must obtain the explicit form of the magnitudes S_0, W_α, U_α and $\vec{V}_\alpha$, using the found potentials $(\mathcal{M}_\alpha,\vec{\Omega}_\alpha)$.

(v) Finally, by using (2.9) one gets explicit expressions for the original field variables of heterotic string theory.

At the end of this section let us compute the doublets $(\mathcal{M}_\alpha,\vec{\Omega}_\alpha)$. By making use of Eqs. (2.4) and (3.12), after some algebraic calculations, one obtains

$$\mathcal{M}_1=\Sigma+\Sigma\tilde{\mathcal{M}}_3\Sigma,\quad \vec{\Omega}_1=-\Sigma\tilde{\vec{\Omega}}_3\Sigma,$$

$$\mathcal{M}_2=-\Sigma\tilde{\mathcal{M}}_2^TT,\quad \vec{\Omega}_2=-\Sigma\tilde{\vec{\Omega}}_2^TT, \tag{3.22}$$

$$\mathcal{M}_3=T^T(\tilde{\mathcal{M}}_1+1)T,\quad \vec{\Omega}_3=-T^T\tilde{\vec{\Omega}}_1T.$$

In the next section we shall exploit these formulas in order to construct a subspace of solutions for the heterotic string theory with $d=2k+1$ and arbitrary n starting from the stationary Einstein theory with k Maxwell fields.

IV. SOLUTIONS VIA KERR–MULTI-NEWMAN–NUT FAMILY

In order to calculate the potentials S_0, W_α, U_α and $\vec{V}_\alpha$ for the heterotic string fields, which correspond to the EmM ones, according to the scheme developed in the previous section, let us parametrize the potential $\tilde{\mathcal{Z}}$ and the symmetry operator T in the appropriate form. For $\tilde{\mathcal{Z}}$ is convenient to set

$$\tilde{\mathcal{Z}}=(\tilde{\mathcal{Z}}_I\ \tilde{\mathcal{Z}}_{II}), \tag{4.1}$$

where $\tilde{\mathcal{Z}}_I$ is a 2×1-column and $\tilde{\mathcal{Z}}_{II}$ is a $2\times(2k+1)$-matrix that read

$$\tilde{\mathcal{Z}}_I=\begin{pmatrix}\tilde{z}'_1\\ \tilde{z}''_1\end{pmatrix},\quad \tilde{\mathcal{Z}}_{II}=\begin{pmatrix}-\tilde{z}''_1 & \tilde{z}'_{1+p} & -\tilde{z}''_{1+p}\\ \tilde{z}'_1 & \tilde{z}''_{1+p} & \tilde{z}'_{1+p}\end{pmatrix}. \tag{4.2}$$

Therefore, for T we choose the following segmentation,

$$T=(T_I\ T_{II}\ T_{III}), \tag{4.3}$$

where T_I is a 2×1-column, T_{II} is a $2\times(2k+1)$-matrix, and T_{III} is a $2\times n$-matrix, i.e.,

$$\begin{gathered}T_I=\mathcal{K}^{-1}\mathcal{Q}_I,\quad \tilde{\mathcal{Q}}_I=\begin{pmatrix}1\\0\end{pmatrix},\\ T_{II}=\mathcal{K}^{-1}\mathcal{Q}_{II},\quad Q_{II}=\begin{pmatrix}0 & r_1^T\\ 1 & r_2^T\end{pmatrix},\\ T_{III}=\mathcal{K}^{-1}\mathcal{Q}_{III},\quad \tilde{\mathcal{Q}}_{III}=\begin{pmatrix}l_1^T\\ l_2^T\end{pmatrix},\end{gathered} \tag{4.4}$$

where we have naturally decomposed $n_a^T=(r_a^T\ l_a^T)$ into the rows r_a^T and l_a^T of dimension $1\times 2k$ and $1\times n$, respectively. It is worth noticing that the block representation (4.1) and (4.3) of the magnitudes $\tilde{\mathcal{Z}}$ and T is directly related to the number of compactified dimensions and Abelian vector fields ($2k+1$ and n, respectively) and, thus, is actually fruitful for the application of Eqs (2.9). Thus, after some algebraic computations, Eqs. (2.7) yield the following expression for the scalar S_0:

$$S_0=1-T_I^TT_I-\tilde{h}^{-1}(\tilde{\mathcal{Z}}_I-T_I)^T(\tilde{\mathcal{Z}}_I-T_I), \tag{4.5}$$

whereas for the columns W_α one obtains

$$\begin{gathered}W_1=T_I^TT_{II}+\tilde{h}^{-1}(\tilde{\mathcal{Z}}_I-T_I)^T(\tilde{\mathcal{Z}}_{II}-T_{II}),\\ W_2=-[T_I^TT_{II}+\tilde{h}^{-1}(\tilde{\mathcal{Z}}_I+T_I)^T(\tilde{\mathcal{Z}}_{II}+T_{II})]G_0,\\ W_3=\sqrt{2}[T_I+\tilde{h}^{-1}(\tilde{\mathcal{Z}}_I+T_I)]^TT_{III};\end{gathered} \tag{4.6}$$

finally, for the matrix potentials U_α one gets

$$U_1 = G_0 + T_{II}^T T_{II} + \tilde{h}^{-1}(\tilde{\mathcal{Z}}_{II} - T_{II})^T(\tilde{\mathcal{Z}}_{II} - T_{II}),$$

$$U_2 = -[T_{II}^T T_{II} - \tilde{h}^{-1}(\tilde{\mathcal{Z}}_{II} - T_{II})^T(\tilde{\mathcal{Z}}_{II} + T_{II})]G_0, \tag{4.7}$$

$$U_3 = \sqrt{2}[T_{II} - \tilde{h}^{-1}(\tilde{\mathcal{Z}}_{II} - T_{II})]^T T_{III}.$$

On the other hand, the vector matrices $\tilde{\tilde{\Omega}}_\alpha$ possess the following parametrization,

$$\tilde{\tilde{\Omega}}_1 = \vec{\omega}\epsilon, \quad \tilde{\tilde{\Omega}}_2 = (\tilde{\tilde{\Omega}}_{2,I}\ \tilde{\tilde{\Omega}}_{2,II}), \quad \tilde{\tilde{\Omega}}_3 = \begin{pmatrix} 0 & \tilde{\tilde{\Omega}}_{3,I\ II} \\ \tilde{\tilde{\Omega}}_{3,II\ I} & \tilde{\tilde{\Omega}}_{3,II\ II} \end{pmatrix}, \tag{4.8}$$

where $\vec{\omega} = \tilde{\tilde{\omega}}_1''$ (the magnitude $\tilde{\tilde{\omega}}_1$ is purely imaginary, i.e., $\tilde{\tilde{\omega}}_1' = 0$), ϵ is the antisymmetric 2×2-matrix with $\epsilon_{12} = -1$, the block components of $\tilde{\tilde{\Omega}}_2$ read

$$\tilde{\tilde{\Omega}}_{2,I} = \begin{pmatrix} \tilde{\tilde{\omega}}_{2,1}' \\ \tilde{\tilde{\omega}}_{2,1}'' \end{pmatrix}, \quad \tilde{\tilde{\Omega}}_{2,II} = \begin{pmatrix} -\tilde{\tilde{\omega}}_{2,1}'' & \tilde{\tilde{\omega}}_{2,1+p}' & -\tilde{\tilde{\omega}}_{2,1+p}'' \\ \tilde{\tilde{\omega}}_{2,1}' & \tilde{\tilde{\omega}}_{2,1+p}'' & \tilde{\tilde{\omega}}_{2,1+p}' \end{pmatrix}, \tag{4.9}$$

whereas $\tilde{\tilde{\Omega}}_{3,II\ I} = -\tilde{\tilde{\Omega}}_{3,I\ II}^T$, $\tilde{\tilde{\Omega}}_{3,II\ II} = -\tilde{\tilde{\Omega}}_{3,II\ II}^T$ ($\tilde{\tilde{\Omega}}_3 = -\tilde{\tilde{\Omega}}_3^T$) and

$$\tilde{\tilde{\Omega}}_{3,I\ II} = (-\tilde{\tilde{\omega}}_{3,1\ 1}''\ \ \tilde{\tilde{\omega}}_{3,1\ 1+p}'\ \ -\tilde{\tilde{\omega}}_{3,1\ 1+p}''). \tag{4.10}$$

Note that, in view of Eqs. (2.11) and (3.22), only the magnitudes $\tilde{\tilde{\omega}}$, $\tilde{\tilde{\Omega}}_{2,I}$, $\tilde{\tilde{\Omega}}_{2,II}$ and $\tilde{\tilde{\Omega}}_{3,I\ II}$ are necessary for the explicit construction of the potential $\vec{V}_\alpha$. Finally, the explicit expressions for these vectors read

$$\vec{V}_1 = \tilde{\tilde{\omega}} T_{II}^T \epsilon T_I - \tilde{\tilde{\Omega}}_{2,II}^T T_I + T_{II}^T \tilde{\tilde{\Omega}}_{2,I} - \tilde{\tilde{\Omega}}_{3,I\ II}^T,$$

$$\vec{V}_2 = -\mathcal{G}_0(\tilde{\tilde{\omega}} T_{II}^T \epsilon T_I + \tilde{\tilde{\Omega}}_{2,II}^T T_I + T_{II}^T \tilde{\tilde{\Omega}}_{2,I} + \tilde{\tilde{\Omega}}_{3,I\ II}^T), \tag{4.11}$$

$$\vec{V}_3 = \sqrt{2}(\tilde{\tilde{\omega}}\epsilon T_I + \tilde{\tilde{\Omega}}_{2,I})^T T_{III}.$$

At this stage some remarks are in order: Eqs. (4.5), (4.7), and (4.11) also possess another parametrization which is based on the identities $\mathcal{K}\mathcal{K}^T = -\kappa$ and $\mathcal{K}\epsilon\mathcal{K}^T = \sqrt{\det \kappa}\epsilon$. In both representations the potentials S_0, W_α, U_α and $\vec{V}_\alpha$ become trivial ($S_0 = 1$, $U_1 = G_0$ and other fields vanish) for a starting EmM solution corresponding to $\tilde{\mathcal{Z}} = 0$. This fact reflects the underlying property of the primordial symmetry map (3.12) in the language of the potentials which define the components of the physical fields of string theory. As a last remark let us point out that the appearance of the $(2k+1)\times(2k+1)$-matrix $G_0 = \mathrm{diag}(-1,1,1,\ldots,1)$, which describes the flat metric corresponding to extra dimensions, in Eq. (4.7) is very natural.

As a matter of fact, our solution-generating procedure, based on the use of Eq. (3.12) and the special choice of the starting matrix potential $\tilde{\mathcal{Z}}$ in an EmM form [see Eqs. (4.1) and (4.2)], breaks the complex structure of the starting theory. Actually, in the general case, the $2\times[2(k+1)+n]$-dimensional symmetry operator T does not represent any complex magnitude t of dimension $1\times(k+1+n/2)$. In particular, the number of Abelian gauge fields n can be odd. However, if n is even, i.e., $n = 2J$, and also $r_{2,2p} = r_{1,2p-1} \equiv r_p'$, $r_{2,2p-1} = -r_{1,2p} \equiv r_p''$, $l_{2,2j} = l_{1,2j-1} \equiv l_j'$, $l_{2,2j-1} = -l_{1,2j} \equiv l_j''$ ($p = 1,2,\ldots,k; j = 1,2,\ldots,J$), then

$$T=\frac{1}{\sqrt{1-\mathcal{N}^2}}\begin{pmatrix}1 & 0 & r'_p & -r''_p & l'_j & -l''_j\\ 0 & 1 & r''_p & r'_p & l''_j & l'_j\end{pmatrix}, \tag{4.12}$$

where $\mathcal{N}^2=n_1^T n_1=n_2^T n_2$. In this special case, vectors n_1 and n_2 have the same length and are mutually orthogonal $(n_1^T n_2=0)$. Therefore, from Eq. (4.12) it immediately follows that the operator T is a real matrix representation of the complex $1\times(k+1+J)$ row $t=|1-\mathcal{N}^2|^{-1/2}(1\ r_p\ l_j)$ where $r_p=r'_p+ir''_p$ and $l_j=l'_j+il''_j$. Notice that in the special case under consideration it is possible to express Eq. (3.22) in a complex form by substituting $\mathcal{M}_\alpha\to m_\alpha$, $\tilde{\mathcal{M}}_\alpha\to\tilde{m}_\alpha$, $T\to t$ and $\Sigma\to\tilde{\sigma}_3$. Thus, in this special case it is possible to keep pure complex notations.

As an example of a concrete class of solutions of the EmM theory one can consider the solution which arises in the framework of the ansatz

$$\tilde{z}=\lambda\tilde{q}, \tag{4.13}$$

where λ is a complex function and $\tilde{q}$ is a $1\times(k+1)$ constant complex row. The corresponding effective system is related to the Lagrangian

$$L_3=2\tilde{\kappa}\frac{|\nabla\lambda|^2}{(1-\tilde{\kappa}|\lambda|^2)}, \tag{4.14}$$

in the case of $\tilde{\kappa}\neq 0$, where

$$\tilde{\kappa}=\tilde{q}\tilde{\sigma}_3\tilde{q}^\dagger. \tag{4.15}$$

When $\tilde{\kappa}=0$ one obtains a decoupled three-dimensional flat space and a harmonic field λ. The parameter $\tilde{\kappa}$ plays the role of a coupling constant between three-dimensional gravity and the complex scalar field λ. We claim that the following concrete choice of the scalar field and the three metric

$$\begin{gathered}\lambda=\frac{1}{R-ia\cos\theta},\\ ds_3^2=\Delta\left(\frac{dR^2}{R^2+a^2-\tilde{\kappa}}+d\theta^2\right)+(R^2+a^2-\tilde{\kappa})\sin^2\theta d\varphi^2,\end{gathered} \tag{4.16}$$

where $\Delta=R^2+a^2\cos^2\theta-\tilde{\kappa}$ and a is a constant, gives a solution of the corresponding equations of motion. Note that in Eq. (4.16) the value of the parameter $\tilde{\kappa}$ is arbitrary. In what follows, this concrete class of solutions will be considered as the typical starting one in the framework of the developed solution-generating scheme.

To start with, we need explicit expressions for the magnitudes $\tilde{m}_\alpha$ and $\tilde{\tilde{\omega}}_\alpha$. For the scalar sector one immediately gets

$$\begin{gathered}\tilde{m}_1=-\left(1+\frac{\tilde{\kappa}}{\Delta}\right),\\ \tilde{m}_2=-\tilde{q}\frac{R+ia\cos\theta}{\Delta},\\ \tilde{m}_3=-\tilde{q}^\dagger\tilde{q}\frac{1}{\Delta},\end{gathered} \tag{4.17}$$

whereas for the vector one, after the corresponding integration, one finds that

$$\tilde{\vec{\omega}}_{1\,\varphi}=-i\frac{a\tilde{\kappa}\sin^2\theta}{\Delta},$$

$$\tilde{\vec{\omega}}_{2\,\varphi}=\tilde{q}\left(-\cos\theta+ia\sin^2\theta\frac{R+ia\cos\theta}{\Delta}\right), \tag{4.18}$$

$$\tilde{\vec{\omega}}_{3\,\varphi}=-i\tilde{q}\dagger\tilde{q}\frac{a\sin^2\theta}{\Delta},$$

and other vector components vanish. These relations define the extension of the solution (4.16) to the realm of the heterotic string theory according to the relations (2.6)–(2.8), (4.5)–(4.7), and (4.11). Let us discuss both, the starting EmM family of solutions and the resulting heterotic string theory fields.

First of all, let us compute the Ernst potentials (3.18) corresponding to the solution (4.16):

$$\mathcal{E}=1-\frac{2(M+iN)}{r+i(N-a\cos\theta)},$$

$$\mathcal{F}_p=\sqrt{2}\,\frac{(e_p+ig_p)}{r+i(N-a\cos\theta)}, \tag{4.19}$$

where

$$\tilde{q}_1=M+iN,\quad \tilde{q}_{1+p}=e_p+ig_p, \tag{4.20}$$

and $r=R+M$ and $\tilde{\kappa}=-M^2-N^2+\Sigma_p(e_p^2+g_p^2)$. It is clear that our starting solution is precisely the Kerr–multi-Newman family of solutions with nontrivial NUT parameter. Thus, (r,θ,φ) stand for conventional oblate spheroidal coordinates, whereas the parameters M, N, e_p and g_p are the mass, NUT, electric and magnetic charges, respectively. Another interesting issue concerns the asymptotical flatness of the resulting multidimensional field configuration in the framework of our solution-generating method in the general case. It turns out that the generating field configurations contain the so-called ''Dirac strings'' and are not asymptotically flat, i.e., they contain a term which is proportional to $\cos\theta$ at spatial infinity $(R\to\infty)$. The same situation takes place for the starting four-dimensional metric of the EmM theory: the corresponding term is proportional to the NUT parameter and it vanishes if $N=0$. Thus, in the starting solution this Dirac string peculiarity is removable. From Eqs. (4.11) and (4.18) it follows that the Dirac string for the metric (i.e., for the magnitude $\vec{V}_1$) is absent if one imposes the restriction

$$\tilde{\mathcal{Q}}_I^T T_{II}=T_I^T\tilde{\mathcal{Q}}_{II} \tag{4.21}$$

on the starting charge configuration and the operator of the symmetry transformation. Here $\tilde{\mathcal{Q}}_I$ and $\tilde{\mathcal{Q}}_{II}$ are, respectively, 2×1 and $2\times(2k+1)$ block components of the charge matrix $\tilde{\mathcal{Q}}=(\tilde{\mathcal{Q}}_I\ \tilde{\mathcal{Q}}_{II})$ which realizes a real matrix representation of the complex charge parameter $\tilde{q}$. Notice that all the relations which involve the matrix $\tilde{\mathcal{Q}}$ can be obtained from the relations for $\tilde{\mathcal{Z}}$ by replacing $z_{\mathcal{P}}\to q_{\mathcal{P}}$ in $\tilde{\mathcal{Z}}$; notice that we have used a decomposition of $\tilde{\mathcal{Q}}$ similar to that of Eqs. (4.1) and (4.2).

It is possible to solve the algebraic restriction (4.21) for the general case. However, for the special case (4.12), when the symmetry operator can be represented in complex form, this can be done in an easy and elegant way. Actually, a simple algebraic analysis shows that in this case Eq. (4.21) leads to $N=0$ and the relations

$$e_p=r'_pM,\quad g_p=r''_pM, \tag{4.22}$$

i.e., to the NUT-less starting solution and to hard relations between the electromagnetic charges and the nonelectromagnetic sector of the symmetry operator T. In this special case, up to construction, the resulting metric is asymptotically flat at spatial infinity. Notice that the resulting matter fields of heterotic string theory also contain Dirac strings. In order to remove them one must impose the corresponding restrictions on the magnitudes $\vec{V}_2$ and $\vec{V}_3$ (to eliminate, in turn, the terms proportional to $\cos\theta$). Here we will not discuss these pure algebraic topics; thus, our final solutions will include, for instance, magnetically charged field configurations.

At the end of this section let us note that our solution-generating procedure, based on Eq. (3.12), maps the full EmM theory into the pure bosonic string theory sector in the case $l_a \equiv 0$. Actually, this last restriction can be imposed independently of our generation scheme. This fact is also reflected in the number of compactified space–time dimensions, which is equal to $2k+1$, where k is precisely the number of starting Maxwell fields. Thus, a surprising fact is that the Abelian gauge field sector of heterotic string theory is not related to the Maxwell sector of the starting EmM theory: all the string theory gauge fields depend only on the structure of the symmetry operator T. Namely, one obtains n Abelian vector fields $U(1)$ if one chooses the parameter l_a of height n.

V. CONCLUSION AND DISCUSSION

The main result of this article is the presentation of a new and explicit scheme of generation of heterotic string theory solutions from stationary fields of the EmM theory. Namely, one can start with an arbitrary stationary solution of Einstein theory coupled to k Maxwell fields and obtain a solution of heterotic string theory with n Abelian gauge fields which lives in $2(k+2)$ dimensions by making use of the procedure developed in this article. It is worth noticing that our symmetry approach is based on pure algebraic calculations only as far as all the potentials of the starting EmM theory have been already computed.

Let us make two remarks concerning the properties of the underlying symmetry map (3.12) [or (4.5)–(4.7) and (4.11) in an equivalent and physically meaningful form]. First of all, it is interesting to notice that for the case $k=3$, the resulting heterotic string theory becomes ten-dimensional. However, the complete theory with $k=3$ (we refer to a theory with arbitrary potential $\tilde{\mathcal{Z}}$ of dimension 2×8, not to the Einstein theory with three Maxwell fields) corresponds to the bosonic sector of $N=4$ supergravity in four dimensions. Thus, when $n=16$, our procedure relates $N=D=4$ and $N=1$, $D=10$ supergravities in a transparent form. Keeping this in mind, it will be interesting to study the problem of supersymmetric, and therefore BPS saturated, solutions in the framework of the established correspondence. Namely, a question that naturally arises is whether or not supersymmetric solutions of the four-dimensional theory map into supersymmetric solutions of the ten-dimensional one. If they do so, how many supersymmetries will preserve under this correspondence? Notice that some classes of four-dimensional supersymmetric solutions have been extensively studied during last several years (see, for instance, Refs. 20 and 19); some special classes of ten-dimensional supersymmetric solutions have also been obtained (see Refs. 21 and 3) and the topic is still under active investigation now.

Our second remark is related to the level of generality of the map (3.12). We consider this issue in the framework of asymptotically flat field configurations in the three-dimensional sense. Namely, we consider that the fields which are encoded in the potential $\mathcal{Z}$ vanish at spatial infinity. In this sense our map (3.12) is complete with respect to the total group of three-dimensional charging symmetries, i.e., to the transformations that preserve the asymptotical triviality of the matrix potential $\mathcal{Z}$. Thus, if in Eq. (3.12) the potential $\tilde{\mathcal{Z}}$ and the symmetry operator T have the most general form, our procedure is nongeneralizable by making use of hidden symmetries that act in the subspace of three-dimensional asymptotically flat field solutions. However, if one starts with the potential $\tilde{\mathcal{Z}}$ and the symmetry operator T given in the matrix representation which corresponds to the complex $\tilde{z}$ and t, one partially loses the charging symmetry self-invariance of the resulting solutions of the heterotic string theory. In fact, one loses the part of the total charging symmetry group of the heterotic string theory which breaks the special (complex) structure of the matrix

potential $\tilde{\mathcal{Z}}$ and the symmetry operator T given by Eqs. (4.2) and (4.12). This lost symmetry sector is evidently nontrivial and can be used for the further generalization of the solutions obtained in the framework of the pure complex generating scheme developed at the end of the previous section.

In this article we have constructed as well the string theory extension of the Kerr–multi-Newman solution of the EmM theory. This extension was presented as some simple and natural application of the developed general formalism. It was also shown how to remove all the Dirac string peculiarities from the resulting multi-dimensional metric field, so that the resulting space-time of the heterotic string theory is asymptotically flat. Note that the constructed family of solutions constitutes the first example of extension of the Kerr-multi-Newman solution to the realm of the heterotic string theory. The obtained class of solutions is really interesting from the point of view of black hole physics and can be studied in detail in a conventional manner.[3,18,19]

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Holography and SL(2,$\mathbb{R}$) symmetry in 2D Rindler space–time

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It is shown that it is possible to define quantum field theory of a massless scalar free field on the Killing horizon of a 2D Rindler space–time. Free quantum field theory on the horizon enjoys diffeomorphism invariance and turns out to be unitarily and algebraically equivalent to the analogous theory of a scalar field propagating inside Rindler space–time, no matter the value of the mass of the field in the bulk. More precisely, there exists a unitary transformation that realizes the bulk-boundary correspondence upon an appropriate choice for Fock representation spaces. Second, the found correspondence is a subcase of an analogous algebraic correspondence described by injective $*$-homomorphisms of the abstract algebras of observables generated by abstract quantum free-field operators. These field operators are smeared with suitable test functions in the bulk and exact one-forms on the horizon. In this sense the correspondence is independent from the chosen vacua. It is proven that, under that correspondence, the ''hidden'' SL(2,$\mathbb{R}$) quantum symmetry found in a previous work gets a clear geometric meaning, it being associated with a group of diffeomorphisms of the horizon itself. © *2004 American Institute of Physics.*
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I. INTRODUCTION

This article deals with some holographic properties of quantum field theory (QFT) in a manifold that admits a (Killing) horizon. The holographic correspondence holds between QFT in the manifold and QFT suitably defined on the horizon itself. It is shown that these holographic properties enjoy a nice interplay with the hidden SL(2,$\mathbb{R}$) symmetry found in Ref. 1.

In the context of the problem of the microscopic origin of black-hole entropy, holographic principle[2–4] arose by the idea that gravity near the horizon should be described by a low dimensional theory with a higher dimensional group of symmetry. On the other hand, in a very famous paper, Brown and Henneaux[5] described the entropy of an asymptotically AdS_3 black hole in terms of diffeomorphisms preserving the space–time structure at spatial infinity. After that, the correspondence between quantum field theories of different dimensions was conjectured by Maldacena in his celebrated work about AdS/Cft correspondence.[6] Using the machinery of string theory, he argued that there is a correspondence between quantum field theory in an asymptotically AdS, $d+1$-dimensional space–time—the ''bulk''—and a conformal theory in a d-dimensional manifold—the (conformal) ''boundary'' at spacelike infinity. Afterwards, Witten[7] described the above correspondence in terms of relations of observables of the two theories. See also Ref. 8 for further details. The correspondence in the two dimensional case was studied in Ref. 9. Results that arose from those works were proven rigorously by Rehren for local quantum fields in an AdS background, establishing the existence of a correspondence between bulk observables and boundary observables (usually called algebraic holography) without employing string technology.[10,11] Finally, Strominger[12] proposed to enlarge the found results by showing that there is an analogous

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correspondence between dS space and a possible conformal field theory on its timelike boundary. In another work,[13] making use of the optical metric, the near horizon limit of a massless theory in Schwarzschild-like space–time has been intepreted as a theory in an asymptotic AdS space–time, giving rise to holographic properties.

A crucial point to explain the holographic correspondence in Rehren's version is that, in AdS_{d+1} space, the conformal group which acts in d dimensions can be realized as the group of the isometries of the AdS_{d+1} bulk. In this way, from a pure geometric point of view, the nature of the bulk-boundary correspondence has a straightforward explanation. This is not the case of manifolds with bifurcate Killing horizon such as Kruskal and Minkowski space–times. In Schwarzschild space–time embedded in Kruskal manifold, the proper boundary relevant to state holographic theorems (dropping the boundary at infinity) seems to be made of the event horizon of the black hole. Obviously a first and intriguing problem is the definition of a quantum field theory on a manifold—as an (event or Killing) horizon—whose metric is degenerate. This problem is considered in this article among other related issues. To approach the general issue in the simplest version, we notice that two-dimensional Rindler space–time embedded in Minkowski space–time approximates the nontrivial part of the space–time structure near a bifurcate horizon as that of a Schwartzschild black hole embedded in Kruskal space–time. The remaining transverse manifold is not so relevant in several interesting quantum effects as Hawking's radiation and it seems that it can be dropped in the simplest approximation. In that context, we have argued in a recent work[1] that free quantum field theory in two-dimensional Rindler space presents a ''hidden'' SL(2,$\mathbb{R}$) symmetry. In other words the theory turns out to be invariant under a unitary representation of SL(2,$\mathbb{R}$) but such a quantum symmetry cannot be induced by the geometric background which enjoys a different group of isometries. SL(2,$\mathbb{R}$) is the group of symmetry of the zero-dimensional conformal field theory in the sense of Ref. 14, so, as for the case of AdS space–time, it suggests the existence of a possible correspondence between quantum field theory in Rindler space and a conformal field theory defined on its (Killing) horizon. In fact, as it is shown within this work, the found hidden symmetry becomes manifest when one examines, after an appropriate definition, quantum field theory on the (Killing) horizon. That theory enjoys diffeomorphism invariance and the SL(2,$\mathbb{R}$) symmetry represents, in the quantum context, the geometric invariance of the theory under a little group of diffeomorphisms of the horizon. (We stress that invariance under isometries makes no sense since the metric is degenerate.) We address in Sec. II technical details concerning the structure of quantum field theory on the horizon that, in a sense, is the limit of the bulk theory toward the horizon. We only say here that, generalizing the symplectic approach valid in the bulk, the theory can be built up by defining a suitable quantum field operator smeared with exact one-forms, which are defined on the horizon, to assure the invariance under diffeomorphisms; moreover the causal propagator (which involves bosonic commutation rules) is naturally defined in spite of the absence, shared with other holographic approaches in other contexts, of any natural evolution equation. The appearance of a manifest quantum SL(2,$\mathbb{R}$) symmetry on the horizon is only a part of the results established in this article. In fact, the manifest SL(2,$\mathbb{R}$) symmetry on the horizon is nothing but a simple result which follows from a holographic boundary-bulk correspondence established in this article for 2D Rindler space–time either in terms of unitary equivalences or in terms of $*$-algebra homomorphisms of free field observables. This operator algebra has a clear geometric interpretation in terms of vector fields defined on the horizon and generating the group of (orientation preserving) diffeomorphisms of the horizon itself. Some overlap with our results could be present in the literature. Guido, Longo, Roberts, and Verch[15] discussed from a general point of view SL(2,$\mathbb{R}$) covariant local QFT defined on a bifurcate Killing horizon and obtained by restriction on the horizon of the net of local (Von Neumann) observables (referred to a Hadamard state with respect to the Killing field) given in the manifold. Along a similar theme, Schroer and Wiesbrock[16] have studied the relationship between QFTs on horizons and QFTs on the ambient space–time. They even use the term ''hidden symmetry'' in a sense similar to we do here and in Ref. 1. In related follow-up works by Schroer[17] and Schroer and Fassarella,[18] the relation to holography and diffeomorphism covariance is also discussed.

This work is organized as follows: the next section is devoted to review and briefly improves

a few results established in Ref. 1, also giving rigorous proofs, concerning hidden $\mathrm{SL}(2,\mathbb{R})$ symmetry for a free quantum scalar field propagating in 2D Rindler space–time. In the third section we present the main achievement of this work: We build up a quantum field theory for a massless scalar field on the horizon which, in a sense, is the limit toward the horizon of the analogous theory developed for a (also massive) field propagating in the bulk. Moreover, we show that any free quantum field theories in the bulk and on the horizon are unitarily and algebraically equivalent (no matter the value of the mass). In other words, there exists a unitary transformation that realizes the bulk-boundary correspondence upon an appropriate choice for Fock representation spaces. In particular, the vacuum expectation values of observables of the free-field theory are invariant under the unitary equivalence. Actually, as we said, the found correspondence is valid in an algebraic sense too, i.e., it is described by injective $*$-homomorphisms of the abstract algebras of observables constructed by products of free-field operators smeared by suitable test functions/one-forms. In this sense the correspondence is independent from the chosen vacua. In the fourth section we show that, as we expected, hidden $\mathrm{SL}(2,\mathbb{R})$ invariance found in Ref. 1 becomes manifast on the horizon. In a forthcoming work[19] we show that the found manifest $\mathrm{SL}(2,\mathbb{R})$ unitary representation defined for the horizon QFT can be extended into a full positive-energy unitary Virasoro algebra representation with nonvanishing central charge which represents the Lie algebra of vector fields on the (compactified) Killing horizon. In the last section we make some remarks and comments on the extension of our result to more complicated space–times containing a bifurcate Killing horizon.

II. HIDDEN $\mathrm{SL}(2,\mathbb{R})$ SYMMETRY NEAR A BIFURCATE KILLING HORIZON

A. Rindler space

In Ref. 1 we have proven that quantum mechanics in a 2D space–time which approximates the space–time near a bifurcate Killing horizon enjoys *hidden* $\mathrm{SL}(2,\mathbb{R})$ invariance. This has been done by using and technically improving some general results on $\mathrm{SL}(2,\mathbb{R})$ invariance in quantum mechanics.[14] Let us review part of the results achieved in Ref. 1 from the point of view of quantum field theory in curved space–time (essentially in the formulation presented in Refs. 20 and 21 but using $*$-algebras instead of C^*-algebras).

Remark: We illustrate the construction of quantum field theory in the considered background in some detail because the general framework will be useful later in developing quantum field theory on a horizon and holography.

Consider a Schwarzschild-like metric

$$-A(r)dt\otimes dt+A^{-1}(r)dr\otimes dr+r^2d\Sigma^2, \tag{1}$$

where Σ denotes angular coordinates. Let $R>0$ denote the radius of the black hole. As the horizon is bifurcate, $A'(R)/2\neq 0$ and we can use the following approximation in the limit $r\to R$,

$$-\kappa^2y^2dt\otimes dt+dy\otimes dy+R^2d\Sigma^2, \tag{2}$$

where $\kappa=A'(R)/2$ and $r=R+A'(R)y^2/4$. Dropping the angular part $R^2d\Sigma$, the metric becomes that of the space–time called *(right) Rindler wedge* $\mathbf{R}$ which is part of Minkowski space–time:

$$g_{\mathbf{R}}:=-\kappa^2y^2dt\otimes dt+dy\otimes dy, \tag{3}$$

with global coordinates $t\in(-\infty,+\infty)$, $y\in(0,+\infty)$. That space–time is static[22] with respect to the timelike Killing vector ∂_t and spacelike surfaces at constant t. Later we shall make use of *Rindler light coordinates* $u,v\in\mathbb{R}$ which cover $\mathbf{R}$ and satisfy

$$u:=t-\frac{\log(\kappa y)}{\kappa}\quad,\quad v:=t+\frac{\log(\kappa y)}{\kappa}\quad,\quad \text{where}\quad t\in\mathbb{R}\ ,y\in(0,+\infty). \tag{4}$$

B. One-particle Hilbert space

As **R** is globally hyperbolic,[22] in particular t-constant surfaces are Cauchy surfaces, quantum field theory can be implemented without difficulties.[21] There is no guarantee for the validity of the approach to quantum field theory for static space–times based on the quadratic form induced by the stress energy tensor presented in Ref. 21 since $-g_{\mathbf{R}}(\partial_t,\partial_t)$ has no positive lower bound. However, we build up quantum field theory of a real scalar field ϕ with mass $m\geqslant 0$ propagating in **R** by following a more direct stationary-mode-decomposition approach. In fact, *a posteriori* it is possible to show that our procedure produces the same quantization as that in Ref. 21. The Klein–Gordon equation reads

$$-\partial_t^2\phi+\kappa^2(y\partial_y y\partial_y-y^2m^2)\phi=0. \tag{5}$$

If $m>0$, $\mathcal{S}$ denotes the vector space of *real wave functions*, i.e., C^∞ real solutions ψ which have Cauchy data with compact support on a Cauchy surface. If $m=0$, (5) reduces to

$$(\partial_t+\kappa y\partial_y)(-\partial_t+\kappa y\partial_y)\phi \quad (=(-\partial_t+\kappa y\partial_y)(\partial_t+\kappa y\partial_y)\phi)=0 \tag{6}$$

and the space of real wave functions we want to consider is defined as $\mathcal{S}:=\mathcal{S}_{\text{out}}+\mathcal{S}_{\text{in}}$ where $\mathcal{S}_{\text{out}}$ and $\mathcal{S}_{\text{in}}$ are, respectively, the space of real C^∞ solutions of $(\partial_t+\kappa y\partial_y)\psi=0$ and $(-\partial_t+\kappa y\partial_y)\psi=0$ with compactly supported Cauchy data. The compactness requirement does not depend on the Cauchy surface.[21] There are solutions of (5) with $m=0$ which do not belong to $\mathcal{S}$ in spite of having compactly supported Cauchy data. [*With the notation used in (7), it is sufficient to fix compact-support Cauchy data* $\psi, n^\mu\partial_\mu\psi$ *on a* t*-constant Cauchy surface* Λ *such that* $\int_\Lambda \partial_\mu\psi\, n^\mu d\sigma\neq 0$.] Define in $\mathcal{S}\times\mathcal{S}$ the following *symplectic form*,[21] which does not depend on the used spacelike Cauchy surface Λ with induced measure $d\sigma$ and unit normal vector n pointing toward the future:

$$\Omega(\psi,\psi'):=\int_\Lambda(\psi'\nabla^\mu\psi-\psi\nabla^\mu\psi')n_\mu\, d\sigma. \tag{7}$$

The definition is well-behaved for a pair of complex-valued wave functions, too, and also if one of these has no compactly supported Cauchy data. Equipped with these tools we can define the one-particle Hilbert space $\mathcal{H}$ associated with the Killing field ∂_t. To this end, consider the two classes of $C^\infty(\mathbf{R};\mathbb{C})$, ∂_t-stationary solutions of (5) where K_a is the usual Bessel–McDonald function:

$$\Phi_E(t,y):=\sqrt{\frac{2E\sinh(\pi E/\kappa)}{\pi^2\kappa}}K_{iE/\kappa}(my)\frac{e^{-iEt}}{\sqrt{2E}} \quad \text{with } E\in\mathbb{R}^+, \qquad \text{if } m>0, \tag{8}$$

$$\Phi_E^{\text{(in)}\atop\text{(out)}}(t,y):=\frac{e^{-iE(t\pm\kappa^{-1}\ln(\kappa y))}}{\sqrt{4\pi E}} \quad \text{with } E\in\mathbb{R}^+, \qquad \text{if } m=0, \tag{9}$$

where $\mathbb{R}^+:=[0,+\infty)$. Modes $\Phi_E^{(\text{in})}$ are associated with particles crossing the future horizon at $t\to+\infty$, modes $\Phi_E^{(\text{out})}$ are associated with particles crossing the past horizon at $t\to-\infty$.

We have a pair of propositions whose proof is straightforward by using properties of K_{ia}, Fourier transform and Lebedev transform.[23]

Proposition 2.1 (completeness of modes): If $m>0$ *and* $\psi\in\mathcal{S}$, *the function on* $\mathbb{R}^+$,

$$E\mapsto\tilde{\psi}_+(E):=-i\Omega(\overline{\Phi_E},\psi), \tag{10}$$

satisfies $\tilde{\psi}_+(E)=\sqrt{E}g(E)$, *and* $\overline{\tilde{\psi}_+(E)}=-\sqrt{E}g(-E)$, *for some* $g\in\mathsf{S}(\mathbb{R};\mathbb{C})$ *(space of complex-valuated Schwartz' functions on the whole* $\mathbb{R}$*). Moreover,*

$$\psi(t,y)=\int_0^{+\infty}\Phi_E(t,y)\tilde{\psi}_+(E)\,dE+\int_0^{+\infty}\overline{\Phi_E(t,y)\tilde{\psi}_+(E)}\,dE \qquad \text{for } (t,y)\in\mathbb{R}\times(0,+\infty). \tag{11}$$

If $m=0$ *and* $\psi\in\mathcal{S}$, *the functions on* $\mathbb{R}^+$ *with* $\alpha=in,\ out$,

$$E\mapsto\tilde{\psi}_+^{(\alpha)}(E):=-i\Omega(\overline{\Phi_E^{(\alpha)}},\psi), \tag{12}$$

satisfy $\tilde{\psi}_+^{(\alpha)}(E)=\sqrt{E}g^{(\alpha)}(E)$, $\overline{\tilde{\psi}_+^{(\alpha)}(E)}=\sqrt{E}g^{(\alpha)}(-E)$, *where* $g^{(\alpha)}\in\mathsf{S}(\mathbb{R};\mathbb{C})$. *Moreover, for* $(t,y)\in\mathbb{R}\times(0,+\infty)$

$$\psi(t,y)=\int_0^{+\infty}\sum_\alpha\Phi_E^{(\alpha)}(t,y)\tilde{\psi}_+^{(\alpha)}(E)\,dE+\int_0^{+\infty}\sum_\alpha\overline{\Phi_E^{(\alpha)}(t,y)\tilde{\psi}_+^{(\alpha)}(E)}\,dE. \tag{13}$$

Proposition 2.2 (associated Hilbert spaces): If $\psi\in\mathcal{S}$, *define the one-to-one associated positive-frequency wave function for* $m>0$ *and* $m=0$, *respectively, as*

$$\psi_+(t,y):=\int_0^{+\infty}\Phi_E(t,y)\tilde{\psi}_+(E)\,dE\ ,\ \psi_+(t,y):=\int_0^{+\infty}\sum_\alpha\Phi_E^{(\alpha)}(t,y)\tilde{\psi}_+^{(\alpha)}(E)\,dE. \tag{14}$$

With that definition, for $\psi_1,\psi_2\in\mathcal{S}$ *it results that* $\Omega(\psi_{1+},\psi_{2+})=0$, *whereas*

$$\langle\psi_{1+},\psi_{2+}\rangle:=-i\Omega(\overline{\psi_{1+}},\psi_{2+}) \tag{15}$$

is well-defined (at least on t-constant surfaces). Notice that, at least for $m=0$, *positive/negative frequency wave functions cannot have Cauchy data with compact support due to known analiticity properties of Fourier transform. Moreover, for* $m>0$ *and* $m=0$, *respectively,*

$$\langle\psi_{1+},\psi_{2+}\rangle=\int_0^{+\infty}\overline{\tilde{\psi}_{1+}(E)}\tilde{\psi}_{2+}(E)\,dE\ ,\ \langle\psi_{1+},\psi_{2+}\rangle=\int_0^{+\infty}\sum_\alpha\overline{\tilde{\psi}_{1+}^{(\alpha)}(E)}\tilde{\psi}_{2+}^{(\alpha)}(E)\,dE. \tag{16}$$

The one-particle Hilbert *space* $\mathcal{H}$ *is defined as the Hilbert completion of the space of finite complex linear combinations of functions* ψ_+, $\psi\in\mathcal{S}$, *equipped with the extension of the scalar product (15) to complex linear combinations of arguments. It results that* $\mathcal{H}\cong L^2(\mathbb{R}^+,dE)$ *if* $m>0$ *or, if* $m=0$, $\mathcal{H}\cong\mathcal{H}_{(\mathrm{in})}\oplus\mathcal{H}_{(\mathrm{out})}$ *with* $\mathcal{H}_{(\alpha)}\cong L^2(\mathbb{R}^+,dE)$, $\alpha=in,out$.

C. Quantum field operators: Symplectic approach

As usual, the whole quantum field is represented in the symmetrized Fock space $\mathfrak{F}(\mathcal{H})$—that is $\cong\mathfrak{F}(\mathcal{H}_{(\mathrm{in})})\otimes\mathfrak{F}(\mathcal{H}_{(\mathrm{out})})$ in the massless case—and referred to a vacuum state $\Psi_{\mathbf{R}}$—namely, $\Psi_{\mathbf{R}}^{(\mathrm{in})}\otimes\Psi_{\mathbf{R}}^{(\mathrm{out})}$ in the massless case—called the *Rindler vacuum state*. $\Psi_{\mathbf{R}}$ does not belong to the Hilbert space of Minkowski particles in the sense that quantum field theory in Rindler space and the Minkowski one are not unitarily equivalent.[21] The *quantum field* $\Omega(\ \cdot\ ,\hat{\phi})$ associated with the real scalar field ϕ in (5) is the linear map[21]

$$\mathcal{S}\ni\psi\mapsto\Omega(\psi,\hat{\phi}):=ia(\overline{\psi_+})-ia^\dagger(\psi_+), \tag{17}$$

where $\psi\in\mathcal{S}$ and $a(\overline{\psi_+})$ and $a^\dagger(\psi_+)$, respectively, denote the annihilation [the conjugation being used just to the get a linear map $\psi_+\mapsto a(\overline{\psi_+})$] and construction operators associated with the one-particle state ψ_+. The right-hand side of (17) is an essentially self-adjoint operator defined in the dense invariant subspace $\mathfrak{F}_0\subset\mathfrak{F}(\mathcal{H})$ spanned by all states containing a finite arbitrarily large number of particles with states given by positive-frequency wave functions. Equation (17) is formally equivalent via (11) to the nonrigorous but popular definition

$$\hat{\phi}(x)\text{“}=\text{”}\int_0^{+\infty}\Phi_E(x)a_E+\overline{\Phi_E(x)}a_E^\dagger\,dE. \tag{18}$$

The given procedure can be generalized to any Klein–Gordon scalar field propagating in a (not necessarily static) globally hyperbolic space–time provided a suitable vacuum state is given.[21] Let $\mathcal{D}(\mathbf{R})$ denote the space of real compactly supported smooth functions in $\mathbf{R}$, in the massless case these functions being also assumed to have zero integral on the Rindler space, and $J(A)$ the union of the *causal past* and *causal future* of a set $A\subset\mathbf{R}$. As $\mathbf{R}$ is globally hyperbolic, there is a uniquely determined *causal propagator* $E:\mathcal{D}(\mathbf{R})\to\mathcal{S}$ of the Klein–Gordon operator K of the field ϕ.[21] E enjoys the following properties. It is linear and surjective, $\mathrm{supp}(Ef)\subset J(\mathrm{supp}f)$, $Ef=0$ only if $f=Kg$ for some $g\in\mathcal{D}(\mathbf{R})$ and E satisfies for all $\psi\in\mathcal{S}$, $f,h\in\mathcal{D}(\mathbf{R})$,

$$\int_{\mathbf{R}}\psi f\,d\mu_g=\Omega(Ef,\psi)\quad\text{and}\quad\int_{\mathbf{R}}h(x)(Ef)(x)\,d\mu_g(x)=\Omega(Ef,Eh), \tag{19}$$

μ_g being the measure induced by the metric in $\mathbf{R}$. Equation (19) suggests to define[21] a quantum-field operator *smeared with functions* f of $\mathcal{D}(\mathbf{R})$ as the linear map

$$f\mapsto\hat{\phi}(f):=\Omega(Ef,\hat{\phi}). \tag{20}$$

It is possible to smear the field operator by means of compactly supported complex-valued functions, whose space will be denoted by $\mathcal{D}(\mathbf{R};\mathbb{C})$, simply by defining $\hat{\phi}(f+ih):=\hat{\phi}(f)+i\hat{\phi}(h)$ when $f,h\in\mathcal{D}(\mathbf{R})$. Equation (20) entails[21]

$$[\hat{\phi}(f),\hat{\phi}(h)]=-iE(f,h):=-i\int_{\mathbf{R}}h(x)(Ef)(x)\,d\mu_g(x), \tag{21}$$

that is the rigorous version of the formal identity $[\hat{\phi}(x),\hat{\phi}(x')]=-iE(x,x')$. As a further result[21] $[\hat{\phi}(f),\hat{\phi}(g)]=0$ if the supports of f and g are *spatially separated*, that is, $\mathrm{supp}f\not\subset J(\mathrm{supp}g)$ [which is equivalent to $\mathrm{supp}g\not\subset J(\mathrm{supp}f)$].

All that we said holds for $m\geqslant 0$. Let us specialize to the massless case giving further details. In Rindler light coordinates (4) the decomposition $\mathcal{S}=\mathcal{S}_{\mathrm{in}}+\mathcal{S}_{\mathrm{out}}$ (see Sec. II B) reads, if $\psi\in\mathcal{S}$, $\psi(u,v)=\psi(v)+\psi'(u)$ where $\psi\in\mathcal{S}_{\mathrm{in}}$ and $\psi'\in\mathcal{S}_{\mathrm{out}}$ are compactly supported. Trivial consequences are that ψ vanishes on the past horizon $v\to-\infty$, and ψ' vanishes on the future horizon $u\to+\infty$ (see Sec. III A) and $\Omega(\psi,\psi')=0$. In the considered case

$$E=E_{\mathrm{in}}+E_{\mathrm{out}}, \tag{22}$$

where, in terms of bi-distributions interpreted as in (21),

$$E_{\mathrm{in}}((u',v'),(u,v))=\tfrac{1}{4}\,\mathrm{sign}(v-v')\quad\text{whereas}\quad E_{\mathrm{out}}((u',v'),(u,v))=\tfrac{1}{4}\,\mathrm{sign}(u-u'). \tag{23}$$

The maps $f\mapsto E_{\mathrm{in/out}}f$ from $\mathcal{D}(\mathbf{R})$ to, respectively, $\mathcal{S}_{\mathrm{in/out}}$ are surjective and $E_{\mathrm{in/out}}f=0$ if and only if, respectively, $\gamma f=\partial_u g$ or $\gamma f=\partial_v g$ for some compactly-supported function g and $\gamma\,du\,dv=d\mu_g$.

In the Fock space associated with Rindler vacuum $\Psi_{\mathbf{R}}$, we have the natural decomposition

$$\hat{\phi}(f)=\hat{\phi}_{\mathrm{in}}(f)+\hat{\phi}_{\mathrm{out}}(f)\quad\text{with}\quad\hat{\phi}_{\mathrm{in/out}}(f):=\Omega(E_{\mathrm{in/out}}f,\hat{\phi}) \tag{24}$$

and the two kinds of field operators commute, i.e., $[\hat{\phi}_{\mathrm{in}}(f),\hat{\phi}_{\mathrm{out}}(g)]=i\Omega(E_{\mathrm{in}}f,E_{\mathrm{out}}g)=0$.

D. SL(2,$\mathbb{R}$) symmetry

If $m>0$ and thus $\mathcal{H}\cong L^2(\mathbb{R}^+,dE)$, the *one-particle (Rindler) Hamiltonian* H is the self-adjoint operator

$$(Hf)(E) := Ef(E) \quad \text{with domain} \quad \mathcal{D}(H) = \left\{ f \in L^2(\mathbb{R}^+, dE) \;\middle|\; \int_0^{+\infty} E^2 |f(E)|^2 dE < +\infty \right\}. \tag{25}$$

If $m=0$ and thus $\mathcal{H} \cong L^2(\mathbb{R}^+, dE) \oplus L^2(\mathbb{R}^+, dE) \cong \mathbb{C}^2 \otimes L^2(\mathbb{R}^+, dE)$, the Hamiltonian H reads $I \otimes H'$, H' being the operator defined on the right-hand side of (25) referred to $L^2(\mathbb{R}^+, dE)$ and *the identity operator I being referred to* $\mathbb{C}^2$.

In Ref. 1 it was argued that the one-particle system enjoys invariance under a unitary representation of $\mathrm{SL}(2,\mathbb{R})$ as a consequence of the form of the spectrum of H which is $\sigma(H) = [0, +\infty)$ with no degeneracy for $m \neq 0$ and double degeneracy if $m=0$. Let us state and prove rigorously some of the statements of Ref. 1 in a form which is relevant for the remaining part of this work. First of all, one has to fix a real constant $\beta > 0$,[1] with the physical dimensions $energy^{-1}$, that is necessary for dimensional reasons in defining the relevant domain of operators as it will be clear from the proof of Theorem 2.1. *We assume to use the same value of β throughout this work*. Fix reals $k, m > 0$ and define the dense subspace $\mathcal{D}_k \subset \mathcal{H} \cong L^2(\mathbb{R}^+, dE)$ spanned by vectors:

$$Z_n^{(k)}(E) := \sqrt{\frac{\Gamma(n-k+1)}{E\,\Gamma(n+k)}}\, e^{-\beta E} (2\beta E)^k \mathsf{L}_{n-k}^{(2k-1)}(2\beta E), \qquad n = k, k+1, \ldots, \tag{26}$$

where $\mathsf{L}_p^{(\alpha)}$ are modified Laguerre's polynomials.[24] Notice that $\mathcal{D}_k \subset \mathcal{D}(H)$. Moreover, $\mathcal{D}_k$ is invariant under the linearly independent symmetric operators defined on $\mathcal{D}_k$:

$$H_0 := H \restriction_{\mathcal{D}_k}, \qquad D := -i\left(\frac{1}{2} + E\frac{d}{dE}\right), \qquad C := -\frac{d}{dE} E \frac{d}{dE} + \frac{(k-\frac{1}{2})^2}{E}, \tag{27}$$

which enjoy the commutation relations of the Lie algebra of $\mathrm{SL}(2,\mathbb{R})$, $\mathrm{sl}(2,\mathbb{R})$,

$$[iH_0, iD] = -iH_0, \quad [iC, iD] = iC, \quad [iH_0, iC] = -2iD. \tag{28}$$

iH_0, iC, iD are operatorial realizations of the basis elements of $\mathrm{sl}(2,\mathbb{R})$

$$h = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad c = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}, \quad d = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{29}$$

As a consequence, one expects that operators in (27) generate a strongly continuous unitary representation of $\mathrm{SL}(2,\mathbb{R})$. A complete treatment of the representations of $\mathrm{SL}(2,\mathbb{R})$ can be found in Ref. 25–27. Let $\mathcal{L}$ indicate the space of finite real linear combinations of operators in (27), let $\rho: \mathrm{sl}(2,\mathbb{R}) \to i\mathcal{L}$ be the unique Lie algebra isomorphism with $\rho(h) = iH_0$, $\rho(c) = iC$, $\rho(d) = iD$, and let $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ denote the universal covering of $\mathrm{SL}(2,\mathbb{R})$.

Theorem 2.1: *The operators of $\mathcal{L}$ are essentially self-adjoint, $\overline{H_0} = H$ in particular, and we have the following.*

(a) $\mathcal{H}$ is irreducible under the unique unitary strongly continuous representation of $\widetilde{\mathrm{SL}}(2,\mathbb{R})$, $g \mapsto U_g : \mathcal{H} \to \mathcal{H}$ such that $U(\exp(tx)) = e^{it\overline{\rho(x)}}$ for all $x \in sl(2,\mathbb{R})$, $t \in \mathbb{R}$. If (and only if) $k \in \{\frac{1}{2}, 1, \frac{3}{2}, \ldots\}$, U is a representation of $\mathrm{SL}(2,\mathbb{R})$ and it is faithful only if $k = 1/2$. U does not depend on $\beta > 0$.

(b) $\{U_g\}_{g \in \widetilde{\mathrm{SL}}(2,\mathbb{R})}$ is a group of symmetries *of the quantum system, that is, for every $t \in \mathbb{R}$ and $g \in \widetilde{\mathrm{SL}}(2,\mathbb{R})$, there is $g(t) \in \widetilde{\mathrm{SL}}(2,\mathbb{R})$ such that*

$$e^{itH}\, U_g\, A\, U_g^\dagger\, e^{-itH} = U_{g(t)}\, e^{itH}\, A\, e^{-itH}\, U_{g(t)}^\dagger, \tag{30}$$

for every observable (i.e., self-adjoint operator) A. If $g = \exp(uh + vc + wd)$, with $u, v, w \in \mathbb{R}$,

$$g(t)=\exp((u+tw+t^2v)h+(w+2tv)d+vc). \tag{31}$$

(c) For every $t\in\mathbb{R}$, consider the linearly independent elements of $\mathcal{L}$

$$H_0(t):=H_0,\quad D(t):=D+tH,\qquad C(t):=C+2tD+t^2H. \tag{32}$$

The time-dependent observables generated by those operators are constants of motion, i.e.,

$$e^{itH}\,\overline{uH_0(t)+vC(t)+wD(t)}\;e^{-itH}=\overline{uH_0+vC+wD}\,,\quad \text{for every}\quad t,u,v,w\in\mathbb{R}. \tag{33}$$

Proof: (a) $\{Z_n^{(k)}\}_{n=k,k+1,\ldots}$ (26) is a Hilbert base of eigenvectors of the operator $K=\frac{1}{2}(\beta H_0+\beta^{-1}C)$.[1] Moreover, $X=\beta^2H_0^2+\beta^{-2}C^2+2D^2$ is essentially self-adjoint in $\mathcal{D}_k$ because $\{Z_n^{(k)}\}_{n=k,k+1,\ldots}$ are analytic vectors for X since $X=4K^2+cI$ from (28) where $c\in\mathbb{R}$. Since X is essentially self-adjoint, general results due to Nelson (Theorem 5.2, Corollary 9.1, Lemma 9.1 and Lemma 5.1 in Ref. 28) imply that the operators in $i\mathcal{L}$ are essentially self-adjoint on $\mathcal{D}_k$, moreover, they imply the existence and uniqueness of a unitary representation on $\mathcal{H}$ of the unique simply connected group with Lie algebra given by the space generated by $\beta h,\beta^{-1}c,2d$ [that is $\widetilde{\mathrm{SL}}(2,\mathbb{R})$] such that $d/dt\,|_{t=0}U(\exp(tx))=i\overline{\rho(x)}$ for all $x\in\mathrm{sl}(2,\mathbb{R})$. The derivative on the left-hand side is evaluated in the strong operator topology sense on a suitable subspace G (Gårding space[28]) and gives a restriction of the Stone generator of the strongly continuous unitary one-parameter subgroup $\mathbb{R}\ni t\mapsto U(\exp(tx))$. As G contains a dense set of analytical vectors for the elements of $\mathcal{L}$,[28] $-i\,d/dt\,|_{t=0}U(\exp(tx))$ is essentially self-adjoint and thus its closure coincides with the usual Stone generator and $U(\exp(tx))=e^{it\overline{\rho(x)}}$. As $\mathcal{D}_k\subset\mathcal{D}(H)$, the unique self-adjoint extension of H_0, $\overline{H_0}$ must coincide with H itself. Suppose that P is the orthogonal projector onto an invariant subspace for each U_g. P must commute with e^{itK} in particular. Using Stone′s theorem and the fact that the spectrum of K is not degenerate, one has that (in strong operator topology sense) $P=\Sigma_{i\in M}Z_n^{(k)}\langle Z_n^{(k)},\cdot\,\rangle$ where $M\subset\mathbb{N}$. Similarly, P must commute with every element of $\mathcal{L}+i\mathcal{L}$, $A_\pm:=\mp iD+\frac{1}{2}(\beta H_0-\beta^{-1}C)$ in particular. Using the fact that, for every $m,n\in\mathbb{N}$ with $m>0$, $Z_{n+1}^{(k)}=c_nA_+Z_n^{(k)}$ and $Z_{m-1}^{(k)}=c_mA_-Z_m^{(k)}$ for some reals $c_n,c_m>0$,[1] one proves that $M=\mathbb{N}$, that is $P=I$ and so the representation is irreducible. The proof of the fact that the representation of $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ reduces to a representation of $\mathrm{SL}(2,\mathbb{R})$ iff $k\in\{\frac{1}{2},1,\frac{3}{2},\ldots\}$ and that the representation is faithful only for $k=\frac{1}{2}$ is based on the representation of the subgroup $\{\exp t(h+c)\}_{t\in\mathbb{R}}\subset\widetilde{\mathrm{SL}}(2,\mathbb{R})$, which is isomorphic to SO(2) and is responsible for the fact that $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ is multiply connected. The proof has been sketched in Sec. 6.2 and footnote 4 in Ref. 1. The self-adjoint extensions of the elements in $\mathcal{L}$ do not depend on the value of $\beta>0$ — and thus it happens for the representation U itself since every $g\in\widetilde{\mathrm{SL}}(2,\mathbb{R})$ is the finite product of elements of some one-parameter subgroups because, if $\beta'\neq\beta$, there is a subspace $\mathcal{D}$ containing, with obvious notation, both $\mathcal{D}_k^{(\beta)}$ and $\mathcal{D}_k^{(\beta')}$ where each element of $\mathcal{L}$ (which is essentially self-adjoint on both $\mathcal{D}_k^{(\beta)}$ and $\mathcal{D}_k^{(\beta')}$) determines the same symmetric extension no matter if one starts with $\mathcal{D}_k^{(\beta)}$ or $\mathcal{D}_k^{(\beta')}$. That extension is essentially self-adjoint since $\mathcal{D}_k^{(\beta)}$ is a dense set of analytic vectors in $\mathcal{D}$. To prove (b) and (c) notice that $e^{itH}=U(\exp(th))$. So, if $g\in\widetilde{\mathrm{SL}}(2,\mathbb{R})$, $g(t):=\exp(th)g(\exp(th))^{-1}$ fulfills (30) by application of the representation U. Define $h(t):=\rho^{-1}(H_0(t))$, $c(t):=\rho^{-1}(C(t))$, $d(t):=\rho^{-1}(D(t))$. These matrices satisfy the commutation rules (28) for every t. Using (28) and uniqueness theorems for matrix-valued differential equations one gets, for $s,t,u,v,w\in\mathbb{R}$,

$$\exp\{th\}\exp\{s(uh(t)+vc(t)+wd(t))\}(\exp\{th\})^{-1}=\exp\{s(uh+vc+wd)\},$$

which is (31) if $s=1$. Applying U on both sides one gets $\exp(itH)\exp[is\,\overline{uH_0(t)+vC(t)+wD(t)}\,\exp(-itH)=\exp(is\,\overline{uH_0+vC+wD})$, which is equivalent to $\exp[is\exp\{itH\}uH_0(t)+vC(t)+wD(t)\exp\{-itH\}]=\exp(is\,uH_0+vC+wD)$. Stone's theorem entails (33) by strongly differentiating both sides in s. □

The generalization to the case $m=0$ is trivial: The theorem holds true separately in each space $L^2(\mathbb{R}^+,dE)$ of $\mathcal{H}\cong L^2(\mathbb{R}^+,dE)\oplus L^2(\mathbb{R}^+,dE)$.

Remarks: (1) From now on we assume to work in the *Heisenberg representation*. Within this picture, by (33), H, $\overline{C}$, $\overline{D}$ coincide with the Heisenberg evolution of, respectively, $\overline{H_0(t)}$, $\overline{C(t)}$, $\overline{D(t)}$ at time t. Moreover, in this picture, $e^{-i\tau H}\psi_+$ must not be seen as the time evolution (at time τ) of the state ψ_+ (given at time 0), but it must be considered as a different state altogether. This turns out to be in accordance with the relationship between states and wave functions (see Sec. II E): ψ and $\alpha_{-\tau}^{(\partial_t)}(\psi)$ are two different wave functions. This point of view will be useful shortly in a context where time evolution makes no sense at all.

(2) The found $\mathrm{SL}(2,\mathbb{R})$ symmetry is only due to the shape of the spectrum of $\sigma(H)$ which is $[0,+\infty)$. The absence of degeneracy implies that the representation is irreducible. From a physical point of view, invariance under the conformal group $\mathrm{SL}(2,\mathbb{R})$ could look very unexpected if $m>0$ since the theory admits the scale m. However, that scale does not affect the spectrum of H. In physical terms this is due to the gravitational energy which is encompassed by H itself since the Rindler frame represents the space–time experienced by an accelerated observer.

(3) It is clear that the found $\mathrm{SL}(2,\mathbb{R})$ symmetry can straightforwardly be extended to the free-field quantization by defining multi-particle operators generated by H,C,D.

(4) Generators iH_0, iD, *differently* from iH_0 and iC, define a basis of the Lie algebra of a subgroup of $\mathrm{SL}(2,\mathbb{R})$, $\mathrm{SL}_+^{\triangle}(2,\mathbb{R})$, made of real 2×2 upper triangular matrices with unitary determinant and positive trace. Equation (30) holds for U_g, $g\in \mathrm{SL}_+^{\triangle}(2,\mathbb{R})$, giving rise to another smaller symmetry of the system. The subgroup generated by iH_0 trivially enjoys the same fact.

E. Hidden and manifest symmetries

A differentiable group of *geometric* symmetries of a classical Klein–Gordon field in $\mathbf{R}$ (however, everything we say can be extended to any globally hyperbolic space–time along the procedures presented in Ref. 21) is defined as follows. Take a differentiable, locally bijective, representation, $G\ni g\mapsto d_g$, of a connected Lie group, G, where $d_g:\mathbf{R}\to\mathbf{R}$ are isometries. The representation automatically induces a group of transformations $\{\alpha_g\}_{g\in G}$ of scalar fields $f:\mathbf{R}\to\mathbb{R}$ (or $\mathbb{C}$), with $(\alpha_g(f))(x):=f(d_{g^{-1}}(x))$. As d_g are (orientation-preserving) isometries, α_g define *geometric symmetries* of the field in the sense that they transform elements of $\mathcal{S}$ into elements of $\mathcal{S}$ not affecting the symplectic form. If quantization is implemented, solutions of the equation of motion in $\mathcal{S}$ are associated with one-particle quantum states through the decompositions (11) and (13). Consider a group of quantum symmetries in the sense of (30), described by a strongly continuous representation of a Lie group G in terms of unitary operators $\{U_g\}_{g\in G}$. In this picture, the one-parameter unitary group generated by the Hamiltonian is assumed to be a subgroup of $\{U_g\}_{g\in G}$. If the symmetry "does not depend on time," i.e., $g(t)=g$ in (30), that assumption can be dropped or, equivalently, the subgroup generated by the Hamiltonian can be considered in the center of $\{U_g\}_{g\in G}$ (i.e., it commutes with the other elements of the group). If $\{U_g\}_{g\in G}$ is related, by means of (11), (13), and (14), to a group of geometric symmetries $\{\alpha_g\}_{g\in G}$, that is $\widetilde{(\alpha_g(\psi))}_+ = U_g\tilde{\psi}_+$ for all $g\in G$ and $\psi\in\mathcal{S}$, we say that the symmetry is *manifest*. Otherwise we say that the symmetry is *hidden*. In Rindler space, the quantum symmetry group $\{e^{i\tau H}\}_{\tau\in\mathbb{R}}$ gives rise to manifest symmetry because it is associated with the geometric group of symmetries $\{\alpha_\tau\}_{\tau\in\mathbb{R}}$, induced by the one-parameter group of isometries generated by the Killing vector ∂_t. The situation changes dramatically if considering the whole $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ symmetry. The space of Killing fields of $\mathbf{R}$ has a basis $\partial_t,\partial_X,\partial_T$ with $\{\partial_T,\partial_X\}=0$, $\{\partial_T,\partial_t\}=\partial_X$ and $\{\partial_X,\partial_t\}=\partial_T$. ($X$ and T are the spatial and temporal coordinates of a Minkowski frame with $\partial_t=X\partial_T+T\partial_X$.) It is trivially proven that no Killing field $a\partial_t+b\partial_X+c\partial_T$ enjoys, with respect to ∂_t, the commutation rule that D enjoys with respect to H_0 in (28) so that no Killing field corresponding to C makes sense. Summarizing, $\mathbf{R}$ cannot support isometry representations of $\mathrm{SL}(2,\mathbb{R})$ [or $\widetilde{\mathrm{SL}}(2,\mathbb{R})$] or the subgroup $\mathrm{SL}_+^{\triangle}(2,\mathbb{R})$ generated by H_0,D. Hence the whole $\mathrm{SL}(2,\mathbb{R})$ symmetry and that associated with D are *hidden*.

III. CONFORMAL FIELD ON THE HORIZON

A. Restriction to horizons

In Ref. 1, a similar analysis is performed for $\mathbf{AdS}_2$ space–time since the spectrum of the Hamiltonian of a particle has the same structure as that in Rindler space. However, as a remarkable difference, SL(2,$\mathbb{R}$) is a *manifest* symmetry of a quantum particle moving in $\mathbf{AdS}_2$ because SL(2,$\mathbb{R}$) admits a representation in terms of $\mathbf{AdS}_2$ isometries.

Coming back to Rindler space viewed as a (open) submanifold of Minkowski space–time, a natural question arises: "*Regardless the found* SL(2,$\mathbb{R}$) *symmetry is hidden, does it become manifest if one considers quantum field theory in an appropriate subregion of* $\mathbf{R}\cup\partial\mathbf{R}$?"

We shall see that investigation on this natural question has several implications with holography because it naturally leads to the formulation of a quantum field theory on the horizon which is algebraically and unitarily related with that formulated in the bulk, but also it suggests that the symmetry of the theory is greater than SL(2,$\mathbb{R}$), it being described by a *Virasoro algebra*. It is clear from Sec. II E that the only region which could give a positive answer to the question is the boundary $\partial\mathbf{R}$ of the Rindler wedge, i.e., a *bifurcate Killing horizon* made of three disjoint parts $\mathbf{F}\cup\mathbf{P}\cup\mathbf{S}$. **S** (a point in our 2D case) is the spacelike submanifold of Minkowski space–time where the limit of the Killing field ∂_t vanishes whereas the lightlike submanifold of Minkowski space–time **F** and **P** (the former in the causal future of the latter) are the *future* and the *past* horizons, respectively, where the limit of ∂_t becomes lightlike but does *not* vanish. Since the induced metric on $\mathbf{F}\cup\mathbf{P}$ is degenerate, the diffeomorphisms of $\mathbf{F}\cup\mathbf{P}$ can be viewed as isometries and the question about a possible *manifest* SL(2,$\mathbb{R}$) symmetry on the horizon must be interpreted in that sense: The unitary representation has to be associated with a group of diffeomorphisms induced by a Lie algebra of vector fields defined on the horizon.

To go on, let us investigate the limit of wave functions when the horizon is approached by Rindler-time evolution. To this end, consider the Rindler light coordinates (4). **F** is represented by $u\to+\infty$, $v\in\mathbb{R}$, whereas **P** is given by $v\to-\infty$, $u\in\mathbb{R}$. Coordinates u,v actually cover the Rindler space only, but, separately, the limit of v is well defined on the lightlike submanifold **F** and the limit of u is well defined on the submanifold **P** and they define well-behaved global coordinate frames on these submanifolds. [*It holds in the* 2D *case. For greater dimension,* v (*resp.,* u) *together with other "transverse" coordinates defines global coordinates on* **F** (*resp.,* **P**) *as well.*] This can be proven by passing to Minkowski light coordinates $U:=T-X, V:=T+X$ which satisfy $V=e^{\kappa v}$, $U=e^{-\kappa u}$ in **R**. So, from now v and u are also interpreted as coordinates on **F** and **P**, respectively. We have the following remarkable technical result (where, if $a\in\mathbb{C}$, "$a+$c.c." means "a $+complex\ conjugation\ of\ a$").

Proposition 3.1: Take $\psi\in\mathcal{S}$, *with associated (Rindler) positive frequency parts* $\tilde{\psi}_+$ *or* $\tilde{\psi}_+^{(\alpha)}$ *as in (11) and (13) and consider the evolution of* ψ *in the whole Minkowski space–time. In coordinate* $v\in\mathbb{R}$, *the restriction of* ψ *to* **F** *reads, respectively, for* $m>0$ *and* $m=0$,

$$\psi(v)=\int_{\mathbb{R}^+}\frac{e^{-iEv}}{\sqrt{4\pi E}}N_{m,\kappa}(E)\,\tilde{\psi}_+(E)\;dE+\text{c.c.},\quad \psi(v)=\int_{\mathbb{R}^+}\frac{e^{-iEv}}{\sqrt{4\pi E}}\,\tilde{\psi}_+^{(\text{in})}(E)\;dE+\text{c.c.}\tag{34}$$

In coordinate $u\in\mathbb{R}$, *the restriction of* ψ *to* **P** *reads, respectively, for* $m>0$ *and* $m=0$,

$$\psi(u)=\int_{\mathbb{R}^+}\frac{e^{-iEu}}{\sqrt{4\pi E}}\overline{N_{m,\kappa}(E)}\,\tilde{\psi}_+(E)\;dE+\text{c.c.},\quad \psi(u)=\int_{\mathbb{R}^+}\frac{e^{-iEu}}{\sqrt{4\pi E}}\,\tilde{\psi}_+^{(\text{out})}(E)\;dE+\text{c.c.}\tag{35}$$

The function $N_{m,\kappa}$ [*that is restricted to* $\mathbb{R}^+$ *in (34) and (35)*] *can be defined on the whole* $\mathbb{R}$ *as*

$$N_{m,\kappa}(E):=e^{-i\,(E/\kappa)\log(m/2\kappa)}\;\text{sign}(E)\;\Gamma\left(\frac{iE}{\kappa}\right)\sqrt{\frac{E}{\kappa\pi}\sinh\frac{\pi E}{\kappa}}\,.\tag{36}$$

It belongs to $C^\infty(\mathbb{R})$ *and satisfies* $|N_{m,\kappa}(E)|=1$ *and* $\overline{N_{m,\kappa}(E)}=-N_{m,\kappa}(-E)$ *for all* $E\in\mathbb{R}$.

Proof: As $t=0$ is part of a Cauchy surface in Minkowski space–time, ψ can uniquely be extended into a smooth solution of the Klein–Gordon equation in Minkowski space–time. Therefore it makes sense to consider its restriction to **P** or **F**. As ψ is smooth, those restrictions can be computed by taking the limit of the function represented in light Rindler coordinates. First consider the case $m=0$ and $u\to\infty$. One has $\Phi_E^{(\mathrm{out})}(t(u,v),y(u,v))=e^{-iEu}/\sqrt{4\pi E}$ and $\Phi_E^{(\mathrm{in})}(t(u,v),y(u,v))=e^{-iEv}/\sqrt{4\pi E}$. Insert these functions in (13) and extend each integration on the whole $\mathbb{R}$ axis by defining $\widetilde{\psi}_+^{(\alpha)}(E)=0$ for $E\leqslant 0$. Using the properties of $\widetilde{\psi}_+^{(\alpha)}$ stated in Proposition 2.1 before (13) one sees that $\psi(u,v)$ can be decomposed as a sum of two functions (one in the variable u and the other in the variable v) which are the real part of the Fourier transform of a couple of $L^1(\mathbb{R})$ functions. Taking the limit $u\to+\infty$ the function containing only modes *out* vanishes as a consequence of Riemann–Lebesgue lemma and (34) with $m=0$ arises. The case $m=0$ and $v\to-\infty$ is strongly analogous. The case $m>0$ is based on the following expansion[24] at $x\to 0$ with ω fixed in $\mathbb{R}$:

$$K_{i\omega}(x)=\frac{i\pi e^{\pi\omega/2}}{2}\left(\frac{ix}{2}\right)^{i\omega}\frac{1+O_\omega(x^2)}{\Gamma(1+i\omega)\sinh(\pi\omega)}-\frac{i\pi e^{-\pi\omega/2}}{2}\left(\frac{ix}{2}\right)^{-i\omega}\frac{1+O'_\omega(x^2)}{\Gamma(1-i\omega)\sinh(\pi\omega)}\,, \tag{37}$$

where, for ω fixed, $|O_\omega(x^2)|\leqslant C_\omega|x|^2$ and $|O'_\omega(x^2)|\leqslant C'_\omega|x|^2$ for some real finite C_ω, C'_ω, whereas for x fixed in $\mathbb{R}$, $\omega\mapsto|O_\omega(x^2)|$ and $\omega\mapsto|O'_\omega(x^2)|$ are bounded. Inserting the expansion above in the expression (8) and taking the limit as $u\to\infty$ in (11), Riemann–Lebesgue's lemma together with some trivial properties of Γ function[24] produces (34) for $m>0$. The function (36) is nothing but $\mathrm{sign}(E)\ \exp[-iE(\log(m/2\kappa))/\kappa]\Gamma(iE/\kappa)|\Gamma(iE/\kappa)|^{-1}$ (Ref. 24) and so $|N_{m,\kappa}(E)|=1$ for $E\neq 0$ is trivially true. $\Gamma(ix)$ is smooth along the real axis with a simple pole in $x=0$ that is canceled out by the zero of $\mathrm{sign}(x)\sqrt{x\sinh x}$ that is smooth in the whole $\mathbb{R}$. Thus $N_{m,\kappa}\in C^\infty((-\infty,+\infty))$. $|N_{m,\kappa}(E)|=1$ for $E=0$ is trivially valid by continuity. $\overline{N_{m,\kappa}(E)}=-N_{m,\kappa}(-E)$ is a straightforward consequence of $\overline{\Gamma(ix)}=\Gamma(-ix)$ for $x\in\mathbb{R}$. The case $v\to-\infty$ can be proven similarly. □

From a pure mathematical point of view perhaps straightforwardly extending known results (see Chap. 5 of Ref. 21), Proposition 3.1 shows that a solution in $\mathcal{S}$ of the massive Klein–Gordon equation in 2D Rindler space is completely determined by its values on *either* the future *or* the past horizon, whereas, in the massless case, a solution $\mathcal{S}$ is completely determined by its values on *both* the future *and* the past horizon.

As $|N_{m,\kappa}(E)|=1$ we can write $N_{m,\kappa}(E)=\exp[i\rho_{m,\kappa}(E)]$ where the phase $\rho_{m,\kappa}(E)$ is real-valued. The restriction of ψ to the horizon **F** (the other case is analogous) depends from the mass of the field through the phase $\rho_{m,\kappa}$ only. As a trivial result we see that two (free scalar QFT) theories in **R** with different strictly positive masses $m\neq m'$ and Rindler vacua $\Psi_m,\Psi_{m'}$ turn out to be unitarily equivalent. This is due to the unitary operator $U:\mathfrak{F}(\mathcal{H}_m)\to\mathfrak{F}(\mathcal{H}_{m'})$ naturally defined by the requirement $U\Psi_m=\Psi_{m'}$ and induced by the scalar-product-preserving map between positive frequency wave functions,

$$\psi_+\mapsto\psi'_+\quad,\quad\text{with}\quad \psi'_+(E):=\exp[+i(\rho_{m,\kappa}(E)-\rho_{m',\kappa}(E))]\psi_+(E)\qquad\text{for all}\quad E\geqslant 0,$$

where $\psi_+\in\mathcal{H}_m$ and $\psi'_+\in\mathcal{H}_{m'}$. Similarly, each theory is unitarily equivalent to the massless theory built up using only *in* modes. Avoiding any choice for the mass, one is naturally lead to consider the class of the "fields defined on the horizon,"

$$\psi(v)=\int_{\mathbb{R}^+}\frac{e^{-iEv}}{\sqrt{4\pi E}}\widetilde{\psi}_+(E)\ dE+\int_{\mathbb{R}^+}\frac{e^{+iEv}}{\sqrt{4\pi E}}\overline{\widetilde{\psi}_+(E)}\ dE, \tag{38}$$

as the object which makes possibles all those crossed unitary identifications and exists independently from the quantum fields defined in the bulk **R** with their own masses. We want to try to consider this object as a *quantum* field in a sense we go to specify.

B. Local quantum field theory on F and P

Following the procedure presented in Secs. II B and C we want to show that it is possible to define a local quantum field theory on **F** which matches with that defined in the bulk. (That idea is not new in the literature and it has been used in important works such as Ref. 29). First of all define the space of ''wave functions'' $\mathcal{S}(\mathbf{F})$. A suitable definition, which will be useful later, is the following: $\mathcal{S}(\mathbf{F})$ is the space $\mathsf{S}(\mathbb{R};\mathbb{R})$ of the real-valued Schwartz' functions on $\mathbb{R}$ where $\mathbb{R}$ is identified with **F** itself by means of the coordinate v. Actually the name ''wave function'' is not appropriate because there is no wave equation to fulfill in our context. As a consequence the correct point of view to interpret the formalism is the Heisenberg's picture. $\mathcal{S}(\mathbf{F})$ has a natural nondegenerate symplectic form which is *invariant under the diffeomorphisms of* **F** *which preserve its orientation*:

$$\Omega_{\mathbf{F}}(\varphi,\varphi') := \int_{\mathbf{F}} \varphi' d\varphi - \varphi d\varphi'. \tag{39}$$

To define the one-particle Hilbert space, consider the modes

$$F_E(v) := \frac{e^{-iEv}}{\sqrt{4\pi E}} \quad \text{with } E \in \mathbb{R}^+. \tag{40}$$

Analogous definitions can be given with analogous notations for the past horizon **P** using modes as in (40) with $-iEv$ replaced for $-iEu$. The following pair of propositions can be simply proven using Fourier transform theory for Schwartz' functions.

Proposition 3.2 (completeness of modes): If φ *belongs to* $\mathcal{S}(\mathbf{F})$*, the function*

$$\mathbb{R}^+ \ni E \mapsto \tilde{\varphi}_+(E) := -i\Omega_{\mathbf{F}}(\overline{F_E},\phi) \tag{41}$$

satisfies $\tilde{\varphi}_+(E) = \sqrt{E}g(E)$, $\overline{\tilde{\varphi}_+(E)} = \sqrt{E}g(-E)$, *where* $g \in \mathsf{S}(\mathbb{R},\mathbb{R})$. *Moreover, for* $v \in \mathbb{R}$ *(38),*

$$\varphi(v) = \int_0^{+\infty} F_E(v)\tilde{\varphi}_+(E)\, dE + \int_0^{+\infty} \overline{F_E(v)\tilde{\varphi}_+(E)}\, dE. \tag{42}$$

Similar results hold replacing **F** *for* **P** *everywhere*.

Proposition 3.3 (associated Hilbert spaces): If φ *belongs to either* $\mathcal{S}(\mathbf{F})$*, define the one-to-one associated* positive-frequency wave function

$$\varphi_+(v) := \int_0^{+\infty} F_E(v)\tilde{\varphi}_+(E)\, dE. \tag{43}$$

With that definition and for φ_1, φ_2 *in* $\mathcal{S}(\mathbf{F})$*, it results that* $\Omega_{\mathbf{F}}(\varphi_{1+},\varphi_{2+}) = 0$ *whereas*

$$\langle \varphi_{1+},\varphi_{2+}\rangle_{\mathbf{F}} := -i\Omega_{\mathbf{F}}(\overline{\varphi_{1+}},\varphi_{2+}), \tag{44}$$

is well-defined and

$$\langle \varphi_{1+},\varphi_{2+}\rangle_{\mathbf{F}} = \int_0^{+\infty} \overline{\tilde{\varphi}_{1+}(E)}\tilde{\varphi}_{2+}(E)\, dE. \tag{45}$$

The one-particle Hilbert space $\mathcal{H}_{\mathbf{F}}$ *is defined as the Hilbert completion of the space of finite complex linear combinations of functions* φ_+, *for all* φ *in* $\mathcal{S}(\mathbf{F})$, *equipped with the extension of the scalar product (44) to complex linear combinations of arguments. It results that* $\mathcal{H}_{\mathbf{F}} \cong L^2(\mathbb{R}^+, dE)$. *Similar results and definitions hold replacing* **F** *for* **P** *everywhere.*

Definition 3.1 (quantum field operators on horizons): Consider the symmetrized Fock space $\mathfrak{F}_{\mathbf{F}}(\mathcal{H}_{\mathbf{F}})$ *with vacuum state* $\Psi_{\mathbf{F}}$ *and scalar product* $\langle\ ,\rangle_{\mathbf{F}}$. *The quantum field operator on* **F**, $\Omega_{\mathbf{F}}(\ .\ , \hat{\phi}_{\mathbf{F}})$, *is the symmetric-operator-valued function*

$$\varphi \mapsto \Omega(\varphi, \hat{\phi}_{\mathbf{F}}) := i a_{\mathbf{F}}(\overline{\varphi_+}) - i a^\dagger_{\mathbf{F}}(\varphi_+), \tag{46}$$

where $\varphi \in \mathcal{S}(\mathbf{F})$. *Here* $a_{\mathbf{F}}(\overline{\varphi_+})$ *and* $a^\dagger_{\mathbf{F}}(\varphi_+)$, *respectively, denote the annihilation and construction operators associated with the one-particle state* φ_+ *which are defined in the dense invariant subspace* $\mathfrak{F}_{0\mathbf{F}}$ *spanned by all states containing a finite, arbitrarily large, number of particles with states given by positive-frequency wave functions. An analogous definition is given replacing* **F** *for* **P** *everywhere.*

Operators $\Omega_{\mathbf{F}}(\varphi, \hat{\phi}_{\mathbf{F}})$ and $\Omega_{\mathbf{P}}(\varphi, \hat{\phi}_{\mathbf{P}})$ are essentially self-adjoint on $\mathfrak{F}_{0\mathbf{F}}$ and $\mathfrak{F}_{0\mathbf{P}}$, respectively, since their elements are analytic vectors.

We want to define an analogous procedure to that in the bulk [see (20)] for smearing field operators by means of ''functions'' instead of ''wave functions.'' The issue is however relevant because it permits us to introduce the analog $E_{\mathbf{F}}$ of the causal propagator E in spite of having no equation of motion in **F**. The idea is that something like (19) should work also in our context. A clear difficulty is that there is no diffeomorphism invariant measure which can be used in the analog of (19) in place of $d\mu_g$. On the other hand, integration of k-forms is diffeomorphism invariant on (oriented manifolds). Therefore, we aspect that the space of ''functions'' used to smear quantum fields should properly be a space of one-forms rather than functions. To go on, we notice that *a posteriori* $E_{\mathbf{F}}$ has to fulfill something like $[\hat{\phi}_{\mathbf{F}}(v), \hat{\phi}_{\mathbf{F}}(v')] = -iE_{\mathbf{F}}(v, v')$. By a formal but straightforward computation which uses $[a_E, a^\dagger_{E'}] = \delta(E - E')$ and the analog of (18) with Φ_E replaced for F_E, one finds that $i[\hat{\phi}_{\mathbf{F}}(v), \hat{\phi}_{\mathbf{F}}(v')] = \frac{1}{4}\text{sign}\,(v - v')$. This v-parametrized distribution actually defines a well-behaved transformation from the space of exact (smooth) one-forms in **F** with compact support to the space of smooth functions on **F**. As the functions $f \in \mathcal{S}(\mathbf{F})$ vanish (with all of their derivatives) as $v \to \infty$, if $\eta = df$,

$$\int_{v' \in \mathbb{R}} \text{sign}\,(v - v')\,\eta(v') = f(v) - (-f(v)) = 2\,f(v).$$

In the following, $\mathcal{D}(\mathbf{F})$ is the real space of the one-forms $\eta = d\varphi$ such that $\varphi \in \mathcal{S}(\mathbf{F})$.

Definition 3.2 (causal propagator and associated quantum field on horizons): With the given notations, the causal propagator *in* **F** *is the mapping* $E_{\mathbf{F}} : \mathcal{D}(\mathbf{F}) \to \mathcal{S}(\mathbf{F})$ *with*

$$(E_{\mathbf{F}}\eta)(v) := \frac{1}{4}\int_{v' \in \mathbb{R}} \text{sign}\,(v - v')\,\eta(v'), \tag{47}$$

and the quantum-field operator on **F** smeared with forms η of $\mathcal{D}(\mathbf{F})$ *is the mapping*

$$\eta \mapsto \hat{\phi}_{\mathbf{F}}(\eta) := \Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta, \hat{\phi}_{\mathbf{F}}). \tag{48}$$

Analogous definitions are given replacing **F** *for* **P** *and* v *for* u *everywhere.*

The given definitions are good generalizations of the analogous tools in the usual quantum field theory [see (19) and (21) in particular] as stated in the following pair of propositions whose proof is trivial. The second item in Proposition 3.5 shows that the theory enjoys *locality* in a suitable way

Proposition 3.4: If $\varphi \in \mathcal{S}(\mathbf{F})$, $\omega = 2d\varphi$ *is the unique element of* $\mathcal{D}(\mathbf{F})$ *such that* $\varphi = E_{\mathbf{F}}(\omega)$. *Moreover, if* $\eta, \omega \in \mathcal{D}(\mathbf{F})$,

$$\int_{\mathbf{F}} \varphi\,\eta = \Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta,\varphi) \quad \text{and} \quad \int_{\mathbf{F}} (E_{\mathbf{F}}\omega)\,\eta = \Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta, E_{\mathbf{F}}\omega)\ . \tag{49}$$

An analogous result holds replacing **F** *for* **P** *everywhere.*

Proposition 3.5: If $\varphi \in \mathcal{S}(\mathbf{F})$ *and* $\eta,\omega \in \mathcal{D}(\mathbf{F})$,

$$[\hat{\phi}_{\mathbf{F}}(\eta), \hat{\phi}_{\mathbf{F}}(\omega)] = -iE(\eta,\omega) := -i\int_{\mathbf{F}} (E_{\mathbf{F}}\eta)\,\omega. \tag{50}$$

In particular, the following locality property holds true:

$$[\hat{\phi}_{\mathbf{F}}(\eta), \hat{\phi}_{\mathbf{F}}(\omega)] = 0 \qquad \text{if } \mathrm{supp}\,\eta \cap \mathrm{supp}\,\omega = \varnothing.$$

An analogous result holds replacing **F** *for* **P** *everywhere.*

C. The algebraic approach

To state holographic theorems it is necessary to reformulate quantum field theory in an algebraic approach either in the bulk and on the horizon. In globally hyperbolic space–times, linear QFT can be formulated independently from a preferred vacuum state and Fock representation. It is worthwhile stressing that[21] physics implies the existence of meaningful quantum states which cannot be represented in the same Hilbert (Fock) representation of the algebra of observables. In this sense the algebraic approach is more fundamental than the usual Fock approach in QFT in curved space–time. Let us summarize the procedure in **R** which, at least for $m>0$, could be replaced by any globally hyperbolic space–time. The basic tool is an abstract $*$-algebra, $\mathcal{A}_{\mathbf{R}}$, made of the linear combinations of products of formal field operators $\phi(f), \phi(f)^*$ ($f \in \mathcal{D}(\mathbf{R};\mathbb{C})$) and the unit I, which enjoy the same properties of operators $\hat{\phi}(f), \hat{\phi}(f)^\dagger$ (and the identity operator I). From a physical point of view, the Hermitian elements of $\mathcal{A}_{\mathbf{R}}$ represent the *local observables* of the free-field theory. For $m>0$, the required properties are

(1) $\phi(f)^* = \phi(\overline{f})$ for all $f \in \mathcal{D}(\mathbf{R};\mathbb{C})$,
(2) $\phi(af+bg) = a\phi(f) + b\phi(g)$ for all $f,g \in \mathcal{D}(\mathbf{R};\mathbb{C})$, $a,b \in \mathbb{C}$,
(3) $[\phi(f),\phi(g)] = -iE(f,g)I$ for all $f,g \in \mathcal{D}(\mathbf{R};\mathbb{C})$, and
(4) $\phi(f) = 0$ if (and only if) $f = Kh$ for some compactly-supported smooth function h.

$\mathcal{A}_{\mathbf{R}}$ is rigorously realized as follows. Consider the complex unital algebra $\mathcal{A}_{0\mathbf{R}}$, freely generated by the unit I, and abstract objects $\phi(f)$ and $\phi(f)^*$ for all $f \in \mathcal{D}(\mathbf{R};\mathbb{C})$. The involution * on $\mathcal{A}_{0\mathbf{R}}$ is the unique antilinear involutive function $^*{}_{:\mathcal{A}_{0\mathbf{R}} \to \mathcal{A}_{0\mathbf{R}}}$ such that $I^* = I$, $(\phi(f))^* = \phi(f)^*$. Let $\mathcal{J} \subset \mathcal{A}_{\mathbf{R}}$ be the double-side ideal whose elements are linear combinations of products containing at least one of the following factors $\phi(f)^* - \phi(\overline{f})$, $\phi(af+bg) - a\phi(f) - b\phi(g)$, $[\phi(f),\phi(g)] + iE(f,g)I$, and $\phi(Kg)$ for $f,g \in \mathcal{D}(\mathbf{R};\mathbb{C})$, $a,b \in \mathbb{C}$. $\mathcal{A}_{\mathbf{R}}$ is defined as the space of equivalence classes with respect to the equivalence relation in $\mathcal{A}_{0\mathbf{R}}$, $A \sim B$ iff $A - B \in \mathcal{J}$ and $\mathcal{A}_{\mathbf{R}}$ is equipped with the $*$-structure induced by $\mathcal{A}_{0\mathbf{R}}$ through $\sim$. If, with little misuse of notation, $\phi(f)$ and I, respectively, denote the classes $[\phi(f)]$ and $[I] \in \mathcal{A}_{\mathbf{R}}$, the properties (1)–(4) are fulfilled.

If $m=0$, there are two relevant algebras $\mathcal{A}_{\mathbf{R}}^{(in)}$ and $\mathcal{A}_{\mathbf{R}}^{(out)}$. $\mathcal{A}_{\mathbf{R}}^{(in)}$ is the unital $*$-algebra generated by I, $\phi_{\mathrm{in}}(f)$ and $\phi_{\mathrm{in}}(f)^*$ for every $f \in \mathcal{D}(\mathbf{R},\mathbb{C})$ whereas $\mathcal{A}_{\mathbf{R}}^{(out)}$ is the unital $*$-algebra generated by I, $\phi_{\mathrm{out}}(f)$ and $\phi_{\mathrm{out}}(f)^*$ for every $f \in \mathcal{D}(\mathbf{R},\mathbb{C})$. By definition these algebras satisfy the constraints (1)–(4) with the difference that, in (3), E must be replaced for E_{in} or E_{out}, respectively, and, in (4), K must be replaced by $\gamma^{-1}\partial_u$ or $\gamma^{-1}\partial_v$, respectively. The rigorous definitions can be given similarly to the case $m>0$, by starting from freely generated algebras and passing to quotient algebras. We recall that if $\mathcal{A}$, $\mathcal{B}$ are $*$-algebras with field $\mathbb{C}$ and units $I_{\mathcal{A}}$, $I_{\mathcal{B}}$, $\mathcal{A}\otimes\mathcal{B}$ denotes (see p. 143 of Ref. 30) the $*$-algebra whose associated vector-space structure is the tensor product $\mathcal{A}\otimes\mathcal{B}$, the unit is $I := I_{\mathcal{A}} \otimes I_{\mathcal{B}}$, and the involution and the algebra product are, respectively, given by $(\Sigma_k A_k \otimes B_k)^* := \Sigma_k A_k^* \otimes B_k^*$ and $(\Sigma_k A_k \otimes B_k)(\Sigma_i A_i' \otimes B_i') := \Sigma_{ki} A_k A_i' \otimes B_k B_i'$

$\otimes B_k B_i'$ with obvious notation. Assuming (24) as the definition of $\phi(f)$, the whole field algebra $\mathcal{A}_{\mathbf{R}}$ is *defined* as $\mathcal{A}_{\mathbf{R}} := \mathcal{A}_{\mathbf{R}}^{(in)} \otimes \mathcal{A}_{\mathbf{R}}^{(out)}$. That unital $*$-algebra satisfies (1)–(4).

An *algebraic state* on a $*$-algebra $\mathcal{A}$ with unit I is a linear map $\mu : \mathcal{A} \to \mathbb{C}$ that is normalized [i.e., $\mu(I) = 1$] and positive [i.e., $\mu(A^*A) \geqslant 0$ for $A \in \mathcal{A}$]. The celebrated GNS theorem (e.g., see Ref. 21) states that for every algebraic state μ on $\mathcal{A}$ there is a triple $(\mathfrak{H}_\mu, \Pi_\mu, \Omega_\mu)$ such that the following facts hold. $\mathfrak{H}_\mu$ is a Hilbert space, and Π_μ is a $*$-algebra representation of $\mathcal{A}$ in terms of operators on $\mathfrak{H}_\mu$ which are defined on a dense invariant subspace $\mathfrak{D}_\mu \subset \mathfrak{H}_\mu$ and such that $\Pi_\mu(A^*) = (\Pi_\mu(A))^\dagger \restriction_{\mathfrak{D}_\mu}$. Finally $\mathfrak{D}_\mu$ is spanned by all the vectors $\Pi_\mu(A)\Omega_\mu$, $A \in \mathcal{A}$, and $\mu(A) = \langle \Omega_\mu, \Pi_\mu(A)\Omega_\mu \rangle$ for all $A \in \mathcal{A}$, $\langle\ ,\ \rangle$ denoting the scalar product in $\mathfrak{H}_\mu$. If $(\mathfrak{H}_\mu', \Pi_\mu', \Omega_\mu')$ is another similar triple associated with the same μ, there is a unitary operator $U : \mathfrak{H}_\mu \to \mathfrak{H}_\mu'$ such that $\Omega_\mu' = U\Omega_\mu$ and $\Pi_\mu' = U\Pi_\mu$. If $\mathcal{A} = \mathcal{A}_{\mathbf{F}}$, by direct inspection one finds that quantum field theory in $\mathbf{R}$ in the Fock space $\mathfrak{F}(\mathcal{H})$ with $\Psi_{\mathbf{R}}$ as vacuum state coincides with that in a GNS representation of $\mathcal{A}_{\mathbf{R}}$ associated with the (*quasifree*[21]) algebraic state $\mu_{\mathbf{R}}$ completely determined by $\mu_{\mathbf{R}}(\phi(f)\phi(g)) := \langle \Psi_{\mathbf{R}}, \hat{\phi}(f)\hat{\phi}(g)\Psi_{\mathbf{R}} \rangle$ via Wick expansion of symmetrized n-point functions. Moreover, it results in $\mathfrak{D}_\mu = \mathfrak{F}_0$.

All the procedure can be used to give an algebraic approach for QFT on $\mathbf{F}$ (or $\mathbf{P}$): Define $\mathcal{D}(\mathbf{F};\mathbb{C}) := \mathcal{D}(\mathbf{F}) + i\mathcal{D}(\mathbf{F})$ and define $\hat{\phi}_{\mathbf{F}}(\omega + i\eta) := \hat{\phi}_{\mathbf{F}}(\omega) + i\hat{\phi}_{\mathbf{F}}(\eta)$ when $\omega, \eta \in \mathcal{D}(\mathbf{F})$. Finally, consider the abstract $*$-algebra $\mathcal{A}_{\mathbf{F}}$ with unit I, generated by I, $\phi_{\mathbf{F}}(\omega)$, $\phi_{\mathbf{F}}(\omega)^*$ for all $\omega \in \mathcal{D}(\mathbf{F};\mathbb{C})$, such that, for all $a, b \in \mathbb{C}$ and $\omega, \eta \in \mathcal{D}(\mathbf{F};\mathbb{C})$,

(1) $\phi_{\mathbf{F}}(\omega)^* = \phi_{\mathbf{F}}(\overline{\omega})$,
(2) $\phi_{\mathbf{F}}(a\omega + b\eta) = a\phi_{\mathbf{F}}(\omega) + b\phi_{\mathbf{F}}(\eta)$, and
(3) $[\phi_{\mathbf{F}}(\omega), \phi_{\mathbf{F}}(\eta)] = -iE_{\mathbf{F}}(\omega, \eta)I$.

(The rigorous definition is given in terms of quotient algebras as usual.) From a physical point of view the (Hermitian) elements of $\mathcal{A}_{\mathbf{F}}$ represent the *(quasi) local observables* of the free-field theory on the future horizon. By direct inspection one finds that quantum field theory in $\mathbf{F}$ in the Fock space referred to the vacuum state $\Psi_{\mathbf{F}}$ and coincides with that in a GNS representation of $*$-algebra $\mathcal{A}_{\mathbf{F}}$ associated with the (quasi-free) algebraic state $\mu_{\mathbf{F}}$ completely determined, via Wick expansion, by $\mu_{\mathbf{F}}(\phi_{\mathbf{F}}(\eta)\phi_{\mathbf{F}}(\omega)) := \langle \Psi_{\mathbf{F}}, \hat{\phi}_{\mathbf{F}}(\eta)\hat{\phi}_{\mathbf{F}}(\omega)\Psi_{\mathbf{F}} \rangle_{\mathbf{F}}$ and $\mathfrak{D}_\mu = \mathfrak{F}_{0\mathbf{F}}$.

Everything can be similarly stated for quantum field theory on $\mathbf{P}$ with trivial changes in notation.

D. Two holographic theorems

Here we prove two *holographic* theorems for the observables of free fields, one in the algebraic approach and the latter in the Hilbert space formulation under the choice of suitable vacuum states. The former theorem says that, in the massive case, there is a one-to-one transformation from the algebra of the fields in the bulk $\mathcal{A}_{\mathbf{R}}$—that is, the local observables of the free field in the bulk—to a subalgebra of fields on the future horizon $\mathcal{A}_{\mathbf{F}}$—that is, the observables of the free field in the future horizon. The mapping preserves the structure of the $*$-algebra and thus the two classes of observables can be identified completely no matter the value of the mass of the field in the bulk and the fact that there is no mass associated with the field on the horizon. Remarkably, this identification does not require any choice for reference vacuum states since it is given at a pure algebraic level. To build up the said mapping, take any compactly supported function f in the bulk, consider the generated wave function $\psi_f = E(f)$ (that is assumed to be defined in the whole Minkowski space), restrict ψ_f on $\mathbf{F}$ obtaining a horizon wave function φ_f and associate with that function the unique form ω_f with $\varphi_f = E_{\mathbf{F}}\omega_f$. Finally, define $\chi_{\mathbf{F}}(\phi(f)) := \phi_{\mathbf{F}}(\omega_f)$. The next step is to extend $\chi_{\mathbf{F}}$ to the whole algebra $\mathcal{A}_{\mathbf{R}}$ by requiring that the $*$-algebra structure is preserved, that is, I is mapped in I, $\phi(f)^*$ is mapped into $\chi_{\mathbf{F}}(\phi(f))^*$, products of fields $\phi(f)\phi(g)$ are mapped into $\chi_{\mathbf{F}}(\phi(f))\chi_{\mathbf{F}}(\phi(g))$ and so on. In the massless case, the procedure is similar but one has to consider also the past evolution of wave functions toward the past horizon $\mathbf{P}$. The theorem says

that the required extensions into algebra homomorphisms actually exists, are uniquely determined and are injective so that the observable algebra in the bulk can be seen as a observable subalgebra on the horizon.

Theorem 3.1 (algebraic holography): *In a 2D Rindler space* $\mathbf{R}$ *viewed as immersed in a corresponding 2D Minkowski space–time, consider quantum field theory of a scalar field with mass* $m \geqslant 0$ *satisfying Klein–Gordon equation (5). Consider the algebra* $\mathcal{A}_{\mathbf{R}}$ *(including* $\mathcal{A}_{\mathbf{R}}^{(out)}$, $\mathcal{A}_{\mathbf{R}}^{(in)}$ *if* $m=0$*) of local observables in the bulk and the algebras* $\mathcal{A}_{\mathbf{F}}$ *and* $\mathcal{A}_{\mathbf{P}}$ *of the observables on the horizons* $\mathbf{F}$ *and* $\mathbf{P}$*. The following statements hold.*

(a) If $m>0$*, there is a unital-*-algebra homomorphism* $\chi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{F}}$ *uniquely determined by*

$$\chi_{\mathbf{F}}:\phi(f)\mapsto\phi_{\mathbf{F}}(\omega_f) \quad with\ \omega_f:=2d((Ef)\restriction_{\mathbf{F}}) \quad for\ all\ f\in\mathcal{D}(\mathbf{R}), \tag{51}$$

$(Ef)\restriction_{\mathbf{F}}$ *denoting the limit of* $E(f)$ *on* $\mathbf{F}$*.* $\chi_{\mathbf{F}}$ *turns out to be injective.*

An analogous statement holds replacing $\mathbf{F}$ *for* $\mathbf{P}$*.*

(b) If $m=0$*, there are two unital-*-algebra homomorphisms* $\pi_{\mathbf{P}}:\mathcal{A}_{\mathbf{R}}^{(out)}\to\mathcal{A}_{\mathbf{P}}$ *and* $\pi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}^{(in)}\to\mathcal{A}_{\mathbf{F}}$ *uniquely determined by*

$$\pi_{\mathbf{F}}:\phi_{in}(f)\mapsto\phi_{\mathbf{F}}(\eta_f) \quad with\ \omega_f:=2d(E(f)\restriction_{\mathbf{F}}) \ for\ all\ f\in\mathcal{D}(\mathbf{R}), \tag{52}$$

$$\pi_{\mathbf{P}}:\phi_{out}(f)\mapsto\phi_{\mathbf{P}}(\omega_f) \quad with\ \eta_f:=2d(E(f)\restriction_{\mathbf{P}}) \ for\ all\ f\in\mathcal{D}(\mathbf{R}). \tag{53}$$

$\pi_{\mathbf{F}}$ *and* $\pi_{\mathbf{P}}$ *turn out to be injective.*

(c) $\pi_{\mathbf{F}}(\mathcal{A}_{\mathbf{R}}^{(in)})\subset\mathcal{A}_{\mathbf{F}}$ *is the subalgebra generated by* I *and abstracts field operators smeared by the elements of* $\mathcal{D}(\mathbf{F},\mathbb{C})$ *with compact support. The analogous statement holds for* $\pi_{\mathbf{P}}(\mathcal{A}_{\mathbf{R}}^{(out)})$.

Proof: (a) The uniqueness of the homomorphism is trivially proven by noticing that the elements of $\mathcal{A}_{\mathbf{R}}$ are of the form $A=aI+\Sigma_k b_k\phi(f_k)+\Sigma_h c_h\phi(g_h)^*+\Sigma_{ls}d_{ls}\phi(h_l)\phi(p_s)+\cdots$ where the overall summation as well as every partial summation is finite. As $\chi_{\mathbf{F}}$ is a homomorphism, $\chi_{\mathbf{F}}(A)=aI+\Sigma_k b_k\chi_{\mathbf{F}}(\phi(f_k))+\Sigma_h c_h\chi_{\mathbf{F}}(\phi(g_h))^*+\Sigma_{ls}d_{ls}\chi_{\mathbf{F}}(\phi(h_l))\chi_{\mathbf{F}}(\phi(p_s))+\cdots$. Moreover, $\chi_{\mathbf{F}}(\phi(h))=\chi_{\mathbf{F}}(\phi(\mathrm{Re}\,h))+i\chi_{\mathbf{F}}(\phi(\mathrm{Im}\,h))$ and thus the values $\chi_{\mathbf{F}}(\phi(f))$ with h real determine the homomorphism provided it exists. Let us prove the existence of the homomorphism. Take $f\in\mathcal{D}(\mathbf{R})$ and consider $\psi_f=Ef$ and the associated function $\tilde{\psi}_{f_+}=\tilde{\psi}_{f_+}(E)$. It holds $\tilde{\psi}_{f_+}(E)=\sqrt{E}f(E)$ with $f\in\mathsf{S}(\mathbb{R},\mathbb{C})$ such that $\overline{f(E)}=-f(-E)$ as stated in Proposition 2.1 and $N_{m,\kappa}\in C^\infty(\mathbb{R})$ [with $|N_{m,\kappa}(E)|=1$] and $\overline{N_{m,\kappa}(E)}=-N_{m,\kappa}(-E)$ as stated in Proposition 3.1. As a consequence $N_{m,\kappa}(E)\tilde{\psi}_+(E)=\sqrt{E}h(E)$ where $\overline{h(E)}=h(-E)$ and $h\in\mathsf{S}(\mathbb{R},\mathbb{C})$. Passing to the function $v\mapsto\psi_f(v)$ in Proposition 3.1 and using these results one gets

$$\psi_f(v)=\mathrm{const}\times\int_0^{+\infty}e^{-iEv}h(E)dE+\mathrm{c.c.}=\mathrm{const}\times\int_{-\infty}^{+\infty}e^{-iEv}h(E)dE.$$

As h belongs to Schwartz' space, ψ_f belongs to the same space because the Fourier transform preserves Schwartz' space. Moreover, ψ_f is real since $h(E)=\overline{h(-E)}$. We have found that $\psi_f\in\mathcal{S}(\mathbf{F})$ and thus $\omega_f:=2d\psi_f=2d[(Ef)\restriction_{\mathbf{F}}]$ is an element of $\mathcal{D}(\mathbf{F})$. Using $f\in\mathcal{D}(\mathbf{R},\mathbb{C})$, the result is preserved trivially by the linear decomposition in the real and imaginary parts. Assume once again that $f\in\mathcal{D}(\mathbf{R})$. Notice that ω_f contains the same information as ψ_f because $\psi_f(v)=2\int_{-\infty}^{v}\omega_f$. In turn ψ_f determines the function $\tilde{\psi}_{f_+}$ which determines Ef. As we said in Sec. II C, Ef determines f up to a term Kh with $h\in\mathcal{D}(\mathbf{R})$. We conclude that $\omega_f=\omega_g$ if and only if $f=g+Kh$ with $h\in\mathcal{D}(\mathbf{R})$. The same result arises for functions $f,g\in\mathcal{D}(\mathbf{R},\mathbb{C})$ by linearity and from the fact that E transforms real functions into real functions. We have found that there is a well-defined linear map $\mathcal{D}(\mathbf{R},\mathbb{C})\ni f\mapsto\omega_f\in\mathcal{D}(\mathbf{F},\mathbb{C})$ that transforms real functions in real forms and such that $\omega_f=\omega_g$ if and only if $f=g+Kh$. Now we define $\chi_{0\mathbf{F}}(\phi(f))=\phi_{\mathbf{F}}(\omega_f)$ and $\chi_{\mathbf{F}}(I)=I$ and $\chi_{\mathbf{F}}(\phi(f)^*)=\phi_{\mathbf{F}}(\omega_f)^*$. That map extends straightforwardly from the $*$-algebra $\mathcal{A}_{0\mathbf{R}}$ freely generated by I, $\phi(f)$, $\phi(f)^*$ (with involution uniquely determined as said in Sec. II D) to the analogous free $*$-algebra on $\mathbf{F}$ giving rise to a $*$-algebra homomorphism $\chi_{0\mathbf{F}}$. However, it is not injective since it

results in $\chi_{0\mathbf{F}}(\phi(f))=\chi_{0\mathbf{F}}(\phi(g))$ whenever $f=g+Kh$, and, more generally, injectivity failure arises for any pair of elements of the algebra which are different from each other because of the presence of factors $\phi(f)$ and $\phi(g)$ with $f-g=Kh$. The injectivity is, however, restored if we take the quotient $*$-algebra $\mathcal{A}_{1\mathbf{R}}$ in $\mathcal{A}_{0\mathbf{R}}$ with respect to the both-side ideal containing linear combinations of products with at least one factor $\phi(Kf)$ or $\phi(Kf)^*$ for any $f\in\mathcal{D}(\mathbf{F},\mathbb{C})$ and redefine the injective map $\chi_{1\mathbf{F}}:\mathcal{A}_{1\mathbf{R}}\to\mathcal{A}_{0\mathbf{F}}$ as the map induced by $\chi_{0\mathbf{F}}$ through the canonical projection of $\mathcal{A}_{0\mathbf{R}}$ onto $\mathcal{A}_{1\mathbf{R}}$. By construction $\chi_{1\mathbf{F}}$ is an injective $*$-algebra isomorphism. In this context and from now on, it is convenient to think of the objects $\phi(f)$ as smeared by the equivalence class $[f]$ rather than f itself, where $[f]$ belongs to the complex vector space obtained by taking the quotient of $\mathcal{D}(\mathbf{R},\mathbb{C})$ with respect to the subspace $K\mathcal{D}(\mathbf{R},\mathbb{C})$. The map $[f]\mapsto\omega_f$ is a well-defined injective vector space isomorphism that preserves the complex conjugation. To conclude we have to extract the algebras $\mathcal{A}_{\mathbf{R}}$ and $\mathcal{A}_{\mathbf{F}}$ by the procedure outlined in Sec. II D, based on the projection on suitable quotient spaces, and prove that the $*$-homeomorphism $\chi_{1\mathbf{F}}$ induces a $*$-homeomorphism $\chi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{F}}$. To this end we have to consider the double-side ideal $\mathcal{J}\subset\mathcal{A}_{1\mathbf{R}}$ whose elements are linear combinations of products containing at least one of the following factors: $\phi(f)^*-\phi(\overline{f})$, $\phi(af+bg)-a\phi(f)-b\phi(g)$, $[\phi(f),\phi(g)]+iE(f,g)I$, for $f,g\in\mathcal{D}(\mathbf{R};\mathbb{C})$, $a,b\in\mathbb{C}$. $\mathcal{A}_{\mathbf{R}}$ is defined as the space of equivalence classes with respect to the equivalence relation in $\mathcal{A}_{1\mathbf{R}}$, $A\sim_{\mathcal{J}}B$ iff $A-B\in\mathcal{J}$ and $\mathcal{A}_{\mathbf{R}}$ is equipped with the $*$-algebra structure induced by $\mathcal{A}_{1\mathbf{R}}$ through the canonical projection. The analogous procedure must be used for $\mathcal{A}_{1\mathbf{F}}$ with respect to an analogous ideal $\mathcal{J}_{\mathbf{F}}\subset\mathcal{A}_{1\mathbf{F}}$ in order to produce $\mathcal{A}_{\mathbf{F}}$. Then the injective $*$-homomorphism $\chi_{1\mathbf{F}}$ induces an injective $*$-homomorphism $\chi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{F}}$ if the equivalence relations induced by $\mathcal{J}$ and $\mathcal{J}_{\mathbf{F}}$ are preserved by $\chi_{1\mathbf{F}}$ itself, i.e., $A\sim_{\mathcal{J}}B$ if and only if $\chi_{1\mathbf{F}}(A)\sim_{\mathcal{J}_{\mathbf{F}}}\chi_{1\mathbf{F}}(B)$. We leave the simple but tedious proof of this fact to the reader, proving the only nontrivial point which concerns factors $[\phi(f),\phi(g)]+iE(f,g)I$. It is simply found that, among other trivially fulfilled conditions, the preservation of the equivalence relation arises if $\chi_{1\mathbf{F}}([\phi(f),\phi(g)]+iE(f,g)I)=[\phi_{\mathbf{F}}(\omega_f),\phi_{\mathbf{F}}(\omega_g)]+iE_{\mathbf{F}}(\omega_f,\omega_g)I$, which is equivalent to $E(f,g)=E_{\mathbf{F}}(\omega_f,\omega_g)$. (Notice that, by the known properties of the causal propagator, both sides are invariant under the addition of a term Kh to f or g.) $E(f,g)=E_{\mathbf{F}}(\omega_f,\omega_g)$ is equivalent to, with obvious notations, $\Omega(\psi_f,\psi_g)=\Omega_{\mathbf{F}}(\varphi_f,\varphi_g)$. It is sufficient to prove that identity for real f,g. By Propositions 2.2 and 3.3 one finds $-i\Omega(\psi_f,\psi_g)=\langle\psi_{f+},\psi_{g+}\rangle-\overline{\langle\psi_{f+},\psi_{g+}\rangle}$ and $-i\Omega_{\mathbf{F}}(\varphi_f,\varphi_g)=\langle\varphi_{f+},\varphi_{g+}\rangle_{\mathbf{F}}-\overline{\langle\varphi_{f+},\varphi_{g+}\rangle_{\mathbf{F}}}$. Passing in energy representation, where the scalar product is simply that of $L^2(\mathbb{R}^+,dE)$ in both spaces, ψ_{f+} and ψ_{g+} are represented by some $E\mapsto\tilde{\psi}_{f+}(E)$ and $E\mapsto\tilde{\psi}_{g+}(E)$, respectively, whereas, by Proposition 3.1, φ_{f+} and φ_{g+} are represented by $E\mapsto N_{m,\kappa}(E)\tilde{\psi}_{f+}(E)$ and $E\mapsto N_{m,\kappa}(E)\tilde{\psi}_{g+}(E)$, respectively. Since $|N_{m,\kappa}(E)|=1$, it results that $\langle\psi_{f+},\psi_{g+}\rangle=\langle\varphi_{f+},\varphi_{g+}\rangle_{\mathbf{F}}$ that entails $\Omega(\psi_f,\psi_g)=\Omega_{\mathbf{F}}(\varphi_f,\varphi_g)$ and concludes the proof. (b) Following a proof very similar to that as in the case (b) (but simpler since the phases $N_{m,\kappa}$ disappear when one uses Proposition 3.1) one sees that $\mathcal{A}_{\mathbf{R}}^{(\mathrm{in})}$ is isomorphic to $\mathcal{A}_{\mathbf{F}}$ under the unique extension, into an injective $*$-algebra-with-unit homomorphism, of the map $\pi_{\mathbf{F}}:\phi_{\mathrm{in}}(f)\mapsto\phi_{\mathbf{F}}(\omega_f)$ with $\omega_f:=2d(E_{\mathrm{in}}(f))$ and this is equivalent to the thesis because $E_{\mathrm{in}}f=E(f)\restriction_{\mathbf{F}}$ since $E_{\mathrm{out}}(f)\restriction_{\mathbf{F}}=0$ and $E_{\mathrm{in}}(f)\restriction_{\mathbf{F}}=E_{\mathrm{in}}f$, for smooth compactly supported f defined in $\mathbf{R}$ (these facts are consequences of Proposition 3.1). The case of $\mathcal{A}_{\mathbf{R}}^{(\mathrm{out})}$ is strongly analogous. (c) Consider the case of $\pi_{\mathbf{F}}$, the other being analogous. If f is smooth and compactly supported in $\mathbf{R}$, $E_{\mathrm{in}}f$ is a compactly supported function of v and thus $\omega_f=2d(E(f)\restriction_{\mathbf{F}})=2d(E_{\mathrm{in}}f)$ is compactly supported on $\mathbf{F}$. Conversely, if $\omega=d\varphi\in\mathcal{D}(\mathbf{F},\mathbb{C})$ is compactly supported on $\mathbf{F}$, φ must be compactly supported and $f(u,v):=2\gamma^{-1}(u,v)\varphi(u)h(u)$ is smooth, compactly supported in $\mathbf{R}$ for every smooth compactly supported function $h:\mathbb{R}\to\mathbb{R}$ and $\omega=2d(E_{\mathrm{in}}(f))$ if $\int_{\mathbb{R}}h(u)du=1$. □

Remarks: (1) We stress that QFT on the horizon is the same no matter the value of the mass of the field in the bulk: Different choices of the mass determine different injective $*$-algebra homomorphisms from the algebra in the bulk to the *same* algebra of observables on the horizon. (2) There are strong differences between the cases $m>0$ and $m=0$. If f is compactly supported in the bulk, the horizon restriction of Ef is compactly supported if $m=0$ but that is not the case when $m>0$. For that reason we have defined $\mathcal{S}(\mathbf{F})$ [and $\mathcal{D}(\mathbf{F})$] as a space of rapidly decreasing functions

(one-forms) rather than a space of compactly supported functions (one-forms). Moreover, if $m>0$, $\mathcal{A}_{\mathbf{R}}$ is isomorphic to a subalgebra of $\mathcal{A}_{\mathbf{F}}$ (or equivalently $\mathcal{A}_{\mathbf{P}}$). Conversely, if $m=0$, $\mathcal{A}_{\mathbf{R}}$ $(=\mathcal{A}_{\mathbf{R}}^{(\mathrm{in})}\otimes\mathcal{A}_{\mathbf{R}}^{(\mathrm{out})})$ is isomorphic to a subalgebra of $\mathcal{A}_{\mathbf{F}}\otimes\mathcal{A}_{\mathbf{P}}$ by means of the injective unital-$*$-algebra homomorphism $\pi_{\mathbf{P}}\otimes\pi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{P}}\otimes\mathcal{A}_{\mathbf{F}}$.

(3) The existence of the $*$-homomorphisms $\chi_{\mathbf{F}}$ and $\pi_{\mathbf{F/P}}$ implies that, for all $f,g\in\mathcal{D}(\mathbf{F},\mathbb{C})$ or $\mathcal{D}(\mathbf{F},\mathbb{C})$ and, respectively, for $m>0$ or $m=0$,

$$[\phi(f),\phi(g)]=[\phi_{\mathbf{F}}(\omega_f),\phi_{\mathbf{F}}(\omega_g)] \quad \text{or} \quad [\phi_{\mathrm{in/out}}(f),\phi_{\mathrm{in/out}}(g)]=[\phi_{\mathbf{F/P}}(\omega_f),\phi_{\mathbf{F/P}}(\omega_g)]. \tag{54}$$

As a consequence, the *causal propagator and the symplectic forms are preserved, too*.

The second theorem concerns the unitary implementation of the $*$-homomorphism given in Theorem 3.1. This theorem states that, if one realizes the algebras of observables $\mathcal{A}_{\mathbf{R}}$ and $\mathcal{A}_{\mathbf{P}}$, $\mathcal{A}_{\mathbf{F}}$ in terms of proper field operators in the Fock spaces constructed over, respectively, the Rindler vacuum $\Psi_{\mathbf{R}}$ and $\Psi_{\mathbf{P}}$, $\Psi_{\mathbf{F}}$, then the injective homomorphisms presented in Theorem 3.1 are implemented by unitary operators which preserve the vacuum states. In other words, *with the said choice of the vacuum states and Fock representation of the algebras of observables*, the theory in the bulk and that on the horizon are *unitarily equivalent*. As an immediate consequence, it arises that the *vacuum expectation values* are preserved passing from the theory in the bulk **R** to the theory on the horizon **F** (or **P**).

Theorem 3.2. (unitary holography): *In the same hypotheses as in Theorem 3.1, consider the realization of the algebra of the local observables of the bulk $\mathcal{A}_{\mathbf{R}}$, in the Fock space $\mathfrak{F}(\mathcal{H})$ with Rindler vacuum $\Psi_{\mathbf{R}}$ $(=\Psi_{\mathbf{R}}^{(\mathrm{out})}\otimes\Psi_{\mathbf{R}}^{(\mathrm{in})}$ if $m=0)$, and the realizations of the algebras of observables of the horizons $\mathcal{A}_{\mathbf{P}}$, $\mathcal{A}_{\mathbf{F}}$ in the Fock spaces $\mathfrak{F}(\mathcal{H}_{\mathbf{P}})$, $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ of Definition 3.1 with horizon vacua $\Psi_{\mathbf{P}},gW_{\mathbf{F}}$. With these realizations, the homomorphisms $\chi_{\mathbf{P/F}}$ and $\pi_{\mathbf{P/F}}$ can be implemented by unitary transformations which preserve the vacuum states. More precisely, we have the following.*

(a) If $m>0$, the map that associates a positive frequency wave function ψ_+ in Rindler space with the element of $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,dE)$, $\phi:E\mapsto M_{m,\kappa}(E)\tilde{\psi}_+(E)$ extends into the unitary operator $U_{\mathbf{F}}:\mathfrak{F}(\mathcal{H})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ such that

$$U_{\mathbf{F}}\Psi_{\mathbf{R}}=\Psi_{\mathbf{F}}, \tag{55}$$

$$\chi_{\mathbf{F}}(\hat{A})=U_{\mathbf{F}}\hat{A}U_{\mathbf{F}}^{-1} \quad \textit{for all } \hat{A}\in\mathcal{A}_{\mathbf{R}}. \tag{56}$$

The analogous statement holds replacing **F** *for* **P**.

(b) If $m=0$, the maps which associate positive frequency wave functions $\psi_+^{(\mathrm{in})}$ and $\psi_+^{(\mathrm{out})}$ in Rindler space with respective elements of $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,dE)$ and $\mathcal{H}_{\mathbf{P}}\cong L^2(\mathbb{R}^+,dE)$, $\phi^{(\mathrm{in})}:E\mapsto\tilde{\psi}_+^{(\mathrm{in})}(E)$ and $\phi^{(\mathrm{out})}:E\mapsto\tilde{\psi}_+^{(\mathrm{out})}(E)$, extend into unitary operators $V_{\mathbf{F}}:\mathfrak{F}(\mathcal{H}_{(\mathrm{in})})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ and $V_{\mathbf{P}}:\mathfrak{F}(\mathcal{H}_{(\mathrm{out})})\to\mathfrak{F}(\mathcal{H}_{\mathbf{P}})$, such that

$$V_{\mathbf{F}}\Psi_{\mathbf{R}}^{(\mathrm{in})}=\Psi_{\mathbf{F}}\ , \qquad V_{\mathbf{P}}\Psi_{\mathbf{R}}^{(\mathrm{out})}=\Psi_{\mathbf{P}}, \tag{57}$$

$$\pi_{\mathbf{F}}(\hat{A})=V_{\mathbf{F}}\ \hat{A}\ V_{\mathbf{F}}^{-1} \quad \textit{for all } \hat{A}\in\mathcal{A}_{\mathbf{R}}^{(\mathrm{in})}, \tag{58}$$

$$\pi_{\mathbf{P}}(\hat{A})=V_{\mathbf{P}}\ \hat{A}\ V_{\mathbf{P}}^{-1} \quad \textit{for all } \hat{A}\in\mathcal{A}_{\mathbf{R}}^{(\mathrm{out})}. \tag{59}$$

Proof: (a) We consider the case of **F**, the case of **P** being similar. Under the identifications $\mathcal{H}\cong L^2(\mathbb{R}^+,dE)$ (Proposition 2.2) and $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,dE)$ (Proposition 3.3), consider the map $V:\mathcal{H}\ni\psi\mapsto\phi\in\mathcal{H}_{\mathbf{F}}$ where we have defined $\phi(E):=N_{m,\kappa}(E)\psi(E)$ for all $\psi\in\mathcal{H}$. V is a unitary transformation by construction since $N_{m,\kappa}$ is a smooth function with $|N_{m,\kappa}(E)|=1$ for all E as stated in Proposition 3.1. That unitary transformation can be extended into a unitary transformation $U_{\mathbf{F}}:\mathfrak{F}(\mathcal{H})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ by defining $U_{\mathbf{F}}\Psi_{\mathbf{R}}:=\Psi_{\mathbf{F}}$ and $U_{\mathbf{F}}\restriction_{\mathcal{H}_s^{\otimes n}}:=U_1\otimes\cdots\otimes U_n$ for all $n=1,2,3,\ldots$, where $\mathcal{H}_s^{\otimes n}$ indicates the symmetrized tensor product of n copies of $\mathcal{H}$ and $U_k=V$ for

$k=1,2,\ldots,n$. $U_{\mathbf{F}}$ preserves the vacuum states by construction and induces a unital-$*$-algebra homomorphism $\rho:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{F}}$ such that $\rho(A)=U_{\mathbf{F}}AU_{\mathbf{F}}^{-1}$ for every $A\in\mathcal{A}_{\mathbf{R}}$. To conclude the proof, by the uniqueness of $\chi_{\mathbf{F}}$ proven in Theorem 3.1, it is sufficient to show that $\rho(\hat{\phi}(f))=\chi_{\mathbf{F}}(\hat{\phi}(f))$ for every $f\in\mathcal{D}(\mathbf{R})$. To this end, take $f\in\mathcal{D}(\mathbf{R})$ and consider the positive-frequency part of $\psi:=Ef$, ψ_+. The construction used to define $U_{\mathbf{F}}$ implies that $U_{\mathbf{F}}a^\dagger(\psi_+)U_{\mathbf{F}}^{-1}=a^\dagger_{\mathbf{F}}(V\psi_+)$ and $U_{\mathbf{F}}a(\overline{\psi_+})U_{\mathbf{F}}^{-1}=a_{\mathbf{F}}(\overline{V\psi_+})$ and thus, by Definitions 3.1 and 3.2, $U_{\mathbf{F}}\hat{\phi}(f)U_{\mathbf{F}}^{-1}=\hat{\phi}_{\mathbf{F}}(\omega_f)$ where $\omega_f=2d\varphi_f$ with $\varphi_f(v)=\int_{\mathbb{R}^+}(e^{-iEv}/\sqrt{4\pi E})\,N_{m,\kappa}(E)\,\tilde{\psi}_+(E)\,dE+\text{c.c.}$. By (a) of Proposition 3.1, $\varphi_f=(Ef)\restriction_{\mathbf{F}}$ and thus it holds $\rho(\hat{\phi}(f))=U_{\mathbf{F}}\hat{\phi}(f)U_{\mathbf{F}}^{-1}=\chi_{\mathbf{F}}(\hat{\phi}(f))$, which concludes the proof. (b) The proof is strongly analogous to that in the massive case with obvious changes. □

Remark: Once again, the crucial difference between the massive and the massless case is that the Hilbert space of the bulk field is isomorphic to either the Fock spaces $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ and $\mathfrak{F}(\mathcal{H}_{\mathbf{P}})$ if $m>0$, whereas it is isomorphic to $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})\otimes\mathfrak{F}(\mathcal{H}_{\mathbf{P}})$ if $m=0$. In the latter case the unitary transformation $V_{\mathbf{F}}\otimes V_{\mathbf{P}}:\mathfrak{F}(\mathcal{H})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F}})\otimes\mathfrak{F}(\mathcal{H}_{\mathbf{P}})$ satisfies $(V_{\mathbf{F}}\otimes V_{\mathbf{P}})\Psi_{\mathbf{R}}=\Psi_{\mathbf{P}}\otimes\Psi_{\mathbf{F}}$ and $(\pi_{\mathbf{F}}\otimes\pi_{\mathbf{P}})(\hat{B})=(V_{\mathbf{F}}\otimes V_{\mathbf{P}})\,\hat{B}\,(V_{\mathbf{F}}^{-1}\otimes V_{\mathbf{P}}^{-1})$ for all $\hat{B}\in\mathcal{A}_{\mathbf{R}}$.

IV. HORIZON MANIFEST SYMMETRY

A. SL(2,$\mathbb{R}$) unitary representations on the horizon

Consider QFT on the future horizon $\mathbf{F}$ in the Fock representation of the algebra $\mathcal{A}_{\mathbf{F}}$ referred to the vacuum state $\Psi_{\mathbf{F}}$. The one-particle space $\mathcal{H}_{\mathbf{F}}$ is isomorphic to $L^2(\mathbb{R}^+,dE)$. An irreducible unitary representation $\widetilde{SL}(2,\mathbb{R})$, $g\mapsto U_{\mathbf{F}}^{(\mathbf{F})}(g)$, generated by the operators (27), $\overline{H_{\mathbf{F}0}}$, $\overline{C_{\mathbf{F}}}$ and $\overline{D_{\mathbf{F}}}$, with

$$H_{\mathbf{F}0}:=E,\qquad D_{\mathbf{F}}:=-i\left(\frac{1}{2}+E\frac{d}{dE}\right),\qquad C_{\mathbf{F}}:=-\frac{d}{dE}E\frac{d}{dE}+\frac{\left(k-\frac{1}{2}\right)^2}{E},\tag{60}$$

can uniquely be defined in $\mathcal{H}_{\mathbf{F}}$ as proven in Theorem 2.1. The operators (60) are defined on the dense invariant subspace $\mathcal{D}_k^{(\mathbf{F})}\subset L^2(\mathbb{R}^+,dE)\cong\mathcal{H}_{\mathbf{F}}$ which has the same definition as $\mathcal{D}_k$. If $m>0$, that representation induces an analogous representation in the one-bulk-particle space $\mathcal{H}$ through unitary holography. That is $SL(2,\mathbb{R})\ni g\mapsto U_g^{(\mathbf{F})}:=U_{\mathbf{F}}^{-1}U_gU_{\mathbf{F}}$ whose generators are $U_{\mathbf{F}}^{-1}\overline{H_{\mathbf{F}0}}U_{\mathbf{F}}$, $U_{\mathbf{F}}^{-1}\overline{D_{\mathbf{F}}}U_{\mathbf{F}}$ and $U_{\mathbf{F}}^{-1}\overline{C_{\mathbf{F}}}U_{\mathbf{F}}$. We stress that $g\mapsto U_g$ does *not* coincide with the analogous representation given in Theorem 2.1, but it is unitarily equivalent to that and thus (a) of Theorem 2.1 can be restated with trivial changes. Moreover (see below), $U_{\mathbf{F}}^{-1}\overline{H_{\mathbf{F}0}}U_{\mathbf{F}}$ still coincides with the Hamiltonian H of the bulk theory. As a consequence, also the analogs of points (b) and (c) in Theorem 2.1 can be restated for the representation $g\mapsto U_g^{\mathbf{F}}$ which, in turn, defines a $\widetilde{\mathrm{SL}}(2,\mathbb{R})$-*symmetry* of the system in the bulk by unitary holography. We are interested in *that* $\widetilde{\mathrm{SL}}(2,\mathbb{R})$-*symmetry* which is induced by the $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ unitary representation on the horizon QFT via (unitary) holography no matter the mass of the field in the bulk. We stress that this $\widetilde{\mathrm{SL}}(2,\mathbb{R})$-symmetry is *hidden* in the bulk because the same argument used in Sec. II E applies to this case, too; however, it could be manifest, in the sense of Sec. II E, when examined on the horizon. That is the issue we want to discuss in the following.

Everything we have said for $\mathbf{F}$ can be restated for $\mathbf{P}$ with obvious changes. If $m=0$ and using (b) of Theorem 3.2, everything we said above concerning the representations of $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ in $\mathcal{H}_{\mathbf{F}}$ and those induced on $\mathcal{H}$ by means of $U_{\mathbf{F}}$ can be restated concerning the triples $\mathcal{H}_{\mathbf{F}}$, $\mathcal{H}_{(\mathrm{in})}$, $V_{\mathbf{F}}$ and $\mathcal{H}_{\mathbf{P}}$, $\mathcal{H}_{(\mathrm{out})}$, $V_{\mathbf{P}}$ separately. Moreover, by the comment after Theorem 3.2, one sees that a pair of $\mathrm{SL}(2,\mathbb{R})$ representations in $\mathcal{H}_{\mathbf{F}}$ and $\mathcal{H}_{\mathbf{P}}$ naturally induces a *reducible* $\mathrm{SL}(2,\mathbb{R})$ on $\mathcal{H}$ by means of $V_{\mathbf{F}}\otimes V_{\mathbf{P}}$.

B. Horizon analysis of the bulk symmetry associated with $H_{\mathbf{F}0}$

Let us focus attention on the first generator $H_{\mathbf{F}0}$ in the case $m>0$. Concerning QFT on $\mathbf{P}$ and the case $m=0$, there are completely analogous results. From now on we use the following conventions referring to a representation of an algebra of observables $\mathcal{A}$ in a symmetrized Fock space $\mathfrak{F}(\mathcal{H})$. If X is a self-adjoint operator in the one-particle Hilbert space $\mathcal{H}$ and $\hat{A}\in\mathcal{A}$, $\hat{A}_\tau^{(X)} := e^{i\tau\mathbf{X}}\hat{A}e^{-i\tau\mathbf{X}}$, where $\mathbf{X}:=0\oplus X\oplus(X\otimes I+I\otimes X)\oplus\cdots$ is the operator naturally associated with X in the Fock space $\mathfrak{F}(\mathcal{H})=\mathbb{C}\oplus\mathcal{H}\oplus(\mathcal{H}\otimes\mathcal{H})_s\oplus\cdots$. In other words, $\hat{A}_\tau^{(X)}$ is the *Heisenberg evolution* of $\hat{A}$ at time τ with respect to the noninteracting multiparticle Hamiltonian $\mathbf{X}$ induced by the one-particle Hamiltonian X. We have the following theorems.

Theorem 4.1: *Unitary holography associates the self-adjoint operator* $\overline{H_{\mathbf{F}0}}$ *with the one-particle Hamiltonian in the bulk H (25), i.e.,*

$$U_{\mathbf{F}}^{-1}\overline{H_{\mathbf{F}0}}U_{\mathbf{F}}=H. \tag{61}$$

Defining $H_{\mathbf{F}}:=\overline{H_{\mathbf{F}0}}$, *the following further statements hold.*

(a) Referring to Fock representations of algebras of observables $\mathcal{A}_{\mathbf{R}}$ *and* $\mathcal{A}_{\mathbf{F}}$ *on vacuum states* $\Psi_{\mathbf{R}}$ *and* $\Psi_{\mathbf{F}}$, *Heisenberg-like evolution is preserved by unitary holography:*

$$U_{\mathbf{F}}\hat{A}_\tau^{(H)}U_{\mathbf{F}}^{-1}=(U_{\mathbf{F}}\hat{A}U_{\mathbf{F}}^{-1})_\tau^{(H_{\mathbf{F}})}. \tag{62}$$

(b) $\{e^{i\tau H_{\mathbf{F}}}\}_{\tau\in\mathbb{R}}$ *induces, via (42), a group of transformations* $\{\alpha_\tau^{(\partial_v)}\}_{\tau\in\mathbb{R}}$ *of horizon wave functions* φ *such that*

$$(\alpha_\tau^{(\partial_v)}(\varphi))(v):=\varphi(v-\tau)\quad \text{for all } \varphi\in\mathcal{S}(\mathbf{F}) \text{ and } v\in\mathbb{R}. \tag{63}$$

That is the same group of transformations of functions induced by the group of diffeomorphisms of $\mathbf{F}$ *generated by the vector field* ∂_v.

(c) If $\{\alpha_\tau^{(\partial_t)}\}_{\tau\in\mathbb{R}}$ *denotes the one-parameter group of Rindler-time displacements of Rindler wave functions (see Sec. II D),*

$$\alpha_\tau^{(\partial_v)}(\psi\restriction_{\mathbf{F}})=(\alpha_\tau^{(\partial_t)}(\psi))\restriction_{\mathbf{F}}\quad \text{for all } \psi\in\mathcal{S}. \tag{64}$$

Proof: Consider the self-adjoint operator on $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,dE)$:

$$(H_{\mathbf{F}}f)(E):=Ef(E)\quad \text{for}\quad f\in\mathcal{D}(H_{\mathbf{F}})=\left\{h\in L^2(\mathbb{R}^+,dE)\;\middle|\;\int_0^{+\infty}E^2|h(E)|^2dE<+\infty\right\}. \tag{65}$$

Since $\mathcal{D}_k^{(\mathbf{F})}\subset\mathcal{D}(H_{\mathbf{F}})$ and $H_{\mathbf{F}0}=H$ in $\mathcal{D}_k^{(\mathbf{F})}$ where $H_{\mathbf{F}0}$ is essentially self-adjoint, it must hold $H_{\mathbf{F}}=\overline{H_{\mathbf{F}0}}$. The definition of $U_{\mathbf{F}}$ (its restriction to $\mathcal{H}$ is sufficient) given in (a) in Theorem 3.2, (25) and (65) entail (61). (a) is an immediate consequence of (61). (b) By Proposition 3.2 and (42), $\varphi\in\mathcal{S}(\mathbf{F})$ is the Fourier (anti)transform of a Schwartz' function f with $\tilde{\varphi}_+(E)=\sqrt{E}f(E)$ if $E\geqslant 0$ and the application of $e^{i\tau H_{\mathbf{F}}}$ on $\tilde{\varphi}_+$ changes f into $\mathbb{R}\ni E\mapsto e^{iE\tau}f(E)$ which still is a Schwartz' function. Hence, $\alpha_\tau^{(\partial_t)}(\varphi)$ is constructed by (1) Fourier transforming φ into f, (2) replacing $f(E)$ by $e^{iE\tau}f(E)$ and (3) transforming back that function into $\alpha_\tau^{(\partial_t)}(\varphi)$ via Fourier transformation. By direct inspection one finds $(\alpha_\tau^{(\partial_t)}(\varphi))(v)=\varphi(v-\tau)$ trivially. (c) In $\mathcal{H}\cong L^2(\mathbb{R}^+,dE)$ and $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,dE)$, (61) states that both $e^{i\tau H}$ and $e^{i\tau H_{\mathbf{F}}}$ are represented by the same multiplicative operator $e^{i\tau E}$ in the respective spaces. Then (14) and (34) imply (64). □

Remark: Since the one-parameter unitary group generated by $H_{\mathbf{F}}$ turns out to be associated with a vector field of $\mathbf{F}$, ∂_v, which induces a group of (orientation-preserving) diffeomorphisms, the bulk-symmetry generated by $H_{\mathbf{F}}$ via unitary holography is *manifest* also on the horizon.

The machinery can be implemented at algebraic level. To this end, using the relation (see Proposition 3.4) $\omega=2dE_{\mathbf{F}}\omega$, define the one-parameter group of transformations of forms ω

$\in \mathcal{D}(\mathbf{F})$ $\{\beta_\tau^{(\partial_v)}\}_{\tau\in\mathbb{R}}$, where $(\beta_\tau^{(\partial_v)}(\omega))(v) := 2d(\alpha_\tau^{(\partial_v)}(E_{\mathbf{F}}\omega))$. Finally, define the action of $\beta_\tau^{(\partial_v)}$ on quantum fields as $\gamma_\tau^{(\partial_v)}(\phi_{\mathbf{F}}(\omega)) := \phi_{\mathbf{F}}(\beta_{-\tau}^{(\partial_v)}(\omega))$, for $\omega \in \mathcal{D}(\mathbf{F},\mathbb{C})$. One has the following result.

Theorem 4.2: *The transformations $\gamma_\tau^{(\partial_v)}$, $\tau\in\mathbb{R}$, uniquely extended into a group of automorphisms of $\mathcal{A}_{\mathbf{F}}$, $\{\gamma_\tau^{(\partial_v)}\}_{\tau\in\mathbb{R}}$ such that*

(a) if $\{\gamma_\tau^{(\partial_t)}\}_{\tau\in\mathbb{R}}$ denotes the analogous group of automorphisms of the bulk algebra $\mathcal{A}_{\mathbf{R}}$ generated by Rindler time-displacements,

$$(\chi_{\mathbf{F}}\circ\gamma_\tau^{(\partial_t)})(A) = (\gamma_\tau^{(\partial_v)}\circ\chi_{\mathbf{F}})(A) \quad \text{for all} \quad A\in\mathcal{A}_{\mathbf{F}} \quad \text{and} \quad \tau\in\mathbb{R}. \tag{66}$$

(b) In the Fock space realization of $\mathcal{A}_{\mathbf{F}}$ referred to $\Psi_{\mathbf{F}}$,

$$(\hat{B})_\tau^{(H_{\mathbf{F}})} = \gamma_\tau^{(\partial_v)}(\hat{B}) \quad \text{for all} \quad \hat{B}\in\mathcal{A}_{\mathbf{F}} \quad \text{and} \quad \tau\in\mathbb{R}. \tag{67}$$

Sketch of proof: $\alpha_\tau^{(\partial_v)}(E_{\mathbf{F}}\omega) = E_{\mathbf{F}}\beta_\tau^{(\partial_v)}(\omega)$, the preservation of the symplectic form under the action of $\alpha_\tau^{(\partial_v)}$ and Proposition 3.4 entail $E_{\mathbf{F}}(\beta_\tau^{(\partial_v)}(\omega),\beta_\tau^{(\partial_v)}(\omega')) = E_{\mathbf{F}}(\omega,\omega')$. This property trivially extended to complex valued forms. $\gamma_\tau^{(\partial_v)}$ must be extended on the whole algebra $\mathcal{A}_{\mathbf{F}}$ requiring the preservation of the unital $*$-algebra structure. The proof of the existence of such an extension is based on the preservation of the causal propagator established above. If $A=\phi(f)$, (66) is an immediate consequence of (64) and the definition of $\chi_{\mathbf{F}}$ in Theorem 3.2. Then (66) extends to the whole algebra since $\gamma_\tau^{(\partial_v)}$, $\gamma_\tau^{(\partial_t)}$ and $\chi_{\mathbf{F}}$ are homomorphisms. Equation (67) is an immediate consequence of the fact that $\gamma_\tau^{(\partial_v)}(\hat{\phi}_{\mathbf{F}}(\omega))$ is the Heisenberg-like evolution of $\hat{\phi}_{\mathbf{F}}(\omega)$ induced by the "Hamiltonian" $H_{\mathbf{F}}$ and evaluated at "time" τ. □

C. Horizon analysis of the bulk symmetry associated with $D_{\mathbf{F}}$

Let us examine the properties of the unitary one-parameter group, $\{e^{i\,\overline{\mu D_{\mathbf{F}}}}\}_{\mu\in\mathbb{R}}$.

Theorem 4.3: *The unitary one-parameter group, $\{e^{i\,\overline{\mu D_{\mathbf{F}}}}\}_{\mu\in\mathbb{R}}$ enjoys the following properties.*
(a) If $\tilde{\varphi}\in L^2(\mathbb{R}^+,dE)\cong\mathcal{H}_{\mathbf{F}}$, *for all* $\mu\in\mathbb{R}$ and $E\in\mathbb{R}^+$,

$$(e^{i\mu\,\overline{D_{\mathbf{F}}}}\tilde{\varphi})(E) = e^{\mu/2}\tilde{\varphi}(e^{\mu}E). \tag{68}$$

(b) By means of (42), $\{e^{i\,\overline{\mu D_{\mathbf{F}}}}\}_{\mu\in\mathbb{R}}$ induces a group $\{\alpha_\mu^{(v\partial_v)}\}_{\mu\in\mathbb{R}}$ of transformations of horizon wave functions φ with

$$(\alpha_\mu^{(v\partial_v)}(\varphi))(v) := \varphi(e^{-\mu}v) \tag{69}$$

for all $\varphi\in\mathcal{S}(\mathbf{F})$ and $\mu\in\mathbb{R}$. $\{\alpha_\mu^{(v\partial_v)}\}_{\mu\in\mathbb{R}}$ is the same group of transformations of functions associated with the group of diffeomorphisms of $\mathbf{F}$ induced by the vector field $v\partial_v$.

Sketch of proof: (a) Consider the one-parameter group of unitary operators $\{V_\mu\}_{\mu\in\mathbb{R}}$ with $V_\mu(\tilde{\varphi})(E) = e^{\mu/2}\tilde{\varphi}(e^{\mu}E)$, for $\tilde{\varphi}\in L^2(\mathbb{R}^+,dE)$. For every $f\in\mathcal{D}_k^{(\mathbf{F})}$, $\langle f, V_\mu\tilde{\varphi}\rangle = \langle V_{-\mu}f,\tilde{\varphi}\rangle$. On the other hand, using the definition of Schwartz space and Lebesgue's dominated-convergence theorem, it is simply proven that $V_{-\mu}f\to f$ as $\mu\to 0$ and so $\langle f,V_\mu\tilde{\varphi}\rangle\to\langle f,\tilde{\varphi}\rangle$ as $\mu\to 0$ for every $f\in\mathcal{D}_k^{(\mathbf{F})}$ which is dense in $L^2(\mathbb{R}^+,dE)$. As a consequence $\{V_\mu\}_{\mu\in\mathbb{R}}$ is weakly continuous, and thus strongly continuous it being made of unitary operators, and Stone's theorem can be used. With a similar procedure (also using Lagrange's theorem to estimate an incremental ratio) one gets that, if $\tilde{\varphi}\in\mathcal{D}_k^{(\mathbf{F})}$ and interpreting the derivative in the topology of $L^2(\mathbb{R}^+,dE)$, $d/d\mu\,|_{\mu=0}(V_\mu\tilde{\varphi})$ can be computed pointwisely. A straightforward calculation of the pointwise derivative gives $d/d\mu\,|_{\mu=0}(V_\mu\tilde{\varphi}) = i(D_{\mathbf{F}})\tilde{\varphi}$. Stone's theorem implies that generator G of $V_\mu = e^{i\mu G}$ is well-defined on $\mathcal{D}_k^{(\mathbf{F})}$ and coincides with $D_{\mathbf{F}}$ therein. Since $D_{\mathbf{F}}$ is essentially self-adjoint on that domain it must be $G=\overline{D_{\mathbf{F}}}$ and this proves (a). (b) Take $\varphi\in\mathcal{S}(\mathbf{F})$, use the decomposition (42) as in the proof of Theorem 4.1, and transform $\tilde{\varphi}_+\in L^2(\mathbb{R},dE)$ under the action of $e^{i\,\overline{\mu D_{\mathbf{F}}}}$ taking (68) into account.

With a trivial change of variables in the decomposition (42) one sees that, if φ belongs to Schwartz' space, the obtained transformed wave function is just $\varphi(e^{-\mu}v)$ which still is in $\mathcal{S}(\mathbf{F})$.□

Remark: Since the one-parameter unitary group generated by $D_{\mathbf{F}}$ turns out to be associated with the vector field of $\mathbf{F}$, $v\partial_v$, which induces a group of (orientation-preserving) diffeomorphisms, the bulk-symmetry generated by $D_{\mathbf{F}}$ via unitary holography is *manifest* on the horizon.

Once again the machinery can be implemented at algebraic level. We consider the group associated with $v\partial_v$ only. Define the one-parameter group of transformations of forms $\omega \in \mathcal{D}(\mathbf{F})$, $\{\beta_\tau^{(v\partial_v)}\}_{\tau\in\mathbb{R}}$, with $(\beta_\tau^{(v\partial_v)}(\omega))(v) := 2d(\alpha_\tau^{(v\partial_v)}(E_{\mathbf{F}}\omega))$. Finally, extend the action of $\beta_\tau^{(v\partial_v)}$ on quantum fields as $\gamma_\tau^{(v\partial_v)}(\phi_{\mathbf{F}}(\omega)) := \phi_{\mathbf{F}}(\beta_{-\tau}^{(v\partial_v)}(\omega))$, for $\omega\in\mathcal{D}(\mathbf{F},\mathbb{C})$. The following result, whose proof is essentially the same as that of the relevant part of Theorem 4.2, holds.

Theorem 4.4: *Transformations $\gamma_\tau^{(v\partial_v)}$ uniquely extended into a one-parameter group of automorphisms of $\mathcal{A}_{\mathbf{F}}$, $\{\gamma_\tau^{(v\partial_v)}\}_{\tau\in\mathbb{R}}$ such that in the Fock space realization of $\mathcal{A}_{\mathbf{F}}$ referred to $\Psi_{\mathbf{F}}$,*

$$(\hat{B})_\tau^{(\overline{D_{\mathbf{F}}})} = \gamma_\tau^{(v\partial_v)}(\hat{B}) \quad \textit{for all} \quad \hat{B}\in\mathcal{A}_{\mathbf{F}} \quad \textit{and} \quad \tau\in\mathbb{R}. \tag{70}$$

D. Horizon analysis of the unitary group generated by $C_{\mathbf{F}}$

The analysis of the action of the group generated by $C_{\mathbf{F}}$ is much more complicated than the other considered cases. The point is the following. A necessary condition to associate with a transformed state $e^{i\overline{tC_{\mathbf{F}}}}\psi$ ($\psi\in\mathcal{H}_{\mathbf{F}}$) a wave function of $\mathcal{S}(\mathbf{F})$ by (43) (with $\tilde{\varphi}_+ = e^{i\overline{tC_{\mathbf{F}}}}\psi$ and taking the real part of the right-hand side) is that $e^{i\overline{tC_{\mathbf{F}}}}\psi$ belong to the domain of $H_{\mathbf{F}}^{-1/2}$. Indeed in the general case (43) must be interpreted as the Fourier–Plancherel transform of the $L^2(\mathbb{R},dE)$ function given by 0 if $E<0$ and $((4\pi H_{\mathbf{F}})^{-1/2}e^{i\overline{tC_{\mathbf{F}}}}\psi)(E)$ if $E\geqslant 0$. Notice that this is the unique unitary extension of the Fourier transform defined on $L^2(\mathbb{R},dE)$. That requirement is, in fact, fulfilled concerning $e^{i\overline{uH_{\mathbf{F}}+vD_{\mathbf{F}}}}\psi$ if $\psi\in\mathcal{S}(\mathbf{F})$ because $e^{i\overline{uH_{\mathbf{F}}+vD_{\mathbf{F}}}}\psi\in\mathcal{S}(\mathbf{F})$ and so the usual Fourier transformation is sufficient to interpret the formalism. Concerning $C_{\mathbf{F}}$ the situation needs a careful treatment and the space $\mathcal{S}(\mathbf{F})$ must, in fact, be changed in order to assure that $e^{i\overline{tC_{\mathbf{F}}}}\psi$ belongs to the domain of $H_{\mathbf{F}}^{-1/2}$. There are several possibilities to do it at least in the case $k=1$ in the definition of $C_{\mathbf{F}}$. To go on we need some preliminary results. If $k=1$, focus attention on the operator analogous to K in the proof of Theorem 2.1, $K_{\mathbf{F}} := (\frac{1}{2})(\beta H_{\mathbf{F}0} + \beta^{-1}C_{\mathbf{F}})$. It is known[1] that $\sigma(\overline{K_{\mathbf{F}}}) = \{1,2,\ldots\}$ (no matter the value of $\beta>0$) with corresponding eigenvectors $Z_1^{(1)}, Z_2^{(1)},\ldots$ (which do depend on β) given in (26). Thus defining $\Theta := e^{i\pi\overline{K_{\mathbf{F}}}}$ one also gets $\Theta = \Theta^\dagger = \Theta^{-1}$. $\{\Theta, I\}$ is the image under $U^{\mathbf{F}}$ of the discrete subgroup $\{\vartheta, \vartheta^2 = -I, \vartheta^3 = -\vartheta, \vartheta^4 = I\} \subset \mathrm{SL}(2,\mathbb{R})$ with

$$\vartheta = \begin{bmatrix} 0 & \beta \\ -\beta^{-1} & 0 \end{bmatrix} = e^{\pi(\beta h + \beta^{-1}c)/2}\,. \tag{71}$$

Proposition 4.1: Fix $k=1$ in the definition (60) so that the representation of $\widetilde{\mathrm{SL}}(2,\mathbb{R})$ is in fact a representation of $\mathrm{SL}(2,\mathbb{R})$. For every $\beta>0$,

$$\Theta\ \beta H_{\mathbf{F}}\ \Theta = \frac{1}{\beta}\overline{C_{\mathbf{F}}} \quad , \quad \Theta\ \overline{D_{\mathbf{F}}}\ \Theta = -\overline{D_{\mathbf{F}}}\,, \tag{72}$$

$-\Theta$ is nothing but the J_1-Hankel unitary transform:

$$(-\Theta\psi)(E) := \beta \lim_{M\to+\infty} \int_0^M J_1(\beta\sqrt{4EE'})\psi(E')dE', \quad \textit{for all} \quad \psi\in L^2(\mathbb{R}^+,dE), \tag{73}$$

where the limit is computed in the norm of $L^2(\mathbb{R}^+,dE)$ and coincides with the L^1 integral over $\mathbb{R}^+$ if $E\mapsto E^{-1/4}\psi(E)$ belongs to $L^1(\mathbb{R}^+,dE)$ and $E\mapsto\sqrt{E}\psi(E)$ belongs to $L^1([0,1],dE)$.

Sketch of proof: By Stone's theorem, identities in (72) are equivalent to analog identities with self-adjoint operators $H_{\mathbf{F}}$, $\overline{C_{\mathbf{F}}}$ and $\overline{D_{\mathbf{F}}}$ replaced by the respectively generated one-parameter uni-

tary groups. In that form, the thesis can be proven, first for the corresponding one-parameter groups in SL(2,$\mathbb{R}$), using simple analytic procedures based on the uniqueness theorem of the matrix-valued solutions of differential equations, and then the result can be extended to unitary operators using the representation introduced in Theorem 2.1. The second part arises straightforwardly from Chap. 9 in Ref. 31 with trivial adaptations of the definitions. □

Proposition 4.2: Take $\varphi \in \mathcal{S}(\mathbf{F})$ *using notation as in (42), define* $\widetilde{\varphi}_{\beta+} := \Theta\widetilde{\varphi}_+$ *and*

$$\varphi_\beta(v) = \varphi\left(-\frac{\beta^2}{v}\right) - \varphi(0) \quad \text{for all} \quad v \in \mathbf{F}. \tag{74}$$

(a) $\varphi \mapsto \varphi_\beta$ *is the transformation induced by* Θ *on wave functions, i.e., (42) holds by replacing* φ *for* φ_β *and* $\widetilde{\varphi}_+$ *for* $\widetilde{\varphi}_{\beta+}$.

(b) If $X := (\beta/2)\,\partial_v + (1/2\beta)\,v^2\partial_v$ *and* $\alpha^{(X)}_\epsilon(\varphi)$ *denotes the natural action of the local one-parameter group of diffeomorphisms generated by X on* φ, *the first term in the right-hand side of (74) is*

$$\lim_{\epsilon\to\pi}(\alpha^{(X)}_\epsilon(\varphi))(v)\,, \quad \text{for all} \quad v \in \mathbf{F}. \tag{75}$$

Sketch of proof: By hypotheses $\widetilde{\varphi}_+$ satisfies the conditions which enables us to represent $\Theta\widetilde{\varphi}_+$ as in (73). In that case, by the expansion of $J_1(x)$ at $x=0$, one sees that the L^2, and continuous on $(0,+\infty)$, function $E \mapsto (\Theta\widetilde{\varphi}_+)(E)$ is $O(E^{1/2})$ as $E \to 0^+$ and thus it belongs to the domain of $H_{\mathbf{F}}^{-1/2}$. Using Fubini–Tonelli's and dominated convergence theorems we have that $\varphi_\beta(v)$ reads (where the limit in the left-hand side is in the L^2-convergence sense)

$$\lim_{\epsilon\to 0^+}\int_0^\infty e^{-iE(v-i\epsilon)}\frac{(\Theta\widetilde{\varphi}_+)(E)}{\sqrt{4\pi E}}dE = -\beta\int_0^\infty \lim_{\epsilon\to 0^+}\left(\int_0^\infty e^{-iE(v-i\epsilon)}\frac{J_1(\beta\sqrt{4EE'})}{\sqrt{4\pi E}}dE\right)\widetilde{\varphi}_+(E')dE'.$$

The limit on the right-hand side can explicitly be computed by using known results,[24] obtaining that it is $(e^{iE'\beta^2/v}-1)/\sqrt{4\pi E'}$. This result produces $\varphi_\beta(v) = \varphi(-\beta^2/v) - \varphi(0)$. Concerning the second statement, it is simply proven that, for $\epsilon \in (-\pi,\pi)$,

$$(\alpha^{(X)}_\epsilon(\varphi))(v) = \varphi\left(\frac{-\beta^2\tan(\epsilon/2)+\beta v}{\beta + v\tan(\epsilon/2)}\right).$$

With our hypotheses for φ, the limit as $\epsilon \to \pi$ is well defined for every $v \in \mathbb{R}$ and proves the statemet in (b). □

By direct inspection and using (74) one sees that, if $\varphi \in \mathcal{S}(\mathbf{F})$, usually $\varphi_\beta \notin \mathcal{S}(\mathbf{F})$, but $\varphi_\beta \in \mathsf{W}_\infty(\mathbb{R})$ in any case, the latter being the Sobolev space of the C^∞ complex-valued functions which are $L^2(\mathbb{R},dv)$ with all of derivatives of every order.

Now, using (72), the geometric action of $e^{i\lambda\,\overline{C_{\mathbf{F}}}} = \Theta e^{i\lambda\beta^2 H_{\mathbf{F}}}\Theta$ can easily be computed for wave functions φ of $\mathcal{S}(\mathbf{F})$ such that $\varphi(0)=0$ and $v \mapsto \varphi(-1/v)$ still belongs to $\mathcal{S}(\mathbf{F})$. Take such a φ, extract $\widetilde{\varphi}_+$ and apply Θ. The resulting wave function is an element of $\mathcal{S}(\mathbf{F})$ by Proposition 4.2. The application of the one-parameter group generated by $\beta^2 H_{\mathbf{F}}$, $e^{i\lambda\beta^2 H_{\mathbf{F}}}$, gives rise to wave functions (see Theorem 4.1) $v \mapsto \varphi(-\beta^2/(v-\beta^2\lambda))$ which still belongs to $\mathcal{S}(\mathbf{F})$. Finally, since it is possible, apply Θ once again. All that procedure is equivalent to applying the group $e^{i\lambda\,\overline{C_{\mathbf{F}}}} = \Theta e^{i\lambda\beta^2 H_{\mathbf{F}}}\Theta$, on the initial $\widetilde{\varphi}_+$. By this way one gets that the following theorem.

Theorem 4.5: *Consider the horizon wave functions* $\varphi \in \mathcal{S}(\mathbf{F})$ *such that* $\varphi(0)=0$ *and* $v \mapsto \varphi(-1/v)$ *still belongs to* $\mathcal{S}(\mathbf{F})$. *The unitary group,* $\{e^{i\lambda\,\overline{C_{\mathbf{F}}}}\}_{\lambda\in\mathbb{R}}$ *induces a class* $\{\alpha^{(v^2\partial_v)}_\lambda\}_{\lambda\in\mathbb{R}}$ *of transformations of the said wave functions by means of (42), with*

$$(\alpha^{(v^2\partial_v)}_\lambda(\varphi))(v) := \varphi\left(\frac{v}{1+\lambda v}\right) - \varphi\left(\frac{1}{\lambda}\right), \quad \text{for all} \quad \lambda \in \mathbb{R}. \tag{76}$$

The transformation of wave functions defined by the first term on the right-hand side of (76) is that generated by the local *group of diffeomorphisms of* $\mathbf{F}$ *associated with the field* $v^2\partial_v$.

Remarks: (1) In our hypotheses, $\alpha_\lambda^{(v^2\partial_v)}(\varphi)\in \mathsf{W}_\infty(\mathbb{R})$, but in general $\alpha_\lambda^{(v^2\partial_v)}(\varphi)\notin \mathcal{S}(\mathbf{F})$ so that the class of transformations does not define a group of transformations of wave functions in $\mathcal{S}(\mathbf{F})$. It is worthwhile stressing that these transformations define a group when working on the space $\mathcal{E}_\mathbf{F}$ of complex wave functions $\psi=\psi(v)$ whose positive-frequency and negative-frequency parts of Fourier transform are linear combinations of functions $E\mapsto Z_n^{(1)}(|E|)/\sqrt{4\pi|E|}$. In fact $\mathcal{E}_\mathbf{F}$ is invariant under (76). On the other hand, $\mathcal{E}_\mathbf{F}\cap(\mathcal{S}(\mathbf{F})+i\mathcal{S}(\mathbf{F}))=\varnothing$.

(2) The integral curves of the field $v^2\partial_v$, $v(t)=v(0)/(1-tv(0))$, have domain which *depends on the initial condition*: That is, $\mathbb{R}\backslash\{1/v(0)\}$, and $v(t)$ diverges if t approaches the singular point [barring the initial condition $v(0)=0$ that produces a constant orbit]. Thus the one-parameter group of (orientation-preserving) diffeomorphisms generated by $v^2\partial_v$ is only *local*. However, as the functions in $\mathcal{S}(\mathbf{F})$ vanish at infinity with all their derivatives, the singular point of the domain is harmless in (76).

(3) It makes sense to extend the definition of symplectically smeared field operator when $\varphi\in \mathsf{W}_\infty(\mathbb{R})$ by means of Definition 3.1. Indeed the Fourier–Plancherel transform of φ, f satisfies $\int_{\mathbb{R}^+}(1+|E|^k)^2|f(E)|^2dE<\infty$, for $k=0,1,2,\ldots$, and so $\mathbb{R}^+\ni E\to\tilde{\varphi}_+(E):=\sqrt{4\pi E}f(E)$ is a one-particle quantum state of $L^2(\mathbb{R}^+,dE)$. With the same hypotheses $E_\mathbf{F}d\varphi$ is well-defined, in particular $d^k\varphi(v)/dv^k\to 0$ as $v\to\pm\infty$ for $k=0,1,2,\ldots$: by elementary calculus and Cauchy–Schwartz inequality, every $d^k\varphi(v)/dv^k$ is uniformly continuous. If $d^k\varphi(v)/dv^k\not\to 0$ as $v\to\pm\infty$ for some k, there are $\epsilon>0$ and a sequence of intervals I_n with $\int_{I_n}dv=l>0$ and $|d^k\varphi(v)/dv^k\restriction_{I_n}|>\epsilon$. Thus $\int_\mathbb{R}|d^k\varphi(v)/dv^k|^2dv=\infty$ which is impossible. Moreover, $E_\mathbf{F}d\varphi$ enjoys the relevant properties stated in Proposition 3.4 and 3.5. Then enlarging $\mathcal{D}(\mathbf{F},\mathbb{C})$ to include elements $\omega=d\varphi$ where φ is real and belongs to $\mathsf{W}_\infty(\mathbb{R})$, one can define $\hat{\phi}(\omega)$ as in Definition 3.2, not affecting the relevant properties stated in Proposition 3.4 and 3.5. By this way, the algebraic approach can be implemented in terms of formal quantum fields smeared by functions of $\mathsf{W}_\infty(\mathbb{R})$.

The action of the one-group generated by $C_\mathbf{F}$ can be implemented at algebraic level. If $\omega\in\mathcal{D}(\mathbf{F})$ [without the enlargement said in the remark (3) above], one can define $(\beta_\tau^{(v^2\partial_v)}(\omega)):=2d(\alpha_\tau^{(v^2\partial_v)}(E_\mathbf{F}\omega))$. By direct inspection one sees that each $\alpha_\tau^{(v^2\partial_v)}$ preserves the symplectic form $\Omega_\mathbf{F}$ and each $\beta_\tau^{(v^2\partial_v)}$ preserves the causal propagator $E_\mathbf{F}$. Notice that these results are not evident *a priori* since the action of $\alpha_\tau^{(v^2\partial_v)}$ (76) is not that canonically induced by a vector field. Finally, extend the action of $\beta_\tau^{(v^2\partial_v)}$ on quantum fields as $\gamma_\tau^{(v^2\partial_v)}(\phi_\mathbf{F}(\omega)):=\phi_\mathbf{F}(\beta_{-\tau}^{(v\partial_v)}(\omega))$, for $\omega\in\mathcal{D}(\mathbf{F},\mathbb{C})$. The following result, whose proof is essentially the same as that of the relevant part of Theorem 4.2, holds.

Theorem 4.6: *Transformations* $\gamma_\tau^{(v^2\partial_v)}$ *uniquely extended into a one-parameter class of automorphisms of* $\mathcal{A}_\mathbf{F}$, $\{\gamma_\tau^{(v^2\partial_v)}\}_{\tau\in\mathbb{R}}$ *such that in the Fock space realization of* $\mathcal{A}_\mathbf{F}$ *referred to* $\Psi_\mathbf{F}$,

$$(\hat{B})_\tau^{(\overline{C_\mathbf{F}})}=\gamma_\tau^{(v^2\partial_v)}(\hat{B})\quad \textit{for all}\quad \hat{B}\in\mathcal{A}_\mathbf{F}\ \textit{and}\ \tau\in\mathbb{R}. \tag{77}$$

E. The full SL(2,$\mathbb{R}$) action

To conclude we show the general action of $\{U_g^{(\mathbf{F})}\}_{g\in \mathrm{SL}(2,\mathbb{R})}$ on horizon wave functions. With a strightforward generalization of the notion of manifest symmetry due to the appearance of the addend on the right-hand side of (79) below, the symmetry associated with the whole group SL(2,$\mathbb{R}$) can be considered as *manifest*. We leave possible comments on the field algebra extension to the reader. Remind that $\vartheta:=e^{\pi(\beta h+\beta^{-1}c)/2}\in\mathrm{SL}(2,\mathbb{R})$ and consider

$$A=\begin{bmatrix} a & b\\ c & d\end{bmatrix}\in\mathrm{SL}(2,\mathbb{R}). \tag{78}$$

Referring to (71) and generators (29), only one of the following facts holds for suitable λ,μ,τ uniquely determined by a,b,c,d in the examined cases: If $a>0$, $A=e^{\lambda c}e^{\mu d}e^{\tau h}$ or, if $a<0$, $A=\vartheta e^{\lambda c}e^{\mu d}e^{\tau h}$, or, if $a=0$ and $b>0$, $A=\vartheta e^{\mu d}e^{\tau h}$, or, if $a=0$ and $b<0$, $A=\vartheta^3 e^{\mu d}e^{\tau h}$. Using these decompositions, part of Theorems 4.1, 4.3, and 4.5, and Proposition 4.2, the following final theorem can simply be proven.

Theorem 4.7: *Take $\varphi\in\mathcal{S}(\mathbf{F})$ such that $\varphi(0)=0$ and $v\mapsto\varphi(-1/v)$ still belongs to $\mathcal{S}(\mathbf{F})$. If $A\in \mathrm{SL}(2,\mathbb{R})$ has the form (78), let $\alpha^{(A)}(\varphi)$ denote the right-hand side of (42) with $\tilde{\varphi}_+$ replaced for $U_A^{(\mathbf{F})}\tilde{\varphi}_+$ where $\tilde{\varphi}_+$ is defined as in* (41). *For $v\in\mathbb{R}$ it holds*

$$(\alpha^{(A)}(\varphi))(v)=\varphi\left(\frac{dv-b}{a-cv}\right)-\varphi\left(-\frac{d}{c}\right). \tag{79}$$

The second term on the right-hand side disappears if either $d=0$ or $c=0$. Finally, the transformation of wave functions defined by the first term on the right-hand side of (79) is that generated by the local group of diffeomorphisms of **F** *generated by the basis of fields $\partial_v, v\partial_v, v^2\partial_v$.*

Remark: From a pure geometric point of view, the $\mathrm{SL}(2,\mathbb{R})$ symmetry is associated to the Lie algebra of fields ∂_v, $v\partial_v$, $v^2\partial_v$. This suggests to focus on the set of fields defined on **F**, $\{\mathcal{L}_n\}_{n\in\mathbb{Z}}$ with

$$\mathcal{L}_n := -v^{n+1}\partial_v, \qquad n\in\mathbb{Z}. \tag{80}$$

By direct inspection one gets that, if $\{\,,\}$ denotes the Lie bracket of vector fields,

$$\{\mathcal{L}_n,\mathcal{L}_m\}=(n-m)\ \mathcal{L}_{n+m}, \tag{81}$$

that is, the generators $\mathcal{L}_n$ span a Virasoro algebra without central charge. We remark that, in fact, the fields $\mathcal{L}_n$ with $n<0$ are not smooth since a singularity arises at $v=0$. It is anyway interesting to investigate the issue of the quantum representation of that Lie algebra in terms of one-particle operators of a quantum field defined on the horizon perhaps in the whole Fock space. At quantum level a central charge could appear. This is just the main goal of the subsequent paper.[19] In that paper we show that, in fact, a suitable and natural enlargement in the Fock space of the hidden $\mathrm{SL}(2,\mathbb{R})$ symmetry gives rise to a positive-energy unitary Virasoro algebra representation. That representation has quantum central charge $c=1$. The Virasoro algebra of operators gets a manifest geometrical meaning if referring to the holographically associated QFT on the event horizon: It is nothing but a representation of the algebra of vector fields defined on the event horizon equipped with a point at infinity. All that happens provided the Virasoro ground energy $h:=\mu^2/2$ vanishes and, in that case, the Rindler Hamiltonian is associated with a certain Virasoro generator. It seems that for $h=\frac{1}{2}$ the ground state of the generator K corresponds to a thermal state when examined in the Rindler wedge with respect to the Rindler evolution. Moreover, that state has inverse temperature equal to $1/(2\beta)$. Finally, under Wick rotation in Rindler time, the pair of QF theories which are built up on the future and past horizon defines a proper two-dimensional conformal quantum field theory on a cylinder.

V. DISCUSSION, OVERVIEW AND OPEN PROBLEMS

In this article we have rigorously proven that it is possible to define a diffeomorphism invariant local quantum field theory for a massless free scalar field defined on the Killing horizon of a Rindler space–time. Actually all of the procedure could be implemented in a manifold diffeomorphic to $\mathbb{R}$ without fixing any metric structure. The diffeomorphism invariance is a consequence of the fact that the field operators and the symplectic form act on exact one-forms instead of smooth smearing functions and thus they do not need a metric invariant measure. Moreover, when the theory is realized on the (future and/or past) Killing horizon in Rindler space–time, there is a natural injective $*$-algebra homomorphism from any quantum field theory of a (generally massive)

scalar field propagating in the bulk. This holographic identification can be implemented in terms of unitary equivalences if the algebras of the fields are represented in suitable Fock spaces. In this case the vacuum state in the bulk is that associated to Rindler quantization. In an approximated picture where Rindler space corresponds to the space–time near the horizon of a Schwarzschild black hole, Rindler particles are just the Poincaré-invariant particles we experience everyday. Conversely, if the Rindler background is taken seriously as part of the actual space–time (Minkowski space–time) without approximation, the Rindler vacuum has to be thought of as the vacuum state of an accelerated observer in Minkowski space–time and Rindler particles have nothing to do with ordinary Poincaré invariant particles. Actually a problem arises from a pure physical point of view and it deserves further investigation in relation with the *unitary* holographic theorem where vacuum states play a relevant role. Indeed, the Rindler vacuum as well as the Boulware vacuum in the Schwarzschild manifold are states which cannot be defined in the natural extension of the manifold (respectively, Minkowski space–time and Kruskal space–time). Essentially speaking, this is due to the behavior of n-point functions on the Killing horizon which is not Hadamard. In this context it would be interesting to investigate the holographic meaning of the Hadamard states (Minkowski vacuum and Hartle-Hawking state) also to make contact with results found in Refs. 15–18 where the net of Von Neumann algebras are defined with respect to Hadamard states.

Another achieved result in this work is that the hidden SL(2,$\mathbb{R}$) symmetry of the bulk theory corresponds to an analogous symmetry for the horizon theory and this horizon symmetry has a clear geometric interpretation in terms of invariance under diffeomorphisms. However, it is possible to show that this symmetry can be enlarged to include a full Virasoro algebra which represents, in the Hilbert space of the system, the algebra of generators of one-parameter groups of local diffeomorphisms of the horizon. That is the subject of another work.[19]

All the work has been developed in the case of a two-dimensional space–time. Nevertheless, we expect that the result obtained for this simple case can be generalized to encompass some four-dimensional cases. Considering a four-dimensional Schwartzschild black hole manifold within the near horizon approximation, angular degrees of freedom are embodied in the solutions of Klein–Gordon equation by multiplication of a two-dimensional solution and a spherical harmonic $Y^l_m(\theta,\phi)$. All field states are elements of an appropriate tensor product of Hilbert spaces. For instance, in the massive case, the final space is the direct sum of spaces $\mathbb{C}^{2l+1}\otimes L^2(\mathbb{R}^+,dE)$ with $l=0,1,\ldots$. (The "square angular momentum" eigenvalue l defines an effective mass of the field when considered at fixed value of l. In this way the massless theory behaves as the massive one when $l\neq 0$.) With simple adaptations [e.g., the appropriate causal propagator on $\mathbf{F}$ reads

$$E_{\mathbf{F}}(x,x')=(\tfrac{1}{4})\text{sign }(v-v')\,\delta(\theta-\theta')\,\delta(\phi-\phi')\sqrt{g_{\,S^2}(\theta,\phi)}$$

and the horizon field operator $\hat{\phi}_{\mathbf{F}}$ has to be smeared with 3-forms as $df(v,\theta,\phi)\wedge d\theta\wedge d\phi$] all the results found in this article can be restated for that apparently more general case. The same conclusion can be achieved when considering a four-dimensional Rindler space–time.

Some comments can be supplied for the case of the exact Schwartzschild space–time dropping the near-horixon approximation in spite of the absence of exact solutions of the Klein–Gordon equation. By the analysis of the effective potential—which depends on the angular momentum—of either a massive or massless particle propagating in the external region of the black hole space–time, one sees that the energy spectrum is $\sigma(H)=[0,+\infty)$ once again for any values of the angular momentum. If the particle is massive, no degeneracy affects a value E of the energy if the mass is greater than E; otherwise twice the degeneracy arises. That is the only possible case for a massless particle. Therefore, we expect that our results, with appropriate adaptations, may hold for the massless case but they could need some substantial change dealing with the massive case.

Another interesting topic that deserves investigation is if, and how, the holographic procedure can be extended in order to encompass a larger algebra of fields containing Wick monomials "ϕ^n" which naturally arise dealing with perturbative interacting quantum field theory.

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Virasoro algebra with central charge $c=1$ on the horizon of a two-dimensional-Rindler space–time

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Using the holographic machinery built up in a previous work, we show that the hidden $SL(2,\mathbb{R})$ symmetry of a scalar quantum field propagating in a Rindler space–time admits an enlargement in terms of a unitary positive-energy representation of Virasoro algebra defined in the Fock representation. That representation has central charge $c=1$. The Virasoro algebra of operators gets a manifest geometrical meaning if referring to the holographically associated quantum field theory on the horizon: It is nothing but a representation of the algebra of vector fields defined on the horizon equipped with a point at infinity. All that happens provided the Virasoro ground energy $h:=\mu^2/2$ vanishes and, in that case, the Rindler Hamiltonian is associated with a certain Virasoro generator. If a suitable regularization procedure is employed, for $h=1/2$, the ground state of that generator seems to correspond to a thermal state when examined in the Rindler wedge, taking the expectation value with respect to Rindler time. Finally, under Wick rotation in Rindler time, the pair of quantum field theories which are built up on the future and past horizon defines a proper two-dimensional conformal quantum field theory on a cylinder. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629396]

I. INTRODUCTION AND SUMMARY OF PREVIOUSLY OBTAINED RESULTS

A number of papers have been concerned with the issue of the statistical origin of black-hole entropy. The holographic principle[1–3] arose from the idea that gravity near the horizon should be described by a low dimensional theory with a higher dimensional group of symmetry. Maldacena and Witten[4,5] showed that there is a correspondence between quantum field theory (QFT) in an asymptotically AdS space–time, the ''bulk,'' and a conformal theory on its ''boundary'' at space–like infinity. Rehren proved rigorously some holographic results for local quantum fields in an AdS background, establishing a correspondence between bulk observables and boundary observables without employing string machinery.[6,7] Dealing with QFT in two-dimensional (2D)-Rindler space–time, we have proved in a recent work[8] that it is possible to define a free quantum theory on the horizon of a two-dimensional Rindler space. That theory enjoys holographic interplay with the analogous theory defined in the bulk. More precisely, there are two holographic theorems. The former shows that there is a $*$-algebra injective homomorphism from the algebra of the bulk observables associated with the Rindler free field to the algebra of the horizon observables associated with the horizon free field. The latter identifies the observables of the theories from the point of view of unitary equivalences whenever the theory is represented in suitable Fock spaces

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(in that case also the vacuum states are in correspondence through the unitary operator which realizes holography). An interesting consequence is that the ''hidden'' $SL(2,\mathbb{R})$ symmetry of free quantum field theory in the bulk found in Ref. 9 becomes manifest when transposed on the Killing horizon by means of unitary holography. In fact, due to the spectrum of the Hamiltonian operator, QFT theory in the bulk turns out to be invariant under a unitary representation of $SL(2,\mathbb{R})$ but such a quantum symmetry cannot be induced by the geometric background because the isometries of Rindler space have a Lie algebra different from that of $SL(2,\mathbb{R})$.[9] Nevertheless, the unitary representation of $SL(2,\mathbb{R})$ realizes that bulk symmetry becomes manifest, i.e., it reveals a clear geometric meaning, if it is examined on the horizon by means of the holographic machinery. All that is summarized later in this section in some detail.

Overlap with ideas and results of Ref. 8 is present in the literature, especially due to Schroer,[10] Schroer and Wiesbrock,[11] and Schroer and Fassarella.[12] In those papers an approach to holography similar to ours is implemented in the framework of LightFront Holography developed at an algebraic level using nets of local observable algebras. From a very elementary point of view, a relevant difference with our machinery is the fact that the quantization of the bulk field used by Schroer and collaborators is that referred to as Minkowski vacuum and Minkowski time instead of Rindler vacuum and time. From a pure physical point of view, perhaps, the quantization with respect to the Rindler frame is more interesting if one tries to use our machinery as a starting point to investigate quantum field theory (QFT) near the bifurcate Killing horizon of a black hole: Rindler quantization corresponds to quantization in a reference frame that gives rise to Minkowski coordinates far from the black hole and the associated particles should be those things are made of. However the interplay of Schroer and collaborators' ideas and achievements and procedures and results presented in our paper deserves further investigation. Another relevant paper which merits particular quotation is that by Guido, Longo, Roberts, and Verch.[13] Overlap with some results arising from our approach is present in Sec. 4 of Ref. 13. In that section, in the very general context of QFT in curved space–time in terms of nets of local C^* algebras (and Von Neumann representations) and making use of very general theorems by Wiesbrock on local quantum field theory defined on $\mathbb{S}^1$ and covariant with respect to $PSL(2,\mathbb{R}) := SL(2,\mathbb{R})/\pm I$, the existence of a local quantum field theory (covariant with respect to $PSL(2,\mathbb{R})/\pm I$) defined on the bifurcate Killing horizon is proven. This is done by considering a net of Von Neumann algebras in the representation of a state which is, in restriction to the subnet of observables which are localized at the horizon, a KMS state at Hawking temperature for the Killing flow.

In Ref. 8 we found some clues for the existence of a whole unitary representation of Virasoro algebra which extends the $SL(2,\mathbb{R})$ unitary representation on the horizon. In this paper we prove the very existence of a full unitary representation of Virasoro algebra with central charge $c=1$ for quantum field theory defined on the horizon. That fact is interesting for several reasons in relation to the problem of the statistical interpretation of black hole entropy. In fact, there are several attempts to give a statistical explanation to black hole entropy by counting microstates in terms of the degeneracy of an eigenspace of a certain Virasoro generator in a suitable irreducible unitary representation of Virasoro algebra.[14,15] This is done by means of the so-called ''Cardy's formula.'' These approaches are, in fact, based on the existence of a Virasoro algebra (with central charge $c\neq 0$) in terms of generators of diffeomorphisms of the black hole manifolds considering the horizon as a boundary. The algebra of the associated generators in the Hamiltonian ADM formulation of gravity gets a nonvanishing central charge. Under the supposition that a quantum version of that Virasoro representation exists, that the value of central charge is not affected by the quantization procedure and that the actual value of the black hole mass is an eigenvalue of the Virasoro generator L_0, it is possible to compute the degeneracy of that eigenspace by means of Cardy's formula because of the presence of a central charge. The logarithm of the degeneracy gives the very black-hole entropy law barring logarithmic corrections.

The main problem of all of those approaches is that the Virasoro algebra representation with nonvanishing central charge is proven to exist at classical level only in the Hamiltonian formulation. All derivations of black hole entropy by that way are based on the found classical formulas

and on the supposition that there is a quantum version of the found Hamiltonian structure (in order to use Cardy's formula).

To make contact with the content of this paper where a quantum scalar field propagating in a 2D-Rindler space is considered, we notice that in the above-outlined approaches, the only near-horizon structure is sufficient to use the Virasoro–Cardy machinery.[15,14,16] Moreover, for a Schwarzschild black-hole manifold, the relevant algebra of diffeomorphisms is that of diffeomorphisms in the plane r,t which preserve the horizon structure. Hence it seems that 2D-Rindler models are relevant to this context. On the other hand, a scalar field arises naturally in these 2D-Rindler space approaches by dimensional reduction[16] from the gravitational theory in four dimensions (4D) in the presence of spherical symmetry. That field supports information of part of the 4D-dimensional gravity in the 2D model. Concerning the problem of the existence of a Virasoro representation at quantum level we stress that, in this paper, we prove that a very positive-energy unitary representation of Virasoro algebra does exist at quantum level for the quantum field defined on the horizon. That algebra of operators can be defined also for the scalar field propagating in the bulk via unitary holography.

In fact, Sec. II of this paper is devoted to showing that the bulk hidden $SL(2,\mathbb{R})$ symmetry admits an enlargement in terms of a unitary representation of Virasoro algebra with central charge $c=1$ defined in Fock representation. The Virasoro algebra of operators gets a manifest geometrical meaning if referring to the holographically associated QFT on the horizon: It gives rise to a unitary representation of a group of automorphisms of the $*$-algebra generated by field operators. This representation is induced by a group of diffeomorphisms of the horizon compactified by adding a point at infinity. Moreover, a subrepresentation which is generated by three certain Virasoro generators reduces to the $SL(2,\mathbb{R})$ representation previously found. Under Wick rotation with respect to Rindler time, the pair of QF theories which are built up on the future and past horizon defines a proper two-dimensional conformal quantum field theory. That CFT can be realized on the Riemann surface given by a two-dimensional cylinder. In Sec. III we see that, with a suitable choice of the weight of the found Virasoro algebra of operators, a certain generator which generalizes Rindler Hamiltonian, admits a ground state Ψ which seems to enjoy thermodynamic properties: When that state is examined in the bulk via holography, and a suitable regularized mean is computed with respect to Rindler-time evolution, Ψ reveals itself as a thermal state whose inverse temperature is 2β, β being the parameter initially used to build up the unitary $SL(2,\mathbb{R})$ representation in the bulk.

We summarize part of the content of Ref. 8 relevant to this work within the following five steps.

[a] Consider the globally hyperbolic space–time **R** called the two-dimensional *Rindler wedge* with metric $ds^2_{\mathbf{R}}=-\kappa^2y^2dt^2+dy^2$, which can be obtained by a suitable near horizon approximation of a general Schwarzschild-like metric also dropping the angular coordinates,[8] above $t\in\mathbb{R}$, $y\in(0,+\infty)$ are global coordinates. A free Klein–Gordon (KG) scalar field ϕ in **R** satisfies the equation of motion $-\partial_t^2\phi+\kappa^2(y\partial_y y\partial_y-y^2m^2)\phi=0$. In Rindler quantization, the one-particle Hilbert space $\mathcal{H}$ consists of the space of complex linear combinations of the positive frequency parts of smooth real solutions ψ of the KG equation with compact Cauchy data. The natural *symplectic form* on that space is $\Omega(\psi,\psi'):=\int_\Lambda(\psi'\nabla^\mu\psi-\psi\nabla^\mu\psi')n_\mu d\sigma$, Λ being any Cauchy surface, $d\sigma$ the induced measure, and n a unit future-oriented normal vector. Every ψ decomposes into ∂_t-stationary modes as

$$\psi(t,y)=\psi_+(t,y)+\text{c.c.}=\int_0^{+\infty}e^{-iEt}\sum_\alpha\Phi_E^{(\alpha)}(y)\,\tilde{\psi}_+^{(\alpha)}(E)\,dE+\text{c.c.} \tag{1}$$

The index α distinguishes between two cases: if $m>0$ there is a single mode $\Phi_E^{(\alpha)}=\Phi_E$. If $m=0$ there are two values of α, corresponding to *ingoing* and *outgoing* modes, $\Phi_E^{(\text{in})/(\text{out})}=e^{\mp iE\ln(\kappa y)/\kappa}/\sqrt{4\pi E}$. In that case both ingoing and outgoing components in (1) must have Cauchy compact support. The one-particle Hilbert space of wave functions is obtained by taking the

completion of the space of complex linear combinations of positive frequency wave functions (obtained from Cauchy support compactly real wave functions) with respect to the Hermitian scalar product $-i\Omega(\overline{\psi'_+},\psi_+)$. ∂_t evolution of a wave function ψ is equivalent to the action of the one-parameter subgroup generated by a Hamiltonian H on the associated $\psi_+ \in \mathcal{H}$. $\sigma(H)=[0, +\infty)$ for $m \geqslant 0$. If $m>0$ there is no energy degeneration and the one-particle Hilbert space $\mathcal{H}$ is isomorphic to $L^2(\mathbb{R}^+,\mathrm{d}E)$ via spectral decomposition of H. In the other case ($m=0$), twofold degeneracy implies that $\mathcal{H}\cong L^2(\mathbb{R}^+,\mathrm{d}E)\oplus L^2(\mathbb{R}^+,\mathrm{d}E)$. Let us pass to the bosonic Fock space, $\mathfrak{F}(\mathcal{H})$, associated with $\mathcal{H}$. The *quantum field* $\Omega(\,\cdot\,,\hat{\phi})$ of our theory is the map

$$\psi \mapsto \Omega(\psi,\hat{\phi}) := ia(\overline{\psi_+}) - ia^\dagger(\psi_+)\ , \tag{2}$$

where ψ is any real compactly supported wave function and $a(\overline{\psi_+})$ and $a^\dagger(\psi_+)$, respectively, denote the annihilation and construction operator associated with the one-particle states $\overline{\psi_+}$ and ψ_+, defined in $\mathfrak{F}(\mathcal{H})$ and referred to the Rindler vacuum $|0\rangle$ (that is $|0\rangle_{\mathrm{in}}\otimes|0\rangle_{\mathrm{out}}$ if $m=0$). $\Omega(\psi,\hat{\phi})$ is essentially self-adjoint in the dense invariant subspace spanned by all states containing a finite arbitrarily large number of particles with states given by positive-frequency wave functions. Every wave function ψ in (1) can be obtained as $\psi=E(f)$ where f is an associated compactly supported smooth function in $\mathbf{R}$ and E is the *causal propagator* (the "advanced-minus-retarded" two point function) of Klein–Gordon operator. Moreover

$$\int_{\mathbf{R}} \psi f \,\mathrm{d}\mu_g = \Omega(Ef,\psi), \quad \int_{\mathbf{R}} h(x)(Ef)(x)\,\mathrm{d}\mu_g(x) = \Omega(Ef,Eh)\ , \tag{3}$$

μ_g being the measure induced by the metric in $\mathbf{R}$. Equation (3) suggests defining[18] a quantum-field operator smeared with compactly supported complex-valued functions f, as the linear map

$$f \mapsto \hat{\phi}(f) := \Omega(Ef,\hat{\phi})\ , \tag{4}$$

which is formally equivalent to the nonrigorous but popular definition

$$\hat{\phi}(t,y) = \int_0^\infty \sum_\alpha \ e^{-iEt}\Phi_E^{(\alpha)}(y)a_{E\alpha} + e^{iEt}\overline{\Phi_E^{(\alpha)}(y)}a^\dagger_{E\alpha}\mathrm{d}E\ . \tag{5}$$

The rigorous version of the formal identity $[\hat{\phi}(x),\hat{\phi}(x')]=-iE(x,x')$ is

$$[\hat{\phi}(f),\hat{\phi}(h)] = -iE(f,h) := -i\int_{\mathbf{R}} h(x)(Ef)(x)\,\mathrm{d}\mu_g(x)\ . \tag{6}$$

[b] In Refs. 9 and 8 we have established that, if $m>0$, $\mathcal{H}$ is irreducible under a (uniquely determined) strongly continuous unitary representation of $SL(2,\mathbb{R})$ whose Lie algebra is given by the (uniquely determined) self-adjoint extension of the real linear combinations of operators H_0, D, C:

$$H_0 := E\ , \quad D := -i\left(\frac{1}{2}+E\frac{\mathrm{d}}{\mathrm{d}E}\right)\ , \quad C := -\frac{\mathrm{d}}{\mathrm{d}E}E\frac{\mathrm{d}}{\mathrm{d}E} + \frac{\left(k-\frac{1}{2}\right)^2}{E}\ . \tag{7}$$

k can arbitrarily be fixed in $\{1/2, 1, 3/2,...\}$. iH_0, iC, iD enjoy the commutation relations of the Lie algebra of $SL(2,\mathbb{R})$ in a suitable dense and invariant domain $\mathcal{D}_k$ where they, and their real linear combinations, are essentially self-adjoint[8] and $\overline{H_0}=H$. $\mathcal{D}_k$ is the subspace spanned by the eigenvectors of the operator

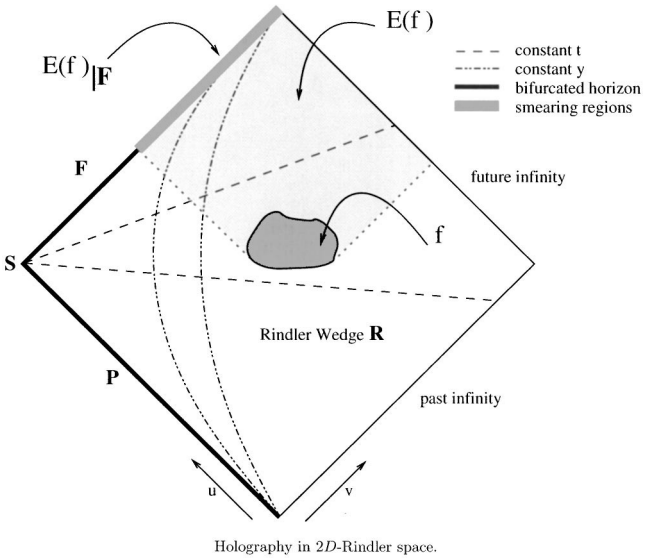

FIG. 1. Holography in 2D-Rindler space.

$$K_\beta := \frac{1}{2}\left(\beta H_0 + \frac{1}{\beta} C\right), \tag{8}$$

β being a constant with the dimensions of an inverse energy. The unitary representation does not depend on the value of β. The spectrum of the self-adjoint operator $\overline{K_\beta}$ (initially defined on $\mathcal{D}_k$) is a pure point spectrum without degeneracy, it does not depend on β itself and is $\sigma(K_\beta) = \{\lambda_n \mid \lambda_n = n,\ \ n = k, k+1, k+2, \ldots\}$. If $\mathrm{L}_p^{(\alpha)}$ are modified Laguerre's polynomials,[17] the associated normalized eigenvectors (which are the same as those of K_β) are

$$Z_n^{(k)}(E) := \eta_n \sqrt{\frac{\Gamma(n-k+1)}{E\,\Gamma(n+k)}}\, e^{-\beta E} (2\beta E)^k \mathrm{L}_{n-k}^{(2k-1)}(2\beta E), \quad n = k, k+1, \ldots, \tag{9}$$

η_n being a pure phase which can be arbitrarily fixed (in Refs. 9 and 8 we used $\eta_n = 1$). As noticed in Ref. 9, if β is interpreted as an inverse temperature, the exponential $e^{-\beta E}$ suggests an interpretation in terms of a canonical ensemble of the energetic content of these states. In this paper we examine in depth this possibility finding out very interesting results.

If $m = 0$ and so $\mathcal{H} \cong L^2(\mathbb{R}^+, \mathrm{d}E) \oplus L^2(\mathbb{R}^+, \mathrm{d}E)$, an analogue representation exists in each space $L^2(\mathbb{R}^+, \mathrm{d}E)$. Making use of the Heisenberg representation it is simply proven that the algebra generated by $H, \overline{D}, \overline{C}$, with depending-on-time coefficients, is made of constant of motions.[8] Thus $SL(2,\mathbb{R})$ is a *symmetry* of the one-particle system. That can straightforwardly be extended to the free quantum field in Fock space. The crucial point is that the found symmetry is *hidden*: It cannot be induced by the background geometry since the Killing fields of Rindler space–time enjoy a different Lie algebra from that of H_0, D, C and no representation of $SL(2,\mathbb{R})$ exists in terms of isometries of **R** (see Ref. 8 for definitions and details). The picture changes dramatically when the found $SL(2,\mathbb{R})$ symmetry is examined on the horizon as noted in [e] below.

[c] The space **R** is naturally embedded in a Minkowski space–time which contains the horizon associated with the Rindler metric. Rindler *light coordinates* $u = t - \log(\kappa y)/\kappa$, $v = t + \log(\kappa y)/\kappa$ (where $u, v \in \mathbb{R}$) cover the (open) Rindler space **R**. Separately, v is well defined on the *future horizon* **F**, $u \to +\infty$, and u is well defined on the *past horizon* **P**, $v \to -\infty$ (see Fig. 1). A wave function in (1) admits well-defined limits toward the future horizon $u \to +\infty$:

$$\psi(v)=\int \frac{e^{-iEv}}{\sqrt{4\pi E}} e^{i\rho_{m,\kappa}(E)}\widetilde{\psi}_+(E)\ \mathrm{d}E+\mathrm{c.c.}, \tag{10}$$

$e^{i\rho_{m,\kappa}(E)}$ being a pure phase.[8] In coordinate $u\in\mathbb{R}$, the restriction of ψ to $\mathbf{P}$ is similar with v replaced for u and $\rho_{m,\kappa}(E)$ replaced by $-\rho_{m,\kappa}(E)$. If $m=0$ restrictions to $\mathbf{F}$ and $\mathbf{P}$ are similar to (10) with the difference that $e^{i\rho_{m,\kappa}(E)}$ is replaced by 1, only ingoing components survive in the limit toward $\mathbf{F}$ and only outgoing components survive in the limit toward $\mathbf{F}$ (v must be replaced for u in that case). Discarding the phase it is possible to consider the following real "*wave function on the (future) horizon* $\mathbf{F}$":

$$\varphi(v)=\int_{\mathbb{R}^+}\frac{e^{-iEv}}{\sqrt{4\pi E}}\widetilde{\varphi}_+(E)\ \mathrm{d}E+\int_{\mathbb{R}^+}\frac{e^{+iEv}}{\sqrt{4\pi E}}\overline{\widetilde{\varphi}_+(E)}\ \mathrm{d}E, \tag{11}$$

where φ *is any real function in Schwartz' space on* $\mathbb{R}\equiv\mathbf{F}$, as the basic object in defining a quantum field theory on the future horizon. The same is doable concerning $\mathbf{P}$. The space of horizon wave functions can be equipped with a diffeomorphism invariant symplectic form $\Omega_{\mathbf{F}}(\varphi,\varphi')\coloneqq\int_{\mathbf{F}}\varphi'\mathrm{d}\varphi-\varphi\mathrm{d}\varphi'$. A suitable causal propagator can also be defined $E_{\mathbf{F}}(v,v')=(1/4)\mathrm{sign}(v-v')$ and used as noted in the following. First of all define the Hermitian scalar product $\langle\varphi'_+,\varphi_+\rangle_{\mathbf{F}}\coloneqq -i\Omega_{\mathbf{F}}(\overline{\varphi'_+},\varphi_+)$. The one-particle Hilbert space $\mathcal{H}_{\mathbf{F}}$ is the completion with respect to that scalar product of the space of complex combinations of positive frequency parts $\widetilde{\varphi}_+(E)$, of horizon wave functions φ. As $\langle\varphi'_+,\varphi_+\rangle_{\mathbf{F}}=\int_{\mathbb{R}^+}\overline{\widetilde{\varphi}'_+(E)}\widetilde{\varphi}_+(E)\mathrm{d}E$, $\mathcal{H}_{\mathbf{F}}$ turns out to be isomorphic to $L^2(\mathbb{R}^+,\mathrm{d}E)$ once again. The field operator is defined in the symmetrized Fock space $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$, with vacuum state $|0\rangle_{\mathbf{F}}$, with rigorous symplectic definition given by

$$\varphi\mapsto\Omega_{\mathbf{F}}(\varphi,\hat{\phi}_F)\coloneqq ia(\overline{\varphi_+})-ia^\dagger(\varphi_+)\ , \tag{12}$$

where φ is any horizon wave function in the above-specified space. With these definitions, in spite of the absence of any equation of motion the essential features of free quantum field theory are preserved by that definition.[8] Degeneracy of the metric on the horizon prevents one from smearing field operators by functions due to the ill-definiteness of the induced volume measure. However, employing the symplectic approach,[18] a well-defined smearing procedure is that of field operators and exact one-forms $\eta=df$ where $f=f(v)$, $v\in\mathbb{R}\equiv\mathbf{F}$, is any real function in Schwartz's space. More precisely, $\eta(v)\mapsto E_{\mathbf{F}}(\eta)=\frac{1}{4}\int_{\mathbb{R}}\mathrm{sign}(v-v')\,\eta(v')=\psi_\eta(v)$ defines a one-to-one correspondence between exact one-forms and horizon wave functions of the form (11) and $\eta=2d\psi_\eta$. Thus, if $\eta=\mathrm{d}\varphi$ with $\varphi=\varphi(v)$ in Schwartz' space, one can define

$$\eta\mapsto\hat{\phi}_{\mathbf{F}}(\eta)\coloneqq\Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta,\hat{\phi}_{\mathbf{F}})\ , \tag{13}$$

which is the rigorous meaning of

$$\hat{\phi}_{\mathbf{F}}(\eta)=\int_0^\infty\frac{\mathrm{d}E}{\sqrt{4\pi E}}\left(\int_{\mathbb{R}}e^{-iEv}\,\eta(v)\right)a_E+\left(\int_{\mathbb{R}}e^{iEv}\,\eta(v)\right)a_E^\dagger. \tag{14}$$

Horizon wave functions φ and one-forms η,η' in the above-noted spaces enjoy the same properties as in the bulk. More precisely one has

$$\int_{\mathbf{F}}\varphi\,\eta=\Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta,\varphi),\qquad\int_{\mathbf{F}}(E_{\mathbf{F}}\eta)\,\eta'=\Omega_{\mathbf{F}}(E_{\mathbf{F}}\eta,E_{\mathbf{F}}\eta')\ , \tag{15}$$

$$[\hat{\phi}_{\mathbf{F}}(\eta),\hat{\phi}_{\mathbf{F}}(\eta')]=-iE_{\mathbf{F}}(\eta,\eta')=\int_{\mathbf{F}}\psi_{\eta'}\mathrm{d}\psi_\eta-\psi_\eta\mathrm{d}\psi_{\eta'}\,. \tag{16}$$

The latter is nothing but the rigorous meaning of the formal equation $[\hat{\phi}(v),\hat{\phi}(v')] = -iE_{\mathbf{F}}(v,v')$. Finally a "locality property" holds true:

$$[\hat{\phi}_{\mathbf{F}}(\eta),\hat{\phi}_{\mathbf{F}}(\eta')]=0 \quad \text{if} \quad \mathrm{supp}(\eta)\cap\mathrm{supp}(\eta')=\varnothing.$$

Everything we have stated for **F** can analogously be stated for **P**.

[d] It is possible to prove the existence of a unitary equivalence between the theory in the bulk and that on the horizon in the sense we are going to describe.

Theorem 1.1: *If f is any real smooth compactly supported function f used to smear the bulk field, define $\eta_f := 2\mathrm{d}(E(f)\restriction_{\mathbf{F}})$, and $\omega_f := 2\mathrm{d}(E(f)\restriction_{\mathbf{P}})$, $E(f)\restriction_{\mathbf{F/P}}$ being the limit toward* **F**, *respectively,* **P**, *of $E(f)$ (see Fig. 1).*

(a) If $m>0$, there is a unitary map $U_{\mathbf{F}}:\mathfrak{F}(\mathcal{H})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ such that

$$U_{\mathbf{F}}|0\rangle=|0\rangle_{\mathbf{F}}, \quad \textit{and} \quad U_{\mathbf{F}}^{-1}\hat{\phi}_{\mathbf{F}}(\eta_f)U_{\mathbf{F}}=\hat{\phi}(f)\ .$$

(b) If $m=0$ two unitary operators arise $V_{\mathbf{F/P}}:\mathfrak{F}(\mathcal{H}_{\mathrm{in/out}})\to\mathfrak{F}(\mathcal{H}_{\mathbf{F/P}})$ such that

$$V_{\mathbf{F/P}}|0\rangle_{\mathrm{in/out}}=|0\rangle_{\mathbf{F/P}}$$

and

$$V_{\mathbf{F}}^{-1}\hat{\phi}_{\mathbf{F}}(\eta_f)V_{\mathbf{F}}=\hat{\phi}_{\mathrm{in}}(f)\ , \quad \textit{and} \quad V_{\mathbf{P}}^{-1}\hat{\phi}_{\mathbf{P}}(\omega_f)V_{\mathbf{P}}=\hat{\phi}_{\mathrm{out}}(f)\ .$$

$\mathcal{H}_{\mathrm{in/out}}$ is the bulk Hilbert space associated with the ingoing/outgoing modes and $\hat{\phi}_{\mathrm{in/out}}(f)$ is the part of bulk field operator built up using only ingoing/outgoing modes.

Details on the construction of $U_{\mathbf{F}}$, $V_{\mathbf{F}}$, $V_{\mathbf{P}}$ are supplied in Ref. 8. Similar to the extent in the bulk case, one focuses on the algebra $\mathcal{A}_{\mathbf{F}}$ of linear combinations of product of field operators $\hat{\phi}_{\mathbf{F}}(\omega)$ varying ω in the space of allowed complex one-forms. We assume that $\mathcal{A}_{\mathbf{F}}$ also contains the unit operator I. The Hermitian elements of $\mathcal{A}_{\mathbf{F}}$ are the natural observables associated with the horizon field. From an abstract point of view the found algebra is a unital $*$-algebra of formal operators $\phi_{\mathbf{F}}(\eta)$ with the additional properties $[\phi_{\mathbf{F}}(\eta),\phi_{\mathbf{F}}(\eta)]=-iE_{\mathbf{F}}(\eta,\eta')$, $\phi_{\mathbf{F}}(\eta)^* = \phi_{\mathbf{F}}(\overline{\eta})$ and linearity in the form η. (The analogous algebra of operators in the bulk fulfill the further requirement $\phi(f)=0$ if (and only if) $f=Kg$, K being the Klein–Gordon operator. No analogous requirement makes sense for $\mathcal{A}_{\mathbf{F}}$ since there is no equation of motion on the horizon.) $\mathcal{A}_{\mathbf{F}}$ can be studied no matter any operator representation in any Fock space. Operator representations are obtained via the GNS theorem once an algebraic state has been fixed.[18] $\mathcal{A}_{\mathbf{P}}$ can analogously be defined. Below $\mathcal{A}_{\mathbf{R}}$ denotes the unital $*$-algebra associated with the bulk field operator. If $m=0$, $\mathcal{A}_{\mathbf{R}}$ naturally decomposes as $\mathcal{A}_{\mathrm{in}}\otimes\mathcal{A}_{\mathrm{out}}$ (see Ref. 8) with obvious notation. We have the following result which is independent of any choice of vacuum state and Fock representation. The proof can be found in Ref. 8.

Theorem 1.2: *Assume the same notation as in Theorem 1.1 concerning η_f and ω_f.*

(a) If $m>0$, there is a unique injective unital $*$-algebras homomorphism $\chi_{\mathbf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathbf{F}}$ such that $\chi_{\mathbf{F}}(\phi(f))=\phi_{\mathbf{F}}(\eta_f)$. Moreover in GNS representations in the respectively associated Fock spaces $\mathfrak{F}(\mathcal{H})$, $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ built up over $|0\rangle$ and $|0\rangle_{\mathbf{F}}$, respectively, $\chi_{\mathbf{F}}$ has a unitary implementation naturally induced by $U_{\mathbf{F}}$ (e.g., $\chi_{\mathbf{F}}(\hat{\phi}(f))=U_{\mathbf{F}}\hat{\phi}(f)U_{\mathbf{F}}^{-1}$).

(b) If $m=0$, there are two injective unital $*$-algebras homomorphisms $\Pi_{\mathbf{F/P}}:\mathcal{A}_{\mathrm{in/out}}\to\mathcal{A}_{\mathbf{F/P}}$ such that $\Pi_{\mathbf{F}}(\phi(f))=\phi_{\mathbf{F}}(\eta_f)$ and $\Pi_{\mathbf{P}}(\phi(f))=\phi_{\mathbf{P}}(\omega_f)$. Moreover in GNS representations in the respectively associated Fock spaces $\mathfrak{F}(\mathcal{H}_{\mathrm{in/out}})$, $\mathfrak{F}(\mathcal{H}_{\mathbf{F/P}})$ built up over $|0\rangle_{\mathrm{in/out}}$ and $|0\rangle_{\mathbf{F/P}}$, respectively, $\Pi_{\mathbf{F}}$ and $\Pi_{\mathbf{P}}$ have unitary implementations and reduce to $V_{\mathbf{F}}$ and $V_{\mathbf{P}}$, respectively.

Notice that, in particular $\chi_{\mathbf{F}}$ preserves the causal propagator, in the sense that it must be $-iE(f,g)=[\phi(f),\phi(g)]=[\phi_{\mathbf{F}}(f),\phi_{\mathbf{F}}(g)]=-iE_{\mathbf{F}}(\eta_f,\eta_g)$.

[e] Consider quantum field theory on **F**, but the same result holds concerning **P**. In $\mathcal{H}_{\mathbf{F}} \cong L^2(\mathbb{R}^+,\mathrm{d}E)$ define operators $H_{\mathbf{F}0},D_{\mathbf{F}},C_{\mathbf{F}}$ as the right-hand side of the equation that, respec-

tively, defines H_0, D, C in (7). They and their real linear combinations are essentially self-adjoint if restricted to the invariant dense domain $\mathcal{D}_k^{(\mathbf{F})}$ defined with the same definition as $\mathcal{D}_k$ in [b]. Exactly as in the bulk case, operators $iH_{\mathbf{F}}=iH_{\mathbf{F}0}$, $i\overline{D}_{\mathbf{F}}, i\overline{C}_{\mathbf{F}}$ generate a strongly continuous unitary $SL(2,\mathbb{R})$ representation $\{U_g^{(\mathbf{F})}\}_{g\in SL(2,\mathbb{R})}$. Hence, varying $g\in SL(2,\mathbb{R})$, the unitary operators obtained by unitary holography $(U_{\mathbf{F}}\restriction_{\mathcal{H}})^{-1}\, U_g^{(\mathbf{F})}\, U_{\mathbf{F}}\restriction_{\mathcal{H}}$ define a representation of $SL(2,\mathbb{R})$ for the system in the bulk. By construction $(U_{\mathbf{F}}\restriction_{\mathcal{H}})^{-1}\, H_{\mathbf{F}}\, U_{\mathbf{F}}\restriction_{\mathcal{H}}=H$. As a consequence every $U_g^{(\mathbf{F})}$ gives rise to a $SL(2,\mathbb{R})$ symmetry of the bulk field and the group of these symmetries is unitary equivalent to that generated by $iH, i\overline{D}, i\overline{C}$. In particular the one-parameter group associated with $H_{\mathbf{F}}$ generates v displacements of horizon wave functions which are equivalent, under unitary holography, to t displacements of bulk wave functions. Now, it makes sense to investigate the *geometrical nature* of the $SL(2,\mathbb{R})$ representation $\{U_g^{(\mathbf{F})}\}$ that, as we said, induces, up to unitary equivalences, the original $SL(2,\mathbb{R})$ symmetry in the bulk, but now can be examined on the horizon. In fact, the symmetry has a geometrical meaning: The action of every $U_g^{(\mathbf{F})}$ on a state $\tilde{\varphi}_+=\tilde{\varphi}_+(E)$ is essentially equivalent to the action of a corresponding **F**-diffeomorphism on the associated [by (11)] horizon wave function φ. More precisely:[8]

Theorem 1.3: *Assume $k=1$ in (7), take a matrix $g\in SL(2,\mathbb{R})$. Let $\varphi=\varphi(v)$ be a real Schwartz's horizon wave function with positive frequency part $\tilde{\varphi}_+=\tilde{\varphi}_+(E)$ and such that $\varphi(0)=0$ and $v\mapsto\varphi(1/v)$ belongs to Schwartz's space too.*

The wave function φ_g associated with $U_g^{(\mathbf{F})}\tilde{\varphi}_+$ reads

$$\varphi_g(v)=\varphi\left(\frac{av+b}{cv+d}\right)-\varphi\left(\frac{b}{d}\right),\quad \begin{pmatrix} a & b\\ c & d\end{pmatrix}=g^{-1}. \tag{17}$$

Moreover one has the particular cases:

(a) The unitary one-parameter group generated by $iH_{\mathbf{F}}$ is associated with the one-parameter group of **F** *diffeomorphisms generated by ∂_v.*
In other words, for every $t\in\mathbb{R}$ and positive-frequency part wave function $\tilde{\varphi}_+$, the positive-frequency part wave function $e^{itH_{\mathbf{F}}}\tilde{\varphi}_+$ is associated with the horizon wave function φ_{g_t} such that

$$\left.\frac{\partial\varphi_{g_t}}{\partial t}\right|_{t=0}=-\partial_v\varphi\ .$$

(b) With the same terminology as in case (a), the unitary one-parameter group generated by $i\overline{D}_{\mathbf{F}}$ is associated with the one-parameter group of **F** *diffeomorphisms generated by $v\partial_v$.*

(c) With the same terminology as in case (a), the unitary one-parameter group generated by $i\overline{C}_{\mathbf{F}}$ is associated with the one-group of **F** *diffeomorphisms generated by $v^2\partial_v$.*

The term $-\varphi(b/d)$ in (17) assures that φ_g vanishes as $v\to\pm\infty$. Notice that the added term disappears when referring to $\mathrm{d}\varphi$ rather than φ. The group of diffeomorphisms of $\mathbf{F}\equiv\mathbb{R}$ used above,

$$v\mapsto\frac{av+b}{cv+d},\quad \begin{pmatrix} a & b\\ c & d\end{pmatrix}\in SL(2,\mathbb{R}), \tag{18}$$

in fact gives a representation of $SL(2,\mathbb{R})$. It can be obtained by finite composition of one-parameter subgroups associated with the following three vector fields on **F**: $\partial_v, v\partial_v, v^2\partial_v$. It is simply proven that the Lie brackets of $-\partial_v, -v\partial_v, -v^2\partial_v$ produce the same algebra as the Lie algebra of $SL(2,\mathbb{R})$. We conclude that the bulk $SL(2,\mathbb{R})$-symmetry is manifest when examined on the horizon, in the sense that it is induced by the geometry.

II. FROM THE LINE TO THE CIRCLE: THE FULL VIRASORO ALGEBRA

Noli tangere circulos meos. (Archimedes' last words.)

The algebra of vector fields $\partial_v, v\partial_v, v^2\partial_v$ can be extended to include the class of fields defined on the horizon $v^{n+1}\partial_v$ with $n\in\mathbb{Z}$. It is interesting to notice that these fields (more precisely the fields $-v^{n+1}\partial_v$) enjoy Virasoro commutation relations without central charge. In fact there is a central representation of Virasoro algebra which presents a central charge and is directly defined in terms of operators acting in the Fock space of the horizon particles. The representation can be introduced after one has given a convenient definition of quantum field operator on the circle $\mathsf{F}=\mathbf{F}\cup\{\infty\}$.

A. QFT on the circle $\mathsf{F}=\mathsf{F}\cup\{\infty\}$

Consider the vector field on $\mathbf{F}$,

$$\mathcal{K}:=\frac{1}{2}\left(\beta\partial_v+\frac{1}{\beta}v^2\partial_v\right). \tag{19}$$

That field is associated with the essentially self-adjoint operator that is defined on $\mathcal{D}_1^{(\mathbf{F})}$,

$$K_{\mathbf{F}\beta}:=\frac{1}{2}\left(\beta H_{\mathbf{F}}+\frac{1}{\beta}C_{\mathbf{F}}\right), \tag{20}$$

in the Lie algebra of the unitary representation of $SL(2,\mathbb{R})$ because of Theorem 1.4. It is simply proven that the integral line of $\mathcal{K}$ with origin in $v=0$ is $v=\beta\tan(\theta/2)$ with $\theta\in(-\pi,\pi)$ and $v=0$ corresponding to $\theta=0$. One can use θ as a new coordinate on $\mathbf{F}$ with the advantage that this new coordinate gets finite values in the whole compactified manifold $\mathbf{F}\cup\{\infty\}\equiv\mathsf{F}$ (in the sense of Alexandrov's procedure), the added point ∞ corresponding to $\theta=\pi\equiv-\pi$ in the circle. As a consequence of our definitions, it turns out that

$$\mathcal{K}=\partial_\theta. \tag{21}$$

In fact this formula smoothly extends the left-hand side on the whole circle F. By construction, there is the natural submanifold embedding $\mathbf{F}\subset\mathsf{F}$. We want to show that such an inclusion can be extended to free quantum field theory if a suitable definition of QFT on F is given. We follow a procedure very similar to that used for the horizon. As a final result we show that more strongly, the ''inclusion'' of QFT on $\mathbf{F}$ into QFT on F is actually a unitary equivalence as well as a $*$-algebras inclusion. The observable $K_{\mathbf{F}\beta}$ plays a central role in that identification. The associated quantum field theory on F will be proved to support a nice unitary Virasoro's algebra representation with an explicit geometric meaning that extends the unitary representation of $SL(2,\mathbb{R})$.

Consider the space of real C^∞ functions ρ on F, $C^\infty(\mathsf{F};\mathbb{R})$, and define a subsequent real vector space $\mathcal{S}(\mathsf{F})$ by taking the quotient with respect to the equivalence relation, for $\rho,\rho'\in C^\infty(\mathsf{F};\mathbb{R})$,

$$\rho\sim\rho' \quad \text{iff} \quad d(\rho-\rho')=0. \tag{22}$$

From now on, the elements of $\mathcal{S}(\mathsf{F})$ are called *circle wave functions*. The following symplectic form on $\mathcal{S}(\mathsf{F})$ is well-defined and nondegenerate [the latter is not true on $C^\infty(\mathsf{F};\mathbb{R})$]:

$$\Omega_{\mathsf{F}}(\rho,\rho'):=\int_{\mathsf{F}}\rho'\,\mathrm{d}\rho-\rho\,\mathrm{d}\rho'. \tag{23}$$

The elements of $C^\infty(\mathsf{F};\mathbb{C})$ can be expanded in Fourier series. If $\rho\in C^\infty(\mathsf{F};\mathbb{R})$, with a rearrangement of the Fourier coefficients it holds either in $L^2(\mathsf{F},\mathrm{d}\theta)$ and in the uniform sense

$$\rho(\theta)=\rho_0+\sum_{n=1}^{\infty}\frac{e^{-in\theta}\,\tilde{\rho}_+(n)}{\sqrt{4\pi n}}+\frac{e^{in\theta}\,\overline{\tilde{\rho}_+(n)}}{\sqrt{4\pi n}}.$$

As $\tilde{\rho}_+(n)$ is proportional to $\int_{\mathsf{F}} e^{-in\theta}\rho(\theta)\mathrm{d}\theta$ and $\int_{\mathsf{F}} e^{-in\theta}\mathrm{d}\theta = 0$, if $n>0$, the coefficients $\tilde{\rho}(n)$ are not affected if ρ is replaced by ρ' with $\rho-\rho' =$ constant, and thus the coefficients $\tilde{\rho}_+(n)$, *for* $n>0$, are well-associated with an element of $\mathcal{S}(\mathsf{F})$. In the following we indicate the elements of $\mathcal{S}(\mathsf{F})$ simply by ρ instead of $[\rho]$. In the sense clarified above, if $\rho \in \mathcal{S}(\mathsf{F})$ we have

$$\rho(\theta) = \sum_{n=1}^{\infty} \frac{e^{-in\theta}\,\tilde{\rho}_+(n)}{\sqrt{4\pi n}} + \text{c.c.} = \rho_+(\theta) + \text{c.c.} \tag{24}$$

To define the one-particle Hilbert space, define the Hermitian scalar product

$$\langle \rho'_+, \rho_+ \rangle_{\mathsf{F}} := -i\Omega_{\mathsf{F}}(\overline{\rho'_+}, \rho_+) \ .$$

The one-particle Hilbert space $\mathcal{H}_{\mathsf{F}}$ is the completion with respect to that scalar product of the space of complex combinations of positive frequency parts $\{\tilde{\rho}_+(n)\}$, of circle wave functions ρ. It is simply proven that, if $\rho \in C^\infty(\mathsf{F};\mathbb{C})$ with Fourier coefficients $\{C_n\}_{n\in\mathbb{Z}}$, for every $p=0,1,\ldots$ there is a real K_p such that $|n|^p|C_n| \leqslant K_p$ for all $n \in \mathbb{Z}$. As a consequence, $\sum_{n\in\mathbb{Z}} n|C_n|^2 < \infty$. We conclude that, if $\rho \in \mathcal{S}(\mathsf{F})$, the sequence of complex numbers $\{\tilde{\rho}_+(n) = \sqrt{2n}C_n\}_{n=1,2,\ldots}$ is an element of $\ell^2(\mathbb{C})$. A direct computation shows that $\mathcal{H}_{\mathsf{F}}$ turns out to be isomorphic to $\ell^2(\mathbb{C})$ because

$$\langle \rho'_+, \rho_+ \rangle_{\mathsf{F}} = \sum_{n=1}^{\infty} \overline{\tilde{\rho}'_+(n)}\tilde{\rho}_+(n).$$

Using the Hilbert base of $\mathcal{H}_{\mathbf{F}}$ given by the eigenvectors of the operator $K_{\beta\mathbf{F}}$, $\{Z_n^{(1)}\}_{n=1,2,\ldots}$ [where the phase of $Z_n^{(1)}$ in (9) is fixed to be $\eta_n = (-1)^{n+1}$], the unitary map $M: \mathcal{H}_{\mathbf{F}} \to \mathcal{H}_{\mathsf{F}}$ can be defined such that

$$M: \varphi \mapsto \{\langle Z_n^{(1)}, \varphi\rangle\}_{n=1,2,\ldots} . \tag{25}$$

That isomorphism has a natural geometric interpretation stated in the former part of the theorem below.

Theorem 2.1: *Let $\varphi = \varphi(v)$ be a real horizon wave function (which belongs to Schwartz's space on $\mathbb{R} \equiv \mathbf{F}$) associated with a quantum state $\tilde{\varphi}_+$. If ρ is the circle wave function associated with φ by means of the unitary transformation (25), that is $\tilde{\rho}_+ := M(\tilde{\varphi}_+)$, one has*

$$\rho(\theta) = \varphi(v(\theta)) \ , \tag{26}$$

where $v(\theta) = \beta\tan(\theta/2)$, $\theta \in (-\pi, \pi]$. In other words

$$\varphi(v(\theta)) = \sum_{n=1}^{\infty} \frac{\langle Z_n^{(1)}, \tilde{\varphi}_+\rangle}{\sqrt{4\pi n}} e^{-in\theta} + \text{c.c.} + \text{const.}$$

The linear map $\varphi \mapsto \rho$ defined in (26) is injective and preserves the symplectic forms of the respective spaces, that is, if ρ' is associated with φ' by the map (26) itself,

$$\Omega_{\mathsf{F}}(\rho, \rho') = \Omega_{\mathbf{F}}(\varphi, \varphi') \ . \tag{27}$$

Proof: Notice that, if the real horizon wave function $\varphi = \varphi(v)$ is in Schwartz's space, the function $(-\pi, \pi] \ni \theta \mapsto \varphi(v(\theta))$ is well-defined and belongs to $C^\infty(\mathsf{F};\mathbb{R})$ with $\varphi(v(\pm\pi)) = 0$ with all its derivatives of any order. So the thesis makes sense. The second part can straightforwardly be proven by using the given definitions, so we focus on the former only. If the real horizon wave function $\varphi = \varphi(v)$ is in Schwartz's space, the associated positive frequency part $\tilde{\varphi}_+(E)$ is such that $\tilde{\varphi}_+(E)/\sqrt{4\pi E}$ is the restriction to $\mathbb{R}^+$ of Schwartz's function. As a consequence $\varphi_+(v) = \int_0^{+\infty} \mathrm{d}E\, e^{-iEv}\tilde{\varphi}_+(E)/\sqrt{4\pi E}$ is smooth and

$$\varphi_+(v(\theta)) \sim \text{const} \times \frac{\tilde{\varphi}_+(E)}{\sqrt{E}}\bigg|_{E=0} (\theta \mp \pi)^2$$

as $\theta \to \pm\pi$. So the Fourier expansion of φ_+ makes sense and each coefficient of the Fourier expansion of φ is the sum of the corresponding coefficients of the Fourier expansion of φ_+ and $\overline{\varphi_+}$, it being $\varphi = \varphi_+ + \overline{\varphi_+}$. We want to evaluate the Fourier coefficients of φ_+. First consider the Fourier coefficients with $n>0$. By direct computation[17] one finds

$$\int_0^{+\infty} \frac{e^{-iE\beta \tan(\theta/2)} Z_n^{(1)}(E)}{\sqrt{4\pi E}} \mathrm{d}E = \frac{1}{\sqrt{4\pi n}} ((-1)^{n+1} + e^{-in\theta}) \ , \tag{28}$$

with $\theta \in (-\pi, \pi]$ [notice that the dependence form β cancels out due the shape (9) of functions $Z_n^{(1)}$ by passing to the new variable of integration βE in the integral]. As a consequence, defining $Z_n^{(1)}(E)=0$ if $E<0$, inverting the Fourier(-Plancherel) transform (and changing the integration variable $v \to -v$),

$$\frac{Z_n^{(1)}(E)}{\sqrt{2E}} = \lim_{L\to+\infty} \int_{-L}^{L} \mathrm{d}v \, e^{-ivE} \frac{(-1)^{n+1} + e^{2in \tan^{-1}(v/\beta)}}{\sqrt{4\pi n}} \ , \tag{29}$$

the limit being computed in the sense of $L^2(\mathbb{R}, \mathrm{d}E)$. Since $E \mapsto \tilde{\varphi}_+(E)/\sqrt{E}$ is the restriction to $\mathbb{R}^+$ of a Schwartz function, $E \mapsto \psi(E) = \sqrt{2E}\tilde{\varphi}_+(E)$ ($\psi(E) := 0$ for $E<0$!) is a function in $L^1(\mathbb{R}, \mathrm{d}E) \cap L^2(\mathbb{R}, \mathrm{d}E)$. The functions $E \mapsto Z_n^{(1)}(E)$ and $E \mapsto Z_n^{(1)}(E)/\sqrt{2E}$ (assumed to vanish for $E<0$) are real and belong to $L^1(\mathbb{R}, \mathrm{d}E) \cap L^2(\mathbb{R}, \mathrm{d}E)$. It holds

$$\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle = \int_0^{\infty} \overline{Z_n^{(1)}(E)} \tilde{\varphi}_+(E) \mathrm{d}E = \int_{-\infty}^{\infty} \frac{Z_n^{(1)}(E)}{\sqrt{2E}} \psi(E) \mathrm{d}E \ .$$

Using (29) and taking the L^2-continuity of the scalar product into account, one gets

$$\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle = \lim_{L\to+\infty} \int_{-\infty}^{\infty} \mathrm{d}E \, \psi(E) \int_{-L}^{L} \mathrm{d}v \, e^{-ivE} \frac{(-1)^{n+1} + e^{2in \tan^{-1}(v/\beta)}}{\sqrt{4\pi n}} \ ,$$

that is

$$\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle = \lim_{L\to+\infty} \int_{0}^{\infty} \mathrm{d}E \, \tilde{\varphi}_+(E) \int_{-L}^{L} \mathrm{d}v \, 2E \frac{e^{-ivE}}{\sqrt{2E}} \frac{(-1)^{n+1} + e^{in\theta(v)}}{\sqrt{4\pi n}} \ .$$

Using $E e^{-ivE} = i(\partial/\partial v) e^{-ivE}$ and integrating by parts it arises

$$\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle = C(L) + \lim_{L\to+\infty} \sqrt{2n} \int_0^{\infty} \mathrm{d}E \, \tilde{\varphi}_+(E) \int_{-L}^{L} \mathrm{d}v \, \frac{e^{-iEv}}{\sqrt{4\pi E}} \frac{e^{in\theta(v)}}{\sqrt{2\pi}} \frac{\mathrm{d}\theta}{\mathrm{d}v} \ ,$$

where $C(L)$ is a boundary term which vanishes in the limit $L\to\infty$ by Riemann–Lebesgue's lemma. Interchanging the integration symbols and taking the limit as $L\to\infty$ we finally get the nth Fourier coefficient of φ_+ and the $(-n)$th Fourier coefficient of $\overline{\varphi_+}$,

$$\int_{-\pi}^{\pi} \varphi_+(v(\theta)) \frac{e^{in\theta}}{\sqrt{2\pi}} \mathrm{d}\theta = \frac{\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle}{\sqrt{2n}} \quad , \quad \int_{-\pi}^{\pi} \overline{\varphi_+(v(\theta))} \frac{e^{-in\theta}}{\sqrt{2\pi}} \mathrm{d}\theta = \frac{\overline{\langle Z_n^{(1)}, \tilde{\varphi}_+ \rangle}}{\sqrt{2n}} \ .$$

Now we pass to consider the remaining Fourier coefficients. Since in (29) $Z_n^{(1)}(E)$ is defined to vanish for $E<0$, one has that, if $n>0$,

$$\lim_{L\to+\infty}\int_{-\infty}^{0} dE\, f(E)\int_{-L}^{L} dv\, e^{-ivE}\frac{(-1)^{n+1}+e^{2in\tan^{-1}(v/\beta)}}{\sqrt{4\pi n}}=0\,,$$

which, after complex conjugation and change of variables $E\to -E$, is equivalent to

$$\lim_{L\to+\infty}\int_{0}^{+\infty} dE\, g(E)\int_{-L}^{L} dv\, e^{-ivE}\frac{(-1)^{m+1}+e^{2im\tan^{-1}(v/\beta)}}{\sqrt{4\pi|m|}}=0\,, \tag{30}$$

where $m=-n<0$ and $g\in L^2(\mathbb{R},dE)$. Using $g(E)=\sqrt{2E}\tilde{\varphi}_+(E)$ for $E\geqslant 0$ and $g(E)=0$ otherwise and following the same procedure as for the case $n>0$, (30) implies that, if $n<0$,

$$\int_{-\pi}^{\pi}\varphi_+(v(\theta))\frac{e^{in\theta}}{\sqrt{2\pi}}d\theta=0\,.$$

As a consequence,

$$\int_{-\pi}^{\pi}\overline{\varphi_+(v(\theta))}\frac{e^{-in\theta}}{\sqrt{2\pi}}d\theta=0\,.$$

Putting all together we get

$$\varphi(v(\theta))=\varphi_+(v(\theta))+\overline{\varphi_+(v(\theta))}=\text{constant}+\sum_{n=1}^{\infty}\frac{\langle Z_n^{(1)},\tilde{\varphi}_+\rangle}{\sqrt{4\pi n}}e^{-in\theta}+\sum_{n=1}^{\infty}\overline{\frac{\langle Z_n^{(1)},\tilde{\varphi}_+\rangle}{\sqrt{4\pi n}}}e^{in\theta}$$

which concludes the proof. □

The result stated in Theorem 2.1 suggests to define a quantum field on the circle $\mathsf{F}:=\mathbf{F}\cup\{\infty\}$ whose Hilbert space is the symmetrized Fock space $\mathfrak{F}(\mathcal{H}_\mathsf{F})\cong\mathfrak{F}(\mathcal{H}_\mathbf{F})$, where the isomorphism is that naturally induced by M of Eq. (25) and the vacuum $|0\rangle_\mathsf{F}$ is associated with $|0\rangle_\mathbf{F}$ by the isomorphism itself. Formally the quantum field operator on F reads

$$\hat{\phi}(\theta)=\sum_{n=1}^{\infty}\frac{e^{-in\theta}\,\alpha_n}{\sqrt{4\pi n}}+\frac{e^{in\theta}\,\alpha_n^\dagger}{\sqrt{4\pi n}}\,, \tag{31}$$

where α_n and $\alpha_n^\dagger$ are the annihilator and constructor operator of modes $Z_n^{(1)}$.

The field operator is defined in the symmetrized Fock space $\mathfrak{F}(\mathcal{H}_\mathsf{F})$, with rigorous symplectic definition given by

$$\rho\mapsto\Omega_\mathsf{F}(\rho,\hat{\phi}_F):=i\alpha(\overline{\rho_+})-i\alpha^\dagger(\rho_+)\,, \tag{32}$$

where ρ is any circle wave function and, respectively, $\alpha(\overline{\rho_+})$, $\alpha^\dagger(\rho_+)$ annihilates and creates the states $\overline{\rho_+}$ and ρ_+. Once again a well-defined smearing procedure is that of field operators and exact one-forms $\eta=d\rho$ where $\rho\in\mathcal{S}(\mathsf{F})$. Notice that $d\rho$ does not depend on the chosen element of the class of equivalence associated with ρ. More precisely, we introduce the "*causal propagator*" on F

$$\eta(\theta)\mapsto E_\mathsf{F}(\eta)=\frac{1}{4}\int_\mathsf{F}[\text{sign}(\theta-\theta')+(\theta'-\theta)/\pi]\,\eta(\theta')\,,$$

where it is understood that one has to take the quotient with respect to the equivalence relation defining $\mathcal{S}(\mathsf{F})$ after the action of E_{F}. Moreover the used function $x\to \mathrm{sign}x$ and $x\to x$ are first defined in $[-\pi,\pi]$ and then are extended in the whole $\mathbb{R}$ as periodic functions with period 2π. E_{F} gives rise to a bijective linear map from the space of real exact C^∞ one-forms on F [which will be denoted by $\mathcal{D}(\mathsf{F})$] and $\mathcal{S}(\mathsf{F})$ itself. Indeed, it results that if $\rho\in\mathcal{S}(\mathsf{F})$,

$$E_{\mathsf{F}}(\omega)=\rho \qquad \text{if and only if} \qquad \omega=2d\rho\ . \tag{33}$$

We can define the field operator smeared by elements of $\mathcal{D}(\mathsf{F};\mathbb{R})$ as

$$\eta\mapsto\hat{\phi}_{\mathsf{F}}(\eta):=\Omega_{\mathsf{F}}(E_{\mathsf{F}}\eta,\hat{\phi}_{\mathsf{F}})\ , \tag{34}$$

which is the rigorous meaning of

$$\hat{\phi}_{\mathsf{F}}(\eta)=\sum_{n=1}^{\infty}\left(\int_{\mathsf{F}}e^{-in\theta}\eta(\theta)\right)\frac{\alpha_n}{\sqrt{4\pi n}}+\left(\int_{\mathsf{F}}e^{in\theta}\eta(\theta)\right)\frac{\alpha_n^\dagger}{\sqrt{4\pi n}}\ . \tag{35}$$

Circle wave functions ρ and one-forms η,η' in the above-noted spaces enjoy the same properties as in the bulk. More precisely one has

$$\int_{\mathsf{F}}\rho\,\eta=\Omega_{\mathsf{F}}(E_{\mathsf{F}}\eta,\rho),\qquad \int_{\mathsf{F}}(E_{\mathsf{F}}\eta)\,\eta'=\Omega_{\mathsf{F}}(E_{\mathsf{F}}\eta,E_{\mathsf{F}}\eta')\ , \tag{36}$$

$$[\hat{\phi}_{\mathsf{F}}(\eta),\hat{\phi}_{\mathsf{F}}(\eta')]=-iE_{\mathsf{F}}(\eta,\eta')\ . \tag{37}$$

The latter is nothing but the rigorous meaning of the formal equation $[\hat{\phi}_{\mathsf{F}}(\theta),\hat{\phi}_{\mathsf{F}}(\theta')]=-iE_{\mathsf{F}}(\theta,\theta')$. Notice that as a consequence of (33), (36), (37), a "locality property" holds

$$[\hat{\phi}_{\mathsf{F}}(\eta),\hat{\phi}_{\mathsf{F}}(\eta')]=0 \qquad \text{if} \qquad \mathrm{supp}(\eta)\cap\mathrm{supp}(\eta')=\varnothing.$$

Everything we said about the future circle $\mathsf{F}=\mathbf{F}\cup\{\infty\}$ can be restated, with obvious changes of notation, for the past circle $\mathsf{P}:=\mathbf{P}\cup\{\infty\}$.

Theorem 2.1 together with Theorems 1.1 and 1.2 has two straightforward consequences.

Theorem 2.2: *If f is any real smooth compactly supported function f used to smear the bulk field, extend on F and P the forms η_f and ω_f defined in Theorem 1.1 by putting $\eta_f(\infty):=0$ and $\omega_f(\infty):=0$ and consider these forms as elements of $\mathcal{D}(\mathsf{F})$ and $\mathcal{D}(\mathsf{P})$ respectively.*

(a) If $m>0$, there is a unitary map $U_{\mathsf{F}}:\mathfrak{F}(\mathcal{H})\to\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ such that

$$U_{\mathsf{F}}|0\rangle=|0\rangle_{\mathsf{F}},\quad \textit{and}\quad U_{\mathsf{F}}^{-1}\hat{\phi}_{\mathsf{F}}(\eta_f)U_{\mathsf{F}}=\hat{\phi}(f)\ .$$

(b) If $m=0$, two unitary operators arise $V_{\mathsf{F/P}}:\mathfrak{F}(\mathcal{H}_{\mathrm{in/out}})\to\mathfrak{F}(\mathcal{H}_{\mathsf{F/P}})$ such that

$$V_{\mathsf{F/P}}|0\rangle_{\mathrm{in/out}}=|0\rangle_{\mathsf{F/P}}$$

and

$$V_{\mathsf{F}}^{-1}\hat{\phi}_{\mathsf{F}}(\eta_f)V_{\mathsf{F}}=\hat{\phi}_{\mathrm{in}}(f)\ ,\quad \textit{and}\quad V_{\mathsf{P}}^{-1}\hat{\phi}_{\mathsf{P}}(\omega_f)V_{\mathsf{P}}=\hat{\phi}_{\mathrm{out}}(f)\ .$$

$\mathcal{H}_{\mathrm{in/out}}$ is the bulk Hilbert space associated with the ingoing/outgoing modes and $\hat{\phi}_{\mathrm{in/out}}(f)$ is the part of bulk field operator built up using only ingoing/outgoing modes.

Sketch of proof: The unitary operator $U_{\mathbf{F}}$ in Theorem 1.1 is obtained (see Ref. 8) as the unitary operator that fulfills the following pair of conditions. (1) $U_{\mathbf{F}}|0\rangle=|0\rangle_{\mathbf{F}}$; (2) for every natural n, consider the subspace of $\mathfrak{F}(\mathcal{H})$, $\mathcal{H}^{n\otimes}$, spanned by (symmetrized) states with n particles; on every $\mathcal{H}^{n\otimes}$, $U_{\mathbf{F}}$ reduces to the tensor product of n copies of the unitary operator $\mathcal{U}_{\mathbf{F}}:\mathcal{H}\to\mathcal{H}_{\mathbf{F}}$, where,

under the identifications (working in the energy representations) $\mathcal{H}\cong L^2(\mathbb{R}^+,\mathrm{d}E)$, $\mathcal{H}_{\mathbf{F}}\cong L^2(\mathbb{R}^+,\mathrm{d}E)$, $\mathcal{U}_{\mathbf{F}}$ is nothing but the identity operator. Now consider the composite unitary operator $\mathcal{U}_{\mathsf{F}}:=M\circ\mathcal{U}_{\mathbf{F}}:\mathcal{H}\to\mathcal{H}_{\mathsf{F}}$, where M is as in Eq. (25), and define U_{F} such that $U_{\mathsf{F}}|0\rangle=|0\rangle_{\mathsf{F}}$ and the restriction of U_{F} to every $\mathcal{H}^{n\otimes}$ coincides with the tensor product of n copies of the unitary operator $\mathcal{U}_{\mathsf{F}}$. Theorems 1.1 and 2.1 and the definition of $\hat{\phi}_{\mathsf{F}}$ immediately imply the validity of the thesis. The case of $m=0$ can be proven by the same way. □

Similar to the extent on the horizon case, one can focus on the algebra $\mathcal{A}_{\mathsf{F}}$ of linear combinations of product of field operators $\hat{\phi}_{\mathsf{F}}(\omega)$, varying ω in the space $\mathcal{D}(\mathsf{F};\mathbb{C}):=\mathcal{D}(\mathsf{F})+i\mathcal{D}(\mathsf{F})$ and defining $\hat{\phi}_{\mathsf{F}}(\omega+i\omega'):=\hat{\phi}_{\mathsf{F}}(\omega)+i\hat{\phi}_{\mathsf{F}}(\omega')$. We assume that $\mathcal{A}_{\mathsf{F}}$ also contains the unit operator I. The Hermitian elements of $\mathcal{A}_{\mathsf{F}}$ are the natural observables associated with the horizon field. From an abstract point of view the found algebra is a unital $*$-algebra of formal operators $\phi_{\mathsf{F}}(\eta)$ with the additional properties $[\phi_{\mathsf{F}}(\eta),\phi_{\mathsf{F}}(\eta')]=-iE_{\mathsf{F}}(\eta,\eta')$, $\phi_{\mathsf{F}}(\eta)^*=\phi_{\mathsf{F}}(\overline{\eta})$ and linearity in the form η. $\mathcal{A}_{\mathsf{F}}$ can be studied no matter any operator representation in any Fock space. Operator representations are obtained via GNS theorem once an algebraic state has been fixed.[18] Everything we said can be extended to the analogous $*$-algebra defined on P, $\mathcal{A}_{\mathsf{P}}$. We have a second result.

Theorem 2.3. *Assume the same notation as in Theorem 2.2 concerning η_f and ω_f.*

(a) If $m>0$, there is a unique injective unital $*$-algebras homomorphism $\chi_{\mathsf{F}}:\mathcal{A}_{\mathbf{R}}\to\mathcal{A}_{\mathsf{F}}$ such that $\chi_{\mathsf{F}}(\phi(f))=\phi_{\mathsf{F}}(\eta_f)$. Consider the GNS representations in the Fock spaces $\mathfrak{F}(\mathcal{H})$, $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ built up over $|0\rangle$ and $|0\rangle_{\mathsf{F}}$, respectively associated with $\mathcal{A}_{\mathbf{R}}$ and $\mathcal{A}_{\mathsf{F}}$, in these representations χ_{F} has a unitary implementation naturally induced by U_{F} (e.g. $\chi_{\mathsf{F}}(\hat{\phi}(f))=U_{\mathsf{F}}\hat{\phi}(f)U_{\mathsf{F}}^{-1}$).

(b) If $m=0$, there are two injective unital $*$-algebras homomorphisms $\Pi_{\mathsf{F/P}}:\mathcal{A}_{\mathrm{in/out}}\to\mathcal{A}_{\mathsf{F/P}}$ such that $\Pi_{\mathsf{F}}(\phi(f))=\phi_{\mathsf{F}}(\eta_f)$ and $\Pi_{\mathsf{P}}(\phi(f))=\phi_{\mathsf{P}}(\omega_f)$. Moreover, considering the GNS representations in the Fock spaces $\mathfrak{F}(\mathcal{H}_{\mathrm{in/out}})$, $\mathfrak{F}(\mathcal{H}_{\mathsf{F/P}})$ built up over $|0\rangle_{\mathrm{in/out}}$ and $|0\rangle_{\mathsf{F/P}}$ respectively associated with $\mathcal{A}_{in/out}$ and $\mathcal{A}_{\mathsf{F/P}}$, Π_{F} and Π_{P} have unitary implementations and reduce to V_{F} and V_{P}, respectively.

Sketch of proof: Consider the map $\chi'_{\mathsf{F}}:\hat{\phi}_{\mathbf{F}}(\eta)\mapsto\hat{\phi}_{\mathsf{F}}(\eta)$ where $\eta=\mathrm{d}\varphi$, φ being any real Schwartz function on $\mathbf{F}\equiv\mathbb{R}$. In $\hat{\phi}_{\mathbf{F}}(\eta)$, η is supposed extended to the whole F by means of $\eta(\infty):=0$ so that $\eta\in\mathcal{D}(\mathsf{F};\mathbb{R})$. Using the fact that it holds $[\hat{\phi}_{\mathsf{F}}(\eta),\hat{\phi}_{\mathsf{F}}(\eta')]=-i\Omega_{\mathsf{F}}(E_{\mathsf{F}}(\eta'),E_{\mathsf{F}}(\eta))=-i\Omega_{\mathbf{F}}(E_{\mathbf{F}}(\eta'),E_{\mathbf{F}}(\eta))=[\hat{\phi}_{\mathbf{F}}(\eta),\hat{\phi}_{\mathbf{F}}(\eta')]$, one proves that χ'_{F} uniquely extends into an injective $*$-algebra homomorphism from $\mathcal{A}_{\mathbf{F}}$ to $\mathcal{A}_{\mathsf{F}}$. The injective $*$-algebra homomorphism χ_{F} is nothing but $\chi'_{\mathsf{F}}\circ\chi_{\mathbf{F}}$. The remaining properties are strightforward consequences of the properties of $\chi_{\mathbf{F}}$ stated in Theorem 1.2. The case $m=0$ is analogous. □

B. Virasoro algebra with $c=1$ in the Fock space of the circle

The unitary map $M:\mathcal{H}_{\mathbf{F}}\to\mathcal{H}_{\mathsf{F}}$ associates the essentially self-adjoint operators $H_{\mathbf{F}0},D_{\mathbf{F}},C_{\mathbf{F}}$ defined on $\mathcal{D}_1^{(\mathbf{F})}\subset\mathcal{H}_{\mathbf{F}}$ with analogous essentially self-adjoint operators acting on one-particle circle states $\mathcal{H}_{\mathsf{F}}$, respectively, $H_{\mathsf{F}0},D_{\mathsf{F}},C_{\mathsf{F}}$. More precisely, the real linear combinations of these operators are essentially self-adjoint in the dense invariant domain $\mathcal{D}_1^{(\mathsf{F})}=M(\mathcal{D}_1^{(\mathbf{F})})$ spanned by the eigenvectors of $K_{\beta\mathsf{F}}$ associated with the analogous operator $K_{\beta\mathbf{F}}$ (20). The Lie algebra spanned by the operators above in F gives rises to a strongly continuous unitary $SL(2,\mathbb{R})$ representation $\{U_g^{(\mathsf{F})}\}_{g\in SL(2,\mathbb{R})}$ on the Hilbert space of the circle that is related, by means of M, with the analogous unitary representation $\{U_g^{(\mathbf{F})}\}_{g\in SL(2,\mathbb{R})}$ found on the horizon $\mathbf{F}$ discussed earlier in [e]. And thus, in turn, it induces just the bulk symmetry induced by $\{U_g^{(\mathbf{F})}\}_{g\in SL(2,\mathbb{R})}$ (see [e] discussed earlier) by means of unitary holography. In particular $H_{\mathsf{F}}:=H_{\mathsf{F}0}$ turns out to be associated with the generator of Rindler-time displacements H.

$H_{\mathsf{F}0},D_{\mathsf{F}},C_{\mathsf{F}}$ are a basis of the Lie algebra of $SL(2,\mathbb{R})$. An equivalent, but more useful in the following, basis of the Lie algebra of $SL(2,\mathbb{R})$ made of essentially self-adjoint operators in $\mathcal{D}_1^{(\mathsf{F})}$ is that of the operators $K_{\beta\mathsf{F}},D_{\mathsf{F}},S_{\mathsf{F}}$ with

$$S_{\mathsf{F}}:=\frac{1}{2}\left(\beta H_{\mathsf{F}0}-\frac{1}{\beta}C_{\mathsf{F}}\right). \tag{38}$$

Now, it makes sense to investigate the *geometrical nature* of the $SL(2,\mathbb{R})$ representation $\{U_g^{(\mathsf{F})}\}$ on *the circle* F *instead of the horizon* **F**. First of all one has to notice that the vector fields $\partial/\partial v$, $v\,(\partial/\partial v)$, $v^2\,(\partial/\partial v)$, which give rise to the geometric interpretation of $\{U_g^{(\mathbf{F})}\}$ when working on **F**, span in **F** the same space as that spanned by the three smooth vector fields defined on the whole circle F,

$$\partial_\theta, \cos(\theta)\partial_\theta, \sin(\theta)\partial_\theta .$$

The proof is straightforward using the relation $v=\beta\tan(\theta/2)$ only. Then consider the transformations (18) of the line **F**, translate them in the variable $\theta=2\arctan(v/\beta)$ extended to the domain $(-\pi,\pi]$ so to include ∞. The new transformations so obtained define a representation of $SL(2,\mathbb{R})$ in terms of orientation-preserving diffeomorphisms d_g of the circle F:

$$d_g:\theta\mapsto 2\arctan\left(\frac{a\beta\tan(\theta/2)+b}{c\beta^2\tan(\theta/2)+\beta d}\right), \quad g:=\begin{pmatrix} a & b \\ c & d\end{pmatrix}\in SL(2,\mathbb{R}) \ . \tag{39}$$

There is another, more elegant, way to write the elements of same diffeomorphism group:

$$\delta_h:e^{i\theta}\mapsto \frac{\zeta e^{i\theta}+\overline{\eta}}{\eta e^{i\theta}+\overline{\zeta}}, \quad h:=\begin{pmatrix} \zeta & \overline{\eta} \\ \eta & \overline{\zeta}\end{pmatrix}\in SU(1,1) \ , \tag{40}$$

where we have used the group isomorphism $SL(2,\mathbb{R})\ni g\mapsto h\in SU(1,1)$ with

$$\zeta:=\frac{\beta a+\beta d+i(b-\beta^2 c)}{2}, \quad \eta:=\frac{\beta d-\beta a-i(b+\beta^2 c)}{2} .$$

The condition $h\in SU(1,1)$, when h has the form in (40), can equivalently be written

$$|\zeta|^2-|\eta|^2=1 . \tag{41}$$

Remark: Notice that the transformation $\rho\mapsto\rho_g$ does not mix Fourier components with positive frequency and Fourier components with negative frequency and vice versa. (This fact allows one to look for unitary representations of the considered group in the one-particle Hilbert space which is constructed by using positive frequency part of wave functions.) Indeed, using (40), $e^{-in\theta}$ is mapped into

$$\left(\frac{\zeta e^{i\theta}+\overline{\eta}}{\eta e^{i\theta}+\overline{\zeta}}\right)^{-n} .$$

Fourier coefficients with strictly ''negative frequency'' $-m$ are proportional to the integrals, where $m,n\geqslant 1$ are integers,

$$\int_{-\pi}^{\pi}\left(\frac{\zeta e^{i\theta}+\overline{\eta}}{\eta e^{i\theta}+\overline{\zeta}}\right)^{-n} e^{-im\theta}\mathrm{d}\theta = \oint_{+\mathbb{S}^1}\frac{-i}{z^{m+1}}\left(\frac{\eta z+\overline{\zeta}}{\zeta z+\overline{\eta}}\right)^{n}\mathrm{d}z = \oint_{+\mathbb{S}^1}\frac{-i}{z^{m+1}}\left(\frac{\eta}{\zeta}+\frac{1/\zeta}{\zeta z+\overline{\eta}}\right)^{n}\mathrm{d}z \ ,$$

where $+\mathbb{S}^1$ is the circle $|z|=1$ with positive orientation. Expanding the expression under the last integration symbol using the binomial formula one reduces to a linear combination of contributions of integrals with form

$$\oint_{+\mathbb{S}^1}\frac{\mathrm{d}z}{z^{m+1}(z-z_0)^p}$$

with $p=0,1,\ldots,n\geqslant 1$, $m\geqslant 1$ and where $z_0=-\overline{\eta}/\zeta$ with $\zeta\neq 0$ [due to (41)]. If $p>0$, using condition (41) one sees that, whatever the values of η and ζ and barring the pole at $z=0$ with order $m+1$, there is another pole of order p inside the region with boundary $\mathbb{S}^1$, at $z=-\overline{\eta}/\zeta$. Cauchy formula for $p>0$ proves that the contribution of the two residues in each integral cancel out each other and the final result is zero. The case $p=0$ gives the same result automatically. So it makes sense to look for unitary representation of the group in the one-particle space.

Exactly as in the case of Theorem 1.3, if ρ is a real circle wave function, with associated one-particle quantum state $\tilde{\rho}_+=\tilde{\rho}_+(n)$, the action of every $U_g^{(\mathsf{F})}$ on $\tilde{\rho}_+$ is equivalent to the action of a corresponding F diffeomorphism, d_g, on the horizon wave function ρ itself.

Theorem 2.4: *Assume $k=1$ in the definition of $\mathcal{D}_k^{(\mathsf{F})}$, that is, in (7). If $g\in SL(2,\mathbb{R})$ and $\tilde{\rho}_+=\tilde{\rho}_+(n)$ is the positive frequency part of $\rho\in\mathcal{S}(\mathsf{F})$, the state $U_g^{(\mathsf{F})}\tilde{\rho}_+$ can be associated with the wave function $\rho_g\in\mathcal{S}(\mathsf{F})$ with*

$$\rho_g(\theta)=\rho(d_g^{-1}\theta)\quad,\quad \text{for all } \theta\in(-\pi,\pi]. \tag{42}$$

In particular (with the same terminology as that used in (a) of Theorem 1.3):
(a) The unitary one-parameter group generated by $i\overline{K_{\mathsf{F}\beta}}$ is associated with the one-group of F diffeomorphisms generated by ∂_θ;
(b) the unitary one-parameter group generated by $i\overline{D_{\mathsf{F}}}$ is associated with the one-parameter group of F diffeomorphisms generated by $\sin\theta\partial_\theta$;
(c) the unitary one-parameter group generated by $i\overline{S_{\mathsf{F}}}$ is associated with the one-group of F diffeomorphisms generated by $\cos\theta\partial_\theta$.

The Lie algebra spanned by fields ∂_θ, $\cos\theta\partial_\theta$, $\sin\theta\partial_\theta$ is a realization of the Lie algebra of $SL(2,\mathbb{R})$.

Proof: The first part can be proven as follows. Take $\rho\in C^\infty(\mathsf{F};\mathbb{R})$. As $\mathcal{H}_{\mathsf{F}}=\ell^2(\mathbb{C})$, the associated positive frequency part in "frequency picture" $\tilde{\rho}_+\in\mathcal{H}_{\mathsf{F}}$ is a sequence $\{C_n\}_{n=1,2,\ldots}$. The associated positive frequency part in "θ picture" can be written

$$\rho_+(\theta)=\mathcal{F}(W\tilde{\rho}_+)(\theta),$$

where $\mathcal{F}:\ell^2(\mathbb{C})\to L^2((-\pi,\pi),d\theta)$ and $W:\ell^2(\mathbb{C})\to\ell^2(\mathbb{C})$ are, respectively, the *continuous* linear operators,

$$\mathcal{F}:\{C_n\}_{n=1,2,\ldots}\mapsto\sum_{n=1}^{+\infty}C_n\frac{e^{-in\theta}}{\sqrt{2\pi}}, \tag{43}$$

$$W:\{C_n\}_{n=1,2,\ldots}\mapsto\left\{\frac{C_n}{\sqrt{2n}}\right\}_{n=1,2,\ldots}. \tag{44}$$

On the other hand, in the sense of the topology of $\ell^2(\mathbb{C})$,

$$\tilde{\rho}_+=\sum_{m=1}^{\infty}C_m\Psi_m$$

where $\{\Psi_m\}_{m=1,2,\ldots}$ is the Hilbert base $\Psi_m=\{\delta_{mn}\}_{n=1,2,\ldots}$. By linearity, continuity, and the absence of positive-negative frequency mixing,

$$(\rho_g)_+=\mathcal{F}(WU_g^{(\mathsf{F})}\tilde{\rho}_+)=\mathcal{F}\left(WU_g^{(\mathsf{F})}\sum_n C_n\Psi_n\right)=\sum_n\mathcal{F}(WU_g^{(\mathsf{F})}C_n\Psi_n)\,. \tag{45}$$

Now one notices that Theorem 1.3 holds true also for the horizon wave function $\varphi^{(n)}$ with positive frequency part, in the "frequency picture" given by $Z_n^{(1)}(E)$ (with $k=1,2,\ldots$) as the

associated positive frequency wave function. (The proof of this fact is, in fact, the same proof as that of Theorem 1.3, that is Theorem 4.7 in Ref. 8, with trivial adaptations which make sense in the considered case. In particular Proposition 4.2 in Ref. 8 can directly be proven by using (28). It is useful to notice that $\Theta Z_n^{(1)}=(-1)^n Z_n^{(1)}$.) By (28),

$$\varphi^{(n)}(v(\theta))=\frac{1}{\sqrt{4\pi n}}[(-1)^{n+1}(C_n+\overline{C_n})+C_n e^{-in\theta}+\overline{C_n}e^{in\theta}]\ , \tag{46}$$

and thus, Theorem 1.3 says that

$$\varphi_g^{(n)}(v(\theta))=\frac{1}{\sqrt{4\pi n}}[C_n e^{-ind_g^{-1}\theta}-e^{-ind_g^{-1}\pi}C_n]+\text{c.c.} \tag{47}$$

Since, by Theorem 2.1, Z_n in $\mathcal{H}_{\mathbf{F}}$ is transformed into Ψ_n of $\mathcal{H}_{\mathsf{F}}$ and the same transformation associates $U_g^{(\mathbf{F})}$ with $U_g^{(\mathsf{F})}$, (47) can be re-written in the space $\mathcal{H}_{\mathsf{F}}$ and in the circle F:

$$\mathcal{F}(WU_g^{(\mathsf{F})}C_n\Psi_n)(\theta)+\text{c.c.}=C_n\varphi_g^{(n)}(v(\theta))+\text{c.c.}=\frac{1}{\sqrt{4\pi n}}[C_n e^{-ind_g^{-1}\theta}-C_n e^{-ind_g^{-1}\pi}]+\text{c.c.} \tag{48}$$

Inserting it in (45), one concludes that

$$\rho_g(\theta)=\sum_{n=1}^{+\infty} C_n\frac{e^{-ind_g^{-1}\theta}}{\sqrt{4\pi n}}-C_n\frac{e^{-ind_g^{-1}\pi}}{\sqrt{4\pi n}}+\text{c.c.} \tag{49}$$

The convergence must be understood in the sense of $L^2(\mathsf{F},\mathrm{d}\theta)$. However since $\rho\in C^\infty(\mathsf{F})$ and thus $\rho\circ d_g^{-1}\in C^\infty(\mathsf{F})$, the latter admit a uniformly convergent Fourier series and the series $\Sigma_n|C_n|/\sqrt{4\pi n}$ converges too. By the uniqueness property of Fourier series it must hold,

$$\rho_g(\theta)=\rho(d_g^{-1}\theta)+\text{const}\quad \text{for all } \theta\in\mathsf{F}\ .$$

This concludes the proof if the functions are considered as elements of $\mathcal{S}(\mathsf{F})$.

Let us pass to prove the statement in (b), the remaining cases can be proven following a strongly analogous proof [which is much more simple in case (a)]. If $t\mapsto g_t$ is the one-parameter subgroup of $SL(2,\mathbb{R})$ whose associated one-parameter group of diffeomorphisms is that generated by the field $\sin\theta\,\partial_\theta$, consider the transformed wave function $\rho_{g(t)}(\theta):=\rho(d_t^{-1}(\theta))=\rho(d_{-t}(\theta))$ and the associated positive frequency part $\widetilde{\rho_{g(t)+}}$ in "frequency representation." Since $SL(2,\mathbb{R})$ acts on positive frequency wave functions by means of a strongly continuous unitary representation, there must be some self-adjoint generator A (not depending on ρ_+) such that $\widetilde{\rho_{g(t)+}}=e^{itA}\widetilde{\rho}_+$. Our thesis states that $A=\overline{D_{\mathsf{F}}}$. With the above-introduced formalism, the statement turns out to be proved if it holds for all the states $\widetilde{\rho^{(k)}}_+=\Psi_k=\{\delta_{nk}\}_{n=1,2,\ldots}\in\ell^2(\mathbb{R})$, $k=1,2,\ldots$. Hence we want to show that for $k=1,2,\ldots$, $\widetilde{\rho_{g(t)+}^{(k)}}=e^{it\overline{D_{\mathsf{F}}}}\Psi_k$. To this end it is sufficient to show that in the topology of $\mathcal{H}_{\mathsf{F}}\cong\ell^2(\mathbb{C})$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho_{g(t)+}^{(k)}}\bigg|_{t=0}=iD_{\mathsf{F}}\Psi_k\,. \tag{50}$$

Indeed, by Stone's theorem the derivative on the left-hand side is $iA\Psi_k$, on the other hand, since D_{F} is essentially self-adjoint in the linear space finitely spanned by the vectors Ψ_k, it must be $A=\overline{D_{\mathsf{F}}}$. Let us prove (50). From now on $\widetilde{\rho_{g(t)+}^{(k)}}=\{C_n(t)\}_{n=1,2,\ldots}$. Defining $\theta_t(\theta):=d_{-t}(\theta)$, one has

$$C_n(t) = \sqrt{\frac{n}{k}} \int_{-\pi}^{\pi} \frac{e^{-i(k\theta_t(\theta)-n\theta)}}{2\pi} \mathrm{d}\theta \,, \tag{51}$$

because of (47) where, by construction, $\rho^{(k)}_{g(t)}(\theta) = \varphi^{(k)}_{g(t)}(v(\theta))$ and using the fact that there is no mixing of positive end negative frequencies under the action of the group. By direct computation one finds that $C_n(0) = 0$ and $\mathrm{d}C_n(t)/\mathrm{d}t|_{t=0} = 0$ if $n \neq k, k \pm 1$. So if the derivative on the left-hand side of (50) is computed term by term, (50) can be re-written

$$\frac{\delta_{n,k-1}\sqrt{k(k-1)} - \delta_{n,k+1}\sqrt{k(k+1)}}{2} = \langle \Psi_n, iD_{\mathsf{F}}\Psi_k \rangle_{\mathsf{F}}, \tag{52}$$

where we have computed the derivatives of $\mathrm{d}C_n(t)/\mathrm{d}t|_{t=0}$ using (51). However, it also holds

$$\langle \Psi_n, iD_{\mathsf{F}}\Psi_k \rangle_{\mathsf{F}} = \langle Z^{(1)}_n, iD_{\mathbf{F}} Z^{(1)}_k \rangle_{\mathbf{F}},$$

and the right-hand side can be computed trivially (for instance by employing the formalism on p. 137 of Ref. 9) and it turns out to coincide with the left-hand side of (52), so (52) holds true. To conclude the proof, it is sufficient to show that the derivative on the left-hand side of (50), which is computed with respect to the topology of $\ell^2(\mathbb{C})$, can equivalently be computed deriving term by term the sequence of complex which defines $\widetilde{\rho^{(k)}_{g(t)^+}}$. Expanding the term under the integral symbol in (51) by means of Taylor formula in the variable t about $t=0$, using the Lagrange formula for the remnant and, finally, using integration by parts and the fact that the integrated functions are smooth and periodic on $\mathbb{S}^1$, one proves that for some constant A, for all t in a neighborhood of 0 and for all $n \neq k, k \pm 1$:

$$\left| \frac{C_n(t)}{t} \right|^2 \leqslant \frac{A}{n^2} \,. \tag{53}$$

Thus

$$\sum_{n=1}^{\infty} \left| \frac{C_n(t) - C_n(0)}{t} - \frac{\mathrm{d}C_n(t)}{\mathrm{d}t}\bigg|_{t=0} \right|^2 = \sum_{n \neq k, k\pm 1} \left| \frac{C_n(t)}{t} \right|^2 + \sum_{n=k,k\pm 1} \left| \frac{C_n(t) - C_n(0)}{t} - \frac{\mathrm{d}C_n(t)}{\mathrm{d}t}\bigg|_{t=0} \right|^2 .$$

$C_n(t)/t \to 0$ in our hypotheses for $0 < n \neq k, k \pm 1$ and so the sum of the corresponding series above vanishes too due to Lebesgue's dominated convergence theorem with respect to the Dirac measure with support on the points $n \neq k, k \pm 1$ as a consequence of (53). We finally get

$$\lim_{t\to 0} \sum_{n=1}^{\infty} \left| \frac{C_n(t) - C_n(0)}{t} - \frac{\mathrm{d}C_n(t)}{\mathrm{d}t}\bigg|_{t=0} \right|^2 = \lim_{t\to 0} \sum_{n=k,k\pm 1} \left| \frac{C_n(t) - C_n(0)}{t} - \frac{\mathrm{d}C_n(t)}{\mathrm{d}t}\bigg|_{t=0} \right|^2 = 0 \,.$$

We conclude that the derivative on the left-hand side of (50) computed with respect to the topology of $\ell(\mathbb{C})$ coincides with that computed term by term. This concludes the proof because the last statement can straightforwardly be proven by direct inspection. □

The theorem states that, in fact, the bulk $SL(2,\mathbb{R})$ symmetry becomes manifest when examined on the circle $\mathsf{F} = \mathbf{F} \cup \{\infty\}$. However that is not the whole story because the found circle unitary $SL(2,\mathbb{R})$ representation is just a little part of a larger unitary representation with geometrical meaning. We can, in fact, consider the Lie algebra $\mathrm{Vect}(\mathbb{S}^1)$ of the infinite dimensional Lie group[19] of orientation-preserving diffeomorphisms of the circle $\mathrm{Diff}^+(\mathbb{S}^1)$, where $\mathbb{S}^1 = \mathsf{F}$ in our case. To make contact with Virasoro algebra we have to consider an associated *complex* Lie algebra.[20] Consider the complex Lie algebra $\mathrm{d}(\mathsf{F}) := \mathrm{Vect}(\mathsf{F}) \oplus i\ \mathrm{Vect}(\mathsf{F})$ equipped with usual Lie

brackets $\{\cdot,\cdot\}$ and the involution $\omega: X \mapsto -\overline{X}$ for $X \in \mathrm{d}(\mathsf{F})$, so that $\omega(\{X,Y\})=\{\omega(Y),\omega(X)\}$. An algebraic basis of that algebra is made of the complex smooth fields on F:

$$\mathcal{F}_n := ie^{in\theta}\partial_\theta \quad \text{with } n \in \mathbb{Z}. \tag{54}$$

The vector fields $\mathcal{F}_n$ enjoy the celebrated *Virasoro commutation rules* with central charge $c=0$:

$$\{\mathcal{F}_n, \mathcal{F}_m\} = (n-m)\mathcal{F}_{n+m}, \tag{55}$$

and the Hermiticity condition

$$\omega(\mathcal{F}_n) = \mathcal{F}_{-n}. \tag{56}$$

In the presented picture Vect(F) is nothing but the sub-algebra of d(F) containing all of the vectors fixed under $-\omega$. An algebraic basis of Vect(F) is that made of the fields

$$\mathcal{F}_n^{(+)} := \frac{\omega(\mathcal{F}_n)+\mathcal{F}_n}{2i} = \cos(n\theta)\partial_\theta, \quad \mathcal{F}_m^{(-)} := \frac{\omega(\mathcal{F}_m)-\mathcal{F}_m}{2} = \sin(n\theta)\partial_\theta, \tag{57}$$

where $n=0,1,\ldots$ while $m=1,2,\ldots$. Conversely, the base of d(F), $\{\mathcal{F}_n\}_{n\in\mathbb{Z}}$ can be obtained from the base above as, where $n=1,2,\ldots$,

$$\mathcal{F}_0 := i\mathcal{F}_0^{(+)}, \quad \mathcal{F}_n := \mathcal{F}_n^{(+)} + i\mathcal{F}_n^{(-)}, \quad \mathcal{F}_{-n} := \mathcal{F}_{-n}^{(+)} - i\mathcal{F}_{-n}^{(-)}. \tag{58}$$

Notice that the three fields $\mathcal{F}_0^{(+)}, \mathcal{F}_1^{(+)}, \mathcal{F}_1^{(-)}$ are in fact generators of a finite-dimensional sub-algebra of Vect(F), namely the representation of the Lie algebra of $SL(2,\mathbb{R})$ found above, which is equivalently generated by the three fields $v^{n+1}\partial_v$ with $n=-1,0,1$. However for $|n|>1$, the algebras spanned by generators $v^{n+1}\partial_v$ and $\mathcal{F}_n^{(\pm)}$ are different and we focus attention on the latter ones.

By direct inspection one proves that each of the fields $\mathcal{F}_n^{(\pm)} \in \mathrm{Vect}(\mathsf{F})$ generate a *global* one-parameter group of F orientation-preserving diffeomorphisms (this fact does not hold for fields $v^{n+1}\partial_v$ in **F**). Global means here that the additive parameter which labels the group ranges over the entire real line $\mathbb{R}$. In turn, that group of diffeomorphisms generates a group of automorphisms of the algebra of the quantum field $\mathcal{A}_\mathsf{F}$. Let us explain how it happens. If $d_\lambda^{(\mathcal{F}_n^{(\pm)})}: \mathsf{F} \to \mathsf{F}$ is an element of the one-parameter (orientation-preserving) diffeomorphism group generated by $\mathcal{F}_n^{(\pm)}$, $\lambda \in \mathbb{R}$ being the additive parameter, and $\rho \in \mathcal{S}(\mathsf{F})$, as usual we define the associated group of wave function transformations: $(\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}\rho)(\theta) := \rho(d_{-\lambda}^{(\mathcal{F}_n^{(\pm)})}(\theta))$. Notice that the transformations $\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}$ are, in fact, automorphisms of the real vector space $\mathcal{S}(\mathsf{F})$ equipped with the symplectic form Ω_F because the latter is orientation-preserving diffemorphism invariant.

Remark: By direct inspection one realizes that, if $n>1$ the transformation $\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}$ does *not* admit the space of positive frequency wave functions as invariant space. As a consequence it is not possible to represent $\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}$ unitarily in the one-particle space $\mathcal{H}_\mathsf{F}$. To implement the transformation $\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}$ at quantum level, the entire Fock space is necessary if $n>1$.

As we want to deal with quantum fields smeared by exact one-forms of $\mathcal{D}(\mathsf{F})$, we define a natural action of the diffeomorphisms $d_\lambda^{(\mathcal{F}_n^{(\pm)})}$ also on these forms by using (33): If $\omega \in \mathcal{D}(\mathsf{F})$ and $\rho := E_\mathsf{F}(\omega)$, we define the one-parameter group of transformations of one-forms $\{\beta_\lambda^{(\mathcal{F}_n^{(\pm)})}\}_{\lambda\in\mathbb{R}}$, such that

$$\beta_\lambda^{(\mathcal{F}_n^{(\pm)})}(\omega) := 2\mathrm{d}\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}(E_\mathsf{F}(\omega)). \tag{59}$$

Finally we can define the action of quantum fields by means of

$$\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega)) := \hat{\phi}_{\mathsf{F}}(\beta_{-\lambda}^{(\mathcal{F}_n^{(\pm)})}(\omega)) \ . \tag{60}$$

Using the given definitions, the fact that $\alpha_\lambda^{(\mathcal{F}_n^{(\pm)})}$ preserves Ω_{F} as well as (36) and (37), one finds

$$[\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega)), \ \ \gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega'))] = [\hat{\phi}_{\mathsf{F}}(\omega), \hat{\phi}_{\mathsf{F}}(\omega')] \ . \tag{61}$$

It is possible to prove by that identity that $\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}$ naturally extends into a $*$-algebra automorphism of the algebra $\mathcal{A}_{\mathsf{F}}$. The procedure to do it is very similar to those used in Ref. 8 to extend transformations of field operators into $*$-algebra homomorphisms. So, in fact, every field $\mathcal{F}_n^{(\pm)}$ gives rise to a one-parameter group of automorphisms of the algebra $\mathcal{A}_{\mathsf{F}}$ that we indicate by $\{\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}\}_{\lambda \in \mathbb{R}}$ once again. A natural question arises:

Is there a representation of the (infinite dimensional complex) Lie algebra d(F)*, in terms of operators defined in* $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ *such that the fields* $\mathcal{F}_n^{(\pm)}$ *are mapped into (essentially) anti-self-adjoint operators* $-iF_n^{(\pm)}$*, whose associated unitary one-parameter groups implement the respective one-parameter group of* $\mathcal{A}_{\mathsf{F}}$ *automorphisms* $\{\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}\}_{\lambda \in \mathbb{R}}$ *(at least at the first order)? That is*

$$e^{-i\lambda \overline{F_n^{(\pm)}}} \overline{\hat{\phi}_{\mathsf{F}}(\omega)} e^{i\lambda \overline{F_n^{(\pm)}}} = \overline{\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega))} \ , \tag{62}$$

or some other formally related, but perhaps weaker, identity holds.

The answer is yes provided one uses an operator algebra which represents *central extensions* of the algebra d(F). In other words one has to permit to change, at quantum level, the relation (55) by adding in the right-hand side a further term which commutes with the elements of the representation itself. The obtained algebra is properly called *Virasoro's algebra.*

More precisely, the quantum representation on the one hand is a straightforward extension of that previously found for the group $SL(2,\mathbb{R})$. On the other hand it is, in fact, a *positive-energy* and *unitary* representation of Virasoro algebra with *central charge* $c=1$.[20] To build up such a representation the entire Fock space, and not only the one-particle Hilbert space, is necessary. A relevant point is that the found unitary representation of the Virasoro algebra can be exported in the bulk via unitary holography.

In the circle Fock space $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$, consider the basis obtained by taking all the symmetrized tensor products of one-particle states $Z_n^{(1)}$, namely, the eigenvectors of the operator $K_{\mathsf{F}\beta}$. Henceforth α_n and $\alpha_n^\dagger$ are, respectively, the creation and annihilation operator associated with the one-particle state $Z_n^{(1)}$ with $n=1,2,\ldots$. As a consequence

$$[\alpha_n, \alpha_m^\dagger] = \delta_{n,m} I \ , \quad [\alpha_n, \alpha_m] = [\alpha_n^\dagger, \alpha_m^\dagger] = 0 \ . \tag{63}$$

Now, fix $\mu \in \mathbb{R}$ and introduce the operators, a_n, with $n \in \mathbb{Z}$ such that

$$a_n = \begin{cases} \mu I & \text{if } \ n=0 \ , \\ i\sqrt{n}\ \alpha_n & \text{if } \ n>0 \ , \\ -i\sqrt{-n}\ \alpha_{-n}^\dagger & \text{if } \ n<0 . \end{cases} \tag{64}$$

By (63) these operators satisfy the *oscillator algebra* commutation relations[20]

$$[a_m, a_n] = m\, \delta_{m,-n} I \ , \tag{65}$$

and the so-called *Hermiticity conditions*

$$a_n^\dagger = a_{-n} \tag{66}$$

(actually on the left-hand side is considered only the restriction of $a_n^\dagger$ to the domain of a_{-n}). With these definitions, the formal expression for $\hat{\phi}_{\mathsf{F}}$ (31) takes the form

$$\hat{\phi}_{\mathsf{F}}(\theta) = \frac{1}{i\sqrt{4\pi}} \sum_{n \in \mathbb{Z}\setminus\{0\}} \frac{e^{-in\theta}}{n} a_n , \tag{67}$$

moreover, formally *but also with a rigorous meaning in terms of a field operator smeared by an exact one-form* (35), it holds

$$a_n = \frac{1}{\sqrt{\pi}} \int_{\mathsf{F}} \hat{\phi}_{\mathsf{F}}(\theta)\ \mathrm{d}e^{in\theta} \quad \text{if } n \in \mathbb{Z}\setminus\{0\} . \tag{68}$$

Finally, define the operators (denoted by L_k in Ref. 20)

$$F_k := \frac{\epsilon_k}{2} a_{k/2}^2 + \sum_{n > -k/2} a_{-n} a_{n+k} , \qquad k \in \mathbb{Z}, \tag{69}$$

where $\epsilon_k = 0$ if k is odd, $\epsilon_k = 1$ if k is even (including $k=0$). The various sums are, in fact, finite when acting on a vector, since we adopt as a common domain of those operators, the dense subspace $\mathfrak{D}_1^{(\mathsf{F})} \subset \mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ made of the finite linear combination of vectors containing any finite number of particles in states $Z_n^{(1)}$.

Theorem 2.5: *The operators F_k, $k \in \mathbb{Z}$ enjoy the following properties on their domain $\mathfrak{D}_1^{(\mathsf{F})}$. (a) The complex Lie algebra finitely spanned by operators F_k (equipped with the usual operator commutator and Hermitian conjugation) is a positive-energy unitary Virasoro algebra representation* $\mathrm{Vir}(\mathsf{F})$ *with central charge $c=1$. Indeed it holds*

$$[F_m, F_n] = (m-n)F_{m+n} + \delta_{m,-n} \frac{m^3 - m}{12} I \quad \text{for } n, m \in \mathbb{Z} , \tag{70}$$

Hermiticity relations are fulfilled

$$F_m^\dagger \Psi = F_{-m} \Psi \quad \text{for every } \Psi \in \mathfrak{D}_1^{(\mathsf{F})} , \tag{71}$$

F_0 is essentially self-adjoint and $\overline{F_0}$ is positive defined with discrete spectrum

$$\sigma(\overline{F_0}) = \left\{ \frac{\mu^2}{2} + N \;\middle|\; N = 0,1,\ldots \right\} . \tag{72}$$

(b) For $n = 1,2,\ldots$, the operators

$$F_0^{(+)} := F_0 , \quad F_n^{(+)} := \frac{F_{-n} + F_n}{2} \quad \textit{and} \quad F_n^{(-)} := i\frac{F_{-n} - F_n}{2} \tag{73}$$

are essentially self-adjoint in $\mathfrak{D}_1^{(\mathsf{F})}$. (It is worth stressing that the interplay of fields $\mathcal{F}_n^{(\pm)}$ and $\mathcal{F}_n$ is the same as that operators $-iF_n^{(\pm)}$ and F_n and not *$F_n^{(\pm)}$ and F_n, this is because the operator involution † corresponds to the field involution ω instead of the simpler complex conjugation.)*

Proof: Barring the statements on F_0, the properties in (a) are proven in Ref. 20 (see Secs. II A–II C and III A) as consequences of (65), (66), and (69). The operators F_0, $F_m + F_{-m}$ and $i(F_m - F_{-m})$ are symmetric by construction and one can prove by direct inspection that the

elements of $\mathfrak{D}_1^{(\mathsf{F})}$ are analytic vectors for these operators. Thus they are essentially self-adjoint. This proves (b) and the essential self-adjointness of F_0. By direct inspection and using (64), one finds

$$F_0=\frac{\mu^2}{2}I+\sum_{n=1}^{\infty} n\alpha_n^\dagger\alpha_n . \tag{74}$$

The Hilbert basis of $\mathfrak{F}(\mathcal{H}_\mathsf{F})$, $\{|L\rangle\}_{L\in\mathbb{N}}$ made of the vectors (labeled with an arbitrary order by the index L) containing any finite number of states $Z_m^{(1)}$ is a basis of eigenvectors of F_0. The eigenvalue associated with $|L\rangle$ is of the form $\mu^2/2+N_L$ where N_L ranges everywhere in $\mathbb{N}$. This fact suggests to consider the self-adjoint operator

$$F_0' := \sum_{L=0}^{\infty} N_L |L\rangle\langle L|,$$

where now the sum is interpreted in the strong operator topology in the domain $\mathcal{D}(F_0')$ containing the vectors $|\Psi\rangle\in\mathfrak{F}(\mathcal{H}_\mathsf{F})$ with

$$\sum_{l=0}^{\infty} N_L^2 |\langle L|\Psi\rangle|^2<\infty .$$

By construction, F_0' has the spectrum (72). On the other hand, since $F_0\subset F_0'$ by construction, uniqueness of self-adjoint extensions of F_0 implies $\overline{F_0}=F_0'$. □

Finally we show that (1) the whole Virasoro representation extends the circle $SL(2,\mathbb{R})$ unitary representation and (2) it has the geometric meaning (62).

Theorem 2.6: *Referring to the Virasoro representation of Theorem 2.5,*
(a) if (and only if) $\mu=0$, the operators $F_0^{(+)},F_1^{(+)},F_1^{(-)}$ admit $\mathcal{D}_1^{(\mathsf{F})}\subset\mathcal{H}_\mathsf{F}$ as invariant space and

$$F_0^{(+)}\restriction_{\mathcal{H}_\mathsf{F}}=K_{\beta\mathsf{F}}, \tag{75}$$

$$F_1^{(+)}\restriction_{\mathcal{H}_\mathsf{F}}=S_\mathsf{F}, \tag{76}$$

$$F_1^{(-)}\cdot\restriction_{\mathcal{H}_\mathsf{F}}=D_\mathsf{F}, \tag{77}$$

and so these operators generate the $SL(2,\mathbb{R})$ representation $\{U_g^{(\mathsf{F})}\}_{g\in SL(2,\mathbb{R})}$.
(b) If (and only if) $\mu=0$, for every $n\in\mathbb{N}$ ($n>0$ in the case $^{(-)}$), (62) holds true at the first order at least,

$$[F_n^{(\pm)},\hat\phi_\mathsf{F}(\omega)]=i\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0}\gamma_\lambda^{(\mathcal{F}_n^{(\pm)})}(\hat\phi_\mathsf{F}(\omega)) \tag{78}$$

for every $\omega=\eta+i\eta'\in\mathcal{D}(\mathsf{F};\mathbb{C})$ such that the real wave functions $E_\mathsf{F}\eta$ and $E_\mathsf{F}\eta'$ are associated with states in $\mathcal{D}^{(\mathsf{F})}$ and the derivative is computed in the strong operator topology in $\mathfrak{D}_1^{(\mathsf{F})}$.

Proof: (a) The proof of the first case is a trivial consequence of (74). Concerning the second and third cases, we notice that using operators α_n and $\alpha_n^\dagger$,

$$F_{-1}=-i\mu\alpha_1^\dagger+\sum_{n=1}^{\infty}\sqrt{n(n+1)}\,\alpha_{n+1}^\dagger\alpha_n \tag{79}$$

$$F_1=i\mu\alpha_1+\sum_{n=1}^{\infty}\sqrt{n(n+1)}\,\alpha_n^\dagger\alpha_{n+1}. \tag{80}$$

It is obvious that, because of the terms containing $\mu(\alpha_1^\dagger \pm \alpha_1)$, the operators above admit $\mathcal{D}_1^{(\mathsf{F})}$ as an invariant space if and only if $\mu=0$. In that case, the restrictions to $\mathcal{D}_1^{(\mathsf{F})}$ coincide, respectively, with the operators A_+ and A_- defined in Ref. 21 or (23) of Ref. 9 (where the coefficient β is indicated by λ/κ and $k=1$). With our notations

$$A_\pm = \frac{1}{2}\left(\beta H_{\mathsf{F}0} - \frac{1}{\beta} C_{\mathsf{F}}\right) \mp i D_{\mathsf{F}}, \tag{81}$$

so that $A_- Z_1^{(1)} = 0$ and $A_+ Z_n^{(1)} = \sqrt{n(n+1)} Z_{n+1}^{(1)}$. Equation (81) implies (76) and (77) straightforwardly taking (38) into account.

Let us come to the last part. It is simply proven that every exact one-form $\omega = \eta + i\eta'$, where the real exact one-forms η, η' determine circle wave functions with positive frequency in $\mathcal{D}_1^{(\mathsf{F})}$, is a finite complex linear combination of forms $\omega_m(\theta) := \mathrm{d}e^{im\theta}$ with $m \in \mathbb{Z}\backslash\{0\}$. Hence it is sufficient to prove (78) for every $\hat{\phi}(\omega_m)$ with $m \in \mathbb{Z}\backslash\{0\}$. Fix $m \in \mathbb{Z}\backslash\{0\}$ and $k \in \mathbb{Z}$. By direct computation and using (68) and (2.12) in Ref. 20, one finds that, for every $\Psi \in \mathfrak{D}_{\mathsf{F}}^{(1)}$,

$$[L_k^{(\pm)}, \hat{\phi}(\omega_m)]\Psi = -\frac{m\sqrt{\pi}}{2}(i)_\pm (a_{m-k} \pm a_{m+k})\Psi, \tag{82}$$

where $(i)_j := 1$ if $j=+$, $(i)_j := i$ if $j=-$. *The identity above holds provided a_{m-m} and a_{-m+m} are interpreted as the multiplicative operator μI.*[20] On the other hand,

$$\gamma_\lambda^{(\mathcal{F}_k^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega_m)) = i\alpha(\phi_{m\lambda}) - i\alpha^\dagger(\psi_{m\lambda}) \ ,$$

where the vectors $\psi_{m\lambda}$ and $\phi_{m\lambda}$ are defined by

$$\psi_{m\lambda} := \left\{\sqrt{n}\int_{-\pi}^{\pi} e^{in\theta} e^{im\theta_t(\theta)} \mathrm{d}\theta\right\}_{n=1,2,\ldots}, \quad \phi_{m\lambda} := \left\{\sqrt{n}\int_{-\pi}^{\pi} e^{-in\theta} e^{im\theta_t(\theta)} \mathrm{d}\theta\right\}_{n=1,2,\ldots} \tag{83}$$

and $\lambda \mapsto \theta_\lambda(\theta)$ is the integral curve of $\mathcal{F}_k^{(\pm)}$ starting from θ. Notice that the linear maps $\psi \mapsto \alpha(\psi)\Psi$ and $\psi \mapsto \alpha^\dagger(\psi)\Psi$ are continuous for every fixed vector $\Psi \in \mathfrak{D}_{\mathsf{F}}^{(1)}$, so that

$$\left.\frac{\mathrm{d}}{\mathrm{d}\lambda}\right|_{\lambda=0} \gamma_\lambda^{(\mathcal{F}_k^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega_m))\Psi = i\alpha\left(\left.\frac{\mathrm{d}}{\mathrm{d}\lambda}\right|_{\lambda=0} \phi_{m\lambda}\right)\Psi - i\alpha^\dagger\left(\left.\frac{\mathrm{d}}{\mathrm{d}\lambda}\right|_{\lambda=0} \psi_{m\lambda}\right)\Psi \ .$$

In turn, using a procedure very similar to that used in the proof of (b) in Theorem 2.4, one sees that the derivatives $(\mathrm{d}/\mathrm{d}\lambda)|_{\lambda=0}\phi_{m\lambda}$ and $(\mathrm{d}/\mathrm{d}\lambda)|_{\lambda=0}\psi_{m\lambda}$ evaluated by using the topology of $\ell^2(\mathbb{C})$ coincide with the analogous derivatives computed term-by-term for the sequences of $\ell^2(\mathbb{C})$ which define $\phi_{m\lambda}$ and $\psi_{m\lambda}$ (83). These derivatives can be computed straightforwardly and give rise to

$$\left.\frac{\mathrm{d}}{\mathrm{d}\lambda}\right|_{\lambda=0} \gamma_\lambda^{(\mathcal{F}_k^{(\pm)})}(\hat{\phi}_{\mathsf{F}}(\omega_m))\Psi = -\frac{im\sqrt{\pi}}{2}(i)_\pm (a_{m-k} \pm a_{m+k})\Psi \ ,$$

where, on the right-hand side, a_{m-m} and a_{-m+m} must be interpreted as the null operator. By comparison with (82) we find that (78) holds true provided $\mu=0$. □

Remarks: (1) A natural question concerns whether or not $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ is irreducible with respect to the found Virasoro representation. The answer depends on the value of μ. If and only if $\mu\sqrt{2} \in \mathbb{Z}$ (and in particular if $\mu=0$) the answer is negative because of several results by Kac, Segal, and Wakimoto-Yamada (see Theorem 6.2 in Ref. 20 where the parameter l used below is indicated by μ which differs from the parameter μ used herein). If $\mu\sqrt{2} = -m \in \mathbb{Z}$, one has the orthogonal decomposition

$$\mathfrak{F}(\mathcal{H}_{\mathsf{F}}) = \bigoplus_{k\in\mathbb{Z}^+, k\geqslant -m} V(1,(m+2k)^2/4)\ ,$$

where $V(c,h)$ is the up-to-isomorphism unique highest-weight unitary Virasoro representation (which is irreducible by consequence) with central charge c and weight h. We recall for the reader that if $c=1$ and $h=l^2/4$ with $l\in\mathbb{Z}$, $V(c,h)$ is not a *Verma representation*. In other words the system of generators of $V(c,h)$ built up over the singular vector of $V(c,h)$ by application of products of Virasoro generators contains linearly dependent vectors. Conversely, if $c=1$ and $h\neq l^2/4$ with $l\in\mathbb{Z}$, $V(c,h)$ is a Verma representation.

(2) It is possible to build up a free scalar standard 2D-CFT by using $\hat{\phi}_{\mathsf{F}}$ and the analogous field $\hat{\phi}_{\mathsf{P}}$ defined on $\mathsf{P}:=\mathbf{P}\cup\{\infty\}$. In fact, consider the Wick rotation in Rindler coordinates $t\mapsto it$. Under that continuation, light-Rindler coordinates transform into $v\to it+\log(\kappa y)/\kappa$, $u\to it-\log(\kappa y)/\kappa$ and so $\theta=2\arctan(v/\beta)\to z$, $\theta'=2\arctan(u/\beta)\to-\overline{z}$. θ' is the coordinate on P which is defined analogously to θ. With the given definitions, z turns out to be defined on a cylinder C obtained by taking $\mathrm{Im}(z)\in\mathbb{R}$ and $\mathrm{Re}(z)\in(-\pi,\pi]$ with the identification $-\pi\equiv\pi$. By this way the fields $\hat{\phi}_{\mathsf{F}}$ and $\hat{\phi}_{\mathsf{P}}$ become, respectively, the Euclidean *holomorphic* and *antiholomorphic* fields in $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})\otimes\mathfrak{F}(\mathcal{H}_{\mathsf{P}})$:

$$\hat{\phi}(w)=\sum_{n\in\mathbb{Z}\setminus\{0\}}\frac{w^n}{n}a_n\,,\quad \hat{\phi}(\overline{w})=\sum_{n\in\mathbb{Z}\setminus\{0\}}\frac{\overline{w}^n}{n}b_n\,,$$

where $w:=e^{-iz}$, the operators b_n are defined on P similarly to operators a_n and $[a_n,b_{\underline{m}}]=0$. The operators F_n and the analogues P_n defined in P are those usually denoted by L_n and $\overline{L}_n$, respectively.

(3) The bulk evolution is generated by the Hamiltonian H which is the quantum generator associated with the bulk killing vector ∂_t. Consider the operator H_{F} associated with H by holography and naturally extending it in the whole Fock space $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ by assuming to work with massive noninteracting particles in the bulk. The obtained operator $H^{\otimes}_{\mathsf{F}}$ coincides with the self-adjoint Virasoro generator

$$H^{\otimes}_{\mathsf{F}}:=\frac{1}{\beta}\overline{(2F_1^{(+)}+F_0)}\qquad(\text{where}\mu=0)\tag{84}$$

provided $\mu=0$. Under this hypothesis, $F_0^{(+)},F_1^{(\pm)}$ span a finite-dimensional Lie algebra and $H^{\otimes}$ is the closure of an element of the algebra. [That is nothing but the Lie algebra of a unitary representation of $SL(2,\mathbb{R})$.] As a consequence it is possible to define time-depending observables $F_0(t),F_1^{(\pm)}(t)$ which are constant of motion in Heisenberg picture. These are finite linear combinations of generators $F_0(t),F_1^{(\pm)}(t)$. The proof of that fact is essentially the same as that of Theorem 2.1—item (b) in particular—in Ref. 8. We conclude that $F_0(t),F_1^{(\pm)}(t)$ generate a *symmetry of the system* when they are realized, by unitary holography, as operators acting in the bulk. Conversely, this result does not apply as it stands for $F_n^{(\pm)}$ if $n>1$. This is because there is no finite-dimensional Lie algebra containing both $F_n^{(\pm)}$ and $H^{\otimes}_{\mathsf{F}}$. However if one assumes that $F_0^{(+)}$ (which is associated with $K_{\beta\mathbf{F}}$ in the bulk) is the Hamiltonian of the theory on F, the observables $F_n^{(\pm)}$ with $n>1$ can be considered as symmetries of the system. This is because, for every fixed integer $n>0$ and also if $\mu\neq 0$, $F_0^{(+)},F_n^{(+)},F_n^{(-)}$ span a finite-dimensional Lie algebra [which is, in fact, a representation of the Lie algebra of $SL(2,\mathbb{R})$].

III. APPEARANCE OF THERMAL STATES FROM VIRASORO GENERATORS

Let us focus on the class of ''Hamiltonian operators'' defined for the theory on the circle F,

$$H^{\otimes}_{\mathsf{F}\,\mu}:=\frac{1}{\beta}\overline{(2F_1^{(+)}+F_0)}\ ,\tag{85}$$

where, differently from (84), now $\mu \in \mathbb{R}$ and thus, barring the value $\mu=0$, $H^{\otimes}_{\mathsf{F}\,\mu}$ cannot be associated with the Rindler Hamiltonian in the bulk by means of holography. In the following we study some properties of these Hamiltonians and associated ground states which can be considered as operators and states of the theory in the bulk. We shall not give rigorous proofs since the treatment of the issue involves a singular Bogoliubov transformation as well as a regularization procedure. We have formally

$$H^{\otimes}_{\mathsf{F}\,\mu}=\frac{\mu^2}{2\beta}I+H^{\otimes}_{\mathsf{F}}+i\,\frac{\mu}{2\beta}(\alpha_1-\alpha_1^{\dagger}). \tag{86}$$

We look for a, formally unitary, transformation U_μ such that

$$H^{\otimes}_{\mathsf{F}}=U_\mu H^{\otimes}_{\mathsf{F}\,\mu}U_\mu^{\dagger}.$$

It is convenient to work in the Fock space $\mathfrak{F}(\mathcal{H}_{\mathbf{F}})$ which is isomorphic to $\mathfrak{F}(\mathcal{H}_{\mathsf{F}})$ by means of the isomorphism $M:\mathcal{H}_{\mathbf{F}}\to\mathcal{H}_{\mathsf{F}}$ used in Theorem 2.1. In this representation

$$H^{\otimes}_{\mathsf{F}\,\mu}=\frac{\mu^2}{2\beta}I+\int_{\mathbb{R}^+}\mathrm{d}E\,E\;\; a_E^{\dagger}a_E+i\,\frac{\mu}{2\beta}\int_{\mathbb{R}^+}\mathrm{d}E\;\; Z_1^{(1)}(E)(a_E-a_E^{\dagger})\ , \tag{87}$$

where a_E and $a_E^{\dagger}$ are as in Eq. (14). By that way, it turns out that formally

$$U_\mu=\exp\left(-i\int_0^{\infty}Z_1^{(1)}(E)\,\frac{\mu}{2\beta}(a_E+a_E^{\dagger})\,\frac{\mathrm{d}E}{E}\right)\ . \tag{88}$$

Notice that when μ is equal to zero the unitary transformation becomes the identity and $H^{\otimes}_{\mathsf{F}\,0}=H^{\otimes}_{\mathsf{F}}$ as is due. For completeness we say that it is possible to rewrite U_μ in terms the operators α_n as follows:

$$U_\mu=\exp\left(-i\sum_{n>0}\,(-1)^{(n+1)}\,\frac{\mu}{\sqrt{n}}(\alpha_n+\alpha_n^{\dagger})\right)\ . \tag{89}$$

The ground state of $H^{\otimes}_{\mathsf{F}\,\mu}$, can be obtained as

$$\Psi_\mu:=U_\mu^{\dagger}|0\rangle_{\mathsf{F}}. \tag{90}$$

Ψ_μ is not invariant under Rindler evolution generated by $H^{\otimes}_{\mathsf{F}}$ but it enjoys interesting thermal properties when one considers expectation values of observables also averaged during a long period of Rindler time $T\to\infty$. Consider the expectation value of the operator A:

$$\langle A\rangle_\mu:=\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\frac{\langle\Psi_\mu(t),A\Psi_\mu(t)\rangle_{\mathsf{F}}}{\langle\Psi_\mu(t),\Psi_\mu(t)\rangle_{\mathsf{F}}}\mathrm{d}t\ , \tag{91}$$

where $\Psi_\mu(t):=\exp\{-itH^{\otimes}_{\mathsf{F}}\}\Psi_\mu$. The direct computation is affected by mathematical problems which can be made harmless by making discrete the energy spectrum and taking the limit toward the continuous case after the evaluation of the expectation value. The discrete spectrum can be obtained by reducing to a known regularization procedure, consisting of a suitable version of the so-called ''box quantization.'' Start from (88) noticing that it can be rewritten, by using the adimensional parameter $\lambda=\log(E/E^*)$, E^* being an arbitrarily fixed energy scale,

$$U_\mu=\exp\left(-i\int_{-\infty}^{+\infty}Z_1^{(1)}(E(\lambda))\,\frac{\mu}{2\beta}(a_{E(\lambda)}+a_{E(\lambda)}^{\dagger})\mathrm{d}\lambda\right)\ . \tag{92}$$

Now, differently from E, λ ranges over the whole real line and box-quantization can be used as follows. First of all define the operators $c_\lambda = \sqrt{E'(\lambda)}a_{E(\lambda)}$ and $c^\dagger_\lambda = \sqrt{E'(\lambda)}a^\dagger_{E(\lambda)}$ so that bosonic commutation relations of a_E and $a^\dagger_E$ turns out to be equivalent to

$$[c_\lambda, c^\dagger_{\lambda'}] = \delta(\lambda - \lambda'), \quad [c_\lambda, c_{\lambda'}] = 0, \quad [c^\dagger_\lambda, c^\dagger_{\lambda'}] = 0. \tag{93}$$

Finally, to get the discrete spectrum in λ, assume that values λ describe the spectrum of a "momentum operator." These values can be made discrete by working a 1D box with length L with periodic boundary conditions, the continuous spectrum being restored in the limit $L \to \infty$. Within this framework, if $\lambda_n = 2\pi n/L$ with $n \in \mathbb{Z}$, the operators $c_j := c_{\lambda_j}$ enjoy the commutation relations

$$[c_i, c^\dagger_j] = \delta_{ij}, \quad [c_i, c_j] = 0, \quad [c^\dagger_i, c^\dagger_j] = 0. \tag{94}$$

With that regularization procedure, the Hamiltonian $H^\otimes_{\mathsf{F}}$ can be rewritten as

$$H^\otimes_{\mathsf{F}} = \int_{\mathbb{R}^+} E \;\; a^\dagger_E \;\; a_E \;\; \mathrm{d}E = \int_{\mathbb{R}} E(\lambda) \;\; c^\dagger_\lambda \;\; c_\lambda \;\; \mathrm{d}\lambda \to \sum_j \; E_j c^\dagger_j c_j, \tag{95}$$

where $E_j := E(\lambda_j)$. Similarly, using $E = E * e^\lambda$ and (9) for $k = n = 1$, the regularized unitary transformation U_μ reads

$$U_\mu = \prod_j \;\; \exp(-i\mu e^{-\beta E_j}(c_j + c^\dagger_j)) \tag{96}$$

and so the state Ψ_μ can be expanded as

$$\Psi_\mu = \prod_j \;\; \exp\left(\frac{\mu^2}{2} e^{-2\beta E_j}\right) \;\; \sum_n \; i^n \mu^n e^{-\beta E_j n} \frac{c^{\dagger n}_j}{n!} |0\rangle_{\mathsf{F}}. \tag{97}$$

We are now ready to compute $\langle A \rangle_\mu$. Using (97) in (91) one gets straightforwardly

$$\langle A \rangle_\mu = Z^{-1}_\beta \sum_{\{n_j\}} \; e^{-2\beta \Sigma_j E_j n_j} \mu^{2\Sigma_j n_j} \langle \{n_j\} | A | \{n_j\} \rangle, \tag{98}$$

with

$$Z_\beta = \sum_{\{n_j\}} \; e^{-2\beta \Sigma_j E_j n_j} \mu^{2\Sigma_j n_j}, \tag{99}$$

and the final limit $L \to \infty$ is understood. Let us consider all the developed machinery as referred to the theory in the bulk making use of the holographic theorem (Theorem 2.2) for a *massive* field. In that way, A must be considered as an observable for an observer in the Rindler wedge and Ψ_μ is a state for a quantum field propagating in the Rindler wedge. If μ is equal to 1, (98) states that the time-averaged state $\Psi_{\mu=1}$ viewed by an observer in the bulk who uses Rindler time-evolution, is a thermal state with inverse temperature $1/(2\beta)$. In particular, if we also choose $\beta = \beta_U/2$, where β_U is the inverse Unruh temperature, we get formally and in the sense of the pointed regularization-procedure out,

$$\langle A \rangle_{\mu=1} = \mathrm{tr}(\rho_{\beta_U} A), \tag{100}$$

where

$$\rho_{\beta_U} := \frac{e^{-\beta_U H_F^{\otimes}}}{\mathrm{tr} e^{-\beta_U H_F^{\otimes}}}$$

is the density matrix of a thermal state, which coincides with the restriction of Minkowski vacuum to Rindler wedge because of celebrated results of QFT (Bisognano–Wichmann–Sewell theorems, see Ref. 22 for a general discussion). In the case $\mu \neq 1$, (98) suggests to interpret

$$\frac{\log \mu^2}{2\beta}$$

as a chemical potential and the associated state can be seen as a grand canonical ensemble state.

IV. OVERVIEW AND OPEN PROBLEMS

In this paper we have shown that quantum field theory for free fields propagating in a 2D-Rindler background is unitary equivalent to the analogue defined on the compactified Killing horizons. The same equivalence can be implemented at the algebraic level. The key point of this holographic description is the hidden $SL(2,\mathbb{R})$ symmetry found in Ref. 9 for the fields propagating in the bulk. Indeed that hidden representation of $SL(2,\mathbb{R})$ becomes geometrically manifest when the theory is represented on the Killing horizon. Preserving a clear geometric meaning, the representation can be enlarged up to include a positive-energy unitary representation of Virasoro algebra with central charge $c=1$. Notice that the Virasoro algebra is realized in the many particles description of the fields, namely it describes a representation in the Fock space. The appearance of the pair of Virasoro algebras in the future and past horizon leads naturally to an (Euclidean) 2D conformal field theory on a cylinder which is holograpically associated with QFT in the bulk. In the last section we have proposed the idea that, for a particular choice of the parameter β and the ground energy $h=\mu^2/2$ of the Virasoro Hamiltonian F_0, the ground state $\Psi_\mu(t)$ of another Virasoro generator which generalizes Rindler Hamiltonian has thermal properties. $\Psi_\mu(t)$, seen in Fock space built up over the Rindler vacuum $|0\rangle$, is revealed to be an infinite particle state in thermal equilibrium temperature $1/(2\beta)$. It can be useful to describe the Hawking effect. These thermal properties are shown here without rigorous proof because of the use of a necessary regularization procedure in computing the mean value of the state with respect to Rindler time. Further investigation in that direction, perhaps based on KMS condition, is necessary.

Another issue which deserves investigation is the existence of any relation between the results of this paper and the attempts to give a statistical explanation to black hole entropy by counting microstates of irreducible unitary representations of Virasoro algebra.[15] This is done by means of the so-called Cardy's formula after a suitable dimensional regularization which gives rise to a scalar field (supporting part of information of 4D gravity) propagating in a 2D space–time. The main problem of those approaches is that they must assume the existence of a quantum Virasoro representation. The existence of such a representation has been established in this paper: It is worthwhile to investigate about the possible interplay between the quantum Virasoro representation found here and that necessary in those approaches.

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Searching for a connection between matroid theory and string theory

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We make a number of observations about matter-ghost string phase, which may eventually lead to a formal connection between matroid theory and string theory. In particular, in order to take advantage of the already established connection between matroid theory and Chern–Simons theory, we propose a generalization of string theory in terms of some kind of Kahler metric. We show that this generalization is closely related to the Kahler–Chern–Simons action due to Nair and Schiff. In addition, we discuss matroid/string connection via matroid bundles and a Schild type action, and we add new information about the relationship between matroid theory, $D=11$ supergravity and Chern–Simons formalism. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1625416]

I. INTRODUCTION

Although the key principle in M-theory[1–3] and string theory[4] is unknown, there is accumulating evidence for the existence of some kind of duality principle. In fact, duality is the key physical concept that relates the five known superstring theories in $9+1$ dimensions (i.e., nine space and one time), Type I, Type IIA, Type IIB, Heterotic SO(32) and Heterotic $E_8\times E_8$, which may now be understood as different manifestations of M-theory. Thus, anticipating the possibility that duality is the basic principle in M-theory, one may be interested in the mathematical structure necessary to make sense of such a duality principle. The idea is similar to the role played by tensor analysis which gives a mathematical sense to the postulate of relativity ''the laws of physics are the same for every observer.'' In two previous works we proposed the possibility that such a mathematical structure could be realized through the so-called matroid theory.[5] Matroid theory, which can be understood as a generalization of graph theory and matrix theory, has the duality symmetry among its key basic concepts. In fact, in contrast to graphs in which duality can only be considered in connection with planar graphs, matroid theory has the remarkable property that every matroid has a unique dual matroid. As an example of the importance of the duality property in matroid theory let us just mention a theorem due to Whitney:[5] if $M_1,\ldots,M_p$ and $M_1',\ldots,M_p'$ are the components (blocks) of the matroids M and M', respectively, and if M_i' is the dual of M_i $(i=1,\ldots,p)$, then M' is the dual of M and, conversely, if M and M' are dual matroids, then M_i' is the dual of M_i. Moreover, in a general context, we have the remarkable proposition that if a statement μ in the theory of matroids has been proved true, then also its dual μ^* is true.

Of course, the question is how to achieve such a relationship between matroid theory and M-theory, especially if we do not even know the formal partition function associated to M-theory. As a first step in this direction, one may attempt to see if matroid theory is linked somehow to $D=11$ supergravity which is one of the manifestations of M-theory. In fact, it has been shown[6] that the Fano matroid and its dual are closely related to Englert's compactification[7] of $D=11$ supergravity. This result is physically interesting because it allows a connection between the fundamental Fano matroid or its dual[8] and octonions which, at the same time, are one of the

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alternative division algebras.[9] In Ref. 10, we made further progress on this program, incorporating matroid theory on quantum Yang–Mills theory in the context of Chern–Simons action. Our mechanism was based on a theorem due to Thistlethwaite[11] which connects the Jones polynomial for alternating knots with the Tutte polynomial for graphs. Since Witten[12] showed that Jones polynomial can be understood in three dimensional terms through a Chern–Simons formalism, it became evident that we achieved a bridge between matroid theory and Chern–Simons formalism.

In this article, we further pursue the idea of relating matroid theory with M-theory. Since the five fundamental strings are different vacuum limits of M-theory, it seems natural to try to find first a link between matroid theory and string theory. In this context there are a number of observations that indicate that this idea makes sense. First, since Chern–Simons formalism is closely linked to conformal field theory and matrix theory, which in turn are related to string theory, one should expect a connection of the form: matroid-theory→Chern–Simons-theory→string-theory. Second, since strings are closely related to knots, which in turn are related in one-to-one correspondence to signed graphs, one should expect a link of the form: matroids→signed graphs→knots→strings. Finally, we can in effect combine the two previous observations in the form: matroids→signed graphs→knots→Chern–Simons-formalism→strings.

In order to achieve our goal, we study the possibility that, in the string phase of matter-ghost coupling, the world sheet metric and the target space–time metric become unified in just one metric. We show, in some detail, that such a unified metric may be a certain kind of Kahler metric. This observation lead us to consider the Kahler–Chern–Simons action as the key bridge to connect matroid theory and string theory.

An alternative matroid/string connection can be achieved via the Schild type action.[13] In fact, we show that writing the Nambu–Goto action in the context of Schild formulation, such a connection seems to be a straightforward extension of the chirotope notion of oriented matroids. We prove that a local description of the chirotope concept becomes part of the structure of the Schild action. The relevant structure in this process is the concept of matroid bundle which has already been developed by the mathematicians.[14–17] Finally, we show that in order to complete the desired connection between matroids and strings it appears necessary to use the Chern–Simons formulation for strings as proposed by Zaikov.[18]

The plan of this work is as follows. In Sec. II, we briefly review matroid theory. In Sec. III, we closely follow Ref. 6 by adding new information about the connection between matroid theory and $D=11$ supergravity. In Sec. IV, we briefly review Ref. 10 and propose a possible extension of the relation between matroid theory and Witten's partition function for knots. In Sec. V, we propose a generalized Polyakov string action with the property of unifying the world-sheet metric and the target space–time metric. In Sec. VI, we discuss an alternative matroid/string connection via the concept of a chirotope of oriented matroids and Schild type action. Finally, in Sec. VII, we make some final comments.

II. A BRIEF REVIEW OF MATROID THEORY

At present matroid theory, also called combinatorial geometry or pregeometry, can be understood as the combinatorial analog of K-theory. In fact, the axioms of K-theory are very similar to the properties achieved with the Tutte–Gotendiek invariants for matroids. This interpretation emerged from a great number of contributions from several mathematicians since 1935 with the pioneer work of Whitney[5] on ''abstract properties of linear dependence.'' In the same year, Birkhoff[19] established the connection between simple matroids and geometric lattices. In 1936, MacLane[20] gave an interpretation of matroids in terms of projective geometry. And an important progress to the subject was given in 1958 by Tutte[8] who introduced the concept of homotopy for matroids. The fascination of this subject among the combinatorial mathematicians can be appreciated from the large body of information about matroid theory. In fact, there is a large number of books about matroid theory. For background information on this subject the reader should consult Oxley[21] and Welsh.[22] We also recommend the books by Wilson,[23] Kung,[24] and Ribnikov.[25]

It is known that in graph theory only planar graphs have an associated dual graph. For instance, the Kuratowski theorem assures that the complete graph K_5 and the bipartita graph $K_{3,3}$,

which are not planar, do not have an associated dual graph. In a sense, matroid theory arose as an attempt to solve this lack of duality symmetry. The attractive feature is that in matroid theory every matroid has an associated unique dual matroid. In particular the matroid associated to K_5, let us say $M(K_5)$, has a dual $M^*(K_5)$. The important aspect is that $M^*(K_5)$ is not graphic, that is, it can not be represented by a graph. This is, of course, an indication that matroid theory is a generalization of graph theory. Therefore, the great advantage of matroid theory is that it provides us with a mathematical structure in which the concepts of duality of planar graphs is extended to graphs that are not planar.

Another interesting aspect that motivates the subject is that linear dependence in algebra can be understood as a particular case of matroid theory. In fact, matroid theory leads to matroids that are not even representable by a finite set of vectors in a vector space or by matrices, extending the concept of orthogonality in vector spaces. Summarizing, we can say that by extending the concept of duality in vector spaces and planar graphs, matroid theory accomplishes a generalization of both graph theory and matrix theory.

Mathematically, a matroid is defined as follows: a matroid M is a pair (E,I), where E, called the ground set, is a nonempty finite set, and I is a nonempty collection of subsets of E satisfying the following two properties:

$(I\ i)$ Any subset of an independent set is independent.

$(I\ ii)$ If K and J are independent sets with $K\subseteq J$, then there is an element e contained in J but not in K such that $K\cup\{e\}$ is independent.

Members of I are called independent sets of M; other sets are called dependent. Therefore, the definition itself of a matroid divides all possible subsets of E in two types: independent and dependent subsets. Thus, we see that, even from the beginning, matroids have the dual structure independent–dependent. From this point of view, it is not a surprise to find eventually that every matroid has an associated dual matroid.

A base is defined to be any maximal independent set. Similarly, the minimal dependent set is called a circuit. By repeatedly using the property $(I\ ii)$ it is straightforward to show that any two bases have the same number of elements.

An alternative definition of a matroid in terms of bases is as follows:

A matroid M is a pair $(E,\mathcal{B})$, where E is a nonempty finite set and $\mathcal{B}$ is a nonempty collection of subsets of E (called bases) satisfying the following properties:

$(\mathcal{B}\ i)$ No base properly contains another base.

$(\mathcal{B}\ ii)$ If B_1 and B_2 are bases and if b is any element of B_1, then there is an element g of B_2 with the property that $(B_1-\{b\})\cup\{g\}$ is also a base.

A matroid can also be defined in terms of circuits:

A matroid M is a pair (E, C), where E is a nonempty finite set, and C is a nonempty collection of subsets of E (called circuits) satisfying the following properties.

$(C\ i)$ No circuit properly contains another circuit.

$(C\ ii)$ If C_1 and C_2 are two distinct circuits each containing an element c, then there exists a circuit in $C_1\cup C_2$ which does not contain c.

If we start with any of the three definitions, then one finds that the other two follow as theorems. For example, it is possible to prove that (I) implies $(\mathcal{B})$ and (C). In other words, these three definitions are equivalent. There are other definitions also equivalent to these three, but for the purpose of this work it is not necessary to consider all of them.

As we noticed previously, even from the initial structure of a matroid theory we find relations such as independent–dependent structure which suggests duality. The dual of M, denoted by M^*, is defined as a pair $(E,\mathcal{B}^*)$, where $\mathcal{B}^*$ is a nonempty collection of subsets of E formed with the complements of the bases of M. An immediate consequence of this definition is that every matroid has a dual and this dual is unique. It also follows that the double-dual M^{**} is equal to M. Moreover, if S is a subset of E, then the size of the largest independent set contained in S is called the rank of S and is denoted by $\rho(S)$. If $M=M_1+M_2$ and $\rho(M)=\rho(M_1)+\rho(M_2)$, we shall say that M is separable. Any maximal nonseparable part of M is a block of M. An important theorem due to Whitney[5] is that if $M_1,\ldots,M_p$ and $M_1',\ldots,M_p'$ are the blocks of the matroids M and M',

respectively, and if M_i' is the dual of M_i $(i=1,\ldots,p)$, then M' is dual of M. Conversely, let M and M' be dual matroids, and let $M_1,\ldots,M_p$ be blocks of M. Let $M_1',\ldots,M_p'$ be the corresponding submatroids of M'. Then $M_1',\ldots,M_p'$ are the blocks of M', and M_i' is the dual of M_i.

Over the last years matroid theory has been growing very rapidly. There are already well established formalisms for oriented matroids[26] and bias matroids.[27] The former can be understood as a generalization of oriented graphs and the latter as an extension of signed graphs. In each one of these branches of matroid theory there are very interesting theorems and results, some of which we shall mention in the next sections.

III. MATROID THEORY AND SUPERGRAVITY

Here, we briefly review the main results of Ref. 6 and add some new observations. In Ref. 6 we showed that the Fano matroid F_7 may be connected with octonions which, in turn, are related to the Englert's compactification of $D=11$ supergravity.

A Fano matroid F_7 is the matroid defined on the ground set

$$E=\{1,2,3,4,5,6,7\} \tag{1}$$

whose bases are all those subsets of E with three elements except $f_1=\{1,2,3\}$, $f_2=\{5,1,6\}$, $f_3=\{6,4,2\}$, $f_4=\{4,3,5\}$, $f_5=\{4,7,1\}$, $f_6=\{6,7,3\}$ and $f_7=\{5,7,2\}$. The circuits of the Fano matroid are precisely these subsets and its complements. It follows that these circuits define the dual F_7^* of the Fano matroid.

Let us write the set E in the form $E=\{e_1,e_2,e_3,e_4,e_5,e_6,e_7\}$. Thus, the subsets used to define the Fano matroid now become $f_1=\{e_1,e_2,e_3\}$, $f_2=\{e_5,e_1,e_6\}$, $f_3=\{e_6,e_4,e_2\}$, $f_4=\{e_4,e_3,e_5\}$, $f_5=\{e_4,e_7,e_1\}$, $f_6=\{e_6,e_7,e_3\}$ and $f_7=\{e_5,e_7,e_2\}$. The key idea in Ref. 6 was to identify the quantities e_i, where $i=1,\ldots,7$, with the octonionic imaginary units. Specifically, we write an octonion q in the form

$$q=q_0e_0+q_1e_1+q_2e_2+q_3e_3+q_4e_4+q_5e_5+q_6e_6+q_7e_7,$$

where q_0 and q_i are real numbers. Here, e_0 denotes the identity. The product of two octonions can be obtained from the formula

$$e_ie_j=-\delta_{ij}+\psi_{ij}^k e_k, \tag{2}$$

where δ_{ij} is the Kronecker delta and $\psi_{ijk}=\psi_{ij}^l\delta_{lk}$ is the fully antisymmetric structure constants, with $i,j,k=1,\ldots,7$. By taking the ψ_{ijk} equal to 1 or -1 for each one of the seven combinations f_i we may derive all the values of ψ_{ijk}.

The octonion (Cayley) algebra is not associative, but alternative. This means that the basic associator of any three imaginary units is

$$\langle e_i,e_j,e_k\rangle=(e_ie_j)e_k-e_i(e_je_k)=\varphi_{ijkm}e_m, \tag{3}$$

where φ_{ijkl} is a fully antisymmetric four index tensor. It turns out that φ_{ijkl} and ψ_{ijk} are related by the expression

$$\varphi_{ijkl}=(1/3!)\,\epsilon_{ijklmnr}\psi_{mnr}, \tag{4}$$

where $\epsilon_{ijklmnr}$ is the completely antisymmetric Levi–Civita tensor, with $\epsilon_{12\ldots7}=1$. It is interesting to observe that given the numerical values f_i for the indices of ψ_{mnr} and using (4) we get the other seven subsets of E with four elements of the dual Fano matroid F_7^*. For instance, if we take f_1, then we have ψ_{123} and (4) gives φ_{4567} which leads to the circuit subset $\{4,5,6,7\}$ of F_7^*.

Therefore, this shows that the Fano matroid and its dual are closely related to octonions which at the same time are an essential part of Englert's solution of absolute parallelism on S^7 of $D=11$ supergravity. It is important to mention that the Fano matroid is the only minimal binary

irregular matroid. Just as octonions are central mathematical objects in division algebras, this property makes the Fano matroid a central mathematical object in matroid theory. $D=11$ supergravity is on the other hand an important physical structure in M-theory. Therefore, we have here a link between three apparently unrelated important objects in its own field: Fano matroid (matroid theory)$\leftrightarrow$ octonions (algebra)$\leftrightarrow D=11$ supergravity (unify fundamental physics).

We would like to make some further observations about the link between the Fano matroid and octonions. Consider the subsets $h_1=\{v_1,v_2,v_3\}$, $h_2=\{v_5,v_1,v_6\}$, $h_3=\{v_6,v_2,v_4\}$, $h_4=\{v_4,v_3,v_5\}$, $h_5=\{v_4,v_7,v_1\}$, $h_6=\{v_6,v_7,v_3\}$ and $h_7=\{v_5,v_7,v_2\}$. If we identify v_i, where $i=1,\ldots,7$, of these subsets with the columns of the matrix

$$A=\begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 \end{pmatrix}, \tag{5}$$

we notice that the matrix A provides a representation (or realization) of the Fano matroid F_7. Now, suppose that the Fano matroid is extended to a structure in which the sets $\{v_i,v_j,v_k\}$ corresponding to the h_i are replaced by the completely antisymmetric object

$$(v_i,v_j,v_k)=-(v_i,v_k,v_j)=-(v_j,v_i,v_k). \tag{6}$$

For instance, we may replace $h_1=\{v_1,v_2,v_3\}$ by $\hat{h}_1=(v_1,v_2,v_3)$. Specifically, we define the extended Fano matroid $\hat{F}_7$ as the pair $(E,\hat{\mathcal{B}})$ in which $\hat{\mathcal{B}}$ is the set of three elements (v_i,v_j,v_k) except the completely antisymmetric quantities $\hat{h}_1=(v_1,v_2,v_3)$, $\hat{h}_2=(v_5,v_1,v_6)$, $\hat{h}_3=(v_6,v_2,v_4)$, $\hat{h}_4=(v_4,v_3,v_5)$, $\hat{h}_5=(v_4,v_7,v_1)$, $\hat{h}_6=(v_6,v_7,v_3)$ and $\hat{h}_7=(v_5,v_7,v_2)$. The generalization from F_7 to $\hat{F}_7$ is very similar to the transition from graphs to digraphs (or oriented graphs) in which the edges of the original graph, let us say $\{a,b\}$, are changed to an ordering set, $(a,b)=-(b,a)$. The important point is that if there exists such a transition between F_7 and $\hat{F}_7$, then we discover that $\hat{F}_7$ almost determine completely the octonion algebra, essentially because (v_i,v_j,v_k) for the different h_i become closely related to the structure constants ψ_{mnr} associated to octonions. In fact, there is an extension of matroid theory which seems to be what these observations suggest for the Fano matroid, namely oriented matroids.[26]

In order to define oriented matroids it is necessary to define first what signed circuits are. A signed circuit X is a circuit with the partition (X^+,X^-) into two sets: X^+ the set of positive elements of X, and X^- its set of negative elements.

An oriented matroid $\mathcal{M}$ is a pair $(E,\mathcal{C})$, where E is a nonempty finite set, and $\mathcal{C}$ is a nonempty collection of subsets of E (called signed circuits) satisfying the following properties.

($\mathcal{C}$ *i*) No circuit properly contains another circuit.

($\mathcal{C}$ *ii*) If $\mathcal{C}_1$ and $\mathcal{C}_2$ are two distinct signed circuits, $\mathcal{C}_1\neq-\mathcal{C}_2$ and $c\in\mathcal{C}_1^+\cap\mathcal{C}_2^-$, then there exists a third circuit $\mathcal{C}_3\in\mathcal{C}$ with $\mathcal{C}_3^+\subseteq(\mathcal{C}_1^+\cap\mathcal{C}_2^+)\backslash\{c\}$ and $\mathcal{C}_3^-\subseteq(\mathcal{C}_1^-\cap\mathcal{C}_2^-)\backslash\{c\}$.

It is not difficult to see that by forgetting signs, this definition of oriented matroids reduces to the definition of ordinary (nonoriented) matroids.

An alternative but equivalent way to define an oriented matroid is as follows: An oriented matroid $\mathcal{M}$ is a pair (E,χ), where E is a nonempty finite set and χ (called chirotope) is a mapping $E^r\rightarrow\{-1,0,1\}$, with r the rank on E, satisfying the following properties.

(χi) χ is not identically zero.

(χii) χ is alternating.

(χiii) For all $x_1,x_2,\ldots,x_r$ and $y_1,y_2,\ldots,y_r$ such that

$$\chi(x_1,x_2,\ldots,x_r)\chi(y_1,y_2,\ldots,y_r)\neq 0, \tag{7}$$

there exists an $i\in\{1,2,3,4,5,6,7\}$ such that

$$\chi(y_i,x_2,\ldots,x_r)\chi(y_1,y_2,\ldots,y_{i-1},x_1,y_{i+1,}\ldots,y_r)=\chi(x_1,x_2,\ldots,x_r)\chi(y_1,y_2,\ldots,y_r). \tag{8}$$

For a vector configuration χ can be identified as

$$\chi(i_1,\ldots,i_r)\equiv \text{sign det}(v_{i_1},\ldots,v_{i_r})\in\{-1,0,1\} \tag{9}$$

and (χiii) turns out to be related to the Grassmann–Plucker relation.

Returning to the case of the Fano matroid, it is tempting to identify h_i with the chirotope

$$\chi(i_1,i_2,i_3)=\text{sign det}(v_{i_1},v_{i_2},v_{i_3}). \tag{10}$$

But, in Ref. 28 it is noted that the Fano matroid is not orientable. Specifically, one can verify that the Fano matroid does not satisfy the property (χiii). Nevertheless, it is interesting to observe that one may write the formula[29]

$$\psi_{i_1i_2i_3}+\chi(i_1,i_2,i_3)=C_{i_1i_2i_3}, \tag{11}$$

where $C_{i_1i_2i_3}\in\{-1,1\}$ may be identified with the uniform matroid $U_{3,7}$ which is an excluded minor for $GF(5)$-representability, where $GF(q)$ denotes a finite field of order q. In this sense the Fano matroid and the octonions look like complementary concepts of the oriented uniform matroid $M(U_{3,7})$ structure.

It is worth remarking that the structure of $\hat{F}_7$ does not necessarily correspond, in a straightforward way, to oriented matroids for the following observations. An important problem in matroid theory is to see which matroids can be mapped into a set of vectors in a vector space over a given field. When such a map exists we are speaking about a coordinatization (or representation) of the matroid over the field. A matroid which has a coordinatization over $GF(2)$ is called binary. Furthermore, a matroid which has a coordinatization over every field is called regular. It turns out that regular matroids are of fundamental importance in matroid theory, among other things, because they play a similar role as planar graphs in graph theory.[23] It is known that a graph is planar if and only if it contains no subgraph homeomorphic to K_5 or $K_{3,3}$. The analog of this theorem for matroids was proved by Tutte.[8] In fact, Tutte proved that a matroid is regular if and only if it is binary and has no minor isomorphic to the Fano matroid or the dual of this.

The important point is that an algebra, like the octonion algebra, is a vector space with an additional multiplicative operation. If it could be possible to identify this additional product with a kind of rule for the bases of $\mathcal{B}$ in a given matroid, then we could speak about a representation of a matroid (with this additional product) in terms of an algebra instead of just the corresponding vector space. At present, we have not been able to find in the literature this kind of structure for matroids. But it seems to us that our identification of $\hat{F}_7$ with octonions may provide an example of matroids associated with an algebra rather than with just the corresponding vector space.

IV. MATROID THEORY AND CHERN–SIMONS THEORY

Here, we shall briefly review the main results of Ref. 10 about the connection between matroid theory and Chern–Simons theory and make additional comments. For this purpose let us introduce the Witten's partition function

$$Z(L,k)=\int DA\,\exp(S_{cs})\prod_{r=1}^{n} W(L_r,\rho_r), \tag{12}$$

where S_{CS} is the Chern–Simons action

$$S_{CS}=\frac{k}{2\pi}\int_{M^3} Tr\left(A\wedge dA+\frac{2}{3}A\wedge A\wedge A\right), \tag{13}$$

and $W(C_i,\rho_i)$ is the Wilson line

$$W(L_r,\rho_r)=Tr_{\rho_r}P\exp\left(\int_{L_r}A_i^aT_a dx^i\right). \tag{14}$$

Here, $A=A_i^aT_a dx^i$, with T_a the generators of the Lie algebra of G and the symbol P means the path-ordering along the knots L_r. If we choose $M^3=S^3$, $G=SU(2)$ and $\rho_r=C^2$ for all the link components, then the Witten's partition function (12) reproduces the Jones polynomial

$$Z(L,k)=V_L(t), \tag{15}$$

where

$$t=e^{2\pi i/k} \tag{16}$$

and $V_L(t)$ denotes the Jones polynomial satisfying the skein relation,

$$t^{-1}V_{L_+}-tV_{L_-}=\left(\sqrt{t}-\frac{1}{\sqrt{t}}\right)V_{L_0}, \tag{17}$$

where L_+, L_- and L_0 are the standard notation for overcrossing, undercrossing and zero crossing.

On the other hand, Thistlethwaite[11] showed that if L is an alternating link and $G(L)$ the corresponding planar graph, then the Jones polynomial $V_L(t)$ is equal to the Tutte polynomial $T_G(-t,-t^{-1})$ up to a sign and a factor power of t. Specifically, we have

$$V_L(t)=(-t^{3/4})^{w(L)}t^{-(\rho-n)/4}T_G(-t,-t^{-1}), \tag{18}$$

where $w(L)$ is the writhe and ρ and n are the rank and the nullity of G, respectively. Here, $V_L(t)$ is the Jones polynomial of alternating link L. The Tutte polynomial associated to each graph G is a polynomial $T_G(x,x^{-1})$ with the property that if G is composed solely of isthmus and loops then $T_G(x,x^{-1})=x^Ix^{-l}$, where I is the number of isthmuses and l is the number of loops. The polynomial T_G satisfies the skein relation

$$T_G=T_{G'}+T_{G''}, \tag{19}$$

where G' and G'' are obtained by respectively delating and contracting an edge that is neither a loop nor an isthmus of G.

On the other hand, a theorem due to Tutte allows us to compute $T_G(-t,-t^{-1})$ from the maximal trees of G. In fact, Tutte proved that if $\mathcal{B}$ denotes the set of maximal trees in a graph G, $i(\mathcal{B})$ denotes the number of internally active edges in G, and $e(B)$ refers to the number of the externally active edges in G (with respect to a given maximal tree $B\in\mathcal{B}$), then the Tutte polynomial is given by the formula

$$T_G(-t,-t^{-1})=\sum_{B\subseteq\mathcal{B}}x^{i(B)}x^{-e(B)}, \tag{20}$$

where the sum is over all elements of $\mathcal{B}$.

The important point is that the Tutte polynomial $T_G(-t,-t^{-1})$ computed according to (20) uses the concept of a graphic matroid $M(G)$ defined as the pair $(E,\mathcal{B})$, where E is the set of edges of G. This remarkable connection between the Tutte polynomial and a matroid allows in fact a relation between the partition function $Z(L,k)$ given in (12) and matroid theory. This is because according to (18) the Tutte polynomial $T_G(-t,-t^{-1})$ is related to the Jones polynomial $V_L(t)$ which in turn according to (15) is connected to the partition function $Z(L,k)$. Specifically, for $M^3=S^3$, $G=SU(2)$, $\rho_r=C^2$ for all alternating link components of L, we have the relation

$$Z(L,k)=V_L(t)=(-t^{3/4})^{w(L)}t^{-(\rho-n)/4}T_G(-t,-t^{-1}). \tag{21}$$

Thus, the matroid $(E,\mathcal{B})$ used to compute $T_G(-t,-t^{-1})$ can be associated not only to $V_L(t)$, but also to $Z(L,k)$. Therefore, we have found a bridge which links the matroid formalism $(E,\mathcal{B})$ and the partition function $Z(L,k)$. This may allow us to bring many concepts of matroid theory to fundamental physics and, conversely, different results in fundamental physics may be used as an inspiration to further develop matroid theory. As an example of the former remark let us just mention how the duality concept in matroid theory can be used as a symmetry of $Z(L,k)$.

First of all, it is known that in matroid theory the concept of duality is of fundamental importance. For example, there is a remarkable theorem that assures that every matroid has a dual. So, the question arises about what are the implications of this theorem in Chern–Simons formalism. In order to address this question let us first make a change of notation $T_G(-t,-t^{-1})\rightarrow T_{M(G)}(t)$ and $Z(L,k)\rightarrow Z_{M(G)}(k)$. The idea of this notation is to emphasize the connection between matroid theory, Tutte polynomial and Chern–Simons partition function. Consider the planar dual graph G^* of G. In matroid theory we have $M(G^*)=M^*(G)$. Therefore, the duality property of the Tutte polynomial

$$T_G(-t,-t^{-1})=T_{G^*}(-t^{-1},-t) \tag{22}$$

can be expressed as

$$T_{M(G)}(t)=T_{M^*(G)}(t^{-1}) \tag{23}$$

and consequently from (15) and (18) we discover that for the partition function $Z_{M(G)}(k)$ we should have the dual property

$$Z_{M(G)}(k)=Z_{M^*(G)}(-k). \tag{24}$$

As a second example let us first mention another theorem due to Withney:[5] If $M_1,\ldots,M_p$ and $M_1',\ldots,M_p'$ are the components (or blocks) of the matroids M and M', respectively, and if M_i' is the dual of M_i $(i=1,\ldots,p)$, then M' is dual of M. Conversely, let M and M' be dual matroids, and let $M_1,\ldots,M_p$ be components of M. Let $M_1',\ldots,M_p'$ be the corresponding submatroids of M'. Then $M_1',\ldots,M_p'$ are the components of M', and M_i' is dual of M_i. Thus, according to (24) we find that

$$Z_{M_i(G_i)}(k)=Z_{M_i'(G_i)}(-k) \tag{25}$$

if and only if

$$Z_{M(G)}(k)=Z_{M'(G)}(-k), \tag{26}$$

where G_i are the components or blocks of G.

Our discussion has been, so far, based on alternating links L. This kind of link is an important, but relatively small, subclass of links. In fact, there is a one-to-one correspondence between links and signed graphs and a link is alternating if the signed graph representation has all edges with the same sign. Therefore, in order to generalize the procedure, it turns necessary to have a generalized Thustlethwaite's[11] theorem for any signed graph not just for those of the same sign. Fortunately, Thustlethwaite himself,[11] and later Kauffman,[30] precisely generalized the original Thustlethwaite's theorem for planar unsigned graphs.

Theorem: Let G be a planar signed graph. Let $K(G)$ be the knot/link diagram corresponding to G. Then $\langle K(G)\rangle=T_G(A,B,x,y)$. The bracket polynomial for knots and links is a specialization of the generalized Tutte polynomial for signed graphs.

Here, A, B, and d are commuting variables associated to the link. A and B correspond to A-channel, B-channel, respectively, while the parameter d is used as a factor of normalization in order to make $T_G(A,B,d)$ invariant under the Reidemeister moves II and III.

Furthermore, Kauffman showed that $T_G = T_G(A,B,x,y)$ has a spanning tree expansion of the form

$$T_G = \sum_{H \subseteq \mathcal{B}} \Lambda(H), \tag{27}$$

where $\Lambda(H)$ denotes the product of the contribution of the edges of G relative activities of the maximal trees H in G.

In principle, since up to a normalized factor, measuring the orientability of the link, $\langle K(G)\rangle \leftrightarrow CS$, in order to find a generalization of our procedure we need to relate T_G with matroid theory. A $T_G \leftrightarrow matroids$ connection is given by (27) in the sense that the sum is over all maximal trees H in G. Notice, however, that the maximal trees H are associated to the underlying graph (without signs) of the signed graph and not to the signed graph itself.

It is known that matroids associated to signed graphs are called bias matroids.[27] It turns out that bias matroids are interesting by themselves, but unfortunately the subject about this kind of matroid has not been developed for our purpose and it appears that many of the interesting properties of ordinary matroids are lost. Nevertheless, the idea of writing T_G as a sum over bias matroids seems interesting and deserves further study.

It may help to mention in this direction that Crapo[31] proposed an alternative possibility to write T_G as a sum over all spanning subsets of E, rather than over maximal trees. This idea is motivated from the observation that in this case the rank function ρ becomes an important concept and can be used to generalize T_G to matroid theory. A generalization for signed graphs of the Crapo's polynomial has been proposed by Murasugi[32] and by Shwarzler and Welsh.[33] Let us briefly mention these two polynomials.

Murasugi introduced the following polynomial. Let $\Gamma(r,s)$ denote the set of all spanning subgraph S of G. Then $T_G(x,y,z)$ is defined by

$$T_G(x,y,z) = \sum_{k,\rho} \left\{ \sum_{S \in \Gamma(r,s)} x^{P(S)-N(S)} \right\} y^{k(S)-1} z^{|S|-\rho(S)}, \tag{28}$$

where $P(S)$ and $N(S)$ denote the number of positive and negative edges in S, respectively. It is interesting to note that $\beta_0 = k = r+1$ and $\beta_1 = n = |S| - \rho(S)$, where n is the nullity and β_i denotes the i Betti number of S as a 1-complex. Although this polynomial uses the rank and the nullity concepts, the fact that the sum is over all spanning subgraphs Γ means that $T_G(x,y,z)$ is also applied only to the underlying unsigned graph G associated to the signed graph. Furthermore, the Murasugi polynomial does not have a direct relation with the Kauffmann polynomial.

On the other hand, Shwarzler and Welsh[33] proved that the Kauffmann polynomial associated to a link L can be expressed in terms of the associated signed graph $G(L)$ as follows,

$$T_G(A,B) = A^{|E^-|-|E^+|}(-A^2 - A^{-2})^{\rho(G)} \sum_{S \subseteq E} A^{4(\rho(S)-|S^-|)} B^{\rho(G)+|S|-2\rho(S)}, \tag{29}$$

where $B = -A^4 - 1$ and for any subset $S \subseteq E(G)$, S^+ and S^- denote the positive and negative signed parts, respectively. It is important to remark that Shwarzler and Welsh showed that (29) is a specialization of a more general polynomial for signed matroids. In fact, Shwarzler and Welsh proposed an eight variables polynomial which contains as specialization not only the Kauffman bracket polynomial but also the Tutte polynomial of a matroid, the partition function of the anisotropic Ising model and the Kauffman-Murasugi polynomial of signed graphs (for further details, see Ref. 33).

V. MATROID THEORY AND STRING THEORY

In the literature,[34–36] several attempts have been done to connect Chern–Simons formalism with string theory. One of the most interesting[37] comes from the idea that at some level the

decoupling of ghost and matter does not hold. In this case, matter fields and ghosts become mixed and the standard string theory should be replaced by some kind of topological string theory.[38] It has been shown[35] that some topological string theories perturbatively coincide with Chern–Simons theory. So, in this sense Chern–Simons theory is equivalent to topological string theory. However, the problem arises when it is attempted to relate Chern–Simons theory with fundamental strings. In fact, it has been shown[38] that in the pure Chern–Simons formalism there are not enough degrees of freedom to reproduce not only the induced gravity but the toroidal compactification of heterotic string.

These observations are, of course, important in order to find a matroid theory and string theory connection and eventually M-theory connection. In the previous section we explained a matroid theory–Chern–Simons theory relation via Tutte and Jones polynomials. It is clear then that what we should look for is some kind of generalization of fundamental strings which may provide the bridge between fundamental strings and topological strings.

The generalized fundamental strings could be the topological membrane[39] itself, but this is likely to be reduced to the topological strings rather than to fundamental strings. Another possibility is the membrane theory or any other p-brane,[40] but it has been shown[41] that through double dimensional reduction these are reduced to fundamental strings rather than to topological strings. So, although there is the hope that at some level 3D topological field theory may lead to fundamental strings, the correct formulation of such a theory is at present unknown.

In this section, we propose an alternative generalization of fundamental strings which seems closer to our purpose than the already known alternative of topological membranes or p-branes.

The idea comes from the observation that in the Polyakov type action the world sheet metric and the target space–time metrics are decoupled. But it seems natural to think that at a more fundamental level when ghost and matter fields are mixed the decoupling between two such metrics is no longer true. Therefore the desired generalization of string theory must be based on a unified metric of the world sheet and target space–time metrics.

Let us clarify these observations. For this purpose, let us first consider the Polyakov action

$$S=\frac{1}{2}\int d^2\xi\sqrt{-g}g^{ab}(\xi)\partial_a x^\mu\partial_b x^\nu G_{\mu\nu}(x), \tag{30}$$

where $g_{ab}(\xi)$ and $G_{\mu\nu}(x)$, with $\mu,\nu=1,\ldots,D$, are the world sheet metric and the target space–time metric, respectively. We observe from (30) that the two metrics $g_{ab}(\xi)$ and $G_{\mu\nu}(x)$ play very different roles; $g_{ab}(\xi)$ determines the world sheet metric swept out by the string in its dynamical evolution, while $G_{\mu\nu}(x)$ determines the background metric where the string is moving. Therefore, classically $g_{ab}(\xi)$ and $G_{\mu\nu}(x)$ are unrelated. However, this is no longer true at the quantum level. For instance, it is well known that in a consistent quantum string theory $g_{ab}(\xi)$ plays an essential role to fix the size of the matrix $G_{\mu\nu}(x)$: $D=26$ in the bosonic case. This kind of relation between $g_{ab}(\xi)$ and $G_{\mu\nu}(x)$ is, however, in a certain sense superficial because in the critical dimension 26 matter fields decouple from the corresponding ghost with associated central charge $c=-26$. The important observation is that, as it was mentioned in the Introduction, at a deeper level the decoupling between matter fields and ghost must be no longer true and therefore one should expect that in such a case there must be a unified framework for the two metrics $g_{ab}(\xi)$ and $G_{\mu\nu}(x)$.

Consider the line element

$$ds^2=G_{(\hat{\mu}\hat{\nu})}(x^{\hat{\alpha}})dx^{\hat{\mu}}\otimes dx^{\hat{\nu}}, \tag{31}$$

where the indices $\hat{\mu},\hat{\nu}$ run from 1 to $2D$, the symbol $\otimes$ means tensor product and $G_{(\hat{\mu}\hat{\nu})}=G_{(\hat{\nu}\hat{\mu})}$. Suppose that (31) can be written as

$$ds^2=G_{(\mu\nu)}(x^{\hat{\alpha}})dx^\mu\otimes dx^\nu+G_{(\mu\nu)}(x^{\hat{\alpha}})dy^\mu\otimes dy^\nu. \tag{32}$$

Here, we assume that $G_{(\mu A)}=G_{(A\mu)}=0$, with $A=D+1,\ldots,2D$ and we identify $x^A\rightarrow y^\mu$ and $G_{(AB)}\rightarrow G_{(\mu\nu)}$. It is not difficult to see that (32) can be rewritten as

$$ds^2=G^{ab}_{(\mu\nu)}(x^{\hat{\alpha}})dx^\mu_a\otimes dx^\nu_b, \tag{33}$$

where $x^\mu_1\equiv x^\mu$ and $x^\mu_2=y^\mu$ and we assumed that $G^{11}_{(\mu\nu)}=G^{22}_{(\mu\nu)}$ and $G^{12}_{(\mu\nu)}=G^{21}_{(\mu\nu)}=0$.

On the other hand, if we use the definition

$$z^\mu=x^\mu+iy^\mu, \tag{34}$$

we find that (32) can be written in the alternative way

$$ds^2=G_{(\mu\nu)}(x^{\hat{\alpha}})dz^\mu\otimes d\overline{z}^\nu. \tag{35}$$

In this scenario, since $dx^{\hat{\mu}}\otimes dx^{\hat{\nu}}$ is a second-rank symmetric tensor, the same results follow if we consider the most general Hermitian metric

$$G_{\hat{\mu}\hat{\nu}}(x^{\hat{\alpha}})=G_{(\hat{\mu}\hat{\nu})}(x^{\hat{\alpha}})+iG_{[\hat{\mu}\hat{\nu}]}(x^{\hat{\alpha}}). \tag{36}$$

Here, $G_{[\hat{\mu}\hat{\nu}]}$ denotes an antisymmetric tensor metric. Of course, $G_{\hat{\mu}\hat{\nu}}$ in (36) satisfies the Hermitian condition $G_{\hat{\mu}\hat{\nu}}=G^\dagger_{\hat{\mu}\hat{\nu}}$.

Now, consider the metric $G_{\hat{\mu}\hat{\nu}}(x^{\hat{\alpha}})$ given in (36), in connection with the exterior product

$$\Omega=\tfrac{1}{2}G_{\hat{\mu}\hat{\nu}}(x^{\hat{\alpha}})dx^{\hat{\mu}}\wedge dx^{\hat{\nu}}. \tag{37}$$

Using the exterior product property $dx^{\hat{\mu}}\wedge dx^{\hat{\nu}}=-dx^{\hat{\nu}}\wedge dx^{\hat{\mu}}$, we see that (37) leads to

$$\Omega=\frac{i}{2}G_{[\hat{\mu}\hat{\nu}]}(x^{\hat{\alpha}})dx^{\hat{\mu}}\wedge dx^{\hat{\nu}}. \tag{38}$$

Assuming that $G_{[\mu A]}=G_{[A\mu]}=0$ we find that (38) becomes

$$\Omega=\frac{i}{2}G_{[\mu\nu]}(x^{\hat{\alpha}})dx^\mu\wedge dx^\nu+\frac{i}{2}G_{[AB]}(x^{\hat{\alpha}})dy^A\wedge dy^B. \tag{39}$$

We again make the identification $x^A\rightarrow y^\mu$ and $G_{[AB]}\rightarrow G_{[\mu\nu]}$. The formula (39) can be rewritten as

$$\Omega=\frac{i}{2}G_{[\mu\nu]}(x^{\hat{\alpha}})(dx^\mu\wedge dx^\nu+dy^\mu\wedge dy^\nu). \tag{40}$$

Introducing $x^\mu_1\equiv x^\mu$ and $x^\mu_2=y^\mu$ and assuming that $G^{12}_{[\mu\nu]}=G^{21}_{[\mu\nu]}=0$ and $G^{11}_{[\mu\nu]}=G^{22}_{[\mu\nu]}\neq 0$ we find that (40) leads to

$$\Omega=\frac{i}{2}G^{ab}_{[\mu\nu]}(x^{\hat{\alpha}})dx^\mu_a\wedge dx^\nu_b. \tag{41}$$

On the other hand, using the definition (34) for z^μ we find that (40) can also be written as

$$\Omega=\frac{i}{2}G_{[\mu\nu]}(x^{\hat{\alpha}})dz^\mu\wedge d\overline{z}^\nu. \tag{42}$$

Summarizing we have shown that if $G^{11}_{(\mu\nu)}=G^{22}_{(\mu\nu)}\neq 0$ and $G^{12}_{(\mu\nu)}=G^{21}_{(\mu\nu)}=0$, and $G^{11}_{[\mu\nu]}=G^{22}_{[\mu\nu]}\neq 0$ and $G^{12}_{[\mu\nu]}=G^{21}_{[\mu\nu]}=0$, then

$$ds^2=G^{ab}_{\mu\nu}(x^\alpha_c)dx^\mu_a\otimes dx^\nu_b \tag{43}$$

is equivalent to

$$ds^2 = G_{\mu\nu}(z^\alpha, \overline{z}^\beta) dz^\mu \otimes d\overline{z}^\nu, \tag{44}$$

and that

$$\Omega = \frac{i}{2} G^{ab}_{\mu\nu}(x^\alpha_c) dx^\mu_a \wedge dx^\nu_b \tag{45}$$

is equivalent to

$$\Omega = \frac{i}{2} G_{\mu\nu}(z^\alpha, \overline{z}^\beta) dz^\mu \wedge d\overline{z}^\nu. \tag{46}$$

We recognize in (44) and (46) the formulas used to define the Kahler metric which in addition satisfies the condition $d\Omega = 0$. Therefore we have shown that under certain anzats the metric $G^{ab}_{\mu\nu}(x^\alpha_c)$ can be identified with the Kahler metric. This shows that it makes mathematical sense to consider a metric of the form $G^{ab}_{\mu\nu}(x^\alpha_c)$.

Our goal is now to use the metric $G^{ab}_{\mu\nu}(x^\alpha_c)$ in connection with string theory. We find that there are at least two different ways to achieve this. In fact, in the first case we have the action

$$S_1 = \frac{1}{2} \int d^2\xi \sqrt{-g} g^{ab}(\xi) \partial_a x^\mu_c \partial_b x^\nu_d G^{cd}_{\mu\nu}(x), \tag{47}$$

while in the second case we have[42]

$$S_2 = \frac{1}{2} \int d^2\xi G^{ab}_{\mu\nu}(\xi, x) \partial_a x^\mu \partial_b x^\nu. \tag{48}$$

For our purpose to relate matroid theory with string theory both possibilities look attractive. The action S_1 may be useful to understand T-duality or S-duality because of its property of being symmetric under the interchange of coordinates $x \leftrightarrow y$. However, S_2 is closer to our idea of unified worldsheet–target space–time metrics when matter and ghost mix.

In fact, in the particular case

$$G^{ab}_{\mu\nu} = \sqrt{g} g^{ab} G_{\mu\nu}, \tag{49}$$

one sees that S_2 is reduced to the Polyakov action (30). This shows that ordinary bosonic string theory is contained in a theory associated to (48). Another particular case for $G^{ab}_{\mu\nu}$ is

$$G^{ab}_{\mu\nu} = \sqrt{g} g^{ab} G_{\mu\nu} + i\varepsilon^{ab} B_{\mu\nu}, \tag{50}$$

where $B_{\mu\nu} = -B_{\nu\mu}$ is a two form and ε^{ab} is the completely antisymmetric tensor with $\varepsilon^{12} = 1$. The choice (50) leads to a generalized bosonic string theory, the so-called nonlinear sigmal model in two dimensions, in which the string propagates in a background determined not only by gravity but by the antisymmetric two form gauge field B with associated field strength $H = dB$. Finally, the third example is provided precisely for what we have already discussed when $G^{ab}_{\mu\nu}$ is identified with a Kahler metric.

Here, we are not particularly interested in developing the full theory implied by S_2, but to point out how S_2 can be related to matroid theory via Chern–Simons theory. For this purpose it seems to be convenient to start by recalling briefly how the Kahler structure is related to Chern–Simons theory.

There are a number of restrictions which a background field must satisfy in order to have a consistent string theory. Perhaps one of the most important is the anomaly cancellation fixed by the constraint[4]

$$dH = trR \wedge R - trF \wedge F, \tag{51}$$

where R is the curvature associated to $G_{\mu\nu}$. The formula (51) is an important restriction for the possible compactifications. One of the most attractive solutions of (51) is when the ten dimensional space–time vacuum state is given by $T^4 \times K$, where T^4 is a maximally symmetric four dimensional space–time and K is a six dimensional Kahler manifold.

Now, it is known that a Kahler metric determines a Kahler manifold, so Kahler metric is related to string theory through (51). In turn (51) contains the second Chern class $\int trF \wedge F$ which reduces to the Chern–Simons form. Therefore, the Kahler metric is closely related to Chern–Simons formalism in string theory. Consequently, the action S_2 with the choice of $G^{ab}_{\mu\nu}$ as a Kahler metric establishes a connection between matroid theory and string theory via Chern–Simons formalism.

VI. ALTERNATIVE CONNECTION BETWEEN MATROID THEORY AND STRING THEORY

The observations in the previous section may motivate us to look for a Chern–Simons formulation for strings. An attempt in this direction has been proposed by Zaikov.[18] Dolan and Tchrakian[43] have proposed a similar structure which has been extensively studied by Castro.[44] One of the roots of these developments is the Schild type construction for strings. In this section we shall show that this kind of construction offers a more direct connection between matroid theory and string theory.

Let us first recall the Schild type construction for strings. It is well known that from the action (30) one can derive the Nambu–Goto action

$$S = T \int d^2\xi \sqrt{-h}, \tag{52}$$

where h is the determinant of

$$h_{ab} = \partial_a x^\mu \partial_b x^\nu G_{\mu\nu}(x). \tag{53}$$

Here, we have restored the tension T of the string.

It is not difficult to see that h can be written as

$$h = \sigma^{\mu\nu}\sigma_{\mu\nu}, \tag{54}$$

where

$$\sigma^{\mu\nu} = \frac{1}{[2!]^{1/2}} \varepsilon^{ab} v^\mu_a(\xi) v^\nu_b(\xi). \tag{55}$$

Here, $v^\mu_a(\xi)$ is defined by

$$v^\mu_a(\xi) = \partial_b x^\mu(\xi). \tag{56}$$

One can show that the action (52) is equivalent to

$$S^{(1)}_p = \int d^2\xi \left(\sigma^{\mu\nu} p_{\mu\nu} - \frac{\gamma}{2}(p^{\mu\nu} p_{\mu\nu} + T^2) \right), \tag{57}$$

where γ is a Lagrange multiplier and $p_{\mu\nu}$ is a linear momentum associated to $\sigma^{\mu\nu}$. If we eliminate $p_{\mu\nu}$ from this action, we get

$$S^{(1)}_p = \frac{1}{2} \int d^2\xi (\gamma^{-1} \sigma^{\mu\nu}\sigma_{\mu\nu} - \gamma T). \tag{58}$$

By eliminating γ from (58) we recover action (52). The importance of (57) or (58) is that it now makes sense to set $T=0$. In this case (58) is reduced to the Schild type null 1-brane action.[13] Here, we are interested in connecting (58) with matroid theory.

Observe that we can relate (58) with matroid theory if we connect $\sigma^{\mu\nu}$ with a matroid structure. Therefore, the question is how expression (55) is related to matroids.

Consider the matrix

$$D=\begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & -1 \end{pmatrix}. \tag{59}$$

The matrix D is a realization of the matroid $E=\{1,2,3,4\}$ and

$$\mathcal{B}=\{\{1,2\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,4\}\}. \tag{60}$$

This is the uniform matroid $U_{2,4}$. The elements of E are identified with the columns of D in the form $1\rightarrow b_a^1$, $2\rightarrow b_a^2$, $3\rightarrow b_a^3$ and $4\rightarrow b_a^4$ where b_a^μ are the four columns of D and the index a runs from 1 to 2. In this case the chirotope formula (9) reads as

$$\chi(\mu,\nu)\equiv \operatorname{sign}\det(\mathbf{b}^\mu,\mathbf{b}^\nu)\in\{-1,0,1\}. \tag{61}$$

In tensor notation we can write (61) in the form

$$\chi(\mu,\nu)\equiv \operatorname{sign}(\varepsilon^{ab}b_a^\mu b_a^\nu)\in\{-1,0,1\}. \tag{62}$$

Let us define

$$\Sigma^{\mu\nu}\equiv\varepsilon^{ab}b_a^\mu b_a^\nu \tag{63}$$

so that $\chi(\mu,\nu)\equiv\operatorname{sign}\Sigma^{\mu\nu}$. Comparing (55) and (63) we observe the great similarity between the two formulas. The main difference is the local property of (55). This is in a certain sense similar to the relation between the flat Minkowski metric $\eta_{\mu\nu}=\operatorname{diag}(-1,\ldots,1)$ and a curved metric $g_{\mu\nu}=g_{\mu\nu}(x)$. Let us discuss this analogy in more detail.

Consider an n-dimensional manifold M. A tangent bundle associated to M can be defined as

$$TM=\bigcup_{x\in M} T_x(M), \tag{64}$$

where $T_x(M)$ is the tangent space attached at each point x of M. The cotangent bundle

$$T^*M=\bigcup_{x\in M} T_x^*(M) \tag{65}$$

is defined through the isomorphism $w:T_x(M)\rightarrow R$, where $w\in T_x^*(M)$. The curved metric $g_{\mu\nu}(x)$ can be understood as the symmetric positive definite map

$$g:T_x(M)\rightarrow T_x^*(M). \tag{66}$$

In tensor notation (45) becomes

$$a_\mu=g_{\mu\nu}a^\nu, \tag{67}$$

where $a^\nu\in T_x(M)$ and $a_\mu\in T_x^*(M)$. A tangent bundle is an example of fiber bundles. In this case the fiber is the tangent space $T_x(M)$.

Therefore, the transition from $\eta_{\mu\nu}$ to $g_{\mu\nu}(x)$ is determined by the transition from flat vector space to a fiber bundle. Similarly, we may say that the transition from $\Sigma^{\mu\nu}$ to $\sigma^{\mu\nu}(\xi)$ is determined by the transition form matroid structure to matroid bundle structure. But the question is now

to understand what we mean by matroid bundle. Fortunately, the mathematicians have already developed such a concept.[14–17] The matroid bundle concept can be understood as the combinatorial analog of a fiber bundle. In a matroid bundle the fiber of a bundle is replaced by a matroid. It is worth mentioning that, recently, matroid bundle structure was used to combine the concepts of matroid and gravity in a proposed theory called gravitoid.[29]

Summarizing, we may start with a rank-two realizable matroid M such as the example in (59). We construct the chirotope $\chi(\mu,\nu)$ by means of the tensor $\Sigma^{\mu\nu}$ as in the formula (63). We then make the transition from a matroid structure to matroid bundle structure in such a way that $\Sigma^{\mu\nu} \rightarrow \sigma^{\mu\nu}(\xi)$. If we can go from (55) to (56), our task is finished.

Consider the object

$$F^{\mu}_{ab} = \partial_a v^{\mu}_b(\xi) - \partial_b v^{\nu}_a(\xi). \tag{68}$$

If F^{μ}_{ab} vanishes, then a solution of (68) is $v^{\mu}_a(\xi) = \partial x^{\mu}/\partial \xi^a$ where x^{μ} is in this context a gauge function. In this case, one says that $v^{\mu}_a(\xi)$ is a pure gauge. This kind of scenario can be derived from an Abelian Chern–Simons action for F^{μ}_{ab} in the form

$$S_{CS} = \frac{k}{2\pi} \int d^3\xi \varepsilon^{ijk} v^{\mu}_i F_{jk\mu}. \tag{69}$$

This shows once again the great importance of Chern–Simons formulation for a matroid/string connection. In fact, if we substitute expression (56) into (69), then the Zaikov's Chern–Simons type action for strings is obtained.

It is worth mentioning that in general a p-form F that can be written as $F = v_1 \wedge \cdots \wedge v_p$ for some $v_1, \ldots, v_p \in R^n$ is called decomposable. This means that the two form $\sigma^{\mu\nu}(\xi)$ given in (55) is decomposable. It turns out that decomposable forms may be considered as the starting point to construct the realization space of an oriented matroid (see Ref. 26, Chap. 8). These observations provide an additional evidence for the close relation between $\sigma^{\mu\nu}(\xi)$ and oriented matroids.

VII. COMMENTS

In the present work we have shown that the Kahler metric may provide an important bridge to connect matroid theory and string theory. Specifically using a generalized string theory we established the following identifications: $string\text{-}theory \leftrightarrow Kahler\text{-}structure$; $Chern\text{–}Simons\text{-}theory \leftrightarrow Kahler\text{-}structure$ and $matroid\text{-}theory \leftrightarrow Chern\text{–}Simons\text{-}theory$. Moreover, it is natural to expect that this kind of relation suggests a direct link between the generalized string theory described by (48), which by convenience we shall call Kahler-string action, and the pure Chern–Simons theory. But at first sight it is improbable that this more direct relation exists. The reason is that pure Chern–Simons theory does not provide us enough degrees of freedom to describe the dynamics even for the heterotic string theory. Therefore, these observations suggest that there must exist a generalized Chern–Simons action which is reduced to the Kahler-string action (48). Of course, the Kahler structure must play an important role in this generalized Chern–Simons theory. Happily, such a theory along this idea has already been proposed. In fact, some years ago Nair and Schiff[45] proposed what they called Kahler–Chern–Simons theory. The action proposed by Nair and Schiff has the form

$$S_{KCS} = \frac{k}{2\pi} \int_{M^3 \times R} Tr\left(A \wedge dA + \frac{2}{3} A \wedge A \wedge A \right) \Omega, + Tr(F\Phi + \Phi F), \tag{70}$$

where F is the field strength in $B^4 \times R$, Φ is a Lie algebra value (2,0) form and M^4 is a Kahler manifold of real dimension four. It turns out that S_{KCS} provides an action description of anti-self-dual gauge fields (instantons) on a four dimensional Kahler manifolds. Here, we are interested in seeing if under quantization S_{KCS} is reduced to the Kahler-string action (48). It can be shown, however, that up to WSW term, S_{KCS} leads to the action

$$S_3=\frac{1}{2}\int d^{2+2}\xi\sqrt{-g}g_{ij}^{ab}(\xi)\frac{\partial x^{\mu}}{\partial\xi_i^a}\frac{\partial x^{\nu}}{\partial\xi_i^a}G_{\mu\nu}(x), \tag{71}$$

rather than (48). Here, g_{ij}^{ab} can be identified with a Kahler metric on B^4, while $G_{\mu\nu}(x)$ is given by $G_{\mu\nu}(x)=\partial_{\mu}U\partial_{\nu}U^{-1}$, where U is a locally defined G-valued function related to the gauge field A by $A=U^{-1}dU$. Therefore, we conjecture that there must be a slightly different action from (70), with the property of reducing to (48).

Nevertheless, the action S_{KCS} may be of special interest to relate matroid theory not only to string theory but to M-theory itself. In fact, it is known that S_{KCS} leads to a theory in terms of fields in a target space of $N=2$ strings.[46] In turn, $N=2$ strings is one of the main proposals of M-theory.[47] Moreover, it has been pointed out in Ref. 48 that a number of similarities exist between the other main proposal of M-theory, namely, matrix theory.[49] In principle, for S_{KCS} one may repeat the formalism of Sec. IV. In fact, consider the partition function

$$Z_{KCS}(L,k)=\int DA\,\exp(S_{KCS})\prod_{r=1}^{n}W(L_r,\rho_r), \tag{72}$$

where $W(L_i,\rho_i)$ are the Wilson lines defined in (14). It is tempting to speculate that $Z_{KCS}(L,k)$ must be related to some knot invariant in a similar way that $Z_{CS}(L,k)$ is related to the Jones polynomials. From this idea, since knots are in one-to-one correspondence with signed graphs, one should expect to find the desired relation between matroid theory and $Z_{KCS}(L,k)$, which may lead eventually to a matroid theory and M-theory connection.

In Sec. VI, we discussed an alternative possibility to connect matroids and strings. The idea is to consider the Schild type action for strings. (This action is equivalent to the Nambu–Goto action and may be considered as the starting point for the Zaikov and Dolan–Tchrakian constructions for p-branes.) We identify the $\sigma^{\mu\nu}$ factor in (55) with the tensor $\Sigma^{\mu\nu}$ associated to the chirotope $\chi(\mu,\nu)$ via the matroid bundle notion. Such identification may lead to the matroid/string connection if one consider the Chern–Simons structure in (69), which becomes a Zaikov type action after using (56). It is important to mention that the discussion of Sec. VI can be generalized in a straightforward way to any p-brane.[50]

Another possible route to connect matroid theory with M-theory comes from the work of Gopakumar and Vafa[51,52] who have proved that topological strings are closely related to M-theory. Since Chern–Simons formalism is linked to topological strings,[35] it seems that we are closer to make the matroid theory the underlying mathematical structure of M-theory (see Ref. 53 for interesting observations about M-theory).

Finally, besides the possible connection between matroid theory, and string theory, the present formalism may be of special interest for quantum gravity based on the Ashtekar formalism[54] (see also Ref. 55 and references therein). The most interesting solutions of the Ashtekar constraints correspond to Witten's partition function. Consequently, the duality symmetries (24) may also play an important role in such solutions. It is known that the Vasiliev invariants become an important tool in the loop solutions of quantum canonical gravity in the Ashtekar formalism. Since the Vasiliev invariants can be understood as a generalization of the Jones polynomials, it may be interesting for further research to investigate whether matroid theory can be connected to such invariants.

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Monopole–antimonopole solutions of the Skyrmed SU(2) Yang–Mills–Higgs model

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Axially symmetric monopole–antimonopole dipole solutions to the second-order equations of a simple SU(2) Yang–Mills–Higgs model featuring a quartic Skyrme-like term are constructed numerically. The effect of varying the Skyrme coupling constant on these solutions is studied in some detail. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1630703]

I. INTRODUCTION

The SU(2) Georgi–Glashow model in the Bogomol'nyi–Prasad–Sommerfield (BPS) limit supports monopoles[1,2] which are solutions of the first-order self-duality equations.[3,4] Away from the BPS limit, when new gauge invariant and positive definite terms are added, the resulting monopoles are described by the solutions to the second-order Euler–Lagrange equations, and not to the first-order self-duality equations. Once these terms are introduced to the model, the BPS topological bound cannot be saturated.

BPS and non-BPS monopoles differ in two remarkable respects. First, the BPS multimonopoles can be constructed analytically[5–8] while the non-BPS monopoles, e.g., when the Higgs potential is present,[1,2] can only be constructed numerically. Second, and perhaps physically more interestingly, BPS monopoles do not interact while non-BPS monopoles interact. In the presence of a Higgs potential this interaction is known to be repulsive[9,10] and has been verified to be so numerically,[11] while in the presence of Skyrme-like terms, higher order in both the Yang–Mills (YM) curvature and the Higgs covariant derivatives, this interaction can be both repulsive and attractive.[12] In a particularly simple such (Skyrme-like) model, this interaction was found[13] to be strictly attractive, and moreover it was found,[13] rather unexpectedly, that the lowest energy bound states were the axially symmetric ones and not those with Platonic symmetries. (It was unexpected since this feature contrasts with that for Skyrmion bound states.[14])

All the above-mentioned monopole solutions discussed are stable relative to the topological lower bound whether they saturate this bound, as for the BPS monopoles, or not, as for non-BPS ones. There is however another class of non-self-dual solutions to the second-order Euler–Lagrange equations which are not stable and represent states of monopoles and antimonopoles in equilibrium. The existence of such solutions was first proved by Taubes[15] for the model featuring no Higgs potential (and of course no higher order terms in the curvature and covariant derivative), namely, for the model which supports BPS multimonopoles. Such a non-BPS solution, namely, an unstable solution of the second-order equations, was first constructed for this system with SU(3) gauge group and subject to spherical symmetry by Burzlaff.[16] More recently Ioannidou and Sutcliffe[17] employed a harmonic map anstaz to construct such spherically symmetric solutions to the same (BPS) system with gauge groups SU(3), SU(4), and SU(N). Using results on sigma

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model instantons, these authors[17] also argued that the zero charge solutions they constructed described monopole–antiimonopole pairs.

A direct approach to constructing zero charge monopole–antimonopole pairs for the SU(2) BPS model was used sometime ago by Rüber.[18] This was the numerical construction of axially symmetric solutions with suitable boundary value conditions. More recently Kleihaus and Kunz[19] constructed this zero charge solution for the full Georgi–Glashow model featuring a Higgs potential, and they studied the effect of the Higgs potential in detail. To date, no such study has been reported in the literature pertaining to the model featuring higher order Skyrme-like terms. In the background of the above-described scenario it is pertinent to carry out such a study.

This is the aim of the present work. We will consider the zero charge axially symmetric monopole–antimonopole solutions as in Refs. 18 and 19, for the simple skyrmed Higgs model studied in Ref. 13 whose axially symmetric charge-2 monopoles are mutually attractive. This contrasts with the monopole–antimonopole solutions studied in Ref. 19 for the model whose charge-2 monopoles are mutually repulsive, which makes the comparison of our results with those of Ref. 19 interesting. In addition to constructing the vorticity-1 monopole–antimonopole solutions, as in Refs. 18 and 19, but now for the Skyrmed model here, we also construct the corresponding vorticity-2 solutions.

II. SKYRMED SU(2) YANG–MILLS–HIGGS MODEL

The static energy of the simplified Skyrme-like model considered is

$$\mathcal{E}=\int\left\{\frac{1}{2}\mathrm{Tr}\{F_{\mu\nu}F^{\mu\nu}\}+\frac{1}{4}\mathrm{Tr}\{D_\mu\Phi D^\mu\Phi\}+\frac{\kappa}{8}\mathrm{Tr}\{[D_\mu\Phi,D_\nu\Phi][D^\mu\Phi,D^\nu\Phi]\}\right.$$
$$\left.+\frac{\lambda}{2}\mathrm{Tr}\{(\Phi^2-\eta^2)^2\}\right\}d^3r \tag{1}$$

with field strength tensor of the su(2) gauge potential $A_\mu=\frac{1}{2}\tau_a A_\mu^a$,

$$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu+ig[A_\mu,A_\nu]\ , \tag{2}$$

and covariant derivative of the Higgs field $\Phi=\tau_a\phi^a$ in the adjoint representation

$$D_\mu\Phi=\partial_\mu\Phi+ig[A_\mu,\Phi]\ \ , \tag{3}$$

and g denotes the gauge coupling constant, κ the coupling strength of the quartic Skyrme-like Higgs kinetic term, λ the strength of the Higgs potential, and η the vacuum expectation value of the Higgs field.

The topological charge Q is the well-known quantity

$$Q=\frac{1}{4\pi\eta}\varepsilon^{ijk}\int\mathrm{Tr}\{F_{ij}D_k\Phi\}d^3r\ \ , \tag{4}$$

corresponding to the magnetic charge $m=Q/g$, and takes integer values that equal the winding number of the Higgs field.[20] The latter is encoded with the boundary conditions which yield the value of this integer.

To construct axially symmetric solutions that describe systems of monopoles and multimonopoles, specific boundary conditions must be imposed at the Higgs field at infinity. For usual multimonopoles, the Higgs field at infinity is described by the vortex number n winding the azimuthal angle φ, n times and the polar angle θ does not wind. Zero magnetic charge monopoles on the other hand, namely those we seek to construct, can be achieved by requiring that in the asymptotic Higgs field the polar angle is enhanced by another integer m. This can also be achieved automatically by incorporating this integer m in the ansatz[18,19] as will be in the following. The integral (4) can be evaluated for a system with m zeros of the Higgs field (i.e., with m monopole and antimonopole centers), and with vorticity n, yielding

$$Q=4\pi n\eta^3[1-(-1)^m] \ . \tag{5}$$

In this paper we will restrict to the charge zero case $m=2$ with vorticity $n=1$, to carry out our detailed analysis of the system, with special attention to the κ dependence of the solutions. After that, we will also briefly study the case of $n=2$ vorticity, again with $m=2$. These are both monopole–antimonopole solutions to the second-order equations carrying $Q=0$.

III. STATIC AXIALLY SYMMETRIC $Q=0$ ANSATZ

We choose the static, axially symmetric, purely magnetic ansatz employed in Ref. 18 for the monopole–antimonopole solution and in Refs. 21 and 22 for the sphaleron–antisphaleron solution of the Weinberg–Salam model. Here the gauge field is parametrized by

$$A_0=0 \ , \quad A_r=\frac{H_1}{2gr}\tau_\varphi^{(n)} \ , \quad A_\theta=\frac{(1-H_2)}{g}\tau_\varphi^{(n)} , \quad A_\varphi=-n\frac{\sin\theta}{g}(H_3\tau_r^{(2,n)}+(1-H_4)\tau_\theta^{(2,n)}), \tag{6}$$

and the Higgs field by

$$\Phi=\eta(\Phi_1\tau_r^{(2,n)}+\Phi_2\tau_\theta^{(2,n)}) \ . \tag{7}$$

All functions H_1, H_2, H_3, H_4, Φ_1, and Φ_2 depend on (r,θ) or equivalently on ($\rho=r\sin\theta$, $z=r\cos\theta$), with the su(2) matrices $\tau_r^{(2,n)}$, $\tau_\theta^{(2,n)}$, and $\tau_\varphi^{(n)}$ defined in terms of the Pauli matrices τ_1,τ_2,τ_3 as

$$\begin{aligned}
\tau_r^{(2,n)}&=\sin 2\theta(\cos n\varphi\tau_1+\sin n\varphi\tau_2)+\cos 2\theta\tau_3 \ , \\
\tau_\theta^{(2,n)}&=\cos 2\theta(\cos n\varphi\ \tau_1+\sin n\varphi\ \tau_2)-\sin 2\theta\ \tau_3 \ , \\
\tau_\varphi^{(n)}&=-\sin n\varphi\ \tau_1+\cos n\varphi\ \tau_2 \ ,
\end{aligned} \tag{8}$$

and for later convenience we define

$$\tau_\rho^{(n)}=\cos n\varphi\ \tau_1+\sin n\varphi\ \tau_2 \ . \tag{9}$$

Note that the dependence on the vorticity n is encoded through $\tau_r^{(2,n)}$ and $\tau_\theta^{(2,n)}$, and of course $\tau_\rho^{(n)}$.

We change to dimensionless coordinates, Higgs field, and coupling parameters by rescaling

$$r\to\frac{r}{g\eta} \ , \quad \Phi\to\eta\Phi \ , \quad \kappa\to\frac{\kappa}{g^2\eta^4} \ , \quad \lambda\to\frac{\lambda}{g^2} \ ,$$

respectively. Then this ansatz leads to the field strength tensor

$$F_{r\theta}=-\frac{1}{2r}(\partial_\theta H_1+2r\partial_r H_2)\tau_\varphi^{(n)} \ ,$$

$$\begin{aligned}
F_{r\varphi}=\frac{n}{2r}\{&(\sin 2\theta H_1-2\sin\theta H_1(1-H_4)-\sin\theta r\partial_r H_3)\tau_r^{(2,n)} \\
&+(\cos 2\theta H_1+2\sin\theta H_1H_3+2\sin\theta r\partial_r H_4)\tau_\theta^{(2,n)}\},
\end{aligned} \tag{10}$$

$$F_{\theta\varphi}=-\frac{n}{2}\{(2\sin 2\theta(H_2-1)+2\cos\theta H_3-2\sin\theta H_2(1-H_4)+2\sin\theta\partial_\theta H_3)\tau_r^{(2,n)}$$
$$+(2\cos 2\theta(H_2-1)+2\cos\theta(1-H_4)+2\sin\theta H_2H_3-2\sin\theta\partial_\theta H_4)\tau_\theta^{(2,n)}\}\ ,$$

and the covariant derivative of the Higgs field

$$D_r\Phi=\frac{1}{r}\{(r\partial_r\Phi_1+H_1\Phi_2)\tau_r^{(2,n)}+(r\partial_r\Phi_2-H_1\Phi_1)\tau_\theta^{(2,n)}\}\ ,$$

$$D_\theta\Phi=(\partial_\theta\Phi_1-2H_2\Phi_2)\tau_r^{(2,n)}+(\partial_\theta\Phi_2+2H_2\Phi_1)\tau_\theta^{(2,n)}\ , \tag{11}$$

$$D_\varphi\Phi=n\{(\sin 2\theta-2\sin\theta(1-H_4))\Phi_1+(\cos 2\theta+2\sin\theta H_3)\Phi_2\}\tau_\varphi^{(n)}\ .$$

The dimensionless energy density then becomes

$$\varepsilon=\mathrm{Tr}\left\{\frac{1}{r^2}F_{r\theta}^2+\frac{1}{r^2\sin^2\theta}F_{r\varphi}^2+\frac{1}{r^4\sin^2\theta}F_{\theta\varphi}^2\right\}+\frac{1}{4}\mathrm{Tr}\left\{(D_r\Phi)^2+\frac{1}{r^2}(D_\theta\Phi)^2+\frac{1}{\sin^2\theta r^2}(D_\varphi\Phi)^2\right\}$$
$$-\frac{\kappa}{4}\mathrm{Tr}\left\{\frac{1}{r^2}[D_r\Phi,D_\theta\Phi]^2+\frac{1}{r^2\sin^2\theta}[D_r\Phi,D_\varphi\Phi]^2+\frac{1}{r^4\sin^2\theta}[D_\theta\Phi,D_\varphi\Phi]^2\right\}$$
$$+\lambda((|\Phi|^2-1)^2), \tag{12}$$

where $|\Phi|=\sqrt{\Phi_1^2+\Phi_2^2}$ denotes the modulus of the Higgs field.

For a monopole–antimonopole pair we expect a magnetic dipole field for the asymptotic gauge potential. The dipole moment $C_{\mathbf{m}}$ can be extracted from the gauge field function H_3, in the gauge where the Higgs field approaches asymototically a constant. Like in Ref. 19 we find

$$H_3=\frac{C_{\mathbf{m}}}{r}\sin\theta\ , \tag{13}$$

while all other gauge field functions decay faster.

IV. NUMERICAL RESULTS

As noted in Ref. 19 the ansatz Eqs. (6) and (7) possess a residual $U(1)$ gauge symmetry. To obtain an unique solution we use the gauge fixing condition[19]

$$G_f=\frac{1}{r^2}(r\partial_rH_1-2\partial_\theta H_2)=0\ . \tag{14}$$

The system of partial differential equations is solved numerically subject to the following boundary conditions, which respect finite energy and finite energy density conditions as well as regularity and symmetry requirements. These boundary conditions are at the origin

$$H_1(0,\theta)=H_3(0,\theta)=0\ ,\quad H_2(0,\theta)=H_4(0,\theta)=1\ , \tag{15}$$

$$\sin 2\theta\Phi_1(0,\theta)+\cos 2\theta\Phi_2(0,\theta)=0\ ,\quad \partial_r(\cos 2\theta\Phi_1(0,\theta)-\sin 2\theta\Phi_2(0,\theta))=0\ , \tag{16}$$

at infinity

$$H_1(\infty,\theta)=H_2(\infty,\theta)=0\ ,\quad H_3(\infty,\theta)=\sin\theta\ ,\ (1-H_4(\infty,\theta))=\cos\theta, \tag{17}$$

$$\Phi_1(\infty,\theta)=1\ ,\quad \Phi_2(\infty,\theta)=0\ , \tag{18}$$

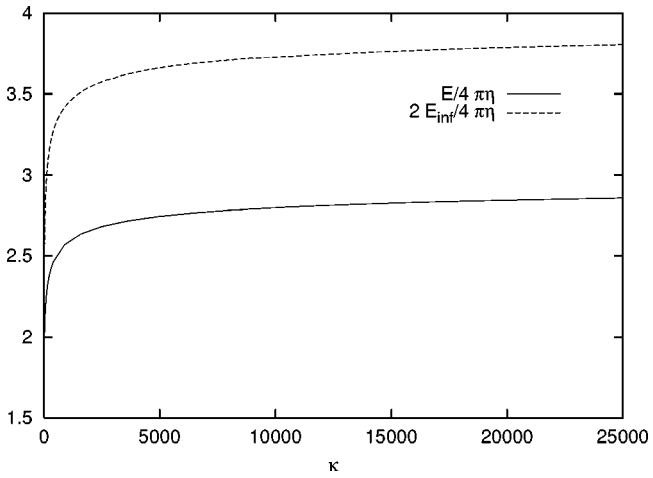

FIG. 1. The energy of the monopole–antimonopole solution (solid line) and the energy of a monopole–antimonopole pair with infinite separation (dashed line), for $n=1$.

and on the z axis

$$H_1(r,\theta=0,\pi)=H_3(r,\theta=0,\pi)=\partial_\theta H_2(r,\theta=0,\pi)=\partial_\theta H_4(r,\theta=0,\pi)=0 \quad , \tag{19}$$

$$\Phi_2(r,\theta=0,\pi)=\partial_\theta \Phi_1(r,\theta=0,\pi)=0 \quad . \tag{20}$$

The numerical calculations were performed with the software package CADSOL, based on the Newton–Raphson method.[23] We have carried out the main part of the numerical analysis for the case of unit vortex number $n=1$ in (8) as in Refs. 18 and 19. In addition we have also studied more briefly, the case of $n=2$.

Starting with the case of vorticity $n=1$, we have constructed monopole–antimonopole solutions for a large range of values of the coupling constant κ. For vanishing coupling constant κ the monopole–antimonopole solution corresponds to a non-Bogomol'nyi solution of the BPS system, for which our results are in good agreement with those of Ref. 19. Our numerical analysis was carried out for the Skyrmed model in the absence of the Higgs potential, namely with $\lambda=0$ in (12). We did however check that the presence of nonvanishing λ does not change the qualitative properties of our solutions. As expected the only effect it has is in the large r asymptotic region, where the modulus of the Higgs field, for example, reaches its asymptotic value faster, namely exponentially.

In Fig. 1 we show the normalized energy of the solitons $E/4\pi\eta$ and the energy $E_{\rm inf}/4\pi\eta$, of the monopole–antimonopole pair with infinite separation corresponding to twice the energy of a

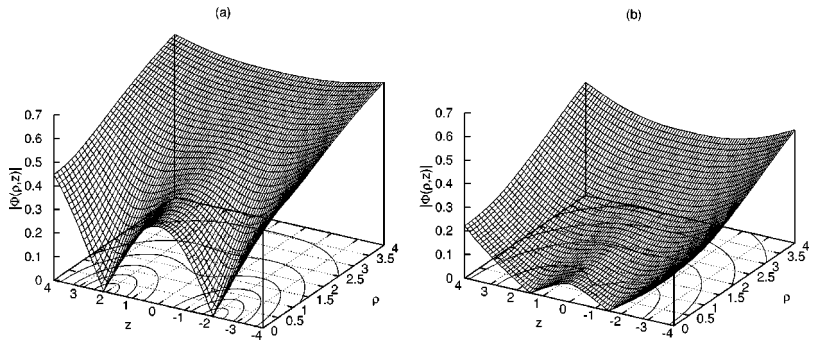

FIG. 2. The modulus of the Higgs field as a function of ρ and z for $\kappa=0$ (a) and $\kappa=100$ (b), for $n=1$.

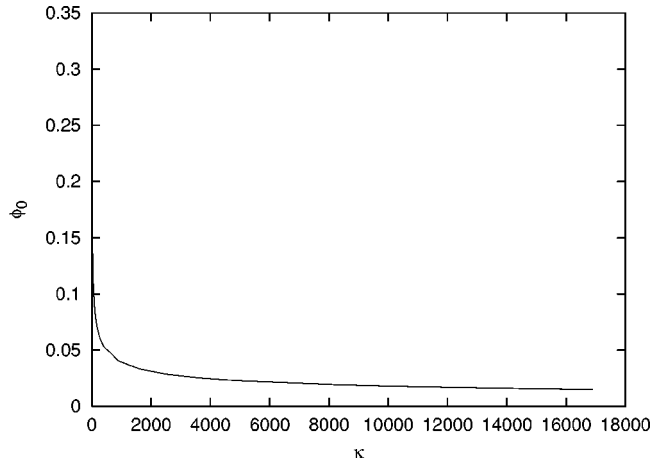

FIG. 3. The modulus of Higgs fields at the origin as a function of κ, for $n=1$.

charge-1 monopole, as functions of the coupling constant κ. As can be seen from Fig. 1 the energy of the monopole–antimonopole solution is less than the energy of a monopole–antimonopole pair with infinite separation for all values of κ.

In Fig. 2 we exhibit the modulus of the Higgs field $|\Phi(\rho,z)|$ as a function of the coordinates $\rho=\sqrt{x^2+y^2}$ and z for $\kappa=0$ and $\kappa=100$. The zeros of $|\Phi(\rho,z)|$ are located on the positive and negative z axis at $\pm z_0 \approx 2.1$ for $\kappa=0$ and at $\pm z_0 \approx 1.5$ for $\kappa=100$. The distance d of the two zeros of the Higgs field decreases monotonically with increasing κ.

Asymptotically $|\Phi(\rho,z)|$ approaches the value 1. But at the origin the value of the modulus of the Higgs field decreases monotonically with increasing κ (see Fig. 3). In the limit $\kappa\to\infty$ $|\phi_0| \approx 0.015$, and we expect the modulus of the Higgs field to be very small for $|z|\leqslant 4$.

In Fig. 4 we show the energy density of the monopole–antimonopole solution as a function of the coordinates $\rho=\sqrt{x^2+y^2}$ and z for $\kappa=0$ and $\kappa=100$. At the locations of the Higgs field the energy density posesses maxima.

For small values of coupling constant κ the equal energy density surfaces near the locations of the zeros of the Higgs field assume a shape close to a sphere, centered at the location of the respective zero [see Fig. 4(a)]. This presents further support for the conclusion that at the two zeros of the Higgs field a monopole and an antimonopole are located, which can be clearly distinguished from each other, and which together form a bound state.

With increasing κ the distance d between the monopole–antimonopole centers becomes smaller tending to a limit as $\kappa\to\infty$. At the same time the spherical equal energy surfaces in Fig. 4(b) become larger, and the equal energy density surfaces assume a shape that looks like the intersection of two spheres [see Fig. 4(b)], thus making it more difficult to distinguish the monopole from the antimonopole. The dependence of the separation length d is given in Table I below as a function of κ.

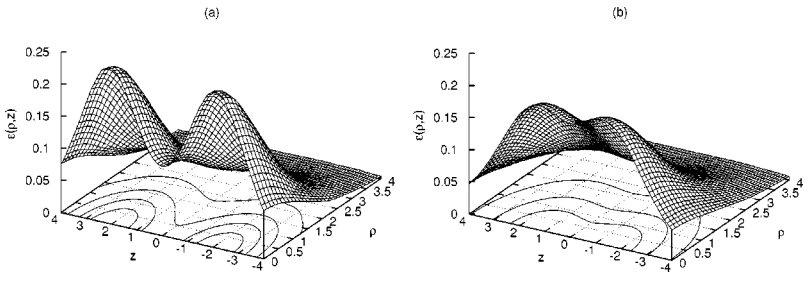

FIG. 4. The dimensionless energy density as a function of ρ and z for $\kappa=0$ (a) and $\kappa=100$ (b), for $n=1$.

TABLE I. Monopole–antimonopole separation d and dipole moment $C_{\mathbf{m}}$ as a functions of κ.

κ	0	9	16	25	36	49	64	100	8100	10 000
d	4.19	3.64	3.49	3.38	3.29	3.21	3.16	3.06	2.54	2.53
$C_{\mathbf{m}}$	2.36	2.27	2.23	2.19	2.15	2.11	2.07	2.02	1.66	1.65

Having exibited the qualitative properties of our *dipole* solutions, we give the values of the dipole moment that we calculated as a function of the coupling constant κ, again in Table I. As expected, with decreasing d the dipole moment $C_{\mathbf{m}}$ also decreases.

Finally we constructed solutions for the case of vorticity $n=2$. Most of the qualitative properties of these solutions do not differ from those of the $n=1$ case just described. The most noticeable quantitative difference concerns the value of the modulus of the Higgs field at the origin, analogous with Figs. 1(a) and 1(b). We do not exhibit here these analogous figures, but simply note that the the moduli of the Higgs fields at the origin are *smaller* than those in Figs. 1(a) and 1(b) for the same values of the coupling constant κ.

Another difference, qualitative though expected, is that the surfaces of equal energy are not spheres centered on the z axis but describe rings or tori around it. This is exhibited in Figs. 5(a) and 5(b), analogously with Figs. 4(a) and 4(b).

Again, as κ grows, the distiction between the monopole and antimonopole rings gets blurred.

V. SUMMARY

We have contructed axially symmetric solutions to a simple SU(2) Skyrmed YM–Higgs model, with such boundary conditions that result in the description of a monopole–antimonopole pair with zero magnetic charge. These solutions have lower mass than two infinitely separated charge-1 monopoles, and since they are characterized by zero magnetic charge, are not topologically stable.

When the usual boundary conditions are imposed, the Skyrmed SU(2) YM–Higgs model employed here supports mutually attractive monopoles, including axially symmetric charge-2 monopoles. This is in contrast to the Georgi–Glashow model studied in Ref. 19 where due to the Higgs potential the monopoles are mutually repulsive.[11] Nevertheless, the qualitative features of the monopole–antimonopole solutions in the two models are similar. Increasing the Skyrme coupling constant κ in the present model results in the approaching of the monopole and the antimonopole centers down to a limiting value 2.53 as $\kappa\to\infty$, just as it does to the limiting value 3.0 as $\lambda\to\infty$ in the Georgi–Glashow model λ being the Higgs coupling constant. (Our results are for $\lambda=0$.)

Another parallel property in the two models is the changing dipole moment with respect to the change in the Skyrme coupling constant κ and the Higgs coupling constant λ, in the two models,

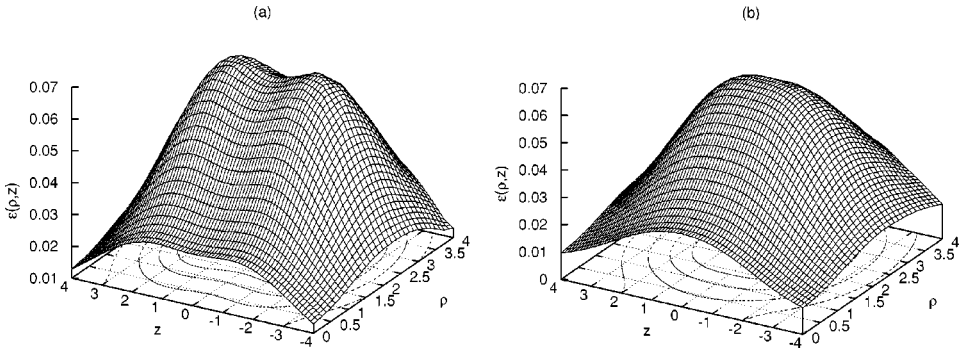

FIG. 5. The dimensionless energy density as a function of ρ and z for $\kappa=0$ (a) and $\kappa=100$ (b), for $n=2$.

respectively. Specifically in the present model the magnetic moment decreases with increasing κ, with limiting value 1.64, while in the Georgi–Glashow model it decreases with increasing λ, with limiting value 1.55, in the same units.

Finally, we also studied the case of a zero charge monopole which has vortex number $n=2$ rather than $n=1$. The qualitative properties again stay unchanged. The most noticeable quantitative difference of the $n=2$ solution is that the value of the modulus of the Higgs field at the origin is smaller than that of the $n=1$ solution, for the same value of κ, and the distance between the two centers is also smaller. For example at $\kappa=25$ the distance $d=3.38$ for the $n=1$ solutions while that for the $n=2$ is $d=1.33$.

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The Weyl–Lanczos relations and the four-dimensional Lanczos tensor wave equation and some symmetry generators

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We examine symmetry generators for exterior differential systems and for systems of partial differential equations and apply the Cartan theory of exterior differential systems to the Weyl–Lanczos equations and to the Lanczos wave equation in four dimensions. We look at a number of examples of symmetries for the Weyl–Lanczos equations in four dimensions and give examples of isovectors when the solution manifold is the Schwarzschild, Kasner or Gödel space–time. Solutions of the Weyl–Lanczos system are automatically solutions of the Lanczos wave equation. We give examples of symmetry generators for the Lanczos wave equation and find that they are not automatically symmetry generators for the Weyl–Lanczos equations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1625076]

I. INTRODUCTION

A. The Weyl–Lanczos equations and the Lanczos tensor wave equation in four dimensions

Lanczos[13] generated the space–time Weyl conformal tensor C_{abcd} from a tensor potential L_{abc} by covariant differentiation and it is given by

$$C_{abcd}=L_{[ab][c;d]}+L_{[cd][a;b]}-{}^{*}L^{*}_{[ab][c;d]}-{}^{*}L^{*}_{[cd][a;b]}, \tag{1}$$

where ";" denotes covariant differentiation. The index symmetries of the Lanczos tensor L_{abc} have to match the symmetries of (1) and so it is usual to add to the property

$$L_{abc}=L_{[ab]c}, \tag{2}$$

the antisymmetric condition

$$L_{[abc]}=0, \tag{3}$$

and the trace-free (gauge) condition

$$L_{as}{}^{s}=0. \tag{4}$$

The space–time Weyl–Lanczos equations (1) can also be expressed as

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}+g_{bc}L_{(ad)}+g_{ad}L_{(bc)}-g_{bd}L_{(ac)}-g_{ac}L_{(bd)} + \tfrac{2}{3}L^{ms}{}_{m;s}(g_{ac}g_{bd}-g_{ad}g_{bc}), \tag{5}$$

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where $L_{ad}=L_{asd;}{}^{s}-L_{as}{}^{s}{}_{;d}$ and round brackets indicate symmetrization. We call (5) the **Weyl–Lanczos equations**. The algebraic equations (2)–(4) leave us with only 16 independent components for the L_{abc}. If we then introduce the differential gauge condition

$$L_{abs;}{}^{s}=0, \tag{6}$$

which we will denote by $f_{ab}^{(DG)}=L_{abs;}{}^{s}=0$, we can simplify (5) considerably to get

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}-g_{bc}L_{sad;}{}^{s}-g_{ad}L_{sbc;}{}^{s}+g_{bd}L_{sac;}{}^{s}+g_{ac}L_{sbd;}{}^{s}. \tag{7}$$

The Weyl–Lanczos equations in solved form, which we denote by $f_{abcd}^{(W)}=0$, are then given by

$$f_{abcd}^{(W)}=C_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}+g_{bc}L_{sad;}{}^{s}+g_{ad}L_{sbc;}{}^{s}-g_{bd}L_{sac;}{}^{s}-g_{ac}L_{sbd;}{}^{s}=0. \tag{8}$$

Theoretically, we could completely solve the six differential gauge conditions (6) for six further components L_{abc} and have only ten L_{abc} components for ten independent space–time Weyl–Lanczos equations. But here, we examine the most general situation first. We note that Eqs. (6) and (7) constitute a system of linear first-order partial differential equations in four dimensions which can easily be rewritten as an exterior differential system (EDS) in involution as was shown in Ref. 1. Using the Janet–Riquier theory we could confirm these results.[9] This theory only applies in four dimensions as the Weyl–Lanczos problem in two and three dimensions does not exist and for five and maybe higher dimensions, we expect extra conditions to apply as we will point out in later papers.

From the Weyl–Lanczos problem it is possible to generate a tensor wave equation for the (space–time) Lanczos potential from which the Penrose wave equation for the Weyl tensor C_{abcd} can be derived.[8,18] Arising from the Weyl–Lanczos equations is the tensor wave equation

$$\Box L_{abc}+2R_{c}{}^{s}L_{abs}-R_{a}{}^{s}L_{bcs}-R_{b}{}^{s}L_{cas}-g_{ac}R^{ls}L_{lbs}+g_{bc}R^{ls}L_{las}-\tfrac{1}{2}RL_{abc}=J_{abc}, \tag{9}$$

where

$$J_{abc}=\tfrac{1}{2}R_{c[a;b]}-\tfrac{1}{6}g_{c[a}R_{;b]} \tag{10}$$

and

$$\Box L_{abc}=g^{sm}L_{abc;sm}. \tag{11}$$

A new comprehensive survey of the Lanczos tensor also using spinors can be found in Ref. 16. A standard derivation of Penrose's wave equation for the space–time Weyl tensor

$$\Box C_{abcd}-C_{absm}C_{cd}{}^{sm}-4C_{asm[c}C_{d]}{}^{sm}{}_{b}+\frac{R}{4}C_{abcd}=J_{[ab][c;d]}+J_{[cd][a;b]}-{}^{*}J^{*}_{[ab][c;d]}-{}^{*}J^{*}_{[cd][a;b]} \tag{12}$$

is given in Ref. 18. The Lanczos wave equation in solved form can be written as

$$\mathcal{W}_{abc}=\Box L_{abc}+2R_{c}{}^{s}L_{abs}-R_{a}{}^{s}L_{bcs}-R_{b}{}^{s}L_{cas}-g_{ac}R^{ls}L_{lbs}+g_{bc}R^{ls}L_{las}-\tfrac{1}{2}RL_{abc}-J_{abc}=0. \tag{13}$$

It was shown in Refs. 6 and 9 that the Lanczos tensor wave equation in four dimensions is also a system in involution. Here, we are going to look at solutions with symmetries and find some symmetry generators for both the Weyl–Lanczos equations and the Lanczos wave equation in four dimensions. The knowledge of symmetries of a system of partial differential equations can help in finding further solutions of its equations. Before suggesting *Ansätze* for symmetry generators, we introduce exterior differential systems (EDS) and isovectors.

B. Historical comments

Over many papers culminating in 1962 Lanczos[13] explored the analogy between electromagnetism as a field theory and general relativity. Thereby the following correspondences were generally established

$$\textit{field}\ \ F_{ab}\leftrightarrow C_{abcd},$$

$$\textit{potential}\ \ A_a\leftrightarrow L_{abc},$$

$$\textit{current}\ \ J_a\leftrightarrow J_{abc}.$$

In the 1962 paper[13] the gravitational analog of the potential field relations

$$F_{ab}=A_{a;b}-A_{b;a} \tag{14}$$

was found to be given by (1) with L_{abc} satisfying (2)–(4) in order to make L_{abc} algebraically irreducible. Further, we have an electromagnetic gauge condition $A^s{}_{;s}=0$ and analogously the differential gauge condition (6) for L_{abc}. The electric current relation J^a satisfies

$$J^a=F^{ab}{}_{;b}, \tag{15}$$

which is equivalent to a wave equation for the potential A_a. Of course, it is the vanishing of the covariant derivatives of the electromagnetic gauge conditions that permit the causal propagation of A_a and so analogously the wave equation (9) for the Lanczos tensor propagates L_{abc} causally because the covariant derivatives of the gauge conditions (6) have been removed. In the same way the Schouten tensor J_{abc} acts as a source for the Lanczos potential wave equation (9). From the potential wave equation for A_a it is well known that we can obtain a field wave equation for the field F_{ab}. The wave equation (9) for the Lanczos potential can also generate the corresponding field wave equation (12). The interest in the study of the Lanczos potential and its wave equation is based on these analogies between electromagnetism and gravity. Fuller details are given in Ref. 8.

II. LANCZOS POTENTIALS AND ISOVECTORS

An **exterior differential system** (EDS) Σ over a formal N-dimensional manifold $\mathcal{M}$ is given by a set of differential forms $\{\alpha^{(1)}_{i_1},\ \alpha^{(2)}_{i_2},\ldots,\alpha^{(p)}_{i_p}\}$ with

$$\begin{aligned}
&\alpha^{(0)}_{i_0}\quad \textit{zero-forms},\quad 1\leqslant i_0\leqslant k_0,\\
&\alpha^{(1)}_{i_1}\quad \textit{one-forms},\quad 1\leqslant i_1\leqslant k_1,\\
&\alpha^{(2)}_{i_2}\quad \textit{two-forms},\quad 1\leqslant i_2\leqslant k_2,\\
&\qquad\vdots\quad\ \vdots\quad\ \vdots\\
&\alpha^{(p)}_{i_p}\quad \textit{p-forms},\quad 1\leqslant i_p\leqslant k_p,
\end{aligned}$$

where the $k_0,k_1,\ldots,k_p$ give the number of zero-forms, one-forms and so on in the EDS. A **Pfaffian system** $\mathcal{P}$ is a special case of an EDS containing only zero-forms and one-forms. A good account of the theory of EDS can be found in Refs. 4, 5, 14, and 25.

We will assume that we are working on a formal manifold $\mathcal{M}$ with dimension $N=84$ with local jet coordinates (x^a,L_{bcd},P_{efgh}), where we have 4 independent variables x^e, 16 variables L_{abc} and 64 P_{abcd} at our disposal so that $N=4+16+64=84$ on the first-order jet bundle $\mathcal{J}^1(\mathbb{R}^4,\mathbb{R}^{16})$. An introduction to jet bundles can be found in Ref. 19. When the P_{abcd} are projected

onto the space–time manifold M they become the partial derivatives $P_{abcd}=\partial L_{abc}/\partial x^d$. We can write the Weyl–Lanczos equations as an EDS Σ with independence condition Ω, which is given by $\Omega=dx^1\wedge dx^2\wedge dx^3\wedge dx^4\neq 0$ when local coordinates (x^1,x^2,x^3,x^4) are used. The EDS is given by

$$df^{(W)}_{abcd}=d(L_{[ab][c;d]})+d(L_{[cd][a;b]})-d(*L^{*}_{[ab][c;d]})-d(*L^{*}_{[cd][a;b]}),$$

$$df^{(DG)}_{ab}=d(L_{abs;}{}^{s}), \tag{16}$$

$$K_{abc}=dL_{abc}-P_{abce}dx^e,$$

where details can be found in Refs. 6 and 9. Solutions to the Weyl–Lanczos equations then correspond to integral manifolds on which all forms in (16) vanish when restricted to submanifolds with $f^{(W)}_{abcd}=0, f^{(DG)}_{ab}=0$. Tangent spaces to such integral manifolds are usually spanned by four **Vessiot vector fields** which we will denote by $V^{(1)},\ldots,V^{(4)}$. A Vessiot vector field V is defined as an annihilator of all one-forms in a Pfaffian system. This means that $V\in\mathcal{D}=\mathcal{P}^{\perp}$ and we can write in local components

$$V=V^e\frac{\partial}{\partial x^e}+V^{abc}\frac{\partial}{\partial L_{abc}}+V^{abcd}\frac{\partial}{\partial P_{abcd}}+V^{abcde}\frac{\partial}{\partial S_{abcde}}.$$

If we consider the Lanczos wave equation, we need to incorporate a further 160 second-order jet variables S_{abcde} so that our jet bundle is given by $\mathcal{J}^2(\mathbb{R}^4,\mathbb{R}^{16})$ with local coordinates $(x^a,L_{bcd},P_{efgh},S_{ijklm})$ and formal dimension $N=4+16+64+160=244$. The S_{abcde} become the partial derivatives $S_{abcde}=\partial^2 L_{abc}/\partial x^d\partial x^e$ when projected onto the space–time manifold M. The Pfaffian system for the Lanczos wave equation is given by

$$d\mathcal{W}_{abc}=d(f^{(W)}_{abcs}{}^{;s}),$$

$$K_{abc}=dL_{abc}-P_{abce}dx^e, \tag{17}$$

$$K_{abcd}=dP_{abcd}-S_{abcde}dx^e,$$

and the details can be found in Refs. 6 and 9. Because of the way the Lanczos wave equation was derived from the Weyl–Lanczos equations, any solutions to the Weyl–Lanczos equations are automatically solutions to the Lanczos wave equation.[7,8]

One can now examine whether such an EDS Σ or a Pfaffian system $\mathcal{P}$ possesses symmetries. The infinitesimal generators of the symmetries of an exterior differential system (EDS) Σ or of a Pfaffian system $\mathcal{P}$ are called *isovectors*. Isovectors X for either of the above systems have to make the Lie derivatives with respect to X of all one-forms involved in the Pfaffian system be linear combinations of the one-forms of the corresponding Pfaffian system itself. They are defined as follows:

Definition 1: Isovectors. X is an isovector of the EDS Σ means that the set of all Lie derivatives of the differential forms in Σ with respect to the vector field X are also differential forms in Σ: $\pounds_X\Sigma\subset\Sigma$. Dually, X is an isovector of the vector field system $\mathcal{V}$ means that $\pounds_X\mathcal{V}\subset\mathcal{V}$.

In order to check whether a given vector field X is an isovector, it is useful to apply the H. Cartan formula

$$\pounds_X\alpha=X\rfloor d\alpha+d(X\rfloor\alpha), \tag{18}$$

where $\rfloor$ denotes the inner product operator and α is any differential form in the EDS Σ. If we specialize Σ to be a Pfaffian system $\mathcal{P}$, then a **subset of** the set of isovectors is given by the set of **Cauchy characteristic vector fields** X which are given by Ref. 2.

Definition 2: X is a Cauchy characteristic vector field of a vector field system $\mathcal{D}$, where we normally have $\mathcal{D}=\mathcal{P}^{\perp}$ for a given Pfaffian system $\mathcal{P}$, means that

$$X\rfloor\alpha=0\,,\quad X\rfloor d\alpha=0\ (mod\ \mathcal{P}),$$

for all one-forms α in $\mathcal{P}$, where $\rfloor$ denotes the inner product operator.

We can also write our equations as systems of partial differential equations (PDEs) directly and find **symmetry generators** for these systems, where details on this approach can be found in Refs. 3, 17, and 22. A generator $Y^{(P)}$ of a **point symmetry** for the Weyl–Lanczos equations is necessarily of the form

$$Y^{(P)}=Y^{f}(x^{e},L_{a'b'c'})\frac{\partial}{\partial x^{f}}+Y_{abc}(x^{e},L_{a'b'c'})\frac{\partial}{\partial L_{abc}}+Y_{abcd}\frac{\partial}{\partial P_{abcd}} \tag{19}$$

with

$$Y_{abcd}=\frac{\partial Y_{abc}}{\partial x^{d}}+P_{a'b'c'd}\frac{\partial Y_{abc}}{\partial L_{a'b'c'}}-P_{abcf}\frac{\partial Y^{f}}{\partial x^{d}}-P_{a'b'c'd}P_{abcf}\frac{\partial Y^{f}}{\partial L_{a'b'c'}}. \tag{20}$$

More generally, we can look at generators $Z^{(C)}$ of **contact symmetries** which are of the form

$$Z^{(C)}=Z^{f}(x^{e},L_{a'b'c'},P_{a'b'c'd'})\frac{\partial}{\partial x^{f}}+Z_{abc}(x^{e},L_{a'b'c'},P_{a'b'c'd'})\frac{\partial}{\partial L_{abc}}+Z_{abcd}\frac{\partial}{\partial P_{abcd}}, \tag{21}$$

but now with

$$\begin{aligned}Z_{abcd}=&\frac{\partial Z_{abc}}{\partial x^{d}}+P_{a'b'c'd}\frac{\partial Z_{abc}}{\partial L_{a'b'c'}}-P_{abcf}\frac{\partial Z^{f}}{\partial x^{d}}-P_{a'b'c'd}P_{abcf}\frac{\partial Z^{f}}{\partial L_{a'b'c'}}+S_{a'b'c'dk}\frac{\partial Z_{abc}}{\partial P_{a'b'c'k}}\\&-P_{abcf}S_{a'b'c'dk}\frac{\partial Z^{f}}{\partial P_{a'b'c'k}}.\end{aligned} \tag{22}$$

The conditions for either vector fields $Y^{(P)}$ or $Z^{(C)}$ to be symmetry generators are then given by

$$\begin{aligned}Y^{(P)}f^{(W)}_{abcd}&\equiv 0\quad \mathrm{mod}\ (f^{(W)}_{abcd})\,,\\ Z^{(C)}f^{(W)}_{abcd}&\equiv 0\quad \mathrm{mod}\ (f^{(W)}_{abcd})\,,\end{aligned} \tag{23}$$

where $f^{(W)}_{abcd}$ is given by (8). If we are determining symmetry generators $Y^{(P)}$ or $Z^{(C)}$ for the Lanczos wave equation, then they have to satisfy

$$\begin{aligned}Y^{(P)}\mathcal{W}_{abc}&\equiv 0\quad \mathrm{mod}(\mathcal{W}_{abc})\,,\\ Z^{(C)}\mathcal{W}_{abc}&\equiv 0\quad \mathrm{mod}(\mathcal{W}_{abc})\,,\end{aligned} \tag{24}$$

where $\mathcal{W}_{abc}$ is given by (13), and the corresponding second-order components Y_{abcde}, Z_{abcde} have to obey conditions which can be found in Refs. 3 and 22. The equations (20) and (22) respectively for the components Y_{abcd}, Z_{abcd}, and, if we are looking at second-order equations, the corresponding equations for the Y_{abcde}, Z_{abcde} as well, ensure that we obtain a contact structure on $\mathcal{J}^{1}(\mathbb{R}^{4},\mathbb{R}^{16})$ and on $\mathcal{J}^{2}(\mathbb{R}^{4},\mathbb{R}^{16})$, respectively.

Now, we wish to consider a number of candidates for isovectors for the Weyl–Lanczos equations and then for the Lanczos wave equation. In Ref. 9 it is shown that the Weyl–Lanczos equations and the Lanczos wave equation possess no Cauchy characteristic vector fields which means that we have to look for isovectors which are not Cauchy characteristic vector fields. We do

not attempt to give a complete discussion of the symmetry groups of the Weyl–Lanczos equations and of the Lanczos wave equation here but to consider some examples. Consider the following *Ansätze*:

$$(1) \quad Y = c^e \frac{\partial}{\partial x^e},$$

$$(2) \quad Y = c_{abc} \frac{\partial}{\partial L_{abc}}, \tag{25}$$

$$(3) \quad Y = Y_{abc}(x^f) \frac{\partial}{\partial L_{abc}} + Y_{abc,d}(x^f) \frac{\partial}{\partial P_{abcd}},$$

where c^e and c_{abc} are arbitrary constants. The reader should note that the coefficients in types 1 and 2 are only constants. This makes type 2 a special case of type 3 when the Y_{abc} are constants. The presence of a nonvanishing coefficient for $\partial/\partial P_{abcd}$ in type 3 forces both its coefficients to have the form given in (25) if Eqs. (20) or (22) are to hold, respectively.

We know that Killing vector fields (KVs) are isometries of our underlying space–time manifold and symmetry generators for Einstein's field equations.[22] KVs are good candidates for symmetry generators because for any KV ξ we always have $\pounds_\xi \nabla = \nabla \pounds_\xi$, where we used ∇ here to indicate covariant differentiation. If we look at the Weyl–Lanczos equations (7) and the differential gauge condition (6), we see that they consist of terms all involving covariant derivatives. For KVs we know that $\pounds_\xi C_{abcd} = 0$. It is obvious that particular KVs present examples of symmetry generators of type 1 for the Weyl–Lanczos equations as well as for the Lanczos wave equation. It is well known that a KV ξ is always a symmetry generator when it is based on *ignorable coordinates*. Such ξ generate isovectors of type 1 for the Weyl–Lanczos equations and for the Lanczos wave equation.

III. EXAMPLES OF SOLUTIONS AND ISOVECTORS FOR THE WEYL–LANCZOS EQUATIONS

First, we look at those solutions, where we *impose* $\pounds_\xi L_{abc} = 0$ for some or for all KVs of a given space–time. Then, we discuss some isovectors of type 3 for Kasner, Schwarzschild and Gödel space–times and it will be shown that no isovectors of type 2 exist for these space–times.

A. Kasner space–time

A line element for Kasner space–time can be given locally as

$$ds^2 = dt^2 - t^{2p_1} dx^2 - t^{2p_2} dy^2 - t^{2p_3} dz^2 \tag{26}$$

with $p_1 + p_2 + p_3 = 1$ and $p_1^2 + p_2^2 + p_3^2 = 1$. We look at those solutions $L_{abc}(t)$ which fulfill the conditions $\pounds_\xi L_{abc} := 0$ for **all** 3 spatial KVs $(\partial/\partial x, \partial/\partial y, \partial/\partial z)$ which the Kasner space–time admits. The only nonvanishing independent components of the Weyl tensor are C_{txtx}, C_{tyty}. Using $L_{txx} = t^{2p_1}(t^{-2p_2} L_{tyy} + t^{-2p_3} L_{tzz})$ resulting from solving (4) for the component L_{txx}, a solution for the components L_{abc} is as given in Ref. 7,

$$\begin{aligned} L_{txx} &= \tfrac{1}{3}(p_1 - \tfrac{1}{3}) t^{2p_1 - 1}, \\ L_{tyy} &= \tfrac{1}{3}(p_2 - \tfrac{1}{3}) t^{2p_2 - 1}, \\ L_{tzz} &= \tfrac{1}{3}(p_3 - \tfrac{1}{3}) t^{2p_3 - 1}, \end{aligned} \tag{27}$$

while all other components are identically zero. This solution (27) corresponds to a particular integral manifold of which the tangent spaces are spanned by the four Vessiot vector fields

$$V^{(1)}=\frac{\partial}{\partial t}+P_{tyyt}\frac{\partial}{\partial L_{tyy}}+P_{tzzt}\frac{\partial}{\partial L_{tzz}}+V^{(1)}_{tyyt}\frac{\partial}{\partial P_{tyyt}}+V^{(1)}_{tzzt}\frac{\partial}{\partial P_{tzzt}},$$

$$V^{(2)}=\frac{\partial}{\partial x},$$

$$V^{(3)}=\frac{\partial}{\partial y},\tag{28}$$

$$V^{(4)}=\frac{\partial}{\partial z}.$$

The $V^{(1)}_{tyyt}$ and $V^{(1)}_{tzzt}$ are given by

$$V^{(1)}_{tyyt}=t^{-1}(p_2+p_3)P_{tyyt}-t^{2p_2-2p_3-1}(p_1-p_3)P_{tzzt}-\frac{\partial f^{(W)}_{tyty}}{\partial t},$$

$$V^{(1)}_{tzzt}=t^{2p_3-2p_2-1}(p_2-p_1)P_{tyyt}+t^{-1}(p_2+p_3)P_{tzzt}+t^{2(p_3-p_1)}\cdot\left(\frac{\partial f^{(W)}_{txtx}}{\partial t}+\frac{\partial f^{(W)}_{tyty}}{\partial t}\right),\tag{29}$$

where the $f^{(W)}_{abcd}$ are given by (8). Solution (27) is not the most general solution as $V^{(1)},\ldots,V^{(4)}$ do not span the most general integral elements but correspond to a particular solution of the general solution. If a system is not in involution, singular solutions can still exist. A solution is a **singular solution** to the original system if for its characters $s_i(\mathbf{x})$ we have

$$s_i(\mathbf{x})<s_i \text{ at any point } \mathbf{x}\tag{30}$$

of the space–time manifold so that they do not adopt their maximal values. The maximal values for the $s_i(\mathbf{x})$ were computed in Refs. 6 and 9 which are given by $(s_0,s_1,s_2,s_3,s_4)=(32,16,16,16,0)$, but when restricted to the submanifold $f^{(W)}_{abcd}=0, f^{(DG)}_{ab}=0$ we get $s_0=16$ while the other characters remain unchanged $s_1=s_2=s_3=16, s_4=0$. We can find a modified Pfaffian system for which the solution (27) turns into the general solution when we look at the integral manifold characterized by

$$df^{(W)}_{abcd}(V^{(i)})=0,$$

$$df^{(DG)}_{ab}(V^{(i)})=0,$$

$$K_{abc}(V^{(i)})=0,$$

$$dP_{abcx}(V^{(i)})=0,\tag{31}$$

$$dP_{abcy}(V^{(i)})=0,$$

$$dP_{abcz}(V^{(i)})=0,$$

where $i=1,2,3,4$. For this Pfaffian system, the $V^{(1)},\ldots,V^{(4)}$ of (28) span a general integral element. The solution (27) now corresponds to the submanifold of (31) on which $f^{(W)}_{abcd}=0$, $f^{(DG)}_{ab}=0$. For our modified Pfaffian system leading to (31) the **only** nonvanishing Cartan character is s_0 which is simply the number of remaining independent one-forms. This is because

$$dK_{abc}(V^{(i)},V^{(j)})=0$$

vanishes identically for any of the above $V^{(i)},V^{(j)}$ in (28). Therefore, the modified system corresponding to (31) consists of a *complete system* to which the Frobenius theorem applies. However, the original system given only by $df^{(W)}_{abcd},df^{(DG)}_{ab},K_{abc}$ does **not** form a complete system.

We can also obtain this result using Janet–Riquier theory. Details of this theory, which involves the *symbol* $\mathcal{M}_q$ of a given system of PDEs of order q denoted by $\mathcal{R}_q$, can be found in Refs. 6, 12, 20, and 21. There, we obtain that the quantities $\alpha^{(k)}_q$ correspond to the Cartan characters s_k, $k=1,2,3,4$, in this case and these are also identically zero for a modified system given by

$$\begin{aligned} f^{(W)}_{abcd}&=0 \quad (1)-(10),\\ f^{(DG)}_{ab}&=0 \quad (11)-(16),\\ P_{abcx}&=0 \quad (17)-(32),\\ P_{abcy}&=0 \quad (33)-(48),\\ P_{abcz}&=0 \quad (49)-(64). \end{aligned} \tag{32}$$

It is easy to show that this modified system (32) consists of a complete system with $\alpha^{(1)}_1=\alpha^{(2)}_1=\alpha^{(3)}_1=\alpha^{(4)}_1=0$.

Lastly, we wish to determine some isovectors for Kasner space–time. A trivial calculation shows that no isovectors of type 2 exist. Apart from the 3 isovectors $\partial/\partial x,\partial/\partial y,\partial/\partial z$ of type 1, we look for isovectors of type 3 of the form

$$Y=Y_{abc}(x^e)\frac{\partial}{\partial L_{abc}}+Y_{abc,d}(x^e)\frac{\partial}{\partial P_{abcd}}. \tag{33}$$

Using algebraic computing as described in detail in Ref. 9, we see that the Weyl–Lanczos equations together with the differential gauge condition (6) can be divided into eight groups of two equations each, where each group only involves two distinct components of the L_{abc}. This leads to the groups:

1: L_{tyy} and L_{tzz} in equations $f^{(W)}_{txtx},f^{(W)}_{tyty}$;

2: L_{txy} and L_{tyx} in equations $f^{(W)}_{txty},f^{(DG)}_{xy}$;

3: L_{xyx} and L_{yzz} in equations $f^{(W)}_{txxy},f^{(DG)}_{ty}$;

4: L_{xyy} and L_{xzz} in equations $f^{(W)}_{tyxy},f^{(DG)}_{tx}$;

5: L_{txz} and L_{tzx} in equations $f^{(W)}_{txtz},f^{(DG)}_{xz}$;

6: L_{tyz} and L_{tzy} in equations $f^{(W)}_{tytz},f^{(DG)}_{yz}$;

7: L_{xzx} and L_{yzy} in equations $f^{(W)}_{txxz},f^{(DG)}_{tz}$;

8: L_{xyz} and L_{xzy} in equations $f^{(W)}_{txyz},f^{(W)}_{tyxz}$.

Solving the determining equations for such isovectors for each group separately leads to 16 distinct isovectors already given in Ref. 9. Here, we are only interested in group 1 for which we obtain the isovector

$$\begin{aligned} Y=t^{(\alpha-2p_3)}\frac{\partial}{\partial L_{tyy}}+\frac{(p_3+2-p_2-\alpha)}{p_2-1}t^{(\alpha-2p_2)}\frac{\partial}{\partial L_{tzz}}+(\alpha-2p_3)t^{(\alpha-2p_3-1)}\frac{\partial}{\partial P_{tyyt}}\\ +(\alpha-2p_2)\frac{(p_3+2-p_2-\alpha)}{p_2-1}t^{(\alpha-2p_2-1)}\frac{\partial}{\partial P_{tzzt}}, \end{aligned} \tag{34}$$

where α adopts either of the values

$$\alpha=(2p_2+3p_3)\pm(3p_2^2+4p_3^2+9p_2p_3-3p_2-5p_3+1)^{1/2}. \tag{35}$$

The α in (35) are solutions of the quadratic equation

$$\alpha^2-2(2p_2+3p_3)\alpha+C=0, \tag{36}$$

where

$$C=p_2^2+3(p_2p_3+p_2)+5(p_3^2+p_3)-1. \tag{37}$$

They are real only for particular choices of p_1,p_2,p_3. This isovector generates an exchange amongst the components L_{txx},L_{tyy},L_{tzz} and their derivatives for solutions of the Weyl–Lanczos equations of the form $L_{txx}(t),L_{tyy}(t),L_{tzz}(t)$.

B. Schwarzschild space–time

Next, we look at Schwarzschild space–time for which the line element in curvature coordinates is

$$ds^2=\left(1-\frac{2m}{r}\right)dt^2-\left(1-\frac{2m}{r}\right)^{-1}dr^2-r^2d\theta^2-r^2\sin^2(\theta)d\phi^2. \tag{38}$$

Schwarzschild space–time admits four well known Killing vector fields;[24] two of them are based on ignorable coordinates. When we impose the cyclic, trace-free and differential gauge conditions (3), (4) and (6) as well as $\pounds_\xi L_{abc}:=0$ for all four KVs ξ, we obtain the well known solution given in Ref. 24. It is given by

$$\begin{aligned} L_{r\theta\theta}&=-\frac{rm}{3(r-2m)},\\ L_{r\phi\phi}&=-\frac{rm}{3(r-2m)}\sin^2(\theta), \end{aligned} \tag{39}$$

where all other components can be chosen to be identically zero. The four Vessiot vector fields spanning the integral elements $(E^4)_{\mathbf{x}}$ of the solution manifold corresponding to (38) can be given as

$$\begin{aligned} V^{(1)}&=\frac{\partial}{\partial t},\\ V^{(2)}&=\frac{\partial}{\partial r}+(P_{abcr}+P_{abc\theta})\frac{\partial}{\partial L_{abc}}+V^{(r)}_{abcr}\frac{\partial}{\partial P_{abcr}}+V^{(r)}_{abc\theta}\frac{\partial}{\partial P_{abc\theta}},\\ V^{(3)}&=\frac{\partial}{\partial \theta}+(P_{abcr}+P_{abc\theta})\frac{\partial}{\partial L_{abc}}+V^{(\theta)}_{abcr}\frac{\partial}{\partial P_{abcr}}+V^{(\theta)}_{abc\theta}\frac{\partial}{\partial P_{abc\theta}},\\ V^{(4)}&=\frac{\partial}{\partial \phi}, \end{aligned} \tag{40}$$

where $V^{(r)}_{abcr},V^{(r)}_{abc\theta},V^{(\theta)}_{abcr},V^{(\theta)}_{abc\theta}$ are given in the Appendix. The above solution corresponds to a submanifold of the integral manifold characterized by

$$\begin{aligned} df^{(W)}_{abcd}(V^{(i)}) &= 0, \\ df^{(DG)}_{ab}(V^{(i)}) &= 0, \\ K_{abc}(V^{(i)}) &= 0, \\ d(\pounds_{\xi} L_{abc})(V^{(i)}) &= 0, \end{aligned} \tag{41}$$

where $i=1,2,3,4$ and on which $f^{(W)}_{abcd}=f^{(DG)}_{ab}=\pounds_{\xi}L_{abc}=0$. This modified system is complete and therefore trivially in involution with only $s_0=s_0'$ nonvanishing. Using Janet–Riquier theory we could confirm this result, where we obtained that $\alpha_1^{(1)}=\alpha_1^{(2)}=\alpha_1^{(3)}=\alpha_1^{(4)}=0$ holds again.

Now, we wish to determine some isovectors for Schwarzschild space–time. We found that again no isovectors of type 2 exist and we look at an *Ansatz* of type 3 which is given by

$$Y=Y_{abc}(r,\theta)\frac{\partial}{\partial L_{abc}}+Y_{abc,r}\frac{\partial}{\partial P_{abcr}}+Y_{abc,\theta}\frac{\partial}{\partial P_{abc\theta}}. \tag{42}$$

Using algebraic computing based on REDUCE[9] we see that the ten Weyl–Lanczos equations and the six differential gauge conditions form four groups each only involving four different components of all the 16 distinct Lanczos components L_{abc}. These groups are:

[1] $L_{r\theta r},L_{r\theta\theta},L_{r\phi\phi},L_{\theta\phi\phi}$ in equations $f^{(W)}_{trtr},f^{(W)}_{trt\theta},f^{(W)}_{t\theta t\theta},f^{(DG)}_{r\theta}$;

[2] $L_{tr\theta},L_{t\theta r},L_{t\theta\theta},L_{t\phi\phi}$ in equations $f^{(W)}_{t\theta r\theta},f^{(W)}_{trr\theta},f^{(DG)}_{tr},f^{(DG)}_{t\theta}$;

[3] $L_{r\theta\phi},L_{r\phi\theta},L_{r\phi r},L_{\theta\phi\theta}$ in equations $f^{(W)}_{trt\phi},f^{(W)}_{t\theta t\phi},f^{(DG)}_{r\phi},f^{(DG)}_{\theta\phi}$;

[4] $L_{tr\phi},L_{t\phi r},L_{t\theta\phi},L_{t\phi\theta}$ in equations $f^{(W)}_{trr\phi},f^{(W)}_{tr\theta\phi},f^{(W)}_{t\theta r\phi},f^{(DG)}_{t\phi}$.

We give 4 examples of isovectors for the Weyl–Lanczos equations for Schwarzschild space–time corresponding to the four groups [1] to [4] above. Note that unfamiliar factors such as $e^{r^2/2}$ may occur because $Y^{(1)}$ to $Y^{(4)}$ are examples of *symmetry generators* for the *Weyl–Lanczos equations* for Schwarzschild space–time. For group [1], we obtain an isovector

$$Y^{(1)}=\frac{1}{r\sin^2(\theta)}\frac{\partial}{\partial L_{r\theta\theta}}-\frac{1}{r}\frac{\partial}{\partial L_{r\phi\phi}}-\frac{1}{r^2\sin^2(\theta)}\frac{\partial}{\partial P_{r\theta\theta r}}-\frac{2}{r}\frac{\cos(\theta)}{\sin^3(\theta)}\frac{\partial}{\partial P_{r\theta\theta\theta}}+\frac{1}{r^2}\frac{\partial}{\partial P_{r\phi\phi r}}. \tag{43}$$

For group [2], an isovector has the form

$$Y^{(2)}=\frac{(2m-r)}{\sin^2(\theta)}\frac{\partial}{\partial L_{t\theta\theta}}-(2m-r)\frac{\partial}{\partial L_{t\phi\phi}}-\frac{1}{\sin^2(\theta)}\frac{\partial}{\partial P_{t\theta\theta r}}+2(2m-r)\frac{\cos(\theta)}{\sin^3(\theta)}\frac{\partial}{\partial P_{t\theta\theta\theta}}+\frac{\partial}{\partial P_{t\phi\phi r}}, \tag{44}$$

whereas an isovector for group [3] is given by

$$\begin{aligned} Y^{(3)}=&\frac{e^{r^2/2}}{\sin(\theta)}\frac{\partial}{\partial L_{r\theta\phi}}+\frac{e^{r^2/2}}{\sin(\theta)}\frac{\partial}{\partial L_{r\phi\theta}}+\frac{re^{r^2/2}}{\sin(\theta)}\frac{\partial}{\partial P_{r\theta\phi r}}-\frac{e^{r^2/2}\cos(\theta)}{\sin^2(\theta)}\frac{\partial}{\partial P_{r\theta\phi\theta}}+\frac{re^{r^2/2}}{\sin(\theta)}\frac{\partial}{\partial P_{r\phi\theta r}} \\ &-\frac{e^{r^2/2}\cos(\theta)}{\sin^2(\theta)}\frac{\partial}{\partial P_{r\phi\theta\theta}}. \end{aligned} \tag{45}$$

Lastly, an isovector for group [4] is of the form

$$Y^{(4)}=\frac{r^{3/2}(r-2m)^{1/2}}{\sin(\theta)}\frac{\partial}{\partial L_{t\theta\phi}}+\frac{r^{3/2}(r-2m)^{1/2}}{\sin(\theta)}\frac{\partial}{\partial L_{t\phi\theta}}+\frac{1}{2\sin(\theta)}[3r^{1/2}(r-2m)^{1/2}$$
$$+r^{3/2}(r-2m)^{-1/2}]\frac{\partial}{\partial P_{t\theta\phi r}}-r^{3/2}(r-2m)^{1/2}\frac{\cos(\theta)}{\sin^2(\theta)}\frac{\partial}{\partial P_{t\theta\phi\theta}}+\frac{1}{2\sin(\theta)}[3r^{1/2}(r-2m)^{1/2}$$
$$+r^{3/2}(r-2m)^{-1/2}]\frac{\partial}{\partial P_{t\phi\theta r}}-r^{3/2}(r-2m)^{1/2}\frac{\cos(\theta)}{\sin^2(\theta)}\frac{\partial}{\partial P_{t\phi\theta\theta}}. \tag{46}$$

Each of these isovectors generates exchanges amongst some of the corresponding Lanczos components L_{abc} given in [1] to [4] and their partial derivatives.

C. Gödel space–time

Next, we examine a space–time with nondiagonalizable metric tensor and a G_5 as its isometry group, namely the Gödel space–time. The line element can be given as

$$ds^2=a^2(dt^2-dx^2-dz^2+\tfrac{1}{2}e^{2x}dy^2+2e^x dt dy)\,, \tag{47}$$

where a is an arbitrary constant. Gödel space–time admits a G_5 of motions of which three KVs commute as they are based on ignorable coordinates along t, y and z.[11] We look for a solution which only depends on x and we use an *Ansatz* based on exponentials of x. Such a solution exists and is given by

$$L_{txy}=\frac{a^2}{18}e^x\,,$$
$$L_{tyx}=-\frac{a^2}{18}e^x\,, \tag{48}$$
$$L_{xyy}=-\frac{a^2}{6}e^{2x}\,,$$

while all other independent components vanish identically. This solution coincides with the solution in Ref. 15, where a different set of local coordinates was used. We can look at the modified system which is again of the form (41). This modified system is again a complete system, a result which is confirmed using Janet–Riquier theory here as well. The integral manifold corresponding to (48) possesses tangent spaces which are spanned by the four Vessiot vector fields

$$V^{(1)}=\frac{\partial}{\partial t},$$
$$V^{(2)}=\frac{\partial}{\partial x}+P_{txyx}\frac{\partial}{\partial L_{txy}}+P_{tyxx}\frac{\partial}{\partial L_{tyx}}+P_{xyyx}\frac{\partial}{\partial L_{xyy}}+V^{(2)}_{txyx}\frac{\partial}{\partial P_{txyx}}+V^{(2)}_{tyxx}\frac{\partial}{\partial P_{tyxx}}+V^{(2)}_{xyyx}\frac{\partial}{\partial P_{xyyx}}, \tag{49}$$
$$V^{(3)}=\frac{\partial}{\partial y},$$
$$V^{(4)}=\frac{\partial}{\partial z},$$

where the components $V^{(2)}_{txyx}, V^{(2)}_{tyxx}, V^{(2)}_{xyyx}$ are given by

$$V^{(2)}_{txyx}=e^{-x}P_{xyyx}+P_{txyx}-e^{-x}L_{xyy}+\tfrac{1}{6}a^2e^{x},$$

$$V^{(2)}_{tyxx}=-P_{txyx}, \tag{50}$$

$$V^{(2)}_{xyyx}=e^{x}L_{tyx}-\tfrac{7}{2}e^{x}L_{txy}-4L_{xyy}+\tfrac{5}{2}e^{x}P_{txyx}-2e^{x}P_{tyxx}+3P_{xyyx}-\tfrac{1}{3}a^2e^{2x}.$$

Now, we wish to determine a number of isovectors for Gödel space–time and look at an *Ansatz* of type 3 as no isovectors of type 2 do exist here either. Such an *Ansatz* can be given by

$$Y=e^{\alpha x}c_{abc}\frac{\partial}{\partial L_{abc}}+\alpha e^{\alpha x}c_{abc}\frac{\partial}{\partial P_{abcx}} \tag{51}$$

for some constants α and c_{abc}. We see that the ten Weyl–Lanczos equations and the six differential gauge conditions can be split into four groups each containing only four distinct components L_{abc} this time given by

1 $L_{txy},L_{tyx},L_{xyy},L_{xzz}$ in equations $f^{(W)}_{txtx},f^{(W)}_{tyty},f^{(W)}_{txxy},f^{(DG)}_{ty}$;

2 $L_{tyy},L_{tzz},L_{xyx},L_{yzz}$ in equations $f^{(W)}_{txty},f^{(W)}_{tyxy},f^{(DG)}_{tx},f^{(DG)}_{xy}$;

3 $L_{tyz},L_{tzy},L_{xzx},L_{yzy}$ in equations $f^{(W)}_{txtz},f^{(W)}_{txyz},f^{(W)}_{tyxz},f^{(DG)}_{xz}$;

4 $L_{txz},L_{tzx},L_{xyz},L_{xzy}$ in equations $f^{(W)}_{tytz},f^{(W)}_{txxz},f^{(DG)}_{tz},f^{(DG)}_{yz}$.

Here, we are again only interested in finding an example of the above type for group 1. After some calculations we find the isovector

$$\begin{aligned}Y=&e^{\alpha x}\frac{\partial}{\partial L_{txy}}-\frac{2(2\alpha-3)}{D(\alpha)}e^{\alpha x}\frac{\partial}{\partial L_{tyx}}+\left(\alpha+\frac{2(3\alpha+1)}{D(\alpha)}\right)e^{(\alpha+1)x}\frac{\partial}{\partial L_{xyy}}+\frac{2(2\alpha^2+1)}{D(\alpha)}e^{(\alpha-1)x}\frac{\partial}{\partial L_{xzz}}\\&+\alpha e^{\alpha x}\frac{\partial}{\partial P_{txyx}}-\frac{2(2\alpha-3)\alpha}{D(\alpha)}e^{\alpha x}\frac{\partial}{\partial P_{tyxx}}+(\alpha+1)\left(\alpha+\frac{2(3\alpha+1)}{D(\alpha)}\right)e^{(\alpha+1)x}\frac{\partial}{\partial P_{xyyx}}\\&+(\alpha-1)\frac{2(2\alpha^2+1)}{D(\alpha)}e^{(\alpha-1)x}\frac{\partial}{\partial P_{xzzx}},\end{aligned} \tag{52}$$

where $D(\alpha)=2\alpha^2-6\alpha-1$ and α has to satisfy the quartic equation

$$\alpha^4-2\alpha^3+7\alpha^2-20\alpha-\tfrac{5}{4}=0. \tag{53}$$

From numerical approximations based on REDUCE using the Newton–Raphson method we find that there are two real roots which satisfy (53). They are given by

$$\begin{aligned}\alpha_1&=-0.061\,166\,927\,586\,6,\\ \alpha_2&=2.492\,142\,058\,35,\end{aligned} \tag{54}$$

whereas the other two roots are complex and therefore not relevant for us for forming isovectors. The isovectors corresponding to α_1 and α_2 lead to an exchange amongst the solution components $L_{txy}(x),L_{tyx}(x),L_{xyy}(x),L_{xzz}(x)$.

D. pp-wave space–times with a G_5

Here, we will see that it is impossible to find a solution to the Weyl–Lanczos equations for pp-space–times for which we impose $\pounds_\xi L_{abc}:=0$ for *all* KVs ξ at the same time. Plane-wave space–times which admit a G_5 as an isometry group can be found in Ref. 23. We write the line element of a plane-wave space–time like

$$ds^2 = 2dudr + (h_{11}X^2 + 2h_{12}XY + h_{22}Y^2)du^2 - dX^2 - dY^2, \tag{55}$$

with h_{11}, h_{12}, h_{22} being functions of u only. Following Ref. 10 we can perform a coordinate transformation so that the line element turns into

$$ds^2 = 2dudv - e^{-U}(e^V \cosh(W)dx^2 - 2\sinh(W)dxdy + e^{-V}\cosh(W)dy^2), \tag{56}$$

where now U, V and W are functions of u only. For linearly polarized gravitational waves, we can always set $W := 0$.[10] The five Killing vector fields are given in Ref. 10, where three of them are given by $\xi^1 = \partial/\partial x$, $\xi^2 = \partial/\partial y$, $\xi^3 = \partial/\partial v$ based on ignorable coordinates and the other two are

$$\begin{aligned} \xi^4 &= x\frac{\partial}{\partial v} + P_-(u)\frac{\partial}{\partial x} + N(u)\frac{\partial}{\partial y}, \\ \xi^5 &= y\frac{\partial}{\partial v} + N(u)\frac{\partial}{\partial x} + P_+(u)\frac{\partial}{\partial y}, \end{aligned} \tag{57}$$

where

$$P_\pm(u) = \int e^{(U\pm V)}\cosh(W)du, \quad N(u) = \int e^U \sinh(W)du.$$

A solution, where $\pounds_\xi L_{abc} := 0$ was imposed only for ξ_1, ξ_2 and ξ_3, is given in Ref. 24. We wish to see whether we can obtain a solution, where $\pounds_\xi L_{abc} := 0$ is imposed for all 5 KVs. This leads to the expressions

$$\begin{aligned} L_{uxx} &= e^V \frac{\cosh(W)}{\sinh(W)}(L_{uyx} - 2L_{uxy}), \\ L_{uyy} &= \frac{1}{e^V \sinh(W)}\left[L_{uxy}\left(\sinh(W) - \frac{2}{\sinh(W)}\right) + L_{uyx}\left(\frac{1}{\sinh(W)} - 2\sinh(W)\right)\right], \\ L_{uvu} &= \frac{e^U}{\sinh(W)}(2L_{uxy} - L_{uyx}), \end{aligned} \tag{58}$$

where $L_{uxu}, L_{uyu}, L_{uxy}, L_{uyx}$ can be chosen arbitrarily and all other components vanish identically. The trace-free condition (4) leads to equations of the form "$0 = 0$" except for $L_u{}^s{}_s = 0$ so that all L_{abc} apart from L_{uxu} and L_{uyu} can be expressed in terms of L_{uxy} with

$$L_{uyx} = 2\left(\frac{3 - \sinh^2(W)}{3\sinh^2(W) + 1}\right)L_{uxy}. \tag{59}$$

We now have to check whether this *Ansatz* satisfies the Weyl–Lanczos equations. The only nonvanishing components remaining are $f_{uxux}, f_{uxuy}, f_{uyuy}$. But this *Ansatz* fails to satisfy all three equations $f_{uxux}, f_{uxuy}, f_{uyuy}$ *at the same time* as it is shown in detail in Ref. 9. Therefore, no solutions to the Weyl–Lanczos equations for pp-space–times, which at the same time admit vanishing Lie derivatives along **all** 5 KVs, do exist but other solutions such as the solution in Ref. 24 can be found.

IV. SOME SOLUTIONS AND ISOVECTORS FOR THE LANCZOS WAVE EQUATION

The Lanczos wave equation in four dimensions (9) consists of a system in involution as shown in Ref. 9. Some solutions for (9) are given in Ref. 7 for Kasner, Schwarzschild and Bondi

space–times. They are also solutions to the Weyl–Lanczos equations such that the one for Kasner corresponds to (27), the one for Schwarzschild to (39) and the one for Gödel to (48).

As for examples of isovectors for the Lanczos wave equation, we see that *KVs based on ignorable coordinates are isovectors for the Lanczos wave equation.* Further symmetry generators for Kasner, Schwarzschild and Gödel space–times can be constructed in the same way as for the Weyl–Lanczos equations except that we have to use the prolonged second-order version

$$Y=Y^e\frac{\partial}{\partial x^e}+Y_{abc}\frac{\partial}{\partial L_{abc}}+Y_{abcd}\frac{\partial}{\partial P_{abcd}}+Y_{abcde}\frac{\partial}{\partial S_{abcde}}, \tag{60}$$

where the general expression for the Y_{abcde} can be found in Refs. 17 and 22. The prolonged form of symmetry generators of the same form as (33) is given by

$$Y=Y_{abc}(x^e)\frac{\partial}{\partial L_{abc}}+Y_{abcd}(x^e)\frac{\partial}{\partial P_{abcd}}+Y_{abcde}(x^e)\frac{\partial}{\partial S_{abcde}} \tag{61}$$

for any space–time and its components Y_{abcd}, Y_{abcde} simply are

$$Y_{abcd}=\frac{\partial Y_{abc}}{\partial x^d}, \quad Y_{abcde}=\frac{\partial Y_{abcd}}{\partial x^e}.$$

But they are not necessarily symmetry generators for the Lanczos wave equation as we will see. Solving the equations $\pounds_Y d\mathcal{W}_{abc}=0$ for **Kasner space–time** using *Ansatz* (61), we obtain

$$\begin{aligned}Y=&t^\beta\frac{\partial}{\partial L_{tyy}}+f(\beta,p_1,p_2,p_3)t^\gamma\frac{\partial}{\partial L_{tzz}}+\beta t^{(\beta-1)}\frac{\partial}{\partial P_{tyyt}}+f(\beta,p_1,p_2,p_3)\gamma t^{(\gamma-1)}\frac{\partial}{\partial P_{tzzt}}\\&+\beta(\beta-1)t^{(\beta-2)}\frac{\partial}{\partial S_{tyytt}}+f(\beta,p_1,p_2,p_3)\gamma(\gamma-1)t^{(\gamma-2)}\frac{\partial}{\partial S_{tzztt}},\end{aligned} \tag{62}$$

where $\gamma=\beta-2p_2+2p_3$ and $f(\beta,p_1,p_2,p_3)$ is given by

$$f(\beta,p_1,p_2,p_3)=\frac{(\beta^2-4p_2\beta-p_1^2-4p_1p_2-3p_2p_3+3p_2-p_3)}{(p_3-p_1+p_1p_2-p_2p_3+p_1^2-p_3^2)}. \tag{63}$$

The quantity β has to satisfy the quartic equation

$$\begin{aligned}0=&\beta^4-8p_2\beta^3+\beta^2(16p_2^2-2p_1^2+4p_3^2+6p_2+2p_3-4p_1p_2-8p_1p_3-10p_2p_3)-4p_2\beta(4-6p_1^2\\&-4p_1p_2-4p_1p_3-6p_2p_3+2-2p_1)+1-16p_2p_3^3+16p_2p_3^2-8p_2p_3+8p_2-32p_3^4+48p_3^3\\&-32p_3^2+8p_3.\end{aligned} \tag{64}$$

We note that depending on particular choices of p_1,p_2,p_3, we can obtain for β four real, two real and two complex, or four complex solutions to (64). We are not going to specify the conditions on p_1,p_2,p_3 because this leads to rather cumbersome calculations. However, using polynomial division, we find that the two solutions for α given by (35) for isovectors for the Weyl–Lanczos equations are *not* solutions to (64) when prolonged to second order because we cannot factorize (36) out of (64) without a remainder term.

If we determine isovectors for **Gödel space–time** using an *Ansatz* of type (61) as well, we obtain isovectors of the form

$$Y = e^{\beta x}\frac{\partial}{\partial L_{txy}} + f_1(\beta)e^{\beta x}\frac{\partial}{\partial L_{tyx}} + f_2(\beta)e^{(\beta+1)x}\frac{\partial}{\partial L_{xyy}} + f_3(\beta)e^{(\beta-1)x}\frac{\partial}{\partial L_{xzz}} + \beta e^{\beta x}\frac{\partial}{\partial P_{txyx}}$$
$$+ f_1(\beta)\beta e^{\beta x}\frac{\partial}{\partial P_{tyxx}} + f_2(\beta)(\beta+1)e^{(\beta+1)x}\frac{\partial}{\partial P_{xyyx}} + f_3(\beta)(\beta-1)e^{(\beta-1)x}\frac{\partial}{\partial P_{xzzx}}$$
$$+ \beta^2 e^{\beta x}\frac{\partial}{\partial S_{txyxx}} + f_1(\beta)\beta^2 e^{\beta x}\frac{\partial}{\partial S_{tyxxx}} + f_2(\beta)(\beta+1)^2 e^{(\beta+1)x}\frac{\partial}{\partial S_{xyyxx}}$$
$$+ f_3(\beta)(\beta-1)^2 e^{(\beta-1)x}\frac{\partial}{\partial S_{xzzxx}}, \tag{65}$$

and, where $f_1(\beta), f_2(\beta), f_3(\beta)$ are given by

$$f_1(\beta) = 8\,\frac{(\beta^4 + 2\beta^3 + \frac{5}{2}\beta^2 + \frac{3}{2}\beta - 7)}{D(\beta)},$$
$$f_2(\beta) = \frac{(4\beta^4 - 8\beta^3 + 32\beta^2 + 8\beta + 69)}{D(\beta)}, \tag{66}$$
$$f_3(\beta) = \frac{(4\beta^6 + 4\beta^5 - 2\beta^4 - 16\beta^3 + 29\beta^2 + 5\beta + \frac{267}{2})}{D(\beta)},$$

where $D(\beta)$ is given by

$$D(\beta) = 4\beta^4 + 16\beta^3 - 28\beta^2 + 12\beta - 109. \tag{67}$$

Because β has to be such that $\pounds_Y d\mathcal{W}_{abc} = 0$, β has to satisfy the equation

$$\beta^9 - \tfrac{3}{2}\beta^8 - 2\beta^6 + \tfrac{31}{2}\beta^5 - \tfrac{107}{4}\beta^4 + 33\beta^3 - 53\beta^2 + \tfrac{573}{16}\beta - \tfrac{171}{32} = 0\,. \tag{68}$$

Using numerical computing based on REDUCE applying the Newton–Raphson method to this equation, we find that (68) possesses three distinct real roots which are given by

$$\beta_1 = 0.204\,256\,218\,397,$$
$$\beta_2 = 0.782\,257\,036\,153, \tag{69}$$
$$\beta_3 = 1.5,$$

of which $\beta_3 = 1.5$ is an exact result and from which we can form three distinct isovectors. Again, we see that these isovectors for $\beta_1, \beta_2, \beta_3$ are not just prolonged versions of the isovectors for the Weyl–Lanczos equations.

An *Ansatz* of type (61) could be used for Schwarzschild space–time as well but this is a rather cumbersome calculation and we will not carry it out explicitly. It remains future work to examine the symmetry groups of both the Weyl–Lanczos equations and of the Lanczos wave equation more systematically.

V. CONCLUSIONS

For Kasner, Schwarzschild and Gödel space–times there exist solutions of the Weyl–Lanczos equations with Lie symmetries along all Killing directions. For pp-space–times no such solutions exist, which shows that not all KVs are symmetry generators for the Weyl–Lanczos equations but only those which are based on *ignorable coordinates*. Some isovectors for the Weyl–Lanczos

equations which indicate an exchange amongst some of the components L_{abc} were given for Kasner, Schwarzschild and Gödel space–times.

All solutions for the Weyl–Lanczos equations in four dimensions are automatically solutions for the Lanczos wave equation, and KVs based on ignorable coordinates are also isovectors for the Lanczos wave equation. We found that isovectors for the Weyl–Lanczos equations are **not** automatically isovectors for the Lanczos wave equation when prolonged to second order. We gave some examples for Kasner and Gödel space–times. A more thorough examination of the respective symmetry groups of the Weyl–Lanczos equations and of the Lanczos wave equation remains future work though.

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APPENDIX: VESSIOT VECTOR FIELDS

Here, we give the components $V^{(e)}_{abcr}, V^{(e)}_{abc\theta}$ of the Vessiot vector fields $V^{(2)}, V^{(3)}$ for Schwarzschild space–time for a solution to the Weyl–Lanczos equations, where $e = r, \theta$:

$$
\begin{aligned}
V^{(e)}_{t\theta\theta r} &= -P_{t\theta\theta e}\frac{m}{r(2m-r)} - P_{t\phi\phi e}\frac{m-r}{\sin^2\theta r(2m-r)} - r^2\frac{\partial f^{(DG)}_{tr}}{\partial e} - \left(\frac{\partial f^{(W)}_{t\theta r\theta}}{\partial e}\right)\frac{1}{2m-r},\\
V^{(e)}_{t\theta\theta\theta} &= P_{t\phi\phi e}\frac{\cot(\theta)}{\sin^2(\theta)} - P_{t\theta\theta e}\cot(\theta) + \frac{\partial f^{(DG)}_{t\theta}}{\partial e},\\
V^{(e)}_{t\phi\phi r} &= P_{t\theta\theta e}\frac{(r-m)\sin^2(\theta)}{r(2m-r)} - P_{t\phi\phi e}\frac{m}{r(2m-r)} + \left(\frac{\partial f^{(W)}_{t\theta r\theta}}{\partial e}\right)\frac{\sin^2(\theta)}{2m-r},\\
V^{(e)}_{t\phi\phi\theta} &= P_{t\theta\theta e}\cos(\theta)\sin(\theta) + P_{t\phi\phi e}\cot(\theta) + \left(\frac{\partial f^{(W)}_{trr\theta}}{\partial e}\right) r\sin^2(\theta),\\
V^{(e)}_{t\theta\phi r} &= -P_{t\theta\phi e}\frac{2m-3}{r(2m-r)} - P_{t\phi\theta e}\frac{3m-r}{r(2m-r)} - \frac{\partial f^{(W)}_{t\theta r\phi}}{\partial e},\\
V^{(e)}_{t\theta\phi\theta} &= -P_{t\phi\theta e}\cot(\theta) - \left(\frac{\partial f^{(W)}_{trr\phi}}{\partial e}\right) r(2m-r),\\
V^{(e)}_{t\phi\theta r} &= P_{t\phi\theta e}\frac{3m-2r}{r(2m-r)} + P_{t\theta\phi e}\frac{3r-8m+3}{r(2m-r)} + \frac{\partial f^{(W)}_{tr\theta\phi}}{\partial e} - \frac{\partial f^{(W)}_{t\theta r\phi}}{\partial e},\\
V^{(e)}_{t\phi\theta\theta} &= P_{t\theta\phi e}\cot(\theta) - r^2\frac{\partial f^{(DG)}_{t\phi}}{\partial e},\\
V^{(e)}_{r\theta\theta r} &= P_{r\theta\theta e}\frac{(10m^2-19mr+4r^2)}{r(2m-r)^2} + P_{r\phi\phi e}\frac{(6m^2-5mr+r^2)}{r(2m-r)^2\sin^2(\theta)} + \frac{r^3}{2m-r}\left(\frac{\partial f^{(W)}_{trtr}}{\partial e}\right)\\
&\quad - \frac{r^2}{(2m-r)^2}\left(\frac{\partial f^{(W)}_{t\theta t\theta}}{\partial e}\right),\\
V^{(e)}_{r\theta\theta\theta} &= P_{r\theta\theta e}\cot(\theta) + P_{r\phi\phi e}\frac{\cot(\theta)}{\sin^2(\theta)} + \frac{\partial f^{(DG)}_{r\theta}}{\partial e},
\end{aligned}
\tag{A1}
$$

$$V^{(e)}_{r\phi\phi r}=P_{r\theta\theta e}\frac{(6m^2-5mr+r^2)}{r(2m-r)^2}\sin^2(\theta)+P_{r\phi\phi e}\frac{(10m^2-9mr+2r^2)}{r(2m-r)^2}+\left(\frac{\partial f^{(W)}_{t\theta t\theta}}{\partial e}\right)\frac{(r)^2\sin^2(\theta)}{(2m-r)^2},$$

$$V^{(e)}_{r\phi\phi\theta}=P_{r\theta\theta e}\cos(\theta)\sin(\theta)+P_{r\phi\phi e}\cot(\theta)+\left(\frac{\partial f^{(W)}_{trt\theta}}{\partial e}\right)\frac{r^3\sin^2(\theta)}{2m-r},$$

$$V^{(e)}_{r\theta\phi r}=P_{r\theta\phi e}\frac{m}{r(2m-r)}+P_{r\phi\theta e}\frac{r-m}{r(r-2m)}-\left(\frac{\partial f^{(W)}_{t\theta t\phi}}{\partial e}\right)\frac{r^2}{(r-2m)^2},$$

$$V^{(e)}_{r\theta\phi\theta}=P_{r\phi\theta e}\cot(\theta)+\frac{r^3}{r-2m}\left(\frac{\partial f^{(W)}_{trt\phi}}{\partial e}\right),$$

$$V^{(e)}_{r\phi\theta r}=P_{r\theta\phi e}\frac{r-m}{r(r-2m)}-P_{r\phi\theta e}\frac{m}{r(r-2m)}+\frac{r}{(r-2m)}\frac{\partial f^{(DG)}_{\theta\phi}}{\partial e}-\left(\frac{\partial f^{(W)}_{t\theta t\phi}}{\partial e}\right)\frac{r^2}{(r-2m)^2},$$

$$V^{(e)}_{r\phi\theta\theta}=r^2\frac{\partial f^{(DG)}_{r\phi}}{\partial e}-P_{r\theta\phi e}\cot(\theta),$$

where $f^{(DG)}_{ab}=L_{abs}{}^{;s}$ as defined before.

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WKB analysis of the Regge–Wheeler equation down in the frequency plane

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The Regge–Wheeler equation for black-hole gravitational waves is analyzed for large negative imaginary frequencies, leading to a calculation of the cut strength for waves outgoing to infinity. In the—limited—region of overlap, the results agree well with numerical findings [Leung *et al.*, Class. Quantum Grav. **20**, L217 (2003)]. Requiring these waves to be outgoing into the horizon as well subsequently yields an analytic formula for the highly damped Schwarzschild quasinormal modes, *including* the leading correction. Just as in the WKB quantization of, e.g., the harmonic oscillator, solutions in different regions of space have to be joined through a connection formula, valid near the boundary between them where WKB breaks down. For the oscillator, this boundary is given by the classical turning points; fascinatingly, the connection here involves an expansion around the black-hole singularity $r=0$. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Black-hole axial gravitational waves of angular momentum $\ell \geqslant 2$ are described (in units $c=G=2M=1$) by the Regge–Wheeler equation[1,2] (RWE)

$$[d_x^2+\omega^2-V(x)]\psi(x,\omega)=0, \tag{1}$$

$$V(r)=\left(1-\frac{1}{r}\right)\left[\frac{\ell(\ell+1)}{r^2}-\frac{3}{r^3}\right], \tag{2}$$

where $x=r+\ln(r-1)$ is the tortoise coordinate and r the circumferential radius; $V(r)$ accounts for the Schwarzschild background. The long-range nature of this potential, $V(x)-\ell(\ell+1)/x^2 \sim 2\ell(\ell+1)\ln x/x^3$ for $x\to\infty$ (Ref. 3), is well known to cause a branch cut in the (retarded) Green's function of (1) on the negative imaginary axis (NIA) in the ω plane.

For damping $\gamma \equiv i\omega \downarrow 0$, this cut causes an algebraically decaying late-time tail in the gravitational-wave signal.[4,5] For moderate γ and $2\leqslant\ell\leqslant 4$, it has recently been investigated numerically,[6] leading to a clear conjecture for the large-γ behavior. In a separate development, the strings of quasinormal modes (QNMs) parallel on both sides of the cut and close to it seem to offer clues to the quantum theory, in particular to a calculation of the Bekenstein entropy in loop quantum gravity and to the quantum of area.[7] These motivate studying also the branch cut asymptotically, which will turn out to have ample independent interest.

In each ℓ sector and in the frequency domain, the RWE is one dimensional, so the above-mentioned Green's function $\bar{G}(x,y)=\bar{G}(y,x)$ can be written as

$$\bar{G}(x,y;\omega)=\frac{f(y,\omega)g(x,\omega)}{J(\omega)}, \quad y<x. \tag{3}$$

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Here, f solves (1) with the left outgoing-wave boundary condition (OWC) $f(x\to-\infty,\omega)\sim 1\cdot e^{-i\omega x}$ and thus represents waves going into the horizon, while $g(x\to\infty,\omega)\sim 1\cdot e^{i\omega x}$ corresponds to waves going to infinity; $J=gf'-fg'$ is their Wronskian. In the physical region $x\in\mathbb{R}$, these asymptotic definitions are unambiguous only for $\mathrm{Im}\,\omega\geqslant 0$, from where the functions are continued analytically. The normalizations of f,g have been fixed for definiteness, but J in the denominator renders (3) normalization independent. Since $V(x\to-\infty)\sim e^{x}$, the function $f(x,\omega)$ is single valued in ω. Thus it is intuitively clear, and readily shown,[6] that the branch cut in $\overline{G}$ can be expressed in terms of the one in g.

Focusing on the latter, we define $g_{\pm}(\omega)$ as the continuations from $\mathrm{Re}\pm\omega>0$ and $\Delta g\equiv g_{+}-g_{-}$. Since $g_{\pm}(x,-i\gamma)\sim 1\cdot e^{\gamma x}$ satisfy the *same* (linear, second-order) wave equation, $\Delta g(x,-i\gamma)\sim 0\cdot e^{\gamma x}$ is the small solution $\propto g(x,+i\gamma)$. The simple symmetry $g(-\omega^{*})=g^{*}(\omega)$ renders Δg imaginary, so we introduce the real cut strength q through[4,8]

$$\Delta g(x,-i\gamma)=iq(\gamma)g(x,+i\gamma). \tag{4}$$

Since g is defined by the OWC at $x\to\infty$, (4) defines q not merely x independent, but rather independent of $V(x)$ at any finite x: if, say, $V_1(x>L)=V_2(x>L)$, the corresponding q_1 and q_2 are identical. Thus, q economically characterizes Δg (and ultimately $\Delta\overline{G}$), and our task can now be specified as calculating the asymptotics of $q(\gamma\to\infty)$.

II. WKB SOLUTIONS

For $\mathrm{Im}\,\omega<0$, in particular on the NIA, the simple asymptotic definition of $g(\omega)$ becomes all but meaningless, since it is impossible to distinguish the decaying component $\sim e^{-\gamma x}$ (to be set to zero) from the ''pure'' outgoing wave $\sim e^{\gamma x}$, where this limiting form, however, has algebraic corrections to all orders in V. One way out is to complement the analytic continuation in frequency with one in *space*,[8–10] so that the product $i\omega x$ retains a negative real part. However, in terms of x, the very equation (1) is multiple valued, so that the analysis henceforth will proceed in the complex r plane, viz.,

$$[r^2(r-1)^2d_r^2+r(r-1)d_r-(r-1)\{\ell(\ell+1)r-3\}+\omega^2r^4]g=0. \tag{5}$$

It is possible to impose the OWC for $g_{+}(r,-i\gamma)$ $[g_{-}(r,-i\gamma)]$ directly and stably for $r\to-\infty$ and continue the solutions to the physical $r>1$ in the upper (lower) half plane.[8] That is, apart from a trivial overall phase, $g_{\pm}$ are the *same* solutions as r grows from $-\infty$, until they are prescribed to encircle the singularity $r=0$ in opposite directions. Hence, closer study of this point should shed light on their difference Δg.

At least away from the singularities $r=0,1$ and the anti-Stokes lines (*v.i.*), one expects to have asymptotic expansions $g_{\mathrm{a}}(r,\omega)$ and $g_{\mathrm{a}}(r,-\omega)$, with

$$g_{\mathrm{a}}(r,\omega)\sim[(r-1)e^{r}]^{i\omega}\left\{1+\frac{g_1(r)}{\omega}+\frac{g_2(r)}{\omega^2}+\cdots\right\}, \tag{6}$$

where the first factor is just a plane wave in the tortoise coordinate. Substitution yields

$$g_1(r)=\frac{1}{2i}\int_{\infty}^{r}\frac{ds\,s}{s-1}V(s)=i\left[\frac{\ell(\ell+1)}{2r}-\frac{3}{4r^2}\right],$$

$$g_2(r)=\frac{1}{4}V(r)-\frac{1}{8}\left[\int_{\infty}^{r}\frac{ds\,s}{s-1}V(s)\right]^2=-\frac{3N}{8r^2}+\frac{\ell(\ell+1)-6}{8r^3}+\frac{15}{32r^4}, \tag{7}$$

where

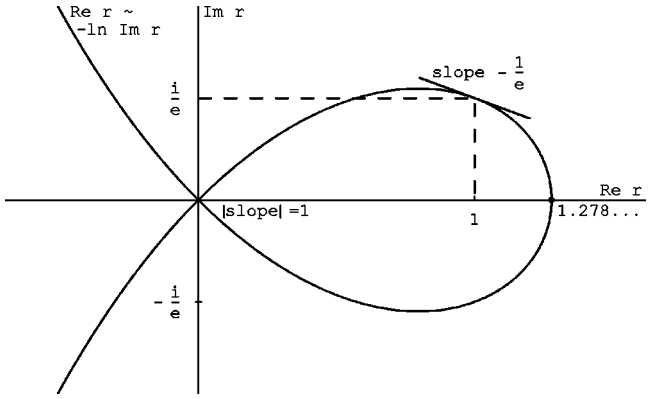

FIG. 1. Anti-Stokes lines of the RWE for negative imaginary frequencies.

$$N=8\binom{\ell+2}{4}=\frac{4}{3}\nu(\nu+1)$$

with $\nu\equiv\frac{1}{2}(\ell-1)(\ell+2)$. That is, these two orders still agree with the upshot of ω expanding the standard WKB expression, though this is no longer true for g_3, which involves V' (of course, there are higher-order corrections to WKB as well).

The anti-Stokes lines of the RWE on the NIA for this expansion are shown in Fig. 1. They are the curves where $|(r-1)e^r|=1$ (i.e., $\mathrm{Re}\,x=0$); for $\gamma\to\infty$, these are the boundaries where the solutions (6) change between exponentially growing and decaying characters.

Thus, the solution which is small for $r\to-\infty$ can be continued to the region including $x>0$, but this only yields the exponentially growing part one knew all along. From there, the solution *cannot* be continued back to $x<0$ (where its imaginary part could be identified) because of the Stokes phenomenon. For the latter continuation, we apparently have to pass through the eye of the storm—the black-hole singularity $r=0$ (Ref. 11). Near $r=0$, the expansion (6) is not valid, for higher-order terms only become small if $|r|\gg 1/\sqrt{\gamma}$. One therefore has to match (possibly different) expansions in terms of g_a in the regions $|\arg r-\pi|\leqslant\pi/4$ and $|\arg r|\leqslant\pi/4$, respectively. This is similar to the connection procedure near classical turning points in Bohr–Sommerfeld quantization. However, near the latter it is merely the asymptotic expansion which breaks down, while the original (Schrödinger) wave equation is perfectly regular. In our case, the connection has to be carried out across a singularity of the RWE.

III. CONNECTION FORMULA

Series expansion around $r=0$ is standard:[12]

$$\psi_1(r)=r^3+\frac{6-\ell(\ell+1)}{5}r^4+\mathcal{O}(r^5), \tag{8}$$

$$\psi_2(r)=r^{-1}+\frac{2\nu}{3}+\frac{N}{4}r+\frac{\ell(\ell+1)N}{12}r^2+\frac{\Omega^2-\omega^2}{4}\psi_1(r)\ln r+\mathcal{O}(r^4), \tag{9}$$

where both error terms are single valued and where we introduced the *algebraically special frequency* $\Omega=-iN/2$ (Refs. 8 and 13). However, because of the large term $\propto\omega^2$ in the RWE (5), higher-order terms in these expansions can only be omitted if $|r^2\omega|\ll 1$ (cf. the given terms of ψ_2). Thus, there is no overlap with the region of validity of g_a, where matching could be carried out. Still, the above series for $\psi_{1,2}$ will be useful for comparison, *inter alia*, yielding the exact monodromy[14] $\psi_2(re^{2\pi i})=\psi_2(r)+i(\pi/2)(\Omega^2-\omega^2)\psi_1(r)$ and $\psi_1(re^{2\pi i})=\psi_1(r)$.

A usable matching solution follows by effectively resumming the large-γ parts of higher-order terms in (8),(9). In practice, it is more convenient to set $r \equiv t/\sqrt{\gamma}$ and sort powers of γ:

$$[t^2 d_t^2 - t d_t - 3 - t^4]\psi = \frac{1}{\sqrt{\gamma}}[2t^3 d_t^2 - t^2 d_t - \{\ell(\ell+1)+3\}t]\psi + \mathcal{O}(\gamma^{-1}) \equiv R(t), \tag{10}$$

$$\psi = \psi^{(0)} + \psi^{(1)} + \cdots .$$

The lowest order follows by equating the right-hand side of (10) to zero:

$$\psi_1^{(0)}(t) = \frac{4it}{\gamma^{3/2}} J_1\left(\frac{t^2}{2i}\right), \tag{11}$$

$$\psi_2^{(0)}(t) = \frac{i\pi\sqrt{\gamma}}{4} t Y_1\left(\frac{t^2}{2i}\right). \tag{12}$$

These have not been written in terms of modified Bessel functions, since the subsequent matching is best done on the anti-Stokes lines where $t^2/2i$ is real. Subsequently, $\psi_1^{(0)}$ figures as an inhomogeneous term in the equation for $\psi_1^{(1)}$, solved by

$$\psi_1^{(1)}(t) = \frac{\pi}{4} t \int_0^t \frac{ds}{s^2}\left[Y_1\left(\frac{t^2}{2i}\right) J_1\left(\frac{s^2}{2i}\right) - J_1\left(\frac{t^2}{2i}\right) Y_1\left(\frac{s^2}{2i}\right)\right] R_1(s), \tag{13}$$

$$R_1(s) = \frac{4i}{\gamma^2}\left\{ 2[s^6 - \nu s^2] J_1\left(\frac{s^2}{2i}\right) - i s^4 J_0\left(\frac{s^2}{2i}\right)\right\}. \tag{14}$$

Note that the occurrence of Y_1 does not spoil the analyticity of $\psi_1^{(1)}$. In particular, for $t \to 0$ the above readily reproduces the t^4 term found in (8) by direct expansion. The counterpart for ψ_2 reads

$$\psi_2^{(1)}(t) = \frac{\pi}{4} t Y_1\left(\frac{t^2}{2i}\right) \int_0^t \frac{ds}{s^2} J_1\left(\frac{s^2}{2i}\right) R_2(s) + \frac{\pi}{4} t J_1\left(\frac{t^2}{2i}\right)\left[\int_0^t ds \left\{ \frac{8i\nu}{\pi s^4} - Y_1\left(\frac{s^2}{2i}\right)\frac{R_2(s)}{s^2}\right\} + \frac{8i\nu}{3\pi t^3}\right], \tag{15}$$

$$R_2(s) = \frac{i\pi}{4}\left\{ 2[s^6 - \nu s^2] Y_1\left(\frac{s^2}{2i}\right) - i s^4 Y_0\left(\frac{s^2}{2i}\right)\right\}, \tag{16}$$

where we introduced a "counterterm" in order to keep the second integral finite near $s = 0$. Again, one verifies that the leading small-t correction [$\propto t^0$ in (9)] is reproduced correctly. Using the standard branching properties of the Y_n one now finds that, up to this second order, $\psi_2(te^{2\pi i}) = \psi_2(t) + i(\pi/2)\gamma^2 \psi_1(t)$, so that the exact monodromy is approached for $|\omega| \gg |\Omega|$.

In fact, we can follow the transformation of $\psi_{1,2}^{(i)}$ under rotation in more detail by using the standard $J_n(-z) = (-)^n J_n(z)$ and $Y_n(e^{\pm i\pi} z) = (-)^n [Y_n(z) \pm 2iJ_n(z)]$, implying

$$\psi_1^{(0)}(it) = -i\psi_1^{(0)}(t), \tag{17}$$

$$\psi_1^{(1)}(it) = \psi_1^{(1)}(t), \tag{18}$$

$$\psi_2^{(0)}(it) = -i\psi_2^{(0)}(t) + \frac{\pi\gamma^2}{8}\psi_1^{(0)}(t), \tag{19}$$

$$\psi_2^{(1)}(it) = \psi_2^{(1)}(t) + i\frac{\pi\gamma^2}{8}\psi_1^{(1)}(t). \tag{20}$$

These relations streamline the asymptotic expansion. Namely, look along $\arg t=\pi/4$, where $\psi_{1,2}^{(0)}e^{-3\pi i/4}\in\mathbb{R}$ and $\psi_{1,2}^{(1)}\in\mathbb{R}$, so that their expansions will read

$$\psi_1(t)\sim\frac{4}{\sqrt{\pi\gamma^3}}\left[e^{t^2/2}\left\{1+\frac{\alpha}{\sqrt{\gamma}}\right\}+e^{-t^2/2}\left\{-i+\frac{\alpha^*}{\sqrt{\gamma}}\right\}+\mathcal{O}(t^{-2})+\mathcal{O}\left(\frac{t^3}{\sqrt{\gamma}}\right)+\mathcal{O}(\gamma^{-1})\right], \quad (21)$$

$$\psi_2(t)\sim\frac{\sqrt{\pi\gamma}}{4}\left[e^{t^2/2}\left\{-i+\frac{\beta}{\sqrt{\gamma}}\right\}+e^{-t^2/2}\left\{1+\frac{\beta^*}{\sqrt{\gamma}}\right\}+\mathcal{O}(t^{-2})+\mathcal{O}\left(\frac{t^3}{\sqrt{\gamma}}\right)+\mathcal{O}(\gamma^{-1})\right]. \quad (22)$$

The occurrence of $\mathcal{O}(t^3/\sqrt{\gamma})$ (which, however, does *not* generate additional $t^0/\sqrt{\gamma}$ terms) means that these hold for $1\ll t\ll\gamma^{1/6}$ or $\gamma^{-1/2}\ll r\ll\gamma^{-1/3}$, conveniently handled as a double asymptotic expansion in t and $\lambda\equiv\gamma/t^6$. The power-law asymptotic corrections in t follow directly from the RWE; the real nonlocal information is contained in α, β.

We can use the general rules (17)–(20) to transform (21),(22) to $\arg t=3\pi/4$ and demand consistency for the ($\propto e^{-t^2/2}$) part that dominates for $\pi/4<\arg t<3\pi/4$. This leads to $\alpha\in\mathbb{R}$ and $\mathrm{Im}\,\beta=-\alpha$. By subsequently demanding consistency also for the combination of ψ_1 and ψ_2 which is minimal in the same sector, one finds

$$\beta=-(2+i)\alpha\ . \quad (23)$$

Thus, this algebraic exercise circumvented directly expanding the integrals (15) for $\psi_2^{(1)}$.

IV. MATCHING

For $|\arg t-\pi|<3\pi/4$ one can do the analogous expansion of $g_+(t,-i\gamma)=g_a(t,-i\gamma)$ in (6). Again, one finds a Gaussian form if $t\ll\gamma^{1/6}$ (Ref. 15):

$$g_+(t,-i\gamma)\sim e^{i\pi\gamma}e^{-t^2/2}\left[1+\frac{3}{4t^2}-\frac{15}{32t^4}-\frac{t^3}{3\sqrt{\gamma}}-\frac{t}{4\sqrt{\gamma}}+\frac{5-16\ell(\ell+1)}{32t\sqrt{\gamma}}+\frac{t^6}{18\gamma}+\text{h.o.t.}\right]; \quad (24)$$

the first factor comes from encircling the horizon $r=1$. The leading corrections verify the consistency of expansions (21),(22), and (24), obtained in very different ways; all that matters for the matching is $[\cdots]=1+0\cdot t^0/\sqrt{\gamma}+\cdots$.

Comparison shows that

$$g_+e^{-i\pi\gamma}=\frac{\sqrt{\pi}}{8}[3i\gamma^{3/2}+(2-3i)\alpha\gamma+\mathcal{O}(\sqrt{\gamma})]\psi_1+\frac{2}{\sqrt{\pi}}\left(-\frac{1}{\sqrt{\gamma}}+\frac{\alpha}{\gamma}+\mathcal{O}(\gamma^{-3/2})\right)\psi_2, \quad (25)$$

which can be matched back to solutions in terms of g_a on $\arg t=\pi/4$, yielding

$$g_+(-i\gamma)=g_a(-i\gamma)+2e^{2\pi i\gamma}\left(i+\frac{\alpha}{\sqrt{\gamma}}\right)g_a(+i\gamma) \quad (26)$$

in the region (bounded by anti-Stokes lines) including $r=1$. Hence, in particular in the physical part $x<0$ of that region, one has

$$\Delta g(-i\gamma)=2i\,\mathrm{Im}\,g_+(-i\gamma)=4i\left[\cos(2\pi\gamma)+\frac{\alpha}{\sqrt{\gamma}}\sin(2\pi\gamma)\right]g(+i\gamma)\equiv iq(\gamma)g(+i\gamma). \quad (27)$$

Already, the numerically observed asymptotics[6] of $q(\gamma)$ have been confirmed. For the corrections, it remains to calculate α in closed form. Let us start with the ν-dependent term in (14), which clearly cannot be combined with the other two. Straightforward manipulations yield its contribution to $\psi_1^{(1)}$ as ($\arg t=\pi/4$)

$$\psi_1^{(1)}(t)\sim\frac{\sqrt{8\pi}}{\gamma^2}\nu\left[\cos\left(\frac{t^2}{2i}+\frac{\pi}{4}\right)\int_0^\infty\frac{dz}{\sqrt{z}}J_1(z)Y_1(z)+\cos\left(\frac{t^2}{2i}+\frac{3\pi}{4}\right)\int_0^\infty\frac{dz}{\sqrt{z}}J_1^2(z)\right]. \quad (28)$$

By considering the asymptotics of $\int_0^K(dz/\sqrt{z})J_1(z)H_1^{(1)}(z)$ (H are Hankel functions) in the upper-half K plane [again using the formula for $Y_1(e^{i\pi}z)$ above (17)], one convinces oneself that in fact $\int_0^\infty(dz/\sqrt{z})J_1(z)Y_1(z)=-\int_0^\infty(dz/\sqrt{z})J_1^2(z)$, which is also necessary for this contribution to α to be real. The latter integral is tabulated as $\int_0^\infty(dz/\sqrt{z})J_1^2(z)=\Gamma(\frac{1}{4})^4/12\pi^{5/2}$ (Ref. 16). Thus, the present contribution to α reads

$$\alpha_1=-\frac{\nu\Gamma(\frac{1}{4})^4}{24\pi^{3/2}}. \quad (29)$$

The last term of (14) analogously leads to the integrals $\int_0^\infty dz\,\sqrt{z}J_1(z)J_0(z)=-\int_0^\infty dz\,\sqrt{z}Y_1(z)J_0(z)=\Gamma(\frac{1}{4})^4/16\pi^{5/2}$, for a contribution

$$\alpha_2=\frac{\Gamma(\frac{1}{4})^4}{32\pi^{3/2}}. \quad (30)$$

However, the first term of (14), with its higher power of s, leads to diverging integrals:

$$\int_0^K dz\,z^{3/2}J_1^2(z)\sim\frac{2}{3\pi}K^{3/2}+\frac{1}{2\pi}\sqrt{K}\cos(2K)+c_3+\mathcal{O}(K^{-1/2}), \quad (31)$$

$$\int_0^K dz\,z^{3/2}J_1(z)Y_1(z)\sim\frac{1}{2\pi}\sqrt{K}\sin(2K)+d_3+\mathcal{O}(K^{-1/2}). \quad (32)$$

If $d_3=-c_3$, these lead to a real contribution

$$\alpha_3=-2\pi c_3. \quad (33)$$

Unfortunately, the general $\int_0^K dz\,z^{3/2}J_1^2(z)=(K^{9/2}/18)\,{}_2F_3(\frac{3}{2},\frac{9}{4};2,3,\frac{13}{4};-K^2)$ does not help directly, since not enough seems to be known about the asymptotics of ${}_2F_3$. Instead, one can proceed as follows: $d_3=-c_3$ can again be proven by studying $\int_0^K dz\,z^{3/2}J_1(z)H_1^{(1)}(z)$ in the upper-half plane. It is then logical to also consider $\int_0^K dz\,z^{3/2}H_1^{(1)}(z)^2$, in which one can take $K\to i\infty$. One finds

$$c_3=\frac{\sqrt{2}}{\pi^2}\int_0^\infty dw\,w^{3/2}K_1^2(w)=\frac{5\Gamma(\frac{1}{4})^4}{192\pi^{5/2}}. \quad (34)$$

The rest is straightforward: (29), (30), and (33) with (34) can be added and substituted into (27), from which one can read off our final answer

$$q(\gamma)\sim 4\cos(2\pi\gamma)+\frac{\Gamma(\frac{1}{4})^4}{12\pi^{3/2}}[1-\ell(\ell+1)]\frac{\sin(2\pi\gamma)}{\sqrt{\gamma}}+\mathcal{O}(\gamma^{-1}), \tag{35}$$

where $\Gamma(\frac{1}{4})^4/12\pi^{3/2}=2.586\ldots$. The *result* for the leading term has appeared before in Ref. 6; preliminary results from a transmission-amplitude calculation seem support the form for the corrections, in particular, the ℓ dependence.[17]

V. DISCUSSION

The above analysis, for $r,\gamma\to\infty$, is the third instance where the mathematics of the RWE near $r=0$ has been seen to influence the goings-on in our universe $r>1$. The first instance is the question of ''anomalous'' vs ''miraculous'' waves outgoing into the horizon, i.e., $r\downarrow 1$ and $2\gamma\in\mathbb{N}$ (Ref. 8, Sec. VI). The second instance is the dynamics at and around the algebraically special frequency $\gamma=N/2$, where the RWE has closed-form solutions, whose global behavior in the r plane can therefore be traced.[6,8]

Besides the axial waves described by the RWE (1), (2) there are also polar waves, described by the Zerilli equation.[18] However, the latter's ''intertwining'' or supersymmetry relation to the RWE yields its cut strength as $\tilde{q}(\gamma)=[(N/2-\gamma)/(N/2+\gamma)]q(\gamma)$ (Ref. 8). Thus, q and $\tilde{q}$ agree up to an overall sign, plus $\mathcal{O}(\gamma^{-1})$ corrections immaterial to (35).

For an outlook, the first obvious item is the numerical verification of (35), in particular of the subleading correction. A brute-force increase of numerical precision in the existing method is unlikely to suffice, especially for $\ell\geqslant 3$. More promising is to calculate $g_{\pm}(-i\gamma)$ directly on the NIA, instead of through extrapolation to this axis. In the series for $g(\omega)$ (Refs. 6 and 12), the problem for $\mathrm{Re}\,\omega\to 0$ is not convergence but rather obtaining the individual (irregular-hypergeometric) terms reliably. Working this out should be mainly a matter of time, but it remains to be seen if it would sufficiently extend the range of validity in γ.

Related to this, it is worth re-emphasizing[8] that the present method involves two conceptually separate steps: (a) the continuation in r, stabilizing the OWC at infinity in the lower-half ω plane, leading to a well-defined computational problem, and (b) the asymptotics, by which one can actually solve this problem analytically for large γ. The second step is optional,[9] and numerical integration of g_+ from $r=-\infty$ (combined with standard series solutions for f) should soon open up the third ω quadrant (i.e., behind the cut) to direct exploration, especially for at most moderate damping.

It would also be interesting if this work could be compared to the closed-form expression for $q(\gamma)$ in (31)–(33) of Ref. 4, through the coefficients $d_L^{(\nu)}$ of an expansion $g\propto\Sigma_{L=-\infty}^{\infty}d_L^{(\nu)}u_{L+\nu}$; here, $u_{L+\nu}$ are Coulomb wave functions. As usual, the $d_L^{(\nu)}$ satisfy a three-term recursion relation (given in a simplified form, which can be made purely real on the NIA, in Sec. VI F of Ref. 12); $0\leqslant\nu<1$ is to be chosen such that $d_L^{(\nu)}$ is the minimal solution to this relation for both $L\to\infty$ and $-\infty$. The adiabatic ansatz of slowly varying $d_{L+1}^{(\nu)}/d_L^{(\nu)}$ readily yields asymptotic solutions for $\gamma\to\infty$, except near $L=\pm\gamma$ and $L=0$. Following Ref. 19, one can try to develop connection formulas near these three points, which would determine ν analytically. At the ''turning points'' $L=\pm\gamma$, the three-term recursion asymptotically degenerates into a *two*-term one, and the connection proceeds exactly as in Ref. 19. Near $L=0$, however, all three terms are of the same order (in γ), and the recursion remains in the form of analytically intractable continued fractions (i.e., without simplifying to products). Thus, this route for now seems unfeasible.

At least to leading order, the method of continuation through the vicinity of $r=0$ has meanwhile independently been used to calculate the high-damping QNM frequencies.[11] On the one hand, this yields more information on the QNM *wave functions* than the continued-fraction technique.[19] On the other, this clearly establishes a relation to the present problem of the branch-cut strength $q(\gamma)$. Thus one can expect also *numerical* results for these two high-damping aspects of the RWE to bear on each other, and an extension to other black-hole models. Conversely, this work's progress on the corrections should help finding the $\mathcal{O}(|\omega|^{-1/2})$ terms for the asymptotic QNM frequencies. Meanwhile, this has indeed been possible; see the Appendix.

In particular, these developments render it urgent to study the branch cut of the RWE's Green's function also for other values of the spin s, where (2) corresponds to $s=2$. Notably, the highly damped electromagnetic ($s=1$) QNMs are predicted[11,19] to approach the NIA asymptotically so that one expects an even closer, though yet unknown, relation to the branch cut in that case.

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APPENDIX: HIGH-DAMPING QNMs

For frequencies close to the NIA, it should certainly be possible to analytically continue (26) and find those γ for which g_+ also satisfies the OWC into the horizon, i.e., $g_+(\omega)\propto f(\omega)$. These should identify the highly damped QNMs. Here, f is characterized by its monodromy around the horizon:

$$f((r-1)e^{2\pi i},\omega)=e^{2\pi\omega}f(r-1,\omega). \tag{A1}$$

Inspecting (6), it seems that $f(\omega)=g_{\mathrm{a}}(-\omega)$, but this is deceptive. While it *is* true that $f(-\omega)=g_{\mathrm{a}}(\omega)$ in the lower-half ω plane, the asymptotic nature of the large (near $r=1$) solution $g_{\mathrm{a}}(-\omega)$ means that naive rotation of $r-1$ only confirms the desired monodromy to dominant order, whereas f is required to obey it exactly.

The solution is to, in the spirit of Refs. 11 and 17, do the rotation along the anti-Stokes contour in Fig. 1, where neither solution dominates the other (skipping $r=0$ on the inside). By the normalization of f one knows the dominant component, so we take the ansatz

$$f(-i\gamma)=g_{\mathrm{a}}(i\gamma)+c(\gamma)g_{\mathrm{a}}(-i\gamma). \tag{A2}$$

Continuing this from the physical $x=0$ to $1/\sqrt{\gamma}\ll|r|\ll 1$ with $\arg r=\pi/4$, one finds

$$\begin{aligned} f(-i\gamma)&\sim e^{-i\pi\gamma}e^{t^2/2}+c(\gamma)e^{i\pi\gamma}e^{-t^2/2}\\ &\sim\frac{\sqrt{\pi\gamma^3}}{8}\left[e^{-i\pi\gamma}\left\{1+\frac{(i-2)\alpha}{\sqrt{\gamma}}\right\}+c(\gamma)e^{i\pi\gamma}\left\{i+\frac{(2+i)\alpha}{\sqrt{\gamma}}\right\}\right]\psi_1\\ &\quad+\frac{2}{\sqrt{\pi\gamma}}\left[e^{-i\pi\gamma}\left\{i-\frac{\alpha}{\sqrt{\gamma}}\right\}+c(\gamma)e^{i\pi\gamma}\left\{1+\frac{\alpha}{\sqrt{\gamma}}\right\}\right]\psi_2; \end{aligned} \tag{A3}$$

the second line followed by comparison with (21),(22). As before, (17)–(20) make quick work of continuing this to $\arg r=-\pi/4$, where it can be matched back to a combination of $g_{\mathrm{a}}(\pm i\gamma)$. One thus finds $f((r-1)e^{2\pi i},-i\gamma)=e^{-2\pi i\gamma}g_{\mathrm{a}}(r-1,i\gamma)+[2i(1-\alpha/\sqrt{\gamma})+c(\gamma)e^{2\pi i\gamma}]g_{\mathrm{a}}(r-1,-i\gamma)$. Indeed f as in (A2) obeys (A1) to dominant order for any c, while the subdominant ($\propto c$) term by itself has the opposite monodromy, corresponding to incoming waves—both as stipulated above. Equation (A1) holds exactly for

$$c(\gamma)\sim-\frac{1-\alpha/\sqrt{\gamma}}{\sin(2\pi\gamma)}. \tag{A4}$$

As required, $c(\gamma\in\mathbb{R})\in\mathbb{R}$, since the exponential tail of $V(x\to-\infty)$ does not generate a branch cut in $f(\omega)$. Also the poles for $2\gamma\in\mathbb{N}$ are not surprising, since the RWE is known to have such *anomalous points* for $2\gamma=1,2,\ldots$, with exactly *one* exception at $2\gamma=N$ (Ref. 8); clearly, the latter

is beyond the reach of the present asymptotics. Expressing $f(\pm\omega)$, $g(\pm\omega)$ not through g_a but in terms of each other, the S matrix could be read off; cf. Ref. 17 for the leading order.

Combining (26), (A2), and (A4), all that remains is to asymptotically solve

$$0=J(-i\gamma)\propto\sin(2\pi\gamma)+2e^{2\pi i\gamma}\left(i+\frac{\alpha}{\sqrt{\gamma}}\right)\left(1-\frac{\alpha}{\sqrt{\gamma}}\right)\approx\sin(2\pi\gamma)+2ie^{2\pi i\gamma}\left(1-\frac{(1+i)\alpha}{\sqrt{\gamma}}\right). \tag{A5}$$

Reexpressing the answer in terms of ω and substituting α from the main text, one obtains

$$\omega_n=\frac{\ln 3}{4\pi}-\left(\frac{n}{2}+\frac{1}{4}\right)i+\frac{\sqrt{2}\Gamma(\frac{1}{4})^4}{144\pi^{5/2}}(1+i)\,\frac{\ell(\ell+1)-1}{\sqrt{n}}+\mathcal{O}(n^{-1}), \tag{A6}$$

where the prefactor of the correction evaluates to 0.097 007... . The ω_n have automatically come out on the physical sheet of g_+; contrast Ref. 19, which is not sheet-specific. Agreement with (29) and (30) in Ref. 20 is excellent; as anticipated in the discussion, this numerical confirmation of the value of α via the *QNMs* greatly supports (35) for the *cut*. To my knowledge, this is the first time that the correction to the highly damped Schwarzschild QNM frequencies has been calculated analytically.

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Continuous symmetries of Lagrangians and exact solutions of discrete equations

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One of the difficulties encountered when studying physical theories in discrete space–time is that of describing the underlying continuous symmetries (like Lorentz, or Galilei invariance). One of the ways of addressing this difficulty is to consider point transformations acting simultaneously on difference equations and lattices. In a previous article we have classified ordinary difference schemes invariant under Lie groups of point transformations. The present article is devoted to an invariant Lagrangian formalism for scalar single-variable difference schemes. The formalism is used to obtain first integrals and explicit exact solutions of the schemes. Equations invariant under two- and three-dimensional groups of Lagrangian symmetries are considered. © *2004 American Institute of Physics.*
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I. INTRODUCTION

A recent article was devoted to a symmetry classification of second-order ordinary difference equations.[1] This was modeled on a paper by Sophus Lie, in which he provided a symmetry classification of second order ordinary differential equations (ODEs).[2] As a matter of fact, the classification of difference schemes goes over into Lie's classification of ODEs in the continuous limit.[1]

Lie showed that a second-order ODE can be invariant under a group G_r of dimension $N=0,1,2,3$, or 8. For $N\geqslant 2$ the equation can be integrated in quadratures. This can be done by transforming the equation to one of the ''canonical'' forms, integrated by Lie himself.[2] Virtually all standard methods of integrating second-order ODEs analytically can be interpreted in this manner (though this is not mentioned in most elementary textbooks).

The situation with difference equations is much less developed. This is not surprising, since applications of Lie group theory to difference equations are much more recent.[3–27] Several different approaches are being pursued. One possibility is to consider the difference equations on a fixed lattice[3–13] and consider only transformations that do not act on the lattice. In order to obtain physically interesting symmetries in this approach, it is necessary to go beyond point symmetries and to let the transformations act on more than one point of the lattice. Lie algebra contractions occur in the continuous limit and some ''generalized'' symmetries may ''contract'' to point ones.[10]

The second possibility is to consider group transformations acting both on the difference equations and on the lattice.[1,17–27] Technically, for systems involving one dependent and one

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independent variable, this is achieved by considering a difference scheme, consisting of two equations, one representing the actual difference equation, the other the lattice.

This is the approach that we will follow in the present article. More specifically, we will consider the same three-point scheme as in our previous article.[1] The continuous limit of the scheme, if it exists, will be a second-order ODE.

Thus, we consider two variables, x and y, with x the independent one and y dependent. The variable x runs through an infinite set of values $\{x=x_k,\ k\in\mathbb{Z}\}$ that are not necessarily equally spaced and are not prescribed *a priori*. Instead, we give two relations between any three neighboring points

$$F(x,x_-,x_+,y,y_-,y_+)=0, \tag{1.1}$$

$$\Omega(x,x_-,x_+,y,y_-,y_+)=0 \tag{1.2}$$

and also specify some initial conditions like x_0, x_1, $y_0=y(x_0)$, $y_1=y(x_1)$. In the continuous limit Eq. (1.1) goes into an ODE, (1.2) into an identity (like $0=0$), if the continuous limit exists.

The group transformations considered in this approach are of the same type as for ODEs. They are generated by a Lie algebra of vector fields of the form

$$X=\xi(x,y)\frac{\partial}{\partial x}+\eta(x,y)\frac{\partial}{\partial y}. \tag{1.3}$$

The corresponding transformations are purely point ones, since the coefficients ξ and η depend only on (x,y), not on the shifted points (x_+,y_+) or (x_-,y_-).

In Ref. 1 we showed how Lie group theory can be used to classify such pairs of equations as (1.1) and (1.2). Possible dimensions of the symmetry group G of Eqs. (1.1) and (1.2) are $N=0,1,2,3,4,5$, and 6. The highest dimension, $N=6$, occurs only for difference schemes equivalent to

$$\frac{y_+-2y+y_-}{(x_+-x)^2}=0,\quad x_+-2x+x_-=0.$$

The purpose of this article is to provide a Lagrange formalism and difference analog of Noether's theorem for second-order difference schemes of the form (1.1) and (1.2), admitting Lie point symmetry groups. The Lagrangians will be used to obtain first integrals and exact analytic solutions of the difference schemes.

II. GENERAL THEORY

A. Definitions and notations

We study the difference system (1.1) and (1.2). In general, we assume that these equations can be solved to express x_+ and y_+ explicitly in terms of (x,y,x_-,y_-) and also vice versa, i.e. (x_-,y_-) in terms of the other quantities. We also make use of the following quantities:

$$h_+=x_+-x,\quad h_-=x-x_-,\quad y_x=\frac{y_+-y}{h_+},\quad y_{\bar{x}}=\frac{y-y_-}{h_-},$$
$$y_{x\bar{x}}=\frac{2}{h_++h_-}(y_x-y_{\bar{x}}), \tag{2.1}$$

i.e., the up and down spacings in x, the right and left discrete first derivatives and the discrete second derivative, respectively. It is also convenient to use the following total shift and discrete differentiation operators:

$$\underset{\pm h}{S} f(x)=f(x_{\pm}), \quad \underset{\pm h}{D}=\frac{\overset{\pm h}{S}-1}{\pm h_{\pm}}.$$

Continuous first and second derivatives are denoted y' and y'', respectively.

When acting on differential equations, the vector fields (1.3) must be prolonged to act on derivatives. For difference schemes, the prolongation of a vector field acts on variables at other points of the lattice. It is obtained by shifting the coefficients to the corresponding points. For three point schemes we have

$$\mathbf{pr}\, X=X+\xi(x_-,y_-)\frac{\partial}{\partial x_-}+\xi(x_+,y_+)\frac{\partial}{\partial x_+}+\eta(x_-,y_-)\frac{\partial}{\partial y_-}+\eta(x_+,y_+)\frac{\partial}{\partial y_+}. \tag{2.2}$$

B. Lagrangian formulation for second-order ODEs

It has been known since Noether's fundamental work that conservation laws for differential equations are connected with their symmetry properties.[28–31] For convenience we present here some well-known results adapted to the case of second-order ODEs.

Let us consider the functional

$$\mathbb{L}(y)=\int_I L(x,y,y')\mathrm{d}x, \quad I\subset\mathbb{R}^1, \tag{2.3}$$

where $L(x,y,y')$ is called a first-order Lagrangian. The functional (2.3) achieves its extremal values when $y(x)$ satisfies the Euler–Lagrange equation

$$\frac{\delta L}{\delta y}=\frac{\partial L}{\partial y}-D\left(\frac{\partial L}{\partial y'}\right)=0, \quad D=\frac{\partial}{\partial x}+y'\frac{\partial}{\partial y}+y''\frac{\partial}{\partial y'}+\cdots, \tag{2.4}$$

where D is the total derivative operator. Equation (2.4) is an ODE that can be rewritten as

$$y''=f(x,y,y'). \tag{2.5}$$

Let us consider a Lie point transformation G generated by the vector field (1.3). The group G is a ''variational symmetry'' of the functional $\mathbb{L}$ if and only if the Lagrangian satisfies

$$\mathrm{pr}\, X(L)+LD(\xi)=0, \tag{2.6}$$

when $\mathrm{pr}\, X$ is the first prolongation of the vector field X for y'. We will actually need a weaker invariance condition than given by Eq. (2.6). The vector field X is an ''infinitesimal divergence symmetry'' of the functional $\mathbb{L}(y)$ if there exists a function $V(x,y)$ such that[28]

$$\mathrm{pr}\, X(L)+LD(\xi)=D(V), \quad V=V(x,y). \tag{2.7}$$

The two important statements for us follow.

(1) If X is an infinitesimal divergence symmetry of the functional $\mathbb{L}$, it generates a symmetry group of the corresponding Euler–Lagrange equation. The symmetry group of Eq. (2.4) can of course be larger than the one generated by symmetries of the Lagrangian.

(2) Noether's theorem[28–31] can be based on the following Noether-type identity,[31] which holds for any vector field and any function L:

$$\mathrm{pr}\, X(L)+LD(\xi)=(\eta-\xi y')\frac{\delta L}{\delta y}+D\left(\xi L+(\eta-\xi y')\frac{\partial L}{\partial y'}\right). \tag{2.8}$$

It follows that if X is a divergence symmetry of L, i.e., (2.6) or (2.7) is satisfied, then there exists a first integral

$$\xi L+(\eta-\xi y')\frac{\partial L}{\partial y'}-V=K=\text{const} \tag{2.9}$$

of the corresponding Euler–Lagrange equation.

The above considerations tell us how to obtain invariant ODEs and conservation laws from divergence invariant Lagrangians. They do not tell us how to obtain invariant Lagrangians for invariant equations. This amounts to ''variational integration,'' as opposed to variational differentiation.

A procedure that we shall use in the following to find invariant Lagrangians for differential equations can be summed up as follows.

Start from a given ODE $y''=f(x,y,y')$ and its symmetry algebra with basis

$$X_\alpha=\xi_\alpha(x,y)\frac{\partial}{\partial x}+\eta_\alpha(x,y)\frac{\partial}{\partial y},\quad \alpha=1,\ldots,k.$$

Find the invariants of X_α in the space $\{x,y,y',\Lambda\}$, where Λ is the Lagrangian. The appropriate prolongation in this case is

$$\mathrm{pr}\,X=\xi\frac{\partial}{\partial x}+\eta\frac{\partial}{\partial y}+\zeta^1\frac{\partial}{\partial y'}-(D\xi)\Lambda\frac{\partial}{\partial\Lambda},\quad \zeta^1=D(\eta)-y'D(\xi) \tag{2.10}$$

and we require that $L(x,y,y')$ should satisfy

$$\mathrm{pr}\,X(\Lambda-L)|_{\Lambda=L}=0. \tag{2.11}$$

Each basis element X_α provides us with an equation of the form

$$\xi_\alpha\frac{\partial L}{\partial x}+\eta_\alpha\frac{\partial L}{\partial y}+\zeta^1_\alpha\frac{\partial L}{\partial y'}-LD(\xi_\alpha)=0. \tag{2.12}$$

Solve the partial differential equations (2.12). This will give us the general form of an invariant Lagrangian. It may involve arbitrary functions of the invariants of X.

Request that the Euler–Lagrange equation (2.4) should coincide with the equation we started from. This will further restrict the invariant Lagrangian and determine whether one exists.

If this procedure does not yield a suitable Lagrangian, then step 1 can be weakened. We can request that the Lagrangian be invariant under some subgroup of the symmetry group of the given ODE, rather then the entire group. We then go through step 2, then verify whether the obtained Lagrangian is divergence invariant under the entire group, or at least a larger subgroup. In any case, each divergence symmetry of the Lagrangian will provide a first integral of the ODE.

For ODEs the Lagrangian formalism is not the only integration method. The existence of one-parameter symmetry group provides a reduction to a first-order ODE directly. The existence of a two-parameter symmetry group makes it possible to integrate in quadratures. An invariant Lagrangian provides an alternative. Indeed, assume that we know two first integrals

$$f_1(x,y,y')=A,\quad f_2(x,y,y')=B, \tag{2.13}$$

then we eliminate y' from these two equations and obtain the general solution

$$y=F(x,A,B), \tag{2.14}$$

of the corresponding ODE (2.5) by purely *algebraic* manipulations. It is this method of invariant Lagrangians that generalizes to difference equations and is particularly useful when direct methods fail.

C. Lagrangian formalism for second-order difference equations

The variational formulation of discrete equations and a discrete analog of Noether's theorem are much more recent.[19,25–27] Here we briefly overview the results that we shall need in the following.

Let us consider a finite difference functional

$$\mathbb{L}_h=\sum_{\Omega}\ \mathcal{L}(x,x_+,y,y_+)h_+, \tag{2.15}$$

defined on some one-dimensional lattice Ω with step h_+ that generally can depend on the solution

$$h_+=\varphi(x,y,x_+,y_+). \tag{2.16}$$

The functional (2.15) must be considered together with a lattice (2.16). On different lattices it can have different continuous limits and in this limit the lattice equation itself vanishes (turns into an identity like $0=0$)

In the continuous case, a Lagrangian L provides an equation (the Euler–Lagrange equation) that inherits all the symmetries of L. In the discrete case we wish the Lagrangian (2.15) to provide two equations: the entire difference system (1.1), (1.2). Moreover, the three-point difference system should inherit the symmetries of two-point Lagrangian.

Let us again consider a Lie group of point transformations, generated by a Lie algebra of vector fields X_α of the form (1.3). The infinitesimal invariance condition of the functional (2.15) on the lattice (2.16) is given by two equations:[19,25,27]

$$\begin{gathered}\xi\frac{\partial\mathcal{L}}{\partial x}+\xi^+\frac{\partial\mathcal{L}}{\partial x_+}+\eta\frac{\partial\mathcal{L}}{\partial y}+\eta^+\frac{\partial\mathcal{L}}{\partial y_+}+\mathcal{L}\underset{+h}{D}(\xi)=0,\\ \underset{+h}{S}(\xi)-\xi=X(\varphi),\end{gathered} \tag{2.17}$$

where

$$\xi^+=\xi(x_+,y_+),\quad \eta^+=\eta(x_+,y_+). \tag{2.18}$$

Let us consider a variation of the difference functional (2.15) along some curve $y=\phi(x)$ at some point (x,y). The variation will effect only two terms in the sum (2.15):

$$\mathbb{L}_h=\cdots+\mathcal{L}(x,x_-,y,y_-)h_-+\mathcal{L}(x,x_+,y,y_+)h_++\cdots, \tag{2.19}$$

so we get the following expression for the variation of the difference functional:

$$\delta\mathbb{L}_h=\frac{\delta\mathcal{L}}{\delta x}\delta x+\frac{\delta\mathcal{L}}{\delta y}\delta y, \tag{2.20}$$

where $\delta y=\phi'\,\delta x$ and

$$\frac{\delta\mathcal{L}}{\delta x}=h_+\frac{\partial\mathcal{L}}{\partial x}+h_-\frac{\partial\mathcal{L}^-}{\partial x}+\mathcal{L}^--\mathcal{L},\quad \frac{\delta\mathcal{L}}{\delta y}=h_+\frac{\partial\mathcal{L}}{\partial y}+h_-\frac{\partial\mathcal{L}^-}{\partial y},$$

where $\mathcal{L}^-=S_{-h}(\mathcal{L})$.

Thus, for an arbitrary curve the stationary value of difference functional is given by any solution of the *two* equations, called *quasiextremal equations*,

$$\frac{\delta \mathcal{L}}{\delta x}=0, \quad \frac{\delta \mathcal{L}}{\delta y}=0. \tag{2.21}$$

Both of them tend to the differential Euler–Lagrange equation in the continuous limit. Together they represent the entire difference scheme and could be called ''the discrete Euler–Lagrange system.'' The difference between these two equations, or some other function of them that vanishes in the continuous limit will represent the lattice.

Now let us consider a vector field (1.3) with given coefficients $\xi(x,y)$ and $\eta(x,y)$. Variations along the integral curves of this vector field are given by $\delta x=\xi da$ and $\delta y=\eta da$, where da is a variation of a group parameter. A stationary value of the difference functional (2.15) along the flow generated by this vector field is given by

$$\xi \frac{\delta \mathcal{L}}{\delta x}+\eta \frac{\delta \mathcal{L}}{\delta y}=0, \tag{2.22}$$

which depends explicitly on the coefficients of the generator.

If we have a Lie algebra of vector fields of dimension 2 or more, then a stationary value of the difference functional (2.15) along the entire flow will be achieved on the intersection of the solutions of all equations of the type (2.22), i.e., on the quasiextremals (2.21).

On the other hand, Eq. (2.21) can be interpreted as a three-point difference scheme of the form (1.1) and (1.2). For instance, given two points (x,y) and (x_-,y_-), we can calculate (x_+,y_+). In the continuous limit both of these equations will provide the same second-order differential equation. Thus, one of the quasiextremal equations can be identified with Eq. (1.1) and the difference between the two of them with the lattice equation (1.2).

It has been shown elsewhere,[19,25,27] that if the functional (2.15) is invariant under some group G, then the quasiextremal equations (2.21) are also invariant with respect to G. As in the continuous case, the quasiextremal equations can be invariant with respect to a larger group than the corresponding Lagrangian.

A useful operator identity, valid for any Lagrangian $\mathcal{L}(x,x_+,y,y_+)$ and any vector field X is (Refs. 19 and 25)

$$\xi \frac{\partial \mathcal{L}}{\partial x}+\xi^+ \frac{\partial \mathcal{L}}{\partial x_+}+\eta \frac{\partial \mathcal{L}}{\partial y}+\eta^+ \frac{\partial \mathcal{L}}{\partial y_+}+\mathcal{L} \underset{+h}{D}(\xi)=\xi\left(\frac{\partial \mathcal{L}}{\partial x}+\frac{h_-}{h_+}\frac{\partial \mathcal{L}^-}{\partial x}-\underset{+h}{D}(\mathcal{L}^-)\right)+\eta\left(\frac{\partial \mathcal{L}}{\partial y}+\frac{h_-}{h_+}\frac{\partial \mathcal{L}^-}{\partial y}\right)$$
$$+\underset{+h}{D}\left(h_-\eta\frac{\partial \mathcal{L}^-}{\partial y}+h_-\xi\frac{\partial \mathcal{L}^-}{\partial x}+\xi\mathcal{L}^-\right). \tag{2.23}$$

From Eq. (2.23) we obtain the following discrete analog of Noether's theorem.

Theorem 2.1: Let the Lagrangian density $\mathcal{L}$ be divergence invariant under a Lie group G of local point transformations generated by vector fields X of the form (1.3), i.e., let us have

$$\mathbf{pr}\,X(\mathcal{L})+\mathcal{L}\underset{+h}{D}(\xi)=\underset{+h}{D}(V) \tag{2.24}$$

for some function $V(x,y)$. Then each element X of the Lie algebra corresponding to G provides us with a first integral of the quasiextremal equations (2.21), namely,

$$K=h_-\eta\frac{\partial \mathcal{L}^-}{\partial y}+h_-\xi\frac{\partial \mathcal{L}^-}{\partial x}+\xi\mathcal{L}^- -V. \tag{2.25}$$

Proof:[19,25] On solutions of the quasiextremal equations (2.21) Eq. (2.23) reduces to

$$\underset{+h}{D}\left(h_-\eta\frac{\partial\mathcal{L}^-}{\partial y}+h_-\xi\frac{\partial\mathcal{L}^-}{\partial x}+\xi\mathcal{L}^-\right)=\underset{+h}{D}(V) \tag{2.26}$$

[we have used Eq. (2.23)]. The result (2.25) follows immediately. □

The fundamental equation (2.25) is the discrete analog of Eq. (2.9) for ODEs.

Let us compare the situation for second-order ODEs and for three-point difference schemes. For a second-order ODE a Lagrangian that is divergence invariant under a two-dimensional symmetry group provides two integrals of motion. From them we can eliminate the remaining first derivative and obtain the general solution, depending on two arbitrary constants (the two first integrals). Moreover, we do not really need a Lagrangian. Once we have a two-dimensional symmetry group of the ODE, we can integrate in quadratures.

For three-point difference schemes we have two equations to solve, namely, the system (1.1) and (1.2). Equivalently, we have a set of points (x_n,y_n), labeled by an integer n. Any three neighboring points are related by two equations that we can write, e.g., as

$$y_{n+1}=F_1(x_n,y_n,x_{n-1},y_{n-1}),\quad x_{n+1}=\Omega_1(x_n,y_n,x_{n-1},y_{n-1}). \tag{2.27}$$

Alternatively, the system could be solved for x_{n-1},y_{n-1}. We mention that we use notations like $x_{n-1}=x_-$, $x_n=x$, $x_{n+1}=x_+$, $y_{n-1}=y_-$, $y_n=y$, $y_{n+1}=y_+$ interchangeably.

Given some starting values (x_0,y_0,x_{-1},y_{-1}), we can solve (2.27) for (x_n,y_n) with $n\geqslant 1$, and $n\leqslant -2$. The solution will depend on four constants $K_i, i=1,\ldots,4$, and can be written as

$$y_n=y_n(x_n,K_1,K_2,K_3,K_4), \tag{2.28}$$

$$x_n=x_n(K_1,K_2,K_3,K_4). \tag{2.29}$$

The two quasiextremal equations (2.21) correspond to the system (2.27).

A one-parameter symmetry group of the Lagrangian $\mathcal{L}$ will provide us with a first integral (2.25), i.e., an equation of the form

$$f(x_n,y_n,x_{n+1},y_{n+1})=K_1, \tag{2.30}$$

compatible with the system (2.21). We can solve (2.30) for, e.g., y_{n+1}, substitute into (2.27) and thus simplify this system.

A two-dimensional symmetry group will provide two first integrals of the form (2.25). We can solve for x_{n+1} and y_{n+1}. Then system (2.27) is reduced to a two-point difference scheme. Quite often it is possible to solve it by integration methods that allow one to integrate a two-point difference scheme explicitly.

A three-dimensional symmetry group provides three first integrals of the type (2.25). From them we can express x_{n-1},y_{n-1} and y_n in terms of x_n. This provides us with the solution (2.28) and a two-point difference equation relating x_{n+1} and x_n. If this equation can be solved, we have a complete solution of the problem. Finally, if we have four first integrals, then we get the general solution of the system by purely algebraic manipulations.

An alternative method can be proposed when the Lagrangian is invariant with respect to a two-dimensional Lie group. The discrete Lagrangian corresponding to a given continuous one is not unique and it is possible to introduce a family of Lagrangians:

$$\mathcal{L}_i=\mathcal{L}_i(x,x_+,y,y_+,\alpha_i,\beta_i),\quad i=1,2,3,\ldots \tag{2.31}$$

depending on parameters α_i,β_i, all satisfying

$$\lim_{(x_+,y_+)\to(x,y)}\mathcal{L}_i(x,x_+,y,y_+,\alpha_i,\beta_i)=L(x,y,y')$$

for the same continuous Lagrangian $L(x,y,y')$.

Let us take three different Lagrangians in the family (2.31), corresponding to constants $\alpha_1,\beta_1,\alpha_2,\beta_2$ and α_3,β_3. Each of them will lead to two first integrals and two quasiextremals. In the examples considered in the following we will show that it is possible to fine-tune the constants α_i,β_i in such a manner as to get a system of two invariant equations of the form (1.1) and (1.2) and three first integrals, yielding a set of solutions to the two quasiextremal equations. It is these two equations that will constitute the invariant difference system.

In Sec. II B we described a procedure for obtaining invariant Lagrangians for given second-order differential equation. For difference equations our starting point will be a discretization of the continuous Lagrangian. This is obviously not unique and we shall make use of the inherent arbitrariness. Once an invariant difference Lagrangian with a correct continuous limit is chosen we construct the invariant difference scheme in the above-described manner.

In our previous article[1] we gave a classification of difference schemes and used all realizations of Lie algebras that provide such schemes. Any algebra containing a two-dimensional subalgebra realized by linearly connected vector fields such as

$$\left(\frac{\partial}{\partial x},\, y\frac{\partial}{\partial x}\right),\quad \left(\frac{\partial}{\partial x},\, x\frac{\partial}{\partial x}\right),$$

leads to a linear differential equation and its discretization.

In the following we shall consider only genuinely nonlinear difference schemes presented in Ref. 1 that have nonlinear differential equations as their limit.

III. EQUATIONS CORRESPONDING TO LAGRANGIANS INVARIANT UNDER ONE- AND TWO-DIMENSIONAL GROUPS

A. One-dimensional symmetry group

We start with the simplest case of a symmetry group, namely a one-dimensional group. Its Lie algebra is generated by one vector field of the form (1.3). By an appropriate change of variables we take this vector field into its rectified form. Thus we have

$$\mathbf{D_{1,1}}:\quad X_1=\frac{\partial}{\partial y}. \tag{3.1}$$

The most general second-order ODE invariant under X_1 is

$$y''=F(x,y'), \tag{3.2}$$

where F is an arbitrary given function.

Equation (3.2) is actually already reduced to a first-order equation for $u=y'$. If X_1 is a variational symmetry of Eq. (3.2) and we know the Lagrangian L that it comes from, we can do better. An invariant Lagrangian density will by necessity have the form $L=L(x,y')$ [see Eq. (2.6)]. The Euler–Lagrange equation (2.4) reduces to

$$\frac{\partial^2 L}{\partial x\partial y'}+y''\frac{\partial^2 L}{\partial y'^2}=0. \tag{3.3}$$

Substituting for y'' from Eq. (3.2), we obtain a linear partial differential equation for $L(x,y')$. This of course has an infinity of solutions. Let us assume that we know a solution $L(x,y)$ explicitly. Equation (2.9), i.e., Noether's theorem, provides us with a first integral

$$\frac{\partial L}{\partial y'}(x,y')=K. \tag{3.4}$$

We can solve (in principle) Eq. (3.4) for y' as a function of x (and K). The general solution is then obtained by a quadrature:

$$y' = \phi(x,K), \quad y(x) = y_0 + \int_0^x \phi(x,K)\,\mathrm{d}t. \tag{3.5}$$

In the discrete case the situation is similar. Let us assume that we know a Lagrangian $\mathcal{L}(x,x_+,y,y_+)$, invariant under the group of transformations of y, generated by X_1 of Eq. (3.1). It will have the form

$$\mathcal{L} = \mathcal{L}(x,x_+,y_x), \quad y_x = \frac{y_+ - y}{x_+ - x}. \tag{3.6}$$

The corresponding quasiextremal equations, to be identified with the system (1.1) and (1.2), are

$$\frac{\delta \mathcal{L}}{\delta y} = -\frac{\partial \mathcal{L}}{\partial y_x}(x,x_+,y_x) + \frac{\partial \mathcal{L}}{y_{\bar{x}}}(x_-,x,y_{\bar{x}}) = 0, \tag{3.7}$$

$$\frac{\delta \mathcal{L}}{\delta x} = h_+ \frac{\partial \mathcal{L}}{\partial x}(x,x_+,y_x) + y_x \frac{\partial \mathcal{L}}{\partial y_x}(x,x_+,y_x) - \mathcal{L}(x,x_+,y_x) + h_- \frac{\partial \mathcal{L}}{\partial x}(x_-,x,y_{\bar{x}}) - y_{\bar{x}} \frac{\partial \mathcal{L}}{\partial y_{\bar{x}}}(x_-,x,y_{\bar{x}}) + \mathcal{L}(x_-,x,y_{\bar{x}}) = 0. \tag{3.8}$$

The first integral (2.25) can be read off form Eq. (3.7) and is

$$\frac{\partial \mathcal{L}}{\partial y_x}(x,x_+,y_x) = K. \tag{3.9}$$

We can solve Eq. (3.9) for y_x and by downshifting obtain $y_{\bar{x}}$:

$$y_x = \phi(x,x_+,K), \quad y_{\bar{x}} = \phi(x_-,x,K). \tag{3.10}$$

Substituting into the quasiextremal equation (3.8), we obtain a relation between x_+, x_- and x, i.e., a single three-point relation for the variable x. For y we then obtain a two point equation

$$y_+ - y = (x_+ - x)\,\phi(x,x_+,K). \tag{3.11}$$

Equation (3.11) is really a discrete quadrature: a first-order inhomogeneous linear equation for y.

Example 3.1: Consider the Lagrangian

$$\mathcal{L} = x_n^a x_{n+1}^b \exp(y_x). \tag{3.12}$$

The quasiextremal equations are

$$-x_n^a x_{n+1}^b \exp(y_x) + x_{n-1}^a x_n^b \exp(y_{\bar{x}}) = 0, \tag{3.13}$$

$$h_+ a x_n^{a-1} x_{n+1}^b \exp(y_x) + y_x x_n^a x_{n+1}^b \exp(y_x) - x_n^a x_{n+1}^b \exp(y_x) + h_- b x_{n-1}^a x_n^{b-1} \exp(y_{\bar{x}}) - y_{\bar{x}} x_{n-1}^a x_n^b \exp(y_{\bar{x}}) + x_{n-1}^a x_n^b \exp(y_{\bar{x}}) = 0. \tag{3.14}$$

The first integral is

$$x_n^a x_{n+1}^b \exp(y_x) = K. \tag{3.15}$$

From (3.15) we have

$$y_x = \ln(K x_n^{-a} x_{n+1}^{-b}), \quad y_{\bar{x}} = \ln(K x_{n-1}^{-a} x_n^{-b}). \tag{3.16}$$

Equation (3.13) is satisfied identically. Equation (3.14) reduces to a three-point equation for x:

$$ax_{n+1}+(b-a)x_n-bx_{n-1}+x_n(-b\ln(x_{n+1})+(b-a)\ln(x_n)+a\ln(x_{n-1}))=0. \quad (3.17)$$

This lattice equation can be reduced to a two-point equation for a new variable $\lambda_n=x_{n+1}/x_n$:

$$a\lambda_n+(b-a)-\frac{b}{\lambda_{n-1}}=a\ln(\lambda_{n-1})+b\ln(\lambda_n). \quad (3.18)$$

In particular, one can choose the solution $\lambda_n=\lambda_{n+1}=\lambda$, where λ satisfies

$$a\lambda+(b-a)-\frac{b}{\lambda}=(a+b)\ln(\lambda).$$

It provides us with the lattice $x_n=x_0\lambda^n$.

Substituting the lattice into (3.15), we obtain a two-point equation for y:

$$y_{n+1}-y_n=(x_{n+1}-x_n)\ln(Kx_n^{-a}x_{n+1}^{-b}). \quad (3.19)$$

The fact that we could solve Eq. (3.17) explicitly is specific for the considered example. The fact that we obtain a three-point equation involving only the independent variables is true in general.

B. Two-dimensional symmetry groups

$\mathbf{D_{2,1}}$: The Abelian Lie algebra with nonconnected basis elements

$$X_1=\frac{\partial}{\partial x}, \quad X_2=\frac{\partial}{\partial y} \quad (3.20)$$

corresponds to the invariant ODE

$$y''=F(y'), \quad (3.21)$$

where F is an arbitrary function.

The equation can be obtained from the Lagrangian

$$L=y+G(y'), \quad F(y')=\frac{1}{G''(y')}. \quad (3.22)$$

The Lagrangian admits symmetries X_1 and X_2:

$$\mathrm{pr}\,X_1L+LD(\xi_1)=0,$$

$$\mathrm{pr}\,X_2L+LD(\xi_2)=1=D(x).$$

With the help of Noether's theorem we obtain the following first integrals:

$$J_1=y+G(y')-y'G'(y'), \quad J_2=G'(y')-x. \quad (3.23)$$

As we mentioned in Sec. II B, it is sufficient to have two first integrals to write out the general solution of a second-order ODE without quadratures. More explicitly, we can solve the second equation (3.23) for y' in terms of x and obtain

$$y'=H(J_2+x), \quad H(J_2+x)=[G']^{-1}(J_2+x). \quad (3.24)$$

Substituting into the first equation, we obtain

$$y(x)=J_1-G[H(J_2+x)]+(J_2+x)H(J_2+x). \quad (3.25)$$

Now we are in a position to show how one can find a variational discrete model and its conservation laws by means of Lagrange-type technique. Let us choose a difference Lagrangian in the form

$$\mathcal{L}=\frac{y+y_+}{2}+G(y_x), \tag{3.26}$$

then

$$\mathbf{pr}\,X_1\mathcal{L}+\mathcal{L}\underset{+h}{D}(\xi_1)=0,$$

$$\mathbf{pr}\,X_2\mathcal{L}+\mathcal{L}\underset{+h}{D}(\xi_2)=1=\underset{+h}{D}(x).$$

The variations of $\mathcal{L}$ yield the following quasiextremal equations:

$$\frac{\delta\mathcal{L}}{\delta y}:\quad G'(y_x)-G'(y_{\bar{x}})=\frac{h_+ + h_-}{2}, \tag{3.27}$$

$$\frac{\delta\mathcal{L}}{\delta x}:\quad -\frac{y+y_+}{2}-G(y_x)+y_xG'(y_x)+\frac{y+y_-}{2}+G(y_{\bar{x}})-y_{\bar{x}}G'(y_{\bar{x}})=0. \tag{3.28}$$

Due to the invariance of the Lagrangian with respect to the operators X_1 and X_2, the difference analog of Noether's theorem yields two first integrals

$$I_1=y+G(y_x)-y_xG'(y_x)+\frac{x_+-x}{2}y_x, \tag{3.29}$$

$$I_2=G'(y_x)-\frac{x+x_+}{2}. \tag{3.30}$$

As in the case of the algebra $\mathbf{D_{1,1}}$ we can solve for y_x to obtain

$$y_x=\Phi_1(I_2,x+x_+). \tag{3.31}$$

Substituting into the equation for I_1 we obtain

$$y=\Phi_2(I_1,I_2,x,x_+). \tag{3.32}$$

Calculating y_x from Eq. (3.32) and setting it equal to (3.31), we obtain a three-point recursion relation for x. Solving it (if we can), we turn Eq. (3.32) into an explicit general solution of the difference scheme (3.27) and (3.28).

Example 3.2: Let us consider the case

$$\mathcal{L}=\frac{y+y_+}{2}+\exp(y_x). \tag{3.33}$$

The two first integrals (3.29) and (3.30) in this case are the following:

$$I_1=y+\exp(y_x)-y_x\exp(y_x)+\frac{x_{n+1}-x_n}{2}y_x,$$

$$I_2=\exp(y_x)-\frac{x_{n+1}+x_n}{2}. \tag{3.34}$$

Equation (3.31) and (3.32) reduce to

$$y_x=\ln\left(I_2+\frac{x_{n+1}+x_n}{2}\right), \tag{3.35}$$

$$y=I_1-I_2-\frac{x_{n+1}+x_n}{2}+(I_2+x_n)\ln\left(I_2+\frac{x_{n+1}+x_n}{2}\right). \tag{3.36}$$

The recursion relation for x is

$$\frac{-x_{n+1}+x_{n-1}}{2}+(I_2+x_n)[\ln(2I_2+x_{n+1}+x_n)-\ln(2I_2+x_n+x_{n-1})]. \tag{3.37}$$

The last equation is difficult to solve. We have however reduced a system of two three-point equations to a single three-point one. We shall return to this case in Sec. V using an alternative method.

$\mathbf{D_{2,2}}$: The non-Abelian Lie algebra with nonconnected elements

$$X_1=\frac{\partial}{\partial y},\quad X_2=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y} \tag{3.38}$$

yields the invariant ODE

$$y''=\frac{1}{x}F(y'). \tag{3.39}$$

We define a function $G(y')$ by

$$F(y')=\frac{G'(y')}{G''(y')}. \tag{3.40}$$

Then the ODE (3.39) is the Euler–Lagrangian equation for the Lagrangian

$$L=\frac{1}{x}G(y'), \tag{3.41}$$

which admits X_1 and X_2 as variational symmetries:

$$\mathrm{pr}\,X_1L+LD(\xi_1)=0,$$

$$\mathrm{pr}\,X_2L+LD(\xi_2)=0.$$

Noether's theorem provides us with two first integrals:

$$J_1=\frac{1}{x}G'(y'),\quad J_2=G(y')+\left(\frac{y}{x}-y'\right)G'(y').$$

Let us take the difference Lagrangian

$$\mathcal{L}=\frac{2}{x+x_+}G(y_x),$$

which satisfies

$$\mathbf{pr}\, X_1 \mathcal{L} + \mathcal{L} \underset{+h}{D}(\xi_1) = 0,$$

$$\mathbf{pr}\, X_2 \mathcal{L} + \mathcal{L} \underset{+h}{D}(\xi_2) = 0.$$

Then the variations of $\mathcal{L}$ yield the following quasiextremal equations:

$$\frac{\delta \mathcal{L}}{\delta y}: \quad \frac{2}{x+x_+} G'(y_x) - \frac{2}{x_-+x} G'(y_{\bar{x}}) = 0,$$

$$\begin{aligned} \frac{\delta \mathcal{L}}{\delta x}: \quad & -\frac{2h_+}{(x+x_+)^2} G(y_x) + \frac{2}{(x+x_+)} G'(y_x) y_x - \frac{2}{(x+x_+)} G(y_x) \\ & - \frac{2h_-}{(x_-+x)^2} G(y_{\bar{x}}) - \frac{2}{(x_-+x)} G'(y_{\bar{x}}) y_{\bar{x}} + \frac{2}{(x_-+x)} G(y_{\bar{x}}) = 0. \end{aligned} \tag{3.42}$$

Since the Lagrangian is invariant with respect to the operators X_1 and X_2, we find the first integrals

$$I_1 = \frac{2G'(y_x)}{x+x_+}, \quad I_2 = \frac{4xx_+}{(x+x_+)^2} G(y_x) + \frac{2G'(y_x)}{x+x_+}(y - xy_x) \tag{3.43}$$

for the solutions of (3.42).

As in the case of the algebra $\mathbf{D_{2,1}}$, we can solve for y_x, using the integral I_1. We obtain

$$y_x = \Phi_1(I_1, x+x_+). \tag{3.44}$$

The second integral allows us to express y as a function of x and x_+,

$$y = x\Phi_1 + \frac{I_2}{I_1} - \frac{4xx_+}{I_1(x+x_+)^2} G(\Phi_1). \tag{3.45}$$

IV. EQUATIONS CORRESPONDING TO LAGRANGIANS INVARIANT UNDER THREE-DIMENSIONAL LIE GROUPS

Among the ''prototype equations'' of our previous article,[1] many have three-dimensional symmetry groups. In this section we shall consider two of these cases. Both of them come from Lagrangians that also have three-dimensional symmetry groups, i.e., all these symmetries are Lagrangian ones.

$\mathbf{D_{3,1}}$: Let us first consider a family of solvable Lie algebras depending on one constant k:

$$X_1 = \frac{\partial}{\partial x}, \quad X_2 = \frac{\partial}{\partial y}, \quad X_3 = x\frac{\partial}{\partial x} + ky\frac{\partial}{\partial y}, \quad k \neq 0, \frac{1}{2}, 1, 2. \tag{4.1}$$

The invariant equation has the form

$$y'' = y'^{(k-2)/(k-1)}. \tag{4.2}$$

This equation can be obtained by the usual variational procedure from the Lagrangian

$$L = \frac{(k-1)^2}{k}(y')^{k/(k-1)} + y, \tag{4.3}$$

which admits operators X_1 and X_2 for any parameter k and X_3 for $k=-1$:

$$\mathrm{pr}\,X_1L+LD(\xi_1)=0,$$

$$\mathrm{pr}\,X_2L+LD(\xi_2)=1=D(x),$$

$$\mathrm{pr}\,X_3L+LD(\xi_3)=(k+1)L.$$

It is possible to show that there is no Lagrangian function $L(x,y,y')$ which gives Eq. (4.2) with $k\neq-1$ as its Euler's equation and is divergence invariant for all three symmetries (4.1).

For arbitrary k there are two first integrals

$$J_1=\frac{(1-k)}{k}(y')^{k/(k-1)}+y=A^0,\quad J_2=(k-1)(y')^{1/(k-1)}-x=B^0.$$

Eliminating y' we find the general solution:

$$y=\frac{1}{k}\left(\frac{1}{k-1}\right)^{(k-1)}(x+B^0)^k+A^0. \tag{4.4}$$

In the case $k=-1$ we have the further first integral corresponding to the symmetry X_3:

$$J_3=\frac{2}{\sqrt{y'}}(y-xy')+xy=C^0.$$

It is functionally dependent on J_1 and J_2 since a second-order ODE can possess only two functionally independent first integrals. Let us mention that the first integral J_3 is basic:

$$J_1=X_1(J_3),\quad J_2=-X_2(J_3),$$

since

$$[X_1,X_3]=X_1,\quad [X_2,X_3]=kX_2.$$

In this case we have the following relation:

$$4-J_1J_2-J_3=0. \tag{4.5}$$

Thus, the integral J_3 is not independent and is of no use in the present context.

Now let us turn to the discrete case and consider $k=-1$ only. Other values of k will be considered in Sec. V, using a different approach. Let us choose the Lagrangian to be

$$\mathcal{L}=-4\sqrt{y_x}+\frac{y+y_+}{2} \tag{4.6}$$

as a discrete Lagrangian, which is invariant for X_1 and X_3 and divergence invariant for X_2:

$$\mathbf{pr}\,X_1\mathcal{L}+\underset{+h}{\mathcal{L}D}(\xi_1)=0,$$

$$\mathbf{pr}\,X_2\mathcal{L}+\underset{+h}{\mathcal{L}D}(\xi_2)=1=\underset{+h}{D}(x), \tag{4.7}$$

$$\mathbf{pr}\,X_3\mathcal{L}+\underset{+h}{\mathcal{L}D}(\xi_3)=0.$$

From the Lagrangian we obtain the quasiextremal equations:

$$\begin{aligned}\frac{\delta\mathcal{L}}{\delta y}:&\quad -\frac{4}{h_-+h_+}\left(\frac{1}{\sqrt{y_x}}-\frac{1}{\sqrt{y_{\bar{x}}}}\right)=1,\\ \frac{\delta\mathcal{L}}{\delta x}:&\quad 4(\sqrt{y_x}-\sqrt{y_{\bar{x}}})-\frac{y+y_+}{2}+\frac{y_-+y}{2}=0.\end{aligned}\tag{4.8}$$

This system of equations is invariant with respect to all three operators (4.1). The application of the difference analog of the Noether theorem gives us three first integrals:

$$\begin{aligned}&I_1=-2\sqrt{y_x}+\frac{y+y_+}{2}=A,\quad I_2=-\frac{2}{\sqrt{y_x}}-\frac{x+x_+}{2}=B,\\ &I_3=\frac{2(x_+y-y_+x)}{h_+\sqrt{y_x}}+\frac{x_+y+y_+x}{2}=C.\end{aligned}\tag{4.9}$$

In contrast to the continuous case the three difference first integrals I_1, I_2, and I_3 are functionally independent and instead of Eq. (4.5) we have the following relation:

$$4-I_1I_2-I_3=\frac{1}{4}h_+^2y_x=\frac{4\varepsilon^2}{(\varepsilon+2)^2}.\tag{4.10}$$

This coincides with Eq. (4.5) in the continuous limit $\varepsilon\to 0$. We see that the expression $h_+^2y_x$ is also a first integral of (4.8). This allows one to introduce a convenient lattice, namely,

$$\frac{1}{4}h_-^2y_{\bar{x}}=\frac{1}{4}h_+^2y_x=\frac{4\varepsilon^2}{(\varepsilon+2)^2},\quad \varepsilon=\text{const},\quad 0<\varepsilon\ll 1.\tag{4.11}$$

Substituting y_x from Eq. (4.11) into I_2, we obtain a two-term recursion relation for x, namely,

$$x_{n+1}-(1+\varepsilon)x_n-\varepsilon B=0,\tag{4.12}$$

or

$$-(1+\varepsilon)x_{n+1}+x_n-\varepsilon B=0,\tag{4.13}$$

depending on the sign choice for $\sqrt{y_x}$. These equations can be solved and we obtain a lattice satisfying

$$x_n=(x_0+B)(1+\varepsilon)^n-B,\quad x_0>-B\tag{4.14}$$

for the first equation and a lattice satisfying

$$x_n=(x_0+B)(1+\varepsilon)^{-n}-B,\quad x_0<-B\tag{4.15}$$

for the second equation. Using the expressions for I_1, we get the general solution for y [the same for both lattices (4.14) and (4.15)] as

$$y_n=A-\frac{4}{x_n+B}\frac{1+\varepsilon}{\left(1+\frac{\varepsilon}{2}\right)^2}.\tag{4.16}$$

This agrees with the continuous case up to order ε.

We have used the three integrals I_1, I_2, and I_3 to obtain the general solution of the difference scheme (4.8). Indeed, the solution (4.14) and (4.16) for x_n, y_n depends on four constants (A,B,x_0,ε), as it should.

The difference scheme is not compatible with a regular lattice, but requires an exponential one, as in Eq. (4.14). The only nonalgebraic step in the integration was the solution of Eq. (4.12): a linear two point equation with constant coefficients.

$\mathbf{D_{3,2}}$: The group given by the operators

$$X_1=\frac{\partial}{\partial x},\quad X_2=2x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y},\quad X_3=x^2\frac{\partial}{\partial x}+xy\frac{\partial}{\partial y} \tag{4.17}$$

corresponds to the invariant differential equation

$$y''=y^{-3}. \tag{4.18}$$

This equation can be obtained from the Lagrangian function

$$L=y'^2-\frac{1}{y^2}, \tag{4.19}$$

which admits all three operators:

$$\begin{gathered}\mathrm{pr}\,X_1L+LD(\xi_1)=0,\\ \mathrm{pr}\,X_2L+LD(\xi_2)=0,\\ \mathrm{pr}\,X_3L+LD(\xi_3)=2y'y=D(y^2).\end{gathered} \tag{4.20}$$

Consequently, the symmetries yield the following first integrals:

$$\begin{gathered}J_1=y'^2+\frac{1}{y^2}=A^0,\quad J_2=2\frac{x}{y^2}-2(y-y'x)y'=2B^0,\\ J_3=\frac{x^2}{y^2}+(y-xy')^2=C^0.\end{gathered} \tag{4.21}$$

Using the integrals A^0 and B^0 we write the general solution $y(x)$ as

$$A^0y^2=(A^0x-B^0)^2+1. \tag{4.22}$$

We see that the third integral, denoted J_3 is not needed, is not useful and indeed, is not independent. The integrals J_1, J_2, and J_3 are related as follows:

$$\left(\frac{J_2}{2}\right)^2-J_1J_3+1=0. \tag{4.23}$$

Now let us consider the discrete case. Let us consider the discrete Lagrangian function

$$\mathcal{L}=y_x^2-\frac{1}{yy_+}, \tag{4.24}$$

which admits the same symmetries as the continuous one:

$$\mathbf{pr}\, X_1\mathcal{L}+\mathcal{L}\underset{+h}{D}(\xi_1)=0,$$

$$\mathbf{pr}\, X_2\mathcal{L}+\mathcal{L}\underset{+h}{D}(\xi_2)=0, \tag{4.25}$$

$$\mathbf{pr}\, X_3\mathcal{L}+\mathcal{L}\underset{+h}{D}(\xi_3)=\underset{+h}{D}(y^2).$$

The Lagrangian generates the invariant quasiextremal equations:

$$\frac{\delta\mathcal{L}}{\delta y}:\ 2(y_x-y_{\bar{x}})=\frac{h_+}{y^2y_+}+\frac{h_-}{y^2y_-},$$

$$\frac{\delta\mathcal{L}}{\delta x}:\ (y_x)^2+\frac{1}{yy_+}-(y_{\bar{x}})^2-\frac{1}{yy_-}=0. \tag{4.26}$$

The quasiextremal equations have three functionally independent first integrals

$$I_1=y_x^2+\frac{1}{yy_+}=A,\quad I_2=\frac{x+x_+}{yy_+}+2y_x(x_+y_x-y_+)=2B,$$

$$I_3=\frac{xx_+}{yy_+}+(x_+y_x-y_+)^2=C. \tag{4.27}$$

In the discrete case the integrals I_1, I_2, and I_3 are independent. Equation (4.23) no longer holds and instead we have

$$\left(\frac{I_2}{2}\right)^2-I_1I_3+1=\frac{1}{4}\left(\frac{h_+}{yy_+}\right)^2. \tag{4.28}$$

In order to integrate the system (4.26) we will use three first integrals A, B and the one in Eq. (4.28), namely,

$$\frac{h_+}{yy_+}=\varepsilon. \tag{4.29}$$

Eliminating y_x, x_+, and y_+, we obtain the solution

$$Ay^2=(Ax-B)^2+1-\frac{\varepsilon^2}{4}. \tag{4.30}$$

This agrees with the continuous limit (4.22) up to order ε^2.

Calculating y_x from Eq. (4.30) and substituting into the expression for A in Eq. (4.27) we obtain a two-point difference equation for x and hence we obtain the lattice. In this case the equation has the form of a fractional linear mapping, i.e., it is a discrete version of the Riccati equation (with constant coefficients).

Explicitly we obtain

$$x_{n+1}=\frac{\alpha x_n+\beta}{\gamma x_n+\delta}, \tag{4.31}$$

$$\alpha=1-\varepsilon B-\frac{1}{2}\varepsilon^2,\quad \beta=\frac{\varepsilon}{A}\left(1+B^2-\frac{1}{4}\varepsilon^2\right),$$
$$\gamma=-\varepsilon A,\quad \delta=1+\varepsilon B-\frac{1}{2}\varepsilon^2. \tag{4.32}$$

We see that the coefficients in the discrete Riccati equation (4.31) satisfy

$$\alpha\delta-\beta\gamma=1,\quad \alpha+\delta=2-\varepsilon^2. \tag{4.33}$$

Like the continuous Riccati equation, Eq. (4.31) can be linearized. To do this we introduce a linear system

$$\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix}=\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{4.34}$$

If u and v satisfy Eq. (4.34), then

$$x=\frac{u}{v} \tag{4.35}$$

will satisfy Eq. (4.31). Equation (4.34) can be solved by standard methods. Indeed, both u and v must satisfy

$$u_{n+2}-(\alpha+\delta)u_{n+1}+(\alpha\delta-\beta\gamma)u_n=0. \tag{4.36}$$

The characteristic equation

$$\lambda^2-(\alpha+\delta)\lambda+(\alpha\delta-\beta\gamma)=0 \tag{4.37}$$

is obtained by putting $u_n=\lambda^n$.

In view of Eq. (4.33) the roots of Eq. (4.37) are complex. The final result is that the solution of Eq. (4.31) is

$$x_n=\frac{1}{A}\sqrt{1-\frac{\varepsilon^2}{4}}\tan(\omega n+\rho)+\frac{B}{A}, \tag{4.38}$$

where ρ is an integration constant and ω satisfies

$$\tan\omega=\frac{2\varepsilon}{2-\varepsilon^2}\sqrt{1-\frac{\varepsilon^2}{4}}. \tag{4.39}$$

Equations (4.30) and (4.38) provide an explicit analytic solution of the system (4.26). It is the general solution and involves four constants: A, B, ε, and ρ. It follows from Eq. (4.38) that the independent variable x varies between $-$ and $+$ infinity as $\omega n+\rho$ varies between $\pm\pi/2$.

V. INTEGRATION OF DIFFERENCE SCHEMES WITH TWO VARIATIONAL SYMMETRIES

A. The method of perturbed Lagrangians

We have mentioned in Sec. III B that a two-dimensional group of Lagrangian symmetries is always sufficient to reduce the original system of two three-point equations to a single three-point equation for the independent variable alone.

Here we shall show that in some cases we can do better. Using a different approach, we will actually obtain a complete solution of a difference scheme approximating a differential equation with a Lagrangian, divergence invariant under a two-dimensional symmetry group.

The case we shall consider is Eq. (3.21) and hence the two-dimensional Abelian group $\mathbf{D_{2,1}}$ corresponding to the algebra (3.20). We shall make use of the fact that the Lagrangian is not unique. Indeed we will consider three different Lagrangians, all having the same continuous limit (3.22). Instead of writing the Lagrangian (3.26) in the discrete case, we shall use a family of Lagrangians, parametrized by two constants, α and β:

$$\mathcal{L}=\alpha G(y_x)+\beta y+(1-\beta)y_+, \quad \alpha\approx 1, \quad 0\leqslant\beta\leqslant 1. \tag{5.1}$$

Each Lagrangian provides its own quasiextremal system

$$\alpha[-G'(y_x)+G'(y_{\bar{x}})]+\beta h_+ +(1-\beta)h_-=0, \tag{5.2}$$

$$\alpha[y_xG'(y_x)-y_{\bar{x}}G'(y_{\bar{x}})-G(y_x)+G(y_{\bar{x}})]-\beta(y-y_-)-(1-\beta)(y_+-y)=0. \tag{5.3}$$

We shall view one Lagrangian, with $\alpha_3=1$ and $\beta_3=0.5$, as the basic one, the other two as its perturbations.

Each Lagrangian in the family is divergence invariant under $X_1=\partial_x$ and $X_2=\partial_y$ and hence provides two first integrals of the corresponding quasiextremal equations (5.2) and (5.3):

$$\alpha[-y_xG'(y_x)+G(y_x)]+y+(1-\beta)h_+y_x=A, \tag{5.4}$$

$$\alpha G'(y_x)-x-\beta h_+=B. \tag{5.5}$$

Let us now choose three different pairs (α_i,β_i). They provide six integrals (and six quasiextremal equations). We shall show that by appropriately fine-tuning the constants α_i and β_i and choosing some of the constants A_i and B_i we can manufacture a consistent difference system, representing both the equation and the lattice. Moreover, we can explicitly integrate the equations in a manner that approximates the exact solution obtained in the continuous limit.

Let us take one equation of the form (5.4) and two of the form (5.5). In these three equations we choose $\alpha_3=1$, $\beta_3=0.5$, and $B_2=B_3=B$. We then take the difference between the two equations involving B to finally obtain the following system of three two-point equations:

$$\alpha_1[-y_xG'(y_x)+G(y_x)]+y+(1-\beta_1)h_+y_x=A, \tag{5.6}$$

$$G'(y_x)-x-\tfrac{1}{2}h_+=B, \tag{5.7}$$

$$(1-\alpha_2)G'(y_x)-(\tfrac{1}{2}-\beta_2)h_+=0. \tag{5.8}$$

From Eqs. (5.7) and (5.8) we have

$$G'(y_x)=\frac{x_++x+2B}{2}, \tag{5.9}$$

$$x_+-(1+\varepsilon)x-\varepsilon B=0, \tag{5.10}$$

where we have put

$$\varepsilon=\frac{2(1-\alpha_2)}{\alpha_2-2\beta_2}. \tag{5.11}$$

The continuous limit will correspond to $\varepsilon\to 0$.

Equation (5.10) coincides with Eq. (4.12) obtained using three Lagrangian symmetries in a special case. Here it appears in a much more general setting. The general solution of Eq. (5.10),

$$x_n=(x_0+B)(1+\varepsilon)^n-B, \tag{5.12}$$

depends on one integration constant x_0. This solution gives a lattice satisfying $h_- > 0$ and $h_+ > 0$ for $x_0 > -B$ if $\varepsilon > 0$ and for $x_0 < -B$ if $\varepsilon < 0$. For the other cases, namely $x_0 < -B$ if $\varepsilon > 0$ and for $x_0 > -B$ if $\varepsilon < 0$, formula (5.12) gives a lattice with a reverse order of points: $h_- < 0$ and $h_+ < 0$.

Using (5.12) and (5.9), we can express y_x in terms of x. We have

$$G'(y_x) = \left(1 + \frac{\varepsilon}{2}\right)(B + x). \tag{5.13}$$

Denoting the inverse function of $G'(y_x)$ as H, we have

$$y_x = H\left[\left(1 + \frac{\varepsilon}{2}\right)(B + x)\right]. \tag{5.14}$$

Using (5.6) and (5.14), we can now write the general solution of the system (5.6), (5.7), and (5.8) as

$$y(x) = A - \alpha_1 G(H) + (x + B)H, \tag{5.15}$$

where we have put

$$\alpha_1\left(1 + \frac{\varepsilon}{2}\right) - (1 - \beta_1)\varepsilon = 1. \tag{5.16}$$

The value of α_1, still figuring in the solution (5.15), must be so chosen as to obtain a consistent scheme. Indeed, x_n and y_n given in Eqs. (5.12) and (5.15) will satisfy the system (5.6), (5.7), and (5.8). We must however assure that y_x of Eq. (5.14) and $y_x = (y_{n+1} - y_n)/(x_{n+1} - x_n)$ coincide. A simple computation shows that this equality requires that α_1 should satisfy

$$\alpha_1 = (1 + \varepsilon)^{n+1}(x_0 + B)\,\frac{H_{n+1} - H_n}{G(H_{n+1}) - G(H_n)}. \tag{5.17}$$

This equation is consistent only if the right-hand side is a constant (independent on n). The constants α_i and β_i can depend upon the constant ε and for $\varepsilon \to 0$ we must have $\alpha_1, \alpha_2 \to 1$; $\beta_1, \beta_2 \to 0.5$.

From Eq. (5.8) we have

$$\frac{h_+}{G'(y_x)} = \frac{2(1 - \alpha_2)}{1 - 2\beta_2}. \tag{5.18}$$

This expression must vanish for $\varepsilon \to 0$. To achieve this while respecting Eq. (5.11) we put

$$\alpha_2 = 1 + \varepsilon^2, \quad \beta_2 = \frac{1}{2} + \varepsilon + \frac{\varepsilon^2}{2}. \tag{5.19}$$

Equation (5.11) is satisfied exactly and we have

$$\frac{h_+}{G'(y_x)} = \frac{2\varepsilon}{\varepsilon + 2}. \tag{5.20}$$

We can view Eqs. (5.12) and (5.15) as the general solution of the following three-point difference scheme:

$$G'(y_x)-G'(y_{\bar{x}})-\frac{x_+-x_-}{2}=0,$$
$$\frac{h_+}{G'(y_x)}=\frac{h_-}{G'(y_{\bar{x}})}. \tag{5.21}$$

The system (5.21) is invariant under the group corresponding to $\mathbf{D_{2,1}}$. Strictly speaking, this is not a quasiextremal system, since it cannot be derived from any single Lagrangian. The arbitrary constants A, B and ε come from three first integrals (5.6), (5.7), and (5.20) that are associated with three different Lagrangians.

We have not proven that Eq. (5.17) is consistent for arbitrary functions $G(y_x)$. We shall however show below that in at least two interesting special cases the above integration scheme is consistent.

The results of this section can be summed up as a theorem.

Theorem 5.1: The ODE (3.21) obtained from the Lagrangian (3.22) can be approximated by the difference system (5.21). If α_1 of Eq. (5.17) is constant, then the general solution of this system is given by

$$x_n=(x_0+B)(1+\varepsilon)^n-B,$$
$$y(x_n)=A-\alpha_1 G(H_n)+(x_n+B)H_n, \tag{5.22}$$

where A, B, ε and x_0 are arbitrary constants. For $\varepsilon\to 0$, $y(x_n)$ agrees with the solution (3.25) of the ODE (3.21).

As applications of this theorem let us consider two different equations, each invariant under a three-dimensional group with $\mathbf{D_{2,1}}$ as an invariant subgroup. In both cases the Lagrangian is only divergence invariant under the subgroup $\mathbf{D_{2,1}}$.

B. A polynomial nonlinearity

$\mathbf{D_{3,1}}$:

$$X_1=\frac{\partial}{\partial x},\quad X_2=\frac{\partial}{\partial y},\quad X_3=x\frac{\partial}{\partial x}+ky\frac{\partial}{\partial y},\quad k\neq 0,\frac{1}{2},\pm 1,2. \tag{5.23}$$

This algebra for $k=-1$ was treated in Sec. IV, now we consider the generic case. We take

$$G(y_x)=\frac{(k-1)^2}{k}{y_x}^{k/(k-1)} \tag{5.24}$$

and hence

$$G'(y_x)=(k-1){y_x}^{1/(k-1)}=\left(1+\frac{\varepsilon}{2}\right)(x+B). \tag{5.25}$$

Equation (5.14) reduces to

$$y_x=H_n(x)=\left(\frac{x+B}{k-1}\right)^{k-1}\left(1+\frac{\varepsilon}{2}\right)^{k-1} \tag{5.26}$$

and we have

$$G(H_n)=\frac{(k-1)^2}{k}\left(\frac{x+B}{k-1}\right)^k\left(1+\frac{\varepsilon}{2}\right)^k. \tag{5.27}$$

Substituting into (5.17), we find

$$\alpha_1=\frac{k(1+\varepsilon)((1+\varepsilon)^{k-1}-1)}{(k-1)\left(1+\frac{\varepsilon}{2}\right)((1+\varepsilon)^k-1)} \tag{5.28}$$

so that we have $\alpha_1=1+O(\varepsilon^2)$.

Thus, α_1 is a constant, close to $\alpha_1=1$ for $\varepsilon\ll 1$. The solution y_n of (5.22) specializes to

$$y_n=A+\frac{(x+B)^k}{(k-1)^{k-1}}\frac{\varepsilon\left(1+\frac{\varepsilon}{2}\right)^{k-1}}{(1+\varepsilon)^k-1}. \tag{5.29}$$

This agrees with the solution (4.4) of the ODE (4.2) up to $O(\varepsilon^2)$.

It is interesting to note that for $k=-1$ α_1 becomes independent on ε and we obtain $\alpha_1=1$, $\beta_1=0.5$. The solution (5.29) provides us with the solution (4.16), which was obtained in Sec. IV with the help of a different method.

C. An exponential nonlinearity

We consider another three-dimensional group and its Lie algebra, namely,

$$\mathbf{D_{3,3}}: \quad X_1=\frac{\partial}{\partial x}, \quad X_2=\frac{\partial}{\partial y}, \quad X_3=x\frac{\partial}{\partial x}+(x+y)\frac{\partial}{\partial y}. \tag{5.30}$$

The corresponding invariant ODE is

$$y''=\exp(-y') \tag{5.31}$$

and can be obtained from the Lagrangian

$$L=\exp(y')+y. \tag{5.32}$$

We have

$$\begin{gathered}\mathrm{pr}\,X_1L+LD(\xi_1)=0,\\ \mathrm{pr}\,X_2L+LD(\xi_2)=1=D(x).\end{gathered} \tag{5.33}$$

The corresponding first integrals of Eq. (5.31) are

$$\exp(y')(1-y')+y=A, \quad \exp(y')-x=B. \tag{5.34}$$

Finally, the general solution of Eq. (5.31) is

$$y=(x+B)(\ln(x+B)-1)+A. \tag{5.35}$$

Now let us consider the discrete case, following the method of Sec. V A. We have

$$G(y_x)=\exp(y_x) \tag{5.36}$$

and hence

$$G'(y_x)=\exp(y_x)=(x_n+B)\left(1+\frac{\varepsilon}{2}\right),$$
$$H_n=y_x=\ln(x_n+B)+\ln\left(1+\frac{\varepsilon}{2}\right). \tag{5.37}$$

Substituting into Eq. (5.17), we find

$$\alpha_1=\frac{(1+\varepsilon)\ln(1+\varepsilon)}{\varepsilon\left(1+\frac{\varepsilon}{2}\right)} \tag{5.38}$$

so that α_1 is indeed a constant and moreover we have $\alpha_1=1+O(\varepsilon^2)$.

The solution $y(x)$ on the lattice given in Eq. (5.22) is

$$y_n=A+(x_n+B)\ln(x_n+B)+(x_n+B)\left[\ln\left(1+\frac{\varepsilon}{2}\right)-\frac{(1+\varepsilon)\ln(1+\varepsilon)}{\varepsilon}\right]. \tag{5.39}$$

This agrees with the solution (5.35) of the ODE (5.31) up to $O(\varepsilon^2)$.

VI. CONCLUDING REMARKS

We see that variational symmetries, and the first integrals they provide, play a crucial role in the study of exact solutions of invariant difference schemes. Much more so than in the theory of ordinary differential equations.

The procedure that we followed in this article can be reformulated as follows. We start from the continuous case where we know a Lagrangian density $L(x,y,y')$, invariant under a group G_0 of local point transformations, i.e., satisfying condition (2.6), or (2.7). We hence also know the corresponding Euler–Lagrange equation, invariant under the same group, or a larger group containing G_0 as a subgroup.

Let us assume that we can approximate this Lagrangian by a ''discrete Lagrangian density'' $\mathcal{L}(x,y,x_+,y_+)$ invariant under the same group G_0. Even in the absence of any symmetry group, the Lagrangian will provide us with the quasiextremal equations (2.21), i.e. with a discrete Euler–Lagrange system. This system can be identified with the difference system (1.1) and (1.2).

If the Lagrangian is invariant under a one-dimensional symmetry group, we can reduce the quasiextremal system to a three-point relation for x alone, plus a ''discrete quadrature'' for y (see Sec. III A). If the symmetry group of the Lagrangian is two-dimensional, we can always reduce the quasiextremal system to one three-point equation for x alone, and write the solution $y_n(x)$ directly (see Sec. III B).

If the invariance group of the Lagrangian is (at least) three-dimensional then we can integrate the system explicitly (Sec. IV).

Finally, we have shown that if the symmetry group of the Lagrangian is two-dimensional, but the quasiextremal system has a third (non-Lagrangian) symmetry, we can also integrate explicitly.

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Lagrangian–Hamiltonian unified formalism for field theory

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The *Rusk–Skinner formalism* was developed in order to give a geometrical unified formalism for describing mechanical systems. It incorporates all the characteristics of Lagrangian and Hamiltonian descriptions of these systems (including dynamical equations and solutions, constraints, Legendre map, evolution operators, equivalence, etc.). In this work we extend this unified framework to first-order classical field theories, and show how this description comprises the main features of the Lagrangian and Hamiltonian formalisms, both for the regular and singular cases. This formulation is a first step toward further applications in optimal control theory for partial differential equations. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In ordinary autonomous classical theories in mechanics there is a unified formulation of Lagrangian and Hamiltonian formalisms,[1] which is based on the use of the *Whitney sum* of the tangent and cotangent bundles $W=TQ\oplus T^*Q\equiv TQ\times_Q T^*Q$ (the *velocity* and *momentum phase spaces* of the system). In this space, velocities and momenta are independent coordinates. There is a canonical presymplectic form Ω (the pull-back of the canonical form in T^*Q), and a natural *coupling function*, locally expressed as p_iv^i, is defined by contraction between vectors and covectors. Given a Lagrangian $L\in C^\infty(TQ)$, a Hamiltonian function, locally given by $H=p_iv^i-L(q,v)$, is determined, and, using the usual constraint algorithm for the geometric equation $i(X)\Omega=\mathrm{d}H$ associated to the Hamiltonian system (W,Ω,H), we obtain that

(1) The first constraint submanifold W_1 is isomorphic to TQ, and the momenta $\partial L/\partial v^i=p_i$ are determined as constraints.
(2) The geometric equation contains the second order condition $v^i=dq^i/dt$.
(3) The identification $W_1\equiv TQ$ allows us to recover the Lagrangian formalism.
(4) The projection to the cotangent bundle generates the Hamiltonian formalism, including constraints. The Legendre map and the time evolution operator are straightforwardly obtained by the previous identification and projection.[2]

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It is also worth noticing that this space is also appropriate for the formulation of different kinds of problems in optimal control.[3–7] Furthermore, in Refs. 8 and 9 this unified formalism has been extended for nonautonomous mechanical systems.

Our aim in this paper is to reproduce the same construction for first-order field theories, generating a unified description of Lagrangian and Hamiltonian formalisms and its correspondence, starting from the multisymplectic description of such theories. (See, for instance, Refs. 10–18, for some general references on this formalism. See, also, Refs. 19–25, for other geometric formulations of field theories.) As is shown throughout the paper, characteristics analogous to those pointed out for mechanical systems can be stated in this context. In Ref. 9, a first approach to this subject has been made, focusing mainly on the constraint algorithm for the singular case.

The organization of the paper is as follows: Sec. II is devoted to reviewing the main features of the multisymplectic description of Lagrangian and Hamiltonian field theories. In Sec. III we develop the unified formalism for field theories: starting from the *extended jet-multimomentum bundle* (analogous to the Whitney sum in mechanics), we introduce the so-called *extended Hamiltonian system* and state the field equations for sections, *m*-vector fields, connections, and jet fields in this framework. It is also shown how the standard Lagrangian and Hamiltonian descriptions are recovered from this unified picture. As a typical example, the *minimal surface problem* is described in this formalism in Sec. IV. Finally, we include an Appendix where basic features about connections, jet fields, and *m*-vector fields are displayed.

Throughout this paper $\pi:E\to M$ will be a fiber bundle ($\dim M=m$, $\dim E=N+m$), where M is an oriented manifold with volume form $\omega\in\Omega^m(M)$. $\pi^1:J^1E\to E$ is the jet bundle of local sections of π, and $\overline{\pi}^1=\pi\circ\pi^1:J^1E\to M$ gives another fiber bundle structure. $(x^\alpha,y^A,v^A_\alpha)$ will denote natural local systems of coordinates in J^1E, adapted to the bundle $E\to M$ ($\alpha=1,...,m$; $A=1,...,N$), and such that $\omega=\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^m\equiv\mathrm{d}^mx$. Manifolds are real, paracompact, connected, and C^∞. Maps are C^∞. Sum over crossed repeated indices is understood.

II. GEOMETRIC FRAMEWORK FOR CLASSICAL FIELD THEORIES

A. Lagrangian formalism

(For details concerning the contents of this and the next section, see, for instance, Refs. 10–13, 17, 18, and 26–31. See, also, the Appendix).

A *classical field theory* is described by giving a *configuration fiber bundle* $\pi:E\to M$ and a *Lagrangian density*, which is a $\overline{\pi}^1$-semibasic m-form on J^1E usually written as $\mathcal{L}=L\,\overline{\pi}^{1*}\omega$, where $L\in C^\infty(J^1E)$ is the *Lagrangian function* determined by $\mathcal{L}$ and ω. The *Poincaré–Cartan m and* $(m+1)$*-forms* associated with the Lagrangian density $\mathcal{L}$ are defined using the *vertical endomorphism* $\mathcal{V}$ of the bundle J^1E (see Ref. 30)

$$\Theta_{\mathcal{L}}:=i(\mathcal{V})\mathcal{L}+\mathcal{L}\in\Omega^m(J^1E);\qquad \Omega_{\mathcal{L}}:=-\mathrm{d}\Theta_{\mathcal{L}}\in\Omega^{m+1}(J^1E).$$

A *Lagrangian system* is a couple $(J^1E,\Omega_{\mathcal{L}})$. It is *regular* if $\Omega_{\mathcal{L}}$ is a multisymplectic $(m+1)$-form (a closed m-form, $m>1$, is called *multisymplectic* if it is one-nondegenerate; elsewhere it is *pre-multisymplectic*). In natural charts in J^1E we have

$$\mathcal{V}=(\mathrm{d}y^A-v^A_\alpha\mathrm{d}x^\alpha)\otimes\frac{\partial}{\partial v^A_\nu}\otimes\frac{\partial}{\partial x^\nu},$$

and

$$\Theta_{\mathcal{L}}=\frac{\partial L}{\partial v^A_\mu}\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\mu-\left(\frac{\partial L}{\partial v^A_\mu}v^A_\mu-L\right)\mathrm{d}^mx,$$

$$\Omega_{\mathcal{L}}=-\frac{\partial^2 L}{\partial v^B_\nu \partial v^A_\alpha}\mathrm{d}v^B_\nu\wedge\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha-\frac{\partial^2 L}{\partial y^B\partial v^A_\alpha}\mathrm{d}y^B\wedge\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha+\frac{\partial^2 L}{\partial v^B_\nu\partial v^A_\alpha}v^A_\alpha\mathrm{d}v^B_\nu\wedge\mathrm{d}^m x$$
$$+\left(\frac{\partial^2 L}{\partial y^B\partial v^A_\alpha}v^A_\alpha-\frac{\partial L}{\partial y^B}+\frac{\partial^2 L}{\partial x^\alpha\partial v^B_\alpha}\right)\mathrm{d}y^B\wedge\mathrm{d}^m x$$

(where $\mathrm{d}^{m-1}x_\alpha\equiv i(\partial/\partial x^\alpha)\mathrm{d}^m x$); the regularity condition is equivalent to $\det(\partial^2 L/\partial v^A_\alpha\partial v^B_\nu(\overline{y}))\neq 0$, for every $\overline{y}\in J^1E$.

The *Lagrangian problem* associated with a Lagrangian system $(J^1E,\Omega_{\mathcal{L}})$ consists in finding sections $\phi\in\Gamma(M,E)$, the set of sections of π, which are characterized by the condition

$$(j^1\phi)^* i(X)\Omega_L=0,\quad \text{for every } X\in\mathfrak{X}(J^1E).$$

In natural coordinates, if $\phi(x)=(x^\alpha,\phi^A(x))$, this condition is equivalent to demanding that ϕ satisfy the *Euler–Lagrange equations*

$$\left.\frac{\partial L}{\partial y^A}\right|_{j^1\phi}-\left.\frac{\partial}{\partial x^\alpha}\left(\frac{\partial L}{\partial v^A_\alpha}\right)\right|_{j^1\phi}=0\quad(\text{for } A=1,\ldots,N).\tag{1}$$

The problem of finding these sections can be formulated equivalently as follows: finding a distribution D of $T(J^1E)$ such that it is integrable (that is, *involutive*), m-dimensional, $\overline{\pi^1}$-transverse, and the integral manifolds of D are the image of sections solution of the above equations (therefore, lifting of π-sections). This is equivalent to stating that the sections solution to the Lagrangian problem are the integral sections of one of the following equivalent elements:

- A class of holonomic m-vector fields $\{X_{\mathcal{L}}\}\subset\mathfrak{X}^m(J^1E)$, such that $i(X_{\mathcal{L}})\Omega_{\mathcal{L}}=0$, for every $X_{\mathcal{L}}\in\{X_{\mathcal{L}}\}$.
- A holonomic connection $\nabla_{\mathcal{L}}$ in $\overline{\pi^1}:J^1E\to M$ such that $i(\nabla_{\mathcal{L}})\Omega_{\mathcal{L}}=(m-1)\Omega_{\mathcal{L}}$.
- A holonomic jet field $\Psi_{\mathcal{L}}:J^1E\to J^1J^1E$, such that $i(\Psi_{\mathcal{L}})\Omega_{\mathcal{L}}=0$ (the contraction of jet fields with differential forms is defined in Ref. 11).

Semi-holonomic locally decomposable m-vector fields, jet fields, and connections which are solution to these equations are called *Euler–Lagrange m-vector fields, jet fields*, and *connections* for $(J^1E,\Omega_{\mathcal{L}})$. In a natural chart in J^1E, the local expressions of these elements are

$$X_{\mathcal{L}}=f\bigwedge_{\alpha=1}^{m}\left(\frac{\partial}{\partial x^\alpha}+F^A_\alpha\frac{\partial}{\partial y^A}+G^A_{\alpha\nu}\frac{\partial}{\partial v^A_\nu}\right),$$

$$\nabla_{\mathcal{L}}=\mathrm{d}x^\alpha\otimes\left(\frac{\partial}{\partial x^\alpha}+F^A_\alpha\frac{\partial}{\partial y^A}+G^A_{\alpha\nu}\frac{\partial}{\partial v^A_\nu}\right),$$

$$\Psi_{\mathcal{L}}=(x^\alpha,y^A,v^A_\alpha,F^A_\alpha,G^A_{\alpha\eta}),$$

with $F^A_\alpha=v^A_\alpha$ (which is the local expression of the semi-holonomy condition), and where the coefficients $G^A_{\alpha\nu}$ are related by the system of linear equations

$$\frac{\partial^2 L}{\partial v^A_\alpha\partial v^B_\nu}G^A_{\alpha\nu}=\frac{\partial L}{\partial y^B}-\frac{\partial^2 L}{\partial x^\nu\partial v^B_\nu}-\frac{\partial^2 L}{\partial y^A\partial v^B_\nu}v^A_\nu\quad(A,B=1,\ldots,N).\tag{2}$$

$f \in C^\infty(J^1E)$ is an arbitrary nonvanishing function. A representative of the class $\{X_{\mathcal{L}}\}$ can be selected by the condition $i(X_{\mathcal{L}})(\overline{\pi}^1{}^*\omega)=1$, which leads to $f=1$ in the above local expression. Therefore, if $j^1\phi=(x^\mu,\phi^A,\partial\phi^A/\partial x^\nu)$ is an integral section of $X_{\mathcal{L}}$, then $v^A_\alpha=\partial\phi^A/\partial x^\alpha$, and hence, the coefficients $G^B_{\alpha\nu}$ must satisfy the equations

$$G^A_{\nu\eta}\left(x^\alpha,\phi^A,\frac{\partial\phi^A}{\partial x^\alpha}\right)=\frac{\partial^2\phi^A}{\partial x^\eta\partial x^\nu} \quad (A=1,...,N;\quad \eta,\nu=1,...,m).$$

As a consequence, the system (2) is equivalent to the Euler–Lagrange Eq. (1) for ϕ.

If $(J^1E,\Omega_{\mathcal{L}})$ is a regular Lagrangian system, the existence of classes of Euler–Lagrange m-vector fields for $\mathcal{L}$ (or what is equivalent, Euler–Lagrange jet fields or connections) is assured. For singular Lagrangian systems, the existence of this kind of solutions is not assured except perhaps on some submanifold $S\hookrightarrow J^1E$. Furthermore, solutions of the field equations can exist (in general, on some submanifold of J^1E), but none of them are semi-holonomic (at any point of this submanifold). In both cases, the integrability of these solutions is not assured, except perhaps on a smaller submanifold I such that the integral sections are contained in I.

B. Hamiltonian formalism

For the Hamiltonian formalism of field theories, we have the *extended multimomentum bundle* $\mathcal{M}\pi$, which is the bundle of m-forms on E vanishing by contraction with two π-vertical vector fields [or equivalently, the set of affine maps from J^1E to $\pi^*\Lambda^mT^*M$ (Refs. 10 and 32)], and the *restricted multimomentum bundle* $J^1{}^*E\equiv\mathcal{M}\pi/\pi^*\Lambda^mT^*M$. We have the natural projections

$$\tau^1:J^1{}^*E\to E,\quad \overline{\tau}^1=\pi\circ\tau^1:J^1{}^*E\to M,\quad \mu:\mathcal{M}\pi\to J^1{}^*E,\quad \hat{\mu}=\overline{\tau}^1\circ\mu:\mathcal{M}\pi\to M.$$

Given a system of coordinates adapted to the bundle $\pi:E\to M$, we can construct natural coordinates $(x^\alpha,y^A,p^\alpha_A,p)$ $(\alpha=1,...,m;\ A=1,...,N)$ in $\mathcal{M}\pi$, corresponding to the m-covector $\mathbf{p}=p\,\mathrm{d}^mx+p^\alpha_A\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha\in\mathcal{M}\pi$, and $(x^\alpha,y^A,p^\alpha_A)$ in $J^1{}^*E$, for the class $[\mathbf{p}]=p^\alpha_A\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha+\langle\mathrm{d}^mx\rangle\in J^1{}^*E$.

Now, if $(J^1E,\Omega_{\mathcal{L}})$ is a Lagrangian system, the *extended Legendre map* associated with $\mathcal{L}$, $\widetilde{\mathcal{FL}}:J^1E\to\mathcal{M}\pi$, is defined as

$$[\widetilde{\mathcal{FL}}(\overline{y})](Z_1,\ldots,Z_m):=(\Theta_{\mathcal{L}})_{\overline{y}}(\overline{Z}_1,\ldots,\overline{Z}_m), \tag{3}$$

where $Z_1,\ldots,Z_m\in T_{\pi^1(\overline{y})}E$, and $\overline{Z}_1,\ldots,\overline{Z}_m\in T_{\overline{y}}J^1E$ are such that $T_{\overline{y}}\pi^1\overline{Z}_\alpha=Z_\alpha$. Then the *restricted Legendre map* associated with $\mathcal{L}$ is $\mathcal{FL}:=\mu\circ\widetilde{\mathcal{FL}}$. Their local expressions are

$$\widetilde{\mathcal{FL}}{}^*x^\alpha=x^\alpha,\quad \widetilde{\mathcal{FL}}{}^*y^A=y^A,\quad \widetilde{\mathcal{FL}}{}^*p^\alpha_A=\frac{\partial L}{\partial v^A_\alpha},\quad \widetilde{\mathcal{FL}}{}^*p=L-v^A_\alpha\frac{\partial L}{\partial v^A_\alpha},$$

$$\mathcal{FL}^*x^\alpha=x^\alpha,\quad \mathcal{FL}^*y^A=y^A,\quad \mathcal{FL}^*p^\alpha_A=\frac{\partial L}{\partial v^A_\alpha}.$$

Therefore, $(J^1E,\Omega_{\mathcal{L}})$ is a *regular* Lagrangian system if $\mathcal{FL}$ is a local diffeomorphism (this definition is equivalent to that given above). Elsewhere $(J^1E,\Omega_{\mathcal{L}})$ is a *singular* Lagrangian system. As a particular case, $(J^1E,\Omega_{\mathcal{L}})$ is a *hyper-regular* Lagrangian system if $\mathcal{FL}$ is a global diffeomorphism. A singular Lagrangian system $(J^1E,\Omega_{\mathcal{L}})$ is *almost-regular* if: $\mathcal{P}:=\mathcal{FL}(J^1E)$ is a closed submanifold of $J^1{}^*E$ (we will denote the natural imbedding by $j:\mathcal{P}\hookrightarrow J^1{}^*E$), $\mathcal{FL}$ is a submersion onto its image, and for every $\overline{y}\in J^1E$, the fibres $\mathcal{FL}^{-1}(\mathcal{FL}(\overline{y}))$ are connected submanifolds of J^1E.

In order to construct a *Hamiltonian system* associated with $(J^1E,\Omega_{\mathcal{L}})$, recall that the multicotangent bundle Λ^mT^*E is endowed with a natural canonical form $\mathbf{\Theta}\in\Omega^m(\Lambda^mT^*E)$, which is

the tautological form defined as follows: let $\tau_E : T^*E \to E$ be the natural projection, and $\Lambda^m \tau_E : \Lambda^m T^*E \to E$ its natural extension; then, for every $\overline{\mathbf{p}} \in \Lambda^m T^*E$ (where $\overline{\mathbf{p}} = (y, \beta)$, with $y \in E$ and $\beta \in \Lambda^m T^*_y E$), and for every $X_1, \ldots, X_m \in \mathfrak{X}(\Lambda^m T^*E)$ we have

$$[\mathbf{\Theta}(X_1, \ldots, X_m)]_{\overline{\mathbf{p}}} := [(\Lambda^m \tau_E)^* \beta](X_{1_{\overline{\mathbf{p}}}}, \ldots, X_{m_{\overline{\mathbf{p}}}}) = \beta(T_{\overline{\mathbf{p}}} \Lambda^m \tau_E(X_{1_{\overline{\mathbf{p}}}}), \ldots, T_{\overline{\mathbf{p}}} \Lambda^m \tau_E(X_{m_{\overline{\mathbf{p}}}})).$$

Thus we also have the multisymplectic form $\mathbf{\Omega} := -\mathrm{d}\mathbf{\Theta} \in \Omega^{m+1}(\Lambda^m T^*E)$. But $\mathcal{M}\pi \equiv \Lambda^m_1 T^*E$ is a subbundle of $\Lambda^m T^*E$. Then, if $\lambda : \Lambda^m_1 T^*E \hookrightarrow \Lambda^m T^*E$ is the natural imbedding, $\Theta := \lambda^* \mathbf{\Theta}$ and $\Omega := -\mathrm{d}\Theta = \lambda^* \mathbf{\Omega}$ are canonical forms in $\mathcal{M}\pi$, which are called the *multimomentum Liouville m* and $(m+1)$ *forms*. In particular, we have that $\Theta(\mathbf{p}) = (\tau_1 \circ \mu)^* \mathbf{p}$, for every $\mathbf{p} \in \mathcal{M}\pi$. Their local expressions are

$$\Theta = p^\alpha_A \mathrm{d}y^A \wedge \mathrm{d}^{m-1} x_\alpha + p\, \mathrm{d}^m x, \quad \Omega = -\mathrm{d}p^\alpha_A \wedge \mathrm{d}y^A \wedge \mathrm{d}^{m-1} x_\alpha - \mathrm{d}p \wedge \mathrm{d}^m x. \tag{4}$$

Observe that $\widetilde{\mathcal{FL}}^* \Theta = \Theta_{\mathcal{L}}$, and $\widetilde{\mathcal{FL}}^* \Omega = \Omega_{\mathcal{L}}$.

Now, if $(J^1E, \Omega_{\mathcal{L}})$ is a hyper-regular Lagrangian system, then $\widetilde{\mathcal{P}} := \widetilde{\mathcal{FL}}(J^1E)$ is a one-codimensional and μ-transverse imbedded submanifold of $\mathcal{M}\pi$ (we will denote the natural imbedding by $\widetilde{\jmath} : \widetilde{\mathcal{P}} \hookrightarrow \mathcal{M}\pi$), which is diffeomorphic to $J^1{}^*E$. This diffeomorphism is μ^{-1}, when μ is restricted to $\widetilde{\mathcal{P}}$, and also coincides with the map $h := \widetilde{\mathcal{FL}} \circ \mathcal{FL}^{-1}$, when it is restricted onto its image (which is just $\widetilde{\mathcal{P}}$). This map h is called a *Hamiltonian section*, and can be used to construct the *Hamilton-Cartan m* and $(m+1)$ *forms* of $J^1{}^*E$ by making

$$\Theta_h = h^* \Theta \in \Omega^m(J^1{}^*E), \quad \Omega_h = h^* \Omega \in \Omega^{m+1}(J^1{}^*E).$$

The couple $(J^1{}^*E, \Omega_h)$ is said to be the *Hamiltonian system* associated with the hyper-regular Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$. Locally, the Hamiltonian section h is specified by the *local Hamiltonian function* $H = p^\alpha_A (F\mathcal{L}^{-1})^* v^A_\alpha - (F\mathcal{L}^{-1})^* L$, that is, $h(x^\alpha, y^A, p^\alpha_A) = (x^\alpha, y^A, p^\alpha_A, -H)$. Then we have the local expressions

$$\Theta_h = p^\alpha_A \mathrm{d}y^A \wedge \mathrm{d}^{m-1} x_\alpha - H \mathrm{d}^m x, \quad \Omega_h = -\mathrm{d}p^\alpha_A \wedge \mathrm{d}y^A \wedge \mathrm{d}^{m-1} x_\alpha + \mathrm{d}H \wedge \mathrm{d}^m x.$$

Of course $\mathcal{FL}^* \Theta_h = \Theta_{\mathcal{L}}$ and $\mathcal{FL}^* \Omega_h = \Omega_{\mathcal{L}}$.

The *Hamiltonian problem* associated with the Hamiltonian system $(J^1{}^*E, \Omega_h)$ consists in finding sections $\psi \in \Gamma(M, J^1{}^*E)$, which are characterized by the condition

$$\psi^* i(X) \Omega_h = 0, \quad \text{for every } X \in \mathfrak{X}(J^1{}^*E).$$

In natural coordinates, if $\psi(x) = (x^\alpha, y^A(x), p^\alpha_A(x))$, this condition leads to the so-called *Hamilton–De Donder–Weyl equations* (for the section ψ).

The problem of finding these sections can be formulated equivalently as follows: finding a distribution D of $T(J^1{}^*E)$ such that D is integrable (that is, *involutive*), m-dimensional, $\overline{\tau}^1$-transverse, and its integral manifolds are the sections solution to the above equations. This is equivalent to stating that the sections solution to the Hamiltonian problem are the integral sections of one of the following equivalent elements:

- A class of integrable and $\overline{\tau}^1$-transverse m-vector fields $\{X_{\mathcal{H}}\} \subset \mathfrak{X}^m(J^1{}^*E)$ satisfying that $i(X_{\mathcal{H}})\Omega_h = 0$, for every $X_{\mathcal{H}} \in \{X_{\mathcal{H}}\}$.
- An integrable connection $\nabla_{\mathcal{H}}$ in $\overline{\tau}^1 : J^1{}^*E \to M$ such that $i(\nabla_{\mathcal{H}})\Omega_h = (m-1)\Omega_h$.
- An integrable jet field $\Psi_{\mathcal{H}} : J^1{}^*E \to J^1 J^1{}^*E$, such that $i(\Psi_{\mathcal{H}})\Omega_h = 0$.

$\overline{\tau}^1$-transverse and locally decomposable m-vector fields, orientable jet fields, and orientable connections, which are solutions of these equations, are called *Hamilton–De Donder–Weyl (HDW) m-vector fields, jet fields*, and *connections* for $(J^1{}^*E, \Omega_h)$. Their local expressions in natural coordinates are

$$X_{\mathcal{H}}=f\bigwedge_{\alpha=1}^{m}\left(\frac{\partial}{\partial x^{\alpha}}+F_{\alpha}^{A}\frac{\partial}{\partial y^{A}}+G_{A\alpha}^{\eta}\frac{\partial}{\partial p_{A}^{\eta}}\right),$$

$$\Psi_{\mathcal{H}}=(x^{\alpha},y^{A},p_{A}^{\alpha};F_{\alpha}^{A},G_{A\alpha}^{\eta}),$$

$$\nabla_{\mathcal{H}}=\mathrm{d}x^{\alpha}\otimes\left(\frac{\partial}{\partial x^{\alpha}}+F_{\alpha}^{A}\frac{\partial}{\partial y^{A}}+G_{A\alpha}^{\nu}\frac{\partial}{\partial p_{A}^{\nu}}\right),$$

where $f\in C^{\infty}(J^{1}{}^{*}E)$ is a nonvanishing function, and the coefficients F_{α}^{A}, $G_{A\alpha}^{\eta}$ are related by the system of linear equations

$$F_{\alpha}^{A}=\frac{\partial H}{\partial p_{A}^{\alpha}},\quad G_{A\nu}^{\nu}=-\frac{\partial H}{\partial y^{A}}.$$

Now, if $\psi(x)=(x^{\alpha},y^{A}(x)=\psi^{A}(x),p_{A}^{\alpha}(x)=\psi_{A}^{\alpha}(x))$ is an integral section of $X_{\mathcal{H}}$ then

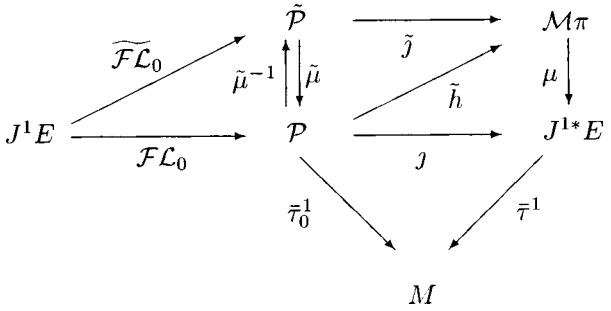
$$\left.\frac{\partial H}{\partial p_{A}^{\alpha}}\right|_{\psi}=F_{\alpha}^{A}\circ\psi=\frac{\partial\psi^{A}}{\partial x_{\alpha}};\quad -\left.\frac{\partial H}{\partial y^{A}}\right|_{\psi}=G_{A\alpha}^{\alpha}\circ\psi=\frac{\partial\psi_{A}^{\alpha}}{\partial x^{\alpha}},$$

which are the Hamilton–De Donder–Weyl equations for ψ. As above, a representative of the class $\{X_{\mathcal{H}}\}$ can be selected by the condition $i(X_{\mathcal{H}})(\overline{\tau}^{1}{}^{*}\omega)=1$, which leads to $f=1$ in the above local expression. The existence of classes of HDW m-vector fields, jet fields, and connections is assured.

In an analogous way, if $(J^{1}E,\Omega_{\mathcal{L}})$ is an almost-regular Lagrangian system, the submanifold $j:\mathcal{P}\hookrightarrow J^{1}{}^{*}E$, is a fiber bundle over E and M. In this case the μ-transverse submanifold $\tilde{\mathcal{P}}\hookrightarrow\mathcal{M}\pi$ is diffeomorphic to $\mathcal{P}$. This diffeomorphism is denoted by $\tilde{\mu}:\tilde{\mathcal{P}}\to\mathcal{P}$, and it is just the restriction of the projection μ to $\tilde{\mathcal{P}}$. Then, taking the Hamiltonian section $\tilde{h}:=\tilde{j}\circ\tilde{\mu}^{-1}$, we define the Hamilton–Cartan forms

$$\Theta_{h}^{0}=\tilde{h}^{*}\Theta;\quad \Omega_{h}^{0}=\tilde{h}^{*}\Omega,$$

which verify that $\mathcal{FL}_{0}^{*}\Theta_{h}^{0}=\Theta_{\mathcal{L}}$ and $\mathcal{FL}_{0}^{*}\Theta_{h}^{0}=\Omega_{\mathcal{L}}$ (where $\mathcal{FL}_{0}$ is the restriction map of $\mathcal{FL}$ onto $\mathcal{P}$). Then $(\mathcal{P},\Omega_{h}^{0})$ is the *Hamiltonian system* associated with the almost-regular Lagrangian system $(J^{1}E,\Omega_{\mathcal{L}})$, and we have Diagram 1.



(5)

Then, the *Hamiltonian problem* associated with the Hamiltonian system $(\mathcal{P},\Omega_{h}^{0})$, and the equations for the sections of $\Gamma(M,\mathcal{P})$ solution to the Hamiltonian problem are stated as in the regular case. Now, the existence of the corresponding Hamilton–De Donder–Weyl m-vector fields, jet fields, and connections for $(\mathcal{P},\Omega_{h}^{0})$ is not assured, except perhaps on some submanifold P of $\mathcal{P}$, where the solution is not unique.

From now on we will consider only regular or almost-regular systems.

III. UNIFIED FORMALISM

A. Extended Hamiltonian system

Given a fiber bundle $\pi:E\to M$ over an oriented manifold (M,ω), we define the *extended jet-multimomentum bundle* $\mathcal{W}$ and the *restricted jet-multimomentum bundle* $\mathcal{W}_r$ as

$$\mathcal{W}:=J^1E\times_E\mathcal{M}\pi,\quad \mathcal{W}_r:=J^1E\times_E J^1{}^*E,$$

whose natural coordinates are $(x^\alpha,y^A,v^A_\alpha,p^\alpha_A,p)$ and $(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)$, respectively. We have the natural projections (submersions)

$$\begin{gathered}\rho_1:\mathcal{W}\to J^1E,\quad \rho_2:\mathcal{W}\to\mathcal{M}\pi,\quad \rho_E:\mathcal{W}\to E,\quad \rho_M:\mathcal{W}\to M,\\ \rho_1^r:\mathcal{W}_r\to J^1E,\quad \rho_2^r:\mathcal{W}_r\to J^1{}^*E,\quad \rho_E^r:\mathcal{W}_r\to E,\quad \rho_M^r:\mathcal{W}_r\to M.\end{gathered}\tag{6}$$

Note that $\pi^1\circ\rho_1=\tau^1\circ\mu\circ\rho_2=\rho_E$. In addition, there is also the natural projection

$$\mu_{\mathcal{W}}:\mathcal{W}\to\mathcal{W}_r,$$

$$(\overline{y},\mathbf{p})\mapsto(\overline{y},[\mathbf{p}]).$$

The bundle $\mathcal{W}$ is endowed with the following canonical structures:

Definition 1:

(1) *The* coupling *m*-form *in* $\mathcal{W}$, *denoted by* $\mathcal{C}$, *is an m-form along* ρ_M *which is defined as follows: for every* $\overline{y}\in J^1_yE$, *with* $\overline{\pi^1}(\overline{y})=\pi(y)=x\in E$, *and* $\mathbf{p}\in\mathcal{M}_y\pi$, *let* $w\equiv(\overline{y},\mathbf{p})\in\mathcal{W}_y$, *then*

$$\mathcal{C}(w):=(T_x\phi)^*\mathbf{p},$$

where $\phi:M\to E$ *satisfies that* $j^1\phi(x)=\overline{y}$.

Then, we denote by $\hat{\mathcal{C}}\in\Omega^m(\mathcal{W})$ *the* ρ_M*-semibasic form associated with* $\mathcal{C}$.

(2) *The* canonical *m*-form $\Theta_{\mathcal{W}}\in\Omega^m(\mathcal{W})$ *is defined by* $\Theta_{\mathcal{W}}:=\rho_2^*\Theta$, *and it is therefore* ρ_E*-semibasic*.

The canonical $(m+1)$-form *is the pre-multisymplectic form* $\Omega_{\mathcal{W}}:=-\mathrm{d}\Theta_{\mathcal{W}}=\rho_1^*\Omega\in\Omega^{m+1}(\mathcal{W})$.

Being $\hat{\mathcal{C}}$ a ρ_M-semibasic form, there is $\hat{C}\in C^\infty(\mathcal{W})$ such that $\hat{\mathcal{C}}=\hat{C}(\rho_M^*\omega)$. Note also that $\Omega_{\mathcal{W}}$ is not one-nondegenerate, its kernel being the ρ_2-vertical vectors; then, we call $(\mathcal{W},\Omega_{\mathcal{W}})$ a pre-multisymplectic structure. This definition of the coupling form is in fact an alternative (obviously equivalent) presentation of the extended multimomentum bundle as the set of affine maps from the jet bundle J^1E to π-basic *m*-forms.

The local expressions for $\Theta_{\mathcal{W}}$ and $\Omega_{\mathcal{W}}$ are the same as (4), and for $\hat{\mathcal{C}}$ we have

$$\hat{\mathcal{C}}(w)=(p+p^\alpha_Av^A_\alpha)\mathrm{d}^mx.$$

Given a Lagrangian density $\mathcal{L}\in\Omega^m(J^1E)$, we denote $\hat{\mathcal{L}}:=\rho_1^*\mathcal{L}\in\Omega^m(\mathcal{W})$, and we can write $\hat{\mathcal{L}}=\hat{L}(\rho_M^*\omega)$, with $\hat{L}=\rho_1^*L\in C^\infty(\mathcal{W})$. We define a *Hamiltonian submanifold*

$$\mathcal{W}_0:=\{w\in\mathcal{W}\,|\,\hat{\mathcal{L}}(w)=\hat{\mathcal{C}}(w)\}.$$

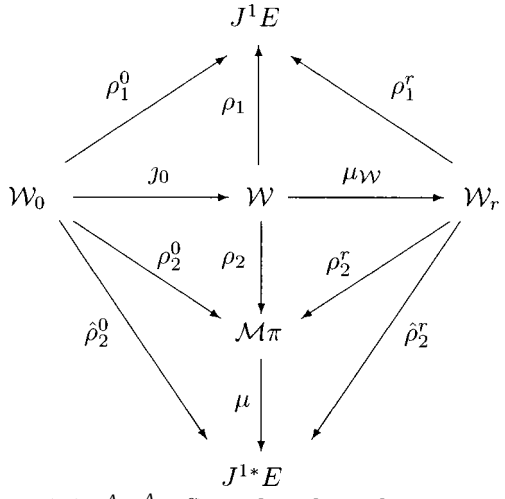
So, $\mathcal{W}_0$ is the submanifold of $\mathcal{W}$ defined by the constraint function $\hat{C}-\hat{L}=0$. In local coordinates this constraint function is

$$p+p^\alpha_Av^A_\alpha-\hat{L}(x^\nu,y^B,v^B_\nu)=0.$$

We have the natural imbedding $J_0:\mathcal{W}_0\hookrightarrow\mathcal{W}$, as well as the projections (submersions)

$$\rho_1^0:\mathcal{W}_0\to J^1E,\quad \rho_2^0:\mathcal{W}_0\to\mathcal{M}\pi,\quad \rho_E^0:\mathcal{W}_0\to E,\quad \rho_M^0:\mathcal{W}_0\to M,$$

which are the restrictions to $\mathcal{W}_0$ of the projections (6), and $\hat{\rho}_2^0=\mu\circ\rho_2^0:\mathcal{W}_0\to J^{1*}E$. So we have Diagram 2.



Local coordinates in $\mathcal{W}_0$ are $(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)$, and we have that

$$\rho_1^0(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)=(x^\alpha,y^A,v^A_\alpha),$$

$$J_0(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)=(x^\alpha,y^A,v^A_\alpha,p^\alpha_A,L-v^A_\alpha p^\alpha_A),$$

$$\rho_2^0(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)=(x^\alpha,y^A,p^\alpha_A,L-v^A_\alpha p^\alpha_A),$$

$$\hat{\rho}_2^0(x^\alpha,y^A,v^A_\alpha,p^\alpha_A)=(x^\alpha,y^A,p^\alpha_A).$$

Proposition 1: $\mathcal{W}_0$ is a one-codimensional $\mu_{\mathcal{W}}$-transversal submanifold of $\mathcal{W}$, diffeomorphic to $\mathcal{W}_r$.

(*Proof*) For every $(\overline{y},\mathbf{p})\in\mathcal{W}_0$, we have $L(\overline{y})\equiv\hat{L}(\overline{y},\mathbf{p})=\hat{C}(\overline{y},\mathbf{p})$,

and

$$(\mu_{\mathcal{W}}\circ J_0)(\overline{y},\mathbf{p})=\mu_{\mathcal{W}}(\overline{y},\mathbf{p})=(\overline{y},\mu(\mathbf{p}))=(\overline{y},[\mathbf{p}]).$$

First, $\mu_{\mathcal{W}}\circ J_0$ is injective: let $(\overline{y}_1,\mathbf{p}_1)$, $(\overline{y}_2,\mathbf{p}_2)\in\mathcal{W}_0$, then we have

$$(\mu_{\mathcal{W}}\circ J_0)(\overline{y}_1,\mathbf{p}_1)=(\mu_{\mathcal{W}}\circ J_0)(\overline{y}_2,\mathbf{p}_2)\Rightarrow(\overline{y}_1,\mu(\mathbf{p}_1))=(\overline{y}_2,\mu(\mathbf{p}_2))\Rightarrow\overline{y}_1=\overline{y}_2,\mu(\mathbf{p}_1)=\mu(\mathbf{p}_2),$$

hence,

$$L(\overline{y}_1)=L(\overline{y}_2)=\hat{C}(\overline{y}_1,\mathbf{p}_1)=\hat{C}(\overline{y}_2,\mathbf{p}_2).$$

In a local chart, third equality gives

$$p(\mathbf{p}_1)+p^\alpha_A(\mathbf{p}_1)v^A_\alpha(\overline{y}_1)=p(\mathbf{p}_2)+p^\alpha_A(\mathbf{p}_2)v^A_\alpha(\overline{y}_2),$$

but $\mu(\mathbf{p}_1)=\mu(\mathbf{p}_2)$ implies that

$$p_A^\alpha(\mathbf{p}_1)=p_A^\alpha([\mathbf{p}_1])=p_A^\alpha([\mathbf{p}_2])=p_A^\alpha(\mathbf{p}_2),$$

therefore, $p(\mathbf{p}_1)=p(\mathbf{p}_2)$, and hence, $\mathbf{p}_1=\mathbf{p}_2$.

Second, $\mu_{\mathcal{W}}\circ J_0$ is onto: Let $(\overline{y},\mathbf{p})\in\mathcal{W}_r$, then there exists $(\overline{y},\mathbf{q})\in J_0(\mathcal{W}_0)$ such that $[\mathbf{q}]=[\mathbf{p}]$. In fact, it suffices to take $[\mathbf{q}]$ in such a way that, in a local chart of $J^1E\times_E\mathcal{M}\pi=\mathcal{W}$

$$p_A^\alpha(\mathbf{q})=p_A^\alpha([\mathbf{p}]),\quad p(\mathbf{q})=p_A^\alpha([\mathbf{p}])v_\alpha^A(\overline{y})-L(\overline{y}).$$

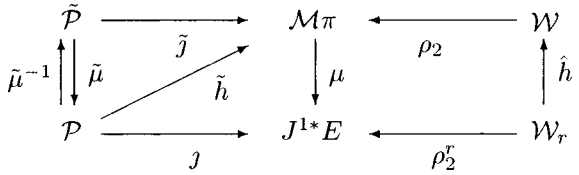
Finally, observe that $\mathcal{W}_0$ is defined by the constraint function $\hat{L}-\hat{C}$ and, as $\ker\mu_{\mathcal{W}*}=\{\partial/\partial p\}$ and $\partial/\partial p(\hat{L}-\hat{C})=1$, then $\mathcal{W}_0$ is a 1-codimensional submanifold of $\mathcal{W}$ and $\mu_{\mathcal{W}}$-transversal. ■

As a consequence of this property, the submanifold $\mathcal{W}_0$ induces a section $\hat{h}:\mathcal{W}_r\to\mathcal{W}$ of the projection $\mu_{\mathcal{W}}$. Locally, $\hat{h}$ is specified by giving the local *Hamiltonian function* $\hat{H}=-\hat{L}+p_A^\alpha v_\alpha^A$; that is, $\hat{h}(x^\alpha,y^A,v_\alpha^A,p_A^\alpha)=(x^\alpha,y^A,v_\alpha^A,p_A^\alpha,-\hat{H})$. In this sense, $\hat{h}$ is said to be a *Hamiltonian section* of $\mu_{\mathcal{W}}$.

Remark: It is important to point out that, from every Hamiltonian $\mu_{\mathcal{W}}$-section $\hat{h}:\mathcal{W}_r\to\mathcal{W}$ in the extended unified formalism, we can recover a Hamiltonian μ-section $h:\mathcal{P}\to\mathcal{M}\pi$ in the standard Hamiltonian formalism. In fact, given $[\mathbf{p}]\in J^{1*}E$, the section $\hat{h}$ maps every point $(\overline{y},[\mathbf{p}])\in(\rho_2^r)^{-1}([\mathbf{p}])$ into $\rho_2^{-1}[\rho_2(\hat{h}(\overline{y},[\mathbf{p}]))]$. So, the crucial point is the projectability of the local function $\hat{H}$ by ρ_2. But, being $\partial/\partial v_\alpha^A$ a local basis for $\ker\rho_{2*}$, $\hat{H}$ is ρ_2-projectable if, and only if, $p_A^\alpha=\partial L/\partial v_A^\alpha$, and this condition is fulfilled when $[\mathbf{p}]\in\mathcal{P}=\operatorname{Im}\mathcal{FL}\subset J^{1*}E$, which implies that $\rho_2[\hat{h}(\rho_2^r)^{-1})([\mathbf{p}]))]\in\widetilde{\mathcal{P}}=\operatorname{Im}\mathcal{FL}\subset\mathcal{M}\pi$. Hence, the Hamiltonian section $\tilde{h}$ is defined as follows:

$$\overline{h([\mathbf{p}])}=(\rho_2\circ\hat{h})[(\rho_2^r)^{-1}(J([\mathbf{p}]))],\quad\text{for every } [\mathbf{p}]\in\mathcal{P}.$$

So we have Diagram 3 (see also Diagram 1).



(For (hyper) regular systems this diagram is the same with $\operatorname{Im}\mathcal{FL}=J^{1*}E$.)

Finally, we can define the forms

$$\Theta_0:=j_0^*\Theta_{\mathcal{W}}=\rho_2^{0*}\Theta\in\Omega^m(\mathcal{W}_0),\quad\Omega_0:=j_0^*\Omega_{\mathcal{W}}=\rho_2^{0*}\Omega\in\Omega^{m+1}(\mathcal{W}_0),$$

with local expressions

$$\begin{aligned}\Theta_0&=(L-p_A^\alpha v_\alpha^A)\mathrm{d}^mx+p_A^\alpha\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha,\\ \Omega_0&=\mathrm{d}(p_A^\alpha v_\alpha^A-L)\wedge\mathrm{d}^mx-\mathrm{d}p_A^\alpha\wedge\mathrm{d}y^A\wedge\mathrm{d}^{m-1}x_\alpha,\end{aligned}\tag{7}$$

and we have obtained a (pre-multisymplectic) Hamiltonian system $(\mathcal{W}_0,\Omega_0)$, or equivalently $(\mathcal{W}_r,\hat{h}^*\Omega_{\mathcal{W}})$.

B. Field equations for sections

The *Lagrange-Hamiltonian problem* associated with the system $(\mathcal{W}_0,\Omega_0)$ consists in finding sections $\psi_0\in\Gamma(M,\mathcal{W}_0)$ which are characterized by the condition

$$\psi_0^*i(Y_0)\Omega_0=0,\quad\text{for every } Y_0\in\mathfrak{X}(\mathcal{W}_0).\tag{8}$$

This equation gives different kinds of information, depending on the type of the vector fields Y_0 involved. In particular, using vector fields Y_0 which are $\hat{\rho}_2^0$-vertical, we have:

Lemma 1: If $Y_0 \in \mathfrak{X}^{V(\hat{\rho}_2^0)}(\mathcal{W}_0)$ (i.e., Y_0 is $\hat{\rho}_2^0$-vertical), then $i(Y_0)\Omega_0$ is ρ_M^0-semibasic.

(*Proof*) A simple calculation in coordinates leads to this result. In fact, taking $\{\partial/\partial v_\alpha^A\}$ as a local basis for the $\hat{\rho}_2^0$-vertical vector fields, and bearing in mind (7) we obtain

$$i\left(\frac{\partial}{\partial v_\alpha^A}\right)\Omega_0 = \left(p_A^\alpha - \frac{\partial L}{\partial v_\alpha^A}\right)\mathrm{d}^m x,$$

which are obviously ρ_M^0-semibasic forms. ■

As an immediate consequence, when $Y_0 \in \mathfrak{X}^{V(\hat{\rho}_2^0)}(\mathcal{W}_0)$, condition (8) does not depend on the derivatives of ψ_0: is a pointwise (algebraic) condition. We can define the submanifold

$$\mathcal{W}_1 = \{(\overline{y},\mathbf{p}) \in \mathcal{W}_0 \,|\, i(V_0)(\Omega_0)_{(\overline{y},\mathbf{p})} = 0, \quad \text{for every} \quad V_0 \in V(\hat{\rho}_2^0)\},$$

which is called the *first constraint submanifold* of the Hamiltonian pre-multisymplectic system $(\mathcal{W}_0,\Omega_0)$, as every section ψ_0 solution to (8) must take values in $\mathcal{W}_1$. We denote by $j_1 : \mathcal{W}_1 \hookrightarrow \mathcal{W}_0$ the natural embedding.

Locally, $\mathcal{W}_1$ is defined in $\mathcal{W}_0$ by the constraints $p_A^\alpha = \partial L/\partial v_\alpha^A$. Moreover:

Proposition 2: $\mathcal{W}_1$ is the graph of $\widetilde{\mathcal{FL}}$; that is, $\mathcal{W}_1 = \{(\overline{y},\widetilde{\mathcal{FL}}(\overline{y})) \in \mathcal{W} | \overline{y} \in J^1E\}$.

(*Proof*) Consider $\overline{y} \in J^1E$, let $\phi : M \to E$ be a representative of $\overline{y}$, and $\mathbf{p} = \widetilde{\mathcal{FL}}(\overline{y})$. For every $U \in T_{\overline{\pi^1}(\overline{y})}M$, consider $V = T_{\overline{\pi^1}(\overline{y})}\phi(U)$ and its canonical lifting $\overline{V} = T_{\overline{\pi^1}(\overline{y})}j^1\phi(U)$. From the definition of the extended Legendre map (3) we have that $(T_{\overline{y}}\pi)^*(\widetilde{\mathcal{FL}}(\overline{y})) = (\Theta_{\mathcal{L}})_{\overline{y}}$, then

$$i(\overline{V})[(T_{\overline{y}}\pi^1)^*(\widetilde{\mathcal{FL}}(\overline{y}))] = i(\overline{V})(\Theta_{\mathcal{L}})_{\overline{y}}.$$

Furthermore, as $\mathbf{p} = \widetilde{\mathcal{FL}}(\overline{y})$, we also have that

$$\begin{aligned} i(\overline{V})[(T_{\overline{y}}\pi^1)^*(\widetilde{\mathcal{FL}}(\overline{y}))] &= i(T_{\overline{\pi^1}(\overline{y})}j^1\phi(U))[(T_{\overline{y}}\pi^1)^*\mathbf{p}) \\ &= i(T_{\pi^1(\overline{y})}[(T_{\overline{\pi^1}(\overline{y})}j^1\phi(U)])\mathbf{p} = i(T_{\overline{\pi^1}(\overline{y})}\phi(U))\mathbf{p} = i(V)\mathbf{p}. \end{aligned}$$

Therefore, we obtain

$$i(U)(\phi^*\mathbf{p}) = i(U)[(j^1\phi)^*(\Theta_{\mathcal{L}})_{\overline{y}}],$$

and bearing in mind the definition of the coupling form $\mathcal{C}$, this condition becomes

$$i(U)(\mathcal{C}(\overline{y},\mathbf{p})) = i(U)[(j^1\phi)^*\Theta_{\mathcal{L}})_{\overline{y}}].$$

Since it holds for every $U \in T_{\overline{\pi^1}(\overline{y})}M$, we conclude that $\mathcal{C}(\overline{y},\mathbf{p}) = [(j^1\phi)^*\Theta_{\mathcal{L}}]_{\overline{y}}$, or equivalently, $\hat{\mathcal{C}}(\overline{y},\mathbf{p}) = \hat{L}(\overline{y},\mathbf{p})$, where we have made use of the fact that $\Theta_{\mathcal{L}}$ is the sum of the Lagrangian density $\mathcal{L}$ and a contact form $i(\mathcal{V})\mathcal{L}$ (vanishing by pull-back of lifted sections). This is the condition defining $\mathcal{W}_0$, and thus we have proved that $(\overline{y},\widetilde{\mathcal{FL}}(\overline{y})) \in \mathcal{W}_0$, for every $\overline{y} \in J^1E$; that is, graph $\widetilde{\mathcal{FL}} \subset \mathcal{W}_0$. Furthermore, graph $\mathcal{FL}$ and $\mathcal{W}_1$ are defined as subsets of $\mathcal{W}_0$ by the same local conditions: $p_A^\alpha - \partial L/\partial v_\alpha^A = 0$. So we conclude that graph $\widetilde{\mathcal{FL}} = \mathcal{W}_1$. ■

Being $\mathcal{W}_1$ the graph of $\mathcal{FL}$, it is diffeomorphic to J^1E. Every section $\psi_0 : M \to \mathcal{W}_0$ is of the form $\psi_0 = (\psi_{\mathcal{L}},\psi_{\mathcal{H}})$, with $\psi_{\mathcal{L}} = \rho_1^0 \circ \psi_0 : M \to J^1E$, and if ψ_0 takes values in $\mathcal{W}_1$ then $\psi_{\mathcal{H}} = \widetilde{\mathcal{FL}} \circ \psi_{\mathcal{L}}$. In this way, every constraint, differential equation, etc., in the unified formalism can be translated to the Lagrangian or the Hamiltonian formalisms by restriction to the first or the second factors of the product bundle.

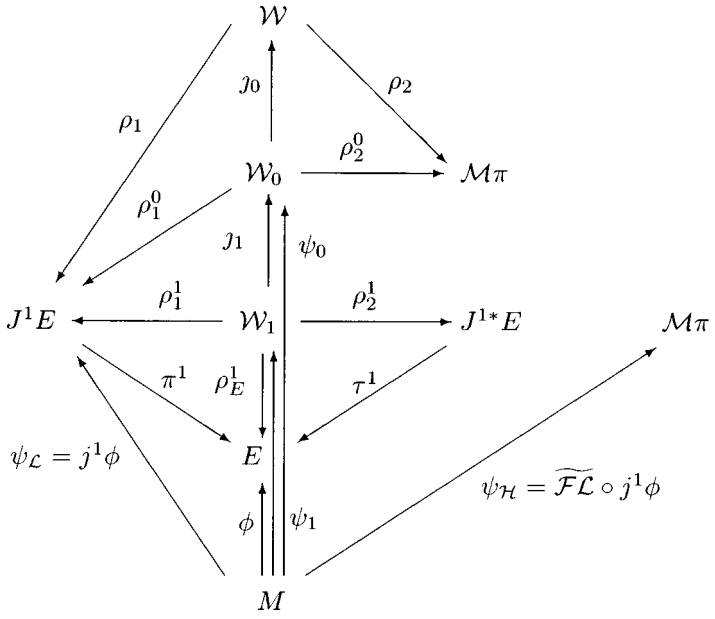
However, as was pointed out before, the geometric condition (8) in $\mathcal{W}_0$, which can be solved only for sections $\psi_0 : M \to \mathcal{W}_1 \subset \mathcal{W}_0$, is stronger than the Lagrangian condition $\psi_{\mathcal{L}}^* i(Z)\Omega_{\mathcal{L}} = 0$, [for every $Z \in \mathfrak{X}(J^1E)$] in J^1E, which can be translated to $\mathcal{W}_1$ by the natural diffeomorphism between them. The reason is that $T_{\mathcal{W}_1}\mathcal{W}_0 = T\mathcal{W}_1 \oplus V_{\mathcal{W}_1}(\rho_1^0)$, so the additional information comes therefore from the ρ_1^0-vertical vectors, and it is just the holonomic condition. In fact:

Theorem 1: *Let $\psi_0 : M \to \mathcal{W}_0$ be a section fulfilling Eq. (8), $\psi_0 = (\psi_{\mathcal{L}}, \psi_{\mathcal{H}}) = (\psi_{\mathcal{L}}, \widetilde{\mathcal{FL}} \circ \psi_{\mathcal{L}})$, where $\psi_{\mathcal{L}} = \rho_1^0 \circ \psi_0$. Then*:

(1) $\psi_{\mathcal{L}}$ is the canonical lift of the projected section $\phi = \rho_E^0 \circ \psi_0 : M \to E$ (that is, $\psi_{\mathcal{L}}$ is a holonomic section).

(2) The section $\psi_{\mathcal{L}} = j^1\phi$ is a solution to the Lagrangian problem, and the section $\mu \circ \psi_{\mathcal{H}} = \mu \circ \widetilde{\mathcal{FL}} \circ \psi_{\mathcal{L}} = \mathcal{FL} \circ j^1\phi$ is a solution to the Hamiltonian problem.

Conversely, for every section $\phi : M \to E$ such that $j^1\phi$ is solutions to the Lagrangian problem (and hence $\mathcal{FL} \circ j^1\phi$ is solution to the Hamiltonian problem) we have that the section $\psi_0 = (j^1\phi, \widetilde{\mathcal{FL}} \circ j^1\phi)$, is a solution to (8) (see Diagram 4).



(*Proof*)

(1) Taking $\{\partial/\partial p_A^\alpha\}$ as a local basis for the ρ_1^0-vertical vector fields:

$$i\left(\frac{\partial}{\partial p_A^\alpha}\right)\Omega_0 = v_\alpha^A \mathrm{d}^m x - \mathrm{d}y^A \wedge \mathrm{d}^{m-1}x_\alpha,$$

so that for a section ψ_0, we have

$$0 = \psi_0^*\left[i\left(\frac{\partial}{\partial p_A^\alpha}\right)\Omega_0\right] = \left(v_\alpha^A(x) - \frac{\partial y^A}{\partial x^\alpha}\right)\mathrm{d}^m x,$$

and thus the holonomy condition appears naturally within the unified formalism, and it is not necessary to impose it by hand to ψ_0. Thus, we have that $\psi_0 = (x^\alpha, y^A, \partial y^A/\partial x^\alpha, \partial L/\partial v_\alpha^A)$, since ψ_0 takes values in $\mathcal{W}_1$, and hence, it is of the form $\psi_0 = (j^1\phi, \widetilde{\mathcal{FL}} \circ j^1\phi)$, for $\phi = (x^\alpha, y^A) = \rho_E^0 \circ \psi_0$.

(2) Since sections $\psi_0 : M \to \mathcal{W}_0$ solution to (8) take values in $\mathcal{W}_1$, we can identify them with sections $\psi_1 : M \to \mathcal{W}_1$. These sections ψ_1 verify, in particular, that $\psi_1^* i(Y_1)\Omega_1 = 0$ holds for every $Y_1 \in \mathfrak{X}(\mathcal{W}_1)$. Obviously, $\psi_0 = J_1 \circ \psi_1$. Moreover, as $\mathcal{W}_1$ is the graph of $\widetilde{\mathcal{FL}}$, denoting by $\rho_1^1 = \rho_1^0 \circ J_1 : \mathcal{W}_1 \to J^1E$ the diffeomorphism which identifies $\mathcal{W}_1$ with J^1E, if we define $\Omega_1 = J_1^* \Omega_0$, we have that $\Omega_1 = \rho_1^{1*} \Omega_{\mathcal{L}}$. In fact; as $(\rho_1^1)^{-1}(\overline{y}) = (\overline{y}, \widetilde{\mathcal{FL}}(\overline{y}))$, for every $\overline{y} \in J^1E$, then $(\rho_0^2 \circ J_1 \circ (\rho_1^1)^{-1})(\overline{y}) = \widetilde{\mathcal{FL}}(\overline{y}) \in \mathcal{M}\pi$, and hence,

$$\Omega_{\mathcal{L}} = (\rho_0^2 \circ J_1 \circ (\rho_1^1)^{-1})^* \Omega = [((\rho_1^1)^{-1})^* \circ J_1^* \circ \rho_0^{2*}]\Omega = [((\rho_1^1)^{-1})^* \circ J_1^*]\Omega_0 = ((\rho_1^1)^{-1})^* \Omega_1 .$$

Now, let $X \in \mathfrak{X}(J^1E)$. We have

$$\begin{aligned}(j^1\phi)^* i(X)\Omega_{\mathcal{L}} &= (\rho_1^0 \circ \psi_0)^* i(X)\Omega_{\mathcal{L}} = (\rho_1^0 \circ J_1 \circ \psi_1)^* i(X)\Omega_{\mathcal{L}} \\ &= (\rho_1^1 \circ \psi_1)^* i(X)\Omega_{\mathcal{L}} = \psi_1^* i((\rho_1^1)_*^{-1} X)(\rho_1^{1*}\Omega_{\mathcal{L}}) = \psi_1^* i(Y_1)\Omega_1 \qquad (9) \\ &= \psi_1^* i(Y_1)(J_1^*\Omega_0) = (\psi_1^* \circ J_1^*) i(Y_0)\Omega_0 = \psi_0^* i(Y_0)\Omega_0 ,\end{aligned}$$

where $Y_0 \in \mathfrak{X}(\mathcal{W}_0)$ is such that $Y_0 = J_{1*} Y_1$. But as $\psi_0^* i(Y_0)\Omega_0 = 0$, for every $Y_0 \in \mathfrak{X}(\mathcal{W}_0)$, then we conclude that $(j^1\phi)^* i(X)\Omega_{\mathcal{L}} = 0$, for every $X \in \mathfrak{X}(J^1E)$.

Conversely, let $j^1\phi : M \to J^1E$ such that $(j^1\phi)^* i(X)\Omega_{\mathcal{L}} = 0$, for every $X \in \mathfrak{X}(J^1E)$, and define $\psi_0 : M \to \mathcal{W}_0$ as $\psi_0 := (j^1\phi, \widetilde{\mathcal{FL}} \circ j^1\phi)$ (observe that ψ_0 takes its values in $\mathcal{W}_1$). Taking into account that, on the points of $\mathcal{W}_1$, every $Y_0 \in \mathfrak{X}(\mathcal{W}_0)$ splits into $Y_0 = Y_0^1 + Y_0^2$, with $Y_0^1 \in \mathfrak{X}(\mathcal{W}_0)$ tangent to $\mathcal{W}_1$, and $Y_0^2 \in \mathfrak{X}^{V(\rho_1^0)}(\mathcal{W}_0)$, we have that

$$\psi_0^* i(Y_0)\Omega_0 = \psi_0^* i(Y_0^1)\Omega_0 + \psi_0^* i(Y_0^2)\Omega_0 = 0,$$

because for Y_0^1, the same reasoning as in (9) leads to

$$\psi_0^* i(Y_0^1)\Omega_0 = (j^1\phi)^* i(X_0^1)\Omega_{\mathcal{L}} = 0$$

[where $X_0^1 = (\rho_1^1)_*^{-1} Y_0^1$] and for Y_0^2, following also the same reasoning as in (9), a local calculus gives

$$\psi_0^* i(Y_0^2)\Omega_0 = (j^1\phi)^* \left[\left(f_A^\alpha(x) \left(v_\alpha^A - \frac{\partial y^A}{\partial x^\alpha} \right) \right) \mathrm{d}^m x \right] = 0,$$

since $j^1\phi$ is a holonomic section.

The result for the sections $\mathcal{FL} \circ j^1\phi$ is a direct consequence of the *equivalence theorem* between the Lagrangian and Hamiltonian formalisms (see, for instance, Refs. 12 and 31). ■

Remark: The results in this section can also be recovered in coordinates taking an arbitrary local vector field $Y_0 = f^A(\partial/\partial y^A) + g_\alpha^A(\partial/\partial v_\alpha^A) + h_A^\alpha(\partial/\partial p_A^\alpha) \in \mathfrak{X}(\mathcal{W}_0)$, then

$$\begin{aligned}i(Y_0)\Omega_0 = &- f^A(\partial L/\partial y^A)\mathrm{d}^m x + f^A \mathrm{d}p_A^\alpha \wedge \mathrm{d}^{m-1}x_\alpha + g_\alpha^A(p_A^\alpha - (\partial L/\partial v_\alpha^A))\mathrm{d}^m x \\ &+ h_A^\alpha v_\alpha^A \mathrm{d}^m x - h_A^\alpha \mathrm{d}y^A \wedge \mathrm{d}^{m-1}x_\alpha\end{aligned}$$

and, for a section ψ_0 fulfilling (8),

$$0=\psi_0^*i(Y_0)\Omega_0=\left[f^A\left(\frac{\partial p_A^\alpha}{\partial x^\alpha}-\frac{\partial L}{\partial y^A}\right)+g_\alpha^A\left(p_A^\alpha-\frac{\partial L}{\partial v_\alpha^A}\right)+h_A^\alpha\left(v_\alpha^A-\frac{\partial y^A}{\partial x^\alpha}\right)\right]\mathrm{d}^m x$$

reproduces the Euler–Lagrange equations, the restricted Legendre map (that is, the definition of the momenta), and the holonomy condition.

Summarizing, Eq. (8) gives different kinds of information, depending on the type of verticallity of the vector fields Y_0 involved. In particular, we have obtained equations of three different classes:

(1) Algebraic (not differential) equations, determining a subset $\mathcal{W}_1$ of $\mathcal{W}_0$, where the sections solution must take their values. These can be called *primary Hamiltonian constraints*, and in fact they generate, by $\hat{\rho}_2^0$ projection, the primary constraints of the Hamiltonian formalism for singular Lagrangians, i.e., the image of the Legendre transformation, $\mathcal{FL}(J^1E)\subset J^{1*}E$.
(2) The holonomic differential equations, forcing the sections solution ψ_0 to be lifting of π-sections. This property is similar to the one in the unified formalism of Classical Mechanics, and it reflects the fact that the geometric condition in the unified formalism is stronger than the usual one in the Lagrangian formalism.
(3) The classical Euler–Lagrange equations.

C. Field equations for *m*-vector fields, connections, and jet fields

The problem of finding sections solution to (8) can be formulated equivalently as follows: finding a distribution D_0 of $T(\mathcal{W}_0)$ such that it is integrable (that is, *involutive*), *m*-dimensional, ρ_M^0-transverse, and the integral manifolds of D_0 are the sections solution to the above equations. (Note that we do not ask them to be lifting of π-sections; that is, the holonomic condition.) This is equivalent to stating that the sections solution to this problem are the integral sections of one of the following equivalent elements:

- A class of integrable and ρ_M^0-transverse *m*-vector fields $\{X_0\}\subset\mathfrak{X}^m(\mathcal{W}_0)$ satisfying that

$$i(X_0)\Omega_0=0,\quad \text{for every } X_0\in\{X_0\}. \tag{10}$$

- An integrable connection ∇_0 in $\rho_M^0:\mathcal{W}_0\to M$ such that

$$i(\nabla_0)\Omega_0=(m-1)\Omega_0. \tag{11}$$

- An integrable jet field $\Psi_0:\mathcal{W}_0\to J^1\mathcal{W}_0$, such that

$$i(\Psi_0)\Omega_0=0. \tag{12}$$

Locally decomposable and ρ_M^0-transverse *m*-vector fields, orientable jet fields, and orientable connections, which are solutions of these equations will be called *Lagrange–Hamiltonian m-vector fields, jet fields*, and *connections* for $(\mathcal{W}_0,\Omega_0)$.

Recall that, in a natural chart in $\mathcal{W}_0$, the local expressions of a connection form, its associated jet field, and the *m*-multivector fields of the corresponding associated class are

$$\nabla_0=\mathrm{d}x^\alpha\otimes\left(\frac{\partial}{\partial x^\alpha}+F_\alpha^A\frac{\partial}{\partial y^A}+G_{\alpha\nu}^A\frac{\partial}{\partial v_\nu^A}+H_{\alpha A}^\nu\frac{\partial}{\partial p_A^\nu}\right),$$

$$\Psi_0=(x^\alpha,y^A,v_\alpha^A,F_\alpha^A,G_{\alpha\eta}^A,H_{\alpha A}^\nu), \tag{13}$$

$$X_0=f\bigwedge_{\alpha=1}^m\left(\frac{\partial}{\partial x^\alpha}+F_\alpha^A\frac{\partial}{\partial y^A}+G_{\alpha\nu}^A\frac{\partial}{\partial v_\nu^A}+H_{\alpha A}^\nu\frac{\partial}{\partial p_A^\nu}\right),$$

where $f \in C^\infty(J^1E)$ is an arbitrary nonvanishing function. A representative of the class $\{X\}$ can be selected by the condition $i(X)(\overline{\rho_M^0}^* \omega) = 1$, which leads to $f = 1$ in the above local expression.

Now, the equivalence of the unified formalism with the Lagrangian and Hamiltonian formalisms can be recovered as follows:

Theorem 2: *Let $\{X_0\}$ be a class of integrable Lagrange–Hamiltonian m-vector fields in $\mathcal{W}_0$, whose elements $X_0 : \mathcal{W}_0 \to \Lambda^m T\mathcal{W}_0$ are solutions to (10), and let $\nabla_0 : \mathcal{W}_0 \to \rho_M^{0*} T^*M \otimes_{\mathcal{W}_0} T\mathcal{W}_0$ be its associated Lagrange–Hamiltonian connection form [which is a solution to (11)], and $\Psi_0 : \mathcal{W}_0 \to J^1\mathcal{W}_1$ its associated Lagrange–Hamiltonian jet field [which is a solution to (12)].*

(1) For every $X_0 \in \{X_0\}$, the m-vector field $X_{\mathcal{L}} : J^1E \to \Lambda^m TJ^1E$ defined by

$$X_{\mathcal{L}} \circ \rho_1^0 = \Lambda^m T\rho_1^0 \circ X_0,$$

is a holonomic Euler–Lagrange m-vector field for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$ (where $\Lambda^m T\rho_1^0 : \Lambda^m T\mathcal{W}_0 \to \Lambda^m TJ^1E$ is the natural extension of $T\rho_1^0$).

Conversely, every holonomic Euler–Lagrange m-vector field for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$ can be recovered in this way from an integrable Lagrange–Hamiltonian m-vector field $X_0 \in \mathfrak{X}^m_{\mathcal{W}_1}(\mathcal{W}_0)$.

(2) The Ehresmann connection form $\nabla_{\mathcal{L}} : J^1E \to \overline{\pi^1}^* T^*M \otimes_{J^1E} TJ^1E$ defined by

$$\nabla_{\mathcal{L}} \circ \rho_1^0 = \kappa_{\mathcal{W}_0} \circ \nabla_0,$$

is a holonomic Euler–Lagrange connection form for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$ (where $\kappa_{\mathcal{W}_0}$ is defined as the map making the following diagram commutative) (see Diagram 5).

$$\begin{array}{ccc} \rho_M^{0*}\mathrm{T}^*M \otimes_{\mathcal{W}_0} \mathrm{T}\mathcal{W}_0 & \xrightarrow{\kappa_{\mathcal{W}_0}} & \bar{\pi}^{1*}\mathrm{T}^*M \otimes_{J^1E} \mathrm{T}J^1E \\ \downarrow & & \downarrow \\ \mathcal{W}_0 & \xrightarrow{\rho_1^0} & J^1E \end{array}$$

Conversely, every holonomic Euler–Lagrange connection form for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$ can be recovered in this way from an integrable Lagrange–Hamiltonian connection form ∇_0.

(3) The jet field $\Psi_{\mathcal{L}} : J^1E \to J^1J^1E$ defined by

$$\Psi_{\mathcal{L}} \circ \rho_1^0 = j^1\rho_1^0 \circ \Psi_0,$$

is a holonomic Euler–Lagrange jet field for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$. Conversely, every holonomic Euler–Lagrange jet field for the Lagrangian system $(J^1E, \Omega_{\mathcal{L}})$ can be recovered in this way from an integrable Lagrange–Hamiltonian jet field Ψ_0.

(*Proof*) Let X_0 be a ρ_M^0-transversal *m*-vector field on $\mathcal{W}_0$ solution to (10). As sections $\psi_0 : M \to \mathcal{W}_0$ solution to the geometric equation (8) must take value in $\mathcal{W}_1$, then X_0 can be identified with a *m*-vector field $X_1 : \mathcal{W}_0 \to \Lambda^m T\mathcal{W}_1$ (i.e., $\Lambda^m TJ_1 \circ X_1 = X_0|_{\mathcal{W}_1}$), and hence, there exists $X_{\mathcal{L}} : J^1E \to \Lambda^m TJ^1E$ such that $X_1 = \Lambda^m T(\rho_1^1)^{-1} \circ X_{\mathcal{L}} \in \mathfrak{X}^m(\mathcal{W}_1)$. Therefore as a consequence of item (1) in theorem 1, for every section ψ_0 solution to (8), there exists $X_{\mathcal{L}}^0 \in \mathfrak{X}^m(j^1\phi(M))$ such that $\Lambda^m TJ_\phi \circ X_{\mathcal{L}}^0 = X_{\mathcal{L}}|_{j^1\phi(M)}$, where $J_\phi : j^1\phi \to E$ is the natural imbedding. So, $X_{\mathcal{L}}$ is $\overline{\pi^1}$-transversal and holonomic. Then, bearing in mind that $J_1^* \Omega_0 = \rho_1^{1*} \Omega_{\mathcal{L}}$, we have

$$J_1^* i(X_0)\Omega_0 = i(X_1)(J_1^* \Omega_0) = i(X_1)(\rho_1^{1*} \Omega_{\mathcal{L}}) = \rho_1^{1*} i(X_{\mathcal{L}})\Omega_{\mathcal{L}},$$

then $i(X_0)\Omega_0=0\Rightarrow i(X_{\mathcal{L}})\Omega_{\mathcal{L}}=0$.

Conversely, given an holonomic Euler–Lagrange m-vector field $X_{\mathcal{L}}$, from $i(X_{\mathcal{L}})\Omega_{\mathcal{L}}=0$, and taking into account the above chain of equalities, we obtain that $i(X_0)\Omega_0\in[\mathfrak{X}(\mathcal{W}_1)]^0$ [the annihilator of $\mathfrak{X}(\mathcal{W}_1)$]. Moreover, being $X_{\mathcal{L}}$ holonomic, X_0 is holonomic, and then the extra condition $i(Y_0)i(X_0)\Omega_0=0$ is also fulfilled for every $Y_0\in\mathfrak{X}^{V(\rho_1^0)}(\mathcal{W}_0)$. Thus, remembering that $T_{\mathcal{W}_1}\mathcal{W}_0=T\mathcal{W}_1\oplus \mathrm{V}_{\mathcal{W}_1}(\rho_1^0)$, we conclude that $i(X_0)\Omega_0=0$.

The proof for Ehresmann connections and jet fields is straightforward, taking into account that they are equivalent alternative descriptions in the Lagrangian formalism. ■

This statement also holds for nonintegrable classes of m-vector fields, connections, and jet fields in $\mathcal{W}_0$, but now the corresponding classes of Euler–Lagrange m-vector fields, connections and jet fields in J^1E will not be holonomic (but only semi-holonomic). To prove this assertion it suffices to compute Eq. (10) in coordinates, using the local expressions (7) and (13), concluding then that, in the expressions (13), $F_\alpha^A=v_\alpha^A$, which is the local expression of the semi-holonomy condition (see, also, Ref. 9).

Finally, the Hamiltonian formalism is recovered in the usual way, by using the following:

Theorem 3: *Let* $(J^1{}^*E,\Omega_h)$ *be the Hamiltonian system associated with a (hyper) regular Lagrangian system* $(J^1E,\Omega_{\mathcal{L}})$.

(1) (Equivalence theorem for m-vector fields*) Let* $X_{\mathcal{L}}\in\mathfrak{X}^m(J^1E)$ *and* $X_{\mathcal{H}}\in\mathfrak{X}^m(J^1{}^*E)$ *be the* m*-vector fields solution to the Lagrangian and the Hamiltonian problems respectively. Then*

$$\Lambda^m T\mathcal{FL}\circ X_{\mathcal{L}}=fX_{\mathcal{H}}\circ\mathcal{FL},$$

for some $f\in C^\infty(J^1{}^*E)$ *(we say that the classes* $\{X_{\mathcal{L}}\}$ *and* $\{X_{\mathcal{H}}\}$ *are* $\mathcal{FL}$*-related).*

(2) (Equivalence theorem for jet fields and connections) Let $\mathcal{Y}_{\mathcal{L}}$ *and* $\mathcal{Y}_{\mathcal{H}}$ *be the jet fields solution of the Lagrangian and the Hamiltonian problems respectively. Then*

$$j^1\mathcal{FL}\circ\mathcal{Y}_{\mathcal{L}}=\mathcal{Y}_{\mathcal{H}}\circ\mathcal{FL}$$

(we say that the jet fields $\mathcal{Y}_{\mathcal{L}}$ *and* $\mathcal{Y}_{\mathcal{H}}$ *are* $\mathcal{FL}$*-related). As a consequence, their associated connection forms,* $\nabla_{\mathcal{L}}$ *and* $\nabla_{\mathcal{H}}$ *respectively, are* $\mathcal{FL}$*-related, too.*

(For almost-regular systems the statement is the same, but changing $J^1{}^*E$ *for* $\mathcal{P}$*).*

(*Proof*) See Ref. 31. (The proof for the almost-regular case follows in a straight-forward way.) ■

As a consequence of these latter theorems, similar comments to those made at the end of Secs. II A and II B about the existence, integrability, and nonuniqueness of Euler–Lagrange and Hamilton–de Donder–Weyl m-vector fields, connections, and jet fields, can be applied to their associated elements in the unified formalism. In particular, for singular systems, the existence of these solutions is not assured, except perhaps on some submanifold $\mathcal{S}\hookrightarrow\mathcal{W}_1$, and the number of arbitrary functions which appear depends on the dimension of $\mathcal{S}$ and the rank of the Hessian matrix of L (an algorithm for finding this submanifold is outlined in Ref. 9). The integrability of these solutions is not assured (even in the regular case), except perhaps on a smaller submanifold $\mathcal{I}\hookrightarrow\mathcal{S}$ such that the integral sections are contained in $\mathcal{I}$.

IV. EXAMPLE: MINIMAL SURFACES (in $\mathbb{R}^3$)

[In Ref. 9 we find another interesting example, the *bosonic string* (which is a singular model), described in this unified formalism.]

A. Statement of the problem: Geometric elements

The problem consists in looking for mappings $\varphi:U\subset\mathbb{R}^2\to$ such that their graphs have minimal area as sets of $\mathbb{R}^3$, and satisfy certain boundary conditions.

For this model, we have that $M=\mathbb{R}^2$, $E=\mathbb{R}^2\times\mathbb{R}$, and

$$J^1E=\pi^*T^*\mathbb{R}^2\otimes\mathbb{R}=\pi^*T^*M=\pi^*T^*\mathbb{R}^2,$$

$$\mathcal{M}\pi=\pi^*(TM\times_M E)\ \text{(affine maps from } J^1E \text{ to } \pi^*\Lambda^2T^*M),$$

$$J^{1*}E=\pi^*TM=\pi^*T\mathbb{R}^2\ \text{(classes of affine maps from } J^1E \text{ to } \pi^*\Lambda^2T^*M).$$

The coordinates in J^1E, $J^{1*}E$ and $\mathcal{M}\pi$ are denoted (x^1,x^2,y,v_1,v_2), (x^1,x^2,y,p^1,p^2), and (x^1,x^2,y,p^1,p^2,p), respectively. If $\omega=\mathrm{d}x^1\wedge\mathrm{d}x^2$, the Lagrangian density is

$$\mathcal{L}=[1+(v_1)^2+(v_2)^2]^{1/2}\mathrm{d}x^1\wedge\mathrm{d}x^2\equiv L\,\mathrm{d}x^1\wedge\mathrm{d}x^2,$$

and the Poincaré–Cartan forms are

$$\Theta_{\mathcal{L}}=\frac{v_1}{L}\mathrm{d}y\wedge\mathrm{d}x^2-\frac{v_2}{L}\mathrm{d}y\wedge\mathrm{d}x^1+L\left(1-\left(\frac{v_1}{L}\right)^2-\left(\frac{v_2}{L}\right)^2\right)\mathrm{d}x^1\wedge\mathrm{d}x^2,$$

$$\Omega_{\mathcal{L}}=-\mathrm{d}\left(\frac{v_1}{L}\right)\wedge\mathrm{d}y\wedge\mathrm{d}x^2+\mathrm{d}\left(\frac{v_2}{L}\right)\wedge\mathrm{d}y\wedge\mathrm{d}x^1-\mathrm{d}\left[L\left(1-\left(\frac{v_1}{L}\right)^2-\left(\frac{v_2}{L}\right)^2\right)\right]\wedge\mathrm{d}x^1\wedge\mathrm{d}x^2.$$

The Legendre maps are

$$\mathcal{FL}(x^1,x^2,y,v_1,v_2)=\left(x^1,x^2,y,\frac{v_1}{L},\frac{v_2}{L}\right),$$

$$\widetilde{\mathcal{FL}}(x^1,x^2,y,v_1,v_2)=\left(x^1,x^2,y,\frac{v_1}{L},\frac{v_2}{L},L-\frac{(v_1)^2}{L}-\frac{(v_2)^2}{L}\right),$$

and then $\mathcal{L}$ is hyperregular. The Hamiltonian function is

$$H=-[1-(p^1)^2-(p^2)^2]^{1/2}. \tag{14}$$

So the Hamilton–Cartan forms are

$$\Theta_h=p^1\mathrm{d}y\wedge\mathrm{d}x^2-p^2\mathrm{d}y\wedge\mathrm{d}x^1-H\mathrm{d}x^1\wedge\mathrm{d}x^2,$$

$$\Omega_h=-\mathrm{d}p^1\wedge\mathrm{d}y\wedge\mathrm{d}x^2+\mathrm{d}p^2\wedge\mathrm{d}y\wedge\mathrm{d}x^1+\mathrm{d}H\wedge\mathrm{d}x^1\wedge\mathrm{d}x^2.$$

B. Unified formalism

For the unified formalism we have

$$\mathcal{W}=\pi^*T^*M\times_E\pi^*(TM\times_M E),\quad \mathcal{W}_r=\pi^*T^*M\times_E\pi^*TM=\pi^*(T^*M\times_M TM).$$

If

$$w=(x^1,x^2,y,v_1,v_2,p^1,p^2,p)\in\mathcal{W},$$

the coupling form is

$$\hat{\mathcal{C}}=(p^1v_1+p^2v_2+p)\mathrm{d}x^1\wedge\mathrm{d}x^2,$$

therefore,

$$\mathcal{W}_0=\{(x^1,x^2,y,v_1,v_2,p^1,p^2,p)\in\mathcal{W}|[1+(v_1)^2+(v_2)^2]^{1/2}-p^1v_1-p^2v_2-p=0\},$$

and we have the forms

$$\Theta_0=([1+(v_1)^2+(v_2)^2]^{1/2}-p^1v_1-p^2v_2)\mathrm{d}x^1\wedge\mathrm{d}x^2-p^2\mathrm{d}y\wedge\mathrm{d}x_1+p^1\mathrm{d}y\wedge\mathrm{d}x_2,$$

$$\Omega_0=-\mathrm{d}([1+(v_1)^2+(v_2)^2]^{1/2}-p^1v_1-p^2v_2)\wedge\mathrm{d}x^1\wedge\mathrm{d}x^2+\mathrm{d}p^2\wedge\mathrm{d}y\wedge\mathrm{d}x_1-\mathrm{d}p^1\wedge\mathrm{d}y\wedge\mathrm{d}x_2.$$

Taking first $\hat{\rho}_2^0$-vertical vector fields $\partial/\partial v_\alpha$ we obtain

$$0=i\left(\frac{\partial}{\partial v_\alpha}\right)\ \Omega_0=\left(p^\alpha-\frac{v_\alpha}{L}\right)\mathrm{d}x^1\wedge\mathrm{d}x^2,$$

which determines the submanifold $\mathcal{W}_1=\mathrm{graph}\,\widetilde{\mathcal{FL}}$ (diffeomorphic to J^1E), and reproduces the expression of the Legendre map. Now, taking ρ_1^0-vertical vector fields $\partial/\partial p^\alpha$, the contraction $i(\partial/\partial p^\alpha)\Omega_0$ gives, for $\alpha=1,2$, respectively,

$$v_1\mathrm{d}x^1\wedge\mathrm{d}x^2-\mathrm{d}y\wedge\mathrm{d}x^2,\quad v_2\mathrm{d}x^1\wedge\mathrm{d}x^2+\mathrm{d}y\wedge\mathrm{d}x^1,$$

so that, for a section

$$\psi_0=(x^1,x^2,y(x^1,x^2),v_1(x^1,x^2),v_2(x^1,x^2),p^1(x^1,x^2),p^2(x^1,x^2)),$$

taking values in $\mathcal{W}_1$, we have that the condition

$$\psi_0^*\left[i\left(\frac{\partial}{\partial p^\alpha}\right)\Omega_0\right]=0$$

leads to

$$\left(v_1-\frac{\partial y}{\partial x^1}\right)\mathrm{d}x^1\wedge\mathrm{d}x^2=0,\quad \left(v_2-\frac{\partial y}{\partial x^2}\right)\mathrm{d}x^1\wedge\mathrm{d}x^2=0,$$

which is the holonomy condition. Finally, taking the vector field $\partial/\partial y$ we have

$$i\left(\frac{\partial}{\partial y}\right)\Omega_0=-\mathrm{d}p^2\wedge\mathrm{d}x^1+\mathrm{d}p^1\wedge\mathrm{d}x^2,$$

and, for a section ψ_0 fulfilling the former conditions, the equation

$$0=\psi_0^*\left[i\left(\frac{\partial}{\partial y}\right)\Omega_0\right],$$

leads to

$$\begin{aligned}0&=\left(\frac{\partial p^2}{\partial x^2}+\frac{\partial p^1}{\partial x^1}\right)\mathrm{d}x^1\wedge\mathrm{d}x^2\\&=\left[\frac{\partial}{\partial x^1}\left(\frac{v_1}{L}\right)+\frac{\partial}{\partial x^2}\left(\frac{v_2}{L}\right)\right]\mathrm{d}x^1\wedge\mathrm{d}x^2\\&=\frac{1}{L^3}\left[\left(1+\left(\frac{\partial y}{\partial x^1}\right)^2\right)\frac{\partial^2y}{\partial x^2\partial x^2}+\left(1+\left(\frac{\partial y}{\partial x^2}\right)^2\right)\frac{\partial^2y}{\partial x^1\partial x^1}-2\,\frac{\partial y}{\partial x^1}\,\frac{\partial y}{\partial x^2}\,\frac{\partial^2y}{\partial x^1\partial x^2}\right]\mathrm{d}x^1\wedge\mathrm{d}x^2,\end{aligned}$$

which gives the Euler–Lagrange equation of the problem.

Now, bearing in mind (14), and the expression of the Legendre map, from the Euler–Lagrange equations we get

$$\frac{\partial y}{\partial x^1}=-\frac{p^1}{H},\quad \frac{\partial y}{\partial x^2}=-\frac{p^2}{H};\quad \frac{\partial p^1}{\partial x^1}=-\frac{\partial p^2}{\partial x^2},$$

which are the Hamilton–De Donder–Weyl equations of the problem.

The *m*-vector fields, connections and jet fields which are the solutions to the problem in the unified formalism are

$$X_0=f\left(\frac{\partial}{\partial x^1}+v_1\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^1}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^1}\frac{\partial}{\partial v_2}+\frac{\partial p^1}{\partial x^1}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^1}\frac{\partial}{\partial p^2}\right)$$
$$\wedge\left(\frac{\partial}{\partial x^2}+v_2\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^2}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^2}\frac{\partial}{\partial v_2}+\frac{\partial p^1}{\partial x^2}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^2}\frac{\partial}{\partial p^2}\right),$$

$$\Psi_0=\left(x^1,x^2,y,p^1,p^2;v_1,v_2,\frac{\partial v_1}{\partial x^1},\frac{\partial v_1}{\partial x^2},\frac{\partial v_2}{\partial x^1},\frac{\partial v_2}{\partial x^2},\frac{\partial p^1}{\partial x^1},\frac{\partial p^1}{\partial x^2},\frac{\partial p^2}{\partial x^1},\frac{\partial p^2}{\partial x^2}\right),$$

$$\nabla_0=dx^1\otimes\left(\frac{\partial}{\partial x^1}+v_1\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^1}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^1}\frac{\partial}{\partial v_2}+\frac{\partial p^1}{\partial x^1}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^1}\frac{\partial}{\partial p^2}\right)$$
$$+dx^2\otimes\left(\frac{\partial}{\partial x^2}+v_2\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^2}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^2}\frac{\partial}{\partial v_2}+\frac{\partial p^1}{\partial x^2}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^2}\frac{\partial}{\partial p^2}\right)$$

(f being a nonvanishing function), where the coefficients $\partial v_\alpha/\partial x^\nu=\partial^2 y/\partial x^\nu\partial x^\alpha$ are related by the Euler–Lagrange equations, and the coefficients $\partial p^\alpha/\partial x^\nu$ are related by the Hamilton–De Donder–Weyl equations (the third one). Hence, the associated Euler–Lagrange *m*-vector fields, connections and jet fields which are the solutions to the Lagrangian problem are

$$X_{\mathcal{L}}=f\left(\frac{\partial}{\partial x^1}+v_1\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^1}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^1}\frac{\partial}{\partial v_2}\right)\wedge\left(\frac{\partial}{\partial x^2}+v_2\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^2}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^2}\frac{\partial}{\partial v_2}\right),$$

$$\Psi_{\mathcal{L}}=\left(x^1,x^2,y,p^1,p^2;v_1,v_2,\frac{\partial v_1}{\partial x^1},\frac{\partial v_1}{\partial x^2},\frac{\partial v_2}{\partial x^1},\frac{\partial v_2}{\partial x^2}\right),$$

$$\nabla_{\mathcal{L}}=dx^1\otimes\left(\frac{\partial}{\partial x^1}+v_1\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^1}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^1}\frac{\partial}{\partial v_2}\right)+dx^2\otimes\left(\frac{\partial}{\partial x^2}+v_2\frac{\partial}{\partial y}+\frac{\partial v_1}{\partial x^2}\frac{\partial}{\partial v_1}+\frac{\partial v_2}{\partial x^2}\frac{\partial}{\partial v_2}\right),$$

and the corresponding Hamilton–De Donder–Weyl *m*-vector fields, connections, and jet fields which are the solutions to the Hamiltonian problem are

$$X_{\mathcal{H}}=f\left(\frac{\partial}{\partial x^1}-\frac{p^1}{H}\frac{\partial}{\partial y}+\frac{\partial p^1}{\partial x^1}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^1}\frac{\partial}{\partial p^2}\right)\wedge\left(\frac{\partial}{\partial x^2}-\frac{p^2}{H}\frac{\partial}{\partial y}+\frac{\partial p^1}{\partial x^2}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^2}\frac{\partial}{\partial p^2}\right),$$

$$\Psi_{\mathcal{H}}=\left(x^1,x^2,y,p^1,p^2;-\frac{p^1}{H},-\frac{p^2}{H},\frac{\partial p^1}{\partial x^1},\frac{\partial p^1}{\partial x^2},\frac{\partial p^2}{\partial x^1},\frac{\partial p^2}{\partial x^2}\right),$$

$$\nabla_{\mathcal{H}}=\mathrm{d}x^1\otimes\left(\frac{\partial}{\partial x^1}-\frac{p^1}{H}\frac{\partial}{\partial y}+\frac{\partial p^1}{\partial x^1}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^1}\frac{\partial}{\partial p^2}\right)+\mathrm{d}x^2\otimes\left(\frac{\partial}{\partial x^2}-\frac{p^2}{H}\frac{\partial}{\partial y}+\frac{\partial p^1}{\partial x^2}\frac{\partial}{\partial p^1}+\frac{\partial p^2}{\partial x^2}\frac{\partial}{\partial p^2}\right).$$

V. CONCLUSIONS AND OUTLOOK

We have generalized the *Rusk–Skinner unified formalism* to first-order classical field theories. Corresponding to the Whitney sum $TQ\times_Q T^*Q$ in autonomous mechanics, here we take $J^1E\times_E\mathcal{M}\pi$ as standpoint, but the field equations are stated in a submanifold $\mathcal{W}_0\subset J^1E\times_E\mathcal{M}\pi$. As a particular case of this situation, the unified formalism for nonautonomous mechanics is recovered, the Whitney sum being now $J^1E\times_E T^*E$, where $\pi:E\to\mathbb{R}$ is the configuration bundle.[8,9] Once the suitable (pre) multisymplectic structures are introduced, the field equations can be written in several equivalent ways: using sections and vector fields (8) in $\mathcal{W}_0$, m-vector fields (10), connections (11), or jet fields (12).

Starting from Eq. (8), we have seen how, when different kinds of vertical vector fields in $\mathcal{W}_0$ are considered, this equation gives a different type of information. In particular, using $\hat{\rho}_2^0$-vertical vector fields, we can define a submanifold $\mathcal{W}_1\hookrightarrow\mathcal{W}_0$, which turns out to be the graph of the (extended) Legendre transformation (and hence diffeomorphic to J^1E). Furthermore, the field equations are only compatible in $\mathcal{W}_1$. As sections solution to the field equations take values in $\mathcal{W}_1$, they split in a natural way into two components, $\psi_0=(\psi_{\mathcal{L}},\psi_{\mathcal{H}})$, (with $\psi_{\mathcal{L}}:M\to J^1E$, and $\psi_{\mathcal{H}}=\widetilde{\mathcal{FL}}\circ\psi_{\mathcal{L}}$). Then, taking ρ_1^0-vertical vector fields in (8), we have proved that the sections solution to the field equations in the unified formalism are automatically holonomic, even in the singular case. They are so in the following sense: for every section ψ_0 solution in the unified formalism, the corresponding section $\psi_{\mathcal{L}}$ is holonomic. (As a special case, nonintegrable m-vector fields, connections and jet fields which are solutions to the field equations are semi-holonomic.) These solutions only exist in general in a submanifold of $\mathcal{W}_1$. Finally, considering (8) for a generic vector field, the Euler–Lagrange equations for $\psi_{\mathcal{L}}$, and the Hamilton–De Donder–Weyl equations for $\mu\circ\psi_{\mathcal{H}}=\mathcal{FL}\circ\psi_{\mathcal{L}}$ arise in a natural way. Conversely, starting from sections $\psi_{\mathcal{L}}=j^1\phi$ and $\mathcal{FL}\circ\psi_{\mathcal{L}}$ solutions to the corresponding field equations, we can recover sections ψ_0 solution to (8). Thus, we have shown the equivalence between the standard Lagrangian and Hamiltonian formalisms and the unified one. This equivalence has been also proved for m-vector fields, connections and jet fields.

Although the subject is not considered in this work, $\mathcal{K}$ operators (i.e., the analogous operators in field theories to the so-called *evolution operator* in mechanics), in their different alternative definitions,[33] can easily be recovered from the unified formalism, similarly to the case of classical mechanics.

In a forthcoming paper, this formalism will be applied to give a geometric framework for optimal control with partial differential equations. Although this subject has been dealt with in the context of functional analysis, to our knowledge there has been no geometric treatment of it to date.

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APPENDIX: *m*-VECTOR FIELDS, JET FIELDS, AND CONNECTIONS IN JET BUNDLES

(See Refs. 17 and 27 for the proofs and other details of the following assertions.)

Let E be a n-dimensional differentiable manifold. For $m\leqslant n$, sections of $\Lambda^m(TE)$ are called *m-vector fields* in E (they are contravariant skew-symmetric tensors of order m in E). We denote by $\mathfrak{X}^m(E)$ the set of m-vector fields in E. $Y\in\mathfrak{X}^m(E)$ is said to be *locally decomposable* if, for every $p\in E$, there exists an open neighborhood $U_p\subset E$ and $Y_1,\ldots,Y_m\in\mathfrak{X}(U_p)$ such that $Y\simeq_{U_p}Y_1\wedge\cdots\wedge Y_m$. Contraction of m-vector fields and tensor fields in E is the usual one.

We can define the following equivalence relation: if $Y, Y' \in \mathfrak{X}^m(E)$ are nonvanishing m-vector fields, then $Y \sim Y'$ if there exists a nonvanishing function $f \in C^\infty(E)$ such that $Y' = fY$ (perhaps only in a connected open set $U \subseteq E$). Equivalence classes will be denoted by $\{Y\}$. There is a one-to-one correspondence between the set of m-dimensional orientable distributions D in TE and the set of the equivalence classes $\{Y\}$ of nonvanishing, locally decomposable m-vector fields in E. Then, there is a bijective correspondence between the set of classes of locally decomposable and π-transverse m-vector fields $\{Y\} \subset \mathfrak{X}^m(E)$, and the set of orientable jet fields $\Psi: E \to J^1E$; that is, the set of orientable Ehresmann connection forms ∇ in $\pi: E \to M$. This correspondence is characterized by the fact that the horizontal subbundle associated with Ψ (and ∇) coincides with $\mathcal{D}(Y)$.

If $Y \in \mathfrak{X}^m(E)$ is nonvanishing and locally decomposable, the distribution associated with the class $\{Y\}$ is denoted $\mathcal{D}(Y)$. A nonvanishing, locally decomposable m-vector field $Y \in \mathfrak{X}^m(E)$ is said to be *integrable* (respectively, *involutive*) if its associated distribution $\mathcal{D}_U(Y)$ is integrable (respectively, involutive). Of course, if $Y \in \mathfrak{X}^m(E)$ is integrable (respectively, involutive), then so is every m-vector field in its equivalence class $\{Y\}$, and all of them have the same integral manifolds. Moreover, *Frobenius' theorem* allows us to say that a nonvanishing and locally decomposable m-vector field is integrable if, and only if, it is involutive. Of course, the orientable jet field Ψ, and the connection form ∇ associated with $\{Y\}$ are integrable if, and only if, so is Y, for every $Y \in \{Y\}$.

Let us consider the following situation: if $\pi: E \to M$ is a fiber bundle, we are concerned with the case where the integral manifolds of integrable m-vector fields in E are sections of π. Thus, $Y \in \mathfrak{X}^m(E)$ is said to be *π-transverse* if, at every point $y \in E$, $(i(Y)(\pi^*\beta))_y \neq 0$, for every $\beta \in \Omega^m(M)$ such that $\beta(\pi(y)) \neq 0$. Then, if $Y \in \mathfrak{X}^m(E)$ is integrable, it is π-transverse if its integral manifolds are local sections of π. In this case, if $\phi: U \subset M \to E$ is a local section with $\phi(x) = y$ and $\phi(U)$ is the integral manifold of Y through y, then $T_y(\mathrm{Im}\,\phi)$ is $\mathcal{D}_y(Y)$. Integral sections ϕ of the class $\{Y\}$ can be characterized by the condition $\Lambda^m T\phi = fY \circ \phi \circ \sigma_M$, where $\sigma_M: \Lambda^m TM \to M$ is the natural projection, and $f \in C^\infty(E)$ is a nonvanishing function.

As a particular case, let $\{X\}: J^1E \to D^m TJ^1E \subset \{\Lambda^m TJ^1E\}$ be a class of nonvanishing, locally decomposable and $\overline{\pi^1}$-transverse m-vector fields in J^1E, $\Psi: J^1E \to J^1J^1E$ its associated jet field, and $\nabla: J^1E \to \overline{\pi^1}^*TM \otimes_{J^1E} TJ^1E$ its associated connection form. Then, these elements are said to be *holonomic* if they are integrable and their integral sections $\varphi: M \to J^1E$ are holonomic. Furthermore, consider the $(1,m)$-tensor field in J^1E defined by $\mathcal{J} := i(\mathcal{V})(\overline{\pi^1}^*\omega)$, whose local expression is $\mathcal{J} = (\mathrm{d}y^A - v^A_\alpha \mathrm{d}x^\alpha) \wedge \mathrm{d}^{m-1}x_\nu \otimes \partial/\partial v^A_\nu$. A connection form ∇ in $\overline{\pi^1}: J^1E \to M$ (and its associated jet field $\Psi: J^1E \to J^1J^1E$) are said to be *semi-holonomic* (or a *second order partial differential equation*), if

$$\overbrace{\mathcal{J}(h^\nabla, \ldots, h^\nabla)}^{m} = 0,$$

where h^∇ denotes the horizontal projector associated with ∇. If $\{X\} \subset \mathfrak{X}^m(J^1E)$ is the associated class of $\overline{\pi^1}$-transverse multivector fields, then this condition is equivalent to $\mathcal{J}(X) = 0$, for every $X \in \{X\}$. Then the class $\{X\}$, and its associated jet field Ψ and connection form ∇ are holonomic if, and only if, they are integrable and semi-holonomic.

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Unsteady equipartition MHD solutions

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The unsteady equipartition solutions are introduced that describe a plasma relaxation in regime of a strong interaction between the plasma velocity **V** and the magnetic field **B** and depend on all four variables t,x,y,z. The solutions exist when the kinematic viscosity ν is equal to the magnetic diffusivity η and $\mathbf{V}=\pm\mathbf{B}/\sqrt{\rho\mu}$. The exact equipartition solutions to the boundary value problem with the "no-slip" boundary condition are derived. The solutions depend on infinitely many parameters and describe the plasma relaxation in a ball with a constant pressure at the boundary. The translationally invariant exact solutions are obtained for $\nu\neq\eta$ for which plasma is confined in cylindrical domains by the magnetic field **B** only while the plasma pressure P is zero at the boundary and is positive inside the domains. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629137]

I. INTRODUCTION

The magnetohydrodynamics equations have the form

$$\frac{\partial\mathbf{V}}{\partial t}+(\mathbf{V}\cdot\operatorname{grad})\mathbf{V}=-\frac{1}{\rho}\operatorname{grad}P+\nu\Delta\mathbf{V}+\frac{1}{\rho\mu}\operatorname{curl}\mathbf{B}\times\mathbf{B}+\frac{1}{\rho}\mathbf{f}, \tag{1.1}$$

$$\frac{\partial\mathbf{B}}{\partial t}=\operatorname{curl}(\mathbf{V}\times\mathbf{B})+\eta\Delta\mathbf{B}, \tag{1.2}$$

$$\operatorname{div}\mathbf{V}=0,\quad \operatorname{div}\mathbf{B}=0, \tag{1.3}$$

where **B** is the magnetic vector field, **V** is the plasma velocity and P is the pressure. We suppose that the plasma density ρ, its kinematic viscosity ν, magnetic permeability μ, and the resistivity (or magnetic diffusivity) η are constant and assume that **f** is the vector field of the external gravitational force, $\mathbf{f}=-\rho\operatorname{grad}\Phi$, where $\Phi(t,\mathbf{x})$ is the gravitational potential and denote $\mathbf{x}=(x,y,z)$. For $\mathbf{B}=0$, the MHD equations turn into the Navier–Stokes equations (NSE):

$$\frac{\partial\mathbf{V}}{\partial t}+(\mathbf{V}\cdot\operatorname{grad})\mathbf{V}=-\frac{1}{\rho}\operatorname{grad}P+\nu\Delta\mathbf{V}+\frac{1}{\rho}\mathbf{f},\quad \operatorname{div}\mathbf{V}=0. \tag{1.4}$$

The NSE were intensively studied in the literature, see the Leray paper[1] and the monographs.[2,3] There are well-known exact parallel shear or unidirectional flows for which all streamlines are parallel to the axis z and velocity **V** is independent of z; this class contains the steady Couette flow and Poiseuille flow. There are exact cylindrically symmetric solutions with closed plane streamlines.[4] The known Landau[5] and Squire[6] exact solution describes a steady and axially symmetric laminar jet; the solution has singularity at $r=0$, infinite total kinetic energy and has the asymptotics $|\mathbf{V}(x,y,z)|=r^{-1}f(\theta)$ as $r\to\infty$ where r, θ, ϕ are the spherical coordinates.

Cole[7] and Hopf[8] demonstrated that the Burgers equation[9]

$$\frac{\partial\mathbf{V}}{\partial t}+(\mathbf{V}\cdot\operatorname{grad})\mathbf{V}=\nu\Delta\mathbf{V} \tag{1.5}$$

has exact potential solutions $\mathbf{V}=-2\nu\,\mathrm{grad}(\log\Psi)$ where function $\Psi(t,\mathbf{x})$ satisfies the diffusion equation $\Psi_t=\nu\Delta\Psi$. The incompressibility condition $\mathrm{div}\,\mathbf{V}=0$ and the pressure P are ignored in the Burgers equation (1.5).

In the paper[10] we presented the following exact solutions to the complete system of the viscous MHD equations with the necessary constraints $\mathrm{div}\,\mathbf{V}=0$, $\mathrm{div}\,\mathbf{B}=0$:

$$\mathbf{V}(t,\mathbf{x})=e^{-\alpha^2\nu t}\int\int_{S^2}[\sin(\alpha\mathbf{k}\cdot\mathbf{x})\mathbf{T}(\mathbf{k})+\cos(\alpha\mathbf{k}\cdot\mathbf{x})\mathbf{k}\times\mathbf{T}(\mathbf{k})]\,\mathrm{d}\sigma, \tag{1.6}$$

$$\mathbf{B}(t,\mathbf{x})=C_1\exp[-\alpha^2(\eta-\nu)t]\mathbf{V}(t,\mathbf{x}),$$

$$P(t,\mathbf{x})=C_2-\rho\mathbf{V}^2(t,\mathbf{x})-\rho\Phi(t,\mathbf{x}).$$

Here the integral is taken with respect to an arbitrary measure $\mathrm{d}\sigma$ on the two-dimensional unit sphere S^2: $\mathbf{k}\cdot\mathbf{k}=1$ and $\mathbf{T}(\mathbf{k})$ is an arbitrary smooth vector field tangent to the unit sphere, $\mathbf{T}(\mathbf{k})\cdot\mathbf{k}=0$ and $\alpha\neq0$ is an arbitrary parameter. The solutions satisfy the Beltrami equation $\mathrm{curl}\,\mathbf{V}=\alpha\mathbf{V}$. For $C_1=0$, we get the exact solutions to the Navier–Stokes equations (1.4). For the special vector fields $\mathbf{T}(\mathbf{k})$ and the Euclidean measure $\mathrm{d}\sigma$, solutions (1.6) have the solitonlike properties, see Refs. 11 and 12.

In this paper we introduce the unsteady field-aligned equipartition solutions to the MHD equations (1.1)–(1.3) that describe the plasma relaxation in the regime of a strong interaction between the magnetic field $\mathbf{B}(t,\mathbf{x})$ and the plasma velocity $\mathbf{V}(t,\mathbf{x})$ (these solutions were first announced in Refs. 13 and 14). The interaction causes the equality of the densities of the plasma magnetic and kinetic energies and the collinearity of the fields $\mathbf{B}(t,\mathbf{x})$ and $\mathbf{V}(t,\mathbf{x})$. The solutions exist when the kinematic viscosity ν is equal to the resistivity η. As an application we construct for $\nu=\eta>0$ the nonequipartition solutions describing a plasma relaxation to an equilibrium with a constant magnetic field $\mathbf{B}$. For the unsteady equipartition solutions with $\nu=\eta>0$, the viscous MHD equations are reduced to the linear system of the vector diffusion equation and the incompressibility equation:

$$\frac{\partial\mathbf{V}}{\partial t}=\nu\Delta\mathbf{V},\quad \mathrm{div}\,\mathbf{V}=0. \tag{1.7}$$

We derive the global equipartition solutions in $\mathbb{R}^3$ for which the total plasma magnetic and kinetic energies are finite and equal. The obtained solutions are different from the small Alfvénic fluctuations or waves[15–18] that satisfy the equation $\delta\mathbf{B}=\pm\sqrt{\rho\mu}\,\delta\mathbf{V}$ for the variations $\delta\mathbf{B}$, $\delta\mathbf{V}$.

We present the exact nonsymmetric equipartition solutions to the boundary value problem

$$\frac{\partial\mathbf{V}}{\partial t}=\nu\Delta\mathbf{V},\quad \mathrm{div}\,\mathbf{V}=0,\quad \mathbf{V}|_{\partial\mathcal{D}}=0 \tag{1.8}$$

with the "no-slip" boundary condition which describe the viscous plasma relaxation in a ball $\mathcal{D}$ with a constant pressure at the boundary. We show that the corresponding initial-boundary value problem is overdetermined. The steady ideal MHD equilibria in a ball with $\nu=\eta=0$ and $\mathbf{V}=0$ were first found by Wu and Chen[19] and by Kaiser and Lortz.[20]

For the generic case $\nu\neq\eta$, we derive the exact translationally invariant solutions that model the plasma relaxation inside cylindrical domains $\mathcal{D}$. An important property of these solutions is that the pressure $P(t,\mathbf{x})$ is positive inside the plasma volume $\mathcal{D}$ and is zero at the boundary $\partial\mathcal{D}$. Hence it is the magnetic field $\mathbf{B}(t,\mathbf{x})$ that confines plasma inside the domain $\mathcal{D}$ but not the external pressure that is zero.

II. UNSTEADY EQUIPARTITION SOLUTIONS

The magnetohydrodynamics equations (1.1)–(1.3) for $\nu=\eta$ have the following exact field-aligned equipartition solutions

$$\mathbf{V}(t,\mathbf{x})=\frac{1}{(4\pi\nu t)^{3/2}}\operatorname{curl}\int_{R^3}\mathbf{A}(\mathbf{x}')\exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|^2}{4\nu t}\right)\mathrm{d}\tau', \tag{2.1}$$

$$\mathbf{B}(t,\mathbf{x})=\pm\sqrt{\rho\mu}\,\mathbf{V}(t,\mathbf{x}), \tag{2.2}$$

where $\mathrm{d}\tau'=\mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}z'$ and the vector field $\mathbf{A}(\mathbf{x}')$ is arbitrary and coincides with the vector potential of the initial vector field $\mathbf{V}(0,\mathbf{x}')$: $\operatorname{curl}\mathbf{A}(\mathbf{x}')=\mathbf{V}(0,\mathbf{x}')$. The pressure P has the form

$$P(t,\mathbf{x})=C-\rho\mathbf{V}^2(t,\mathbf{x})/2-\rho\Phi(t,\mathbf{x}). \tag{2.3}$$

Using the known identity

$$(\mathbf{V}\cdot\operatorname{grad})\mathbf{V}=\operatorname{curl}\mathbf{V}\times\mathbf{V}+\operatorname{grad}(\mathbf{V}^2/2), \tag{2.4}$$

one transforms equations (1.1) to the form

$$\frac{\partial\mathbf{V}}{\partial t}=\mathbf{V}\times\operatorname{curl}\mathbf{V}+\nu\Delta\mathbf{V}+\frac{1}{\rho\mu}\operatorname{curl}\mathbf{B}\times\mathbf{B}-\operatorname{grad}\frac{1}{\rho}\left(P+\frac{1}{2}\mathbf{V}^2+\Phi\right). \tag{2.5}$$

Equations (2.5) and (1.2) after substitution of (2.2) take the form

$$\frac{\partial\mathbf{V}}{\partial t}=\nu\Delta\mathbf{V}-\operatorname{grad}\left(\frac{1}{\rho}P+\frac{1}{2}\mathbf{V}^2+\Phi\right),\quad \frac{\partial\mathbf{V}}{\partial t}=\eta\Delta\mathbf{V}.$$

Applying operator curl to these two equations we find the conditions of their compatibility

$$\nu=\eta,\quad \frac{1}{\rho}P(t,\mathbf{x})+\frac{1}{2}\mathbf{V}^2(t,\mathbf{x})+\Phi(t,\mathbf{x})=\text{const}.$$

For this case, the equations (1.1)–(1.3) are reduced to the linear equations (1.7). The solutions to the scalar diffusion equation $\partial u/\partial t=\nu\Delta u$ have the form[1]

$$u(t,\mathbf{x})=\frac{1}{(4\pi\nu t)^{3/2}}\int_{R^3}f(\mathbf{x}')\exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|^2}{4\nu t}\right)\mathrm{d}\tau',$$

where $f(\mathbf{x}')=u(0,\mathbf{x}')$ are the initial data. Substituting here an arbitrary vector field $\mathbf{A}(\mathbf{x}')$ instead of the function $f(\mathbf{x}')$ we get a solution to the vector diffusion equation (1.7). Applying to this solution operator curl we obtain the vector field (2.1) that is divergence free and hence satisfies both equations (1.7) and therefore the MHD equations (1.1)–(1.3).

Remark 1: The exact solutions (2.1), (2.2) are the unsteady equipartition solutions because the densities of the kinetic and magnetic energies are equal: $\rho\mathbf{V}^2(t,\mathbf{x})=\mathbf{B}^2(t,\mathbf{x})/\mu$. It is evident that if the vector field $\mathbf{A}(\mathbf{x}')$ is square integrable then the solutions (2.1), (2.2) are square integrable also; hence the total kinetic and magnetic energies are finite and equal.

Remark 2: The derived exact solutions (2.1)–(2.3) describe a plasma relaxation in a regime of a strong interaction between the plasma velocity $\mathbf{V}$ and the magnetic field $\mathbf{B}$. Indeed, the very fact of the equality of the densities of the plasma kinetic and magnetic energies and the collinearity (2.2) mean a strong interaction between the magnetic field $\mathbf{B}(t,\mathbf{x})$ and the plasma velocity $\mathbf{V}(t,\mathbf{x})$.

Remark 3: Solutions (2.1) can be represented also in the form

$$\mathbf{V}(t,\mathbf{x})=\int_{R^3}\exp(-\nu\mathbf{k}^2t)[\cos(\mathbf{k}\cdot\mathbf{x})\mathbf{S}(\mathbf{k})+\sin(\mathbf{k}\cdot\mathbf{x})\mathbf{T}(\mathbf{k})]\mathrm{d}\tau, \tag{2.6}$$

where $\mathrm{d}\tau=\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3$ and the vector fields $\mathbf{S}(\mathbf{k})$ and $\mathbf{T}(\mathbf{k})$ are tangent to the spheres $\mathbf{k}\cdot\mathbf{k}=\text{const}$, or the equations $\mathbf{k}\cdot\mathbf{S}(\mathbf{k})=0$, $\mathbf{k}\cdot\mathbf{T}(\mathbf{k})=0$ hold. Indeed, a direct calculation proves that the vector field (2.6) satisfies both equations (1.7).

III. AN APPLICATION TO THE PLASMA RELAXATION TO A CONSTANT MAGNETIC FIELD

As a first application of the equipartition solutions (2.1)–(2.3) we construct the following exact solutions for $\nu=\eta$:

$$\mathbf{V}_2(t,\mathbf{x})=\frac{1}{(4\pi\nu t)^{3/2}}\operatorname{curl}\int_{R^3}\mathbf{A}(\mathbf{x}')\exp\left(-\frac{|\mathbf{x}\pm\mathbf{B}_0t/\sqrt{\rho\mu}-\mathbf{x}'|^2}{4\nu t}\right)\mathrm{d}\tau', \tag{3.1}$$

$$\mathbf{B}_2(t,\mathbf{x})=\pm\sqrt{\rho\mu}\,\mathbf{V}_2(t,\mathbf{x})+\mathbf{B}_0,$$

$$P_2(t,\mathbf{x})=C-\frac{\rho}{2}\left(\mathbf{V}_2(t,\mathbf{x})\pm\frac{1}{\sqrt{\rho\mu}}\mathbf{B}_0\right)^2-\rho\Phi\left(t,\mathbf{x}\pm\frac{1}{\sqrt{\rho\mu}}\mathbf{B}_0t\right).$$

To prove that (3.1) is an exact solution, we consider first for any square integrable vector field $\mathbf{V}(t,\mathbf{x})$ (2.1) the following equipartition solution:

$$\mathbf{V}_1(t,\mathbf{x})=\mathbf{V}(t,\mathbf{x})\pm\frac{1}{\sqrt{\rho\mu}}\mathbf{B}_0,\quad \mathbf{B}_1(t,\mathbf{x})=\pm\sqrt{\rho\mu}\,\mathbf{V}(t,\mathbf{x})+\mathbf{B}_0, \tag{3.2}$$

$$P_1(t,\mathbf{x})=C-\rho\mathbf{V}_1^2(t,\mathbf{x})/2-\rho\Phi(t,\mathbf{x}),$$

where $\mathbf{B}_0$ is an arbitrary constant vector. The formulas (3.2) define a solution to the equations (1.1)–(1.3) because the equations (1.7), (2.2), and (2.3) are satisfied.

As is known, the magnetohydrodynamics equations (1.1)–(1.3) are invariant with respect to the Galilean transforms

$$\mathbf{V}_2(t,\mathbf{x})=\mathbf{V}_1(t,\mathbf{x}-\mathbf{u}t)+\mathbf{u},\quad \mathbf{B}_2(t,\mathbf{x})=\mathbf{B}_1(t,\mathbf{x}-\mathbf{u}t), \tag{3.3}$$

$$P_2(t,\mathbf{x})=P_1(t,\mathbf{x}-\mathbf{u}t),$$

where $\mathbf{u}$ is an arbitrary constant vector. Applying the Galilean transform (3.3) with the vector $\mathbf{u}=\mp\mathbf{B}_0/\sqrt{\rho\mu}$ to the exact solutions (3.2), we obtain the solutions (3.1).

The exact solutions (3.1) evidently are not the equipartition ones and not the field-aligned ones. For these solutions the plasma velocity $\mathbf{V}_2(t,\mathbf{x})\to0$ as $t\to\infty$ and as $|\mathbf{x}|\to\infty$ and is square integrable. At the same time the magnetic field $\mathbf{B}_2(t,\mathbf{x})\to\mathbf{B}_0$. Therefore the derived noncollinear and nonequipartition solutions (3.1) describe a plasma relaxation to an equilibrium with a constant magnetic field $\mathbf{B}_0$.

IV. PLASMA RELAXATION IN A BALL

The steady MHD equilibria in a ball are constructed in Refs. 19 and 20 where the authors consider the ideal plasma ($\nu=\eta=0$) with zero velocity $\mathbf{V}(t,\mathbf{x})=0$. In Ref. 21 we generalize these solutions to the ideal MHD equilibria with dynamics of plasma with a steady velocity $\mathbf{V}(t,\mathbf{x})=\mathbf{V}(\mathbf{x})\neq0$ using the newly discovered symmetry transform.[21,22] In this section we present the unsteady equipartition solutions in a ball that take into account the effects of the plasma viscosity and the finite electric conductivity ($\nu=\eta\neq0$) and have spherical magnetic surfaces $|\mathbf{x}|=r$.

For the equipartition solutions (2.2) in a domain $\mathcal{D}\subset\mathbb{R}^3$, the initial-boundary value problem with the "no-slip" boundary condition $\mathbf{V}(t,\mathbf{x})|_{\partial\mathcal{D}}=0$ is overdetermined.

Indeed, since the equipartition solutions satisfy the system of equations (1.7), the initial-boundary value problem for them takes the form

$$\frac{\partial\mathbf{V}}{\partial t}=\nu\Delta\mathbf{V},\quad \operatorname{div}\mathbf{V}=0,\quad \mathbf{V}(t,\mathbf{x})|_{\partial\mathcal{D}}=0,\quad \mathbf{V}(0,\mathbf{x})=\mathbf{U}(\mathbf{x}),\tag{4.1}$$

where the vector field $\mathbf{U}(\mathbf{x})$ is the initial plasma velocity in the domain $\mathcal{D}$. The presence of the additional incompressibility condition $\operatorname{div}\mathbf{V}=0$ makes the problem (4.1) overdetermined. Indeed, let us consider the solutions independent of the variable z. Then the incompressibility equation implies $\mathbf{V}(t,x,y)=-\psi_y\mathbf{e}_x+\psi_x\mathbf{e}_y$ where $\psi(t,x,y)$ is a streamfunction and $\psi_x=\partial\psi/\partial x$, $\psi_y=\partial\psi/\partial y$. For this case the initial-boundary value problem (4.1) takes the form

$$\psi_t=\nu(\psi_{xx}+\psi_{yy}),\quad \psi_x|_{\partial\mathcal{D}}=0,\quad \psi_y|_{\partial\mathcal{D}}=0,\quad \psi(0,x,y)=f(x,y).\tag{4.2}$$

The two boundary conditions in (4.2) are equivalent to the taken simultaneously Dirichlet's and Neumann's conditions,

$$\psi(t,x,y)|_{\partial\mathcal{D}}=\text{const},\quad \left.\frac{\partial\psi(t,x,y)}{\partial\mathbf{n}}\right|_{\partial\mathcal{D}}=0.$$

Here $\mathbf{n}$ is the unit normal vector field to the boundary $\partial\mathcal{D}$. As is known,[23] for each of these two boundary conditions separately the initial-boundary value problem for the diffusion equation $\psi_t=\nu(\psi_{xx}+\psi_{yy})$ has a unique solution (up to a constant), and the two solutions are different in general. Hence the problem (4.2) is overdetermined.

Therefore we construct some solutions to the boundary value problem (1.8) without prescribed initial conditions. Let the domain $\mathcal{D}$ be a ball of radius R. Function

$$F_\alpha(\mathbf{x})=\frac{\sin(\alpha|\mathbf{x}|)}{\alpha|\mathbf{x}|}$$

satisfies the Helmholtz equation $\Delta F_\alpha(\mathbf{x})=-\alpha^2F_\alpha(\mathbf{x})$ where α is an arbitrary parameter. Hence for an arbitrary vector $\mathbf{a}$ the vector field $\mathbf{A}(\mathbf{x})=F_\alpha(\mathbf{x})\mathbf{a}$ satisfies the vector Helmholtz equation $\Delta\mathbf{A}(\mathbf{x})=-\alpha^2\mathbf{A}(\mathbf{x})$. Therefore the vector field

$$\mathbf{V}(t,\mathbf{x},\mathbf{a})=e^{-\alpha^2\nu t}\operatorname{curl}(F_\alpha(\mathbf{x})\mathbf{a})=e^{-\alpha^2\nu t}h_\alpha(\mathbf{x})\mathbf{x}\times\mathbf{a}\tag{4.3}$$

satisfies the first two equations (1.8). Here

$$h_\alpha(\mathbf{x})=h_\alpha(|\mathbf{x}|)=F'_\alpha(|\mathbf{x}|)|\mathbf{x}|^{-1}=\cos(\alpha|\mathbf{x}|)|\mathbf{x}|^{-2}-\sin(\alpha|\mathbf{x}|)\alpha^{-1}|\mathbf{x}|^{-3}\tag{4.4}$$

is a smooth function of $\mathbf{x}$.

The zeros of the function $h_\alpha(z\alpha^{-1})$ satisfy the equation

$$\tan z=z.\tag{4.5}$$

Let $z_1,\dots,z_k,\dots$ be the positive roots of equation (4.5). As is known,

$$z_k\approx k\pi+\frac{\pi}{2}-\frac{2}{(2k+1)\pi}\quad\text{as}\quad k\to\infty,\quad k\pi+\frac{\pi}{4}<z_k<k\pi+\frac{\pi}{2}.$$

Formula (4.4) yields that $h_\alpha(z_k\alpha^{-1})=0$. Therefore the vector field $\mathbf{V}(t,\mathbf{x},\mathbf{a})$ (4.3) vanishes on the spheres $|\mathbf{x}|=z_k\alpha^{-1}$. Hence for the discrete values of α: $\alpha_1=z_1R^{-1}$, $\alpha_2=z_2R^{-1},\dots$ and for the arbitrary vectors $\mathbf{a}=\mathbf{a}_k$ the vector fields (4.3) vanish on the sphere $|\mathbf{x}|=R$. Thus the vector fields

$$\mathbf{V}_k(t,\mathbf{x},\mathbf{a}_k)=e^{-z_k^2R^{-2}\nu t}\left[\frac{\cos(z_kR^{-1}|\mathbf{x}|)}{|\mathbf{x}|^2}-R\frac{\sin(z_kR^{-1}|\mathbf{x}|)}{z_k|\mathbf{x}|^3}\right]\mathbf{x}\times\mathbf{a}_k \tag{4.6}$$

satisfy the boundary value problem (1.8) in the ball $|\mathbf{x}|\leqslant R$. The vector fields (4.6) have two first integrals $f_1(t,\mathbf{x})=|\mathbf{x}|$ and $f_2(t,\mathbf{x})=\mathbf{x}\cdot\mathbf{a}_k$; hence their magnetic field lines are circumferences in the planes orthogonal to the vectors $\mathbf{a}_k$. A more general solution to the boundary value problem (1.8) is represented by the convergent series

$$\mathbf{V}(t,\mathbf{x})=\sum_{k=1}^{\infty}e^{-z_k^2R^{-2}\nu t}\left[\frac{\cos(z_kR^{-1}|\mathbf{x}|)}{|\mathbf{x}|^2}-R\frac{\sin(z_kR^{-1}|\mathbf{x}|)}{z_k|\mathbf{x}|^3}\right]\mathbf{x}\times\mathbf{a}_k, \tag{4.7}$$

where we suppose that the series $\Sigma_{k=1}^{\infty}|\mathbf{a}_k|$ is convergent. The unsteady equipartition solutions (2.2), (2.3), (4.7) satisfy the boundary value problem (1.8) in the ball $|\mathbf{x}|\leqslant R$. The pressure (2.3) is $P(t,\mathbf{x})=P_0-\rho\mathbf{V}^2(t,\mathbf{x})/2$ where P_0 is an arbitrary constant. Hence we find at the boundary $|\mathbf{x}|=R$:

$$P(t,\mathbf{x})=P_0,\quad \text{grad } P(t,\mathbf{x})=0.$$

The solution is continued in the outer space by the trivial solution $P=P_0$, $\mathbf{B}=0$, $\mathbf{V}=0$.

A direct calculation using the equations $\tan z_k=z_k$ proves that the total kinetic energy of the field (4.7) inside the ball $\mathcal{D}$ has the simple form

$$E=\frac{\rho}{2}\int_{\mathcal{D}}\mathbf{V}^2\,dx\,dy\,dz=\frac{2\pi\rho R}{3}\sum_{k=1}^{\infty}e^{-2z_k^2R^{-2}\nu t}|\mathbf{a}_k|^2\frac{z_k^2}{1+z_k^2},$$

for arbitrary vectors $\mathbf{a}_k$. The total plasma kinetic plus magnetic energy for the solutions (2.2), (4.7) is equal to $2E$.

The solutions (2.2), (4.7) possess invariant magnetic surfaces that are the spheres $|\mathbf{x}|=r=\text{const}$. We have $\mathbf{V}(t,\mathbf{x})=\mathbf{x}\times\mathbf{\Omega}(t,|\mathbf{x}|)$ where

$$\mathbf{\Omega}(t,r)=\sum_{k=1}^{\infty}e^{-z_k^2R^{-2}\nu t}\left[\frac{\cos(z_kR^{-1}r)}{r^2}-R\frac{\sin(z_kR^{-1}r)}{z_kr^3}\right]\mathbf{a}_k. \tag{4.8}$$

Therefore on each sphere $|\mathbf{x}|=r$ the vector field $\mathbf{V}(t,\mathbf{x})$ (4.7) defines a rotation around the vector $\mathbf{\Omega}(t,r)$ (4.8) that depends on t and r. Hence the solutions (2.2), (4.7) have no geometrical symmetries provided that some of the vectors $\mathbf{a}_k$ are noncollinear. It is evident that the solutions (2.2), (4.7) have spherical magnetic surfaces $|\mathbf{x}|=r\leqslant R$. The boundary value problem (1.8) is transformed to that for the vector $\mathbf{\Omega}(t,r)$:

$$\mathbf{\Omega}_t=\nu(4r^{-1}\mathbf{\Omega}_r+\mathbf{\Omega}_{rr}),\quad \mathbf{\Omega}(t,0)=0,\quad \mathbf{\Omega}(t,R)=0,$$

where $\mathbf{\Omega}_t=\partial\mathbf{\Omega}/\partial t$, $\mathbf{\Omega}_r=\partial\mathbf{\Omega}/\partial r$.

V. TRANSLATIONALLY INVARIANT SOLUTIONS FOR $\nu\neq\eta$

The viscous MHD equations (1.1)–(1.3) for arbitrary constants ρ, μ, ν, η have an infinite-dimensional family of exact solutions

$$\mathbf{V}(t,\tilde{\mathbf{x}})=e^{-\alpha^2\nu t}[-a\psi_y(\tilde{\mathbf{x}})\hat{\mathbf{e}}_x+a\psi_x(\tilde{\mathbf{x}})\hat{\mathbf{e}}_y+b\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z]+c\hat{\mathbf{e}}_z, \tag{5.1}$$

$$\mathbf{B}(t,\tilde{\mathbf{x}})=e^{-\alpha^2\eta t}[-k\psi_y(\tilde{\mathbf{x}})\hat{\mathbf{e}}_x+k\psi_x(\tilde{\mathbf{x}})\hat{\mathbf{e}}_y+\ell\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z]+m\hat{\mathbf{e}}_z, \tag{5.2}$$

where $\tilde{\mathbf{x}}=(x,y)$ and a,b,c,k,ℓ,m and α are arbitrary parameters, $\psi_x=\partial\psi/\partial x$, $\psi_y=\partial\psi/\partial y$ and the flux function $\psi(\tilde{\mathbf{x}})$ satisfies the two-dimensional Helmholtz equation

$$\Delta\psi(\tilde{\mathbf{x}}) = -\alpha^2\psi(\tilde{\mathbf{x}}). \tag{5.3}$$

The pressure P is

$$P = C - \frac{a^2\rho}{2}E^2(\psi_x^2+\psi_y^2+\alpha^2\psi^2) + \frac{\alpha^2k^2-\ell^2}{2\mu}E_m^2\psi^2 - \frac{\ell m}{\mu}E_m\psi, \tag{5.4}$$

where $E=\exp(-\alpha^2\nu t)$ and $E_m=\exp(-\alpha^2\eta t)$. The solutions possess invariant magnetic surfaces that are defined by the equations $\psi(\tilde{\mathbf{x}})=\text{const}$. For $k=\ell=m=0$, the formulas (5.1)–(5.4) describe exact solutions to the Navier–Stokes equations (1.4).

It is evident that the vector fields (5.1), (5.2) have the form

$$\mathbf{V} = b\mathbf{U} - a\,\text{curl}\,\mathbf{U} + c\hat{\mathbf{e}}_z, \quad \mathbf{B} = e^{-\alpha^2(\eta-\nu)t}(\ell\mathbf{U} - k\,\text{curl}\,\mathbf{U}) + m\hat{\mathbf{e}}_z, \tag{5.5}$$

where vector field $\mathbf{U}=\exp(-\alpha^2\nu t)\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z$ satisfies the equations $\text{div}\,\mathbf{U}=0$, $\Delta\mathbf{U}=-\alpha^2\mathbf{U}$. Hence using the identity $\text{curl}\,\text{curl}\,\mathbf{U}=\text{grad}\,\text{div}\,\mathbf{U}-\Delta\mathbf{U}$ we find

$$\text{curl}\,\mathbf{V} = -\alpha^2 a\mathbf{U} + b\,\text{curl}\,\mathbf{U}, \quad \text{curl}\,\mathbf{B} = e^{-\alpha^2(\eta-\nu)t}(-\alpha^2 k\mathbf{U} + \ell\,\text{curl}\,\mathbf{U}). \tag{5.6}$$

The formulas (5.5)–(5.6) imply

$$\text{curl}\,\mathbf{V}\times\mathbf{V} = (b^2-\alpha^2a^2)\text{curl}\,\mathbf{U}\times\mathbf{U} + bc\,\text{curl}\,\mathbf{U}\times\hat{\mathbf{e}}_z = \text{grad}[(\alpha^2a^2-b^2)E^2\psi^2/2 - bcE\psi]. \tag{5.7}$$

Hence using the identity (2.4) we get

$$(\mathbf{V}\cdot\text{grad})\mathbf{V} = a^2E^2\,\text{grad}(\psi_x^2+\psi_y^2+\alpha^2\psi^2)/2. \tag{5.8}$$

Analogously we obtain

$$\text{curl}\,\mathbf{B}\times\mathbf{B} = \text{grad}[(\alpha^2k^2-\ell^2)E_m^2\psi^2/2 - \ell mE_m\psi], \tag{5.9}$$

$$\mathbf{V}\times\mathbf{B} = \text{grad}[(a\ell-bk)EE_m\psi^2/2 + (amE-ckE_m)\psi]. \tag{5.10}$$

For the vector fields (5.1)–(5.2), equations (1.3) hold identically. A substitution of the formulas (5.8)–(5.10) shows that equations (1.1)–(1.2) reduce to the form

$$\frac{\partial\mathbf{B}}{\partial t} = \eta\Delta\mathbf{B}, \quad \frac{\partial\mathbf{V}}{\partial t} = \nu\Delta\mathbf{V} - \text{grad}\left(\frac{P}{\rho} + \frac{a^2E^2}{2}(\psi_x^2+\psi_y^2+\alpha^2\psi^2) - \frac{\alpha^2k^2-\ell^2}{2\rho\mu}E_m^2\psi^2 + \frac{\ell m}{\rho\mu}E_m\psi\right). \tag{5.11}$$

An inspection proves that the vector fields (5.1), (5.2) satisfy equations (5.11) provided that the pressure P has form (5.4) and function $\psi(\tilde{\mathbf{x}})$ is any solution to the Helmholtz equation (5.3). Such solutions can be taken in the form

$$\psi(\tilde{\mathbf{x}}) = \int_0^{2\pi}[\sin(\alpha\mathbf{k}\cdot\tilde{\mathbf{x}})f_1(\phi) + \cos(\alpha\mathbf{k}\cdot\tilde{\mathbf{x}})f_2(\phi)]\,\mathrm{d}\phi. \tag{5.12}$$

Here vector $\mathbf{k}=(\cos\phi)\mathbf{e}_x+(\sin\phi)\mathbf{e}_y$, $0\leqslant\phi\leqslant2\pi$, and $f_1(\phi)$, $f_2(\phi)$ are any integrable functions.

The exact solutions (5.1)–(5.4) were first announced in Ref. 24. For the special case $b=c=0$, $k=\ell=m=0$, they become the Taylor two-dimensional flows of viscous fluid.[25]

VI. MAGNETIC CONFINEMENT OF PLASMA IN CYLINDRICAL DOMAINS

For $a=c=0$ and arbitrary constants ρ, μ, ν, η, the solutions (5.1)–(5.4) take the form

$$\mathbf{V}(t,\tilde{\mathbf{x}})=be^{-\alpha^2\nu t}\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z, \tag{6.1}$$

$$\mathbf{B}(t,\tilde{\mathbf{x}})=e^{-\alpha^2\eta t}[-k\psi_y(\tilde{\mathbf{x}})\hat{\mathbf{e}}_x+k\psi_x(\tilde{\mathbf{x}})\hat{\mathbf{e}}_y+\ell\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z]+m\hat{\mathbf{e}}_z, \tag{6.2}$$

$$P(t,\tilde{\mathbf{x}})=\frac{\alpha^2k^2-\ell^2}{2\mu}e^{-2\alpha^2\eta t}\psi^2(\tilde{\mathbf{x}})-\frac{\ell m}{\mu}e^{-\alpha^2\eta t}\psi(\tilde{\mathbf{x}}). \tag{6.3}$$

For $\alpha^2k^2\geqslant\ell^2$ and $\ell m\leqslant 0$, the solutions (6.1)–(6.3) describe a relaxation of the plasma flow inside the z-invariant cylindrical domains $\mathcal{D}$ where $\psi(\tilde{\mathbf{x}})\geqslant 0$. The function $\psi(\tilde{\mathbf{x}})$ satisfies the Helmholtz equation (5.3). At the boundary $\psi(\tilde{\mathbf{x}})=0$, the necessary boundary conditions $\mathbf{V}(t,\tilde{\mathbf{x}})=0$ and $P(t,\tilde{\mathbf{x}})=0$ hold (the pressure P is defined up to an arbitrary constant C). The magnetic field $\mathbf{B}(t,\tilde{\mathbf{x}})$ lines and the electric current $\mathbf{J}(t,\tilde{\mathbf{x}})$ lines preserve the magnetic surfaces $\psi(\tilde{\mathbf{x}})=\text{const}$. The electric current is

$$\mathbf{J}(t,\tilde{\mathbf{x}})=\mu^{-1}\operatorname{curl}\mathbf{B}(t,\tilde{\mathbf{x}})=\mu^{-1}e^{-\alpha^2\eta t}[\ell\psi_y(\tilde{\mathbf{x}})\hat{\mathbf{e}}_x-\ell\psi_x(\tilde{\mathbf{x}})\hat{\mathbf{e}}_y-\alpha^2k\psi(\tilde{\mathbf{x}})\hat{\mathbf{e}}_z].$$

For example, let the function $\psi(\tilde{\mathbf{x}})$ be

$$\psi_1(\tilde{\mathbf{x}})=\cos(\beta x)\cos(\sqrt{\alpha^2-\beta^2}\,y),\quad \beta>0,\ \alpha^2>\beta^2. \tag{6.4}$$

The Helmholtz equation $\Delta\psi_1(\tilde{\mathbf{x}})=-\alpha^2\psi_1(\tilde{\mathbf{x}})$ evidently holds. The corresponding cylindrical domain $\mathcal{D}$ has the rectangular form

$$|x|\leqslant\frac{\pi}{2\beta},\quad |y|\leqslant\frac{\pi}{2\sqrt{\alpha^2-\beta^2}},\quad -\infty<z<\infty. \tag{6.5}$$

A more general class of solutions to the Helmholtz equation has the form

$$\psi_2(\tilde{\mathbf{x}})=\int_0^{|\alpha|}f(\tau)\cos(\tau x)\cos(\sqrt{\alpha^2-\tau^2}\,y)\,\mathrm{d}\tau, \tag{6.6}$$

where $f(\tau)$ is a distribution. The solution (6.4) corresponds to $f(\tau)=\delta(\tau-\beta)$. Any function $\psi_2(\tilde{\mathbf{x}})$ (6.6) specifies a domain $\mathcal{D}$: $\psi_2(\tilde{\mathbf{x}})\geqslant 0$. It is plausible that any smooth closed curve in a neighborhood of the rectangle (6.5) can be defined by the equation $\psi_2(\tilde{\mathbf{x}})=0$ for an appropriate distribution $f(\tau)$ in (6.6).

Remark 4: The exact solutions (6.1)–(6.3) exist for arbitrary values of the physical constants ρ, μ, ν, and η and describe a relaxation as $t\to\infty$ of the plasma flows inside the cylindrical domains $\mathcal{D}$ where $\psi(\tilde{\mathbf{x}})\geqslant 0$. An important property of the exact solutions (6.1)–(6.3) is that the pressure $P(t,\tilde{\mathbf{x}})$ (6.3) for $\alpha^2k^2\geqslant\ell^2$ and $\ell m\leqslant 0$ attains its minimum 0 at the boundary $\partial\mathcal{D}$, $\psi(\tilde{\mathbf{x}})=0$, and is positive inside the domain $\mathcal{D}$. Hence the plasma is confined inside the cylindrical domain $\mathcal{D}$ only by the magnetic field $\mathbf{B}(t,\tilde{\mathbf{x}})$ (6.2) and not by an external pressure that is zero.

VII. TRANSLATIONALLY INVARIANT NONEQUIPARTITION SOLUTIONS FOR $\nu=\eta$

The viscous MHD equations (1.1)–(1.3) for $\nu=\eta$ and $\mathbf{f}=0$ have an infinite-dimensional family of z-translationally invariant exact solutions

$$\mathbf{V}(t,x,y)=-a\psi_y\hat{\mathbf{e}}_x+a\psi_x\hat{\mathbf{e}}_y+(b\psi+c)\hat{\mathbf{e}}_z, \tag{7.1}$$

$$\mathbf{B}(t,x,y)=-k\psi_y\hat{\mathbf{e}}_x+k\psi_x\hat{\mathbf{e}}_y+(\ell\psi+m)\hat{\mathbf{e}}_z, \tag{7.2}$$

where $\psi_x=\partial\psi/\partial x$, $\psi_y=\partial\psi/\partial y$, a,b,c,k,ℓ,m *are arbitrary parameters satisfying the equation* $a^2=k^2/(\rho\mu)$ *and the flux function* $\psi(t,x,y)$ *satisfies the diffusion equation*

$$\frac{\partial\psi}{\partial t}=\nu\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right). \tag{7.3}$$

The pressure P *is*

$$P=C-\frac{a^2\rho}{2}(\psi_x^2+\psi_y^2)-\frac{\ell^2}{2\mu}\psi^2-\frac{\ell m}{\mu}\psi. \tag{7.4}$$

Indeed, the formulas (7.1)–(7.2) imply

$$(\mathbf{V}\cdot\operatorname{grad})\mathbf{V}=a^2\operatorname{grad}(\psi_x^2+\psi_y^2)/2-a^2\Delta\psi\operatorname{grad}\psi, \tag{7.5}$$

$$\operatorname{curl}\mathbf{B}\times\mathbf{B}=-\operatorname{grad}(\ell^2\psi^2/2+\ell m\psi)-k^2\Delta\psi\operatorname{grad}\psi, \tag{7.6}$$

$$\mathbf{V}\times\mathbf{B}=\operatorname{grad}[(a\ell-bk)\psi^2/2+(am-ck)\psi], \tag{7.7}$$

$$\operatorname{curl}\mathbf{V}\times\mathbf{V}=-\operatorname{grad}(b^2\psi^2/2+bc\psi)-a^2\Delta\psi\operatorname{grad}\psi. \tag{7.8}$$

A substitution of the formulas (7.5)–(7.7) reduces the equations (1.1) and (1.2) for $a^2=k^2/(\rho\mu)$ to the form

$$\frac{\partial\mathbf{V}}{\partial t}=\nu\Delta\mathbf{V}-\operatorname{grad}\left(\frac{P}{\rho}+\frac{a^2}{2}(\psi_x^2+\psi_y^2)+\frac{\ell^2\psi^2}{2\rho\mu}+\frac{\ell m\psi}{\rho\mu}\right),\quad \frac{\partial\mathbf{B}}{\partial t}=\eta\Delta\mathbf{B}. \tag{7.9}$$

Substituting the vector fields (7.1), (7.2) we find that equations (1.3) hold identically and equations (7.9) are satisfied if and only if $\nu=\eta$, the pressure P has form (7.4) and the flux function $\psi(t,x,y)$ satisfies the two-dimensional diffusion equation (7.3). The solutions to this equation have the form[1]

$$\psi(t,\tilde{\mathbf{x}})=\frac{1}{4\pi\nu t}\int_{R^2}f(\tilde{\mathbf{x}}')\exp\left(-\frac{|\tilde{\mathbf{x}}-\tilde{\mathbf{x}}'|^2}{4\nu t}\right)d\tilde{\mathbf{x}}', \tag{7.10}$$

where $\tilde{\mathbf{x}}=(x,y)$, $\tilde{\mathbf{x}}'=(x',y')$, and $f(\tilde{\mathbf{x}}')=\psi(0,\tilde{\mathbf{x}}')$ are the initial data.

Remark 5: The z-invariant solutions (7.1)–(7.4) are rather general for they do not belong to any simpler class of exact solutions. Indeed, formula (7.6) implies that the solutions are not force-free, formula (7.7) shows that they are not field-aligned and formula (7.8) yields that the flows $\mathbf{V}(t,x,y)$ are not the Beltrami flows. The solutions are not the equipartition ones either because

$$\frac{1}{2}\rho\mathbf{V}^2(t,\mathbf{x})-\frac{1}{2\mu}\mathbf{B}^2(t,\mathbf{x})=\frac{1}{2}\rho(b\psi+c)^2-\frac{1}{2\mu}(\ell\psi+m)^2\neq 0.$$

The derived exact solutions are unidirectional only for $a=k=0$. The exact solutions (7.1)–(7.4) are uniformly bounded and for $c=m=0$ tend to zero as $x^2+y^2\to\infty$ if it was so for the initial data $\psi(0,x,y)$.

VIII. SUMMARY

We have introduced the unsteady equipartition solutions to the viscous MHD equations. The solutions exist when the plasma kinematic viscosity is equal to the magnetic diffusivity, $\nu=\eta$, and the plasma velocity and the magnetic field are collinear, $\mathbf{V}=\pm\mathbf{B}/\sqrt{\rho\mu}$. We have constructed the smooth solutions (2.1)–(2.3) in $\mathbb{R}^3$ with finite and equal kinetic and magnetic energies. The

solutions turn into the ideal and steady Chandrasekhar equipartition equilibria[26] when $\nu=\eta=0$ in formula (2.6). Applying the Galilean transform to some special equipartition solutions we have derived the nonequipartition solutions (3.1) that describe plasma relaxation to an equilibrium with a constant magnetic field **B**.

We have shown that the initial-boundary value problem with the ''no-slip'' boundary condition $\mathbf{V}(t,\mathbf{x})|_{\partial\mathcal{D}}=0$ is overdetermined for the equipartition solutions. An infinite family of the exact solutions (4.7) is constructed that satisfy the boundary value problem (1.8) in a ball of radius R. The solutions describe the viscous plasma relaxation in a ball with a constant pressure at the boundary and have spherical magnetic surfaces $|\mathbf{x}|=r$. On each sphere $|\mathbf{x}|=r\leqslant R$, the plasma dynamics is a rotation with the angular velocity $\mathbf{\Omega}(t,r)$ (4.8) and $\mathbf{\Omega}(t,R)=0$.

For the arbitrary values of the parameters ρ, μ, ν, and η, we have derived the exact translationally invariant solutions (5.1)–(5.3). The solutions are rather general since they are not field-aligned, are not force-free ($\operatorname{curl}\mathbf{B}\times\mathbf{B}\neq 0$) and do not satisfy the Beltrami equation since $\operatorname{curl}\mathbf{V}\times\mathbf{V}\neq 0$. The exact solutions (6.1)–(6.3) model the magnetic confinement of viscous plasma in cylindrical domains $\mathcal{D}$. They satisfy the ''no-slip'' boundary condition $\mathbf{V}(t,\mathbf{x})|_{\partial\mathcal{D}}=0$. An important property of these solutions is that the plasma pressure P is positive inside the domain $\mathcal{D}$ (if $\alpha^2k^2\geqslant\ell^2$, $\ell m\leqslant 0$) and is zero at the boundary. Hence plasma is confined inside the domain $\mathcal{D}$ by the magnetic field **B**.

For $\nu=\eta$, we have derived a larger class of translationally invariant solutions (7.1)–(7.3) that are defined by an arbitrary solution to the two-dimensional diffusion equation (7.3). The solutions are non-field-aligned and nonequipartition ones.

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Continuity of Bethe solutions with respect to chain length N and winding numbers $\{\lambda_l\}$

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Bethe solutions for r reversed spins are characterized by a set of winding numbers $\{\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_r\}$. Such classification is, however, not unique since the same sequences can describe different solutions and different sequences yield essentially equivalent states. These ambiguities should find their resolution in a complete configuration. We demonstrate here that in general a solution with a fixed sequence of winding numbers evolves in a quasicontinuous way as the function of N, the number of spins. This property could be disturbed in some cases at special transition point N_{tr}. We explain analytically the origin of this discontinuity. Consideration was addressed for three and four spin deviations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623614]

I. INTRODUCTION

A lot of modern problems in theoretical physics, particularly in statistical physics, nonlinear science, and condensed matter physics are transformed so that they might assume the one-dimensional (1D) Heisenberg model. Such a wide applicability in completely distinct areas of physics emerges from the fact that this model belongs to a little family of quantum systems, which offer exact solutions. Moreover, the classical 1D Heisenberg chain is a very interesting nonlinear dynamical system, which manifests such unique properties like coherency or chaos, depending on the imposed magnetic interactions. The adaptation of this method was very fruitful in classical statistical physics on two-dimensional lattices,[1] by giving a new approach to such subjects like, e.g., BCS theory,[2] solitons,[3] Bloch particles in magnetic field,[4,5] etc. Bethe ansatz (BA) stimulated the giant development of mathematical methods applicable in the field of integrable systems, leading to the quantum inverse scattering methods[6–8] as well as to important contributions to combinatorics.[9–11] Nowadays BA is still extensively studied and developed from both physical and mathematical points of view.[12–14]

The examination of solutions of Bethe equations is a difficult task in physical and mathematical investigations because of strange nonlinearity of these equations. For a small number of overturned spins (particularly for $r=2$), these solutions (introduced for the first time by Bethe[15]) have an analytical form. For finite systems the solutions of Bethe equations can be found using numerical methods. Only in the case of very small systems, the solutions of the Heisenberg chain can be obtained by solving the Bethe equations by hand or by straight diagonalization of the Hamiltonian. In many cases for small N these methods collapse to numerical procedure. Moreover, a serious difficulty arises when the relation between diagonalization results and Bethe parameters (momenta and phases of pseudoparticles) should be established. We have proposed in the former paper[16] a new method for the determination of solutions of Bethe equations. This method is especially applicable for large, but finite length of the Heisenberg chain N, e.g., $N \leqslant 1000$. The need for exact results for the 1D Heisenberg chain of a finite size is motivated nowadays by the great development in science and technology of materials of mesoscopic as well as nanoscopic

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size and their application in an electronics of the future such as spintronics, quantum computing, as well as in biochemistry and biophysics. One should emphasize that for $100 \leqslant N \leqslant 1000$ even the usual numerical computer method fails. That is why the proposed method of solving the Bethe equations presented in Ref. 16 seems to be promising in science of small systems. The method not only determines the solutions but also provides some information about their form and origin. The method is based on the principal assumption that the solutions have quasicontinuous properties with respect to N. A starting point of the procedure is the asymptotic solution. Furthermore we make the hypothesis that this solution is also valid for sufficiently large N, e.g., $N=1000$ as chosen in our previous paper.[16] That assumption preserves proper action of the procedure. In that paper we have established that in the range of $N \in (10,1000)$ the solutions are changing in a quasicontinuous way as functions of N. The same behavior was independently noticed by Fujita *et al.*,[17] but only for the two-magnon case. However for small systems some discontinuities arise at the so-called special points:[18] critical N_{cr}, limiting N_{lim}, and transition N_{tr}. In the case of $N = N_{\mathrm{tr}}$, the transition of winding numbers sequence $\{\lambda_l\}$ into a new one $\{\lambda_l'\}$ is also observed.

In Sec. II of the present paper we introduce Bethe equations briefly and we pay attention especially to winding numbers, showing that for some cases they describe equivalent solutions. Section III presents the above-mentioned method, which enables finding solutions of Bethe equations for a wide range of chain lengths for a selected set of winding numbers. For some special chain length the procedure fails. Therefore in such cases the method should be modified (Sec. IV). Furthermore in that section we illustrate graphically the evolution of Bethe parameters as the function of chain length. The cases were selected to demonstrate transition points clearly.

II. WINDING NUMBERS AND EQUIVALENCY OF SOLUTIONS

The 1D Heisenberg model[19–26] consists of identical particles with spin 1/2 on each site, with interaction only between nearest neighbors. The Hamiltonian of such a system has the form

$$\hat{H} = \sum_{n=1}^{N} (4\mathbf{S}^n \cdot \mathbf{S}^{n+1} - 1), \tag{1}$$

where $\mathbf{S}^n$ denotes a spin vector at the nth position in the chain. Furthermore we have

$$\mathbf{S}^N \equiv \mathbf{S}^1, \tag{2}$$

so the periodic boundary condition is satisfied.

Considering the Heisenberg chain, we write the stationary states in following the form:

$$\Psi = \sum_{1 \leqslant n_1 \leqslant n_2 \leqslant \cdots \leqslant n_r \leqslant N} a(n_1, n_2, \ldots, n_r) |n_1 n_2 \cdots n_r\rangle, \tag{3}$$

with coefficients of the form

$$a(n_1, n_2, \ldots, n_r) = \sum_P \exp\left[i \left(\sum_{l=1}^{r} k_{P(l)} n_l + \frac{1}{2} \sum_{j<l} \phi_{P(j)P(l)} \right) \right]. \tag{4}$$

In formula (4) there are two characteristic parameters describing solutions: k_l—pseudomomenta of pseudoparticles and $\phi_{l,j}$—phases between interacting pseudoparticles. The sum runs over all permutations P of positions r occupied by these pseudoparticles. Furthermore $|n_1 n_2 \cdots n_r\rangle$ describes magnetic configuration containing r spin deviation (overturned spins) on chain nodes $n_1, n_2, \cdots, n_r$. The two referred parameters satisfy the following conditions:

$$2 \cot \frac{\phi_{l,j}}{2} = \cot \frac{k_l}{2} - \cot \frac{k_j}{2}, \quad \phi_{l,j} = -\phi_{j,l}, \quad 1 \leqslant l \leqslant j \leqslant N, \tag{5}$$

TABLE I. Equivalent solutions with respect to symmetry of sets $\{\lambda_l\}$ for $N=6$ and $r=3$. Sets with an asterisk are obtained from the other ones because of the appearance of N_{tr}. For further details see Sec. IV.

$\{\lambda_l\}$	k_1	k_2	k_3	$\phi_{1,2}$	$\phi_{1,3}$	$\phi_{2,3}$
$(-3,-1,1)$	$-\pi$	$-1{,}72$	$1{,}72$	$2{,}33$	$-2{,}33$	$-1{,}72$
$(-1,1,3)$	$-1{,}72$	$1{,}72$	π	$-1{,}72$	$-2{,}33$	$2{,}33$
$(-3,0,0)$	$-\pi$	0	0	0	0	0
$(0,0,3)$	0	0	π	0	0	0
$(-2,1,1)$	$-\pi$	$\pi/2-i\infty$	$\pi/2+i\infty$	$-\pi+1{,}10i$	$-\pi+1{,}10i$	$-i\infty$
$(-1,-1,2)$	$-\pi/2-i\infty$	$-\pi/2+i\infty$	π	$-i\infty$	$-\pi+1{,}10i$	$-\pi+1{,}10i$
$(-2,-1,0)$	$-\pi/2-i\infty$	$-\pi/2+i\infty$	0	$\pi+i\infty$	0	0
$(0,1,2)$	0	$\pi/2-i\infty$	$\pi/2+i\infty$	0	0	$\pi+i\infty$
$(-3,0,0)^*$	$-\pi$	$-1{,}09i$	$1{,}09i$	$5{,}44i$	$-5{,}44i$	$-1{,}09i$
$(0,0,3)^*$	$-1{,}09i$	$1{,}09i$	π	$-1{,}09i$	$-5{,}44i$	$5{,}44i$

and

$$Nk_l=2\pi\lambda_l+\sum_{j\neq l}\phi_{l,j},\quad l=1,2,\ldots,r. \tag{6}$$

The first one is a set of reflection conditions, whereas the second one expresses boundary condition. In formula (6) N and the integer λ_l are, respectively, chain length and winding numbers, where

$$-\frac{N}{2}\leqslant\lambda_1\leqslant\lambda_2\leqslant\cdots\leqslant\frac{N}{2}. \tag{7}$$

The winding numbers $\{\lambda_l\}$ parametrize the Bethe equations but not unequivocally. One can consider two types of equivalency. First, the different sets of $\{\lambda_l\}$ classify in some cases solutions that differ only in sign, but these may describe the same physical state for certain N. Second, there are cases where the same winding numbers result in different solutions. Both possibilities can be addressed to the form of Bethe equations.

Let us consider this problem for the case of the Heisenberg chain with three spin deviations $(r=3)$. The transformation $\{\lambda_1,\lambda_2,\lambda_3\}\rightarrow\{-\lambda_3,-\lambda_2,-\lambda_1\}$ introduced to the B-H equations (5) and (6) results in the following changes in Bethe parameters:

$$k_1\rightarrow -k_3,\quad \phi_{1,2}\rightarrow\phi_{2,3},$$

$$k_2\rightarrow -k_2,\quad \phi_{1,3}\rightarrow\phi_{1,3},$$

$$k_3\rightarrow -k_1,\quad \phi_{2,3}\rightarrow\phi_{1,2}.$$

But equivalent solutions can be observed only for the cases where total $|\lambda|=\pm N/2$ or $|\lambda|=0$.

In Table I results for selected winding numbers for the case $N=6$, $r=3$ are collected as an illustration of this quasiequivalency.

In Table II we present an example of the second type of equivalency. There are the results of solutions for various N starting from $N=1000$ down to $N=6$ for two sets of winding numbers: $(-3,0,0)$ and $(-1,-1,-1)$. In the range $N\in(1000,N_{\mathrm{tr}}=8)$ these parameters result in different solutions, but for $N<N_{\mathrm{tr}}$ different solutions are obtained for the same set $(-3,0,0)$. The way by which the parameter set $\{\lambda_l\}$ is changed in the transition point is described in Sec. IV.

TABLE II. Comparison of solutions for two different sets $\{\lambda_l\}$ for the case $r=3$.

N	$\{\lambda_l\}$	k_1	k_2	k_3	$\phi_{1,2}$	$\phi_{1,3}$	$\phi_{2,3}$
1000	$(-3,0,0)$	$-0{,}0188$	0	0	0	0	0
	$(-1,-1,-1)$	$-0{,}0063$	$-0{,}0063$	$-0{,}0063$	$-0{,}0042$	$-0{,}0042$	0
			$-0{,}0003i$	$+0{,}0003i$	$+0{,}2302i$	$-0{,}2302i$	$-0{,}1148i$
100	$(-3,0,0)$	$-0{,}1885$	0	0	0	0	0
	$(-1,-1,-1)$	$-0{,}0637$	$-0{,}0624$	$-0{,}0624$	$-0{,}0455$	$-0{,}0455$	0
			$-0{,}0111i$	$+0{,}0111i$	$+0{,}7509i$	$-0{,}7509i$	$-0{,}3640i$
50	$(-3,0,0)$	$-0{,}3770$	0	0	0	0	0
	$(-1,-1,-1)$	$-0{,}1296$	$-0{,}1237$	$-0{,}1237$	$-0{,}0990$	$-0{,}0990$	0
			$-0{,}0323i$	$+0{,}0323i$	$+1{,}1013i$	$-1{,}1013i$	$-0{,}5158i$
30	$(-3,0,0)$	$-0{,}6283$	0	0	0	0	0
	$(-1,-1,-1)$	$-0{,}2218$	$-0{,}2032$	$-0{,}2032$	$-0{,}1861$	$-0{,}1861$	0
			$-0{,}0721i$	$+0{,}0721i$	$+1{,}4972i$	$-1{,}4972i$	$-0{,}6660i$
10	$(-3,0,0)$	$-1{,}8850$	0	0	0	0	0
	$(-1,-1,-1)$	$-0{,}8681$	$-0{,}5084$	$-0{,}5084$	$-1{,}1987$	$-1{,}1987$	0
			$-0{,}4663i$	$+0{,}4663i$	$+3{,}5888i$	$-3{,}5888i$	$-1{,}0740i$
8	$(-3,0,0)$	$-2{,}3562$	0	0	0	0	0
	$(-1,-1,-1)$	$-1{,}3399$	$-0{,}5082$	$-0{,}5082$	$-2{,}2179$	$-2{,}2179$	0
			$-0{,}7176i$	$+0{,}7176i$	$+4{,}6264i$	$-4{,}6264i$	$-1{,}1148i$
7	$(-3,0,0)$	$-2{,}6928$	0	0	0	0	0
	$(-3,0,0)$	$-1{,}9007$	$-0{,}3961$	$-0{,}3961$	2,7724	2,7724	0
			$-0{,}9233i$	$+0{,}9233i$	$+5{,}3525i$	$-5{,}3525i$	$-1{,}1105i$
6	$(-3,0,0)$	$-\pi$	0	0	0	0	0
	$(-3,0,0)$	$-\pi$	0	0	0	0	0
			$-1{,}0871i$	$+1{,}0871i$	$+5{,}4354i$	$-5{,}4354i$	$-1{,}10871i$

III. QUASICONTINUITY AND RECURRENCE-NUMERICAL DETERMINATION OF BETHE SOLUTIONS

Numerical computations concerning solutions of large systems are not efficient because for large N the set of a great number of equations which should be solved is either impossible to be solved at all using usual computer programs, or the result of computations consists of many additional solutions, which are inappropriate from a physical point of view. It is known that the numerical procedures for solving nonlinear equations are very sensitive to the correct prediction of the range in which the solutions are expected to be obtained (ΔS) or exact establishment of the starting point of the inner computations. For large N, especially for $r \gg 2$, the fulfillment of these conditions must be particularly precise and restricted. Observed quasicontinuity of solutions provides the opportunity to satisfy described requirements fully for the determination of the proper range as well as the starting point. As such a point choosing the asymptotic solutions one can assume that $N=1000$ is also a good point at which start calculations. Solution obtained become the starting point for following smaller N. For $N \in (100,1000)$ values of solutions for two different N's are small even for every N from this range, which is why for the calculation of solutions of any N it is possible to assume $N=1000$ as the starting point. Thus for $N<100$ the differences are more and more distinct for N and $N-\Delta N$ even for small ΔN (keep in mind that the x axis in Fig. 1 is in logarithmic scale). Therefore in this range we have to be careful in choosing the starting point to be sure that the ΔN is small enough to also provide small ΔS. We have absolute conviction that the starting point was picked correctly when we chose $N+1$ as a starting point of the studied point N.

Of course it is not necessary to derive all solutions for all possible N, going by step 1 from $N=1000$ to very small N. We have the opportunity to choose the proper steps, taking care to be sure that the expected solutions for $N-\Delta N$ are from the assumed range ΔS. For large N it is necessary to realize this condition even for large ΔN, but for small lengths of systems we have to apply smaller steps that provide that ΔS is sufficiently small. However we observed that in some ranges of N the continuity of solutions is broken. There are so-called special points like critical

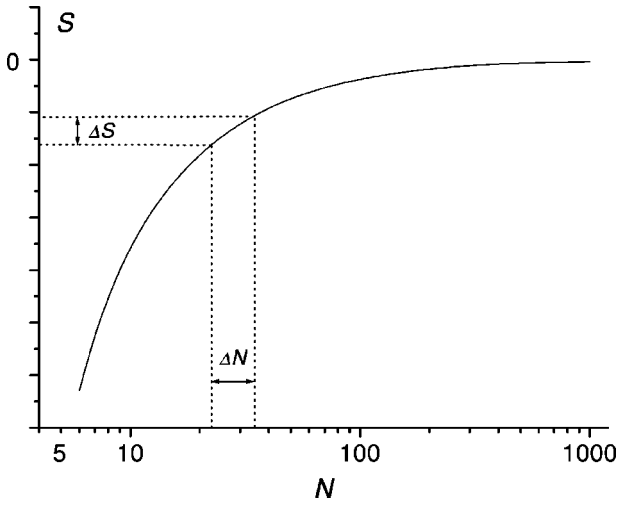

FIG. 1. Continuity of Bethe solutions for selected set of winding numbers in a wide range of N. Here S denotes one of the parameters k_l or $\phi_{l,j}$ describing the solution.

N_{cr}, limiting N_{lim}, and transition N_{tr} points. The relevant property of N_{tr} is that for this value of N the set $\{\lambda_l\}$ should be changed into another one $\{\lambda_l'\}$ in order to keep the real parts of wave numbers and phases within the proper bounds $(-\pi,\pi)$. It is important to note that such modification does not disturb the behavior of remaining parameters in relation to N.

IV. BREAK OF QUASICONTINUITY

In Sec. III it was noticed that in transition point N_{tr} quasicontinuity of some parameters describing solutions is broken, as they leave $(-\pi,\pi)$ range, where we expected to get results, which disables using the above-described method. To remove this problem one has to change the set of winding numbers related to the solutions studied into another one according to the equivalency resulting from the Bethe equations (see Sec. II). Such modification enables one to bring all parameters to the $(-\pi,\pi)$ range again.

As an example let us consider the system with $r=3$ overturned spins. Then the set of three winding numbers $\{\lambda_1,\lambda_2,\lambda_3\}$ should satisfy relation (7). The Bethe equations enable us to find the relation between the sets of winding numbers on both sides of the transition point N_{tr}. The simplest case we consider for finding this relation is the one of real solutions (Sec. IV A). Another one is the complex solution (Sec. IV B). Calculations conducted by our recurrency-numerical method point out that values of $\phi_{l,j}$ leave the $(-\pi,\pi)$ range for $N=N_{\mathrm{tr}}$, but there are indications that k_l also leaves that range. In Fig. 2 one can notice that other parameters preserve quasicontinuity very well.

A. The case of real solutions

In the case of real solutions we can rewrite Bethe equations (5) and (6) in the form

$$Nk_1=2\pi\lambda_1+\phi_{1,2}+\phi_{13}, \tag{8}$$

$$Nk_2=2\pi\lambda_2-\phi_{1,2}+\phi_{2,3}, \tag{9}$$

$$Nk_3=2\pi\lambda_3-\phi_{1,3}-\phi_{2,3}, \tag{10}$$

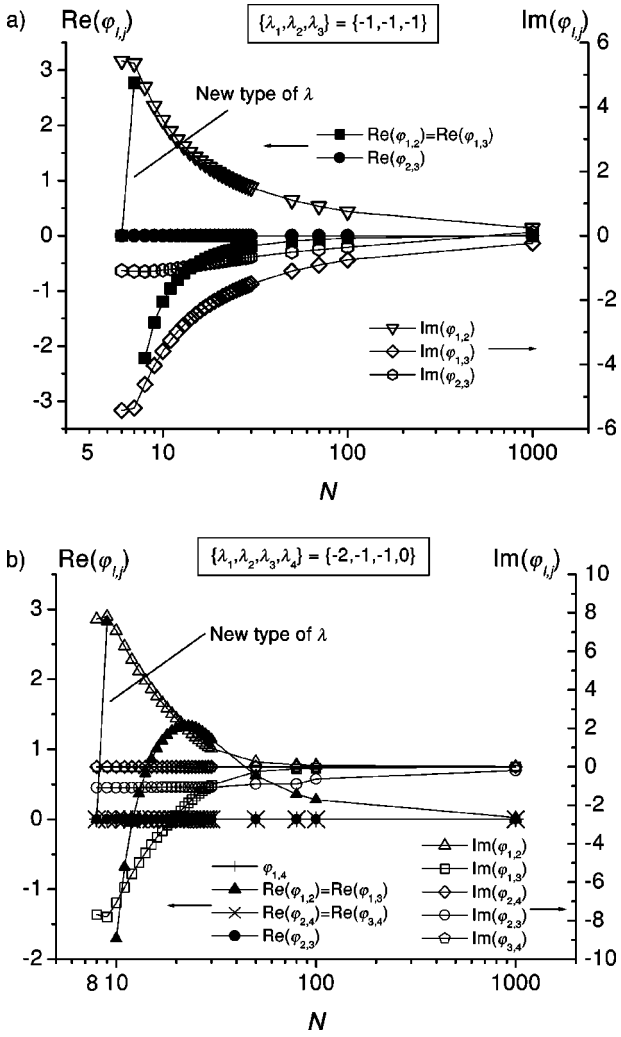

FIG. 2. Quasicontinuous form of changes in Bethe solutions starting from $N=1000$; (a) $r=3$, set $\{-1,-1,-1\}$ changes into $\{-3,0,0\}$ in $N_{\mathrm{tr}}=8$ (b) $r=4$, the set $\{-2,-1,-1,0\}$ changes into $\{-4,0,0,0\}$ in $N_{\mathrm{tr}}=9$.

$$\cot\frac{\phi_{1,2}}{2}=\frac{\sin\dfrac{k_1-k_2}{2}}{\cos\dfrac{k_1+k_2}{2}-\cos\dfrac{k_1-k_2}{2}}, \tag{11}$$

$$\cot\frac{\phi_{1,3}}{2}=\frac{\sin\dfrac{k_1-k_3}{2}}{\cos\dfrac{k_1+k_3}{2}-\cos\dfrac{k_1-k_3}{2}}, \tag{12}$$

$$\cot\frac{\phi_{2,3}}{2}=\frac{\sin\dfrac{k_2-k_3}{2}}{\cos\dfrac{k_2+k_3}{2}-\cos\dfrac{k_2-k_3}{2}}. \tag{13}$$

Let us assume that $\phi_{l,j}=\phi_{1,2}$ leaves the $(-\pi,\pi)$ range by passing the limit π. Thus we can write

$$\phi_{1,2}=\phi'_{1,2}+2\pi, \tag{14}$$

where $\phi'_{1,2}$ belongs to the range. Then from (8) and (9) we get

$$Nk_1=2\pi\lambda_1+\phi'_{1,2}+2\pi+\phi_{1,3}, \tag{15}$$

$$Nk_2=2\pi\lambda_2-\phi'_{1,2}-2\pi+\phi_{2,3}. \tag{16}$$

Now we can see that

$$Nk_1=2\pi(\lambda_1+1)+\phi'_{1,2}+\phi_{1,3}, \tag{17}$$

$$Nk_2=2\pi(\lambda_2-1)-\phi'_{1,2}+\phi_{2,3}. \tag{18}$$

It means that we get new winding numbers

$$\lambda_1+1\equiv\lambda'_1, \tag{19}$$

$$\lambda_2-1\equiv\lambda'_2. \tag{20}$$

Thus from (8) and (9) we can write

$$Nk_1=2\pi\lambda'_1+\phi'_{1,2}+\phi_{1,3}, \tag{21}$$

$$Nk_2=2\pi\lambda'_2-\phi'_{1,2}+\phi_{2,3}. \tag{22}$$

Looking at the change of set of winding numbers $\{\lambda_l\}$ into $\{\lambda'_l\}$ one can see that it does not influence the total λ and k:

$$\lambda'_1+\lambda'_2=\lambda_1+1+\lambda_2-1=\lambda_1+\lambda_2. \tag{23}$$

The form of Eqs. (8)–(13), especially the properties of trigonometric functions, preserves the quasicontinuous form of the other parameters, despite the change $\phi_{1,2}\rightarrow\phi'_{1,2}$.

B. The case of complex solutions

In such a case we assume that two parameters are complex conjugated:[18]

$$k_1=A-ib,\ \ k_2=A+ib,\ \ \phi_{1,3}=P-iq,\ \ \phi_{2,3}=P+iq,\ \ \phi_{1,2}=-il. \tag{24}$$

Rewriting Eqs. (8)–(10) and having in mind relations (24) we have

$$N(A-ib)=2\pi\lambda_1-il+P-iq, \tag{25}$$

$$N(A+ib)=2\pi\lambda_1+il+P+iq, \tag{26}$$

$$Nk_3=2\pi\lambda_3-2P, \tag{27}$$

and after simplification we get

$$NA=2\pi\lambda_1+P, \tag{28}$$

$$Nb=l-q, \tag{29}$$

$$Nk_3 = 2\pi\lambda_3 - 2P. \tag{30}$$

Now we assume that P leaves the range. Similar to the first case we write

$$P = P' + 2\pi. \tag{31}$$

Thus finally we get

$$NA = 2\pi(\lambda_1 + 1) + P', \tag{32}$$

$$Nk_3 = 2\pi(\lambda_3 - 2) - 2P'. \tag{33}$$

From (32) and (33) we can observe that

$$\lambda_1' = \lambda_1 + 1, \quad \lambda_2' = \lambda_2 + 1, \quad \lambda_3' = \lambda_3 - 2. \tag{34}$$

Both cases (a) and (b) show how to change the set of winding numbers to another one to make sure that all seeking solutions are within the $(-\pi, \pi)$ range, even when transition point appears.

Analogous considerations applied to the case with $r=4$ overturned spins results in the following: In Fig. 2 we show quasicontinuity of solutions for selected examples with $r=3$ and $r=4$ including the situation where N_{tr} appears.

V. CONCLUSIONS

Solutions of the Bethe equations manifest the quasicontinuous property with respect to N for an established set of winding numbers. Our studies reveal that for some chain length N (special points) the quasicontinuity is disturbed because some pseudomomenta and phases lose quasicontinuity in the range $(-\pi, \pi)$. In the paper we examine in detail one such type of point, i.e., the transition point N_{tr}.

For this point and below it the solution does not exist in the $(-\pi, \pi)$ range for the initial set of $\{\lambda_l\}$ (for sufficiently large N) and changing it into $\{\lambda_l'\}$ is required to ensure the quasicontinuity below N_{tr}. The method for finding such a new set $\{\lambda_l'\}$ for both real and complex cases has been described. Nevertheless it should be emphasized that changing of $\{\lambda_l\} \to \{\lambda_l'\}$ does not influence the quasicontinuity for all other Bethe parameters (k, ϕ) in N_{tr}.

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Quantum stochastic equation for a test particle interacting with a dilute Bose gas

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We use the stochastic limit method to study long time quantum dynamics of a test particle interacting with a dilute Bose gas. The case of arbitrary form factors and an arbitrary, not necessarily equilibrium, quasifree low density state of the Bose gas is considered. Starting from microscopic dynamics we derive in the low density limit a quantum white noise equation for the evolution operator. This equation is equivalent to a quantum stochastic equation driven by a quantum Poisson process with intensity $S-1$, where S is a one-particle S matrix. The novelty of our approach is that the equations are derived directly in terms of correlators, without use of a Fock–anti-Fock (or Gel'fand–Naimark–Segal) representation. Advantages of our approach are the simplicity of derivation of the limiting equation and that the algebra of the master fields and the Ito table do not depend on the initial state of the Bose gas. The notion of a causal state is introduced. We construct master fields (white noise and number operators) describing the dynamics in the low density limit and prove the convergence of chronological (causal) correlators of the field operators to correlators of the master fields in the causal state. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1626806]

I. INTRODUCTION

The fundamental equations in quantum theory are the Heisenberg and Schrödinger equations. However, it is a very difficult problem to solve explicitly these equations for realistic physical models and one uses various approximations or limiting procedures such as weak coupling, low density, and hydrodynamical limits. These scaling limits describe the long time behavior of physical systems in different physical regimes.

One of the powerful methods to study the long time behavior in quantum theory is the stochastic limit method developed by Accardi, Lu, and Volovich.[1] Many interesting physical models have been investigated by using this method. In particular, it has been applied to study the long time quantum dynamics of a system interacting with a reservoir in the case of a weak interaction between the system and reservoir, i.e., in the weak coupling limit. It was applied to study the spin-boson model,[2] polaron model and nonrelativistic quantum electrodynamics,[3,4] quantum Hall effect,[5] relations between Hepp–Lieb and Alli–Sewell laser models,[6] bifurcation phenomenon in a spin relaxation,[7] etc.

An important problem is to study the long time dynamics of a quantum system interacting with a reservoir in the case the interaction is not weak but the density of particles of the reservoir is small, i.e., in the low density limit. To describe a quantum physical model to which the low density limit can be applied let us consider an N-level atom (test particle) immersed in a free gas whose molecules can collide with the atom; the gas is supposed to be very dilute. Then the reduced time evolution for the atom will be Markovian, since the characteristic time t_S for appreciable action of the surroundings on the atom (time between collisions) is much larger than the characteristic time t_R for relaxation of correlations in the surroundings. The dynamics of the

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N-level atom interacting with the free gas should converge, in the low density limit, to the solution of a quantum stochastic differential equation driven by quantum Poisson noise. The quantum Poisson process, introduced by Hudson and Parthasarathy[8] (for a description of the quantum Poisson process see also Kumerrer[9]), should arise naturally in the low density limit, as conjectured by Frigerio and Maassen[10] and later by Alicki and Frigerio.[11] For a general survey of quantum stochastic calculus we refer to the review by Attal.[12]

The quantum stochastic equation for the low density limit was derived by Accardi and Lu[13–15] using perturbation series for the evolution operator. A nonperturbative white noise approach for the investigation of dynamics in the low density limit is developed in Refs. 16 and 17, where the mathematical procedure, the so-called stochastic golden rule for the low density limit, was formulated. This derivation uses the white noise technique developed for the case of the weak coupling limit by Accardi, Lu, and Volovich.[1] The approach to derivation of the stochastic equations in Refs. 13–17 is based on use of the Fock–anti-Fock [or Gel'fand–Naimark–Segal (GNS)] representation for the canonical commutation relations (CCR) algebra of the Bose gas. The approach of the present paper does not use the Fock–anti-Fock representation.

We study the low density limit for an N-level atom (test particle) interacting with a Bose gas. Starting from microscopic quantum dynamics we derive quantum white noise and quantum stochastic differential equations for the limiting evolution operator. A useful tool is the energy representation introduced in Refs. 16 and 17 where the case of orthogonal form factors was considered. In the present paper we consider the case of arbitrary form factors and an arbitrary, not necessarily equilibrium, quasifree low density state of the reservoir. To each initial low density state of the Bose gas we associate in the low density limit a special ''state'' (which is called a causal state) on the limiting master field algebra. We prove the convergence of time-ordered (or causal) correlators of the initial Bose field to the correlators of master fields (which are number operators constructed from some white noise operators) in these causal states. These states are determined by the diagrams which give a nontrivial contribution to the limit. The leading diagrams can be interpreted as a new statistics arising in the low density limit (new statistics arising in the weak coupling limit is discussed in Refs. 1 and 18).

One of the main results of the paper is that the dynamics in the low density limit is given by the solution of a quantum white noise equation, which is equivalent to the quantum stochastic equation

$$dU_t = dN_t(S-1)U_t, \tag{1}$$

where U_t is the evolution operator at time t describing the limiting dynamics, S is a one-particle S matrix describing scattering of the test particle on one particle of the reservoir, and $N_t(S-1)$ is the quantum Poisson (number or gauge) process with intensity $S-1$. The equation describes the evolution of the total system+reservoir and can be applied, in particular, to the important problem of derivation of the linear quantum Boltzmann equation describing the irreversible reduced dynamics of the test particle in the low density limit. Such an equation for the reduced density matrix can be easily obtained from the quantum Langevin equation, which can be derived by using the quantum stochastic differential equation and quantum Ito table (see Sec. VII) for stochastic differential dN_t (for a derivation of the quantum Langevin equation see Ref. 17). However, in the present paper we are mainly concentrated on further understanding in what sense the Poisson process is an approximation of the usual quantum field (Theorem 1) and in mechanism through which the quantum stochastic equation arises as a limit of the usual Hamiltonian equation.

In order to describe the objects appearing in (1) let us introduce two Hilbert spaces $\mathcal{H}_S$ and $\mathcal{H}$, which are called in this context the system and one-particle reservoir Hilbert spaces, and the Fock space $\Gamma(L^2(\mathbb{R}_+;\mathcal{H}))$ over the Hilbert space of square-integrable measurable vector-valued functions from $\mathbb{R}_+=[0,\infty)$ to $\mathcal{H}$. With these notations the solution of the equation is a family of operators $U_t; t\geqslant 0$ in $\mathcal{H}_S\otimes\Gamma(L^2(\mathbb{R}_+;\mathcal{H}))$ (adapted process); S is a unitary operator in $\mathcal{H}_S\otimes\mathcal{H}$, which is explicitly defined in Sec. VI.

Let us introduce the notion of a Poisson process. Let X be a self-adjoint operator in a Hilbert space $\mathcal{K}$ and $\Psi(f)$ the normalized coherent vector in the Fock space $\Gamma(\mathcal{K})$ with test function $f \in \mathcal{K}$. The *number operator* is the generator of one-parameter unitary group $\Gamma(e^{i\lambda X})$ characterized by

$$\Gamma(e^{i\lambda X})\Psi(f)=\Psi(e^{i\lambda X}f), \quad \lambda \in \mathbb{R}.$$

The number operator is characterized by the property

$$\langle \Psi(f), N(X)\Psi(g)\rangle = \langle f, Xg\rangle \langle \Psi(f), \Psi(g)\rangle.$$

The definition of $N(X)$ is extended by complex linearity to any bounded operator X on $\mathcal{K}$. Let us consider $\mathcal{K}$ of the form $L^2(\mathbb{R}_+;\mathcal{H}) \cong L^2(\mathbb{R}_+)\otimes\mathcal{H}$. For any bounded operators $X_0 \in B(\mathcal{H}_S)$, $X_1 \in B(\mathcal{H})$, and for any $t \geqslant 0$ we define $N_t(X_0\otimes X_1) := X_0 \otimes N(\chi_{[0,t]}\otimes X_1)$, extend this definition by linearity to any bounded operator K in $\mathcal{H}_S\otimes\mathcal{H}$, and call the family $N_t(K); t\geqslant 0$ of operators in $\mathcal{H}_S\otimes\Gamma(L^2(\mathbb{R}_+;\mathcal{H}))$ a *quantum Poisson process with intensity K*. The existence and uniqueness of the solution of the equation in this case follows from the general theory of quantum stochastic differential equations. Moreover, unitarity of S leads to the conclusion that, for each $t\geqslant 0$, U_t is a unitary operator (see Lemma 2).

For the vacuum state of the reservoir (zero density) such an equation was derived by Accardi and Lu.[14] In the present paper we derive this equation for an arbitrary quasifree initial state of the Bose gas. The main feature of the present paper is that the stochastic equations are derived directly in terms of correlators, without use of a Fock–anti-Fock (or GNS) representation. This simplifies the derivation of the limiting quantum white noise equation and allows us to express the intensity of the quantum Poisson process directly in terms of a one-particle S matrix. In our approach the limiting equation, the algebra of the master fields, and the Ito table do not depend on the initial state of the Bose gas.

We obtain that the dynamics of the compound system in the low density limit is described by the solution of quantum white noise equation (36) or, equivalently, quantum stochastic differential equation in forms (44) and (1) and the family of causal states φ_L on the algebra of master fields.

The reduced dynamics of the system (test particle) in the low density limit for the model under consideration, with completely different methods, based on a quantum Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy, has been investigated by Dümcke,[19] where it is proved that, under some conditions, the reduced dynamics is given by a quantum Markovian semigroup.

In the approach of the present paper the reduced dynamics can be easily derived from the solution of the limiting quantum stochastic differential equation. Namely, the limiting evolution operator U_t and the limit state φ_L determine the reduced dynamics by

$$T_t(X)=\varphi_L(U_t^\dagger(X\otimes 1)U_t),$$

where X is any system observable (bounded operator in $\mathcal{H}_S$), $\varphi_L(\cdot)$ denotes partial expectation, and T_t is the limiting semigroup. This equality shows that U_t is a stochastic dilation of the limiting Markovian semigroup. Using the quantum Ito table for stochastic differential dN_t one can derive a quantum Langevin equation for the quantity $U_t^\dagger(X\otimes 1)U_t$. Then taking partial expectation one gets an equation for $T_t(X)$; in particular, one can get the generator of the semigroup. This is a general feature of the white noise approach: one at first obtains the equation for the evolution operator of the total system and then gets the reduced dynamics of the test particle. Let us note that although quantum stochastic equations, which are derived in Refs. 13 and 17 are different from (1) they give the same reduced dynamics.

The low density limit can be applied to the model of a test particle moving through an environment of randomly placed, infinitely heavy scatterers (Lorentz gas) (see the review of Spohn[20]). In the Boltzmann–Grad limit successive collisions become independent and the averaged over the positions of the scatterers the position and velocity distribution of the particle

converges to the solution of the linear Boltzmann equation. An advantage of the stochastic limit method is that it allows us to derive equations not only for averaged over reservoir degrees of freedom dynamics of the test particle but for the total system+reservoir. For a rigorous treatment of a classical Lorentz gas we refer to Refs. 21–26. The convergence results and derivation of the linear Boltzmann equation for a quantum Lorentz gas in the low density and weak coupling limits are presented in Refs. 27 and 28. The Coulomb gas at low density is considered in Ref. 29.

The hydrodynamical limit is described by the Euler equation. In Ref. 30 the Euler equation for fermions in the hydrodynamical limit is derived under some assumptions.

Let us describe the plan of the paper. In Sec. III we construct the master fields, which are number operators acting in some Hilbert space, and the limit causal states on the master field's algebra. We prove that the time-ordered (or causal) correlators of the free evolution of the initial field converge in the low density limit to the correlators of the master field in these causal states. In Sec. IV the stochastic Schrödinger equation which describes the dynamics in the low density limit is derived. In Sec. V we bring this equation to the causally normally ordered form. This form is convenient for study of reduced dynamics of the system. In Sec. VI the expressions for the one-particle S matrix and T operator are given. In Sec. VII quantum stochastic differential equation (1) for the limiting evolution operator is derived.

II. MODEL OF AN ATOM INTERACTING WITH A DILUTE BOSE GAS

Let us explain our notations. We consider a quantum model of a system (test particle) interacting with a boson reservoir (heat bath). Let $\mathcal{H}_{\mathrm{S}}$ be the Hilbert space of the system. For an example, for an N-level atom $\mathcal{H}_{\mathrm{S}}=\mathbb{C}^N$. The system Hamiltonian H_{S} is a self-adjoint operator in $\mathcal{H}_{\mathrm{S}}$. The reservoir is described by the boson Fock space $\Gamma(\mathcal{H})$ over the one-particle Hilbert space $\mathcal{H}=L^2(\mathbb{R}^d)$ (with scalar product $\langle\cdot,\cdot\rangle$), where $d=3$ in the physical case. Moreover, the Hamiltonian of the reservoir is given by $H_{\mathrm{R}}:=\mathrm{d}\Gamma(H_1)$ (the second quantization of the one-particle Hamiltonian H_1) and the total Hamiltonian H_{tot} of the compound system is given by a self–adjoint operator on the total Hilbert space $\mathcal{H}_{\mathrm{S}}\otimes\Gamma(\mathcal{H})$:

$$H_{\mathrm{tot}}:=H_{\mathrm{free}}+H_{\mathrm{int}}=H_{\mathrm{S}}\otimes 1+1\otimes H_{\mathrm{R}}+H_{\mathrm{int}}.$$

Here H_{int} is the interaction Hamiltonian between the system and reservoir. The one-particle Hamiltonian H_1 is the operator of multiplication by some real-valued function $\omega(k)$. The interaction Hamiltonian will be assumed to have the following form:

$$H_{\mathrm{int}}:=\mathrm{i}(D\otimes A^{\dagger}(g_0)A(g_1)-D^{\dagger}\otimes A^{\dagger}(g_1)A(g_0)),$$

where D is a bounded operator in $\mathcal{H}_S$, $D\in\mathbf{B}(\mathcal{H}_S)$; $A(g_n)$ and $A^{\dagger}(g_n)$, $n=0,1$, are annihilation and creation operators, and $g_0,g_1\in\mathcal{H}$ are form factors describing the interaction of the system with the reservoir. This Hamiltonian describes scattering of particles of the Bose gas on the test particle (N-level atom) and can be obtained by quantization of the classical interaction potential between particles of two different types with an infinite number of particles of one type (particles of the gas) and finite number of particles of the second type (atoms). This Hamiltonian preserves the particle number of the reservoir, and therefore the particles of the reservoir are only scattered on the test particle and not created or destroyed. Such a Hamiltonian was considered by Davies[31] in the analysis of the weak coupling limit.

The initial state of the compound system is supposed to be of the form

$$\rho=\rho_{\mathrm{S}}\otimes\varphi_{L,\xi}.$$

Here ρ_{S} is an arbitrary density matrix of the system and the initial state of the reservoir $\varphi_{L,\xi}$ is the gauge-invariant mean-zero Gaussian state, characterized by

$$\varphi_{L,\xi}(A^{\dagger}(f)A(g))=\xi\left\langle g,\frac{L}{1-\xi L}f\right\rangle \tag{2}$$

for each $f,g \in \mathcal{H}$. Here $\xi>0$ is a small positive number and L is a bounded positive operator in $\mathcal{H}$ commuting with S_t [an operator of multiplication by some function $L(k)$]. In the case $L=\mathrm{e}^{-\beta H_1}$, where $\beta>0$ is a positive number, the state $\varphi_{L,\xi}$ is just the Gibbs state, at inverse temperature β and fugacity ξ, of the free evolution. The fugacity $\xi=\mathrm{e}^{\beta\mu}$; μ is the chemical potential.

The dynamics of the total system is determined by the evolution operator which in interaction representation has the form

$$U(t) := \mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}\mathrm{e}^{-\mathrm{i}tH_{\mathrm{tot}}}.$$

It satisfies the differential equation

$$\frac{dU(t)}{dt} = -\mathrm{i}H_{\mathrm{int}}(t)U(t),$$

where the quantity $H_{\mathrm{int}}(t)$ will be called the evolved interaction and defined as

$$H_{\mathrm{int}}(t) = \mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}H_{\mathrm{int}}\mathrm{e}^{-\mathrm{i}tH_{\mathrm{free}}}.$$

The iterated series for the evolution operator is

$$U(t) = 1 + \sum_{n=1}^{\infty} (-\mathrm{i})^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n H_{\mathrm{int}}(t_1)\cdots H_{\mathrm{int}}(t_n). \tag{3}$$

With the notations

$$S_t := \mathrm{e}^{\mathrm{i}tH_1}, \quad D(t) := \mathrm{e}^{\mathrm{i}tH_S} D \mathrm{e}^{-\mathrm{i}tH_S},$$

the evolved interaction can be written in the form

$$H_{\mathrm{int}}(t) := \mathrm{i}(D(t)\otimes A^{\dagger}(S_t g_0)A(S_t g_1) - D^{\dagger}(t)\otimes A^{\dagger}(S_t g_1)A(S_t g_0)). \tag{4}$$

We assume the rotating wave approximation

$$\mathrm{e}^{\mathrm{i}tH_S} D \mathrm{e}^{-\mathrm{i}tH_S} = D,$$

although generalization to the case of arbitrary D is not difficult.

We study the dynamics generated by the Hamiltonian (4) in the low density limit: $n\to 0$, $t \sim 1/n$ (n is the density of particles of the reservoir). The density of particles with momentum k in the state $\varphi_{L,\xi}$ is equal to

$$\frac{\xi L(k)}{1-\xi L(k)}$$

and goes to zero as $\xi\to 0$. Therefore the limit $n\to 0$, $t\sim 1/n$ is equivalent to the limit $\xi\to 0$, $t \sim 1/\xi$.

Let us consider the time rescaling $t\to t/\xi$ so that $U(t)\to U(t/\xi)$. With the notation

$$N_{f,g,\xi}(t) = \frac{1}{\xi} A^{\dagger}(S_{t/\xi} f) A(S_{t/\xi} g) \tag{5}$$

for any $f,g \in \mathcal{H}$, the equation for the evolution operator $U(t/\xi)$ becomes

$$\frac{\mathrm{d}U(t/\xi)}{\mathrm{d}t} = (D\otimes N_{g_0,g_1,\xi}(t) - D^{\dagger}\otimes N_{g_1,g_0,\xi}(t))U(t/\xi). \tag{6}$$

The reduced dynamics of any test particle's observable X in the low density limit is defined by the limit

$$\lim_{\xi\to 0}\varphi_{L,\xi}(U^{\dagger}(t/\xi)(X\otimes 1)U(t/\xi)),$$

where $\varphi_{L,\xi}(\cdot)$ denotes partial expectation. In Ref. 19 it was proved that, under some conditions, the limit exists in a small time interval and is equal to $T_t(X)$, where $\{T_t;t\geqslant 0\}$ is a quantum Markovian semigroup. The dynamics of the reduced density matrix $\rho_S(t)$ is determined through the duality $\mathrm{Tr}(\rho_S T_t(X))=\mathrm{Tr}(\rho_S(t)X)$. As was mentioned in the Introduction, in the approach of the present paper the limiting semigroup can be obtained by using the solution U_t of the quantum stochastic equation as

$$T_t(X)=\varphi_L(U_t^{\dagger}(X\otimes 1)U_t)$$

and the generator of the semigroup can be easily derived from quantum Langevin equation. The limiting semigroup can be obtained also from quantum Langevin equation in Ref. 17, which is based on a quantum stochastic equation similar to (1) but much more complicated.

The first step to study the low density limit of the model is to find the limit of the field $N_{f,g,\xi}(t)$. This limit we call master fields or number operators.

III. MASTER FIELDS AND THE LIMIT STATES

In this section we construct the algebra of the master fields arising in the low density limit and the limit causal states on this algebra. We prove (Theorem 1) that time-ordered correlators of initial fields (5) converge in the low density limit to correlators of number operators constructed from some white noise operators. Theorem 2 states a useful factorization property of the limiting causal states.

It is convenient to use the ''projections''

$$P_E:=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}tS_t\mathrm{e}^{-\mathrm{i}tE}=\delta(H_1-E),$$

with the properties

$$P_EP_{E'}=\delta(E-E')P_E,\quad P_E^*=P_E,\quad S_t=\int \mathrm{d}EP_E\mathrm{e}^{\mathrm{i}tE}.$$

For the δ function of a self-adjoint operator cf. Definition (1.2.1) in Ref. 1.

Let us construct the master space (which is Fock space over some Hilbert space) and master fields. For a given Hilbert space $\mathcal{H}$ and a self-adjoint operator H_1 in $\mathcal{H}$ we define the Hilbert space $\mathcal{X}_{\mathcal{H},H_1}$ as the completion of the quotient of the set

$$\left\{F:\mathbb{R}\to\mathcal{H}\ \text{ s.t.}\|F\|^2:=2\pi\int \mathrm{d}E\langle F(E),P_EF(E)\rangle<\infty\right\},$$

with respect to the zero-norm elements. The inner product in $\mathcal{X}_{\mathcal{H},H_1}$ is defined as

$$\langle F,G\rangle=2\pi\int \mathrm{d}E\langle F(E),P_EG(E)\rangle.$$

We denote by $B_f^{\dagger}(E,t)$, $B_g(E',t')$ time-energy white noise creation and annihilation operators acting in the symmetric Fock space $\Gamma(L^2(\mathbb{R}_+,\mathcal{X}_{\mathcal{H},H_1}))$ where $L^2(\mathbb{R}_+,\mathcal{X}_{\mathcal{H},H_1})$ is the Hilbert space of square integrable functions $f:\mathbb{R}_+\to\mathcal{X}_{\mathcal{H},H_1}$. These operators (operator-valued distributions) satisfy the canonical commutation relations

$$[B_g(E,t), B_f^\dagger(E',t')] = \delta(t'-t)\,\delta(E'-E)\,\tilde{\gamma}_{g,f}(E) \tag{7}$$

and causal commutation relations

$$[B_g(E,t), B_f^\dagger(E',t')] = \delta_+(t'-t)\,\delta(E'-E)\,\gamma_{g,f}(E), \tag{8}$$

where $\delta_+(t'-t)$ is the causal δ function and

$$\gamma_{g,f}(E) = \int dE' \frac{\langle g, P_{E'} f\rangle}{\mathrm{i}(E'-E-i0)},$$

$$\tilde{\gamma}_{g,f}(E) = 2\pi\langle g, P_E f\rangle.$$

In the Appendix we review the definition of the causal δ function: for a detailed discussion of distributions over the simplex and the meaning of two different commutators (7) and (8) for the same operators we refer to Sec. VII in Ref. 1. These operators are called time-energy quantum white noise due to the presence of $\delta(t'-t)\,\delta(E'-E)$ in (7).

For any positive bounded operator L in $\mathcal{H}$ we define the causal gauge-invariant mean zero Gaussian state φ_L by the properties (9)–(12):

$$\text{for } n=2k, \quad \varphi_L(B_1^{\epsilon_1}\cdots B_n^{\epsilon_n}) = \sum \varphi_L(B_{i_1}^{\epsilon_{i_1}} B_{j_1}^{\epsilon_{j_1}})\cdots\varphi_L(B_{i_k}^{\epsilon_{i_k}} B_{j_k}^{\epsilon_{j_k}}), \tag{9}$$

where the sum is taken over all permutations of the set $(1,\ldots,2k)$ such that $i_\alpha < j_\alpha$, $\alpha = 1,\ldots,k$, $i_1 < i_2 < \cdots < i_k$; $B_m^{\epsilon_m} := B_{f_m}^{\epsilon_m}(E_m,t_m)$, for $m=1,\ldots,n$, are time-energy quantum white noise operators with causal commutation relations (8), and ϵ_m means either creation or annihilation operator;

$$\text{for } n=2k+1 \quad \varphi_L(B_1^{\epsilon_1}\cdots B_n^{\epsilon_n}) = 0, \tag{10}$$

$$\varphi_L(B_f(E,t)B_g(E',t')) = \varphi_L(B_f^\dagger(E,t)B_g^\dagger(E',t')) = 0, \tag{11}$$

$$\varphi_L(B_f^\dagger(E,t)B_g(E',t')) = \chi_{[0,t]}(t')\langle g, P_E L f\rangle. \tag{12}$$

Notice that the "state" φ_L does not satisfy the positivity condition. This is a well-known situation for the weak coupling limit (see Ref. 1) and is due to the fact that we work with time-ordered, or causal, correlators. Therefore it is natural to call such "states" causal states.

Definition 1: Causal time-energy white noise is a pair $(B_f(E,t),\varphi_L)$, *where* $B_f(E,t)$ *satisfy the causal commutation relations (8) and* φ_L *is a causal gauge invariant mean zero Gaussian state characterized by (9)–(12).*

Using the operators $B_f^\dagger(E,t)$, $B_g(E,t)$ we define the number operators as

$$N_{f,g}(t) = \int dE B_f^\dagger(E,t)B_g(E,t). \tag{13}$$

Finally, for a given Hilbert space $\mathcal{H}$ and a self-adjoint operator H_1 we have the following objects: for any $\xi > 0$ the family of operators $N_{f,g,\xi}(t)$ defined by (5) together with the gauge-invariant quasifree mean-zero Gaussian state $\varphi_{L,\xi}$ and the number operators $N_{f,g}(t)$ together with the causal state φ_L.

The following theorem describes the relation between these objects and states the master field in the low density limit.

Theorem 1: *There exists causal time-energy white noise* $(B_f(E,t),\varphi_L)$ *such that* $\forall n\in\mathbb{N}$

$$\lim_{\xi\to 0}\varphi_{L,\xi}(N_{f_1,g_1,\xi}(t_1)\cdots N_{f_n,g_n,\xi}(t_n))=\varphi_L(N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)),$$

where the equality is understood in the sense of distributions over simplex $t_1\geqslant t_2\geqslant\cdots\geqslant t_n\geqslant 0$. *The limit causal state* φ_L *is characterized by (9)–(12) and the number operators are defined by (13).*

Remark 1: This convergence is called convergence in the sense of time ordered correlators. The fact that we use the distributions over simplex is motivated by iterated series (3) for the evolution operator.

Proof: Notice that

$$N_{f,g,\xi}(t)=\int \mathrm{d}E N_{f,g,\xi}(E,t),$$

where

$$N_{f,g,\xi}(E,t):=\frac{\mathrm{e}^{\mathrm{i}tE/\xi}}{\xi}A^\dagger(P_E f)A(S_{t/\xi}g).$$

Therefore

$$\varphi_{L,\xi}(N_{f_1,g_1,\xi}(t_1)\cdots N_{f_n,g_n,\xi}(t_n))=\int \mathrm{d}E_1\cdots\mathrm{d}E_n\varphi_{L,\xi}(N_{f_1,g_1,\xi}(E_1,t_1)\cdots N_{f_n,g_n,\xi}(E_n,t_n)).$$

Let us denote for shortness of notation for $l=1,\ldots,n$,

$$A_l^\dagger:=\frac{\mathrm{e}^{\mathrm{i}t_lE_l/\xi}}{\sqrt{\xi}}A^\dagger(P_{E_l}f_l),\quad A_l:=\frac{1}{\sqrt{\xi}}A(S_{t_l/\xi}g_l).$$

In this notation,

$$\varphi_{L,\xi}(N_{f_1,g_1,\xi}(E_1,t_1)\cdots N_{f_n,g_n,\xi}(E_n,t_n))=\varphi_{L,\xi}(A_1^\dagger A_1\cdots A_n^\dagger A_n). \tag{14}$$

The state $\varphi_{L,\xi}$ is a gauge-invariant mean-zero Gaussian state. Therefore (14) equals the sum of terms of the form

$$\varphi_{L,\xi}(A_{i_1}^\dagger A_{j_1})\cdots\varphi_{L,\xi}(A_{i_k}^\dagger A_{j_k})\varphi_{L,\xi}(A_{j_{k+1}}A_{i_{k+1}}^\dagger)\cdots\varphi_{L,\xi}(A_{j_n}A_{i_n}^\dagger), \tag{15}$$

where $k=1,\ldots,n$, $1=i_1<i_2<\cdots<i_k$, $j_{k+1}<\cdots<j_n$, $i_l\leqslant j_l$ for $l=1,\ldots,k$ and $j_l<i_l$ for $l=k+1,\ldots,n$. We say that (15) corresponds to a nonconnected diagram if there exists $m\in\{1,\ldots,n\}$ such that $i_l\leqslant m\Leftrightarrow j_l\leqslant m$. Otherwise we say that (15) corresponds to a connected diagram.

Let us prove that all the connected diagrams except only one corresponding to the case $k=1$ are equal to zero in the limit. One can write (15) as

$$\frac{1}{\xi^n}\exp\{i[(t_1-t_{j_1})E_1+\cdots+(t_{i_n}-t_{j_n})E_{i_n}]/\xi\}(\xi^k F(E)+O(\xi^{k+1}))$$

$$=\frac{1}{\xi^n}\exp\{i[t_n(E_n-E_{\alpha_n})+\cdots+t_1(E_1-E_{\alpha_1})]/\xi\}(\xi^k F(E)+O(\xi^{k+1}))$$

$$=\frac{1}{\xi^{n-1}}\exp\{i[(t_n-t_{n-1})\omega_n(E)+\cdots+(t_2-t_1)\omega_2(E)]/\xi\}(\xi^{k-1}F(E)+O(\xi^k))$$

$$=\frac{e^{i(t_n-t_{n-1})\omega_n(E)/\xi}}{\xi}\cdots\frac{e^{i(t_2-t_1)\omega_2(E)/\xi}}{\xi}(\xi^{k-1}F(E)+O(\xi^k)), \tag{16}$$

where $(\alpha_1,\ldots,\alpha_n)$ is the permutation of the set $(1,\ldots,n)$, $\omega_l(E)=E_n+\cdots+E_l-E_{\alpha_n}-\cdots-E_{\alpha_l}$ for $l=2,\ldots,n$, and

$$F(E)=\prod_{l=1}^{k}\langle g_{j_l},P_{E_l}Lf_{i_l}\rangle\prod_{l=k+1}^{n}\langle g_{j_l},P_{E_{i_l}}f_{i_l}\rangle.$$

Notice that for a connected diagram all the functions $\omega_l(E)$ are not identically zero. In fact, suppose that $\omega_m(E)\equiv 0$ for some $m\in\{2,\ldots,n\}$. In this case one has the identity

$$E_m+\cdots+E_n\equiv E_{\alpha_m}+\cdots+E_{\alpha_n}$$

(where $E_\alpha, E_{\alpha'}$ for $\alpha\neq\alpha'$ are independent variables) which means that $(\alpha_m,\ldots,\alpha_n)$ is a permutation of the set $\{m,\ldots,n\}$ and hence $(\alpha_1,\ldots,\alpha_{m-1})$ is a permutation of the set $\{1,\ldots,m-1\}$. Let us choose any $l\in\{1,\ldots,n\}$ and consider the term $t_{j_l}(E_{j_l}-E_{i_l})$ in the exponent in the second line of (16). If $j_l<m$, then since $i_l\equiv\alpha_{j_l}$ and α_{j_l} belongs to the set $\{1,\ldots,m-1\}$, one has $i_l\equiv\alpha_{j_l}\in\{1,\ldots,m-1\}$, and vice versa if $\alpha_{j_l}\equiv i_l\in\{1,\ldots,m-1\}$, then $j_l\leqslant m-1$. This means that if ω_l are not identically zero, then (15) corresponds to a connected diagram.

Let us consider the case $k>1$. Then, if (15) corresponds to a connected diagram, the functions $\omega_l(E)$ are not identically zero. In this case, since there exists the limit

$$\lim_{\xi\to 0}\frac{e^{i(t_l-t_{l-1})\omega_l(E)/\xi}}{\xi}=\delta_+(t_l-t_{l-1})\frac{1}{i(\omega_l(E)-i0)}$$

and the limit of the product of such terms in (16), and $k-1>0$, the limit of (16) is equal to zero.

Now let us consider the case $k=1$. In this case (15) has the form

$$\varphi_{L,\xi}(A_1^\dagger A_n)\varphi_{L,\xi}(A_1A_2^\dagger)\cdots\varphi_{L,\xi}(A_{n-1}A_n^\dagger)$$

$$=\frac{1}{\xi^n}\exp\{i[(t_1-t_n)E_1+(t_2-t_1)E_2+\cdots+(t_n-t_{n-1})E_n]/\xi\}(\xi F(E)+O(\xi^2))$$

$$=\frac{e^{i(t_n-t_{n-1})\omega_n(E)/\xi}}{\xi}\cdots\frac{e^{i(t_2-t_1)\omega_2(E)/\xi}}{\xi}(F(E)+O(\xi)), \tag{17}$$

where $\omega_l(E)=E_l-E_1$. Using the limit (A2) one finds that the limit of the right-hand side (RHS) of (17) is equal to

$$\delta_+(t_2-t_1)\cdots\delta_+(t_n-t_{n-1})\langle g_n,P_{E_1}Lf_1\rangle\frac{\langle g_1,P_{E_2}f_2\rangle}{i(E_2-E_1-i0)}\cdots\frac{\langle g_{n-1},P_{E_n}f_n\rangle}{i(E_n-E_1-i0)}.$$

After integration over $E_1\cdots E_n$ it becomes equal to

$$\delta_+(t_2-t_1)\cdots\delta_+(t_n-t_{n-1})\int \mathrm{d}E\langle g_n, P_E L f_1\rangle \gamma_{g_1,f_2}(E)\cdots\gamma_{g_{n-1},f_n}(E). \tag{18}$$

This proves that only one connected diagram survives in the limit.

Now let us consider the quantity

$$\varphi_L(N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)).$$

With the notation

$$B_l^\dagger := B_{f_l}^\dagger(E_l,t_l), \quad B_l := B_{g_l}(E_l,t_l),$$

it can be written as

$$\int \mathrm{d}E_1\cdots\mathrm{d}E_n \varphi_L(B_1^\dagger B_1\cdots B_n^\dagger B_n). \tag{19}$$

Notice that on the simplex $t_1\geqslant t_2\geqslant\cdots\geqslant t_n\geqslant 0$ causal δ functions $\delta_+(t_{l+m}-t_l)$ for $m\geqslant 2$ are equal to zero. Therefore for $m\geqslant 2$ one has $\varphi_L(B_{t_l}B_{t_{l+m}}^\dagger)\propto\delta_+(t_{l+m}-t_l)=0$ and hence the integrand in (19) can be written as

$$\begin{aligned}\varphi_L(B_1^\dagger B_1\cdots B_n^\dagger B_n)=&\sum_{k=1}^{n-1}\varphi_L(B_1^\dagger B_k)\varphi_L(B_1B_2^\dagger)\cdots\varphi_L(B_{k-1}B_k^\dagger)\varphi_L(B_{k+1}^\dagger B_{k+1}\cdots B_n^\dagger B_n)\\&+\varphi_L(B_1^\dagger B_n)\varphi_L(B_1B_2^\dagger)\cdots\varphi_L(B_{n-1}B_n^\dagger).\end{aligned} \tag{20}$$

The terms in the sum correspond to nonconnected diagrams. The last term corresponds to a unique nonzero connected diagram. Moreover,

$$\begin{aligned}&\int \mathrm{d}E_1\cdots\mathrm{d}E_n\varphi_L(B_1^\dagger B_n)\varphi_L(B_1B_2^\dagger)\cdots\varphi_L(B_{n-1}B_n^\dagger)\\&\quad=\delta_+(t_2-t_1)\cdots\delta_+(t_n-t_{n-1})\int\mathrm{d}E\langle g_n,P_E L f_1\rangle\gamma_{g_1,f_2}(E)\cdots\gamma_{g_{n-1},f_n}(E),\end{aligned}$$

which is equal to (18).

For $n=1$ the statement of the theorem is clear. In fact,

$$\lim_{\xi\to 0}\varphi_{L,\xi}(N_{f,g,\xi}(t))=\lim_{\xi\to 0}\left\langle g,\frac{L}{1-\xi L}f\right\rangle=\langle g,Lf\rangle=\int \mathrm{d}E\,\varphi_L(B_f^\dagger(E,t)B_g(E,t)).$$

Then proof of the theorem follows by induction using the fact that only one connected diagram survives in the limit.

Remark 2: The fact that in each order of iterated series only one connected diagram survives in the limit can be interpreted as emergence of a new statistics (different from Bose) in the low density limit. For a discussion of new statistic arising in the weak coupling limit we refer to Ref. 1 (see also Ref. 18).

The following theorem is important for investigation of the limiting white noise equation for the evolution operator.

Theorem 2: *The limit state φ_L has the following factorization property*: $\forall n\in\mathbb{N}$,

$$\varphi_L(B_f^\dagger(E,t)N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)B_g(E,t))=\varphi_L(B_f^\dagger(E,t)B_g(E,t))\varphi_L(N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)), \tag{21}$$

where the equality is understood in the sense of distributions over simplex $t \geqslant t_1 \geqslant t_2 \geqslant \cdots \geqslant t_n \geqslant 0$.

Proof: From Gaussianity of the causal state φ_L [property (9)] it follows that

$$\varphi_L(B_f^\dagger(E,t)N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)B_g(E,t))$$

$$= \varphi_L(B_f^\dagger(E,t)B_g(E,t))\varphi_L(N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)) + \int dE_1\cdots dE_n$$

$$\times \sum \varphi_L(B_f^\dagger(E,t)B_{g_i}(E_i,t_i))\cdots\varphi_L(B_{f_j}^\dagger(E_j,t_j)B_g(E,t)).$$

The sum is equal to zero since the last multiplier

$$\varphi_L(B_{f_j}^\dagger(E_j,t_j)B_g(E,t)) = \chi_{[0,t_j]}(t)\langle g, P_{E_j}Lf_j\rangle$$

is equal to zero almost everywhere on the simplex $t \geqslant t_1 \geqslant t_2 \geqslant \cdots \geqslant t_n \geqslant 0$ and hence is equal to zero in the sense of distributions on the simplex. This proves the theorem.

Theorem 1 allows us to calculate, in particular, the partial expectation of the evolution operator and Heisenberg evolution of any system observable in the low density limit. In fact, partial expectation of the nth term of the iterated series for the evolution operator (3) (or equivalent series for Heisenberg evolution of a system observable) after time rescaling $t \to t/\xi$ includes the quantity

$$\int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \varphi_{L,\xi}(N_{f_1,g_1,\xi}(t_1)\cdots N_{f_n,g_n,\xi}(t_n))$$

(where f_α, g_α are equal to g_0 or g_1). The limit as $\xi \to 0$ of this quantity can be calculated using Theorem 1. For example, the contribution of the connected diagram is equal to

$$\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \delta_+(t_2 - t_1) \int_0^{t_2} \mathrm{d}t_3 \delta_+(t_3 - t_2) \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \delta_+(t_n - t_{n-1})$$

$$\times \int \mathrm{d}E \langle g_n, P_E L f_1\rangle \gamma_{g_1,f_2}(E)\cdots\gamma_{g_{n-1},f_n}(E) = t \int \mathrm{d}E \langle g_n, P_E L f_1\rangle \gamma_{g_1,f_2}(E)\cdots\gamma_{g_{n-1},f_n}(E).$$

Similarly one can calculate the contribution of nonconnected diagrams (they give terms proportional to higher orders of t). Summing over all orders of the iterated series one can find the reduced dynamics of the system. But in the present paper we will get the limiting dynamics in a nonperturbative way, without direct summation of the iterated series. This procedure includes derivation of the white noise equation for the limiting evolution operator and then bringing this equation to the causally normally ordered form. After that one can easily find, for example, the reduced dynamics of the system. For the weak coupling limit such a procedure was developed in Ref. 1. A nontrivial generalization to the low density limit was developed in Ref. 16 and 17, where the derivation is based on the Fock–anti-Fock representation for the CCR algebra of the Bose field determined by the state $\varphi_{L,\xi}$. The approach of the present paper does not require a GNS representation and is different from approach of Ref. 16 and 17.

IV. WHITE NOISE SCHRÖDINGER EQUATION

In this section we derive, using the results of previous section, the white noise Schrödinger equation for the limiting evolution operator.

The evolution operator $U(t/\xi)$ satisfies Eq. (6) which can be written as

$$\frac{\mathrm{d}U(t/\xi)}{\mathrm{d}t} = -\mathrm{i}H_\xi(t)U(t/\xi),$$

where

$$H_\xi(t)=\mathrm{i}(D\otimes N_{g_0,g_1,\xi}(t)-D^\dagger\otimes N_{g_1,g_0,\xi}(t)).$$

The results of the preceding section allow us to write the limit as $\xi\to 0$ of the Hamiltonian $H_\xi(t)$. In the notation (13) the limiting Hamiltonian is the following operator in $\mathcal{H}_S \otimes\Gamma(L^2(\mathbb{R}_+,\mathcal{X}_{\mathcal{H},H_1}))$:

$$\begin{aligned}H(t)&=\mathrm{i}(D\otimes N_{g_0,g_1}(t)-D^\dagger\otimes N_{g_1,g_0}(t))\\&=\mathrm{i}\int \mathrm{d}E(D\otimes B^\dagger_{g_0}(E,t)B_{g_1}(E,t)-D^\dagger\otimes B^\dagger_{g_1}(E,t)B_{g_0}(E,t)).\end{aligned}\tag{22}$$

The dynamics of the total system (system+reservoir) in the low density limit $\xi\to 0$ is given by a new evolution operator U_t which is the solution of the white noise Schrödinger equation

$$\frac{\mathrm{d}U_t}{\mathrm{d}t}=-\mathrm{i}H(t)U_t,\quad U_0=1,\tag{23}$$

or equivalent integral equation

$$U_t=1+\int_0^t \mathrm{d}t_1(D\otimes N_{g_0,g_1}(t_1)-D^\dagger\otimes N_{g_1,g_0}(t_1))U_{t_1}.\tag{24}$$

V. NORMALLY ORDERED FORM OF THE WHITE NOISE EQUATION

Our next step is to bring the white noise Schrödinger equation to the causally normally ordered form (Theorem 3), i.e., the form in which all annihilation operators are on the right side of the evolution operator and all creation operators are on the left side. Such a form is convenient for study of the limiting dynamics (see remark 3 and text after remark). In particular, it can be used for derivation of (linear) Boltzmann equation.

We assume that for each $E\in\mathbb{R}$, the inverse operators

$$T_0(E):=(1+\gamma_{g_0,g_1}(E)D^\dagger-\gamma_{g_1,g_0}(E)D+(\gamma_{g_0,g_0}\gamma_{g_1,g_1}-\gamma_{g_1,g_0}\gamma_{g_0,g_1})(E)DD^\dagger]^{-1},$$

$$T_1(E):=(1+\gamma_{g_0,g_1}(E)D^\dagger-\gamma_{g_1,g_0}(E)D+(\gamma_{g_0,g_0}\gamma_{g_1,g_1}-\gamma_{g_1,g_0}\gamma_{g_0,g_1})(E)D^\dagger D)^{-1}$$

exist.

Lemma 1: If the evolution operator U_t satisfies (23) with $H(t)$ given by (22), then one has

$$B_{g_0}(E,t)U_t=\gamma_{g_0,g_0}(E)T_0(E)DU_tB_{g_1}(E,t)+T_0(E)(1-\gamma_{g_1,g_0}(E)D)U_tB_{g_0}(E,t),\tag{25}$$

$$B_{g_1}(E,t)U_t=-\gamma_{g_1,g_1}(E)T_1(E)D^\dagger U_tB_{g_0}(E,t)+T_1(E)(1+\gamma_{g_0,g_1}(E)D^\dagger)U_tB_{g_0}(E,t).\tag{26}$$

Notice that in the RHS of these equalities the annihilation operators $B_f(E,t)$ are on the right of the evolution operator.

Proof: It follows from (8) and (13) that

$$[B_{f'}(E,t),N_{f,g}(t_1)]=\delta_+(t_1-t)\gamma_{f',f}(E)B_g(E,t).\tag{27}$$

Therefore using the integral equation (24) for the evolution operator one gets

$$B_f(E,t)U_t=[B_f(E,t),U_t]+U_tB_f(E,t)$$
$$=\int_0^t \mathrm{d}t_1(D\otimes[B_f(E,t),N_{g_0,g_1}(t_1)]-D^\dagger\otimes[B_f(E,t),N_{g_1,g_0}(t_1)])U_{t_1}+U_tB_f(E,t)$$
$$=(D\gamma_{f,g_0}(E)B_{g_1}(E,t)-D^\dagger\gamma_{f,g_1}(E)B_{g_0}(E,t))U_t+U_tB_f(E,t). \tag{28}$$

The second equality in (28) holds because, due to the time consecutive principle,

$$[B_f(E,t),U_{t_1}]=0 \quad \text{for } t_1<t.$$

In fact, let us consider the quantity

$$\int_0^t \mathrm{d}t_1[B_f(E,t),U_{t_1}^{(n-1)}]=(-i)^{n-1}\int_0^t \mathrm{d}t_1\cdots\int_0^{t_{n-1}}\mathrm{d}t_n[B_f(E,t),H(t_2)\cdots H(t_n)], \tag{29}$$

where the nth term of the iterated series (3) for U_t has the form

$$U_t^{(n)}:=(-i)^n\int_0^t \mathrm{d}t_1\cdots\int_0^{t_{n-1}}\mathrm{d}t_nH(t_1)\cdots H(t_n).$$

The commutator $[B_f(E,t),H(t_k)]$ is proportional to $\delta_+(t_k-t)$; hence the commutator $[B_f(E,t),H(t_2)\cdots H(t_n)]$ is equal to zero on the simplex $t\geqslant t_1\geqslant t_2\geqslant\cdots\geqslant t_n\geqslant 0$ and therefore (29) is equal to zero.

The third equality in (28) holds since from (27) and the definition of the causal δ function one has

$$\int_0^t \mathrm{d}t_1\delta_+(t_1-t)B_f(E,t_1)U_{t_1}=B_f(E,t)U_t.$$

For a detailed discussion of the time consecutive principle and causal δ function we refer to Ref. 1.

After the substitution $f=g_0$ and $f=g_1$ in (28) one gets

$$B_{g_0}(E,t)U_t=(D\gamma_{g_0,g_0}(E)B_{g_1}(E,t)-D^\dagger\gamma_{g_0,g_1}(E)B_{g_0}(E,t))U_t+U_tB_{g_0}(E,t),$$

$$B_{g_1}(E,t)U_t=(D\gamma_{g_1,g_0}(E)B_{g_1}(E,t)-D^\dagger\gamma_{g_1,g_1}(E)B_{g_0}(E,t))U_t+U_tB_{g_1}(E,t),$$

or equivalently

$$(1+\gamma_{g_0,g_1}(E)D^\dagger)B_{g_0}(E,t)U_t=\gamma_{g_0,g_0}(E)DB_{g_1}(E,t)U_t+U_tB_{g_0}(E,t), \tag{30}$$

$$(1+\gamma_{g_1,g_0}(E)D)B_{g_1}(E,t)U_t=-\gamma_{g_1,g_1}(E)D^\dagger B_{g_0}(E,t)U_t+U_tB_{g_1}(E,t). \tag{31}$$

After left multiplication of both sides of equality (30) by $(1+\gamma_{g_1,g_0}(E)D)$ and both sides of (31) by $\gamma_{g_0,g_0}(E)D$ one gets

$$(1+\gamma_{g_1,g_0}(E)D)(1+\gamma_{g_0,g_1}(E)D^\dagger)B_{g_0}(E,t)U_t$$
$$=\gamma_{g_0,g_0}(E)D(1+\gamma_{g_1,g_0}(E)D)B_{g_1}(E,t)U_t+(1+\gamma_{g_1,g_0}(E)D)U_tB_{g_0}(E,t), \tag{32}$$

$$\gamma_{g_0,g_0}(E)D(1+\gamma_{g_1,g_0}(E)D)B_{g_1}(E,t)U_t$$
$$=-\gamma_{g_0,g_0}(E)DD^\dagger\gamma_{g_1,g_1}(E)B_{g_0}(E,t)U_t+\gamma_{g_0,g_0}(E)DU_tB_{g_1}(E,t). \tag{33}$$

Now after substitution of expression (33) into (32) one has

$$(1+\gamma_{g_0,g_1}(E)D^\dagger-\gamma_{g_1,g_0}(E)D+(\gamma_{g_0,g_0}\gamma_{g_1,g_1}-\gamma_{g_1,g_0}\gamma_{g_0,g_1})(E)DD^\dagger)B_{g_0}(E,t)U_t$$
$$=\gamma_{g_0,g_0}(E)DU_tB_{g_1}(E,t)+(1-\gamma_{g_1,g_0}(E)D)U_tB_{g_0}(E,t). \tag{34}$$

One can show by similar computations that

$$(1+\gamma_{g_0,g_1}(E)D^\dagger-\gamma_{g_1,g_0}(E)D+(\gamma_{g_0,g_0}\gamma_{g_1,g_1}-\gamma_{g_1,g_0}\gamma_{g_0,g_1})(E)D^\dagger D)B_{g_1}(E,t)U_t$$
$$=-\gamma_{g_1,g_1}(E)D^\dagger U_tB_{g_0}(E,t)+(1+\gamma_{g_0,g_1}(E)D^\dagger)U_tB_{g_1}(E,t). \tag{35}$$

Now since we suppose that the inverse operators $T_0(E)$ and $T_1(E)$ exist, we can solve the above equations (34) and (35) with respect to $B_{g_0}(E,t)U_t$ and $B_{g_1}(E,t)U_t$. The solutions are given by (25) and (26), and that proves the lemma.

Denote

$$R_{0,0}(E):=\gamma_{g_1,g_1}(E)DT_1(E)D^\dagger,$$

$$R_{1,1}(E):=\gamma_{g_0,g_0}(E)D^\dagger T_0(E)D,$$

$$R_{0,1}(E):=-DT_1(E)(1+\gamma_{g_0,g_1}(E)D^\dagger),$$

$$R_{1,0}(E):=D^\dagger T_0(E)(1-\gamma_{g_1,g_0}(E)D).$$

Theorem 3: *The normally ordered form of Eq. (23) is*

$$\frac{\mathrm{d}U_t}{\mathrm{d}t}=-\sum_{n,m=0,1}\int \mathrm{d}E R_{m,n}(E)B^\dagger_{g_m}(E,t)U_tB_{g_n}(E,t). \tag{36}$$

Proof: Using (22) white noise Schrödinger equation (23) can be rewritten in a more detailed form

$$\frac{\mathrm{d}U_t}{\mathrm{d}t}=\int \mathrm{d}E(D\otimes B^\dagger_{g_0}(E,t)B_{g_1}(E,t)-D^\dagger\otimes B^\dagger_{g_1}(E,t)B_{g_0}(E,t))U_t. \tag{37}$$

It follows from Lemma 1 that

$$D^\dagger B_{g_0}(E,t)U_t=R_{1,1}(E)U_tB_{g_1}(E,t)+R_{1,0}(E)U_tB_{g_0}(E,t),$$

$$DB_{g_1}(E,t)U_t=-R_{0,0}(E)U_tB_{g_0}(E,t)-R_{0,1}(E)U_tB_{g_1}(E,t).$$

The statement of the theorem is obtained after substitution of these expressions in (37).

Remark 3: An immediate consequence of Theorem 2 is the following factorization property of the limiting state φ_L:

$$\varphi_L(B^\dagger_{g_m}(E,t)U_tB_{g_n}(E,t))=\varphi_L(B^\dagger_{g_m}(E,t)B_{g_n}(E,t))\varphi_L(U_t).$$

This property of the state φ_L *similar to the factorization property of the state determined by a coherent vector* $\Psi,\|\Psi\|=1$:

$$(\Psi,B^\dagger_{g_m}(E,t)U_tB_{g_n}(E,t)\Psi)=(\Psi,B^\dagger_{g_m}(E,t)B_{g_n}(E,t)\Psi)(\Psi,U_t\Psi),$$

which is usually used to define quantum stochastic differential equations (the general notion of adaptedness and adapted domains which are much larger than the coherent ones is given in Ref. 12).

Taking the partial expectation of both sides of Eq. (36) in the state φ_L, using the factorization property and noticing that

$$\varphi_L(B^\dagger_{g_m}(E,t)B_{g_n}(E,t))=\langle g_n, P_E L g_m\rangle,$$

one gets the equation

$$\frac{\mathrm{d}\varphi_L(U_t)}{\mathrm{d}t}=-\Gamma\varphi_L(U_t), \tag{38}$$

where Γ is being called drift and is equal to

$$\Gamma=\sum_{n,m=0,1}\int \mathrm{d}E R_{m,n}(E)\langle g_n, P_E L g_m\rangle.$$

The solution of (38) is

$$\varphi_L(U_t)=\mathrm{e}^{-\Gamma t}.$$

In the case of orthogonal test functions, i.e., $\langle g_0, S_t g_1\rangle=0$, this expectation value for the evolution operator was obtained in Ref. 16. Let us note that the expectation value is obtained in a nonpertrubative way, without direct summation of the iterated series for the evolution operator, and is a result of the procedure of causal normal ordering.

VI. ONE-PARTICLE *T* OPERATOR AND *S* MATRIX

In the low density limit the role of multiparticle collisions is negligible and the dynamics of the test particle should be determined by the interaction of the test particle with one particle of the reservoir. In the present section we give the expressions for the one-particle T operator and S matrix. In the next section we will rewrite normally ordered white noise equation (36) in a form of the quantum stochastic equation (44) and show (Theorem 5) that the coefficients of this equation can be expressed in terms of the one-particle S matrix.

Because of number conservation, the closed subspace of $\mathcal{H}_S\otimes\Gamma(\mathcal{H})$ generated by vectors of the form $u\otimes A^\dagger(f)\Phi$ ($u\in\mathcal{H}_S$, $f\in\mathcal{H}=L^2(\mathbb{R}^d)$, Φ is the vacuum vector), which is naturally isomorphic to $\mathcal{H}_S\otimes\mathcal{H}$, is globally invariant under the time evolution operator $\exp[\mathrm{i}(H_S\otimes 1+1\otimes H_R+V)t]$. The restriction of the time evolution operator to this subspace corresponds to the evolution operator on $\mathcal{H}_S\otimes\mathcal{H}$ given by

$$\exp[\mathrm{i}(H_S\otimes 1+1\otimes H_1+V_1)t],$$

where

$$V_1=\mathrm{i}(D\otimes|g_0\rangle\langle g_1|-\mathrm{H.c.}). \tag{39}$$

The one-particle Møller wave operators are defined as

$$\Omega_\pm=s-\lim_{t\to\mp\infty}\exp[\mathrm{i}(H_S\otimes 1+1\otimes H_1+V_1)t]\exp[-\mathrm{i}(H_S\otimes 1+1\otimes H_1)t].$$

The one-particle T operator is defined as

$$T=V_1\Omega_+ \tag{40}$$

and the one-particle S matrix as

$$S=\Omega_-^*\Omega_+ . \tag{41}$$

Theorem 4: *For the interaction (39) the one-particle T operator and S matrix have the form*

$$T=-\mathrm{i}\sum_{n,m\in\{0,1\}}\int \mathrm{d}E R_{m,n}(E)\otimes|g_m\rangle\langle g_n|P_E , \tag{42}$$

$$S=1-2\pi\sum_{n,m\in\{0,1\}}\int \mathrm{d}E R_{m,n}(E)\otimes|P_E g_m\rangle\langle P_E g_n|. \tag{43}$$

Proof: For the case $\langle g_0,S_t g_1\rangle=0$ equality (42) was proved in Ref. 17. The proof of (42) and (43) for the general case can be done in a similar way.

Expression (43) will be used in the next section for derivation of Eq. (47).

VII. QUANTUM STOCHASTIC EQUATION FOR THE LIMITING EVOLUTION OPERATOR

Normally ordered white noise equation (36) equivalent, through identification

$$B_m^\dagger(E,t)U_t B_n(E,t)\mathrm{d}t=2\pi\mathrm{d}N_t(|P_E g_m\rangle\langle P_E g_n|)U_t$$

to the quantum stochastic differential equation

$$\mathrm{d}U_t=-2\pi\sum_{n,m\in\{0,1\}}\int \mathrm{d}E R_{m,n}(E)\mathrm{d}N_t(|P_E g_m\rangle\langle P_E g_n|)U_t , \tag{44}$$

where N_t is the quantum Poisson process in $\Gamma(L^2(\mathbb{R}_+)\otimes\mathcal{H})$ defined by $N_t(X):=N(\chi_{[0,t]}\otimes X)$, if X is an operator in $\mathcal{H}$. The stochastic differential $\mathrm{d}N_t$ satisfies the usual Ito table

$$\mathrm{d}N_t(X)\mathrm{d}N_t(Y)=\mathrm{d}N_t(XY), \tag{45}$$

where X, Y are operators in $\mathcal{H}$, and the limit state φ_L characterized by the property

$$\varphi_L(2\pi\mathrm{d}N_t(|P_E f\rangle\langle P_E g|))=\langle g,P_E L f\rangle\mathrm{d}t.$$

The coefficients of quantum stochastic equation (44) can be expressed in terms of a one-particle S matrix describing scattering of the test particle on one particle of the reservoir. To show this we will use Hilbert module notation. For any pair of Hilbert spaces $\mathcal{X}_0,\mathcal{X}_1$, if N_t denotes the Poisson process on the Fock space $\Gamma(L^2(\mathbb{R}_+)\otimes\mathcal{X}_1)$, then for bounded operators $X_0\in B(\mathcal{X}_0)$, $X_1\in B(\mathcal{X}_1)$, the Hilbert module notation is[10]

$$N_t(X_0\otimes X_1):=X_0\otimes N_t(X_1).$$

With this notation Eq. (44) can be written as

$$\mathrm{d}U_t=\mathrm{d}N_t\left(-2\pi\sum_{n,m\in\{0,1\}}\int \mathrm{d}E R_{m,n}(E)\otimes|P_E g_m\rangle\langle P_E g_n|\right)U_t . \tag{46}$$

An immediate conclusion from (43) and (46) is the following theorem which is one of the main results of the paper.

Theorem 5: *The evolution operator in the low density limit satisfies the quantum stochastic equation driven by the quantum Poisson process with intensity $S-1$:*

$$\mathrm{d}U_t=\mathrm{d}N_t(S-1)U_t . \tag{47}$$

Equation (47) describes the dynamics of the compound system in the low density limit. Using this equation and the Ito table for stochastic differentials one can obtain a quantum Langevin equation for the Heisenberg evolution of any system observable. Then the corresponding master equation or, equivalently, quantum (linear) Boltzmann equation for reduced density matrix of the system can be obtained simply by taking the partial expectation of this Langevin equation in the causal state φ_L.

Lemma 2: The solution of (47) is unitary.

Proof: Let us show that $\mathrm{d}(U_t^\dagger U_t)=0$. The operator $U_t^\dagger$ satisfies the equation

$$\mathrm{d}U_t^\dagger = U_t^\dagger \mathrm{d}N_t(S^\dagger - 1).$$

One has

$$\begin{aligned}\mathrm{d}(U_t^\dagger U_t) &= \mathrm{d}U_t^\dagger U_t + U_t^\dagger \mathrm{d}U_t + \mathrm{d}U_t^\dagger \mathrm{d}U_t \\ &= U_t^\dagger \mathrm{d}N_t(S^\dagger - 1)U_t + U_t^\dagger \mathrm{d}N_t(S-1)U_t + U_t^\dagger \mathrm{d}N_t(S^\dagger - 1)\mathrm{d}N_t(S-1)U_t .\end{aligned}$$

Using the Ito table (45) one gets

$$\mathrm{d}N_t(S^\dagger - 1)\mathrm{d}N_t(S-1) = \mathrm{d}N_t[(S^\dagger - 1)(S-1)].$$

This and unitarity of S leads to

$$\mathrm{d}(U_t^\dagger U_t) = U_t^\dagger \mathrm{d}N_t[S^\dagger - 1 + S - 1 + (S^\dagger - 1)(S-1)]U_t = 0.$$

Now it follows from the initial condition $U_{t=0}=1$ that, for any $t \geqslant 0$, $U_t^\dagger U_t = 1$. The proof of $U_t U_t^\dagger = 1$ can be done in a similar way.

VIII. CONCLUSIONS

In the present paper we consider the dynamics of a test particle (N-level atom) interacting with a dilute Bose gas. It is proved that the dynamics of the total system converges in the low density limit to the solution of the quantum stochastic equation driven by a quantum Poisson process with intensity $S-1$, where S is a one-particle scattering matrix. The limiting equation is derived in a nonpertrubative way, without use of iterated series for the evolution operator. The derivation is based on the white noise approach and on the procedure of causal normal ordering developed for the weak coupling limit by Accardi, Lu, and Volovich.[1] The novelty of the present derivation is that we do not use the Fock–anti-Fock (or GNS) representation for the CCR algebra of the boson gas, determined by the state $\varphi_{L,\xi}$. This simplifies the derivation and allows us to express the intensity of the Poisson process directly in terms of a one-particle S matrix. The notion of causal states is introduced and the convergence of the correlators of the free evolution of the initial number operators to correlators of quantum white noise operators in causal states is proved. The causal states satisfy the factorization property similar to that satisfied by states determined by coherent vectors. This property is crucial for study of the reduced dynamics of the system.

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APPENDIX: CAUSAL δ FUNCTION

Let us recall the construction for distributions on the standard simplex (cf. Ref. 1). Define

$$C_0 := \{\phi : \mathbb{R}_+ \to \mathbb{C} \,|\, \phi = 0 \ \text{ a.e.}\},$$

$$C_1 := \{\phi : \mathbb{R}_+ \to \mathbb{C} \mid \phi \text{ is bounded and left-continuous at any } t>0\},$$

$$C := \text{ linear span of } \{C_0 \cup C_1\}.$$

For any $a>0$ define $\delta_+(\cdot - a)$ as the unique linear extension of the map:

$$\delta_+(\cdot - a) : \phi \in C_1 \to \phi(a),$$

$$\delta_+(\cdot - a) : \phi \in C_0 \to 0.$$

In Ref. 1 the following results are proved.

Lemma 3: In the sense of distributions one has the limit

$$\lim_{\lambda \to 0} \frac{e^{i(t'-t)E/\lambda^2}}{\lambda^2} = 2\pi \delta(t'-t)\,\delta(E). \tag{A1}$$

Lemma 4: In the sense of distributions over the simplex $t \geqslant t' \geqslant 0$ one has the limit

$$\lim_{\lambda \to 0} \frac{e^{i(t'-t)E/\lambda^2}}{\lambda^2} = \delta_+(t'-t)\,\frac{1}{i(E-i0)}. \tag{A2}$$

The last equality means, in particular, that for any $f \in C$, $g \in S(\mathbb{R})$, one has the limit

$$\lim_{\lambda \to 0} \int_0^t dt' \int_{\mathbb{R}} dE\, \frac{e^{i(t'-t)E/\lambda^2}}{\lambda^2} f(t') g(E) = f(t) \lim_{\varepsilon \to 0+} \int dE\, \frac{g(E)}{i(E-i\varepsilon)}.$$

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Positive operator valued measures covariant with respect to an Abelian group

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Given a unitary representation U of an Abelian group G and a subgroup H, we characterize the positive operator valued measures based on the quotient group G/H and covariant with respect to U. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Usually, the observables in quantum mechanics are represented by self-adjoint operators acting in the Hilbert space of states, or, equivalently, by projection valued operator measures. However, in quantum theory of measurement and in its applications (such as quantum optics or theory of measurement in phase-space) one needs to consider a more general setting in which projectivity is dropped and generalized observables are described in terms of positive operator valued measures (for a review see, for example, Refs. 1, 2, 6, 10, 13, and 14). Among these measures, the physically significant ones satisfy certain properties of covariance with respect to a symmetry group of the theory.

More precisely, consider a topological group G and a closed subgroup H. Given a unitary representation U of G, it is of interest both in quantum mechanics and in wavelet analysis to describe the positive operator valued measures Q defined on the quotient space G/H and covariant with respect to U.

In his seminal papers,[11,12] Holevo classifies the covariant positive operator valued measures if G is of type I and $H=\{e\}$, and if G is compact and H is arbitrary.

In this article we extend the above result to the case G Abelian and H arbitrary. Moreover, we give a more feasible description of covariant positive operator valued measures in terms of a family $W_x : E_x \to E$ of isometries, where the index x runs over the dual group of G, dim E_x equals the multiplicity of the character x in U and E is a fixed (infinite dimensional) Hilbert space. As a byproduct, we define a unitary operator Σ that diagonalizes the representation of G unitarily induced by a representation of H with uniform multiplicity.

As an application of our characterization, in the final section we give three examples of physical interest:

(1) the *regular* representation of the real line, where the positive operator valued measures describe the *position observables* in one dimension;

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(2) the *number*-representation of the torus, where the positive operator valued measures describe the *phase observables*;[3] and
(3) the tensor product of two *number*-representations of the torus, where the positive operator valued measures describe the *phase difference observables*.[9]

II. NOTATIONS

In this article, by *Hilbert space* we mean a separable complex Hilbert space with scalar product $\langle\cdot,\cdot\rangle$ linear in the first argument, by *group* we mean a locally compact second countable Abelian group and by *representation* a continuous unitary representation of a group acting on a Hilbert space. If X is a locally compact second countable topological space, we denote by $\mathcal{B}(X)$ the Borel σ-algebra of X and by $C_c(X)$ the space of continuous complex functions on X with compact support. By *measure* we mean a positive measure defined on $\mathcal{B}(X)$ and finite on compact sets.

In the sequel we shall use rather freely basic results of harmonic analysis on Abelian groups, as exposed, for example, in Refs. 7 and 8.

We fix a group G and a closed subgroup H. We denote by $\hat{G}$ and $\hat{H}$ the corresponding dual groups and by $\langle x,g\rangle$ the canonical pairing.

We denote by

$$q:G\to G/H,\quad q(g)=\dot{g}$$

the canonical projection onto the quotient group G/H. If $a\in G$ and $\dot{g}\in G/H$, we let $a[\dot{g}]=q(ag)=\dot{a}\dot{g}$ be the natural action of a on the point $\dot{g}$.

Let $H^\perp$ be the annihilator of H in $\hat{G}$, that is,

$$H^\perp=\{y\in\hat{G}\,|\,\langle y,h\rangle=1\ \forall h\in H\}.$$

The group $H^\perp$ is a closed subgroup of $\hat{G}$ and $\widehat{G/H}$ can be identified (and we will do that) with $H^\perp$ by means of

$$\langle y,\dot{g}\rangle:=\langle y,g\rangle\quad \forall y\in H^\perp,\forall\dot{g}\in G/H.$$

Since $H^\perp$ is closed, we can consider the quotient group $\hat{G}/H^\perp$. We denote by

$$\pi:\hat{G}\to\hat{G}/H^\perp,\quad \pi(x)=\dot{x}$$

the canonical projection. The group $\hat{H}$ can be identified (and we will do that) with the quotient group $\hat{G}/H^\perp$ by means of

$$\langle\dot{x},h\rangle:=\langle x,h\rangle\quad \forall\dot{x}\in\hat{G}/H^\perp,\forall h\in H.$$

Let μ_G, μ_H and $\mu_{G/H}$ be fixed Haar measures on G, H and G/H, respectively.

We denote by $\mu_{H^\perp}$ the Haar measure on $H^\perp$ such that the Fourier–Plancherel cotransform $\overline{\mathcal{F}}_{G/H}$ is unitary from $L^2(G/H,\mu_{G/H})$ onto $L^2(H^\perp,\mu_{H^\perp})$, where $\overline{\mathcal{F}}_{G/H}$ is given by

$$(\overline{\mathcal{F}}_{G/H}f)(y)=\int_{G/H}\langle y,\dot{g}\rangle f(\dot{g})\,\mathrm{d}\mu_{G/H}(\dot{g}),\quad y\in H^\perp,$$

for all $f\in(L^1\cap L^2)(G/H,\mu_{G/H})$.

Given $\varphi\in C_c(\hat{G})$, let

$$\tilde{\varphi}(\dot{x}) := \int_{H^\perp} \varphi(xy)\,\mathrm{d}\mu_{H^\perp}(y) \quad \forall \dot{x} \in \hat{G}/H^\perp.$$

It is well known that $\tilde{\varphi}$ is in $C_c(\hat{G}/H^\perp)$ and that $\tilde{\varphi} \geqslant 0$ if $\varphi \geqslant 0$. Given a measure ν on $\hat{G}/H^\perp$, the map

$$C_c(\hat{G}) \ni \varphi \mapsto \int_{\hat{G}/H^\perp} \tilde{\varphi}(\dot{x})\,\mathrm{d}\nu(\dot{x}) \in \mathbb{C} \tag{1}$$

is linear and positive. Hence, by Riesz–Markov theorem, there is a unique measure $\tilde{\nu}$ on $\hat{G}$ such that

$$\int_{\hat{G}} \phi(x)\,\mathrm{d}\tilde{\nu}(x) = \int_{\hat{G}/H^\perp} \mathrm{d}\nu(\dot{x}) \int_{H^\perp} \phi(xy)\,\mathrm{d}\mu_{H^\perp}(y)$$

for all $\phi \in L^1(\hat{G}, \tilde{\nu})$. One can check that the correspondence $\nu \mapsto \tilde{\nu}$ preserves equivalence and orthogonality of measures.

Given a finite measure μ on $\hat{G}$, we denote by μ^π the image measure of μ with respect to π, i.e., the measure on $\hat{G}/H^\perp$ given by

$$\mu^\pi(A) = \mu(\pi^{-1}(A)) \quad \forall A \in \mathcal{B}(\hat{G}/H^\perp).$$

We fix a representation U of G acting on a Hilbert space $\mathcal{H}$. Let Q be a positive operator valued measure (POVM) defined on G/H and acting on $\mathcal{H}$. If Q satisfies the following properties,

(1) $Q(G/H) = I$,
(2) for all $X \in \mathcal{B}(G/H)$,

$$U(g)Q(X)U(g^{-1}) = Q(g[X]) \quad \forall g \in G,$$

it is called *covariant* and (U, Q) is said to be a *covariance system*. In particular, if Q is a projective measure, (U, Q) is called an *imprimitivity system.*

For $\omega \in C_c(G/H)$, we define the operator

$$M(\omega) := \int_{G/H} \omega(\dot{g})\,\mathrm{d}Q(\dot{g}).$$

The map $\omega \mapsto M(\omega)$ defines uniquely the POVM Q. In the following we use M instead of Q.

Finally, given a representation σ of H, we denote by $(\mathrm{ind}_H^G(\sigma), M_0)$ the imprimitivity system induced by σ from H to G.

The aim of this article is to describe all the positive operator valued measures covariant with respect to U. The generalized imprimitivity theorem (see, for example, Refs. 4 and 5) states the following.

Theorem 1: *A POVM M based on G/H and acting on $\mathcal{H}$ is covariant with respect to U if and only if there exists a representation σ of H and an isometry W intertwining U with* $\mathrm{ind}_H^G(\sigma)$ *such that*

$$M(\omega) = W^* M_0(\omega) W$$

for all $\omega \in C_c(G/H)$.

If σ' is another representation of H such that σ is contained (as subrepresentation) in σ, then $(\mathrm{ind}_H^G(\sigma), M_0)$ is contained (as an imprimitivity system) in $(\mathrm{ind}_H^G(\sigma'), M_0')$. Hence, we can always assume that σ in the previous theorem has infinite multiplicity.

Moreover, there exist a measure ν on $\hat{G}/H^{\perp}$ and an infinite dimensional Hilbert space E such that, up to a unitary equivalence, σ acts diagonally on $L^2(\hat{G}/H^{\perp},\nu;E)$. The first step of our construction is to diagonalize the representation $\mathrm{ind}_H^G(\sigma)$.

III. DIAGONALIZATION OF $\mathrm{ind}_H^G(\sigma)$

In this section, given a representation of H with uniform multiplicity, we diagonalize the corresponding induced representation.

Let ν be a measure on $\hat{G}/H^{\perp}$ and E be a Hilbert space. Let σ^{ν} be the diagonal representation of H acting on the space $L^2(\hat{G}/H^{\perp},\nu;E)$, that is,

$$(\sigma^{\nu}(h)\xi)(\dot{x})=\langle \dot{x},h\rangle \xi(\dot{x}), \quad \dot{x}\in \hat{G}/H^{\perp},$$

where $h\in H$.

We denote by $\mathcal{H}^{\nu}$ the space of functions $f:G\times \hat{G}/H^{\perp}\to E$ such that

(i) f is weakly $(\mu_G\otimes\nu)$-measurable;

(ii) for all $h\in H$,

$$f(gh,\dot{x})=\overline{\langle \dot{x},h\rangle} f(g,\dot{x}) \quad \forall (g,\dot{x})\in G\times \hat{G}/H^{\perp}; \tag{2}$$

(iii)

$$\int_{G/H\times \hat{G}/H^{\perp}} \|f(g,\dot{x})\|_E^2 \,\mathrm{d}(\mu_{G/H}\otimes\nu)(\dot{g},\dot{x})<+\infty.$$

We identify functions in $\mathcal{H}^{\nu}$ that are equal $(\mu_G\otimes\nu)$-a.e.. Let G act on $\mathcal{H}^{\nu}$ as

$$(\lambda^{\nu}(a)f)(g,\dot{x}):=f(a^{-1}g,\dot{x}), \quad (g,\dot{x})\in G\times \hat{G}/H^{\perp},$$

for all $a\in G$. Define

$$(M_0^{\nu}(\omega)f)(g,\dot{x}):=\omega(\dot{g})f(g,\dot{x}), \quad (g,\dot{x})\in G\times \hat{G}/H^{\perp}$$

for all $f\in\mathcal{H}^{\nu}$, $\omega\in C_c(G/H)$.

One can easily prove the following fact.

Proposition 2: The space $\mathcal{H}^{\nu}$ is a Hilbert space with respect to the inner product

$$\langle f_1,f_2\rangle_{\mathcal{H}^{\nu}}=\int_{G/H\times \hat{G}/H^{\perp}} \langle f_1(g,\dot{x}),f_2(g,\dot{x})\rangle_E \mathrm{d}(\mu_{G/H}\otimes\nu)(\dot{g},\dot{x}).$$

If $\varphi\in C_c(G\times \hat{G}/H^{\perp};E)$, let

$$f_{\varphi}(g,\dot{x}):=\int_H \langle \dot{x},h\rangle \varphi(gh,\dot{x})\mathrm{d}\mu_H(h) \quad \forall (g,\dot{x})\in G\times \hat{G}/H^{\perp}.$$

Then f_{φ} is a continuous function in $\mathcal{H}^{\nu}$ such that $(q\times \mathrm{id}_{\hat{G}/H^{\perp}})(\mathrm{supp}\ f_{\varphi})$ is compact, and the set

$$\mathcal{H}_0^{\nu}=\{f_{\varphi}|\varphi\in C_c(G\times \hat{G}/H^{\perp};E)\}$$

is a dense subspace of $\mathcal{H}^{\nu}$. The couple $(\lambda^{\nu},M_0^{\nu})$ is the imprimitivity system induced by σ^{ν} from H to G.

We now diagonalize the representation λ^{ν}. First of all, we let $\tilde{\nu}$ be the measure defined in $\hat{G}$ by Eq. (1). Let Λ^{ν} be the diagonal representation of G acting on $L^2(\hat{G},\tilde{\nu};E)$ as

$$(\Lambda^{\nu}(g)\phi)(x)=\langle x,g\rangle\phi(x),\quad x\in\hat{G},$$

for all $g\in G$.

Moreover, given $\phi:\hat{G}\to E$ and fixed $x\in\hat{G}$, define ϕ_x from $H^{\perp}$ to E as

$$\phi_x(y):=\phi(xy)\quad \forall y\in H^{\perp}.$$

Theorem 3: *There is a unique unitary operator Σ from $\mathcal{H}^{\nu}$ onto $L^2(\hat{G},\tilde{\nu};E)$ such that, for all $f\in\mathcal{H}_0^{\nu}$,*

$$(\Sigma f)(x)=\int_{G/H}\langle x,g\rangle f(g,\dot{x})\mathrm{d}\mu_{G/H}(\dot{g}),\quad x\in\hat{G}. \tag{3}$$

The operator Σ intertwines λ^{ν} with Λ^{ν}. Moreover,

$$(\Sigma^{*}\varphi)(g,\dot{x})=\int_{H^{\perp}}\overline{\langle xy,g\rangle}\varphi(xy)\mathrm{d}\mu_{H^{\perp}}(y),\quad (g,\dot{x})\in G\times\hat{H}, \tag{4}$$

for all $\varphi\in C_c(\hat{G};E)$.

Proof: We first define Σ on $\mathcal{H}_0^{\nu}$. Let $f\in\mathcal{H}_0^{\nu}$. Fix $x\in\hat{G}$. By virtue of Eq. (2) the function

$$g\mapsto\langle x,g\rangle f(g,\dot{x})$$

depends only on the equivalence class $\dot{g}$ of g and we let f^x be the corresponding map on G/H. Due to the properties of f, f^x is continuous and has compact support, so it is $\mu_{G/H}$-integrable and we define Σf by means of Eq. (3).

We claim that Σf is in $L^2(\hat{G},\tilde{\nu};E)$ and $\|\Sigma f\|_{L^2(\hat{G},\tilde{\nu};E)}=\|f\|_{\mathcal{H}^{\nu}}$. Since the map

$$(x,\dot{g})\mapsto f^x(\dot{g})$$

is continuous, by a standard argument Σf is continuous. Moreover, if $x\in\hat{G}$ and $y\in H^{\perp}$,

$$(\Sigma f)(xy)=\int_{G/H}\langle xy,g\rangle f(g,\dot{x})\mathrm{d}\mu_{G/H}(\dot{g})=\int_{G/H}\langle y,\dot{g}\rangle\langle x,g\rangle f(g,\dot{x})\mathrm{d}\mu_{G/H}(\dot{g})=\overline{\mathcal{F}}_{G/H}(f^x)(y).$$

Indeed,

$$\begin{aligned}
\|\Sigma f\|^2_{L^2(\hat{G},\tilde{\nu};E)}&=\int_{\hat{G}}\|\Sigma f(x)\|_E^2\mathrm{d}\tilde{\nu}(x)\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\|(\Sigma f)(xy)\|_E^2\mathrm{d}\mu_{H^{\perp}}(y)\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\|\overline{\mathcal{F}}_{G/H}(f^x)(y)\|_E^2\mathrm{d}\mu_{H^{\perp}}(y)\ \ (\text{unitarity of }\overline{\mathcal{F}}_{G/H})\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\|f^x(\dot{g})\|_E^2\mathrm{d}\mu_{G/H}(\dot{g})\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\|f(g,\dot{x})\|_E^2\mathrm{d}\mu_{G/H}(\dot{g})\\
&=\int_{G/H\times\hat{G}/H^{\perp}}\|f(g,\dot{x})\|_E^2\mathrm{d}(\mu_{G/H}\otimes\nu)(\dot{g},\dot{x})\\
&=\|f\|^2_{\mathcal{H}^{\nu}}.
\end{aligned}$$

By density, Σ extends to an isometry from $\mathcal{H}^{\nu}$ to $L^2(\hat{G},\tilde{\nu};E)$. Clearly, Eq. (3) holds and it defines uniquely Σ.

The second step is computing the adjoint of Σ. Let $\varphi\in C_c(\hat{G};E)$. By standard arguments the right hand side of Eq. (4) is a continuous function of $(g,\dot{x})$. Moreover, it satisfies Eq. (2). We have

$$\int_{H^{\perp}}\overline{\langle xy,g\rangle}\varphi(xy)\mathrm{d}\mu_{H^{\perp}}(y)=\overline{\langle x,g\rangle}\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g}),\quad (g,\dot{x})\in G\times\hat{H}.$$

First of all, we show that the above function is in $\mathcal{H}^{\nu}$. Indeed,

$$\begin{aligned}
&\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\|\overline{\langle x,g\rangle}\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g})\|_E^2\mathrm{d}\mu_{G/H}(\dot{g})\\
&\quad=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\|\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g})\|_E^2\mathrm{d}\mu_{G/H}(\dot{g})\quad(\text{unitarity of }\overline{\mathcal{F}}_{G/H})\\
&\quad=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\|\varphi_x(y)\|_E^2\mathrm{d}\mu_{H^{\perp}}(y)\\
&\quad=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\|\varphi(xy)\|_E^2\mathrm{d}\mu_{H^{\perp}}(y)\\
&\quad=\|\varphi\|^2_{L^2(\hat{G},\tilde{\nu};E)}.
\end{aligned}\tag{5}$$

Moreover, for all $f\in\mathcal{H}^{\nu}_0$, we have

$$\begin{aligned}
\langle\Sigma^{*}\varphi,f\rangle_{\mathcal{H}^{\nu}}&=\langle\varphi,\Sigma f\rangle_{L^2(\hat{G},\tilde{\nu};E)}\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\langle\varphi(xy),(\Sigma f)(xy)\rangle_E\mathrm{d}\mu_{H^{\perp}}(y)\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\langle\varphi_x(y),\overline{\mathcal{F}}_{G/H}(f^x)(y)\rangle_E\mathrm{d}\mu_{H^{\perp}}(y)\quad(\text{unitarity of }\overline{\mathcal{F}}_{G/H})\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\langle\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g}),f^x(\dot{g})\rangle_E\mathrm{d}\mu_{G/H}(\dot{g})\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\langle\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g}),\langle x,g\rangle f(g,\dot{x})\rangle_E\mathrm{d}\mu_{G/H}(\dot{g})\\
&=\int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\langle\overline{\langle x,g\rangle}\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g}),f(g,\dot{x})\rangle_E\mathrm{d}\mu_{G/H}(\dot{g})\\
&=\int_{G/H\times\hat{G}/H^{\perp}}\langle\overline{\langle x,g\rangle}\overline{\mathcal{F}}^{*}_{G/H}(\varphi_x)(\dot{g}),f(g,\dot{x})\rangle_E\mathrm{d}(\mu_{G/H}\otimes\nu)(\dot{g},\dot{x}).
\end{aligned}$$

Since $\mathcal{H}^{\nu}_0$ is dense, Eq. (4) follows. By Eq. (5) Σ^{*} is isometric, hence Σ is unitary.

Finally, we show the intertwining property. Let $a\in G$ and $f\in\mathcal{H}^{\nu}_0$. Then $\lambda^{\nu}(a)f\in\mathcal{H}^{\nu}_0$, and so one has

$$
\begin{aligned}
(\Sigma\lambda^{\nu}(a)f)(x) &= \int_{G/H}\langle x,g\rangle f(a^{-1}g,\dot{x})\,\mathrm{d}\mu_{G/H}(\dot{g}) \\
&= \langle x,a\rangle\int_{G/H} f^{x}(a^{-1}[\dot{g}])\,\mathrm{d}\mu_{G/H}(\dot{g})\quad(\dot{g}\to a[\dot{g}]) \\
&= \langle x,a\rangle\int_{G/H}\langle x,g\rangle f(g,\dot{x})\,\mathrm{d}\mu_{G/H}(\dot{g}) \\
&= (\Lambda^{\nu}(a)\Sigma f)(x),\quad x\in\hat{G}.
\end{aligned}
$$

By density of $\mathcal{H}_0^{\nu}$, it follows that $\Sigma\lambda^{\nu}(a)=\Lambda^{\nu}(a)\Sigma$. ■

Given $\omega\in C_c(G/H)$, let $\widetilde{M_0^{\nu}}(\omega)=\Sigma M_0^{\nu}(\omega)\Sigma^*$. Then we have the following proposition.

Proposition 4: For all $\omega\in C_c(G/H)$ and $\phi\in L^2(\hat{G},\tilde{\nu};E)$,

$$
(\widetilde{M_0^{\nu}}(\omega)\phi)(x)=\int_{H^{\perp}}\overline{\mathcal{F}}_{G/H}(\omega)(y)\,\phi(xy^{-1})\,\mathrm{d}\mu_{H^{\perp}}(y),\quad x\in\hat{G}. \tag{6}
$$

Proof: Let $\omega\in C_c(G/H)$. We compute the action of $\widetilde{M_0^{\nu}}(\omega)$ on $C_c(\hat{G};E)$. If $\varphi\in C_c(\hat{G};E)$, let

$$
\xi(x):=\int_{H^{\perp}}\overline{\mathcal{F}}_{G/H}(\omega)(y)\,\varphi(xy^{-1})\,\mathrm{d}\mu_{H^{\perp}}(y)\quad\forall x\in\hat{G},
$$

which is well defined and continuous. Moreover, for all $x\in\hat{G}$ and $y\in H^{\perp}$,

$$
\begin{aligned}
\xi(xy) &= \int_{H^{\perp}}\overline{\mathcal{F}}_{G/H}(\omega)(y')\,\varphi(xyy'^{-1})\,\mathrm{d}\mu_{H^{\perp}}(y') \\
&= \int_{H^{\perp}}\overline{\mathcal{F}}_{G/H}(\omega)(y')\,\varphi_x(yy'^{-1})\,\mathrm{d}\mu_{H^{\perp}}(y')=(\overline{\mathcal{F}}_{G/H}(\omega)*\varphi_x)(y).
\end{aligned} \tag{7}
$$

Here and in the following, convolutions are always taken in $H^{\perp}$. If $\varphi,\psi\in C_c(\hat{G};E)$,

$$
\begin{aligned}
\langle\widetilde{M_0^{\nu}}(\omega)\varphi,\psi\rangle_{L^2(\hat{G},\tilde{\nu};E)} &= \langle M_0^{\nu}(\omega)\Sigma^*\varphi,\Sigma^*\psi\rangle_{\mathcal{H}^{\nu}} \\
&= \int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\mathrm{d}\mu_{G/H}(\dot{g}) \\
&\quad\times\langle\omega(\dot{g})\overline{\langle x,g\rangle}\,\overline{\mathcal{F}}^*_{G/H}(\varphi_x)(\dot{g}),\overline{\langle x,g\rangle}\,\overline{\mathcal{F}}^*_{G/H}(\psi_x)(\dot{g})\rangle_E \\
&= \int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{G/H}\mathrm{d}\mu_{G/H}(\dot{g})\langle\omega(\dot{g})\overline{\mathcal{F}}^*_{G/H}(\varphi_x)(\dot{g}),\overline{\mathcal{F}}^*_{G/H}(\psi_x) \\
&\quad\times(\dot{g})\rangle_E\ \text{(unitarity of } \overline{\mathcal{F}}_{G/H}\text{ and properties of convolution)} \\
&= \int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\mathrm{d}\mu_{H^{\perp}}(y)\langle(\overline{\mathcal{F}}_{G/H}(\omega)*\varphi_x)(y),\psi_x(y)\rangle_E \\
&= \int_{\hat{G}/H^{\perp}}\mathrm{d}\nu(\dot{x})\int_{H^{\perp}}\mathrm{d}\mu_{H^{\perp}}(y)\langle\xi(xy),\psi(xy)\rangle_E,
\end{aligned}
$$

hence Eq. (6) holds on $C_c(\hat{G};E)$.

Let now $\phi\in L^2(\hat{G},\tilde{\nu};E)$. Since

$$\|\phi\|^2_{L^2(\hat{G},\tilde{\nu};E)}=\int_{\hat{G}/H^\perp}\mathrm{d}\nu(\dot{x})\int_{H^\perp}\|\phi(xy)\|^2_E\mathrm{d}\mu_{H^\perp}(y)<+\infty,$$

by virtue of the Fubini theorem there is a ν-negligible set $Y_1\subset\hat{G}/H^\perp$ such that, for all $x\in\hat{G}$ with $\dot{x}\notin Y_1$, $\phi_x\in L^2(H^\perp,\mu_{H^\perp};E)$. Moreover, using the definition of $\tilde{\nu}$, one can check that $\pi^{-1}(Y_1)$ is $\tilde{\nu}$-negligible. Then, for $\tilde{\nu}$-almost all $x\in\hat{G}$, ϕ_x is in $L^2(H^\perp,\mu_{H^\perp};E)$. We observe that the map

$$\dot{g}\mapsto\omega(\dot{g})(\overline{\mathcal{F}}^*_{G/H}(\phi_x))(\dot{g})$$

is then in $(L^1\cap L^2)(G/H,\mu_{G/H};E)$ for $\tilde{\nu}$-almost all $x\in\hat{G}$, hence its Fourier cotransform is continuous, and we have

$$\overline{\mathcal{F}}_{G/H}(\omega\overline{\mathcal{F}}^*_{G/H}(\phi_x))(e)=(\overline{\mathcal{F}}_{G/H}(\omega)*\phi_x)(e)=\int_{H^\perp}\overline{\mathcal{F}}_{G/H}(\omega)(y)\phi(xy^{-1})\mathrm{d}\mu_{H^\perp}(y).\tag{8}$$

Now, we let $(\varphi_k)_{k\geqslant 1}$ be a sequence in $C_c(\hat{G};E)$ converging to ϕ in $L^2(\hat{G},\tilde{\nu};E)$. Then

$$\int_{\hat{G}/H^\perp}\mathrm{d}\nu(\dot{x})\int_{H^\perp}\|(\varphi_k)_x(y)-\phi_x(y)\|^2_E\mathrm{d}\mu_{H^\perp}(y)\to 0$$

and so, possibly passing to a subsequence, there is a ν-negligible set $Y_2\subset\hat{G}/H^\perp$ such that

$$\int_{H^\perp}\|(\varphi_k)_x(y)-\phi_x(y)\|^2_E\mathrm{d}\mu_{H^\perp}(y)\to 0$$

for all $x\in\hat{G}$ with $\dot{x}\notin Y_2$. This fact means that, for $\tilde{\nu}$-almost all $x\in\hat{G}$,

$$(\varphi_k)_x\to\phi_x$$

in $L^2(H^\perp,\mu_{H^\perp};E)$. It follows that

$$\omega\overline{\mathcal{F}}^*_{G/H}((\varphi_k)_x)\to\omega\overline{\mathcal{F}}^*_{G/H}(\phi_x)$$

in $L^1(G/H,\mu_{G/H};E)$. Then, for $\tilde{\nu}$-almost all $x\in\hat{G}$,

$$\overline{\mathcal{F}}_{G/H}(\omega\overline{\mathcal{F}}^*_{G/H}((\varphi_k)_x))\to\overline{\mathcal{F}}_{G/H}(\omega\overline{\mathcal{F}}^*_{G/H}(\phi_x))$$

uniformly, and, using Eqs. (7), and (8),

$$\begin{aligned}(\widetilde{M^\nu_0})(\omega)\varphi_k)(x)&=\overline{\mathcal{F}}_{G/H}(\omega\overline{\mathcal{F}}^*_{G/H}((\varphi_k)_x))(e)\to\overline{\mathcal{F}}_{G/H}(\omega\overline{\mathcal{F}}^*_{G/H}(\phi_x))(e)\\&=\int_{H^\perp}\overline{\mathcal{F}}_{G/H}(\omega)(y)\phi(xy^{-1})\mathrm{d}\mu_{H^\perp}(y).\end{aligned}$$

Since $\widetilde{M^\nu_0}(\omega)\varphi_k$ converges to $\widetilde{M^\nu_0}(\omega)\phi$ in $L^2(\hat{G},\tilde{\nu};E)$, Eq. (6) follows from unicity of the limit. ■

IV. CHARACTERIZATION OF COVARIANT POVMs

We fix in the following an *infinite dimensional* Hilbert space E. According to the results of the previous sections, the generalized imprimitivity theorem for Abelian groups can be stated in the following way.

Theorem 5: *A POVM M based on G/H and acting on $\mathcal{H}$ is covariant with respect to U if and only if there exist a measure ν on $\hat{G}/H^\perp$ and an isometry W intertwining U with Λ^ν such that*

$$M(\omega)=W^{*}\widetilde{M_0^{\nu}}(\omega)W$$

for all $\omega\in C_c(G/H)$.

To get an explicit form of W, we assume that U acts diagonally on $\mathcal{H}$. This means that $\mathcal{H}$ is the orthogonal sum of invariant subspaces

$$\mathcal{H}=\bigoplus_{k\in I} L^2(\hat{G},\rho_k;F_k), \tag{9}$$

where I is a denumerable set, $(\rho_k)_{k\in I}$ is a family of measures on $\hat{G}$, $(F_k)_{k\in I}$ is a family of Hilbert spaces, and the action of U is given by

$$(U(g)\phi_k)(x)=\langle x,g\rangle\phi_k(x),\quad x\in\hat{G},$$

where $\phi_k\in L^2(\hat{G},\rho_k;F_k)$ and $g\in G$. We will denote by P_k the orthogonal projector onto the subspace $L^2(\hat{G},\rho_k;F_k)$.

The assumption (9) is not restrictive. Indeed, it is well known that there are a family of disjoint measures $(\rho_k)_{k\in\mathbb{N}\cup\{\infty\}}$ and a family of Hilbert spaces $(F_k)_{k\in\mathbb{N}\cup\{\infty\}}$ such that $\dim F_k=k$ and, up to a unitary equivalence, Eq. (9) holds.

Given the decomposition (9), let ρ be a measure on $\hat{G}$ such that

$$\rho(N)=0\Leftrightarrow\rho_k(N)=0\quad\forall k\in I. \tag{10}$$

We recall that the equivalence class of ρ is uniquely defined by the family $(\rho_k)_{k\in I}$.

Finally, we observe also that the equivalence class of ρ is independent of the choice of decomposition (9). Indeed, if G acts diagonally on another decomposition,

$$\mathcal{H}=\bigoplus_{k\in I'} L^2(\hat{G},\rho_k';F_k'),$$

then

$$\rho_k'(N)=0\quad\forall k\in I'\Leftrightarrow\rho_k(N)=0\quad\forall k\in I.$$

It follows that the representation U defines uniquely an equivalence class $\mathcal{C}_U$ of measures ρ such that relation (10) holds. Chosen in this equivalence class a *finite* measure ρ, we denote by $\mathcal{C}_U^{\pi}$ the equivalence class of the image measure ρ^{π}. Clearly $\mathcal{C}_U^{\pi}$ depends only on $\mathcal{C}_U$.

We now give the central result of this section.

Theorem 6: *Let U be a representation of G acting diagonally on*

$$\mathcal{H}=\bigoplus_{k\in I} L^2(\hat{G},\rho_k;F_k).$$

Given $\nu_U\in\mathcal{C}_U^{\pi}$, let $\widetilde{\nu}_U$ be the measure given by Eq. (1). The representation U admits covariant positive operator valued measures based on G/H if and only if, for all $k\in I$, ρ_k has density with respect to $\widetilde{\nu}_U$. In this case, for every $k\in I$, let α_k be the densities of ρ_k with respect to $\widetilde{\nu}_U$.

Let E be a fixed infinite dimensional Hilbert space. For each $k\in I$, let

$$\hat{G}\ni x\mapsto W_k(x)\in\mathcal{L}(F_k;E)$$

be a weakly measurable map such that $W_k(x)$ are isometries for ρ_k-almost all $x\in\hat{G}$. For $\omega\in C_c(G/H)$, let $M(\omega)$ be the operator given by

$$(P_j M(\omega) P_k \phi)(x) = \int_{H^\perp} \mathrm{d}\mu_{H^\perp}(y) \overline{\mathcal{F}}_{G/H}(\omega)(y) \sqrt{\frac{\alpha_k(xy^{-1})}{\alpha_j(x)}} \times W_j(x) * W_k(xy^{-1})(P_k\phi)(xy^{-1}), \quad x \in \hat{G}, \tag{11}$$

for all $\phi \in \mathcal{H}$ and $k,j \in I$. Then, M is a POVM covariant with respect to U.

Conversely, any POVM based on G/H and covariant with respect to U is of the form given by Eq. (11).

We add some comments before the proof of the theorem.

Remark 7: We observe that Eq. (11) is invariant with respect to the choice of the measure $\nu_U \in \mathcal{C}_U^\pi$. Indeed, let $\nu'_U \in \mathcal{C}_U^\pi$, and $\beta > 0$ be the density of ν_U with respect to ν'_U. Clearly,

$$\widetilde{\nu_U} = (\beta \circ \pi)\widetilde{\nu'_U},$$

so that the densities α'_k of ρ_k with respect to $\widetilde{\nu'_U}$ are

$$\alpha'_k = (\beta \circ \pi)\alpha_k .$$

It follows that Eq. (11) does not depend on the choice of $\nu_U \in \mathcal{C}_U^\pi$.

Corollary 8: Let H be the trivial subgroup $\{e\}$. The representation U admits covariant positive operator valued measures based on G if and only if the measures ρ_k have densities with respect to the Haar measure $\mu_{\hat{G}}$. In this case, the functions α_k in Eq. (11) are the densities of ρ_k with respect to $\mu_{\hat{G}}$.

Remark 9: The content of the previous corollary was first shown by Holevo in Ref. 11 for non-normalized POVM. In order to compare the two results, observe that, if $\phi \in (L^1 \cap L^2) \times (\hat{G}, \rho_k; F_k)$ and $\psi \in (L^1 \cap L^2)(\hat{G}, \rho_j; F_j)$, Eq. (11) becomes

$$\begin{aligned} \langle M(\omega)\phi, \psi \rangle_{\mathcal{H}} &= \int_G \mathrm{d}\mu_G(g)\, \omega(g) \int_{\hat{G}\times\hat{G}} \langle x, g\rangle \overline{\langle y, g\rangle} \sqrt{\alpha_k(y)\alpha_j(x)} \\ &\quad \times \langle W_j(x) * W_k(y)\phi(y), \psi(x)\rangle \mathrm{d}(\mu_{\hat{G}} \otimes \mu_{\hat{G}})(x,y) \\ &= \int_G \mathrm{d}\mu_G(g)\, \omega(g) \int_{\hat{G}\times\hat{G}} K_{U(g^{-1})\psi, U(g^{-1})\phi}(x,y) \mathrm{d}(\mu_{\hat{G}} \otimes \mu_{\hat{G}})(x,y), \end{aligned}$$

where

$$K_{\psi,\phi}(x,y) = \sqrt{\alpha_k(y)\alpha_j(x)} \langle W_k(y)\phi(y), W_j(x)\psi(x)\rangle$$

is a bounded positive definite measurable field of forms [compare with Eqs. (4.2) and (4.3) in Ref. 11].

In order to prove Theorem 6, we need the following lemma.

Lemma 10: Let ρ be a finite measure on $\hat{G}$. Assume that there is a measure ν on $\hat{G}/H^\perp$ such that ρ has density with respect to $\widetilde{\nu}$. Then ρ has density with respect to $\widetilde{\rho^\pi}$. In this case, ν uniquely decomposes as

$$\nu = \nu_1 + \nu_2,$$

where ν_1 is equivalent to ρ^π and $\nu_2 \perp \rho^\pi$.

Proof: Suppose that ν is a measure on $\hat{G}/H^\perp$ such that $\rho = \alpha\widetilde{\nu}$, where α is a non-negative $\widetilde{\nu}$-integrable function on $\hat{G}$. Then, for all $\varphi \in C_c(\hat{G}/H^\perp)$,

$$\rho^\pi(\varphi) = \int_{\hat{G}} \varphi(\pi(x)) \mathrm{d}\rho(\dot{x}) = \int_{\hat{G}/H^\perp} \mathrm{d}\nu(\dot{x}) \int_{H^\perp} \varphi(\dot{x})\alpha(xy)\mathrm{d}\mu_{H^\perp}(y) = \int_{\hat{G}/H^\perp} \varphi(\dot{x})\alpha'(\dot{x})\mathrm{d}\nu(\dot{x}),$$

where the function

$$\alpha'(\dot{x}) := \int_{H^\perp} \alpha(xy)\mathrm{d}\mu_{H^\perp}(y) \geqslant 0$$

is ν-integrable by virtue of Fubini theorem. It follows that

$$\rho^\pi = \alpha' \nu. \tag{12}$$

Using the Lebesgue theorem, we can uniquely decompose

$$\nu = \nu_1 + \nu_2,$$

where ν_1 has base ρ^π and $\nu_2 \perp \rho^\pi$. From Eq. (12), it follows that ν_1 and ρ^π are equivalent, and this proves the second statement of the lemma. If $A, B \in \mathcal{B}(\hat{G}/H^\perp)$ are disjoint sets such that ν_2 is concentrated in A and ν_1 is concentrated in B, then $\widetilde{\nu_2}$ and $\widetilde{\nu_1}$ are respectively concentrated in the disjoint sets $\tilde{A} = \pi^{-1}(A)$ and $\tilde{B} = \pi^{-1}(B)$. By definition of ρ^π, we also have

$$\rho(\tilde{A}) = \rho^\pi(A) = 0.$$

Since ρ has density with respect to $\widetilde{\nu} = \widetilde{\nu_1} + \widetilde{\nu_2}$ and $\widetilde{\nu_2}$ is concentrated in $\tilde{A}$, it follows that ρ has density with respect to $\widetilde{\nu_1} \cong \widetilde{\rho^\pi}$. The claim is now clear. ■

Proof of Theorem 6: Let ρ be a finite measure in $\mathcal{C}_U$. By virtue of Theorem 5, U admits a covariant POVM $\Leftrightarrow$ there exists a measure ν in $\hat{G}/H^\perp$ such that U is a subrepresentation of $\Lambda^\nu \Leftrightarrow$ each measure ρ_k has density with respect to $\widetilde{\nu} \Leftrightarrow \rho$ has density with respect to $\widetilde{\nu}$. From Lemma 10, U admits a covariant POVM if and only if ρ has density with respect to $\widetilde{\rho^\pi}$. Since $\rho^\pi \in \mathcal{C}_U^\pi$, the first claim follows.

Let now M be a covariant POVM. By Theorem 5, there is a measure ν on $\hat{G}/H^\perp$ and an isometry W intertwining U with Λ^ν such that

$$M(\omega) = W^* \widetilde{M_0^\nu}(\omega) W \quad \forall \omega \in C_c(G/H).$$

Using Lemma 10, we (uniquely) decompose

$$\nu = \nu_1 + \nu_2,$$

where ν_1 is equivalent to ν_U and $\nu_2 \perp \nu_U$. Then we have

$$\sigma^\nu \cong \sigma^{\nu_U} \oplus \sigma^{\nu_2} \Rightarrow (\Lambda^\nu, \widetilde{M_0^\nu}) \cong (\Lambda^{\nu_U}, \widetilde{M_0^{\nu_U}}) \oplus (\Lambda^{\nu_2}, \widetilde{M_0^{\nu_2}}),$$

i.e., the imprimitivity system $(\Lambda^\nu, \widetilde{M_0^\nu})$ preserves the decomposition

$$L^2(\hat{G}, \widetilde{\nu}; E) \cong L^2(\hat{G}, \widetilde{\nu_U}; E) \oplus L^2(\hat{G}, \widetilde{\nu_2}; E).$$

Moreover, since each ρ_k has density with respect to $\widetilde{\nu_U}$ and $\widetilde{\nu_U}$ is disjoint from $\widetilde{\nu_2}$, it follows that $W(\mathcal{H}) \subset L^2(\hat{G}, \widetilde{\nu_U}; E)$, then we can always assume that the measure ν on $\hat{G}/H^\perp$ which occurs in Theorem 5 is ν_U.

We now characterize the form of W. For $k \in I$, we can always fix an isometry $T_k : F_k \to E$ such that $T_k(F_k)$ are mutually orthogonal subspaces of E. Hence, if we define, for $\phi_k \in L^2(\hat{G}, \rho_k; F_k)$,

$$(T\phi_k)(x) := \sqrt{\alpha_k(x)} T_k \phi_k(x), \quad x \in \hat{G},$$

T is an isometry intertwining U with Λ^{ν_U}. We define $W_k = WP_k$. The operator $V = WT^*$ is a partial isometry commuting with Λ^{ν_U}, hence there exists a weakly measurable correspondence $\hat{G} \ni x \mapsto V(x) \in \mathcal{L}(E)$ such that $V(x)$ are partial isometries for $\widetilde{\nu_U}$-almost all $x \in \hat{G}$ and

$$(V\phi)(x) = V(x)\phi(x), \quad x \in \hat{G},$$

where $\phi \in L^2(\hat{G}, \widetilde{\nu_U}; E)$. We have $W = WT^*T = VT$. Then

$$(W_k\phi_k)(x) = \sqrt{\alpha_k(x)}V(x)T_k\phi_k(x) = \sqrt{\alpha_k(x)}W_k(x)\phi_k(x), \quad x \in \hat{G}, \tag{13}$$

where we set

$$W_k(x) = V(x)T_k \quad \forall x \in \hat{G}.$$

Since W is isometric, then $W_k^* W_k$ is the identity operator on $L^2(\hat{G}, \rho_k; F_k)$, hence

$$T_k^* V(x)^* V(x) T_k = I_k, \quad x \in \hat{G},$$

ρ_k-almost everywhere, where I_k is the identity operator on F_k. Since T_k is isometric and $V(x)$ is a partial isometry for $\widetilde{\nu_U}$-almost every $x \in \hat{G}$ (that is for ρ_k-almost every $x \in \hat{G}$), it follows that $V(x)^*V(x)$ is the identity on $\mathrm{ran}T_k$ and that $W_k(x)$ is isometric, for ρ_k-almost every $x \in \hat{G}$. Weak measurability of the maps $x \mapsto W_k(x)$ is immediate.

The explicit form of M is then given by

$$(P_j M(\omega) P_k \phi)(x) = (W_j^* \widetilde{M_0^\nu}(\omega) W_k \phi)(x) = \frac{1}{\sqrt{\alpha_j(x)}} W_j(x)^* \int_{H^\perp} \overline{\mathcal{F}}_{G/H}(\omega)(y) \times \sqrt{\alpha_k(xy^{-1})} W_k(xy^{-1})(P_k\phi)(xy^{-1}) \mathrm{d}\mu_{H^\perp}(y), \quad x \in \hat{G},$$

where $\phi \in \mathcal{H}$, $\omega \in C_c(G/H)$.

Conversely, let $\hat{G} \ni x \mapsto W_k(x) \in \mathcal{L}(F_k; E)$ be a weakly measurable map such that $W_k(x)$ are isometries for ρ_k-almost every $x \in \hat{G}$ and for all $k \in I$. We define, for $\phi_k \in L^2(\hat{G}, \rho_k; F_k)$,

$$(W\phi_k)(x) := \sqrt{\alpha_k(x)} W_k(x) \phi_k(x) \quad \forall x \in \hat{G}.$$

Then W is clearly an intertwining isometry between U and Λ^{ν_U} and Eq. (11) defines a covariant POVM. ■

We now study the problem of equivalence of covariant POVMs. To simplify the exposition, we assume that the measures ρ_k in decomposition (9) are orthogonal.

Let M and M' be two covariant positive operator valued measures that are equivalent, i.e., there exists an unitary operator $S: \mathcal{H} \to \mathcal{H}$ such that

$$SU(g) = U(g)S \quad \forall g \in G, \tag{14}$$

$$SM(\omega) = M'(\omega)S \quad \forall \omega \in C_c(G/H). \tag{15}$$

We have the following result.

Proposition 11: Let $(W_j)_{j \in I}$ and $(W'_j)_{j \in I}$ be families of maps such that Eq. (11) holds for M and M', respectively.

The POVMs M and M' are equivalent if and only if, for each $k \in I$, there exists a weakly measurable map $x \mapsto S_k(x) \in \mathcal{L}(F_k)$ such that $S_k(x)$ are unitary operators for ρ_k-almost all x and

$$\sqrt{\alpha_k(xy)} W_j(x)^* W_k(xy) = \sqrt{\alpha_k(xy)} S_j(x)^* W'_j(x)^* W'_k(xy) S_k(xy) \tag{16}$$

for $(\rho_j \otimes \mu_{H^\perp})$*-almost all* (x,y).

Proof: By virtue of condition (14) and orthogonality of the measures ρ_k, S preserves decomposition (9). Moreover, for each $k \in I$, there exists a weakly measurable map $x \mapsto S_k(x) \in \mathcal{L}(F_k)$ such that $S_k(x)$ is unitary for ρ_k-almost all x and, if $\phi_k \in L^2(\hat{G}, \rho_k; F_k)$,

$$(S\phi_k)(x) = S_k(x)\phi_k(x), \quad x \in \hat{G}.$$

Condition (15) is equivalent to

$$P_j M(\omega) P_k \phi = P_j S^* M'(\omega) S P_k \phi$$

for all $\phi \in \mathcal{H}$, $\omega \in C_c(G/H)$ and $j,k \in I$. It is not restrictive to assume that the densities α_k are measurable functions. Let

$$\Omega_{j,k}(x,x') = \sqrt{\frac{\alpha_k(x')}{\alpha_j(x)}} (W_j(x)^* W_k(x') - S_j(x)^* W_j'(x)^* W_k'(x') S_k(x')).$$

Using Eq. (11), the previous condition becomes

$$\int_{H^\perp} \mathcal{F}_{G/H}(\omega)(y) \Omega_{j,k}(x, xy^{-1}) (P_k \phi)(xy^{-1}) \mathrm{d}\mu_{H^\perp}(y) = 0, \tag{17}$$

ρ_j-almost everywhere for all $\phi \in \mathcal{H}$, $\omega \in C_c(G/H)$ and $j,k \in I$.

Let K be a compact set of $\hat{G}$ and $v \in F_k$. In Eq. (17) we choose

$$\phi = \chi_K v \in L^2(\hat{G}, \rho_k; F_k)$$

and $\omega \in C_c(G/H)$ running over a denumerable subset dense in $L^2(G/H, \mu_{H^\perp})$. It follows that there exists a ρ_j-null set $N \subset \hat{G}$ such that, for all $x \notin N$,

$$\chi_K(xy^{-1}) \Omega_{j,k}(x, xy^{-1}) v = 0$$

for $\mu_{H^\perp}$-almost all $y \in H^\perp$. Since $\Omega_{j,k}$ is weakly measurable, the last equation holds in a measurable subset $Y \subset \hat{G} \times H^\perp$ whose complement is a $(\rho_j \otimes \mu_{H^\perp})$-null set. Define

$$m(x,y) = xy^{-1} \quad \forall (x,y) \in G^\perp.$$

For all $(x,y) \in Y \cap m^{-1}(K)$ we then have

$$\Omega_{j,k}(x, xy^{-1}) v = 0.$$

Since F_k is separable and $\hat{G}$ is σ-compact, we get

$$\Omega_{j,k}(x, xy) = 0$$

for $(\rho_j \otimes \mu_{H^\perp})$-almost all $(x,y) \in \hat{G} \times H^\perp$, that is,

$$\sqrt{\alpha_k(xy)} W_j(x)^* W_k(xy) = \sqrt{\alpha_k(xy)} S_j(x)^* W_j'(x)^* W_k'(xy) S_k(xy)$$

for $(\rho_j \otimes \mu_{H^\perp})$-almost all (x,y).

Conversely, if condition (16) is satisfied for all $j,k \in I$, then clearly M is equivalent to M'. ■

V. EXAMPLES

A. Generalized covariant position observables

Let $\mathcal{H}=L^2(\mathbb{R},\mathrm{d}x)$, where $\mathrm{d}x$ is the Lebesgue measure on $\mathbb{R}$. We consider the representation U of the group $\mathbb{R}$ acting on $\mathcal{H}$ as

$$(U(a)\phi)(x)=e^{iax}\phi(x), \quad x\in\mathbb{R},$$

for all $a\in\mathbb{R}$. By means of Fourier transform, U is clearly equivalent to the regular representation of $\mathbb{R}$. We classify the POVMs based on $\mathbb{R}$ and covariant with respect to U. With the notations of the previous sections, we have

$$G=\mathbb{R}, \quad H=\{0\}, \quad G/H=\mathbb{R}, \quad \hat{G}=H^\perp=\mathbb{R}, \quad \hat{G}/H^\perp=\{0\}.$$

We choose $\mu_{G/H}=(1/2\pi)\mathrm{d}x$, so that $\mu_{H^\perp}=\mathrm{d}x$, and $E=\mathcal{H}$.

The representation U is already diagonal with multiplicity equal to 1, so that in the decomposition (9) we can set $I=\{1\}$, $\rho_1=\mathrm{d}x$, $F_1=\mathbb{C}$. Hence, by Corollary 8, U admits covariant POVMs based on $\mathbb{R}$ and $\alpha_1=1$.

According to Theorem 6, any covariant POVM M is defined in terms of a weakly measurable map $x\mapsto W_1(x)$ such that $W_1(x):\mathbb{C}\to\mathcal{H}$ is an isometry for every $x\in\mathbb{R}$. This is equivalent to selecting a weakly measurable map $x\mapsto h_x\in\mathcal{H}$, with $\|h_x\|_{\mathcal{H}}=1$ $\forall x\in\mathbb{R}$, such that $W_1(x)=h_x$ $\forall x\in\mathbb{R}$. Explicitly, if $\phi\in L^2(\mathbb{R},\mathrm{d}x)$,

$$\begin{aligned}(M(\omega)\phi)(y)&=\int_{\mathbb{R}}\overline{\mathcal{F}_{\mathbb{R}}}(\omega)(x)\langle h_{y-x},h_y\rangle\phi(y-x)\mathrm{d}x\\&=\int_{\mathbb{R}}\overline{\mathcal{F}_{\mathbb{R}}}(\omega)(y-x)\langle h_x,h_y\rangle\phi(x)\mathrm{d}x\\&=\int_{\mathbb{R}}\left(\int_{\mathbb{R}}e^{i(y-x)z}\omega(z)\langle h_x,h_y\rangle\phi(x)\frac{\mathrm{d}z}{2\pi}\right)\mathrm{d}x, \quad y\in\mathbb{R}.\end{aligned}$$

B. Generalized covariant phase observables

We give a complete characterization of the covariance systems based on the one-dimensional torus

$$\mathbb{T}=\{z\in\mathbb{C}\,|\,|z|=1\}=\{e^{i\theta}|\,\theta\in[0,2\pi]\}.$$

We have

$$G=\mathbb{T}, \quad H=\{1\}, \quad G/H=\mathbb{T},$$

$$\hat{G}=H^\perp=\{(\mathbb{T}\ni z\mapsto z^n\in\mathbb{C})\,|\,n\in\mathbb{Z}\}\cong\mathbb{Z},$$

$$\hat{G}/H^\perp=\{1\}.$$

We choose $\mu_{G/H}=(1/2\pi)\,d\theta=:\mu_{\mathbb{T}}$, so that $\mu_{H^\perp}$ is the counting measure $\mu_{\mathbb{Z}}$ on $\mathbb{Z}$.

Let U be a representation of $\mathbb{T}$. Since $\mathbb{T}$ is compact, we can always assume that U acts diagonally on

$$\mathcal{H}=\bigoplus_{k\in I}F_k,$$

where $I \subset \mathbb{Z}$, and F_k are Hilbert spaces such that $\dim F_k$ is the multiplicity of the representation $k \in \mathbb{Z}$ in U. Explicitly,

$$(U(z)\phi_k) = z^k \phi_k$$

for all $z \in \mathbb{T}$ and $\phi_k \in F_k$.

In order to use Eq. (9), we notice that $F_k = L^2(\mathbb{Z}, \delta_k; F_k)$ (where δ_k is the Dirac measure at k), so that $\rho_k = \delta_k$, By Corollary 8, one has that U admits covariant POVMs based on $\mathbb{T}$ and that $\alpha_k(j) = \delta_{k,j}$ (where $\delta_{k,j}$ is the Kronecker delta).

Choose an infinite dimensional Hilbert space E and, for each $k \in I$, fix an isometry W_k from F_k to E. The corresponding covariance system is given by

$$P_j M(\omega) P_k \phi = \overline{\mathcal{F}_{\mathbb{T}}}(\omega)(j-k) W_j^* W_k P_k \phi = \frac{1}{2\pi} \int_0^{2\pi} \omega(e^{i\theta}) e^{i(j-k)\theta} W_j^* W_k P_k \phi \, \mathrm{d}\theta,$$

where $\phi \in \mathcal{H}$ and $\omega \in \mathcal{C}(\mathbb{T})$.

If $I = \mathbb{Z}$ and $\dim F_k = 1$ $\forall k \in \mathbb{Z}$, U is the number representation and M represents the phase observable (compare with the result obtained in Ref. 3).

C. Covariant phase difference observables

Let $\mu_{\mathbb{T}}$ as in the previous section. We consider the following representation U of the direct product $G = \mathbb{T} \times \mathbb{T}$ acting on the space $\mathcal{H} = L^2(\mathbb{T} \times \mathbb{T}, \mu_{\mathbb{T}} \otimes \mu_{\mathbb{T}})$ as

$$(U(a,b)f)(z_1, z_2) = f(az_1, b^{-1} z_2), \quad (z_1, z_2) \in \mathbb{T} \times \mathbb{T},$$

for all $(a,b) \in \mathbb{T} \times \mathbb{T}$.

Let H be the closed subgroup

$$H = \{(a,b) \in \mathbb{T} \times \mathbb{T} \mid b = a\} \cong \mathbb{T}.$$

We classify all the POVMs based on G/H and covariant with respect to U (for a different approach to the same problem, see Ref. 9).

We have

$$G = \mathbb{T} \times \mathbb{T}, \quad G/H \cong \mathbb{T}, \quad \hat{G} = \hat{\mathbb{T}} \times \hat{\mathbb{T}} \cong \mathbb{Z} \times \mathbb{Z},$$

$$H^\perp = \{(j,k) \in \mathbb{Z} \times \mathbb{Z} \mid k = -j\} \cong \mathbb{Z},$$

$$\hat{G}/H^\perp \cong \mathbb{Z}.$$

We fix $\mu_{G/H} = \mu_{\mathbb{T}}$, so that $\mu_{H^\perp} = \mu_{\mathbb{Z}}$.

We choose the following orthonormal basis $(e_{i,j})_{i,j \in \mathbb{Z}}$ of $\mathcal{H}$,

$$e_{i,j}(z_1, z_2) = z_1^i z_2^{-j}, \quad (z_1, z_2) \in \mathbb{T} \times \mathbb{T},$$

so that

$$U(a,b) e_{i,j} = a^i b^j e_{i,j} \quad \forall (a,b) \in \mathbb{T} \times \mathbb{T}.$$

Let $F_{i,j} = \mathbb{C} e_{i,j}$, Then U acts diagonally on $F_{i,j}$ as the character $(i,j) \in \mathbb{Z} \times \mathbb{Z}$. Then, one can choose as decomposition (9)

$$\mathcal{H} = \bigoplus_{i,j \in \mathbb{Z}} F_{i,j} \cong \bigoplus_{i,j \in \mathbb{Z}} L^2(\mathbb{Z} \times \mathbb{Z}, \delta_i \otimes \delta_j; F_{i,j}).$$

With the notations of Sec. IV, we have $I=\mathbb{Z}\times\mathbb{Z}$ and $\rho_{i,j}=\delta_i\otimes\delta_j$. It follows that $\mathcal{C}_U^{\pi}$ is the equivalence class of $\mu_{\mathbb{Z}}$. With the choice $\nu_U=\mu_{\mathbb{Z}}$, it follows that $\tilde{\nu}=\mu_{\mathbb{Z}}\otimes\mu_{\mathbb{Z}}$. According to Theorem 6, U admits covariant POVMs and $\alpha_{i,j}(n,m)=\delta_{n,i}\delta_{m,j}$.

With the choice $E=\mathcal{H}$, we select a map $(i,j)\mapsto W_{i,j}$, where $W_{i,j}$ is an isometry from $F_{i,j}$ to $\mathcal{H}$. Since $F_{i,j}$ are one dimensional, there exists a family of vectors $(h_{i,j})_{i,j\in\mathbb{Z}}$ in $\mathcal{H}$, with $\|h_{i,j}\|_{\mathcal{H}}=1\ \forall(i,j)\in\mathbb{Z}\times\mathbb{Z}$, such that

$$W_{i,j}e_{i,j}=h_{i,j}\quad\forall(i,j)\in\mathbb{Z}\times\mathbb{Z}.$$

The corresponding covariant POVM M is given, for every $\phi\in\mathcal{H}$, by

$$\begin{aligned}P_{l,m}M(\omega)P_{i,j}\phi&=\sum_{h\in\mathbb{Z}}\mathcal{F}_{\mathbb{T}}(\omega)(h)\,\delta_{l-h,i}\delta_{m+h,j}\langle h_{i,j},h_{l,m}\rangle\langle\phi,e_{i,j}\rangle e_{l,m}\\&=\delta_{l+m,i+j}\ \mathcal{F}_{\mathbb{T}}(\omega)(j-m)\langle h_{i,j},h_{l,m}\rangle\ \langle\phi,e_{i,j}\rangle e_{l,m}.\end{aligned}$$

In particular, if $l+m=i+j$, we have

$$\langle M(\omega)e_{i,j},e_{l,m}\rangle=\overline{\mathcal{F}_{\mathbb{T}}}(\omega)(j-m)\langle h_{i,j},h_{l,m}\rangle=\frac{1}{2\pi}\int_0^{2\pi}\omega(e^{i\theta})e^{i(j-m)\theta}\langle h_{i,j},h_{l,m}\rangle\mathrm{d}\theta.$$

If $l+m\neq i+j$, one has

$$\langle M(\omega)e_{i,j},e_{l,m}\rangle=0.$$

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Hopf structure of the Yangian $Y(\mathrm{sl}_n)$ in the Drinfel'd realization

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The Yangian of the Lie algebra sl_n is known to have different presentations, in particular the RTT realization and the Drinfel'd realization. Using the isomorphism between them, the explicit expressions of the comultiplication, the antipode and the counit in the Drinfel'd realization of the Yangian $Y(\mathrm{sl}_n)$ are given. As examples, the cases of $Y(\mathrm{sl}_2)$ and $Y(\mathrm{sl}_3)$ are worked out. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1633024]

I. TWO REALIZATIONS OF THE YANGIAN $Y(\mathrm{sl}_n)$

The Yangian $Y(\mathfrak{a})$ based on a simple Lie algebra $\mathfrak{a}$ is defined[1,2] as the (unique) homogeneous quantization of the algebra $\mathfrak{a}[u]=\mathfrak{a}\otimes\mathbb{C}[u]$ endowed with its standard bialgebra structure, where $\mathbb{C}[u]$ is the ring of polynomials in the indeterminate u. This algebra has a structure of a noncocomutative Hopf algebra, which partially explains the importance of Yangians and their representations in the study of quantum inverse problem. Among the different presentations of the Yangians, the one known as the Drinfel'd realization is well adapted for the study of their representations.[3] No explicit formula for the Hopf structure in this realization was known yet, except for sl_2[4] and for $\mathrm{osp}(1|2)$.[5] The aim of this paper is to give an explicit expression of the comultiplication, the antipode and the counit in the Drinfel'd realization for $Y(\mathrm{sl}_n)$. Note that partial results were given in Refs. 6 and 7. The comultiplication given in this paper can be extended to the double Yangian $DY(\mathrm{sl}_n)$. One can show that the so-called Drinfel'd comultiplication defined only for the double Yangian is the twist of this extended comultiplication (see, for example, Refs. 7 and 8).

This paper is organized as follows. In this section, the RTT formalism[9] and Drinfel'd realization of $Y(\mathrm{sl}_n)$ are presented, which allow us to give the normalization of the generators as well as the exact form of the R-matrix and of the quantum determinant. In the second section, some properties about the quantum minors, needed in the following, are explained. The expressions of the isomorphism using the quantum minors or the Gauss decomposition are then presented. The main theorem of this paper, i.e., the explicit form of the Hopf structure, is exposed in the next two sections. Finally, as illustrative examples, the $Y(\mathrm{sl}_2)$ and $Y(\mathrm{sl}_3)$ cases are worked out.

In this section, two well-known realizations of the Yangian based on the Lie algebra sl_n are presented: the RTT formalism and the Drinfel'd realization.[3]

The first realization uses the RTT formalism.[3,4,9] Let $V^{(n)}$ denote the n-dimensional fundamental vector space representation of sl_n. The Yang's R-matrix is given by

$$R_{12}^{(n)}(u)=I\otimes I+\sum_{1\leqslant i,j\leqslant n}\frac{E_{ij}\otimes E_{ji}}{u}\in \mathrm{End}(V^{(n)}\otimes V^{(n)}), \tag{1.1}$$

where E_{ij} is the elementary matrix with entry 1 in row i and column j and 0 elsewhere. This R-matrix satisfies the following properties:

$$R_{12}^{(n)}(u)R_{13}^{(n)}(u+v)R_{23}^{(n)}(v)=R_{23}^{(n)}(v)R_{13}^{(n)}(u+v)R_{12}^{(n)}(u) \quad \text{(Yang–Baxter equation)}, \tag{1.2}$$

$$R_{12}^{(n)}(u)R_{21}^{(n)}(-u)=\frac{u^2-1}{u^2}\ \ (I\otimes I)\quad (\text{unitarity}). \tag{1.3}$$

Definition 1.1: The Yangian of gl_n, $Y(\mathrm{gl}_n)$, *is the associative algebra, generated by the unit and the elements* $\{T_{i,j}^{(k)}|1\leqslant i,j\leqslant n,k\in\mathbb{Z}_{>0}\}$ *gathered in the formal series*

$$T(u)=1+\sum_{i,j=1}^{n}\ \sum_{k\in\mathbb{Z}_{>0}}\ T_{i,j}^{(k)}\,u^{-k}\,E_{ij}=\sum_{i,j=1}^{n}\ T_{i,j}(u)\,E_{ij} \tag{1.4}$$

subject to the defining relations

$$R_{12}^{(n)}(u-v)(T(u)\otimes 1)(1\otimes T(v))=(1\otimes T(v))(T(u)\otimes 1)R_{12}^{(n)}(u-v). \tag{1.5}$$

The defining relations (1.5) as commutators of $T_{ij}(u)$ are

$$-(u-v)[T_{i,j}(u),T_{k,l}(v)]=T_{k,j}(u)\,T_{i,l}(v)-T_{k,j}(v)\,T_{i,l}(u). \tag{1.6}$$

The Yangian $Y(\mathrm{gl}_n)$ has a Hopf algebra structure and the explicit forms of comultiplication, antipode and counit are

$$\Delta(T_{i,j}(u))=\sum_{k=1}^{n}\ T_{i,k}\otimes T_{k,j},\quad S(T(u))=T^{-1}(u)\quad \text{and}\ \ \epsilon(T_{i,j}(u))=\delta_{ij}\ \ . \tag{1.7}$$

By definition, the quantum determinant is the following formal series with coefficients in $Y(\mathrm{gl}_n)$:

$$q\det T(u)=\sum_{\sigma\in\mathfrak{S}_n}\ \mathrm{sgn}(\sigma)\ T_{\sigma(1),1}(u)\cdots T_{\sigma(n),n}(u+n-1). \tag{1.8}$$

Remark: To avoid ambiguity, let us stress that

$$q\det T(-u)=\sum_{\sigma\in\mathfrak{S}_n}\ \mathrm{sgn}(\sigma)\ T_{\sigma(1),1}(-u)\cdots T_{\sigma(n),n}(-u+n-1)$$

is different from the quantum determinant of the matrix $\tilde{T}(u)=T(-u)$,

$$q\det\tilde{T}(u)=\sum_{\sigma\in\mathfrak{S}_n}\ \mathrm{sgn}(\sigma)\ T_{\sigma(1),1}(-u)\cdots T_{\sigma(n),n}(-u-n+1). \tag{1.9}$$

A well-known result (see, e.g., Ref. 4) is that the coefficients of $q\det T(u)$ generate the center of $Y(\mathrm{gl}_n)$ and furthermore

$$\Delta(q\det T(u))=q\det T(u)\otimes q\det T(u). \tag{1.10}$$

These results justify the following definition.

Definition 1.2: The Yangian of the Lie algebra sl_n, $Y(\mathrm{sl}_n)$, *is the quotient of the algebra* $Y(\mathrm{gl}_n)$ *by the ideal generated by* $q\det T(u)=1$ *with the Hopf algebra structure (1.7).*

Let us note that the Yangian $Y(\mathrm{sl}_n)$ can also be viewed as a subalgebra of $Y(\mathrm{gl}_n)$; for more details, see, for example, Ref. 4. In the following, $T(u)$ will denote the generators of the Yangian $Y(\mathrm{sl}_n)$.

The map

$$T(u)\mapsto T^{-1}(-u)\equiv T^{*}(u) \tag{1.11}$$

defines an automorphism of $Y(\mathrm{sl}_n)$.

The second realization of the Yangian uses the so-called Drinfel'd generators. Let $\{\alpha_i|1\leqslant i\leqslant n-1\}$ be the set of simple roots of sl_n and $(\cdot,\cdot)$ be the standard nondegenerate symmetric

invariant bilinear form on sl_n. For each simple root α_i, e_{α_i}, and f_{α_i} are the corresponding root vectors, such that $(e_{\alpha_i},f_{\alpha_i})=1$, and $h_{\alpha_i}=[e_{\alpha_i},f_{\alpha_i}]$ are the Cartan generators. The Drinfel'd realization of the Yangian is given by the following theorem.[3]

Theorem 1.3: The Yangian of sl_n, $Y(\mathrm{sl}_n)$, *is isomorphic to the associative algebra* $\mathcal{A}$, *generated by the unit and the elements* $\{e_i^{(k)},f_i^{(k)},h_i^{(k)} \mid 1\leqslant i\leqslant n-1, k\in\mathbb{Z}_{\geqslant 0}\}$ *subject to the defining relations*

$$[h_i^{(k)},h_j^{(l)}]=0, \quad [e_i^{(k)},f_j^{(l)}]=\delta_{i,j}\ \ h_i^{(k+l)}, \tag{1.12}$$

$$[h_i^{(0)},e_j^{(l)}]=(\alpha_i,\alpha_j)e_j^{(l)}, \quad [h_i^{(0)},f_j^{(l)}]=-(\alpha_i,\alpha_j)f_j^{(l)}, \tag{1.13}$$

$$[h_i^{(k+1)},e_j^{(l)}]-[h_i^{(k)},e_j^{(l+1)}]=\tfrac{1}{2}(\alpha_i,\alpha_j)\ \ (h_i^{(k)}e_j^{(l)}+e_j^{(l)}h_i^{(k)}), \tag{1.14}$$

$$[h_i^{(k+1)},f_j^{(l)}]-[h_i^{(k)},f_j^{(l+1)}]=-\tfrac{1}{2}(\alpha_i,\alpha_j)\ \ (h_i^{(k)}f_j^{(l)}+f_j^{(l)}h_i^{(k)}), \tag{1.15}$$

$$[e_i^{(k+1)},e_j^{(l)}]-[e_i^{(k)},e_j^{(l+1)}]=\tfrac{1}{2}(\alpha_i,\alpha_j)\ \ (e_i^{(k)}e_j^{(l)}+e_j^{(l)}e_i^{(k)}), \tag{1.16}$$

$$[f_i^{(k+1)},f_j^{(l)}]-[f_i^{(k)},f_j^{(l+1)}]=-\tfrac{1}{2}(\alpha_i,\alpha_j)\ \ (f_i^{(k)}f_j^{(l)}+f_j^{(l)}f_i^{(k)}), \tag{1.17}$$

and to the Serre relations, for $i\neq j$ *and* $n_{ij}=1-2[(\alpha_i,\alpha_j)/(\alpha_i,\alpha_i)]$:

$$\sum_{\sigma\in\mathfrak{S}_{n_{ij}}}[e_i^{(k_{\sigma(1)})},[\cdots,[e_i^{(k_{\sigma(n_{ij})})},e_j^{(l)}]\cdots]=0, \tag{1.18}$$

$$\sum_{\sigma\in\mathfrak{S}_{n_{ij}}}[f_i^{(k_{\sigma(1)})},[\cdots,[f_i^{(k_{\sigma(n_{ij})})},f_j^{(l)}]\cdots]=0. \tag{1.19}$$

For later conveniences, we define the following formal series:

$$e_i(u)=\sum_{k=0}^{+\infty}\frac{e_i^{(k)}}{u^{k+1}}, \quad f_i(u)=\sum_{k=0}^{+\infty}\frac{f_i^{(k)}}{u^{k+1}}, \quad \text{and} \quad h_i(u)=1+\sum_{k=0}^{+\infty}\frac{h_i^{(k)}}{u^{k+1}} \quad \text{for} \quad 1\leqslant i\leqslant n-1. \tag{1.20}$$

The mapping $e_{\alpha_i}\mapsto e_i^{(0)}$, $f_{\alpha_i}\mapsto f_i^{(0)}$, $h_{\alpha_i}\mapsto h_i^{(0)}$ defines an embedding $\mathrm{U}(\mathrm{sl}_n)\hookrightarrow\mathcal{A}$, where $\mathrm{U}(\mathrm{sl}_n)$ is the universal enveloping algebra of sl_n.

II. QUANTUM MINORS

Before giving the expression of the isomorphism that relates the two Yangian presentations, in the next section, we introduce the notion of quantum minors and recall some of their properties (see, e.g., Refs. 4 and 8, for the proofs).

Let $I=\{a_1,a_2,\ldots,a_m\}$ and $J=\{b_1,b_2,\ldots,b_m\}$ such that $I,J\subset\{1,\ldots,n\}$ and $\mathrm{card}(I)=\mathrm{card}(J)=m$ with $1\leqslant m\leqslant n$. The set of generators $\{T_{a_i,b_j}(u)\mid 1\leqslant i,j\leqslant m\}$ defines a subalgebra of $Y(\mathrm{sl}_n)$ with the following commutation relations:

$$\begin{aligned}R_{12}^{(m)}(u-v)&\left(T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)\otimes 1\right)\left(1\otimes T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(v)\right)\\ &=\left(1\otimes T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(v)\right)\left(T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)\otimes 1\right)R_{12}^{(m)}(u-v),\end{aligned} \tag{2.1}$$

where $T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\sum_{i,j=1}^{m}T_{a_ib_j}(u)\ \ E_{ij}$.

Definition 2.1: The quantum minor $t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)$ *of* $T(u)$ *is defined by*

$$t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=q\det T\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\sum_{\sigma\in\mathfrak{S}_m}\operatorname{sgn}(\sigma)T_{a_{\sigma(1)},b_1}(u)\cdots T_{a_{\sigma(m)},b_m}(u+m-1). \quad (2.2)$$

The quantum minors can also be given by[4]

$$t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\sum_{\sigma\in\mathfrak{S}_m}\operatorname{sgn}(\sigma)T_{a_1,b_{\sigma(1)}}(u+m-1)\cdots T_{a_m,b_{\sigma(m)}}(u). \quad (2.3)$$

By convention, when $m<1$, the quantum minor is equal to 1. Quantum minors satisfy some properties which are analogous to those of numerical matrices minors (for more details, see, for example, Refs. 4 and 8).

Proposition 2.2: The quantum minor $t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)$ *verifies the following properties:*

(1) It is antisymmetric, i.e., for $\rho\in\mathfrak{S}_m$,

$$t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\operatorname{sgn}(\rho)t\left(\begin{smallmatrix}\rho(a_1)\cdots\rho(a_m)\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\operatorname{sgn}(\rho)t\left(\begin{smallmatrix}a_1\cdots a_m\\ \rho(b_1)\cdots\rho(b_m)\end{smallmatrix}\right)(u). \quad (2.4)$$

(2) It is alternated, i.e., if there exists $i\neq j$ *such that* $a_i=a_j$ *or* $b_i=b_j$, *then* $t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=0$.

(3) It can be expanded with respect to its last column or its last row as follows:

$$t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)=\sum_{k=1}^{m}(-1)^{k+m}\,t\left(\begin{smallmatrix}a_1\cdots a_{k-1}\,a_{k+1}\cdots a_{m-1}\,a_m\\ b_1\cdots b_{k-1}\,b_k\cdots b_{m-2}\,b_{m-1}\end{smallmatrix}\right)(u)\;T_{a_k,b_m}(u+m-1) \quad (2.5)$$

$$=\sum_{k=1}^{m}(-1)^{k+m}\;T_{a_m,b_k}(u+m-1)\;t\left(\begin{smallmatrix}a_1\cdots a_{k-1}\,a_k\cdots a_{m-2}\,a_{m-1}\\ b_1\cdots b_{k-1}\,b_{k+1}\cdots b_{m-1}\,b_m\end{smallmatrix}\right)(u). \quad (2.6)$$

From the defining relations (1.6), the commutation relations of the quantum minors with $T_{i,j}(u)$ can be computed:

$$(u-v)[T_{i,j}(u),t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(v)]=\sum_{k=1}^{m}\Big(t\left(\begin{smallmatrix}a_1\cdots a_{k-1}\,a_k a_{k+1}\cdots a_m\\ b_1\cdots b_{k-1}\,j\,b_{k+1}\cdots b_m\end{smallmatrix}\right)(v)\;\;T_{i,b_k}(u)$$

$$-T_{a_k,j}(u)t\left(\begin{smallmatrix}a_1\cdots a_{k-1}\,i\,a_{k+1}\cdots a_m\\ b_1\cdots b_{k-1}\,b_k\,b_{k+1}\cdots b_m\end{smallmatrix}\right)(v)\Big). \quad (2.7)$$

A corollary of (2.7) is that the quantum minor $t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(u)$ lies in the center of the subalgebra generated by $\{T_{a_i,b_j}(u)\,|\,1\leqslant i,j\leqslant m\}$, i.e.,

$$[T_{a_i,b_j}(u),\;\;t\left(\begin{smallmatrix}a_1\cdots a_m\\ b_1\cdots b_m\end{smallmatrix}\right)(v)]=0\qquad\text{for }\;1\leqslant i,j\leqslant m. \quad (2.8)$$

The map

$$T_{i,j}(u)\mapsto t\left(\begin{smallmatrix}1\cdots p\;\,p+i\\ 1\cdots p\;\,p+j\end{smallmatrix}\right)(u) \quad (2.9)$$

defines an algebra homomorphism $Y(\mathrm{sl}_{n-p})\to Y(\mathrm{sl}_n)$, for $1\leqslant p\leqslant n-1$ and $1\leqslant i,j\leqslant n-p$. Note that this homomorphism allows us to compute a simple way the commutation relations among the $t\left(\begin{smallmatrix}1\cdots p\;\,p+i\\ 1\cdots p\;\,p+j\end{smallmatrix}\right)(u)$ minors.

Finally, quantum minors allow us to express some elements of the inverse matrix of $T(u)$ thanks to the following proposition (see, e.g., Ref. 4).

Proposition 2.3: For $1\leqslant i,j\leqslant n$, *the following equality holds:*

$$(T^{-1}(u+n-1))_{i,j}=(-1)^{i+j}\;t\left(\begin{smallmatrix}1\cdots j-1\;\,j+1\cdots n\\ 1\cdots i-1\;\,i+1\cdots n\end{smallmatrix}\right)(u). \quad (2.10)$$

III. ISOMORPHISMS BETWEEN THE TWO REALIZATIONS OF $Y(\mathrm{sl}_n)$

For clarity purposes, the isomorphism between the two previous realizations is recalled (see, e.g., Refs. 3 and 8). Two presentations of this isomorphism are possible. The first one uses the quantum minors and the second one uses the Gauss decomposition.

Theorem 3.1: *The map* $\phi:\mathcal{A}\to Y(\mathrm{sl}_n)$,

$$e_i\left(u+\frac{i-2}{2}\right)\mapsto(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i-1\ i}_{1\cdots i-1\ i+1})(u), \tag{3.1}$$

$$f_i\left(u+\frac{i-2}{2}\right)\mapsto t(^{1\cdots i-1\ i+1}_{1\cdots i-1\ i})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}, \tag{3.2}$$

$$h_i\left(u+\frac{i-2}{2}\right)\mapsto(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i-1}_{1\cdots i-1})(u)t(^{1\cdots i+1}_{1\cdots i+1})(u-1)(t(^{1\cdots i}_{1\cdots i})(u-1))^{-1}, \tag{3.3}$$

defines an algebra isomorphism.

Note that the image of $h_i(u)$ can be written differently as, by using the proposition 2.2,

$$\phi\left(h_i\left(u+\frac{i-2}{2}\right)\right)=(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i-1\ i+1}_{1\cdots i-1\ i+1})(u)-\phi\left(f_i\left(u+\frac{i}{2}\right)e_i\left(u+\frac{i-2}{2}\right)\right) \tag{3.4}$$

$$=t(^{1\cdots i-1\ i+1}_{1\cdots i-1\ i+1})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}-\phi\left(f_i\left(u+\frac{i-2}{2}\right)e_i\left(u+\frac{i}{2}\right)\right). \tag{3.5}$$

The other presentation of the isomorphism ϕ uses the Gauss decompositions of the matrix $T(u)$,

$$T(u)=\begin{pmatrix}1 & & & 0\\ f_{2,1}(u) & 1 & & \\ \vdots & \ddots & \ddots & \\ f_{n,1}(u) & \cdots & f_{n,n-1}(u) & 1\end{pmatrix}\begin{pmatrix}k_1(u) & & 0\\ & \ddots & \\ 0 & & k_n(u)\end{pmatrix}\begin{pmatrix}1 & e_{1,2}(u) & \cdots & e_{1,n}(u)\\ & 1 & \ddots & \vdots\\ & & \ddots & e_{n-1,n}(u)\\ 0 & & & 1\end{pmatrix} \tag{3.6}$$

$$=\begin{pmatrix}1 & \tilde{e}_{1,2}(u) & \cdots & \tilde{e}_{1,n}(u)\\ & 1 & \ddots & \vdots\\ & & \ddots & \tilde{e}_{n-1,n}(u)\\ 0 & & & 1\end{pmatrix}\begin{pmatrix}\tilde{k}_1(u) & & 0\\ & \ddots & \\ 0 & & \tilde{k}_n(u)\end{pmatrix}\begin{pmatrix}1 & & & 0\\ \tilde{f}_{2,1}(u) & 1 & & \\ \vdots & \ddots & \ddots & \\ \tilde{f}_{n,1}(u) & \cdots & \tilde{f}_{n,n-1}(u) & 1\end{pmatrix}. \tag{3.7}$$

The expression of the elements of the Gauss decomposition (3.6) in terms of quantum minors has been computed by Iohara.[8] For the alternative Gauss decomposition (3.7), the computations are similar and one obtains the following.

Proposition 3.2: Let $1\leqslant i<j\leqslant n$ *and* $1\leqslant p\leqslant n$. *The formal series* $e_{i,j}(u)$, $\tilde{e}_{i,j}(u)$, $f_{j,i}(u)$, $\tilde{f}_{j,i}(u)$, $k_p(u)$ *and* $\tilde{k}_p(u)$ *in the Gauss decompositions, can be expressed in terms of quantum minors,*

$$e_{i,j}(u+i-1)=(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i-1\ i}_{1\cdots i-1\ j})(u), \tag{3.8}$$

$$f_{j,i}(u+i-1)=t(^{1\cdots i-1\ j}_{1\cdots i-1\ i})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}, \tag{3.9}$$

$$k_j(u+j-1)=t(^{1\cdots j}_{1\cdots j})(u)(t(^{1\cdots j-1}_{1\cdots j-1})(u))^{-1}, \tag{3.10}$$

$$k_1(u)=t\binom{1}{1}(u)=T_{1,1}(u) \tag{3.11}$$

and

$$\tilde{e}_{i,j}(u+n-j)=t\binom{i\ \ j+1\cdots n}{j\ \ j+1\cdots n}(u)\left(t\binom{j+1\cdots n}{j+1\cdots n}(u)\right)^{-1}, \tag{3.12}$$

$$\tilde{f}_{j,i}(u+n-j)=\left(t\binom{j+1\cdots n}{j+1\cdots n}(u)\right)^{-1}t\binom{j\ \ j+1\cdots n}{i\ \ j+1\cdots n}(u), \tag{3.13}$$

$$\tilde{k}_i(u+n-i)=\left(t\binom{i+1\cdots n}{i+1\cdots n}(u)\right)^{-1}t\binom{i\cdots n}{i\cdots n}(u), \tag{3.14}$$

$$\tilde{k}_n(u)=t\binom{n}{n}(u)=T_{n,n}(u). \tag{3.15}$$

Remark: Proposition 3.2 proves the existence of the two Gauss decomposition.

Then, proposition 3.2 implies that the map $\tilde{\phi}:\mathcal{A}\to Y(\mathrm{sl}_n)$,

$$e_i(u)\mapsto e_{i,i+1}\left(u+\frac{i}{2}\right), \tag{3.16}$$

$$f_i(u)\mapsto f_{i+1,i}\left(u+\frac{i}{2}\right), \tag{3.17}$$

$$h_i(u)\mapsto k_{i+1}\left(u+\frac{i}{2}\right)k_i^{-1}\left(u+\frac{i}{2}\right) \tag{3.18}$$

is an algebra isomorphism, for $1\leqslant i\leqslant n-1$.

Let $T^*(u)$ denote $T(-u)^{-1}$. Then, thanks to the map (1.11), the quantum minors of $T^*(u)$ has a meaning and is denoted by $t^*\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)$.

Corollary 3.3: For $1\leqslant m\leqslant n$, *the following equalities hold:*

$$t^*\binom{1\cdots m}{1\cdots m}(-u-n+1)=t\binom{m+1\cdots n}{m+1\cdots n}(u), \tag{3.19}$$

$$t^*\binom{1\cdots m-1\ \ m+1}{1\cdots m-1\ \ m}(-u-n+1)=-t\binom{m+1\ \ m+2\cdots n}{m\ \ m+2\cdots n}(u), \tag{3.20}$$

$$t^*\binom{1\cdots m-1\ \ m}{1\cdots m-1\ \ m+1}(-u-n+1)=-t\binom{m\ \ m+2\cdots n}{m+1\ \ m+2\cdots n}(u), \tag{3.21}$$

$$t^*\binom{1\cdots m-1\ \ m+1}{1\cdots m-1\ \ m+1}(-u-n+1)=t\binom{m\ \ m+2\cdots n}{m\ \ m+2\cdots n}(u). \tag{3.22}$$

Proof: Let $T(u)$ decomposed according to (3.7). Then, $T^*(u)$ decomposes as in (3.6). Using the relation $T^*(u)=T(-u)^{-1}$, we deduce

$$e^*_{i,i+1}(u)=-e_{i,i+1}(-u), \tag{3.23}$$

$$f^*_{i+1,i}(u)=-f_{i+1,i}(-u),\quad \text{for}\quad 1\leqslant i\leqslant n-1, \tag{3.24}$$

$$k^*_i(u)=(k_i(-u))^{-1},\quad \text{for}\quad 1\leqslant i\leqslant n, \tag{3.25}$$

with obvious notations. Finally, using proposition 3.2, the equalities are proven. ■

For $1\leqslant i<j\leqslant n$, the elements $e^{(0)}_{i,j}=T^{(1)}_{i,j}$ and $f^{(0)}_{j,i}=T^{(1)}_{j,i}$ are root generators of the algebra sl_n, which can be expressed in terms of simple root generators, $e^{(0)}_i$ and $f^{(0)}_i$, as follows:

$$e^{(0)}_{i,j}=[\cdots[e^{(0)}_{j-1},e^{(0)}_{j-2}],e^{(0)}_{j-3}],\cdots],e^{(0)}_{i+1}],e^{(0)}_i], \tag{3.26}$$

$$f^{(0)}_{j,i}=[f^{(0)}_i,[f^{(0)}_{i+1},[\cdots,[f^{(0)}_{j-3},[f^{(0)}_{j-2},f^{(0)}_{j-1}]\cdots]. \tag{3.27}$$

Remark: In (3.26) and (3.27), the isomorphism $\tilde{\phi}$ has been omitted for simplicity. In the following, this notation is always used, i.e., the isomorphisms between two realizations of the same algebra are omitted.

IV. THE HOPF STRUCTURE OF $Y(\mathrm{sl}_n)$ IN THE DRINFEL'D BASIS

Before giving the Hopf structure of $Y(\mathrm{sl}_n)$ in the Drinfel'd basis, the images of any quantum minor under the coproduct, the antipode and the counit are needed. Let us recall that $T^*(u)$ denotes $T(-u)^{-1}$ and $t^*\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)$ denotes its quantum minors.

Proposition 4.1: Let $1\leqslant m\leqslant n, 1\leqslant a_1<\cdots<a_m\leqslant n$ *and* $1\leqslant b_1<\cdots<b_m\leqslant n$. *The images of a quantum minor under the coproduct, the antipode and the counit are given by*

$$\Delta\left(t\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)\right)=\sum_{1\leqslant c_1<\cdots<c_m\leqslant n} t\binom{a_1\cdots a_m}{c_1\cdots c_m}(u)\otimes t\binom{c_1\cdots c_m}{b_1\cdots b_m}(u), \tag{4.1}$$

$$S\left(t\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)\right)=(-1)^{[m/2]}t^*\binom{a_1\cdots a_m}{b_1\cdots b_m}(-u-m+1), \tag{4.2}$$

$$\varepsilon\left(t\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)\right)=\delta_{a_1,b_1}\cdots\delta_{a_m,b_m}, \tag{4.3}$$

where $[m/2]$ *is the integer part of* $m/2$.

Proof: The result for the coproduct is well known (see, e.g., Ref. 4). For the antipode, one gets

$$S\left(t\binom{a_1\cdots a_m}{b_1\cdots b_m}(u)\right)=S\left(\sum_{\sigma\in\mathfrak{S}_m}\mathrm{sgn}(\sigma)T_{a_{\sigma(1)},b_1}(u)\cdots T_{a_{\sigma(m)},b_m}(u+m-1)\right) \tag{4.4}$$

$$=\sum_{\sigma\in\mathfrak{S}_m}\mathrm{sgn}(\sigma)S(T_{a_{\sigma(m)},b_m}(u+m-1))\cdots S(T_{a_{\sigma(1)},b_1}(u))$$

(S is an antimorphism) (4.5)

$$=\sum_{\sigma\in\mathfrak{S}_m}\mathrm{sgn}(\sigma)T^*_{a_{\sigma(m)},b_m}(-u-m+1)\cdots T^*_{a_{\sigma(1)},b_1}(-u) \tag{4.6}$$

$$=(-1)^{[m/2]}\sum_{\sigma\in\mathfrak{S}_m}\mathrm{sgn}(\sigma)T^*_{a_{\sigma(m)},b_1}(-u-m+1)\cdots T^*_{a_{\sigma(1)},b_m}(-u)$$

[Eq. (2.4)], (4.7)

which proves the relation (4.2). The computation for the antipode is obvious. ■

The comultiplication, the antipode and the counit are established in the Drinfel'd basis thanks to the isomorphism ϕ (see theorem 3.1) between $\mathcal{A}$ and $Y(\mathrm{sl}_n)$.

A. Comultiplication

The adjoint actions of the elements of the algebra sl_n on $X\in Y(\mathrm{sl}_n)$ will be denoted by, for $1\leqslant i\leqslant j\leqslant n$,

$$\mathrm{Ad}^{\pm}_{e_{i,j}}(X)=\begin{cases}\pm[e^{(0)}_{i,j},X], & i<j,\\ X, & i=j,\end{cases}\quad\text{and}\quad \mathrm{Ad}^{\pm}_{f_{j,i}}(X)=\begin{cases}\pm[f^{(0)}_{j,i},X], & i<j,\\ X, & i=j.\end{cases} \tag{4.8}$$

To determine the explicit form of the comultiplication, the following generalization of the adjoint action, depending on a spectral parameter, is useful.

Definition 4.2: Let $1\leqslant i\leqslant j\leqslant n$, $1\leqslant\alpha\leqslant n$ *and* X *an element of* $Y(\mathrm{sl}_n)$. *The generalized adjoint actions are defined by*

$$ {}^{\alpha}\mathcal{E}_{i,j}(u)(X)=\mathrm{Ad}^{+}_{e_{i,j}}(X)+\delta_{i\leqslant\alpha<j}\,\mathrm{Ad}^{-}_{e_{i,\alpha}}(\mathrm{Ad}^{+}_{e_{\alpha+1,j}}(e_{\alpha}(u)))\;X, \tag{4.9}$$

$$ \mathcal{E}^{\alpha}_{i,j}(u)(X)=\mathrm{Ad}^{+}_{e_{i,j}}(X)+\delta_{i\leqslant\alpha<j}\,X\;\;\mathrm{Ad}^{-}_{e_{i,\alpha}}(\mathrm{Ad}^{+}_{e_{\alpha+1,j}}(e_{\alpha}(u))), \tag{4.10}$$

and

$$ {}^{\alpha}\mathcal{F}_{j,i}(u)(X)=\mathrm{Ad}^{-}_{f_{j,i}}(X)+\delta_{i\leqslant\alpha<j}\,\mathrm{Ad}^{+}_{f_{\alpha,i}}(\mathrm{Ad}^{-}_{f_{j,\alpha+1}}(f_{\alpha}(u)))X, \tag{4.11}$$

$$ \mathcal{F}^{\alpha}_{j,i}(u)(X)=\mathrm{Ad}^{-}_{f_{j,i}}(X)+\delta_{i\leqslant\alpha<j}\,X\;\;\mathrm{Ad}^{+}_{f_{\alpha,i}}(\mathrm{Ad}^{-}_{f_{j,\alpha+1}}(f_{\alpha}(u))), \tag{4.12}$$

where

$$ \delta_{i\leqslant\alpha<j}=\begin{cases}1 & \text{if } i\leqslant\alpha<j,\\ 0 & \text{otherwise.}\end{cases}$$

Let us give examples of the generalized adjoint actions (4.9),

$$ {}^{1}\mathcal{E}_{13}(u)(X)=\mathrm{Ad}^{+}_{e_{13}}(X)+\mathrm{Ad}^{-}_{e_{11}}(\mathrm{Ad}^{+}_{e_{23}}(e_1(u)))X=[e^{(0)}_{13},X]+[e^{(0)}_{23},e_1(u)]X, \tag{4.13}$$

$$ {}^{2}\mathcal{E}_{13}(u)(X)=\mathrm{Ad}^{+}_{e_{13}}(X)+\mathrm{Ad}^{-}_{e_{12}}(\mathrm{Ad}^{+}_{e_{33}}(e_2(u)))X=[e^{(0)}_{13},X]-[e^{(0)}_{12},e_2(u)]X, \tag{4.14}$$

$$ {}^{3}\mathcal{E}_{13}(u)(X)=\mathrm{Ad}^{+}_{e_{13}}(X)=[e^{(0)}_{13},X]. \tag{4.15}$$

Let ${}^{\alpha}\mathcal{G}$, $\mathcal{G}^{\beta}$ be any actions on $Y(\mathrm{sl}_n)$. Hereafter, for simplicity, the notation ${}^{\alpha}\mathcal{G}^{\beta}$ means either ${}^{\alpha}\mathcal{G}$ or $\mathcal{G}^{\beta}$.

To compute the comultiplication, we also need the following definition.

Definition 4.3: For $1\leqslant m\leqslant n$, $1\leqslant k_1<k_2<\cdots<k_m\leqslant n$ *and* $k_m\neq m$, ${}^{\alpha}E^{\beta}_{k_1,k_2,\cdots,k_m}(u)$ *and* ${}^{\alpha}F^{\beta}_{k_1,k_2,\cdots,k_m}(u)(X)$ *are defined by for* $X\in Y(\mathrm{sl}_n)$:

$$ {}^{\alpha}E^{\beta}_{k_1,k_2,\cdots,k_m}(u)(X)=\left(\overrightarrow{\prod_{1\leqslant i\leqslant m-1}}\;{}^{\alpha}\mathcal{E}^{\beta}_{i,k_i}(u)\right)({}^{\alpha}\mathcal{E}^{\beta}_{m+1,k_m}(u)(X)), \tag{4.16}$$

$$ {}^{\alpha}F^{\beta}_{k_1,k_2,\cdots,k_m}(u)(X)=\left(\overrightarrow{\prod_{1\leqslant i\leqslant m-1}}\;{}^{\alpha}\mathcal{F}^{\beta}_{k_i,i}(u)\right)({}^{\alpha}\mathcal{F}^{\beta}_{k_m,m+1}(u)(X)), \tag{4.17}$$

where, for $\{\mathcal{G}_p|1\leqslant p\leqslant m-1\}$, *a set of actions on* $Y(\mathrm{sl}_n)$, *we denote*

$$ \overrightarrow{\prod_{1\leqslant i\leqslant m-1}}\;\mathcal{G}_i(X)=\mathcal{G}_1(\cdots(\mathcal{G}_{m-2}(\mathcal{G}_{m-1}(X))\cdots). \tag{4.18}$$

In particular, one gets for $k>1$

$$ {}^{\alpha}E^{\beta}_{k}(u)(X)={}^{\alpha}\mathcal{E}^{\beta}_{2,k}(u)(X),\quad {}^{\alpha}F^{\beta}_{k}(u)(X)={}^{\alpha}\mathcal{F}^{\beta}_{k,2}(u)(X). \tag{4.19}$$

By convention, if the set of indices $\{k_1,k_2,\ldots,k_m\}$ is empty, then ${}^{\alpha}E^{\beta}_{k_1,k_2,\ldots,k_m}(u)(X)=1$ and ${}^{\alpha}F^{\beta}_{k_1,k_2,\ldots,k_m}(u)(X)=1$. Remark that these generators can be expressed only in terms of the elements of the Drinfel'd basis, thanks to Eqs. (3.26) and (3.27).

These generalized actions show up in the following lemma.

Lemma 4.4: For $1\leqslant i\leqslant n-1$, $1\leqslant a_1<\cdots<a_i\leqslant n$ *and* $a_i\neq i$, *one gets*

$$(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots\ i}_{a_1\cdots\ a_i})(u)={}^{i}E_{a_1,\ldots,a_i}\left(u+\frac{i-2}{2}\right)\left(e_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.20}$$

$$t(^{1\ \cdots\ i}_{a_1\cdots\ a_i})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}=E^{i}_{a_1,\ldots,a_i}\left(u+\frac{i}{2}\right)\left(e_i\left(u+\frac{i}{2}\right)\right), \tag{4.21}$$

$$(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{a_1\cdots a_i}_{1\ \cdots i})(u)={}^{i}F_{a_1,\ldots,a_i}\left(u+\frac{i}{2}\right)\left(f_i\left(u+\frac{i}{2}\right)\right), \tag{4.22}$$

$$t(^{a_1\cdots a_i}_{1\ \cdots i})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}=F^{i}_{a_1,\ldots,a_i}\left(u+\frac{i-2}{2}\right)\left(f_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.23}$$

$$(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\ \cdots i-1\ \ i+1}_{a_1\cdots a_{i-1}\ \ a_i})(u)={}^{i}E_{a_1,\ldots,a_i}\left(u+\frac{i-2}{2}\right)\left(\tilde{g}_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.24}$$

$$t(^{1\ \cdots i-1\ \ i+1}_{a_1\cdots a_{i-1}\ \ a_i})(u)(t(^{1\cdots i}_{1\cdots i})(u))^{-1}=E^{i}_{a_1,\ldots,a_i}\left(u+\frac{i}{2}\right)\left(g_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.25}$$

$$(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{a_1\cdots a_{i-1}\ \ a_i}_{1\ \cdots i-1\ \ i+1})(u)={}^{i}F_{a_1,\ldots,a_i}\left(u+\frac{i}{2}\right)\left(\tilde{g}_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.26}$$

$$t(^{a_1\cdots a_{i-1}\ \ a_i}_{1\ \cdots i-1\ \ i+1})(u)\ \ (t(^{1\cdots i}_{1\cdots i})(u))^{-1}=F^{i}_{a_1,\ldots,a_i}\left(u+\frac{i-2}{2}\right)\left(g_i\left(u+\frac{i-2}{2}\right)\right), \tag{4.27}$$

where

$$g_i(u)=h_i(u)+f_i(u)e_i(u+1), \tag{4.28}$$

$$\tilde{g}_i(u)=h_i(u)+f_i(u+1)e_i(u). \tag{4.29}$$

Proof: The proof is only given for (4.20). Let i and $\{a_1,\ldots,a_i\}$ fixed as in the lemma. The first step is to evaluate the quantum minor $t(^{1\cdots i}_{a_1\cdots a_i})(u)$ in terms of the quantum minor $t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u)$ and in terms of some generators of the sl_n algebra. Selecting the coefficient of u^0v^{-1} in Eq. (2.7), the following relation is obtained for $1\leqslant b_1<\cdots<b_i\leqslant n$, $1\leqslant p\leqslant i$ and $1\leqslant m\leqslant n-b_p$:

$$\mathrm{Ad}^{+}_{e_{b_p,b_p+m}}(t(^{1\cdots p\ \cdots i}_{b_1\cdots b_p\cdots b_i})(v))=[T^{(1)}_{b_p,b_p+m},t(^{1\cdots p\ \cdots i}_{b_1\cdots b_p\cdots b_i})(v)]=t(^{1\cdots p\ \ \cdots i}_{b_1\cdots b_p+m\cdots b_i})(v). \tag{4.30}$$

This relation allows us to increase the parameters of the quantum minor. Using this relation, the indices $\{1,\ldots,i-1,\ i+1\}$ of $t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u)$ can be increased up to $\{a_1,\ldots,a_i\}$:

$$\left(\prod_{1\leqslant p\leqslant i-1}^{\rightarrow}\mathrm{Ad}^{+}_{e_{p,a_p}}\right)(\mathrm{Ad}^{+}_{e_{i+1,a_i}}(t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u)))=t(^{1\cdots i}_{a_1\cdots a_i})(u). \tag{4.31}$$

The second step of the proof consists in determining the commutator of $(t(^{1\cdots i}_{1\cdots i})(u))^{-1}$ with $e^{(0)}_{j,j+1}$. The commutation relations are computed using equation (2.7),

$$(u-v)[T_{j,j+1}(u),t(^{1\cdots i}_{1\cdots i})(v)]=\delta_{ij}\ t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(v)T_{ii}(u)+O\left(\frac{1}{u}\right). \tag{4.32}$$

Multiplying by $(t(^{1\cdots i}_{1\cdots i})(v))^{-1}$ both sides of the u^0 coefficient in (4.32), one gets

$$[e^{(0)}_{j,j+1},(t(^{1\cdots i}_{1\cdots i})(v))^{-1}]=-\delta_{ij}\ \ e_i\left(v+\frac{i-2}{2}\right)(t(^{1\cdots i}_{1\cdots i})(v))^{-1}. \tag{4.33}$$

Thus, thanks to the relations (3.26) and (4.33), one obtains for $X\in Y(\mathrm{sl}_n)$,

$$(t(^{1\cdots i}_{1\cdots i})(u))^{-1}\,\mathrm{Ad}^{+}_{e_{p,a_p}}(X)={}^{i}\mathcal{E}_{p,a_p}\left(u+\frac{i-2}{2}\right)((t(^{1\cdots i}_{1\cdots i})(u))^{-1}X). \tag{4.34}$$

This proves the Eq. (4.20). Equation (4.21) is proven along the same lines. Indeed, one remarks that

$$t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u-1)(t(^{1\cdots i}_{1\cdots i})(u-1))^{-1}=(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u), \tag{4.35}$$

by using the commutation relations deduced from the map (2.9). This explains the shift of the spectral parameter between (4.20) and (4.21). For the relations (4.22)–(4.27), the proof is analogous. ■

Now we can state the main theorem of the paper.

Theorem 4.5: *Let* $1\leqslant i\leqslant n-1$. *The comultiplication in the Drinfel'd basis is given by*

$$\Delta(e_i(u))=\sum_{m=0}^{+\infty}(-1)^m\left(\sum_{\substack{1\leqslant b_1<\cdots<b_i\leqslant n\\ b_i\neq i}}{}^{i}E_{b_1,\ldots,b_i}(u)(e_i(u))\otimes{}^{i}F_{b_1,\ldots,b_i}(u+1)(f_i(u+1))\right)^m$$
$$\times\left(1\otimes e_i(u)+\sum_{\substack{1\leqslant a_1<\cdots<a_i\leqslant n\\ a_i\neq i}}{}^{i}E_{a_1,\ldots,a_i}(u)(e_i(u))\ \otimes\ {}^{i}F_{a_1,\ldots,a_i}(u+1)(\tilde{g}_i(u))\right), \tag{4.36}$$

$$\Delta(f_i(u))=\left(f_i(u)\otimes 1+\sum_{\substack{1\leqslant a_1<\cdots<a_i\leqslant n\\ a_i\neq i}}E^{i}_{a_1,\ldots,a_i}(u+1)(g_i(u))\otimes F^{i}(a_1\cdots a_i)(u)(f_i(u))\right)$$
$$\times\sum_{m=0}^{+\infty}(-1)^m\left(\sum_{\substack{1\leqslant b_1<\cdots<b_i\leqslant n\\ b_i\neq i}}E^{i}_{b_1,\ldots,b_i}(u+1)(e_i(u+1))\otimes F^{i}_{b_1,\ldots,b_i}(u)(f_i(u))\right)^m, \tag{4.37}$$

$$\Delta(h_i(u))=\left(f_i(u)\otimes e_i(u+1)+\sum_{\substack{1\leqslant a_1<\cdots<a_i\leqslant n\\ a_i\neq i}}E^{i}_{a_1,\ldots,a_i}(u+1)(g_i(u))\otimes F^{i}_{a_1,\ldots,a_i}(u)(g_i(u))\right)$$
$$\times\sum_{m=0}^{+\infty}(-1)^m\left(\sum_{\substack{1\leqslant b_1<\cdots<b_i\leqslant n\\ b_i\neq i}}E^{i}_{b_1,\ldots,b_i}(u+1)(e_i(u+1))\otimes F^{i}_{b_1,\ldots,b_i}(u+1)(f_i(u))\right)^m$$
$$-\Delta(f_i(u))\Delta(e_i(u+1)). \tag{4.38}$$

Proof: The full proof is presented only for $e_i(u)$, the outline of proofs for $f_i(u)$ and $h_i(u)$ being similar. The comultiplication in the Drinfel'd realization is constructed thanks to the isomorphism given in the theorem 3.1,

$$\Delta\left(e_i\left(u+\frac{i-2}{2}\right)\right)=\Delta(t(^{1\cdots i}_{1\cdots i})(u))^{-1}\Delta(t(^{1\cdots i-1\ \ i}_{1\cdots i-1\ \ i+1})(u)) \tag{4.39}$$

$$=\left(\sum_{b_1<\cdots<b_i} t(^{1\cdots i}_{b_1\cdots b_i})(u)\otimes t(^{b_1\cdots b_i}_{1\cdots i})(u)\right)^{-1}\sum_{a_1<\cdots<a_i} t(^{1\cdots i}_{a_1\cdots a_i})(u)\otimes t(^{a_1\cdots a_{i-1}\ \ a_i}_{1\cdots i-1\ \ i+1})(u) \tag{4.40}$$

$$=\sum_{m\leqslant 0}(-1)^m\left(\sum_{\substack{b_1<\cdots<b_i\\ b_i\neq i}}(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i}_{b_1\cdots b_i})(u)\otimes(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{b_1\cdots b_i}_{1\cdots i})(u)\right)^m$$

$$\times\sum_{a_1<\cdots<a_i}(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{1\cdots i}_{a_1\cdots\ a_i})(u)\otimes(t(^{1\cdots i}_{1\cdots i})(u))^{-1}t(^{a_1\cdots a_{i-1}\ \ a_i}_{1\cdots i-1\ \ i+1})(u). \tag{4.41}$$

The lemma 4.4 allows us to evaluate all the terms of Eq. (4.41), which proves (4.36). ■

B. Antipode and counit

As for the comultiplication, generalized adjoint actions must be introduced to express the antipode.

Definition 4.6: Let $1\leqslant i,\ j\leqslant n,\ 1\leqslant\alpha\leqslant n$. *X denotes an element of* $Y(\mathrm{sl}_n)$. *The generalized adjoint actions are defined by*

$${}^{\alpha}\mathcal{H}_{i,j}(u)(X)=\begin{cases}1 & \text{if } i>j,\\ X & \text{if } i=j,\\ X+{}^{\alpha}\mathcal{E}_{i,j}(u)({}^{\alpha}\mathcal{F}_{j,i}(u+1)(X)) & \text{otherwise,}\end{cases} \tag{4.42}$$

$$\mathcal{H}^{\alpha}_{i,j}(u)(X)=\begin{cases}1 & \text{if } i>j,\\ X & \text{if } i=j,\\ X+\mathcal{E}^{\alpha}_{i,j}(u+1)(\mathcal{F}^{\alpha}_{j,i}(u)(X)) & \text{otherwise.}\end{cases} \tag{4.43}$$

Let $1\leqslant m\leqslant n-1$ *and* $1\leqslant k_1<k_2<\cdots<k_m\leqslant n$. *Then, one has*

$${}^{\alpha}H^{\beta}_{k_1,k_2,\ldots,k_m}(u)(X)=\left(\overrightarrow{\prod_{1\leqslant p\leqslant m-1}}{}^{\alpha}\mathcal{H}^{\beta}_{p,k_p}(u)\right)({}^{\alpha}\mathcal{H}^{\beta}_{m+1,k_m}(u)(X)). \tag{4.44}$$

Similary, $\hat{E}_m(u)(X)$ *is defined as*

$$\mathcal{E}^1_{2,n}(u+1)(\mathcal{F}^1_{n-1,1}(u)(X)) \quad \text{if} \quad m=1,$$

$$\mathcal{E}^m_{1,n-m+1}(u+1)\mathcal{F}^m_{n-m,1}(u)\left(\overrightarrow{\prod_{2\leqslant p\leqslant m-1}}\mathcal{H}^m_{p,n-m+p}(u)\right)\mathcal{E}^m_{m+1,n}(u+1)\mathcal{F}^m_{n,m}(u)(X) \quad \text{otherwise,} \tag{4.45}$$

and $\hat{F}_m(u)(X)$ *as*

$${}^1\mathcal{E}_{1,n-1}(u)({}^1\mathcal{F}_{n,2}(u+1)(X)) \quad \text{if} \quad m=1,$$

$${}^m\mathcal{E}_{1,n-m}(u+1)^m\mathcal{F}_{n-m+1,1}(u)\left(\overrightarrow{\prod_{2\leqslant p\leqslant m-1}}{}^m\mathcal{H}_{p,n-m+p}(u)\right)^m\mathcal{E}_{m,n}(u+1)^m\mathcal{F}_{n,m+1}(u)(X)$$

otherwise. (4.46)

To find the image under the antipode, the following lemma is needed.

Lemma 4.7: For $1\leqslant i\leqslant n-1$ *and* $1\leqslant j\leqslant i+1$, *one has*

$$t\binom{j\ \ i+2\cdots n}{i+2\cdots n}(u)\left(t\binom{1\cdots n-i}{1\cdots n-i}(u)\right)^{-1}=H^{n-i}_{j,i+2,\ldots,n}\left(u+\frac{n-i-2}{2}\right)\left(g_{n-i}\left(u+\frac{n-i-2}{2}\right)\right), \quad (4.47)$$

$$\left(t\binom{1\cdots n-i}{1\cdots n-i}(u)\right)^{-1}t\binom{j\ \ i+2\cdots n}{i+2\cdots n}(u)={}^{n-i}H_{j,i+2,\ldots,n}\left(u+\frac{n-i-2}{2}\right)\left(\tilde{g}_{n-i}\left(u+\frac{n-i-2}{2}\right)\right) \quad (4.48)$$

and

$$t\binom{i\ \ i+2\cdots n}{i+1\ \ i+2\cdots n}(u)\left(t\binom{1\cdots n-i}{1\cdots n-i}(u)\right)^{-1}=\hat{E}_{n-i}\left(u+\frac{n-i-2}{2}\right)\left(e_{n-i}\left(u+\frac{n-i}{2}\right)\right), \quad (4.49)$$

$$\left(t\binom{1\cdots n-i}{1\cdots n-i}(u)\right)^{-1}t\binom{i+1\ \ i+2\cdots n}{i\ \ i+2\cdots n}(u)=\hat{F}_{n-i}\left(u+\frac{n-i-2}{2}\right)\left(f_{n-i}\left(u+\frac{n-i}{2}\right)\right). \quad (4.50)$$

Proof: This lemma is proven along the same lines as the lemma 4.4. ■

Theorem 4.8: *The antipode and the counit in the Drinfel'd basis are given by, for* $1\leqslant i\leqslant n-1$,

$$S\left(e_i\left(u+\frac{n}{2}\right)\right)=-\hat{E}_{n-i}(u)(e_{n-i}(u+1))\left(H^{n-i}_{i+1,\ldots,n}(u)(g_{n-i}(u))\right)^{-1}, \quad (4.51)$$

$$S\left(f_i\left(u+\frac{n}{2}\right)\right)=-\left({}^{n-i}H_{i+1,i+2,\ldots,n}(u)(\tilde{g}_{n-i}(u))\right)^{-1}\hat{F}_{n-i}(u)(f_{n-i}(u+1)), \quad (4.52)$$

$$S\left(h_i\left(u+\frac{n}{2}\right)\right)=\left({}^{n-i}H_{i+1,i+2,\ldots,n}(u)(\tilde{g}_{n-i}(u))\right)^{-1}{}^{n-i}H_{i,i+2,\ldots,n}(u)(\tilde{g}_{n-i}(u)) - S(e_{n-i}(u+1))S(f_{n-i}(u)), \quad (4.53)$$

and

$$\epsilon(e_i(u))=0,\quad \epsilon(f_i(u))=0,\quad \epsilon(h_i(u))=1. \quad (4.54)$$

Proof: The proof is given for $S(e_{n-i}(u))$. $S(h_{n-i}(u))$ and $S(f_{n-i}(u))$ are proven analogously,

$$S\left(e_i\left(u+\frac{i-2}{2}\right)\right)=S\left(t\binom{1\cdots i-1\ \ i}{1\cdots i-1\ \ i+1}(u)\right)S\left(\left(t\binom{1\cdots i}{1\cdots i}(u)\right)\right)^{-1}=t^*\binom{1\cdots i-1\ \ i}{1\cdots i-1\ \ i+1}(u)\left(t^*\binom{1\cdots i}{1\cdots i}(u)\right)^{-1} \quad (4.55)$$

$$=-t\binom{i\ \ i+2\cdots n}{i+1\ \ i+2\cdots n}(u-n+i)\left(t\binom{1\cdots n-i}{1\cdots n-i}(u-n+i)\right)^{-1}\left(t\binom{i+1\cdots n}{i+1\cdots n}(u-n+i)\right. \times\left.\left(t\binom{1\cdots n-i}{1\cdots n-i}(u-n+i)\right)^{-1}\right)^{-1} \quad \text{[Eq. (2.10) and corollary 3.3]}. \quad (4.56)$$

The terms in the relation (4.56) can be expressed thanks to the lemma 4.7, which proves the relation for $S(e_{n-i}(u))$.

The proof for the counit is obvious. ■

Remark: This Hopf structure can be extended to the double Yangian $DY(\mathrm{sl}_n)$. The image of the generators $x(u)\in Y(sl_n)\subset DY(\mathrm{sl}_n)$ under the comultiplication, the antipode or the counit are unchanged. For the dual generator $x^*(u)$ of $x(u)$, its image is given by the same formula where all the generators are replaced by their dual.

C. Examples

We give two examples to show explicit computations using the theorems 4.5 and 4.8. The comultiplication of $Y(\mathrm{sl}_2)$ is given by

$$\Delta(e_1(u))=\sum_{m=0}^{+\infty}(-e_1(u)\otimes f_1(u+1))^m(1\otimes e_1(u)+e_1(u)\otimes(h_1(u)+f_1(u+1)e_1(u))) \tag{4.57}$$

$$=1\otimes e_1(u)+\sum_{m=0}^{+\infty}(-1)^m e_1(u)^{m+1}\otimes f_1(u+1)^m h_1(u), \tag{4.58}$$

$$\Delta(f_1(u))=(f_1(u)\otimes 1+(h_1(u)+f_1(u+1)e_1(u))\otimes f_1(u))\sum_{m=0}^{+\infty}(-e_1(u+1)\otimes f_1(u))^m \tag{4.59}$$

$$=f_1(u)\otimes 1+\sum_{m=0}^{+\infty}(-1)^m h_1(u)e_1(u+1)^m\otimes f_1(u)^{m+1}, \tag{4.60}$$

$$\Delta(h_1(u))=(f_1(u)\otimes e_1(u+1)+(h_1(u)+f_1(u)e_1(u+1))\otimes(h_1(u)+f_1(u)e_1(u+1)))\times\sum_{m=0}^{+\infty}(-e_1(u+1)\otimes f_1(u))^m-\Delta(f_1(u))\Delta(e_1(u+1)) \tag{4.61}$$

$$=\sum_{m=0}^{+\infty}(-1)^m(m+1)h(u)\quad e_1(u+1)^m\otimes f_1(u+1)^m h(u). \tag{4.62}$$

The explicit forms (4.58), (4.60), and (4.62) allows us to show that the comultiplication, introduced in this paper, is the opposite of the comultiplication used by Molev.[4] Remark that the proof of the relation (4.62) from (4.61) is not obvious. A simpler way consists in using the form (3.3) instead of the form (3.5) in the proof of the theorem 4.5. Despite its simpler form, the generalization to sl_n of the form given by Molev does not seem possible.

The antipode and the counit of $Y(\mathrm{sl}_2)$ are given by

$$S(e_1(u+1))=-e_1(u+1)(h_1(u)+f_1(u)e_1(u+1))^{-1}, \tag{4.63}$$

$$S(f_1(u+1))=-(h_1(u)+f_1(u+1)e_1(u))^{-1}f_1(u+1), \tag{4.64}$$

$$S(h_1(u+1))=(h_1(u)+f_1(u+1)e_1(u))^{-1}-S(e_1(u+1))S(f_1(u)), \tag{4.65}$$

and

$$\epsilon(e_1(u))=0,\quad \epsilon(f_1(u))=0,\quad \text{and}\quad \epsilon(h_1(u))=1. \tag{4.66}$$

For $Y(\mathrm{sl}_3)$, the comultiplication in the Drinfel'd basis is given by

$$\Delta(e_1(u))=\sum_{m=0}^{+\infty}(-1)^m(e_1(u)\otimes f_1(u+1)-[e_2^0,e_1(u)]\otimes[f_2^0,f_1(u+1)])^m\times(1\otimes e_1(u)+e_1(u)\otimes(h_1(u)+f_1(u+1)e_1(u))-[e_2^0,e_1(u)]\otimes[f_2^0,h_1(u)+f_1(u+1)e_1(u)]), \tag{4.67}$$

$$\Delta(f_1(u))=(f_1(u)\otimes 1+(h_1(u)+f_1(u)e_1(u+1))\otimes f_1(u)-[e_2^0,h_1(u)+f_1(u)e_1(u+1)]\otimes[f_2^0,f_1(u)])\sum_{m=0}^{+\infty}(-1)^m(e_1(u+1)\otimes f_1(u)-[e_2^{(0)},e_1(u+1)]\otimes[f_2^{(0)},f_1(u)])^m, \tag{4.68}$$

$$\Delta(h_1(u))=(f_1(u)\otimes e_1(u)+(h_1(u)+f_1(u)e_1(u+1))\otimes(h_1(u)+f_1(u)e_1(u+1))-[e_2^{(0)},h_1(u)+f_1(u)e_1(u+1)]\otimes[f_2^{(0)},h_1(u)+f_1(u)e_1(u+1)])\sum_{m=0}^{+\infty}(-1)^m(e_1(u+1)\otimes f_1(u)-[e_2^{(0)},e_1(u+1)]\otimes[f_2^{(0)},f_1(u)])^m-\Delta(f_1(u))\Delta(e_1(u+1)), \tag{4.69}$$

$\Delta(e_2(u))$ [respectively, $\Delta(f_2(u))$, $\Delta(h_2(u))$] is obtained by exchanging the subscripts 1 and 2 in Eq. (4.67) [respectively, (4.68), (4.69)]. Of course, the antipode and the counit for $Y(\mathrm{sl}_3)$ can be computed thanks to theorem 4.8, however we leave it to the reader.

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Lie symmetry analysis and some new exact solutions of the Wu–Zhang equation

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The Lie symmetry analysis and the basic similarity reductions are performed for the Wu–Zhang equation, a $2+1$ dimensional nonlinear dispersive wave equation. Some new exact solutions generated from the similarity transformation are provided. They demonstrate some new three-dimensional features of a single solitary wave and two interacting solitary waves. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629779]

I. INTRODUCTION

The $2+1$ dimensional nonlinear dispersive wave equation

$$u_t+uu_x+vu_y+w_x=0,$$

$$v_t+uv_x+vv_y+w_y=0, \tag{1}$$

$$w_t+(uw)_x+(vw)_y+\tfrac{1}{3}(u_{xxx}+u_{xyy}+v_{xxy}+v_{yyy})=0,$$

where (u,v) is the horizontal projection of the surface velocity of a water particle, w is the total water depth ($w-1$ being the wave elevation), is regarded as Wu–Zhang (WZ) equation by Ref. 1. The WZ equation is derived in Ref. 2 from the Euler equation with a perturbation scheme under the assumption that the amplitude of wave elevation is small and the wave is long compared with the water depth (scaled to be 1). The WZ equation can be used to model the three dimensional behavior of solitary waves on a uniform layer of water, such as oblique interaction, oblique reflection from a vertical wall and turning in a curved channel.

If the waves propagate in only one dimension, e.g., along y coordinate, then the WZ equation is reduced to the classical Boussinesq equation

$$v_t+vv_y+w_y=0,$$

$$w_t+(vw)_y+\tfrac{1}{3}v_{yyy}=0, \tag{2}$$

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which is known to be integrable and equivalent to Broer–Kaup (BK) system[3,4] and a member of Ablowitz–Kaup–Newell–Segur (AKNS) system[5] that has a tri-Hamiltonian structure. Its exact bidirectional N-soliton solution has been provided by Ref. 5.

Reference 1 provides the Painlevé analysis of the WZ equation. It obtains some exact solutions by using the standard Weiss–Tabor–Carnevale Painlevé truncation expansion. However, the Lie symmetry analysis of the WZ equation is not available yet.

Since the WZ equation is a physical extension of the classical Boussinesq equation, it allows bidirectional soliton solution in any direction in the (x,y) plane. It might have an exact solution that can be used to describe obliquely interacting solitons. This paper is one of a series study towards a good understanding of the WZ equation.

We perform the Lie symmetry analysis in Sec. II, present the $1+1$ similarity reductions in Sec. III and provide a few new exact solutions of the WZ equation in Sec. IV. Finally we summarize the paper in Sec. V.

II. LIE POINT SYMMETRIES

In this section we perform Lie symmetry analysis for the $2+1$-dimensional system (1). Let us consider a one-parameter Lie group of infinitesimal transformation[6]

$$\begin{aligned} x&\to x+\epsilon X(x,y,t,u,v,w),\\ y&\to y+\epsilon Y(x,y,t,u,v,w),\\ t&\to t+\epsilon T(x,y,t,u,v,w),\\ u&\to u+\epsilon U(x,y,t,u,v,w),\\ v&\to v+\epsilon V(x,y,t,u,v,w),\\ w&\to w+\epsilon W(x,y,t,u,v,w) \end{aligned} \tag{3}$$

with a small parameter $\epsilon \ll 1$. The vector field associated with the above group of transformations can be written as

$$\underline{u}=X\frac{\partial}{\partial x}+Y\frac{\partial}{\partial y}+T\frac{\partial}{\partial t}+U\frac{\partial}{\partial u}+V\frac{\partial}{\partial v}+W\frac{\partial}{\partial w}. \tag{4}$$

An invariance of system (1) under transformation (3) leads to the expressions for the functions X, Y, T, U, V,W of the form (throughout this paper we use symbolic package MAPLE to perform all calculation)

$$\begin{aligned} X&=c_8xt+c_7x+c_6y+c_4t+c_1,\\ Y&=c_8yt+c_7y-c_6x+c_5t+c_2,\\ T&=c_8t^2+2c_7t+c_3,\\ U&=-(c_8ut+c_7u-c_6v-c_8x-c_4),\\ V&=-(c_8vt+c_7v+c_6u-c_8y-c_5),\\ W&=-(2c_8wt+2c_7w), \end{aligned} \tag{5}$$

where c_i, $i=1,\ldots,8$ are arbitrary constants. The presence of these arbitrary constants leads to a finite-dimensional Lie algebra of symmetries. A general element of this algebra is written as

$$\underline{v}=\underline{v}_1c_1+\underline{v}_2c_2+\underline{v}_3c_3+\underline{v}_4c_4+\underline{v}_5c_5+\underline{v}_6c_6+\underline{v}_7c_7+\underline{v}_8c_8, \tag{6}$$

where

$$\underline{v}_1=\frac{\partial}{\partial x},$$

$$\underline{v}_2=\frac{\partial}{\partial y},$$

$$\underline{v}_3=\frac{\partial}{\partial t},$$

$$\underline{v}_4=\frac{\partial}{\partial u}+t\frac{\partial}{\partial x},$$

$$\underline{v}_5=t\frac{\partial}{\partial y}+\frac{\partial}{\partial v},$$

$$\underline{v}_6=y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}-u\frac{\partial}{\partial v}+v\frac{\partial}{\partial u},$$

$$\underline{v}_7=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+2t\frac{\partial}{\partial t}-u\frac{\partial}{\partial u}-v\frac{\partial}{\partial v}-2w\frac{\partial}{\partial w},$$

$$\underline{v}_8=xt\frac{\partial}{\partial x}+yt\frac{\partial}{\partial y}+t^2\frac{\partial}{\partial t}+(y-vt)\frac{\partial}{\partial v}+(x-ut)\frac{\partial}{\partial u}-2wt\frac{\partial}{\partial w}, \tag{7}$$

construct a basis of the vector space. The associated Lie algebra among these vector fields becomes

	$\underline{v}_1$	$\underline{v}_2$	$\underline{v}_3$	$\underline{v}_4$	$\underline{v}_5$	$\underline{v}_6$	$\underline{v}_7$	$\underline{v}_8$
$\underline{v}_1$	0	0	0	0	0	$-\underline{v}_2$	$\underline{v}_1$	$\underline{v}_4$
$\underline{v}_2$		0	0	0	0	$\underline{v}_1$	$\underline{v}_2$	$\underline{v}_5$
$\underline{v}_3$			0	$\underline{v}_1$	$\underline{v}_2$	0	$2\underline{v}_3$	$\underline{v}_7$
$\underline{v}_4$				0	0	$-\underline{v}_5$	$-\underline{v}_4$	0
$\underline{v}_5$					0	$\underline{v}_4$	$-\underline{v}_5$	0
$\underline{v}_6$						0	0	0
$\underline{v}_7$							0	$2\underline{v}_8$
$\underline{v}_8$								0

where the entry in jth row and kth column represents the commutator $[v_j,v_k]$, and $\{\underline{v}_1,\underline{v}_2,\underline{v}_3\}$, $\{\underline{v}_4,\underline{v}_5\}$, $\{\underline{v}_7,\underline{v}_8\}$, $\{\underline{v}_1,\underline{v}_2,\underline{v}_4,\underline{v}_5,\underline{v}_6\}$ are some of the subalgebras.

We now consider a point transformation

$$G:(x,y,t,u,v,w)\mapsto(\xi,\eta,\zeta,P,Q,R). \tag{8}$$

From the transformation (1), we have the corresponding one-parameter group of symmetries of the WZ equation

$$
\begin{aligned}
&G_1:(x,y,t,u,v,w)\mapsto(x+\epsilon,y,t,u,v,w),\\
&G_2:(x,y,t,u,v,w)\mapsto(x,y+\epsilon,t,u,v,w),\\
&G_3:(x,y,t,u,v,w)\mapsto(x,y,t+\epsilon,u,v,w),\\
&G_4:(x,y,t,u,v,w)\mapsto(x+t\epsilon,y,t,u+\epsilon,v,w),\\
&G_5:(x,y,t,u,v,w)\mapsto(x,y+t\epsilon,t,u,v+\epsilon,w),\\
&G_6:(x,y,t,u,v,w)\mapsto(x\cos\epsilon+y\sin\epsilon,-x\sin\epsilon+y\cos\epsilon,t,u\cos\epsilon+v\sin\epsilon,-u\sin\epsilon\\
&\qquad +v\cos\epsilon,w),\\
&G_7:(x,y,t,u,v,w)\mapsto(xe^{\epsilon},ye^{\epsilon},te^{2\epsilon},ue^{-\epsilon},ve^{-\epsilon},we^{-2\epsilon}),\\
&G_8:(x,y,t,u,v,w)\mapsto\left(\frac{x}{1-t\epsilon},\frac{y}{1-t\epsilon},\frac{t}{1-t\epsilon},u(1-t\epsilon)+x\epsilon,v(1-t\epsilon)+y\epsilon,w(1-t\epsilon)^2\right).
\end{aligned}
\tag{9}
$$

We observe that G_1 and G_2 are space translations, G_3 is a time translations, G_4 and G_5 are Galilean boost, G_6 is a rotation, G_7 is a scaling for all variables with different ratios. G_8 is a time-dependent scaling. The entire symmetry group is obtained by composing one-dimensional subgroups G_i, $i=1,\ldots,8$. When G is an element of this group, if $u(x,y,t)$, $v(x,y,t)$, $w(x,y,t)$ is a solution of WZ equation, then $P(\xi,\eta,\zeta)$, $Q(\xi,\eta,\zeta)$, $R(\xi,\eta,\zeta)$ is also a solution of WZ equation.

III. 1+1 SIMILARITY REDUCTIONS

After determining the infinitesimal generators, the similarity variables can be found by solving the characteristic equations[6]

$$
\frac{\mathrm{d}x}{X}=\frac{\mathrm{d}y}{Y}=\frac{\mathrm{d}t}{T}=\frac{\mathrm{d}u}{U}=\frac{\mathrm{d}v}{V}=\frac{\mathrm{d}w}{W}. \tag{10}
$$

It is easy to know that the generator $\underline{v}_1$ has an invariance

$$
\xi=y,\quad \eta=t,\quad P=u,\quad Q=v,\quad R=w.
$$

Under this transformation, WZ equation is reduced to a system of PDE with two independent variables ξ and η and three dependent variables P, Q, and R. The reduced equation is WZ equation but with u, v, and w independent of x, i.e., $u_x=v_x=w_x=0$. In fact the set of two equations on v and w is identical to the system (2) and the other one is a linear equation on u

$$
u_t+vu_y=0, \tag{11}
$$

which can be solved with a method of characteristic line. Therefore one can obtain a solution of WZ equation (1) from a solution of the classical Boussinesq equation (2).

For the generator $\underline{v}_2$, we have a similar result except now the solution is independent of y.

For the generator $\underline{v}_3$, WZ equation is reduced to its steady case.

For the generator of Galilean transformation $\underline{v}_4=(\partial/\partial u)+t(\partial/\partial x)$, we have the following similarity variables:

$$
\xi=y,\quad \eta=t,\quad P=ut-x,\quad Q=v,\quad R=w. \tag{12}
$$

The reduced PDE becomes

$$P_\eta + QP_\xi = 0,$$

$$Q_\eta + QQ_\xi + R_\xi = 0,$$

$$R_\eta + \frac{R}{\eta} + Q_\xi R + QR_\xi + \frac{1}{3}Q_{\xi\xi\xi} = 0. \tag{13}$$

One may notice that the second and third equations are very closely related to the classical Boussinesq equation (2) except the extra term R/η.

The generator $\underline{v}_5$ has a similar result as $\underline{v}_4$.

For the rotation transformation $\underline{v}_6$, the similarity variables are

$$\xi = x^2 + y^2, \quad \eta = t, \quad P = -xv + yu, \quad Q = yv + xu, \quad R = w. \tag{14}$$

Then WZ equation is reduced to

$$P_\eta + 2QP_\xi = 0,$$

$$\xi Q_\eta + 2\xi^2 R_\xi + 2\xi QQ_\xi - (P^2 + Q^2) = 0,$$

$$R_\eta + 2QR_\xi + 2RQ_\xi + \tfrac{8}{3}Q_{\xi\xi} + \tfrac{8}{3}\xi Q_{\xi\xi\xi} = 0. \tag{15}$$

Of course one may choose another set of invariants to be the similarity variables and obtain a different reduced system. For example, if we take

$$\xi = x^2 + y^2, \quad \eta = t, \quad P = \frac{-xv + yu}{x^2 + y^2}, \quad Q = \frac{yv + xu}{x^2 + y^2}, \quad R = w, \tag{16}$$

then the reduced system reads

$$P_\eta - 2QP_\xi\xi - 2QP = 0,$$

$$Q_\eta + Q^2 + 2QQ_\xi\xi - P^2 + 2R_\xi = 0, \tag{17}$$

$$2RQ + 2QR_\xi\xi + 2RQ_\xi\xi + R_\eta + \tfrac{16}{3}Q_\xi + \tfrac{8}{3}Q_{\xi\xi\xi}\xi^2 + \tfrac{32}{3}Q_{\xi\xi}\xi = 0,$$

which is equivalent to the system (15).

For the scaling transformation generated by $\underline{v}_7$, the similarity variables are

$$\xi = \frac{x}{\sqrt{t}}, \quad \eta = \frac{y}{\sqrt{t}}, \quad P = u\sqrt{t}, \quad Q = v\sqrt{t}, \quad R = wt. \tag{18}$$

The WZ equation is reduced to a system with two independent variables but in a more complicated form

$$(\xi - 2P)P_\xi + (\eta - 2Q)P_\eta + P - 2R_\xi = 0,$$

$$(\xi - 2P)Q_\xi + (\eta - 2Q)Q_\eta + Q - 2R_\eta = 0, \tag{19}$$

$$6R(Q_\eta + P_\xi - 1) - 3(\eta - 2Q)R_\eta - 3(\xi - 2P)R_\xi + 2(P_{\xi\xi\xi} + P_{\eta\eta\xi} + Q_{\eta\eta\eta} + Q_{\eta\xi\xi}) = 0.$$

The similarity variables corresponding to $\underline{v}_8$ are

$$\xi=\frac{x}{t},\quad \eta=\frac{y}{t},\quad P=ut-\xi t,\quad Q=vt-\eta t,\quad R=wt^2. \tag{20}$$

The WZ equation is also reduced to its steady case.

We would like to point out that in this section we have only reported the $1+1$ similarity reduction generated by the single but different basic infinitesimal generators v_j. More $1+1$ reduced systems can be obtained by considering a proper linear combination of different basic generators. We may also implement the symmetry analysis and similarity reduction upon a $1+1$ reduced system and obtain a corresponding ODE system.

IV. SOME NEW EXACT SOLUTIONS

In this section, we present some new exact particular solutions of WZ system (1) obtained from the three kinds of reduction transformation studied in the last section.

A. Solutions from v_3 reduction

The system generated by v_3 is the steady WZ system. Here we are looking for a particular steady solution with a similarity variable $z=k_1x+k_2y$, where the two constants k_1 and k_2 are assumed to satisfy $k_1^2+k_2^2=1$ without a loss of generality. The velocity field (u,v) and the total wave depth w are assumed to be functions of z only. The WZ equation becomes a system of ODE

$$k_1uu'+k_2vu'+k_1w'=0, \tag{21}$$

$$k_1uv'+k_2vv'+k_2w'=0, \tag{22}$$

$$(k_1u+k_2v)w'+(k_1u'+k_2v')w+\tfrac{1}{3}(k_1u'''+k_2v''')=0. \tag{23}$$

Integrating the first two equations gives

$$v=\frac{k_2}{k_1}u+d_1,\quad w=-\frac{1}{2k_1^2}u^2-\frac{k_2}{k_1}d_1u+d_2+k_2^2d_1^2.$$

Substituting into Eq. (23) and integrating it twice yields a single equation for u,

$$u'^2=\frac{3}{4k_1^2}u^4+3\frac{k_2}{k_1}d_1u^3-3d_2u^2+d_3u+d_4,$$

where the four integration constants d_i, $i=1,2,3,4$ are determined by the boundary condition at infinity. For a set of d_i's with four real parameters, $\lambda_1>\lambda_2>\lambda_3>\lambda_4$,

$$d_1=-\frac{1}{4k_2}\sum_{i=1}^{4}\lambda_i,\quad d_2=-\frac{1}{4}\sum_{i,j=1,i<j}^{4}\lambda_i\lambda_j,\quad d_3=-\frac{3}{4}k_1\sum_{j=1}^{4}\frac{1}{\lambda_j}\lambda_1\lambda_2\lambda_3\lambda_4,$$

$$d_4=\tfrac{3}{4}k_1^2\lambda_1\lambda_2\lambda_3\lambda_4.$$

the ODE is written as

$$u'^2=\frac{3}{4k_1^2}(u-k_1\lambda_1)(u-k_1\lambda_2)(u-k_1\lambda_3)(u-k_1\lambda_4),$$

and the solution can be written in terms of a Jacobi elliptic function

$$u=k_1\left(\lambda_4+\frac{\Delta_{24}\Delta_{34}}{\Delta_{24}-\Delta_{23}\,\mathrm{sn}^2(s,m)}\right),\quad \text{or}\quad u=k_1\left(\lambda_2+\frac{\Delta_{24}\Delta_{12}}{\Delta_{24}-\Delta_{14}\,\mathrm{sn}^2(s,m)}\right),$$

$$v=\frac{k_2}{k_1}u-\frac{1}{4k_2}\sum_{i=1}^{4}\lambda_i, \tag{24}$$

$$w=-\frac{1}{2k_1^2}u^2+\frac{1}{4k_1}\sum_{i=1}^{4}\lambda_i u-\frac{1}{4}\sum_{i,j=1,i<j}^{4}\lambda_i\lambda_j+\frac{1}{16}\left(\sum_{i=1}^{4}\lambda_i\right)^2,$$

where

$$s=\frac{1}{4}\sqrt{3\Delta_{13}\Delta_{24}}(z-z_0),\quad m=\sqrt{\frac{\Delta_{14}\Delta_{23}}{\Delta_{13}\Delta_{24}}},\quad \Delta_{ij}=\lambda_i-\lambda_j.$$

For a particular set of integration constants with one parameter λ,

$$d_1=0,\quad d_2=1+\tfrac{1}{2}\lambda^2,\quad d_3=6k_1\lambda,\quad d_4=\tfrac{3}{4}k_1^2\lambda^4-3k_1^2\lambda^2, \tag{25}$$

the solution given by

$$u=k_1\left(\lambda-\frac{2(\lambda^2-1)}{\lambda+\cosh\sqrt{3(\lambda^2-1)}(z-z_0)}\right),\quad v=\frac{k_2}{k_1}u, \tag{26}$$

$$w=1+\frac{2(\lambda^2-1)(1+\lambda\cosh\sqrt{3(\lambda^2-1)}(z-z_0))}{(\lambda+\cosh\sqrt{3(\lambda^2-1)}(z-z_0))^2}, \tag{27}$$

describes a steady solitary wave on a uniform layer of water. For the same set of constants as (25), we have another solution

$$u=k_1\left(\lambda+\frac{2(1-\lambda^2)}{\lambda\pm\sin\sqrt{3(1-\lambda^2)}(z-z_0)}\right),\quad v=\frac{k_2}{k_1}u,$$

$$w=1-\frac{2(1-\lambda^2)(1\pm\lambda\sin\sqrt{3(1-\lambda^2)}(z-z_0))}{(\lambda\pm\sin\sqrt{3(1-\lambda^2)}(z-z_0))^2}, \tag{28}$$

which has a singularity in a finite domain.

With some other choices of the constants, we have more steady solutions listed below.

Case 1:

$$d_1=-\frac{1}{2k_2}(\lambda+\mu),\quad d_2=-\frac{1}{4}(\lambda^2+4\lambda\mu+\mu^2),$$

$$d_3=-\tfrac{3}{2}k_1\lambda\mu(\lambda+\mu),\quad d_4=\tfrac{3}{4}k_1^2\lambda^2\mu^2,$$

$$u=k_1\frac{\lambda-\mu\exp\left(\pm\frac{\sqrt{3}}{2}(\lambda-\mu)(z-z_0)\right)}{1-\exp\left(\pm\frac{\sqrt{3}}{2}(\lambda-\mu)(z-z_0)\right)},\quad v=\frac{k_2}{k_1}u-\frac{1}{2k_2}(\lambda+\mu), \tag{29}$$

$$w=-\frac{1}{8}(\lambda-\mu)^2\,\mathrm{csch}^2\frac{\sqrt{3}}{4}(\lambda-\mu)(z-z_0),$$

or

$$u=k_1\frac{\mu+\lambda\exp\left(\pm\frac{\sqrt{3}}{2}(\lambda-\mu)(z-z_0)\right)}{1+\exp\left(\pm\frac{\sqrt{3}}{2}(\lambda-\mu)(z-z_0)\right)},\quad v=\frac{k_2}{k_1}u-\frac{1}{2k_2}(\lambda+\mu),$$

$$w=\frac{1}{8}(\lambda-\mu)^2\,\mathrm{sech}^2\frac{\sqrt{3}}{4}(\lambda-\mu)(z-z_0). \tag{30}$$

Case 2:

$$d_1=-\frac{1}{k_2}(\lambda\mp1),\quad d_2=-\frac{3}{2}\lambda(\lambda\mp2),$$

$$d_3=-3k_1\lambda^2(\lambda\mp3),\quad d_4=\tfrac{3}{4}k_1^2\lambda^3(\lambda\mp4),$$

$$u=k_1\left(\lambda\pm\frac{4}{3(z-z_0)^2-1}\right),\quad v=\frac{k_2}{k_1}u-\frac{1}{k_2}(\lambda\mp1), \tag{31}$$

$$w=1-\frac{4(3(z-z_0)^2+1)}{(3(z-z_0)^2-1)^2}.$$

Case 3:

$$d_1=-\frac{\lambda}{k_2},\quad d_2=-\frac{3}{2}\lambda^2,\quad d_3=-3k_1\lambda^3,\quad d_4=\frac{3}{4}k_1^2\lambda^4,$$

$$u=k_1\left(\lambda\mp\frac{2}{\sqrt{3}(z-z_0)}\right),\quad v=\frac{k_2}{k_1}u-\frac{\lambda}{k_2},\quad w=\frac{-2}{3(z-z_0)^2}. \tag{32}$$

Case 4:

$$d_1=0,\quad d_2=\tfrac{1}{4}(\lambda^2-\mu^2),\quad d_3=0,\quad d_4=-\tfrac{3}{2}k_1^2\lambda^2\mu^2,$$

$$u=\frac{k_1\lambda}{\sqrt{1-\mathrm{sn}^2(s,m)}},\quad v=\frac{k_2}{k_1}u,\quad w=\frac{1}{4}(\lambda^2-\mu^2)-\frac{\lambda^2}{2(1-\mathrm{sn}^2(s,m))}, \tag{33}$$

$$s=\tfrac{1}{2}\sqrt{3(\lambda^2+\mu^2)}(z-z_0),\quad m^2=\frac{\mu^2}{\lambda^2+\mu^2}.$$

Case 5:

$$d_1=-\frac{1}{k_2}\mu,\quad d_2=-\frac{1}{4}(6\mu^2+\lambda^2),$$

$$d_3=-\tfrac{3}{2}k_1\mu(2\mu^2+\lambda^2),\quad d_4=\tfrac{3}{4}k_1^2\mu^2(\mu^2+\lambda^2),$$

$$u=k_1\left(\mu\mp\frac{\lambda}{\sinh\frac{\sqrt{3}}{2}\lambda(z-z_0)}\right),\quad v=\frac{k_2}{k_1}u-\frac{\mu}{k_2},\tag{34}$$

$$w=-\frac{\lambda^2}{4}\left(1+\frac{2}{\sinh^2\frac{\sqrt{3}}{2}\lambda(z-z_0)}\right).$$

Case 6:

$$d_1=0,\quad d_2=-\tfrac{1}{4}(\lambda^2+\mu^2),\quad d_3=0,\quad d_4=\tfrac{3}{4}k_1^2\lambda^2\mu^2,$$

$$u=k_1\lambda\frac{\mathrm{sn}(s,m)}{\mathrm{cn}(s,m)},\quad v=\frac{k_2}{k_1}u,\quad w=\frac{1}{4}(\lambda^2-\mu^2)-\frac{\lambda^2}{2\,\mathrm{cn}^2(s,m)},\tag{35}$$

$$s=\frac{\sqrt{3}}{2}\mu(z-z_0),\quad m^2=1-\frac{\lambda^2}{\mu^2}\quad(\lambda^2<\mu^2).$$

Case 7:

$$d_1=\frac{\lambda}{2k_2},\quad d_2=-\tfrac{1}{8}(3\lambda^2+b^2),\quad d_3=\tfrac{3}{8}k_1\lambda(\lambda^2+b^2),\quad d_4=\tfrac{3}{64}k_1^2(\lambda^2+b^2)^2,$$

$$u=-\frac{k_1}{2}\left(\lambda\mp b\tan\frac{\sqrt{3}}{4}b(z-z_0)\right),\quad v=\frac{k_2}{k_1}u+\frac{\lambda}{2k_2},\tag{36}$$

$$w=-\frac{1}{8}b^2\left(1+\tan^2\frac{\sqrt{3}}{4}b(z-z_0)\right).$$

These solutions are of mathematical interests, even though some of them are not physically meaningful for the water wave because the total water depth w either goes to zero at infinity or has a singularity in a finite domain.

B. Solutions from v_4 reduction

The last two equations in the reduced system (13) from the generator v_4 are closely related to the classical Boussinesq equation except the extra term R/η. Their relation is very similar to that of KdV and cKdV equations. In fact, with the following transformation

$$\bar{\xi}=\frac{\xi+d_1}{d_1\eta}+d_2,\quad \bar{\eta}=-\frac{1}{d_1^2\eta}+d_3,$$

$$\bar{P}=d_4P+d_5,\quad \bar{Q}=\left(Q-\frac{\xi+d_1}{\eta}\right)d_1\eta,\quad \bar{R}=Rd_1^2\eta^2\tag{37}$$

the system (13) is converted to

$$\overline{P}_{\overline{\eta}}+\overline{\overline{Q}\overline{P}_{\overline{\xi}}}=0,$$

$$\overline{Q}_{\overline{\eta}}+\overline{\overline{Q}\overline{Q}_{\overline{\xi}}}+\overline{R}_{\overline{\xi}}=0, \tag{38}$$

$$\overline{R}_{\overline{\eta}}+\overline{Q}_{\overline{\xi}}\overline{R}+\overline{\overline{Q}\overline{R}_{\overline{\xi}}}+\tfrac{1}{3}\overline{Q}_{\overline{\xi\xi\xi}}=0,$$

where the last two equations are the classical Boussinesq equation. We can make use of the property to construct new solutions of WZ equation. For example, starting with a single soliton solution of the classical Boussinesq equation

$$\overline{Q}=\frac{2\,(\lambda^2-1)}{\lambda+\cosh(\sqrt{3\,\lambda^2-3}\,(\overline{\xi}-\lambda\,\overline{\eta}))}, \tag{39}$$

$$\overline{R}=\frac{2\,(\lambda^2-1)[1+\lambda\,\cosh(\sqrt{3\,\lambda^2-3}(\overline{\xi}-\lambda\,\overline{\eta}))]}{[\lambda+\cosh(\sqrt{3\,\lambda^2-3}(\overline{\xi}-\lambda\,\overline{\eta}))]^2}+1, \tag{40}$$

we are able to obtain a particular solution of WZ equation

$$u=\frac{1}{d_4 t}(d_4 x+\overline{P}-d_5), \tag{41}$$

$$v=\frac{2(\lambda^2-1)}{d_1 t[\lambda+\cosh(\sqrt{3\,\lambda^2-3}\;\;s)]}+\frac{y+d_1}{t}, \tag{42}$$

$$w=\frac{2(\lambda^2-1)[1+\lambda\,\cosh(\sqrt{3\,\lambda^2-3}\;\;s)]}{d_1^2 t^2[\lambda+\cosh(\sqrt{3\,\lambda^2-3}\;\;s)]^2}+\frac{1}{d_1^2 t^2}, \tag{43}$$

where the phase function s is given by

$$s=\overline{\xi}-\lambda\,\overline{\eta}=\frac{1}{d_1 t}\left[y-d_1(\lambda d_3-d_2)t+d_1+\frac{\lambda}{d_1}\right]$$

and $\overline{P}$ is a solution of linear equation

$$\overline{P}_{\overline{\eta}}+\overline{\overline{Q}\overline{P}_{\overline{\xi}}}=0$$

with $\overline{Q}$ given by (39) and d_j, $j=1,\ldots,5$ are arbitrary constants but $d_1 d_4\neq 0$. The solution describes a single solitary wave that is uniform along x direction and travels along y direction. The wave travels with a speed $d_1(\lambda d_3-d_2)$. Since d_2 and d_3 are two free parameters, the solitary wave can be made still by choosing $d_2=\lambda d_3$. It is double-peaked when $\lambda>2$ just like the solution of the classical Boussinesq equation. Its amplitude of the total water depth for the case of $\lambda<2$ is $(2\lambda-1)/(d_1 t)^2$, which is singular at time $t=0$ and decreases as time goes on from 0 to $+\infty$, and its wavelength increases like $d_1 t$. For $t>0$, the mass loss under the solitary wave is due to the sinks at infinity. One may notice that the velocity $u\to\pm\infty$ as $x\to\pm\infty$ and $v\to\pm\infty$ as $y\to\pm\infty$. The solitary wave solution of the WZ equation has a three-dimensional feature that has not been presented before for other $2+1$ dimensional nonlinear dispersive wave equations.

We now start with the solution of two-soliton head-on collision of the classical Boussinesq equation[5]

$$\overline{Q}=\frac{2(\lambda_1+\lambda_2)(\lambda_2^2-\lambda_1^2-k_2^2\tanh^2\xi_2+k_1^2\tanh^2\xi_1)}{(k_2\tanh\xi_2-k_1\tanh\xi_1)^2-(\lambda_1+\lambda_2)^2}, \tag{44}$$

$$\overline{R}=\frac{1}{\sqrt{3}}\overline{Q}_{\overline{\xi}}+\frac{k_2\tanh\xi_2-k_1\tanh\xi_1-\lambda_1-\lambda_2}{k_2\tanh\xi_2-k_1\tanh\xi_1+\lambda_1+\lambda_2}\times\left[1+2\frac{(\lambda_1+\lambda_2)(k_1\tanh\xi_1-\lambda_1)(k_2\tanh\xi_2+\lambda_2)}{k_2\tanh\xi_2-k_1\tanh\xi_1+\lambda_1+\lambda_2}\right], \tag{45}$$

$$\xi_1=\frac{\sqrt{3}}{2}k_1(\overline{\xi}-\lambda_1\overline{\eta}),\quad \xi_2=\frac{\sqrt{3}}{2}k_2(\overline{\xi}+\lambda_2\overline{\eta}),\quad k_i=\sqrt{\lambda_i^2-1},\quad \lambda_i>1,\quad i=1,2,$$

and construct a new solution of the WZ equation

$$u=\frac{1}{d_4t}(d_4x+\overline{P}-d_5),\quad v=\frac{\overline{Q}}{d_1t}+\frac{y+d_1}{t},\quad w=\frac{\overline{R}}{d_1^2t^2}, \tag{46}$$

where $\overline{P}$ solves $\overline{P}_{\overline{\eta}}+\overline{QP}_{\overline{\xi}}=0$, $\overline{Q}$ and $\overline{R}$ are given by (44) and (45) with

$$\overline{\xi}=\frac{y+d_1}{d_1t}+d_2,\quad \overline{\eta}=-\frac{1}{d_1^2t}+d_3.$$

The two phase functions are

$$s_1=\overline{\xi}-\lambda_1\overline{\eta}=\frac{1}{d_1t}\left[y-d_1(\lambda_1d_3-d_2)t+d_1+\frac{\lambda_1}{d_1}\right],$$

$$s_2=\overline{\xi}+\lambda_2\overline{\eta}=\frac{1}{d_1t}\left[y-d_1(-\lambda_2d_3-d_2)t+d_1-\frac{\lambda_2}{d_1}\right].$$

The two wave speeds are

$$c_1=d_1(\lambda_1d_3-d_2),\quad c_2=d_1(-\lambda_2d_3-d_2).$$

If we pick $d_2=-\lambda_2d_3$, then $c_1=d_1d_3(\lambda_1+\lambda_2)$ and $c_2=0$, solitary wave 2 will stand still and solitary wave 1 will pass through solitary wave 2. Like the single solitary wave solution, the amplitude of the total water depth of both solitary waves decreases like $1/(d_1t)^2$, the wave length increases like d_1t for $t>0$. The mass loss under the two solitary waves is due to the sinks at infinity of both x and y directions.

Figure 1 shows the total water depth $w(y,t)$ from (46) for the interaction of two single-peak solitary waves. The parameters are chosen to ensure that the solitary wave 2 with higher amplitude stands still near the origin and solitary wave 1 with lower amplitude passes through the solitary wave 2 as time goes on. After the elastic collision, each one experiences a backward phase shift. The phase shift of solitary wave 2 is visible in Fig. 1 by comparing the lowerest dashed and solid lines. Figure 2 shows the same solution with λ_1 and λ_2 larger than 2, so that the two solitary waves are double peaked. The phase shift of solitary wave 2 is more visible because the two solitary waves have larger amplitude.

Similarly we can obtain a new exact solution of the WZ equation by using the multisoliton solution of the classical Boussinesq equation.[5]

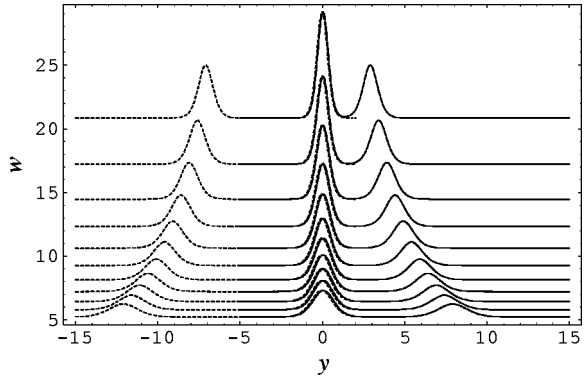

FIG. 1. The interaction of two single-peak solitary waves, $\lambda_1=1.1$, $\lambda_2=1.2$, $d_1=\sqrt{\lambda_2}$, $d_3=10$, $d_2=-\lambda_2 d_3$. The dashed lines are for the total water depth w as a function of space y for the time instances of $t=-0.4$, -0.38, -0.36, -0.34, -0.32, -0.3, -0.28, -0.26, -0.24, -0.22, and -0.2 bottom up. The solid lines are for the time instances of $t=0.2$, 0.22, 0.24, 0.26, 0.28, 0.3, 0.32, 0.34, 0.36, 0.38, 0.4 top down.

C. Solution from v_8 reduction

The system generated by v_8 is also the steady WZ system. With the steady solution (26) and (27) and the similarity variables (20), we obtain a new solution of the WZ equation

$$u=\frac{x}{t}+\frac{k_1}{t}\left(\lambda-\frac{2(\lambda^2-1)}{\lambda+\cosh\sqrt{3(\lambda^2-1)}\ \dfrac{k_1x+k_2y-z_0t}{t}}\right),\quad k_1^2+k_2^2=1,$$

$$v=\frac{y}{t}+\frac{k_2}{t}\left(\lambda-\frac{2(\lambda^2-1)}{\lambda+\cosh\sqrt{3(\lambda^2-1)}\ \dfrac{k_1x+k_2y-z_0t}{t}}\right),$$

$$w=\frac{1}{t^2}+\frac{2(\lambda^2-1)\left(1+\lambda\cosh\sqrt{3(\lambda^2-1)}\ \dfrac{k_1x+k_2y-z_0t}{t}\right)}{t^2\left(\lambda+\cosh\sqrt{3(\lambda^2-1)}\ \dfrac{k_1x+k_2y-z_0t}{t}\right)^2}.$$

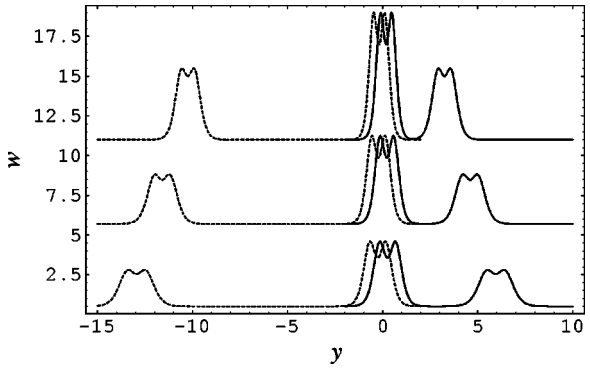

FIG. 2. The interaction of two double-peak solitary waves, $\lambda_1=3$, $\lambda_2=4$, $d_1=\sqrt{\lambda_2}$, $d_3=1$, $d_2=-\lambda_2 d_3$. The dashed lines are for the total water depth w as a function of space y for the time instances of $t=-0.7$, -0.6, and -0.5 bottom up. The solid lines are for the time instances of $t=0.5$, 0.6, and 0.7 top down.

The solution describes a solitary wave with an amplitude of the total water depth decreasing like $1/t^2$ and wavelength increasing like t. The wave speed of the solitary wave is z_0, which can be an arbitrary number.

V. SUMMARY

We have performed Lie symmetry analysis for the Wu–Zhang (WZ) equation and found its algebraic structure. The WZ equation is shown to have a finite dimension of Lie algebra, which means that the equation is less integrable than other integrable $2+1$ dimensional system, such as Kadomtsev–Petviashvili (KP) equation, Davey–Stewartson (DS) equation, Nizhnik–Novikov–Veselov (NNV) equation and $2+1$ dimensional sine-Gorden (sG) system,[7–14] which have infinite dimension of Lie algebra. The result agrees with that from Painlevé analysis.[1]

We have also obtained some new exact solutions of WZ equation by using the similarity transformation approach. They are of mathematical interest even though most of them are not physically meaningful. The solution demonstrate that a solitary wave could travel with arbitrary speed, its amplitude decreases and wave-length increases with time, and solitary waves with any kind of amplitudes could take over each other. These new features are due to the velocity sinks at infinity in both x and y directions. The three-dimensional feature of solitary waves seems to be a new phenomenon to us.

Since the WZ equation has a rotation symmetry, it admits a solitary wave solution along any direction in (x,y) plane. Two such solitary waves on two different directions could have an oblique interaction. The WZ equation can be used to model the process, but the question remains open whether the obliquely interacting solitary wave solution can be written in a closed-form. This is left for further research.

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Theta functions on noncommutative T^4

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We construct the so-called theta vectors on noncommutative T^4, which correspond to the theta functions on commutative tori with complex structures. Following the method of Dieng and Schwarz, we first construct holomorphic connections and then find the functions satisfying the holomorphic conditions, the theta vectors. The holomorphic structure in the noncommutative T^4 case is given by a 2×2 complex matrix, and the consistency requires its off-diagonal elements to be the same. We also construct the tensor product of these functions satisfying the consistency requirement. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629778]

I. INTRODUCTION

Classical theta functions have played an important role in the string loop calculation.[1,2] Recently, noncommutative geometry[3] became an important ingredient of string/M theory (for instance, see Ref. 4) starting with the work of Ref. 5.

Along this direction, the noncommutative torus[6,7] and its varieties,[8–11] and physics on noncommutative $\mathbb{R}^4$ (Refs. 12–14) have been studied intensively. However, noncommutative tori with complex structures have been rarely studied.[15–17] Noncommutative geometry with complex structures has been also studied recently with the algebraic geometry approach for Calabi–Yau three folds,[18–20] and for K3 surfaces.[21]

Classical theta functions can be regarded as state functions over commutative tori with complex structures. The noncommutative generalization of this has been initiated in mathematics in the quantized theta function approach by Manin,[15] and with the so-called theta vectors by Schwarz.[16] In the physics literature, this has appeared in the context of noncommutative solitons[22–24] but mostly in the so-called integral torus case. Recently, Dieng and Schwarz[17] have computed the theta vectors and their tensor products on noncommutative T^2 explicitly without any restriction.

In this paper, we follow the method of Dieng and Schwarz and calculate the theta vectors and their tensor products in the case of noncommutative T^4. In Sec. II, we construct modules on the noncommutative four torus. In Sec. III, we deal with connections with complex structures. In Sec. IV, we deal with tensor product of these modules. In Sec. V, we conclude with a discussion.

II. MODULES ON NONCOMMUTATIVE T^4

In this section, we construct the modules on noncommutative T^4 following the method of Rieffel.[7]

Recall that T^d_θ is the deformed algebra of the algebra of smooth functions on the torus T^d with the deformation parameter θ, which is a real $d\times d$ anti-symmetric matrix. This algebra is generated by operators $U_1,\ldots,U_d$ obeying the following relations:

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$$U_iU_j=e^{2\pi i\theta_{ij}}U_jU_i \quad \text{and} \quad U_i^*U_i=U_iU_i^*=1, \quad i,j=1,\ldots,d.$$

The above relations define the presentation of the involutive algebra,

$$\mathcal{A}_\theta^d=\left\{\sum a_{i_1\cdots i_d}U_1^{i_1}\cdots U_d^{i_d}\middle| a=(a_{i_1\cdots i_d})\in\mathcal{S}(\mathbb{Z}^d)\right\},$$

where $\mathcal{S}(\mathbb{Z}^d)$ is the Schwartz space of sequences with rapid decay.

Every projective module over a smooth algebra $\mathcal{A}_\theta^d$ can be represented by a direct sum of modules of the form $\mathcal{S}(\mathbb{R}^p\times\mathbb{Z}^q\times F)$, the linear space of Schwartz functions on $\mathbb{R}^p\times\mathbb{Z}^q\times F$, where $2p+q=d$ and F is a finite Abelian group. The module action is specified by operators on $\mathcal{S}(\mathbb{R}^p\times\mathbb{Z}^q\times F)$ and the commutation relation of these operators should be matched with that of elements in $\mathcal{A}_\theta^d$.

Recall that there is the dual action of the torus group T^d on $\mathcal{A}_\theta^d$ which gives a Lie group homomorphism of T^d into the group of automorphisms of $\mathcal{A}_\theta^d$. Its infinitesimal form generates a homomorphism of Lie algebra L of T^d into Lie algebra of derivations of $\mathcal{A}_\theta^d$. Note that the Lie algebra L is Abelian and is isomorphic to $\mathbb{R}^d$. Let $\delta: L\to\mathrm{Der}(\mathcal{A}_\theta^d)$ be the homomorphism. For each $X\in L$, $\delta(X):=\delta_X$ is a derivation i.e., for $u,v\in\mathcal{A}_\theta^d$,

$$\delta_X(uv)=\delta_X(u)v+u\delta_X(v). \tag{1}$$

Derivations corresponding to the generators $\{e_1,\ldots,e_d\}$ of L will be denoted by $\delta_1,\ldots,\delta_d$. For the generators U_i's of T_θ^d, it has the following property:

$$\delta_i(U_j)=2\pi i\delta_{ij}U_j. \tag{2}$$

If E is a projective $\mathcal{A}_\theta^d$-module, a connection ∇ on E is a linear map from E to $E\otimes L^*$ such that for all $X\in L$,

$$\nabla_X(\xi u)=(\nabla_X\xi)u+\xi\delta_X(u), \quad \xi\in E, \ u\in\mathcal{A}_\theta^d. \tag{3}$$

It is easy to see that

$$[\nabla_i,U_j]=2\pi i\delta_{ij}U_j. \tag{4}$$

We now consider the endomorphisms algebra of a module over $\mathcal{A}_\theta^d$. Let Λ be a lattice in $G=M\times\hat{M}$, where $M=\mathbb{R}^p\times\mathbb{Z}^q\times F$ and $\hat{M}$ is its dual. Let Φ be an embedding map such that Λ is the image of $\mathbb{Z}^d$ under the map Φ. This determines a projective module which will be denoted by E_Λ.[7] The dual lattice of Λ can be defined as

$$\Lambda^\perp:=\{(n,\hat{t})\in M\times\hat{M}\,|\,\theta((m,\hat{s}),(n,\hat{t}))=\langle m,\hat{t}\rangle-\langle n,\hat{s}\rangle\in\mathbb{Z}, \quad \text{for all } (m,\hat{s})\in\Lambda\}, \tag{5}$$

since in the Heisenberg representation the operators are defined by

$$\mathcal{U}_{(m,\hat{s})}f(r)=e^{2\pi i\langle r,\hat{s}\rangle}f(r+m), \tag{6}$$

for $f\in E_\Lambda$, $r\in M$. Namely, the operators defined in the dual lattice, $\mathcal{U}_{(n,\hat{t})}$ for $(n,\hat{t})\in\Lambda^\perp$, commute with all the operators defined in the original lattice, $\mathcal{U}_{(m,\hat{s})}$ for $(m,\hat{s})\in\Lambda$.

It is known that the algebra of endomorphisms on E_Λ, denoted by $\mathrm{End}_{\mathcal{A}_\theta}(E_\Lambda)$, is a C^*-algebra obtained by C^*-completion of the space spanned by operators $\mathcal{U}_{(n,\hat{t})}$, $(n,\hat{t})\in\Lambda^\perp$. The algebra $\mathrm{End}_{\mathcal{A}_\theta}(E_\Lambda)$ can be identified with a noncommutative torus $\mathcal{A}_{\tilde{\theta}}$, i.e., $\mathcal{A}_{\tilde{\theta}}$ is Morita equivalent to $\mathcal{A}_\theta$.[7] Recall that a C^*-algebra A is said to be Morita equivalent to A' if $A'\cong\mathrm{End}_A(E)$ for some finite projective module E. In general, a noncommutative torus $\mathcal{A}_{\tilde{\theta}}$ is Morita equivalent to $\mathcal{A}_\theta$ if θ and $\tilde{\theta}$ are related by $\tilde{\theta}=(A\theta+B)(C\theta+D)^{-1}$, where $\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)\in\mathrm{SO}(d,d|\mathbb{Z})$.[25]

In this paper, we consider a projective module of the form $\mathcal{S}(\mathbb{R}^p\times\mathbb{Z}^q)\otimes\mathcal{S}(F)$ with $p=2$, $q=0$.

For the real part, we choose our embedding map as

$$\Phi_{\text{inf}}=\begin{pmatrix} \theta_1+\dfrac{n_1}{m_1} & 0 & 0 & 0 \\ 0 & 0 & \theta_2+\dfrac{n_2}{m_2} & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\equiv(x_{ij}), \tag{7}$$

then using the previous expression for the Heisenberg representation with $s_1,s_2\in\mathbb{R}$,

$$(V_if)(s_1,s_2)=(V_{e_i}f)(s_1,s_2):=\exp(2\pi i(s_1x_{3i}+s_2x_{4i}))f(s_1+x_{1i},s_2+x_{2i}),$$

we get

$$(V_1f)(s_1,s_2)=f\left(s_1+\theta_1+\frac{n_1}{m_1},s_2\right),$$

$$(V_2f)(s_1,s_2)=\exp(2\pi is_1)f(s_1,s_2),$$

$$(V_3f)(s_1,s_2)=f\left(s_1,s_2+\theta_2+\frac{n_2}{m_2}\right),$$

$$(V_4f)(s_1,s_2)=\exp(2\pi is_2)f(s_1,s_2).$$

For the finite part, let $F=\mathbb{Z}_{m_1}\times\mathbb{Z}_{m_2}$, where $\mathbb{Z}_{m_i}=\mathbb{Z}/m_i\mathbb{Z}$, $(i=1,2)$ and consider the space $\mathbb{C}^{m_1}\otimes\mathbb{C}^{m_2}$ as the space of functions on $C(\mathbb{Z}_{m_1}\times\mathbb{Z}_{m_2})$. For all $m_i\in\mathbb{Z}$ and $n_i\in\mathbb{Z}/m_i\mathbb{Z}$ such that m_i and n_i are relatively prime. We define the operators W_i on $C(\mathbb{Z}_{m_1}\times\mathbb{Z}_{m_2})$ corresponding to our embedding map,

$$\Phi_{\text{fin}}=\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & \dfrac{n_1}{m_1} & 0 & 0 \\ 0 & 0 & 0 & \dfrac{n_2}{m_2} \end{pmatrix}, \tag{8}$$

with $k_i\in\mathbb{Z}_{m_i}$ $(i=1,2)$ as follows:

$$(W_1f)(k_1,k_2)=f(k_1-1,k_2),$$

$$(W_2f)(k_1,k_2)=\exp\left(2\pi i\frac{n_1k_1}{m_1}\right)f(k_1,k_2),$$

$$(W_3f)(k_1,k_2)=f(k_1,k_2-1),$$

$$(W_4f)(k_1,k_2)=\exp\left(2\pi i\frac{n_2k_2}{m_2}\right)f(k_1,k_2).$$

Thus, we define operators $U_i = V_i \otimes W_i$ acting on the space $E_T := \mathcal{S}(\mathbb{R}^2) \otimes \mathbb{C}^{m_1} \otimes \mathbb{C}^{m_2}$ as

$$\begin{aligned}
(U_1 f)(s_1,s_2,k_1,k_2) &= f\left(s_1 + \theta_1 + \frac{n_1}{m_1}, s_2, k_1 - 1, k_2\right), \\
(U_2 f)(s_1,s_2,k_1,k_2) &= e^{2\pi i (s_1 + n_1 k_1/m_1)} f(s_1,s_2,k_1,k_2), \\
(U_3 f)(s_1,s_2,k_1,k_2) &= f\left(s_1, s_2 + \theta_2 + \frac{n_2}{m_2}, k_1, k_2 - 1\right), \\
(U_4 f)(s_1,s_2,k_1,k_2) &= e^{2\pi i (s_2 + n_2 k_2/m_2)} f(s_1,s_2,k_1,k_2).
\end{aligned} \tag{9}$$

One can now see that they satisfy

$$\begin{aligned}
U_2 U_1 &= e^{2\pi i \theta_1} U_1 U_2, \\
U_4 U_3 &= e^{2\pi i \theta_2} U_3 U_4,
\end{aligned} \tag{10}$$

and otherwise $U_i U_j = U_j U_i$.

In order to find operators which commute with the U_i's, we recall the definition of the dual lattice $\Lambda^\perp$:

$$\langle m, \hat{t} \rangle - \langle n, \hat{s} \rangle \in \mathbb{Z}, \quad \text{for all } (m,\hat{s}) \in \Lambda \text{ and } (n,\hat{t}) \in \Lambda^\perp.$$

If we express the embedding map Φ as

$$\Phi = \begin{pmatrix} m & \cdots \\ \hat{s} & \cdots \end{pmatrix}, \tag{11}$$

and the embedding map Ψ for the dual lattice as

$$\Psi = \begin{pmatrix} n & \cdots \\ \hat{t} & \cdots \end{pmatrix}, \tag{12}$$

then the duality condition above can be written as

$$\langle m, \hat{t} \rangle - \langle n, \hat{s} \rangle = \Phi^t J \Psi \in \mathbb{Z},$$

where

$$J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{13}$$

Hence, we obtain the relation between the two embedding maps:

$$\Psi = -J \Phi^{-t} \mathbb{Z}. \tag{14}$$

Using the above relation, the dual map for the real part is now given by

$$\Psi_{\text{inf}}=\begin{pmatrix} 0 & \frac{1}{m_1} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{m_2} \\ \frac{1}{m_1\theta_1+n_1} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{m_2\theta_2+n_2} & 0 \end{pmatrix}, \tag{15}$$

and the finite part is given by

$$\Psi_{\text{fin}}=\begin{pmatrix} 0 & -a_1 & 0 & 0 \\ 0 & 0 & 0 & -a_2 \\ \frac{1}{m_1} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{m_2} & 0 \end{pmatrix}. \tag{16}$$

Here, $a_i \in \mathbb{Z}$ and $a_i n_i - b_i m_i = 1$ for some $b_i \in \mathbb{Z}$ $(i=1,2)$.

The generators of operators corresponding to the embedding map for the dual lattice are thus defined by

$$\begin{aligned} (Z_1 f)(s_1,s_2,k_1,k_2) &= e^{2\pi i(s_1/(m_1\theta_1+n_1)+k_1/m_1)} f(s_1,s_2,k_1,k_2), \\ (Z_2 f)(s_1,s_2,k_1,k_2) &= f\left(s_1+\frac{1}{m_1},s_2,k_1-a_1,k_2\right), \\ (Z_3 f)(s_1,s_2,k_1,k_2) &= e^{2\pi i(s_2/(m_2\theta_2+n_2)+k_2/m_2)} f(s_1,s_2,k_1,k_2), \\ (Z_4 f)(s_1,s_2,k_1,k_2) &= f\left(s_1,s_2+\frac{1}{m_2},k_1,k_2-a_2\right). \end{aligned} \tag{17}$$

Here,

$$\begin{aligned} Z_1 Z_2 &= e^{2\pi i\theta_1'} Z_2 Z_1, \\ Z_3 Z_4 &= e^{2\pi i\theta_2'} Z_4 Z_3, \end{aligned} \tag{18}$$

where

$$\theta_i' = \frac{a_i\theta_i+b_i}{m_i\theta_i+n_i}, \quad i=1,2, \tag{19}$$

and otherwise $Z_i Z_j = Z_j Z_i$. One can check that the Z_i's commute with the U_i's, i.e., $U_i Z_j = Z_j U_i$.

III. CONNECTIONS WITH COMPLEX STRUCTURES

In the previous section, connections on a projective $\mathcal{A}_\theta^d$-module satisfies the condition (4)

$$[\nabla_i, U_j] = 2\pi i \delta_{ij} U_j.$$

A connection ∇_i is called a constant curvature connection if $[\nabla_i,\nabla_j]=iF_{ij}$ for constants F_{ij}. This condition is satisfied if ∇_i is expressed as $\nabla_i=\partial_i-(i/2)F_{ij}s_j$ where ∂_i is a derivative with respect to s_i. Note that the condition (4) can be regarded as a compactification condition. This can be seen by considering an operator $\overline{X_i}=-\nabla_i$ with which the condition is expressed as

$$U_j\overline{X_i}U_j^{-1}=\overline{X_i}+2\pi i\delta_{ij}, \tag{20}$$

and this relation is comparable to a compactification with radius R_i, $U_jX_iU_j^{-1}=X_i+2\pi\delta_{ij}R_i$.

We thus let

$$(\overline{X_i}f)(s_1,s_2,k_1,k_2)=2\pi iA_{i1}s_1f(s_1,s_2,k_1,k_2)+2\pi iA_{i2}s_2f(s_1,s_2,k_1,k_2)$$
$$-A_{i3}\frac{\partial f(s_1,s_2,k_1,k_2)}{\partial s_1}-A_{i4}\frac{\partial f(s_1,s_2,k_1,k_2)}{\partial s_2},$$

where $A_{ik}\in\mathbb{R}$ are constants. If we denote the embedding maps as $\Phi_{\text{inf}}\equiv(x_{ij})$ and $\Phi_{\text{fin}}\equiv(y_{ij})$, then U_i action is expressed as

$$(U_if)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1x_{3i}+s_2x_{4i}+k_1y_{3i}+k_2y_{4i})}f(s_1+x_{1i},s_2+x_{2i},k_1+y_{1i},k_2+y_{2i}).$$

The condition (20) is satisfied if

$$x_{1i}x_{3i}+x_{2i}x_{4i}+y_{1i}y_{3i}+y_{2i}y_{4i}=0, \tag{21}$$

and

$$A_{ik}=(\Phi_{\text{inf}}^{-1})_{ik}. \tag{22}$$

The embedding maps (7), (8) satisfy the condition (21), and the condition (22) gives

$$(A_{ik})=\begin{pmatrix} \dfrac{1}{\theta_1+\dfrac{n_1}{m_1}} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & \dfrac{1}{\theta_2+\dfrac{n_2}{m_2}} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Therefore the following operators specify a constant curvature connection of right T^4_θ-module $E_{N,M}$:

$$\nabla_1=-\frac{2\pi is_1}{\theta_1+\dfrac{n_1}{m_1}},$$

$$\nabla_2=\frac{\partial}{\partial s_1},$$

$$\nabla_3 = -\frac{2\pi i s_2}{\theta_2 + \frac{n_2}{m_2}},$$

$$\nabla_4 = \frac{\partial}{\partial s_2}. \tag{23}$$

In general, a constant curvature connection can be obtained by adding some constants: $\nabla_i \to \nabla_i + d_i$, $i=1,\ldots,4$, where $d_i \in \mathbb{R}$ are constants.

A complex structure on the module $E_{N,M}$ can be introduced by fixing a $\overline{\partial}$-connection,

$$\overline{\nabla_1} = \lambda_{11}\nabla_1 + \lambda_{12}\nabla_2 + \lambda_{13}\nabla_3 + \lambda_{14}\nabla_4,$$

$$\overline{\nabla_2} = \lambda_{21}\nabla_1 + \lambda_{22}\nabla_2 + \lambda_{23}\nabla_3 + \lambda_{24}\nabla_4,$$

where $\lambda_{ij} \in \mathbb{C}$. Choosing an appropriate basis such that (λ_{ij}) becomes

$$\begin{pmatrix} \tau_{11} & 1 & \tau_{12} & 0 \\ \tau_{21} & 0 & \tau_{22} & 1 \end{pmatrix} = \begin{pmatrix} \lambda_{12} & \lambda_{14} \\ \lambda_{22} & \lambda_{24} \end{pmatrix}^{-1} \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} & \lambda_{24} \end{pmatrix},$$

the (2×2) matrix $\left(\begin{smallmatrix} \tau_{11} & \tau_{12} \\ \tau_{21} & \tau_{22} \end{smallmatrix}\right)$, $\tau_{ij} \in \mathbb{C}$ represents the complex structure of the T^4_θ-module and 1–1 corresponds to the complex structure on T^4_θ via the $\overline{\partial}$-derivative, $\overline{\delta_i} = \Sigma_j \lambda_{ij}\delta_j$ where δ_j is defined by (2).[16]

Now we consider holomorphic vectors in T^4_θ-module. A vector $\Theta \in E_{N,M}$ is called holomorphic[16] if it satisfies

$$(\overline{\nabla_i} - c_i)\Theta = 0, \quad \text{for } i=1,2, \tag{24}$$

where $c_i \in \mathbb{C}$ are constants. The above holomorphic condition for $f \in E_{N,M}$ now takes the form

$$\begin{aligned} \left(\frac{2\pi i \tau_{11}}{\theta_1 + \frac{n_1}{m_1}} s_1 + \frac{2\pi i \tau_{12}}{\theta_2 + \frac{n_2}{m_2}} s_2 + c_1 \right) f &= \frac{\partial f}{\partial s_1}, \\ \left(\frac{2\pi i \tau_{21}}{\theta_1 + \frac{n_1}{m_1}} s_1 + \frac{2\pi i \tau_{22}}{\theta_2 + \frac{n_2}{m_2}} s_2 + c_2 \right) f &= \frac{\partial f}{\partial s_2}. \end{aligned} \tag{25}$$

In order for the two equations in (25) to be consistent τ_{ij} should satisfy

$$\frac{\tau_{12}}{\theta_2 + \frac{n_2}{m_2}} = \frac{\tau_{21}}{\theta_1 + \frac{n_1}{m_1}}. \tag{26}$$

If $\mathrm{Re}\,\Omega < 0$, Eq. (25) has $m_1 \times m_2$ linearly independent solutions, the so-called theta vectors[16,17] on noncommutative T^4,

$$f_{(\alpha_1,\alpha_2)}(s_1,s_2,k_1,k_2) = \exp\left[\frac{1}{2} S^t \Omega S + C^t S\right] \delta^{k_1}_{\alpha_1} \delta^{k_2}_{\alpha_2}, \tag{27}$$

where $C = \left(\begin{smallmatrix} c_1 \\ c_2 \end{smallmatrix}\right)$, $S = \left(\begin{smallmatrix} s_1 \\ s_2 \end{smallmatrix}\right)$, $c_i \in \mathbb{C}$, $s_i \in \mathbb{R}$, $k_i \in \mathbb{Z}_{m_i}$ $(i=1,2)$, and

$$\Omega=\begin{pmatrix} \dfrac{2\pi i\tau_{11}}{\theta_1+\dfrac{n_1}{m_1}} & \dfrac{2\pi i\tau_{12}}{\theta_2+\dfrac{n_2}{m_2}} \\ \dfrac{2\pi i\tau_{21}}{\theta_1+\dfrac{n_1}{m_1}} & \dfrac{2\pi i\tau_{22}}{\theta_2+\dfrac{n_2}{m_2}} \end{pmatrix}.$$

IV. TENSOR PRODUCT

In this section we consider a tensor product of two bimodules. The tensor product of a (C,Y)-bimodule E and a (Y,D)-bimodule E' over Y results in a (C,D)-bimodule F for algebras C,Y,D;

$$_CE_Y\otimes_YE'_D={}_CF_D,$$

where the tensor product over Y is obtained by identifying $ey\otimes e'\sim e\otimes ye'$ for $y\in Y$, $e\in E,e'\in E'$. Note that in this identification, E behaves as a right Y-module and E' behaves as a left Y-module. Thus, we will denote $E_{N,M}$ as a right T^4_θ-module and $E'_{K,L}$ as a left T^4_θ-module. Here, we recall that $T^4_{\tilde\theta}$ is Morita equivalent to T^4_θ if θ and $\tilde\theta$ are related by $\tilde\theta=(A\theta+B)(M\theta+N)^{-1}$ where $\left(\begin{smallmatrix}A & B\\ M & N\end{smallmatrix}\right)\in \mathrm{SO}(4,4|\mathbb{Z})$, and $T^4_{\tilde\theta}\cong \mathrm{End}_{T^4_\theta}(E)$ for some finite projective module E. In this notation, a right module $E_{N,M}$ is identified with a left module $E'_{A,M}$. Let us calculate the tensor product $E_{N,M}\otimes_{T^4_\theta}E'_{K,L}$ which forms a vector space $S(\mathbb{R}\times\mathbb{Z}_{n_1l_1+m_1k_1}\times\mathbb{Z}_{n_2l_2+m_2k_2})$, when each N,M,K,L is reducible into two blocks represented by the values $N\sim(n_1,n_2)$, $M\sim(m_1,m_2)$, $K\sim(k_1,k_2)$, $L\sim(l_1,l_2)$.[26] For $f(s_1,s_2,\mu_1,\mu_2)\in E_{N,M}$, and $g(t_1,t_2,\nu_1,\nu_2)\in E'_{K,L}$ where $s_i,t_i\in\mathbb{R}$, $\mu_i\in\mathbb{Z}_{m_i}$, $\nu_i\in\mathbb{Z}_{l_i}(i=1,2)$ the actions of $U_i\in T^4_\theta$ and $Z_i\in T^4_{\tilde\theta}$ are given as follows.

The right U_i actions on $E_{N,M}$ are defined as

$$\begin{aligned}
(U_1f)(s_1,s_2,\mu_1,\mu_2)&=f\left(s_1+\theta_1+\frac{n_1}{m_1},s_2,\mu_1-1,\mu_2\right),\\
(U_2f)(s_1,s_2,\mu_1,\mu_2)&=e^{2\pi i(s_1+n_1\mu_1/m_1)}f(s_1,s_2,\mu_1,\mu_2),\\
(U_3f)(s_1,s_2,\mu_1,\mu_2)&=f\left(s_1,s_2+\theta_2+\frac{n_2}{m_2},\mu_1,\mu_2-1\right),\\
(U_4f)(s_1,s_2,\mu_1,\mu_2)&=e^{2\pi i(s_2+n_2\mu_2/m_2)}f(s_1,s_2,\mu_1,\mu_2).
\end{aligned}\tag{28}$$

The left U_i actions on $E'_{K,L}$ are defined as

$$\begin{aligned}
(U_1g)(t_1,t_2,\nu_1,\nu_2)&=g\left(t_1-\theta_1+\frac{k_1}{l_1},t_2,\nu_1-1,\nu_2\right),\\
(U_2g)(t_1,t_2,\nu_1,\nu_2)&=e^{2\pi i(t_1+k_1\nu_1/l_1)}g(t_1,t_2,\nu_1,\nu_2),\\
(U_3g)(t_1,t_2,\nu_1,\nu_2)&=g\left(t_1,t_2-\theta_2+\frac{k_2}{l_2},\nu_1,\nu_2-1\right),\\
(U_4g)(t_1,t_2,\nu_1,\nu_2)&=e^{2\pi i(t_2+k_2\nu_2/l_2)}g(t_1,t_2,\nu_1,\nu_2).
\end{aligned}\tag{29}$$

The left Z_i actions on $E_{N,M}$ are defined as

$$
\begin{aligned}
(Z_1 f)(s_1,s_2,\mu_1,\mu_2) &= e^{2\pi i(s_1/(m_1\theta_1+n_1)+\mu_1/m_1)} f(s_1,s_2,\mu_1,\mu_2),\\
(Z_2 f)(s_1,s_2,\mu_1,\mu_2) &= f\left(s_1+\frac{1}{m_1},s_2,\mu_1-a_1,\mu_2\right),\\
(Z_3 f)(s_1,s_2,\mu_1,\mu_2) &= e^{2\pi i(s_2/(m_2\theta_2+n_2)+\mu_2/m_2)} f(s_1,s_2,\mu_1,\mu_2),\\
(Z_4 f)(s_1,s_2,\mu_1,\mu_2) &= f\left(s_1,s_2+\frac{1}{m_2},\mu_1,\mu_2-a_2\right),
\end{aligned}
\tag{30}
$$

where $a_i \in \mathbb{Z}$ and $a_i n_i - b_i m_i = 1$ for some $b_i \in \mathbb{Z}$ $(i=1,2)$.

Following Ref. 17, we define the tensor product $f \otimes g \equiv h \in E_{N,M} \otimes_{T^4_\theta} E'_{K,L}$ as

$$
\begin{aligned}
h(r_1,r_2,j_1,j_2) = \sum_{q_1\in\mathbb{Z}} \sum_{q_2\in\mathbb{Z}} & f\Bigg((n_1+m_1\theta_1)r_1+\frac{n_1+m_1\theta_1}{m_1}q_1-\frac{l_1(n_1+m_1\theta_1)}{m_1(n_1l_1+m_1k_1)}j_1,(n_2+m_2\theta_2)r_2\\
&+\frac{n_2+m_2\theta_2}{m_2}q_2-\frac{l_2(n_2+m_2\theta_2)}{m_2(n_2l_2+m_2k_2)}j_2,-q_1+a_1j_1,-q_2+a_2j_2\Bigg)\\
&\times g\Bigg((n_1+m_1\theta_1)r_1-\frac{k_1-l_1\theta_1}{l_1}q_1+\frac{k_1-l_1\theta_1}{n_1l_1+m_1k_1}j_1,(n_2+m_2\theta_2)r_2-\frac{k_2-l_2\theta_2}{l_2}q_2\\
&+\frac{k_2-l_2\theta_2}{n_2l_2+m_2k_2}j_2,q_1,q_2\Bigg),
\end{aligned}
\tag{31}
$$

for $r_i \in \mathbb{R}$, $j_i \in \mathbb{Z}$ $(i=1,2)$. Then, one can check that

$$
\begin{aligned}
(U_i f)\otimes g &\sim f\otimes(U_i)g,\\
(Z_i h) &\sim (Z_i f)\otimes g,\\
h(r_i, j_i+n_il_i+m_ik_i) &= h(r_i,j_i),
\end{aligned}
$$

for $i=1,2$. Notice that in the above calculation Z_i's act on h as left actions, since h is regarded here as an element of a left module E'. So far, we have only defined the left actions of Z_i on a right module E. Thus, we define left Z_i actions on a left module E' as

$$
\begin{aligned}
(Z_1 g) &= (U_2 g),\\
(Z_2 g) &= (U_1 g),\\
(Z_3 g) &= (U_4 g),\\
(Z_4 g) &= (U_3 g),
\end{aligned}
$$

where $U_i g$ are defined in (29).

If $E_{N,M}$ is a right module expression of a $(T^4_{\tilde\theta}, T^4_\theta)$-bimodule and $E'_{K,L}$ is a left module expression of a $(T^4_\theta, T^4_{\theta'})$-bimodule, then one can also show that h belongs to $E'_{AK+BL,NL+MK}(\tilde\theta)$ where $\tilde\theta = (A\theta+B)(M\theta+N)^{-1}$ and $\theta = (K\theta'+D)(L\theta'+C)^{-1}$ with $CK-DL \sim 1$, $AN-BM \sim 1$, when each A,B,M,N,K,D,L,C is reducible into 2 blocks in the sense that we described earlier.

Let us consider the tensor product (31) between the two theta vectors, $f \in E_{N,M}$ and $g \in E'_{K,L}$,

$$f_{(\alpha_1,\alpha_2)}(s_1,s_2,\mu_1,\mu_2)=\exp[\tfrac{1}{2}S^t\Omega S+C^tS]\,\delta^{\mu_1}_{\alpha_1}\delta^{\mu_2}_{\alpha_2},$$
$$g_{(\beta_1,\beta_2)}(t_1,t_2,\nu_1,\nu_2)=\exp[\tfrac{1}{2}T^t\Omega' T+C'^tT]\,\delta^{\nu_1}_{\beta_1}\delta^{\nu_2}_{\beta_2}, \tag{32}$$

where $C=\binom{c_1}{c_2}$, $C'=\binom{c_1'}{c_2'}$, $S=\binom{s_1}{s_2}$, $T=\binom{t_1}{t_2}$, $c_i,c_i'\in\mathbb{C}$, $s_i,t_i\in\mathbb{R}$, $\mu_i\in\mathbb{Z}_{m_i}$, $\nu_i\in\mathbb{Z}_{l_i}$ $(i=1,2)$,

$$\Omega=\begin{pmatrix} \dfrac{2\pi i\tau_{21}}{\theta_1+\dfrac{n_1}{m_1}} & \dfrac{2\pi i\tau_{11}}{\theta_1+\dfrac{n_1}{m_1}} \\ \dfrac{2\pi i\tau_{22}}{\theta_2+\dfrac{n_2}{m_2}} & \dfrac{2\pi i\tau_{12}}{\theta_2+\dfrac{n_2}{m_2}} \end{pmatrix},\quad \text{and}\quad \Omega'=\begin{pmatrix} \dfrac{2\pi i\tau'_{21}}{-\theta_1+\dfrac{k_1}{l_1}} & \dfrac{2\pi i\tau'_{11}/}{-\theta_1+\dfrac{k_1}{l_1}} \\ \dfrac{2\pi i\tau'_{22}}{-\theta_2+\dfrac{k_2}{l_2}} & \dfrac{2\pi i\tau'_{12}}{-\theta_2+\dfrac{k_2}{l_2}} \end{pmatrix}.$$

The resulting function now takes the form

$$h_{\alpha_1,\alpha_2,\beta_1,\beta_2}(r_1,r_2,j_1,j_2)=\sum_{q_1\in\mathbb{Z}}\sum_{q_2\in\mathbb{Z}}\exp\left(\frac{1}{2}\tilde{\mathcal{A}}^t\Omega\tilde{\mathcal{A}}+C^t\tilde{\mathcal{A}}\right)\delta^{-q_1+a_1j_1,-q_2+a_2j_2}_{\alpha_1,\alpha_2}$$
$$\times\exp\left(\frac{1}{2}\tilde{\mathcal{A}}'^t\Omega'\tilde{\mathcal{A}}'+C'^t\tilde{\mathcal{A}}'\right)\delta^{q_1,q_2}_{\beta_1,\beta_2},$$

where $r_i\in\mathbb{R}$, $j_i\in\mathbb{Z}_{n_il_i+m_ik_i}$ $(i=1,2)$ and

$$\tilde{\mathcal{A}}=\begin{pmatrix} (n_1+m_1\theta_1)r_1+\dfrac{n_1+m_1\theta_1}{m_1}q_1-\dfrac{l_1(n_1+m_1\theta_1)}{m_1(n_1l_1+m_1k_1)}j_1 \\ (n_2+m_2\theta_2)r_2+\dfrac{n_2+m_2\theta_2}{m_2}q_2-\dfrac{l_2(n_2+m_2\theta_2)}{m_2(n_2l_2+m_2k_2)}j_2 \end{pmatrix},$$

$$\tilde{\mathcal{A}}'=\begin{pmatrix} (n_1+m_1\theta_1)r_1-\dfrac{k_1-l_1\theta_1}{l_1}q_1+\dfrac{k_1-l_1\theta_1}{n_1l_1+m_1k_1}j_1 \\ (n_2+m_2\theta_2)r_2-\dfrac{k_2-l_2\theta_2}{l_2}q_2+\dfrac{k_2-l_2\theta_2}{n_2l_2+m_2k_2}j_2 \end{pmatrix}.$$

From the delta function relations, we rewrite q_i as $q_i=p_i+u_im_il_i/v_i$, $u_i\in\mathbb{Z}$ $(i=1,2)$ for some integers p_i where $v_i=\text{g.c.d.}(m_i,l_i)$. Then, h can be written as

$$h_{\alpha_1,\alpha_2,\beta_1,\beta_2}(r_1,r_2,j_1,j_2)=\sum_{u_1\in\mathbb{Z}}\sum_{u_2\in\mathbb{Z}}\exp\left(\frac{1}{2}(\mathcal{A}+\mathcal{U})^t\Omega(\mathcal{A}+\mathcal{U})+C^t\mathcal{U}+C^t\mathcal{A}\right.$$
$$\left.+\frac{1}{2}(\mathcal{A}'+\mathcal{U}')^t\Omega'(\mathcal{A}'+\mathcal{U}')+C'^t\mathcal{U}'+C'^t\mathcal{A}'\right),$$

where

$$\mathcal{A}=\begin{pmatrix} (n_1+m_1\theta_1)r_1+\dfrac{n_1+m_1\theta_1}{m_1}p_1-\dfrac{l_1(n_1+m_1\theta_1)}{m_1(n_1l_1+m_1k_1)}j_1 \\ (n_2+m_2\theta_2)r_2+\dfrac{n_2+m_2\theta_2}{m_2}p_2-\dfrac{l_2(n_2+m_2\theta_2)}{m_2(n_2l_2+m_2k_2)}j_2 \end{pmatrix},$$

$$\mathcal{A}'=\begin{pmatrix}(n_1+m_1\theta_1)r_1-\dfrac{k_1-l_1\theta_1}{l_1}p_1+\dfrac{k_1-l_1\theta_1}{n_1l_1+m_1k_1}j_1\\ (n_2+m_2\theta_2)r_2-\dfrac{k_2-l_2\theta_2}{l_2}p_2+\dfrac{k_2-l_2\theta_2}{n_2l_2+m_2k_2}j_2\end{pmatrix},$$

$$\mathcal{U}=\begin{pmatrix}\dfrac{(n_1+m_1\theta_1)l_1}{v_1}u_1\\ \dfrac{(n_2+m_2\theta_2)l_2}{v_2}u_2\end{pmatrix},\quad \mathcal{U}'=\begin{pmatrix}-\dfrac{(k_1-l_1\theta_1)m_1}{v_1}u_1\\ -\dfrac{(k_2-l_2\theta_2)m_2}{v_2}u_2\end{pmatrix}.$$

This can be decomposed into two parts, including the classical theta function,

$$h=\vartheta(\mathcal{T},\mathcal{Z})\xi(r_1,r_2,j_1,j_2). \tag{33}$$

Here, the classical theta function ϑ is given by

$$\vartheta(\mathcal{T},\mathcal{Z})=\sum_{u_1,u_2\in\mathbb{Z}}\exp(\pi i U^t\mathcal{T}U+2\pi i\mathcal{Z}^tU),$$

where

$$U=\begin{pmatrix}u_1\\u_2\end{pmatrix},\quad \mathcal{T}=\begin{pmatrix}\mathcal{B}_1\mathcal{O}_{11}\mathcal{B}_1+\mathcal{B}_1'\mathcal{O}_{11}'\mathcal{B}_1' & \mathcal{B}_1\mathcal{O}_{12}\mathcal{B}_2+\mathcal{B}_1'\mathcal{O}_{12}'\mathcal{B}_2'\\ \mathcal{B}_2\mathcal{O}_{21}\mathcal{B}_1+\mathcal{B}_2'\mathcal{O}_{21}'\mathcal{B}_1' & \mathcal{B}_2\mathcal{O}_{22}\mathcal{B}_2+\mathcal{B}_2'\mathcal{O}_{22}'\mathcal{B}_2'\end{pmatrix},$$

$$\mathcal{Z}=\begin{pmatrix}\mathcal{B}_1\mathcal{O}_{11}\mathcal{A}_1+\mathcal{B}_1\mathcal{O}_{12}\mathcal{A}_2+\mathcal{B}_1'\mathcal{O}_{11}'\mathcal{A}_1'+\mathcal{B}_1'\mathcal{O}_{12}'\mathcal{A}_2'\\ \mathcal{B}_2\mathcal{O}_{21}\mathcal{A}_1+\mathcal{B}_2\mathcal{O}_{22}\mathcal{A}_2+\mathcal{B}_2'\mathcal{O}_{21}'\mathcal{A}_1'+\mathcal{B}_2'\mathcal{O}_{22}'\mathcal{A}_2'\end{pmatrix}+\frac{1}{2\pi i}\begin{pmatrix}c_1\mathcal{B}_1+c_1'\mathcal{B}_1'\\ c_2\mathcal{B}_2+c_2'\mathcal{B}_2'\end{pmatrix},$$

with

$$\mathcal{O}=\frac{1}{2\pi i}\Omega,\quad \mathcal{O}'=\frac{1}{2\pi i}\Omega',\quad \mathcal{B}=\begin{pmatrix}\mathcal{B}_1\\ \mathcal{B}_2\end{pmatrix}=\begin{pmatrix}\dfrac{(n_1+m_1\theta_1)l_1}{v_1}\\ \dfrac{(n_2+m_2\theta_2)l_2}{v_2}\end{pmatrix},$$

$$\mathcal{B}'=\begin{pmatrix}\mathcal{B}_1'\\ \mathcal{B}_2'\end{pmatrix}=\begin{pmatrix}-\dfrac{(k_1-l_1\theta_1)m_1}{v_1}\\ -\dfrac{(k_2-l_2\theta_2)m_2}{v_2}\end{pmatrix},$$

and function ξ is given by

$$\xi(r_1,r_2,j_1,j_2)=\exp(\tfrac{1}{2}\mathcal{A}^t\Omega\mathcal{A}+\tfrac{1}{2}\mathcal{A}'^t\Omega'\mathcal{A}'+C^t\mathcal{A}+C'^t\mathcal{A}').$$

Requiring that $E_{N,M}$ and $E'_{K,L}$ have the same complex structure for consistency of the tensor product, i.e., $(\tau_{ij})=(\tau'_{ij})$, and the consistency condition (26) the resulting function h becomes

$$h_{\alpha_1,\alpha_2,\beta_1,\beta_2}(r_1,r_2,j_1,j_2)=\sum_{\gamma_1,\gamma_2}c^{\gamma_1,\gamma_2}_{\alpha_1,\alpha_2,\beta_1,\beta_2}\varphi_{\gamma_1,\gamma_2}(r_1,r_2,j_1,j_2). \tag{34}$$

Here, the function $\varphi_{\gamma_1,\gamma_2}$ is given by

$$\varphi_{\gamma_1,\gamma_2}(r_1,r_2,j_1,j_2)=\exp(\pi i R^t\tilde{\mathcal{O}}R+(C+C')^t\tilde{R})\delta^{j_1}_{\gamma_1}\delta^{j_2}_{\gamma_2},$$

with

$$R=\begin{pmatrix} r_1 \\ r_2 \end{pmatrix},\quad \tilde{\mathcal{O}}=\begin{pmatrix} \dfrac{\tau_{11}(n_1+m_1\theta_1)(n_1l_1+m_1k_1)}{(k_1-l_1\theta_1)} & \dfrac{\tau_{12}(n_1+m_1\theta_1)(n_2l_2+m_2k_2)}{(k_2-l_2\theta_2)} \\ \dfrac{\tau_{21}(n_2+m_2\theta_2)(n_1l_1+m_1k_1)}{(k_1-l_1\theta_1)} & \dfrac{\tau_{22}(n_2+m_2\theta_2)(n_2l_2+m_2k_2)}{(k_2-l_2\theta_2)} \end{pmatrix},$$

$$\tilde{R}=\begin{pmatrix} (n_1+m_1\theta_1)r_1 \\ (n_2+m_2\theta_2)r_2 \end{pmatrix},$$

and the constants $c^{\gamma_1,\gamma_2}_{\alpha_1,\alpha_2,\beta_1,\beta_2}$ are given by

$$c^{\gamma_1,\gamma_2}_{\alpha_1,\alpha_2,\beta_1,\beta_2}=\vartheta(\Xi,\Lambda)e^{\mathcal{K}},$$

where

$$\mathcal{K}=\pi i\tilde{Q}^t\tilde{P}+C^t\tilde{M}+C'^t\tilde{L},$$

with

$$\tilde{Q}=\begin{pmatrix} \tau_{11}p_1+\tau_{12}p_2-\dfrac{\tau_{11}l_1j_1}{n_1l_1+m_1k_1}-\dfrac{\tau_{12}l_2j_2}{n_2l_2+m_2k_2} \\ \tau_{21}p_1+\tau_{22}p_2-\dfrac{\tau_{21}l_1j_1}{n_1l_1+m_1k_1}-\dfrac{\tau_{22}l_2j_2}{n_2l_2+m_2k_2} \end{pmatrix},\quad \tilde{P}=\begin{pmatrix} \dfrac{n_1l_1+m_1k_1}{l_1m_1}p_1-\dfrac{j_1}{m_1} \\ \dfrac{n_2l_2+m_2k_2}{l_2m_2}p_2-\dfrac{j_2}{m_2} \end{pmatrix},$$

$$\tilde{M}=\begin{pmatrix} \dfrac{n_1+m_1\theta_1}{m_1}p_1-\dfrac{l_1(n_1+m_1\theta_1)}{m_1(n_1l_1+m_1k_1)}j_1 \\ \dfrac{n_2+m_2\theta_2}{m_2}p_2-\dfrac{l_2(n_2+m_2\theta_2)}{m_2(n_2l_2+m_2k_2)}j_2 \end{pmatrix},\quad \tilde{L}=\begin{pmatrix} -\dfrac{k_1-l_1\theta_1}{l_1}q_1+\dfrac{k_1-l_1\theta_1}{n_1l_1+m_1k_1}j_1 \\ -\dfrac{k_2-l_2\theta_2}{l_2}q_2+\dfrac{k_2-l_2\theta_2}{n_2l_2+m_2k_2}j_2 \end{pmatrix},$$

and

$$\vartheta(\Xi,\Lambda)=\sum_{u_1,u_2\in\mathbb{Z}}\exp(\pi i U^t\Xi U+2\pi i\Lambda^t U),$$

with

$$U=\begin{pmatrix} u_1 \\ u_2 \end{pmatrix},\quad \Xi=\begin{pmatrix} \dfrac{\tau_{11}(n_1l_1+m_1k_1)l_1m_1}{v_1^2} & \dfrac{\tau_{12}(n_1l_1+m_1k_1)l_2m_2}{v_1v_2} \\ \dfrac{\tau_{21}(n_2l_2+m_2k_2)l_1m_1}{v_1v_2} & \dfrac{\tau_{22}(n_2l_2+m_2k_2)l_2m_2}{v_2^2} \end{pmatrix},$$

$$\Lambda=\begin{pmatrix} \frac{\tau_{11}}{v_1}((l_1n_1+m_1k_1)p_1-l_1j_1)+\frac{\tau_{12}}{v_1}(l_1n_1+m_1k_1)\left(p_2-\frac{l_2j_2}{l_2n_2+m_2k_2}\right) \\ \frac{\tau_{21}}{v_2}(l_2n_2+m_2k_2)\left(p_1-\frac{l_1j_1}{l_1n_1+m_1k_1}\right)+\frac{\tau_{22}}{v_2}((l_2n_2+m_2k_2)p_2-l_2j_2) \end{pmatrix} + \frac{1}{2\pi i}\begin{pmatrix} c_1\mathcal{B}_1+c_1'\mathcal{B}_1' \\ c_2\mathcal{B}_2+c_2'\mathcal{B}_2' \end{pmatrix},$$

where $c_i, c_i', \mathcal{B}_i, \mathcal{B}_i'$ are the same as given before.

Notice that the function $\varphi_{\gamma_1,\gamma_2}(r_1,r_2,j_1,j_2)$ is a theta vector (32) and belongs to $E'_{AK+BL,NL+MK}(\tilde{\theta})$ with $\tilde{\theta}=(A\theta+B)/(M\theta+N)$ as we expected.

V. DISCUSSION

In this paper, we first construct a module on noncommutative T^4 and its dual. Then we define the complex structure on this module and construct the theta vector which is a solution for a holomorphic connection. We then consider the tensor product of the theta vectors satisfying the consistency requirement.

Here, we want to notice what has not been apparent in the noncommutative T^2 case.[17] When we require the holomorphic condition (24), the symmetry appears not in the complex structure itself but in the Ω-matrix which appears in the theta vector (27), i.e., $\Omega_{12}=\Omega_{21}$ instead of $\tau_{12}=\tau_{21}$ in the commutative 4-torus case. We consider that this difference comes from noncommutativity.

As in the noncommutative T^2 case, the tensor products of modules on the noncommutative 4-torus with complex structures become very restrictive in order to satisfy the consistency requirement. We consider this consistency requirement as another aspect of noncommutativity compared with the commutative case in which there is no restriction.

So far, theta functions on noncommutative tori have not been utilized in the physics literature except for the integral torus case.[22–24] With the theta functions on noncommutative tori without any restriction, one can hope to explore the physical states on noncommutative tori in more general cases.

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Import of a set of solutions of the homogeneous Bloch equation

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We show for a class of time-varying magnetic fields that a generalized solution of precession is decomposed by two ways into two solutions of the homogeneous Bloch equation, thus having four solutions of which three are independent and form the fundamental systems. These solutions are found by solving the Riccati equation to which the homogeneous Bloch equation reduces. A brief discussion of the magnectic field class characteristics and an illustrative exmaple are given. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1629136]

I. INTRODUCTION

Recently we succeeded in finding a solution of the inhomogeneous Bloch equation.[1] This was completed by giving the fundamental system in terms of a set of the three independent solutions of the homogeneous Bloch equation. These three solutions were found by solving the Riccati equation to which the homogeneous Bloch equation reduces.

The purpose of this paper is to clarify the import of a set of solutions of the homgeneous Bloch equation. Of immediate utility to us are the solvable cases of the Riccati equation. Equating the Riccati equation of Abel's type[2] to the Riccati equation above we can find the fourth solution of it. By this finding we show that a generalized solution of precession is decomposed by two ways into two solutions of the homogeneous Bloch equation, thus having four solutions of which three are independent and form the fundamental systems. Two sets of the two decomposed solutions are related to each other through the formula to find a general solution when two independent special solutions of the Riccati equation are known. The same arguments hold for the Riccati equation of Chini's type.[3] In this soluble case the real parameter C is contained in the solutions to form the fundamental system. By setting the parameter on the special value all the solutions reduce to those of the Riccati equation of Abel's type.

Although we cannot solve the Riccati equation in general, we can do for a class of time-varying magnetic fields. This class is distinguished by requiring a nonlinear relation between one of the magnetic field components and the other two components and their derivatives. This restriction seems to arise in the solvable cases of the Riccati equation.

In Secs. II and III we solve the Riccati equation using the Riccati equation of Abel's type and Chini's type, respectively. A brief discussion of the magnetic field class characteristics and an illustrative example of precession are given in Sec. IV. The final section is devoted to our conclusions.

II. THE RICCATI EQUATION OF ABEL'S TYPE

The Bloch equation for magnetization with infininite relaxation times is a homogeneous system of three first-order linear differential equations given by

$$\dot{\vec{M}} = -\gamma(\vec{B}\times\vec{M}), \tag{1}$$

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where a dot means differentiation with respect to time. Here $\vec{M}$ and $\vec{B}$ are the magnetization vector and the applied magnetic field, respectively, and γ is the constant gyromagnetic ratio in some substance. Since the magnitude of the magnetization vector is constant in time, as is clear from Eq. (1), the normalized magnetization vector obeys the Bloch equation,

$$\dot{\vec{m}} = -\gamma(\vec{B}\times\vec{m}), \tag{2}$$

with

$$\vec{m} = \frac{\vec{M}}{|\vec{M}|}. \tag{3}$$

Introducing the two complex variables, ξ and η, given by

$$m_1 + i\, m_2 = \xi(1-m_3) \tag{4}$$

and

$$m_1 - i\, m_2 = \frac{1}{\eta}(m_3 - 1), \tag{5}$$

we derive the following ordinary differential equation for ξ (and η) from the Bloch equation (2):

$$\dot{\xi} = \tfrac{1}{2}\gamma(B_2 + i\, B_1)\xi^2 - i\,\gamma B_3\,\xi + \tfrac{1}{2}\gamma(B_2 - iB_1). \tag{6}$$

This is a form of the general Riccati equation which can be cast in the form

$$\dot{\xi} = i\dot{\chi}\, e^{-i\psi}\xi^2 - i\dot{\chi}_3\,\xi - i\dot{\chi}\, e^{i\psi}. \tag{7}$$

Here χ and χ_3 are defined by

$$\chi = \frac{1}{2}\gamma\int_{t_0}^{t} B_0(\tau)\,\mathrm{d}\tau \tag{8}$$

and

$$\chi_3 = \gamma\int_{t_0}^{t} B_3(\tau)\,\mathrm{d}\tau, \tag{9}$$

with

$$B_2 \pm iB_1 = \pm iB_0\, e^{\mp i\psi} \tag{10}$$

and

$$B_0 = \sqrt{B_1^2 + B_2^2}. \tag{11}$$

Also,

$$\psi = \tan^{-1}\left(\frac{B_2}{B_1}\right). \tag{12}$$

The Riccati equation of Abel's type is of the form

$$\dot{u}=\frac{\dot{f}}{g}u^2-\frac{\dot{g}}{f}, \tag{13}$$

and the solution is given by[2]

$$u=-\frac{g}{f}+\frac{1}{f^2}\left[C_1-\int_{t_0}^{t}\frac{\dot{f}(\tau)}{g(\tau)f^2(\tau)}\,\mathrm{d}\tau\right]^{-1}, \tag{14}$$

where C_1 is a constant of integration.

The Riccati equation (7) has the form

$$\dot{u}=\dot{\chi}\,e^{-i(\psi+\chi_3)}u^2+\dot{\chi}\,e^{i(\psi+\chi_3)}, \tag{15}$$

and an equation of this form results from the substitution

$$\xi=-iu\,e^{-i\chi_3}. \tag{16}$$

Equating Eq. (15) to Eq. (13), we find

$$\dot{\chi}\,e^{-i(\psi+\chi_3)}=\frac{\dot{f}}{g} \tag{17}$$

and

$$\dot{\chi}\,e^{i(\psi+\chi_3)}=-\frac{\dot{g}}{f}, \tag{18}$$

which reduce to two second-order linear differential equations

$$\ddot{f}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-i(\dot{\psi}+\dot{\chi}_3)\right]\dot{f}+(\dot{\chi})^2 f=0 \tag{19}$$

and

$$\ddot{g}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+i(\dot{\psi}+\dot{\chi}_3)\right]\dot{g}+(\dot{\chi})^2 g=0. \tag{20}$$

Notice that the linearized Riccati equation has the form [Eq. (20) in Ref. 4]

$$\ddot{u}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-i(\dot{\psi}+\dot{\chi}_3)\right]\dot{u}+(\dot{\chi})^2 u=0, \tag{21}$$

where we have substituted ξ given by

$$\xi=i\frac{1}{\dot{\chi}}\left(\frac{\dot{u}}{u}\right)e^{i\psi}, \tag{22}$$

into Eq. (7). Equation (21) can be solved[4] under the restriction [Eq. (46) in Ref. 4]

$$\dot{\psi}+\dot{\chi}_3=C\dot{\chi}, \tag{23}$$

with

$$C=\pm 2. \tag{24}$$

This restriction was imposed to eliminate unwanted derivative differential equations arising from differentiating the original coupled differential equations.

We immediately find two independent solutions of the second-order linear differential equation for both f and g by using the solutions obtained by solving Eq. (21). [See Eqs. (57) and (58) in Ref. 4.] A specific combination is required for g in order to satisfy Eqs. (17) and (18) when choosing one of two independent solutions of Eq. (19) as f. We thus find two sets of the solutions for f and g such that

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} \cos(\sqrt{2}\chi)e^{-i\chi} \\ -[i+\sqrt{2}\tan(\sqrt{2}\chi)]\cos(\sqrt{2}\chi)e^{i\chi} \end{pmatrix} \tag{25}$$

and

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} \sin(\sqrt{2}\chi)e^{-i\chi} \\ -[i-\sqrt{2}\cot(\sqrt{2}\chi)]\sin(\sqrt{2}\chi)e^{i\chi} \end{pmatrix}, \tag{26}$$

where we have chosen C as

$$C=2\,. \tag{27}$$

Substituting Eqs. (25) and (26) back into Eq. (14) and arranging them, we arrive at two independent special solutions of Eq. (7),

$$\xi_3 = e^{i\psi}\left[1-i\sqrt{2}\,\frac{1+\tan(\sqrt{2}\chi)}{1-\tan(\sqrt{2}\chi)}\right] \tag{28}$$

and

$$\xi_4 = e^{i\psi}\left[1+i\sqrt{2}\,\frac{1-\tan(\sqrt{2}\chi)}{1+\tan(\sqrt{2}\chi)}\right], \tag{29}$$

where we have used the relationship (16) and C_1 has been chosen as

$$C_1+\frac{1}{\sqrt{2}}\tan(\sqrt{2}\chi_0)=\frac{1}{\sqrt{2}} \tag{30}$$

and

$$C_1-\frac{1}{\sqrt{2}}\cot(\sqrt{2}\chi_0)=\frac{1}{\sqrt{2}}, \tag{31}$$

respectively, with

$$\chi_0=\chi(t_0)\,. \tag{32}$$

Let $\xi_a\,(a=i,j)$ be two special solutions of Eq. (7), then

$$\frac{\dot{\xi}-\dot{\xi}_i}{\xi-\xi_i}-\frac{\dot{\xi}-\dot{\xi}_j}{\xi-\xi_j}=i\dot{\chi}\,e^{-i\psi}(\xi_i-\xi_j)\,. \tag{33}$$

Thus, we find that a general solution of the differential equation (33) is

$$\frac{\xi-\xi_i}{\xi-\xi_j}=C_2\exp\left\{i\int_{t_0}^{t}\dot{\chi}(\tau)e^{-i\psi(\tau)}[\xi_i(\tau)-\xi_j(\tau)]\,\mathrm{d}\tau\right\}, \tag{34}$$

where C_2 is a constant of integration.

Substituting the two independent special solutions (28) and (29) into Eq. (34) and choosing C_2,

$$C_2=-\frac{1+\tan(\sqrt{2}\chi_0)}{1-\tan(\sqrt{2}\chi_0)} \tag{35}$$

and

$$C_2=\frac{1+\tan(\sqrt{2}\chi_0)}{1-\tan(\sqrt{2}\chi_0)}, \tag{36}$$

we find the other two special solutions

$$\xi_1=e^{i\psi}[1-i\sqrt{2}\tan(\sqrt{2}\chi)] \tag{37}$$

and

$$\xi_2=e^{i\psi}[1+i\sqrt{2}\cot(\sqrt{2}\chi)], \tag{38}$$

respectively. These two special solutions (37) and (38) are exactly the same ones [Eqs. (61) and (62) in Ref. 4] as were derived from the linearized Riccati equation (21).[4] Inversely, we obtain the special solutions (28) and (29) by substituting Eqs. (37) and (38) back into Eq. (34) and choosing C_2 as

$$C_2=\tan(\sqrt{2}\chi_0) \tag{39}$$

and

$$C_2=-\tan(\sqrt{2}\chi_0), \tag{40}$$

respectively. We thus find the relationship between a couple of the special solutions (ξ_1, ξ_2) and (ξ_3, ξ_4).

Notice that the special solutions ξ_i $(i=1,2)$ were already found as stated above and ξ_3 is contained in the fundamental system[1] [Eq. (52) in Ref. 1] which we have found as a special case. Thus, the special solution of ξ_4 is unknown so far.

As mentioned in the beginning of this section, the homogeneous Bloch equation is a system of the three first-order linear differential equations, thus having three independent magnetization vectors. While we have found four special solutions ξ_i $(i=1,2,3,4)$, each of which has the one to one correspondence to the magnetization vector. This fact strongly suggests that the four magnetization vectors are not independent, but a constraint exists. To see this we express the magnetization vectors, $\vec{m}^{(i)}$ $(i=1,2,3,4)$, in terms of ξ_i $(i=1,2,3,4)$,

$$m_1^{(i)}=\frac{\xi_i+\xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{41}$$

$$m_2^{(i)}=-i\,\frac{\xi_i-\xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{42}$$

and

$$m_3^{(i)} = -\frac{1-\xi_i\,\xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{43}$$

where we have used the definition of ξ, Eq. (4).

Though the explicit forms of the magnetization vectors are easily obtained by using Eqs. (41), (42), and (43), we do not list them in this section, because those are contained in the corresponding expressions in Sec. III as the parameter C being the specific value, i.e., $C=2$. Instead we display the relation among the magnetization vectors,

$$\vec{m}^{(1)}+\vec{m}^{(2)}=\vec{m}^{(3)}+\vec{m}^{(4)}=\sqrt{2}\vec{m}^{(5)}, \tag{44}$$

where

$$\vec{m}^{(5)}=\left(\frac{1}{\sqrt{2}}\cos\psi,\frac{1}{\sqrt{2}}\sin\psi,\frac{1}{\sqrt{2}}\right)^T. \tag{45}$$

It is worth noticing that the fifth magnetization vector is a generalized solution of the classical precession. We thus find the correct number of magnetization vectors.

The fundamental matrix is defined by

$$(K)_{ij}=K_{ij}=m_i^{(j)} \quad (i,j=1,2,3). \tag{46}$$

The equivalent fundamental systems appear in a set of magnetization vectors by denoting j: $j=2,3,4;3,4,1;4,1,2$. Thus we have four fundamental systems. In each of the fundamental systems, the determinant of the fundamental matrix turns out, up to a sign, to be

$$\det K=\frac{1}{\sqrt{2}}. \tag{47}$$

This means that the fundamental matrices are nonsingular and then three of the four solutions of the homogeneous Bloch equation are linearly independent.

The homogeneous Bloch equation (2) can be written in a matrix form

$$\dot{K}=A\,K, \tag{48}$$

where K is the fundamental matrix defined by Eq. (46) and a matrix A is given by

$$A=\begin{pmatrix} 0 & \gamma B_3 & -\gamma B_2 \\ -\gamma B_3 & 0 & \gamma B_1 \\ \gamma B_2 & -\gamma B_1 & 0 \end{pmatrix}, \tag{49}$$

which is antisymmetric and singular. Moreover, we find

$$\det\dot{K}=\mathrm{tr}\,A\,\det K=0, \tag{50}$$

and solving Eq. (50) for $\det K$ we have

$$\det K=\det K(t_0). \tag{51}$$

The inhomogeneous Bloch equation has the form[5]

$$\dot{\vec{m}}=A\,\vec{m}+\vec{b}. \tag{52}$$

The fundamental system of solutions of the homogeneous system is a set of three linearly independent magnetization vectors $\vec{m}^{(j)}$. Using the fundamental matrix defined by Eq. (46), the unique solution to the inhomogeneous system (52) is

$$\vec{m}=K\,K^{-1}(t_0)\,\vec{m}(t_0)+K\int_{t_0}^{t}K^{-1}(\tau)\vec{b}(\tau)\,\mathrm{d}\tau\,. \tag{53}$$

III. THE RICCATI EQUATION OF CHINI'S TYPE

The Riccati equation of Chini's type is in the form

$$\dot{u}=\frac{1}{(ag+b)^2}\frac{\dot{g}}{f}u^2+\frac{\dot{f}}{f}u+f\dot{g}=0\,, \tag{54}$$

where a and b are arbitrary constants.

The Riccati equation (7) is rewritten in the form

$$\dot{u}=\dot{\chi}u^2-i(\dot{\psi}+\dot{\chi}_3)\,u+\dot{\chi}\,, \tag{55}$$

which results from the substitution of

$$\xi=-iu\,e^{i\psi} \tag{56}$$

into Eq. (7). Equating Eq. (55) to Eq. (54), we find

$$\dot{\chi}=\frac{1}{(ag+b)^2}\frac{\dot{g}}{f}=f\dot{g} \tag{57}$$

and

$$-i(\dot{\psi}+\chi_3)=\frac{\dot{f}}{f}. \tag{58}$$

It follows from Eq. (57) that

$$f=\frac{1}{ag+b} \tag{59}$$

and

$$\dot{\chi}=\frac{1}{ag+b}\dot{g}\,. \tag{60}$$

Solving the differential equation (60), we obtain

$$ag+b=A\,e^{a\chi}\,, \tag{61}$$

where A is a constant of integration. Thus we find

$$\dot{f}=-a\dot{\chi}f\,. \tag{62}$$

By setting $a=iC$ (C, real number), Eq. (58) yields

$$\dot{\psi}+\dot{\chi}_3=C\,\dot{\chi}\,. \tag{63}$$

This produces a separation of the variables, u and χ, and leads to

$$\dot{u}=\dot{\chi}\,(u^2-iC\,u+1)\,, \tag{64}$$

where we have used Eq. (55).

Solving Eq. (64), we find two solutions [Eqs. (42) and (43) in Ref. 1]

$$\xi_1=e^{i\psi}[\,\alpha-i\beta\tan(\beta\chi)] \tag{65}$$

and

$$\xi_2=e^{i\psi}[\,\alpha+i\beta\cot(\beta\chi)]\,, \tag{66}$$

where α and β are given by

$$\alpha=\tfrac{1}{2}C \tag{67}$$

and

$$\beta=\sqrt{1+\alpha^2}\,. \tag{68}$$

The same procedure to find another couple of special solutions developed in Sec. II is applicable to this case. We thus find

$$\xi_3=e^{i\psi}\left[\,\alpha-i\beta\frac{1+\tan(\beta\chi)}{1-\tan(\beta\chi)}\right] \tag{69}$$

and

$$\xi_4=e^{i\psi}\left[\,\alpha+i\beta\frac{1-\tan(\beta\chi)}{1+\tan(\beta\chi)}\right], \tag{70}$$

where use has been made of the relation (34) and C_2 has been chosen as

$$C_2=\tan(\beta\chi_0) \tag{71}$$

and

$$C_2=-\tan(\beta\chi_0)\,, \tag{72}$$

respectively. Note that Eq. (69) corresponds to Eq. (52) in Ref. 1. Inversely, substituting Eqs. (69) and (70) into Eq. (34) and choosing C_2 as

$$C_2=-\frac{1+\tan(\beta\chi_0)}{1-\tan(\beta\chi_0)} \tag{73}$$

and

$$C_2=\frac{1+\tan(\beta\chi_0)}{1-\tan(\beta\chi_0)}, \tag{74}$$

respectively, we find Eqs. (65) and (66). Thus a couple of the special solutions (ξ_1,ξ_2) and (ξ_3,ξ_4) are transferable through the relationship in (34).

Using Eqs. (41), (42), and (43), we find the explicit forms of the magnetization vectors $\vec{m}^{(i)}$ $(i=1,2,3,4)$ corresponding to the special solutions of the Riccati equation (55) as follows:

$$\vec{m}^{(1)},$$

$$m_1^{(1)}=\frac{1}{\beta^2}\{\alpha[1+\cos(2\beta\chi)]\cos\psi+\beta\sin(2\beta\chi)\sin\psi\}, \tag{75}$$

$$m_2^{(1)}=\frac{1}{\beta^2}\{\alpha[1+\cos(2\beta\chi)]\sin\psi-\beta\sin(2\beta\chi)\cos\psi\}, \tag{76}$$

$$m_3^{(1)}=-\frac{1}{\beta^2}(1-\alpha^2)\frac{1}{2}[1+\cos(2\beta\chi)]+\frac{1}{2}[1-\cos(2\beta\chi)], \tag{77}$$

$$\vec{m}^{(2)},$$

$$m_1^{(2)}=\frac{1}{\beta^2}\{\alpha[1-\cos(2\beta\chi)]\cos\psi-\beta\sin(2\beta\chi)\sin\psi\}, \tag{78}$$

$$m_2^{(2)}=\frac{1}{\beta^2}\{\alpha[1-\cos(2\beta\chi)]\sin\psi+\beta\sin(2\beta\chi)\cos\psi\}, \tag{79}$$

$$m_3^{(2)}=-\frac{1}{\beta^2}(1-\alpha^2)\frac{1}{2}[1-\cos(2\beta\chi)]+\frac{1}{2}[1+\cos(2\beta\chi)], \tag{80}$$

$$\vec{m}^{(3)},$$

$$m_1^{(3)}=\frac{1}{\beta^2}\{\alpha[1-\sin(2\beta\chi)]\cos\psi+\beta\cos(2\beta\chi)\sin\psi\}, \tag{81}$$

$$m_2^{(3)}=\frac{1}{\beta^2}\{\alpha[1-\sin(2\beta\chi)]\sin\psi-\beta\cos(2\beta\chi)\cos\psi\}, \tag{82}$$

$$m_3^{(3)}=-\frac{1}{\beta^2}(1-\alpha^2)\frac{1}{2}[1-\sin(2\beta\chi)]+\frac{1}{2}[1+\sin(2\beta\chi)], \tag{83}$$

$$\vec{m}^{(4)},$$

$$m_1^{(4)}=\frac{1}{\beta^2}\{\alpha[1+\sin(2\beta\chi)]\cos\psi-\beta\cos(2\beta\chi)\sin\psi\}, \tag{84}$$

$$m_2^{(4)}=\frac{1}{\beta^2}\{\alpha[1+\sin(2\beta\chi)]\sin\psi+\beta\cos(2\beta\chi)\cos\psi\}, \tag{85}$$

$$m_3^{(4)}=-\frac{1}{\beta^2}(1-\alpha^2)\frac{1}{2}[1+\sin(2\beta\chi)]+\frac{1}{2}[1-\sin(2\beta\chi)]. \tag{86}$$

A key relationship appears to be

$$\vec{m}^{(1)}+\vec{m}^{(2)}=\vec{m}^{(3)}+\vec{m}^{(4)}=\frac{2\alpha}{\beta}\vec{m}^{(5)}, \tag{87}$$

where

$$\vec{m}^{(5)}=\left(\frac{1}{\beta}\cos\psi,\frac{1}{\beta}\sin\psi,\frac{\alpha}{\beta}\right)^{T}. \tag{88}$$

The fifth magnetization vector (a special solution of the homogeneous Bloch equation) is a generalized solution of the classical precession, as will be illustrated in Sec. IV. Thus the relation (87) tells us that a generalized solution of precession can be decomposed by two ways into two special solutions of the homgeneous Bloch equation and then three of the four special solutions $\vec{m}^{(j)}$ ($j=1,2,3,4$) are independent and form the fundamental systems. Whole, the special solutions of the homogeneous Bloch equation, reduce to those obtained in the preceding section by setting $C=2$, as was stated.

The fundamental systems are obtained by using a set of three special solutions of the homogeneous Bloch equation if and only if the fundamental matrices are nonsingular.

Using the definition of fundamental matrix (46), we evaluate the determinant of the fundamental matrix as

$$\det K=\frac{2\alpha}{\beta^3}=C\left(\frac{2}{\sqrt{4+C^2}}\right)^3, \tag{89}$$

as is expected from Eq. (51). This means that the fundamental matrix is nonsingular and the set of three special solutions, denoting by $j=1,2,3$, consists of the three linearly independent ones. We also find the other fundamental systems $j=2,3,4$; 3,4,1; 4,1,2. The determinant of each fundamental matrix becomes the same as Eq. (89) up to a sign.

Using the fundamental matrix, we can find the unique solution to the inhomogeneous system (52). [See Eq. (53).]

IV. THE MAGNETIC FIELD CLASS CHARACTERISTICS AND AN ILLUSTRATIVE EXAMPLE

Using Eq. (12), the constraint (63) yields

$$\gamma B_3=\frac{\dot{B}_1B_2-B_1\dot{B}_2}{B_1^2+B_2^2}+\frac{1}{2}C\gamma\sqrt{B_1^2+B_2^2}. \tag{90}$$

The third component of magnetic field is expressed by the other two independent time-varying magnetic field components.

To discuss the characteristics of the magnetic field class we give some insight to the meaning of the restriction (90) which must be satisfied by the applied magnetic field in order to obtain the solution which is devloped in this paper.

The simplest practical discussion would center on the behavior of the third component when the first two components are harmonically varying,

$$\vec{B}(t)=(B_0(t)\cos\omega t, B_0(t)\sin\omega t, B_3(t)), \tag{91}$$

with ω being a constant angular velocity (harmonic frequency). The restriction (90) leads to the relation

$$B_3(t)=-\frac{\omega}{\gamma}+\frac{1}{2}CB_0(t). \tag{92}$$

This immediately suggests the effect of the variation of the constant C as a controlling influence on the third component of the applied magnetic field; the effects of variation harmonic frequency, gyromagnetic ratio and the magnitude of the harmonic field thus being easily interpreted.

The fifth magnetization vector (88) in this case turns out to be

$$\vec{m}^{(5)}=\left(\frac{1}{\beta}\cos\omega t,\frac{1}{\beta}\sin\omega t,\frac{\alpha}{\beta}\right)^{T}, \tag{93}$$

where we have used Eq. (12). This is the well-known solution of classical precession.

V. CONCLUSIONS

We clarify the import of a set of the special solutions of the Riccati equation as follows.

A set of special solutions has been obtained for a class of time-varying magnetic fields by solving the Riccati equation to which the homogeneous Bloch equation reduces. The finding of the fourth special solution allows us to interpret a set of the four special solutions as

$$\vec{m}^{(1)}+\vec{m}^{(2)}=\vec{m}^{(3)}+\vec{m}^{(4)}=\frac{2\alpha}{\beta}\vec{m}^{(5)}, \tag{94}$$

i.e., a generalized solution of the classical precession is decomposed by two ways into the two special solutions of the Riccati equation (7), thus having the four special solutions of which three special solutions are independent and form the fundamental system. Thus we have found a solution of the inhomogeneous Bloch equation for a class of time-varying magnetic fields.

Notice that a couple of the special solutions (ξ_1,ξ_2) and (ξ_3,ξ_4) are transferable to each other through the relationship (34). This is the characteristics of the Riccati equation.

Also note that we have found four (eight when including the fifth special solution) fundamental systems which are equivalent.

In most of the soluble cases of the Riccati equation the restriction (63) would appear to be a key of solvability. We have not yet succeeded in finding an unknown solution of the Riccati equation.

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Towards a general solution of the inhomogeneous Bloch equation

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A general form of solution of the inhomogeneous Bloch equation is given in terms of a solution of the homogeneous Bloch equation which is assumed to be known. The fundamental system of the homogeneous Bloch equation is derived from the method inherent to the Riccati equation to which the homogeneous Bloch equation reduces. The fundamental matrix is an orthogonal matrix. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1633023]

I. INTRODUCTION

Very recently, an interesting solution was found to the inhomogeneous Bloch equation.[1] The fundamental matrix in terms of a set of three independent solutions of the homogeneous Bloch equation became an orthogonal matrix. A simple question arose whether or not a fundamental matrix can always be chosen to be an orthogonal matrix.

The aim of this article is to show that a general form of solution of the inhomogeneous Bloch equation is obtained and the fundamental matrix is an orthogonal matrix. The key to demonstrating this is to make use of well-known properties of the Riccati equation.

The homogeneous Bloch equation reduces to a form of Riccati equation by introducing two complex variables. The same Riccati equation is satisfied by each of these variables. If a solution of the homogeneous Bloch equation is assumed to be known, then another solution may be automatically found. Whenever two special solutions are found, further special solutions can be derived from using a method inherent to the Riccati equation.[1–3] This leads to expressions for a set of three independent special solutions without solving the Riccati equation explicitly. We can show that the resulting normalized magnetization vectors obey the homogeneous Bloch equation by using the differential equations which the real and imaginary parts of an assumed solution must satisfy. Thus we arrive at a general form of solution of the inhomogeneous Bloch equation by finding the fundamental system of the homogeneous Bloch equation. The fundamental matrix turns out to be orthogonal.

In Sec. II we give a set of special solutions of the homogeneous Bloch equation in terms of an assumed known solution. In Sec. III the fundamental system of the homogeneous Bloch equation is given, thereby providing a general form of solution of the inhomogeneous Bloch equation. The differential equation which must be solved in order to obtain a general solution of the homogeneous Bloch equation is given in Sec. IV. The final section is devoted to conclusions.

II. A SET OF SPECIAL SOLUTIONS OF THE RICCATI EQUATION

The Bloch equation for magnetization with infinite relaxation times is a homogeneous system of three first-order linear differential equations given by

$$\dot{\vec{M}} = -\gamma(\vec{B}\times\vec{M}), \tag{1}$$

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where an overdot means differentiation with respect to time. Here $\vec{M}$ and $\vec{B}$ are the magnetization vector and the time-dependent applied magnetic field, respectively. Also γ is the constant gyromagnetic ratio in some substance. Since the magnitude of the magnetization vector is preserved, as is clear from Eq. (1), the normalized magnetization vector obeys the Bloch equation

$$\dot{\vec{m}} = -\gamma(\vec{B}\times\vec{m}), \tag{2}$$

with

$$\vec{m} = \frac{\vec{M}}{|\vec{M}|}. \tag{3}$$

Introducing the two complex variables ξ and η given by

$$m_1 + i\, m_2 = \xi(1 - m_3) \tag{4}$$

and

$$m_1 - i\, m_2 = \frac{1}{\eta}(m_3 - 1), \tag{5}$$

we can derive the following ordinary differential equation for both ξ and η from the Bloch equation (2):

$$\dot{\xi} = i\dot{\chi}e^{-i\psi}\xi^2 - i\dot{\chi}_3\xi - i\dot{\chi}e^{i\psi}, \tag{6}$$

where χ and χ_3 are defined by

$$\chi = \frac{1}{2}\gamma\int_{t_0}^{t} B_0(\tau)\,\mathrm{d}\tau \tag{7}$$

and

$$\chi_3 = \gamma\int_{t_0}^{t} B_3(\tau)\,\mathrm{d}\tau, \tag{8}$$

with

$$B_2 \pm iB_1 = \pm iB_0\, e^{\mp i\psi}, \tag{9}$$

and

$$B_0 = \sqrt{B_1^2 + B_2^2}. \tag{10}$$

Also,

$$\psi = \cos^{-1}\left(\frac{B_1}{B_0}\right) = \sin^{-1}\left(\frac{B_2}{B_0}\right) = \tan^{-1}\left(\frac{B_2}{B_1}\right). \tag{11}$$

The Riccati equation (6) can be cast in the form

$$\dot{u} = \dot{\chi}u^2 - i(\dot{\psi} + \dot{\chi}_3)u + \dot{\chi}, \tag{12}$$

where the variable u is introduced by

$$\xi = -ie^{i\psi}u\,. \tag{13}$$

Let u_1 be a solution assumed to be known of the form

$$u_1 = \mathrm{Re}\,u_1 + i\,\mathrm{Im}\,u_1 = \beta_1 + i\alpha_1\,, \tag{14}$$

then the Riccati equation (12) yields

$$\dot{\alpha}_1 = 2\dot{\chi}\beta_1(\alpha_1 - a) \tag{15}$$

and

$$\dot{\beta}_1 = -2\dot{\chi}\alpha_1(\alpha_1 - a) + \dot{\chi}\left(1 + \frac{1}{\lambda}\right), \tag{16}$$

where the variables a and λ are defined by

$$a = \frac{\dot{\psi} + \dot{\chi}_3}{2\dot{\chi}} \tag{17}$$

and

$$\frac{1}{\lambda} = u_1 u_1^* = \alpha_1^2 + \beta_1^2\,. \tag{18}$$

By differentiating Eq. (18) with respect to time together with Eqs. (15) and (16), we find

$$\dot{\lambda} = -2\dot{\chi}\beta_1\lambda(\lambda + 1)\,. \tag{19}$$

Since the variables ξ and η satisfy the relationship; $\xi^*\eta = -1$, a second special solution is immediately obtained from

$$u_2 = -\frac{1}{u_1^*} = -\lambda u_1\,. \tag{20}$$

By using Eq. (19), we can directly show that u_2 is a solution of the Riccati equation (12) when u_1 is a solution.

Another solution of the Riccati equation, when two independent special solutions are known, is of the form

$$\frac{u - u_1}{u - u_2} = C_2 \exp\left\{\int_{t_0}^{t} \dot{\chi}(\tau)[u_1(\tau) - u_2(\tau)]\,\mathrm{d}\tau\right\}, \tag{21}$$

where C_2 is a constant of integration. An appropriate choice of the integration constant leads to a third solution in the form

$$\frac{u_3 - u_1}{u_3 - u_2} = \frac{1}{\sqrt{\lambda}} e^{i\chi_1}, \tag{22}$$

where χ_1 is given by

$$\chi_1 = \int_{t_0}^{t} \dot{\chi}(\tau)\alpha_1(\tau)[1 + \lambda(\tau)]\mathrm{d}\tau\,, \tag{23}$$

namely,

$$\dot{\chi}_1=\dot{\chi}\alpha_1(1+\lambda)\,. \tag{24}$$

Here use has been made of the relationship

$$\dot{\chi}(u_1-u_2)=i\dot{\chi}\alpha_1(1+\lambda)-\frac{1}{2}\frac{\dot{\lambda}}{\lambda}. \tag{25}$$

We thus find

$$u_3=\lambda_1 u_1\,, \tag{26}$$

where

$$\lambda_1=\frac{1+\sqrt{\lambda}e^{i\chi_1}}{1-\dfrac{1}{\sqrt{\lambda}}e^{i\chi_1}}. \tag{27}$$

Again a further solution of the Riccati equation when three independent special solutions are known is given by

$$\frac{u-u_1}{u-u_2}=C_3\frac{u_3-u_1}{u_3-u_2}, \tag{28}$$

where C_3 is a constant of integration. A fourth special solution is obtained by choosing

$$C_3=-i\,. \tag{29}$$

Thus we find a fourth special solution in the form

$$u_4=\lambda_2 u_1\,, \tag{30}$$

where

$$\lambda_2=\frac{1-i\sqrt{\lambda}e^{i\chi_1}}{1+i\dfrac{1}{\sqrt{\lambda}}e^{i\chi_1}}. \tag{31}$$

Thus we find four independent special solutions of the Riccati equation (12). Noticing that the magnetization vectors derived from these four special solutions are not always independent, we expect that three of them are independent and form a fundamental system.

III. THE FUNDAMENTAL SYSTEM OF THE HOMOGENEOUS BLOCH EQUATION

The special solutions of the Riccati equation (6) are found in terms of u_i $(i=1,2,3,4)$, which are given by Eqs. (14), (20), (26), and (30), such that

$$\xi_i=-ie^{i\psi}u_i \quad (i=1,2,3,4)\,. \tag{32}$$

The normalized magnetization vectors, $\vec{m}^{(i)}$ $(i=1,2,3,4)$, corresponding to the special solutions (32) are obtained from the definition of ξ, Eq. (4), and given by

$$m_1^{(i)}=\frac{\xi_i+\xi_i^*}{1+\xi_i\xi_i^*}, \tag{33}$$

$$m_2^{(i)} = -i\frac{\xi_i - \xi_i^*}{1+\xi_i\xi_i^*}, \tag{34}$$

and

$$m_3^{(i)} = -\frac{1-\xi_i\xi_i^*}{1+\xi_i\xi_i^*}. \tag{35}$$

Writing out Eqs. (33), (34), and (35), we find the magnetization vectors as follows:

$$\vec{m}^{(1)} = -\vec{m}^{(2)} \tag{36}$$

and

$$\vec{m}^{(1)},$$

$$m_1^{(1)} = (1-\lambda_0)(\alpha_1\cos\psi + \beta_1\sin\psi), \tag{37}$$

$$m_2^{(1)} = (1-\lambda_0)(\alpha_1\sin\psi - \beta_1\cos\psi), \tag{38}$$

$$m_3^{(1)} = \lambda_0, \tag{39}$$

$$\vec{m}^{(3)},$$

$$m_1^{(3)} = \sqrt{\lambda}[(-\alpha_1\lambda_0\cos\chi_1 + \beta_1\sin\chi_1)\cos\psi - (\alpha_1\sin\chi_1 + \beta_1\lambda_0\cos\chi_1)\sin\psi], \tag{40}$$

$$m_2^{(3)} = \sqrt{\lambda}[(\alpha_1\sin\chi_1 + \beta_1\lambda_0\cos\chi_1)\cos\psi + (-\alpha_1\lambda_0\cos\chi_1 + \beta_1\sin\chi_1)\sin\psi], \tag{41}$$

$$m_3^{(3)} = \frac{1}{\sqrt{\lambda}}(1-\lambda_0)\cos\chi_1, \tag{42}$$

and

$$\vec{m}^{(4)},$$

$$m_1^{(4)} = \sqrt{\lambda}[-(\alpha_1\lambda_0\sin\chi_1 + \beta_1\cos\chi_1)\cos\psi + (\alpha_1\cos\chi_1 - \beta_1\lambda_0\sin\chi_1)\sin\psi], \tag{43}$$

$$m_2^{(4)} = \sqrt{\lambda}[(-\alpha_1\cos\chi_1 + \beta_1\lambda_0\sin\chi_1)\cos\psi - (\alpha_1\lambda_0\sin\chi_1 + \beta_1\cos\chi_1)\sin\psi], \tag{44}$$

$$m_3^{(4)} = \frac{1}{\sqrt{\lambda}}(1-\lambda_0)\sin\chi_1, \tag{45}$$

where λ_0 is given by

$$\lambda_0 = -\frac{1-\frac{1}{\lambda}}{1+\frac{1}{\lambda}}. \tag{46}$$

As is obvious from Eq. (36), the magnetization vector corresponding to the second special solution is not independent. Thus we find the fundamental system in terms of $\vec{m}^{(i)}$ $(i=1,3,4)$.

Differentiating the magnetization vectors (37)–(45) with respect to time and using the first-order nonlinear differential equations (15), (16), and (19) together with the definitions (7), (8),

(11), (17), (24), and (46), we can show, after some tedious but straightforward manipulation, that the magnetization vectors (37)–(45) obey the homogeneous Bloch equation (2). Note that using Eq. (19) we find

$$\dot{\lambda}_0 = 2\dot{\chi}\beta_1(1-\lambda_0)\,. \tag{47}$$

For later convenience, we replace from now on $\vec{m}^{(3)}$ and $\vec{m}^{(4)}$ by $\vec{m}^{(2)}$ and $\vec{m}^{(3)}$, respectively. We thus define the fundamental matrix K by

$$(K)_{ij} = K_{ij} = m_i^{(j)} \quad (i,j=1,2,3)\,. \tag{48}$$

The cofactors of each element of the fundamental matrix are given by

$$K_{ij}^C = K_{ij} \quad (i,j=1,2,3)\,, \tag{49}$$

where K_{ij}^C is the cofactor of K_{ij}. This beautiful relationship is obtained after a straightforward manipulation using Eqs. (37)–(46) and the useful relation

$$(1-\lambda_0)\frac{1}{\lambda} - (1+\lambda_0) = 0\,. \tag{50}$$

Thus, we find that the determinant of the fundamental matrix is

$$\det K = K_{i1}K_{i1}^C = K_{i2}K_{i2}^C = K_{i3}K_{i3}^C = 1\,, \tag{51}$$

where we assume summation over repeated indices. Here we have used the fact that the magnetization vectors are normalized. The fundamental matrix is nonsingular and therefore the three special solutions of the homogeneous Bloch equation, $\vec{m}^{(i)}$ $(i=1,2,3)$, are linearly independent.

The homogeneous Bloch equation (2) is written in the matrix form

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{m} = A\,\vec{m}\,, \tag{52}$$

where the normalized magnetization vector $\vec{m}$ is a column vector and A is a 3×3 matrix given by

$$A = \begin{pmatrix} 0 & \gamma B_3 & -\gamma B_2 \\ -\gamma B_3 & 0 & \gamma B_1 \\ \gamma B_2 & -\gamma B_1 & 0 \end{pmatrix}. \tag{53}$$

The homogeneous Bloch equation turns out to be

$$\dot{K}_{ij} = \dot{m}_i^{(j)} = A_{ik}m_k^{(j)} = A_{ik}K_{kj} \quad (i,j=1,2,3)\,, \tag{54}$$

where

$$(A)_{ij} = A_{ij}\,. \tag{55}$$

We thus find

$$\dot{K} = AK\,. \tag{56}$$

Differentiating the determinant of the fundamental matrix with respect to time, we find

$$\det \dot{K} = \dot{K}_{ij}K_{ij}^C = A_{ik}K_{kj}K_{ij}^C = A_{ik}\delta_{ki}\det K = \mathrm{tr}\,A\,\det K\,, \tag{57}$$

where

$$K_{ik}K^{C}_{jk}=\delta_{ij}\det K\,. \tag{58}$$

The solution of the differential equation (57) is

$$\det K=\det K(t_0)\exp\left[\int_{t_0}^{t}\mathrm{tr}\,A(\tau)\,\mathrm{d}\tau\right], \tag{59}$$

with

$$\mathrm{tr}\,A=0\,. \tag{60}$$

Thus we find that Eq. (51) is exactly the solution we want.

The inhomogeneous Bloch equation has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{m}=A\vec{m}+\vec{b}\,, \tag{61}$$

where the column vector $\vec{b}$ is given by

$$b_i=-\frac{m_i}{T_2}\quad(i=1,2) \tag{62}$$

and

$$b_3=-\frac{m_3-m_0}{T_1}, \tag{63}$$

where T_i $(i=1,2)$ are the relaxation times and m_0 is the equilibrium magnetization vector.

The fundamental system of the homogeneous Bloch equation is a set of three linearly independent magnetization vectors. Using the fundamental matrix K defined by Eq. (48), the unique solution to the inhomogeneous system (61) is given by[4]

$$\vec{m}=KK^{-1}(t_0)\vec{m}(t_0)+K\int_{t_0}^{t}K^{-1}(\tau)\vec{b}(\tau)\,d\tau\,, \tag{64}$$

where the inverse matrix of K is defined by

$$K^{-1}=\frac{\mathrm{adj}\,K}{\det K}, \tag{65}$$

with

$$(\mathrm{adj}\,K)_{ij}=K^{C}_{ji}\,. \tag{66}$$

Using Eq. (48) we find

$$K^{-1}=K^{T}\,. \tag{67}$$

This means that the fundamental matrix is an orthogonal matrix with

$$\det K=1\,. \tag{68}$$

IV. THE SPECIAL SOLUTIONS OF THE RICCATI EQUATION

To find a general solution of the Riccati equation (12), we have to solve the system of two first-order nonlinear differential equations (15) and (16). Combining them yields

$$\beta_1=\frac{\dot{\alpha}_1}{2\dot{\chi}(\alpha_1-a)} \tag{69}$$

and

$$\ddot{\alpha}_1[2\dot{\chi}(\alpha_1-a)]-\dot{\alpha}_1\left\{\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)[2\dot{\chi}(\alpha_1-a)]-2\dot{\chi}a\left(\frac{\dot{a}}{a}\right)\right\}-3\dot{\chi}(\dot{\alpha}_1)^2+\{\alpha_1[2\dot{\chi}(\alpha_1-a)]$$
$$-\dot{\chi}(1+\alpha_1^2)\}[2\dot{\chi}(\alpha_1-a)]^2=0\,. \tag{70}$$

This highly nonlinear differential equation (70) seems very difficult to solve in general. This is the main difficulty of solving the homogeneous Bloch equation.

Now we briefly review the soluble cases in this section. Two special solutions of the Riccati equation (12) have been found so far.[1,3] These solutions were obtained by imposing constraints

(1) $a=\alpha=\alpha_1$, for the case in Ref. 3 and
(2) $a=(\alpha_1^2+\alpha^2)/2\alpha_1$ and $\alpha_1=\sqrt{\alpha^2+2[1+\tan^2(\beta\chi)]}$, for the case in Ref. 1,

where α and β are arbitrary real constants satisfying:

$$\beta^2-\alpha^2=1\,. \tag{71}$$

The differential equation (16) for both cases reduces to

$$\dot{\beta}_1=\dot{\chi}(\beta^2+\beta_1^2)\,, \tag{72}$$

where we have used the useful relationship

$$\alpha_1(\alpha_1-a)=1+\tan^2(\beta\chi)\,. \tag{73}$$

We thus find the solution of Eq. (72) as

$$\beta_1=\beta\tan(\beta\chi)\,. \tag{74}$$

Notice that χ_1 defined by Eq. (23) can be evaluated and given by

$$\chi_1=\tan^{-1}\left[\frac{\beta\tan(\beta\chi)}{\alpha}\right] \quad \text{for the case (1)}\,, \tag{75}$$

and

$$\chi_1=\frac{\sqrt{2}}{\beta}\ln\left\{\frac{1}{\sqrt{1+\beta^2}}[\alpha_1+\sqrt{2}\tan(\beta\chi)]\right\}-\tan^{-1}\left[\frac{\alpha_1\cot(\beta\chi)}{\beta}\right] \quad \text{for the case (2)}\,. \tag{76}$$

V. CONCLUSIONS

We have found a general form of solution of the inhomogeneous Bloch equation by finding the fundamental system in terms of a solution of the homogeneous Bloch equation which is assumed to be known. In other words, whenever a special solution of the homogeneous Bloch equation is known, a solution of the inhomogeneous Bloch equation is given by Eq. (64) for which the fundamental matrix is of the form (48).

The reason why we have succeeded in finding a general form of the fundamental matrix is due to the fact that the second special solution is obtained in the form of Eq. (20). This is one of the characteristics of the Riccati equation to which the homogeneous Bloch equation reduces.

The problem which remains is the biggest one: to solve the highly nonlinear differential equation (70).

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Confluence expansions of the generalized hypergeometric function

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By confluencing a subset of upper and lower parameters in the generalized hypergeometric function ${}_PF_Q(a_1,\ldots,a_P,c_1,\ldots,c_Q;z)$ with the variable z one obtains a lower-order hypergeometric function in the limit when the confluence parameters go to infinity. It is shown that this function is the first term in a convergent expansion in terms of functions of the same type with parameters increasing stepwise by integers ν and coefficients which are polynomials in the reciprocals of the confluence parameters. These polynomials have nonvanishing lowest degree terms whose power increases with ν. The expansion can hence be used to derive asymptotic expansions for large but finite absolute values of the confluence parameters. [DOI: 10.1063/1.1629777]

I. INTRODUCTION AND SUMMARY

The hypergeometric function ${}_2F_1(a,b,c;z)$ and its various limiting and special cases are of great importance in mathematical and theoretical physics. By confluence of one or two of the upper parameters (say b, and a and b, respectively) with the variable z one obtains the confluent hypergeometric function ${}_1F_1(a,c;z)$, or the function ${}_0F_1(c;z)$, closely related to the Bessel function. In some applications one may be interested in the behavior of the hypergeometric function when the confluence is not taken "all the way," i.e., to obtain an asymptotic expansion in $1/b$, or $1/a$ and $1/b$, in the two cases mentioned. This has been done in two recent articles,[1,2] where the asymptotic expansions including second order have been derived and applied to a study of various aspects of the Coulomb excitation of atomic systems by passing charged particles.

In a previous article[3] I showed that in the second of the cases mentioned above (the one addressed in Ref. 1) the asymptotic expansion could be derived from a convergent expansion of the hypergeometric function in Bessel functions, with expansion coefficients which are polynomials in $1/a$ and $1/b$; rearrangement of this convergent expansion would in principle give the asymptotic expansion to any order. In a similar way an asymptotic expansion corresponding to the confluence of the parameter b can be derived; see the end of Sec. II below.

Here, I shall show that by an extension of the method in Ref. 3 one can derive a confluence expansion corresponding to confluence of a general subset of upper and lower parameters in the generalized hypergeometric function defined by the series

$$ {}_PF_Q(a_1,\ldots a_P,c_1,\ldots,c_Q;z)=\sum_{n=0}^{\infty}\frac{(a_1)_n\cdots(a_P)_n}{n!(c_1)_n\cdots(c_Q)_n}z^n,\quad (a)_n=\Gamma(a+n)/\Gamma(a). \tag{1}$$

Provided $P\leqslant Q+1$ (1) defines a function of z and the parameters which is holomorphic for all complex values of the parameters, except nonpositive integer c parameters, and (at least) for $|z|<1$ (or arbitrary complex z if $P\leqslant Q$). If $P>Q+1$ we must assume one of the upper parameters to be equal to a nonpositive integer, say $a_1=-m$, to get a polynomial of degree m in z.

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With the view of confluencing p' of the upper and q' of the lower parameters, we put $P=p+p'$, $Q=q+q'$, divide each of the upper and lower parameter sets into the two corresponding subsets [some subset(s) may be empty], and introduce the notations

$$[a]=a_1,\ldots,a_p,\quad [b]=b_1,\ldots,b_{p'},\quad [c]=c_1,\ldots,c_q,\quad [d]=d_1,\ldots,d_{q'};$$

$$[a+\nu]=a_1+\nu,\ldots,a_p+\nu,\quad p[a]=a_1\cdots a_p;\quad s[a]=a_1+\cdots+a_p; \tag{2}$$

$$f([a])=f(a_1)\cdots f(a_p),\ \text{etc.}$$

Confluencing the b and d parameters with z in each of the terms in the series (1), we get, at least formally, the confluence relation (all b and d parameters go to infinity)

$$\lim_{p+p'}{}_{q+q'}F([a],[b],[c],[d];p[d]z/p[b])={}_pF_q([a],[c];z). \tag{3}$$

We shall see that (3) gives the first term in a convergent series expansion of the following form:

$$\begin{aligned}&{}_{p+p'}F_{q+q'}([a],[b],[c],[d];p[d]z/p[b])\\&\quad=\sum_{\nu=0}^{\infty}(-1)^{\nu}{}_{p'+1}F_{q'}(-\nu,[b],[d];p[d]/p[b])\,\frac{([a])_\nu}{\nu!([c])_\nu}z^\nu\,{}_pF_q([a+\nu],[c+\nu];z).\end{aligned} \tag{4}$$

Here, we assume, as always, that no c or d parameter is a nonpositive integer, so that in particular $p[d]\neq 0$; besides, we assume $p[b]\neq 0$, but a and b parameters may take negative integer values.

Equation (4) is first derived formally by introducing in each term of the series expansion (1) for upper and lower confluence parameters standard integral representations for the gamma functions $\Gamma(b+n)$ and the reciprocals $1/\Gamma(d+n)$, inverting order of summation and integration, and expanding the integrand around the resulting multiple saddle point, assuming in this derivation the b and d parameters real, positive, and large. This gives a $(p'+q')$-dimensional mixed integral representation for the hypergeometric polynomial ${}_{p'+1}F_{q'}(-\nu,\ldots)$, which is useful in the study of this function.

To establish validity of the expansion (4) inside some radius of convergence in z, and for general complex parameters, we first show that it is a formal power series identity if we expand each ${}_pF_q$ function on the right-hand side in a power series and rearrange terms. (In particular, if one of the a parameters is a nonpositive integer, we have a polynomial identity.) It then follows from well-known theorems about series of holomorphic functions that if we get a common nonzero radius of convergence in z for the series on both sides, equality holds inside this radius. This turns out to be always possible, provided the general necessary conditions $P\leqslant Q+1$, $p\leqslant q+1$ are fulfilled. The asymptotic behavior as $\nu\to\infty$ of the functions ${}_pF_q([a+\nu],[c+\nu];z)$ and ${}_{p'+1}F_{q'}(-\nu,[b],[d];p[d]/p[b])$ is studied in the Appendix. It turns out that if $p\leqslant q$ the validity of (4) is given by the convergence radius of the left-hand side: $|p[d]z/p[b]|<1$ if $P=Q+1$, all complex z if $P\leqslant Q$. Compare the end section of Appendix 1, combined with (A13) and (A15). If $p=q+1$, the functions ${}_{q+1}F_q$ have the finite convergence radius 1, and a singularity for $z=1$ with a dominating asymptotic ν behavior $(1-z)^{-\nu}$. As a consequence in this case the factors depending on [a] and [c] in the terms on the right-hand side of (4) have essentially an asymptotic $(z/[1-z])^\nu$ behavior. This means that if $P\leqslant Q$, i.e., $q'-p'\geqslant 1$, we have the conditions $|z|<1$, $|z/(1-z)|<1$, cf. the comment after Eq. (A31). In the case $P=Q+1$, i.e., $q'=p'$ we find from (A25) and (A26) the further condition $|1-p[d]/p[b]||z/(1-z)|<1$ if $|1-p[d]/p[b]|>1$.

As a by-product of the results derived or quoted in the Appendix we get asymptotic estimates, large ν, of the behavior of the generalized hypergeometric polynomials ${}_pF_q(-\nu,.;z)$, generalizing among other things classical results for the Laguerre polynomials.

The dependence on the confluence parameters is contained in the generalized hypergeometric polynomial ${}_{p'+1}F_{q'}(-\nu,[b],[d];p[d]/p[b])=F(-\nu)$, for short. It is easily seen that $F(0)=1$, $F(-1)=0$, and that for $\nu\geqslant 2$ the limiting value of $F(-\nu)$ as all parameters go to infinity is $(1-1)^{\nu}=0$, so that (4) implies (3). To get a polynomial in the reciprocals of all the parameters we can form $F'(-\nu)=([d])_{\nu}/p[d]^{\nu}\,F(-\nu)$, which is seen to be a symmetric polynomial in the reciprocals of the b parameters and the reciprocals of the d parameters, separately, of degrees $p'(\nu-1)$ and $q'(\nu-1)$. If $p'\neq q'$ the largest of these two numbers gives the degree of $F'(-\nu)$. The largest degree terms of this type are seen to come from the last and first terms in the expansion of $F'(-\nu)$ and are $(-1)^{\nu}[(\nu-1)!]^{p'}/p[b]^{\nu-1}$ and $-(\nu-1)[(\nu-1)!]^{q'}/p[d]^{\nu-1}$. If $p'=q'$, so that these two terms are of the same degree, the highest degree terms can be derived to be of the following form:

$$\frac{([d])_{\nu}}{p[d]^{\nu}}F(-\nu)=\cdots[(\nu-1)!]^{p'}(p[b]/p[d]-1)\left[\left(\frac{1}{p[d]}-\frac{1}{p[b]}\right)^{\nu-1}-\frac{1}{p[d]^{\nu-1}}\right]. \tag{5}$$

It could be remarked that the results for $p'\neq q'$ given above can be obtained from (5) by letting $p[d]$ or $p[b]$ go to infinity, in the last case also changing the exponent p' to q'.

To derive from (4) an asymptotic expansion in the reciprocals of the confluence parameters, it is of importance to verify that the lowest degree terms in $F'(-\nu)$, or, which is the same, in $F(-\nu)$, have a degree which increases with ν (they turn out to be of degree $[(\nu+1)/2]$, where $[\cdots]$ here stands for integer part) and to find expressions for these lowest degree terms. To do this directly from the series expression seems less trivial; we do it by a saddle-point estimate—all parameters real, positive, and large—of the multiple integral representation of $F(-\nu)$ obtained in the formal derivation of the expansion (4). The result is different for even and odd ν: (we use the notation $s[1/b^m]=\Sigma_i 1/b_i^{\,m}$, $m=1,2$ etc.)

$$F(-2\kappa)\approx\frac{2^{\kappa}\Gamma(\kappa+1/2)}{\sqrt{\pi}}(s[1/b]-s[1/d])^{\kappa}+\cdots, \tag{6a}$$

$$F(-2\kappa-1)\approx-\frac{2^{\kappa+1}\kappa\Gamma(\kappa+3/2)}{\sqrt{\pi}}(s[1/b]-s[1/d])^{\kappa-1}\left[(s[1/b]-s[1/d])^2-\frac{1}{3}(s[1/b^2]-s[1/d^2])\right]. \tag{6b}$$

These formulas agree with the special case treated in Ref. 3, except for the fact that there is an error in formula (5) in that paper: the factor $\Gamma(2\kappa+1)$ should be replaced by $-\Gamma(2\kappa+2)$. In the derivation of (18) of Ref. 3 the correct form of (5) has been used.

In the second section the details of the derivations indicated above are carried through. We also give the explicit result of the asymptotic expansion in $1/b$ including third order of ${}_2F_1(a,b,c;z/b)$, the case studied in Ref. 2. As already mentioned, in the Appendix the asymptotic behavior or asymptotic bounds as $\nu\to\infty$ of the functions on the right-hand side of (4) are derived.

A final cautionary remark is that in view of the enormous amount of papers treating various aspects of the hypergeometric function and its generalizations, dating back over two centuries, it is possible that expansions such as (4), or at least special cases of it, have been derived earlier. For the usefulness of these expansions for asymptotic estimates it is also essential to know the degree of the lowest order terms, as contained in the relations (6a) and (6b).

In a true asymptotic expansion in reciprocals of a lower confluence parameter evidently in each order all the "previous" ${}_pF_q([a+\nu]\ldots)$ will appear, because of the factor $p[d]^{\nu}/([d])_{\nu}$ difference between $F'(-\nu)$ and $F(-\nu)$. In an explicit computation it might be preferrable to attach this factor to the z-dependent part of the expansion terms.

II. DERIVATION OF FORMULAS (4)–(6)

Let us first make a formal derivation of the expansion (4), not caring about convergence or conditions for inverting summation and integration. Start from the series expansion of the left-hand side of (4)

$$F \equiv {}_{p+p'}F_{q+q'}([a],[b],[c],[d];p[d]z/p[b]) = \sum_{n=0}^{\infty} \frac{([a])_n([b])_n p[d]^n}{n!([c])_n([d])_n p[b]^n} z^n. \tag{7}$$

Here, we assume the confluence parameters b and d real and positive, sometimes even large and going to infinity.

In the sum in (7) we introduce for the confluence Pochhammer symbols standard integral representations for the gamma function and the reciprocal of the gamma function[4] and make a variable change $s=bx$, $t=dy$, as follows:

$$(b)_n = \frac{1}{\Gamma(b)} \int_0^{\infty} ds e^{-s} s^{b+n-1} = \frac{b^{b+n}}{\Gamma(b)} \int_0^{\infty} dx e^{-bx} x^{b+n-1}, \tag{8}$$

$$\frac{1}{(d)_n} = \frac{\Gamma(d)}{2\pi i} \int_{-\infty}^{(0^+)} dt e^t t^{-d-n} = \frac{\Gamma(d)}{d^{d+n-1} 2\pi i} \int_{-\infty}^{(0^+)} dy e^{dy} y^{-d-n}. \tag{9}$$

The integration path in (9) is from $-\infty$ below the real axis (whose negative part is a branch cut for noninteger d) around zero and back to $-\infty$ above the real axis, with the argument of the integration variable zero on the positive real axis.

Introducing (8) and (9) into (7) and inverting order of integration and summation, we get, using the notations introduced in (2) and considering x and y as p'- and q'-dimensional vectors, so that, e.g., $bx=\Sigma_{i=1}^{p'} b_i x_i$, $dx=dx_1 \cdots dx_{p'}$ etc.

$$F = \frac{p[b^b]\Gamma([d])}{\Gamma([b])p[d^{d-1}]} \frac{1}{(2\pi i)^{q'}} \int_0^{\infty} \cdot \int_0^{\infty} dx \int_{-\infty}^{(0^+)} \cdot \int_{-\infty}^{(0)^+} dy e^{-bx+dy}$$
$$\times p[x^{b-1}] p[y^{-d}] \sum \frac{([a])_n}{n!([c])_n} \left(\frac{p[x]}{p[y]} z \right)^n. \tag{10}$$

Here, the sum under the integrations gives, with $X=p[x]$, etc., ${}_pF_q([a],[c];Xz/Y)$. As we shall see, the a and c parameters play a sort of dummy role in the (formal) power series identity (4).

For large positive values of the b and d parameters the dominant factor in the multiple integrand can be written $\exp[-\Sigma b_i f(x_i)+\Sigma d_k f(y_k)]$, where the function $f(\varsigma)=\varsigma-\ln\varsigma=1+(\varsigma-1)^2/2-(\varsigma-1)^3/3+\cdots$ takes its minimum (maximum) value at the saddle point 1 for the x (y) variables along the respective paths of integration. We expand the ${}_pF_q$ function in its Taylor series around the common saddle point 1, and using the easily derived formula for the νth derivative

$${}_pF_q^{(\nu)}([a],[c]:z) = \frac{([a])_\nu}{([c])_\nu} {}_pF_q([a+\nu],[c+\nu];z), \tag{11}$$

we can write

$${}_pF_q([a],[c];Xz/Y) = \sum_{\nu=0}^{\infty} (-1)^\nu (1-X/Y)^\nu \frac{([a])_\nu}{\nu!([c])_\nu} z^\nu \, {}_pF_q([a+\nu],[c+\nu];z). \tag{12}$$

Introducing (12) in (10), inverting order of integration and summation, expanding

$$(1-X/Y)^{\nu}=\sum_{n=0}^{\nu}\frac{(-\nu)_n}{n!}(X/Y)^n, \tag{13}$$

and using the formulas (8) and (9) ''backwards'' in performing the integrations, we get the desired expansion formula (4), where as an intermediate result we obtain an integral representation for the function $F(-\nu)$

$$\begin{aligned}F(-\nu)&\equiv{}_{p'+1}F_{q'}(-\nu,[b],[d];p[d]/p[b])\\&=\frac{p[b^b]\Gamma([d])}{\Gamma([b])p[d^{d-1}]}\frac{1}{(2\pi i)^{q'}}\int_0^{\infty}\cdots\int_0^{\infty}dx\int_{-\infty}^{(0^+)}\cdots\int_{-\infty}^{(0)^+}dy e^{-bx+dy}\\&\quad\times p[x^{b-1}]p[y^{-d}](1-p[x]/p[y])^{\nu}.\end{aligned} \tag{14}$$

To further investigate the formula (4) we use the fact that the two sides, if they both make sense, should have identical power series expansions in z. Comparing the nth power of z, one observes that due to the relation $(a)_k(a+k)_{n-k}=(a)_n$ the expressions containing the a and c parameters are the same on both sides, and introducing the notation $B_n=([b])_n p[d]^n/\{([d])_n p[b]^n\}$ we get, expanding the ${}_{p'+1}F_{q'}$ function

$$B_n=\sum_{k=0}^{n}\binom{n}{k}(-1)^k\sum_{l=0}^{k}\frac{(-k)_l}{l!}B_l,\quad \binom{n}{k}=\frac{n!}{k!(n-k)!}. \tag{15}$$

This relation is an identity, i.e., the right-hand side is equal to B_n independent of the other B_l values: Introduce a new summation variable $k'=k-l$ and use $(-k)_l/l!=(-1)^l\binom{k}{l}$ to rewrite the right-hand side of (15) as

$$\sum_{l=0}^{n}\binom{n}{l}B_l\sum_{k'=0}^{n-l}(-1)^{k'}\binom{n-l}{k'}. \tag{15$'$}$$

Now, the sum over k' is the binomial expansion of $(1-1)^{n-l}$; thus$=0$ except for $l=n$, when the ''sum'' is 1.

Generalizing the crucial property of the a and c parameters used above, we can extract the essentials of relation (4) as a formal power series identity in the form

$$\sum_{n=0}^{\infty}\frac{1}{n!}A_n(a)B_n z^n=\sum_{\nu=0}^{\infty}\left[(-1)^{\nu}\left(\sum_{\mu=0}^{\nu}\frac{(-\nu)_\mu}{\mu!}B_\mu\right)\frac{1}{\nu!}A_\nu(a)z^{\nu}\left(\sum_{m=0}^{\infty}\frac{1}{m!}A_m(a+\nu)z^m\right)\right], \tag{16}$$

where $\{B_n\}$ is an arbitrary sequence and the expressions $\{A_n(a)\}$ defined for (complex) N-dimensional vectors a fulfill $A_{m+n}(a)=A_m(a)A_n(a+m)$, where $a+m$ stands for componentwise addition of m.

One could argue that since our basic derivation of (4) from the integral representations (8) and (9) was only formal anyhow, one could directly use the basic elementary relation (15) and the formula (16) to get (4). This is of course correct, but is somewhat of a ''put'' derivation. Besides, for deriving the lowest order term of the expansion of $F(-\nu)$ in reciprocal powers of the parameters we use the multiple integral representation, which is the starting point for the asymptotic estimate.

Since the verification of the validity of (4) with a common radius of convergence in z is based on asymptotic estimates of the functions on the right-hand side of (4) obtained in the Appendix, and the derivation of the relation (5) giving the highest order terms in the reciprocals of the b and d parameters in the special case $p'=q'$ is rather straightforward, we proceed to the derivation of the crucial formulas (6a) and (6b).

These formulas are obtained by making a first nonvanishing order saddle-point estimate[5] of the integral representation (14) for large positive values of the b and d parameters. The saddle points for both types of integrals is 1, and as noted in the text before formula (11) the dominant exponential function has the argument $\varsigma-\ln\varsigma$ multiplied by the b and d variables. In the spirit of the standard saddle-point estimate procedure we introduce new variables (vector notation!)

$$x=1+\xi/\sqrt{b},\quad y=1+i\,\eta/\sqrt{d}. \tag{17}$$

We should then integrate in the variables ξ and η from $-\infty$ to $+\infty$. Since in the case of odd ν the lowest order terms in ξ and η are odd, and give zero contribution by symmetry, we have to expand to relative order $1/\sqrt{b}$ and $1/\sqrt{d}$ everywhere. For the further calculation it is advantageous to introduce new (''small'') parameters $u_i=-1/\sqrt{b_i}$, $w_k=i/\sqrt{d_k}$. The resulting formulas are easily seen to be even polynomials in these new parameters. Since we want to calculate integrals giving the coefficients of these polynomials, it is clear that for the purpose of this calculation we can assume the u and w parameters to be real. The resulting expression is given for clarity in a mixed vector and component presentation:

$$\begin{aligned}F(-\nu)\approx{}&\frac{p[b^{b-1/2}e^{-b}]\Gamma([d])}{\Gamma([b])p[d^{d-1/2}e^{-d}](2\pi)^{q'}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}d\xi\,d\eta\,e^{-(\xi^2+\eta^2)/2}\\&\times\left[\sum u_i\xi_i+\sum w_k\eta_k-\frac{1}{2}\sum_{i\neq j}u_iu_j\xi_i\xi_j+\frac{1}{2}\sum_{k\neq l}w_kw_l\eta_k\eta_l+\cdots\right]^{\nu}\\&\times\left[1+\sum u_i(\xi_i-\xi_i^3/3)-\sum w_k(\nu\eta_k-\eta_k^3/3)+\cdots\right].\end{aligned} \tag{18}$$

The various terms in the two $[\cdots]$ brackets come from the expansions to first relative order of $p[y]-p[x],1/p[x]p[y]^{\nu}$, and the third power term $-(\varsigma-1)^3/3$ in the dominating exponential obtained in the expression (14).

For the case of even $\nu=2\kappa$, the leading contribution comes from the linear terms in the first $[\cdots]$ raised to power 2κ. Assuming that the u and w parameters are real we can make an orthogonal coordinate transformation of the $p'+q'$ ξ, η variables, taking $(u\xi+w\eta)/\sqrt{u^2+w^2}$ (again vector notation!) as one of the transformed variables, and the other transformed variables as a set of complementary orthogonal expressions, so that the exponent expression $\xi^2+\eta^2$ and the volume product $d\xi d\eta$ are invariant. As noted earlier the result is an even polynomial in the u and w parameters, and can be carried over to the actual expressions for u and w. The integrations are elementary, and using the asymptotic forms of the Γ functions in front of the integrals we obtain as leading asymptotic term

$$F(-2\kappa)\approx\frac{2^{\kappa}\Gamma(\kappa+1/2)}{\sqrt{\pi}}\left(\sum {u_i}^2+\sum {w_k}^2\right)^{\kappa}, \tag{19}$$

which gives (6a).

For the case $\nu=2\kappa+1$, odd, the leading terms are odd, and one has to calculate the next order terms. This can easily be done by suitable differentiations of the previously obtained result for even $\nu=2\kappa+2,2\kappa+4$ with respect to the u and w parameters. The resulting calculations lead to (6b).

The five possible confluence expansions for the ordinary hypergeometric function are

$${}_2F_1(a,b,c,z/b)=\sum_{\nu=0}^{\infty}(-1)^{\nu}\,{}_2F_0(-\nu,b;1/b)\frac{(a)_{\nu}}{\nu!(c)_{\nu}}z^{\nu}\,{}_1F_1(a+\nu,c+\nu;z), \tag{20a}$$

$$ {}_2F_1(a,b,c,cz)=\sum_{\nu=0}^{\infty}(-1)^{\nu}\,{}_1F_1(-\nu,c;c)\,\frac{(a)_{\nu}(b)_{\nu}}{\nu!}z^{\nu}\,{}_2F_0(a+\nu,b+\nu;z), \tag{20b} $$

$$ {}_2F_1(a,b,c,z/ab)=\sum_{\nu=0}^{\infty}(-1)^{\nu}\,{}_3F_0(-\nu,a,b;1/ab)\,\frac{1}{\nu!(c)_{\nu}}z^{\nu}\,{}_0F_1(c+\nu;z), \tag{20c} $$

$$ {}_2F_1(a,b,c,cz/b)=(1-z)^{-a}\sum_{\nu=0}^{\infty}(-1)^{\nu}\,{}_2F_1(-\nu,b,c;c/b)\,\frac{(a)_{\nu}}{\nu!}(z/[1-z])^{\nu}. \tag{20d} $$

$$ {}_2F_1(a,b,c,cz/ab)=e^{z}\sum_{\nu=0}^{\infty}(-1)^{\nu}\,{}_3F_1(-\nu,a,b,c;c/ab)\,\frac{1}{\nu!}z^{\nu}. \tag{20e} $$

Equation (20b) makes sense only if a (or b) is a nonpositive integer.

The three possible confluence expansion formulas for the confluent hypergeometric function ${}_1F_1(a,c:z)$ are obtained by confluencing the b parameter on both sides of the three last relations.

Equation (20c) is the case studied in Ref. 3, with argument and parameter adjusted to give an expansion in Bessel functions, resulting in Eq. (1) of that paper

$$ \frac{(z/2)^{c}}{\Gamma(c+1)}\,{}_2F_1(a,b,c+1;-z^2/4ab)=\sum_{\nu=0}^{\infty}\frac{1}{\nu!}\,{}_3F_0(-\nu,a,b;1/ab)(z/2)^{\nu}J_{c+\nu}(z). \tag{21} $$

Finally, I give the resulting asymptotic expansion including third-order terms in $1/b$ for the case (20a), which is the case addressed in Ref. 2. It is seen that the resulting formula involves ${}_2F_0(-\nu,b;1/b)$ functions with $\nu=2,...,6$, and that the expressions for the highest and lowest order terms given in formulas (5) and (6a) and (6b) suffice to give the necessary terms. If we want to include fourth-order terms, we should go to $\nu=8$, and that would only require explicit calculation of the fourth-order $1/b$ term of $F(-6)$, the middle one of its three terms of order 3, 4, and 5. Since we know the coefficients of the other two powers, we can determine the value of the missing coefficient by calculating the $F(-6)$ function for a special value of b, say $b=1$.

The result to order three is

$$ \begin{aligned} {}_2F_1(a,b,c:z/b)=&\,{}_1F_1(a,c:z)+\frac{(a)_2}{(c)_2}\frac{z^2}{2}\,{}_1F_1(a+2,c+2;z)\,\frac{1}{b}\\ &+\left[\frac{(a)_3}{(c)_3}\frac{z^3}{3}\,{}_1F_1(a+3,c+3;z)+\frac{(a)_4}{(c)_4}\frac{z^4}{8}\,{}_1F_1(a+4,c+4;z)\right]\frac{1}{b^2}\\ &+\left[\frac{(a)_4}{(c)_4}\frac{z^4}{4}\,{}_1F_1(a+4,c+4;z)+\frac{(a)_5}{(c)_5}\frac{z^5}{6}\,{}_1F_1(a+5,c+5;z)\right.\\ &\left.+\frac{(a)_6}{(c)_6}\frac{z^6}{48}\,{}_1F_1(a+6,c+6;z)\right]\frac{1}{b^3}+O\left(\frac{1}{b^4}\right). \end{aligned} \tag{22} $$

Equation (22) agrees to second order with the result of Ref. 2, Eq. (2.7).

APPENDIX

In this appendix we shall often use two different asymptotic estimates of the Pochhammer symbol $(a+\nu)_n=\Gamma(a+\nu+n)/\Gamma(a+\nu)$, which can be derived from the asymptotic estimate of $\Gamma(a+z)$ as $z\to\infty, |\arg z|<\pi$

$$ \Gamma(a+z)=\sqrt{2\pi}(z/e)^{z}z^{a-1/2}[1+A(a)/z+B(a)/z^2+O(1/z^3)], \tag{A1} $$

where $A(a)=1/12+a(a-1)/2$ and $B(a)$ is a fourth-degree polynomial in a. In (A1) a is assumed finite, or more general, $|a|^2 \ll |z|$.

From (A1) with $z=\nu$ and $z=\nu+n$, we get when $\nu\to\infty$, any positive n

$$(a+\nu)_n=\left(\frac{\nu+n}{e}\right)^n\left(\frac{\nu+n}{\nu}\right)^{\nu+a-1/2}\left[1-A(a)\frac{n}{n+\nu}\frac{1}{\nu}+\frac{n}{n+\nu}O(1/\nu^2)\right]. \tag{A2}$$

If n stays finite, the first correction term is actually of order $1/\nu^2$, the second of order $1/\nu^3$, and (A2) then gives, including the first correction term, the first three terms in the polynomial $(a+\nu)_n=\nu^n+a_1\nu^{n-1}+\cdots$.

Assuming instead $n\to\infty$ and ν finite, or $\nu^2 \ll n$, we get from (A1)

$$(a+\nu)_n=\frac{\sqrt{2\pi}}{\Gamma(a+\nu)}(n/e)^n n^{a+\nu-1/2}[1+A(a+\nu)/n+B(a+\nu)/n^2+O(1/n^3)]. \tag{A3}$$

It should be noted that the definition of $(a+\nu)_n$ as a quotient of gamma functions actually defines $(a+\nu)_n$ as a holomorphic function for general complex n and ν. We shall sometimes use this extension in connection with the estimate of a sum over n by a corresponding integral over (continuous) n, and even deforming the integration path into the complex n plane.

1. Study of the asymptotic behavior, $\nu\to\infty$, of ${}_pF_q([a+\nu],[c+\nu],z)$

Unless one of the a's is a nonpositive integer, we must have $p\leqslant q+1$.

Let us first state the result in some simple cases, using well-known transformation formulas for the hypergeometric and confluent hypergeometric functions

$${}_1F_0(a+\nu;z)=(1-z)^{-a-\nu}, \tag{A4a}$$

$$\begin{aligned}{}_2F_1(a+\nu,b+\nu,c+\nu;z)&=(1-z)^{c-a-b-\nu}\,{}_2F_1(c-a,c-b,c+\nu;z)\\&=(1-z)^{c-a-b-\nu}[1+O(1/\nu)],\end{aligned} \tag{A4b}$$

$${}_1F_1(a+\nu,c+\nu;z)=e^z\,{}_1F_1(c-a,c+\nu;-z)=e^z+O(1/\nu)], \tag{A4c}$$

$${}_0F_1(c+\nu;z)=1+\frac{z}{c+\nu}\sum_{n=1}\frac{z^{n-1}}{n!(c+\nu+1)_{n-1}}=1+O(1/\nu). \tag{A4d}$$

The order terms $O(1/\nu)$ in (A4c) and (A4d) hold uniformly in z for z bounded, say $|z|<R$, but the "order constant" will increase with increasing R.

From (A2) follows for large ν

$$([a+\nu])_n=\left(\frac{\nu+n}{e}\right)^{pn}\left(\frac{\nu+n}{\nu}\right)^{p(\nu-1/2)+s[a]}\left[1-s[A(a)]\frac{n}{n+\nu}\frac{1}{\nu}+\cdots\right]. \tag{A5}$$

This implies that one can for large ν "multiply" and "divide" Pochhammer symbols between numerator and denominator in the expansion coefficients of the ${}_pF_q$ functions.

One should thus expect that asymptotically for large ν

$${}_{q+1}F_q([a+\nu],[c+\nu];z)\approx{}_1F_0(s[a]-s[c]+\nu;z)=(1-z)^{-s[a]+s[c]-\nu}, \tag{A6a}$$

$${}_qF_q([a+\nu],[c+\nu];z)\approx{}_1F_1(s[a]+\nu,s[c]+\nu;z)=e^z+O(1/\nu), \tag{A6b}$$

$${}_pF_{p+1}([a+\nu],[c+\nu];z)\approx{}_0F_1(s[c]-s[a]+\nu;z)=1+O(1/\nu). \tag{A6c}$$

For $q\geqslant p+1$ one finds in the same way as in (A4d) that

$$ {}_pF_{p+l}([a+\nu],[c+\nu];z)=1+O(1/\nu^l), l\geqslant 1. \tag{A7}$$

$O(1/\nu^l)$ should be interpreted in the way that is indicated after (A4d).

Using (A5) it is possible to show the estimates (A6b)–(A6c) and (A7); to prove (A6a) seems to be more difficult. However, all the estimates in (A6) and (A7) have been derived by Knottnerus,[6] as quoted and presented in Ref. 7, Chap. VII, 7.3, Eqs. (3), (4), and (5).

So, summing up we see that the functions ${}_pF_q([a+\nu],[c+\nu];z)$ influence the convergence of the right-hand side of (4) only in the limiting case $p=q+1$, where, besides the necessary restriction $|z|<1$, the essential asymptotic behavior is $(1-z)^{-\nu}$.

2. Asymptotic behavior, $\nu\to\infty$, of ${}_{p'+1}F_{q'}(-\nu,[b],[d],p[d]/p[b])$

Although some of the results below are contained in, or can be derived from results presented in Ref. 7, Chap. VII, I give an independent presentation, only sometimes checking against or using results from this reference.

For simplicity of notation let us drop the primes on p' and q' and use $-n$ instead of $-\nu$ as the first parameter and ν as the summation index. Recall that according to the assumptions stated after Eq. (4) $p[d]/p[b]$ is finite and stays away from zero. We can write for a general argument z

$$ {}_{p+1}F_q(-n[b],[d]:z)=\frac{\Gamma([d]}{\Gamma([b])}\sum_{\nu=0}^{n} A_\nu(n)(-z)^\nu, \tag{A8}$$

where from (A1), with the notation $k=q-p$

$$ A_\nu(n)=\binom{n}{\nu}\frac{\Gamma([b+\nu])}{\Gamma([d+\nu])}=\binom{n}{\nu}(2\pi)^{-k/2}\left(\frac{\nu}{e}\right)^{-k\nu}\nu^{s[b]-s[d]+k/2}[1+O(1/\nu)]. \tag{A9}$$

As we shall see, the main contribution to the asymptotic behavior for large n of the ${}_{p+1}F_q(-n,\ldots)$ function comes from terms with large ν (at worst a fractional power of n, see below), so that (A9) can be used in the estimate. This means that the asymptotic form of such a function, apart from the gamma function factors in front of (A8), depends only on k and the combination $s[b]-s[d]$ of parameters.

The binomial coefficient $\Gamma(n+1)/\Gamma(\nu+1)\Gamma(n-\nu+1)$ satisfies the inequality

$$ 1\leqslant\binom{n}{\nu}\leqslant\binom{n}{n/2}\approx\sqrt{2/\pi n}\cdot 2^n, \tag{A10}$$

and has the asymptotic behavior, large ν and $n-\nu$

$$ \binom{n}{\nu}=\frac{\exp\left[\nu(\ln(n/\nu)+1)-(\nu^2/n)\sum_{\mu=0}^{\infty}\frac{1}{(\mu+1)(\mu+2)}\left(\frac{\nu}{n}\right)^\mu\right]}{\sqrt{2\pi\nu(1-\nu/n)}}\left[1+O\left(\max\left\{\frac{1}{\nu},\frac{1}{n-\nu}\right\}\right)\right], \tag{A11}$$

and in particular in a more symmetrical form between ν and $n-\nu$

$$ \binom{n}{yn}\approx\frac{\exp\{n[-y\ln y-(1-y)\ln(1-y)]\}}{\sqrt{2\pi ny(1-y)}}[1+O(1/n)],\quad \varepsilon<y<1-\varepsilon. \tag{A12}$$

If we ignore the actual value of $z=p[d]]p[b]$ we see from (A8) and (A9) that the most ''unfavorable'' case is z real and negative, since all terms then have essentially the same sign; this is strictly true if all the parameters $[b]$ and $[d]$ are positive. The estimate for this case then gives a majorization for general parameters and general complex z (which we shall assume stays away a

positive distance from zero) as argument. The asymptotic estimates in (A9)–(A12) then imply a qualitatively different behavior for the two cases $k>0$ and $k<0$. In the first case the terms in the lower part of the series give the dominant contribution, whereas in the second case the final terms dominate. $k=0$ is an intermediate case where there is a sharp peak of dominant terms near the middle of the series; here, the estimate in (A12) turns out to be useful.

We start with the case with negative k, where the dominant contribution for large n is expected to come from the end of the series, cf. (A9). To explore this we use the "reversed summation" formula, following from $(b)_n=(-1)^{n-\nu}(b)_\nu(1-b-n)_{n-\nu}$

$$ {}_{p+1}F_q(-n,[b],[d];z)=\frac{([b])_n}{([d])_n}(-z)^n\,{}_{q+1}F_p(-n,[1-d-n],[1-b-n];(-1)^{p-q}/z). \tag{A13}$$

Since

$$ {}_{q+1}F_p(-n,[1-d-n],[1-b-n];y)=\sum_{\nu=0}^{n}\frac{(-n)_\nu([1-d-n])_\nu}{([1-b-n])_\nu}\frac{y^\nu}{\nu!}, \tag{A14}$$

we would, by going to the limit in each term, expect the following asymptotic behavior as $n\to\infty$:

$$ {}_{q+1}F_{q+1}(-n,\ldots:y)\approx e^y;\quad {}_{q+1}F_p(-n,\ldots;y)\approx 1 \ \text{ for } \ p-q\geqslant 2. \tag{A15}$$

This behavior can be verified by a closer examination, as follows.

We write

$$ {}_{q+1}F_{q+1}(-n,[1-d-n],[1-b-n];y)=\sum_{\nu=0}^{n}a_\nu(n)\frac{y^\nu}{\nu!}, \tag{A16}$$

where—use $(b)_\nu=(-1)^\nu(1-b-\nu)_\nu$—

$$\begin{aligned} a_\nu(n)&=(-n)_\nu([1-d-n])_\nu/([1-b-n])_\nu\\ &=\frac{\Gamma(n+1)\Gamma([n+d])\Gamma([n-\nu+b])}{\Gamma(n-\nu+1)\Gamma([n-\nu+d])\Gamma([n+b])}\\ &\approx(1-\nu/n)^{s[b]-s[d]-1}\ \text{ for } \ n \ \text{ and } \ n-\nu \ \text{ large.} \end{aligned} \tag{A17}$$

Subtracting the series for the exponential and making obvious majorizations, we get

$$ \left|{}_{q+1}F_{q+1}(-n,\ldots;y)-e^y\right|\leqslant\sum_{\nu=0}^{m}|a_\nu(n)-1|\frac{|y|^\nu}{\nu!}+\sum_{m+1}^{n}|a_\nu(n)|\frac{|y|^\nu}{\nu!}+\sum_{m+1}^{\infty}\frac{|y|^\nu}{\nu!}, \tag{A18}$$

where m is large but small compared to n. Evidently, assuming $|y|<R$ and choosing m large enough, the last term can be made as small as we like, and by then taking n large enough the first term can also be made as small as desired. To handle the middle term one can check that the terms are monotonously decreasing with increasing ν, for large enough m, and divide the summation into two parts, using the asymptotic estimate in (A17) in the first part and monotonicity in the second, giving

$$ \sum_{m+1}^{n}\cdots<\max[1,2^{1-s[\mathrm{Re}\,b]+s[\mathrm{Re}\,d]}]\sum_{m+1}^{n/2}\frac{|y|^\nu}{\nu!}+(n/2)a_{n/2}(n)\frac{|y|^{n/2}}{(n/2)!}. \tag{A19}$$

Evidently this term can also be made arbitrarily small by picking for a given m a large enough n.

A similar argument for the case $p-q\geqslant 2$ verifies the second estimate in (A15). It should be observed that these estimates assume y bounded, which means in the actual application that the argument $p[d]/p[b]$ should stay away from zero, as we have already assumed.

For $k\geqslant 0$ we put temporarily $z=-x$, x real and positive, in (A8), and find the location of the peak value of the terms by the condition

$$1/x=A_{\nu+1}(n)/A_{\nu}(n)=\frac{n-\nu}{\nu+1}\frac{p[b+\nu]}{p[d+\nu]}\approx\frac{n-\nu}{\nu^{k+1}},\quad \text{large } n \text{ and } \nu. \tag{A20}$$

For $k=0$ we then get the maximum for $\nu_0=nx/(1+x)$, for $k\geqslant 1$ $\nu_0=\sqrt[k+1]{nx}$.

Let us first look at the case $k=0$. Generalizing to a complex z and approximating the sum by an integral, using the asymptotic approximations (A9) and (A12) and changing integration variable by $\nu=ny$ we get, with $A=s[b]-s[d]$

$$\sum_{\nu=0}^{n}A_{\nu}(n)z^{\nu}\approx\sum_{\nu=0}^{n}\binom{n}{\nu}\nu^{A}z^{\nu}\approx\int_0^n\binom{n}{\nu}\nu^{A}z^{\nu}\,d\nu\approx\frac{n^{A+1/2}}{\sqrt{2\pi}}\int_0^1\frac{e^{ng(y)}}{\sqrt{y(1-y)}}y^{A}dy, \tag{A21}$$

where

$$g(y)=-y\ln y-(1-y)\ln(1-y)+y\ln z, \tag{A22}$$

goes from 0 to $\ln z$ as y goes from 0 to 1. For $z=x$, real and positive, $g(y)$ takes its maximum value $\ln(1+x)$ at $\nu_0/n=x/(1+x)$. In the general case we get $g'(y_0)=0$ for $y_0=z/(1+z)$, and $g(y_0)=\ln(1+z)$, $g''(y_0)=-(1+z)^2/z$. So, we can write

$$g(y)=\ln(1+z)-\frac{(1+z)^2}{2z}(y-y_0)^2+\cdots \tag{A23}$$

in the vicinity of the saddle point of the dominating factor in the integral. Extending the integral to complex y values, and using the standard saddle-point asymptotic evaluation of the integral, introducing a new integration variable $t=(1+z)\sqrt{n/2z}(y-y_0)$, we get the asymptotic estimate

$$\int_0^1\frac{e^{ng(y)}}{\sqrt{y(1-y)}}y^{A}dy=\sqrt{2\pi/n}(1+z)^{n-A}z^{A}[1+O(1/n)], \tag{A24}$$

which finally leads to the estimate

$${}_{p+1}F_p(-n,[b],[d];-z)=\frac{\Gamma([d])}{\Gamma([b])}(nz)^{s[b]-s[d]}(1+z)^{n-s[b]+s[d]}[1+O(1/n)]. \tag{A25}$$

The error estimate $O(1/n)$ comes from (A9), (A11), and the two approximations in (A21) and (A24): the approximation of a sum by an integral—in most cases seen the other way around—gives a relative error of the order of the discretization interval squared times the quotient of the second derivative of the function to the function itself, which gives $(1/\sqrt{n})^2\cdot 1$; and the next to leading term in the evaluation of the integral in (A24), which is also of relative order $1/n$ $\propto(1/\sqrt{n})^2$, since an integral over odd powers of t gives zero by symmetry.

The condition for the application of the saddle-point evaluation in (A24) is that $\mathrm{Re}\,g(y)$ takes its maximum value on the deformed integration path in the saddle point y_0, which means $\ln|1+z|>\ln|z|$, $\ln|1+z|>0$, i.e., $|1+z|>\max(1,|z|)$. Expressed in the argument $\varsigma=-z$ this means the left half-plane $\mathrm{Re}\,\varsigma<1/2$ outside the circle $|\varsigma-1|=1$.

Equation (A25) can be shown to be correct under the weaker condition $|1+z|>1$ according to the result in Ref. 7 7.4, (8), p. 265. In this reference a completely different and more rigorous

derivation of the asymptotic behavior is given. I have chosen to reproduce my own derivation as a test for the similar derivation in the cases $k>0$, where the results are not given except for $k=1$, at least not explicitly, in Ref. 7.

For $|1+z|<1$, it is shown in the same formula that the dominating asymptotic behavior is proportional to $(nz)^{-b'}$, where b' is the b parameter with the numerically smallest real part. If several have the same real part, there contributions are added, with coefficients depending on the b and d parameters. From our point of view the essential result is that, being powers of n, they don't influence the convergence of the right-hand side of (4).

For the case $p=1$, the formula reads ($|1-\varsigma|<1$)

$$ {}_2F_1(-n,b,d;\varsigma)=\frac{\Gamma(d)}{\Gamma(d-b)}(n\varsigma)^{-b}[1+O(1/n)], \tag{A26}$$

and can, for the restricted domain, be derived from (A25) by the transformation formula $F(-n,b,d:z)=(1-z)^nF[-n,d-b,d;z/(z-1)]$. For this special case (A25) and (A26) can be verified by asymptotic estimates of one of the standard integral representations of the hypergeometric function, involving integration from 0 to 1 over the integrand $(1-t)^{b-1}(1-t)^{d-b-1}(1-tz)^n$, simplest in the case where $\mathrm{Re}\,d>\mathrm{Re}\,b>0$. The dominant asymptotic contribution comes from the integration near 1, or 0, in the case (A25), or (A26), respectively.[8]

Let us now look at the cases with $k\geqslant 1$. Here, we have again

$$ {}_{p+1}F_{p+k}(-n,[b],[d];-z)=\frac{\Gamma([d])}{\Gamma([b])}\sum_{\nu=0}^{n}A_\nu(n)z^\nu. \tag{A27}$$

For large n and $z=x$, real and positive, the maximum term of the sum corresponds, as we have seen from (A20), to $\nu_0=\sqrt[k+1]{nx}$. With the aim of approximating the sum with an integral, we write $\nu=t\nu_0$, $0<t<n/\nu_0$, put $z=x\cdot e^{i\varphi}$, $|\varphi|<\pi$, and combine (A9) and (A11) to obtain

$$\begin{aligned}\ln[A_\nu(n)z^\nu]=&-(k+1)\nu_0 t[\ln t-1-i\varphi/(k+1)]-(1/2n)\nu_0{}^2t^2+[s[b]-s[d]\\&+(k-1)/2](\ln\nu_0+\ln t)-\ln(2\pi)^{(k+1)/2}+O(1/\nu)+O(\nu^3/n^2).\end{aligned} \tag{A28}$$

The dominating terms of order $\nu_0\ln\nu_0$ from (A9) and (A11) have been canceled, and the leading term of order ν_0 is multiplied with the function $f(t)=t[\ln t-1-i\varphi/(k+1)]$, which goes from 0 at $t=0$ to ∞ at $t=\infty$. $f'(t)=0$ for $t=t_0=e^{i\varphi/(k+1)}$, which corresponds to a negative $\mathrm{Re}\,f(t_0)=-\cos[\varphi/(k+1)]$. $f(t)$ can be expanded around t_0 as $f(t)=-t_0+(t-t_0)^2/2t_0-(t-t_0)^3/6t_0^2+\cdots$. Making a standard asymptotic saddle-point evaluation of the integral corresponds to introducing a new variable by $t-t_0=\tau/\sqrt{(k+1)\nu_0/t_0}$, integrating the resulting function $e^{-\tau^2/2}$ from $-\infty$ to $+\infty$ while putting $t=t_0$ in all other factors of the integrand. Since we have the partly symbolic differential relation ''$d\nu$''$=\nu_0dt=\sqrt{\nu_0t_0/(k+1)}d\tau$, we can estimate

$$\sum_\nu A_\nu(n)z^\nu\approx\nu_0\int_0^{n/\nu_0}\cdots dt\approx\sqrt{\nu_0t_0/(k+1)}\int_{-\infty}^{\infty}\cdots d\tau, \tag{A29}$$

which finally leads to the asymptotic estimate

$$\sum_{\nu=0}^{n}A_\nu(n)z^\nu=\frac{1}{(2\pi)^{k/2}\sqrt{k+1}}e^{(k+1)\nu_0t_0}e^{-\nu_0^2t_0{}^2/2n}(\nu_0t_0)^{s[b]-s[d]+k/2}[1+O(1/\nu_0)]. \tag{A30}$$

The error estimate $O(1/\nu_0)$ comes from (A9), (A11), and the two approximations in (A29) and (A30): the approximation of a sum by an integral—as argued earlier—gives a relative error of the order of the discretization interval squared times the quotient of the second derivative of the function to the function itself, which, if seen relative to the integral over t, gives $(1/\nu_0)^2\cdot\nu_0$ (or in

the τ variable $(1/\sqrt{\nu_0})^2 \cdot 1)$, and the next to leading term in the asymptotic saddle-point estimate of the integral which is also of relative order $1/\nu_0 \propto (1/\sqrt{(k+1)\nu_0})^2$, since an integral over odd powers of τ gives zero by symmetry.

From (A30) we get for the generalized hypergeometric polynomial the estimate for large n, $k \geqslant 1$, and $|\arg z| < \pi$

$$ {}_{p+1}F_{p+k}(-n,[b].[d];-z) = \frac{\Gamma([d])}{\Gamma([b])} \frac{1}{(2\pi)^{k/2}\sqrt{k+1}} (nz)^{[s[b]-s[d]+k/2]/(k+1)} e^{(k+1)^{k+1}\sqrt{nz}} \times e^{-z/2\delta_{1k}} [1 + O(1/^{k+1}\sqrt{nx})]. \tag{A31} $$

Equation (A31) shows that for the cases $k \geqslant 1$ the functions ${}_{p'+1}F_{q'}(-\nu,\ldots)$ give a harmless, slower than exponential ν behavior to the convergence of the right-hand side series in Eq. (4).

Finally, we shall make a comment on the special case of (A31) with $k=1$, $p=0$:

$$ {}_1F_1(-n,d;-z) = \frac{\Gamma(d)}{2\sqrt{\pi}} (nz)^{1/4-d/2} e^{-z/2} e^{2\sqrt{nz}} [1 + O(1/\sqrt{nz})]. \tag{A32} $$

This function is essentially a generalized Laguerre polynomial

$$ L_n^{\alpha}(x) = \frac{\Gamma(n+\alpha+1)}{\Gamma(\alpha+1)n!} {}_1F_1(-n,\alpha+1;x) \approx \frac{n^{\alpha}}{\Gamma(\alpha+1)} {}_1F_1(-n,\alpha+1;x). \tag{A33} $$

Some known asymptotic formulas, large n, for the Laguerre polynomial lead to the following corresponding formulas for the confluent hypergeometric polynomial: Fejer's formula[9] for the behavior on the positive real axis

$$ {}_1F_1(-n,d;x) = \frac{\Gamma(d)}{\sqrt{\pi}} (nx)^{1/4-d/2} e^{x/2} \cos[2\sqrt{nx} + (1/4 - d/2)\pi] + O(n^{1/4-d/2}), \tag{A34} $$

valid for fixed positive x, or uniformly in a finite interval staying away from 0.

A formula by Perron[10] gives the behavior in the complex plane cut along the positive real axis

$$ {}_1F_1(-n,d;z) = \frac{\Gamma(d)}{2\sqrt{\pi}} (-nz)^{1/4-d/2} e^{x/2} \exp[2\sqrt{-nz}]\{1 + O(1/\sqrt{n})\}, \tag{A35} $$

which agrees with (A32). Equations (A34) and (A35) show that we get the behavior on the positive real axis by adding the limiting values from above and below in the complex plane [which makes more sense if we look the other way, extending the formula on the real axis up (or down) into the complex plane]. This probably holds also for the general case (A31).

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[8] The asymptotic estimates given in Ref. 4, Chap. 2.32, (14) and (15), p. 77, are not correct. For one thing they evidently do not satisfy the transformation formula for the hypergeometric function quoted above. The mistake made in the derivation is that the original error estimate in formula (13) is incorrect, so the transformation to the asymptotics for the

confluent hypergeometric function is not valid. The formulas should be corrected by substituting the factor $(1-z)^{c-a-b}$ for the factor e^{bz} in the two formulas. The results in Ref. 4 have been quoted also in later references, such as Abramowitz, Stegun: *Handbook of Mathematical Functions*, and Magnus, Oberhettinger, Soni: *Formulas and Theorems for the Special Functions of Mathematical Physics*.

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Low dimensional cohomology of general conformal algebras gc_N

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We compute the low dimensional cohomologies $\tilde{H}^q(gc_N,\mathbb{C})$, $H^q(gc_N,\mathbb{C})$ of the infinite rank general Lie conformal algebras gc_N with trivial coefficients for $q\leqslant 3$, $N=1$ or $q\leqslant 2$, $N\geqslant 2$. We also prove that the cohomology of gc_N with coefficients in its natural module is trivial, i.e., $H^*(gc_N,\mathbb{C}[\partial]^N)=0$, and thus partially solve an open problem of Bakalov–Kac–Voronov [Commun. Math. Phys., **200**, 561–598 (1999)]. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The notion of a conformal algebra, introduced by Kac in Ref. 12, encodes an axiomatic description of the operator product expansion of chiral fields in conformal field theory. Conformal algebras play important roles in quantum field theory and vertex operator algebras (e.g., Ref. 12), whose study has drawn much attention in the literature (e.g., Refs. 1–7, 12–14, and 20–23). As is pointed out in Ref. 1, on one hand, it is an adequate tool for the study of infinite-dimensional Lie algebras satisfying the locality property (cf. Refs. 5, 12, and 14). On the other hand, conformal modules over a conformal algebra R correspond to conformal modules over the associated Lie algebra Lie R (cf. Ref. 3). The main examples of Lie algebras Lie R are the Lie algebras "based" on the punctured complex plane $\mathbb{C}^\times$, namely, the Lie algebra $Vect\mathbb{C}^\times$ of vector fields on $\mathbb{C}^\times$ (the Virasoro algebra) and the Lie algebra of maps of $\mathbb{C}^\times$ to a finite-dimensional Lie algebra (the loop algebra). Their irreducible conformal modules are the spaces of densities on $\mathbb{C}^\times$ and loop modules, respectively (cf. Ref. 3). Since complete reducibility does not hold in this case (cf. Refs. 4 and 10), one may expect that their cohomology theory is very interesting and important (cf. Ref. 1), just as the cohomology theory of Lie algebras has played important roles in the structure and representation theories of Lie algebras (cf. Refs. 8–11 and 15–19).

A general theory of cohomology of Lie conformal algebras was established by Bakalov, Kac, and Voronov in Ref. 1. They also computed the cohomologies for the finite simple Lie conformal algebras. However the problem for the general Lie conformal algebra gc_N, which is an infinite Lie conformal algebra, remains open. It is well-known that the general Lie conformal algebra gc_N plays the same important role in the theory of Lie conformal algebras as the general Lie algebra gl_N does in the theory of Lie algebras: any module $M=\mathbb{C}[\partial]^N$ over a Lie conformal algebra R is obtained via a homomorphism $R\to gc_N$ (cf. Refs. 5 and 12), thus the study of Lie conformal algebras gc_N has drawn some authors' attentions (cf. Refs. 1, 2, 6, 13, and 14). It seems to us that the computation of cohomology of gc_N is important.

In this paper, we compute the low-dimensional basic cohomologies $\tilde{H}^q(gc_N,\mathbb{C})$ and the reduced cohomology $\tilde{H}^q(gc_N,\mathbb{C})$ of gc_N with trivial coefficients for $q\leqslant 3$, $N=1$ or $q\leqslant 2$, $N\geqslant 2$. We also prove that the cohomology of gc_N with coefficients in its natural module is trivial, i.e., $H^*(gc_N,\mathbb{C}[\partial]^N)=0$; thus we partially solve an open problem in Ref. 1.

In Sec. II, we shall recall definitions of conformal algebras, their modules and cohomology,

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and present the main theorem of this paper (Theorem 2.5). Sections III and IV are devoted to the proof of the main theorem.

II. NOTATIONS AND MAIN RESULTS

We shall briefly recall definitions of conformal algebras, their modules and cohomology. More details can be found in, say, Ref. 1.

Definition 2.1: A *Lie conformal algebra* is a $\mathbb{C}[\partial]$-module A with a λ-bracket $[a_\lambda b]$ which defines a linear map $A\times A\to A[\lambda]$, where $A[\lambda]=\mathbb{C}[\lambda]\otimes A$ is the space of polynomials of λ with coefficients in A, satisfying

$$[\partial a_\lambda b]=-\lambda[a_\lambda b],\quad [a_\lambda \partial b]=(\partial+\lambda)[a_\lambda b]\quad \text{(conformal sesquilinearity)}, \tag{2.1}$$

$$[a_\lambda b]=-[b_{-\lambda-\partial}a]\quad \text{(skew-symmetry)}, \tag{2.2}$$

$$[a_\lambda[b_\mu c]]=[[a_\lambda b]_{\lambda+\mu}c]+[b_\mu[a_\lambda c]]\quad \text{(Jacobi identity)}, \tag{2.3}$$

for $a, b, c\in A$. A subset $S\subset A$ is called a *generating set* if S generates A as a $\mathbb{C}[\partial]$-module. If there exists a finite generating set, then A is called *finite*. Otherwise, it is called *infinite*. □

There is a similar notion of associative conformal algebras, which we shall not introduce in this paper. Below we shall only work with Lie conformal algebras, thus we shorten the term ''Lie conformal algebra'' to ''conformal algebra.'' The simplest nontrivial conformal algebra is the *Virasoro conformal algebra* Vir, which is a rank one free $\mathbb{C}[\partial]$-module generated by a symbol L such that

$$\text{Vir}=\mathbb{C}[\partial]L,\quad [L_\lambda L]=(\partial+2\lambda)L. \tag{2.4}$$

Note that, using (2.1), it suffices to define λ-brackets on a generating set. Let $N\geqslant 1$ be an integer. The *general conformal algebra* gc_N can be defined (see, e.g., Ref. 14) as an infinite rank free $\mathbb{C}[\partial]$-module with a generating set

$$S_N=\{J_A^n | n\in\mathbb{Z}_+, A\in gl_N\}, \tag{2.5}$$

where gl_N is the space of $N\times N$ matrices (note that the set S_N is not $\mathbb{C}$-linearly independent, for example, $J_{aA}^m=aJ_A^m$ for $a\in\mathbb{C}$), such that the λ-bracket is defined by

$$[J_{A\lambda}^m J_B^n]=\sum_{s=0}^{m}\binom{m}{s}(\lambda+\partial)^s J_{AB}^{m+n-s}-\sum_{s=0}^{n}\binom{n}{s}(-\lambda)^s J_{BA}^{m+n-s}, \tag{2.6}$$

for $m, n\in\mathbb{Z}_+$, $A, B\in gl_N$, where $\binom{m}{s}=m(m-1)\cdots(m-s+1)/s!$ if $s\geqslant 0$ and $\binom{m}{s}=0$ otherwise, is the binomial coefficient.

Definition 2.2: A *module* over a conformal algebra A is a $\mathbb{C}[\partial]$-module M with a λ-action $a_\lambda v$ which defines a map $A\times M\to M[[\lambda]]$, where $M[[\lambda]]$ is the set of formal power series of λ with coefficients in M, such that

$$a_\lambda(b_\mu v)-b_\mu(a_\lambda v)=[a_\lambda b]_{\lambda+\mu}v, \tag{2.7}$$

$$(\partial a)_\lambda v=-\lambda a_\lambda v,\quad a_\lambda(\partial v)=(\partial+\lambda)a_\lambda v, \tag{2.8}$$

for $a, b\in A$, $v\in M$. If $a_\lambda v\in M[\lambda]$ for all $a\in A$, $v\in M$, then the A-module M is called *conformal*. If M is finitely generated over $\mathbb{C}[\partial]$, then M is simply called *finite*.

Below we shall only consider ''conformal modules,'' thus we drop the word ''conformal'' and simply call a ''conformal module'' a ''module.'' Clearly, the one-dimensional vector space $\mathbb{C}$ can be defined as a module (called a *trivial module*) over any conformal algebra A with both the action

of ∂ and the action of A being zero. Furthermore, for $a\in\mathbb{C}$, $a\neq 0$, one can define a $\mathbb{C}[\partial]$-module $\mathbb{C}_a$, which is the one-dimensional vector space $\mathbb{C}$ such that $\partial v=av$ for $v\in\mathbb{C}_a$. Then $\mathbb{C}_a$ becomes an A-module with trivial action of A.

Let $\alpha\in\mathbb{C}$. The space $\mathbb{C}^N[\partial]$ (a rank N free $\mathbb{C}[\partial]$-module) can be defined as a gc_N-module with λ-action

$$J^m_{A\lambda}v=(\partial+\lambda+\alpha)^mAv \quad \text{for } A\in gl_N,\ m\in\mathbb{Z}_+,\ v\in\mathbb{C}^N \tag{2.9}$$

[cf. the statement after (2.4)]. We denote this module by $\mathbb{C}^N_\alpha[\partial]$. When $\alpha=0$, the module $\mathbb{C}^N[\partial]=\mathbb{C}^N_0[\partial]$ is called the *natural module of* gc_N.

Definition 2.3: Let $q\in\mathbb{Z}_+$. A *q-cochain of a conformal algebra A with coefficients in a module M* is a $\mathbb{C}$-linear map $\gamma: A^{\otimes q}\to M[\lambda_1,\dots,\lambda_q]$,

$$\gamma(a_1\otimes\cdots\otimes a_q)=\gamma_{\lambda_1,\dots,\lambda_q}(a_1,\dots,a_q), \tag{2.10}$$

satisfying

$$\gamma_{\lambda_1,\dots,\lambda_q}(a_1,\dots,\partial a_i,\dots,a_q)=-\lambda_i\gamma_{\lambda_1,\dots,\lambda_q}(a_1,\dots,a_i,\dots,a_q) \quad \text{(conformal antilinearity)}, \tag{2.11}$$

$$\begin{aligned}&\gamma_{\lambda_1,\dots,\lambda_{i-1},\lambda_{i+1},\lambda_i,\lambda_{i+2},\dots,\lambda_q}(a_1,\dots,a_{i-1},a_{i+1},a_i,a_{i+2},\dots,a_q)\\ &\quad=-\gamma_{\lambda_1,\dots,\lambda_{i-1},\lambda_i,\lambda_{i+1},\lambda_{i+2},\dots,\lambda_q}\\ &\qquad\times(a_1,\dots,a_{i-1},a_i,a_{i+1},a_{i+2},\dots,a_q) \quad \text{(skew-symmetry)},\end{aligned} \tag{2.12}$$

for $a_1,\dots,a_q\in A$ and all possible i. We let $A^{\otimes 0}=\mathbb{C}$, so that a zero-cochain γ is simply an element of M. □

We define a *differential d of a cochain* γ as follows:

$$\begin{aligned}(d\gamma)_{\lambda_1,\dots,\lambda_{q+1}}(a_1,\dots,a_{q+1})&=\sum_{i=1}^{q+1}(-1)^{i+1}a_{i\lambda_i}\gamma_{\lambda_1,\dots,\hat{\lambda}_i,\dots,\lambda_{q+1}}(a_1,\dots,\hat{a}_i,\dots,a_{q+1})\\ &\quad+\sum_{1\leq i<j\leq q+1}(-1)^{i+j}\gamma_{\lambda_i+\lambda_j,\lambda_1,\dots,\hat{\lambda}_i,\dots,\hat{\lambda}_j,\dots,\lambda_{q+1}}\\ &\quad\times([a_{i\lambda_i}a_j],a_1,\dots,\hat{a}_i,\dots,\hat{a}_j,\dots,a_{q+1}),\end{aligned} \tag{2.13}$$

where γ is extended linearly over the polynomials in λ_i, and where, the symbol $\hat{}$ means the element below it is missing. In particular,

$$(d\gamma)_\lambda(a)=a_\lambda\gamma \quad \text{if } \gamma\in M \text{ is a zero-cochain.} \tag{2.14}$$

By Ref. 1, the operator d preserves the space of cochains and $d^2=0$, so that the cochains form a complex, which will be denoted by $\widetilde{C}^*=\widetilde{C}^*(A,M)=\oplus_{q\in\mathbb{Z}_+}\widetilde{C}^q(A,M)$, and called the *basic complex* for the A-module M.

Define the structure of a $\mathbb{C}[\partial]$-module on $\widetilde{C}^*(A,M)$ by

$$(\partial\gamma)_{\lambda_1,\dots,\lambda_q}(a_1,\dots,a_q)=\left(\partial_M+\sum_{i=1}^q\lambda_i\right)\gamma_{\lambda_1,\dots,\lambda_q}(a_1,\dots,a_q), \tag{2.15}$$

where ∂_M denotes the action of ∂ on M. Then $d\partial=\partial d$ (see Ref. 1) and so the graded subspace $\partial\widetilde{C}^*\subset\widetilde{C}^*$ forms a subcomplex. Define the quotient complex $C^*=C^*(A,M)=\widetilde{C}^*(A,M)/\partial\widetilde{C}^*(A,M)=\oplus_{q\in\mathbb{Z}_+}C^q(A,M)$, called the *reduced complex*.

Definition 2.4: The *basic cohomology* $\widetilde{H}^*(A,M)$ *of a conformal algebra A with coefficients in a module M* is the cohomology of the basic complex $\widetilde{C}^*$. The *(reduced) cohomology* $H^*(A,M)$ is the cohomology of the reduced complex C^*. □

Note that the basic cohomology $\widetilde{H}^*(A,M)$ is naturally a $\mathbb{C}[\partial]$-module, whereas the reduced cohomology $H^*(A,M)$ is a complex vector space.

The main results of this paper are the following theorem.

Theorem 2.5: *(1) For the general conformal algebra* gc_1*, we have*

$$\dim \widetilde{H}^q(gc_1,\mathbb{C})=\begin{cases}1 & \text{if } q=0 \text{ or } 3,\\ 0 & \text{if } q=1 \text{ or } 2,\end{cases} \tag{2.16}$$

and

$$\dim H^q(gc_1,\mathbb{C})=\begin{cases}1 & \text{if } q=0,2 \text{ or } 3,\\ 0 & \text{if } q=1.\end{cases} \tag{2.17}$$

(2) Equations (2.16) and (2.17) also hold for the general conformal algebra gc_N *if* $q\leqslant 2$.

(3) $H^*(gc_N,\mathbb{C}_a)=0$ *if* $a\neq 0$.

(4) $H^*(gc_N,\mathbb{C}_\alpha^N[\partial])=0$ *for* $\alpha\in\mathbb{C}$*. Furthermore, for any* gc_N*-module M which is freely generated over* $\mathbb{C}[\partial]$ *such that there exists nonzero* $c\in\mathbb{C}$ *satisfying* $J^0_{I\lambda}v|_{\lambda=0}=cv$ *for* $v\in M$*, where I is the* $N\times N$ *identity matrix, we have* $H^*(gc_N,M)=0$.

Remark 2.6: (1) Equations (2.16) and (2.17) show that the cohomologies $\widetilde{H}^q(gc_1,\mathbb{C})$, $H^*(gc_1,\mathbb{C})$, $q\leqslant 3$, of the general conformal algebra gc_1 with trivial coefficients are isomorphic to those of the Virasoro conformal algebra with trivial coefficients.

(2) Theorem 2.5(2) in particular shows that there is a unique nontrivial universal central extension of the general conformal algebra gc_N, which agrees with that of the Lie algebra $\mathcal{D}^N$ of $N\times N$ matrix differential operators on the circle (cf. Refs. 16 and 18). (It is well-known that $\mathcal{D}^N$ is the distribution Lie algebra associated with gc_N, cf. Ref. 14.) A nontrivial reduced two-cocycle ψ' of gc_N is given in (3.36), and the universal central extension $\widetilde{g}c_N$ of gc_N corresponding to ψ' is given by

$$[J^m_{A\lambda}J^n_B]=\sum_{s=0}^{m}\binom{m}{s}(\lambda+\partial)^s J^{m+n-s}_{AB}-\sum_{s=0}^{n}\binom{n}{s}(-\lambda)^s J^{m+n-s}_{BA}$$

$$+(-1)^n\frac{m!n!}{(m+n+1)!}\operatorname{tr}(AB)\lambda^{m+n+1}C, \tag{2.18}$$

where C is a nonzero *central element* of $\widetilde{g}c_N$ (i.e., $[C_\lambda a]=[a_\lambda C]=0$ for all $a\in\widetilde{g}c_N$) such that $\mathbb{C}C$ is a trivial $\mathbb{C}[\partial]$-module.

(3) In Theorem 2.5(4), note that if we define the zero-bracket by $[a_0b]=[a_\lambda b]|_{\lambda=0}$ for a, $b\in gc_N$, and define the zero-action of gc_N on a module M by $a_0v=a_\lambda v|_{\lambda=0}$ for $a\in gc_N$, $v\in M$, then J^0_I is *central under zero-bracket*, i.e., $[J^0_{I0}a]=[a_0J^0_I]$ for $a\in gc_N$, and so the zero-action of J^0_I on any indecomposable gc_N-module M is a scalar. □

We shall give the proof of Theorem 2.5 in the next two sections.

III. PROOF OF THEOREM 2.5(2)–(4)

We shall keep the notation of the previous section. For a q-cochain $\gamma\in\widetilde{C}^q(A,M)$, we call γ a *q-cocycle* if $d\gamma=0$; a *q-coboundary* or a *trivial q-cocycle* if there is a $(q-1)$-cochain $\phi\in\widetilde{C}^{q-1}(A,M)$ such that $\gamma=d\phi$. Two cochains γ and ψ are *equivalent* if $\gamma-\psi$ is a coboundary. Denote by $\widetilde{D}^q(A,M)$ and by $\widetilde{B}^q(A,M)$ the spaces of q-cocycles and q-coboundaries, respectively. Then, by Definition 2.4, we have

$$\widetilde{H}^q(A,M)=\widetilde{D}^q(A,M)/\widetilde{B}^q(A,M)=\{\text{equivalent classes of } q\text{-cocycles}\}. \tag{3.1}$$

We shall divide the proof of Theorem 2.5(2)–(4) into several lemmas. (Although we are unable to give the general result for gc_N in this paper, Lemmas 3.1–4 below may be helpful in determining $\widetilde{H}^*(gc_N,\mathbb{C})$ and $H^*(gc_N,\mathbb{C})$ in the future.)

First suppose $\gamma\in\widetilde{C}^q(gc_N,\mathbb{C})$. Clearly, by (2.11), γ is uniquely determined by the right-hand side of (2.10) for $a_1,\ldots,a_q\in S_N$, where S_N is defined in (2.5). We can regard the right-hand side of (2.10) as a polynomial in $\lambda_1,\ldots,\lambda_q$. For any fixed $p\in\mathbb{Z}$, we define a $\mathbb{C}$-linear map $\gamma^{(p)}:gc_N^{\otimes q}\to\mathbb{C}[\lambda_1,\ldots,\lambda_q]$ such that (2.11) holds for $\gamma^{(p)}$ and such that

$$\gamma^{(p)}(J_{A_1}^{n_1}\otimes\cdots\otimes J_{A_q}^{n_q})=\gamma^{(p)}_{\lambda_1,\ldots,\lambda_q}(J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q}) \tag{3.2}$$

is a homogenous polynomial in $\lambda_1,\ldots,\lambda_q$ consisting of all monomials of total degree p' which appear in $\gamma_{\lambda_1,\ldots,\lambda_q}(J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q})$, where

$$p'=p+\sum_{i=1}^{q}n_i. \tag{3.3}$$

Then it is straightforward to see that $\gamma^{(p)}\in\widetilde{C}^q(gc_N,\mathbb{C})$ and

$$\gamma=\sum_{p\in\mathbb{Z}}\gamma^{(p)}. \tag{3.4}$$

Note that (3.4) is possibly an infinite sum, however for given $J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q}\in S_N$, there are only finite many p's such that (3.2) is not zero; we call such a sum *summable*. From (2.6), (2.11) and (2.13) [note that in (2.6), if we informally regard the right-hand side as a polynomial in λ, ∂, J_{AB}, J_{BA}, then it is a homogenous polynomial of the total degree $m+n$; also note that (2.13) now takes the form such that the first sum in the right-hand side is missing since $\mathbb{C}$ is a trivial module and note from (2.11) that when we substitute (2.6) into (2.13), ∂ in (2.6) can be replaced by $-\lambda_i$ for some i], we immediately obtain the following lemma.

Lemma 3.1: A q-cochain $\gamma\in\widetilde{C}^q(gc_N,\mathbb{C})$ is a q-cocycle (resp., q-coboundary)⇔all $\gamma^{(p)}$ are q-cocycles (resp., q-coboundaries). □

A q-cochain of the form $\gamma^{(p)}$ is called a *homogenous q-cochain of degree p*.

Following Ref. 1, we define an operator $\tau_1:\widetilde{C}^q(gc_N,\mathbb{C})\to\widetilde{C}^{q-1}(gc_N,\mathbb{C})$ as follows: If $q=0$, we set $\tau_1\gamma=0$; otherwise, we set

$$(\tau_1\gamma)_{\lambda_1,\ldots,\lambda_{q-1}}(a_1,\ldots,a_{q-1})=(-1)^{q-1}\frac{\partial}{\partial\lambda}\gamma_{\lambda_1,\ldots,\lambda_{q-1},\lambda}(a_1,\ldots,a_{q-1},J)|_{\lambda=0}, \tag{3.5}$$

for $a_1,\ldots,a_{q-1}\in S_N$, where $J=J_I^1$ and I is the $N\times N$ identity matrix. Noting that, by (2.6),

$$[J_{A_i\lambda_i}^{n_i}J]=\sum_{s=1}^{n_i}\binom{n_i}{s}(\lambda_i+\partial)^sJ_{A_i}^{n_i+1-s}-(-\lambda_i)J_{A_i}^{n_i}, \tag{3.6}$$

we obtain

$$
\begin{aligned}
&((d\tau_1+\tau_1 d)\gamma^{(p)})_{\lambda_1,\ldots,\lambda_q}(J^{n_1}_{A_1},\ldots,J^{n_q}_{A_q})\\
&\quad=(-1)^q\frac{\partial}{\partial\lambda}\sum_{i=1}^{q}(-1)^{i+q+1}\gamma^{(p)}_{\lambda_i+\lambda,\lambda_1,\ldots,\hat{\lambda_i},\ldots,\lambda_q}([J^{n_i}_{A_i\lambda_i}J],J^{n_1}_{A_1},\ldots,\hat{J}^{n_i}_{A_i},\ldots,J^{n_q}_{A_q})|_{\lambda=0}\\
&\quad=\frac{\partial}{\partial\lambda}\sum_{i=1}^{q}\gamma^{(p)}_{\lambda_1,\ldots,\lambda_{i-1},\lambda_i+\lambda,\lambda_{i+1},\ldots,\lambda_q}(J^{n_1}_{A_1},\ldots,J^{n_{i-1}}_{A_{i-1}},[J^{n_i}_{A_i\lambda_i}J],J^{n_{i+1}}_{A_{i+1}},\ldots,J^{n_q}_{A_q})|_{\lambda=0},\quad(3.7)
\end{aligned}
$$

where the first equality follows from the fact that all terms appearing in $d\tau_1\gamma^{(p)}$ are canceled with the corresponding terms in $\tau_1 d\gamma^{(p)}$ and the terms left are all appearing in $\tau_1 d\gamma^{(p)}$ [cf. (2.13)]; the second equality follows from (2.12). Note that for a polynomial P, $\partial P/\partial\lambda|_{\lambda=0}$ is simply the coefficient of λ^1 in P. Now we substitute (3.6) into (3.7). By (2.11), $(\lambda_i+\partial)^s$ can be replaced by $(-\lambda)^s$. Since we only need coefficients of λ^1, the terms with $s\geqslant 2$ in (3.6) do not contribute to the calculation. Thus $[J^{n_i}_{A_i\lambda_i}J]$ in (3.7) can be replaced by $(\lambda_i-n_i\lambda)J^{n_i}_{A_i}$. Thus (3.7) is equal to

$$
\frac{\partial}{\partial\lambda}\sum_{i=1}^{q}(\lambda_i-n_i\lambda)\gamma^{(p)}_{\lambda_1,\ldots,\lambda_{i-1},\lambda_i+\lambda,\lambda_{i+1},\ldots,\lambda_q}(J^{n_1}_{A_1},\ldots,J^{n_q}_{A_q})|_{\lambda=0}=p\,\gamma^{(p)}_{\lambda_1,\ldots\lambda_q}(J^{n_1}_{A_1},\ldots,J^{n_q}_{A_q}),\quad(3.8)
$$

which follows from (3.3) and the fact that for a homogenous polynomial $P(\lambda_1,\ldots,\lambda_q)$ of total degree p', we have

$$
\frac{\partial}{\partial\lambda}\sum_{i=1}^{q}(\lambda_i-n_i\lambda)P(\lambda_1,\ldots,\lambda_{i-1},\lambda_i+\lambda,\lambda_{i+1},\ldots,\lambda_q)|_{\lambda=0}=\left(p'-\sum_{i=1}^{q}n_i\right)P.\quad(3.9)
$$

From (3.7) and (3.8), we obtain

$$
(d\tau_1+\tau_1 d)\gamma^{(p)}=p\,\gamma^{(p)}.\quad(3.10)
$$

So if $d\gamma=0$, then (3.10) shows that $\gamma'=\Sigma_{p\neq 0}\gamma^{(p)}=d(\Sigma_{p\neq 0}p^{-1}\tau_1\gamma^{(p)})$ [note that this is summable, cf. the statement after (3.4)] is a coboundary, and $\gamma-\gamma'=\gamma^{(0)}$. Thus, we obtain the following lemma.

Lemma 3.2: A q-cocycle in $\widetilde{D}^q(gc_N,\mathbb{C})$ is equivalent to a homogenous q-cocycle of degree zero. □

Now suppose γ is a homogenous q-cocycle of degree zero. For $1\leqslant j,\ k\leqslant N$, denote by $E_{j,k}$ the $N\times N$ matrix with entry 1 at (j,k) and 0 otherwise. Then

$$
S'_N=\{J^n_{E_{j,k}}|n\in\mathbb{Z}_+,1\leqslant j,k\leqslant N\}\quad(3.11)
$$

is a free generating set of gc_N over $\mathbb{C}[\partial]$. Let $h=\Sigma_{j=1}^{N}jE_{j,j}$. We define another operator $\tau_2:\widetilde{C}^q(gc_N,\mathbb{C})\to\widetilde{C}^{q-1}(gc_N,\mathbb{C})$ as follows: We set $\tau_2\gamma=0$ if $q=0$, otherwise we set

$$
(\tau_2\gamma)_{\lambda_1,\ldots,\lambda_{q-1}}(a_1,\ldots,a_{q-1})=(-1)^{q-1}\gamma_{\lambda_1,\ldots,\lambda_{q-1},0}(a_1,\ldots,a_{q-1},J^0_h),\quad(3.12)
$$

for $a_1,\ldots,a_{q-1}\in S_N$. Now note that, by (2.6),

$$
[J^{n_i}_{E_{j_i,k_i}\lambda_i}J^0_h]=\sum_{s=0}^{n_i}\binom{n_i}{s}k_i(\lambda_i+\partial)^s J^{n_i-s}_{E_{j_i,k_i}}-j_i J^{n_i}_{E_{j_i,k_i}}.\quad(3.13)
$$

Thus as discussed in (3.7) and (3.8), the terms with $s\geqslant 1$ do not contribute to the following calculation, and, as in (3.7), we have

$$
\begin{aligned}
&((d\tau_2+\tau_2 d)\gamma)_{\lambda_1,\ldots,\lambda_q}(J^{n_1}_{E_{j_1,k_1}},\ldots,J^{n_q}_{E_{j_q,k_q}})\\
&\quad=\sum_{i=1}^{q}\gamma_{\lambda_1,\ldots,\lambda_q}(J^{n_1}_{E_{j_1,k_1}},\ldots,J^{n_{i-1}}_{E_{j_{i-1},k_{i-1}}},[J^{n_i}_{E_{j_i,k_i}\lambda_i}J^0_h],J^{n_{i+1}}_{E_{j_{i+1},k_{i+1}}},\ldots,J^{n_q}_{E_{j_q,k_q}})\\
&\quad=\sum_{i=1}^{q}(k_i-j_i)\gamma_{\lambda_1,\ldots,\lambda_q}(J^{n_1}_{E_{j_1,k_1}},\ldots,J^{n_q}_{E_{j_q,k_q}}).
\end{aligned}
\tag{3.14}
$$

Thus as in Lemma 2.2, we obtain the following lemma.

Lemma 3.3: A q-cocycle in $\widetilde{D}^q(gc_N,\mathbb{C})$ is equivalent to a homogenous q-cocycle γ of degree zero satisfying

$$
\gamma_{\lambda_1,\ldots,\lambda_q}(J^{n_1}_{E_{j_1,k_1}},\ldots,J^{n_q}_{E_{j_q,k_q}})=0 \quad \text{if } \sum_{i=1}^{q}(j_i-k_i)\neq 0. \tag{3.15}
$$

□

For a q-cochain $\gamma\in\widetilde{C}^q(gc_N,\mathbb{C})$, we define a linear map $\Delta\gamma: gc_N^{\otimes q}\to\mathbb{C}[\lambda_1,\ldots,\lambda_{q-1}]$ by

$$
\Delta\gamma(a_1\otimes\cdots\otimes a_q)=\gamma_{\lambda_1,\ldots,\lambda_q}(a_1,\ldots,a_q)|_{\lambda_q=-\lambda_1-\ldots-\lambda_{q-1}}=\gamma_{\lambda_1,\ldots,\lambda_{q-1},-\lambda_1-\ldots-\lambda_{q-1}}(a_1,\ldots,a_q), \tag{3.16}
$$

for $a_1,\ldots,a_q\in gc_N$ [we define $\Delta\gamma=\gamma$ if $q=0$, and define $\Delta\gamma(a_1)=\gamma_{\lambda_1}(a_1)|_{\lambda_1=0}$ if $q=1$]. Let $C'^q(gc_N,\mathbb{C})=\{\Delta\gamma|\,\gamma\in\widetilde{C}^q(gc_N,\mathbb{C})\}$. Then we obtain a linear map $\Delta:\widetilde{C}^q(gc_N,\mathbb{C})\to C'^q(gc_N,\mathbb{C})$. If $\gamma\in\partial\widetilde{C}^q(gc_N,\mathbb{C})=(\Sigma_{i=1}^{q}\lambda_i)\widetilde{C}^q(gc_N,\mathbb{C})$ [note that $\partial_{\mathbb{C}}=0$, cf. (2.15)], then clearly $\Delta\gamma=0$. Thus Δ factors to a map $\Delta:C^q(gc_N,\mathbb{C})\to C'^q(gc_N,\mathbb{C})$.

Lemma 3.4: The map $\Delta:C^q(gc_N,\mathbb{C})\to C'^q(gc_N,\mathbb{C})$ is an isomorphism as spaces.

Proof: Suppose $\Delta\gamma=0$ for a q-cochain γ. For $a_1,\ldots,a_q\in gc_N$, regarding $\gamma_{\lambda_1,\ldots,\lambda_q}(a_1,\ldots,a_q)$ as a polynomial in λ_q, we see that it has a root $\lambda_q=-\Sigma_{i=1}^{q-1}\lambda_i$, i.e., it is divided by $\Sigma_{i=1}^{q}\lambda_i$. Thus

$$
\phi(a_1\otimes\cdots\otimes a_q)=\left(\sum_{i=1}^{q}\lambda_i\right)^{-1}\gamma_{\lambda_1,\ldots,\lambda_q}(a_1,\ldots,a_q) \tag{3.17}
$$

defines a map $\phi: gc_N^{\otimes N}\to\mathbb{C}[\lambda_1,\ldots,\lambda_q]$. Obviously, ϕ is a q-cochain, and $\gamma=(\Sigma_{i=1}^{q}\lambda_i)\phi\in\partial\widetilde{C}^q(gc_N,\mathbb{C})$. □

Thus we can identify $C^q(gc_N,\mathbb{C})$ with the space $C'^q(gc_N,\mathbb{C})$. We call an element in $C'^q(gc_N,\mathbb{C})$ a *reduced q-cochain*. We define the operator $d:C'^q(gc_N,\mathbb{C})\to C'^{q+1}(gc_N,\mathbb{C})$ by $d\Delta\gamma=\Delta d\gamma$, and then we have similar notions of *reduced q-cocycles, reduced q-coboundaries*.

Lemma 3.5: Theorem 2.5(2) holds.

Proof: Clearly, by (2.14), $\widetilde{D}^0(gc_N,\mathbb{C})=\widetilde{C}^0(gc_N,\mathbb{C})=\mathbb{C}$, and $\widetilde{B}^0(gc_N,\mathbb{C})=0$. Thus $\widetilde{H}^0(gc_N,\mathbb{C})=\mathbb{C}$. Also by (2.15), $\partial\widetilde{C}^0(gc_N,\mathbb{C})=0$ and we have $H^0(gc_N,\mathbb{C})=\mathbb{C}$.

Suppose $\gamma\in\widetilde{C}^1(gc_N,\mathbb{C})$ such that $d\gamma\in\partial\widetilde{C}^2(gc_N,\mathbb{C})$, i.e., there is $\phi\in\widetilde{C}^2(gc_N,\mathbb{C})$ such that

$$
\begin{aligned}
\gamma_{\lambda_1+\lambda_2}([u_{\lambda_1}v]) &= -(d\gamma)_{\lambda_1,\lambda_2}(u,v)\\
&= -(\partial\phi)_{\lambda_1,\lambda_2}(u,v)\\
&= -(\partial_{\mathbb{C}}+\lambda_1+\lambda_2)\phi_{\lambda_1,\lambda_2}(u,v)\\
&= -(\lambda_1+\lambda_2)\phi_{\lambda_1,\lambda_2}(u,v)
\end{aligned}
\tag{3.18}
$$

[cf. (2.13) and (2.15)] for $u, v\in S_N$. By (2.6), we have

$$[J^n_{A\lambda_1}J^0]=\sum_{s=1}^{n}\binom{n}{s}(\lambda_1+\partial)^s J^{n-s}_A, \tag{3.19}$$

for $A\in gl_N$, $n\in\mathbb{Z}_+$, where $J^0=J^0_I$. Thus by (2.11), (3.18), and (3.19), we have

$$\sum_{s=1}^{n}\binom{n}{s}(-\lambda_2)^s\gamma_{\lambda_1+\lambda_2}(J^{n-s}_A)=\gamma_{\lambda_1+\lambda_2}[J^n_{A\lambda_1}J^0]=-(\lambda_1+\lambda_2)\phi_{\lambda_1,\lambda_2}(u,v). \tag{3.20}$$

Let $\lambda_1=\lambda-\lambda_2$. Then expressions in (3.20) are polynomials in λ, λ_2 and the right-hand side is divided by λ, thus each term in the left-hand side is divided by λ. Therefore we can set

$$\gamma'_\lambda(J^n_A)=\lambda^{-1}\gamma_\lambda(J^n_A)\quad\text{for } a\in gl_N,\ n\in\mathbb{Z}_+. \tag{3.21}$$

Clearly, (3.21) defines a one-cochain $\gamma'\in\widetilde{C}^1(gc_N,\mathbb{C})$, and we have $\gamma=\partial\gamma'\in\partial\widetilde{C}^1(gc_N,\mathbb{C})$. This proves that $H^1(gc_N,\mathbb{C})=0$.

Now suppose $\gamma\in\widetilde{D}^1(gc_N,\mathbb{C})$ is a one-cocycle. This means that $\phi=0$ in (3.18) and (3.20), and, so, we obtain $\gamma=0$. Thus $\widetilde{H}^1(gc_N,\mathbb{C})=0$.

Next suppose $\psi\in\widetilde{D}^2(gc_N,\mathbb{C})$ is a homogenous two-cocycle of degree zero. We define a one-cochain f which is uniquely determined by

$$f_{\lambda_1}(J^n_A)=(n+1)^{-1}\frac{\partial}{\partial\lambda}\psi_{\lambda_1,\lambda}(J^{n+1}_A,J^0)|_{\lambda=0}. \tag{3.22}$$

Set $\gamma=\psi+df$, which is also a homogenous two-cocycle of degree zero. Then

$$\frac{\partial}{\partial\lambda}\gamma_{\lambda_1,\lambda}(J^n_A,J^0)|_{\lambda=0}=\frac{\partial}{\partial\lambda}\psi_{\lambda_1,\lambda}(J^n_A,J^0)|_{\lambda=0}-\frac{\partial}{\partial\lambda}f_{\lambda_1+\lambda}([J^n_{A\lambda_1}J^0])|_{\lambda=0}=0, \tag{3.23}$$

where the last equality follows from (3.19), (2.11) and (3.22) if $n\geqslant 1$, or from the fact that $\psi_{\lambda_1,\lambda}(J^0_A,J^0)$ is a constant polynomial [cf. (3.3)] if $n=0$. Thus we have

$$\begin{aligned}0&=\frac{\partial}{\partial\lambda}(d\gamma)_{\lambda_1,\lambda_2,\lambda}(J^m_A,J^n_B,J^0)|_{\lambda=0}\\&=\frac{\partial}{\partial\lambda}(-\gamma_{\lambda_1+\lambda_2,\lambda}([J^m_{A\lambda_1}J^n_B],J^0)\\&\quad+\gamma_{\lambda_1+\lambda,\lambda_2}([J^m_{A\lambda_1}J^0],J^n_B)-\gamma_{\lambda_2+\lambda,\lambda_1}([J^n_{B\lambda_2}J^0],J^m_A))|_{\lambda=0}\\&=m\gamma_{\lambda_1,\lambda_2}(J^{m-1}_A,J^n_B)+n\gamma_{\lambda_1,\lambda_2}(J^m_A,J^{n-1}_B),\end{aligned} \tag{3.24}$$

for A, $B\in gl_N$, m, $n\in\mathbb{Z}_+$, where the second equality follows from (2.13) and the last equality follows from (3.23), (3.19) and (2.11). Induction on $n\geqslant 0$ in (3.24) proves $\gamma_{\lambda_1,\lambda_2}(J^m_A,J^n_B)=0$. Thus $\gamma=0$ and so $\widetilde{H}^2(gc_N,\mathbb{C})=0$.

Finally, suppose $\psi'=\Delta\psi\in C'^2(gc_N,\mathbb{C})$ is a reduced two-cochain. By (2.13) and (3.16),

$$(d\psi')_{\lambda_1,\lambda_2}(a_1,a_2,a_3)=-\psi'_{\lambda_1+\lambda_2}([a_{1\lambda_1}a_2],a_3)+\psi'_{-\lambda_2}([a_{1\lambda_1}a_3],a_2)-\psi'_{-\lambda_1}([a_{2\lambda_2}a_3],a_1), \tag{3.25}$$

for $a_1,a_2,a_3\in gc_N$. We define a reduced one-cochain $f'=\Delta f\in C'^1(gc_N,\mathbb{C})$ as follows [note from (3.16) that $f'(a)=f_\lambda(a)|_{\lambda=0}=f_0(a)$ is simply a linear function $f':gc_N\to\mathbb{C}$, and it is not necessary to write down explicitly its representative (basic) one-cochain f]

$$f'(J_A^m)=(m+1)^{-1}\frac{d}{d\lambda}\psi'_\lambda(J_A^m,J)|_{\lambda=0} \tag{3.26}$$

[recall (3.6) that $J=J_I^1$] for $A\in gl_N$, $m\in\mathbb{Z}_+$ [note from (2.11) that $f'(\partial a)=f_0(\partial a)=0$]. By (2.13) and (3.16),

$$(df')_\lambda(a_1,a_2)=-f'([a_{1\lambda}a_2]), \tag{3.27}$$

for a_1, $a_2\in gc_N$.

Now suppose ψ' is a reduced two-cocycle. Then $\gamma'=\psi'+df'$ is a reduced two-cocycle equivalent to ψ'. By (3.26), (3.27), and (3.6),

$$\frac{d}{d\lambda}\gamma'_\lambda(J_A^m,J)|_{\lambda=0}=0 \quad \text{for } A\in gl_N,\ m\in\mathbb{Z}_+. \tag{3.28}$$

Thus, by (3.25),

$$\begin{aligned}0&=\frac{\partial}{\partial\lambda}(d\gamma')_{\lambda_1,\lambda}(J_A^m,J_B^n,J)|_{\lambda=-\lambda_1}\\&=\frac{\partial}{\partial\lambda}(-\gamma'_{\lambda_1+\lambda}([J^m_{A\lambda_1}J^n_B],J)+\gamma'_{-\lambda}([J^m_{A\lambda_1}J],J^n_B)-\gamma'_{-\lambda_1}([J^n_{B\lambda}J],J^m_A))|_{\lambda=-\lambda_1}\\&=\frac{\partial}{\partial\lambda}((m(\lambda_1+\lambda)+\lambda_1)\gamma'_{-\lambda}(J_A^m,J_B^n)-((n(\lambda+\lambda_1)+\lambda)\gamma'_{-\lambda_1}(J_B^n,J_A^m))|_{\lambda=-\lambda_1},\end{aligned} \tag{3.29}$$

where the last equality follows from (3.28) and (3.6) [similarly to the discussion after (3.7), $\lambda_1+\partial$ and $\lambda+\partial$ can be replaced by $\lambda+\lambda_1$ and the terms with $s\geqslant 2$ do not contribute to the calculation]. Using (2.12) and (3.16), the right-hand side of (3.29) is equal to

$$(m+n+1)\gamma'_{\lambda_1}(J_A^m,J_B^n)-\lambda_1\frac{\partial}{\partial\lambda_1}\gamma'_{\lambda_1}(J_A^m,J_B^n)=0. \tag{3.30}$$

From (3.30), we obtain

$$\gamma'_\lambda(J_A^m,J_B^n)=c_{A,B}^{(m,n)}\lambda^{m+n+1} \quad \text{for some } c_{A,B}^{(m,n)}\in\mathbb{C}. \tag{3.31}$$

In particular,

$$\frac{d}{d\lambda}\gamma'_\lambda(J_A^m,J^0)|_{\lambda=0}=\delta_{m,0}c_A, \tag{3.32}$$

where $c_A=c_{A,I}^{(0,0)}$. Similarly to (3.29) [also cf. (3.24)],

$$\begin{aligned}0&=\frac{\partial}{\partial\lambda}(d\gamma')_{\lambda_1,\lambda}(J_A^m,J_B^n,J^0)|_{\lambda=-\lambda_1}\\&=-\frac{\partial}{\partial\lambda}\gamma'_{\lambda_1+\lambda}([J^m_{A\lambda_1}J^n_B],J^0)|_{\lambda=-\lambda_1}+m\gamma'_{\lambda_1}(J_A^{m-1},J_B^n)+n\gamma'_{\lambda_1}(J_A^m,J_B^{n-1})\\&=-\binom{m}{m+n}\lambda_1^{m+n}c_{AB}+\binom{n}{m+n}(-\lambda_1)^{m+n}c_{BA}+(mc_{A,B}^{(m-1,n)}+nc_{A,B}^{(m,n-1)})\lambda_1^{m+n},\end{aligned} \tag{3.33}$$

where the last equality follows from (2.6), (2.11), (3.16), (3.31), and (3.32). Taking $m=n=0$, we obtain $c_{AB}=c_{BA}$. Thus

$$mc_{A,B}^{(m-1,n)}+nc_{A,B}^{(m,n-1)}=\left(\binom{m}{m+n}-(-1)^{m+n}\binom{n}{m+n}\right)c_{AB}. \tag{3.34}$$

Thus we solve

$$c_{A,B}^{(m,n)}=(-1)^n\frac{m!n!}{(m+n+1)!}c_{AB}\quad \text{for } A,B\in gl_N, m,n\in\mathbb{Z}_+. \tag{3.35}$$

From (3.31) and the fact that $c_A=c_{A,I}^{(0,0)}$ and that $c_{AB}=c_{BA}$, we see that the map $A\mapsto c_A$ is a trace of gl_N, i.e., c_A is a scalar multiple of $\mathrm{tr}(A)$ for $A\in gl_N$. Thus (3.31) and (3.35) show that γ' is a multiple of ψ' which is defined by

$$\psi'_\lambda(J_A^m,J_B^n)=(-1)^n\frac{m!n!}{(m+n+1)!}\mathrm{tr}(AB)\lambda^{m+n+1}. \tag{3.36}$$

To see that ψ' is a nontrivial reduced two-cocycle, first define

$$\psi_{\lambda_1,\lambda_2}(J_A^m,J_B^n)=(-1)^n\frac{m!n!}{(m+n+1)!}((-1)^m\lambda_1^{m+n+1}-(-1)^n\lambda_2^{m+n+1})\mathrm{tr}(AB)\lambda^{m+n+1}. \tag{3.37}$$

Clearly, ψ is a two-cochain [recall the second sentence in the paragraph before (3.2)], and $\psi'=\Delta\psi$ is a reduced two-cochain. One can easily check that $d\psi'=0$ and that $\psi'\neq df'$ for any reduced one-cochain f'. This proves that $H^2(gc_N,\mathbb{C})=\mathbb{C}\psi'$. □

Lemma 3.6: Theorem 2.5(3) holds.

Proof: We define an operator $\tau:\widetilde{C}^q(gc_N,\mathbb{C}_a)\to\widetilde{C}^{q-1}(gc_N,\mathbb{C}_a)$ by

$$(\tau\gamma)_{\lambda_1,\ldots,\lambda_{q-1}}(a_1,\ldots,a_{q-1})=(-1)^{q-1}\gamma_{\lambda_1,\ldots,\lambda_{q-1},\lambda}(a_1,\ldots,a_{q-1},J)|_{\lambda=0}, \tag{3.38}$$

for $a_1,\ldots,a_{q-1}\in gc_N$. Similarly to the discussions in (3.7) and (3.8), we have

$$\begin{aligned}((d\tau+\tau d)\gamma)_{\lambda_1,\ldots,\lambda_q}(J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q})&=\left(\sum_{i=1}^q\lambda_q\right)\gamma_{\lambda_1,\ldots,\lambda_q}(J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q})\\&\equiv -a\,\gamma_{\lambda_1,\ldots,\lambda_q}(J_{A_1}^{n_1},\ldots,J_{A_q}^{n_q})(\mathrm{mod}\,\partial\widetilde{C}^q(gc_N,\mathbb{C}_a)).\end{aligned} \tag{3.39}$$

[Note that $\partial\widetilde{C}^q(gc_N,\mathbb{C}_a)=(a+\Sigma_{i=1}^q\lambda_i)\widetilde{C}^q(gc_N,\mathbb{C}_a)$ by (2.15), since $\partial_{\mathbb{C}_a}=a$.] Now suppose $\gamma\in\widetilde{C}^q(gc_N,\mathbb{C}_a)$ such that $d\gamma\in\partial\widetilde{C}^{q+1}(gc_N,\mathbb{C}_a)$, i.e., there exists a $(q+1)$-cochain ϕ such that $d\gamma=(a+\Sigma_{i=1}^{q+1}\lambda_i)\phi$. Clearly, by (3.38) $\tau d\gamma=(a+\Sigma_{i=1}^q\lambda_i)\tau\phi\in\partial\widetilde{C}^q(gc_N,\mathbb{C}_a)$. Thus (3.39) shows that $\gamma\equiv -d(a^{-1}\tau\gamma)(\mathrm{mod}\,\partial\widetilde{C}^q(gc_N,\mathbb{C}_a))$ is a reduced coboundary (note that we assume $a\neq 0$), i.e., $H^q(gc_N,\mathbb{C}_a)=0$. □

Lemma 3.7: Theorem 2.5(4) holds.

Proof: Note that as spaces, we have $\mathbb{C}_a^N[\partial][\lambda_1,\ldots,\lambda_q]=\mathbb{C}^N[\lambda_1,\ldots,\lambda_q,\partial]$, and a q-cochain $\widetilde{\gamma}\in\widetilde{C}^q(gc_N,\mathbb{C}_\alpha^N[\partial])$ can be regarded as a map $\widetilde{\gamma}:gc_N^{\otimes q}\to\mathbb{C}^N[\lambda_1,\ldots,\lambda_q,\partial]$,

$$\widetilde{\gamma}(a_1\otimes\cdots\otimes a_q)=\widetilde{\gamma}_{\lambda_1,\ldots,\lambda_q,\partial}(a_1,\ldots,a_q), \tag{3.40}$$

for $a_1,\ldots,a_q\in gc_N$. Regarding (3.40) as a polynomial in $\lambda_1,\ldots,\lambda_q,\partial$ with coefficients in $\mathbb{C}^N$, then similarly to Lemma 3.4, a reduced q-cochain

$$\gamma\in C^q(gc_N,\mathbb{C}_\alpha^N[\partial])=\widetilde{C}^q(gc_N,\mathbb{C}_\alpha^N[\partial])/\left(\partial+\sum_{i=1}^q\lambda_i\right)\widetilde{C}^q(gc_N,\mathbb{C}_\alpha^N[\partial]) \tag{3.41}$$

is uniquely determined by the coefficient of ∂^0 in (3.40). Thus a reduced q-cochain γ can be regarded as a map $\gamma: gc_N^{\otimes q} \to \mathbb{C}^N[\lambda_1,\dots,\lambda_q]$,

$$\gamma(a_1\otimes\cdots\otimes a_q)=\gamma_{\lambda_1,\dots,\lambda_q}(a_1,\dots,a_q). \tag{3.42}$$

Define an operator $\tau_0: C^q(gc_N,\mathbb{C}_\alpha^N[\partial]) \to C^{q-1}(gc_N,\mathbb{C}_\alpha^N[\partial])$ by [cf. (3.38)]

$$(\tau_0\gamma)_{\lambda_1,\dots,\lambda_{q-1}}(a_1,\dots,a_{q-1})=(-1)^{q-1}\gamma_{\lambda_1,\dots,\lambda_{q-1},\lambda}(a_1,\dots,a_{q-1},J^0)|_{\lambda=0}. \tag{3.43}$$

Similarly to the discussions in (3.7) and (3.8), using (3.19), we have [comparing with (3.7), all terms corresponding to the right-hand side of (3.7) are now zero because J has been replaced by J^0 and we do not take partial derivative $\partial/\partial\lambda$; but note that since the first sum in (2.13) is not zero in this case, we have one more term here]

$$((d\tau_0+\tau_0 d)\gamma)_{\lambda_1,\dots,\lambda_q}(J_{A_1}^{n_1},\dots,J_{A_q}^{n_q})=J_\lambda^0\gamma_{\lambda_1,\dots,\lambda_q}(J_{A_1}^{n_1},\dots,J_{A_q}^{n_q})|_{\lambda=0}. \tag{3.44}$$

Now by (2.9), the λ-action of gc_N on its module $\mathbb{C}_\alpha^N[\partial]$ in particular satisfies $J_\lambda^0 v=v$ for $v\in\mathbb{C}_\alpha^N[\partial]$. Thus the right-hand side of (3.44) is simply $-\gamma_{\lambda_1,\dots,\lambda_q}(J_{A_1}^{n_1},\dots,J_{A_q}^{n_q})$, i.e., we obtain

$$\gamma=(d\tau_0+\tau_0 d)\gamma. \tag{3.45}$$

In particular, if γ is a reduced cocycle, (3.45) gives that $\gamma=d(\tau_0\gamma)$ is a coboundary, i.e., $H^q(gc_N,\mathbb{C}_\alpha^N[\partial])=0$.

Clearly, the above proof works for any gc_N-module M satisfying the condition stated in Theorem 2.5(4). □

Thus Theorem 2.5(2)–(4) is proved.

IV. PROOF OF THEOREM 2.5(1)

This section is devoted to the proof of Theorem 2.5(1). By Lemma 3.5, it remains to consider the case $q=3$. Since some of the following arguments also work for general q-cocycles, we shall first consider q-cocycles with $q\geqslant 3$ so that it may be possible to use these arguments to determine higher dimensional cohomologies in the future.

Let $gc=gc_1$. It has a free generating set $S=\{J^n|n\in\mathbb{Z}_+\}$, such that

$$[J_\lambda^m J^n]=\sum_{s=1}^{m}\binom{m}{s}(\lambda+\partial)^s J^{m+n-s}-\sum_{s=1}^{n}\binom{n}{s}(-\lambda)^s J^{m+n-s}, \tag{4.1}$$

for m, $n\in\mathbb{Z}_+$. We shall give some more notations. An element in $\mathbb{Z}_+^q$ is denoted by

$$\underline{n}=\underline{n}[q]=(n_1,\dots,n_q),\quad n_1,\dots,n_q\in\mathbb{Z}_+ \tag{4.2}$$

(when there is no confusion we denote it by $\underline{n}$, otherwise we denote it by $\underline{n}[q]$). Denote $J^{\underline{n}}=J^{n_1}\otimes\cdots\otimes J^{n_q}=(J^{n_1},\dots,J^{n_q})\in gc^{\otimes q}$. Denote $\underline{\lambda}=\underline{\lambda}[q]=(\lambda_1,\dots,\lambda_q)$. For $\underline{n}\in\mathbb{Z}_+^q$, let $|\underline{n}|=\Sigma_{i=1}^q n_i$, called the *level of* $\underline{n}$. We define a total ordering on $\mathbb{Z}_+^q$ by the *level-lexicographical order*, i.e.,

$$\underline{m}<\underline{n}\Leftrightarrow|\underline{m}|<|\underline{n}|,\quad \text{or}\quad |\underline{m}|=|\underline{n}|\ \text{ and }\ \exists p\ \text{ such that }\ m_i=n_i\ \text{ for }\ i<p\ \text{ and }\ m_p<n_p, \tag{4.3}$$

for $\underline{m}$, $\underline{n}\in\mathbb{Z}_+^q$. Set

$$\mathcal{N}_q=\{\underline{n}\in\mathbb{Z}_+^q|n_1\leqslant n_2\leqslant\cdots\leqslant n_q\}. \tag{4.4}$$

For $m, n \in \mathbb{Z}$, we denote $[m,n]=\{m,m+1,...,n\}$. Let $\mathcal{S}_q$ be the permutation group on the index set $[1,q]$, which acts on $\mathbb{C}^q$ by $\sigma(v)=(v_{\sigma(1)},\ldots,v_{\sigma(q)})$ for $v=(v_1,\ldots,v_q)\in\mathbb{C}^q$. Then for any $\underline{n} \in \mathbb{Z}_+^q$, there is a unique $\underline{n}^* \in \mathcal{N}_q$ and some $\sigma \in \mathcal{S}_q$ such that $\underline{n}^*=\sigma(\underline{n}) \in \mathcal{N}_q$ and $\underline{n}^* \leqslant \tau(n)$ for τ in S_q. In fact,

$$\underline{n}^*=\min\{\sigma(\underline{n})|\sigma\in\mathcal{S}_q\} \tag{4.5}$$

is the minimal element in $\mathcal{S}_q(\underline{n})=\{\sigma(\underline{n})|\sigma\in\mathcal{S}_q\}$.

A q-cochain γ is uniquely determined by $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ for $\underline{n}\in\mathcal{N}_q$ and

$$\gamma_{\underline{\lambda}}(J^{\underline{n}})=\mathrm{sgn}(\sigma)\,\gamma_{\sigma(\underline{\lambda})}(J^{\sigma(\underline{n})}), \tag{4.6}$$

for $\underline{n}\in\mathbb{Z}_+^q$, $\sigma\in\mathcal{S}_q$, where $\mathrm{sgn}(\sigma)$ is the signature of the permutation σ. In fact, $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ can be arbitrary polynomial in $\underline{\lambda}$ satisfying (4.6) for all σ such that $\sigma(\underline{n})=\underline{n}$.

First we construct a three-cochain $\overline{\gamma}$ as follows:

$$\overline{\gamma}_{\underline{\lambda}}(J^{\underline{n}})=\begin{cases}\lambda_2^{n_3}-\lambda_1^{n_3} & \text{if } n_1=n_2=0,\ n_3\neq 0,\\ 0 & \text{otherwise,}\end{cases} \tag{4.7}$$

for $\underline{n}\in\mathcal{N}_3$ (note that in the first case, we let $n_3\neq 0$ in order to avoid the problem on how to deal with 0^0 when we set $\lambda_1=0$).

Lemma 4.1: $\overline{\gamma}$ is a nontrivial three-cocycle.

Proof: One can define a *Leibniz q-cochain* by removing the skew-symmetric condition (2.12), and define the *Leibniz differential operator* d_L by changing (2.13) into

$$\begin{aligned}(d_L\gamma)_{\lambda_1,\ldots,\lambda_{q+1}}(a_1,\ldots,a_{q+1})=&\sum_{i=1}^{q+1}(-1)^{i+1}a_{i\lambda_i}\gamma_{\lambda_1,\ldots,\hat{\lambda}_i,\ldots,\lambda_{q+1}}(a_1,\ldots,\hat{a}_i,\ldots,a_{q+1})\\ &+\sum_{1\leqslant i<j\leqslant q+1}(-1)^i\gamma_{\lambda_1,\ldots,\hat{\lambda}_i,\ldots,\lambda_{j-1},\lambda_i+\lambda_j,\lambda_{j+1},\ldots,\lambda_{q+1}}\\ &\times(a_1,\ldots,\hat{a}_i,\ldots,a_{j-1},[a_{i\lambda_i}a_j],a_{j+1},\ldots,a_{q+1}).\end{aligned} \tag{4.8}$$

[Note that if γ is a (regular) q-cochain, then (4.8) coincides with (2.13), i.e., $d=d_L$ in this case.] Then we obtain *Leibniz cohomology* (cf. Ref. 1). We shall not discuss Leibniz cohomology here, but we define a Leibniz two-cochain f by

$$f_{\lambda_1,\lambda_2}(J^0,J^0)=1 \quad\text{and}\quad f_{\lambda_1,\lambda_2}(J^m,J^n)=0 \quad\text{if } (m,n)\neq(0,0). \tag{4.9}$$

One can immediately check that $\overline{\gamma}=d_Lf$ (thus $\overline{\gamma}$ is a Leibniz three-coboundary). Therefore $d\overline{\gamma}=dd_Lf=d_L^2f=0$, i.e., $\overline{\gamma}$ is a (regular) three-cocycle. However, there is no two-cochain ϕ such that $d\phi=\overline{\gamma}$ because if $d\phi=\overline{\gamma}$, then we also have $\phi_{\lambda_1,\lambda_2}(J^0,J^0)=1$ and so ϕ is not a (regular) two-cochain [(2.12) is not satisfied]. Thus $\overline{\gamma}$ is a nontrivial three-cocycle. □

Now let γ be a q-cocycle with $q\geqslant 3$. By Lemma 3.2, we can suppose γ is homogenous with degree zero. First we have the following lemma.

Lemma 4.2: If $q=3$, by replacing γ by $\gamma-c\overline{\gamma}$ for some $c\in\mathbb{C}$, we can suppose $\gamma_{\underline{\lambda}}(J^0,J^0,J)=0$.

Proof: Note that $\gamma_{\underline{\lambda}}(J^0,J^0,J)$ is a linear polynomial in $\underline{\lambda}$ [cf. (3.3)] which is skew-symmetric with respect to λ_1,λ_2 by (2.12). Thus $\gamma_{\underline{\lambda}}(J^0,J^0,J)=c(\lambda_2-\lambda_1)$ for some $c\in\mathbb{C}$. Replacing γ by $\gamma-c\overline{\gamma}$, we have the lemma. □

To prove (2.16), our strategy is the following: We want to prove by induction on $\underline{n}\in\mathcal{N}_q$ [with respect to the order (4.3)] that after a number of steps, in each of which γ is replaced by $\gamma-\gamma'$ for some q-coboundaries γ', we obtain that $\gamma_{\underline{\lambda}}(J^{\underline{m}})=0$ for all $\underline{m}\in\mathcal{N}_q$, $\underline{m}\leqslant\underline{n}$ [Thus we obtain that $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ for all $\underline{n}\in\mathcal{N}_q$, i.e., $\gamma=0$, after a countably infinite number of steps; this amounts to

saying that γ is subtracted by an infinite sum of q-coboundaries, but from the following proof we see that this infinite sum is summable, cf. the statement after (3.4).] For the case $q=3$, this will be done by a number of lemmas (unfortunately, not all arguments work for $q\geqslant 4$, cf. the proof of Lemma 4.6).

Lemma 4.3: $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ *if* $|\underline{n}|\leqslant 1$.

Proof: Note that $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ is a polynomial in $\underline{\lambda}$ on degree $|\underline{n}|$. If $|\underline{n}|=0$, we have $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ by (4.6). If $|\underline{n}|=1$, then $\underline{n}=(0,...,0,1)$ and $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ is skew-symmetric with respect to $\lambda_1,\dots,\lambda_{q-1}$, thus divided by $\Pi_{1\leqslant i<j\leqslant q-1}(\lambda_i-\lambda_j)$, which has degree $(q-1)(q-2)/2>1$ if $q>3$. Thus $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ if $q>3$. If $q=3$, then $\gamma_{\underline{\lambda}}(J^{\underline{n}})=\gamma_{\underline{\lambda}}(J^0,J^0,J)=0$ by Lemma 4.2. □

Now suppose $|\underline{n}|\geqslant 2$. We set $i_0=\#\{i\in[1,q]|n_i=0\}\geqslant 0$ (where $\#X$ stands for the size of the finite set X), $i_2=q-\#\{i\in[1,q]|n_i=n_q\}\leqslant q-1$. If $i_0\neq i_2$, we set i_1 to satisfy

$$0=n_1=\cdots=n_{i_0}<n_{i_0+1}\leqslant\cdots\leqslant n_{i_1}<n_{i_1+1}=\cdots=n_{i_2}<n_{i_2+1}=\cdots=n_q; \tag{4.10}$$

if $i_0=i_2$, we set $i_1=0$.

Let $\underline{m}\in\mathcal{N}_{q+1}$ be such that $|\underline{m}|=|\underline{n}|+1$. Consider $(d\gamma)_{\underline{\lambda}[q+1]}(J^{\underline{m}})$ [cf. notation (4.2)]. Note that when we substitute (4.1) into (2.13), using (2.11) and (2.12), we obtain that $(d\gamma)_{\underline{\lambda}[q+1]}\times(J^{\underline{m}})$ is a combination of $\gamma_{\underline{\lambda}'}(J^{\underline{k}})$ with coefficients being polynomials in $\underline{\lambda}[q+1]$, where $\underline{k}\in\mathcal{N}_q$, $|\underline{k}|\leqslant|\underline{n}|$, and $\underline{\lambda}'=(\lambda_1',\dots,\lambda_q')$ such that each λ_i' is a linear polynomial in $\underline{\lambda}[q+1]$. Using the inductive assumption, $\gamma_{\underline{\lambda}'}(J^{\underline{k}})=0$ if $|\underline{k}|<|\underline{n}|$. Thus the terms with $s\geqslant 2$ in (4.1) do not contribute to (2.13) [cf. the discussion after (3.7)], and so we have [here we use (4.8) instead of (2.13)]

$$0=(d\gamma)_{\underline{\lambda}[q+1]}(J^{\underline{m}})=\sum_{1\leqslant i<j\leqslant q+1}(-1)^i(m_j\lambda_i-m_i\lambda_j)\gamma_{\lambda_1,\dots,\hat{\lambda}_i,\dots,\lambda_{j-1},\lambda_i+\lambda_j,\lambda_{j+1},\dots,\lambda_{q+1}}(J^{\underline{m}(i,j)}), \tag{4.11}$$

where

$$\underline{m}(i,j)=(m_1,\dots,\hat{m}_i,\dots,m_{j-1},m_i+m_j-1,m_{j+1},\dots,m_{q+1}), \tag{4.12}$$

and the right-hand side of (4.11) is a combination of $\gamma_{\underline{\lambda}'}(J^{\underline{m}(i,j)^*})$ [cf. (4.5) and (4.6)].

Lemma 4.4: $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ *if* $n_1\geqslant 1$ (*i.e.*, $i_0=0$).

Proof: In (4.11), take $\underline{m}=(0,n_1,\dots,n_{q-1},n_q+1)\in\mathcal{N}_{q+1}$. In (4.12), if $i\neq 1$, then $m_1=0<n_1$ and so $\underline{m}(i,j)^*\leqslant\underline{m}(i,j)<\underline{n}$; by induction, $\gamma_{\underline{\lambda}'}(J^{\underline{m}(i,j)^*})=0$. Similarly, $\gamma_{\underline{\lambda}'}(J^{\underline{m}(i,j)^*})=0$ if $j\neq q+1$. Thus the only possible nonzero term in (4.11) is the one with $(i,j)=(1,q+1)$. Since $\underline{m}(1,q+1)=\underline{n}$, (4.11) gives

$$-(n_q+1)\lambda_1\gamma_{\lambda_2,\dots,\lambda_q,\lambda_1+\lambda_{q+1}}(J^{\underline{n}})=0. \tag{4.13}$$

This gives the lemma. □

From now on, we assume that $n_1=0$.

Lemma 4.5: $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ *if* $i_2=q-1$ *and* $n_q\geqslant n_{q-1}+2$ *[cf. (4.10)].*

Proof: As above, now (4.11) gives [cf. (4.13)]

$$\sum_{i=1}^{i_0+1}(-1)^i(n_q+1)\lambda_i\gamma_{\lambda_1,\dots,\hat{\lambda}_i,\dots,\lambda_q,\lambda_i+\lambda_{q+1}}(J^{\underline{n}})=0. \tag{4.14}$$

Replacing $(\lambda_1,\dots,\lambda_{q+1})$ by $(\lambda,\lambda_1,\dots,\lambda_q)$ and applying the operator $\partial/\partial\lambda|_{\lambda=0}$ to (4.14), we obtain

$$\gamma_{\underline{\lambda}}(J^{\underline{n}})=-\sum_{i=1}^{i_0}(-1)^i\lambda_i\frac{\partial}{\partial\lambda}\gamma_{\lambda,\lambda_1,\ldots,\hat{\lambda_i},\ldots,\lambda_{q-1},\lambda_i+\lambda_q}(J^{\underline{n}})|_{\lambda=0}. \tag{4.15}$$

We define a $(q-1)$-cochain f as follows:

$$f_{\underline{\lambda}[q-1]}(J^{\underline{k}})=\begin{cases}-n_q^{-1}\dfrac{\partial}{\partial\lambda}\gamma_{\lambda,\lambda_1,\ldots,\lambda_{q-1}}(J^{\underline{n}})|_{\lambda=0} & \text{if } \underline{k}=\underline{n}^-,\\ 0 \quad \text{otherwise,}\end{cases} \tag{4.16}$$

for $\underline{k}\in\mathcal{N}_{q-1}$, where $\underline{n}^-=(n_2,\ldots,n_{q-1},n_q-1)\in\mathcal{N}_{q-1}$ [cf. (4.10)]. Indeed, f is a $(q-1)$-cochain [cf. the statement after (4.6)]: Write $\underline{n}^-$ as $\underline{n}^-=(n_1^-,\ldots,n_{q-1}^-)$, then $n_i^-=n_j^-\Leftrightarrow n_{i+1}=n_{i+1}$. Thus the skew-symmetric condition (4.6) for f follows from the skew-symmetric condition for γ. We claim that

$$\gamma_{\underline{\lambda}}(J^{\underline{k}})=(df)_{\underline{\lambda}}(J^{\underline{k}}), \tag{4.17}$$

for all $\underline{k}\in\mathcal{N}_q$ with $\underline{k}\leqslant\underline{n}$. If $\underline{k}=\underline{n}$, similarly to (4.14), we have

$$(df)_{\underline{\lambda}}(J^{\underline{n}})=\sum_{i=1}^{i_0}(-1)^i n_q\lambda_i f_{\lambda_1,\ldots,\hat{\lambda_i},\ldots,\lambda_{q-1},\lambda_i+\lambda_q}(J^{\underline{n}^-})=\gamma_{\underline{\lambda}}(J^{\underline{n}}), \tag{4.18}$$

where the last equality follows from (4.15) and (4.16). If $\underline{k}<\underline{n}$, when we substitute (4.1) into (2.13) for $(df)_{\underline{\lambda}}(J^{\underline{k}})$, as in (4.11), $(df)_{\underline{\lambda}}(J^{\underline{k}})$ is a combination of the form $f_{\underline{\lambda}'}(J^{\underline{k}(i,j)})$, and we see that $\underline{k}(i,j)<\underline{n}^-$ [cf. (4.12)], i.e., the term $f_{\underline{\lambda}'}(J^{\underline{n}^-})$ does not appear in $(df)_{\underline{\lambda}}(J^{\underline{k}})$, thus $(df)_{\underline{\lambda}}(J^{\underline{k}})=0$, which is the same as $\gamma_{\underline{\lambda}}(J^{\underline{k}})$ by inductive assumption. This proves (4.17). Thus by replacing γ by $\gamma-df$, we have the lemma. □

Lemma 4.6: $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$ *if* $q=3$.

Proof: When $q=3$, by Lemmas 4.3–5, we are left to consider the cases $\underline{n}=(0,n_2,n_2)$ and $\underline{n}=(0,n_2,n_2+1)$ for $n_2\geqslant 1$. First suppose $\underline{n}=(0,n_2,n_2)$. As in (4.14), we have

$$0=(d\gamma)_{\underline{\lambda}[4]}(J^0,J^0,J^{n_2},J^{n_2+1})=(n_2+1)(-\lambda_1\gamma_{\lambda_2,\lambda_3,\lambda_1+\lambda_4}(J^{\underline{n}})+\lambda_2\gamma_{\lambda_1,\lambda_3,\lambda_2+\lambda_4}(J^{\underline{n}})). \tag{4.19}$$

Setting $\lambda_4=0$, it gives that $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ can be divided by λ_1. So we can write $\gamma_{\underline{\lambda}}(J^{\underline{n}})=\lambda_1\gamma'_{\underline{\lambda}}$ for some polynomial $\gamma'_{\underline{\lambda}}$, and (4.19) shows that $\gamma'_{\lambda_2,\lambda_3,\lambda_1+\lambda_4}=\gamma'_{\lambda_1,\lambda_3,\lambda_2+\lambda_4}$. Setting $\lambda_1=0$, this gives that $\gamma'_{\lambda_2,\lambda_3,\lambda_4}=\gamma'_{0,\lambda_3,\lambda_2+\lambda_4}$. Thus

$$\gamma_{\underline{\lambda}}(J^{\underline{n}})=\lambda_1\gamma'_{0,\lambda_2,\lambda_1+\lambda_3}. \tag{4.20}$$

But $\gamma_{\underline{\lambda}}(J^{\underline{n}})$ is skew-symmetric with respect to λ_2,λ_3, we obtain $\gamma'_{0,\lambda_2,\lambda_1+\lambda_3}=-\gamma'_{0,\lambda_3,\lambda_1+\lambda_2}$. Setting $\lambda_1=0$ and $\lambda_3=0$, respectively, we obtain that $\gamma'_{0,\lambda_2,\lambda_3}=-\gamma'_{0,\lambda_3,\lambda_2}$ and $\gamma'_{0,\lambda_2,\lambda_1}=-\gamma'_{0,0,\lambda_1+\lambda_2}$, which gives that $\gamma'_{\underline{\lambda}}=0$. Thus $\gamma_{\underline{\lambda}}(J^{\underline{n}})=0$.

Next suppose $\underline{n}=(0,n_2,n_2+1)$. We still have (4.20) for some polynomial $\gamma'_{\underline{\lambda}}$. We assume that $n_2\geqslant 2$ (the proof for the case $n_2=1$ is similar and we leave it to the reader). For $1\leqslant i<n_2$, by (2.13) and the inductive assumption, we have

$$\begin{aligned}0&=(d\gamma)_{\underline{\lambda}[4]}(J^0,J,J^{n_2-i},J^{n_2+i+1})\\&=(n_2-i)\lambda_1\gamma_{\lambda_2,\lambda_1+\lambda_3,\lambda_4}(J,J^{n_2-i-1},J^{n_2+i+1})+(n_2+i+1)\lambda_1\gamma_{\lambda_2,\lambda_3,\lambda_1+\lambda_4}(J,J^{n_2-i},J^{n_2+i}).\end{aligned} \tag{4.21}$$

Note that when $i=n_2-1$, the first term of the right-hand side is zero since $\gamma_\lambda(J,J^0,J^{2n_2})=-\gamma_{\lambda_2,\lambda_1,\lambda_3}(J^0,J,J^{2n_2})$ and $(0,1,2n_2)<\underline{n}$. Thus induction on i gives that $\gamma_\lambda(J,J^{n_2-i},J^{n_2+i})=0$. Then by (2.13) and the inductive assumption,

$$\begin{aligned}0&=(d\gamma)_{\lambda[4]}(J^0,J,J^{n_2},J^{n_2+1})\\&=-\lambda_1\gamma_{\lambda_1+\lambda_2,\lambda_3,\lambda_4}(J^a)-(n_2+1)\lambda_1\gamma_{\lambda_2,\lambda_3,\lambda_1+\lambda_4}(J,J^{n_2},J^{n_2})+(n_2\lambda_2-\lambda_3)\gamma_{\lambda_1,\lambda_2+\lambda_3,\lambda_4}(J^a)\\&\quad+((n_2+1)\lambda_2-\lambda_4)\gamma_{\lambda_1,\lambda_3,\lambda_2+\lambda_4}(J^a).\end{aligned}\tag{4.22}$$

Substituting (4.20) into (4.22), cancelling the common factor λ_1, then setting $\lambda_1=\lambda_2=0$, we obtain that $0=-(n_2+1)\gamma_{0,\lambda_3,\lambda_4}(J,J^{n_2},J^{n_2})-(\lambda_3+\lambda_4)\gamma'_{0,\lambda_3,\lambda_4}$, which shows that $\gamma'_{0,\lambda_3,\lambda_4}$ is skew-symmetric with respect to λ_3, λ_4. Thus

$$f_{\lambda_1,\lambda_2}(J^{m_1},J^{m_2})=\begin{cases}-n_2^{-1}\gamma'_{0,\lambda_1,\lambda_2} & \text{if } (m_1,m_2)=(n_2,n_2),\\ 0 \quad \text{otherwise,}\end{cases}\tag{4.23}$$

defines a two-cochain f [cf. (4.16)]. Now as in the proof of Lemma 4.5, by replacing γ by $\gamma-df$, we have the lemma. This also proves (2.16). □

Lemma 4.7: Equation (2.17) holds.

Proof: By Lemma 3.5, it remains to consider the case $q=3$. Let $\overline{\gamma}$ be the three-cocycle defined in (4.7). Let $\overline{\gamma'}=\Delta\overline{\gamma}$ be the corresponding reduced three-cocycle [cf. (3.16)]. Clearly $\overline{\gamma'}$ is non-trivial. Now suppose γ' is an arbitrary reduced three-cocycle. As in the paragraph before Lemma 4.3, we shall prove by induction on $\underline{n}\in\mathcal{N}_3$ that by replacing γ' by $\gamma'-c\overline{\gamma'}-df'$ for some $c\in\mathbb{C}$ and some reduced two-cochain f' we have $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{m}})=0$ for $\underline{m}\leqslant\underline{n}$. Assume that we have proved $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{m}})=0$ for $\underline{m}<\underline{n}$.

First suppose $\underline{n}=(0,0,n_3)$. By (2.13), (3.16) and the inductive assumption, we have

$$0=(d\gamma')_{\lambda[3]}(J^0,J^0,J^0,J^{n_3+1})=(n_3+1)(-\lambda_1\gamma'_{\lambda_2,\lambda_3}(J^a)+\lambda_2\gamma'_{\lambda_1,\lambda_3}(J^a)-\lambda_3\gamma'_{\lambda_1,\lambda_2}(J^a)).\tag{4.24}$$

Thus

$$\gamma'_{\lambda_1,\lambda_2}(J^a)=\lambda_1\gamma'_{1,\lambda_2}(J^a)-\lambda_2\gamma'_{1,\lambda_1}(J^a).\tag{4.25}$$

If $n_3=0$, then by (2.12) and (3.16), $\gamma'_{\lambda_1,\lambda_2}(J^a)=-\gamma'_{\lambda_1,-\lambda_1-\lambda_2}(J^a)$. This together with (4.25) gives that $\gamma'_{\lambda_1,\lambda_2}(J^a)=0$. If $n_3=1$, then by (2.13), (3.16) and the inductive assumption,

$$\begin{aligned}0&=(d\gamma')_{\lambda[3]}(J^0,J^0,J,J)\\&=-\lambda_1(\gamma'_{\lambda_2,\lambda_1+\lambda_3}(J^a)-\gamma'_{\lambda_2,-\lambda_2-\lambda_3}(J^a))\\&\quad+\lambda_2(\gamma'_{\lambda_1,\lambda_2+\lambda_3}(J^a)-\gamma'_{\lambda_1,-\lambda_1-\lambda_3}(J^a)).\end{aligned}\tag{4.26}$$

Using (4.25) in (4.26), we see that γ'_{1,λ_1} can be divided by λ_1. Writing $\gamma'_{1,\lambda_1}=\lambda_1 p(\lambda_1)$ for some polynomial $p(\lambda_1)$ and using this in (4.26), cancelling the common factor $\lambda_1\lambda_2$, and setting $\lambda_2=\lambda_3=0$, we see that $p(\lambda_1)=c\in\mathbb{C}$ is a constant. Thus $\gamma'_{\lambda_1,\lambda_2}(J^a)=c(\lambda_1-\lambda_2)$. Replacing γ' by $\gamma'+c\overline{\gamma'}$, we obtain that $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{m}})=0$ for $\underline{m}\leqslant\underline{n}$.

If $n_3\geqslant 2$, we define a reduced two-cochain f' as follows:

$$f'_{\lambda_1}(J^{m_1},J^{m_2})=\begin{cases}-\gamma'_{1,\lambda_1}(J^a) & \text{if } (m_1,m_2)=(0,n_3-1),\\ 0 \quad \text{otherwise,}\end{cases}\tag{4.27}$$

for $(m_1,m_2)\in\mathcal{N}_2$. Clearly, this indeed defines a reduced two-cochain f'. Using (4.25), by replacing γ' by $\gamma'-df'$ as in the proof of Lemma 4.5, we have $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{m}})=0$ for $\underline{m}\leqslant\underline{n}$.

Next suppose $\underline{n}=(0,n_2,n_2)$ for $n_2\geqslant 1$. As in (4.25), from $(d\gamma')_{\lambda[3]}(J^0,J^0,J^{n_2},J^{n_2+1})=0$ we obtain that $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{n}})=\lambda_1\gamma'_{1,\lambda_2}(J^{\underline{n}})$. But $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{n}})=-\gamma'_{\lambda_1,-\lambda_1-\lambda_2}(J^{\underline{n}})$ by (2.12) and (3.16); we obtain $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{n}})=0$.

Now suppose $\underline{n}=(0,n_2,n_2+1)$ for $n_2\geqslant 1$. From $\gamma'_{\underline{\lambda}[3]}(J^{\underline{k}})=0$ for $\underline{k}=(0,0,n_2,n_2+2)$ and $\underline{k}=(0,0,n_2+1,n_2+1)$, we obtain that $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{n}})=\lambda_1\gamma'_{1,\lambda_2}(J^{\underline{n}})$ and that (4.26) again holds. From this, we obtain that $\gamma'_{\lambda_1,\lambda_2}(J^{\underline{n}})=-\gamma'_{\lambda_1,-\lambda_2}(J^{\underline{n}})$. Thus we can define a reduced two-cochain f' such that $f'_{\lambda_1}(J^{m_1},J^{m_2})=\gamma'_{1,\lambda_1}(J^{\underline{n}})$ if $(m_1,m_2)=(n_2,n_2)$ or $f'_{\lambda_1}(J^{m_1},J^{m_2})=0$ otherwise. Then the rest of the proof is as before.

Finally suppose $\underline{n}=(0,n_2,n_3)$ with $n_3\geqslant n_2+2$ or $\underline{n}=(n_1,n_2,n_3)$ with $n_1\geqslant 1$. Then the proof is the same as that of Lemmas 4.4 and 4.5. □

This completes the proof of Theorem 2.5.

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Classification of derivation-simple color algebras related to locally finite derivations

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We classify the pairs $(\mathcal{A},\mathcal{D})$ consisting of an (ϵ,Γ)-color-commutative associative algebra $\mathcal{A}$ with an identity element over an algebraically closed field $\mathbb{F}$ of characteristic zero and a finite dimensional subspace $\mathcal{D}$ of (ϵ,Γ)-color-commutative locally finite color-derivations of $\mathcal{A}$ such that $\mathcal{A}$ is Γ-graded $\mathcal{D}$-simple and the eigenspaces for elements of $\mathcal{D}$ are Γ-graded. Such pairs are the important ingredients in constructing some simple Lie color algebras which are in general not finitely-graded. As some applications, using such pairs, we construct new explicit simple Lie color algebras of generalized Witt type, Weyl type. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1628837]

I. INTRODUCTION

Lie color algebras, a notion first appeared in mathematical physics,[1,3,5–7,15] are generalizations of Lie algebras and Lie superalgebras. Let us start with the definition. Let $\mathbb{F}$ be an algebraically closed field of characteristic zero and let Γ be an additive group. A *skew-symmetric bicharacter* of Γ is a map $\epsilon:\Gamma\times\Gamma\to\mathbb{F}^\times=\mathbb{F}\backslash\{0\}$ satisfying

$$\epsilon(\lambda,\mu)=\epsilon(\mu,\lambda)^{-1},\quad \epsilon(\lambda,\mu+\nu)=\epsilon(\lambda,\mu)\epsilon(\lambda,\nu),\quad \forall\,\lambda,\mu,\nu\in\Gamma. \tag{1.1}$$

It is clear that

$$\epsilon(\lambda,0)=1,\quad \forall\,\lambda\in\Gamma. \tag{1.2}$$

Let $L=\oplus_{\lambda\in\Gamma}L_\lambda$ be a Γ-graded $\mathbb{F}$-vector space. For a nonzero homogeneous element a, denote by $\overline{a}$ the unique group element in Γ such that $a\in L_{\overline{a}}$. We shall call $\overline{a}$ the *color* of a. The $\mathbb{F}$-bilinear map $[\cdot,\cdot]:L\times L\to L$ is called a Lie color bracket on L if the following conditions are satisfied:

$$[a,b]=-\epsilon(\overline{a},\overline{b})[b,a]\quad \text{(skew symmetry)},$$

$$[a,[b,c]]=[[a,b],c]+\epsilon(\overline{a},\overline{b})[b,[a,c]]\quad \text{(Jacobi identity)},$$

for all homogeneous elements $a,b,c\in L$. The algebra structure $(L,[\cdot,\cdot])$ is called an (ϵ,Γ)-*Lie color algebra or simply a Lie color algebra*. If $\Gamma=\mathbb{Z}/2\mathbb{Z}$ and $\epsilon(i,j)=(-1)^{ij},\forall\, i,j\in\mathbb{Z}/2\mathbb{Z}$, then (ϵ,Γ)-Lie color algebras are simply Lie superalgebras. For Lie color algebras, we refer the reader to Ref. 1.

For any Γ-graded $\mathbb{F}$-vector space V, we denote

$$H(V)=\{\text{all homogeneous elements in } V\}.$$

Let $\mathcal{A}=\oplus_{\lambda\in\Gamma}\mathcal{A}_\lambda$ be a Γ-graded associative $\mathbb{F}$-algebra with an identity element 1, i.e., $\mathcal{A}_\lambda\mathcal{A}_\mu\subset\mathcal{A}_{\lambda+\mu}$ for all $\lambda,\mu\in\Gamma$. So $1\in\mathcal{A}_0$. We say that $\mathcal{A}$ is *graded simple* if $\mathcal{A}$ does not have nontrivial Γ-graded ideals. If we define the bilinear product $[\cdot,\cdot]$ on $\mathcal{A}$ by

$$[x,y]=xy-\epsilon(\overline{x},\overline{y})yx,\quad \forall\, x,y\in H(\mathcal{A}),\tag{1.3}$$

then $(\mathcal{A},[\cdot,\cdot])$ becomes a Lie color algebra.

A *Lie color ideal* U of $\mathcal{A}$ is a Γ-graded vector space U of $\mathcal{A}$ such that $[\mathcal{A},U]\subset U$. Sometimes it is called an (ϵ,Γ)-Lie ideal. The *ϵ-center* $Z_\epsilon(\mathcal{A})$ of $\mathcal{A}$ is defined as

$$Z_\epsilon=Z_\epsilon(\mathcal{A})=\{x\in\mathcal{A}\,|\,[x,\mathcal{A}]=0\}.$$

It is easy to see that $Z_\epsilon(\mathcal{A})$ is Γ-graded. We say that $\mathcal{A}$ is *color-commutative* (or ϵ-color-commutative) if $Z_\epsilon(\mathcal{A})=\mathcal{A}$, i.e., $[\mathcal{A},\mathcal{A}]=0$.

Let $\mathcal{A}$ be an (ϵ,Γ)-color-commutative associative algebra with an identity element 1. A nonzero $\mathbb{F}$-linear transformation $\partial:\mathcal{A}\to\mathcal{A}$ is called a *homogeneous color-derivation* of degree $\lambda\in\Gamma$ if

$$\begin{aligned}&\partial(a)\in\mathcal{A}_{\lambda+\mu},\quad \forall\, a\in\mathcal{A}_\mu,\quad \mu\in\Gamma,\\ &\partial(ab)=\partial(a)b+\epsilon(\lambda,\overline{a})a\partial(b),\quad \forall\, a,b\in H(\mathcal{A}).\end{aligned}\tag{1.4}$$

For convenience, we shall often denote $\overline{\partial}=\lambda$ if ∂ has degree λ. Clearly $\partial(c)=0$ for all $c\in\mathbb{F}$. Denote $\mathrm{Der}^\epsilon(\mathcal{A})=\oplus_{\lambda\in\Gamma}\mathrm{Der}^\epsilon_\lambda(\mathcal{A})$, where $\mathrm{Der}^\epsilon_\lambda(\mathcal{A})$ is the $\mathbb{F}$-vector space spanned by all homogeneous color derivations of degree λ. Similar to the Lie algebra case, it is easy to verify that $\mathrm{Der}^\epsilon_\lambda(\mathcal{A})$ becomes a Lie color algebra under the Lie color bracket

$$[\partial,\partial']=\partial\partial'-\epsilon(\overline{\partial},\overline{\partial'})\partial'\partial,\quad \forall\,\partial,\partial'\in H(\mathrm{Der}^\epsilon(\mathcal{A})),$$

where $\partial\partial'$ is the composition of the operators ∂ and ∂'.

Let $\mathcal{D}=\oplus_{\lambda\in\Gamma}\mathcal{D}_\lambda$ be an (ϵ,Γ)-color-commutative subspace of $\mathrm{Der}^\epsilon(\mathcal{A})$, i.e.,

$$\partial\partial'=\epsilon(\overline{\partial},\overline{\partial'})\partial'\partial,\quad \forall\,\partial,\partial'\in H(\mathcal{D}).\tag{1.5}$$

Recall that the associative algebra $\mathcal{A}$ is called *graded $\mathcal{D}$-simple* if $\mathcal{A}$ has no nontrivial graded $\mathcal{D}$-stable ideals.[4]

A linear transformation T on a vector space V is called *locally finite* if

$$\dim(\mathrm{span}\{T^m(v)\,|\,m\in\mathbb{N}\})<\infty,$$

for any $v\in V$. The transformation T is called *locally nilpotent* if for any $v\in V$, we have $T^n(v)=0$ for some $n\in\mathbb{N}$, and T is called *semisimple* if it acts diagonalizably on V.

For a pair $(\mathcal{A},\mathcal{D})$ of an (ϵ,Γ)-color-commutative associative algebra with an identity element and an (ϵ,Γ)-color-commutative subspace $\mathcal{D}$ of $\mathrm{Der}^\epsilon(\mathcal{A})$, Passman[4] proved that the Lie color algebra (including the Lie algebra case) $\mathcal{A}\mathcal{D}=\mathcal{A}\otimes\mathcal{D}$ is simple if and only if $\mathcal{A}$ is graded $\mathcal{D}$-simple and $\mathcal{A}\mathcal{D}$ acts faithfully on $\mathcal{A}$ (except a minor case). The authors of the present paper[11] (see also Refs. 9, 10, and 14) constructed (associative and Lie) color algebras of Weyl type $\mathcal{A}[\mathcal{D}]$, which is the color commutative algebra generated by $\mathcal{A}$ and $\mathcal{D}$ (as operators on $\mathcal{A}$), and proved that $\mathcal{A}[\mathcal{D}]$ is simple as an associative algebra or is *central simple* as a Lie color algebra (i.e., the derived subalgebra modulo its ϵ-center is simple) if and only if $\mathcal{A}$ is graded $\mathcal{D}$-simple (except a minor case in Lie case). However, it is still a question of how to construct new explicit simple Lie color algebras of generalized Witt type or Weyl type.

The problem of classifying all the pairs $(\mathcal{A},\mathcal{D})$ of a commutative associative algebra $\mathcal{A}$ with an identity element and a finite-dimensional locally finite commutative derivation subalgebra $\mathcal{D}$ such that $\mathcal{A}$ is *$\mathcal{D}$-simple* (i.e., $\mathcal{A}$ does not have $\mathcal{D}$-stable ideals), was settled in Ref. 8 (using the pairs

$(\mathcal{A},\mathcal{D})$, Xu constructed explicit simple Lie algebras of generalized Cartan type[12] and of generalized Block type[13]). However, this problem becomes much more complicated in color case.

In order to construct explicit new simple Lie color algebras of generalized Witt, Weyl types, the first aim of the present paper is to give a classification of all the pairs $(\mathcal{A},\mathcal{D})$ of an (ϵ,Γ)-color-commutative associative algebra $\mathcal{A}$ with an identity element over an algebraically closed field $\mathbb{F}$ of characteristic zero and a finite-dimensional subspace $\mathcal{D}$ of (ϵ,Γ)-color-commutative locally finite color derivations of $\mathcal{A}$ such that $\mathcal{A}$ is Γ-graded $\mathcal{D}$-simple and the eigenspaces for elements of $\mathcal{D}$ are Γ-graded (see Theorem 2.2). Then in Sec. III, as some applications, using the pairs $(\mathcal{A},\mathcal{D})$, we construct explicit new simple Lie color algebras (including Lie superalgebras) of generalized Witt, Weyl types (see Theorem 3.1).

II. $\mathcal{D}$-SIMPLE COLOR ALGEBRAS

In this section, we shall classify the pairs $(\mathcal{A},\mathcal{D})$ of an (ϵ,Γ)-commutating associative algebra $\mathcal{A}$ with an identity element 1 and a finite-dimensional subspace $\mathcal{D}$ of (ϵ,Γ)-commutative locally finite color derivations of $\mathcal{A}$ such that $\mathcal{A}$ is graded $\mathcal{D}$-simple and the eigenspaces for elements of $\mathcal{D}$ are Γ-graded.

First we would like to remark that the eigenspace of a derivation is not necessarily Γ-graded. Since we are considering Γ-graded algebras, it is natural that we require the eigenspaces for elements of $\mathcal{D}$ are Γ-graded.

We shall start with constructing explicitly such pairs $(\mathcal{A},\mathcal{D})$. The motivation to construct such pairs will become clear in the proof of Theorem 2.2 below. Actually, the proof of Theorem 2.2 leads us to the way to construct such pairs.

Set

$$\Gamma_+=\{\lambda\in\Gamma\mid \epsilon(\lambda,\lambda)=1\},\quad \Gamma_-=\{\lambda\in\Gamma\mid \epsilon(\lambda,\lambda)=-1\}.$$

Then by (1.1), Γ_+ is a subgroup of Γ with index $\leqslant 2$. For any graded subspace $\mathcal{B}$ of $\mathcal{A}$, we define $\mathcal{B}_+=\oplus_{\lambda\in\Gamma_+}\mathcal{B}_\lambda$, then $\mathcal{B}_+$ is Γ-graded. Similarly we can define $\mathcal{B}_-$. Since $\Gamma=\Gamma_+\cup\Gamma_-$, it follows that $\mathcal{B}=\mathcal{B}_+\oplus\mathcal{B}_-$. By (1.5), we have

$$a^2=0 \quad \text{or} \quad \partial^2=0 \quad \text{if } \overline{a}\in\Gamma_- \quad \text{or} \quad \overline{\partial}\in\Gamma_-. \tag{2.1}$$

For $m,n\in\mathbb{Z}$, we denote

$$\overline{m,n}=\{m,m+1,\ldots,n\}.$$

To construct the pair $(\mathcal{A},\mathcal{D})$, first we construct a Γ-*graded* ϵ-*commutative field extension* $\mathbb{E}$ of $\mathbb{F}$ (i.e., each nonzero homogeneous element of $\mathbb{E}$ is invertible). To do this, let $\Gamma^0\subset\Gamma_+$ be a subgroup of Γ and let $\mathbb{E}_0$ be a field extension of $\mathbb{F}$. Let $e:\Gamma^0\times\Gamma^0\to\mathbb{E}_0^\times=\mathbb{E}_0\backslash\{0\}$ be a 2-variable function $e:(\alpha,\beta)\mapsto e_{\alpha,\beta}$ such that

$$e_{\alpha,\beta}=\epsilon(\alpha,\beta)e_{\beta,\alpha},\quad e_{\alpha,0}=1,\quad e_{\alpha,\beta}e_{\alpha+\beta,\gamma}=e_{\alpha,\beta+\gamma}e_{\beta,\gamma},\quad \forall\ \alpha,\beta,\gamma\in\Gamma^0. \tag{2.2}$$

You will see that these are required by the associativity of the algebra we are going to construct. Let $\mathbb{E}=\mathbb{E}_0[\Gamma^0]=\mathrm{span}_{\mathbb{E}_0}\{E_\alpha\mid\alpha\in\Gamma^0\}$ be a Γ^0-graded ϵ-commutative associative algebra over $\mathbb{E}_0$ such that E_α has color $\overline{E_\alpha}=\alpha$, with the multiplication

$$E_\alpha\cdot E_\beta=e_{\alpha,\beta}E_{\alpha+\beta},\quad \forall\ \alpha,\beta\in\Gamma^0. \tag{2.3}$$

From (2.2) it is easy to see that $\mathbb{E}$ is a Γ-graded ϵ-commutative field extension of $\mathbb{F}$.

Let

$$\underline{k}=(k_1,k_2,k_3,k_4)\in\mathbb{N}^4 \quad \text{such that } k=k_1+k_2+k_3+k_4>0.$$

We also require that $k_4=0$ if $\Gamma_-=\varnothing$. We shall construct $\mathcal{D}$ which will be spanned by color derivations $\partial_p, p\in\overline{1,k}$ such that

$$\partial_p \text{ is semisimple with color } \overline{\partial}_p=0, \quad \forall\ p\in\overline{1,k_1}, \tag{2.4}$$

$$\partial_{k_1+p} \text{ is locally finite but not semisimple with color } \overline{\partial}_{k_1+p}=0, \quad \forall\ p\in\overline{1,k_2}, \tag{2.5}$$

$$\partial_{k_1+k_2+p} \text{ is locally nilpotent with color } \overline{\partial}_{k_1+k_2+p}\in\Gamma_+, \quad \forall\ p\in\overline{1,k_3}, \tag{2.6}$$

$$\partial_{k_1+k_2+k_3+p} \text{ is locally nilpotent with color } \overline{\partial}_{k_1+k_2+k_3+p}\in\Gamma_-, \quad \forall\ p\in\overline{1,k_4} \tag{2.7}$$

[cf. (2.21) and (2.22)]. To this end, we first need to construct $\mathcal{A}$ which will be the tensor product of two algebras $\mathcal{A}=\mathcal{A}_1\otimes\mathcal{A}_2$ [cf. (2.19)] such that $\mathcal{A}_1$ is a ''group-algebra-like'' algebra [cf. (2.12)] and $\mathcal{A}_2$ is a ''polynomial-like'' algebra [cf. (2.16)].

Now we construct $\mathcal{A}_1$ such that $\partial_p|_{\mathcal{A}_1}$ are nonzero semisimple operators for $p\in\overline{1,k_1+k_2}$ and $\partial_{k_1+k_2+p}|_{\mathcal{A}_1}$ are zero operators for $p\in\overline{1,k_3+k_4}$ [cf. (2.4)–(2.7) and (2.21)–(2.22)]. To do this, let G be a *nondegenerate* additive subgroup of $\mathbb{F}^{k_1+k_2}$, i.e., G contains an $\mathbb{F}$-basis of $\mathbb{F}^{k_1+k_2}$. If $k_1+k_2=0$, we take $G=\{0\}$. An element in G is usually denoted by

$$\underline{a}=(a_1,a_2,\ldots,a_k) \quad \text{with } a_p=0,\ \forall\ p>k_1+k_2. \tag{2.8}$$

Let $\hat{}:G\to\Gamma_+$ be a map $\hat{}:\underline{a}\mapsto\hat{\underline{a}}$ satisfying

$$\hat{0}=0, \quad \theta_{\underline{a},\underline{b}}:=\hat{\underline{a}}+\hat{\underline{b}}-\widehat{\underline{a}+\underline{b}}\in\Gamma^0, \quad \forall\ \underline{a},\underline{b}\in G. \tag{2.9}$$

Let $f(\cdot,\cdot):G\times G\to\mathbb{E}_0^\times$ be a map such that

$$f(\underline{a},\underline{b})=\epsilon(\hat{\underline{a}},\hat{\underline{b}})f(\underline{b},\underline{a}), \quad f(\underline{a},0)=1, \tag{2.10}$$

$$e_{\theta_{\underline{a},\underline{b}},\theta_{\underline{a}+\underline{b},\underline{c}}}f(\underline{a},\underline{b})f(\underline{a}+\underline{b},\underline{c})=\epsilon(\hat{\underline{a}},\theta_{\underline{b},\underline{c}})e_{\theta_{\underline{b},\underline{c}},\theta_{\underline{a},\underline{b}+\underline{c}}}f(\underline{b},\underline{c})f(\underline{a},\underline{b}+\underline{c}), \tag{2.11}$$

for $\underline{a},\underline{b},\underline{c}\in G$. Denote by $\mathcal{A}_1=\mathcal{A}(G,\mathbb{E},f)$ the (ϵ,Γ)-color commutative associative algebra with $\mathbb{E}$-basis $\{x^{\underline{a}}\mid\underline{a}\in G\}$ or $\mathbb{E}_0$-basis $\{E_\alpha x^{\underline{a}}\mid(\alpha,\underline{a})\in\Gamma^0\times G\}$ such that $x^{\underline{a}}$ has color $\hat{\underline{a}}$ and

$$x^{\underline{a}}\cdot x^{\underline{b}}=f(\underline{a},\underline{b})E_{\theta_{\underline{a},\underline{b}}}x^{\underline{a}+\underline{b}}, \quad \forall\ \underline{a},\underline{b}\in G, \tag{2.12}$$

and in general

$$E_\alpha x^{\underline{a}}\cdot E_\beta x^{\underline{b}}=\epsilon(\hat{\underline{a}},\beta)e_{\alpha,\beta}e_{\alpha+\beta,\theta_{\underline{a},\underline{b}}}f(\underline{a},\underline{b})E_{\alpha+\beta+\theta_{\underline{a},\underline{b}}}x^{\underline{a}+\underline{b}}, \quad \forall\ \alpha,\beta\in\Gamma^0,\ \underline{a},\underline{b}\in G \tag{2.13}$$

[cf. (2.3)]. The ϵ-commutativity and associativity of $\mathcal{A}_1$ are guaranteed by conditions (2.10) and (2.11).

Now we shall construct $\mathcal{A}_2$ such that $\partial_p|_{\mathcal{A}_2}=0$ for $p\in\overline{1,k_1}$ and $\partial_p|_{\mathcal{A}_2}$ are nonzero locally nilpotent operators for $p\in\overline{k_1+1,k}$ [cf. (2.4)–(2.7) and (2.21)–(2.22)]. To this end, let $t_{k_1+1},\ldots,t_k$ be $k_2+k_3+k_4$ variables such that each t_p has color $\overline{t_p}$ satisfying

$$\overline{t}_{k_1+p}=0, \quad \overline{t}_{k_1+k_2+q}\in\Gamma_+, \quad \overline{t}_{k_1+k_2+k_3+r}\in\Gamma_-, \tag{2.14}$$

for $p\in\overline{1,k_2}$, $q\in\overline{1,k_3}$, $r\in\overline{1,k_4}$. For convenience, we denote $t_p=0$ if $p\leqslant k_1$. Denote $\mathcal{J}=\{0\}^{k_1}\times\mathbb{N}^{k_2+k_3}\times\mathbb{Z}_2^{k_4}$, where $\mathbb{Z}_2=\mathbb{Z}/2\mathbb{Z}$, i.e., $\mathcal{J}$ is the subset of $\mathbb{F}^k$ consisting of the following elements:

$$\underline{i}=(i_1,i_2,\ldots,i_k), \tag{2.15}$$

with $i_p=0$ for $p\leqslant k_1$, and $i_q\in\mathbb{N}$ for $q\in\overline{k_1+1,k_1+k_2+k_3}$, and $i_r=0,1$ for $q>k_1+k_2+k_3$ [(2.1) and (2.16) explain why we shall have $i_q=0,1$ for $q>k_1+k_2+k_3$]. Let $\mathcal{A}_2=\mathbb{E}[t_{k_1+1},\ldots,t_k]$ be the ϵ-commutative algebra of polynomials in $k_2+k_3+k_4$ variables with an $\mathbb{E}$-basis consisting of the elements

$$t^{\underline{i}}=t_{k_1+1}^{i_{k_1+1}}\cdots t_k^{i_k},\quad \forall\ \underline{i}\in\mathcal{J}, \tag{2.16}$$

or $\mathbb{E}_0$-basis $\{E_\alpha t^{\underline{i}}\mid(\alpha,\underline{i})\in\Gamma^0\times\mathcal{J}\}$ such that

$$E_\alpha t^{\underline{i}}\cdot E_\beta t^{\underline{j}}=e_{\alpha,\beta}\prod_{p=k_1+1}^{k}\epsilon(\overline{t_p},\beta)^{i_p}\prod_{k_1<p<q\leqslant k}\epsilon(\overline{t_q},\overline{t_p})^{i_qj_p}E_{\alpha+\beta}t^{\underline{i}+\underline{j}},\quad \forall\ \alpha,\beta\in\Gamma^0,\ \underline{i},\underline{j}\in\mathcal{J} \tag{2.17}$$

[cf. (2.3)], where we use the convention that $t^{\underline{i}}=0$ if $\underline{i}\notin\mathcal{J}$. For convenience, we shall denote

$$\epsilon_{\underline{i},\beta}=\prod_{p=k_1+1}^{k}\epsilon(\overline{t_p},\beta)^{i_p},\quad \widetilde{\epsilon}_{\underline{i},\underline{j}}=\prod_{k_1<p<q\leqslant k}\epsilon(\overline{t_q},\overline{t_p})^{i_qj_p},\quad \forall\ \underline{i},\underline{j}\in\mathcal{J},\ \beta\in\Gamma^0. \tag{2.18}$$

Definition 2.1: We define $\mathcal{A}=\mathcal{A}(\underline{k},G,\mathbb{E},f)$ to be the (ϵ,Γ)-commutative associative algebra with the identity element $1=E_0=x^0$, which is the tensor product of algebras $\mathcal{A}=\mathcal{A}_1\otimes_{\mathbb{E}}\mathcal{A}_2$, having $\mathbb{E}_0$-basis

$$E_\alpha x^{\underline{a},\underline{i}}=E_\alpha x^{\underline{a}}t^{\underline{i}},\quad \forall\ (\alpha,\underline{a},\underline{i})\in\Gamma^0\times G\times\mathcal{J}, \tag{2.19}$$

with the multiplication

$$E_\alpha x^{\underline{a},\underline{i}}\cdot E_\beta x^{\underline{b},\underline{j}}=\epsilon_{\underline{i},\beta}e_{\alpha,\beta}\epsilon_{\underline{i},\hat{\underline{b}}}\widetilde{\epsilon}_{\underline{i},\underline{j}}\epsilon(\hat{\underline{a}},\beta)e_{\alpha+\beta,\theta_{\underline{a},\underline{b}}}f(\underline{a},\underline{b})E_{\alpha+\beta+\theta_{\underline{a},\underline{b}}}x^{\underline{a}+\underline{b},\underline{i}+\underline{j}}, \tag{2.20}$$

for $\alpha,\beta\in\Gamma^0$, $\underline{a}$, $\underline{b}\in G$, $\underline{i},\underline{j}\in\mathcal{J}$ [cf. (2.3), (2.13), (2.17), and (2.18)].

For $a\in\mathbb{F}^k,p\in\overline{1,k}$, we denote

$$a_{[p]}=(0,\ldots,0,\overset{p}{a},0,\ldots,0)\in\mathbb{F}^k.$$

For $p\in\overline{1,k}$, we define the linear transformations $\partial_p,\partial_{t_p},\partial_p^*$ on $\mathcal{A}$ such that they have color $-\overline{t_p}$ [in particular, they have color 0 if $p\leqslant k_1+k_2$, cf. (2.14)], and

$$\partial_p=\partial_p^*+\partial_{t_p}, \tag{2.21}$$

$$\partial_p^*(E_\alpha x^{\underline{a},\underline{i}})=a_pE_\alpha x^{\underline{a},\underline{i}},\quad \partial_{t_p}(E_\alpha x^{\underline{a},\underline{i}})=\epsilon(\overline{\partial_{t_p}},\alpha+\hat{\underline{a}})\prod_{q=1}^{p-1}\epsilon(\overline{\partial_{t_p}},\overline{t_q})^{i_q}\,i_pE_\alpha x^{\underline{a},\underline{i}-1_{[p]}}, \tag{2.22}$$

for $(\alpha,\underline{a},\underline{i})\in\Gamma^0\times G\times\mathcal{J}$. Clearly, $\partial_p^*=0$ if $p>\underline{k_1}+k_2$ by (2.8), and $\partial_q=0$ if $q\leqslant k_1$ by (2.15). Then $\partial_p,\partial_p^*,\partial_{t_p}$ are ϵ-derivations of $\mathcal{A}$ for $p\in\overline{1,k}$. We call ∂_p^* a *grading operator* (or *degree operator*), ∂_{t_p} a *down-grading operator*, and $\partial_p=\partial_p^*+\partial_{t_p}$ a *mixed operator* if both p_p^* and ∂_{t_p} are nonzero. Then

$$\mathcal{D}=\mathrm{span}_{\mathbb{F}}\{\partial_p\mid p\in\overline{1,k}\} \tag{2.23}$$

is a finite-dimensional subspace of ϵ-commutative locally finite color derivations of $\mathcal{A}$ such that the eigenspaces for elements of $\mathcal{D}$ are Γ-graded.

Theorem 2.2: Let $\mathcal{A}=\Sigma_{\alpha\in\Gamma}\mathcal{A}_\alpha$ be an ϵ-commutative associative graded algebra with an identity element over an algebraically closed field $\mathbb{F}$ of characteristic zero and let $\mathcal{D}=\Sigma_{\alpha\in\Gamma}\mathcal{D}_\alpha$ be

a finite-dimensional Γ-graded $\mathbb{F}$-subspace of ϵ-commutative locally finite color-derivations of $\mathcal{A}$ such that the eigenspaces for elements of $\mathcal{D}$ are Γ-graded. Then $\mathcal{A}$ is graded $\mathcal{D}$-simple if and only if $\mathcal{A}$ is isomorphic to the algebra of the form $\mathcal{A}(\underline{k},G,\mathbb{E},f)$ defined in (2.19) and (2.20), and $\mathcal{D}$ is of the form (2.21)–(2.23).

Proof: "⇐:" Let $\mathcal{I}$ be a Γ-graded $\mathcal{D}$-stable nonzero ideal of $\mathcal{A}=\mathcal{A}(\underline{k},G,\mathbb{E},f)$. By (2.21) and (2.22), we see that

$$\left(\bigcup_{(\alpha,\underline{a})\in\Gamma^0\times G}\mathbb{F}(E_\alpha x^{\underline{a}})\right)\Big\backslash\{0\},$$

is the set of the common eigenvectors of $\mathcal{D}$. We also see that if a homogeneous element $\partial\in H(\mathcal{D})$ has a nonzero eigenvalue, then $\partial\in\mathcal{D}_0$. Thus $\Sigma_{0\neq\alpha\in\Gamma}\mathcal{D}_\alpha$ acts locally nilpotently on $\mathcal{I}$. Since $\mathcal{D}_0$ is commutative [cf. (1.2) and (1.5)], and $\mathcal{D}_0$ commutes with $\Sigma_{0\neq\alpha\in\Gamma}\mathcal{D}_\alpha$, and $\Sigma_{0\neq\alpha\in\Gamma}\mathcal{D}_\alpha$ is color-commutative, by linear algebra, $\mathcal{I}$ must contain a common eigenvector of $\mathcal{D}$. Thus $E_\alpha x^{\underline{a}}\in\mathcal{I}$ for some $(\alpha,\underline{a})\in\Gamma^0\times G$. Then

$$1=e_{-\alpha,\alpha}^{-1}f(-\underline{a},\underline{a})^{-1}(E_{-\alpha}x^{-\underline{a}})\cdot(E_\alpha x^{\underline{a}})\in\mathcal{I}$$

[cf. (2.13)]. Hence $\mathcal{I}=\mathcal{A}$. This proves that $\mathcal{A}$ is graded $\mathcal{D}$-simple.

"⇒:" Suppose $\partial\in H(\mathcal{D})$ has a nonzero eigenvalue $\underline{a}\in\mathbb{F}$ such that $u_{\underline{a}}\in H(\mathcal{A})$ is a corresponding eigenvector. Then we have $\partial(u_{\underline{a}})=\underline{a}u_{\underline{a}}$, and so $\overline{\partial}+\overline{u_{\underline{a}}}=\overline{u_{\underline{a}}}$ by (1.4). Thus $\overline{\partial}=0$. In other words, we have

$$\partial\in H(\mathcal{D}),\ \overline{\partial}\neq 0\Rightarrow\ \partial\quad\text{acts locally nilpotent on}\quad\mathcal{A}. \tag{2.24}$$

Since $\mathbb{F}$ is algebraically closed and $\mathcal{D}$ is a finite-dimensional subspace of ϵ-commutative locally finite color derivations of $\mathcal{A}$, from linear algebra, we have

$$\mathcal{A}=\bigoplus_{\underline{a}\in\mathcal{D}^*}\mathcal{A}(\underline{a}),$$

where $\mathcal{D}^*$ is the dual space of $\mathcal{D}$, and

$$\mathcal{A}(\underline{a})=\{u\in\mathcal{A}\,|\,(\partial-\underline{a}(\partial))^m(u)=0\ \text{ for }\ \partial\in H(\mathcal{D})\ \text{ and some } m\in\mathbb{N}\},$$

for $\underline{a}\in\mathcal{D}^*$ [note that $\underline{a}(\partial)=0$ if $\overline{\partial}\neq 0$ by (2.24)]. Denote

$$G=\{\underline{a}\in\mathcal{D}^*\,|\,\mathcal{A}(\underline{a})\neq 0\}.$$

By (2.24), G can be viewed as a subset of $\mathcal{D}_0^*$ by the restriction $\underline{a}\mapsto\underline{a}|_{\mathcal{D}_0}$. For any $\underline{a}\in G$, $n\in\mathbb{N}$, we define

$$\mathcal{A}(\underline{a})^{(n)}=\{u\in\mathcal{A}\,|\,(d_1-\underline{a}(d_1))\cdots(d_{n+1}-\underline{a}(d_{n+1}))(u)=0,\ \forall\, d_1,\cdots,d_{n+1}\in H(\mathcal{D})\}. \tag{2.25}$$

Then

$$\mathcal{A}(\underline{a})=\bigcup_{n=0}^{\infty}\mathcal{A}(\underline{a})^{(n)},\quad\forall\,\underline{a}\in G.$$

A nonzero vector in $\mathcal{A}(\underline{a})^{(0)}$ is called a *root vector* with root $\underline{a}$. For any homogeneous root vector $u\in\mathcal{A}(\underline{a})^{(0)}$, clearly $\mathcal{A}u$ is a Γ-graded $\mathcal{D}$-stable ideal of $\mathcal{A}$. Thus $\mathcal{A}u=\mathcal{A}$. In particular, $vu=1$ for some $v\in\mathcal{A}$. So any homogeneous root vector is invertible. For a root vector $u\in H(\mathcal{A}(\underline{a})^{(0)})$ with $\underline{a}\in G$ and any $\partial\in H(\mathcal{D})$, we have

$$0=\partial(1)=\partial(uu^{-1})=\partial(u)u^{-1}+\epsilon(\overline{\partial},\overline{u})u\partial(u^{-1})=\underline{a}(\partial)uu^{-1}+\epsilon(\overline{\partial},\overline{u})u\partial(u^{-1})$$
$$=\begin{cases}\epsilon(\overline{\partial},\overline{u})u\partial(u^{-1}) & \text{if} \quad \overline{\partial}\neq 0,\\ \underline{a}(\partial)+u\partial(u^{-1}) & \text{if} \quad \overline{\partial}=0,\end{cases}$$

because $\underline{a}(\partial)=0$ if $\overline{\partial}\neq 0$ by (2.24). This implies

$$\partial(u^{-1})=-\underline{a}(\partial)u^{-1}, \tag{2.26}$$

by (2.24). Hence

$$-\underline{a}\in G, \quad \forall \quad \underline{a}\in G. \tag{2.27}$$

For any $x\in H(\mathcal{A}(\underline{a})^{(0)})$, $y\in H(\mathcal{A}(\underline{b})^{(0)})$, and $\partial\in H(\mathcal{D})$, we have

$$\partial(xy)=\partial(x)y+\epsilon(\overline{\partial},\overline{x})x\partial(y)=\begin{cases}0 & \text{if} \quad \overline{\partial}\neq 0,\\ (\underline{a}(\partial)+\underline{b}(\partial))xy & \text{if} \quad \overline{\partial}=0.\end{cases}$$

Hence

$$\mathcal{A}(\underline{a})^{(0)}\cdot\mathcal{A}(\underline{b})^{(0)}\subset\mathcal{A}(\underline{a}+\underline{b})^{(0)}, \quad \forall \quad \underline{a},\underline{b}\in G.$$

Considering the invertibility of root vectors, we have

$$\mathcal{A}(\underline{a})^{(0)}\cdot\mathcal{A}(\underline{b})^{(0)}=\mathcal{A}(\underline{a}+\underline{b})^{(0)}, \quad \forall \quad \underline{a},\underline{b}\in G.$$

In particular, we obtain

$$\underline{a}+\underline{b}\in G, \quad \forall \quad \underline{a},\underline{b}\in G. \tag{2.28}$$

Thus by (2.27) and (2.28), G is an additive subgroup of D^*. Set

$$\mathbb{E}=\mathcal{A}(0)^{(0)}. \tag{2.29}$$

Then $\mathbb{E}$ is a Γ-graded field extension of $\mathbb{F}$ such that $\mathbb{E}_0$ is a field extension of $\mathbb{F}$. We set

$$\Gamma^0=\{\alpha\in\Gamma \mid \mathbb{E}_\alpha\neq\{0\}\}.$$

Clearly, Γ^0 is a subgroup of Γ and $\Gamma^0\subset\Gamma_+$ by (2.1). For any $\alpha\in\Gamma^0$, choose $E_\alpha=1$ if $\alpha=0$, and $E_\alpha\in\mathbb{E}_\alpha\backslash\{0\}$ if $\alpha\neq 0$. Then $\{E_\alpha \mid \alpha\in\Gamma^0\}$ forms an $\mathbb{E}_0$-basis of $\mathbb{E}$. Thus we have (2.3) such that the coefficient $e_{\alpha,\beta}$ satisfies (2.2) by color commutativity and associativity.

First assume that $\mathcal{A}(0)\neq\mathbb{E}$. Since $\underline{a}(\partial)=0$ for any homogeneous derivation ∂ with $\overline{\partial}\neq 0$, for $u\in\mathcal{A}(\underline{a})^{(m)}$, $v\in\mathcal{A}(\underline{b})^{(n)}$ and $d_1,\ldots,d_{m+n+1}\in H(\mathcal{D})$, by induction on $m+n+1$, we can write

$$(d_1-(\underline{a}+\underline{b})(d_1))\cdots(d_{m+n+1}-(\underline{a}+\underline{b})(d_{m+n+1}))(uv), \tag{2.30}$$

as a linear combination of the forms

$$(d_{i_1}-\underline{a}(d_{i_1}))\cdots(d_{i_r}-\underline{a}(d_{i_r}))(u)\cdot(d_{j_1}-\underline{a}(d_{j_1}))\cdots(d_{j_s}-\underline{a}(d_{j_s}))(v), \tag{2.31}$$

where

$$r+s=m+n+1, \quad \{i_1,\ldots,i_r,j_1,\ldots,j_s\}=\{1,\ldots,m+n+1\}.$$

By definition (2.25), we obtain that (2.31) is zero, and so is (2.30). It follows that $uv\in\mathcal{A}(\underline{a}+\underline{b})^{(m+n)}$. Thus

$$\mathcal{A}(\underline{a})^{(m)}\cdot\mathcal{A}(\underline{b})^{(n)}\subset\mathcal{A}(\underline{a}+\underline{b})^{(m+n)},\quad \forall\ \ \underline{a},\underline{b}\in G,\ \ m,n\in\mathbb{N}. \tag{2.32}$$

In particular (since homogeneous root vectors are invertible),

$$\mathbb{E}\mathcal{A}(\underline{a})^{(m)}=\mathcal{A}(\underline{a})^{(m)}=\mathcal{A}(\underline{a})^{(0)}\mathcal{A}(0)^{(m)},\quad \forall\ \ \underline{a}\in G,\ \ m\in\mathbb{N} \tag{2.33}$$

[cf. (2.29)]. Hence each $\mathcal{A}(\underline{a})^{(m)}$ is a vector space over the graded field $\mathbb{E}$. For any $v\in\mathcal{A}(0)^{(1)}$, we have $\mathcal{D}(v)\subset\mathbb{E}$ and

$$\mathcal{D}(v)=0\ \ \Leftrightarrow\ \ v\in\mathbb{E}. \tag{2.34}$$

Set

$$\mathcal{H}=\mathbb{E}\mathcal{D},\quad \mathcal{H}_1=\{\partial\in\mathcal{H}\mid\partial(\mathcal{A}(0)^{(1)})=\{0\}\},\quad k_1=\dim_{\mathbb{E}}\mathcal{H}_1. \tag{2.35}$$

Expression (2.34) implies that $\mathcal{A}(0)^{(1)}/\mathbb{E}$ is isomorphic to a subspace of the space $\mathrm{Hom}_{\mathbb{E}}(\mathcal{H},\mathbb{E})$ over $\mathbb{E}$. By linear algebra, there exist subsets

$$\{\partial_{k_1+1},\partial_{k_1+2},\cdots,\partial_k\}\subset H(\mathcal{D}),\quad \{t_{k_1+1},t_{k_1+2},\cdots,t_k\}\subset H(\mathcal{A}(0)^{(1)}), \tag{2.36}$$

for some $k\in\mathbb{N}$, such that

$$\mathcal{A}(0)^{(1)}=\mathbb{E}+\sum_{l=k_1+1}^{k}\mathbb{E}t_l,\quad \partial_p(t_q)=\delta_{p,q},\quad \forall\ \ p,q\in\overline{k_1+1,k}. \tag{2.37}$$

Set

$$\mathcal{H}_2=\sum_{p=k_1+1}^{k}\mathbb{E}\partial_p.$$

Then we have

$$\mathcal{H}=\mathcal{H}_1\oplus\mathcal{H}_2.$$

For convenience, denote

$$t^{\underline{i}}=t_{k_1+1}^{i_{k_1+1}}\cdots t_k^{i_k}\quad \text{for}\ \ \underline{i}=(i_{k_1+1},\ldots,i_k)\in\mathbb{N}^{\ell},$$

where $\ell=k-k_1$. By (2.1) then

$$t^{\underline{i}}=0\ \text{if}\ \ i_p\geqslant 2\ \text{with}\ \ \overline{t_p}\in\Gamma_-\ \text{for some}\ \ p\in\overline{k_1+1,k},$$

and

$$t^{\underline{i}}\cdot t^{\underline{j}}=\prod_{k_1+1\leqslant p<q\leqslant k}\epsilon(\overline{t_q},\overline{t_p})^{i_qj_p}t^{\underline{i}+\underline{j}},\quad \forall\ \ \underline{i},\underline{j}\in\mathbb{N}^{\ell}.$$

Furthermore, by (2.37), we can deduce by induction on the level $|\underline{i}|:=\Sigma_{p=k_1+1}^{k}i_p$ that

$$t^{\underline{i}}\in\mathcal{A}(0)^{(|\underline{i}|)},\quad \partial_p(t^{\underline{i}})=\prod_{k_1<q<p}\epsilon(\overline{p_p},t_q)^{i_q}\,i_p t^{\underline{i}-1_{[p]}}, \tag{2.38}$$

for $\underline{i}\in\mathbb{N}^{\ell},p\in\overline{k_1+1,k}$. Set

$$\tilde{\mathcal{A}}(0)=\sum_{\underline{i}\in\mathbb{N}^{\ell}}\mathbb{E}t^{\underline{i}}\subset\mathcal{A}(0). \tag{2.39}$$

Then $\tilde{\mathcal{A}}(0)$ forms a subalgebra of $\mathcal{A}$. We want to prove that $\mathcal{A}(0)=\tilde{\mathcal{A}}(0)$. By (2.37), $\mathcal{A}(0)^{(1)}\subset\tilde{\mathcal{A}}(0)$. Suppose $\mathcal{A}(0)^{(m)}\subset\tilde{\mathcal{A}}(0)$ for some $1\leqslant m\in\mathbb{N}$. By (2.25), $\partial(\mathcal{A}(0)^{(m+1)})\subset\mathcal{A}(0)^{(m)}\subset\tilde{\mathcal{A}}(0)$ for any $\partial\in\mathcal{H}$. Thus, for $\partial_{k_1+1}\in H(\mathcal{H})$ and $u\in H(\mathcal{A}(0)^{(m)})$, we may assume that

$$\partial_{k_1+1}(u)=\sum_{\underline{i}\in\mathbb{N}^{\ell}}c_{\underline{i}}t^{\underline{i}}, \tag{2.40}$$

where $c_{\underline{i}}\in H(\mathbb{E})$ and $c_{\underline{i}}=0$ for all but a finite number of $\underline{i}$. If $\overline{\partial}_{k_1+1}\in\Gamma_+$, then we set

$$u_1=\sum_{\underline{i}\in\mathbb{N}^{\ell}}c_{\underline{i}}\epsilon(\overline{\partial}_{k_1+1},\overline{c_{\underline{i}}})^{-1}(i_{k_1+1}+1)^{-1}t^{\underline{i}+1_{[k_1+1]}}\in H(\tilde{\mathcal{A}}(0)), \tag{2.41}$$

and we obtain

$$\partial_{k_1+1}(u)=\partial_{k_1+1}(u_1). \tag{2.42}$$

If $\overline{\partial}_{k_1+1}\in\Gamma_-$, then by (2.1), $\partial_{k_1+1}^2=0$, we must have

$$i_{k_1+1}=0 \quad \text{if } c_{\underline{i}}\neq 0, \tag{2.43}$$

otherwise if (2.43) does not hold, then by (2.38) and (2.40) we would have $\partial_{k_1+1}^2(u)\neq 0$, leading to a contradiction to the fact that $\partial_{k_1+1}^2=0$. Thus we can still choose u_1 as in (2.41) to give (2.42). Similarly, since $\partial_{k_1+2}(u-u_1)\in\mathcal{A}(0)^{(m)}\subset\tilde{\mathcal{A}}(0)$, there exists $u_2\in H(\tilde{\mathcal{A}}(0))$ such that

$$\partial_{k_1+2}(u-u_1)=\partial_{k_1+2}(u_2). \tag{2.44}$$

Assume that $u_2=\Sigma_{\underline{i}\in\mathbb{N}^{\ell}}c'_{\underline{i}}t^{\underline{i}}$, where $c'_{\underline{i}}\in H(\mathbb{E})$. Since $\mathcal{H}$ is color commutative, by (2.42) and (2.44), we have

$$0=\partial_{k_1+1}\partial_{k_1+2}(u_2)=\sum_{\underline{i}\in\mathbb{N}^{\ell}}c'_{\underline{i}}\epsilon(\overline{\partial}_{k_1+1}+\overline{\partial}_{k_1+2},\overline{c'_{\underline{i}}})e(\overline{\partial}_{k_1+2},t_{k_1+1})^{i_{k_1+1}}i_{k_1+1}i_{k_1+2}t^{\underline{i}-1_{[k_1+1]}-1_{[k_1+2]}}.$$

Thus $i_{k_1+1}i_{k_1+2}=0$ if $c'_{\underline{i}}\neq 0$. Hence we can re-choose $u_2\in H(\tilde{\mathcal{A}}(0))$ such that

$$\partial_{k_1+1}(u_2)=0, \quad \partial_{k_1+2}(u-u_1)=\partial_{k_1+2}(u_2).$$

Similarly, we can find $u_2,\ldots,u_{\ell}\in H(\tilde{\mathcal{A}}(0))$ such that

$$\partial_{k_1+p}\left(u-\sum_{q=1}^{p}u_q\right)=0, \quad \partial_{k_1+1}(u_p)=\partial_{k_1+2}(u_p)=\cdots=\partial_{k_1+p-1}(u_p)=0, \quad \forall\ \ p\in\overline{2,\ell},$$

by induction on p. Thus we have

$$\partial_{k_1+p}\left(u-\sum_{q=1}^{\ell}u_q\right)=0, \quad \forall\ \ p\in\overline{1,\ell}. \tag{2.45}$$

For any $\partial,\partial'\in H(\mathcal{H}_1)$, using (2.35) and (2.39) we deduce

$$\partial\partial'\left(u-\sum_{p=1}^{\ell}u_p\right)\in\partial(\mathcal{A}(0)^{(m)})+\partial'(\mathcal{A}(0)^{(m)})\subset\partial(\tilde{\mathcal{A}}(0))+\partial'(\tilde{\mathcal{A}}(0))=\{0\}. \tag{2.46}$$

Now (2.45) and (2.46) show that $u-\Sigma_{p=1}^{\ell}u_p\in\mathcal{A}(0)^{(1)}$. Thus by (2.35),

$$\partial\left(u-\sum_{p=1}^{\ell}u_p\right)=0,\quad \forall\ \ \partial\in H(\mathcal{H}_1). \tag{2.47}$$

Then (2.45), (2.47) and the definition (2.25) show that

$$u-\sum_{p=1}^{\ell}u_p\in\mathcal{A}(0)^{(0)}=\mathbb{E}.$$

Thus $u\in\tilde{\mathcal{A}}(0)$. This proves

$$\mathcal{A}(0)=\tilde{\mathcal{A}}(0).$$

The case $\mathcal{A}(0)=\mathbb{E}$ can be viewed as in the general case $\mathcal{A}(0)=\tilde{\mathcal{A}}(0)$ with $\ell=0$.

We re-choose $\partial_p,t_p,p\in\overline{1,k}$ as follows: Choose a homogeneous $\mathbb{F}$-basis $\{\partial_1,\ldots,\partial_{k_1}\}$ of $\mathcal{D}\cap\mathcal{H}_1$, and set $t_p=0$ for $p\in\overline{1,k_1}$, then ∂_p are semi-simple derivations on $\mathcal{A}$ by (2.33) and (2.35). Let ℓ_1 be the dimension of the maximal locally nilpotent $\mathbb{F}$-subspace of $\mathcal{D}$. Clearly $\ell_1\leqslant\ell=k-k_1$. Let $k_2=\ell-\ell_1$. Now we choose $\partial_{k_1+k_2+1},\ldots,\partial_k$ to be homogeneous locally nilpotent derivations of $\mathcal{D}$ such that the first k_3 derivations have colors in Γ_+ and the last k_4 derivations have colors in Γ_- for some k_3,k_4 with $k_3+k_4=\ell_1$. Extend $\{\partial_p\mid p\in\overline{1,k_1}\cup\overline{k_1+k_2+1,k}\}$ to a homogeneous $\mathbb{F}$-basis $\{\partial_p\mid p\in\overline{1,k}\}$ of $\mathcal{D}$. By the choices of ∂_p, then there exists $t_p\in\mathcal{A}(0)^{(1)}$ for each $p\in\overline{k_1+1,k}$ satisfying (2.36) and (2.37).

For any $\underline{a}\in G$, we identify

$$\underline{a}\ \leftrightarrow\ (\underline{a}(\partial_1),\ldots,\underline{a}(\partial_{k_1+k_2}))\in\mathbb{F}^{k_1+k_2}.$$

Then G is a nondegenerate subgroup of $\mathbb{F}^{k_1+k_2}$ (otherwise, there exists $\partial\in\Sigma_{p=1}^{k_1+k_2}\mathbb{F}\partial_p$ such that $\underline{a}(\partial)=0$ for all $\underline{a}\in G$ and so ∂ is locally nilpotent, which contradicts the maximality of ℓ_1). Taking homogeneous root vector $u\in\mathcal{A}^{(\bar{0})}(\underline{a})$, by (2.26) and (2.32), we have

$$u^{-1}\mathcal{A}(\underline{a})\subset\mathcal{A}(0),\quad u\mathcal{A}(0)\subset\mathcal{A}(\underline{a}).$$

Hence

$$u\mathcal{A}(0)=\mathcal{A}(\underline{a}). \tag{2.48}$$

In particular,

$$\mathcal{A}(\underline{a})^{(0)}=\mathbb{E}u \tag{2.49}$$

is one-dimensional over $\mathbb{E}$. Choose

$$x^0=1,\quad 0\neq x^{\underline{a}}\in\mathcal{A}(\underline{a})^{(0)}\quad\text{for } 0\neq\underline{a}\in G,$$

such that $x^{\underline{a}}$ is homogeneous with color denoted by $\hat{\underline{a}}$. Since $x^{\underline{a}}$ is invertible, we have $\hat{\underline{a}}\in\Gamma_+$. Then we have a map $\hat{}$ satisfying (2.9). By (2.32) and (2.49), we have (2.12) with $f(\underline{a},\underline{b})$ satisfying (2.10) and (2.11) by color commutativity and associativity. By (2.48), we obtain

$$\mathcal{A}=\mathcal{A}^{(\bar{0})}\mathcal{A}(0)\cong\mathcal{A}^{(\bar{0})}\otimes\mathcal{A}(0),$$

where $\mathcal{A}^{(0)}=\oplus_{\underline{a}\in G}\mathcal{A}(\underline{a})^{(0)}$ is isomorphic to the algebra $\mathcal{A}_1$ defined in (2.12) and (2.13), and $\mathcal{A}(0)=\tilde{\mathcal{A}}(0)$ is isomorphic to the algebra $\mathcal{A}_2$ defined in (2.16) and (2.17). Therefore, the algebra $\mathcal{A}$ is isomorphic to the algebra $\mathcal{A}(\underline{k},G,\mathbb{E},f)$ defined in (2.19) and (2.20), and $\mathcal{D}$ is of the form (2.23). This completes the proof of Theorem 2.2. □

III. CONSTRUCTING SIMPLE LIE COLOR ALGEBRAS FROM $\mathcal{D}$-SIMPLE COLOR ALGEBRAS

In this section, as applications, we shall construct some explicit simple Lie color algebras using the pairs $(\mathcal{A},\mathcal{D})$ given in the last section. For simplicity, we assume that the pairs $(\mathcal{A},\mathcal{D})$ in (2.19) and (2.23) satisfies

$$\{u\in\mathcal{A}\mid\mathcal{D}(u)=0\}=\mathbb{F}.$$

This is equivalent to that $\mathbb{E}_0=\mathbb{F}$ and $\Gamma^0=\{0\}$. So the map $\hat{}:G\to\Gamma_+$ in (2.9) is a group homomorphism and $\theta_{\underline{a},\underline{b}}=0$ for all $\underline{a},\underline{b}\in G$. In this case, noting that $\mathbb{F}$ is algebraically closed, we prove that we can choose suitable basis $\{x^{\underline{a}}\mid\underline{a}\in G\}$ such that the coefficient $f(\underline{a},\underline{b})$ determined by (2.12), which satisfies (2.10) and (2.11), has the following form:

$$f(\underline{a},\underline{b})=\epsilon(\hat{\underline{a}},\hat{\underline{b}})^{1/2},\quad\forall\ \ \underline{a},\underline{b}\in G,\tag{3.1}$$

where the right-hand side is a fixed square root such that (2.10) and (2.11) hold.

Let G' be a maximal subgroup of G such that $x^{\underline{a}}$, $\underline{a}\in G'$ can be chosen so that (3.1) holds for $\underline{a},\underline{b}\in G'$. Suppose $G'\neq G$. Let $\underline{c}\in G\backslash G'$ and set $G''=G'+\mathbb{Z}\underline{c}$. If $G'\cap\mathbb{Z}\underline{c}=\{0\}$, we choose any $x^{\underline{c}}\neq 0$, and set $x^{\underline{a}+k\underline{c}}=\epsilon(\hat{\underline{a}},\hat{\underline{c}})^{-k/2}x^{\underline{a}}\cdot(x^{\underline{c}})^k$ for $\underline{a}+k\underline{c}\in G''$. If $G'\cap\mathbb{Z}\neq\{0\}$, then $G'\cap\mathbb{Z}\underline{c}=\mathbb{Z}\underline{d}$ for some $\underline{d}=m\underline{c}$, $m>1$. In this case, since $\mathbb{F}$ is algebraically closed, we can choose $x^{\underline{c}}$ such that $(x^{\underline{c}})^m=x^{\underline{d}}$, and set $x^{\underline{a}+k\underline{c}}$ as above. In any case, the coefficient $f(\underline{a},\underline{b})$ determined by (2.12) satisfies (3.1) for $\underline{a},\underline{b}\in G''$. But $G'\neq G''\supset G'$. This contradicts the maximality of G'. This proves (3.1).

Let $\mathbb{F}[\mathcal{D}]$ be the (ϵ,Γ)-commutative associative algebra with basis

$$\{\partial^{\mu}=\partial_1^{\mu_1}\cdots\partial_k^{\mu_k}\mid\mu=(\mu_1,\ldots,\mu_k)\in\mathcal{M}\},$$

where $\mathcal{M}=\mathbb{N}^{k_1+k_2+k_3}\times\mathbb{Z}_2^{k_4}$. For convenience, we denote $\partial^{\mu}=0$ if $\mu\notin\mathcal{M}$. Denote

$$W=W(\underline{k},G)=\mathcal{A}\otimes\mathcal{D}=\operatorname{span}\{x^{\underline{a},\underline{i}}\partial_p\mid(\underline{a},\underline{i})\in G\times\mathcal{J},p\in\overline{1,k}\},$$

$$\mathcal{W}=\mathcal{W}(\underline{k},G)=\mathcal{A}\otimes\mathbb{F}[\mathcal{D}]=\operatorname{span}\{x^{\underline{a},\underline{i}}\partial^{\mu}\mid(\underline{a},\underline{i},\mu)\in G\times\mathcal{J}\times\mathcal{M}\}.$$

Then as spaces, we have $W\subset\mathcal{W}$. By regarding $\mathcal{W}$ as operators on $\mathcal{A}$, $\mathcal{W}$ becomes a Γ-graded associative algebra whose multiplication is the composition of operators. Thus $\mathcal{W}$ forms an (ϵ,Γ)-Lie color algebra under the bracket (1.3). We call $\mathcal{W}$ a *Lie color algebra of (generalized) Weyl type*. Clearly $\mathbb{F}$ is the center of $\mathcal{W}$. Let $\tilde{\mathcal{W}}=\mathcal{W}/\mathbb{F}$ and let $\overline{\mathcal{W}}=[\tilde{\mathcal{W}},\tilde{\mathcal{W}}]$ the derived algebra of $\tilde{\mathcal{W}}$. Obviously, W forms an (ϵ,Γ)-Lie color subalgebra of $\mathcal{W}$, called a *Lie color algebra of (generalized) Witt type*. Using results in Refs. 4 and 11, we obtain the following.

Theorem 3.1: The Lie color algebras $\overline{\mathcal{W}}$ and W are simple if $k_1+k_2+k_3>0$ or $k_4>1$. Furthermore, $\overline{\mathcal{W}}=\tilde{\mathcal{W}}$ if $k_1+k_2+k_3>0$ or otherwise, $\tilde{\mathcal{W}}=\overline{\mathcal{W}}+\mathbb{F}t^{\underline{n}}\partial^{\lambda}$, where $\underline{n}$ and λ are the largest elements respectively in $\mathcal{J}$ and in $\mathcal{M}$. □

Note that in case $k=k_4=1$, $\overline{\mathcal{W}}=0$ and $W=\mathbb{F}t_1\partial_1$ are not simple. If $k=k_4>1$, then we obtain finite dimensional simple Lie color algebras $\overline{\mathcal{W}}$ and W of dimensions $2^{2n}-2$ and $n2^n$. In particular, if $\Gamma=\mathbb{Z}_2,\epsilon(i,j)=(-1)^{ij},i,j\in\mathbb{Z}_2$, we obtain the finite dimensional simple Lie superalgebras $\overline{\mathcal{W}}=H(2n)$ and $W=W(n)$ (see Ref. 2).

Using the pair $(\mathcal{A},\mathcal{D})$, one might construct other simple Lie color algebras, for example, other series of Lie color algebras of Cartan type.

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The noncommutative Lorentzian cylinder as an isospectral deformation

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We present a new example of a finite-dimensional noncommutative manifold, namely, the noncommutative cylinder. It is obtained by isospectral deformation of the canonical triple associated with the Euclidean cylinder. We discuss Connes' character formula for the cylinder. In the second part, we discuss noncommutative Lorentzian manifolds. Here, the definition of spectral triples involves Krein spaces and operators on Krein spaces. A central role is played by the admissible fundamental symmetries on the Krein space of square integrable sections of a spin bundle over a Lorentzian manifold. Finally, we discuss isospectral deformation of the Lorentzian cylinder and determine all admissible fundamental symmetries of the noncommutative cylinder. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Strict deformation quantization[1–3] provides a powerful mathematical tool to describe the notion of quantization in physics. The central object here is a family of C^*-algebras $\{\mathcal{A}_\hbar\}$, parametrized by some real number $\hbar$. Recall that a C^*-algebra $\mathcal{A}$ is a norm-closed $*$-algebra where the norm satisfies

$$\|a^*a\| = \|a\|^2 \quad (a \in \mathcal{A}).$$

In physics, the commutative algebra of functions on a phase space describes a classical theory. We denote this algebra by $\mathcal{A}_0$. A quantum mechanical theory at value $\hbar$ of Planck's constant, on the other hand, is described by a noncommutative algebra of operators on a Hilbert space, denoted by $\mathcal{A}_\hbar$ $(\hbar \neq 0)$. As we will see, the family $\{\mathcal{A}_\hbar\}$ is a strict deformation quantization if it satisfies certain axioms.

A good example is the noncommutative torus. It is obtained via deformation quantization of the algebra of functions on the torus $\mathbb{T}^d$.[1,4] The noncommutative tori play a role in string theory and M(atrix) theory.[5]

In this article, we will discuss a third example: the noncommutative cylinder. It is defined along the same lines by deformation quantization of the cylinder. In string theory, the cylinder is quite a natural object. There, space–time is a manifold of dimension higher than four. This dimension follows from certain consistency conditions of the theory (see Polchinski, Ref. 6). For example, the superstring can only be defined in a ten-dimensional background, say $\mathbb{R}^{10}$. It is usually toroidally compactified to $\mathbb{R}^4 \times \mathbb{T}^6$ in order for the theory to make sense. This means that six dimensions are rolled up to the 6-torus $\mathbb{T}^6$. As Seiberg and Witten argued in Ref. 7, the effective action of open strings in the presence of a constant magnetic field in the background is described by making space–time noncommutative. In order to describe this noncommutative background, one needs to quantize the (generalized) cylinder $\mathbb{R}^4 \times \mathbb{T}^6$.

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Another motivation to quantize the cylinder comes from an idea of Kamani. In Ref. 8, he studied the worldsheet of a superstring in a background as described before, as a noncommutative geometry. In this case, one quantizes the worldsheet, which is an ordinary cylinder $\mathbb{R}\times\mathbb{T}$.

Apart from such physical arguments, the quantization of the cylinder is also interesting from a mathematical point of view. It turns out that the C^*-algebras occurring in the quantization of the plane and of the torus are rather different. As the cylinder in some sense lies in between the plane and the torus, it will be interesting to study the C^*-algebras occurring in its quantization. Furthermore, the noncommutative cylinder provides another example in the scarce list of finite-dimensional noncommutative geometries.[9]

Having obtained the deformation quantization of the cylinder, it is interesting to consider its K-theory. This requires the K-theory of C^*-algebras, which turns out to be the right noncommutative analogue of topological K-theory. In fact, for the C^*-algebra $C(X)$ of continuous functions on a compact Hausdorff space X we have that

$$K_n(C(X))=K^n(X).$$

The main results in topological K-theory, like Bott periodicity and homotopy invariance, lift to the K-theory of C^*-algebras which has the additional powerful feature of stability.[10]

It is interesting to study the interplay between K-theory and deformation quantization. We say that K-theory is *rigid* under a given deformation when $K(\mathcal{A}_\hbar)$ is independent of $\hbar$.[11] For example, both Bott periodicity[12] and a far-reaching generalization of it, the Baum–Connes conjecture in E-theory,[13] can be seen as examples of such rigidity.[14] For the three examples just mentioned, i.e., Euclidean space, the torus, and the cylinder, rigidity of K-theory turns out to hold. However, in general this is not the case. Let $\mathcal{A}_0=C_0(T^*M)$ and $\mathcal{A}_\hbar=\mathcal{B}_0(L^2(M))$ for al $\hbar>0$. Then for general M, clearly

$$K_n(\mathcal{A}_0)=K^n(T^*M)\neq K_n(\mathcal{A}_\hbar)=\begin{cases}\mathbb{Z} & \text{if } n=0\\ 0 & \text{if } n=1.\end{cases}$$

The Gel'fand–Naimark theorem assures us that we can obtain all topological notions of a locally compact Hausdorff space from the C^*-algebra of continuous functions on it. However, in order to describe the full geometry of a spin manifold, we need more data. It turns out that the right algebraic description of a spin manifold is given by a real spectral triple satisfying Connes' seven axioms.

Definition 1: A *spectral triple* $(\mathcal{A},\mathcal{H},D)$ is given by a unital involutive algebra of operators $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ and a self-adjoint operator $D=D^*$ on $\mathcal{H}$ such that

(1) The resolvent $(D-\lambda)^{-1}$ is compact for all $\lambda\notin \mathrm{sp}(D)$,
(2) The commutators $[D,a]:=Da-aD$ are bounded for any $a\in\mathcal{A}$.

For the formulation of the seven axioms that define a *spin geometry* on $\mathcal{A}$, we refer to Refs. 15–17. A complete reconstruction of the spin structure on a spin manifold M from the spin geometry over $C^\infty(M)$ can be found in Ref. 18.

Spectral triples provide a powerful tool in describing noncommutative geometries but, at least in this definition, it relies heavily on two conditions, namely:

(1) $1\in\mathcal{A}$,
(2) D is self-adjoint.

In (commutative) spin geometry, this is equivalent to the condition that M is a compact Riemannian spin manifold.[18] In physics, however, it is natural to work in a setting where this is not the case. This is illustrated by simple examples. Consider a Minkowski space–time $M=\mathbb{R}^4$ with an indefinite metric $\eta=(-1,1,1,1)$. The Dirac operator on M is neither self-adjoint nor elliptic, and

M is noncompact. Other examples come from string theory. Consider the worldsheet of a string $\mathbb{R}\times\mathbb{T}$, embedded in a compactified background $\mathbb{R}^4\times\mathbb{T}^6$. Both the worldsheet and the background have a semi-Riemannian metric, so that both conditions are unfulfilled.

Thus, in order to describe such physical models in noncommutative geometry, i.e., using a spectral triple, we need to adjust its definition. If the C^*-algebra is nonunital, it is sufficient to replace condition 1 in the definition of a spectral triple by

(1′) The operator $a(D-\lambda)^{-1}$ is compact for any $a\in\mathcal{A}$; $\lambda\notin \mathrm{sp}(D)$.

However, in Lorentzian geometry, the Dirac operator D is not self-adjoint, so that this condition must be dropped. It turns out that the operator D is a Krein-self-adjoint operator in a Krein space $\mathcal{H}$.

Noncompact Lorentzian manifolds are central objects in physics and, therefore, we will discuss here the adjustifications mentioned in the definition of spectral triples. It will turn out that this can be done in a natural way, which allows for a definition of isospectral deformation, similar to what has been done by Connes and Landi.[19] Our key example of a noncommutative noncompact Lorentzian manifold will be the noncommutative cylinder, which is defined by isospectral deformation of the Lorentzian cylinder.

In Sec. II, we discuss deformation quantization of Euclidean space, the torus, and the cylinder. We obtain the family of C^*-algebras as a family of crossed product algebras and discuss their K-theory. We provide new evidence for the idea that K-theory is rigid under deformation quantization by describing the K-theory of the noncommutative cylinder.

In Sec. III, still working in the Euclidean setting, we consider Connes' trace theorem for noncompact manifolds. We construct spectral triples for algebras without a unit and discuss Connes' character formula in the case of the cylinder. It turns out that it is possible to generalize this theorem to noncompact manifolds. Then we obtain the noncommutative cylinder as a spectral triple, via isospectral deformation of the canonical triple of the cylinder, similar to what is done by Connes and Landi.[19] We attempt to construct a spin geometry over the noncommutative cylinder, where Connes' seven axioms are adapted to nonunital algebras as in Ref. 20.

We adjust the definition of the spectral triple to semi-Riemannian spin geometry[21] in Sec. IV, in particular to Lorentzian spin geometry. This involves Krein spaces, and we give a short introduction to the theory of these spaces and operators acting in them. Since the Dirac operator is not self-adjoint, we work with the associated operator Δ_J, which is self-adjoint. It plays a central role in the formulation of the integral in terms of a Dixmier trace.

Finally, we consider the noncommutative Lorentzian cylinder, obtained by isospectral deformation of the semi-Riemannian spectral triple that describes the Lorentzian cylinder. The set of admissible fundamental symmetries for the noncommutative cylinder is shown to be exactly the set of fundamental symmetries coming from spacelike reflections in spinor space.

II. DEFORMATION QUANTIZATION AND K-THEORY

A. Old examples

We start with a brief recapitulation of the definition of strict deformation quantization. Subsequently, we review the strict deformation quantization of Euclidean space and of the torus, both due to Rieffel.[1,2,4,22]

Definition 2: Let M be a Poisson manifold with bracket $\{\,,\}$ and let $\mathcal{A}$ be a dense $*$-subalgebra of $C_0(M)$. A *strict deformation quantization* of M in the direction of $\{,\}$, consists of an open interval $I\subseteq\mathbb{R}$ with 0 as an accumulation point, together with, for each $\hbar\in I$, an associative product $*_\hbar$, an involution $*^\hbar$, and a C^*-norm $\|\ \|_\hbar$ (for $*_\hbar$ and $*^\hbar$) on $\mathcal{A}$, which for $\hbar=0$ are the original pointwise product, complex conjugation involution, and supremum norm, such that

(1) The family $\{\mathcal{A}_\hbar\}_{\hbar\in I}$ forms a continuous field of C^*-algebras over I. Here $\mathcal{A}_\hbar$ denotes the C^*-completion of $\mathcal{A}$ with respect to $\|\ \|_\hbar$.

(2) For every $f,g\in\mathcal{A}$,

$$\lim_{\hbar\to 0}\|(f*_\hbar g-g*_\hbar f)/\mathrm{i}\hbar-\{f,g\}\|_\hbar=0 \quad \text{(Dirac's condition)}.$$

1. Weyl quantization

We consider even-dimensional Euclidean space $\mathbb{R}^{2n}$. Let $\mathcal{S}(\mathbb{R}^{2n})$ denote the commutative algebra of Schwartz functions on $\mathbb{R}^{2n}$ under pointwise multiplication. This pointwise product is deformed to the Moyal star product, which reads, in Fourier space, for any $\hbar \in \mathbb{R}$,

$$(\phi *_\hbar \psi)(p,q) = \int_{\mathbb{R}^{2n}} \mathrm{d}^n p' \mathrm{d}^n q' \, \phi(p',q') \psi(p-p', q-q') e^{-\mathrm{i}\hbar(q'\cdot p - p'\cdot q)}. \tag{1}$$

The involution we use on $\mathcal{S}(\mathbb{R}^{2n})$ is defined by $\phi^*(p,q) = \overline{\phi(-p,-q)}$, which is independent of $\hbar$. We let $\pi_\hbar$ denote the left regular representation of $\mathcal{S}(\mathbb{R}^{2n})$ on $L^2(\mathbb{R}^{2n})$ via $*_\hbar$, i.e., for $\phi \in \mathcal{S}(\mathbb{R}^{2n})$ and $\Psi \in L^2(\mathbb{R}^{2n})$,

$$\pi_\hbar(\phi)\Psi := \phi *_\hbar \Psi.$$

We define a norm $\| \ \|_\hbar$ on $\mathcal{S}(\mathbb{R}^{2n})$ as the operator norm for this representation. The completion of $\mathcal{S}(\mathbb{R}^{2n})$ with respect to this norm is a C^*-algebra, denoted by $\mathbb{R}^{2n}_\hbar$. By rewriting formula (1) in terms of partial Fourier transforms, one can show the following.[3]

Proposition 3: The C^*-algebra $\mathbb{R}^{2n}_\hbar$ is isomorphic to the crossed product algebra

$$C_0(\mathbb{R}^n) \rtimes_\hbar \mathbb{R}^n,$$

where $\mathbb{R}^n$ acts on $\mathbb{R}^n$ by translation, $x \mapsto x + \hbar y$ $(x,y \in \mathbb{R}^n)$, so that it acts on $C_0(\mathbb{R}^n)$ by the pullback of this action.

Theorem 4: *For $\hbar \neq 0$, the C^*-algebra $\mathbb{R}^{2n}_\hbar$ is isomorphic to $\mathcal{B}_0(L^2(\mathbb{R}^n))$, the C^*-algebra of compact operators on $L^2(\mathbb{R}^n)$.*

For a proof of this, we refer to Refs. 3 and 22.

It is now immediate that the C^*-algebras $\mathbb{R}^{2n}_\hbar$ $(\hbar \neq 0)$ are simple, and are all isomorphic to each other. Furthermore, we can conclude that Euclidean space $\mathbb{R}^{2n}$ has rigid K-theory under quantization, i.e., for all $\hbar$ one has

$$K^0(\mathbb{R}^{2n}) \cong K_0(\mathbb{R}^{2n}_\hbar) \cong \mathbb{Z},$$

$$K^1(\mathbb{R}^{2n}) \cong K_1(\mathbb{R}^{2n}_\hbar) \cong 0.$$

2. Noncommutative tori

Let $\mathbb{T}^d$ be the d-dimensional torus, and let θ be a real skew-symmetric $d \times d$ matrix. Instead of deforming the pointwise product in the space of smooth functions on $\mathbb{T}^d$, we deform the product in its Fourier space $\mathcal{S}(\mathbb{Z}^d)$. For $\hbar \in \mathbb{R}$, the star product reads

$$(\phi *_\hbar \psi)(n) = \sum_{m \in \mathbb{Z}^d} \phi(m) \psi(n-m) e^{2\pi \mathrm{i}\hbar\, \theta(m,n)}. \tag{2}$$

Here θ is the skew bilinear form defined by $\theta(m,n) := \Sigma_{j,k} \theta_{jk} m_j n_k$.

We set $\phi^*(n) := \overline{\phi(-n)}$, which is independent of $\hbar$. We let $\mathcal{S}(\mathbb{Z}^d)$ act on $L^2(\mathbb{Z}^d)$ by left multiplication via $*_\hbar$. The completion of $\mathcal{S}(\mathbb{Z}^d)$ with respect to the operator norm $\| \ \|_\hbar$, equipped with this star product is the *noncommutative torus*, denoted by $\mathbb{T}^d_{\hbar\theta}$. For fixed θ, the family $\{\mathbb{T}^d_{\hbar\theta}\}$ provides a strict deformation quantization of $\mathbb{T}^d$.[1] When $d=2$, the skew-symmetric matrix θ is just determined by a real number, denoted by θ as well. It turns out that the noncommutative torus $\mathbb{T}^2_\theta$ is isomorphic to the crossed product algebra $C(\mathbb{T}) \rtimes_\alpha \mathbb{Z}$, where $\alpha(f)(t) := f(t+\theta)$. Furthermore, it is simple if and only if θ is irrational. If $\theta \neq \theta'$, both irrational with $0 < \theta, \theta' < \frac{1}{2}$, then $\mathbb{T}^2_\theta \ncong \mathbb{T}^2_{\theta'}$.[16] It came as a surprise that the K-groups of $\mathbb{T}^d_\theta$ do not depend on θ.

Proposition 5: The torus $\mathbb{T}^d$ has rigid K-theory under quantization, i.e., for all $\hbar$ one has

$$K^0(\mathbb{T}^d) \cong K_0(\mathbb{T}^d_{\hbar\theta}) \cong \mathbb{Z}^{2^{d-1}},$$

$$K^1(\mathbb{T}^d) \cong K_1(\mathbb{T}^d_{\hbar\theta}) \cong \mathbb{Z}^{2^{d-1}}.$$

B. Deformation quantization of cylinders

We consider the cylinder in a generalized form. The (n,d)-*dimensional cylinder* $C^{(n,d)}$ is defined as

$$C^{(n,d)} := \mathbb{R}^n \times \mathbb{T}^d. \tag{3}$$

In the case $n=d=1$ we obtain $C^2 := \mathbb{R}\times S^1$, which is of course the familiar two-dimensional cylinder.

Let Λ be a Poisson structure on $\mathbb{R}^n\times\mathbb{T}^d$. For $j=1,\ldots,n+d$, let ∂_{x_j} denote the vector field on $\mathbb{R}^n\times\mathbb{T}^d$ corresponding to differentiation in the jth direction. We can write the Poisson structure as

$$\Lambda = -\pi^{-1}\sum_{i<j} \theta_{ij}\partial_{x_i}\wedge\partial_{x_j}. \tag{4}$$

The factor π^{-1} has been included for later convenience. Here θ_{ij} is a real skew-symmetric matrix. For later use, we define a skew bilinear form θ on $\mathbb{R}^n\times\mathbb{Z}^d$,

$$\theta(l,k) = \sum_{i,j} \theta_{ij} l_i k_j \quad (l,k \in \mathbb{R}^n\times\mathbb{Z}^d). \tag{5}$$

Let λ denote the Lebesgue measure on $\mathbb{R}^n\times\mathbb{T}^d$. The Fourier transform $\hat{f}$ of a Schwartz function $f\in\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ is given by

$$\hat{f}(k) = \int_{\mathbb{R}^n\times\mathbb{T}^d} \mathrm{d}\lambda(x) e^{-2\pi \mathrm{i} k\cdot x} f(x). \tag{6}$$

For $i=1,\ldots,n$ we have $k_i\in\mathbb{R}$, for $i=n+1,\ldots,n+d$ we have $k_i\in\mathbb{Z}$. In fact, the Fourier transform maps $\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ isomorphically to $\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$.

To integrate over $\mathbb{R}^n$ and sum over $\mathbb{Z}^d$ in the product $\mathbb{R}^n\times\mathbb{Z}^d$, we introduce the measure μ on $\mathbb{R}^n\times\mathbb{Z}^d$, defined as the product of Lebesgue measure on $\mathbb{R}^n$ and the counting measure on $\mathbb{Z}^d$.

For functions in Fourier space, the Poisson bracket is given by

$$\begin{aligned}\{\phi,\psi\}(k) &= 4\pi \int_{\mathbb{R}^n\times\mathbb{Z}^d} \mathrm{d}\mu(l) \sum_{i,j} \theta_{ij} l_i \phi(l)(k_j - l_j)\psi(k-l) \\ &= 4\pi \int_{\mathbb{R}^n\times\mathbb{Z}^d} \mathrm{d}\mu(l)\, \phi(l)\psi(k-l)\theta(l,k),\end{aligned} \tag{7}$$

where $k,l\in\mathbb{R}^n\times\mathbb{Z}^d$ and θ is the bilinear form defined in Eq. (5).

We define a bicharacter $\sigma_\hbar$ on $\mathbb{R}^n\times\mathbb{Z}^d$ by

$$\sigma_\hbar(l,k) = e^{2\pi \mathrm{i}\hbar\,\theta(l,k)}, \tag{8}$$

where $\hbar\in\mathbb{R}$, and introduce a star product $*_\hbar$ on $\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$ by

$$(\phi *_\hbar \psi)(k) = \int_{\mathbb{R}^n\times\mathbb{Z}^d} \mathrm{d}\mu(l)\, \phi(l)\psi(k-l)\sigma_\hbar(l,k). \tag{9}$$

We define an involution on $\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$ by $\phi^*(k):=\overline{\phi(-k)}$, independent of $\hbar$. We represent $\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$ on $L^2(\mathbb{R}^n\times\mathbb{Z}^d)$ by star product multiplication, and define the *noncommutative cylinder* as the completion of $\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$ in the operator norm $\|\ \|_\hbar$, equipped with product $*_\hbar$. This C^*-algebra is denoted by $C^{(n,d)}_{\hbar\theta}$.

We could equally well define the noncommutative cylinder as the (completion of) the algebra $\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ with product, involution, and norm obtained by pulling back the product $*_\hbar$, involution* and norm $\|\ \|_\hbar$ through the inverse Fourier transform. Even though this makes the differences with the ordinary cylinder more clear, we will continue in Fourier space to avoid expressions involving many derivatives.

Theorem 6: *For fixed θ, the family $\{C^{(n,d)}_{\hbar\theta}\}$ provides a strict deformation quantization of $\mathbb{R}^n\times\mathbb{T}^d$ in the direction of $\{\ ,\ \}$.*

Proof: We verify Dirac's condition

$$\|(\phi*_\hbar\psi-\psi*_\hbar\phi)/\mathrm{i}\hbar-\{\phi,\psi\}\|_\hbar\to 0 \quad \text{as } \hbar\to 0, \tag{10}$$

where $\phi,\psi\in\mathcal{S}(\mathbb{R}^n\times\mathbb{Z}^d)$. We define

$$\Delta_\hbar:=(\phi*_\hbar\psi-\psi*_\hbar\phi)/\mathrm{i}\hbar-\{\phi,\psi\}.$$

With formulas (7) and (9), this reads

$$\Delta_\hbar(k)=\int_{\mathbb{R}^n\times\mathbb{Z}^d}\mathrm{d}\mu(l)\,\phi(l)\,\psi(k-l)((\sigma_\hbar(l,k)-\sigma_\hbar(k,l))/\mathrm{i}\hbar-4\pi\theta(l,k)).$$

Similar to Rieffel in Ref. 1, we can estimate the expression inside ( ) so that

$$|\Delta_\hbar(k)|\leqslant\hbar M\int_{\mathbb{R}^n\times\mathbb{Z}^d}\mathrm{d}\mu(l)|\,\phi(l)||\,\psi(k-l)||l|^2|k-l|^2,$$

for some constant M. This last expression is just (proportional to) the convolution product of two functions $\tilde{\phi}$ and $\tilde{\psi}$ where

$$\tilde{\phi}(k):=|k|^2|\,\phi(k)|,\quad \tilde{\psi}(k):=|k|^2|\,\psi(k)|.$$

As the L^1-norm dominates the norm $\|\ \|_\hbar$, we have

$$\|\Delta_\hbar\|_\hbar\leqslant\hbar M\|\tilde{\phi}*\tilde{\psi}\|_1.$$

It follows that $\|\Delta_\hbar\|_\hbar\to 0$ as $\hbar\to 0$.

Continuity of the field $\{C^{(n,d)}_{\hbar\theta}\}$ follows from Corollary 5.6 in Ref. 23 (or Lemma 1 in Ref. 2), in combination with Proposition 7 below. □

C. Properties of noncommutative cylinders

When one observes the major differences between $\mathbb{R}^{2n}_\hbar$ and $\mathbb{T}^d_{\hbar\theta}$, one is led to the questions whether the noncommutative cylinders are simple and whether they are all isomorphic. For this, we connect with the theory of crossed product algebras. At the end, we discuss the K-theory of noncommutative cylinders.

We take the noncommutative cylinder for $n=d$, and denote it by $C^{2d}_\hbar$. We let $l=(x,n)$ and $k=(y,m)$, where $x,y\in\mathbb{R}^d$ and $n,m\in\mathbb{Z}^d$, and choose the following skew bilinear form on $\mathbb{R}^d\times\mathbb{Z}^d$,

$$\theta(l,k)=\frac{1}{2\pi}\sum_{i=1}^{d}y_in_i-m_ix_i\,. \tag{11}$$

We want to rewrite the star product (9) in terms of partial Fourier transforms, defined by

$$\acute{\phi}(x,t) := \sum_{n\in\mathbb{Z}^d} \phi(x,n)e^{in\cdot t} \quad (t\in\mathbb{T}^d), \tag{12}$$

which is a function on $\mathbb{R}^d\times\mathbb{T}^d$. The star product on $\mathcal{S}(\mathbb{R}^d\times\mathbb{T}^d)$ then reads

$$(\acute{\phi}*_\hbar\acute{\psi})(x,t) = \int_{\mathbb{R}^d} dy\, \acute{\phi}(y,t+\hbar(y-x))\,\acute{\psi}(x-y,t+\hbar y), \tag{13}$$

as can be easily verified. We introduce an action β of $\mathbb{R}^d$ on $\mathbb{T}^d$ defined by $\beta_x(t)=t+\hbar x$, and write

$$(\acute{\phi}*_\hbar\acute{\psi})(x,t) = \int_{\mathbb{R}^d} dy\, \acute{\phi}(y,\beta_{y-x}(t))\,\acute{\psi}(x-y,\beta_y(t)). \tag{14}$$

This formulation of the star product in terms of an action β of $\mathbb{R}^d$ on $\mathbb{T}^d$ goes back to Rieffel. As in the examples in his paper,[22] we relate this to crossed product algebras. For more details on the theory of these algebras, we refer to Pedersen.[24] Let $C(\mathbb{T}^d)\rtimes_\hbar\mathbb{R}^d$ denote the crossed product algebra for the $\hbar$-dependent action β_{2x}. Then $\mathcal{S}(\mathbb{R}^d,C^\infty(\mathbb{T}^d))$ is a dense $*$-subalgebra of this crossed product algebra. Define a map $Q:\mathcal{S}(\mathbb{R}^d\times\mathbb{T}^d)\to\mathcal{S}(\mathbb{R}^d,C^\infty(\mathbb{T}^d))$ by

$$Q(\acute{\phi})(x,t) := \acute{\phi}(x,\beta_x(t)). \tag{15}$$

Note that $\mathcal{S}(\mathbb{R}^d\times\mathbb{T}^d)$ is a dense $*$-subalgebra of $C_\hbar^{2d}$. Clearly, Q is an isomorphism, in that

$$\begin{aligned} Q(\acute{\phi}*_\hbar\acute{\psi})(x,t) &= (\acute{\phi}*_\hbar\acute{\psi})(x,\beta_x(t)) \\ &= \int_{\mathbb{R}^d} dy\, Q(\acute{\phi})(y,t)Q(\acute{\psi})(x-y,\beta_{2y}(t)) = Q(\acute{\phi})*Q(\acute{\psi}). \end{aligned} \tag{16}$$

Extension of the map Q to $C_\hbar^{2d}$ yields the following.

Proposition 7: The noncommutative cylinder $C_\hbar^{2d}$ $(\hbar\neq 0)$ is isomorphic to the crossed product $C(\mathbb{T}^d)\rtimes_\hbar\mathbb{R}^d$.

This allows us to use known results on crossed product algebras.

Theorem 8: *The C^*-algebra $C_\hbar^{2d}$ is isomorphic to $\mathcal{B}_0(L^2(\mathbb{T}^d))\otimes C^*(\mathbb{Z}^d)$.*

Proof: We note that $C(\mathbb{T}^d)\rtimes_\hbar\mathbb{R}^d\cong C(\mathbb{T}^d)\rtimes_{\hbar'}\mathbb{R}^d$ for $\hbar,\hbar'\neq 0$. In particular,

$$C(\mathbb{T}^d)\rtimes_\hbar\mathbb{R}^d\cong C(\mathbb{T}^d)\rtimes\mathbb{R}^d$$

for $\hbar\neq 0$. Corollary 2.8 of Green[25] completes the proof. □

With the isomorphism $C^*(\mathbb{Z}^d)\cong C(\mathbb{T}^d)$, we have the following.

Corollary 9: The noncommutative cylinders $C_\hbar^{2d}$ $(\hbar\neq 0)$ are nonsimple C^*-algebras.

It is well known that any C^*-algebra A is Morita equivalent to its stabilization

$$A_S := \mathcal{B}_0(\mathcal{H})\otimes A$$

for some Hilbert space $\mathcal{H}$. In particular, $\mathcal{B}_0(L^2(\mathbb{T}^d))\otimes C(\mathbb{T}^d)$ is Morita equivalent to $C(\mathbb{T}^d)$. Since Morita-equivalent C^*-algebras have isomorphic K-groups, we have the following.

Corollary 10: For the noncommutative cylinder $C_\hbar^{2d}$ one has for all $\hbar\neq 0$,

$$K_0(C_\hbar^{2d})\cong K_1(C_\hbar^{2d})\cong\mathbb{Z}^{2^{d-1}}.$$

In order to compare this with the K-groups of the original cylinder $\mathbb{R}^d\times\mathbb{T}^d$ we need the following Lemma.

Lemma 11: For the cylinder $\mathbb{R}^d\times\mathbb{T}^d$ *the K-groups are*

$$K^0(\mathbb{R}^d\times\mathbb{T}^d)\cong K^1(\mathbb{R}^d\times\mathbb{T}^d)\cong\mathbb{Z}^{2^{d-1}}.$$

Proof: For the K-groups of $\mathbb{T}^d$ we note that

$$K_0(C(\mathbb{T},\mathcal{A}))\cong K_1(C(\mathbb{T},\mathcal{A}))\cong K_0(\mathcal{A})\oplus K_1(\mathcal{A})$$

for any C^*-algebra $\mathcal{A}$ (cf. Exercise 10.1 in Ref. 10). Since

$$C_0(\mathbb{R}^d\times\mathbb{T}^d)\cong C(\mathbb{T},C_0(\mathbb{R}^d\times\mathbb{T}^{d-1})),$$

this yields by induction

$$K_0(C_0(\mathbb{R}^d\times\mathbb{T}^d))\cong K_1(C_0(\mathbb{R}^d\times\mathbb{T}^d))\cong\mathbb{Z}^{2^{d-1}}.$$

Here, one uses $K_0(C_0(\mathbb{R}^d))\oplus K_1(C_0(\mathbb{R}^d))\cong\mathbb{Z}$. An alternative proof can be constructed using Bott periodicity.

Proposition 12: The cylinder $\mathbb{R}^d\times\mathbb{T}^d$ *has rigid K-theory under quantization, i.e., for all* $\hbar$ *one has*

$$K^0(\mathbb{R}^d\times\mathbb{T}^d)\cong K_0(C_\hbar^{2d})\cong\mathbb{Z}^{2^{d-1}},$$

$$K^1(\mathbb{R}^d\times\mathbb{T}^d)\cong K_1(C_\hbar^{2d})\cong\mathbb{Z}^{2^{d-1}}.$$

Note that these groups are the same as the K-groups of the noncommutative torus $\mathbb{T}^d_{\hbar\theta}$.

III. NONCOMMUTATIVE MANIFOLDS AND ISOSPECTRAL DEFORMATION

The description of a manifold in terms of spectral data is provided by the theory of K-cycles (also called spectral triples) developed by Connes. This generalization has been very successful in describing noncommutative manifolds, as shown by examples like the noncommutative torus[13] and the noncommutative 4-sphere S^4_θ.[19] It also admits generalizations to noncompact manifolds, or, in other words, to nonunital algebras.

A. Connes' trace theorem

An important result here is that Connes' trace theorem generalizes to noncompact manifolds.[16] Connes' trace theorem[13,26] relates the Wodzicki residue of an elliptic pseudodifferential operator to the Dixmier trace of this operator. It allows one to compute the integral of any function on a compact Riemannian manifold in terms of an operatorial formula. See for example Ref. 16 for a complete treatment and proof of the theorem.

Proposition 13: Let f *be an integrable function on an* n*-dimensional Riemannian manifold* M*, then*

$$\int_M f(x)\sqrt{|g|}\mathrm{d}x=\frac{n(2\pi)^n}{\Omega_n}\mathrm{Tr}_\omega(f\Delta^{-n/2}),$$

where Δ *is the Laplacian on* M.

The fact that a manifold M is not compact translates into the fact that the C^*-algebra $C_0(M)$ is not unital. So, in order to describe a Riemannian manifold which is only locally compact by a spectral triple, we need a generalization of the definition as given in Ref. 13.

Definition 14: A spectral triple $(\mathcal{A},\mathcal{H},D)$ is given by an involutive algebra of operators $\mathcal{A}$ in a Hilbert space $\mathcal{H}$ and a self-adjoint operator $D=D^*$ in $\mathcal{H}$ such that

(1) $a(D-\lambda)^{-1}$ is compact for any $a\in\mathcal{A}$; $\lambda\notin sp(D)$,
(2) The commutators $[D,a]:=Da-aD$ are bounded for any $a\in\mathcal{A}$.

The triple is said to be *even* if there is a $\mathbb{Z}_2$ grading of $\mathcal{H}$, namely, an operator χ on $\mathcal{H}$ with $\chi^* = \pm\chi$ and $\chi^2 = 1$, such that

$$\chi D + D\chi = 0,$$

$$\chi a - a\chi = 0 \quad \text{for all } a \in \mathcal{A}. \tag{17}$$

If such a grading does not exist, the triple is said to be *odd*, and we set $\chi = 1$.

This was already pointed out by Connes in 1995 (Ref. 27). If $\mathcal{A}$ is unital this yields the familiar definition, because then condition (1) implies that $1_{\mathcal{A}}(D-\lambda)^{-1}$ is compact.

As a special case, we have the Dirac geometry $(C_0^\infty(M), L^2(M,S), \not{D})$ where M is a spin manifold and $\not{D}$ the Dirac operator for a spin bundle $S \to M$. Here, $C_0^\infty(M)$ denotes the algebra of smooth continuous functions on M "vanishing at infinity." For general M this means for $f \in C_0(M)$ that for all $\epsilon > 0$, there exists a compact submanifold K of M such that $f(x) < \epsilon$ for all $x \in M/K$. Note that the principal symbol $\sigma(\Delta)$ of the Laplacian, coincides with $\sigma(\not{D}^2)$.

Definition 15: A spectral triple $(\mathcal{A},\mathcal{H},D)$ is said to be p^+*-summable* $(p>0)$, if $a|D|^{-p} \in \mathcal{L}^{(1,\infty)}$ for any $a \in A$ for some dense subalgebra $A \subset \mathcal{A}$.

For a p^+-summable spectral triple $(\mathcal{A},\mathcal{H},D)$, the *noncommutative integral* of $a \in \mathcal{A}$ is defined by

$$\int a := \frac{n(2\pi)^n}{2^{[n/2]}\Omega_n} \mathrm{Tr}_\omega a|D|^{-n}. \tag{18}$$

If $\mathcal{A} = C_0^\infty(M)$, the $*$-subalgebra A consists of integrable functions with respect to the measure associated to the Riemannian metric on M.

B. Connes' character formula for the cylinder

Another result in noncommutative geometry is Connes' character formula. It provides a link between Hochschild and cyclic cohomology in that it gives a representation of the Hochschild class of the Chern character, i.e., a cyclic cocycle. It turns out that the Hochschild cocycle is much easier to handle than the Chern character. Here, we prove the character formula for the cylinder. As we saw in the previous section, the geometry of the (n,d)-dimensional cylinder can be described by the triple

$$\mathcal{A} := C_c^\infty(\mathbb{R}^n \times \mathbb{T}^d),$$

$$\mathcal{H} := L^2(\mathbb{R}^n \times \mathbb{T}^d) \otimes \mathbb{C}^{2^{[(n+d)/2]}},$$

$$D := \not{D}.$$

For convenience we have restricted $\mathcal{A}$ to functions with compact support, so that all functions in $\mathcal{A}$ are integrable.

The Dirac operator on the cylinder is defined by $\not{D} := \gamma^a \partial_a$ where the gamma-matrices satisfy $\{\gamma^a, \gamma^b\} = 2\delta^{ab}$. Using the spectral theorem for self-adjoint operators we define $F = \mathrm{sign}(\not{D})$, where $\mathrm{sign}(x) = +1(-1)$ for $x \geqslant 0$ $(x<0)$. The couple $(\mathcal{H},F)$, together with a representation σ of $\mathcal{A}$ in $\mathcal{H}$, defines a Fredholm module over $\mathcal{A}$. In the case $n+d$ is even, there is grading operator on $\mathcal{H}$ defined by $\chi := \mathrm{i}^{n+d}\gamma^1 \cdots \gamma^{n+d}$, which makes $(\mathcal{H},F)$ an even Fredholm module. Before we continue, we state some theory on universal differential graded algebras for nonunital algebras, which will be needed later.

1. Universal forms on nonunital algebras

The way to describe the graded differential algebra for nonunital algebras is very similar to the way K-theory is defined for nonunital algebras. Both rely on the notion of unitization. For the

theory of universal graded differential algebras for algebras with unit, we refer to Refs. 16, 28, and 29. A comprehensive introduction is found in Chap. 4 of Ref. 30. The approach we take here is based on Refs. 29 and 31.

Let $\mathcal{A}$ be an algebra. Its unitization $\tilde{\mathcal{A}}$ is defined by $\tilde{\mathcal{A}} := \mathcal{A} \oplus \mathbb{C}$. The quotient map is $\pi: \tilde{\mathcal{A}} \to \mathbb{C}$ with $\mathcal{A} = \ker(\pi)$. Since $1 \in \tilde{\mathcal{A}}$, we can construct the graded universal differential algebra $\Omega\tilde{\mathcal{A}}$ following standard literature. The relation between the differential algebras is similar to K-theory, i.e., $\Omega\tilde{\mathcal{A}} = \mathbb{C} \oplus \Omega\mathcal{A}$. Let δ be the corresponding derivation. By Proposition 3.2 of Ref. 29 we can extend π uniquely to a map $\pi_* : \Omega\tilde{\mathcal{A}} \to \Omega\mathbb{C}$ by

$$\pi_*(\tilde{a}_0 \delta\tilde{a}_1 \cdots \delta\tilde{a}_n) = \pi\tilde{a}_0 \delta(\pi\tilde{a}_1) \cdots \delta(\pi\tilde{a}_n). \tag{19}$$

Immediately, this yields $\pi_*(\Omega^n\tilde{\mathcal{A}}) = \{0\}$ for $n > 0$. For $n = 0$, we have $\pi_*(a + \lambda 1) = \lambda$. Of course, $\Omega\mathbb{C} = \mathbb{C}$.

Similar to what is done in the definition of K-theory for nonunital algebras, we define the graded universal differential algebra $\Omega\mathcal{A}$ of the nonunital algebra $\mathcal{A}$ as a kernel

$$\Omega\mathcal{A} := \ker(\pi_* : \Omega\tilde{\mathcal{A}} \to \Omega\mathbb{C}). \tag{20}$$

From the above observations it is clear that $\Omega^n\mathcal{A} = \Omega^n\tilde{\mathcal{A}}$ for $n > 0$. For $n = 0$, we have $\Omega^0\tilde{\mathcal{A}} = \mathbb{C} \oplus \Omega^0\mathcal{A}$, which yields $\Omega^0\mathcal{A} = \mathcal{A}$.

2. The Chern character

Given a Fredholm module $(\mathcal{H}, F, \sigma)$ over $\mathcal{A}$, we will construct a representation of $\Omega\mathcal{A}$, for $\mathcal{A} = C_c^\infty(\mathbb{R}^n \times \mathbb{T}^d)$. This will use the fact that the map

$$\mathrm{d}: a \mapsto \mathrm{i}[F, \sigma(a)]$$

is a derivation on $\mathcal{A}$, which commutes with the convolution. We can uniquely extend σ to a representation of the unitization $\tilde{\mathcal{A}}$. The couple $(\mathcal{H}, F)$ is a Fredholm module over $\tilde{\mathcal{A}}$, since obviously $[F, \tilde{a}] = [F, a]$ where we have suppressed the representations σ and $\tilde{\sigma}$. We extend $\tilde{\sigma}$ to the universal differential algebra $\Omega\mathcal{A}$ by

$$\tilde{\sigma}: \quad \Omega^k\mathcal{A} \to \mathcal{B}(\mathcal{H}),$$

$$\tilde{a}_0 \delta\tilde{a}_1 \cdots \delta\tilde{a}_k \mapsto \tilde{a}_0 \mathrm{i}^k [F, \tilde{a}_1] \cdots [F, \tilde{a}_k] = \tilde{a}_0 \mathrm{d}a_1 \cdots \mathrm{d}a_k .$$

From Ref. 16 we take the following lemma, generalized to the nonunital case.

Lemma 16: Let $\mathbb{D}$ be the (Euclidean) Dirac operator on the cylinder $\mathbb{R}^n \times \mathbb{T}^d$ and $F = \mathrm{sign}(\mathbb{D})$. Then $[F, \sigma(a)] \in \mathcal{L}^q(\mathcal{H})$, where $q = n + d + 1$.

Besides the Schatten ideals $\mathcal{L}^p(\mathcal{H})$, we define the conditional trace class $\mathcal{L}^1_C(\mathcal{H})$ by

$$\mathcal{L}^1_C(\mathcal{H}) := \{a \in \mathcal{B}(\mathcal{H}) : a + FaF \in \mathcal{L}^1(\mathcal{H})\}. \tag{21}$$

For elements in $\mathcal{L}^1_C(\mathcal{H})$, we define the conditional trace by

$$\mathrm{Tr}_C(a) := \tfrac{1}{2}\mathrm{Tr}(a + FaF). \tag{22}$$

Definition 17: The Chern character of the Fredholm module $(\mathcal{H}, F)$ is the cyclic $(n+d)$ cocycle

$$\tau_F^{(n+d)}(\tilde{a}_0, a_1, \ldots, a_{n+d}) = \mathrm{Tr}_C(\tilde{a}_0 \mathrm{d}a_1 \cdots \mathrm{d}a_{n+d}) \quad (a_i \in \mathcal{A})$$

(with $\chi\tilde{a}_0$ instead of $\tilde{a}_0$ if $n + d$ is even).

Note that since $da_i = i[F,a_i] \in \mathcal{L}^q(\mathcal{H})$, the above expression is indeed in $\mathcal{L}^1_C(\mathcal{H})$, using Hölders inequality. The following lemma brings us back from $\tilde{\mathcal{A}}$ to $\mathcal{A}$.

Lemma 18:

$$\tau_F^{(n+d)}(\tilde{a}_0,a_1,\ldots,a_{n+d}) = \tau_F^{(n+d)}(a_0,a_1,\ldots,a_{n+d}).$$

Proof: This follows immediately by writing out $a+FaF$ for $a=\tilde{a}_0 da_1\cdots da_{n+d}$.

□

Thus, although the Chern character is defined as a cyclic $(n+d)$-cocycle on $\tilde{\mathcal{A}}$, it is essentially a cyclic $(n+d)$-cocycle on $\mathcal{A}$.

Theorem 19: *For all* $a_0,a_1,\ldots,a_{n+d} \in C_c^\infty(\mathbb{R}^n \times \mathbb{T}^d)$, *one has*

$$\tau_F^{(n+d)}(a_0,a_1,\ldots,a_{n+d}) = c_{n+d} \int_{\mathbb{R}^n \times \mathbb{T}^d} a_0 \mathrm{d}_{\mathrm{dR}} a_1 \wedge \cdots \wedge \mathrm{d}_{\mathrm{dR}} a_{n+d},$$

for some constant c_{n+d} *and where* d_{dR} *is the de Rham differential.*

The proof of this theorem is really analogous to the case of $\mathbb{R}^n$, which was proved by Langmann in Ref. 32.

3. Connes' character formula

It was already mentioned in Ref. 16 that Connes' character formula holds for noncompact manifolds. Specifically, we can construct a Hochschild $(n+d)$-cocycle, which agrees with the Chern character $\tau_F^{(n+d)}$ on Hochschild $(n+d)$-cycles to obtain Connes' character formula for the cylinder. In this simple case, this follows directly from Proposition 13 and Theorem 19, if we define a Hochschild $(n+d)$-cocycle by

$$\psi_D^\omega(\tilde{a}_0,a_1,\ldots,a_{n+d}) := \mathrm{Tr}_\omega(\tilde{a}_0[\not{D},a_1]\cdots[\not{D},a_{n+d}]|\not{D}|^{-n-d})$$

(with $\chi\tilde{a}_0$ instead of $\tilde{a}_0$ in the even case). This expression makes sense by the summability properties of the spectral triple. Similar to the Chern character, we can replace $\tilde{a}_0$ by a_0.

Theorem 20: *For all* $a_0,a_1,\ldots,a_{n+d} \in C_c^\infty(\mathbb{R}^n \times \mathbb{T}^d)$, *we have*

$$\psi_D^\omega(a_0,a_1,\ldots,a_{n+d}) = \tau_F^{(n+d)}(a_0,a_1,\ldots,a_{n+d}).$$

C. Isospectral deformation of the cylinder

In Secs. II B and II C, we constructed the noncommutative cylinder as the family of C^*-algebras $C_{\hbar\theta}^{(n,d)}$, $\hbar \in (0,1]$. Here $C_{\hbar\theta}^{(n,d)}$ was defined as the completion of $\mathcal{S}(\mathbb{R}^n \times \mathbb{T}^d)$ with respect to the norm $\| \|_\hbar$, equipped with product $*_\hbar$. Note that we here choose the more natural Fourier transform instead of $\mathcal{S}(\mathbb{R}^n \times \mathbb{Z}^d)$. We now want to describe the geometry of the noncommutative cylinder using the theory of spectral triples developed in the previous sections. The approach we take involves isospectral deformation (see the following) of the (Euclidean) Dirac geometry of the cylinder $\mathbb{R}^n \times \mathbb{T}^d$.

Deformation quantization provides a natural technique to obtain a noncommutative analogue of a function algebra. Starting from the Dirac geometry $(C^\infty(M),\mathcal{H},D)$ of a compact spin manifold M, the simplest noncommutative manifold is the triple $(\mathcal{A}_\hbar,\mathcal{H},D)$, where $\mathcal{A}_\hbar$ is obtained from $C^\infty(M)$ along the lines of deformation quantization. This recipe for noncommutative manifolds is called isospectral deformation, since $\mathcal{H}$ and D are unchanged. The only thing that changes is the algebra and the way it acts on the Hilbert space.

The Dirac geometry of the cylinder is given by $(C_0^\infty(\mathbb{R}^n \times \mathbb{T}^d), \mathcal{H}, \not{D})$, where $\mathcal{H} = L^2(\mathbb{R}^n \times \mathbb{T}^d) \otimes \mathbb{C}^{2^{[(n+d)/2]}}$. However, in order to represent the deformed algebra on the same Hilbert space,

we have to restrict to $\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)\subset C_0^\infty(\mathbb{R}^n\times\mathbb{T}^d)$. Let $\mathcal{C}_{\hbar\theta}^{(n,d)}$ denote the algebra $\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ equipped with product $*_\hbar$. Note the difference with the noncommutative cylinder $C_{\hbar\theta}^{(n,d)}$ as a C^*-algebra which is the completion of $\mathcal{C}_{\hbar\theta}^{(n,d)}$.

We want to construct a spin geometry on the noncommutative cylinder. Recall that a noncommutative spin geometry is a real spectral triple fulfilling Connes' seven axioms.[15] It was shown in Refs. 16 and 33, that when the algebra $\mathcal{A}=C^\infty(M)$ on a compact spin manifold M, the spin structure, metric, and Dirac operator can be recovered from these seven axioms. However, in our case, we need a modification of these conditions. Clearly, both $\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ and $\mathcal{C}_{\hbar\theta}^{(n,d)}$ are nonunital. Hence, the conditions for a spin geometry on the noncommutative cylinder have to be modified. Such a definition of a noncommutative noncompact spin geometry has been proposed in Ref. 20.

Let us start by completing the set of ingredients for a spin geometry on the noncommutative cylinder. The basic element is the spectral triple $(\mathcal{C}_{\hbar\theta}^{(n,d)},\mathcal{H},\not{D})$. A lengthy computation shows that $\pi_\hbar(f)(\not{D}-\lambda)^{-1}$ is compact. Both the grading operator χ and the charge conjugation operator C are inherited from the commutative case.

Regularity, finiteness, and reality follow directly from the commutative case, since we are considering an isospectral deformation. However, the classical dimension cannot be obtained directly from the spectrum of $\not{D}$, since the latter is continuous. Following Ref. 20, it can be extracted from the leading term of the distributional kernel of $|\not{D}|$,[33] so that it follows from the commutative case, i.e., the classical dimension is $n+d$. The first order axiom is fulfilled since $[\not{D},f]\in\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ if $f\in\mathcal{S}(\mathbb{R}^n\times\mathbb{T}^d)$ and

$$C\pi_\hbar(f^*)C^{-1}\psi=\psi *_\hbar f=\pi_\hbar^\circ(f)\psi.$$

For the orientation, we need a Hochschild $(n+d)$-cycle c that satisfies $\pi_{\not{D}}(c)=\chi$. However, $\mathcal{C}_\hbar^{2d}$ is Morita equivalent to $C^\infty(\mathbb{T}^d)$ (see the Appendix) so that with Loday[34]

$$HH(\mathcal{C}_\hbar^{2d})=HH(C^\infty(\mathbb{T}^d))=H_{\mathrm{dR}}(\mathbb{T}^d). \tag{23}$$

Hence, in the case $n=d$, $\pi_{\not{D}}(c)=0$ for any $2d$-cycle.

Poincaré duality is satisfied in the case $n=d$ and the special form of θ described before. Since we are considering an isospectral deformation of $\mathbb{R}^d\times\mathbb{T}^d$, Poincaré duality follows from the commutative case. Indeed, we have

$$K_\bullet(\mathcal{C}_\hbar^{2d})\cong K^\bullet(\mathbb{R}^d\times\mathbb{T}^d)$$

as proved before. Since the pairing in Poincaré duality involves only the K-groups of the algebra and the Dirac operator $\not{D}$, the claim follows.

The real spectral triple $(\mathcal{C}_\hbar^{2d},\mathcal{H},\not{D},C,\chi)$ satisfies almost all conditions for a spin geometry on $\mathcal{C}_\hbar^{2d}$. Only the orientation class does not exist for the dimension prescribed by the Dirac operator. This illustrates again[20] the need for an adjustment of the orientation axiom.

IV. NONCOMMUTATIVE LORENTZIAN MANIFOLDS AND ISOSPECTRAL DEFORMATION

We saw in the previous sections that spectral triples provide a powerful noncommutative description of Riemannian geometry, which allows for generalizations to noncompact manifolds. However, in physics it is more natural to consider Lorentzian manifolds, and more generally semi-Riemannian manifolds. In fact, this is closely related to noncompactness, as illustrated by our key example: the cylinder. In string theory, one thinks of the cylinder $\mathbb{R}\times\mathbb{T}$ as the worldsheet of a string, where the noncompact direction represents the time-axis. In order to give meaning to notions such as time, a causal structure is needed and, therefore, an indefinite metric.

Following Strohmaier,[21] we start by setting up a general theory of Lorentzian manifolds in terms of spectral triples. Then we return to the (Lorentzian) cylinder and study its isospectral deformation. For an introduction to semi-Riemannian and Lorentzian geometry, we refer to Refs. 35 and 36.

The description of a Lorentzian manifold in terms of spectral data requires a more general approach than that of Riemannian manifolds. This is enforced by the fact that the Lorentzian Dirac operator is no longer a self-adjoint operator on the Hilbert space of square integrable sections of the spin bundle. Rather it is Krein-self-adjoint on the Krein space of square integrable sections. Furthermore, the signature of the Lorentzian metric implies nonellipticity of the Dirac operator as a pseudodifferential operator acting on smooth sections. Before we go into details on this, we summarize some definitions concerning Krein spaces. For a more comprehensive overview we refer to Ref. 37 or to the lecture notes by Dritschel and Rovnyak, Ref. 38.

Let V be a nondegenerate indefinite inner product space. It is called *decomposable* if there are subspaces V^-, V^+ with $V=V^-\oplus V^+$ such that the inner product $(\cdot,\cdot)$ is negative definite on V^- and positive definite on V^+. The inner product then defines a norm on these subspaces. If V^- and V^+ are complete in these norms, then V is called a *Krein space*. To every decomposition $V=V^-\oplus V^+$, we can associate an operator $J=-\mathrm{id}\oplus\mathrm{id}$, called a *fundamental symmetry*. This operator defines a positive definite inner product on V by $\langle\cdot,\cdot\rangle_J:=(\cdot,J\cdot)$ which makes V a Hilbert space.

Example 21: Consider flat Minkowski space, $V=\mathbb{R}^n$, with inner product defined by $(x,y)=-x_0y_0+x_1y_1+\cdots+x_{n-1}y_{n-1}$. We have $V=\mathbb{R}\oplus\mathbb{R}^{n-1}$ and $J=\mathrm{diag}(-1,1,\ldots,1)$. Clearly, $\langle x,y\rangle_J=\Sigma_i x_iy_i$ is positive definite.

A. Lorentzian spin geometry

Our starting point will be an n-dimensional spin manifold M, equipped with a Lorentzian metric g, i.e., a metric with signature $(n-1,1)$. Spinors on this space–time are smooth sections of the spin bundle $S\to M$. In the following, we denote by γ^μ the curved gamma-matrices, whereas γ^a are the flat ones.[39] The flat gamma matrix γ^0 plays a special role in that it defines an operator $J:=\mathrm{i}\gamma^0$ satisfying $J^2=1$. In fact, this operator is a fundamental symmetry of the space $L^2(M,S)$ of square integrable sections of the spin bundle. The space $L^2(M,S)$ is a Krein space endowed with the indefinite inner product

$$(\psi,\phi):=\int_M\sum_{i,j}\psi_i^*(x)J_{ij}\phi_j(x)\sqrt{|g|}\mathrm{d}x.$$

1. Operators in Krein spaces

In what follows we will make a clear distinction between self-adjoint operators and Krein-self-adjoint operators in $\mathcal{H}$.

The Krein adjoint $A^{[*]}$ of a densely defined operator A on a Krein space $\mathcal{H}$ is defined with respect to the indefinite inner product $(\cdot,\cdot)$ on $\mathcal{H}$. One shows that $A^{[*]}=JA^*J$ and that A is Krein-self-adjoint if and only if AJ (or JA) is self-adjoint. See Ref. 21 for more details. According to Proposition 4.1 therein, we can formally write the square of a Krein-self-adjoint operator A as

$$(A)_J:=\tfrac{1}{2}(AA^*+A^*A). \tag{24}$$

The J-dependency of this operator appears in the conjugation*. It follows that the operator $(A)_J$ is self-adjoint and commutes with J. Hence, it is Krein-self-adjoint by the above remarks.

2. Spacelike reflections and fundamental symmetries

Spacelike reflections make it possible to introduce a positive definite metric on a Lorentzian manifold (or, more generally, on a semi-Riemannian manifold). We give some of the basic notions and refer to Ref. 21 for a more detailed description.

Definition 22: Let (M,g) be a semi-Riemannian manifold. A *spacelike reflection* r is an automorphism of the vector bundle TM, such that

(1) $g(r.,r.)=g(.,.)$,
(2) $r^2=\mathrm{id}$,
(3) $g^r(.,.):=g(.,r.)$ is a positive definite metric on TM.

This map induces a splitting of TM in a direct sum $F_1\oplus F_2$, such that

$$r(x,k_1\oplus k_2)=(x,-k_1\oplus k_2).$$

The metric g^r is called the *Riemannian metric associated to* r.

If M is a semi-Riemannian spin manifold, we can associate an operator J_r to a spacelike reflection r. Let $e_0,e_1,\ldots,e_k$ be a local oriented orthonormal frame for F_1. We define $J_r:=\mathrm{i}^{k(k+1)}\gamma(e_0)\gamma(e_1)\cdots\gamma(e_{k-1})$. In the case of a Lorentzian manifold, we have $J_r=\mathrm{i}\gamma^0$, which is a fundamental symmetry of the Krein space $L^2(M,S)$ as noted before.

3. The Dirac operator

We define the Dirac operator for a spin bundle $S\to M$ in local coordinates by

$$\not{D}:=\gamma^\mu\nabla^S_\mu=\gamma^a e^\mu_a\nabla^S_\mu \tag{25}$$

acting on smooth sections $\Gamma^\infty(S)$. Here, ∇^S is the lift of the Levi-Civita connection to the spin bundle. Its principal symbol $\sigma(\not{D})$ satisfies the relation

$$\sigma(\not{D})(\xi)^2=g(\xi,\xi). \tag{26}$$

This shows that the Dirac operator on a Lorentzian manifold is a nonelliptic pseudodifferential operator that is not self-adjoint. However, from the fact that $iJ\not{D}$ is self-adjoint, it follows that $D=i\not{D}$ is Krein-self-adjoint.

As ellipticity was an important property of the Dirac operator on a Riemannian manifold, we define an elliptic self-adjoint operator Δ_J using results of Sec. IV A 2:

$$\Delta_J:=((D)_J+1)^{1/2}. \tag{27}$$

Ellipticity of this operator follows from considering its principal symbol:

$$\sigma(\Delta_J)(\xi)=\sqrt{g^r(\xi,\xi)}, \tag{28}$$

where g^r is the Riemannian metric associated to g. Furthermore, Δ_J is a pseudodifferential operator of order 1. This motivates the following definition.

Definition 23: An n^+*-summable semi-Riemannian spectral triple* $(\mathcal{A},\mathcal{H},D)$ is given by an involutive algebra of operators $\mathcal{A}$ in a Krein space $\mathcal{H}$, such that $a^*=a^{[*]}$, and by a Krein-self-adjoint operator $D=D^{[*]}$ in $\mathcal{H}$ such that

(1) The commutators $[D,a]:=Da-aD$ are bounded for any $a\in\mathcal{A}$,
(2) The operator $a\Delta_J^{-n}$ is in $\mathcal{L}^{(1,\infty)}$, for all $a\in\mathcal{A}$.

Similar to Definition 14, the triple is called even if there is a grading operator χ on $\mathcal{H}$ that satisfies the relations stated there with the only adjustification that now $\chi^{[*]}=\pm\chi$.

Of course, the triple $(C_0^\infty(M),L^2(M,S),D)$, where $D=\mathrm{i}\not{D}$, is a semi-Riemannian spectral triple, called the *canonical triple* associated to the Lorentzian spin manifold M. If the dimension n of M is even, there is a $\mathbb{Z}_2$-grading on the Hilbert space given by $\chi=\mathrm{i}^{n/2}\gamma^0\cdots\gamma^{n-1}$ so that the canonical triple is even. If the dimension of M is odd, the canonical triple is odd. Since the self-adjoint operator Δ_J associated to D is an elliptic pseudodifferential operator of order 1 as noted before, we have the following. Compare with Proposition 13.

Proposition 24: Let f be an integrable function on an n-dimensional Lorentzian manifold M, then

$$\int_M f(x)\sqrt{|g|}\,\mathrm{d}x = \frac{n(2\pi)^n}{2^{[n/2]}\Omega_n}\mathrm{Tr}_\omega(f\Delta_J^{-n}).$$

For the canonical triple, the fundamental symmetries of the form J_r for some spacelike reflection r play an important role. The analogue of such fundamental symmetries in the general case is given by the admissible fundamental symmetries as were defined in Ref. 21. Therein, it is proved that the admissible fundamental symmetries of the canonical triple are indeed exactly those of the form J_r.

B. Hochschild cocylces

We associate a Hochschild n-cocycle to the canonical triple $(C_0^\infty(M),\ L^2(M,S),\ D)$ as follows:

$$\psi_D^\omega(a_0,a_1,\ldots,a_n) = \mathrm{Tr}_\omega(a_0[D,a_1]\cdots[D,a_n]|\Delta_J|^{-n}). \tag{29}$$

Another cocycle can be constructed using the following result.

Theorem 25: *Let $(C_0^\infty(M),\ L^2(M,S),\ D)$ be the semi-Riemannian canonical triple as defined before. Then $(C_0^\infty(M),\ L^2(M,S),\ \Delta_J)$ is an n^+-summable spectral triple.*

Proof. The only nontrival condition to prove is the boundedness of $[\Delta_J,f]$ for any $f\in C_0^\infty(M)$. Since Δ_J is a pseudodifferential operator of order 1, $[\Delta_J,f]$ is of order 0, hence it is bounded. □

We define the following Hochschild n-cocyle on $C_0^\infty(M)$:

$$\psi_{\Delta_J}^\omega(a_0,a_1,\ldots,a_n) = \mathrm{Tr}_\omega(a_0[\Delta_J,a_1]\cdots[\Delta_J,a_n]|\Delta_J|^{-n}). \tag{30}$$

Obviously the two Hochschild cocycles do not coincide. We illustrate this by the following example.

Example 26: Let M be a compact two-dimensional manifold, equipped with a Minkowski metric. We evaluate the two 2-cocycles using symbol calculus:

$$\mathrm{Tr}_\omega(f[\Delta_J,g][\Delta_J,h]|\Delta_J|^{-n}) = C\int_M f\ \mathrm{d}g\wedge *(\mathrm{d}h)$$

in contrast to

$$\mathrm{Tr}_\omega(f[D,g][D,h]|\Delta_J|^{-n}) = C'\int_M f\ \mathrm{d}g\wedge \mathrm{d}h$$

for some integration constants C,C'. Note the apperance of a Polyakov type function for ψ_D^ω in this special case.

C. Isospectral deformation of the Lorentzian cylinder

With the theory of semi-Riemannian spectral triples developed in the previous sections in our hands, we are now in a position to describe the geometry of the cylinder equipped with a semi-Riemannian metric. In this section, we will discuss the semi-Riemannian spectral triple that describes the cylinder equipped with a Minkowski metric. Then we discuss isospectral deformation in this case, similar to what has been done before in the Euclidean setting. Finally, we show that the set of admissible fundamental symmetries of the noncommutative cylinder coincides with the set of fundamental symmetries coming from spacelike reflections in spinor space.

The cylinder can be described by the following semi-Riemannian spectral triple:

$$\mathcal{A} := C_0^\infty(\mathbb{R}^n \times \mathbb{T}^d),$$

$$\mathcal{H} := L^2(\mathbb{R}^n \times \mathbb{T}^d) \otimes \mathbb{C}^{2^{[(n+d)/2]}},$$

$$D := i\not{\partial}.$$

Here $\not{\partial} = \gamma^a \partial_a$, where the gamma-matrices satisfy $\{\gamma^a, \gamma^b\} = 2\eta^{ab}$ for the flat (Minkowski) metric $\eta = (-1,1,\ldots,1)$.

In order to obtain a noncommutative manifold, we perform isospectral deformation of the Lorentzian cylinder, along the same lines as we did before for the Euclidean cylinder. We restrict to $\mathcal{S}(\mathbb{R}^n \times \mathbb{T}^d)$ in order to represent the deformed algebra $\mathcal{C}_{\hbar\theta}^{(n,d)}$ on the Hilbert space $\mathcal{H}$.

Theorem 27: *The triple* $(\mathcal{C}_{\hbar\theta}^{(n,d)}, \mathcal{H}, D)$ *is a semi-Riemannian spectral triple, which is an isospectral deformation of* $(\mathcal{S}(\mathbb{R}^n \times \mathbb{T}^d), \mathcal{H}, D)$.

One could very well imitate the construction of the Riemannian spin geometry on $\mathcal{C}_\hbar^{2d}$ to obtain a Lorentzian spin geometry on the noncommutative cylinder. However, it turns out that in order to obtain for example the Lorentzian distance function from a canonical triple, one needs a different approach.[40]

An admissible fundamental symmetry J for the triple $(\mathcal{S}(\mathbb{R}^n \times \mathbb{T}^d), \mathcal{H}, D)$ is also admissible for the noncommutative cylinder. Indeed, $\mathcal{C}_{\hbar\theta}^{(n,d)}$ is invariant under conjugation with J. Invariance of $\pi(\Omega\mathcal{C}_{\hbar\theta}^{(n,d)})$ follows from the following lemma.

Lemma 28: For the semi-Riemannian spectral triple $(\mathcal{C}_{\hbar\theta}^{(n,d)}, \mathcal{H}, D)$ *we have*

$$\pi(\Omega^p \mathcal{C}_{\hbar\theta}^{(n,d)}) = \left\{ \sum_j a^j \gamma(v_1^j) \cdots \gamma(v_p^j) : \quad a^j \in \mathcal{C}_{\hbar\theta}^{(n,d)}, v_i^j \in \mathbb{C}^{2^{[(n+d)/2]}} \right\}.$$

Proof: Recall the theory of universal forms on nonunital algebras described before. Since $[D,a] = i\gamma(da)$ still holds, we have for $a_i \in \mathcal{C}_{\hbar\theta}^{(n,d)}$,

$$\pi(\tilde{a}_0 \delta a_1 \cdots \delta a_p) = \pi(\tilde{a}_0)\pi(\partial_{\mu_1} a_1) \cdots \pi(\partial_{\mu_p} a_p)\gamma(dx_1^\mu) \cdots \gamma(dx_p^\mu),$$

which is of the required form. For $p = 0$ we have $\pi(\Omega^0 \mathcal{C}_{\hbar\theta}^{(n,d)}) = \mathcal{C}_{\hbar\theta}^{(n,d)}$. □

In Sec. IV A, we saw that the set of admissible fundamental symmetries of the semi-Riemannian canonical triple coincides with the set of fundamental symmetries coming from spacelike reflections in $\mathbb{C}^{2^{[(n+d)/2]}}$. Strohmaier[21] showed that this statement also holds for noncommutative tori with trivial center. For the noncommutative cylinder, we restrict to the class described in Sec. II C, where $n = d$. There, we proved the following isomorphism of C^*-algebras:

$$C_\hbar^{2d} \cong \mathcal{B}_0(L^2(\mathbb{T}^d)) \otimes C(\mathbb{T}^d). \tag{31}$$

The appearance of the set of compact operators in the tensor product plays a central role in the following result. It turns out to hold in a slightly more general setting, i.e., in the case of a semi-Riemannian Dirac operator.

Theorem 29: *The set of admissible fundamental symmetries of the noncommutative semi-Riemannian cylinder* $(\mathcal{C}_\hbar^{2d}, \mathcal{H}, D)$ *coincides with the set*

$$\{J_r : r \text{ is a spacelike reflection of } \mathbb{C}^{2^d}\}.$$

Proof: Let r be a spacelike reflection of $\mathbb{C}^{2^d}$. It follows from Lemma 28 that J_r is admissible. For the proof of the converse statement, suppose that J is an admissible fundamental symmetry of $(\mathcal{A}, \mathcal{H}, D)$, where we take $\mathcal{A} := \mathcal{C}_\hbar^{2d}$. Since J commutes with all elements in $\mathcal{A}$, we have

$$J \in \mathcal{A}' \otimes \mathrm{End}(\mathbb{C}^{2^d}),$$

where $\mathcal{A}'$ is the commutant of $\mathcal{A}$ in $\mathcal{B}(L^2(\mathbb{R}^d\times\mathbb{T}^d))$. Since the opposite algebra $\mathcal{A}^\circ$, which acts on $\mathcal{H}$ from the right, is a dense subalgebra of $\mathcal{A}'$, we have for its unitization, with formula (10.82) in Ref. 16,

$$\tilde{\mathcal{A}}^\circ=\{T\in(\mathcal{A}^\circ)'':\quad T\in\mathrm{Dom}^\infty\delta\}=\{T\in\mathcal{A}':\quad T\in\mathrm{Dom}^\infty\delta\},$$

where $\mathrm{Dom}^\infty\delta$ is the smooth domain of the derivation $\delta:=[\Delta_J,.]$. Here we used the fact that $\mathcal{A}'=\tilde{\mathcal{A}}'$. Since J is smooth, $J\in\mathrm{Dom}^\infty\delta$, and it follows that $J\in\tilde{\mathcal{A}}^\circ\otimes\mathrm{End}(\mathbb{C}^{2^d})$. Note that the construction in Ref. 16 relies on finitely generated projective modules so that it does not directly apply to nonunital algebras.

Since $\pi(\Omega^p\mathcal{A})$ is invariant under conjugation with J, we have

$$[J\pi(\Omega^1\mathcal{A})J,\tilde{\mathcal{A}}^\circ]=[\pi(\Omega^1\mathcal{A}),\tilde{\mathcal{A}}^\circ]=0.$$

In particular, for any $\tilde{a}\gamma(v)\in\pi(\Omega^1\mathcal{A})$, we have $\tilde{a}[J\gamma(v)J,\tilde{\mathcal{A}}^\circ]=0$ so that $J\gamma(v)J$ has entries in the center of $\tilde{\mathcal{A}}^\circ$. Since $C(\mathcal{A})=C(C_\hbar^{2d})=0$, as can be seen from formula (30), we infer that $C(\tilde{\mathcal{A}})=\mathbb{C}$. Hence, $J\gamma(v)J$ must be an element of $\mathrm{End}(\mathbb{C}^{2^d})$, so that $J\gamma(v)J=-\gamma(rv)$ for some endomorphism r of $\mathbb{C}^{2^d}$. One checks the conditions of Definition 22 to conclude that r is a spacelike reflection. Hence there exists J_r such that $J\gamma(v)J=J_r\gamma(v)J_r$. Define the operator $a:=JJ_r$. It commutes with all $\gamma(v)$, so that $a\in\tilde{\mathcal{A}}^\circ$. Since $J_r\in\mathrm{End}(\mathbb{C}^{2^d})$, $[a,J_r]=0$. One shows that $a^2=a^{[*]}a=aa^{[*]}=1$ and that

$$\langle\xi,a\xi\rangle_{J_r}=(\xi,J_ra\xi)=(\xi,J\xi)\geqslant 0,\quad(\xi\in\mathcal{H}).$$

We conclude that $a=1$ and $J=J_r$. □

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APPENDIX: MORITA EQUIVALENCE OF $\mathcal{C}_\hbar^{2d}$ AND $\mathcal{S}(\mathbb{Z}^d)$

Theorem 30: *The Fréchet algebras $\mathcal{C}_\hbar^{2d}$ and $\mathcal{S}(\mathbb{Z}^d)$ are Morita equivalent via the Fréchet bimodule $\mathcal{S}(\mathbb{R}^d)$, i.e.,*

$$\mathcal{S}(\mathbb{R}^d)\overline{\otimes}_{\mathcal{S}(\mathbb{Z}^d)}\mathcal{S}(\mathbb{R}^d)\cong\mathcal{C}_\hbar^{2d},$$

$$\mathcal{S}(\mathbb{R}^d)\overline{\otimes}_{\mathcal{C}_\hbar^{2d}}\mathcal{S}(\mathbb{R}^d)\cong\mathcal{S}(\mathbb{Z}^d).$$

Here $\overline{\otimes}_{\mathcal{A}}$ denotes the completion of the tensor product over a Fréchet algebra $\mathcal{A}$ in the projective tensor product topology.

For notational convenience, we restrict to the case $d=1$. Recall that $\mathcal{C}_\hbar^2$ is the Fréchet algebra $\mathcal{S}(\mathbb{R}\times\mathbb{T})$ equipped with the following product:

$$(F*G)(x,t)=\int_{\mathbb{R}}\mathrm{d}y\,F(y,t)G(x-y,t-\pi(y)),$$

where $\pi:\mathbb{R}\to\mathbb{R}/\mathbb{Z}\cong\mathbb{T}$ is the natural projection. We equip it with the following submultiplicative seminorms:[41]

$$p^{\alpha,\beta,\gamma}(F)=\int_{\mathbb{T}}\mathrm{d}t\int_{\mathbb{R}}\mathrm{d}x(1+|x|)^{\alpha}|\partial_x^{\beta}\partial_t^{\gamma}F(x,t)|.$$

The algebra $\mathcal{S}(\mathbb{Z})$ is equipped with the usual convolution product and the corresponding submultiplicative seminorms

$$q^{\alpha}(a)=\sum_{n\in\mathbb{Z}}(1+|n|)^{\alpha}|a(n)|.$$

Proof: The module $\mathcal{S}(\mathbb{R})$ is a Fréchet $\mathcal{C}_\hbar^2-\mathcal{S}(\mathbb{Z})$ bimodule in the following sense. First of all, it consists of differentiable functions on $\mathbb{R}$ with the topology given by the seminorms $\nu^{\alpha,\beta}$,

$$\nu^{\alpha,\beta}(f):=\int_{\mathbb{R}}\mathrm{d}x(1+|x|)^{\alpha}|\partial_x^{\beta}f(x)|. \tag{A1}$$

The left and right actions of $\mathcal{C}_\hbar^2$ and $\mathcal{S}(\mathbb{Z})$ are defined by

$$F\cdot f(x)=\int_{\mathbb{R}}\mathrm{d}y\,F(x-y,\pi(x))f(y), \tag{A2}$$

$$f\cdot a(x)=\sum_n a(n)f(x+n). \tag{A3}$$

One checks that these actions are continuous and that $(F*G)\cdot f=F\cdot(G\cdot f)$, $f\cdot(a*b)=(f\cdot a)\cdot b$. Furthermore, compatibility of both actions, $(F\cdot f)\cdot a=F\cdot(f\cdot a)$ is easily checked. We write ${}_{\mathcal{C}_\hbar^2}\mathcal{S}(\mathbb{R})_{\mathcal{S}(\mathbb{Z})}$.

We will endow $\mathcal{S}(\mathbb{R})$ also with the structure of a $\mathcal{S}(\mathbb{Z})-\mathcal{C}_\hbar^2$ bimodule:

$$f\cdot F(x)=\int_{\mathbb{R}}\mathrm{d}y\,F(y-x,\pi(y))f(y), \tag{A4}$$

$$a\cdot f(x)=\sum_n a(n)f(x-n). \tag{A5}$$

Again, this module satisfies the right properties and we write ${}_{\mathcal{S}(\mathbb{Z})}\mathcal{S}(\mathbb{R})_{\mathcal{C}_\hbar^2}$.

Recall that an essential Fréchet A-modules X satisfies $A\cdot X\subset X$ densely.[42]

Lemma 31: The Fréchet bimodules ${}_{\mathcal{C}_\hbar^2}\mathcal{S}(\mathbb{R})_{\mathcal{S}(\mathbb{Z})}$ *and* ${}_{\mathcal{S}(\mathbb{Z})}\mathcal{S}(\mathbb{R})_{\mathcal{C}_\hbar^2}$ *are essential.*

Proof: Since the algebra $\mathcal{S}(\mathbb{Z})$ is unital for the convolution product, there is nothing to prove there. The algebra $\mathcal{C}_\hbar^2$ has an approximate identity $\{e_\lambda\}_{\lambda\in\Lambda}$ defined by

$$e_\lambda(x,t):=\frac{\lambda}{\sqrt{\pi}}e^{-\lambda x^2}.$$

We have $e_\lambda\cdot f\to f$ and $f\cdot e_\lambda\to f$ for $f\in\mathcal{S}(\mathbb{R})$. □

We proceed by defining bilinear maps,

$$\tilde{\phi}:\mathcal{S}(\mathbb{R})\times\mathcal{S}(\mathbb{R})\to\mathcal{C}_\hbar^2,$$

$$\tilde{\phi}(f,g)(x,t)=\sum_n f(t-n)g(t-x-n), \tag{A6}$$

$$\tilde{\psi}:\mathcal{S}(\mathbb{R})\times\mathcal{S}(\mathbb{R})\to\mathcal{S}(\mathbb{Z}),$$

$$\tilde{\psi}(f,g)(n)=\int_{\mathbb{R}} \mathrm{d}x f(x)g(x-n). \tag{A7}$$

One checks that the maps $\tilde{\phi}$ and $\tilde{\psi}$ are bounded bilinear module maps. They are balanced since one easily computes

$$\tilde{\phi}(f\cdot a,g)=\tilde{\phi}(f,a\cdot g),$$

$$\tilde{\psi}(f\cdot F,g)=\tilde{\psi}(f,F\cdot g). \tag{A8}$$

Therefore, we can extend $\tilde{\phi}$ and $\tilde{\psi}$ to the tensor product:

$$\phi:\mathcal{S}(\mathbb{R})\overline{\otimes}_{\mathcal{S}(\mathbb{Z})}\mathcal{S}(\mathbb{R})\to\mathcal{C}^2_\hbar,$$

$$\psi:\mathcal{S}(\mathbb{R})\overline{\otimes}_{\mathcal{C}^2_\hbar}\mathcal{S}(\mathbb{R})\to\mathcal{S}(\mathbb{Z}). \tag{A9}$$

Note that the maps $\tilde{\phi}$ and $\tilde{\psi}$ satisfy the following properties:

$$\tilde{\phi}(f,g)\cdot h=f\cdot\tilde{\psi}(g,h),$$

$$\tilde{\psi}(f,g)\cdot h=f\cdot\tilde{\phi}(g,h). \tag{A10}$$

Lemma 32: The module morphisms ϕ and ψ are surjective.

Proof: Let $F\in\mathcal{C}^2_\hbar$. Define $H\in\mathcal{S}(\mathbb{R})\overline{\otimes}_{\mathcal{S}(\mathbb{Z})}\mathcal{S}(\mathbb{R})$ by

$$H(x,y):=f(x)F(x-y,\pi(x)),$$

where $f\in\mathcal{S}(\mathbb{R})$ satisfies $\Sigma_n f(t-n)=1$ for all $t\in[0,1)$. Then $\phi(H)=F$. For surjectivity of ψ it is enough to construct a function $f\in\mathcal{S}(\mathbb{R})$ with $\psi(f\otimes f)=\mathbf{1}_{\mathcal{S}(\mathbb{Z})}$. Clearly, this holds for a function f with $\mathrm{supp}f\in(0,1)$ and $\int\mathrm{d}x|f(x)|^2=1$. □

Lemma 33: The module morphisms ϕ and ψ are injective

Proof: Let $\Sigma_i\tilde{\phi}(f_i,g_i)=0$. Then

$$\tilde{\phi}(f,g)\cdot\sum_i f_i\otimes_{\mathcal{S}(\mathbb{Z})}g_i=\sum\tilde{\phi}(f,g)\cdot f_i\otimes_{\mathcal{S}(\mathbb{Z})}g_i=\sum f\cdot\tilde{\psi}(g,f_i)\otimes_{\mathcal{S}(\mathbb{Z})}g_i$$

$$=\sum f\otimes_{\mathcal{S}(\mathbb{Z})}\tilde{\psi}(g,f_i)\cdot g_i=f\otimes_{\mathcal{S}(\mathbb{Z})}g\cdot\sum_i\tilde{\phi}(f_i,g_i)=0, \tag{A11}$$

using formula (A10) twice. Hence, $F\cdot\Sigma_i f_i\otimes_{\mathcal{S}(\mathbb{Z})}g_i=0$ for all $F\in\mathcal{C}^2_\hbar$. Since $\mathcal{C}^2_\hbar$ has an approximate identity it follows that $\Sigma_i f_i\otimes_{\mathcal{S}(\mathbb{Z})}g_i=0$. Since $\mathcal{S}(\mathbb{Z})$ is unital, we find similarly injectivity of ψ. □

This completes the proof of the theorem.

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Eigenvalues of Ruijsenaars–Schneider models associated with A_{n-1} root system in Bethe ansatz formalism

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Ruijsenaars–Schneider models associated with A_{n-1} root system with a discrete *coupling constant* are studied. The eigenvalues of the Hamiltonian are given in terms of the Bethe ansatz formulas. Taking the ''nonrelativistic'' limit, we obtain the spectrum of the corresponding Calogero–Moser systems in the *third formulas* of Felder *et al.* © *2004 American Institute of Physics.*
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I. INTRODUCTION

Ruijsenaars–Schneider (RS) models[1,2] are integrable generalization of Calogero–Moser (CM) models[3,4] at both classical and quantum levels. The integrability of classical RS models associated with various root systems were studied by Lax pair representation for A_{n-1},[1] for D_n,[5] for C_n and BC_n with one coupling constant.[6] The commuting conserved quantities for quantum RS models were discussed in Refs. 2, 7, 8, and 9.

It is well known that the Hamiltonian of RS model with degenerate potentials (trigonometric and rational ones) is one of the commuting families of Macdonald operators,[10] which are also called *Ruijsenaars–Macdonald operators*. The eigenfunctions of the *degenerate* Hamiltonian are given by so-called *Macdonald polynomials*.[10] However, an analogous construction for elliptic generalization of *Macdonald polynomials* is still an open problem.

Bethe ansatz method has proved to be the most powerful and (probably) unified method to construct the common eigenvectors of commuting families of operators (usually called *transfer matrices*) in two-dimensional trigonometric and rational integrable models.[11–15] Recently, after a definition of elliptic quantum groups $E_{\tau,\eta}(\mathfrak{g})$ associated with any simple classical Lie algebra $\mathfrak{g}$ was given,[16] the algebraic Bethe ansatz method has been successfully extended. The method for construction of the eigenvectors of the transfer matrices associated with the module over $E_{\tau,\eta}(sl_2)$ (Ref. 17) is now generalized to apply for those associated with the module over $E_{\tau,\eta}(sl_n)$ with generic n.[18,19]

In particular, the elliptic *Ruijsenaars–Macdonald operator* (3.7) with a discrete *coupling constant* $\gamma=\sqrt{-1}gl$ (l being a non-negative integer) associated with A_{n-1} root system can be rewritten as the *transfer matrices* associated with the symmetric $n\times l$ tensor product evaluation $E_{\tau,\eta}(sl_n)$ module.[20] This enables us to obtain the eigenvalues of the Hamiltonian of elliptic RS models with the discrete *coupling constant* $\gamma=\sqrt{-1}gl$ associated with A_{n-1} root system by the algebraic Bethe ansatz for elliptic quantum group $E_{\tau,\eta}(sl_n)$.

The paper is organized as follows. In Sec. II, we give a brief review of the algebraic Bethe ansatz for elliptic quantum group $E_{\tau,\eta}(sl_n)$ developed in Ref. 19. In Sec. III, choosing the special $E_{\tau,\eta}(sl_n)$-module $W=V_{\Lambda(nl)}(0)$, we give the eigenvalues of elliptic RS model with the discrete *coupling constant* $\gamma=\sqrt{-1}gl$ and the associated Bethe ansatz equations. Taking the degenerate

(trigonometric and rational) limit, we obtain the eigenvalues of Hamiltonian of the degenerate RS models associated with A_{n-1} root system. In Sec. IV, taking the ''nonrelativistic'' limit,[21] we obtain the eigenvalues of elliptic, trigonometric and rational types of CM models associated with A_{n-1} root system with an integer *coupling constant* $\gamma=l+1$ in the Bethe ansatz formulas or the *third formulas* in the sense of Felder *et al.*[22]

II. ALGEBRAIC BETHE ANSATZ FOR ELLIPTIC QUANTUM GROUP $E_{\tau,\eta}(sl_n)$

A. Elliptic quantum group associated with A_{n-1}

We first review the definition of the elliptic quantum group $E_{\tau,\eta}(sl_n)$ associated with A_{n-1}.[16] Let $\{\boldsymbol{\epsilon}_i | i=1,2,...,n\}$ be the orthonormal basis of the vector space $\mathbb{C}^n$ such that $\langle \boldsymbol{\epsilon}_i, \boldsymbol{\epsilon}_j \rangle = \delta_{ij}$. The A_{n-1} simple roots are $\{\alpha_i = \boldsymbol{\epsilon}_i - \boldsymbol{\epsilon}_{i+1} | i=1,...,n-1\}$ and the fundamental weights $\{\Lambda_i | i=1,...,n-1\}$ satisfying $\langle \Lambda_i, \alpha_j \rangle = \delta_{ij}$ are given by

$$\Lambda_i = \sum_{k=1}^{i} \boldsymbol{\epsilon}_k - \frac{i}{n} \sum_{k=1}^{n} \boldsymbol{\epsilon}_k .$$

Set

$$\hat{i} = \boldsymbol{\epsilon}_i - \overline{\boldsymbol{\epsilon}}, \quad \overline{\boldsymbol{\epsilon}} = \frac{1}{n} \sum_{k=1}^{n} \boldsymbol{\epsilon}_k, \quad i=1,...,n, \quad \text{then} \ \sum_{i=1}^{n} \hat{i} = 0. \tag{2.1}$$

For each dominant weight $\Lambda = \Sigma_{i=1}^{n-1} a_i \Lambda_i$, $a_i \in \mathbb{Z}^+$, there exists an irreducible highest weight finite-dimensional representation V_Λ of A_{n-1} with the highest vector $|\Lambda\rangle$. For example, the fundamental vector representation is V_{Λ_1}. In this paper, we consider only the symmetric tensor-product representation of $\overbrace{V_{\Lambda_1} \otimes V_{\Lambda_1} \cdots \otimes V_{\Lambda_1}}^{l}$ (or, the *higher spin-l representation of* A_{n-1}), namely, the one parameter series of highest weight representations $V_{\Lambda^{(l)}}$, with

$$\Lambda^{(l)} = l\Lambda_1, \quad l \in \mathbb{Z} \quad \text{and} \ l>0. \tag{2.2}$$

This corresponds to the Young diagram $\overbrace{\square\square\square\cdots\square}^{l}$.

Let $\mathfrak{h}$ be the Cartan subalgebra of A_{n-1} and $\mathfrak{h}^*$ be its dual. A finite dimensional diagonalizable $\mathfrak{h}$-module is a complex finite dimensional vector space W with a weight decomposition $W = \oplus_{\mu \in h^*} W[\mu]$, so that $\mathfrak{h}$ acts on $W[\mu]$ by $xv = \mu(x)v$, $(x \in \mathfrak{h}, v \in W[\mu])$. For example, the fundamental vector representation $V_{\Lambda_1} = \mathbb{C}^n$, the nonzero weight spaces $W[\hat{i}] = \mathbb{C}\boldsymbol{\epsilon}_i$, $i=1,...,n$.

Let us fix τ such that $\mathrm{Im}(\tau)>0$ and a generic complex number η. For convenience, we introduce another parameter $w = n\eta$ related to η. Let us introduce the following elliptic functions:

$$\theta\begin{bmatrix} a \\ b \end{bmatrix}(u,\tau) = \sum_{m=-\infty}^{\infty} \exp\{\sqrt{-1}\pi[(m+a)^2\tau + 2(m+a)(u+b)]\}, \tag{2.3}$$

$$\sigma(u) = \theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u,\tau), \quad \zeta(u) = \partial_u\{\ln\sigma(u)\}, \quad \wp(u) = -\partial_u\{\zeta(u)\}. \tag{2.4}$$

These functions have the following properties:

$$\sigma(u) = 0 + u\sigma'(0) + \frac{u^3}{6}\sigma'''(0) + \cdots, \quad \text{when} \ u \to 0, \tag{2.5}$$

$$\sigma(-u) = -\sigma(u), \quad \zeta(-u) = -\zeta(u), \quad \wp(-u) = \wp(u), \tag{2.6}$$

where $\sigma'(0)=\partial_u\{\sigma(u)\}|_{u=0}$ and $\sigma'''(0)=\partial_u^3\{\sigma(u)\}|_{u=0}$.

For a generic $\lambda\in\mathbb{C}^n$, define

$$\lambda_i=\langle\lambda,\epsilon_i\rangle,\quad \lambda_{ij}=\lambda_i-\lambda_j=\langle\lambda,\epsilon_i-\epsilon_j\rangle,\quad i,j=1,...,n. \tag{2.7}$$

Let $R(z,\lambda)\in\mathrm{End}(\mathbb{C}^n\otimes\mathbb{C}^n)$ be the R-matrix given by

$$R(z,\lambda)=\sum_{i=1}^{n} R_{ii}^{ii}(z,\lambda)E_{ii}\otimes E_{ii}+\sum_{i\neq j}\{R_{ij}^{ij}(z,\lambda)E_{ii}\otimes E_{jj}+R_{ij}^{ji}(z,\lambda)E_{ji}\otimes E_{ij}\}, \tag{2.8}$$

in which E_{ij} is the matrix with elements $(E_{ij})_k^l=\delta_{jk}\delta_{il}$. The coefficient functions are

$$R_{ii}^{ii}(z,\lambda)=1,\quad R_{ij}^{ij}(z,\lambda)=\frac{\sigma(z)\sigma(\lambda_{ij}+w)}{\sigma(z+w)\sigma(\lambda_{ij})}, \tag{2.9}$$

$$R_{ij}^{ji}(z,\lambda)=\frac{\sigma(w)\sigma(z+\lambda_{ij})}{\sigma(z+w)\sigma(\lambda_{ij})}, \tag{2.10}$$

and λ_{ij} is defined in (2.7). The R-matrix satisfies the dynamical (modified) quantum Yang–Baxter equation.

$$\begin{aligned}&R_{12}(z_1-z_2,\lambda-wh^{(3)})R_{13}(z_1-z_3,\lambda)R_{23}(z_2-z_3,\lambda-wh^{(1)})\\&\quad=R_{23}(z_2-z_3,\lambda)R_{13}(z_1-z_3,\lambda-wh^{(2)})R_{12}(z_1-z_2,\lambda),\end{aligned} \tag{2.11}$$

with the initial condition

$$R_{ij}^{kl}(0,\lambda)=\delta_i^l\delta_j^k. \tag{2.12}$$

We adopt the notation $R_{12}(z,\lambda-wh^{(3)})$ acts on a tensor $v_1\otimes v_2\otimes v_3$ as $R(z,\lambda-w\mu)\otimes Id$ if $v_3\in W[\mu]$.

A representation of the elliptic quantum group $E_{\tau,\eta}(sl_n)$ [an $E_{\tau,\eta}(sl_n)$-module] is by definition a pair (W,L) where W is a diagonalizable $\mathfrak{h}$-module and $L(z,\lambda)$ is a meromorphic function of λ and the spectral parameter $z\in\mathbb{C}$, with values in $\mathrm{End}_{\mathfrak{h}}(\mathbb{C}^n\otimes W)$ (the endomorphisms commuting with the action of $\mathfrak{h}$). It obeys the so-called RLL relation

$$R_{12}(z_1-z_2,\lambda-wh^{(3)})L_{13}(z_1,\lambda)L_{23}(z_2,\lambda-wh^{(1)})=L_{23}(z_2,\lambda)L_{13}(z_1,\lambda-wh^{(2)})R_{12}(z_1-z_2,\lambda), \tag{2.13}$$

where the first and second space are auxiliary spaces ($\mathbb{C}^n$) and the third space plays the role of the quantum space (W). The total weight conservation condition for the L-operator reads

$$[h^{(1)}+h^{(3)},L_{13}(z,\lambda)]=0.$$

In terms of the elements of the L-operator defined by

$$L(z,\lambda)(\epsilon_i\otimes v)=\sum_{j=1}^{n}\epsilon_j\otimes L_i^j(z,\lambda)v,\quad v\in W, \tag{2.14}$$

the above condition can be expressed equivalently as

$$f(h)L_i^j(z,\lambda)=L_i^j(z,\lambda)f(h+\hat{i}-\hat{j}), \tag{2.15}$$

in which $f(h)$ is any meromorphic function of h and h measures the weight of the quantum space (W).

B. Modules over $E_{\tau,\eta}(sl_n)$ and the associated operator algebra

The basic example of an $E_{\tau,\eta}(sl_n)$-module is $(\mathbb{C}^n, L)$ with $L(z,\lambda)=R(z-z_1,\lambda)$, which is called the fundamental vector representation $V_{\Lambda_1}(z_1)$ with the evaluation point z_1. It is obvious that the RLL relation is satisfied as a consequence of the dynamical Yang–Baxter equation (2.11). Other modules can be obtained by taking tensor products: if $(W_1, L^{(1)})$ and $(W_2, L^{(2)})$ are $E_{\tau,\eta}(sl_n)$-modules, where $L^{(j)}$ acts on $(\mathbb{C}^n \otimes W_j)$, then also $(W_1 \otimes W_2, L)$ with

$$L(z,\lambda)=L^{(1)}(z,\lambda-wh^{(2)})L^{(2)}(z,\lambda) \quad \text{acting on } \mathbb{C}^n \otimes W_1 \otimes W_2. \tag{2.16}$$

An $E_{\tau,\eta}(sl_n)$-submodule of an $E_{\tau,\eta}(sl_n)$-module (W,L) is a pair (W_1, L_1) where W_1 is an $\mathfrak{h}$-submodule of W such that $\mathbb{C}^n \otimes W_1$ is invariant under the action of all the $L(z,\lambda)$, and $L_1(z,\lambda)$ is the restriction to this invariant subspace. Namely, the $E_{\tau,\eta}(sl_n)$-submodules are $E_{\tau,\eta}(sl_n)$-modules.

Using the fusion rule of $E_{\tau,\eta}(sl_n)$ (2.16) one can construct the symmetric $E_{\tau,\eta}(sl_n)$-submodule of l-tensors of fundamental vector representations:

$$V_{\Lambda^{(l)}}(z_1)=\text{symmetric subspace of } V_{\Lambda_1}(z_1)\otimes V_{\Lambda_1}(z_1-w)\otimes\cdots\otimes V_{\Lambda_1}(z_1-(l-1)w),$$

where $\Lambda^{(l)}$ is defined by (2.2). We call such an $E_{\tau,\eta}(sl_n)$-module the *higher spin-l representation* with the evaluation point z_1. These series of representations in the case of $\mathbb{Z}_n$ Sklyanin algebra have been studied in Ref. 23 for $n=2$ case and in Refs. 24 and 25 for generic n case.

For any $E_{\tau,\eta}(sl_n)$-module, as in Ref. 17 one can define an associated operator algebra of difference operators on the space $\mathrm{Fun}(W)$ of meromorphic functions of λ with values in W. The algebra is generated by h and the operators $\widetilde{L}(z) \in \mathrm{End}(\mathbb{C}^n \otimes \mathrm{Fun}(W))$ acting as

$$\widetilde{L}(z)(\epsilon_i \otimes f)(\lambda)=\sum_{j=1}^{n} \epsilon_j \otimes L_i^j(z,\lambda) f(\lambda - w\hat{i}). \tag{2.17}$$

One can derive the following exchange relation of the difference operator $\widetilde{L}(z)$ from the RLL relation (2.13), the weight conservation condition $L_i^j(z,\lambda)$ (2.15) and the fact $[h^{(1)}+h^{(2)}, R_{12}(z,\lambda)]=0$,

$$R_{12}(z_1-z_2, \quad \lambda-wh)\widetilde{L}_{13}(z_1)\widetilde{L}_{23}(z_2)=\widetilde{L}_{23}(z_2)\widetilde{L}_{13}(z_1)R_{12}(z_1-z_2,\lambda), \tag{2.18}$$

$$f(h)\widetilde{L}_i^j(z)=\widetilde{L}_i^j(z)f(h+\hat{i}-\hat{j}), \tag{2.19}$$

where $f(h)$ is any meromorphic function of h. Let $W=V_{\Lambda^{(l_1)}}(z_1)\otimes V_{\Lambda^{(l_2)}}(z_2)\otimes\cdots\otimes V_{\Lambda^{(l_m)}}(z_m)$ and $\Lambda=\Lambda^{(l_1)}+\cdots+\Lambda^{(l_m)}$, then $W[\Lambda]=\mathbb{C}|\Lambda\rangle$ with $|\Lambda\rangle=|\Lambda^{(l_1)}\rangle\otimes\cdots\otimes|\Lambda^{(l_m)}\rangle$.

Theorem 1 (Ref. 19): *With generic evaluation points $\{z_i\}$, W is an irreducible highest weight $E_{\tau,\eta}(sl_n)$-module and the vector $|\Lambda\rangle$, viewed as a constant function in Fun(W), obeys the following highest weight conditions:*

$$\widetilde{L}_1^1(z)|\Lambda\rangle=A(z,\lambda)|\Lambda\rangle, \quad \widetilde{L}_1^i(z)|\Lambda\rangle=0, \quad i=2,...,n,$$

$$\widetilde{L}_j^i(z)|\Lambda\rangle=\delta_j^i D_i(z,\lambda)|\Lambda\rangle, \quad i,j=2,...,n, \quad f(h)|\Lambda\rangle=f(N\hat{1})|\Lambda\rangle.$$

The highest weight functions read

$$A(z,\lambda)=1, \quad D_i(z,\lambda)=\left\{\prod_{k=1}^{m}\frac{\sigma(z-p_k)}{\sigma(z-q_k)}\right\}\frac{\sigma(\lambda_{i1}+Nw)}{\sigma(\lambda_{i1})}, \quad i=2,...,n, \tag{2.20}$$

where

$$p_k = z_k, \quad q_k = z_k - l_k w, \quad N = \sum_{k=1}^{m} l_k, \quad k = 1,...,m. \tag{2.21}$$

The *transfer matrices* associated with an $E_{\tau,\eta}(sl_n)$-module (W,L) (Ref. 17) are difference operators acting on the space $\mathrm{Fun}(W)[0]$ of meromorphic functions of λ with values in the zero-weight space of W. They are defined by

$$T(u)f(\lambda) = \sum_{i=1}^{n} \tilde{L}_i^i(u) f(\lambda) = \sum_{i=1}^{n} L_i^i(u,\lambda) f(\lambda - w\hat{i}). \tag{2.22}$$

The exchange relations of $\tilde{L}$-operators (2.18) and (2.19) imply that, for any $E_{\tau,\eta}(sl_n)$-module, the above transfer matrices preserve the space $\mathcal{H} = \mathrm{Fun}(W)[0]$. Moreover, they commute pairwise on $\mathcal{H}$: $[T(u),T(v)]|_{\mathcal{H}} = 0$.

C. Algebraic Bethe ansatz for $E_{\tau,\eta}(sl_n)$

We fix a highest weight $E_{\tau,\eta}(sl_n)$-module W of weight Λ, the functions $A(z,\lambda)$, $D_i(z,\lambda)$ (2.20), with the highest weight vector $|\Lambda\rangle$. We assume that $N = \Sigma_{k=1}^{m} l_k = n \times l$ with l being an integer, so that the zero-weight space $W[0]$ can be nontrivial and that the algebraic Bethe ansatz method can be applied as in Refs. 26, 27, 28, 17, and 19.

Let us adopt the standard notation for convenience:

$$\mathcal{A}(u) = \tilde{L}_1^1(u), \quad \mathcal{B}_i(u) = \tilde{L}_i^1(u), \quad i = 2,...,n, \tag{2.23}$$

$$\mathcal{C}_i(u) = \tilde{L}_1^i(u), \quad \mathcal{D}_i^j(u) = \tilde{L}_i^j(u), \quad i,j = 2,...,n. \tag{2.24}$$

The transfer matrices $T(u)$ become

$$T(u) = \mathcal{A}(u) + \sum_{i=2}^{n} \mathcal{D}_i^i(u). \tag{2.25}$$

Any nonzero vector $|\Omega\rangle \in \mathrm{Fun}(W)[\Lambda]$ is of form $|\Omega\rangle = g(\lambda)|\Lambda\rangle$, for some meromorphic function $g \neq 0$. When $N = n \times l$, the weight Λ can be written in the form

$$\Lambda = nl\Lambda_1 = l \sum_{k=1}^{n-1} (\epsilon_1 - \epsilon_{k+1}). \tag{2.26}$$

Noting (2.19), the zero-weight vector space is spanned by the vectors of the following form:

$$\mathcal{B}_{i_{N_1}}(v_{N_1}) \mathcal{B}_{i_{N_1-1}}(v_{N_1-1}) \cdots \mathcal{B}_{i_1}(v_1)|\Omega\rangle, \tag{2.27}$$

where $N_1 = (n-1) \times l$ and among the indices $\{i_k | k = 1,...,N_1\}$, the number of $i_k = j$, denoted by $\#(j)$, should be

$$\#(j) = l, \quad j = 2,...,n. \tag{2.28}$$

The above states (2.27) actually belong to the zero-weight space $W[0]$.[19] Let us introduce the following set of integers for convenience:

$$N_i = (n-i) \times l, \quad i = 1,2,...,n-1, \tag{2.29}$$

and $[n(n-1)/2]l$ parameters $\{\{v_k^{(i)} | k = 1,2,...,N_{i+1}\}, i = 0,1,...,n-2\}$. The parameters $\{\{v_k^{(i)}\}\}$ will be specified later by the Bethe ansatz equations (2.40). We will seek the common eigenvectors of the *transfer matrices* $T(u)$ in the form

$$|\lambda;\{v_k\}\rangle=\sum_{i_1,\cdots,i_{N_1}=2}^{n} F^{i_1,i_2,\ldots,i_{N_1}}(\lambda;\{v_k\})\mathcal{B}_{i_{N_1}}(v_{N_1})\mathcal{B}_{i_{N_1-1}}(v_{N_1-1})\cdots\mathcal{B}_{i_1}(v_1)|\Omega\rangle, \quad (2.30)$$

with the restriction condition (2.28). We adopt hereafter the convention

$$v_k=v_k^{(0)}, \quad k=1,2,\ldots,(n-1)\times l. \quad (2.31)$$

Let us introduce n parameters $\{\alpha^{(i)}|i=1,\ldots,n\}$ to specify quasivacua of each step of the nested Bethe ansatz,[19] and another set of parameters related to them,

$$\overline{\alpha}^{(i)}=\frac{1}{(n-i-1)}\left\{\alpha^{(i+1)}-\frac{\sum_{k=i+1}^{n}\alpha^{(k)}}{n-i}\right\}, \quad i=0,\ldots,n-2. \quad (2.32)$$

Choosing the function of $g(\lambda)$,

$$g(\lambda)=e^{\sqrt{-1}\pi\langle\alpha^{(1)}\epsilon_1,\lambda\rangle}\prod_{j=2}^{n}\left\{\prod_{k=1}^{l}\frac{\sigma(\lambda_{j1}+kw)}{\sigma(w)}\right\}, \quad (2.33)$$

then we have the following.

Theorem 2 (Ref. 19): *With properly chosen coefficients* $F^{i_1,i_2,\ldots,i_{N_1}}(\lambda;\{v_k\})$, *we obtain eigenvectors of the transfer matrices*

$$T(u)|\lambda;\{v_k\}\rangle=t(u;\{v_k\})|\lambda;\{v_k\}\rangle, \quad (2.34)$$

with the eigenvalue

$$t(u;\{v_k\})=e^{\sqrt{-1}\pi(1-n)\overline{\alpha}w}\left\{\prod_{k=1}^{N_1}\frac{\sigma(v_k-u+w)}{\sigma(v_k-u)}\right\}+e^{\sqrt{-1}\pi\overline{\alpha}w}\left\{\prod_{k=1}^{N_1}\frac{\sigma(u-v_k+w)}{\sigma(u-v_k)}\right\}$$
$$\times\left\{\prod_{k=1}^{m}\frac{\sigma(u-p_k)}{\sigma(u-q_k)}\right\}t^{(1)}(u;\{v_k^{(1)}\}). \quad (2.35)$$

The functions $t^{(i)}(u;\{v_k^{(i)}\})$ *are given recursively,*

$$t^{(i)}(u;\{v_k^{(i)}\})=e^{\sqrt{-1}\pi(i+1-n)\overline{\alpha}^{(i)}w}\left\{\prod_{k=1}^{N_{i+1}}\frac{\sigma(v_k^{(i)}-u+w)}{\sigma(v_k^{(i)}-u)}\right\}+e^{\sqrt{-1}\pi\overline{\alpha}^{(i)}w}\left\{\prod_{k=1}^{N_{i+1}}\frac{\sigma(u-v_k^{(i)}+w)}{\sigma(u-v_k^{(i)})}\right\}$$
$$\times\left\{\prod_{k=1}^{N_i}\frac{\sigma(u-p_k^{(i)})}{\sigma(u-q_k^{(i)})}\right\}t^{(i+1)}(u;\{v_k^{(i+1)}\}), \quad i=0,1,\ldots,n-2, \quad (2.36)$$

$$t^{(n-1)}(u)=1, \quad t^{(0)}(u;\{v_k^{(0)}\})=t(u;\{v_k\}), \quad (2.37)$$

where $\overline{\alpha}^{(i)}$, $i=0,1,\ldots,n-2$ *are given by (2.32),* $\overline{\alpha}^{(0)}=\overline{\alpha}$, $N_0=m$ *and*

$$p_k^{(0)}=p_k=z_k, \quad q_k^{(0)}=q_k=z_k-l_kw, \quad k=1,2,\ldots,m, \quad (2.38)$$

$$p_k^{(i)}=v_k^{(i-1)}, \quad q_k^{(i)}=v_k^{(i-1)}-w, \quad i=1,2,\ldots,n-2, \quad k=1,2,\ldots,N_i. \quad (2.39)$$

The $\{\{v_k^{(i)}\}\}$ *satisfy the following Bethe ansatz equations:*

$$e^{\sqrt{-1}\pi(i-n)\bar{\alpha}^{(i)}w}\left\{\prod_{k=1,k\neq s}^{N_{i+1}}\frac{\sigma(v_k^{(i)}-v_s^{(i)}+w)}{\sigma(v_k^{(i)}-v_s^{(i)}-w)}\right\}=\left\{\prod_{k=1}^{N_i}\frac{\sigma(v_s^{(i)}-p_k^{(i)})}{\sigma(v_s^{(i)}-q_k^{(i)})}\right\}t^{(i+1)}(v_s^{(i)};\{v_k^{(i+1)}\}). \tag{2.40}$$

In principle one can construct explicit expression of the coefficients of $F^{i_1,i_2,\cdots,i_{N_1}}(\lambda;\{v_k\})$ (for details we refer the reader to Ref. 19).

We conclude this section with some remarks on functional dependence of the states $|\lambda;\{v_k\}\rangle$. By construction (2.23), the operators $\{\mathcal{B}_i\}$ are the functions of $\{\lambda_i-\lambda_j\}$ because of the definition of the R-matrix (2.9)–(2.10), and the states can be written in the following form:

$$|\lambda;\{v_k\}\rangle=\exp\left\{\sum_{i=1}^{n}\sqrt{-1}\pi\alpha^{(i)}\lambda_i\right\}\overline{|\lambda;\{v_k\}\rangle}. \tag{2.41}$$

Here $\overline{|\lambda;\{v_k\}\rangle}$ is a meromorphic function of $\{\lambda_i\}$ and has the following properties:

$$\overline{|\lambda_1+c,\ldots,\lambda_n+c;\{v_k\}\rangle}=\overline{|\lambda_1,\ldots,\lambda_n;\{v_k\}\rangle},\quad \text{for } \forall c\in\mathbb{C}, \tag{2.42}$$

$$\overline{|\lambda_1,\ldots,\lambda_{i-1},\lambda_i+1,\lambda_{i+1},\ldots\lambda_n;\{v_k\}\rangle}=(-1)^{l(n-1)}\overline{|\lambda_1,\ldots,\lambda_n;\{v_k\}\rangle},\quad i=1,\ldots,n. \tag{2.43}$$

III. RUIJSENAARS–SCHNEIDER MODELS ASSOCIATED WITH A_{n-1} ROOT SYSTEM

A. The elliptic case

Let us choose an $E_{\tau,\eta}(sl_n)$-module W, a special one which corresponds to the Young diagram $\overbrace{\square\square\cdots\square}^{nl}$,

$$W=V_{\Lambda^{(nl)}}(0), \tag{3.1}$$

in which the evaluation point z_1 is set to 0. Then the zero-weight space of this module is one-dimensional: $|\lambda;\{v_k\}\rangle=\tilde{\Phi}_{\mathrm{RS}}(\lambda;\{\alpha^{(i)}\})e_0$, $e_0\in W[0]$ and it does not depend on λ_i. The associated *transfer matrices* can be written as[20]

$$T(u)=\frac{\sigma(u+lw)}{\sigma(u+nlw)}M. \tag{3.2}$$

The operator M is independent of u and is given by

$$M=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\frac{\sigma(\lambda_{ij}+lw)}{\sigma(\lambda_{ij})}\Gamma_i\right\}. \tag{3.3}$$

Here $\{\Gamma_i\}$ are difference operators: $\Gamma_i f(\lambda)=f(\lambda-w\hat{i})$. Noting (2.41)–(2.43) and (3.14), we find

$$M\tilde{\Phi}_{\mathrm{RS}}=\tilde{H}_{\mathrm{RS}}\tilde{\Phi}_{\mathrm{RS}}=\epsilon_{\mathrm{RS}}\tilde{\Phi}_{\mathrm{RS}}. \tag{3.4}$$

The difference operator $\tilde{H}_{\mathrm{RS}}$ is given by

$$\tilde{H}_{\mathrm{RS}}=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\frac{\sigma(\lambda_{ij}+lw)}{\sigma(\lambda_{ij})}e^{-w(\partial/\partial\lambda_i)}\right\}. \tag{3.5}$$

In order to apply Theorem 2 to RS model, hereafter we restrict the parameters τ and w as follows:

$$\tau=\sqrt{-1}\kappa,\quad \kappa\in\mathbb{R},\quad \kappa>0,\quad w=\sqrt{-1}g, \tag{3.6}$$

where g is a real number. This is necessary for the reality of the Hamiltonian. Because the parameters $\{\lambda_i\}$ will play the role of the canonical coordinates, we further restrict $\lambda_i \in \mathbb{R}$. In terms of the specified parameters, $\tilde{H}_{\mathrm{RS}}$ becomes

$$\tilde{H}_{\mathrm{RS}}=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\frac{\sigma(\lambda_{ij}+\sqrt{-1}gl)}{\sigma(\lambda_{ij})}e^{-\sqrt{-1}g(\partial/\partial\lambda_i)}\right\}. \tag{3.7}$$

The resulting difference operator $\tilde{H}_{\mathrm{RS}}$ will be the Hamiltonian of elliptic A_{n-1} type RS model[2] with the special *coupling constant* $\gamma=\sqrt{-1}gl$, up to conjugation by a function.[25,29] Suppose $\tilde{\Phi}_{\mathrm{RS}}$ and ϵ_{RS} are an eigenfunction and the corresponding eigenvalue of $\tilde{H}_{\mathrm{RS}}$,

$$\tilde{H}_{\mathrm{RS}}\tilde{\Phi}_{\mathrm{RS}}=\epsilon_{\mathrm{RS}}\tilde{\Phi}_{\mathrm{RS}}. \tag{3.8}$$

Let us introduce another function Φ_{RS},

$$\Phi_{\mathrm{RS}}=e^{-\Psi_{\mathrm{RS}}}\tilde{\Phi}_{\mathrm{RS}},\quad \Psi_{\mathrm{RS}}=\frac{1}{2}\ln\prod_{i\neq j}\left\{\prod_{k=1}^{l}\frac{\sigma(\lambda_{ij}-\sqrt{-1}gk)}{\sigma(\sqrt{-1}g)}\right\}, \tag{3.9}$$

associated to $\tilde{\Phi}_{\mathrm{RS}}$. Then Φ_{RS} is an eigenfunction of the similarity transformed Hamiltonian H_{RS} with the same eigenvalue ϵ_{RS},

$$H_{\mathrm{RS}}\Phi_{\mathrm{RS}}=\epsilon_{\mathrm{RS}}\Phi_{\mathrm{RS}},\quad H_{\mathrm{RS}}=e^{-\Psi_{\mathrm{RS}}}\tilde{H}_{\mathrm{RS}}e^{\Psi_{\mathrm{RS}}}, \tag{3.10}$$

$$H_{\mathrm{RS}}=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\frac{\sigma(\lambda_{ji}-\sqrt{-1}gl)}{\sigma(\lambda_{ji})}\right\}^{1/2}e^{-\sqrt{-1}g(\partial/\partial\lambda_i)}\left\{\prod_{j\neq i}\frac{\sigma(\lambda_{ij}-\sqrt{-1}gl)}{\sigma(\lambda_{ij})}\right\}^{1/2}. \tag{3.11}$$

One finds that H_{RS} is the Hamiltonian of elliptic A_{n-1} type RS model[2] with the special *coupling constant* $\gamma=\sqrt{-1}gl$.

Now, we consider the spectrum of $\tilde{H}_{\mathrm{RS}}$. Theorem 2 enables us to obtain the spectrum of the Hamiltonian of the elliptic A_{n-1} Ruijsenaars–Schneider model as well as the eigenfunctions, in terms of the associated transfer matrices (3.2). Since we have already taken the special $E_{\tau,\eta}(sl_n)$-module $W=V_{\Lambda^{(n\times l)}}(0)$, thanks to Theorem 2, the eigenvalues are given by (2.34) and (2.35) but with special values of the parameters

$$m=N_0=1,\quad p_1^{(0)}=z_1=0,\quad q_1^{(0)}=-\sqrt{-1}gnl. \tag{3.12}$$

Since M is independent of u, we can evaluate the eigenvalues of $T(u)$ at $u=z_1=0$. Then the expression of the eigenvalue $t(u;\{v_k\})$ simplifies drastically, for the second term on the right-hand side of (2.35) [the one depending on the eigenvalue of the reduced transfer matrices $t^{(1)}\times(u;\{v_k^{(1)}\})$] vanishes because $u-p_1^{(0)}=0$.

Note that $\tilde{H}_{\mathrm{RS}}(H_{\mathrm{RS}})$ has periodic coefficients with $\lambda_i\to\lambda_i+1$, and therefore preserves the space of Bloch functions such that

$$\psi(\lambda_1,\ldots,\lambda_{i-1},\lambda_i+1,\lambda_{i+1},\ldots,\lambda_n)=\pm(-1)^{l(n-1)}\psi(\lambda_1,\ldots,\lambda_n). \tag{3.13}$$

The (quasi)periodicity requires integer $\alpha^{(i)}$, $\alpha^{(i)}\in\mathbb{Z}$. Noting the relation (2.32), in order to get one-to-one correspondence between $\{\alpha^{(i)}\}$ and $\{\overline{\alpha^{(i)}}\}$, we need further choose

$$\alpha^{(i)}\in\mathbb{Z}^+,\quad i=1,\ldots,n-1,\quad \text{and}\quad \alpha^{(n)}=-\sum_{k=1}^{n-1}\alpha^{(k)}. \tag{3.14}$$

Finally, we obtain the eigenvalues $\epsilon_{RS}(\{v_k\})$ of $\tilde{H}_{RS}$ (3.4):

$$e^{\pi(n-1)\overline{\alpha}g}\frac{\sigma(\sqrt{-1}gnl)}{\sigma(\sqrt{-1}gl)}\left\{\prod_{k=1}^{(n-1)\times l}\frac{\sigma(v_k+\sqrt{-1}g)}{\sigma(v_k)}\right\}, \tag{3.15}$$

where $\{\{v_k^{(i)}\}\}$ satisfy the Bethe ansatz equations

$$e^{\pi(n-i)\overline{\alpha}^{(i)}g}\left\{\prod_{k=1,k\neq s}^{N_{i+1}}\frac{\sigma(v_k^{(i)}-v_s^{(i)}+\sqrt{-1}g)}{\sigma(v_k^{(i)}-v_s^{(i)}-\sqrt{-1}g)}\right\}=\left\{\prod_{k=1}^{N_i}\frac{\sigma(v_s^{(i)}-p_k^{(i)})}{\sigma(v_s^{(i)}-q_k^{(i)})}\right\}t^{(i+1)}(v_s^{(i)};\{v_k^{(i+1)}\}),$$

$$i=0,1,\ldots,n-2. \tag{3.16}$$

The functions $t^{(i)}(u)$ appearing in (3.16) are given by the same recurrence relations as (2.36)–(2.37), but with the special $N_0=1$, $p_1^{(0)}=0$, and $q_1^{(0)}=-\sqrt{-1}gnl$ and replacing w by $\sqrt{-1}g$. Substituting the expression of the function $t^{(i+1)}(u)$ (2.36) into the Bethe ansatz equations (3.16), noting the conditions (3.12) and (2.39), we have the following.

Proposition 1: The eigenvalues of the Hamiltonian (3.11) of the elliptic RS model associated with A_{n-1} root system with the discrete coupling constant $\gamma=\sqrt{-1}gl$ (l being an integer) are

$$\epsilon_{\mathrm{RS}}=e^{\pi(n-1)\overline{\alpha}g}\frac{\sigma(\sqrt{-1}gnl)}{\sigma(\sqrt{-1}gl)}\left\{\prod_{k=1}^{(n-1)\times l}\frac{\sigma(v_k+\sqrt{-1}g)}{\sigma(v_k)}\right\}. \tag{3.17}$$

The $[n(n-1)/2]l$ parameters $\{\{v_k^{(i)}\}\}$ satisfy the Bethe ansatz equations

$$e^{\pi n\overline{\alpha}g}\prod_{k=1,k\neq s}^{N_1}\frac{\sigma(v_k-v_s+\sqrt{-1}g)}{\sigma(v_k-v_s-\sqrt{-1}g)}=e^{\pi(n-2)\overline{\alpha}^{(1)}g}\frac{\sigma(v_s)}{\sigma(v_s+\sqrt{-1}gnl)}\prod_{k=1}^{N_2}\frac{\sigma(v_k^{(1)}-v_s+\sqrt{-1}g)}{\sigma(v_k^{(1)}-v_s)}, \tag{3.18}$$

$$e^{\pi(n-i)\overline{\alpha}^{(i)}g}\prod_{k=1,k\neq s}^{N_{i+1}}\frac{\sigma(v_k^{(i)}-v_s^{(i)}+\sqrt{-1}g)}{\sigma(v_k^{(i)}-v_s^{(i)}-\sqrt{-1}g)}=e^{\pi(n-i-2)\overline{\alpha}^{(i+1)}g}\prod_{k=1}^{N_i}\frac{\sigma(v_s^{(i)}-v_k^{(i-1)})}{\sigma(v_s^{(i)}-v_k^{(i-1)}+\sqrt{-1}g)}$$
$$\times\prod_{k=1}^{N_{i+2}}\frac{\sigma(v_k^{(i+1)}-v_s^{(i)}+\sqrt{-1}g)}{\sigma(v_k^{(i+1)}-v_s^{(i)})},\quad i=1,\ldots,n-3, \tag{3.19}$$

$$e^{2\pi\overline{\alpha}^{(n-2)}g}\prod_{k=1,k\neq s}^{N_{n-1}}\frac{\sigma(v_k^{(n-2)}-v_s^{(n-2)}+\sqrt{-1}g)}{\sigma(v_k^{(n-2)}-v_s^{(n-2)}-\sqrt{-1}g)}=\prod_{k=1}^{N_{n-2}}\frac{\sigma(v_s^{(n-2)}-v_k^{(n-3)}}{\sigma(v_s^{(n-2)}-v_k^{(n-3)}+\sqrt{-1}g)}. \tag{3.20}$$

The parameters $\overline{\alpha}^{(i)}$, $i=0,1,\ldots,n-2$ and $\overline{\alpha}^{(0)}=\overline{\alpha}$ are given by the relation (2.32) from $n-1$ arbitrary non-negative integers $\{\alpha^{(i)}\in\mathbb{Z}^+|i=1,\ldots,n-1\}$.

Our formula of eigenvalues is the elliptic generalization of the *third formulas* in the sense of Felder *et al.*[22] Taking complex conjugation of the Bethe ansatz equations (3.18)–(3.20), noting the property (A5), we find that the solutions $\{\{v_k^{(i)}\}\}$ are all pure imaginary numbers. This ensures that the eigenvalues ϵ_{RS} are real. By construction from the nested Bethe ansatz method and the relation (3.9), we know that the corresponding eigenfunction is a meromorphic function of $\{\lambda_i\}$ and satisfies the following properties:

$$\Phi_{\mathrm{RS}}(\lambda_1,\ldots,\lambda_{i-1},\lambda_i+1,\lambda_{i+1},\ldots,\lambda_n;\{\alpha^{(i)}\})=(-1)^{\alpha^{(i)}}\Phi_{\mathrm{RS}}(\lambda;\{\alpha^{(i)}\}). \tag{3.21}$$

B. The trigonometric case

Here we consider the trigonometric RS model associated with A_{n-1} root system. The corresponding Hamiltonian with the discrete *coupling constant* $\gamma=\sqrt{-1}gl$ is given

$$H_{\mathrm{RS}}=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\frac{\sin\pi(\lambda_{ji}-\sqrt{-1}gl)}{\sin\pi(\lambda_{ji})}\right\}^{1/2}e^{-\sqrt{-1}g(\partial/\partial\lambda_i)}\left\{\prod_{j\neq i}\frac{\sin\pi(\lambda_{ij}-\sqrt{-1}gl)}{\sin\pi(\lambda_{ij})}\right\}^{1/2}. \tag{3.22}$$

Taking the trigonometric limit $\kappa\to+\infty$ ($\tau\to+\sqrt{-1}\infty$), one finds that

$$\frac{\sigma(x)}{\sigma(y)}\to\frac{\sin\pi x}{\sin\pi y},\quad \text{when}\ \ \kappa\to+\infty, \tag{3.23}$$

from the product expression (A1) of the σ-function. The trigonometric Hamiltonian (3.22) can be obtained from the elliptic one (3.11) by taking limit $\kappa\to+\infty$. Consequently, we can find the spectrum of the Hamiltonian of the trigonometric RS model associated with A_{n-1} type root system by taking the trigonometric limit of the elliptic one. Noting that the solutions to the Bethe ansatz equations (3.18)–(3.20) $\{\{v_k^{(i)}\}\}$ are all pure imaginary numbers, let us introduce $[n(n-1)/2]l$ real parameters $\{\{\overline{v}_k^{(i)}\}\}$ associated to $[n(n-1)/2]l$ pure imaginary parameters $\{\{v_k^{(i)}\}\}$ as follows:

$$v_k^{(i)}=\sqrt{-1}\overline{v}_k^{(i)},\quad \overline{v}_k^{(i)}\in\mathbb{R}. \tag{3.24}$$

Finally, we have

Proposition 2: The eigenvalues of the Hamiltonian (3.22) of the trigonometric RS model associated with A_{n-1} root system with the discrete coupling constant $\gamma=\sqrt{-1}gl$ are

$$\epsilon_{\mathrm{RS}}=e^{\pi(n-1)\overline{\alpha}g}\frac{\sinh\pi(nlg)}{\sinh\pi(lg)}\left\{\prod_{k=1}^{(n-1)\times l}\frac{\sinh\pi(\overline{v}_k^{(0)}+g)}{\sinh\pi(\overline{v}_k^{(0)})}\right\}. \tag{3.25}$$

The $[n(n-1)/2]l$ real parameters $\{\{\overline{v}_k^{(i)}\}\}$ satisfy the Bethe ansatz equations

$$e^{\pi n\overline{\alpha}g}\left\{\prod_{k=1,k\neq s}^{N_1}\frac{\sinh\pi(\overline{v}_k^{(0)}-\overline{v}_s^{(0)}+g)}{\sin\pi(\overline{v}_k^{(0)}-\overline{v}_s^{(0)}-g)}\right\}=e^{\pi(n-2)\overline{\alpha}^{(1)}g}\frac{\sinh\pi(\overline{v}_s^{(0)})}{\sinh\pi(\overline{v}_s^{(0)}+nlg)}\times\left\{\prod_{k=1}^{N_2}\frac{\sinh\pi(\overline{v}_k^{(1)}-\overline{v}_s^{(0)}+g)}{\sinh\pi(\overline{v}_k^{(1)}-\overline{v}_s^{(0)})}\right\}, \tag{3.26}$$

$$e^{\pi(n-i)\overline{\alpha}^{(i)}g}\left\{\prod_{k=1,k\neq s}^{N_{i+1}}\frac{\sinh\pi(\overline{v}_k^{(i)}-\overline{v}_s^{(i)}+g)}{\sinh\pi(\overline{v}_k^{(i)}-\overline{v}_s^{(i)}-g)}\right\}=e^{\pi(n-i-2)\overline{\alpha}^{(i+1)}g}\left\{\prod_{k=1}^{N_i}\frac{\sinh\pi(\overline{v}_s^{(i)}-\overline{v}_k^{(i-1)})}{\sinh\pi(\overline{v}_s^{(i)}-\overline{v}_k^{(i-1)}+g)}\right\}\times\left\{\prod_{k=1}^{N_{i+2}}\frac{\sinh\pi(\overline{v}_k^{(i+1)}-\overline{v}_s^{(i)}+g)}{\sinh\pi(\overline{v}_k^{(i+1)}-\overline{v}_s^{(i)})}\right\},$$

$$i=1,\ldots,n-3, \tag{3.27}$$

$$e^{2\pi\overline{\alpha}^{(n-2)}g}\left\{\prod_{k=1,k\neq s}^{N_{n-1}}\frac{\sinh\pi(\overline{v}_k^{(n-2)}-\overline{v}_s^{(n-2)}+g)}{\sinh\pi(\overline{v}_k^{(n-2)}-\overline{v}_s^{(n-2)}-g)}\right\}=\left\{\prod_{k=1}^{N_{n-2}}\frac{\sinh\pi(\overline{v}_s^{(n-2)}-\overline{v}_k^{(n-3)})}{\sinh\pi(\overline{v}_s^{(n-2)}-\overline{v}_k^{(n-3)}+g)}\right\}. \tag{3.28}$$

Here the parameters $\overline{\alpha}^{(i)}$, $i=0,1,\ldots,n-2$ and $\overline{\alpha}=\overline{\alpha}^{0}$ are given by the relation (2.32) from $n-1$ arbitrary non-negative integers $\{\alpha^{(i)}\in\mathbb{Z}^{+}|i=1,\ldots,n-1\}$.

Our formula of eigenvalues is the *trigonometric* generalization of the *third formulas* in the sense of Felder *et al.*[22] Similarly to the elliptic case, we know that the corresponding eigenfunction has the same quasiperiodic properties (3.21).

C. The rational case

The Hamiltonian of the rational RS model associated with A_{n-1} root system reads as

$$H_{RS}=\sum_{i=1}^{n}\left\{\prod_{j\neq i}\left(1-\frac{\sqrt{-1}gl}{\lambda_{ji}}\right)\right\}^{1/2}e^{-\sqrt{-1}g(\partial/\partial\lambda_i)}\left\{\prod_{j\neq i}\left(1-\frac{\sqrt{-1}gl}{\lambda_{ij}}\right)\right\}^{1/2}. \tag{3.29}$$

If one rescales

$$\lambda_i\to\delta\lambda_i,\quad \overline{\alpha}^{(i)}\to\frac{1}{\pi\delta}\overline{\alpha}^{(i)},\quad g\to\delta g, \tag{3.30}$$

$$\overline{v}_k^{(i)}\to\delta\overline{v}_k^{(i)}, \tag{3.31}$$

and takes the limit: $\delta\to 0$ (we call it the rational limit), the Hamiltonian (3.29) of the rational RS model can be obtained from the trigonometric one (3.22). Therefore we can find the spectrum of the Hamiltonian of the rational RS model associated with A_{n-1} root system by taking the rational limit of Proposition 2. Finally we have the following.

Proposition 3: The eigenvalues of the Hamiltonian (3.29) of the rational RS model associated with A_{n-1} root system with the discrete coupling constant $\gamma=\sqrt{-1}gl$ are

$$\epsilon_{\mathrm{RS}}=ne^{(n-1)\overline{\alpha}g}\left\{\prod_{k=1}^{(n-1)\times l}\frac{\overline{v}_k^{(0)}+g}{\overline{v}_k^{(0)}}\right\}. \tag{3.32}$$

The $[n(n-1)/2]l$ real parameters $\{\{\overline{v}_k^{(i)}\}\}$ satisfy the Bethe ansatz equations

$$e^{n\overline{\alpha}g}\left\{\prod_{k=1,k\neq s}^{N_1}\frac{(\overline{v}_k^{(0)}-\overline{v}_s^{(0)}+g)}{(\overline{v}_k^{(0)}-\overline{v}_s^{(0)}-g)}\right\}=e^{(n-2)\overline{\alpha}^{(1)}g}\frac{\overline{v}_s^{(0)}}{\overline{v}_s^{(0)}+nlg}\left\{\prod_{k=1}^{N_2}\frac{(\overline{v}_k^{(1)}-\overline{v}_s+g)}{(\overline{v}_k^{(1)}-\overline{v}_s)}\right\}, \tag{3.33}$$

$$\begin{aligned}e^{(n-i)\overline{\alpha}^{(i)}g}\left\{\prod_{k=1,k\neq s}^{N_{i+1}}\frac{(\overline{v}_k^{(i)}-\overline{v}_s^{(i)}+g)}{(\overline{v}_k^{(i)}-\overline{v}_s^{(i)}-g)}\right\}&=e^{(n-i-2)\overline{\alpha}^{(i+1)}g}\left\{\prod_{k=1}^{N_i}\frac{(\overline{v}_s^{(i)}-\overline{v}_k^{(i-1)})}{(\overline{v}_s^{(i)}-\overline{v}_k^{(i-1)}+g)}\right\}\\&\times\left\{\prod_{k=1}^{N_{i+2}}\frac{(\overline{v}_k^{(i+1)}-\overline{v}_s^{(i)}+g)}{(\overline{v}_k^{(i+1)}-\overline{v}_s^{(i)})}\right\},\quad i=1,\ldots,n-3,\end{aligned} \tag{3.34}$$

$$e^{2\overline{\alpha}^{(n-2)}g}\left\{\prod_{k=1,k\neq s}^{N_{n-1}}\frac{(\overline{v}_k^{(n-2)}-\overline{v}_s^{(n-2)}+g)}{(\overline{v}_k^{(n-2)}-\overline{v}_s^{(n-2)}-g)}\right\}=\left\{\prod_{k=1}^{N_{n-2}}\frac{(\overline{v}_s^{(n-2)}-\overline{v}_k^{(n-3)})}{(\overline{v}_s^{(n-2)}-\overline{v}_k^{(n-3)}+g)}\right\}. \tag{3.35}$$

Here the parameters $\overline{\alpha}^{(i)}$, $i=0,1,\ldots,n-2$ and $\overline{\alpha}^{(0)}=\overline{\alpha}$ are given by the relation (2.32) from $n-1$ arbitrary non-negative real numbers $\{\alpha^{(i)}\in\mathbb{R}^+|i=1,\ldots,n-1\}$.

Our formula of eigenvalues is the rational generalization of the *third formulas* in the sense of Felder *et al.*[22] The rescalings (3.30) and (3.31) and the rational limit lead to that the coefficients of the Hamiltonian (3.29) are no longer periodic (cf. the elliptic and trigonometric case). The (quasi)periodic properties (3.21) of the eigenfunction now are replaced by the following asymptotic properties:

$$\Phi_{\mathrm{RS}}\propto e^{\sqrt{-1}\alpha^i\lambda_i},\quad \lambda_i\to\infty. \tag{3.36}$$

Namely, the corresponding eigenfunctions are bounded when $\lambda_i\to\infty$ on the real axis.

IV. CALOGERO–MOSER SYSTEMS ASSOCIATED WITH A_{n-1} ROOT SYSTEM

In this section, we will study all types of CM models associated with A_{n-1} root system by taking "nonrelativistic" limit:[21] $g\to 0$ of the corresponding RS models which have already been studied in Sec. III.

A. Elliptic potential

Taking the *nonrelativistic limit* of the Hamiltonian (3.7) and noting the asymptotic properties of σ-function (2.5), we obtain

$$\widetilde{H}_{\mathrm{RS}}=n+\frac{g^2}{2}\widetilde{H}_{\mathrm{CM}}+O(g^3),\quad g\to 0. \tag{4.1}$$

The resulting differential operator $\widetilde{H}_{\mathrm{CM}}$ is given by

$$\widetilde{H}_{\mathrm{CM}}=-\sum_{i=1}^{n}\frac{\partial^2}{(\partial\lambda_i)^2}+2l\sum_{i\neq j}^{n}\zeta(\lambda_{ij})\frac{\partial}{\partial\lambda_i}-l^2\sum_{i\neq j}\frac{\sigma''(\lambda_{ij})}{\sigma(\lambda_{ij})}-l^2\sum_{i\neq j\neq k}\zeta(\lambda_{ij})\zeta(\lambda_{ik}), \tag{4.2}$$

where $\sigma''(t)=[\partial^2/(\partial u)^2]\sigma(u)|_{u=t}$ and the function ζ is defined in (2.4). We can further transform $\widetilde{H}_{\mathrm{CM}}$ to a more familiar form. Let us suppose $\widetilde{\Phi}$ and ϵ_{CM} are an eigenfunction and the corresponding eigenvalue of $\widetilde{H}_{\mathrm{CM}}$, namely,

$$\widetilde{H}_{\mathrm{CM}}\widetilde{\Phi}=\epsilon_{\mathrm{CM}}\widetilde{\Phi}. \tag{4.3}$$

At the same time, we introduce another function Φ,

$$\Phi=e^{-\Psi}\widetilde{\Phi},\quad \Psi=\ln\prod_{i<j}(\sigma(\lambda_{ij}))^l, \tag{4.4}$$

associated to $\widetilde{\Phi}$. Then Φ is an eigenfunction of the Hamiltonian H_{CM} with the same eigenvalue ϵ_{CM},

$$H_{\mathrm{CM}}\Phi=\epsilon_{\mathrm{CM}}\Phi,\quad H_{\mathrm{CM}}=e^{-\Psi}\widetilde{H}_{\mathrm{CM}}e^{\Psi}=-\sum_{i=1}^{n}\frac{\partial^2}{(\partial\lambda_i)^2}+l(l+1)\sum_{i\neq j}\wp(\lambda_{ij}), \tag{4.5}$$

where the function $\wp$ is defined in (2.4). One finds that H_{CM} is exactly the Hamiltonian of elliptic CM model associated with A_{n-1} root system[3,4] with the *coupling constant* $l+1$. (Traditionally, the *coupling constant* of the Hamiltonian: $H_{\mathrm{CM}}=-\Sigma_{i=1}^{n}[\partial^2/(\partial\lambda_i)^2]+\gamma(\gamma-1)\Sigma_{i\neq j}\wp(\lambda_{ij})$ of CM model is set to γ.)

Now we study the asymptotic properties of the eigenvalues of $\widetilde{H}_{\mathrm{RS}}$ (3.17) and the associated Bethe ansatz equations (3.18)–(3.20). Let the solution to the Bethe ansatz equations (3.18)–(3.20) have the following form:

$$v_k^{(i)}=x_k^{(i)}+\sqrt{-1}gy_k^{(i)}-g^2z_k^{(i)}+O(g^3),\quad g\to 0. \tag{4.6}$$

Noting the asymptotic properties of σ-function (2.5), the Eq. (3.17) becomes

$$\begin{aligned}\epsilon_{\mathrm{RS}}=n+\sqrt{-1}gn\left((1-n)\sqrt{-1}\pi\overline{\alpha}+\sum_{k=1}^{N_1}\zeta(x_k^{(0)})\right)+\frac{g^2}{2}\left\{n\sum_{k=1}^{N_1}(2y_k^{(0)}+1)\wp(x_k^{(0)})\right.\\ \left.-\frac{(n+1)n(n-1)l^2}{3}\frac{\sigma'''(0)}{\sigma'(0)}-n\left((1-n)\sqrt{-1}\pi\overline{\alpha}+\sum_{k=1}^{N_1}\zeta(x_k^{(0)})\right)^2\right\}+O(g^3).\end{aligned} \tag{4.7}$$

The Bethe ansatz equations (3.18)–(3.20) at the first order of g become

$$2\sum_{k=1,k\neq s}^{N_1}\zeta(x_k^{(0)}-x_s^{(0)})-n\sqrt{-1}\pi\overline{\alpha}=(2-n)\sqrt{-1}\pi\overline{\alpha}^{(1)}-nl\zeta(x_s^{(0)})+\sum_{k=1}^{N_2}\zeta(x_k^{(1)}-x_s^{(0)}), \tag{4.8}$$

$$2\sum_{k=1,k\neq s}^{N_{i+1}}\zeta(x_k^{(i)}-x_s^{(i)})+(i-n)\sqrt{-1}\pi\overline{\alpha}^{(i)} =(i+2-n)\sqrt{-1}\pi\overline{\alpha}^{(i+1)}-\sum_{k=1}^{N_i}\zeta(x_s^{(i)}-x_k^{(i-1)})+\sum_{k=1}^{N_{i+2}}\zeta(x_k^{(i+1)}-x_s^{(i)}),\quad i=1,...,n-3, \tag{4.9}$$

$$2\sum_{k=1,k\neq s}^{N_{n-1}}\zeta(x_k^{(n-2)}-x_s^{(n-2)})-2\sqrt{-1}\pi\overline{\alpha}^{(n-2)}=-\sum_{k=1}^{N_{n-2}}\zeta(x_s^{(n-2)}-x_k^{(n-3)}). \tag{4.10}$$

Sum up with s for each equation of (4.8)–(4.10). Then taking the summation of all the equations and noting the parity property of ζ-function (2.4), we find

$$\sum_{k=1}^{N_1}\zeta(x_k^{(0)})+(1-n)\sqrt{-1}\pi\overline{\alpha}=0. \tag{4.11}$$

This means that the first order of g term of ϵ_{RS} in (4.7) is vanishing which is in conformity with (4.1).

The Bethe ansatz equations (3.18)–(3.20) at the second order of g are

$$4\sum_{k=1,k\neq s}^{N_1}(y_s^{(0)}-y_k^{(0)})\wp(x_k^{(0)}-x_s^{(0)}) =nl(2y_s^{(0)}+nl)\wp(x_s^{(0)})-\sum_{k=1}^{N_2}(2y_k^{(1)}-2y_s^{(0)}+1)\wp(x_k^{(1)}-x_s^{(0)}), \tag{4.12}$$

$$4\sum_{k=1,k\neq s}^{N_{i+1}}(y_s^{(i)}-y_k^{(i)})\wp(x_k^{(i)}-x_s^{(i)})=\sum_{k=1}^{N_i}(2y_s^{(i)}-2y_k^{(i-1)}+1)\wp(x_s^{(i)}-x_k^{(i-1)})-\sum_{k=1}^{N_{i+2}}(2y_k^{(i+1)}-2y_s^{(i)} +1)\wp(x_k^{(i+1)}-x_s^{(i)}),\quad i=1,...,n-3, \tag{4.13}$$

$$4\sum_{k=1,k\neq s}^{N_{n-1}}(y_s^{(n-2)}-y_k^{(n-2)})\wp(x_k^{(n-2)}-x_s^{(n-2)})=\sum_{k=1}^{N_{n-2}}(2y_s^{(n-2)}-2y_k^{(n-3)}+1)\wp(x_s^{(n-2)}-x_k^{(n-3)}). \tag{4.14}$$

Sum up with s for each equation of (4.12)–(4.14). Then taking the summation of all the equations and noting the parity property of $\wp$-function (2.4), we find

$$\sum_{s=1}^{N_1}(2y_s^{(0)}+nl)\wp(x_s^{(0)})=0. \tag{4.15}$$

Substituting the equations (4.11) and (4.15) into (4.7), we finally have the following.

Proposition 4: The eigenvalues of the Hamiltonian (4.5) of the elliptic CM model associated with A_{n-1} root system with the discrete coupling constants $\gamma=l+1$ are

$$\epsilon_{\mathrm{CM}}=(1-nl)n\sum_{k=1}^{N_1}\wp(x_k^{(0)})-\frac{(n+1)n(n-1)}{3}l^2\frac{\sigma'''(0)}{\sigma'(0)}. \tag{4.16}$$

The $[n(n-1)/2]l$ *parameters* $\{\{x_k^{(i)}\}\}$ *satisfy the Bethe ansatz equations*

$$2\sum_{k=1,k\neq s}^{N_1}\zeta(x_k^{(0)}-x_s^{(0)})-n\sqrt{-1}\pi\overline{\alpha}=(2-n)\sqrt{-1}\pi\overline{\alpha}-nl\zeta(x_s^{(0)})+\sum_{k=1}^{N_2}\zeta(x_k^{(1)}-x_s^{(0)}), \tag{4.17}$$

$$2\sum_{k=1,k\neq s}^{N_{i+1}}\zeta(x_k^{(i)}-x_s^{(i)})+(i-n)\sqrt{-1}\pi\overline{\alpha}^{(i)}=(i+2-n)\sqrt{-1}\pi\overline{\alpha}^{(i+1)}-\sum_{k=1}^{N_i}\zeta(x_s^{(i)}-x_k^{(i-1)})$$
$$+\sum_{k=1}^{N_{i+2}}\zeta(x_k^{(i+1)}-x_s^{(i)}),\quad i=1,...,n-3, \tag{4.18}$$

$$2\sum_{k=1,k\neq s}^{N_{n-1}}\zeta(x_k^{(n-2)}-x_s^{(n-2)})-2\sqrt{-1}\pi\overline{\alpha}^{(n-2)}=-\sum_{k=1}^{N_{n-2}}\zeta(x_s^{(n-2)}-x_k^{(n-3)}). \tag{4.19}$$

The parameters $\overline{\alpha}^{(i)}$, $i=0,1,...,n-2$ *and* $\overline{\alpha}^{(0)}=\overline{\alpha}$ *are given by the relation (2.32) from* $n-1$ *arbitrary non-negative integers* $\{\alpha^{(i)}\in\mathbb{Z}^+|i=1,...,n-1\}$.

Our result agrees with the *third formulas* (or Bethe ansatz type) of the eigenvalues of the elliptic CM model associated with A_{n-1} root system.[22] Taking complex conjugation of the Bethe ansatz equations (4.17)–(4.19), noting the property (2.6) and (A5), we find that the solutions $\{\{x_k^{(i)}\}\}$ to the equations are all pure imaginary numbers. This ensures that the eigenvalues ϵ_{CM} are real and positive up to *the ground state energy* $\epsilon_0=-[(n+1)n(n-1)/3]l^2[\sigma'''(0)/\sigma'(0)]$ [the positivity from the expression (A4) of $\wp$-function when the argument is taken on imaginary axis].

B. Trigonometric potential

Here we consider trigonometric CM models associated with A_{n-1} root system. The corresponding Hamiltonian with the discrete *coupling constant* $\gamma=l+1$ is given

$$H_{\mathrm{CM}}=-\sum_{i=1}^{n}\frac{\partial^2}{(\partial\lambda_i)^2}+l(l+1)\sum_{i\neq j}\frac{\pi^2}{\sin^2(\pi\lambda_{ij})}. \tag{4.20}$$

Taking the trigonometric limit $\kappa\to+\infty$, one finds that

$$\zeta(u)\to\pi\cot\pi u, \tag{4.21}$$

$$\wp(u)\to\frac{\pi^2}{\sin^2(\pi u)}, \tag{4.22}$$

from expansions (A2) and (A3). Then the Hamiltonian (4.20) can be obtained from the elliptic type (4.5) by taking the trigonometric limit. Moreover, since the solutions $\{\{x_k^{(i)}\}\}$ to the Bethe ansatz equations (4.17)–(4.19) are all pure imaginary numbers, we can introduce $[n(n-1)/2]l$ real parameters $\{\{\overline{x}_k^{(i)}\}\}$ associated with $\{\{x_k^{(i)}\}\}$,

$$x_k^{(i)}=\sqrt{-1}\overline{x}_k^{(i)}. \tag{4.23}$$

Finally, we can find the spectrum of the Hamiltonian of trigonometric CM model associated with A_{n-1} root system from Proposition 4.

Proposition 5: The eigenvalues of the Hamiltonian (4.20) of the trigonometric CM model associated with A_{n-1} *root system with the discrete coupling constant* $\gamma=l+1$ *are*

$$\epsilon_{\mathrm{CM}}=(nl-1)n\sum_{k=1}^{N_1}\frac{\pi^2}{\sinh^2(\pi\overline{x}_k^{(0)})}+\frac{(n+1)n(n-1)}{3}l^2\pi^2. \tag{4.24}$$

The $[n(n-1)/2]l$ *real parameters* $\{\{\overline{x}_k^{(i)}\}\}$ *satisfy the Bethe ansatz equations*

$$2\sum_{k=1,k\neq s}^{N_1}\coth\pi(\overline{x}_k^{(0)}-\overline{x}_s^{(0)})+n\overline{\alpha}=(n-2)\overline{\alpha}^{(1)}-nl\coth\pi(\overline{x}_s^{(0)})+\sum_{k=1}^{N_2}\coth\pi(\overline{x}_k^{(1)}-\overline{x}_s^{(0)}), \tag{4.25}$$

$$2\sum_{k=1,k\neq s}^{N_{i+1}}\coth\pi(\overline{x}_k^{(i)}-\overline{x}_s^{(i)})+(n-i)\overline{\alpha}^{(i)}=(n-i-2)\overline{\alpha}^{(i+1)}-\sum_{k=1}^{N_i}\coth\pi(\overline{x}_s^{(i)}-\overline{x}_k^{(i-1)})$$
$$+\sum_{k=1}^{N_{i+2}}\coth\pi(\overline{x}_k^{(i+1)}-\overline{x}_s^{(i)}),\quad i=1,\ldots,n-3, \tag{4.26}$$

$$2\sum_{k=1,k\neq s}^{N_{n-1}}\coth\pi(\overline{x}_k^{(n-2)}-\overline{x}_s^{(n-2)})+2\overline{\alpha}^{(n-2)}=-\sum_{k=1}^{N_{n-2}}\coth\pi(\overline{x}_s^{(n-2)}-\overline{x}_k^{(n-3)}). \tag{4.27}$$

Here the parameters $\overline{\alpha}^{(i)}$, $i=0,1,\ldots,n-2$ *and* $\overline{\alpha}^{(0)}=\overline{\alpha}$ *are given by the relation (2.32) from* $n-1$ *arbitrary non-negative integers* $\{\alpha^{(i)}\in\mathbb{Z}^+|i=1,\ldots,n-1\}$.

C. Rational potential

Taking further rational limit of the elliptic Hamiltonian (4.5) as in Sec. III C, we can obtain the Hamiltonian of rational CM model associated with A_{n-1} root system

$$H_{\mathrm{CM}}=-\sum_{i=1}^{n}\frac{\partial^2}{(\partial\lambda_i)^2}+\sum_{i\neq j}\frac{l(l+1)}{(\lambda_i-\lambda_j)^2}. \tag{4.28}$$

Moreover, we have

Proposition 6: The eigenvalues of the Hamiltonian (4.28) of the rational CM model associated with A_{n-1} *root system with the discrete coupling constants* $\gamma=l+1$ *are*

$$\epsilon_{\mathrm{CM}}=\sum_{k=1}^{N_1}\frac{(nl-1)n}{(\overline{x}_k^{(0)})^2}, \tag{4.29}$$

where the $[n(n-1)/2]l$ *real parameters* $\{\{\overline{x}_k^{(i)}\}\}$ *satisfy the Bethe ansatz equations*

$$2\sum_{k=1,k\neq s}^{N_1}\frac{1}{\overline{x}_k^{(0)}-\overline{x}_s^{(0)}}+n\overline{\alpha}=(n-2)\overline{\alpha}^{(1)}-\frac{nl}{\overline{x}_s^{(0)}}+\sum_{k=1}^{N_2}\frac{1}{\overline{x}_k^{(1)}-\overline{x}_s^{(0)}}, \tag{4.30}$$

$$2\sum_{k=1,k\neq s}^{N_{i+1}}\frac{1}{\overline{x}_k^{(i)}-\overline{x}_s^{(i)}}+(n-i)\overline{\alpha}^{(i)}=(n-i-2)\overline{\alpha}^{(i+1)}-\sum_{k=1}^{N_1}\frac{1}{\overline{x}_s^{(i)}-\overline{x}_k^{(i-1)}}+\sum_{k=1}^{N_{i+2}}\frac{1}{\overline{x}_k^{(i+1)}-\overline{x}_s^{(i)}},$$
$$i=1,\ldots,n-3, \tag{4.31}$$

$$2\sum_{k=1,k\neq s}^{N_{n-1}}\frac{1}{\overline{x}_k^{(n-2)}-\overline{x}_s^{(n-2)}}+2\overline{\alpha}^{(n-2)}=-\sum_{k=1}^{N_{n-2}}\frac{1}{\overline{x}_s^{(n-2)}-\overline{x}_k^{(n-3)}}. \tag{4.32}$$

Here the parameters $\overline{\alpha}^{(i)}$, $i=0,1,...,n-2$ *and* $\overline{\alpha}^{(0)}=\overline{\alpha}$ *are given by the relation (2.32) from* $n-1$ *arbitrary non-negative real numbers* $\{\alpha^{(i)}\in\mathbb{R}^+|i=1,...,n-1\}$.

V. SUMMARY AND COMMENTS

Using the nested Bethe ansatz method for $E_{\tau,\eta}(sl_n)$,[19] we obtain the spectrum of the Hamiltonian of all types of (elliptic, trigonometric, rational) RS models associated with A_{n-1} root system with the discrete *coupling constant* $\gamma=\sqrt{-1}gl$. Eigenvalues are given in the Bethe ansatz formulas (or the *third formulas* in sense of Felder *et al.*[22]). The corresponding eigenfunction is a meromorphic function of $\{\lambda_i\}$ and has quasiperiodic properties (3.21) for the elliptic and trigonometric cases, asymptotic properties (3.36) for the rational case. For the special case of $n=2$, our generalized result recovers that of Refs. 17, 30, and 31.

Taking the "*nonrelativistic limit,*" the Hamiltonian of RS model becomes that of the CM model. Then, we give eigenvalues of the Hamiltonian of CM models associated with A_{n-1} root system with the discrete *coupling constant* $\gamma=l+1$ in the Bethe ansatz formulas. Our formulas coincide with those of Ref. 22 and those of $n=2$ case.[30,32] The eigenvalues from our formulas are real and positive up to the *ground state energy* ϵ_0 as physically desired. But, we have not yet got a direct proof of positivity of the eigenvalues of RS models from our formulas. However, we can show that for small *coupling constant* the eigenvalues of RS model associated with A_{n-1} root system are positive, from their asymptotic expansion (4.1). Moreover, we find that the elliptic and trigonometric RS and CM models have *discrete spectrum* which are parametrized by a set of non-negative integers $\{\alpha^{(i)}|i=1,...,n-1\}$. The rational RS and CM models have *continuous spectrum* which are parametrized by a set of non-negative real numbers $\{\alpha^{(i)}|i=1,...,n-1\}$.

If one writes the Hamiltonian of CM model with the *coupling constant* γ as $H_{\mathrm{CM}}(\gamma)$ and the associated eigenvalues as $\epsilon_{\mathrm{CM}}(\gamma)$, from the expression of the Hamiltonian (4.5), (4.20), and (4.28) one can find the following *duality*:

$$H_{\mathrm{CM}}(-\gamma)=H_{\mathrm{CM}}(\gamma-1). \tag{5.1}$$

Then, actually, we have already obtained the spectrum of CM models associated with A_{n-1} root system with the discrete *coupling constants* $\gamma=l$ $(l\in\mathbb{Z})$. Unfortunately, such a *duality* does not exist for RS models associated with A_{n-1} root systems.

There also exists another way (we call *symmetric polynomials approach*) to get eigenfunctions and the corresponding eigenvalues of the *trigonometric and rational* RS models[10] and CM models.[33–36] It would be very interesting to compare our formulas (of trigonometric and rational cases) with those obtained by the *symmetric polynomials approach* (for special A_1 case, it has already been obtained[30]). However, the *symmetric polynomials approach* fails in the elliptic models.

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APPENDIX: FORMULAS FOR ELLIPTIC FUNCTIONS

In this appendix, we give some useful series expansions of the elliptic functions given by (2.4) when $\tau=\sqrt{-1}\kappa$, $\kappa\in\mathbb{R}$, $\kappa>0$. By (2.3), σ-function can be expressed in terms of product form[37] (see Chap. 15)

$$\sigma(u)=q^{1/4}\sin\pi u\prod_{n=1}^{\infty}(1-q^{2n}e^{2\sqrt{-1}\pi u})(1-q^{2n}e^{-2\sqrt{-1}\pi u})(1-q^{2n}),\quad q=e^{-\pi\kappa}. \tag{A1}$$

We can derive the following series expansions from (2.4):

$$\zeta(u)=\frac{\pi\cos\pi u}{\sin\pi u}+\pi\sum_{n=1}^{\infty}\frac{\sin 2\pi u}{\sin\pi(u+\sqrt{-1}n\kappa)\sin\pi(u-\sqrt{-1}n\kappa)}, \tag{A2}$$

$$\wp(u)=\frac{\pi^2}{\sin^2\pi u}+\sum_{n=1}^{\infty}\left\{\frac{\pi^2}{\sin^2\pi(u+\sqrt{-1}n\kappa)}+\frac{\pi^2}{\sin^2\pi(u-\sqrt{-1}n\kappa)}\right\}. \tag{A3}$$

Moreover, the functions have the following properties:

$$\wp(\sqrt{-1}u)=-\left\{\frac{\pi^2}{\sinh^2\pi u}+\sum_{n=1}^{\infty}\left\{\frac{\pi^2}{\sinh^2\pi(u+n\kappa)}+\frac{\pi^2}{\sinh^2\pi(u-n\kappa)}\right\}\right\}, \tag{A4}$$

$$\sigma^*(u)=\sigma(u^*),\quad \zeta^*(u)=\zeta(u^*),\quad \wp^*(u)=\wp(u^*), \tag{A5}$$

where $*$ stands for the complex conjugation.

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Eigenvalue problems of a two-dimensional Schrödinger operator with nonparabolic effective mass

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In this paper, we study the eigenvalue problem for the Schrödinger operator on a two dimensional disk with nonparabolic effective mass approximation. Here the effective mass depends on the energy states. Our results mainly concern with the number of energy states lying in a wire and the monotonicity of energy states with respect to the depth of the wire. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Semiconductor quantum wires (or dots) are nanoscale structures in which the carriers are confined in two (or three) dimensions. The carriers exhibit wavelike properties in quantum wires and dots, and discrete energy states exist for the structures. These structures have recently attracted intensive research, on their physical phenomena and the corresponding practical applications (see, e.g., Ref. 1). Methods like photoluminescence[2] and capacitance-voltage spectroscopy[3] have been used to study the electronic and optical properties of quantum dots. For practical applications, quantum wires and dots play an important role in optoelectronic devices such as infrared photodetectors,[4] quantum dots laser,[5] memory device,[6] and quantum computing systems.[7]

In this paper, we study the eigenvalue problem for the Schrödinger operator on a disk $\mathbb{D}=\{(r,\theta)|\ r\in(0,R_1)\cup(R_1,R_2],\ \theta\in[0,2\pi]\}$:

$$\frac{-\hbar^2}{2m(r,\lambda)}\left(\frac{\partial^2\psi}{\partial r^2}+\frac{1}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}\right)+V(r)\psi(r,\theta)=\lambda\psi(r,\theta), \tag{1.1}$$

where the potential function V is defined by

$$V(r)=\begin{cases}0, & r<R_1\\ c, & R_1<r\leqslant R_2,\end{cases} \tag{1.2}$$

and the nonparabolic effective mass $m(r,\lambda)$ is defined by

$$m(r,\lambda)=\begin{cases}m_1(\lambda), & r<R_1\\ m_2(\lambda), & R_1<r\leqslant R_2.\end{cases} \tag{1.3}$$

Equation (1.1) is equipped with the Dirichlet boundary condition:

$$\psi(R_2,\theta)=0,\qquad \theta\in[0,2\pi]. \tag{1.4}$$

We also impose the interface conditions at $r=R_1$ and $\theta\in[0,2\pi]$:

$$\psi(R_1^-,\theta)=\psi(R_1^+,\theta) \tag{1.5}$$

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and

$$\frac{1}{m_1(\lambda)}\frac{\partial\psi}{\partial r}(R_1^-,\theta)=\frac{1}{m_2(\lambda)}\frac{\partial\psi}{\partial r}(R_1^+,\theta). \tag{1.6}$$

Throughout this paper, we further assume that
($\mathcal{H}1$) The effective mass $m_1(\lambda)$, $m_2(\lambda)>0$ are C^1 and increasing for $\lambda\in[0,c]$.
($\mathcal{H}1$) The product $m_2(\lambda)(c-\lambda)$ is decreasing for $\lambda\in[0,c]$.

Remark 1.1: *In Refs. 8–10, for a quantum wire of small size, the nonparabolic effective mass* $m(r,\lambda)$ *in (1.3) is approximated by*

$$\frac{1}{m_j(\lambda)}=\frac{P_j^2}{\hbar^2}\left(\frac{2}{\lambda+a_j-c_j}+\frac{1}{\lambda+a_j-c_j+\delta_j}\right),\quad j=1,2, \tag{1.7}$$

where P_j, a_j, *and* δ_j *stand for the momentum, main energy gap and spin–orbit splitting in the* j*th region, respectively. The semiconductor band structure parameters are*

$$c_1=0,\ a_1=0.235,\ \delta_1=0.81,\ P_1=0.2875;$$

$$c_2=c=\text{the depth of the potential wire},\ a_2=1.59,\ \delta_2=0.8,\ P_2=0.1993.$$

By taking the derivatives of $m_1(\lambda)$ *and* $m_2(\lambda)(c-\lambda)$ *with respect to* λ, *one can easily verify, for*

$$0<c\leqslant\frac{a_2}{2},$$

that the nonparabolic effective mass approximations $m_j(\lambda)$ $(j=1,2)$ *satisfy* ($\mathcal{H}1$) *and* ($\mathcal{H}2$).

Such problem and its generalization have been studied by many authors (see, e.g., Refs. 11–16 and the work cited therein). Their results mainly focus on the ratios of and the gaps between eigenvalues. We are led to investigate, in this paper, the eigen-states lying in the wire by the following work. In Refs. 17 and 18, the spatial tunneling (from one hole to another) occurs in coupled quantum wells [one-dimensional (1D)] when the energy states in both wells are aligned. In the case of the hole tunneling in the coupled quantum dots, the tunneling mechanisms are significantly more complicated, due to the band mixing effect. When the energy states are approximately aligned between heavy hole and light hole, mixing tunneling occurs. Moreover, it was reported in Ref. 19 that a chaotic tunneling effect was generated when tunneling occurs. Our effort here aims towards understanding these phenomena. Note also that the discretization of the one-dimensional Schrödinger operator with constant effective mass has recently been reported in Ref. 20.

This paper is organized as follows. In Sec. II, we apply separation of variables and derive the secular equations for (1.1):

$$f_k(\lambda)=g_k(\lambda)\qquad(k=0,1,2,\ldots;\ \lambda\in[0,c]),$$

from which λ can be solved. In Sec. III, we show for all k that $f_k(\lambda)$ is decreasing and $g_k(\lambda)$ is increasing. Furthermore, we shall show that $g_k(\lambda)$ is continuous in $[0,c]$. In Sec. IV, we utilize the results in Secs. II and III to find the exact number of energy states lying in the wire, i.e., those eigenvalues in $[0,c]$. We shall give a sufficient and necessary condition which guarantees the existence of at least one energy state in the wire. The monotonicity of the energy state with respect to c, the depth of the wire, is also obtained. Section V contains some brief concluding remarks.

II. SECULAR EQUATIONS

In this section we shall derive the secular equations for the eigenvalue problem (1.1). To this end, we apply the technique of separation of variables, assuming that the wave function ψ satisfies

$$\psi(r,\theta)=u(r)\omega(\theta). \tag{2.1}$$

Substituting (2.1) into (1.1) we get

$$\frac{r^2}{u(r)}\left\{\frac{-\hbar^2}{2}\left(\frac{d^2u}{dr^2}+\frac{1}{r}\frac{du}{dr}\right)+m(r,\lambda)[V(r)-\lambda]u(r)\right\}=\frac{\hbar^2}{2}\frac{1}{\omega(\theta)}\frac{d^2\omega}{d\theta^2}. \tag{2.2}$$

Furthermore, the boundary condition (1.4) becomes

$$u(R_2)=0, \tag{2.3}$$

and the interface conditions (1.5) and (1.6), respectively, become

$$u(R_1^-)=u(R_1^+) \tag{2.4}$$

and

$$\frac{1}{m_1(\lambda)}\frac{du}{dr}(R_1^-)=\frac{1}{m_2(\lambda)}\frac{du}{dr}(R_1^+). \tag{2.5}$$

As (2.2) holds for all values of $r\in[0,R_1)\cup(R_1,R_2]$ and $\theta\in[0,2\pi]$, both sides of the equation equal to a constant. Consequently, the right hand side of (2.2) implies that the function $\omega(\theta)$ satisfies the following boundary value problems:

$$\frac{\omega''(\theta)}{\omega(\theta)}=-k^2, \qquad \omega(0)=\omega(2\pi),\ \ \omega'(0)=\omega'(2\pi),$$

where $k=0,1,2,\ldots$. For convenience, we shall denote

$$\alpha\equiv\sqrt{2m_1(\lambda)\lambda/\hbar^2},\ \ \beta\equiv\sqrt{2m_2(\lambda)(c-\lambda)/\hbar^2}. \tag{2.6}$$

Similarly, the left hand side of (2.2) implies, for $k=0,1,2,\ldots$,

$$r^2u''+ru'+(r^2\alpha^2-k^2)u=0, \quad \text{for } 0<r<R_1 \tag{2.7}$$

and

$$r^2u''+ru'-(r^2\beta^2+k^2)u=0, \quad \text{for } R_1<r<R_2. \tag{2.8}$$

Let J_k be Bessel functions of the first kind of order k, which satisfies the Bessel's equation $r^2u''+ru'+(r^2-k^2)u=0$. Let I_k and K_k, respectively, be the modified Bessel functions of the first and second kind of order k, which are linearly independent solutions of the modified Bessel's equation $r^2u''+ru'-(r^2+k^2)u=0$.

For a given k, (2.7) and (2.8) imply that the solution of (2.2) is given by

$$u(r)=AJ_k(\alpha r), \qquad \text{for } 0<r<R_1 \tag{2.9}$$

and

$$u(r)=BI_k(\beta r)+CK_k(\beta r), \qquad \text{for } R_1<r\leqslant R_2, \tag{2.10}$$

where A, B, and C are constant coefficients to be determined. Note that Bessel functions of the second kind are absent in (2.9) because of the boundedness of the eigenfunction $\psi(r,\theta)=u(r)\omega(\theta)$.

Now, applying the boundary condition (2.3) to (2.10), we obtain

$$C=-D_kB\ ,\ D_k\equiv\frac{I_k(\beta R_2)}{K_k(\beta R_2)}. \tag{2.11}$$

Applying the interface conditions (2.4) and (2.5) to (2.9) and (2.10), we have

$$AJ_k(\alpha R_1)=B[I_k(\beta R_1)-D_kK_k(\beta R_1)] \tag{2.12}$$

and

$$\frac{A}{m_1(\lambda)}\alpha J_k'(\alpha R_1)=\frac{B}{m_2(\lambda)}\beta[I_k'(\beta R_1)-D_kK_k'(\beta R_1)]. \tag{2.13}$$

Dividing (2.13) by (2.12), we can show that an eigenvalue of (1.1) is a root of the secular equations

$$f_k(\lambda)=g_k(\lambda)\quad(k=0,1,2,\ldots), \tag{2.14}$$

where

$$f_k(\lambda)\equiv\frac{1}{m_1(\lambda)}\frac{\alpha J_k'(\alpha R_1)}{J_k(\alpha R_1)} \tag{2.15}$$

and

$$g_k(\lambda)=\frac{1}{m_2(\lambda)}\tilde{g}_k(\lambda)\ \ ,\ \ \tilde{g}_k(\lambda)\equiv\frac{\beta[I_k'(\beta R_1)-D_kK_k'(\beta R_1)]}{I_k(\beta R_1)-D_kK_k(\beta R_1)}. \tag{2.16}$$

Remark 2.1. Assumptions ($\mathcal{H}1$) *and* ($\mathcal{H}2$) *are not involved in the derivation of the secular equations (2.14). Thus, (2.14) holds for any effective mass* $m(r,\lambda)$ *and can be used in numerical computations involving the eigenvalues of (1.1).*

III. MONOTONICITY OF f_k AND g_k

In this section, we shall study the monotonicity of f_k and g_k with respect to λ and c. To this end, we first quote some well-known and useful properties of J_k, I_k, and K_k, as well as the Comparison Theorem [Ref. 21, p. 24] for differential equations.

Proposition 3.1 (Ref. 22, p. 79): Let k be a nonnegative integer. Then the following properties hold.

(i) $J_k(x)=\sum_{n=0}^{\infty}\frac{(-1)^n\left(\frac{x}{2}\right)^{2n+k}}{n!\Gamma(n+k+1)}$, *where* $\Gamma(\cdot)$ *is the gamma function.*

(ii) $I_k(x)=\sum_{n=0}^{\infty}\frac{\left(\frac{x}{2}\right)^{2n+k}}{n!\Gamma(n+k+1)}$.

(iii) $K_k(x)=-I_k(x)\ln\frac{x}{2}+\frac{1}{2}\sum_{n=0}^{k-1}(-1)^n\frac{(k-n-1)!}{n!}\left(\frac{x}{2}\right)^{-k+2n}$

$$+(-1)^{k+1}\frac{1}{2}\sum_{n=0}^{\infty}\frac{\left(\frac{x}{2}\right)^{k+2n}}{n!(n+k)!}\left(\frac{\Gamma'(n+1)}{\Gamma(n+1)}+\frac{\Gamma'(n+k+1)}{\Gamma(n+k+1)}\right),\quad\text{for } k\geqslant 1,$$

$$K_0(x)=-I_0(x)\ln\frac{x}{2}+\frac{1}{2}\sum_{n=0}^{\infty}\frac{\left(\frac{x}{2}\right)^{2n}}{(n!)^2}\frac{\Gamma'(n+1)}{\Gamma(n+1)}.$$

(iv) $I_k(x),\ K_k(x)>0,\ for\ x>0.$

(v) $I_{k+1}+I_{k-1}=2I_k',\quad I_0'=I_1.$

(vi) $K_{k+1}+K_{k-1}=-2K_k',\quad K_0'=-K_1.$

(vi) $W\{I_k(x),K_k(x)\}=-\frac{1}{x}$ *where* $W\{\cdot,\cdot\}$ *denotes the Wronskian of two functions.*

Theorem 3.1 (Comparison Theorem): *Let u and v be, respectively, the solutions of the differential equations*

$$y'=F(y,x),\quad z'=G(z,x)$$

where $F(\eta,x)\leqslant G(\eta,x)$ in the strip $a\leqslant x\leqslant b$, and F and G satisfy the Lipschitz condition. If $u(a)\leqslant v(a)$ then $u(x)\leqslant v(x)$, for all $x\in[a,b]$.

Now, we are ready to prove the monotonicity properties of f_k and g_k, with a modified Prüfer transform[21] for linear second-order boundary value problems.

Proposition 3.2: Assume that ($\mathcal{H}1$) *and* ($\mathcal{H}2$) *in Sec. I hold.*

(i) *For each k, $f_k(\lambda)$ is decreasing.*

(ii) $f_k|_{\lambda=0}=k/m_1(0)R_1$.

Proof: For a given k, denote $u(r)\equiv J_k(\alpha r)$. Then u satisfies the differential equation (2.7). Note that $f_k(\lambda)=u'(R_1)/[m_1(\lambda)u(R_1)]$, and define the modified Prüfer transform

$$\tan\phi(r,\lambda)=\frac{u'(r)}{m_1(\lambda)u(r)}. \tag{3.1}$$

Differentiating (3.1) and with the help of (2.7), we can show that ϕ satisfies the first-order differential equation

$$\phi'=F(\phi,r,\lambda):=\frac{uu''-(u')^2}{m_1(\lambda)\left[1+\frac{1}{m_1(\lambda)^2}\left(\frac{u'}{u}\right)^2\right]u^2}=\left[-\frac{2\lambda}{\hbar^2}+\frac{k^2}{m_1(\lambda)r^2}\right]\cos^2\phi-\frac{1}{r}\sin\phi\cos\phi$$
$$-m_1(\lambda)\sin^2\phi. \tag{3.2}$$

Routine calculations, with the help of Proposition 3.1 (i), then yield

$$\frac{u'}{m_1(\lambda)u}=\sqrt{\frac{2\lambda}{m_1(\lambda)\hbar^2}}\,\frac{J_k'(\sqrt{2m_1(\lambda)\lambda/\hbar^2}\ r)}{J_k(\sqrt{2m_1(\lambda)\lambda/\hbar^2}\ r)}=\frac{k}{m_1(\lambda)r}-\frac{\lambda r}{(k+1)\hbar^2}+O(m_1(\lambda)\lambda^2r^3). \tag{3.3}$$

Consequently, for $\lambda_1>\lambda_2$ and a sufficiently small $r_0>0$, we arrive at

$$\left.\frac{u'(r)}{m_1(\lambda)u(r)}\right|_{r=r_0,\lambda=\lambda_1}\leqslant\left.\frac{u'(r)}{m_1(\lambda)u(r)}\right|_{r=r_0,\lambda=\lambda_2},$$

hence

$$\phi(r_0,\lambda_1)\leqslant\phi(r_0,\lambda_2). \tag{3.4}$$

On the other hand, it follows from (3.2) that F is Lipschitz continuous for $r\in[r_0,R_1]$ and is decreasing with respect to λ. Thus, from (3.4) and Theorem 3.1, we have $\phi(R_1,\lambda_1)\leqslant\phi(R_1,\lambda_2)$. From (2.15), (3.1) and the definition of $u(r)$, assertion (i) follows. Assertion (ii) is a direct consequence of (3.3). □

Remark 3.1. We require the modified Prüfer transform $\tan\Phi(r,\lambda)=u'(r)/[m_1(\lambda)u(r)]$ *in (3.1) in the proof of Proposition 3.1, rather than the traditional Prüfer transform* $\cot\phi(r)=u'(r)/u(r)$.

In the following, we study the continuity and monotonicity of g_k.

Proposition 3.3: Let a, $b>0$, and k be a nonnegative integer. Then

$$I_k(a)-\frac{I_k(b)}{K_k(b)}K_k(a)\begin{cases}>0, & \text{if } a>b\\ =0, & \text{if } a=b\\ <0, & \text{if } a<b.\end{cases}$$

Proof: Since $K_k(x)$ never vanishes, we define $h(x):=I_k(x)/K_k(x)$. Using Proposition 3.1 (vii), it follows that $h'(x)=[xK_k(x)^2]^{-1}>0$, and the assertion follows. □

Proposition 3.4: Assume $m_2(\lambda)>0$, for $\lambda\in[0,c]$. For any nonnegative integer k, we have

(i) $\tilde{g}_k(\lambda)$ *in* (2.16) *is continuous and nonpositive on* $[0,c)$, *and so is* $g_k(\lambda)$.

(ii) $\lim_{\lambda\to c}g_k(\lambda)=\begin{cases}[m_2(c)\ \ R_1\ln R_1/R_2]^{-1}, & k=0\\ k(R_1^{2k}+R_2^{2k})\ \ [m_2(c)\ \ R_1(R_1^{2k}-R_2^{2k})]^{-1}, & k\geqslant 1\end{cases}$.

Proof: Applying Proposition 3.3 to (2.16), together with (2.11), we can show that the denominator of $\tilde{g}_k$ is negative, implying that $\tilde{g}_k$ is continuous. From Proposition 3.1 (v) and (vi), it follows that the numerator of $\tilde{g}_k$ is positive. Thus, $\tilde{g}_k(\lambda)<0$ for $0\leqslant\lambda<c$. As $g_k=\tilde{g}_k/m_2(\lambda)$ and $m_2(\lambda)>0$, assertion (i) holds.

To prove assertion (ii), a straightforward application of MATHEMATICA[23] on Proposition 3.1 (ii) and (iii) produces

$$\begin{aligned}&\frac{K_k(\beta R_2)\ \ I_k'(\beta R_1)-I_k(\beta R_2)\ \ K_k'(\beta R_1)}{K_k(\beta R_2)\ \ I_k(\beta R_1)-I_k(\beta R_2)\ \ K_k(\beta R_1)}\\ &\quad=\begin{cases}\left[\beta\ \ R_1\ln\dfrac{R_1}{R_2}\right]^{-1}+O(\beta), & k=0\\ k(R_1^{2k}+R_2^{2k})\ \ [\beta\ \ R_1(R_1^{2k}-R_2^{2k})]^{-1}+O(\beta), & k\geqslant 1,\end{cases}\end{aligned}$$

when β is sufficiently small. The fact that $\beta\to 0$ as $\lambda\to c$ leads to assertion (ii). □

Proposition 3.5: Assume that $(\mathcal{H}1)$ *and* $(\mathcal{H}2)$ *hold. Then for any nonnegative integer k,*

(i) g_k is increasing with respect to λ for $0\leqslant\lambda\leqslant c$, and

(ii) g_k is decreasing with respect to c.

Proof: We first show that $\tilde{g}_k$ in (2.16) is decreasing with respect to β. Let

$$u(r)\equiv I_k(\beta r)-D_kK_k(\beta r).$$

Define the Prüfer transform $\tan\phi=v=u'/u$. With (2.8) and a similar argument as in the proof of Proposition 3.2, we can show that $\tilde{g}_k(\lambda)=v|_{r=R_1}$ and ϕ satisfies

$$\phi'=\frac{1}{r^2}(\cos^2\phi)(\beta^2r^2+k^2)-\frac{1}{r}\sin\phi\cos\phi-\sin^2\phi. \tag{3.5}$$

From Proposition 3.3, it follows for each β that $u(r,\beta)=0$ only when $r=R_2$. Together with the definitions of the Bessel functions I_k and K_k, we prove that v is continuous for $0<r<R_2$ and

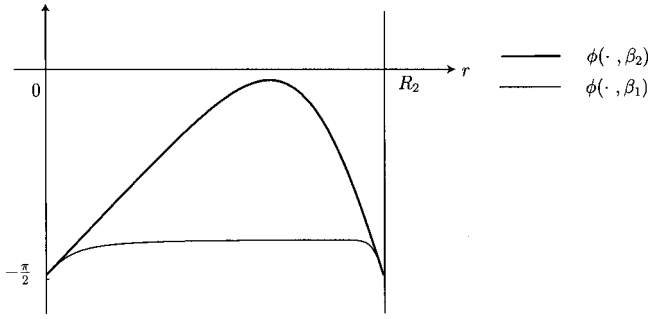

FIG. 1. Illustration of the proof of Proposition 3.5 that ϕ decreases in β.

$$\lim_{r\to 0^+} v(r,\beta)=\lim_{r\to R_2^-} v(r,\beta)=-\infty \quad \text{for all } \beta. \tag{3.6}$$

Using Proposition 3.1 (v) and (vi) and Proposition 3.3, we have $u'>0$ and $u<0$. This implies $v(r,\beta)<0$ for $0<r<R_2$. Thus we may choose $\phi(\cdot,\beta)$ as one branch of $\tan^{-1}(\cdot)$ in $[-\pi/2,\pi/2]$, and (3.6) leads to $\phi(R_2,\beta)=\phi(0,\beta)=-\pi/2$ for all β. Using the change of variable $s=R_2-r$, (3.5) becomes

$$\frac{d\phi}{ds}=G(\phi,s,\beta):=\frac{-\cos^2\phi}{(R_2-s)^2}[\beta^2(R_2-s)^2+k^2]+\frac{\sin\phi\cos\phi}{R_2-s}+\sin^2\phi. \tag{3.7}$$

Pick $\beta_1>\beta_2>0$. We then have

$$\phi(s=0,\beta_1)=\phi(s=0,\beta_2)=-\frac{\pi}{2}$$

and

$$G(\phi,s,\beta_1)\leqslant G(\phi,s,\beta_2) \qquad \text{for} \quad 0\leqslant s<R_2.$$

Applying Theorem 3.1 to (3.7), we conclude that $\phi(s,\beta_1)\leqslant\phi(s,\beta_2)$ for $0\leqslant s<R_2$, i.e., ϕ is decreasing with respect to β (see Fig. 1 for illustration). From ($\mathcal{H}2$) and (2.6), it follows that $\partial\beta/\partial\lambda<0$ and $\partial\beta/\partial c>0$, implying that $\tilde{g}_k$ is increasing with respect to λ and decreasing with respect to c. Together with the result in Proposition 3.4 that $\tilde{g}_k(\lambda)<0$ and assumption ($\mathcal{H}1$) that $m_2(\lambda)>0$ is increasing, we show that g_k is increasing with respect to λ. Since $g_k=\tilde{g}_k/m_2(\lambda)$ and $m_2(\lambda)$ is independent of c, assertion (ii) also holds. □

IV. MAIN RESULTS

In this section, we shall prove the main result of this paper. Denote the eigenvalue of (1.1) by $\lambda_{k,j}$ ($k=0,1,2,\ldots$, $j=1,2,\ldots$), corresponding to the jth root of the kth secular equation (2.14). We also define $s_{k,j}$ ($k=0,1,2,\ldots$, $j=1,2,3,\ldots$) to be the real number such that $\sqrt{2m_1(s_{k,j})s_{k,j}}\ R_1/\hbar$ is the jth root of the kth Bessel function J_k, with $s_{k,0}=0$. It is easy to see that $s_{k,j}$ ($j=1,2,\ldots$) are the singularities of f_k. Note that $\{s_{k,j}\}$ are well-defined, since ($\mathcal{H}1$) implies that the function $\lambda\mapsto m_1(\lambda)\lambda$ is increasing from zero to infinity in $[0,\infty)$. Using the properties of f_k and g_k in Propositions 3.2, 3.4, and 3.5, we sketch $f_k(\lambda)$ and $g_k(\lambda)$ in Fig. 2.

We now prove the first main result that exactly counts the number of eigenvalues of (1.1) which lie in the wire.

Theorem 4.1. *Assume that* ($\mathcal{H}1$) *and* ($\mathcal{H}2$) *hold. Suppose* $s_{k,n}<c<s_{k,n+1}$ *for some* $n\geqslant 0$. *If* $f_k(c)<g_k(c)$, *then* $\lambda_{k,1},\ldots,\lambda_{k,n+1}$ *lie in the wire; otherwise,* $\lambda_{k,1},\ldots,\lambda_{k,n}$ *lie in the wire and*

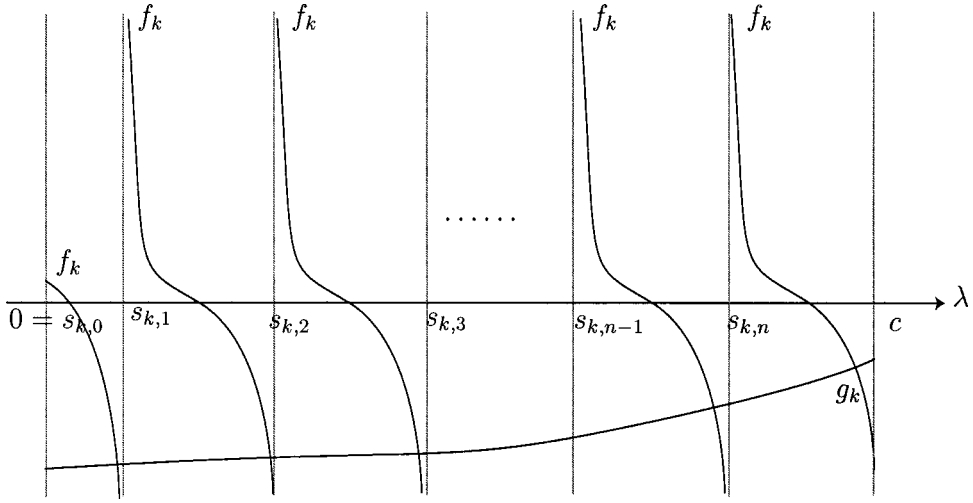

FIG. 2. Illustration for the graphs of f_k and g_k on $[0,c]$.

$\lambda_{k,n+1}$ *is out of the wire. Moreover, for any given size and depth of the wire in (1.1), there exists* $\overline{R_2}$ *such that there is at least one energy state lying in the wire for* $R_2 > \overline{R_2}$.

Proof: For a fixed k, define $d(\lambda) \equiv f_k(\lambda) - g_k(\lambda)$. It follows from Propositions 3.2 and 3.5 that d is decreasing in λ. Since g_k is continuous on $[0,c]$, d has only singularities $s_{k,1},\ldots,s_{k,n}$ in $[0,c]$. But $f_k(0) \geqslant 0$ and $g_k(0) < 0$ imply that $\lambda_{k,j} \in (s_{k,j-1}, s_{k,j})$, $j = 1,2,\ldots,n$. The existence of $\lambda_{k,n+1}$ in $(s_{k,n}, c]$ comes from the inequality $f_k(c) \leqslant g_k(c)$.

To complete the proof, it suffices to consider the case when $s_{0,1} > c$ we see that f_0 is continuous on $[0,c]$, with $f_0(0) = 0$, $f_0(c) < 0$. Using Proposition 3.4, we have $g_0(c) = [m_2(c) \;\; R_1 \ln(R_1/R_2)]^{-1} \to 0$ as $R_2 \to \infty$. The assertion follows. □

Remark 4.1. (i) A direct consequence of the last assertion of Theorem 4.1 is that when the domain of (1.1) is degenerated to the entire plane, i.e., $R_2 = \infty$, *there is at least one energy state lying in the wire.*

(ii) From a computational point of view, all discrete energy states of (1.1) lying in the wire $[0,c]$ *can easily be computed by applying Newton's iteration or the bisection method to the secular equations (2.14), with* $s_{k,j}$ *as initial guesses.*

The second main result shows that the increasing monotonicity of the energy state holds with respect to the depth c of the wire.

Theorem 4.2. *Each energy state lying in the wire increases as* c *increases.*

Proof: Let $d(\lambda) \equiv f_k(\lambda) - g_k(\lambda)$. As in the proof of Theorem 4.1, the result follows from Proposition 3.5 (ii). □

V. CONCLUDING REMARKS

We conclude this paper with some brief remarks and speculation on future works.

The non-parabolic effective mass approximations in (1.7) proposed in Refs. 9 and 10 satisfy satisfy ($\mathcal{H}1$) and ($\mathcal{H}2$) for specified c. These approximations are thus applicable, for some specific c, in our main Theorems. With assumptions ($\mathcal{H}1$) and ($\mathcal{H}2$), the monotonicity properties of f_k and g_k are ensured. Hence, the roots of (2.14) can be computed by classical iterative methods (e.g., Newton's method or bisection method). Without assumptions ($\mathcal{H}1$) and ($\mathcal{H}2$), the monotonicity properties of f_k and g_k does not always hold, so it cannot guarantee that there is a unique root of (2.14) between two consecutive singularities. Hence, the number of energy states lying in the wire from Theorem 4.1 becomes a lower bound.

Analogously, the main results of (1.1) in this paper with Neumann boundary conditions can be proved. It may be of interest to study the eigenvalue problem for the Schrödinger operator (or discretized Schrödinger operator) on a 3D the cylindrical domain with Dirichlet or Neumann boundary condition.

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Transition elements for a non-Hermitian quadratic Hamiltonian

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The non-Hermitian quadratic Hamiltonian $H=\omega a^{\dagger}a+\alpha a^{2}+\beta a^{\dagger 2}$ is analyzed, where $a^{\dagger}$ and a are harmonic oscillator creation and annihilation operators and ω, α, and β are real constants. For the case that $\omega^{2}-4\alpha\beta\geqslant 0$, it is shown using operator techniques that the Hamiltonian possesses real and positive eigenvalues. A generalized Bogoliubov transformation allows the energy eigenstates to be constructed from the algebra and states of the harmonic oscillator. The eigenstates are shown to possess an imaginary norm for a large range of the parameter space. Finding the orthonormal dual space allows the inner product to be redefined using the complexification procedure of Bender *et al.* for non-Hermitian Hamiltonians. Transition probabilities governed by H are shown to be manifestly unitary when the complexification procedure is followed. A specific transition element between harmonic oscillator states is evaluated for both the Hermitian and non-Hermitian cases to identify the differences in time evolution. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1640796]

I. INTRODUCTION

There is a good deal of current interest in extending quantum mechanics to include non-Hermitian Hamiltonians, stemming primarily from the work of Bender and collaborators.[1,2] An example is the Hamiltonian

$$H=p^{2}+x^{2}(ix)^{\nu} \qquad (\nu\geqslant 0), \tag{1}$$

which is known[1] to have a real and positive spectrum. Recent work[2] has found similar non-Hermitian cases that give rise to real and positive spectra. The key step in extending the structures of quantum mechanics to these Hamiltonians in a consistent manner is dealing with the indefinite metric[3] that arises in the Hilbert space of their eigenfunctions. For the eigenfunctions of (1) the standard inner product yields norms that alternate in sign. An indefinite metric threatens unitarity and prevents a probabilistic interpretation of matrix elements. In Bender's approach unitarity is maintained by modifying the inner product of the Hilbert space through the action of an operator, written as the product of time reversal $\mathcal{T}$, parity $\mathcal{P}$, and charge conjugation $\mathcal{C}$, so that the inner product takes the form[4]

$$\langle f|g\rangle=\int_{\mathrm{C}} dx\,[\mathcal{CPT}f(x)]g(x), \tag{2}$$

where both the contour C in the complex x plane and the form for $\mathcal{CPT}$ are determined from the form of the Hamiltonian. For the case that $\nu\to 0$ in (1) the operator $\mathcal{CP}\to 1$ and the inner product (2) reduces to the usual definition since $\mathcal{T}f(x)=f^{*}(-x)$. In general, Hamiltonians that are $\mathcal{PT}$

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symmetric can be treated in this manner. The resulting generalization to a complexified version of quantum mechanics allows a much broader range of Hamiltonians to be considered while maintaining unitary time evolution.

The purpose of this paper is to analyze a simple quadratic non-Hermitian Hamiltonian with operator methods and adapt it to the structure developed by Bender. The Hamiltonian is expressed in terms of bosonic harmonic oscillator creation and annihilation operators $a^\dagger$ and a, which obey the usual commutation relationship

$$[a,a^\dagger]=1. \tag{3}$$

The operator a annihilates the state $|0\rangle$, so that

$$a|0\rangle=0\Rightarrow\langle 0|a^\dagger=0. \tag{4}$$

The set of states given by

$$|n\rangle=\frac{a^{\dagger n}}{\sqrt{n!}}|0\rangle \tag{5}$$

are eigenstates of the Hermitian Hamiltonian $H_0=\omega a^\dagger a$ and are orthonormal and complete. The Hamiltonian to be considered is then given by

$$H=\omega a^\dagger a+\alpha a^2+\beta a^{\dagger 2}+\tfrac{1}{2}\omega, \tag{6}$$

where ω, α, and β are real parameters with the dimensions of inverse time. The Hamiltonian (6) is of course manifestly non-Hermitian when $\alpha\neq\beta$, but it is both $\mathcal{P}$ and $\mathcal{T}$ invariant since $\mathcal{T}$:$a\rightarrow a$ and $\mathcal{P}$:$a\rightarrow -a$ with similar transformation properties for $a^\dagger$. As a result, if eigenstates of (6) can be found they will possess real eigenvalues.[5] The Hermitian version of (6) occurs in the analysis of two photon processes,[6] but to the knowledge of the author the non-Hermitian version and its transition elements have not been considered.

The approach followed is first to find the Hilbert space of energy eigenstates and then to define via Bender's method an inner product that allows unitary time development. This paper will restrict attention to the case that α and β are real and $\omega^2-4\alpha\beta\geqslant 0$. For those restrictions the Hamiltonian (6) possesses eigenstates with real and positive eigenvalues, and therefore, meets the criteria for applying Bender's method. The energy eigenstates will be constructed from the harmonic oscillator states using a generalized Bogoliubov transformation[7] and will be shown to be structurally identical to the harmonic oscillator. It will be seen that the Hilbert space of energy eigenstates possesses an indefinite metric if $\alpha\neq\beta$ corresponding to non-normalizable eigenstates. In order to implement Bender's approach to dealing with the breakdown of unitarity the space dual to these eigenstates will be constructed through the demand of orthonormality. An explicit form for the operator U that maps the energy eigenstates into the orthonormal dual basis is determined and, in order to avoid a breakdown of unitarity, it will be shown that the action of U must be included in the inner product. This operator reduces to unity when the Hermitian limit $\alpha\rightarrow\beta$ is taken, in a manner identical to the result that $\lim_{\nu\rightarrow 0}\mathcal{CP}=1$ for the Hamiltonian (1). The Hilbert space of eigenstates and the modified inner product then allow the definition of a unit projection operator. It will be explicitly demonstrated that time evolution using this inner product is unitary, showing that the non-Hermitian Hamiltonian (6) can be treated by Bender's general method. Transition elements between harmonic oscillator states using (6) will be calculated using both the methods of Bender and the standard inner product. Because the states of the theory are explicitly constructed from the harmonic oscillator states, evaluating the transition elements in either case reduces to an exercise in normal ordering. Transition probabilities calculated without Bender's complexification procedure are oscillatory due to the real and positive energy spectrum but are not time-reversal invariant since $|W_{fi}|^2\neq|W_{if}|^2$ when $\alpha\neq\beta$. The resulting transition elements therefore manifestly violate unitarity when $\alpha\neq\beta$. The origin of this failure is clearly demonstrated for

a specific fixed number transition element in the limit that $\alpha \to 0$ while $\beta \neq 0$. Comparing the Hermitian limit $\alpha = \beta$ of a transition amplitude to the non-Hermitian case shows that for small β the non-Hermitian case is very similar in behavior to the Hermitian case, but that significant differences in time evolution appear as β approaches $\omega/2$.

The outline of the paper is as follows. In Sec. II the Hamiltonian is analyzed using operator techniques to determine the structure of the Hilbert space of eigenstates and the form of the inner product required for unitary time evolution. In Sec. III fixed number transition elements are evaluated to demonstrate the failure of time-reversal invariance in the absence of the modified inner product. A specific transition element governed by the Hamiltonian (6) is then defined and evaluated in several limits. To enhance readability the more tedious aspects of the evaluation are collected in a set of appendices.

II. ENERGY EIGENSTATES AND THE INNER PRODUCT

The first step in evaluating (6) is to find its eigenstates. This process begins by introducing two new operators, c and d, by means of a generalized Bogoliubov transformation[7]

$$c = g_1 a^\dagger - g_3 a, \tag{7}$$

$$d = g_4 a - g_2 a^\dagger, \tag{8}$$

where in the general case the g_j coefficients are complex numbers. It is clear that $c \neq d^\dagger$ unless $g_4 = g_1^*$ and $g_3 = g_2^*$, in which case (7) and (8) reduce to the standard Bogoliubov transformation for the Hermitian case. This yields the Hermitian limits

$$\lim_{\alpha \to \beta} g_1^* = g_4, \tag{9a}$$

$$\lim_{\alpha \to \beta} g_2^* = g_3, \tag{9b}$$

and their complex conjugates. Written in matrix form, the definitions of (7) and (8) become

$$\begin{pmatrix} d \\ c \end{pmatrix} = \begin{pmatrix} g_4 & -g_2 \\ -g_3 & g_1 \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}. \tag{10}$$

The algebra $[a, a^\dagger] = 1$ gives

$$[d, c] = g_1 g_4 - g_2 g_3 = 1, \tag{11}$$

where, to simplify subsequent calculations, (11) has been set to unity. Since (11) is the determinant of the matrix in (10), the matrix is a member of the group SL(2,C) and its inversion gives

$$a = g_1 d + g_2 c, \tag{12}$$

$$a^\dagger = g_3 d + g_4 c. \tag{13}$$

Substituting (12) and (13) into (6) yields

$$H = \Omega c d + \tilde{\alpha} c^2 + \tilde{\beta} d^2 + \epsilon + \tfrac{1}{2}\omega, \tag{14}$$

where the new coefficients are given in terms of the parameters of (6) and the g_j:

$$\Omega = (g_2 g_3 + g_1 g_4)\omega + 2 g_1 g_2 \alpha + 2 g_3 g_4 \beta, \tag{15a}$$

$$\tilde{\alpha} = g_2 g_4 \omega + g_2^2 \alpha + g_4^2 \beta, \tag{15b}$$

$$\tilde{\beta}=g_1g_3\omega+g_1^2\alpha+g_3^2\beta, \tag{15c}$$

$$\epsilon=g_2g_3\omega+g_1g_2\alpha+g_3g_4\beta. \tag{15d}$$

It is important to note that the ordering prescription of moving c to the left in all expressions has been chosen and this choice generates the form for ϵ. While the other option is possible, this choice takes advantage of the similarity of c and d to creation and annihilation operators in the commutator (11) to avoid needless complications.

The g_j are now chosen so that the two complex constraints

$$\tilde{\alpha}=\tilde{\beta}=0, \tag{16}$$

are satisfied. If $\alpha=\beta=0$ in (6), then (7) and (8) can be chosen to reduce to $c=a^\dagger$ and $d=a$, and this yields the boundary conditions

$$\lim_{\alpha,\beta\to 0} g_{2,3}=0, \tag{17}$$

for g_2 and g_3. Condition (11) is then consistent with the limits

$$\lim_{\alpha,\beta\to 0} g_{1,4}=1, \tag{18}$$

which will be true up to an arbitrary phase. The two conditions of (16) and the constraint (11) remove six degrees of freedom from the four complex numbers g_j, which naively possess eight degrees of freedom. However, the g_j actually possess only six physical parameters due to the freedom to adjust the overall phases of the operators in the definitions (12) and (13). The details of this argument are presented in Appendix A. Because all six actual degrees of freedom are now accounted for, solutions to (11) and (16) consistent with the boundary conditions can now be found. It is shown in Appendix B that

$$\Omega=\sqrt{\omega^2-4\alpha\beta}, \tag{19a}$$

$$\epsilon=\tfrac{1}{2}(\Omega-\omega), \tag{19b}$$

and these are real if $\omega^2-4\alpha\beta\geqslant 0$.

The eigenstates of the Hamiltonian (6) can now be constructed from the harmonic oscillator states. Defining the state $|0_d\rangle$ through the relation

$$d|0_d\rangle=0, \tag{20}$$

allows the eigenstates of (6) to be expressed defined in a manner similar to the simple harmonic oscillator

$$|\tilde{n}\rangle=\frac{1}{\sqrt{n!}}c^n|0_d\rangle. \tag{21}$$

Using the algebra (11) and the property (20) gives

$$H|\tilde{n}\rangle=(n+\tfrac{1}{2})\Omega|\tilde{n}\rangle\equiv E_n|\tilde{n}\rangle. \tag{22}$$

It follows that the eigenvalues of H are real and positive as long as $\Omega^2=\omega^2-4\alpha\beta\geqslant 0$ and are formally identical to the simple harmonic oscillator.

The key step in understanding the properties of the eigenstates is to construct the state $|0_d\rangle$ from the states of the harmonic oscillator. The Baker–Campbell–Hausdorff theorem[8] states that if

the commutator of two operators $[A,B]$ commutes with B, then $Ae^{\lambda B^2}=e^{\lambda B^2}(A+\lambda[A,B]B)$, where λ is an arbitrary c-number parameter. In addition, it shows that if A and B are two operators such that $[B,A]=A$, then $e^{\lambda B}A=e^{\lambda}Ae^{\lambda B}$, where λ is a c-number parameter. Using these shows that

$$d\exp\left(\frac{1}{2}\frac{g_2}{g_4}a^{\dagger 2}\right)=(g_4a-g_2a^{\dagger})\exp\left(\frac{1}{2}\frac{g_2}{g_4}a^{\dagger 2}\right)=\exp\left(\frac{1}{2}\frac{g_2}{g_4}a^{\dagger 2}\right)g_4a. \tag{23}$$

It then follows that the state that satisfies (20) is given by

$$|0_d\rangle=N_d\exp\left(\frac{1}{2}\frac{g_2}{g_4}a^{\dagger 2}\right)|0\rangle, \tag{24}$$

where N_d will be used to define a unit projection operator. It is shown in Appendix C that the ground state $|0_d\rangle$ possesses the norm

$$\langle 0_d|0_d\rangle=\frac{|N_d|^2|g_4|^2}{\sqrt{|g_4|^2-|g_2|^2}}. \tag{25}$$

For the case that $-1>g_2/g_4>1$ the ground state possesses an imaginary norm and the Hilbert space possesses an indefinite metric. This is caused by the divergence of the power series (C4) that defines the norm, and so the indefinite metric is signaling that the eigenstates are not normalizable if $-1>g_2/g_4>1$. Using result (B4) shows there are no solutions to this inequality in the Hermitian case. However, for the non-Hermitian case $\alpha<0$ and $\beta>0$ result (B4) shows that imaginary norms occur if $\alpha+\beta<\omega$. As a result, the Hamiltonian (6) suffers difficulties with its metric that are similar to other non-Hermitian cases.[3]

The solution by Bender, Brody, and Hughes[4] to the indefinite metric of other non-Hermitian Hamiltonians is to find the charge conjugation operator $\mathcal{C}$ such that the action of the operator $\mathcal{CPT}$ yields a positive-definite inner product as in (2). In some cases it is necessary to resort to a perturbative construction of this operator.[9] The approach followed in this paper will be to find the orthonormal dual space basis $|\overline{n}\rangle$ first, and then to deduce the form of the operator U that maps the energy eigenstates into the dual states, $|\overline{n}\rangle=U|\tilde{n}\rangle$. By construction this will result in a modified inner product such that $\langle\tilde{n}|U^{\dagger}|\tilde{n}\rangle$ is positive definite. For the case that the dual space is associated with the eigenvectors of $H^{\dagger}$ and the energy spectrum of $H^{\dagger}$ is identical to H, this approach yields an inner product that will preserve unitarity. The proof of this will be given later in this section. This method is easier for the Hamiltonian (6) since the algebra (11) allows the space dual to the Hilbert space of eigenstates (21) to be constructed from the dual space of the harmonic oscillator.

The process begins by defining the dual $\langle 0_c|$ to the ground state $|0_d\rangle$ as the state that satisfies

$$(c^{\dagger}|0_c\rangle)^{\dagger}=\langle 0_c|c=0. \tag{26}$$

As in (24) this state can be constructed from the original harmonic oscillator algebra and its ground state dual $\langle 0|$ by defining

$$\langle 0_c|=N_c\langle 0|\exp\left(\frac{1}{2}\frac{g_3}{g_1}a^2\right). \tag{27}$$

This process yields the dual space basis

$$\langle\overline{m}|=\langle 0_c|\frac{d^m}{\sqrt{m!}}. \tag{28}$$

The notation is intended to reinforce the fact that $\langle\overline{n}| \neq |\tilde{n}\rangle^\dagger$. Using the algebra (11) immediately shows that the dual space basis defined by (28) will be orthonormal to the states of (21), i.e., $\langle\overline{m}|\tilde{n}\rangle = \delta_{mn}$, if $\langle 0_c|0_d\rangle = 1$. This inner product can be evaluated easily because the two states have inherited the inner product of the harmonic oscillator basis. The result (C3) from Appendix C shows that

$$\langle 0_c|0_d\rangle = N_c N_d \sqrt{g_1 g_4}, \tag{29}$$

so that $N_c N_d = 1/\sqrt{g_1 g_4}$ normalizes the inner product. It is convenient to choose

$$N_d = (g_4)^{-1/2}, \tag{30a}$$

$$N_c = (g_1)^{-1/2}, \tag{30b}$$

so that in the limit (18) the normalization factors reduce to unity. The matrix elements of the Hamiltonian are well defined in this basis, yielding

$$\langle\overline{m}|H|\tilde{n}\rangle = (n + \tfrac{1}{2})\Omega\ \delta_{mn}. \tag{31}$$

It is shown in Appendix C that these states and their duals allow the definition of a unit projection operator

$$\sum_{n=0}^{\infty} |\tilde{n}\rangle\langle\overline{n}| = \hat{1}. \tag{32}$$

It is important to note that this process is equivalent to finding the complete set of eigenstates for the Hermitian adjoint $H^\dagger$. Given the explicit form of H and the dual states (28) it is easy to show that

$$H^\dagger|\overline{n}\rangle = (n + \tfrac{1}{2})\Omega|\overline{n}\rangle = E_n|\overline{n}\rangle. \tag{33}$$

Since the eigenvalues are real, nondegenerate, and identical to those for H, the orthonormality statement (31) immediately follows from the relation

$$E_m\langle\overline{m}|\tilde{n}\rangle = (\langle\overline{m}|H)|\tilde{n}\rangle = \langle\overline{m}|(H|\tilde{n}\rangle) = E_n\langle\overline{m}|\tilde{n}\rangle. \tag{34}$$

In order to avoid the indefinite metric an operator U will be found that satisfies

$$\langle\overline{n}| = (U|\tilde{n}\rangle)^\dagger = \langle\tilde{n}|U^\dagger. \tag{35}$$

As long as the states $|\tilde{n}\rangle$ and $|\overline{n}\rangle$ have the same spectrum it will now be shown that

$$H^\dagger U - UH = 0. \tag{36}$$

This follows by using (33) to give

$$E_n|\overline{n}\rangle = H^\dagger U|\tilde{n}\rangle, \tag{37}$$

while from (22) it follows that

$$E_n|\overline{n}\rangle = U^\dagger H|\tilde{n}\rangle, \tag{38}$$

where the equivalence of the eigenvalues has been used. Combining (37) and (38) immediately yields (36). It is shown in Appendix D that for the Hamiltonian (6) the operator U is given explicitly by

$$U=\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}\exp\left(\frac{1}{2}wd^2\right)\exp(cd\ln z), \tag{39}$$

with

$$w=\frac{g_3g_4-g_1^*g_2^*}{g_4^2}, \tag{40a}$$

$$z=\frac{g_4}{g_1^*}. \tag{40b}$$

Appendix D also shows that the operator U has the property that

$$Uc=d^\dagger U, \tag{41a}$$

$$Ud=c^\dagger U, \tag{41b}$$

so that

$$UH=U\Omega cd=\Omega d^\dagger c^\dagger U=H^\dagger U, \tag{42}$$

and its action on the Hamiltonian is precisely that predicted by (36). Result (42) is essential in proving that the theory using the modified inner product is unitary. To demonstrate unitarity the projection operator (32) is rewritten

$$\sum_{n=0}^{\infty}|\tilde{n}\rangle\langle\tilde{n}|U^\dagger=\hat{1}. \tag{43}$$

An arbitrary state $|\tilde{\varphi}\rangle$ is written as a superposition of the energy eigenstates

$$|\tilde{\varphi}\rangle=\sum_{n=0}^{\infty}a_n|\tilde{n}\rangle, \tag{44}$$

with the normalization condition

$$\sum_{n=0}^{\infty}|a_n|^2=1. \tag{45}$$

Using the definition

$$\langle\overline{\varphi}|=(U|\tilde{\varphi}\rangle)^\dagger=\sum_{n=0}^{\infty}\langle\overline{n}|a_n^*, \tag{46}$$

shows that $\langle\overline{\varphi}|\tilde{\varphi}\rangle=1$. The transition element from $|\tilde{\varphi}\rangle$ to the energy eigenstate $|\tilde{n}\rangle$ in Bender's complexified quantum mechanics is defined as

$$W_{\tilde{\varphi}\tilde{n}}\equiv\langle\overline{n}|e^{-iHT}|\tilde{\varphi}\rangle=\langle\tilde{n}|U^\dagger e^{-iHT}|\tilde{\varphi}\rangle, \tag{47}$$

so that its complex conjugate is given by

$$W_{\tilde{\varphi}\tilde{n}}^*=\langle\tilde{\varphi}|e^{iH^\dagger T}U|\tilde{n}\rangle. \tag{48}$$

Unitarity requires that the transition probability satisfies

$$1=\sum_n |W_{\tilde{\varphi}\tilde{n}}|^2=\sum_n \langle\tilde{\varphi}|e^{iH^\dagger T}U|\tilde{n}\rangle\langle\tilde{n}|U^\dagger e^{-iHT}|\tilde{\varphi}\rangle. \tag{49}$$

Using (43) followed by (42) immediately gives

$$\sum_n |W_{\tilde{\varphi}\tilde{n}}|^2=\langle\tilde{\varphi}|e^{iH^\dagger T}Ue^{-iHT}|\tilde{\varphi}\rangle=\langle\tilde{\varphi}|e^{iH^\dagger T}e^{-iH^\dagger T}U|\tilde{\varphi}\rangle=\langle\tilde{\varphi}|U|\tilde{\varphi}\rangle=\langle\overline{\varphi}|\tilde{\varphi}\rangle^*=1. \tag{50}$$

As a result, the use of the modified inner product preserves unitarity in transition probability. The method used in this paper for constructing the operator U requires that H and $H^\dagger$ possess an identical spectrum, and this is the case for (6).

As a result, (35) generalizes the adjoint operation to this particular case of a non-Hermitian Hamiltonian. The operator U is playing a role identical to that of the $\mathcal{CP}$ operator for the Hamiltonian (1) by mapping the eigenstates into a dual space that yields a positive definite and orthonormal inner product. Using the limits (9) shows that the arguments of the exponentials in (39) go to zero when $\alpha\to\beta$. The Hermitian limit, therefore, yields $\lim_{\alpha\to\beta}U=1$ and the standard adjoint operation is recovered, as in the other non-Hermitian Hamiltonians analyzed using Bender's method.

III. TRANSITION ELEMENTS

In this section a specific simple transition element will be evaluated with and without Bender's complexification procedure. The results verify the breakdown of unitarity for the non-Hermitian case $\alpha\neq\beta$ if Bender's procedure is not followed. However, in the Hermitian limit $\alpha=\beta$ and $U=1$, so that the transition element calculated in this manner will coincide with Bender's method. The same transition amplitude for the non-Hermitian case will then be calculated using Bender's method and shown to be manifestly unitary. It is of interest to compare the results of using a non-Hermitian Hamiltonian and Bender's method to the case of using a Hermitian Hamiltonian. Since both cases correspond to unitary time development it is useful through comparison to see what differences emerge in the time evolution of the states. It will be seen that significant differences appear for the case $\beta/\omega\approx 1/2$.

That unitarity will be violated for the non-Hermitian case can be seen from the following general argument. If the inner product is not generalized via Bender's method the transition element from an arbitrary state $|\varphi\rangle$ to a harmonic oscillator eigenstate of the form (5) is defined as

$$W_{\varphi n}=\langle n|e^{-iHT}|\varphi\rangle. \tag{51}$$

Repeating the steps of (49) and (47) gives

$$\sum_n |W_{\varphi n}|^2=\langle\varphi|e^{iH^\dagger T}e^{-iHT}|\varphi\rangle, \tag{52}$$

and this result is not unity if $H^\dagger\neq H$. As a result, the transition element defined by (51) will not give a unitary transition probability in the non-Hermitian case. However, this does not prevent an evaluation of (51) and an explicit examination of the breakdown of unitarity when $\alpha\neq\beta$. Since the operator U of (39) reduces to unity in the Hermitian case, the expression (51) will be the correct definition of the transition amplitude in the limit $\alpha\to\beta$.

In the first step a transition element will be calculated without Bender's complexification procedure. It is simple and instructive to look at the fixed number process

$$W_{02}=\langle 2|e^{-iHT}|0\rangle, \tag{53}$$

where $\langle 2| = \langle 0|a^2/\sqrt{2}$ and H is given by (6). Despite the fact that H is non-Hermitian, evaluating (53) is nothing more than an exercise in normal ordering. This is simplified by using the unit projection operator (32) to find

$$W_{02} = \sum_n \langle 2|\tilde{n}\rangle\langle\overline{n}|0\rangle e^{-in\Omega T} e^{-(1/2)i\Omega T}. \tag{54}$$

It is straightforward to adapt expressions (C13) and (C19) to show that

$$W_{02} = -\left(\frac{\beta}{\sqrt{2}\Omega}\right)(1-e^{-2i\Omega T})(g_1 g_4 - g_2 g_3 e^{-2i\Omega T})^{-3/2} e^{-(1/2)i\Omega T}. \tag{55}$$

Similarly, it is straightforward to show that

$$W_{20} = \langle 0|e^{-iHT}|2\rangle = -\left(\frac{\alpha}{\sqrt{2}\Omega}\right)(1-e^{-2i\Omega T})(g_1 g_4 - g_2 g_3 e^{-2i\Omega T})^{-3/2} e^{-(1/2)i\Omega T}. \tag{56}$$

Interpreting these quantities as the transition probability amplitude shows that the transition probability defined by $P(T) = |W|^2$ would yield two differing rates for these processes as long as $\alpha \neq \beta$. This violates the well known time-reversal invariance of processes driven by Hermitian Hamiltonians, i.e., $|W_{fi}|^2 = |W_{if}|^2$, and is a direct outcome of the fact that the Hamiltonian (6) is non-Hermitian as long as $\alpha \neq \beta$. The origin of this violation is particularly clear in the limit that $\alpha \to 0$ while $\beta \neq 0$. For such a case it is impossible for the Hamiltonian to connect the state $|2\rangle$ to the state $\langle 0|$ since there are no terms quadratic in the destruction operators in the Hamiltonian. Using the results of Appendix B gives the limits for the non-Hermitian transition elements obtained without the complexification procedure as

$$\lim_{\alpha\to 0} W_{20} = 0, \tag{57a}$$

$$\lim_{\alpha\to 0} W_{02} = -\frac{\beta}{\sqrt{2}\omega}(1-e^{-2i\omega T}). \tag{57b}$$

The small T limit of (57b) reduces to the first order term in a perturbative expansion of the transition element (53) where $\alpha = 0$, verifying that the factors in (57b) are correct. Unitarity is, therefore, manifestly violated in the absence of the complexification procedure.

In the Hermitian limit $\alpha = \beta$, (55) and (56) are identical and correspond to unitary time development. Using the results of Appendix B gives

$$\lim_{\alpha\to\beta} W_{20} = -\frac{\beta}{\sqrt{2}\Omega}\left(\frac{\Omega(\omega-\Omega)}{2|\beta|^2}\right)^{3/2}(1-e^{-2i\Omega T})\left(1-\frac{(\omega-\Omega)^2}{4|\beta|^2}e^{-2i\Omega T}\right)^{-3/2} e^{-(1/2)i\Omega T}. \tag{58}$$

The absolute value $|\beta|^2$ appears in (58) to reflect the fact that the expansion is actually in terms of $|\beta|^2 = \alpha\beta$, which is invariant under the phase transformations discussed in Appendix A. For small β/ω (58) reduces to

$$W_{20} \approx -\frac{\beta}{\sqrt{2}\omega}(1-e^{-2i\omega T})\left(1-\frac{|\beta|^2}{\omega^2}e^{-2i\omega T}\right)^{-3/2} e^{-(1/2)i\omega T}. \tag{59}$$

Calculating the same transition element via Bender's method for the non-Hermitian case $\alpha=0$ and $\beta\neq 0$ is particularly simple. For such a case the results of Appendix B show that $\Omega=\omega$, $g_1 g_4=1$, $g_3=0$, and $g_2=-\beta/\omega$. The first step is to express the states $|0\rangle$ and $|2\rangle$ in terms of the energy eigenstates $|\tilde{n}\rangle$, so that

$$|0\rangle=N_0\sum_n\ |\tilde{n}\rangle\langle\overline{n}|0\rangle\equiv N_0\sum_n\ a_n|\tilde{n}\rangle, \tag{60}$$

$$|2\rangle=N_2\sum_n\ |\tilde{n}\rangle\langle\overline{n}|2\rangle\equiv N_2\sum_n\ b_n|\tilde{n}\rangle. \tag{61}$$

The factors N_0 and N_2 are required to normalize the states when the modified transition element of (47) is used. In the limit that $T\to 0$ all transition elements from a state to itself must coincide with unity. This requires fixing

$$|N_0|^{-2}=\sum_n\ |a_n|^2, \tag{62}$$

$$|N_2|^{-2}=\sum_n\ |b_n|^2, \tag{63}$$

which ensures that the inner product is unity:

$$\langle 0|U^\dagger|0\rangle=\langle 2|U^\dagger|2\rangle=1. \tag{64}$$

It is again straightforward to adapt the expressions (C13) and (C19) to show that for $\alpha=0$ and n even the coefficients are given by

$$a_n=\frac{N_c\sqrt{n!}}{2^{n/2}(n/2)!}\left(-\frac{g_2}{g_1}\right)^{n/2}, \tag{65a}$$

$$b_n=\frac{\sqrt{2}N_c\sqrt{n!}}{g_1^2 2^{n/2}(n/2-1)!}\left(-\frac{g_2}{g_1}\right)^{n/2}. \tag{65b}$$

Using the results of Appendixes B and C, the norms are then given by

$$|N_0|^2=\left(1-\frac{|\beta|^2}{\omega^2}\right)^{-1/2}, \tag{66a}$$

$$|N_2|^2=\left(1+\frac{|\beta|^2}{2\omega^2}\right)\left(1-\frac{|\beta|^2}{\omega^2}\right)^{-5/2}, \tag{66b}$$

where it has been assumed that $\beta/\omega<1$ in order for the series to converge. Evaluating the transition amplitude is now straightforward, since

$$W_{20}=\langle 0|U^\dagger e^{-iHT}|2\rangle=N_0^* N_2\sum_{n=0,2,\ldots}\ a_n^* b_n e^{-in\omega T}. \tag{67}$$

Using (65) and (66) and the identity (C2) gives

$$\lim_{\alpha\to 0} W_{20}=-\frac{\beta}{\sqrt{2}\omega}\left(1+\frac{|\beta|^2}{2\omega^2}\right)^{-1/2}\left(\frac{1-(|\beta|^2/\omega^2)}{1-(|\beta|^2/\omega^2)e^{-2i\omega T}}\right)^{3/2} e^{-2i\omega T}, \tag{68}$$

which is true up to the irrelevant arbitrary phase available for β.

It is now possible to compare result (58) to (68). Both expressions are characterized by only two parameters, ω and β, since $\Omega=\sqrt{\omega^2-4|\beta|^2}$ in expression (58). The first point is that (68) does not vanish as did (57a). Result (58) goes to zero at $|\beta|=\omega/2$, while (68) remains well defined for $|\beta|<\omega$. There is a great deal of similarity between (68) and (59) for β small. However, it is clear that the transition amplitude (58) for the Hermitian case deviates significantly from (68) as β increases. In the Hermitian case the frequency Ω is not independent of β, while in the non-Hermitian case (68) ω and β are independent parameters. Thus, as in other cases, the use of a non-Hermitian Hamiltonian has given rise to a well-defined theory but with different dynamics than its Hermitian counterpart.

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APPENDIX A: NORMAL ORDERING, FUNCTIONAL DEPENDENCE, AND DEGREES OF FREEDOM

The process of normal ordering a matrix element results in restrictions on the functional dependence of the matrix element upon its parameters. To illustrate consider the general matrix element

$$W_{00}=\langle 0|\exp\{-i(\omega a^\dagger a+\alpha a^2+\beta a^{\dagger 2})T\}|0\rangle, \tag{A1}$$

where ω, α, and β are real variables with the units of inverse time. In this case the operator U that maps H into $H^\dagger$ and discussed in Sec. III is absent in the definition (A1). The dimensionless operators $a^\dagger$ and a obey the commutation relation $[a,a^\dagger]=1$. Evaluation of (69) consists of normal ordering the a and $a^\dagger$ operators in an arbitrary power of the effective Hamiltonian. In so doing, it is a simple observation that in order to have a nonzero contribution to the matrix element, the product of the a and $a^\dagger$ operators must have equal numbers of a and $a^\dagger$ operators. Only for this case can the process of normal ordering the operators produce a nonzero c-number. In all other cases the process of normal ordering will result in terms with powers of either a or $a^\dagger$, and these have a vanishing matrix element. This is easily seen for low order crossterms such as $aa^{\dagger 2}$ and $aa^\dagger aa^\dagger$, and the general result can be then be established by induction.

This observation can now be coupled with the fact that the commutation relation $[a,a^\dagger]=1$ is invariant under the simultaneous phase transformations $a^\dagger\to e^{i\theta}a^\dagger$ and $a\to e^{-i\theta}a$. However, this transformation does not leave the effective Hamiltonian of (69) invariant, instead inducing the transformations

$$\alpha\to e^{-2i\theta}\alpha, \tag{A2a}$$

$$\beta\to e^{2i\theta}\beta, \tag{A2b}$$

$$\omega\to\omega, \tag{A2c}$$

on the parameters of the Hamiltonian. However, since all terms in the expansion of the exponential that produce nonzero contributions must have equal numbers of a and $a^\dagger$ operators, it follows that (A1) is invariant under this transformation. This means that the final result of evaluating (A1) can depend only upon combinations of parameters that are independent of the transformations (A2a)–(A2c), and this includes terms such as ω and $\alpha\beta$, as well as any combinations determined from the form of the states.

While these restrictions can serve as a consistency check for the form determined for (A1), the phase symmetry also reduces the number of free parameters in the generalized Bogoliubov transformation of (7) and (8). This follows from reexpressing the matrix element (A1) in terms of the

c and d operators. For the same reasons discussed earlier in this appendix, the matrix element (A1) will be independent of the simultaneous phase transformations $c \to e^{i\xi}c$ and $d \to e^{-i\xi}d$ since these also leave invariant the commutator $[a,a^\dagger]$ determined using (7) and (8). As a result, there are two independent arbitrary relative phases present in the generalized Bogoliubov transformation, the one associated with c and d and the one associated with a and $a^\dagger$. In effect, the generalized Bogoliubov transformations (12) and (13) could have been written

$$a = e^{i(\xi+\theta)}g_1 c + e^{-i(\xi-\theta)}g_2 d = e^{i\theta}(e^{i\xi}g_1 c + e^{-i\xi}g_2 d), \tag{A3}$$

$$a^\dagger = e^{i(\xi-\theta)}g_3 c + e^{-i(\xi+\theta)}g_4 d = e^{-i\theta}(e^{i\xi}g_3 c + e^{-i\xi}g_4 d), \tag{A4}$$

where θ and ξ are arbitrary real phases, without affecting the final result of evaluating the matrix element. All resulting expressions in the final form for the matrix element (A1) will therefore possess the symmetries (A2a)–(A2c) when combined with the simultaneous transformations

$$g_1 \to e^{i(\xi+\theta)}g_1, \tag{A5a}$$

$$g_2 \to e^{-i(\xi-\theta)}g_2, \tag{A5b}$$

$$g_3 \to e^{i(\xi-\theta)}g_3, \tag{A5c}$$

$$g_4 \to e^{-i(\xi+\theta)}g_4. \tag{A5d}$$

These symmetries ensure that two of the degrees of freedom in the g_j can always be removed by choosing θ and ξ appropriately, and therefore, these degrees of freedom cannot have any physical significance. This is identical to gauge fixing[10] in field theories, where the gauge symmetry corresponds to unphysical ghost states in the spectrum. Therefore, the g_j possess only six physical degrees of freedom with which to evaluate the matrix element.

APPENDIX B: SOLUTIONS OF THE GENERALIZED BOGOLIUBOV TRANSFORMATION

In this appendix the relevant properties of the g_j will be derived through algebraic manipulation for later use in the paper. The constraints of (16) can be rewritten as two quadratic equations under the assumption that $g_1 \neq 0$ and $g_4 \neq 0$:

$$\omega(g_3/g_1) + \alpha + \beta(g_3/g_1)^2 = 0, \tag{B1}$$

$$\omega(g_2/g_4) + \beta + \alpha(g_2/g_4)^2 = 0. \tag{B2}$$

Consistency with the limits (17) and (18) requires selecting the roots

$$g_3/g_1 = (-\omega + \sqrt{\omega^2 - 4\alpha\beta})/2\beta, \tag{B3}$$

$$g_2/g_4 = (-\omega + \sqrt{\omega^2 - 4\alpha\beta})/2\alpha. \tag{B4}$$

It follows that

$$\frac{g_2 g_3}{g_1 g_4} = (\omega^2 - 2\alpha\beta - \omega\sqrt{\omega^2 - 4\alpha\beta})/2\alpha\beta. \tag{B5}$$

Combining (B5) with condition (11) gives

$$g_1 g_4 = \frac{2\alpha\beta}{(4\alpha\beta - \omega^2 + \omega\sqrt{\omega^2 - 4\alpha\beta})}, \tag{B6}$$

$$g_2 g_3 = \frac{\omega - \sqrt{\omega^2 - 4\alpha\beta}}{2\sqrt{\omega^2 - 4\alpha\beta}}, \tag{B7}$$

$$g_1 g_4 + g_2 g_3 = \frac{\omega}{\sqrt{\omega^2 - 4\alpha\beta}}. \tag{B8}$$

Because (B5)–(B7) are invariant under the transformations of (A4), they can serve as fundamental components of the final form of the transition element. It also follows that $g_1 g_4$ is a real positive number as long as $\omega^2 - 4\alpha\beta \geqslant 0$, while $g_2 g_3$ is real but its sign is that of $\alpha\beta$.

The relationships among the g_j determined so far can now be used to determine other products and ratios. Straightforward algebraic manipulation gives

$$g_1 g_2 = \frac{g_1}{g_3} g_2 g_3 = -\frac{\beta}{\sqrt{\omega^2 - 4\alpha\beta}}, \tag{B9}$$

$$g_3 g_4 = \frac{g_4}{g_2} g_2 g_3 = -\frac{\alpha}{\sqrt{\omega^2 - 4\alpha\beta}}. \tag{B10}$$

The parameters appearing in the transformed Hamiltonian (14) are then given by

$$\Omega = (g_2 g_3 + g_1 g_4)\omega + 2 g_1 g_2 \alpha + 2 g_3 g_4 \beta = \sqrt{\omega^2 - 4\alpha\beta}, \tag{B11}$$

$$\epsilon = g_2 g_3 \omega + g_1 g_2 \alpha + g_3 g_4 \beta = \tfrac{1}{2}\sqrt{\omega^2 - 4\alpha\beta} - \tfrac{1}{2}\omega = \tfrac{1}{2}(\Omega - \omega). \tag{B12}$$

APPENDIX C: PROPERTIES OF THE EIGENSTATES

This appendix analyzes the properties of the states defined by (21) and (28) as well as the states built from them. To begin, the inner product of the states (24) and (27) is evaluated. Using their definitions the inner product reduces to the sum

$$\begin{aligned} \langle 0_c | 0_d \rangle &= N_c N_d \sum_{n,m=0}^{\infty} \frac{\sqrt{(2m)!}}{2^m m!} \frac{\sqrt{(2n)!}}{2^n n!} \left(\frac{g_2}{g_4}\right)^n \left(\frac{g_1}{g_3}\right)^m \langle m | n \rangle \\ &= N_c N_d \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} \left(\frac{g_2 g_3}{g_1 g_4}\right)^n. \end{aligned} \tag{C1}$$

Result (B5) of Appendix B shows that $|g_2 g_3 / g_1 g_4| < 1$, so that the series in (C1) converges absolutely. Using the identity

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta \cos^{2n}\theta = \frac{(2n)!}{4^n (n!)^2}, \tag{C2}$$

allows (C1) to be replaced by a geometric sum and integrated with the desired result that

$$\langle 0_c | 0_d \rangle = \frac{N_c N_d}{2\pi} \int_0^{2\pi} d\theta \frac{g_1 g_4}{g_1 g_4 - g_2 g_3 \cos^2\theta} = N_c N_d \sqrt{g_1 g_4}, \tag{C3}$$

where (11) has been used. The two states have a unit inner product for the conditions of (29). Similarly, the norm of the state (24) can be found to be

$$\langle 0_d|0_d\rangle = |N_d|^2 \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} \left(\frac{|g_2|^2}{|g_4|^2} \right)^n = \frac{|N_d|^2 |g_2|^2}{\sqrt{|g_4|^2 - |g_2|^2}}, \tag{C4}$$

where the assumption that $|g_2|/|g_4| < 1$ has been made.

In proving completeness of the modified states (21) and (28) it will be necessary to evaluate their inner product with the harmonic oscillator ground state $|0\rangle$. This is accomplished by first noting the identity

$$c \exp\left(\frac{1}{2} \frac{g_2}{g_4} a^{\dagger 2} \right) = \exp\left(\frac{1}{2} \frac{g_2}{g_4} a^{\dagger 2} \right) \left(-g_3 a + \frac{a^\dagger}{g_4} \right), \tag{C5}$$

where (11) has again been used. As a result the state $|\tilde{n}\rangle$ can be written

$$|\tilde{n}\rangle = \frac{N_d}{\sqrt{n!}} \exp\left(\frac{1}{2} \frac{g_2}{g_4} a^{\dagger 2} \right) \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n |0\rangle. \tag{C6}$$

The inner product then reduces to evaluating

$$\langle 0|\tilde{n}\rangle = \frac{N_d}{\sqrt{n!}} \langle 0| \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n |0\rangle. \tag{C7}$$

The matrix element can be evaluated to give

$$T_n \equiv \left\langle 0 \left| \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n \right| 0 \right\rangle = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \dfrac{n!}{2^{n/2}(n/2)!} \left(-\dfrac{g_3}{g_4} \right)^{n/2} & \text{if } n \text{ is even.} \end{cases} \tag{C8}$$

The proof is inductive, and begins by noting that (C8) is correct for $n = \{0,1,2,3,4\}$ by direct calculation. Assuming that T_n and T_{n-2} are given by (C8), the next term T_{n+2} can be evaluated inductively by using the formulas

$$a \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n = \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n a + \frac{n}{g_4} \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^{n-1}, \tag{C9}$$

$$\left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n a^\dagger = a^\dagger \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n - n g_3 \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^{n-1}, \tag{C10}$$

with the result that for n an even integer

$$\begin{aligned} T_{n+2} &= -\frac{g_3}{g_4} \langle 0| a \left(-g_3 a + \frac{a^\dagger}{g_4} \right)^n a^\dagger |0\rangle \\ &= \frac{(n+2)!}{2^{(n+2)/2}((n+2)/2)!} \left(-\frac{g_3}{g_4} \right)^{(n+2)/2}, \end{aligned} \tag{C11}$$

which completes the proof of (C8). Using (C8) in (C7) yields the final form for the inner product

$$\langle 0|\tilde{n}\rangle = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \dfrac{N_d \sqrt{n!}}{2^{n/2}(n/2)!} \left(-\dfrac{g_3}{g_4} \right)^{n/2} & \text{if } n \text{ is even.} \end{cases} \tag{C12}$$

A similar result follows for $\langle \overline{n}|0\rangle$

$$\langle\overline{n}|0\rangle=\begin{cases}0 & \text{if } n \text{ is odd}\\ \dfrac{N_c\sqrt{n!}}{2^{n/2}(n/2)!}\left(-\dfrac{g_2}{g_1}\right)^{n/2} & \text{if } n \text{ is even.}\end{cases} \tag{C13}$$

It is critical that the states (21) and (28) can be used to expand the harmonic oscillator states appearing in transition elements. This reduces to showing that the projection operator

$$\hat{P}=\sum_{n=0}^{\infty}|\tilde{n}\rangle\langle\overline{n}| \tag{C14}$$

is a unit operator in the Hilbert space of the harmonic oscillator states. The orthonormality of the states (21) and (28) ensures that the operator (C14) is idempotent, $\hat{P}^2=\hat{P}$. The proof that $\hat{P}$ is a unit projection operator is inductive, and begins by noting that (C12) and (C13) give

$$\langle 0|\hat{P}|0\rangle=N_cN_d\sum_{n=0,2,\ldots}^{\infty}\frac{n!}{2^n\left(\dfrac{n}{2}!\right)^2}\left(\frac{g_2g_3}{g_1g_4}\right)^{n/2}=N_cN_d\sqrt{\frac{g_1g_4}{g_1g_4-g_2g_3}}=1, \tag{C15}$$

where the method employed in summing (C1) has been used as well as using the condition (26) and the norms (30). As a result, $\langle 0|\hat{P}|0\rangle=\langle 0|0\rangle=1$.

The projection operator must also preserve orthonormality of the original harmonic oscillator states. Using the tools developed so far it is straightforward to show that

$$\sum_{n=0}^{\infty}\langle 1|\tilde{n}\rangle\langle\overline{n}|0\rangle=\langle 1|0\rangle=0. \tag{C16}$$

Result (C16) follows from the fact that $\langle 1|\tilde{n}\rangle=0$ for n even, while $\langle\overline{n}|0\rangle=0$ for n odd. The next step is to demonstrate that

$$\langle 2|\hat{P}|0\rangle=\sum_{n=0}^{\infty}\langle 2|\tilde{n}\rangle\langle\overline{n}|0\rangle=0. \tag{C17}$$

From the definitions of the modified states it follows that

$$\langle 2|\tilde{n}\rangle=\frac{N_dn(n-1)}{g_4^2\sqrt{2(n!)}}\langle 0|\left(-g_3a+\frac{1}{g_4}a^{\dagger}\right)^{(n-2)}|0\rangle+\frac{N_d}{\sqrt{2(n!)}}\frac{g_2}{g_4}\langle 0|\left(-g_3a+\frac{1}{g_4}a^{\dagger}\right)^{n}|0\rangle, \tag{C18}$$

where the first term on the right hand side of (C18) is present only if $n\geqslant 2$. Result (C8) can now be used to show that

$$\langle 2|\tilde{n}\rangle=\frac{N_d}{\sqrt{2(n!)}}\frac{n!}{2^{n/2}(n/2)!}\left[\frac{g_2}{g_4}-\frac{n}{g_3g_4}\right]\left(-\frac{g_3}{g_4}\right)^{n/2}+\frac{N_dg_2}{\sqrt{2}g_4}, \tag{C19}$$

where the $n=0$ contribution has been written as the last term on the right hand side of (C19). Result (C19) can now be combined with (C8) to give

$$\sum_{n=0}^{\infty}\langle 2|\tilde{n}\rangle\langle\overline{n}|0\rangle=\frac{N_cN_dg_2}{\sqrt{2}g_4}+\frac{N_cN_dg_2}{\sqrt{2}g_4}\sum_{n=2,4,\ldots}^{\infty}\frac{n!}{2^n((n/2)!)^2}\left(1-\frac{n}{g_2g_3}\right)\left(\frac{g_2g_3}{g_1g_4}\right)^{n/2}. \tag{C20}$$

Using the identities

$$\frac{g_2}{\sqrt{2}g_4}\sum_{n=2,4,\ldots}^{\infty}\frac{n!}{2^n((n/2)!)^2}\left(\frac{g_2g_3}{g_1g_4}\right)^{n/2}=\frac{g_2}{\sqrt{2}g_4}(\sqrt{g_1g_4}-1), \tag{C21}$$

$$\frac{1}{\sqrt{2}g_3g_4}\sum_{n=2,4,\ldots}^{\infty}\frac{n\,n!}{2^n((n/2)!)^2}\left(\frac{g_2g_3}{g_1g_4}\right)^{n/2}=\frac{g_2}{\sqrt{2}g_4}\sqrt{g_1g_4}, \tag{C22}$$

shows that (C20) vanishes. The preservation of orthonormality can now be extended to all the harmonic oscillator states by using induction.

APPENDIX D: THE *U* TRANSFORMATION

The object is to demonstrate that the action of the operator U, given by (39), maps the eigenstates into their orthonormal duals under the adjoint operation. The U operator is invariant under the transformations of (A5a)–(A5d), which is required for consistency. The first two operators in (39) leave the state $|0_d\rangle$ invariant by virtue of the fact that $d|0_d\rangle=0$, so their action is solely upon the c operators that define the eigenstate. The Baker–Campbell–Hausdorff theorem gives

$$\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}\exp\left(\frac{1}{2}wd^2\right)\exp(cd\ln z)c^n|0_d\rangle=\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}(zc+wzd)^n|0_d\rangle. \tag{D1}$$

Using the forms (7) and (8) for c and d allows the action of the remaining operator in (39) to be evaluated, with the result that

$$\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}(zc+wzd)^n|0_d\rangle=N_d\left(z\left[\frac{1}{g_4}+\frac{g_3g_3^*}{g_1^*}-\frac{wg_3^*g_4}{g_1^*}\right]a^\dagger + z[wg_4-g_3]a\right)^n\exp\left(\frac{1}{2}\frac{g_3^*}{g_1^*}a^{\dagger 2}\right)|0\rangle, \tag{D2}$$

where (11) has been used. Using (40), the forms for z and w, and the complex conjugate of (11) yields the desired result that

$$Uc=\left\{z\left[\frac{1}{g_4}+\frac{g_3g_3^*}{g_1^*}-\frac{wg_3^*g_4}{g_1^*}\right]a^\dagger+z[wg_4-g_3]a\right\}U=(g_4^*a^\dagger-g_2^*a)U=d^\dagger U, \tag{D3}$$

while comparison with (27) shows that

$$(U|0_d\rangle)^\dagger=\left(N_d\exp\left(\frac{1}{2}\frac{g_3^*}{g_1^*}a^{\dagger 2}\right)|0\rangle\right)^\dagger=\langle 0_c|. \tag{D4}$$

Combining these results gives

$$\left(U\frac{c^n}{\sqrt{n!}}|0_d\rangle\right)^\dagger=\left(\frac{d^{\dagger n}}{\sqrt{n!}}|0_c\rangle\right)^\dagger=\langle\overline{n}|. \tag{D5}$$

This completes the demonstration of (35).

From (D3) it is clear that (41a) is satisfied. The Baker–Campbell–Hausdorff theorem gives

$$\exp\left(\frac{1}{2}wd^2\right)\exp(cd\ln z)d=\frac{d}{z}\exp\left(\frac{1}{2}wd^2\right)\exp(cd\ln z), \tag{D6}$$

while using (11) shows

$$\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}d=\left(g_4 a-\frac{g_3^* g_4}{g_1^*}a^\dagger\right)\exp\left\{\frac{1}{2}\left(\frac{g_3^*}{g_1^*}-\frac{g_2}{g_4}\right)a^{\dagger 2}\right\}. \tag{D7}$$

Combining these results with $z=g_4/g_1^*$ and noting that (7) gives $c^\dagger=g_1^* a-g_3^* a^\dagger$ immediately yields (41b).

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The Euler characteristic and the first Chern number in the covariant phase space formulation of string theory

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Using a covariant description of the geometry of deformations for extendons, it is shown that the topological corrections for the string action associated with the Euler characteristic and the first Chern number of the normal bundle of the world sheet, although do not give dynamics to the string, modify the symplectic properties of the covariant phase space of the theory. Future extensions of the present results are outlined. © *2004 American Institute of Physics.*
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I. INTRODUCTION

As it is well known, string theory contains two natural topological invariants related with the different topologies of the two-dimensional world surface embedded in a background space–time. Specifically, the Gauss–Bonnet action, which depends only on the purely intrinsic properties of the world surface, corresponds to the Euler characteristic, which counts the number of holes or handles of the world surface. Additionally, the first Chern number of the normal bundle of the world surface, which depends on the extrinsic properties of the world surface embedded in a (four-dimensional) background space–time, gives us essentially the number of self-intersections of the world surface. Such topological invariants do not contribute effectively as Lagrangian terms to the string dynamics, although it is well known also that there is a global contribution in the path integral formulation of the theory, weighting the different topologies in the sum over world surfaces.

On the other hand, in the canonical formulations of the theory for quantization, based on the classical dynamics of the theory, the topological terms will have no any contribution, since the dynamics remains unmodified. The fact that such terms play a nontrivial role in the path integral formulation of the theory, and do not appear at all in the canonical scheme, is somewhat suspicious at first glance. Hence, the aim of this work is to show that, on the basis of a covariant description of the canonical formulation of the theory, the topological terms in the string action may have indeed a physically relevant contribution on the symplectic structure constructed on the corresponding covariant phase space. With these results, we give a new relevant role of the topological terms within a canonical formulation, which is completely unknown in the literature, levelling thus the roles of such terms in both approaches for quantization.

In the next section, we outline the covariant canonical formalism, and in Sec. III we give some remarks on the covariant canonical formulation of the Dirac–Nambu–Goto (DNG) action, in order to prepare the background for the subsequent sections, where the topological terms will be worked out. In Sec. VII we conclude with some discussions about our results and future extensions.

II. COVARIANT PHASE SPACE AND THE EXTERIOR CALCULUS

In this section we summarize the exterior calculus on the covariant phase space given in Ref. 1 but adjusted for the treatment of embeddings.[2]

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According to Ref. 1, in a given physical theory, *the classical phase space is the space of solutions of the classical equations of motion*, which corresponds to a manifestly covariant definition. The basic idea of the covariant description of the canonical formalism is to construct a symplectic structure on such a phase space, instead of choosing p's and q's.

In the present case, the phase space is the space of solutions of Eq. (12), and we shall call it Z. Any background quantity, will be associated with zero-forms on Z. The deformation operator δ (see Sec. III) acts as an exterior derivative on Z, taking k-forms into $(k+1)$-forms, and it should satisfy

$$\delta^2 = 0, \tag{1}$$

and the Leibniz rule

$$\delta(AB) = \delta A B + (-1)^A A\, \delta B. \tag{2}$$

In particular, δX^μ is the exterior derivative of the zero-form X^μ [see Eq. (5)], and it will be closed,

$$\delta^2 X^\mu = 0. \tag{3}$$

Furthermore, since $\phi^i = n^i_\mu \delta X^\mu$, and n^i_μ corresponds to zero-forms on Z, the scalar fields ϕ^i are one-forms on Z, and thus are anticommutating objects: $\phi^i \phi^j = -\phi^j \phi^i$. This property allows us to verify that, being the vector field $\delta = n^i \phi_i$, thus $\delta^2 = n^i n^j \phi_i \phi_j$, which vanishes because of the commutativity of the zero-form n^i and the anticommutativity of the ϕ^i on Z, in full agreement with Eq. (1). It is important to mention, at this point, that the covariant deformation operator D_δ (see Sec. III) also works as an exterior derivative on Z, in the sense that maps k-forms into $(k+1)$-forms; however D_δ^2 does not vanish necessarily.

We can determine certain two-forms on Z that will be useful for our present purposes. Considering that $\delta \equiv \delta X^\mu \partial_\mu$ and $D_\delta \equiv \delta X^\mu D_\mu$, we can show that $D_\delta(\delta X^\mu)$ vanishes,

$$D_\delta(\delta X^\mu) = \delta X^\alpha D_\alpha \delta X^\mu = \delta X^\alpha [\partial_\alpha \delta X^\mu + \Gamma^\mu_{\alpha\lambda} \delta X^\lambda] = \delta^2 X^\mu + \Gamma^\mu_{\alpha\lambda} \delta X^\alpha \delta X^\lambda = 0, \tag{4}$$

where the first term vanishes according to Eq. (3), and the second one because of the symmetry of $\Gamma^\mu_{\alpha\lambda}$ in the indices α and λ, and the anticommutativity of δX^α and δX^λ. Hence, Eq. (4) suggests that D_δ is, as well as δ, a measure of the closeness of δX^μ on Z.

III. COVARIANT CANONICAL FORMULATION FOR DNG *p*-BRANES IN A CURVED BACKGROUND

It will be convenient to do the general treatment for p-branes, and then to consider the particular case of string theory (1-brane), which will show the particularities of string theory as opposed to the other higher-dimensional objects.

In Ref. 2 it is shown that there exists an identically closed two-form on the space of solutions of the classical equations of motion (modulo gauge transformations) for p-branes propagating in a curved background, endowing to the physical phase space $\hat{Z}$ of a symplectic structure. However, a more detailed study[3] shows that such a closed two-form is even an exact two-form, obtained by direct exterior derivative of a *symplectic potential*, a global one-form on the phase space. The strategy in Ref. 3 for obtaining the global symplectic potential directly from the variations of the corresponding Lagrangian is as follows.

In the geometry of deformations of p-branes developed in Ref. 4, it is assumed that an infinitesimal deformation tangent to the world surface is not physically relevant, since it can be identified always with the action of a world surface diffeomorphism. However, as claimed in Ref. 3, it is precisely such an infinitesimal diffeomorphism that plays the role of our global symplectic potential on the phase space (and it is the first example showing that a *spurious* quantity in a

conventional sense, may be physically relevant on the phase space). Hence, we will maintain explicitly a world surface diffeomorphism from the beginning, modifying slightly the original deformation scheme given in Ref. 4.

In this manner, following Ref. 4, the deformation of the world surface swept out by a p-brane (propagating in a curved background) is given by the infinitesimal space–time variation

$$\xi^{\mu} \equiv \delta X^{\mu} = n_i^{\mu} \phi^i + e_a^{\mu} \phi^a, \tag{5}$$

where n_i correspond to vector fields normal to the world surface and, e_a to the vector fields tangent to such a surface.[4] Hence, considering that D_{μ} is the background torsionless covariant derivative, in Ref. 4 the normal deformation operator is defined as

$$D_{\delta} \equiv \delta^{\mu} D_{\mu}, \quad \delta \equiv n_i \phi^i, \tag{6}$$

and it is found that[4]

$$\begin{aligned} D_{\delta} c_a &= (K_{ab}^i \phi_i) e^b + (\tilde{\nabla}_a \phi_i) n^i, \\ D_{\delta} \gamma_{ab} &= 2 K_{ab}^i \phi_i, \\ D_{\delta} \sqrt{-\gamma} &= \sqrt{-\gamma} K^i \phi_i, \end{aligned} \tag{7}$$

which will be useful below. We define here the tangential deformation operator as

$$D_{\Delta} \equiv \Delta^{\mu} D_{\mu}, \quad \Delta \equiv e_a \phi^a, \tag{8}$$

and using the generalized Gauss–Weingarten equations, we find that

$$\begin{aligned} D_{\Delta} e_a &= (\nabla_a \phi^b) e_b - K_{ab}^i \phi^b n_i, \\ D_{\Delta} \gamma_{ab} &= \nabla_a \phi_b + \nabla_b \phi_a, \\ D_{\Delta} \sqrt{-\gamma} &= \sqrt{-\gamma} \nabla_a \phi^a. \end{aligned} \tag{9}$$

In this manner, the action for DNG p-branes,

$$S_0 = -\sigma_0 \int \mathrm{d}^D \xi \sqrt{-\gamma}, \tag{10}$$

considering world surface diffeomorphisms, has as a first variation

$$0 = (D_{\delta} + D_{\Delta}) S_0 = -\sigma_0 \int \mathrm{d}^D \xi \sqrt{-\gamma} K^i \phi_i - \sigma_0 \int \mathrm{d}^D \xi \sqrt{-\gamma} \nabla_a \phi^a, \tag{11}$$

where the last of Eqs. (7) and (9) have been considered; from Eq. (11) we can see that $D_{\Delta} S_0$ is associated with a total divergence that can be indeed negligible, since it does not contribute locally to the dynamics.

Therefore, from Eq. (11), the equations of motion for extremal surfaces are

$$K^i = 0, \tag{12}$$

whose set of solutions defines, in fact, the covariant phase space Z of the theory.

On the other hand, from the deformation dynamics [obtained linearizing Eq. (12)], and using the scheme of (self-) adjoint operators, it is found that the current $j^a = \phi_i \tilde{\nabla}^a \phi^i$ is world surface

covariantly conserved ($\nabla_a j^a = 0$), and corresponds to a closed two-form on the phase space $D_\delta j^a = 0$.[2] Therefore, one can finally construct a covariant and gauge invariant symplectic structure ω for the theory,[2]

$$\omega \equiv \int_\Sigma \sqrt{-\gamma} j^a \, d\Sigma_a , \tag{13}$$

independent on the choice of Σ (a spacelike section of the world surface corresponding to a Cauchy p-surface for the configuration of the p-brane). However, the symplectic current j^a is even an exact two-form,[3] since from Eqs. (4), (5), and the first of Eqs. (7) one finds that

$$\delta\phi^a = D_\delta(e^a_\mu \delta X^\mu) = -j^a, \tag{14}$$

and j^a is in particular a closed form, $\delta j^a = 0$, because of the nilpotency of δ [see Eq. (1)]. Therefore ϕ^a (the tangential projection of the deformation of the embedding), coming directly from the pure divergence term in Eq. (11), plays the role of a global symplectic potential on the phase space. As pointed out above, ϕ^a gives no dynamics to the string, but it is physically relevant on the phase space, in accordance with Eq. (14).

It is important to emphasize here, the significance of a covariant and gauge invariant symplectic structure for the theory. ω in Eq. (13) represents a complete *Hamiltonian* description of the covariant phase space, preserving manifestly all relevant symmetries of the theory. Hence, ω represents a starting point for the study of the symmetry aspects and also a covariant description of the canonical formulation of the theory for quantization. For the general features of the covariant phase space formulation, see, for example, Ref. 1. Note, however, that the concept of symplectic potential does not appear at all in Ref. 1.

In the next section we will follow the same procedure employed in this section for determining the symplectic potential ϕ^a, in order to find the contribution of the Gauss–Bonnet topological term in the action on the covariant phase space of the theory.

IV. THE GAUSS–BONNET TOPOLOGICAL TERM

The Gauss–Bonnet term for an arbitrary closed p-brane without physical boundaries is proportional to the Ricci scalar $\mathcal{R}$ constructed from the world surface metric γ_{ab},

$$\chi \equiv \sigma_1 \int d^D\xi \sqrt{-\gamma}\mathcal{R}, \tag{15}$$

whose first variation, according to the geometry of deformations of Ref. 4, is given by

$$D_\delta(\sqrt{-\gamma}\mathcal{R}) = -2\sqrt{-\gamma}G_{ab}K_i^{ab}\phi^i + \sqrt{-\gamma}\nabla_a\psi_N^a, \tag{16}$$

where G_{ab} is the world surface Einstein tensor

$$G_{ab} = \mathcal{R}_{ab} - \tfrac{1}{2}\gamma_{ab}\mathcal{R}, \tag{17}$$

and

$$\psi_N^a = \gamma^{ab}D_\delta\gamma^c_{bc} - \gamma^{bc}D_\delta\gamma^a_{bc} \tag{18}$$

is the analogous to ϕ^a in Sec. III. Note that in Ref. 4, the pure divergence term involving ψ_N^a is completely ignored (which is correct in a conventional analysis of the brane dynamics), without suspecting the relevant role that such a term will play in a phase space formulation of the theory.

In this manner, Eq. (16) gives the universal contribution of the Gauss–Bonnet term on the brane dynamics (the first term on the right-hand side), and on the covariant phase space through ψ_N^a. In this sense, there is no surprise for an arbitrary p-brane, since χ changes the dynamics and

correspondingly the symplectic structure on the phase space. Nevertheless, as it is well known, in a two-dimensional world surface (and only for such a case), swept out for a string, the world surface Einstein tensor vanishes (for an arbitrary embedding background dimension),

$$G_{ab}=0, \tag{19}$$

and there is not effect on the string dynamics. However, there is a nontrivial contribution of the topological term on the phase space through symplectic potential (18), independently on the null contribution at the level of the string dynamics. For example, in the case considered in Sec. III, if Eqs. (12) are the equations of motion for the closed string dynamics described by external surfaces, the inclusion of the topological term χ in the action leaves Eqs. (12) unchanged (and thus the phase space itself, defined as the space of solutions of the equations of motion, is unaltered), but the corresponding symplectic potential on the phase space is no longer $-\sigma_0\phi^a$, but $-\sigma_0\phi^a+\sigma_1\psi_N^a$, where ψ_N^a is given in Eq. (18).

Although we have considered only the DNG closed strings as the reference Lagrangian term for the inclusion of the GB term, the main idea is to show that $\sigma_1\psi_N^a$ is the universal contribution of the latter on the phase space, and similarly for any action describing strings, for example, some action including terms with curvature corrections.[3] Therefore, if Φ^a is the symplectic potential for such a general action, we can construct the symplectic structure ω as

$$\omega=\int_\Sigma D_\delta\sqrt{-\gamma}(\Phi^a+\sigma_1\psi_N^a)\mathrm{d}\Sigma_a, \tag{20}$$

with the wanted properties of closeness ($\delta\omega=0$). The closeness of ω is equivalent to the Jacobi identity that the Poisson brackets satisfy, in the usual Hamiltonian scheme.[5]

Considering the deformation formulas of Ref. 4, we can determine explicitly the universal contribution of ψ_N^a to the symplectic current of the theory, in terms of ϕ^i, the only measure of the deformation that cannot be gauged away,

$$D_\delta\psi_N^a=-2\phi_i\{K^{abi}\nabla_b(K^j\phi_j)+K^{bci}[\nabla_b(K_c^{aj}\phi_j)+\nabla_c(K_b^{aj}\phi_j)-\nabla^a(K_{bc}^j\phi_j)]\}; \tag{21}$$

which will constitute the universal integral kernel of the Euler characteristic on the symplectic geometry of string theory. Note that even in the simplest case of a DNG closed string dynamics described by Eq. (12), $D_\delta\psi_N^a$ in Eq. (21) does not vanish. Therefore, the topological term modifies drastically the symplectic properties of the phase space of the theory, without changing the dynamics and the phase space itself.

V. THE FIRST CHERN NUMBER OF THE NORMAL BUNDLE OF THE WORLD SHEET

The self-intersection number of the world sheet embedded in a four-dimensional background space–time, given essentially by the first Chen number of the normal bundle of the world sheet, has the analytic expression[6,7]

$$\nu=\sigma_2\int \mathrm{d}^2\xi\,\Omega, \tag{22}$$

in terms of the extrinsic twist curvature,

$$\begin{aligned}\Omega&=\tfrac{1}{2}\epsilon_{ij}\epsilon^{ab}\Omega_{ab}^{ij},\\ \Omega_{ab}^{ij}&=\partial_b\omega_a^{ij}-\partial_a\omega_b^{ij},\end{aligned} \tag{23}$$

where ω_a^{ij} corresponds to the extrinsic twist potential.[4,7] Using Eqs. (23), ν can be rewritten explicitly as a topological invariant in terms of a total divergence,

$$\nu = \sigma_2 \int \mathrm{d}^2\xi \sqrt{-\gamma} \nabla_a (\epsilon_{ij} \epsilon^{ab} \omega_b^{ij}), \tag{24}$$

where $\epsilon^{ab} = \sqrt{-\gamma} \epsilon^{ab}$.[7] In order to determine the variation of ν, we exploit the frame gauge dependence of the potential ω_b^{ij}, which means that it can always be set equal to zero at any single chosen point by an appropriate choice of the normal frame,

$$\delta\nu = \sigma_2 \int \mathrm{d}^2\xi \sqrt{-\gamma} \nabla_a (\epsilon_{ij} \epsilon^{ab} \delta\omega_b^{ij}), \tag{25}$$

where the (normal) variation of the twist potential is given in terms of ϕ^i by[4,7]

$$\delta\omega_b^{ij} = -2K_{cb}^i \tilde{\nabla}^c \phi^j + R_{\mu\nu\alpha\beta} n^{\mu i} n^{\nu j} n^{\alpha\kappa} e_b^\beta \phi_\kappa, \tag{26}$$

where $R_{\mu\nu\alpha\beta}$ is the Riemann tensor of the (four-dimensional) background space–time. In this manner, following the ideas of the present work, from Eq. (25) we can identify to $\Theta^a = \sigma_2 \epsilon_{ij} \epsilon^{ab} \delta\omega_b^{ij}$ as a symplectic potential for ν. Thus, the contribution of ν on the integral Kernel of the symplectic structure of the theory is given by the deformation (exterior derivative) of Θ^a,

$$\delta\Theta^a = -K_i \phi^i \Theta^a, \tag{27}$$

where we have considered that $\delta\sqrt{-\gamma} = \sqrt{-\gamma} K_i \phi^i$.[4] Note that the effect of adding ν to the DNG string action is, in addition to leave unaltered the dynamics governed by $K^i = 0$ [Eq. (12)], to leave unchanged the symplectic structure for the theory (unlike the case of χ in Sec. IV), since in this case $\delta\Theta^a = 0$ in accordance with Eq. (27); of course the situation is different in a more general case than that described by the DNG action, where in general $K^i \neq 0$. Therefore, if Ψ^a is the symplectic potential for such a general action (which may include, for example, the Gauss–Bonnet term χ considered in Sec. IV), the symplectic structure ω of string theory (in four dimensions) including the term ν will take the form

$$\omega = \int_\Sigma D_\delta (\sqrt{-\gamma} \Psi^a) \mathrm{d}\Sigma_a + \int_\Sigma D_\delta \Theta^a \, \mathrm{d}\Sigma_a, \tag{28}$$

which is evidently closed.

The same argument employed in Ref. 2 for demonstrating the nondegeneracy of the symplectic structure for DNG branes works for the contributions of the topological terms on the symplectic structure of the theory. In this manner the ω's in (20) and (28) are nondegenerate and are defined on the reduced phase space Z/G, with G being the volume of the group of infinitesimal space–time diffeomorphisms.[2]

VI. REMARKS ON OPEN AND CLOSED STRINGS

In Ref. 7 open strings with topologically inspired boundary conditions are considered, specifically the topological terms considered here for closed strings. In both cases, such topological terms do not affect the equations of motion; however, in the case of open strings such terms lead to boundary conditions to be implemented in addition to the equations of motion, unlike the case treated here of closed strings, where such complementary conditions do not appear at all, because of the absence of physical boundaries. Thus, it is opportune to emphasize the results presented in this work: the topological terms for closed strings do not modify the classical dynamics, neither imposing any additional condition, but contributing explicitly to the symplectic structure of the theory, and thus they may have possible quantum effects.

It is important to remark also that the symplectic potentials for the topological terms χ and ν are the same for both closed and open strings; however for the former the symplectic structure will

be constructed on the phase space defined by the (unmodified) equations of motion, and for the latter on a *restriction* of the same phase space defined by the complementary conditions mentioned above.

VII. REMARKS AND PROSPECTS

In Ref. 8, it is proved that the topological terms modify drastically the deformation dynamics of string theory, in such a way that the symplectic current obtained as a consequence of the self-adjointness of that deformation dynamics, is in full agreement with the currents obtained in the present treatment calculating the variations of the symplectic potentials. Specifically it is proved that the symplectic currents of the topological terms in Eqs. (20) and (28) are world sheet covariantly conserved: $\nabla_a(D_\delta\sqrt{-\gamma}\psi_N^a)=0=\nabla_a(D_\delta\Theta^a)$, which ensures that the ω's in (20) and (28) are independent on the choice of Σ. It is important to mention that such world sheet conserved currents that play the role of integral kernels for the symplectic structures on Z in the present approach, can be considered, in a more ordinary sense, as Noetherian current for the topological invariants considered, which will allow us in this sense to obtain conserved currents associated with any continuous symmetries of the background. In the context of brane dynamics in the current literature, these conserved currents only have been considered in this conventional sense.[9]

Since a symplectic structure ω governs the transition between the classical and quantum domains, and allows us to consider also the aspects of symmetry of the theory, it may be interesting to study the possible contribution of the topological terms on the Poincaré charges, Poincaré algebra, and the relevant commutation relations of the theory. In this sense, because of the presence of the topological terms, the quantum version of string theory obtained from the unmodified classical dynamics, may be radically different to that obtained from the global description of the phase space given in terms of ω. All these questions will be the subject of forthcoming communications.

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Construction of a family of quantum Ornstein–Uhlenbeck semigroups

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For a given quasi-free state on the CCR algebra over one dimensional Hilbert space, a family of Markovian semigroups which leave the quasi-free state invariant is constructed by means of noncommutative elliptic operators and Dirichlet forms on von Neumann algebras. The generators (Dirichlet operators) of the semigroups are analyzed and the spectrums together with eigenspaces are found. When restricted to a maximal Abelian subalgebra, the semigroups are reduced to a unique Markovian semigroup of classical Ornstein–Uhlenbeck process. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1641150]

I. INTRODUCTION

The purpose of this paper is to find the explicit expressions of the generators of Markovian semigroups on the CCR algebra $\mathcal{A}$ over one dimensional Hilbert space, which leave a given (fixed) quasi-free state ω on $\mathcal{A}$ invariant. By means of noncommutative elliptic operators[1] and Dirichlet forms on standard forms of von Neumann algebras,[2] we construct a family of symmetric Markovian semigroups on the natural standard form associated to the GNS representation of the pair $(\mathcal{A},\omega)$. If one restricts the semigroups to a maximal Abelian subalgebra, then the semigroups are reduced to a unique Markovian semigroup of classical Ornstein–Uhlenbeck (O-U) process. Each generator of the semigroups has a discrete spectrum and a simple lowest eigenvalue. Thus the semigroups are ergodic and tend to the equilibrium exponentially fast.

The need to construct Markovian semigroups on von Neumann algebras, which are symmetric with respect to a nontracial state, is clear for various applications to open systems,[3] quantum statistical mechanics,[4] and quantum probability theory.[5–7] Although on the abstract level we have quite a well-developed theory,[2,8,9] the progress in concrete applications is very slow. We would like to mention a few works in this direction. The completely positive Hamiltonian semigroup for quantum spin chains in the ground state representation has been considered in Ref. 10. In Refs. 11 and 12, the generalized conditional expectation is used to construct generators of spin-flip type dynamics for quantum spin systems. In Ref. 13, one of authors gave a general construction method of Dirichlet forms on standard forms of von Neumann algebras and applied the method to construct translation invariant Markovian semigroups for quantum spin systems. The method of Ref. 13 has been extended to construct symmetric Markovian semigroups on the CCR and CAR algebras with respect to quasi-free states,[14,15] and on quantum mechanical systems.[16] In Ref. 17, quantum O-U semigroups were constructed by means of noncommutative Dirichlet forms. It may be worthwhile to mention that for a given quasi-free state ω on the CCR algebra $\mathcal{A}$, the O-U semigroup constructed in Ref. 17 belongs to the family of semigroups we constructed in this article. See Sec. III for the details.

Let us describe the content of this paper briefly. Let $\mathcal{A}$ be the C^*-algebra generated by the Weyl operators $W(z)$, $z \in \mathbb{C}$. See Sec. 5.2 of Ref. 4 for the details. The quasi-free state ω on $\mathcal{A}$ is given by

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$$\omega(W(z))=\exp\{-\tfrac{1}{4}|z|^2(1+e^{-\beta})(1-e^{-\beta})^{-1}\},\ z\in\mathbb{C}, \tag{1.1}$$

where $\beta\in(0,\infty)$ is the inverse temperature, which is fixed throughout in this article.

Let $(\mathcal{H}_\omega,\pi_\omega,\Omega_\omega)$ be the GNS representation[4] of $(\mathcal{A},\omega)$ and let $\mathcal{M}=\pi_\omega(\mathcal{A})''$. For each $z\in\mathbb{C}$, we denote by $\Phi_\omega(z)$ the infinitesimal generator of the strongly continuous unitary group $\pi_\omega(W(tz)),t\in\mathbb{R}$:

$$\pi_\omega(W(tz))=\exp(it\Phi_\omega(z)). \tag{1.2}$$

Let Q and P be the position and momentum operators given by

$$Q=\Phi_\omega(1),\quad P=\Phi_\omega(i). \tag{1.3}$$

From now on we write $\mathcal{H}=\mathcal{H}_\omega$, $\xi_0=\Omega_\omega$ and $W(z)=\pi_\omega(W(z))$, $\forall z\in\mathbb{C}$. Let σ_t be the group of automorphisms on $\mathcal{M}$ defined by

$$\sigma_t(W(z))=W(e^{-i\beta t}z),\ \forall z\in\mathbb{C}. \tag{1.4}$$

The state ω satisfies the σ-KMS condition[4] and thus σ_t, $t\in\mathbb{R}$, is the group of the modular automorphisms. Let Δ and J be the modular operator and modular conjugation respectively associated to $(\mathcal{M},\xi_0)$. Then $\sigma_t(A)=\Delta^{it}A\Delta^{-it}$, $A\in\mathcal{M}$. Let $\mathcal{M}'$ be the commutant of $\mathcal{M}$. The map $j:\mathcal{M}\to\mathcal{M}'$ is the antilinear $*$-isomorphism defined by $j(A)=JAJ$, $A\in\mathcal{M}$. The natural positive cone $\mathcal{P}$ associated with $(\mathcal{M},\xi_0)$ is the closure of the set $\{Aj(A)\xi_0:A\in\mathcal{M}\}$. Then $(\mathcal{M},\mathcal{H},\mathcal{P},J)$ is the natural standard form associated to $(\mathcal{M},\xi_0)$.

Next let us describe the explicit forms of the generators of Markovian semigroups on $\mathcal{M}$ which leave ω invariant. In Ref. 1, the authors constructed Markovian semigroups on von Neumann algebras by the quantum Feynman–Kac formula. Let $\mathcal{N}$ be a von Neumann algebra and $b=b^*\in\mathcal{N}$. Let δ be a densely defined $*$-derivation on $\mathcal{N}$ such that $\mathbf{1}\in D(\delta)$ and $\delta(\mathbf{1})=0$. Let G^b be an elliptic operator on $\mathcal{N}$ defined by

$$\begin{aligned} &D(G^b)=D(\delta^2),\\ &G^b(A)=-\tfrac{1}{2}\delta^2(A)-b\,\delta(A)-\delta(A)b+\tfrac{1}{2}[b,[b,A]],\ A\in D(G^b), \end{aligned} \tag{1.5}$$

where $[A,B]=AB-BA$, $A,B\in\mathcal{N}$. It was shown that the closed extension of G^b generates a Markovian semigroup on $\mathcal{N}$.[1]

We are searching for elliptic operators on $\mathcal{M}$ which generate Markovian semigroup leaving ω invariant. Let $\alpha_1,\alpha_2,\alpha_3\in\mathbb{R}$ be real parameters. In (1.5), we choose $\delta(A)=i[P,A]$ and $b=\alpha_1 Q$, and let

$$G_1(A):=\tfrac{1}{2}[P,[P,A]]-i\alpha_1(Q[P,A]+[P,A]Q)+\tfrac{1}{2}\alpha_1^2[Q,[Q,A]].$$

Next, choose $\delta(A)=i\alpha_3[Q,A]$ and $b=\alpha_2 P$, and let

$$G_2(A):=\tfrac{1}{2}\alpha_3^2[Q,[Q,A]]-i\alpha_2\alpha_3(P[Q,A]+[Q,A]P)+\tfrac{1}{2}\alpha_2^2[P,[P,A]].$$

Let G be the elliptic operator on $\mathcal{M}$ given by

$$\begin{aligned} G(A):=\gamma\{G_1(A)+G_2(A)\}=&\frac{\gamma}{2}(1+\alpha_2^2)[P,[P,A]]+\frac{\gamma}{2}(\alpha_1^2+\alpha_3^2)[Q,[Q,A]]-i\gamma\alpha_1(Q[P,A]\\ &+[P,A]Q)-i\gamma\alpha_2\alpha_3(P[Q,A]+[Q,A]P), \end{aligned} \tag{1.6}$$

where γ is the normalized constant which will be chosen as $\gamma=(1+\alpha_2^2)^{-1}$. Since P and Q are unbounded operators affiliated to $\mathcal{M}$, the above is a formal expression.

Because of the well-developed theory,[2] it is convenient to construct Markovian semigroups on the standard form $(\mathcal{M},\mathcal{H},\mathcal{P},J)$. Consider the symmetric embedding:[2]

$$\begin{aligned} &i_0:\mathcal{M}\to\mathcal{H},\\ &i_0(A)=\Delta^{1/4}A\xi_0=\sigma_{-i/4}(A)\xi_0, \end{aligned} \tag{1.7}$$

and define the operator H on $\mathcal{H}$ by

$$H\sigma_{-i/4}(A)\xi_0=\sigma_{-i/4}(G(A))\xi_0. \tag{1.8}$$

It follows from (1.8) that

$$\begin{aligned} H=&\frac{\gamma}{2}(1+\alpha_2^2)(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))^2+\frac{\gamma}{2}(\alpha_1^2+\alpha_3^2)(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q)))^2\\ &-i\gamma\alpha_1(\sigma_{-i/4}(Q)+j(\sigma_{-i/4}(Q)))(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))-i\gamma\alpha_2\alpha_3(\sigma_{-i/4}(P)\\ &+j(\sigma_{-i/4}(P)))(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q))). \end{aligned} \tag{1.9}$$

Let the parameters $\alpha_1,\ \alpha_2,\ \alpha_3\in\mathbb{R}$, satisfy the following relations:

$$\begin{aligned} &\tfrac{1}{2}(1+\alpha_2^2)\sinh(\beta/2)=-\alpha_1\cosh(\beta/2),\\ &\tfrac{1}{2}(\alpha_1^2+\alpha_3^2)\sinh(\beta/2)=\alpha_2\alpha_3\cosh(\beta/2). \end{aligned} \tag{1.10}$$

Then the operator H can be written as

$$\begin{aligned} H=&\gamma_1(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))^*(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))+\gamma_2(\sigma_{-i/4}(Q)\\ &-j(\sigma_{-i/4}(Q)))^*(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q))), \end{aligned} \tag{1.11}$$

where $\gamma_1=-\gamma\alpha_1/\sinh(\beta/2)$, $\gamma_2=\gamma\alpha_2\alpha_3/\sinh(\beta/2)$. Recall that $\gamma=(1+\alpha_2^2)^{-1}$. See the proof of Proposition 3.1 in Sec. IV.

Notice that formally the operator H in (1.11) is symmetric and positive. By means of Dirichlet forms on von Neumann algebras[2] and the approximation procedure used in Ref. 14, we will show that H becomes a positive self-adjoint operator on a dense domain in $\mathcal{H}$, which generates a strongly continuous symmetric Markovian semigroup $\{T_t\}_{t\geqslant 0}$ on $\mathcal{H}$. Define the map S_t on $\mathcal{M}$ by

$$S_t:\mathcal{M}\to\mathcal{M},\quad i_0\circ S_t=T_t\circ i_0.$$

Then $\{S_t\}_{t\geqslant 0}$ is a weakly continuous Markovian semigroup on $\mathcal{M}$ which leaves ω invariant. See Remark 3.1.

Let φ be a bounded smooth function on $\mathbb{R}$. It follows from (1.6) and the commutation relation $[P,Q]=-i\mathbf{1}$ that

$$G(\varphi(Q))=-\frac{\gamma}{2}(1+\alpha_2^2)\varphi''(Q)-2\gamma\alpha_1Q\varphi'(Q)=-\tfrac{1}{2}\varphi''(Q)+\tanh(\beta/2)Q\varphi'(Q). \tag{1.12}$$

Thus for any α_1, α_2 and α_3 satisfying (1.10), the restriction of S_t to the maximal Abelian subalgebra $\mathcal{N}\subset\mathcal{M}$ generated by $\exp(ikQ), k\in\mathbb{R}$, is reduced to a unique classical O-U semigroup.

The spectrum of H will be analyzed by a method similar to that used in Ref. 14. It turns out that H has discrete spectrum and H has a simple eigenvalue zero with eigenvector ξ_0.

The article is organized as follows: In Sec. II, we review the theory of noncommutative Dirichlet forms on von Neumann algebras.[2] In Sec. III, we give explicit expressions of Dirichlet forms and state the main results. Section IV is devoted to the proof of the Markov property of

semigroups by means of the theory of noncommutative Dirichlet forms and the approximation procedure used in Ref. 14. In Sec. V, we decompose $\mathcal{H}$ to a direct sum of eigenspaces of Direchlet operators and analyze the spectrum of generators of the semigroups.

II. REVIEW ON THE NONCOMMUTATIVE DIRICHLET FORMS

In this section we give a brief review on the theory of Dirichlet forms and Markovian semigroups on standard forms of von Neumann algebras. For details, we refer the reader to Ref. 2.

Let $\mathcal{M}$ be a σ-finite von Neumann algebra acting on a complex Hilbert space $\mathcal{H}$. A *self-dual cone* $\mathcal{P}$ in $\mathcal{H}$ is a subset satisfying the property:

$$\{\xi \in \mathcal{H}: \langle \xi, \eta \rangle \geqslant 0, \forall\, \eta \in \mathcal{P}\} = \mathcal{P}.$$

Then $\mathcal{P}$ is a closed convex cone and $\mathcal{H}$ is the complexification of the real subspace $\mathcal{H}^J := \{\xi \in \mathcal{H}: \langle \xi, \eta \rangle \in \mathbb{R}, \forall\, \eta \in \mathcal{P}\}$, whose elements are called *J-real*: $\mathcal{H} = \mathcal{H}^J \oplus i\mathcal{H}^J$. For any two elements $\xi, \eta \in \mathcal{H}^J$, $\xi \leqslant \eta$ means $\eta - \xi \in \mathcal{P}$, thus $\mathcal{H}^J$ has an ordered structure. An anti-unitary involution J on $\mathcal{H}$ by $J(\xi + i\eta) := \xi - i\eta, \forall\, \xi, \eta \in \mathcal{H}^J$, preserves $\mathcal{P}$ and $\mathcal{H}^J$. Any J-real element ξ can be decomposed uniquely as a difference, $\xi = \xi_+ - \xi_-$, of two orthogonal, positive elements, called the positive and the negative part of ξ: $\xi_+, \xi_- \in \mathcal{P}$, $\langle \xi_+, \xi_- \rangle = 0$.

A *standard form* $(\mathcal{M}, \mathcal{H}, \mathcal{P}, J)$ of the von Neumann algebra $\mathcal{M}$ acting faithfully on the Hilbert space $\mathcal{H}$ consists of self-dual, closed, convex cone $\mathcal{P}$ in $\mathcal{H}$ and the anti-unitary involution J satisfying the following properties:

(a) $J\mathcal{M}J = \mathcal{M}'$,
(b) $JAJ = A^*, \quad \forall A \in \mathcal{M} \cap \mathcal{M}'$,
(c) $J\xi = \xi, \quad \forall \xi \in \mathcal{P}$,
(d) $AJAJ(\mathcal{P}) \subset \mathcal{P}, \quad \forall A \in \mathcal{M}$,

where $\mathcal{M}'$ is the commutant of $\mathcal{M}$.

A bounded operator A on $\mathcal{H}$ is called *J-real* if $AJ = JA$ and *positive preserving* if $A\mathcal{P} \subset \mathcal{P}$. The semigroup $\{T_t\}_{t \geqslant 0}$ is said to be *J-real* if T_t is J-real for any $t \geqslant 0$ and it is called *positive preserving* if T_t is positive preserving for any $t \geqslant 0$.

Let us fix a cyclic and separating vector ξ_0 in $\mathcal{P}$. A bounded operator $A: \mathcal{H} \to \mathcal{H}$ is called *sub-Markovian* (with respect to ξ_0) if $0 \leqslant \xi \leqslant \xi_0$ implies $0 \leqslant A\xi \leqslant \xi_0$. A is called *Markovian* if it is sub-Markovian and also $A\xi_0 = \xi_0$. A semigroup $\{T_t\}_{t \geqslant 0}$ is said to be *sub-Markovian* (with respect to ξ_0) if T_t is sub-Markovian for every $t \geqslant 0$. The semigroup $\{T_t\}_{t \geqslant 0}$ is called *Markovian* if T_t is Markovian for every $t \geqslant 0$.

Next, we consider a sesquilinear form on some linear manifold of $\mathcal{H}$: $\mathcal{E}(\cdot, \cdot): D(\mathcal{E}) \times D(\mathcal{E}) \to \mathbb{C}$. We also consider the associated quadratic form: $\mathcal{E}[\,\cdot\,]: D(\mathcal{E}) \to \mathbb{C}$, $\mathcal{E}[\xi] := \mathcal{E}(\xi, \xi)$. A real valued quadratic form $\mathcal{E}[\,\cdot\,]$ is said to be *semi-bounded* if $\inf\{\mathcal{E}[\xi]: \xi \in D(\mathcal{E}), \|\xi\| = 1\} = -b > -\infty$. A quadratic form $(\mathcal{E}, D(\mathcal{E}))$ is said to be *J-real* if $JD(\mathcal{E}) \subset D(\mathcal{E})$ and $\mathcal{E}[J\xi] = \overline{\mathcal{E}[\xi]}$ for any $\xi \in D(\mathcal{E})$. For a given semi-bounded quadratic form $\mathcal{E}$, one considers the inner product given by $\langle \xi, \eta \rangle_\lambda := \mathcal{E}(\xi, \eta) + \lambda \langle \xi, \eta \rangle$, for $\lambda > b$. The form $\mathcal{E}$ is *closed* if $D(\mathcal{E})$ is a Hilbert space for some of the above norms. The form $\mathcal{E}$ is called *closable* if it admits a closed extension.

Associated to a semi-bounded closed form $\mathcal{E}$, there are a self-adjoint operator $(H, D(H))$ and a strongly continuous, symmetric semigroup $\{T_t\}_{t \geqslant 0}$. Each of the above objects determines uniquely the others according to well known relations (see Sec. 3.1 of Ref. 4).

From now on we will consider only J-real, real-valued, semi-bounded, densely defined quadratic forms. It is easy to check that these forms satisfy the relation $\mathcal{E}[\xi + i\eta] = \mathcal{E}[\xi] + \mathcal{E}[\eta]$ for all $\xi + i\eta \in D(\mathcal{E})^J + iD(\mathcal{E})^J = D(\mathcal{E})$ where $D(\mathcal{E})^J := D(\mathcal{E}) \cap H^J$.

Let us denote by $\mathrm{Proj}(\xi, \mathcal{Q})$ the projection of the vector $\xi \in \mathcal{H}^J$ onto the closed, convex cone $\mathcal{Q} \subset \mathcal{H}^J$. For $\xi, \eta \in \mathcal{H}^J$, define

$$\xi \vee \eta := \mathrm{Proj}(\xi, \eta + \mathcal{P}),$$

$$\xi \wedge \eta := \mathrm{Proj}(\xi, \eta - \mathcal{P}).$$

Definition 2.1: A J-real, real-valued, densely defined quadratic form $(\mathcal{E}, D(\mathcal{E}))$ *is called Markovian with respect to* $\xi_0 \in \mathcal{P}$ *if*

$$\xi \in D(\mathcal{E})^J \text{ implies } \xi \wedge \xi_0 \in D(\mathcal{E}) \text{ and } \mathcal{E}[\xi \wedge \xi_0] \leqslant \mathcal{E}[\xi].$$

A closed Markovian form is called a Dirichlet form.

Next, we state main results which will be used in the sequel. For the proofs we refer to Ref. 2.

Proposition 2.1: Let $(\mathcal{E}, D(\mathcal{E}))$ *be a J-real, real valued, densely defined closed form. Assume that the following properties hold*:

(a) $\xi_0 \in D(\mathcal{E})$,
(b) $\mathcal{E}(\xi, \xi) \geqslant 0$ *for* $\xi \in D(\mathcal{E})$,
(c) $\xi \in D(\mathcal{E})^J$ *implies* $\xi_\pm \in D(\mathcal{E})$ *and* $\mathcal{E}(\xi_+, \xi_-) \leqslant 0$.

Then $\mathcal{E}$ *is a Dirichlet form if and only if* $\mathcal{E}(\xi, \xi_0) \geqslant 0$ *for all* $\xi \in D(\mathcal{E}) \cap \mathcal{P}$.

The above result follows from Proposition 4.5(b) of Ref. 2 and Proposition 4.10(ii) of Ref. 2.

Theorem 2.1 (*Theorem 4.11 of Ref. 2): Let* $\{T_t\}_{t \geqslant 0}$ *be a J-real, strongly continuous, symmetric semigroup on* $\mathcal{H}$ *and let* $(\mathcal{E}, D(\mathcal{E}))$ *be the associated densely defined J-real, real valued quadratic form. Then the followings are equivalent*:

(a) $\{T_t\}_{t \geqslant 0}$ *is sub-Markovian.*
(b) $(\mathcal{E}, D(\mathcal{E}))$ *is a Dirichlet form.*

III. DIRICHLET FORMS: PRELIMINARIES AND MAIN RESULTS

Let $\mathcal{A}$ be the C^*-algebra generated by the Weyl operators $W(z)$, $z \in \mathbb{C}$, satisfying

$$\begin{aligned} W(z)^* &= W(-z), \\ W(z)W(z') &= e^{-i/2\,\mathrm{Im}(\bar{z}z')} W(z+z'), \forall z, z' \in \mathbb{C}, \end{aligned} \tag{3.1}$$

where $\bar{z}$ is a complex conjugate of z. $\mathcal{A}$ is the CCR algebra over one dimensional Hilbert space. Let ω be a quasi-free state on $\mathcal{A}$ defined by

$$\omega(W(z)) = \exp\{-\tfrac{1}{4}|z|^2(1+e^{-\beta})(1-e^{-\beta})^{-1}\}, \forall z \in \mathbb{C}, \tag{3.2}$$

where $\beta > 0$ is the inverse temperature.

Let $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ be the GNS representation[4] of $(\mathcal{A}, \omega)$, and let $\mathcal{M} = \pi_\omega(\mathcal{A})''$. Denote by $\Phi_\omega(z)$ the infinitesimal generator of the strongly continuous unitary group $\pi_\omega(W(tz))$ for all $z \in \mathbb{C}$:

$$\pi_\omega(W(tz)) = \exp(it\Phi_\omega(z)).$$

The position and momentum operators are defined by

$$Q := \Phi_\omega(1), \quad P := \Phi_\omega(i), \tag{3.3}$$

respectively. Since ω is an entire analytic state[4] by (3.2), the cyclic vector Ω_ω is an entire analytic vector for P and Q. The annihilation and creation operators given by

$$\begin{aligned} D(a_\omega) &= D(P) \cap D(Q) = D(a_\omega^*), \\ a_\omega &:= 2^{-1/2}(Q + iP), \quad a_\omega^* := 2^{-1/2}(Q - iP), \end{aligned} \tag{3.4}$$

are densely defined, closed and $(a_\omega)^* = a_\omega^*$, and satisfy the canonical commutation relation-(CCR): $[a_\omega, a_\omega^*] = \mathbf{1}$. See Sec. 5.2.3 of Ref. 4 for the details.

In the rest of this paper, we write that $\mathcal{H} = \mathcal{H}_\omega$, $\xi_0 = \Omega_\omega$, $W(z) = \pi_\omega(W(z))$, $\Phi(z) = \Phi_\omega(z)$, $\forall z \in \mathbb{C}$, $a = a_\omega$ and $a^* = a_\omega^*$. Let $\sigma_t : \mathcal{M} \to \mathcal{M}$ be the group of automorphisms on $\mathcal{M}$ defined by

$$\sigma_t(W(z)) = W(e^{-i\beta t}z), \forall z \in \mathbb{C}.$$

The state ω in (3.2) satisfies the σ-KMS condtion[4] and thus σ_t, $t \in \mathbb{R}$, is the modular automorphism by Theorem 5.3.10 of Ref. 4. Let Δ and J be the modular operator and modular conjugation respectively associated to the pair $(\mathcal{M}, \xi_0)$.[4] Then $\sigma_t(A) = \Delta^{it} A \Delta^{-it}$, $A \in \mathcal{M}$. Let $\mathcal{M}'$ be the commutant of $\mathcal{M}$. The map $j : \mathcal{M} \to \mathcal{M}'$ is the anti-linear *-isomorphism defined by $j(A) = JAJ$, $A \in \mathcal{M}$. The natural positive cone $\mathcal{P}$ associated with $(\mathcal{M}, \xi_0)$ is the closure of the set $\{Aj(A)\xi_0 : A \in \mathcal{M}\}$. Then $(\mathcal{M}, \mathcal{H}, \mathcal{P}, J)$ is the natural standard form associated to $(\mathcal{M}, \xi_0)$.

Next, we introduce two dense manifolds of $\mathcal{H}$. For any $A \in \mathcal{M}$, define

$$A_n = \left(\frac{n}{\pi}\right)^{1/2} \int \sigma_t(A) e^{-nt^2} dt, \quad n \in \mathbb{N}. \tag{3.5}$$

Then A_n is an entire analytic element for σ_t, $\|A_n\| \leqslant \|A\|$ $\forall n \in \mathbb{N}$ and $A_n \to A$ strongly. See the proof of Proposition 2.5.22 in Ref. 4. Put

$$\mathcal{M}_0 := \text{the algebra generated by } A_n,\ A \in \mathcal{M},\ n \in \mathbb{N}, \tag{3.6}$$

and denote by $\mathcal{H}_{fin}$ the subset of finite linear combinations of the vectors of the following type:

$$\psi_m^n = P^m Q^n \xi_0, \quad m, n = 0,1,2,\ldots .$$

Clearly $\mathcal{M}_0\xi_0$ and $\mathcal{H}_{fin}$ are dense in $\mathcal{H}$, and P, Q and $j(P)$, $j(Q)$ are affiliated with $\mathcal{M}$ and $\mathcal{M}'$, respectively (see Lemma 4.1).

For any $z \in \mathbb{C}$, we write

$$\sigma_z(a) := e^{i\beta z}a, \quad \sigma_z(a^*) := e^{-i\beta z}a^*, \tag{3.7}$$

and

$$\sigma_z(P) := -i2^{-1/2}(e^{i\beta z}a - e^{-i\beta z}a^*), \quad \sigma_z(Q) := 2^{-1/2}(e^{i\beta z}a + e^{-i\beta z}a^*). \tag{3.8}$$

Denote by Φ either P or Q. In fact, one may be able to show that for $\xi \in \mathcal{M}_0\xi_0$ the function $t \mapsto \sigma_t(\Phi)\xi$ has an analytic extension on $\mathbb{C}$, which is denoted by $\sigma_z(\Phi)\xi$, and that $\sigma_z(\Phi)$ is equal to that of (3.8) on $\mathcal{M}_0\xi_0$. See Lemma 4.1 for $D(\Phi)$.

As discussed in the Introduction, for any parameters α_1, α_2, α_3, we introduce a sesquilinear form corresponding to the operator H given in (1.9) by

$$D(\mathcal{E}) = \mathcal{M}_0\xi_0, \tag{3.9}$$

$$\begin{aligned}
\mathcal{E}(\eta, \xi) = {} & \frac{\gamma}{2}(1+\alpha_2^2)\langle(\sigma_{-i/4}(P) - j(\sigma_{-i/4}(P)))^*\eta, (\sigma_{-i/4}(P) - j(\sigma_{-i/4}(P)))\xi \rangle \\
& + \frac{\gamma}{2}(\alpha_1^2+\alpha_3^2)\langle(\sigma_{-i/4}(Q) - j(\sigma_{-i/4}(Q)))^*\eta, (\sigma_{-i/4}(Q) - j(\sigma_{-i/4}(Q)))\xi \rangle \\
& - i\gamma\alpha_1\langle(\sigma_{-i/4}(Q) + j(\sigma_{-i/4}(Q)))^*\eta, (\sigma_{-i/4}(P) - j(\sigma_{-i/4}(P)))\xi \rangle \\
& - i\gamma\alpha_2\alpha_3\langle(\sigma_{-i/4}(P) + j(\sigma_{-i/4}(P)))^*\eta, (\sigma_{-i/4}(Q) - j(\sigma_{-i/4}(Q)))\xi\rangle
\end{aligned}$$

for $\eta, \xi \in \mathcal{M}_0\xi_0$, where $\gamma=(1+\alpha_2^2)^{-1}$. Notice that $\mathcal{E}$ is well defined on $\mathcal{M}_0\xi_0$ by Lemma 4.1.

Proposition 3.1: Let the parameters $\alpha_1, \alpha_2, \alpha_3 \in \mathbb{R}$ satisfy the following relations:

$$\begin{aligned} \tfrac{1}{2}(1+\alpha_2^2)\sinh(\beta/2) &= -\alpha_1 \cosh(\beta/2), \\ \tfrac{1}{2}(\alpha_1^2+\alpha_3^2)\sinh(\beta/2) &= \alpha_2\alpha_3 \cosh(\beta/2). \end{aligned} \tag{3.10}$$

Then the sesquilinear form given by (3.9) equals to

$$\begin{aligned} D(\mathcal{E}) &= \mathcal{M}_0\xi_0, \\ \mathcal{E}(\eta,\xi) &= \gamma_1\langle(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))\eta,(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))\xi\rangle + \gamma_2\langle(\sigma_{-i/4}(Q) \\ &\quad -j(\sigma_{-i/4}(Q)))\eta,(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q)))\xi\rangle, \end{aligned} \tag{3.11}$$

where

$$\gamma_1 = -\gamma\alpha_1/\sinh(\beta/2), \quad \gamma_2 = \gamma\alpha_2\alpha_3/\sinh(\beta/2). \tag{3.12}$$

Thus by (3.11) $\mathcal{E}$ is a positive form.

In the rest of the paper, *we assume that the relations (3.10) hold*. We state the main results.

Theorem 3.1: *The form $(\mathcal{E},D(\mathcal{E}))$ defined as in (3.9) [and so as in (3.11)] is closable. Denote by $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$ the closure of $(\mathcal{E},D(\mathcal{E}))$ and by H the positive self-adjoint operator associated to $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$. Then the following properties hold*:

(a) $\xi_0 \in D(H)$ *and* $H\xi_0=0$,
(b) $\overline{\mathcal{E}}$ *is J-real, that is,* $\overline{\mathcal{E}}[J\xi]=\overline{\mathcal{E}}[\xi]$ *for* $\xi \in D(\overline{\mathcal{E}})$,
(c) $\overline{\mathcal{E}}(\xi_+,\xi_-)\leqslant 0$ *for any* $\xi \in D(\overline{\mathcal{E}})\cap\mathcal{H}^J$.

Furthermore, the form $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$ is a Dirichlet form.

Recall that a symmetric, strongly continuous, positive preserving semigroup $\{T_t\}_{t\geqslant 0}$ on $\mathcal{H}$ is called *ergodic* if for any $\eta, \xi \in \mathcal{P}-\{0\}$, there exists $t>0$ such that $\langle \eta, T_t\xi\rangle > 0$. Let H be the self-adjoint generator of $T_t: T_t=e^{-tH}$, $t\geqslant 0$. An eigenvector of H corresponding to the lowest eigenvalue $\inf \sigma(H)$ will be called a *ground state* for H (or $\{T_t\}_{t\geqslant 0}$). The ergodicity of its semigroup is equivalent to that the lowest eigenvalue of H has multiplicity one and there exists a strictly positive ground state for H (Theorem 4.3 of Ref. 18).

Theorem 3.2: *Let $\{T_t\}_{t\geqslant 0}$ be the symmetric Markovian semigroup associated to the Dirichlet form $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$ and let H be the Dirichlet operator, i.e., $T_t=e^{-tH}$. Then the following results hold*:

(a) H *is essentially self-adjoint on* $\mathcal{H}_{fin}$.
(b) *The spectrum of generator H are discrete, i.e.,* $\sigma(H)=\{m\tau_1+n\tau_2 : m,n=0,1,2,\ldots\}$, *where* $\tau_1=2\gamma_1\sinh(\beta/2)$, $\tau_2=2\gamma_2\sinh(\beta/2)$.
(c) *The zero is a simple eigenvalue of H with eigenvector ξ_0. Thus $\{T_t\}_{t\geqslant 0}$ is ergodic.*

The eigenspaces of H will be given in Theorem 5.2(b). By the spectral theorem, Theorem 3.2(b) implies that for any $\xi \in \mathcal{H}$ and $t>0$

$$\|T_t\xi - \langle\xi_0,\xi\rangle\xi_0\| \leqslant e^{-\tau t}\|\xi - \langle\xi_0,\xi\rangle\xi_0\|,$$

where $\tau=\min\{\tau_1,\tau_2\}$. Thus $\{T_t\}_{t\geqslant 0}$ converges to the equilibrium exponentially fast.

Remark 3.1: Let $\{T_t\}_{t\geqslant 0}$ be a strongly continuous, symmetric Markovian semigroup on $\mathcal{H}$. Consider the symmetric embedding:

$$i_0 : \mathcal{M} \to \mathcal{H},$$

$$i_0(A) = \Delta^{1/4}A\xi_0.$$

Define the maps S_t on $\mathcal{M}$ by

$$S_t:\mathcal{M}\to\mathcal{M},\quad i_0\circ S_t=T_t\circ i_0. \tag{3.13}$$

It follows from Theorem 2.12 of Ref. 2 that $\{S_t\}_{t\geqslant 0}$ is a weakly continuous Markovian semigroup on $\mathcal{M}$.

Remark 3.2: Let $\mathcal{N}$ be the maximal Abelian subalgebra of $\mathcal{M}$ generated by $\exp\{ikQ\}, k\in\mathbb{R}$. *Let S_t be the Markovian semigroup on $\mathcal{M}$ obtained by (3.13). As mentioned in the Introduction, it can be checked that for any $\alpha_1, \alpha_2, \alpha_3\in\mathbb{R}$ satisfying (3.10) the restriction of S_t to $\mathcal{N}$ gives a unique O-U semigroup whose generation satisfies the equation in (1.12).*

Before closing this section, we show that distinct values of the parameters $\alpha_1, \alpha_2, \alpha_3\in\mathbb{R}$ satisfying (3.10) give distinct semigroups on $\mathcal{H}$. It follows from Theorem 3.2(b) that the spectrum of each generator H is characterized by

$$\gamma_1/\gamma_2=-\alpha_1/(\alpha_2\alpha_3).$$

We first consider two special examples and then describe general case.

Example 3.1: the O-U semigroup studied in Ref. 17. Choose $\alpha_3=1$ and $-\alpha_1=\alpha_2$. It follows from (3.10) and (3.12) that

$$\begin{gathered}\gamma_1=\gamma_2,\\ \alpha_2=(\cosh(\beta/2)\pm 1)/\sinh(\beta/2)\equiv\alpha_{2,\pm}(\beta).\end{gathered} \tag{3.14}$$

Using (3.8), we obtain from (3.11) that

$$\mathcal{E}(\xi,\xi)=\gamma(\|(\mu a-\lambda j(a^*))\xi\|^2+\|(\lambda a^*-\mu j(a))\xi\|^2),\forall\,\xi\in\mathcal{M}_0\xi_0,$$

where $\mu=\lambda^{-1}=e^{\beta/4}$ and $\gamma=\gamma_1=\gamma_2$. The above is the form studied in Ref. 17.

Example 3.2: Consider $\alpha_2=1$. It follows from (3.10) and (3.12) that

$$\begin{aligned}\alpha_1&=-\tanh(\beta/2),\\ \alpha_3&=\coth(\beta/2)\pm(\coth^2(\beta/2)-\tanh^2(\beta/2))^{1/2}\\ &=\tanh^2(\beta/2)/[\coth(\beta/2)\mp(\coth^2(\beta/2)-\tanh^2(\beta/2))^{1/2}],\\ \gamma_1/\gamma_2&=\coth(\beta/2)[\coth(\beta/2)\mp(\coth^2(\beta/2)-\tanh^2(\beta/2))^{1/2}]\neq 1.\end{aligned} \tag{3.15}$$

Next, we consider the general case. Consider α_2 as a parameter. Then we get from (3.10) that

$$\begin{gathered}\alpha_1=-\tfrac{1}{2}(1+\alpha_2^2)\tanh(\beta/2),\\ \alpha_3=[\alpha_2\cosh(\beta/2)\pm(\alpha_2^2\cosh^2(\beta/2)-\alpha_1^2\sinh^2(\beta/2))^{1/2}]/\sinh(\beta/2).\end{gathered} \tag{3.16}$$

For real α_3, one requires that $\alpha_2^2\cosh^2(\beta/2)\geqslant\alpha_1^2\sinh^2(\beta/2)$. By the first equation in (3.16), positive solutions α_2 exist if and only if

$$2\alpha_2\cosh^2(\beta/2)\geqslant(1+\alpha_2^2)\sinh^2(\beta/2).$$

Denote

$$\kappa_\pm(\beta):=[\cosh^2(\beta/2)\pm(\cosh^4(\beta/2)-\sinh^4(\beta/2))^{1/2}]/\sinh^2(\beta/2),$$

$$I_\beta:=[\kappa_-(\beta),\kappa_+(\beta)].$$

Thus $\alpha_2\in I_\beta$. Note that

$$\kappa_+(\beta)=[\cosh^2(\beta/2)+(\cosh^2(\beta/2)+\sinh^2(\beta/2))^{1/2}]/\sinh^2(\beta/2),$$

$$\geqslant[\cosh^2(\beta/2)+\cosh(\beta/2)]/\sinh^2(\beta/2),$$

$$=\coth(\beta/2)\alpha_{2,+}(\beta),$$

where $\alpha_{2,+}(\beta)$ has been defined in (3.14). The above implies that $\kappa_+(\beta)>\alpha_{2,+}(\beta)$. An argument similar to that used above yields that $\kappa_-(\beta)<\alpha_{2,-}(\beta)$. Thus we conclude that $1\in[\alpha_{2,-}(\beta),\alpha_{2,+}(\beta)]\subset I_\beta$.

Define

$$f_\pm(\alpha_2):=-\alpha_1(\alpha_2)/\alpha_2\alpha_{3,\pm}(\alpha_2),$$

$$\alpha_{3,\pm}(\alpha_2)=[\alpha_2\cosh(\beta/2)\pm(\alpha_2^2\cosh^2(\beta/2)-\alpha_1^2\sinh^2(\beta/2))^{1/2}]/\sinh(\beta/2)$$

$$=\alpha_2\coth(\beta/2)\pm(\alpha_2^2\coth^2(\beta/2)-\tfrac{1}{4}(1+\alpha_2^2)^2\tanh^2(\beta))^{1/2}.$$

Since $f_\pm$ are continuous on $I_\beta\subset(0,\infty)$, $f_+(I_\beta)$ and $f_-(I_\beta)$ are closed intervals which have common point at $\alpha_2=\kappa_-(\beta)$ and $\alpha_2=\kappa_+(\beta)$. Thus $f_+(I_\beta)\cup f_-(I_\beta)$ is a closed interval containing 1 with nonzero length [by (3.15)]. Therefore there exist infinitely many different semigroups, which contain the semigroups constructed in Ref. 17.

IV. MARKOV PROPERTY OF FORMS: PROOFS OF PROPOSITION 3.1 AND THEOREM 3.1

In this section we produce the proofs of Proposition 3.1 and Theorem 3.1. Since P and Q are unbounded operators, we need to employ the approximation procedure used in Ref. 14. In the rest of this article we denote by Φ either P or Q and by $a^\sharp$ either a or a^*.

Lemma 4.1: (a) $\mathcal{M}_0\xi_0$ and $\mathcal{H}_{fin}$ are dense in $\mathcal{H}$.

(b) The inclusions

$$\mathcal{M}_0\xi_0\subset D(\Phi) \text{ and } \mathcal{H}_{fin}\subset D(\Phi)$$

hold; moreover, the relation

$$\Phi A\xi_0=j(\sigma_{-i/2}(A^*))\Phi\xi_0$$

holds for any $A\in\mathcal{M}_0$. Also we have $\mathcal{M}_0\xi_0\subset D(a^\sharp)$, $\mathcal{H}_{fin}\subset D(a^\sharp)$ and $a^\sharp A\xi_0=j(\sigma_{-i/2}(A^*))a^\sharp\xi_0, A\in\mathcal{M}_0$.

Proof: (a) Since for $A\in\mathcal{M}$, A_n in (3.5) converges strongly to A as $n\to\infty$ and since $\mathcal{M}\xi_0$ is dense in $\mathcal{H}$, $\mathcal{M}_0\xi_0$ is dense in $\mathcal{H}$. It follows from (3.2) that ω is an entire analytic state, and so ξ_0 is an entire analytic vector for $\Phi(z), z\in\mathbb{C}$. Thus $\mathcal{H}_{fin}$ is dense. See Sec. 5.2.3 of Ref. 4 for the details.

(b) Since ξ_0 is an entire analytic vector for Φ, $\mathcal{H}_{fin}\subset D(\Phi)$. Notice that for any $A\in\mathcal{M}_0$, $j(\sigma_{-i/2}(A^*))\xi_0=A\xi_0$. For $z=1,i$ and $n\in\mathbb{N}$, we write that

$$\Phi(z,n)=-in\left(W\left(\frac{1}{n}z\right)-1\right). \tag{4.1}$$

Notice that

$$\Phi(z,n)A\xi_0=\Phi(z,n)j(\sigma_{-i/2}(A^*))\xi_0=j(\sigma_{-i/2}(A^*))\Phi(z,n)\xi_0.$$

Since the sequence $\{\Phi(z,n)\xi_0\}$ converges to $\Phi\xi_0$, it follows that $A\xi_0\in D(\Phi)$ and the relation

$$\Phi A\xi_0=j(\sigma_{-i/2}(A^*))\Phi\xi_0$$

hold for $A \in \mathcal{M}_0$. The rest part of (b) follows from (3.4). □

Recall the definitions of $\sigma_z(\Phi)$, $z \in \mathbb{C}$ in (3.8), i.e.,

$$\sigma_z(P) = -i2^{-1/2}(e^{i\beta z}a - e^{-i\beta z}a^*), \quad \sigma_z(Q) = 2^{-1/2}(e^{i\beta z}a + e^{-i\beta z}a^*).$$

For any $n \in \mathbb{N}$, we write that

$$\Phi_n := -\left(\frac{n}{\pi}\right)^{1/2} \int in\left\{\sigma_t\left(\exp\left(\frac{i}{n}\Phi\right) - \mathbf{1}\right)\right\} e^{-nt^2}\, dt. \tag{4.2}$$

Notice that for any $n \in \mathbb{N}$, Φ_n is an entire analytic element for σ_t and $\sigma_z(\Phi_n)$ is given by

$$\sigma_z(\Phi_n) := -\left(\frac{n}{\pi}\right)^{1/2} \int in\left\{\sigma_t\left(\exp\left(\frac{i}{n}\Phi\right) - \mathbf{1}\right)\right\} e^{-n(t-z)^2}\, dt \tag{4.3}$$

for any $z \in \mathbb{C}$. See the proof of Proposition 2.5.22(1) in Ref. 4.

Lemma 4.2: For any $n \in \mathbb{N}$, $z = t + is \in \mathbb{C}$ and $A \in \mathcal{M}_0$, there exists a constant $M(A,s)$ such that the bound

$$\|\sigma_z(\Phi_n)A\xi_0\| + \|\sigma_z(\Phi)A\xi_0\| \leq M(A,s),$$

and, moreover, $\sigma_z(\Phi)A\xi_0 = \lim_{n\to\infty}\sigma_z(\Phi_n)A\xi_0$ holds.

Proof: By the method used in the proof Lemma 4.1, one can check that

$$\sigma_z(\Phi_n)A\xi_0 = j(\sigma_{-i/2}(A))\sigma_z(\Phi_n)\xi_0,$$

and a similar relation for $\sigma_z(\Phi)$. Since $\sigma_z(\Phi_n)\xi_0$ converges to $\sigma_z(\Phi)\xi_0$, the lemma follows from above relation. □

We first produce the proof of Proposition 3.1. Note that by (3.7)

$$\begin{aligned} \sigma_{-i/4}(a^*) &= e^{-\beta/4}a^*, \quad \sigma_{-i/4}(a) = e^{\beta/4}a, \\ \sigma_{i/4}(a^*) &= e^{\beta/4}a^*, \quad \sigma_{i/4}(a) = e^{-\beta/4}a. \end{aligned} \tag{4.4}$$

Proof of Proposition 3.1: By Lemmas 4.1 and 4.2 the operators $\sigma_{\pm i/4}(P)$ and $\sigma_{\pm i/4}(Q)$ are well defined on $\mathcal{M}_0\xi_0$. We have that

$$\begin{aligned} P = \sigma_{-i/4}(\sigma_{i/4}(P)) &= i2^{-1/2}\sigma_{-i/4}(e^{\beta/4}a^* - e^{-\beta/4}a) \\ &= i2^{-1}e^{\beta/4}(\sigma_{-i/4}(Q) - i\sigma_{-i/4}(P)) - i2^{-1}e^{-\beta/4}(\sigma_{-i/4}(Q) + i\sigma_{-i/4}(P)) \\ &= i\sinh(\beta/4)\sigma_{-i/4}(Q) + \cosh(\beta/4)\sigma_{-i/4}(P). \end{aligned} \tag{4.5}$$

By the method used above, we also have that

$$Q = \cosh(\beta/4)\sigma_{-i/4}(Q) - i\sinh(\beta/4)\sigma_{-i/4}(P). \tag{4.6}$$

It follows from (4.4) and (4.6) that

$$\begin{aligned} &[\sigma_{i/4}(P) \mp j(\sigma_{i/4}(P))] - [\sigma_{-i/4}(P) \mp j(\sigma_{-i/4}(P))] \\ &\quad = i2^{-1/2}[(e^{\beta/4} - e^{-\beta/4})a^* - (e^{-\beta/4} - e^{\beta/4})a] \mp 2^{-1/2}j\{i[(e^{\beta/4} - e^{-\beta/4})a^* - (e^{-\beta/4} - e^{\beta/4})a]\} \\ &\quad = 2i\sinh(\beta/4)Q \mp j(2i\sinh(\beta/4)Q) = 2i\sinh(\beta/4)(Q \pm j(Q)) \\ &\quad = 2i\sinh(\beta/4)\{\cosh(\beta/4)\sigma_{-i/4}(Q) - i\sinh(\beta/4)\sigma_{-i/4}(P)\} \\ &\qquad \pm 2i\sinh(\beta/4)j\{\cosh(\beta/4)\sigma_{-i/4}(Q) - i\sinh(\beta/4)\sigma_{-i/4}(P)\} \\ &\quad = i\sinh(\beta/2)[\sigma_{-i/4}(Q) \pm j(\sigma_{-i/4}(Q))] + 2\sinh^2(\beta/4)[\sigma_{-i/4}(P) \mp j(\sigma_{-i/4}(P))]. \end{aligned} \tag{4.7}$$

Here we have used the equality $2\sinh(\beta/4)\cosh(\beta/4)=\sinh(\beta/2)$. The argument used above yields

$$[\sigma_{i/4}(Q)\mp j(\sigma_{i/4}(Q))]-[\sigma_{-i/4}(Q)\mp j(\sigma_{-i/4}(Q))]=2\sinh^2(\beta/4)[\sigma_{-i/4}(Q)\mp j(\sigma_{-i/4}(Q))] - i\sinh(\beta/2)[\sigma_{-i/4}(P)\pm j(\sigma_{-i/4}(P))]. \tag{4.8}$$

Note that $1+2\sinh^2(\beta/4)=\cosh(\beta/2)$. Thus (4.7) and (4.8) imply

$$\sigma_{i/4}(P)\mp j(\sigma_{i/4}(P))=i\sinh(\beta/2)[\sigma_{-i/4}(Q)\pm j(\sigma_{-i/4}(Q))]+\cosh(\beta/2)[\sigma_{-i/4}(P) \mp j(\sigma_{-i/4}(P))],$$

$$\sigma_{i/4}(Q)\mp j(\sigma_{i/4}(Q))=-i\sinh(\beta/2)[\sigma_{-i/4}(P)\pm j(\sigma_{-i/4}(P))]+\cosh(\beta/2)[\sigma_{-i/4}(Q) \mp j(\sigma_{-i/4}(Q)].$$

Notice that $(\sigma_{-i/4}(\Phi)\pm j(\sigma_{-i/4}(\Phi)))^*=\sigma_{i/4}(\Phi)\pm j(\sigma_{i/4}(\Phi))$ on $\mathcal{M}_0\xi_0$. We substitute the above relations into (3.9) to obtain that for $\eta,\xi\in\mathcal{M}_0\xi_0$,

$$\begin{aligned}\mathcal{E}(\eta,\xi)=&A_1(\alpha_1,\alpha_2,\alpha_3)\langle(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))\eta,(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))\xi\rangle\\ &+A_2(\alpha_1,\alpha_2,\alpha_3)\langle(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q)))\eta,(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q)))\xi\rangle\\ &+A_3(\alpha_1,\alpha_2,\alpha_3)\langle(\sigma_{-i/4}(Q)+j(\sigma_{-i/4}(Q)))\eta,(\sigma_{-i/4}(P)-j(\sigma_{-i/4}(P)))\xi\rangle\\ &+A_4(\alpha_1,\alpha_2,\alpha_3)\langle(\sigma_{-i/4}(P)+j(\sigma_{-i/4}(P)))\eta,(\sigma_{-i/4}(Q)-j(\sigma_{-i/4}(Q)))\xi\rangle,\end{aligned}$$

where

$$A_1(\alpha_1,\alpha_2,\alpha_3)=\gamma[\tfrac{1}{2}(1+\alpha_2^2)\cosh(\beta/2)+\alpha_1\sinh(\beta/2)],$$

$$A_2(\alpha_1,\alpha_2,\alpha_3)=\gamma[\tfrac{1}{2}(\alpha_1^2+\alpha_3^2)\cosh(\beta/2)-\alpha_2\alpha_3\sinh(\beta/2)],$$

$$A_3(\alpha_1,\alpha_2,\alpha_3)=-i\gamma[\tfrac{1}{2}(1+\alpha_2^2)\sinh(\beta/2)+\alpha_1\cosh(\beta/2)],$$

$$A_4(\alpha_1,\alpha_2,\alpha_3)=i\gamma[\tfrac{1}{2}(\alpha_1^2+\alpha_3^2)\sinh(\beta/2)-\alpha_2\alpha_3\cosh(\beta/2)].$$

By the relations (3.10), the form in (3.9) equals that in (3.11). □

In order to prove Theorem 3.1, we employ the approximation procedure similar to that used in Ref. 14. For any $n\in\mathbb{N}$, let $(\mathcal{E}_n,\mathcal{H})$ be the form given by

$$\begin{aligned}\mathcal{E}_n(\eta,\xi)=&\frac{\gamma}{2}(1+\alpha_2^2)\langle(\sigma_{-i/4}(P_n)-j(\sigma_{-i/4}(P_n)))^*\eta,(\sigma_{-i/4}(P_n)-j(\sigma_{-i/4}(P_n)))\xi\rangle\\ &+\frac{\gamma}{2}(\alpha_1^2+\alpha_3^2)\langle(\sigma_{-i/4}(Q_n)-j(\sigma_{-i/4}(Q_n)))^*\eta,(\sigma_{-i/4}(Q_n)-j(\sigma_{-i/4}(Q_n)))\xi\rangle\\ &-i\gamma\alpha_1\langle(\sigma_{-i/4}(Q_n)+j(\sigma_{-i/4}(Q_n)))^*\eta,(\sigma_{-i/4}(P_n)-j(\sigma_{-i/4}(P_n)))\xi\rangle\\ &-i\gamma\alpha_2\alpha_3\langle(\sigma_{-i/4}(P_n)+j(\sigma_{-i/4}(P_n)))^*\eta,(\sigma_{-i/4}(Q_n)-j(\sigma_{-i/4}(Q_n)))\xi\rangle,\end{aligned} \tag{4.9}$$

where $\gamma=(1+\alpha_2^2)^{-1}$ and P_n, Q_n have been defined as in (4.2). Notice that $\mathcal{E}_n$ is bounded.

Lemma 4.3: Let $(\mathcal{E},D(\mathcal{E}))$ *be the form defined by (3.9). For any* $\eta,\xi\in\mathcal{M}_0\xi_0$,

$$\mathcal{E}(\eta,\xi)=\lim_{n\to\infty}\mathcal{E}_n(\eta,\xi).$$

Proof: The lemma follows from Lemma 4.2. □

We write that

$$\delta_-(A) := A - j(\sigma_{-i/2}(A^*)),$$
$$\delta_+(A) := A + j(\sigma_{-i/2}(A^*)), \tag{4.10}$$

where A is an operator on $\mathcal{H}$. By Lemmas 4.1 and 4.2, $\delta_-(\Phi)$ and $\delta_+(\Phi)$ are also well defined on $\mathcal{M}_0\xi_0$. We are ready to prove Theorem 3.1.

Proof of Theorem 3.1: Two operators $\delta_-(\sigma_{-i/4}(P))$ and $\delta_-(\sigma_{-i/4}(Q))$ are defined on $\mathcal{M}_0\xi_0$ and have the adjoint operators $\delta_-(\sigma_{i/4}(P))$ and $\delta_-(\sigma_{i/4}(Q))$, respectively, which are also defined on $\mathcal{M}_0\xi_0$, and so they are closable. Thus by Proposition 3.1 the form $(\mathcal{E}, D(\mathcal{E}))$ is closable. Notice that $(\mathcal{E}, D(\mathcal{E}))$ in (3.11) is positive. Denote by $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$ the closure of $(\mathcal{E}, D(\mathcal{E}))$ and by H the positive self-adjoint operator associated to $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$.

(a) Notice that $\xi_0 \in \mathcal{M}_0\xi_0$ and $\delta_-(\sigma_{-i/4}(\Phi))\xi_0 = 0$ implies $\xi_0 \in D(\overline{\mathcal{E}})$, and so $\xi_0 \in D(H^{1/2})$ and $H^{1/2}\xi_0 = 0$. By the spectral theorem one has $\xi_0 \in D(H)$ and $H\xi_0 = 0$.

(b) Note that $JA\xi_0 = \sigma_{-i/2}(A^*)\xi_0 \in \mathcal{M}_0\xi_0$, $A \in \mathcal{M}_0$. Thus $\xi \in \mathcal{M}_0\xi_0$ implies $J\xi \in \mathcal{M}_0\xi_0$. Consider the form $(\mathcal{E}, D(\mathcal{E}))$ in (3.11). The proof of (b) follows from $\delta_-(\sigma_{-i/4}(\Phi))J\xi = -J\delta_-(\sigma_{-i/4}(\Phi))\xi$, $\xi \in \mathcal{M}_0\xi_0$, and the fact that $\mathcal{M}_0\xi_0$ is a form core of $\overline{\mathcal{E}}$.

(c) We first assert that

$$\xi \in \mathcal{M}_0\xi_0 \cap \mathcal{H}^J \Rightarrow \xi_+, \xi_- \in D(\overline{\mathcal{E}}) \quad \text{and} \quad \overline{\mathcal{E}}[\xi_\pm] = \lim_{n\to\infty} \mathcal{E}_n[\xi_\pm]. \tag{4.11}$$

Let us prove our assertion. Let s_+ and s_- be the projections onto the closure of $\mathcal{M}'\xi_+$ and $\mathcal{M}'\xi_-$ respectively, where $s_+, s_- \in \mathcal{M}$.[19] For $\xi = A\xi_0$, $A \in \mathcal{M}_0$, we write that

$$\xi_{n,\pm} = (s_\pm A)_n \xi_0,$$

where

$$(s_\pm A)_n = \left(\frac{n}{\pi}\right)^{1/2} \int \sigma_t(s_\pm A) e^{-nt^2}\, dt.$$

Notice that $\|(s_\pm A)_n\| \leq \|A\|$, $n \in \mathbb{N}$, and that for any $\eta \in \mathcal{H}$, $(s_\pm A)_n \eta \to s_\pm A\eta$ as $n \to \infty$. See the proof of Proposition 2.5.22 of Ref. 4. Since $\Delta^{it}\mathcal{P} \subset \mathcal{P}$ for $t \in \mathbb{R}$, $\xi_{n,\pm} = (s_\pm A)_n\xi_0 = j((s_\pm A)_n)\xi_0$, and so

$$\sigma_{-i/4}(\Phi)\xi_{n,\pm} = j((s_\pm A)_n)\sigma_{-i/4}(\Phi)\xi_0.$$

Since $\sigma_{-i/4}(\Phi)$ is a closed operator, we take n to infinity to conclude that $\xi_\pm \in D(\sigma_{-i/4}(\Phi))$, and $\sigma_{-i/4}(\Phi)\xi_\pm = j(s_\pm A)\sigma_{-i/4}(\Phi)\xi_0$, and so

$$\delta_-(\sigma_{-i/4}(\Phi))\xi_\pm = j(s_\pm A)\sigma_{-i/4}(\Phi)\xi_0 - (s_\pm A)j(\sigma_{-i/4}(\Phi))\xi_0. \tag{4.12}$$

By the method used above, we also have that $\xi_\pm \in D(\sigma_{i/4}(\Phi))$ and

$$\delta_-(\sigma_{i/4}(\Phi))\xi_\pm = j(s_\pm A)\sigma_{i/4}(\Phi)\xi_0 - (s_\pm A)j(\sigma_{i/4}(\Phi))\xi_0,$$
$$\delta_+(\sigma_{i/4}(\Phi))\xi_\pm = j(s_\pm A)\sigma_{i/4}(\Phi)\xi_0 + (s_\pm A)j(\sigma_{i/4}(\Phi))\xi_0. \tag{4.13}$$

The relations analogous to (4.12) and (4.13) for Φ_n hold. Thus, it follows from (3.9) and Lemma 4.2 that $\overline{\mathcal{E}}[\xi_{m,\pm} - \xi_{n,\pm}] \to 0$ as $m, n \to \infty$. Since $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$ is closed, $\xi_\pm \in D(\overline{\mathcal{E}})$. Next we will prove that $\mathcal{E}_n[\xi_\pm]$ converges to $\overline{\mathcal{E}}[\xi_\pm]$ as n tends to infinity. By (4.12), (4.13) and Lemma 4.2, we conclude that for any $\xi = A\xi_0$, there exists a positive real number M such that the bounds

$$\|\delta_-(\sigma_{-i/4}(\Phi_n))\xi_\pm\|+\|\delta_-(\sigma_{-i/4}(\Phi))\xi_\pm\|\leqslant M,$$
$$\|\delta_-(\sigma_{i/4}(\Phi_n))\xi_\pm\|+\|\delta_-(\sigma_{i/4}(\Phi))\xi_\pm\|\leqslant M, \tag{4.14}$$
$$\|\delta_+(\sigma_{i/4}(\Phi_n))\xi_\pm\|+\|\delta_+(\sigma_{i/4}(\Phi))\xi_\pm|\leqslant M$$

hold uniformly in $n\in\mathbb{N}$. It follows from (3.9), (4.9), (4.12), (4.13) and the above bounds that

$$\begin{aligned}|\mathcal{E}_n[\xi_\pm]-\overline{\mathcal{E}}[\xi_\pm]|&\leqslant 4\alpha M\|(\delta_-(\sigma_{-i/4}(\Phi_n))-\delta_-(\sigma_{-i/4}(\Phi)))\xi_\pm\|+2\alpha M\|(\delta_-(\sigma_{i/4}(\Phi_n))\\&\quad-\delta_-(\sigma_{i/4}(\Phi)))\xi_\pm\|+2\alpha M\|(\delta_+(\sigma_{i/4}(\Phi_n))-\delta_+(\sigma_{i/4}(\Phi)))\xi_\pm\|\\&\leqslant M'(\|\sigma_{-i/4}(\Phi_n)\xi_0-\sigma_{-i/4}(\Phi)\xi_0\|+\|\sigma_{i/4}(\Phi_n)\xi_0-\sigma_{i/4}(\Phi)\xi_0\|)\to 0\\&\quad\text{as}\quad n\to\infty,\end{aligned}$$

where $\alpha=\gamma\max\{(1+\alpha_2^2)/2,(\alpha_1^2+\alpha_3^2)/2,|\alpha_1|+|\alpha_2\alpha_3|\}$. This completes the proof of our assertion (4.11).

Recall the definition of $\mathcal{E}_n$ in (4.9). To show the Dirichlet property, $\mathcal{E}_n(\xi_+,\xi_-)$ in (4.9) can be written as

$$\mathcal{E}_n(\xi_+,\xi_-)=\mathcal{E}_n^{(1)}(\xi_+,\xi_-)+\mathcal{E}_n^{(2)}(\xi_+,\xi_-)=(I^{(1)}+II^{(1)})+(I^{(2)}+II^{(2)}), \tag{4.15}$$

where

$$\begin{aligned}\mathcal{E}_n^{(1)}(\xi_+,\xi_-)&=\frac{\gamma}{2}\langle\delta_-(\sigma_{-i/4}(P_n))^*\xi_+,\delta_-(\sigma_{-i/4}(P_n))\xi_-\rangle\\&\quad+\frac{\gamma}{2}\alpha_1^2\langle\delta_-(\sigma_{-i/4}(Q_n))^*\xi_+,\delta_-(\sigma_{-i/4}(Q_n))\xi_-\rangle\\&\quad-i\gamma\alpha_1\langle\delta_+(\sigma_{-i/4}(Q_n))^*\xi_+,\delta_-(\sigma_{-i/4}(P_n))\xi_-\rangle,\end{aligned}$$

$$\begin{aligned}\mathcal{E}_n^{(2)}(\xi_+,\xi_-)&=\frac{\gamma}{2}\alpha_2^2\langle\delta_-(\sigma_{-i/4}(P_n))^*\xi_+,\delta_-(\sigma_{-i/4}(P_n))\xi_-\rangle\\&\quad+\frac{\gamma}{2}\alpha_3^2\langle\delta_-(\sigma_{-i/4}(Q_n))^*\xi_+,\delta_-(\sigma_{-i/4}(Q_n))\xi_-\rangle\\&\quad-i\gamma\alpha_2\alpha_3\langle\delta_+(\sigma_{-i/4}(P_n))^*\xi_+,\delta_-(\sigma_{-i/4}(Q_n))\xi_-\rangle,\end{aligned}$$

and

$$\begin{aligned}I^{(1)}&=\frac{\gamma}{2}\langle\xi_+,\sigma_{-i/4}(P_n^2+\alpha_1^2Q_n^2)\xi_-\rangle+\frac{\gamma}{2}\langle\sigma_{-i/4}(P_n^2+\alpha_1^2Q_n^2)\xi_-,\xi_+\rangle-\gamma\langle\xi_+,\sigma_{-i/4}(i\alpha_1Q_nP_n)\xi_-\rangle\\&\quad-\gamma\langle(\sigma_{-i/4}(i\alpha_1Q_nP_n)\xi_-,\xi_+\rangle,\end{aligned}$$

$$\begin{aligned}I^{(2)}&=\frac{\gamma}{2}\langle\xi_+,\sigma_{-i/4}(\alpha_2^2P_n^2+\alpha_3^2Q_n^2)\xi_-\rangle+\frac{\gamma}{2}\langle\sigma_{-i/4}(\alpha_2^2P_n^2+\alpha_3^2Q_n^2)\xi_-,\xi_+\rangle\\&\quad-\gamma\langle\xi_+,\sigma_{-i/4}(i\alpha_2\alpha_3P_nQ_n)\xi_-\rangle-\gamma\langle j(\sigma_{-i/4}(i\alpha_2\alpha_3P_nQ_n))\xi_-,\xi_+\rangle,\\II^{(1)}&=-\gamma\langle\xi_+,\sigma_{-i/4}(P_n-i\alpha_1Q_n)j(\sigma_{-i/4}(P_n-i\alpha_1Q_n))\xi_-\rangle,\\II^{(2)}&=-\gamma\langle\xi_+,\sigma_{-i/4}(\alpha_2P_n+i\alpha_3Q_n)j(\sigma_{-i/4}(\alpha_2P_n+i\alpha_3Q_n))\xi_-\rangle.\end{aligned}$$

Here we have used the fact that $\langle \xi_+, j(A)\xi_- \rangle = \langle A\xi_-, \xi_+ \rangle$, $A \in \mathcal{M}$ in $I^{(1)}$, $I^{(2)}$. As a consequence of Theorem 4(7) of Ref. 19, $\mathcal{M}\xi_+ \perp \mathcal{M}\xi_-$, which implies $I^{(1)}=0$ and $I^{(2)}=0$. Since $Aj(A)\xi_- \in \mathcal{P}$ for $A \in \mathcal{M}$, we obtain that $II^{(1)} \leqslant 0$ and $II^{(2)} \leqslant 0$. Therefore $\mathcal{E}_n(\xi_+, \xi_-) \leqslant 0$.

We turn to the proof of the property (c). Since $|\xi| = \xi_+ + \xi_-$, the assertion (4.11) implies that

$$\xi \in \mathcal{M}_0\xi_0 \cap \mathcal{H}^J \Rightarrow |\xi| \in D(\overline{\mathcal{E}}) \quad \text{and} \quad \overline{\mathcal{E}}[|\xi|] = \lim_{n\to\infty} \mathcal{E}_n[|\xi|]. \tag{4.16}$$

Let $\xi \in D(\overline{\mathcal{E}}) \cap \mathcal{H}^J$ be given. Choose a sequence $\{\xi_m\}$ in $\mathcal{M}_0\xi_0 \cap \mathcal{H}^J$ such that $\xi_m \to \xi$ in $\mathcal{H}$ and $\overline{\mathcal{E}}[\xi_m] \to \overline{\mathcal{E}}[\xi]$ as $m \to \infty$. The inequality $\|\xi_\pm - \eta_\pm\| \leqslant \|\xi - \eta\|$, $\forall\, \xi,\ \eta \in \mathcal{H}^J$, implies $|\xi_m| \to |\xi|$ as $m \to \infty$. Notice that $\overline{\mathcal{E}}(\xi_+, \xi_-) \leqslant 0$ is equivalent to $\overline{\mathcal{E}}[|\xi|] \leqslant \overline{\mathcal{E}}[\xi]$, and we have shown that each $\mathcal{E}_n$, $n \in \mathbb{N}$, satisfies the property (c). By the lower semi-continuity of $\overline{\mathcal{E}}$ and (4.16), we obtain that

$$\overline{\mathcal{E}}[|\xi|] \leqslant \underline{\lim}_{m\to\infty} \overline{\mathcal{E}}[|\xi_m|] = \underline{\lim}_{m\to\infty} \left(\lim_{n\to\infty} \mathcal{E}_n[|\xi_m|] \right) \leqslant \underline{\lim}_{m\to\infty} \left(\lim_{n\to\infty} \mathcal{E}_n[\xi_m] \right) = \underline{\lim}_{m\to\infty} \mathcal{E}[\xi_m] = \overline{\mathcal{E}}[\xi].$$

Thus $|\xi| \in D(\overline{\mathcal{E}})$ and $\overline{\mathcal{E}}[|\xi|] \leqslant \overline{\mathcal{E}}[\xi]$. This completes the proof of the property (c).

Since $\overline{\mathcal{E}}(\xi, \xi_0) = 0$ for any $\xi \in D(\overline{\mathcal{E}})$, it follows from the properties (b) and (c) and Proposition 2.1 that $\overline{\mathcal{E}}$ is a Dirichlet form. □

V. SPECTRAL ANALYSIS OF DIRICHLET OPERATORS

In this section we decompose the Hilbert space $\mathcal{H} = \mathcal{H}_\omega$ into direct sum of eigenspaces of Dirichlet operator, and analyze the spectrum of generator (Dirichlet operator) of Markovian semigroup. We also show the ergodicity of its semigroup. The decomposition method we use is essentially the same as that in Ref. 20. See also Example 5.2.20 in Ref. 4.

We write that

$$\begin{aligned} D_1 &:= (2\sinh(\beta/2))^{-1/2}(e^{\beta/4}a - e^{-\beta/4}j(a^*)), \\ D_2 &:= (2\sinh(\beta/2))^{-1/2}(e^{-\beta/4}a^* - e^{\beta/4}j(a)). \end{aligned} \tag{5.1}$$

By Lemma 4.1 the operators D_1 and D_2 are well defined on $\mathcal{M}_0\xi_0$ and also on $\mathcal{H}_{fin}$. It follows from (5.1) that

$$\begin{aligned} D_1^* &= (2\sinh(\beta/2))^{-1/2}(e^{\beta/4}a^* - e^{-\beta/4}j(a)) = (2\sinh(\beta/2))^{1/2}e^{-\beta/4}a^* + e^{-\beta/2}D_2, \\ D_2^* &= -(2\sinh(\beta/2))^{1/2}e^{\beta/4}a + e^{\beta/2}D_1. \end{aligned} \tag{5.2}$$

Note that $j(a^*)\xi_0 = e^{\beta/2}a\xi_0$ and $j(a)\xi_0 = e^{-\beta/2}a^*\xi_0$. Thus $D_i\xi_0 = 0$, $i = 1,2$. A direct calculation shows that for $i, j = 1,2$, the following canonical commutation relations (CCRs),

$$\begin{aligned} &[D_i, D_j] = 0, \quad [D_i^*, D_j^*] = 0, \\ &[D_i, D_j^*] = \delta_{ij}\mathbf{1}, \end{aligned} \tag{5.3}$$

hold on $\mathcal{H}_{fin}$. By (5.1), (5.2) and (3.8), any $P^mQ^n\xi_0$, $m, n = 0,1,2,\ldots$, can be expressed as a finite linear combination of the vectors of the form

$$(D_1^*)^p(D_2^*)^q\xi_0,\ p,q = 0,1,2,\ldots.$$

Thus, as a consequence of (5.2) and the CCRs in (5.3), $\mathcal{H}_{fin}$ is spanned by the vectors of the above form, and also the following decomposition holds,

$$\mathcal{H} = \bigoplus_{m,n=0}^{\infty} \mathcal{H}^{(m,n)},$$

where $\mathcal{H}^{(m,n)}$ is the closure of subspace spanned by the vectors of the type $(D_1^*)^m(D_2^*)^n\xi_0$, $m, n=0,1,2,\ldots$. See also Sec. V of Ref. 14.

To analyze the spectrum of generator H, we introduce the new operators and decomposition of $\mathcal{H}$. Define

$$A_1 := 2^{-1/2}(D_1 - D_2), \quad A_2 := 2^{-1/2}(D_1 + D_2). \tag{5.4}$$

We first collect some properties of A_i, $i=1,2$, which are similar to (5.3).

Proposition 5.1: (*a*) $A_i\xi_0 = 0$ *for* $i=1,2$.

(*b*) *As operators defined on* $\mathcal{H}_{fin}$, *we have the following CCRs: for* $i, j=1,2$,

$$\begin{gathered}[A_i, A_j] = 0, \quad [A_i^*, A_j^*] = 0, \\ [A_i, A_j^*] = \delta_{ij}\mathbf{1}.\end{gathered} \tag{5.5}$$

Proof: (a) The result follows from $D_i\xi_0 = 0$, $i=1,2$, and (5.4). (b) This follows from (5.4) and the CCRs in (5.3). □

We are ready to get another decomposition of the Hilbert space $\mathcal{H}=\mathcal{H}_\omega$, called quasi-free Hilbert space. According to the CCRs in Proposition 5.1, A_i and A_i^*, $i=1,2$, can be thought of as annihilation and creation operators, respectively. The following decomposition of $\mathcal{H}$ will be used to analyze the spectrum of generator H.

Theorem 5.1: *The following decomposition holds*:

$$\mathcal{H} = \bigoplus_{m,n=0}^{\infty} \mathcal{H}_{(m,n)}, \tag{5.6}$$

where $\mathcal{H}_{(m,n)}$ *is the closure of subspace spanned by the vectors of the type* $(A_1^*)^m(A_2^*)^n\xi_0$, $m, n=0,1,2,\ldots$.

Proof: Note that

$$D_1 = 2^{-1/2}(A_1 + A_2), \quad D_2 = -2^{-1/2}(A_1 - A_2).$$

Thus any $(D_1^*)^m(D_2^*)^n\xi_0$, $m,n=0,1,2,\ldots$, can be expressed as a finite linear combination of the vectors of the form

$$(A_1^*)^p(A_2^*)^q\xi_0, \quad p,q=0,1,2,\ldots.$$

Since $\mathcal{H}_{fin}$ is dense in $\mathcal{H}$, we conclude that the set of finite linear combinations of the vectors of the above forms is dense in $\mathcal{H}$. The decomposition follows from the CCRs in Proposition 5.1. □

Let l^2 be the space of sequences $\{z_n\}_{n=0}^{\infty}$ of complex numbers satisfying $\Sigma_{n=0}^{\infty}|z_n|^2<\infty$ and $\{e_n\}_{n=0}^{\infty}$ be the standard orthonormal basis in l^2. Denote by N, a_1 and a_1^* the number, annihilation and creation operator on l^2 as follows. The number operator N is the self-adjoint multiplication operator, $Ne_n = ne_n$, with maximal domain $D(N)=\{\{z_n\}\in l^2 \mid \Sigma_{n=0}^{\infty}|nz_n|^2<\infty\}$. a_1 and a_1^* are given by

$$a_1e_0 = 0, \quad a_1e_n = n^{1/2}e_{n-1}, \quad n=1,2,\ldots,$$

$$a_1^*e_n = (n+1)^{1/2}e_{n+1}, \quad n=0,1,2,\ldots.$$

The operators a_1 and a_1^* are closed and mutually adjoint, $a_1^*a_1 = N$ and $a_1a_1^* = N+\mathbf{1}$.

Proposition 5.2: Let U *be the operator defined by*

$$U:\mathcal{H}\to l^2\otimes l^2, \quad (A_1^*)^m(A_2^*)^n\xi_0 \mapsto (a_1^*)^m e_0 \otimes (a_1^*)^n e_0,$$

for $m,n=0,1,2,\ldots$. *Then* U *is unitary.*

Proof: Since A_i, A_i^*, $i=1,2$ and a_1, a_1^* satisfy the same commutation relation, the unitarity of U is easily checked. □

By (3.8), (4.10) and (5.1) we get that

$$\begin{aligned}\delta_-(\sigma_{-i/4}(P)) &= \sigma_{-i/4}(P) - j(\sigma_{-i/4}(P)) = -i2^{-1/2}\{(e^{\beta/4}a - e^{-\beta/4}a^*) + (e^{\beta/4}j(a) - e^{-\beta/4}j(a^*))\} \\ &= -i2^{-1/2}(2\sinh(\beta/2))^{1/2}(D_1 - D_2) \\ &= -i(2\sinh(\beta/2))^{1/2}A_1. \end{aligned} \tag{5.7}$$

The argument used above yields

$$\delta_-(\sigma_{-i/4}(Q)) = 2^{-1/2}(2\sinh(\beta/2))^{1/2}(D_1 + D_2) = (2\sinh(\beta/2))^{1/2}A_2. \tag{5.8}$$

Define the operator $\tilde{H}$ on $\mathcal{H}_{fin}$ by

$$\begin{aligned}\tilde{H} &= \gamma_1 \delta_-(\sigma_{-i/4}(P))^* \delta_-(\sigma_{-i/4}(P)) + \gamma_2 \delta_-(\sigma_{-i/4}(Q))^* \delta_-(\sigma_{-i/4}(Q)) \\ &= \tau_1 A_1^* A_1 + \tau_2 A_2^* A_2 \equiv \tau_1 H_1 + \tau_2 H_2, \end{aligned} \tag{5.9}$$

where $\tau_1 = 2\gamma_1 \sinh(\beta/2)$, $\tau_2 = 2\gamma_2 \sinh(\beta/2)$. It follows from Proposition 5.1 that

$$\tilde{H}(A_1^*)^m (A_2^*)^n \xi_0 = (m\tau_1 + n\tau_2)(A_1^*)^m (A_2^*)^n \xi_0, \ m,n = 0,1,2,\ldots. \tag{5.10}$$

Proposition 5.3: (*a*) $\mathcal{H}_{fin} \subset D(\overline{\mathcal{E}})$.
(*b*) *For* $\xi \in \mathcal{H}_{fin}$ *the equality*

$$\overline{\mathcal{E}}[\xi] = \gamma_1 \| \delta_-(\sigma_{-i/4}(P))\xi \|^2 + \gamma_2 \| \delta_-(\sigma_{-i/4}(Q))\xi \|^2 = \frac{\tau_1}{2}\|(D_1 - D_2)\xi\|^2 + \frac{\tau_2}{2}\|(D_1 + D_2)\xi\|^2 \tag{5.11}$$

holds.

(*c*) *For* $\eta, \xi \in \mathcal{H}_{fin}$ *the equality*

$$\overline{\mathcal{E}}(\eta, \xi) = \langle \eta, \tilde{H}\xi \rangle$$

holds.

Proof: (a) By the method similar to that used in the proof of Lemma 4.1(b), we get that $W(z)\xi_0 \in D(a^\sharp)$, $z \in \mathbb{C}$, and so $W(z)\xi_0$ belongs to the domain of D_i, $i=1,2$. Denote by $\mathcal{W}$ the algebra generated by $W(z), z \in \mathbb{C}$. Clearly $\mathcal{W}\xi_0$ is dense in $\mathcal{H}$. Using CCRs, one can check that the relations for $z \in \mathbb{C}$,

$$\begin{aligned}[a, W(z)] &= i2^{-1/2} z W(z), \\ [a^*, W(z)] &= -i2^{-1/2}\overline{z} W(z), \end{aligned} \tag{5.12}$$

hold on $\mathcal{W}\xi_0$. Recall the definition of $W_n(z) := (W(z))_n$, $n \in \mathbb{N}$, $z \in \mathbb{C}$ in (3.5). It can be easily checked that for $z \in \mathbb{C}$

$$\overline{\mathcal{E}}[W_n(z)\xi_0 - W(z)\xi_0] \to 0 \quad \text{as} \quad n \to \infty.$$

See also the proof of Lemma 5.3 of Ref. 14. Since $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$ is closed, $W(z)\xi_0 \in D(\overline{\mathcal{E}})$ for any $z \in \mathbb{C}$.

For each $l = 1, \ldots, m$, $m \in \mathbb{N}$, let z_l be either 1 or i. Recall the definition of $\Phi(z,n)$ in (4.1) for $z = 1, i$ and $n \in \mathbb{N}$. We will use the following abbreviated notations:

$$\Phi_l(n) := \Phi(z_l, n), \quad l = 1, \ldots, m,$$

$$\Phi_l := \Phi(z_l), \quad l = 1, \ldots, m, \tag{5.13}$$

$$\xi(n) := \left(\prod_{l=1}^{m} \Phi_l(n) \right) \xi_0 \quad \text{and} \quad \xi := \left(\prod_{l=1}^{m} \Phi_l \right) \xi_0 .$$

Using the relations in (5.12) and (5.1), we obtain that the relations

$$[D_1, \Phi_l(n)] = (2(1 - e^{-\beta}))^{-1/2} z_l W\left(\frac{1}{n} z_l \right),$$

$$[D_1, \Phi_l] = (2(1 - e^{-\beta}))^{-1/2} z_l \tag{5.14}$$

hold on $\mathcal{W}\xi_0$. Notice that $\xi(n) \in D(\overline{\mathcal{E}})$, $n \in \mathbb{N}$ and $\xi \in \mathcal{H}_{fin}$. It is not hard to show that $\xi(n) \to \xi$ as $n \to \infty$. See the method used below. We will show that $\overline{\mathcal{E}}[\xi(n) - \xi] \to 0$ as $n \to \infty$. Since $\overline{\mathcal{E}}$ is closed, this implies that $\mathcal{H}_{fin} \subset D(\overline{\mathcal{E}})$ and

$$\overline{\mathcal{E}}[\xi] = \lim_{n \to \infty} \overline{\mathcal{E}}[\xi(n)]. \tag{5.15}$$

Let ξ and $\xi(n)$, $n \in \mathbb{N}$, be defined as in (5.13). Notice that

$$\xi(n) - \xi = \sum_{p=1}^{m} \left(\prod_{l=1}^{p-1} \Phi_l(n) \right) (\Phi_p(n) - \Phi_p) \left(\prod_{l=p+1}^{m} \Phi_l \right) \xi_0 .$$

We use the Schwarz inequality twice to obtain that

$$\| D_1(\xi(n) - \xi) \|^2 \leq m \sum_{p=1}^{m} \left\| D_1 \left(\prod_{l=1}^{p-1} \Phi_l(n) \right) (\Phi_p(n) - \Phi_p) \left(\prod_{l=p+1}^{m} \Phi_l \right) \xi_0 \right\|^2 . \tag{5.16}$$

It follows from (5.14) and the definition of D_1 that

$$D_1 \left(\prod_{l=1}^{p-1} \Phi_l(n) \right) (\Phi_p(n) - \Phi_p) \left(\prod_{l=p+1}^{m} \Phi_l \right) \xi_0 = (2(1 - e^{-\beta}))^{-1/2} \sum_{q=1}^{m} z_q \Psi(p, q; n), \tag{5.17}$$

where

$$\Psi(p, q; n) := \left(\prod_{l=1}^{q-1} \Phi_l(n) \right) W\left(\frac{1}{n} z_q \right) \left(\prod_{l=q+1}^{p-1} \Phi_l(n) \right) (\Phi_p(n) - \Phi_p) \left(\prod_{l=p+1}^{m} \Phi_l \right) \xi_0, \quad 1 \leq q \leq p-1,$$

$$\Psi(p, q; n) := \left(\prod_{l=1}^{p-1} \Phi_l(n) \right) \left(W\left(\frac{1}{n} z_p \right) - \mathbf{1} \right) \left(\prod_{l=p+1}^{m} \Phi_l \right) \xi_0, \quad q = p,$$

$$\Psi(p, q; n) := \left(\prod_{l=1}^{p-1} \Phi_l(n) \right) (\Phi_p(n) - \Phi_p) \left(\prod_{l=p+1}^{q-1} \Phi_l(n) \right) \left(\prod_{l=q+1}^{m} \Phi_l \right) \xi_0, \quad p+1 \leq q \leq m.$$

We use the Schwarz inequality twice again to (5.17) and substitute the result into (5.16) to conclude that

$$\| D_1(\xi(n) - \xi) \|^2 \leq \frac{1}{2} m^2 (1 - e^{-\beta})^{-1} \sum_{p=1}^{m} \sum_{q=1}^{m} \| \Psi(p, q; n) \|^2 .$$

One notes that each $\Psi(p,q;n)$ contains either $(\Phi_p(n)-\Phi_p)$ or else $(W((1/n)z_p)-\mathbf{1})$, which implies that

$$\|\Psi(p,q;n)\|^2\to 0 \quad \text{as} \quad n\to\infty$$

for any p, q, and so

$$\|D_1(\xi(n)-\xi)\|^2\to 0 \quad \text{as} \quad n\to\infty.$$

The method similar to that used in the above implies that

$$\|D_2(\xi(n)-\xi)\|^2\to 0 \quad \text{as} \quad n\to\infty.$$

By (5.7), (5.8) and (3.11), this proved part (a) of this proposition.

(b) This follows from Theorem 5.1, (3.11) and (5.9).

(c) This follows from (5.4) and part (b) of the proposition. □

Theorem 5.2: (*a*) *The operators* $\tilde{H}$ *and* H_i, $i=1,2$, *are essential self-adjoint and the self-adjoint extension of* $\tilde{H}$ *equals to the Dirichlet operator H given in Theorem 3.1.*

(*b*) *For each* m, $n=0,1,2,\ldots$, $\mathcal{H}_{(m,n)}$ *is an eigenspace of the Dirichlet operator H corresponding to eigenvalue* $\tau_1 m+\tau_2 n$.

Proof: (a) Clearly $\tilde{H}$ and H_i, $i=1,2$, are symmetric on $\mathcal{H}_{fin}$. It follows from (5.5) that the following relations holds: for $\xi=(A_1^*)^m(A_2^*)^n\xi_0$, $m,n=0,1,2,\ldots$,

$$H_1\xi=m\xi, \quad H_2\xi=n\xi. \tag{5.18}$$

By (5.18) any $\xi\in\mathcal{H}_{fin}$ is an analytic vector for $\tilde{H}$ and H_i, $i=1,2$, and $\tilde{H}\mathcal{H}_{fin}\subset\mathcal{H}_{fin}$, $H_i\mathcal{H}_{fin}\subset\mathcal{H}_{fin}$, $i=1,2$. It follows from Corollary 2 of Theorem X.39 in Ref. 21 that $\tilde{H}$ and H_i, $i=1,2$, are essentially self-adjoint on $\mathcal{H}_{fin}$. By Proposition 5.3 (c), $H=\tilde{H}$ on $\mathcal{H}_{fin}$, which implies $H=\tilde{H}$.

(b) By Proposition 5.2 and (5.18), we have that

$$UHU^{-1}=\tau_1 N\otimes\mathbf{1}+\mathbf{1}\otimes\tau_2 N,$$

where N is the number operator on l^2. Thus this completes the proof of (b). □

Finally we are able to produce the proof of Theorem 3.2.

Proof of Theorem 3.2: (a) and (b) follow from Theorem 5.2.

(c) By (b), zero is a simple eigenvalue of H with eigenvector ξ_0. Since ξ_0 is a strictly positive vector, $\{T_t\}_{t\geq 0}$ is ergodic. The proof of Theorem 3.2 is completed. □

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Existence of mesons and mass splitting in strong coupling lattice quantum chromodynamics

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We consider one flavor lattice quantum chromodynamics in the imaginary time functional integral formulation for space dimensions $d=2,3$ with 4×4 Dirac spin matrices, small hopping parameter κ, $0<\kappa\ll1$, and zero plaquette coupling. We determine the energy-momentum spectrum associated with four-component gauge invariant local meson fields which are composites of a quark and an antiquark field. For the associated correlation functions, we establish a Feynman–Kac formula and a spectral representation. Using this representation, we show that the mass spectrum consists of two distinct masses m_a and m_b, given by $m_c=-2\ln\kappa+r_c(\kappa)$, $c=a,b$, where r_c is real analytic. For $d=2$, m_a and m_b have multiplicity two and the mass splitting is $\kappa^4+\mathcal{O}(\kappa^6)$; for $d=3$, one mass has multiplicity one and the other three, with mass splitting $2\kappa^4+\mathcal{O}(\kappa^6)$. In the subspace of the Hilbert space generated by an even number of fermion fields the dispersion curves are isolated (upper gap property) up to near the two-meson threshold of asymptotic mass $-4\ln\kappa$. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1636000]

I. INTRODUCTION

It is fundamental to determine the existence of particles and their spectral properties of quantum field theory. In quantum chromodynamics (QCD), one needs to establish on a rigorous basis the energy-momentum (EM) spectrum of particles and their bound states, in particular, to prove the existence of mesons and baryons and their bound states. These types of spectral properties involve low energies and one way to study them is by using a lattice regularization of the continuum, and to consider the strong coupling regime. Strong coupling lattice QCD models give a good insight into the low-energy behavior of QCD. Indeed, our partial understanding of confinement up to now comes in this way, and in fact was one reason for the introduction of lattice QCD (see Refs. 1–3 for a reference book and Refs. 4 and 5 for recent reviews).

Basically, there have been two routes used in the rigorous studies of the particle spectrum in lattice theories. One is based on methods which are reminiscent of continuum field theories (e.g., decoupling of hyperplanes, Euclidean subtraction)[6–11] and the others are based on statistical mechanical methods (e.g., random surfaces).[12,13] Here, we take the former approach.

As our main result, we prove the existence of meson particles by showing that mesons arise as tightly bound, bound states of a gauge invariant state composed of one quark and one antiquark. The occurrence of mesons is manifested by an isolated dispersion curve in the EM spectrum. The same kind of spectral problems that we consider here were also treated in previous works, for other types of particles. For the pure gauge case, with small coupling g_0^{-2}, the low-lying glueball spectrum is found in Ref. 8. The corresponding glueball mass is $\approx 8\ln g_0$. The determination of the masses in the baryonic sector was considered in Refs. 14 and 15. Recently, a rigorous treat-

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ment allowed to prove the existence of baryons and their multiplicities for a one-flavor lattice QCD model in the infinitely strong coupling regime and for small enough hopping parameter $\kappa > 0$, $0 < g_0^{-2} \ll \kappa \ll 1$. In Ref. 16, this was done for space dimension $d = 2$, using 2×2 Pauli spin matrices, and in Ref. 17 for $d = 2,3$ employing 4×4 Dirac spin matrices. The two-baryon bound state spectrum within the context of Ref. 16 was analyzed more recently in Ref. 18.

Here, we work with the same lattice QCD model as in Ref. 17, but our analysis is restricted to the meson sector of the underlying physical Hilbert space $\mathcal{H}$. The method used in Ref. 17 for baryons is largely applied here, with some adaptations. No approximations are made so our results are exact within this context. We will assume the results of Ref. 17 regarding positivity and the construction of $\mathcal{H}$. We begin directly by introducing a local four-component meson field. For the associated correlation functions (CF's), we establish a Feynman–Kac formula and a spectral representation analogous to the Källen–Lehman representation in quantum field theory. We emphasize that it is this representation that allows us to identify complex momentum space singularities of the two-point function with points in the EM spectrum. To our knowledge, such a representation as given here is not found in the literature. We also point out that determining exponential decay rates of CF's, as in Ref. 13, is *not sufficient* to identify these rates with the mass spectrum, since a connection with the energy-momentum spectrum is not established. This is especially true in the case where there are multiplicities involved and mass splitting, as here.

Let $\mathcal{H}_e \subset \mathcal{H}$ denote the subspace generated by an even number of fermions. We show that there are meson particles, with asymptotic masses $-2 \ln \kappa$, manifested by isolated dispersions curves in the EM spectrum (upper mass gap property) and it is the *only* spectrum in the subspace $\mathcal{H}_e \subset \mathcal{H}$, up to near the two-meson threshold which is asymptotically of order $-4 \ln \kappa$.

Besides its intrinsic importance, the determination and control of the meson spectrum is an essential step towards the understanding of, e.g., meson–meson and meson–baryon bound states from first principles. Indeed, a two-meson bound state analysis is in progress,[25] using, e.g., our techniques from previous works (see Refs. 10, 11, and 18). Also, our results open the way to study the EM spectrum for the more realistic case when the glueball mass is large, but is such that $g_0^{-2} \ll 1$ cannot be neglected in comparison with the small hopping parameter $\kappa \ll 1$.

II. THE RESULTS

We first give a very brief definition of one flavor SU(3) gauge-matter QCD model of Ref. 17 and present our results. We use the same notation as in Ref. 17, and the reader is referred there for all details concerning notation, the definition of the model, the introduction of energy, and momentum operators, the derivation of a Feynman–Kac-type formula for general correlation functions, the construction of the underlying physical Hilbert space $\mathcal{H}$, the computation of gauge and Fermi (Grassmann) integrals, and the analysis of symmetries other than gauge that is the main result of its Theorem 4, namely, the symmetries of charge conjugation, parity, lattice coordinate reflections, and lattice spatial rotations. We omit these and other details here, for the sake of brevity.

We consider the case where the space dimension is $d = 2,3$ and the gauge group is SU(3). The partition function of the model is given formally by

$$Z = \int e^{-S(\psi, \overline{\psi}, g)} \, \mathrm{d}\psi \, \mathrm{d}\overline{\psi} \, \mathrm{d}\mu(g), \tag{2.1}$$

and for a function $F(\overline{\psi}, \psi, g)$, of the single flavor (anti)quark Grassmann fields ψ and $\overline{\psi}$, and the gauge field g, the normalized expectations, in the thermodynamic limit, are denoted by

$$\langle F(\overline{\psi}, \psi, g) \rangle \equiv \frac{1}{Z} \int F(\overline{\psi}, \psi, g) e^{-S(\psi, \overline{\psi}, g)} \, \mathrm{d}\psi \, \mathrm{d}\overline{\psi} \, \mathrm{d}\mu(g).$$

The gauge invariant action $S(\psi, \overline{\psi}, g)$ is given by

$$S(\psi,\overline{\psi},g)=\frac{\kappa}{2}\sum\ \overline{\psi}_{a\alpha}(u)\,\Gamma^{\epsilon e^{\rho}}_{\alpha\beta}(g_{u,u+\epsilon e^{\rho}})_{ab}\,\psi_{b\beta}(u+\epsilon e^{\rho})$$

$$+\sum_{u\in\mathbb{Z}_o^{d+1}}\overline{\psi}_{a\alpha}(u)M_{\alpha\beta}\psi_{a\beta}(u)-\frac{1}{g_0^2}\sum_p\ \chi(g_p), \tag{2.2}$$

where the first sum runs over $u=(u^0,\vec{u})=(u^0,u^1,\ldots,u^d)\in\mathbb{Z}_o^{d+1}\equiv\mathbb{Z}_{1/2}\times\mathbb{Z}^d$, where $\mathbb{Z}_{1/2}=\{\pm 1/2, \pm 3/2,\ldots\}$, $\epsilon=\pm 1$, $\rho=0,1,\ldots,d$, and over repeated indices. For notational simplicity, we sometimes drop U from the gauge matrix $U(g)$ associated with each oriented lattice bond. Concerning the parameters, we take $m>0$, $0<g_0^{-2}\ll\kappa\ll 1$ and $M\equiv M(m,\kappa)=(m+2\kappa)I_4$, I_4 being the 4×4 identity matrix. Also, within the family of actions of Ref. 2, we have $\Gamma^{\pm e^{\rho}}=-1\pm\gamma^{\rho}$. For $d=3$, γ^{ρ} are the 4×4 Hermitian traceless anticommuting Dirac matrices. For $d=2$, all but the γ^3 matrix appear in the action. The measure $\mathrm{d}\mu(g)$ is the product measure over non-oriented bonds of normalized SU(3) Haar measures (see Ref. 19) and the integrals over Grassmann fields are defined according to Ref. 20. In Eq. (2.1), $\mathrm{d}\psi\,\mathrm{d}\overline{\psi}$ means $\Pi_{u,a,\alpha}\,\mathrm{d}\psi_{a\alpha}(u)\,\mathrm{d}\overline{\psi}_{a\alpha}(u)$ such that, with a normalization $\mathcal{N}=\langle 1\rangle$, we have

$$\langle\psi_{a\alpha}(x)\,\overline{\psi}_{b\beta}(y)\rangle=(1/\mathcal{N})\ \int\ \psi_{a\alpha}(x)\,\overline{\psi}_{b\beta}(y)\,e^{-\Sigma_u\overline{\psi}_{a'\alpha'}(u)M_{\alpha'\beta'}\psi_{a'\beta'}(u)}\,\mathrm{d}\psi\,\mathrm{d}\overline{\psi}$$

$$=M^{-1}_{\alpha\beta}\delta_{ab}\delta(x,y),$$

with a Kronecker delta for space–time coordinates. With our restrictions on the parameters, there is a quantum mechanical Hilbert space $\mathcal{H}$ of physical states, for $\kappa>0$; and the condition $m>0$ guarantees that the one-particle free Fermion dispersion curve increases in each positive momentum component. Last, without loss of generality, we set $M=I_4$ in (2.2).

We note that by polymer expansion methods (see Refs. 2, 9, 21), CF's exist and are lattice translational invariant in the thermodynamic limit and truncated correlations have exponential tree decay. Furthermore, the CF's extend to analytic functions in the coupling parameters κ and g_0^{-2}.

To state our results on the existence of meson particles, their masses and dispersion curves, we consider the subspace $\mathcal{H}_m\subset\mathcal{H}$ generated by vectors associated with the gauge invariant meson fields composed of a fermion (quark) and an antifermion (antiquark) given by

$$\mu_{\alpha}(u)=\begin{cases}\dfrac{1}{\sqrt{6}}(\psi_{a3}(u)\overline{\psi}_{a1}(u)+\psi_{a4}(u)\overline{\psi}_{a2}(u)), & \alpha=1,\\[2ex] \dfrac{1}{\sqrt{3}}\psi_{a4}(u)\overline{\psi}_{a1}(u), & \alpha=2,\\[2ex] \dfrac{1}{\sqrt{3}}\psi_{a3}(u)\overline{\psi}_{a2}(u), & \alpha=3,\\[2ex] \dfrac{1}{\sqrt{6}}(\psi_{a3}(u)\overline{\psi}_{a1}(u)-\psi_{a4}(u)\overline{\psi}_{a2}(u)), & \alpha=4\,;\end{cases} \tag{2.3}$$

$$\pi_\beta(v)=\begin{cases}\dfrac{1}{\sqrt{6}}(\overline{\psi}_{a3}(v)\psi_{a1}(v)+\overline{\psi}_{a4}(v)\psi_{a2}(v)), & \beta=1,\\ \dfrac{1}{\sqrt{3}}\overline{\psi}_{a4}(v)\psi_{a1}(v), & \beta=2,\\ \dfrac{1}{\sqrt{3}}\overline{\psi}_{a3}(v)\psi_{a2}(v), & \beta=3,\\ \dfrac{1}{\sqrt{6}}(\overline{\psi}_{a3}(v)\psi_{a1}(v)-\overline{\psi}_{a4}(v)\psi_{a2}(v)), & \beta=4\,.\end{cases} \tag{2.4}$$

The normalization is chosen so that the associated matrix-valued two-point CF (see below), at coincident points and zero hopping parameter κ, equals I_4.

To see the connection with the EM spectrum, we define a two-point CF, establish a Feynman–Kac (FK) formula, and a spectral representation. The normalized two-point CF is defined by (χ here denotes the characteristic function)

$$\begin{aligned}G_{\alpha\beta}(u,v)&=\langle\mu_\alpha(u)\pi_\beta(v)\rangle_T\,\chi_{u^0\leqslant v^0}+\langle\pi_\alpha(u)\mu_\beta(v)\rangle_T^*\,\chi_{u^0>v^0}\\&=\langle\mu_\alpha(u)\pi_\beta(v)\rangle\,\chi_{u^0\leqslant v^0}+\langle\pi_\alpha(u)\mu_\beta(v)\rangle^*\,\chi_{u^0>v^0}\\&=G_{\alpha\beta}(u-v),\end{aligned}$$

where the truncation $\langle\ \rangle_T$ is given by

$$\langle F(u)H(v)\rangle_T=\langle F(u)H(v)\rangle-\langle F(u)\rangle\langle H(v)\rangle\,, \tag{2.5}$$

and we used that the truncation for $G_{\alpha\beta}$ is zero, by parity symmetry.

This seemingly awkward definition has three desirable features. First, the extension to equal times of the $u^0>v^0$ definition agrees with the one for $u^0\leqslant v^0$, by translational invariance and time reversal. Second, its Fourier transform admits a simple spectral representation. Third, it permits us to show the existence of particles, such as the upper mass gap property.

We set $\mathcal{E}(\lambda^0,\vec{\lambda})=\mathcal{E}_0(\lambda^0)\mathcal{E}(\vec{\lambda})$, where $\mathcal{E}_0(\lambda^0)$ is the spectral family for the time translation operator T_0, and $\mathcal{E}(\vec{\lambda})=\Pi_{i=1}^d\mathcal{E}_i(\lambda^i)$ is the product of the spectral families for the ith component self-adjoint momentum operator P^i which generates lattice space translations along the ith direction e^i, $i=1,\ldots,d$. The spectral representation of the next proposition is an important tool. Its proof is omitted here since it follows closely the one for baryons given in Ref. 17.

Proposition 2.1: For $u^0\neq v^0$, $\pi_\alpha\equiv\pi_\alpha(1/2,\vec{0})$, the following FK formula holds for the two-point meson CF [and the right-hand-side is an even function of $\vec{v}-\vec{u}$]:

$$G_{\alpha\beta}(u,v)=\int_{-1}^{1}\int_{\mathbf{T}^d}(\lambda^0)^{|v^0-u^0|-1}e^{i\vec{\lambda}.(\vec{v}-\vec{u})}\mathrm{d}(\pi_\alpha,\mathcal{E}(\lambda^0,\vec{\lambda})\pi_\beta)_{\mathcal{H}}\,. \tag{2.6}$$

We now obtain a spectral representation for the Fourier transform of the two-point function $G_{\alpha\beta}(u,v)$. For $x\in\mathbb{Z}^{d+1}$, with an abuse of notation, we define $G_{\alpha\beta}(x=u-v)\equiv G_{\alpha\beta}(u,v)$. Then, the Fourier transform $\tilde{G}_{\alpha\beta}(p)=\Sigma_{x\in\mathbb{Z}^{d+1}}G_{\alpha\beta}(x)e^{-ipx}$, $p\in\mathbf{T}^{d+1}$, admits the spectral representation

$$\widetilde{G}_{\alpha\beta}(p) = \widetilde{G}_{\alpha\beta}(\vec{p}) + (2\pi)^d \int_{-1}^{1} \int_{\mathbf{T}^d} \delta(\vec{p}-\vec{\lambda}) \frac{2(\cos p^0 - \lambda^0)}{1+(\lambda^0)^2 - 2\lambda^0 \cos p^0} \times \mathrm{d}_{\lambda^0}\mathrm{d}_{\vec{\lambda}}(\pi_\alpha(1/2,\vec{0}), \mathcal{E}_0(\lambda^0)\mathcal{E}(\vec{\lambda})\pi_\beta(1/2,\vec{0}))_{\mathcal{H}}, \tag{2.7}$$

where $\widetilde{G}(\vec{p}) = \Sigma_{\vec{x}\in\mathbb{Z}^d} e^{-i\vec{p}.\vec{x}} G(x^0=0,\vec{x})$. From the above spectral representation, we see that points of nonanalyticity in p^0, on the imaginary axis, are points in the EM spectrum. It is possible that points of nonanalyticity of the form $p^0 = \pm\pi + iq^0$ can occur but this is shown not to be the case in our analysis. We determine the spectrum and show the existence of isolated dispersion curves, up to near the threshold $-4\ln\kappa$, by showing that $\Gamma_{\alpha\beta}(u,v)$, the convolution inverse of the two-point function $G_{\alpha\beta}(u,v)$, decays faster than $G_{\alpha\beta}(u,v)$, and hence the Fourier transform $\widetilde{\Gamma}_{\alpha\beta}(p)$ of $\Gamma_{\alpha\beta}(x=u-v)=\Gamma_{\underline{\alpha}\beta}(u,v)$ has a larger region of analyticity in p^0. Thus, as $\widetilde{G}(p)\widetilde{\Gamma}(p)=I_4$, $\widetilde{\Gamma}^{-1}_{\alpha\beta}(p)=[\mathrm{cof}\,\widetilde{\Gamma}]_{\beta\alpha}(p)/\det[\widetilde{\Gamma}(p)]$ provides a meromorphic extension of $\widetilde{G}_{\alpha\beta}(p)$, and the EM spectrum occurs, for each $\vec{p}$, as points given by the p^0 imaginary axis zeroes of $\det[\widetilde{\Gamma}(p)]$.

The reader may wonder, e.g., for space dimension $d=3$, why composite fields of the form $\overline{\psi}(u)\gamma^5\psi(u)$ and, for $k=1,2,3$, $\overline{\psi}(u)\gamma^k\psi(u)$, $\gamma^5=\gamma^0\gamma^1\gamma^2\gamma^3$, are not employed to form the two-point CF matrix rather than those of Eqs. (2.3) and (2.4). Intuitively, these are the vector and the pseudoscalar meson fields. The reason is that, with our choices, it turns out that the zero spatial momentum matrix $\widetilde{G}_{\alpha\beta}(p^0,\vec{p}=\vec{0})$ is already diagonal (see Sec. IV, Lemma 4.1), so that the masses m_α are determined as the solutions of $\widetilde{\Gamma}_{\alpha\alpha}(p^0=im_\alpha,\vec{p}=\vec{0})=0$, $\alpha=1,2,3,4$.

The zero space momentum improper states we obtain can be classified using the irreducible discrete Z_4 rotation group generated by $\pi/2$ rotations in the x^1x^2 plane and the group Z_2 generated by x^3-coordinate reflections. Using the results of Theorem 4 of Ref. 17, about symmetries, we find that, for $\pi_i' \equiv \Sigma_{\vec{x}\in\mathbb{Z}^{d-1}} \pi_i(1/2,\vec{x})$, the improper zero momentum states π_i', $i=1,2,3,4$, satisfy the following: π_1' and π_4' form a basis for the trivial representation of Z_4, while π_2' (π_3') is a basis for the representation of Z_4 generated by i ($-i$) times the identity; $\pi_1'+\pi_4'$ ($\pi_1'-\pi_4'$) forms a basis for the trivial (nontrivial) representation of Z_2; and π_2' and π_3' form a basis for the trivial representation of Z_2. The commuting groups Z_4 and Z_2 are of course subgroups of the full lattice rotation and reflection group. We note that all the states have parity (-1), so that parity does not distinguish among them.

To analyze $\det\widetilde{\Gamma}(p)$, it suffices to obtain a long range bound for $\Gamma(x)$, but we need its precise short distance behavior, for $|x|\leqslant 2$ to determine the masses and the mass splitting up to and including the order κ^4. However, to control the error, bounds on $\Gamma(x)$ (which improve those obtained by the hyperplane decoupling method) are needed for some x's, with $|x^0|\leqslant 3$. These bounds are obtained by exhibiting cancellations in the Neumann series.

The two-point function convolution inverse $\Gamma(x)$ is defined by the Neumann series $\Gamma = \Sigma_{i=0}^{\infty}(-1)^i[G_d^{-1}G_n]^i G_d^{-1}$, where G_d is the diagonal part of G,

$$G_{d,\alpha\beta}(u,v) = G_{\alpha\alpha}(u,u)\delta_{\alpha\beta}\delta(u,v) \tag{2.8}$$

and G_n is the remainder $G_{n,\alpha\beta}(u,v)=G_{\alpha\beta}(u,v)-G_{d,\alpha\beta}(u,v)$. By the bounds in Theorems 2.1 and 2.2 below, G, G_d, G_n, and Γ are bounded as matrix operators on $\ell_2(\mathbb{C}^4\times\mathbb{Z}_o^{d+1})$.

Moreover, $\Gamma_{\alpha\beta}(x)$ is analytic in κ as $G_{\alpha\beta}(x)$ is, and its short distance behavior is determined by expanding in κ. Long-range bounds on the decay of $G_{\alpha\beta}(x)$ and $\Gamma_{\alpha\beta}(x)$ are obtained by the decoupling of the hyperplane method (see Refs. 6, 7, 9, and 11). Our results hold for all sufficiently small hopping parameter $\kappa>0$, $0<g_0^{-2}\ll\kappa\ll 1$. The short-distance behavior and bounds on G and Γ are given in the next two theorems.

Theorem 2.1: *Let* $0<g_0^{-2}\ll\kappa\ll 1$, c *be a positive constant,* $\rho,\sigma=0,1,\ldots,d$ *and* e^0 *denote the time unit vector,* e^i, e^j $(i,j=1,\ldots,d)$, *denote space unit vectors,* $|\vec{x}|\equiv\Sigma_{i=1}^{d}|x^i|$ *and* $\epsilon,\epsilon'=\pm 1$. *The following properties hold for G:*

(1)

$$G_{\alpha\beta}(x)=\begin{cases}\delta_{\alpha\beta}+\mathcal{O}(\kappa^8), & x=0,\\ \delta_{\alpha\beta}\kappa^2+\mathcal{O}(\kappa^6), & x=\epsilon e^0,\\ c_2\delta_{\alpha\beta}\kappa^2+\mathcal{O}(\kappa^6), & x=\epsilon e^j,\\ \delta_{\alpha\beta}\kappa^4+\mathcal{O}(\kappa^8), & x=2\epsilon e^0,\\ c_2\delta_{\alpha\beta}\kappa^4+\mathcal{O}(\kappa^8), & x=2\epsilon e^j,\\ c_{\alpha\beta}(x)\kappa^4+\mathcal{O}(\kappa^8), & x=\epsilon e^\rho+\epsilon' e^\sigma,\quad \rho<\sigma,\end{cases}\tag{2.9}$$

where the κ *independent constants are given by* $c_2=1/4$, *and*

$$c_{\alpha\beta}(x)=\begin{cases}\delta_{\alpha\beta}/2, & x=\epsilon e^0+\epsilon' e^\rho,\\ c_{\alpha\beta}^{ij}, & x=\epsilon e^i+\epsilon' e^j,\quad i<j,\end{cases}\tag{2.10}$$

where $c_{\alpha\beta}^{ij}$ *is given by* $c_{\alpha\beta}^{12}$, *diagonal with* $4c_{11}^{12}=4c_{44}^{12}=1$ *and* $c_{22}^{12}=c_{33}^{12}=0$, $4c_{11}^{13}=8c_{22}^{13}=8c_{33}^{13}=-8c_{23}^{13}=-8c_{32}^{13}=1$, $4c_{11}^{23}=8c_{22}^{23}=8c_{33}^{23}=8c_{23}^{23}=8c_{32}^{23}=1$, *and the remaining elements are zero.*

(2)

$$|G_{\alpha\beta}(x)|\leqslant c|\kappa|^{2|x^0|+2|\vec{x}|}.\tag{2.11}$$

(3) $G_{\alpha\beta}(x)=d_\alpha G_{\alpha\beta}(x')d_\beta^*$, *where*

$$\begin{aligned}&(a)\ \text{for } x'=(x^0,-x^2,x^1,x^3),\quad d_1=1,\quad d_2=-i,\quad d_3=i,\quad d_4=1;\\ &(b)\ \text{for } x'=(x^0,-x^1,-x^2,x^3),\quad d_1=1,\quad d_2=-1,\quad d_3=-1,\quad d_4=1;\\ &(c)\ \text{for } x'=(x^0,-x^1,-x^2,-x^3),\quad d_\alpha=-1,\quad \text{for } \alpha=1,2,3,4.\end{aligned}$$

Also,

$$G(e^1+e^2)=SG(e^1+e^3)S^\dagger,$$

where $S=S^t$ *and* $S^{-1}=S^\dagger$ (*superscript t means transpose and* † *Hermitian conjugate*). S *has the matrix elements* $S_{11}=1$, $S_{12}=S_{13}=S_{14}=S_{44}=0$, $S_{22}=S_{33}=S_{23}=1/2$, *and* $S_{24}=S_{34}^*=i\sqrt{2}/2$.

Remark 2.1: The equality of the diagonal elements of $c_{\alpha\beta}^{13}$ *and* $c_{\alpha\beta}^{23}$ *follows from the symmetry results of Theorem 4 in Ref. 17, namely rotations by* $\pi/2$ *about the* e^3 *axis.*

Remark 2.2: The third result above follows by using the symmetry results of Theorem 4 in Ref. 17 below and holds to all orders in κ.

The short distance and decay behaviors of $\Gamma(x)$ are given by the following.

Theorem 2.2: *Under the same hypotheses of Theorem 2.1, with* c_2 *and* $c_{\alpha\beta}(x)$ *as given there, we have the following:*

(1)

$$\Gamma_{\alpha\beta}(x)=\begin{cases}\delta_{\alpha\beta}+(2+2dc_2^2)\delta_{\alpha\beta}\kappa^4+\mathcal{O}(\kappa^8), & x=0,\\ -\delta_{\alpha\beta}\kappa^2+\mathcal{O}(\kappa^8), & x=\epsilon e^0,\\ -c_2\delta_{\alpha\beta}\kappa^2+\mathcal{O}(\kappa^6), & x=\epsilon e^j,\\ \mathcal{O}(\kappa^{10}), & x=2\epsilon e^0,\\ (-c_2+c_2^2)\,\delta_{\alpha\beta}\kappa^4+\mathcal{O}(\kappa^8), & x=2\epsilon e^j,\\ [-c_{\alpha\beta}(x)+2c_2^2\delta_{\alpha\beta}](1-\delta_{0\rho})(1-\delta_{0\sigma})\kappa^4+\mathcal{O}(\kappa^8), & x=\epsilon e^\rho+\epsilon' e^\sigma,\quad \rho<\sigma,\\ \mathcal{O}(\kappa^8), & |x^0|=1,\quad |\vec{x}|=2,\\ \mathcal{O}(\kappa^{10}), & |x^0|=2,\quad |\vec{x}|=1,\\ \mathcal{O}(\kappa^{12}), & |x^0|=3,\quad |\vec{x}|=0.\end{cases} \tag{2.12}$$

(2)

$$|\Gamma_{\alpha\beta}(x)|\leqslant\begin{cases}c|\kappa|^{2+4(|x^0|-1)+2|\vec{x}|}, & |x^0|>1,\\ c|\kappa|^{2|x^0|+2|\vec{x}|}, & |x^0|\leqslant 1.\end{cases} \tag{2.13}$$

Remark 2.3: The absence of lower order terms in $\Gamma_{\alpha\beta}$, *as compared to* $G_{\alpha\beta}$, *for* $|x^0|=1,2,3$, *is due to explicit cancellations in the Neumann series and improves the hyperplane method bounds obtained in Theorem 2.2, item (2).*

Concerning the mass spectrum, i.e., the EM spectrum at zero-space momentum, it turns out that the mass is determined up to $\mathcal{O}(\kappa^4)$ by the values of $\Gamma_{\alpha\beta}(x)$ up to distance $|x|\leqslant 2$, and $\alpha=\beta$. The κ^4 contribution to $\Gamma(x)$, for these values of x, comes from the first and second order terms in G_n in the Neumann series. The second order terms are independent of α since they are products of two κ^2 terms of $G_{n,\alpha\beta}(x)$, for points x of distance one, which are diagonal and independent of α. For the first order term in $G_n(x)$, $|x|=2$, the κ^4 contributions come from *straight* contributions and *angle* contributions. Straight contributions have two subsequent sets of two bonds, with opposite orientation, connecting, e.g., the point 0 to ϵe^ρ and then to $2\epsilon e^\rho$; and the property of the Γ matrices given above guarantees that these contributions behave like the κ^2, diagonal and α-independent contributions $G_{n,\alpha\beta}(x)$, $|x|=1$, and do not give rise to mass splitting as well. Angles are contributions to $G_{n,\alpha\beta}$ for points of the form $x=\epsilon e^i+\epsilon' e^j$, $i,j=1,2,\ldots,d$, $i<j$, $\epsilon,\epsilon'=\pm 1$. These are L-type contributions associated with two sets of two lattice bonds, with opposite orientation; one set connecting the points $0\to\epsilon e^i$ and the other connecting $\epsilon e^i\to\epsilon e^i+\epsilon' e^j$, or one set connecting the points $0\to\epsilon' e^j$ and the other connecting $\epsilon' e^j\to\epsilon e^i+\epsilon' e^j$. They contribute to mass splitting in $\mathcal{O}(\kappa^4)$ for $d=2,3$. (See Theorem 2.3.)

Before stating our results on the mass spectrum and dispersion curves, we give an intuitive picture for the *asymptotic* behavior of the mass. Retaining only the diagonal part of $\Gamma_{\alpha\beta}(x)$, $x=0$ and $x=(1,\vec{0})$, the equation for the mass m is

$$\det\tilde{\Gamma}(p^0=im,\vec{p}=\vec{0})\cong(1-\kappa^2 e^m)^4=0,\quad m\in\mathbb{R},$$

so we have a mass m of order $-2\ln\kappa$, with a fourfold degeneracy.

To rigorously determine the EM spectrum, we exploit symmetries for $\vec{p}=\vec{0}$. $\tilde{\Gamma}(p^0=im,\vec{p}=\vec{0})$ is shown to be diagonal. The determination of the nonsingular part can be cast into an analytic implicit function problem. For $\vec{p}\neq\vec{0}$, we have not shown that $\tilde{\Gamma}(p^0=im,\vec{p})$ is diagonal, but the asymptotic form of the dispersion curve can be obtained by a Rouché's theorem argument for the zeroes of $\det\tilde{\Gamma}(p^0=iw(\vec{p}),\vec{p})$. Also, our results in $\mathcal{H}_m$ are extended to the whole Hilbert space $\mathcal{H}_e$ by adapting the subtraction method of Ref. 8.

The results for the EM spectrum are given in the theorem below.

Theorem 2.3: *Under the hypotheses of Theorem 2.1, the following mesonic spectral results hold in the even subspace $\mathcal{H}_e$ of the physical Hilbert space $\mathcal{H}$.*

(1) To any order in κ and for $d=2,3$, the mass spectrum in $\mathcal{H}_e$ and in the energy interval $(0, -(4-\epsilon)\ln\kappa)$, $\epsilon>0$, consists of three masses given by $diag[a+c,b,b,a-c]$, $a+c$ for $\alpha=1$, b for $\alpha=2,3$ and $a-c$ for $\alpha=4$. Up to and including order κ^4, $a-c=b$, for $d=3$, and $c=0$, for $d=2$, and there are only two distinct masses m_a and m_b given by

$$m_j=-2\ln\kappa+r_j(\kappa), \quad j=a \text{ or } j=b,$$

where $r_j(\kappa)\equiv\Sigma_{n=2}^{\infty}b_{j,n}\kappa^n$ is real analytic in κ at 0, for each $d=2,3$. We obtain, with the constants given in Theorem 2.1,

$$r_j(\kappa)=-2\,\mathrm{d}c_2\kappa^2+[-4(c_{\alpha\alpha}^{12}+c_{\alpha\alpha}^{13;23})+(1-2\,\mathrm{d}c_2-24c_2^2+20\,\mathrm{d}c_2^2)-2\,\mathrm{d}^2c_2^2]\kappa^4+\mathcal{O}(\kappa^6),$$

where $c_{\alpha\alpha}^{13;23}\equiv c_{\alpha\alpha}^{13}+c_{\alpha\alpha}^{23}$ is to be omitted for $d=2$. Again, up to and including order κ^4, for $d=3$, the mass m_b is associated with $\alpha=1$ and has multiplicity one; m_a is associated with $\alpha=2,3,4$, and has multiplicity three. The mass splitting is $m_a-m_b=2\kappa^4+\mathcal{O}(\kappa^6)$. For $d=2$, m_b (m_a) is associated with $\alpha=1,4$ $(\alpha=2,3)$, and both have multiplicity two. The mass splitting is $m_a-m_b=\kappa^4+\mathcal{O}(\kappa^6)$.

(2) The EM spectrum in $\mathcal{H}_e$ and in the energy interval $(0,-(4-\epsilon)\ln\kappa)$, $\epsilon>0$, consists of four dispersion curves (not necessarily distinct), each of which has the form

$$w(\vec{p})=-2\ln\kappa-2\,dc_2\kappa^2+c_2\kappa^2\sum_{j=1}^{d}2(1-\cos p^j)+\mathcal{O}(\kappa^4). \tag{2.14}$$

The curves $w(\vec{p})$ are increasing functions of each component p^j of $\vec{p}$, and are convex for small $|\vec{p}|$.

Remark 2.4: The action of the charge conjugation transformation defined below leaves the space $\mathcal{H}_m$ stable, and hence we have the same spectral representation for particles and antiparticles, as given by Eq. (2.7). At the level of CF, the two-point function for the meson antiparticle (which we call G'), is related to G by $G'=TGT^{-1}$, with $T=diag[1,-1,-1,-1]$, for $d=3$. For $d=2$, replace T by U, where $U=diag[-1,-1,-1,1]$. As the mass and dispersion curves are determined by the implicit equation $\det\tilde{\Gamma}(p_0,\vec{p})=0$, the meson particle and antiparticle mass spectrum and dispersion curves are identical.

The organization of the rest of the paper is also patterned by that in Ref. 17. Section III is devoted to the proof of Theorems 2.1 and 2.2. In Sec. IV we prove Theorem 2.3.

III. DECAY BOUNDS AND SHORT-DISTANCE BEHAVIOR OF *G* AND Γ

We now use the decoupling of the hyperplane method to obtain bounds on G and Γ, as given in Theorem 2.1. We assume that the reader has some familiarity with this method and refer to Refs. 6, 9, and 11 for more details.

We will encounter gauge group integrals of monomials in the group matrix elements g_{ij} $(i,j=1,2,3)$, denote SU(3) matrix elements, and we suppress the lattice points from the notation and the inverses g_{ij}^{-1}. These are evaluated following techniques developed in Chap. 8 of Ref. 22 and in Refs. 23 and 24, for the general SU(N) case. In particular, to prove Theorem 2.1, we will need $\int g_{a_1b_1}g^{-1}_{a_2b_2}\,\mathrm{d}\mu(g)=\frac{1}{3}\delta_{a_1b_2}\delta_{a_2b_1}$ and $\int g_{a_1b_1}g^{-1}_{a_2b_2}g_{a_3b_3}g^{-1}_{a_4b_4}\,\mathrm{d}\mu(g)=\frac{1}{8}(\delta_{a_1b_2}\delta_{a_3b_4}\delta_{b_1a_2}\delta_{b_3a_4}+\delta_{a_1b_4}\delta_{a_3b_2}\delta_{b_1a_4}\delta_{b_3a_2})-\frac{1}{24}(\delta_{a_1b_2}\delta_{a_3b_4}\delta_{b_1a_4}\delta_{b_3a_2}+\delta_{a_1b_4}\delta_{a_3b_2}\,\delta_{b_1a_2}\delta_{b_3a_4})$. Also, we use the following properties involving Γ matrices $(\rho,\sigma=0,1,\ldots,d,$ and $\epsilon,\ \epsilon'=\pm1)$ $\Gamma^{\epsilon e^\rho}\Gamma^{-\epsilon e^\rho}=0$, $\Gamma^{\epsilon e^\rho}\Gamma^{\epsilon e^\rho}=-2\Gamma^{\epsilon e^\rho}$, and $\Gamma^{\epsilon e^\rho}\Gamma^{\epsilon' e^\sigma}=2I_4-\Gamma^{-\epsilon' e^\sigma}\Gamma^{-\epsilon e^\rho}$.

We will obtain decay properties for the gauge invariant truncated CF's,

$$\langle F(u)H(v)\rangle_T=\langle[T_0^{u^0-1/2}\vec{T}^{\vec{u}}F(1/2,\vec{0})][T_0^{v^0-1/2}\vec{T}^{\vec{v}}H(1/2,\vec{0})]\rangle_T, \tag{3.1}$$

where $F,H\in\mathcal{H}_e$, T_0 is time translation by e^0 and $\vec{T}^{\vec{u}}=T_1^{u^1}\cdots T_d^{u^d}$ is space translation by $\vec{u}=(u^1,\ldots,u^d)\in\mathbb{Z}^d$.

We discuss explicitly the decoupling procedure for the time (vertical) direction. The space directions are treated similarly, and together with the time direction. The arguments are carried out for CF's in a finite volume $\Lambda\in\mathbb{Z}_o^{d+1}$, with bounds uniform in the volume $|\Lambda|$, and extend to the infinite volume using standard consequences of the polymer expansion (see, e.g., Refs. 9 and 21).

For $u^0<v^0$, $p\in\mathbb{Z}$, $u^0+1/2\leqslant p\leqslant v^0-1/2$ (or, if $u^0>v^0$, $v^0+1/2\leqslant p\leqslant u^0-1/2$), replace the hopping parameter $\kappa>0$ multiplying the nonlocal fermionic part of the action (2.2) (*not* the κ in M) by $\kappa_p\in\mathbb{C}$ and denoting $\partial^r/\partial\kappa_p^r$ by ∂^r and by ∂_0^r its $\kappa_p=0$ value, the following properties hold.

Lemma 3.1: Concerning the derivatives of G, we have the following.

(1) If $u^0\neq v^0$, $\partial_0^r\langle F(u)H(v)\rangle_T=0$, $r=0,1,3$.

(2) If $u^0<v^0$, and $r=2$,

$$\partial_0^2\langle F(u)H(v)\rangle_T=2\sum_{w|w^0=-1/2+p}\langle F(u)\pi_\alpha(w)\rangle_T\langle\mu_\alpha(w+e^0)H(v)\rangle_T|_{\kappa_p=0}.$$

(3) If $u^0>v^0$, and $r=2$,

$$\partial_0^2\langle F(u)H(v)\rangle_T=2\sum_{w|w^0=-1/2+p}\langle F(u)\mu_\alpha(w+e^0)\rangle_T\langle\pi_\alpha(w)H(v)\rangle_T|_{\kappa_p=0}.$$

Proof: Consider $u^0<v^0$; the argument for $v^0<u^0$ is similar. For the truncated two-point function of Eq. (2.5), we introduce a duplicate variable representation (see Ref. 8) depending on the hyperplane decoupling parameters $\{\kappa_p\}$,

$$\begin{aligned}\langle F(u)H(v)\rangle_T=\frac{1}{2Z^2}\int\,&[F(u)-F'(u)][H(v)-H'(v)]\\&\times\exp\Bigg[-\sum_{w|w_0=-1/2+p}\kappa_p(A(\psi,\overline{\psi},g,w)+A(\psi',\overline{\psi}',g',w))\Bigg]\\&\times\exp[-S(\psi,\overline{\psi},g)-S(\psi',\overline{\psi}',g')]\,\mathrm{d}\psi\,\mathrm{d}\overline{\psi}\,\mathrm{d}\mu(g)\,\mathrm{d}\psi'\,\mathrm{d}\overline{\psi}'\,\mathrm{d}\mu(g'),\end{aligned}\tag{3.2}$$

where $A(\psi,\overline{\psi},g,w)=\frac{1}{2}[\overline{\psi}_{a\alpha}(w)\,\Gamma^{\epsilon e^0}_{\alpha\beta}(g_{w,w+e^0})_{ab}\,\psi_{b\beta}(w+\epsilon^0)+\overline{\psi}_{\alpha\alpha}(w+e^0)\Gamma^{-e^0}_{\alpha\beta}(g_{w+e^0,w})\,ab\,\psi_{b\beta}(w)]$ and Z^2 is the normalization factor. The primes in F' and H' mean functions of the duplicate variables ψ', $\overline{\psi}'$, and g'. $S(\psi,\overline{\psi},g)$ is the action for the remaining bonds. We now expand the numerator and denominator of (3.2) in powers of κ_p. For the denominator the κ_p coefficient is a sum of bond terms and each term is a product of expectations containing a single ψ or $\overline{\psi}$ which Fermi integrates to zero. The coefficient of κ_p^2 is a sum of terms with two bounds which must be coincident and of opposite orientation to give a nonzero contribution. For the numerator, we consider the coefficients of κ_p. For the first statement, the κ_p^0 is trivially zero. For κ_p^1 and κ_p^3 the expectation factorizes and each factor has an odd number of fermions and gives zero. The integral over interhyperplane gauge field could also be used to show zero contribution for κ_p^1. For the second statement, the κ_p^2 coefficient has terms with two bonds. For a nonzero contribution performing the gauge integral and the matrix structure of $\Gamma^{\pm e^0}$ gives the result. The proof of the third statement is similar to the second one. □

To calculate the κ_p derivatives of Γ, it is convenient to consider instead $\Gamma'\equiv-\Gamma$, minus the convolution inverse of G, and use the formula

$$\partial^r\Gamma'=\sum_{s=0}^{r-1}\binom{r}{s}\Gamma'\,\partial^{r-s}G\,\partial^s\Gamma'.\tag{3.3}$$

The first three $\kappa=0$ derivatives of Γ are given in the next lemma.

Lemma 3.2: For the derivatives of Γ, we have the following.

(1) If $u^0 \neq v^0$, $\partial_0^r \Gamma(u,v) = 0$, $r = 0,1$.
(2) If $u^0 < v^0$, $\partial_0^2 \Gamma(u,v) = -2\Sigma_{w|w^0=-1/2+p}\ \delta(u,w)\delta(w+e^0,v)$.
(3) If $u^0 > v^0$, $\partial_0^2 \Gamma(u,v) = -2\Sigma_{w|w^0=-1/2+p}\ \delta(u,w+e^0)\delta(w,v)$.
(4) If $|u^0 - v^0| > 1$, $\partial_0^3 \Gamma(u,v) = 0$.

Proof: For the first statement, consider first $u^0 < v^0$. Using Eq. (3.3) and Lemma 3.1, the result follows directly; and similarly for $u^0 > v^0$. For the second statement, using the first one and the second statement of Lemma 3.1, we have

$$\partial_0^2 \Gamma(u,v) = -\sum_{w,z|w^0+1/2\leq p\leq z^0-1/2} \Gamma(u,w)\partial^2 G(w,z)\Gamma(z,v)\Big|_{\kappa_p=0}$$

$$= -2\sum_{w,z|w^0+1/2\leq p\leq z^0-1/2} \Gamma(u,w)\sum_{r|r^0+1/2=p} G(w,r)G(r+e^0,z)\,\Gamma(z,v)\Big|_{\kappa_p=0}. \tag{3.4}$$

Using Lemma 3.1 (first item) for $r=0$ the w and z sums can be taken over all values to give the result. The third statement follows from a similar argument. The fourth statement follows from the first three statements and uses Eq. (3.3) again. □

We are now ready to prove Theorem 2.1.

Proof of Theorem 2.1 (first item): Consider the expansion of the denominator of $G_{\alpha\beta}$ in powers of κ. For a point where the bonds arrive and leave in opposite directions the Fermi integration gives products of Γ's, in which case the above property is used to give zero. The first nonvanishing contribution occurs at κ^8, corresponding to two sets of four bonds going around an elementary square in opposite directions. For the numerator we explicitly carry out two typical calculations: one for the κ^2 contribution to $G_{11}(x)$, associated with $x=\epsilon e^\rho$ ($|x|=1$), and another for the case of an angle contribution to $G_{11}(x)$, when $x=\epsilon e^\rho+\epsilon' e^\sigma$. The case $\epsilon=\epsilon'$ and $\rho=\sigma$ is simpler as the property $\Gamma^{\epsilon e^\rho}\Gamma^{\epsilon e^\rho}=-2\Gamma^{\epsilon e^\rho}$ can be used.

The κ^2 contribution to the case $|x=u-v|=1$, involves two bonds, with opposite orientation connecting u and v. After performing the gauge group integral, we obtain for $G_{11}(u,v)$ with $\langle\ \rangle_0$ denoting the expectation with the hopping parameter set equal to zero in the action of (2.2),

$$\frac{\kappa^2}{12}\langle \mu_1(u)\overline{\psi}_{a_1\alpha_1}(u)\psi_{a_1\beta_2}(u)\rangle_0 \Gamma^{\epsilon e^\rho}_{\alpha_1\beta_1}\Gamma^{-\epsilon e^\rho}_{\alpha_2\beta_2}\langle \psi_{a_2\beta_1}(v)\overline{\psi}_{a_2\alpha_2}(v)\pi_1(v)\rangle_0.$$

Using the definitions (2.3), (2.4) and applying again Wick's theorem for the factors $\langle\ \rangle_0$ we get

$$\frac{\kappa^2}{8}(\Gamma^{-\epsilon e^\rho}_{11}\Gamma^{\epsilon e^\rho}_{33}+\Gamma^{-\epsilon e^\rho}_{12}\Gamma^{\epsilon e^\rho}_{43}+\Gamma^{-\epsilon e^\rho}_{21}\Gamma^{\epsilon e^\rho}_{34}+\Gamma^{-\epsilon e^\rho}_{22}\Gamma^{\epsilon e^\rho}_{44}).$$

By the explicit structure of the matrices Γ the second and third terms above are zero (for all ρ) and the sum of the first and fourth is equal to $8\delta_{\rho 0}+2\delta_{\rho j}$ (remember that $j=1,2,3$) and the result follows.

The κ^4 contribution to $G_{11}(u,v)=G_{11}(x=u-v)$ of the angle $0\to\epsilon e^\rho\to\epsilon e^\rho+\epsilon' e^\sigma\equiv x$ is denoted by $A_{11}^{\epsilon e^\rho,x}\kappa^4$ and has $g_{0,\epsilon e^\rho}$ ($g^{-1}_{0,\epsilon e^\rho}$) emanating from 0 ($\epsilon e^\rho$) in the e^ρ direction and $g_{\epsilon e^\rho,x}(g^{-1}_{\epsilon e^\rho,x})$ arriving at $x(\epsilon e^\rho)$ in the e^σ direction. After gauge integration of $g_{0,\epsilon e^\rho}g_{\epsilon e^\rho,0}$ and $g_{\epsilon e^\rho,x}g_{x,\epsilon e^\rho}$, and Fermi integration of the fields at ϵe^ρ using Wick's theorem, we have

$$A_{11}^{\epsilon e^\rho,x}=\tfrac{1}{48}\langle \mu_1(u)\overline{\psi}_{a_1\alpha_1}(u)\psi_{a_1\beta_2}(u)\rangle_0\,(\Gamma^{\epsilon e^\rho}_{\alpha_1\beta_1}\Gamma^{-\epsilon e^\rho}_{\alpha_2\beta_2}\Gamma^{\epsilon' e^\sigma}_{\beta_1\beta_3}\Gamma^{-\epsilon' e^\sigma}_{\alpha_4\alpha_2}$$
$$-3\Gamma^{\epsilon e^\rho}_{\alpha_1\beta_1}\Gamma^{-\epsilon e^\rho}_{\beta_1\beta_2}\Gamma^{\epsilon' e^\sigma}_{\alpha_3\beta_3}\Gamma^{-\epsilon' e^\sigma}_{\alpha_4\alpha_3})\,\langle \psi_{a_4\beta_3}(v)\overline{\psi}_{a_4\alpha_4}(v)\pi_1(v)\rangle_0.$$

The second product of Γ's above is zero by $\Gamma^{\epsilon e^\rho}\Gamma^{-\epsilon e^\rho}=0$. Using the definitions (2.3), (2.4) and applying again Wick's theorem for the factors $\langle\ \rangle_0$ we get

$$A_{11}^{\epsilon e^\rho,x}=\tfrac{1}{32}[\Lambda_{11}^{-\epsilon' e^\sigma,-\epsilon e^\rho}\Lambda_{33}^{\epsilon e^\rho,\epsilon' e^\sigma}+\Lambda_{12}^{-\epsilon' e^\sigma,-\epsilon e^\rho}\Lambda_{43}^{\epsilon e^\rho,\epsilon' e^\sigma}+\Lambda_{21}^{-\epsilon' e^\sigma,-\epsilon e^\rho}\Lambda_{34}^{\epsilon e^\rho,\epsilon' e^\sigma}$$
$$+\Lambda_{22}^{-\epsilon' e^\sigma,-\epsilon e^\rho}\Lambda_{44}^{\epsilon e^\rho,\epsilon' e^\sigma}],$$

where $\Lambda_{uu'}^{-\epsilon' e^\sigma,-\epsilon e^\rho}\equiv\Gamma_{u\alpha}^{-\epsilon' e^\sigma}\Gamma_{\alpha u'}^{-\epsilon e^\rho}$ and $\Lambda_{\ell\ell'}^{\epsilon e^\rho,\epsilon' e^\sigma}\equiv\Gamma_{\ell\beta}^{\epsilon e^\rho}\Gamma_{\beta\ell'}^{\epsilon' e^\sigma}$. Similarly, we can calculate the contribution of $A_{11}^{\epsilon' e^\sigma,x}$. The expression for $c_{11}(x)$ is

$$c_{11}(x)=A_{11}^{\epsilon e^\rho,x}+A_{11}^{\epsilon' e^\sigma,x},$$

with $x=\epsilon e^\rho+\epsilon' e^\sigma$, and similarly for the other $c_{\alpha\beta}(x)$'s. When $\rho=i$ and $\sigma=j$ $(i,j=1,2,3)$ by the symmetry properties of Theorem 4 in Ref. 17 (namely, rotations by π about e^3 and parity), we can show that $c_{\alpha\beta}(x=\epsilon e^i+\epsilon' e^j)$ is independent of ϵ, ϵ' so, we can write $c_{\alpha\beta}(x)=c_{\alpha\beta}(e^i+e^j)\equiv c_{\alpha\beta}^{ij}$ and we get Eq. (2.10). □

Proof of Theorem 2.1 (second item): Using a Cauchy integral representation for each κ_p and for analogous spatial complex hyperplane decoupling parameters, taking into account the number of vanishing derivatives as given in Lemma 3.1, and using Cauchy estimates on the multiple integral gives the result. An argument based on the maximum modulus theorem could also be used (see Ref. 9 for details). □

Let us now turn to the proof of Theorem 2.2. The corrections to the asymptotic mass value of $-2\ln\kappa$ which we need for the determination of mass splitting require precise values of $\Gamma_{\alpha\beta}(x)$, for small $|x|$. The results go beyond those obtained by the hyperplane method, and rely on explicit cancellations in the Neumann series for Γ. The results below are obtained expanding in powers of κ and controlling the remainders using the analyticity of G and Γ, and the decay of G as given by Theorem 2.1.

Proof of Theorem 2.2 (first item): $\Gamma_{\alpha\beta}$ is obtained from the Neumann series and Theorem 2.1 (first item). We show how the cancellations occur, which improves the hyperplane method bound. We explicitly consider the case $x=\epsilon e^0+\epsilon' e^j$; the other cases where there are one, two or three times units are treated similarly. Recall that [see Eq. (2.8)] $G_{d,\alpha\beta}(u,v)=G_{\alpha\alpha}(u,u)\delta_{\alpha\beta}\delta(u,v)$. From Theorem 2.1, we obtain $G_{\alpha\alpha}(0)=1+\mathcal{O}(\kappa^8)$. Using $\Gamma=\Sigma_{i=0}^{\infty}(-1)^i[G_d^{-1}G_n]^iG_d^{-1}$, for $x=u-v\neq 0$, we write

$$\Gamma_{\alpha\beta}(u,v)=-G_{\alpha\alpha}^{-1}(0)G_{n,\alpha\beta}(u,v)G_{\beta\beta}^{-1}(0)+\sum_w\ G_{\alpha\alpha}^{-1}(0)G_{n,\alpha\gamma}(u,w)$$
$$\times\ G_{\gamma\gamma}^{-1}(0)G_{n,\gamma\beta}(w,v)G_{\beta\beta}^{-1}(0)+\mathcal{O}(G_n^3). \tag{3.5}$$

For $\alpha=\beta$, there are two κ^4 angle contributions to $G_{n,\alpha\beta}(u,v)$ in the first term of Eq. (3.5), and these are cancelled by the product of κ^2 contributions for $w-v=\epsilon e^0$ and $w-v=\epsilon e^j$ in the second term of Eq. (3.5). □

Proof of Theorem 2.2 (second item): Similar to Theorem 2.1 (second item). □

IV. SPECTRAL RESULTS

We now prove Theorem 2.3. To determine the meson masses and dispersion curves, we find the p^0 imaginary axis solutions of $\det\tilde{\Gamma}(p^0,\vec{p})=0$. For the mass spectrum, we find, by the use of symmetries, that $\tilde{\Gamma}_{\alpha\beta}(p^0,\vec{p}=\vec{0})$ is diagonal. Furthermore, we show that $m_c+2\ln\kappa$ is real analytic in κ. For $\vec{p}\neq\vec{0}$, as we have *not* found symmetries which simplify the matrix structure, we determine the dispersion curves $w(\vec{p})$, where $\det\tilde{\Gamma}(p^0=iw(\vec{p}),\vec{p})=0$, by an application of Rouché's theorem.

We state some symmetry properties in the next lemma.

Lemma 4.1: The following symmetry properties are satisfied by the matrices G and Γ.

(1) $G_{\alpha\beta}(x) = [G_{\beta\alpha}(x)]^*$ *and* $\Gamma_{\alpha\beta}(x) = [\Gamma_{\beta\alpha}(x)]^*$,
(2) For $\chi \in \mathbb{R}$, *let* $p^0 = i\chi$. *We have* $\tilde{G}_{\alpha\beta}(i\chi,\vec{p}) = [\tilde{G}_{\beta\alpha}(i\chi,\vec{p})]^*$ *and* $\tilde{\Gamma}_{\alpha\beta}(i\chi,\vec{p}) = [\tilde{\Gamma}_{\beta\alpha}(i\chi,\vec{p})]^*$,
(3) At $\vec{p}=\vec{0}$, $\tilde{G}_{\alpha\beta}(p^0,\vec{p}=\vec{0}) = \mathrm{diag}[a+c, b, b, a-c]$, *with* $a, b, c \in \mathbb{C}$.

Proof: Here we use several symmetries given in Theorem 4 in Ref. 17. By the spectral representation of Proposition 2.1, for $x^0 \neq 0$, item (1) follows. For $x^0 = 0$, the result follows from time reversal and parity. Thus, item (1) holds for all x. The proof of item (2) follows from parity invariance $G_{\alpha\beta}(x^0,\vec{x}) = G_{\alpha\beta}(x^0,-\vec{x})$. To prove item (3), we use reflection symmetry in the coordinate x^1. Here $\vec{x}=(x^1,\ldots,x^d) \mapsto \vec{x}\,' = (-x^1,\ldots,x^d)$, and $\tilde{\psi}_{a1}(x) \mapsto -\tilde{\psi}_{a2}(x')$, $\tilde{\psi}_{a2}(x) \mapsto -\tilde{\psi}_{a1}(x')$, $\tilde{\psi}_{a3}(x) \mapsto \tilde{\psi}_{a4}(x')$, $\tilde{\psi}_{a4}(x) \mapsto \tilde{\psi}_{a3}(x')$. Also rotations of $\pi/2$ and π about e^3 will be used. Considering $\pi/2$ and $d=3$ we have, $x=(x^0,x^1,x^2,x^3) \mapsto x' = (x^0,-x^2,x^1,x^3)$ [$x = (x^0,x^1,x^2) \mapsto x' = (x^0,-x^2,x^1)$, for $d=2$] and $\tilde{\psi}_{a\underline{1}}(x) \mapsto \tilde{\psi}_{a\underline{1}}(x')$, $\psi_{a\underline{2}}(x) \mapsto -i\psi_{a\underline{2}}(x')$, $\tilde{\psi}_{a3}(x) \mapsto \tilde{\psi}_{a3}(x')$, $\psi_{a4}(x) \mapsto -i\psi_{a4}(x')$ and $\overline{\psi}_{a\underline{2}}(x) \mapsto i\overline{\psi}_{a\underline{2}}(x')$, $\psi_{a4}(x) \mapsto i\overline{\psi}_{a4}(x')$. For π and $d=3$ we have, $x=(x^0,x^1,x^2,x^3) \mapsto x' = (x^0,-x^1,-x^2,x^3)$ [$x=(x^0,x^1,x^2) \mapsto x' = (x^0,-x^1,-x^2)$, for $d=2$] and $\tilde{\psi}_{a1}(x) \mapsto \tilde{\psi}_{a1}(x')$, $\tilde{\psi}_{a2}(x) \mapsto -\tilde{\psi}_{a2}(x')$, $\tilde{\psi}_{a3}(x) \mapsto \tilde{\psi}_{a3}(x')$, $\tilde{\psi}_{a4}(x) \mapsto -\tilde{\psi}_{a4}(x')$.

These transformations, taken together with the symmetry results given in Theorem 4 in Ref. 17, are used to obtain the matrix structure stated in the third item, for $d=2,3$. □

After using Theorem 2.2 and taking the Fourier transform, we have

$$\tilde{\Gamma}_{\alpha\beta}(p^0,\vec{0}) = [1-2\,dc_2\kappa^2 + 2(1-dc_2-12c_2^2+10\,dc_2^2)\kappa^4]\delta_{\alpha\beta} - 4(c_{\alpha\beta}^{12}+c_{\alpha\beta}^{13}+c_{\alpha\beta}^{23})\kappa^4 + \mathcal{O}(\kappa^6) - [\delta_{\alpha\beta}\kappa^2 + \mathcal{O}(\kappa^8)](e^{ip^0}+e^{-ip^0}) + \cdots . \tag{4.1}$$

We now introduce an auxiliary function $H_\alpha(w,\kappa)$, jointly analytic in w and κ, for small $|\kappa|$ and $|w|$, such that $H_\alpha(w=1-\kappa^2 e^{-ip^0},\kappa) = \tilde{\Gamma}_{\alpha\alpha}(p^0,\vec{p}=\vec{0})$. $H_\alpha(w,\kappa)$ is defined by

$$H_\alpha(w,\kappa), = w - 2\,dc_2\kappa^2 + 2(1-dc_2-12c_2^2+10\,dc_2^2)\kappa^4 - 4(c_{\alpha\alpha}^{12}+c_{\alpha\alpha}^{13;23})\kappa^4 - \frac{\kappa^4}{1-w} + \sum_{\vec{x}} \Gamma'_{\alpha\alpha}(0,\vec{x}) - \sum_{\vec{x}} \Gamma'_{\alpha\alpha}(1,\vec{x})\left[\frac{\kappa^2}{1-w}+\frac{1-w}{\kappa^2}\right] + \sum_{n\geq 1,\vec{x}|(n,\vec{x})\neq(1,\vec{0})} \Gamma_{\alpha\alpha}(n,\vec{x})\left[\left(\frac{\kappa^2}{1-w}\right)^n + \left(\frac{1-w}{\kappa^2}\right)^n\right], \tag{4.2}$$

where $\Gamma'_{\alpha\alpha}(0,\vec{x})$ [respectively, $\Gamma'_{\alpha\alpha}(1,\vec{x})$] contains the contributions of $\mathcal{O}(\kappa^6)$ [respectively, $\mathcal{O}(\kappa^8)$] or higher and $c_{\alpha\alpha}^{13;23}$ is the sum of angle contributions $0 \to e^i \to e^{13}$ $(i=1,3)$ and $0 \to e^j \to e^{23}$ $(j=2,3)$ which is diagonal. $H_\alpha(0,0)=0$ and $(\partial H_\alpha/\partial w)(0,0)=1$, and hence the analytic implicit function theorem applies and gives us an analytic function $w(\kappa) \equiv w_\alpha(\kappa)$ such that $H_\alpha(w(\kappa),\kappa)=0$. Thus, for κ real positive, the mass is given by

$$m_\alpha = -\ln\kappa^2 + \ln(1-w)\,.$$

By an analysis of the formulas for the implicit function derivatives, with $\mathrm{d}w = -(\partial_w H)^{-1}\partial_k H \equiv -(H_w)^{-1}H_k$, we find $\mathrm{d}_0^r w = 0$, $r=0,1,3,5$ and

$$\mathrm{d}_0^2 w = -\partial_\kappa^2 H(0,0) = 4c_2 d$$

$$\mathrm{d}_0^4 w = -\partial_\kappa^4 H(0,0) = -4![1-2\,dc_2-24c_2^2+20\,dc_2^2-4(c_{\alpha\alpha}^{12}+c_{\alpha\alpha}^{13;23})]\,.$$

Hence, for $d=3$,

$$m_\alpha = -2\ln\kappa - 2\,dc_2\kappa^2 + [-4(c^{12}_{\alpha\alpha}+c^{13;23}_{\alpha\alpha}) + (1-2\,dc_2-24c_2^2+20\,dc_2^2) - 2\,d^2c_2^2]\kappa^4 + \mathcal{O}(\kappa^6)\,,$$

and similarly, for $d=2$, with $c^{13;23}_{\alpha\alpha}=0$.

Thus, up to and including $\mathcal{O}(\kappa^4)$, we have, for $d=3$, $m_a\equiv m_\alpha$ and $m_b\equiv m_1$, $m_a-m_b=2\kappa^4$ and $\alpha=2,3,4$; for $d=2$, $m_a\equiv m_\alpha$ and $m_b\equiv m_\beta$, $m_a-m_b=\kappa^4$, $\alpha=2,3$ and $\beta=1,4$.

Let us now turn to the dispersion curves. They satisfy $\det\tilde{\Gamma}(ip^0=iw(\vec{p}),\vec{p})=0$. To determine them, with $c_2(\vec{p})\equiv c_2\sum_{j=1}^d 2\cos p^j$, we write the Fourier transform of $\Gamma_{\alpha\beta}(x)$ as

$$\tilde{\Gamma}_{\alpha\beta}(p^0,\vec{p}) = [1-c_2(\vec{p})\kappa^2-\kappa^2(e^{-ip^0}+e^{ip^0})]\delta_{\alpha\beta} + \sum_{n,\vec{x}}{}' \;\Gamma_{\alpha\beta}(n,\vec{x})\,e^{-i\vec{p}.\vec{x}}(e^{-ip^0n}+e^{ip^0n})\,, \tag{4.3}$$

where $\Sigma'_{n,\vec{x}}$ means that all terms of order κ^4 or higher in $\Gamma_{\alpha\beta}(x)$ are included. Introduce the auxiliary matrix function $H_{\alpha\beta}(w,\kappa)\equiv H_{\alpha\beta}(w,\kappa,\vec{p})$ such that $H_{\alpha\beta}(w=1-c_2(\vec{p})\kappa^2-\kappa^2e^{-ip^0},\kappa) = \tilde{\Gamma}_{\alpha\beta}(p^0,\vec{p})$. $H_{\alpha\beta}(w,\kappa)$ is defined by

$$H_{\alpha\beta}(w,\kappa) = w\,\delta_{\alpha\beta} + \sum_{n,\vec{x}}{}'' \;\Gamma_{\alpha\beta}(n,\vec{x})\,e^{-i\vec{p}.\vec{x}}\left[\left(\frac{1-w-c_2(\vec{p})\kappa^2}{\kappa^2}\right)^n + \left(\frac{\kappa^2}{1-w-c_2(\vec{p})\kappa^2}\right)^n\right],$$

where $\Sigma''_{n,\vec{x}}$ means that only $\mathcal{O}(\kappa^4)$ terms or higher order terms are to be included. $H(w,\kappa)$ is jointly analytic in κ and w at $(w,\kappa)=(0,0)$.

Letting

$$f(w)\equiv\det H(w,\kappa) = \det wI_4 + [\det H(w,\kappa)-\det wI_4] \equiv g(w)+h(w)\,,$$

we can apply Rouché's theorem to $f(w)$ on the circle $|w|=c|\kappa|^4$, $c\gg>1$, $|g(w)|=c^4|\kappa|^{16}$ and $|h(w)|\leqslant c'|\kappa|^{16}<c^4|\kappa|^{16}=|g(w)|$, so that $f(w)$ has four zeroes inside $|w|=c|\kappa|^4$, as $g(w)=w^4$ has a fourth order zero. Notice that the upper bound for $|h(w)|$ comes from an upper bound on the remaining 23 terms in the difference between the two determinants. Now, for $p^0=iw(\vec{p})$, and κ real positive, each of the four zeroes satisfying $\det\tilde{\Gamma}(p^0=iw(\vec{p}),\vec{p})=0$ has the form

$$w(\vec{p}) = -2\ln\kappa - 2\,dc_2\kappa^2 + 2c_2\kappa^2\sum_{j=1}^d(1-\cos p^j) + \mathcal{O}(\kappa^4)\,.$$

We now extend the spectral results from $\mathcal{H}_m$ to the space $\mathcal{H}_e$, using the Euclidean subtraction method established in Ref. 8. We consider the generalized subtracted two-point CF,

$$\mathcal{F}(u,v) = \mathcal{G}_{LL}(u,v) - \sum_{w,w'\in\mathbb{Z}_0^{d+1}} \mathcal{G}_{L,\Phi}(u,w)\Gamma(w,w')\mathcal{G}_{\Phi,L}(w',v)\,,$$

where $\Phi(u)=(\pi_1(u),\ldots,\pi_4(u))$ has four components; $\Gamma(w,w')$ is given by the convolution inverse of the two-point function G. Finally,

$$\mathcal{G}_{FH}(u,v) = \begin{cases} S_{\Theta T_0^{-1}F,H}(u,v), & u^0\leqslant v^0,\\ S^*_{F,\Theta T_0^{-1}H}(u,v), & u^0>v^0,\end{cases}$$

with $S_{F,H}(u,v)=\langle[T_0^{u^0-1/2}\vec{T}^{\vec{u}}F(1/2,\vec{0})][T_0^{v^0-1/2}\vec{T}^{\vec{v}}H(1/2,\vec{0})]\rangle_T$.

The lemma below guarantees that our results hold in the full space $\mathcal{H}_e$.

Lemma 4.2: For $u^0<v^0$, $p\in\mathbb{Z}$, $u^0+1/2\leqslant p\leqslant v^0-1/2$ (or, if $u^0>v^0$, $v^0+1/2\leqslant p\leqslant u^0-1/2$), and again denoting by ∂_0 the κ_p derivative at $\kappa_p=0$, we have $\partial_0^r\mathcal{F}(u,v)=0$, for $r=0,1,2,3$.

Proof: The proof follows Ref. 8 closely. For $u^0<v^0$ (the case $u^0>v^0$ is similar) and from Lemmas 3.1 and 3.2 the power series expansions in κ_p of the functions appearing in the definition of $\mathcal{F}(u,v)$ are of the form

$$\mathcal{G}_{LL}(u,v)=a_2(u,v)\kappa_p^2+\mathcal{O}(\kappa_p^4),$$

$$\mathcal{G}_{L,\Phi}(u,w)=b_0(u,w)\chi_{w^0\leqslant -1/2+p}+b_2(u,w)\kappa_p^2+\mathcal{O}(\kappa_p^4),$$

$$\Gamma(w,w')=c_0(w,w')(\chi_{w^0\leqslant -1/2+p}\chi_{w'^0\leqslant -1/2+p}+\chi_{w^0>-1/2+p}\chi_{w'^0>-1/2+p})+c_2(w,w')\kappa_p^2+\mathcal{O}(\kappa_p^4),$$

$$\mathcal{G}_{\Phi,L}(w',v)=d_0(w',v)\chi_{w'^0>-1/2+p}+d_2(w',v)\kappa_p^2+\mathcal{O}(\kappa_p^4).$$

Substituting these expressions, it is easy to show that $\partial_0^r\mathcal{F}(u,v)=0$ $(r=0,1,3)$. For $r=2$, proceeding exactly as in Theorem 3.7 of Ref. 8, we have four terms which sum up to zero and the result follows. □

This ends the proof of Theorem 2.3. □

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Warped product approach to universe with nonsmooth scale factor

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In the framework of Lorentzian warped products, we study the Friedmann–Robertson–Walker cosmological model to investigate nonsmooth curvatures associated with multiple discontinuities involved in the evolution of the universe. In particular we analyze nonsmooth features of the spatially flat Friedmann–Robertson–Walker universe by introducing double discontinuities occurred at the radiation-matter and matter-lambda phase transitions in astrophysical phenomenology. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Since the cosmic microwave background was discovered, there have been many ideas and proposals to figure out how the universe has evolved. The standard big bang cosmological model based on the Friedmann–Robertson–Walker (FRW) space–times has led to the inflationary cosmology[1] and nowadays to the M-theory cosmology with bouncing universes.[2] These space–times are foliated by a special set of spacelike hypersurfaces such that each hypersurface corresponds to an instant of time. From a physical point of view, these warped product space–times are interesting since they include classical examples of space–time such as the FRW manifold and the intermediate zone of Reissner–Nordström (RN) manifold.[3,4]

The Lorentzian manifolds with non-smooth metric tensors have been extensively discussed from various view points.[5–9] In a space–time where the metric tensor is continuous but has a jump in its first and second derivatives across a submanifold in an admissible coordinate system, one can have a curvature tensor containing a Dirac delta function.[10] The support of this distribution may be of three, two, or one dimensional or may even consist of a single event. Moreover, Lichnerowicz's formalism[7] for dealing with such tensors is modified so that one can obtain the Riemannian curvature tensor and Ricci curvature tensor defined in the sense of distributions.

A general theory for matching two solutions of the Einstein field equations has been proposed[8,9] at arbitrary shock-wave interface across which the metric tensor is C^0-Lorentzian, namely at smooth surface across which the first derivatives of the metric suffer at worst a jump discontinuity, so that the simplest solution of Einstein equations can incorporate a shock-wave into a standard FRW metric whose equation of state accounts for the Hubble constant and the microwave background radiation temperature. There have been later presented the evolution of the one point probability distribution function of the cosmological density field based on an exact statistical treatment.[11]

On the other hand, the concept of a warped product manifold was introduced by Bishop and O'Neill long ago,[12] and it was later connected to general relativity[13] and semi-Riemannian geometry[14] by elevating warped products to a central role. Warped product spaces has been also

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extended to a richer class of spaces involving multiple product spaces.[5,6] One of the authors has investigated the curvature of a multiply warped product possessing C^0-warping functions with a discontinuity at a single point,[5] and in this paper we will generalize this result to a warped product space–time with multiple discontinuities associated with cosmological phenomenology. Of particular interest are space–times with metric tensors which fail to be C^1 across multiple points on the hypersurface, and is C^∞ off the hypersurface. We will also study the Lorentzian metric which fails to be C^0 across multiple points on the hypersurfaces and is C^∞ off the hypersurfaces.

In this paper, as a cosmological model we will exploit the FRW space–times $M_0\times_f H$, which can be treated as a warped product manifold possessing warping function (or scale factor) f with time dependence, to investigate the nonsmooth curvature associated with the multiple discontinuities involved in the evolution of the universe. We will also analyze nonsmooth features of the spatially flat FRW universe by introducing double discontinuities occurred at the radiation-matter and matter-lambda phase transitions in the astrophysical phenomenology.

In Sec. II we will introduce the warped product space–time with multiple warping functions and extend the warped product scheme to the case with multiple discontinuities in the FRW cosmological model in Sec. III. We will study the realistic cosmological phenomenology in the spatially flat FRW universe associated with the radiation-matter and matter-lambda phase transitions in Sec. IV.

II. WARPED PRODUCT SPACE–TIME WITH MULTIPLE WARPING FUNCTIONS

In this section we briefly recapitulate the curvature of the warped product approach to space–time with multiple C^0-warping functions at a single point.

Definition 2.1 (Ref. 5): A multiply warped products space–time with base $(M_0,-\mathrm{d}t^2)$, fibers (F_i,g_i) $i=1,\ldots,n$ and warping functions $f_i>0$ is the product manifold $(M_0\times F_1\times\cdots\times F_n,g)$ endowed with the Lorentzian metric:

$$g=-\pi_{M_0}^{*}\,\mathrm{d}t^2+\sum_{i=1}^{n}\,(f_i\circ\pi_{M_0})^2\pi_i^{*}g_i,$$

where π_{M_0}, π_i $(i=1,\ldots,n)$ are the natural projections of $M_0\times F_1\times\cdots\times F_n$ onto M_0 and $F_1,\ldots,F_n$, respectively. For a specific case of $M_0=R$ and $g_{M_0}=-\mathrm{d}t^2$, the Lorentzian metric is given by

$$g=-\mathrm{d}t^2+\sum_{i=1}^{n}\,f_i^2g_i\,.$$

Proposition 2.2 (Ref. 5): Let $M=M_0\times_{f_1}F_1\times\cdots\times_{f_n}F_n$ be a multiply warped product with Riemannian curvature tensor R. If $X,\ Y\in\mathfrak{L}(M_0),\ U_i,\ V_i,\ W_i\in\mathfrak{L}(F_i)$ $(n=1,2,\ldots,n)$, $f_i\in C^0(S)$ at a single point $p\in M_0$, and $S=\{p\}\times_{f_1}F_1\times\cdots\times_{f_n}F_n$, then

(i)

$$R_{XU_i}U_j=R_{U_iU_j}X=R_{U_jX}U_i=0\quad\text{for } i\neq j,$$

(ii)

$$R_{U_iX}Y=U_iX^1Y^1\frac{f_i''(t)+\delta(t-p)(f_i'^{+}-f_i'^{-})}{f_i},$$

(iii)

$$R_{XU_i}U_j=R_{U_iU_j}X=R_{U_jX}U_i=0,\quad\text{for } i\neq j,$$

(iv)

$$R_{XY}U_i=0, \quad \text{for } i=1,\ldots,n,$$

(v)

$$R_{U_iV_i}U_j=0, \quad \text{for } i\neq j,$$

(vi)

$$R_{U_iU_j}V_j=U_i\langle U_j,V_j\rangle\frac{(f_i'^{+}+f_i'^{-})(f_j'^{+}+f_j'^{-})}{f_if_j}, \quad \text{for } i\neq j,$$

(vii)

$$R_{U_iV_i}W_i={}^{F_i}R_{U_iV_i}W_i+(\langle U_i,W_i\rangle V_i-\langle V_i,W_i\rangle U_i)\frac{f_i'^{+}\mu(t-p)+f_i'^{-}\mu(p-t)}{f_i^2},$$

where $X=X^1\partial/\partial_t$ and $Y=Y^1\partial/\partial_t$, and $\mu(t-p)$ and $\delta(t-p)$ are the unit step function and the delta function, respectively.

Proposition 2.3 (Ref. 5): Let $M=M_0\times_{f_1}F_1\times\cdots\times_{f_n}F_n$ be a multiply warped products with Riemannian curvature tensor R. If $X,\ Y\in\mathfrak{L}(M_0),\ U_i,\ V_i\in\mathfrak{L}(F_i)\ (n=1,2,\ldots,n),\ d_i=\dim F_i$, $f_i\in C^0(S)$ at a single point $p\in M_0$, and $S=\{p\}\times_{f_1}F_1\times\cdots\times_{f_n}F_n$, then

(i)

$$\mathrm{Ric}(X,Y)=-\sum_{i=1}^{n}d_iX^1Y^1\frac{f_i''(t)+\delta(t-p)(f_i'^{+}-f_i'^{-})}{f_i},$$

(ii)

$$\mathrm{Ric}(X,U_i)=0,$$

(iii)

$$\mathrm{Ric}(U_i,V_i)={}^{F_i}\mathrm{Ric}(U_i,V_i)+\langle U_i,V_i\rangle\frac{f_i''(t)+\delta(t-p)(f_i'^{+}-f_i'^{-})}{f_i}+\langle U_i,V_i\rangle\left[(d_i-1)\frac{f_i'^{+}-f_i'^{-}}{f_i^2}+\sum_{j\neq i}d_j\frac{\langle f_i'^{+}-f_i'^{-},f_j'^{+}-f_j'^{-}\rangle}{f_if_j}\right],$$

(iv)

$$\mathrm{Ric}(U_i,U_j)=0, \quad \text{for } i\neq j,$$

where $X=X^1\partial/\partial_t$ and $Y=Y^1\partial/\partial_t$, and $\delta(t-p)$ is the delta function.

III. FRW METRIC WITH MULTIPLE DISCONTINUITIES

The FRW space–time is one of the *warped product* manifold where the base is an open interval M_0 of R with usual metric reversed $(M_0,-\mathrm{d}t^2)$, the fiber is a three-dimensional Riemannian manifold (F,g_F) and the warping function f is any positive function f on M_0. The Robertson–Walker space–time is then the product manifold $M=M_0\times_f H$ endowed with the Lorentzian metric $g=-\mathrm{d}t^2+f^2(t)g_H$ with f being the scale factor of the FRW universe associated with universal expansion. This warping function f is a function of time alone and it measures how

physical separations change with time. The dynamics of the expanding universe only appears implicitly in the time dependence of the warping function (or scalar factor) f.

Consider the space–time (M, g) with metric $g=-\mathrm{d}t^2+f^2\mathrm{d}\sigma^2$ in the form of warped products. Let $M=M_0\times_f H$ be a warped product with $g_{M_0}=-\mathrm{d}t^2$. Let $f>0$ be smooth functions on $M_0=(t_0, t_\infty)$. Assume $f\in C^\infty$ for $t\neq t_i$ and $f\in C^1$ at $t=t_i$ $(i=1,2,\ldots,n)$. When $f\in C^1$ at points $t_i\in(t_0,t_\infty)$ and $S=\{t_i\}\times_f H$, we define $f\in C^1(S)$ as a collection of functions $\{f^{(i)}\}$ with $f^{(i)}$ piecewisely defined on the intervals $t_i\leqslant t\leqslant t_{i+1}$ $(i=0,1,2,\ldots,n)$ with $t_{n+1}=t_\infty$. Since $f\in C^1(S)$, we have $f^{(i-1)}(t_i)=f^{(i)}(t_i)$, $f^{(i-1)'}(t_i)=f^{(i)'}(t_i)$ but $f^{(i-1)''}(t_i)\neq f^{(i)''}(t_i)$. We shall use the unit step function μ for discontinuity of $f^{(i)''}$ at $t=t_i$.

Consider the FRW metric of the form

$$g=-\mathrm{d}t^2+f^2(t)\left(\frac{\mathrm{d}r^2}{1-kr^2}+r^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2)\right),$$

where k is a parameter denoting the spatially flat $(k=0)$, 3-sphere $(k=1)$ and hyperboloid $(k=-1)$ universes.

Proposition 3.1: Let $M=M_0\times_f H$ be the FRW space–time with Riemannian curvature R and flow vector field $U=\partial_t$. If $f\in C^1(S)$, vector fields $X, Y, Z\in\mathfrak{L}(H)$ satisfy

(i)

$$R_{XY}Z=\frac{f'^2+k}{f^2}(\langle X,Z\rangle Y-\langle Y,Z\rangle X),$$

(ii)

$$R_{XU}U=\frac{f''}{f}X,$$

(iii)

$$R_{XY}U=0,$$

(iv)

$$R_{XU}Y=\frac{f''}{f}\langle X,Y\rangle U,$$

where f'' is given by

$$\begin{aligned}f''=&\left(f^{(n)''}-f^{(n-1)''}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)''}\right)\mu(t-t_n)+\sum_{l=1}^{n-1}\left(-f^{(l-1)''}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)''}\right)\mu(t-t_l)\\&+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)''}\mu(t_n-t)+\sum_{l=1}^{n-1}\left(-f^{(l)''}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)''}\right)\mu(t_l-t),\end{aligned}\tag{1}$$

with $\mu(t-t_i)$ being the unit step function which becomes unity for $t>t_i$ and vanishes otherwise.

Proof: We derive f'' in terms of the collection of functions $\{f^{(i)}\}$ with $f^{(i)}$ piecewisely defined on the intervals $t_i\leqslant t\leqslant t_{i+1}$ $(i=0,1,2,\ldots,n)$ with $t_{n+1}=t_\infty$. For a single discontinuity $n=1$ case, f is trivially given by

$$f''=f^{(1)''}\mu(t-t_1)+f^{(0)''}\mu(t_1-t)$$

which fulfills (1). For double discontinuities $n=2$ case, f is similarly given by

$$f''=(f^{(2)\prime\prime}-\tfrac{1}{2}f^{(1)\prime\prime}+\tfrac{1}{2}f^{(0)\prime\prime})\mu(t-t_2)+(\tfrac{1}{2}f^{(1)\prime\prime}-\tfrac{1}{2}f^{(0)\prime\prime})\mu(t-t_1)+(\tfrac{1}{2}f^{(1)\prime\prime}+\tfrac{1}{2}f^{(0)\prime\prime})\mu(t_2-t)$$
$$+(-\tfrac{1}{2}f^{(1)\prime\prime}+\tfrac{1}{2}f^{(0)\prime\prime})\mu(t_1-t), \tag{2}$$

which also fulfills (1). By using iteration method, one can obtain (1) for an arbitrary n case. □

For the case of $f\in C^0(S)$ we use the derivative of the unit step function $\mu(t_i)$. For all $t\neq t_i$ this is well-defined, $\mu'(t)=0$. However, at $t=t_i$ there exists a jump discontinuity so that we cannot define classical derivative and thus we use the δ-function, $\mu'(t-t_i)=\delta(t-t_i)$ to obtain the follow results.

Proposition 3.2: Let $M=M_0\times_f H$ be the FRW space–time with Riemannian curvature R and flow vector field $U=\partial_t$. If $f\in C^0(S)$, vector fields X, Y, $Z\in\mathfrak{L}(H)$ then satisfy
(i)

$$R_{XY}Z=\frac{f'^2+k}{f^2}(\langle X,Z\rangle Y-\langle Y,Z\rangle X),$$

(ii)

$$R_{XU}U=\frac{f''}{f}X,$$

(iii)

$$R_{XY}U=0,$$

(iv)

$$R_{XU}Y=\frac{f''}{f}\langle X,Y\rangle U,$$

where f' and f'' are given by

$$f'=\left(f^{(n)\prime}-f^{(n-1)\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime}\right)\mu(t-t_n)+\sum_{l=1}^{n-1}\left(-f^{(l-1)\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime}\right)\mu(t-t_l)$$
$$+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime}\mu(t_n-t)+\sum_{l=1}^{n-1}\left(-f^{(l)\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime}\right)\mu(t_l-t), \tag{3}$$

$$f''=\left(f^{(n)\prime\prime}-f^{(n-1)\prime\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime\prime}\right)\mu(t-t_n)+\sum_{l=1}^{n-1}\left(-f^{(l-1)\prime\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime\prime}\right)\mu(t-t_l)$$
$$+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime\prime}\mu(t_n-t)+\sum_{l=1}^{n-1}\left(-f^{(l)\prime\prime}+\frac{1}{n}\sum_{k=0}^{n-1}f^{(k)\prime\prime}\right)\mu(t_l-t)+(f^{(n)\prime}-f^{(n-1)\prime})\delta(t-t_n)$$
$$+\sum_{l=1}^{n-1}(f^{(l)\prime}-f^{(l-1)\prime})\delta(t-t_l), \tag{4}$$

with $\mu(t-t_i)$ and $\delta(t-t_i)$ being the unit step function and the delta function, respectively.

Proof: Similar to (1) in Proposition 3.1, one can readily obtain f'. Differentiating f' with respect to t and using the definition of the delta function $\mu'(t-t_i)=\delta(t-t_i)$ at $t=t_i$, one can also obtain f''. □

Proposition 3.3: Let $M=M_0\times_f H$ be the FRW space–time with Riemannian curvature R and flow vector field $U=\partial_t$. If $f\in C^0(S)$ and X, $Y\in\mathfrak{L}(H)$, then Ricci curvature is given by

(i)

$$\mathrm{Ric}(U,U) = -\frac{3f''}{f},$$

(ii)

$$\mathrm{Ric}(U,X) = 0,$$

(iii)

$$\mathrm{Ric}(X,Y) = \left(\frac{2(f'^2+k)}{f^2} + \frac{f''}{f}\right)\langle X,Y\rangle, \quad \text{if } X,Y \perp U,$$

where f' and f'' are given by (3) and (4).

Proposition 3.4: Let $M = M_0 \times_f H$ be the FRW space–time with Riemannian curvature R and flow vector field $U = \partial_t$. If $f \in C^0(S)$, the Einstein scalar curvature is given by

$$R = 6\left(\frac{f'^2}{f^2} + \frac{f''}{f} + \frac{k}{f^2}\right),$$

where f' and f'' are given by (3) and (4).

Proposition 3.5: For every plane containing a vector field of $U = \partial_t$, if $f \in C^0(S)$ and X, $Y \in \mathfrak{L}(H)$, we have a sectional curvature K on the space–time (M, g) for an arbitrary plane containing a vector field of $U = \partial_t$ and $W = \alpha U + \beta Y$,

$$K(W,X) = \frac{-\alpha^2 f'' + \beta^2(f'+k)}{(-\alpha^2+\beta^2)f^2},$$

where f' and f'' are given by (3) and (4).

Proof: The result follows $K(W,X) = g(R_{WX}W,X)/g(W,W)g(X,X) - [g(W,X)]^2$ of the non-degenerate 2-plane with basis (W,X). □

IV. COSMOLOGY OF SPATIALLY FLAT FRW METRIC WITH DOUBLE DISCONTINUITIES

In the spatially flat FRW cosmology with $k = 0$, the early universe was radiation dominated, the adolescent universe was matter dominated, and the present universe is now entering into lambda-dominate phase in the absence of vacuum energy. If the universe underwent inflation, there was a very early period when the stress-energy was dominated by vacuum energy. The Friedmann equation may be integrated to give the age of the universe in terms of present cosmological parameters. We have the scale factor f as a function of time t which scales as $f(t) \propto t^{1/2}$ for a radiation-dominated (RD) universe, and scales as $f(t) \propto t^{2/3}$ for a matter-dominated (MD) universe, and scales as $f(t) \propto e^{Kt}$ for a lambda-dominated (LD) universe. Note that the transition from the radiation-dominated phase to the matter-dominated is not an abrupt one; neither is the latter transition from the matter-dominated phase to the exponentially growing lambda-dominated phase.

With the above astrophysical phenomenology in mind, consider the spatially flat FRW space–time (M, g) with metric $g = -\mathrm{d}t^2 + f^2(t)\mathrm{d}\sigma^2$ in the form of warped products. Let $M = M_0 \times_f H$ be a warped product with $g_{M_0} = -\mathrm{d}t^2$.

Definition 4.1: A C^0-Lorentzian metric on M is a nondegenerate (0,2) tensor of Lorentzian signature such that

(i) $g \in C^0$ on S
(ii) $g \in C^\infty$ on $M \cap S^c$

(iii) for all $p \in S$, and $U(p)$ partitioned by S, $g|_{U_p^+}$ and $g|_{U_p^-}$ have smooth extensions to U. We call S a C^0-singular hypersurface of (M,g).

Consider M_0 as a C^0-singular hypersurface of (M,g). In the spatially flat FRW space–time, $f>0$ is smooth functions on $M_0=(t_0, t_\infty)$ except at $t\neq t_i$ $(i=1,2)$, that is $f\in C^\infty(S)$ (where $S=\{t_i\}\times_f H$) for $t\neq t_i$ and $f\in C^0(S)$ at $t=t_i\in M_0$ to yield

$$f=\begin{pmatrix} f^{(0)}=c_0t^{1/2}, & \text{for } t<t_1 \\ f^{(1)}=c_1t^{2/3}, & \text{for } t_1\leqslant t\leqslant t_2 \\ f^{(2)}=c_2e^{Kt}, & \text{for } t>t_2 \end{pmatrix} \tag{5}$$

with the boundary conditions

$$c_0t_1^{1/2}=c_1t_1^{2/3}, \quad c_1t_2^{2/3}=c_2e^{Kt_2}. \tag{6}$$

Experimental values for t_1 and t_2 are given by $t_1=4.7\times10^4$ yr and $t_2=9.8$ Gyr.[15] Moreover c_1 and c_2 are given in terms of c_0, t_1 and t_2 as follows:

$$c_1=c_0t_1^{-1/6}, \quad c_2=c_0t_1^{-1/6}t_2^{2/3}e^{-Kt_2}.$$

Note that in the spatially flat FRW model, $f\in C^0(S)$ since if we assume $f\in C^1(S)$ one could have the boundary conditions $\frac{1}{2}c_0t_1^{-1/2}=\frac{2}{3}c_1t_1^{-1/3}$ and $\frac{2}{3}c_1t_2^{-1/3}=Kc_2e^{Kt_2}$, which cannot satisfy the above boundary conditions (6) simultaneously.

Proposition 4.2: Let $M=M_0\times H$ be the spatially flat FRW space–time with Riemannian curvature R, flow vector field $U=\partial_t$ and warping function $f\in C^0(S)$. For vector fields X, Y, $Z\in\mathfrak{L}(H)$ we have

(i)

$$R_{XY}Z=\frac{f'^2}{f^2}(\langle X,Z\rangle Y-\langle Y,Z\rangle X),$$

(ii)

$$R_{XU}U=\frac{f''}{f}X,$$

(iii)

$$R_{XY}U=0,$$

(iv)

$$R_{XU}Y=\frac{f''}{f}\langle X,Y\rangle U,$$

where f is given by (5) and f' and f'' are given by

$$\begin{aligned} f'=&(\tfrac{1}{4}c_0t^{-1/2}-\tfrac{1}{3}c_1t^{-1/3}+Kc_2e^{Kt})\mu(t-t_2)+(-\tfrac{1}{4}c_0t^{-1/2}+\tfrac{1}{3}c_1t^{-1/3})\mu(t-t_1)\\ &+(\tfrac{1}{4}c_0t^{-1/2}+\tfrac{1}{3}c_1t^{-1/3})\mu(t_2-t)+(\tfrac{1}{4}c_0t^{-1/2}-\tfrac{1}{3}c_1t^{-1/3})\mu(t_1-t), \end{aligned} \tag{7}$$

$$f''=(-\tfrac{1}{8}c_0t^{-3/2}+\tfrac{1}{9}c_1t^{-4/3}+K^2c_2e^{Kt})\mu(t-t_2)+(\tfrac{1}{8}c_0t^{-3/2}-\tfrac{1}{9}c_1t^{-4/3})\mu(t-t_1)+(-\tfrac{1}{8}c_0t^{-3/2}-\tfrac{1}{9}c_1t^{-4/3})\mu(t_2-t)+(-\tfrac{1}{8}c_0t^{-3/2}+\tfrac{1}{9}c_1t^{-4/3})\mu(t_1-t)+(-\tfrac{2}{3}c_1t^{-1/3}+Kc_2e^{Kt})\delta(t-t_2)+(-\tfrac{1}{2}c_0t^{-1/2}+\tfrac{2}{3}c_1t^{-1/3})\delta(t-t_1), \tag{8}$$

with $\mu(t-t_i)$ and $\delta(t-t_i)$ being the unit step function and the delta function, respectively.

Proof: Substituting f in (5) into (3) and (4) in Proposition 3.2, one can readily obtain (7) and (8). □

Proposition 4.3: Let $M=M_0\times H$ be the spatially flat FRW space–time with Riemannian curvature R, flow vector field $U=\partial_t$ and warping function $f\in C^0(S)$. For vector fields X, Y, $Z\in\mathfrak{L}(H)$, the Ricci curvature is given by

(i)

$$\mathrm{Ric}(U,U)=-\frac{3f''}{f},$$

(ii)

$$\mathrm{Ric}(U,X)=0,$$

(iii)

$$\mathrm{Ric}(X,Y)=\left(\frac{2f'^2}{f^2}+\frac{f''}{f}\right)\langle X,Y\rangle, \quad \text{if } X,Y\perp U,$$

where f, f', and f'' are given by (5), (7), and (8), respectively.

Proposition 4.4: Let $M=M_0\times H$ be the spatially flat FRW space–time with Riemannian curvature R, flow vector field $U=\partial_t$ and warping function $f\in C^0(S)$. The Einstein scalar curvature is then given by

$$R=6\left(\frac{f'^2}{f^2}+\frac{f''}{f}\right),$$

where f, f', and f'' are given by (5), (7), and (8), respectively.

Proposition 4.5: For every plane containing a vector field of $U=\partial_t$ and $f\in C^0(S)$, if X, $Y\in\mathfrak{L}(H)$ we have a sectional curvature K on the FRW space–time (M, g) for an arbitrary plane containing a vector field of $U=\partial_t$ and $W=\alpha U+\beta Y$,

$$K(W,X)=\frac{-\alpha^2f''+\beta^2f'}{(-\alpha^2+\beta^2)f^2},$$

where f, f', and f'' are given by (5), (7), and (8), respectively.

Proposition 4.6: Let $M=M_0\times H$ be the spatially flat FRW space–time with Riemannian curvature R, flow vector field $U=\partial_t$ and warping function $f\in C^0(S)$. The evolution equations are then given by

(i)

$$\frac{3f'^2}{f^2}=8\pi\rho+\Lambda,$$

(ii)

$$\frac{3f''}{f} = -4\pi(\rho + 3P) + \Lambda,$$

where f, f', and f'' are given by (5), (7), and (8), respectively. Here ρ, P, and Λ are the mass density and pressure of matter and the cosmological constant.

Proof: Consider the Einstein equation,

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = R_{\mu\nu} - \tfrac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi T_{\mu\nu}, \tag{9}$$

where $G_{\mu\nu}$ is the Einstein tensor, and $T_{\mu\nu}$ is the stress-energy tensor for all the field present-matter, radiation and so on. To be consistent with the symmetries of the metric, the total stress-energy tensor $T_{\mu\nu}$ must be diagonal, and by isotropy the spatial components must be equal. The simplest realization of such a stress-energy tensor is that of a perfect fluid characterized by a time-dependent energy density $\rho(t)$ and pressure $p(t)$,

$$T^{\mu}_{\nu} = \mathrm{diag}(\rho, -p, -p, -p). \tag{10}$$

Substituting (10) into (9), together with the Ricci and Einstein curvatures given in Proposition 4.3 and Proposition 4.4, one can readily obtain the above evolution equations. □

Remarks 4.7: The $\mu = 0$ component of the conservation of stress-energy tensor, $T^{\mu\nu}_{;\nu} = 0$, gives the first law of thermodynamics of the familiar form $d(\rho f^3) = -p\,d(f^3)$ or equivalently, $d[f^3(\rho + p)] = f^3\,dp$. The change in energy in a co-moving volume element, $d(\rho f^3)$, is equal to minus the pressure times the change in volume element, $-p\,d(f^3)$. For the simple equation of state $p = \omega\rho$, where ω is independent of time, the energy density evolves as $\rho \propto f^{-3(1+\omega)}$. Examples of interest include: radiation ($p = \frac{1}{3}\rho$, $\rho \propto f^{-4}$), matter ($p = 0$, $\rho \propto f^{-3}$), and vacuum energy ($p = -\rho$, $\rho \propto$ const) phases.

V. CONCLUSIONS

We have considered the FRW cosmological model in the warped product scheme to investigate the nonsmooth curvature associated with the multiple discontinuities involved in the evolution of the universe. In particular we have analyzed the nonsmooth features of the spatially flat FRW universe by introducing double discontinuities occurred at the radiation-matter and matter-lambda phase transitions in the astrophysical phenomenology.

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On the classification of type D space–times

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We give a classification of the type D space–times based on the invariant differential properties of the Weyl principal structure. Our classification is established using tensorial invariants of the Weyl tensor and, consequently, besides its intrinsic nature, it is valid for the whole set of the type D metrics and it applies on both, vacuum and nonvacuum solutions. We consider the Cotton-zero type D metrics and we study the classes that are compatible with this condition. The subfamily of space–times with constant argument of the Weyl eigenvalue is analyzed in more detail by offering a canonical expression for the metric tensor and by giving a generalization of some results about the nonexistence of purely magnetic solutions. The usefulness of these results is illustrated in characterizing and classifying a family of Einstein–Maxwell solutions. Our approach permits us to give intrinsic and explicit conditions that label every metric, obtaining in this way an operational algorithm to detect them. In particular a characterization of the Reissner–Nordström metric is accomplished. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Type D space–times have been widely considered in literature and we can point out not only the large number of known families of exact solutions but also the interest of these solutions from the physical point of view. Let us quote, for example, the Schwarszchild or the Kerr metrics which model the exterior gravitational field produced, respectively, by a nonrotating or a rotating spherically symmetric bounded object. Or also the related metrics in the case of a charged object, the Reissner–Nordström or the Kerr–Newman solutions. However, although some classes of type D metrics have been considered taking into account algebraic properties of the Weyl eigenvalue or differential conditions on the null Weyl principal directions, a classification of the type D solutions involving all the first-order differential properties of the Weyl tensor geometry is a task which has not been totally accomplished yet. In this work we present this classification of the type D metrics and we show the role that it can play in studying geometric properties of known space–times, in looking for new solutions of Einstein equations or in offering new elements which allow us to give intrinsic and explicit characterizations of all these space–times.

At an algebraic level, a type D Weyl tensor determines a complex scalar invariant, the eigenvalue, and a $2+2$ almost-product structure defined by its principal 2–planes. Some classes of type D metrics can be considered by imposing the real or imaginary nature of the Weyl eigenvalue. In this way we find the so-called purely electric or purely magnetic space–times. The purely electric character often appears as a consequence of usual geometric or physical restrictions.[1] This is the case of the static type D vacuum spacetimes found by Ehlers and Kundt,[2] or the Barnes degenerate perfect fluid solutions with shear-free normal flow.[3] On the other hand, some restrictions are

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known on the existence of purely magnetic solutions.[4,5] A wide bibliography about Weyl-electric and Weyl-magnetic space–times can be found in a recent work[6] where these concepts have been generalized.

The most usual approaches to look for exact solutions of the Einstein equations work in frames or local coordinates adapted to some outlined direction of the curvature tensor. For example, in the case of perfect fluid solutions or static metrics the $3+1$ formalism adapted, respectively, to the fluid flow or to the normal timelike Killing vector can be useful. Sometimes one considers that some of the kinematic coefficients associated with the unitary vector are zero. This means that one is searching for new solutions belonging to a class of metrics that are defined by first-order differential conditions imposed on the curvature tensor. A similar situation appears when local coordinates adapted to the multiple Debever direction are considered when looking for algebraically special solutions. Indeed, if the hypotheses of the generalized Goldberg–Sachs theorem hold, the multiple Debever direction defines a shear-free geodesic null congruence. In this case, or when considering nondiverging or nontwisting restrictions on a Debever direction, we are imposing differential conditions on the Weyl tensor.

It is worth pointing out that the kinematic coefficients associated with a unitary vector completely determine the first-order differential properties of the $1+3$ almost-product structure that it defines. Nevertheless, the conditions usually imposed on the two double Debever directions of a type D space–time do not cover all the differential properties of the principal $2+2$ almost-product structure of the Weyl tensor exhaustively. The first goal of this work is to offer a classification of the type D metrics based on all the first-order differential properties of the principal structure, and to reinterpret under this view the usual conditions that can be found in the literature. This classification is not based on the scalar invariants, but on tensorial invariants of the Weyl tensor. These invariants are well adapted to the generic type D metrics, where a Weyl canonical frame is not univocally determined, and where the eigenvalues and the $2+2$ principal structure are the only invariants associated with the Weyl tensor.

The (proper) Riemannian almost-product structures have been classified according the invariant decomposition of their structure tensor,[7] and the classes have been interpreted in terms of the foliation, minimal and umbilical properties.[8] This classification can be generalized to the space–time structures by also considering the causal character of the planes.[9] Almost-product structures have shown their usefulness in studying the underlying geometry of some physical fields. The $1+3$ structures are frequently used in relativity and sometimes the properties of a physical field can be expressed in terms of the kinematic properties of a unitary vector.[10,11] On the other hand, the $2+2$ structure associated with a regular solution of Maxwell equations[12] is a basic concept in building the ''already unified theory'' for the electromagnetic field.[13] It has also allowed a geometric interpretation[14] of the Teukolsky–Press relations[15] used in analyzing incident electromagnetic waves on a Kerr black hole.

In General Relativity we can also find almost-product structures attached to the geometric or physical properties of the spacetime. Indeed, some energy contents (for example, in the Einstein–Maxwell or perfect fluid solutions) define underlying structures that restrict, via Einstein equations, the Ricci tensor. On the other hand, the Weyl tensor also defines almost-product structures associated with its principal bivectors depending on the different Petrov types.[16] These structures determine the Weyl canonical frames.[17] In the type D case, only the *principal structure* is outlined.

Until now we have mentioned two different ways of classifying the type D space–times: The first one is strictly algebraic and takes into account the real or imaginary character of the Weyl eigenvalues; the second one, which we will present here, involves differential conditions of the $2+2$ principal structure, that is, on the Weyl eigenvectors. Nevertheless, there is a third natural manner to impose restrictions on the type D metrics: To take into account the relative position between the principal 2–planes and the gradient of the Weyl scalar invariants. This is a mixed classification, differential in the eigenvalues and algebraic in the principal structure, which affords 16 different classes of type D metrics. In this work we will show the marked relation that exists between this classification and the two previous ones.

A classification of type D space–times taking into account the properties of the $2+2$ principal

structure shows quite interesting advantages. Indeed, the integration of the static type D vacuum equations using an alternative approach based on the Weyl principal structure has allowed us to complete the results by Ehlers and Kundt[2] in order to accomplish an algorithmic and intrinsic identification of the solutions and, in particular, to obtain the equations that define the Schwarzschild space–time explicitly.[18] Moreover, our classification affords a geometric interpretation of the other families of vacuum type D solutions. Starting from this approach two Killing vectors can be determined in terms of Weyl concomitants,[19] a result which shows that a commutative bidimensional group of isometries exists. Although all the type D vacuum solutions were found by Kinnersley[20] a integration method based on our classification permits their intrinsic label, as well as a geometric interpretation of the NUT and acceleration parameters.[21]

In this work we apply our classification to the study of space–times with zero Cotton tensor. For them, the Bianchi identities impose the same restrictions on the Weyl tensor as the vacuum condition. We interpret these restrictions in terms of geometric properties of the principal structure and we show that the compatible classes can be characterized in terms of the relative position between the gradient of some invariant scalars and the principal 2–planes. From a physical point of view these metrics have two interesting properties. Firstly, the two double Debever directions define shear-free geodesic null congruences and, secondly, the principal structure is Maxwellian. This result can be of interest in order to generalize the Teukolsky–Press relations[14,15] and their applications to type D nonvacuum solutions.

In order to show the usefulness of this approach in analyzing properties of known metrics, in integrating Einstein equations and in labeling the solutions, here we study the space–times with the two properties quoted above for the particular classes with integrable structure. In this case, the space–time metric turns out to be conformal to a product metric. Then, as a first consequence, we extend the result by Hall[4] (see also McIntosh *et al.*[5]) concerning the nonexistence of purely magnetic type D vacuum solutions in a double sense: The family of solutions where the new result applies is wider than the vacuum metrics, and the purely magnetic restriction is weakened to an arbitrary constant argument. Elsewhere[22] we have acquired a similar extension for some results concerning the purely magnetic type I solutions. Moreover, starting from a canonical form we begin on the integration of the Einstein–Maxwell equations for the compatible classes, and we recover the charged counterpart of the A, B, C vacuum metrics by Ehlers and Kundt. The integration method at once provides an algorithm to detect the solutions with intrinsic and explicit conditions and, in particular, it offers a characterization of the Reissner–Nordström space–time. The classification of the Kinnersley rotating type D vacuum solutions will be considered elsewhere.[21]

The paper is organized as follows. In Sec. II we introduce some definitions and notations and we give some results about $2+2$ almost-product structures. In Sec. III we present the classification of the type D metrics based on the first-order differential properties of the Weyl principal structure, as well as the mixed classification involving the eigenvalues gradient and the principal structure. The Cotton-zero type D metrics are analyzed in Sec. IV, and we show that the principal 2–planes define an umbilical structure and, consequently, we only have 16 compatible classes which coincide precisely with those defined by the mixed classification. The four classes with integrable structure are studied in detail in Sec. V: We present a canonical form for them and generalize a result about the nonexistence of purely magnetic solutions. Finally, in Sec. VI, we apply our results to recover a family of Einstein–Maxwell solutions, to give an operational algorithm to detect them and to explicitly and intrinsically characterize the Reissner–Nordström space–time. Some of the results in this paper were communicated without proof at the Spanish Relativity Meeting–96.[19]

II. SPACE–TIME ALMOST-PRODUCT STRUCTURES

On a Riemannian manifold (M,g) an almost-product structure is defined by a p-plane field V and its orthogonal complement H. Let v and $h=g-v$ the respective projectors, and let Q_v be the (2,1)-tensor:

$$Q_v(x,y)=h(\nabla_{vx}vy)\,,\quad \forall\ x,y. \tag{1}$$

Let us consider the invariant decomposition of Q_v into its antisymmetric part A_v and its symmetric part $S_v\equiv S_v^T+(1/p)\,v\otimes \mathrm{Tr}S_v$, where S_v^T is a traceless tensor:

$$Q_v=A_v+\frac{1}{p}v\otimes \mathrm{Tr}\ S_v+S_v^T. \tag{2}$$

The plane V is foliation if, and only if, $A_v=0$. In this case $Q_v=S_v$ and it coincides with the second fundamental form of the integral manifolds of the foliation V.[23] Moreover V is minimal, umbilical or geodesic if, and only if, Tr $S_v=0$, $S_v^T=0$ or $S_v=0$, respectively. Then one can generalize these geometric concepts for plane fields which are not necessarily foliation:

Definition 1: *A plane field V is said to be geodesic, umbilical or minimal if the symmetric part* S_v *of its (generalized) second fundamental form* Q_v *satisfies, respectively,* $S_v=0$, $S_v^T=0$ *or* Tr $S_v=0$.

The (proper) Riemannian almost-product structures (V,H) have been classified taking into account the invariant decomposition (2) of the tensors Q_v and Q_h or, equivalently, according with the foliation, minimal, umbilical, or geodesic character of each plane.[7,8] Some of these properties have also been interpreted in terms of invariance along vector fields.[24] A generalization for the spacetime structures follows taking into account the causal character of the planes. We will say that a structure is integrable when both planes are foliation and we will say that it is minimal, umbilical or geodesic if both of the planes are so.

This way, on an oriented space–time (V_4,g) of signature $(-+++)$ we have generically $2^6=64$ different classes of (almost-product) structures depending on the first-order geometric properties. Nevertheless, when $p=1$, V is always an umbilical foliation and, consequently, only 16 possible classes exist. In this case Q_v and Q_h depend on the kinematic coefficients associated with a unitary vector u, and the classes are defined by the vanishing or nonvanishing of the acceleration, rotation, shear, and expansion. Elsewhere this kinematical interpretation has been extended to the $2+2$ space–time structures and, as a consequence, the Maxwell–Rainich equations have been expressed in terms of kinematical variables.[9]

In order to be used in next sections, we now analyze the space–time $2+2$ almost-product structures in detail by giving the characterization of their properties in terms of their canonical 2–form U, and by showing their relation with other usual approaches, the Newmann–Penrose and the self-dual formalisms. We also study the change of these properties for a conformal transformation and we summarize some results about Maxwellian structures.

A. 2+2 structures

In the case of a $2+2$ space–time structure it is useful to work with the *canonical* unitary 2-form U, volume element of the time-like plane V. Then, the respective projectors are $v=U^2$ and $h=-(*U)^2$, where $U^2=U\times U=\mathrm{Tr}_{23}\ U\otimes U$ and $*$ is the Hodge dual operator.

The tensors Q_v and Q_h determine the derivatives of the volume elements U and $*U$ by means of

$$\nabla_\alpha U_{\beta\lambda}=(Q_v)_{\alpha\mu,[\beta}U^{\mu}{}_{\lambda]}+(Q_h)_{\alpha[\beta,}{}^{\mu}\ U_{\lambda]\mu}\,,$$

$$\nabla_\alpha *U_{\beta\lambda}=(Q_h)_{\alpha\mu,[\beta}*U^{\mu}{}_{\lambda]}+(Q_v)_{\alpha[\beta,}{}^{\mu}*U_{\lambda]\mu}\,. \tag{3}$$

Then, if we denote $\delta=-\mathrm{Tr}\ \nabla$, a straightforward calculation leads to

$$\delta U=i(\mathrm{Tr}\ S_h)U-2(U,A_v)\qquad \delta *U=i(\mathrm{Tr}\ S_v)*U-2(*U,A_h), \tag{4}$$

where $2(U,A_v)^\mu=U^{\alpha\beta}(A_v)_{\alpha\beta}{}^{\mu}$. So, the minimal and the foliation character of the planes can be stated in terms of the projections of δU and $\delta *U$ onto V and H. On the other hand, let us consider

$$G_\perp = U\otimes U - *U\otimes *U + G; \quad \eta_\perp = U\tilde{\otimes} *U + \eta, \tag{5}$$

where η is the metric volume element of the space–time, $G=\frac{1}{2}g\owedge g$ is the metric on the 2–forms space, and $\owedge$ denotes the double-forms exterior product, $(A\owedge B)_{\alpha\beta\mu\nu}=A_{\alpha\mu}B_{\beta\nu}+A_{\beta\nu}B_{\alpha\mu}-A_{\alpha\nu}B_{\beta\mu}-A_{\beta\mu}B_{\alpha\nu}$. The tensors (5) satisfy $G_\perp(U)=G_\perp(*U)=0$, $\eta_\perp(U)=\eta_\perp(*U)=0$ and they can be calculated as

$$G_\perp = v\owedge h, \quad \eta_\perp = U\owedge *U. \tag{6}$$

Then, from expressions (3) and (4) we get

$$(2\nabla U - K)_{\lambda\alpha\beta} = (S_v^T)_{\lambda\mu,[\alpha}\ U^\mu{}_{\beta]} + (S_h^T)_{\lambda\mu,[\alpha}\ *U^\mu{}_{\beta]}, \tag{7}$$

$$K \equiv i(\delta U)G_\perp - i(\delta *U)\eta_\perp, \tag{8}$$

and so, the umbilicity of each plane is equivalent to the vanishing of the respective projections of the first member of (7). We summarize these results in the following lemma:

Lemma 1: *Let* (V,H) *be a* $2+2$ *almost-product structure and let* U *be its canonical 2-form. Then, the following conditions hold*:

(1) V $(resp.\ H)$ *is foliation* $\Leftrightarrow i(\delta U)*U=0$ $(resp.\ i(\delta *U)U=0)$;
(2) V $(resp.\ H)$ *is minimal* $\Leftrightarrow i(\delta *U)*U=0$ $(resp.\ i(\delta U)U=0)$;
(3) V *is umbilical* $\Leftrightarrow U\times\{2\nabla U-[i(\delta U)G_\perp - i(\delta *U)\eta_\perp]\}=0$
H *is umbilical* $\Leftrightarrow *U\times\{2\nabla U-[i(\delta U)G_\perp - i(\delta *U)\eta_\perp]\}=0$.

A $2+2$ structure is also determined by the two null directions $l_\pm$ on the plane V. A family of complex null bases $\{l_+, l_-, m, \overline{m}\}$ exists such that $U=l_-\wedge l_+$. This family is fixed up to change $l_\pm \hookrightarrow e^{\pm\phi}l_\pm$, $m\hookrightarrow e^{i\theta}m$. Then, conditions of lemma 1 can be interpreted in terms of the Newman–Penrose coefficients[25] as

Lemma 2: *Let* $U=l_-\wedge l_+$ *be the canonical 2–form of a* $2+2$ *structure. It holds*:

(1) The plane V is umbilical iff $\kappa=0=\nu$;
(2) the plane H is umbilical iff $\lambda=0=\sigma$;
(3) the plane V is minimal iff $\overline{\pi}=\tau$;
(4) the plane H is minimal iff $\rho+\overline{\rho}=0=\mu+\overline{\mu}$;
(5) the plane V is a foliation iff $\overline{\pi}=-\tau$;
(6) the plane H is a foliation iff $\rho-\overline{\rho}=0=\mu-\overline{\mu}$.

Taking into account the significance of the NP coefficients[25] this lemma implies that the umbilical nature of a $2+2$ structure means that its principal directions $l_\pm$ define shear-free geodesic null congruences. The minimal or foliation character of the spacelike 2-plane have also a kinematical interpretation and state, respectively, that both principal directions are expansion-free or vorticity-free. Elsewhere[9] all the geometric properties have been interpreted in terms of kinematic coefficients associated with every direction in a 2–plane (not only the null ones) with respect to the other 2–plane.

When both planes have a specific differential property, it is more convenient to introduce the self-dual unitary 2–form $\mathcal{U}\equiv(1/\sqrt{2})\,(U-i*U)$ associated with U. We have

$$2\ \mathrm{Re}[i(\delta\mathcal{U})\mathcal{U}] = i(\delta U)U - i(\delta *U)*U \equiv \Phi(U),$$

$$2\ \mathrm{Im}[i(\delta\mathcal{U})\mathcal{U}] = -i(\delta U)*U - i(\delta *U)U \equiv \Psi(U). \tag{9}$$

So, the complex 1–form $\delta\mathcal{U}$ collects the information about the minimal and foliation character of the structure. On the other hand, if $\mathcal{G}=\frac{1}{2}(G-\mathrm{i}\eta)$ is the metric on the self-dual 2–forms space, and $\mathcal{K}\equiv(1/\sqrt{2})(K-\mathrm{i}*K)$ is the self-dual 2-form associated to the vector valued 2–form K given in (8), we have

$$\mathcal{K}=i(\delta\mathcal{U})[\mathcal{U}\otimes\mathcal{U}+\mathcal{G}]. \tag{10}$$

Consequently, from lemma 1 and Eqs. (9) and (10), we have

Lemma 3: *Let us consider the* $2+2$ *structure defined by* $\mathcal{U}=(1/\sqrt{2})(U-\mathrm{i}*U)$. *It holds*:

(1) The structure is minimal if, and only if, $\mathrm{Re}[i(\delta\mathcal{U})\mathcal{U}]=0$;
(2) the structure is integrable if, and only if, $\mathrm{Im}[i(\delta\mathcal{U})\mathcal{U}]=0$;
(3) the structure is umbilical, if, and only if, $\nabla\mathcal{U}=i(\delta\mathcal{U})[\mathcal{U}\otimes\mathcal{U}+\mathcal{G}]$.

B. Almost-product structures and conformal transformations

If (V,H) is a $p+q$ almost-product structure for a metric g, then (V,H) is also an almost-product structure for every conformal metric $\hat{g}=e^{2\lambda}g$, and the projectors are related by the conformal factor: If $g=v+h$, then $\hat{g}=\hat{v}+\hat{h}$, where $\hat{v}=e^{2\lambda}v$, $\hat{h}=e^{2\lambda}h$. The generalized second fundamental form change as

$$Q_{\hat{v}}=e^{2\lambda}\,(Q_v-v\otimes h(\mathrm{d}\lambda)). \tag{11}$$

So, the foliation and the umbilical character are conformal invariants, but the minimal character is not. Indeed, taking the trace of the expression above, we have

$$\mathrm{Tr}\;Q_{\hat{v}}=\mathrm{Tr}\;Q_v-ph(\mathrm{d}\lambda). \tag{12}$$

These expressions immediately lead to the following result.

Lemma 4: *Let* (V,H) *be a* $p+q$ *almost-product structure for a metric* $g=v+h$. *The structure* (V,H) *is minimal for a conformal metric* $\hat{g}=e^{2\lambda}g$ *if, and only if,*

$$\frac{1}{p}\mathrm{Tr}\;Q_v+\frac{1}{q}\mathrm{Tr}\;Q_h=\mathrm{d}\lambda. \tag{13}$$

If $p=q$ (as happens for the space–time $2+2$ structures), we conclude that the necessary and sufficient condition for a structure to be minimal for a conformal metric is the sum of the traces of the second fundamental forms to be a closed 1-form, $\mathrm{d}(\mathrm{Tr}\;Q_v+\mathrm{Tr}\;Q_h)=0$. Thus, taking into account (4) and the expression (9) for $\Phi(U)$, lemma 4 can be stated for the $2+2$ case as

Lemma 5: *Let* U *be the canonical 2–form of a* $2+2$ *structure for the space–time metric* g. *The structure is minimal for a conformal metric if, and only if,* $\mathrm{d}\Phi(U)=0$. *More precisely, when this condition hold, let* λ *be such that* $2\mathrm{d}\lambda=\Phi(U)$. *Then, the structure is minimal for the conformal metric* $\hat{g}=e^{2\lambda}g$.

The most degenerated class of almost-product structures are the product ones, which means, those that satisfy $Q_v=0=Q_h$. A metric that admits a product structure is called a product metric. Then, and only then, local coordinates (x^A,x^i), $A=0,1$, $i=2,3$, exist such that $\tilde{g}=\sigma^-+\sigma^+$, being $\sigma^-=\sigma^-_{AB}(x^C)\mathrm{d}x^A\mathrm{d}x^B$ and $\sigma^+=\sigma^+_{ij}(x^k)\mathrm{d}x^i\mathrm{d}x^j$ bidimensional metrics, hyperbolic and elliptic, respectively. Then, if $\tilde{g}$ is a *2+2* product metric and $g=e^{-2\lambda}\tilde{g}$, lemma 5 and expression (11) lead to the following result.

Lemma 6: *The necessary and sufficient condition for a metric* g *to be conformal to a product metric* $\tilde{g}$, *is that an integrable and umbilical almost-product structure* U *exists such that* $\mathrm{d}\Phi(U)=0$. *More precisely, if* $2\mathrm{d}\lambda=\Phi(U)$, *then* $\tilde{g}=e^{2\lambda}g$ *is a product metric*.

C. Maxwellian structures

A regular 2-form F takes the canonical expression $F=e^{\phi}[\cos\psi U+\sin\psi *U]$, where U defines the $2+2$ associated structure, ϕ is the *energetic index* and ψ is the *Rainich index*. When F is solution of the source-free Maxwell equations, $\delta F=0$, $\delta *F=0$, one says that U defines a *Maxwellian structure*. In terms of the canonical elements (U,ϕ,ψ), Maxwell equations become:[12,14]

$$\mathrm{d}\phi=\Phi(U)\equiv i(\delta U)U-i(\delta *U)*U, \tag{14}$$

$$\mathrm{d}\psi=\Psi(U)\equiv -i(\delta U)*U-i(\delta *U)U. \tag{15}$$

Then, from (14) and (15) the Rainich theorem[12] follows:

Lemma 7: *A unitary 2-form U defines a Maxwellian structure if, and only if, it satisfies*:

$$\mathrm{d}\Phi(U)=0; \qquad \mathrm{d}\Psi(U)=0. \tag{16}$$

The Maxwell–Rainich equations (14) and (15) have a simple expression in the self-dual formalism. Indeed, the self-dual 2–form $\mathcal{F}=(1/\sqrt{2})(F-\mathrm{i}*F)$ may be written as $\mathcal{F}=e^{\phi+\mathrm{i}\psi}\mathcal{U}$. Then, from Maxwell equations, $\delta\mathcal{F}=0$, and taking into account that $2\mathcal{U}^2=g$,

$$\mathrm{d}(\phi+\mathrm{i}\psi)=2i(\delta\mathcal{U})\mathcal{U}. \tag{17}$$

This last equation is equivalent to (14) and (15) if we take into account (9). Moreover, from here we recover the complex version of (16) easily

$$\mathrm{d}i(\delta\mathcal{U})\mathcal{U}=0. \tag{18}$$

III. CLASSIFYING TYPE D SPACE–TIMES

The self–dual Weyl tensor $\mathcal{W}=\frac{1}{2}(W-\mathrm{i}*W)$ of a type D space–time takes the canonical expression[17]

$$\mathcal{W}=3\alpha\mathcal{U}\otimes\mathcal{U}+\alpha\mathcal{G}, \tag{19}$$

where $\alpha=-\operatorname{Tr}\mathcal{W}^3/\operatorname{Tr}\mathcal{W}^2$ is the double eigenvalue and $\mathcal{U}$ is the self-dual principal 2–form. This principal 2–form defines a $2+2$ almost-product structure which is called the *principal structure* of a type D space–time. In terms of the canonical 2–form U of the principal structure the self-dual 2–form $\mathcal{U}$ becomes $\mathcal{U}=(1/\sqrt{2})(U-\mathrm{i}*U)$. So, at the algebraic level, a type D Weyl tensor only determines the complex scalar α and the principal structure U. Consequently, any generic classification of the type D metrics must depend on these invariants associated with the Weyl tensor.

The families of purely electric or purely magnetic type D spacetimes are defined, at first glance, by means of alternative conditions, namely, the nullity of the magnetic or the electric Weyl fields associated with an observer u. But, actually, they admit a simple intrinsic characterization in terms of the Weyl scalar invariant: The eigenvalue is real or imaginary.[5] In spite of these strong conditions, the family of Weyl-electric type D space–times contains quite interesting solutions. We can quote, for example, the static vacuum metrics[2] or the degenerate perfect fluids with shear-free normal flow.[3] All the type D silent universes are also known[26,27] as well as other families of purely electric type D perfect fluid solutions.[28,30] Nevertheless, few Weyl-magnetic type D solutions have been found,[29] and some restrictions about their existence are known. Indeed, there are not vacuum metrics with purely magnetic type D Weyl tensor.[4,5] The classification that we present below allows us to give an extension of this result in Sec. 5. On the other hand, the generalization of the purely electric or magnetic concepts to the spacelike or null directions does not afford new classes in the type D case.[6]

But the purely electric or magnetic properties define very narrow subsets of the generic type D metrics because they impose one of the two real scalar invariants to be zero. The large family of known solutions of the Einstein equation recommends us to consider other classifications, based

on less restrictive properties, which afford new intrinsic elements that increase the knowledge of the metrics and permit their explicit characterization. Besides the *intrinsic* nature, the classification must be *generic*, that is, valid for the whole set of the type D metrics. Consequently, it will be independent of the energy content and it will have to be built on the intrinsic geometry associated with a type D Weyl tensor.

The first classification that we propose is based on the geometric properties of the principal 2–planes, that is, it is induced by the geometric classification of the principal structure. Every principal 2–plane can be submitted or not to three properties, so $2^6=64$ classes can be considered.

Definition 2: *Taking into account the foliation, minimal, or umbilical character of each principal 2–plane we distinguish* 64 *different classes of type D space–times*.

We denote the classes as D^{pqr}_{lmn}, *where the superscripts* p,q,r *take the value 0 if the time-like principal plane is, respectively, a foliation, a minimal or an umbilical distribution, and they take the value 1 otherwise. In the same way, the subscripts* l,m,n *collect the foliation, minimal or umbilical nature of the space-like plane.*

The most degenerated class that we can consider is D^{000}_{000} which corresponds to a type D product metric, and the most regular one is D^{111}_{111} which means that neither V nor H are foliation, minimal or umbilical distributions. We will put a dot in place of a fixed script (1 or 0) to indicate the set of metrics that cover both possibilities. So, for example, the metrics of type $\mathrm{D}^{111}_{11\cdot}$ are the union of the classes D^{111}_{111} and D^{111}_{110}; or a metric is of type $\mathrm{D}^{0\,\cdot\,\cdot}_{\cdot\,\cdot\,\cdot}$ if the timelike 2–plane is a foliation.

Taking into account lemma 1, every class is defined by means of first-order differential equations imposed on the canonical 2–form U. On the other hand, U can be written explicitly in terms of the Weyl tensor[17] and, consequently, every class admits an intrinsic and explicit characterization.

The above classification depends on the derivatives of the principal 2–form U. An alternative classification at first order in the Weyl eigenvalues can also be considered by taking into account the four 1-forms defined by the principal 2–planes and the gradient of the modulus and the argument of the eigenvalue. So, we will have $2^4=16$ classes.

Definition 3: *Let* $\alpha=e^{\frac{3}{2}(\rho+\mathrm{i}\theta)}$ *be the Weyl eigenvalue. Taking into account the relative position between the gradients* $d\theta,d\rho$ *and each principal 2–plane we distinguish* 16 *different classes of type D* space–times.

We denote the classes $D[pq,rs]$ *where* p,q,r,s *take the values* 0 *or* 1 *to indicate, respectively, that one of the 1-forms* $U(d\theta),U(d\rho),{*}U(d\theta),{*}U(d\rho)$ *is zero or nonzero*.

The most degenerated class D[00;00] is occupied by the type D metrics with constant eigenvalues, and the most general one D[11;11] by those type D space–times for which both, the modulus and the argument of the Weyl eigenvalue, have nonzero projection onto the principal planes. As above, a dot means that a condition is not fixed. So, for example, we write $\mathrm{D}[0\cdot;\cdot\cdot]$ to indicate the type D metrics for which the argument of the eigenvalues have zero projection onto the timelike principal 2–plane.

The type D metrics with constant modulus, $d\rho=0$, correspond to the classes $D[\,\cdot 0;\cdot 0]$, and those with constant argument, $d\theta=0$, are the metrics of type $D[0\cdot;0\cdot]$. This last family contains the Weyl-electric and the Weyl-magnetic space–times because a real or imaginary eigenvalue means that the argument takes the constant value 0, π or $\pi/2$, $3\pi/2$, respectively.

In the next section we will show the marked relation between the two classifications given in definitions 2 and 3 when some usual restrictions are imposed on the Ricci tensor.

IV. TYPE D METRICS WITH ZERO COTTON TENSOR

The space–time Cotton tensor P is a vector valued 2–form which depends on the Ricci tensor as

$$P_{\mu\nu,\beta}\equiv\nabla_{[\mu}Q_{\nu]\beta},\qquad 2Q\equiv Ric-\tfrac{1}{6}(\mathrm{Tr}\,Ric)g. \tag{20}$$

The Bianchi identities equal the Cotton tensor with the divergence of the Weyl tensor. Indeed, if $\mathcal{W}$ is the self-dual Weyl tensor and $\mathcal{P}=\frac{1}{2}(P-\mathrm{i}*P)$ is the self-dual 2–form associated with the Cotton tensor, Bianchi identities become

$$\mathcal{P}=-\delta\mathcal{W}. \tag{21}$$

So, the vanishing of the Cotton tensor is equivalent to the Weyl tensor to be divergence free, $\delta\mathcal{W}=0$. Taking into account the canonical expression of a type D Weyl tensor (19), a straightforward calculation leads to the following:

Proposition 1: *Let $\mathcal{U}$ and $\alpha=-\operatorname{Tr}\mathcal{W}^3/\operatorname{Tr}\mathcal{W}^2$ be the principal 2–form and the double eigenvalue of a type D Weyl tensor. Then, the space–time Cotton tensor is zero if, and only if,*

$$\nabla\mathcal{U}=i(\delta\mathcal{U})[\mathcal{U}\otimes\mathcal{U}+\mathcal{G}] \quad ; \quad i(\delta\mathcal{U})\mathcal{U}=\tfrac{1}{3}\mathrm{d}\ln\alpha. \tag{22}$$

From the results of the previous section, we know that the first condition means that the principal structure is umbilical, that is, the principal directions are shear free null geodesics accordingly to the Goldberg–Sachs theorem. Consequently, every type D space–time with zero Cotton tensor is of type $\mathrm{D}^{\cdot\cdot 0}_{\cdot\cdot 0}$. The second equation in (22) shows that the principal structure is Maxwellian and the electromagnetic invariant scalars depend on the Weyl eigenvalue. If we take the real and the imaginary parts of this equation and write $\rho+\mathrm{i}\theta=\frac{2}{3}\ln\alpha$, we get

$$\Phi(U)=\mathrm{d}\rho \; ; \qquad \Psi(U)=\mathrm{d}\theta. \tag{23}$$

So the modulus and the argument of the Weyl eigenvalue govern, respectively, the minimal and the foliation character of the principal planes. This relation establishes a bijection between the classes of the two classifications that we have presented. More precisely, we have:

Theorem 1: *Every type D spacetime with zero Cotton tensor is of type $D^{\cdot\cdot 0}_{\cdot\cdot 0}$. Moreover, it is of class D^{pq0}_{lm0} if, and only if, it is of class $D[lm,pq]$.*

So we have just 16 classes of type D space–times with zero Cotton tensor and each one is characterized by the vanishing or not of the projections of the gradient of the Weyl eigenvalue onto the principal planes. The second condition in (22) implies that a solution of the Maxwell equations exists that has $\mathcal{U}$ as its associated structure. Then, taking into account the results of Sec. II C, it holds:

Proposition 2: *The principal structure of a type D space–time with zero Cotton tensor is Maxwellian. More precisely, if $\mathcal{U}$ and $\alpha=-\operatorname{Tr}\mathcal{W}^3/\operatorname{Tr}\mathcal{W}^2$ are the principal 2–form and the double eigenvalue of the Weyl tensor, the self–dual 2–form*

$$\mathcal{F}_M=\alpha^{2/3}\mathcal{U}, \tag{24}$$

is a solution of the source-free Maxwell equations, $\delta\mathcal{F}_M=0$.

In the following D(M) denotes the type D space–times with Maxwellian principal structure, and $\mathrm{D(M)}^{pqr}_{lmn}$ expresses the type D(M) space–times of class D^{pqr}_{lmn}. With this notation, from theorem 1 and proposition 2 it follows: *Every type D space–time with zero Cotton tensor is of type $D(M)^{\cdot\cdot 0}_{\cdot\cdot 0}$.*

It is worth pointing out that the family of type D metrics admitting a conformal Killing–Yano tensor attached to its principal structure are those of type $\mathrm{D(M)}^{\cdot\cdot 0}_{\cdot\cdot 0}$,[31] and this family includes the Cotton-zero type D metrics.

The results of this section have been used elsewhere[21] in offering a new approach to the Kinnersley type D vacuum solutions. An integration of the Einstein vacuum equations based on the classification given above permits the explicit and intrinsic labeling of the solutions as well as to put over interesting geometric properties of these space–times.

V. SOME RESULTS ABOUT TYPE $D(M)^{0\cdot 0}_{0\cdot 0}$ SPACE–TIMES

Now, in this section, we restrict our study to the type D metrics with Maxwellian, integrable and umbilical structure, that is, those of type $D(M)^{0\cdot 0}_{0\cdot 0}$. We can easily obtain a canonical form for these metrics. Indeed, lemma 6 states that the metric is conformal to a product one with a conformal factor determined by the potential of the closed 1–form $\Phi(U)$. More precisely, the metric can be written as

$$g=\frac{1}{\Omega^2}[\sigma^-_{AB}(x^C)\ dx^A dx^B+\sigma^+_{ij}(x^k)\ dx^i dx^j], \tag{25}$$

where Ω satisfies

$$2\ \mathrm{d}\ln\Omega=\Phi(U)\equiv i(\delta U)U-i(\delta *U)*U. \tag{26}$$

Conversely, we can analyze the Petrov type of the metric (25) by studying a product metric $\tilde{g}=\sigma^-+\sigma^+$. Let X_- and X_+ be the Gaussian curvatures of the arbitrary bidimensional metrics, σ^- and σ^+, hyperbolic and elliptic, respectively. The Gauss–Codazzi equations show that the Riemann and the Ricci tensors of $\tilde{g}$ are

$$Riem(\tilde{g})=\tfrac{1}{2}X_-\sigma^-\owedge\sigma^-+\tfrac{1}{2}X_+\sigma^+\owedge\sigma^+;\quad Ric(\tilde{g})=X_-\sigma^-+X_+\sigma^+. \tag{27}$$

So, the Weyl tensor of a product metric is Petrov-type O precisely when $X_-+X_+=0$, and then both curvatures are constant. On the other hand, when $X_-+X_+\neq 0$, the space–time is type D. Moreover U determines the principal structure and the double eigenvalue is given by

$$\tilde{\alpha}=-\tfrac{1}{6}(X_-+X_+). \tag{28}$$

So, we have

Lemma 8: *Every* $2+2$ *product metric* $\sigma^-+\sigma^+$ *is of type D* (*or O*) *with real eigenvalues, and the double eigenvalue is given by (28), where* X_- *and* X_+ *are the Gaussian curvatures of* σ^- *and* σ^+, *respectively. Moreover, it is of type O if, and only if,* $X_-=-X_+=constant$.

A conformal transformation $\tilde{g}=\Omega^2 g$ preserves the Petrov type and the Weyl eigenvalues change as $\tilde{\alpha}=\Omega^{-2}\ \alpha$. Consequently, from Eq. (26) and taking into account lemmas 1 and 8, we can conclude:

Proposition 3: *A space–time is of type* $D(M)^{0\cdot 0}_{0\cdot 0}$ *if, and only if, there exist local coordinates such that the metric g takes the expression (25) with* $X_-+X_+\neq 0$, *where* X_- *and* X_+ *are the Gaussian curvatures of* σ^- *and* σ^+, *respectively. Moreover, it is of class* D^{010}_{010}, D^{000}_{010}, D^{010}_{000}, *or* D^{000}_{000} *if, and only if,* $\sigma^-(d\Omega)\neq 0\neq\sigma^+(d\Omega)$, $\sigma^+(d\Omega)=0\neq\sigma^-(d\Omega)$, $\sigma^+(d\Omega)\neq 0=\sigma^-(d\Omega)$, *or* $d\Omega=0$, *respectively*.

Furthermore, taking into account the expressions (27) for the Ricci and (28) for the eigenvalue of a product metric, and considering the change of these metric concomitants for a conformal transformation, we can state:

Proposition 4: *The Weyl eigenvalue of the metric (25) is real and it is given by*

$$\alpha=-\tfrac{1}{6}\Omega^2(X_-+X_+). \tag{29}$$

The Ricci tensor of this metric is

$$Ric(g)=\frac{2}{\Omega}\nabla d\Omega+X_-\sigma^-+X_+\sigma^+-\left[\frac{1}{\Omega}\Delta\Omega-\frac{3}{\Omega^2}\tilde{g}(d\Omega,d\Omega)\right]\tilde{g}, \tag{30}$$

where $\nabla=\nabla_{\sigma^-}+\nabla_{\sigma^+}$ *is the connection of the product metric* $\tilde{g}=\sigma^-+\sigma^+$.

Let us consider metrics with zero Cotton tensor again. If they have a constant argument, theorem 1 implies that the principal structure is integrable and so, the space–times are of type $\mathrm{D}(\mathrm{M})^{0\cdot 0}_{0\cdot 0}$. Consequently, from proposition 4 the Weyl tensor has real eigenvalues. So we can state:

Theorem 2: *The Weyl eigenvalues of a type D space–time with zero Cotton tensor have constant argument if, and only if, they are real*.

This result generalizes a previous one by Hall[4] (see also McIntosh *et al.*[5]). He showed that there are no purely magnetic Type D vacuum metrics. But the purely magnetic case occurs when the eigenvalue argument is $\frac{3}{2}\theta=\pm\pi/2$, that is to say, a particular value of constant argument. So, from theorem 2 it follows:

Corollary 1: *There is no purely magnetic Type D metric with zero Cotton tensor*.

This corollary shows that not only the purely magnetic vacuum solutions are forbidden, but also the Weyl-magnetic space–times with zero Cotton tensor. On the other hand the Hall result is also generalized in the sense that theorem 2 excludes all the constant arguments that differ from 0 or π. Although this approach could be of interest in studying the existence of purely magnetic type I solutions, the recent results on this subject have been obtained by using the $1+3$ formalism.[22,32,33]

From the results above it is easy to recover the canonical form for the metrics with zero Cotton tensor and real Weyl eigenvalues. Indeed, expressions (23) and (26) show that the conformal factor and the Weyl eigenvalue are related by $\Omega^2=c^2e^{\rho}=c^2\alpha^{2/3}$, c being an arbitrary constant. On the other hand they also satisfy expression (29) and, consequently, Ω coincides, up to a constant factor, with X_-+X_+. So we have

Proposition 5: *Every type D metric with real eigenvalues and zero Cotton tensor may be written*

$$g=\frac{1}{(X_-+X_+)^2}(\sigma^-+\sigma^+),$$

where $\sigma^-=\sigma^-_{AB}(x^C)dx^Adx^B$, $\sigma^+=\sigma^+_{ij}(x^k)dx^idx^j$, *are two arbitrary bidimensional metrics,* σ^- *hyperbolic and* σ^+ *elliptic, with Gaussian curvatures* X_- *and* X_+, *respectively*.

This canonical expression was obtained in a previous work[18] where it was used to integrate the Einstein vacuum equations, in this way getting an intrinsic algorithm to identify every A, B, and C-metric of Ehlers and Kundt.[2] In the following section, starting from the propositions 3 and 4 we present a similar study for the charged counterpart of these vacuum solutions.

VI. ALIGNED EINSTEIN–MAXWELL SOLUTIONS OF TYPE $\mathrm{D}^{0\cdot 0}_{0\cdot 0}$

If (v,h) is the principal structure of the Weyl tensor, the aligned Einstein–Maxwell solutions satisfy

$$Ric(g)=\chi(v-h)=\kappa\ (\sigma^--\sigma^+), \tag{31}$$

where the second equality is satisfied for the type $\mathrm{D}^{0\cdot 0}_{0\cdot 0}$ metrics as a consequence of proposition 3: $\chi=\kappa\Omega^2$, $\sigma^-=\Omega^2v$, $\sigma^+=\Omega^2h$. Moreover, as the principal structure is integrable, it is Maxwellian and the associated Rainich index is a constant. So, (31) is a necessary and sufficient condition for the metric (25) to be an aligned solution of the Einstein–Maxwell equations. Taking into account the expression (30) for the Ricci tensor, condition (31) becomes

$$\Omega=\lambda_-(x^A)+\lambda_+(x^i), \tag{32}$$

$$\nabla d\lambda_\epsilon=\beta_\epsilon\sigma^\epsilon, \tag{33}$$

$$\frac{\Omega^2}{6}(X_-+X_+)+\Omega\ (\beta_-+\beta_+)=\sigma^-(d\lambda_-,d\lambda_-)+\sigma^+(d\lambda_+,d\lambda_+), \tag{34}$$

$$d\beta_\epsilon+X_\epsilon d\lambda_\epsilon=0. \tag{35}$$

Equations (35) are the integrability conditions of (33). Moreover, if we differentiate (34), project on σ_-, differentiate again and take into account (35), we have

$$2(X_- + X_+)\mathrm{d}\lambda_- \wedge \mathrm{d}\lambda_+ + \Omega[\mathrm{d}X_+ \wedge \mathrm{d}\lambda_- - \mathrm{d}X_- \wedge \mathrm{d}\lambda_+] = 0. \tag{36}$$

Then a simple analysis of the expressions (32)–(36) leads to

Lemma 9: *The following conditions are equivalent*: (i) $dX_\epsilon = 0$, (ii) $\beta_\epsilon = 0$, (iii) $d\lambda_\epsilon = 0$, (iv) $\sigma^\epsilon(d\Omega) = 0$. *Moreover, these conditions hold if* $\sigma^\epsilon(d\lambda_\epsilon, d\lambda_\epsilon) = 0$ *everywhere.*

A. The solutions: A, B, and C charged metrics

Proposition 3 states that the classes D^{0q0}_{0m0} can be discriminated using the vectors $\sigma^\epsilon(\mathrm{d}\Omega)$. Then, lemma 9 implies that, as happens in the vacuum case,[18] the four classes can be characterized by σ^- or σ^+ to be bidimensional metrics that have constant curvature or not.

If g is in class D^{010}_{010}, lemma 9 implies that λ_ϵ can be taken as coordinate in the plane σ^ϵ. Then, Eqs. (34)–(36) say that β_ϵ, X_ϵ, and $\sigma^\epsilon(d\lambda_\epsilon, d\lambda_\epsilon)$ depend just on λ_ϵ, and that $X_\epsilon = -\beta'_\epsilon$. Then, from (34) we have $\beta'''_-(\lambda_-) + \beta'''_+(\lambda_+) = 0$ and, consequently, β_ϵ is a polynomial in λ_ϵ of degree less than or equal to three. But lemma 9 also states that $d\lambda_\epsilon$ is not a null vector everywhere. Then, Einstein–Maxwell equations (32)–(36) finally lead to

$$\sigma^\epsilon = \frac{1}{\epsilon f(\epsilon\lambda_\epsilon)}\mathrm{d}\lambda_\epsilon^2 + f(\epsilon\lambda_\epsilon)dZ^2, \tag{37}$$

with $f(\lambda)$ a fourth degree polynomial. Then, putting (37) and (32) into (25) we recover the known expression of the charged C-metrics.[25]

If g is in class D^{000}_{010}, lemma 9 implies that λ_- can be taken as a coordinate in the plane σ^- and, moreover, σ^+ must be of constant curvature. Thus, a redefinition of Ω and σ^- allows us to consider $X_+ \in \{-1,0,1\}$ and $\Omega = \lambda_-$. Then, if we introduce the coordinate transformation $r = -1/\lambda_-$, a similar procedure that leads in the general case to the charged counterpart of the A_i-metrics:

$$g = -a(r)\mathrm{d}t^2 + \frac{1}{a(r)}\mathrm{d}r^2 + r^2\mathrm{d}\sigma^2, \qquad a(r) \equiv X - \frac{C}{r} + \frac{D}{r^2}, \tag{38}$$

$\mathrm{d}\sigma^2$ being the bidimensional elliptic metric of constant curvature X, with $X = 1,-1,0$ depending on the A_1, A_2, or A_3 case.

If g is in the class D^{010}_{000}, in a similar way λ_+ can be taken as a coordinate in the plane σ^+, and σ^- must be of constant curvature $X_- \in \{-1,0,1\}$. Then, the coordinate transformation $r = -1/\lambda_+$, leads to the charged counterpart of the B_i-metrics:

$$g = r^2\mathrm{d}\sigma^2 + a(r)\mathrm{d}z^2 + \frac{1}{a(r)}\mathrm{d}r^2, \qquad a(r) \equiv X - \frac{C}{r} + \frac{D}{r^2}, \tag{39}$$

$\mathrm{d}\sigma^2$ being the bidimensional hyperbolic metric of constant curvature X, with $X = 1,-1,0$ depending on the B_1, B_2, or B_3 case.

Finally, in class D^{000}_{000} both bidimensional metrics have a constant curvature and Eq. (34) implies that $X_- + X_+ = 0$. This means that the space–times is conformally flat and the metric becomes $g = \sigma^- + \sigma^+$, where σ^ϵ are bidimensional metrics, hyperbolic, and elliptic, respectively, with a constant curvature ϵX. The metrics of this more degenerated class are the only ones that have zero Cotton tensor.

B. The intrinsic characterization

The metrics of type $\mathrm{D(M)}^{0\cdot 0}_{0\cdot 0}$, which take the canonical form (25), admit an intrinsic identification by means of conditions involving the principal 2–form $\mathcal{U}$. These characterization equa-

tions that we have given in previous sections could be written explicitly in terms of metric concomitants because $\mathcal{U}$ can be determined from the Weyl tensor.[17] Nevertheless, as a consequence of the Bianchi identities some of the above conditions can be satisfied identically taking into account the properties of the Ricci tensor. This is the case of vacuum metrics: As $Ric=0$ implies the nullity of the Cotton tensor, the principal planes always define an umbilical and Maxwellian structure as a consequence of the results in Sec. IV. Actually we want to characterize aligned Einstein–Maxwell solutions that are conformal to a product metric. So, the Weyl tensor must have real eigenvalues and the principal planes are the eigenspaces of the Ricci tensor, that is,

$$W=3\alpha(U\otimes U-*U\otimes *U)+\alpha G, \quad Ric=\chi(v-h), \tag{40}$$

where $v=U^2$, $h=-*U^2$. Then, taking into account the expressions in Sec. II about $2+2$ almost-product structures, a straightforward calculation shows that the Bianchi identities (21) can be written

$$(3\alpha+2\chi)\ Q_v=v\otimes h(d\alpha); \quad (3\alpha-2\chi)\ Q_h=h\otimes v(d\alpha), \tag{41}$$

$$v(d\chi)-2\chi i(\delta U)U=0; \quad h(d\chi)+2\chi i(\delta *U)*U=0. \tag{42}$$

From these expressions we find that, under the scalar restriction $(3\alpha)^2\neq(2\chi)^2$, the properties of the structure follow just by imposing that the Weyl and the Ricci tensor take expressions (40). On the other hand, the case $(3\alpha)^2=(2\chi)^2$ leads to the *exceptional* metrics considered by Plebański and Hacyan.[34] Nevertheless, it can easily be shown that $(3\alpha)^2\neq(2\chi)^2$ for the solutions recovered in the subsection above. So we get the following characterization:

Lemma 10: *The charged counterpart of the A, B, and C-metrics are the only aligned Einstein–Maxwell solutions of type D with real eigenvalues that satisfy* $(3\alpha)^2\neq(2\chi)^2$, α *and* χ *being, respectively, the Weyl and the Ricci eigenvalues*.

Elsewhere,[18] conditions for g to be of type D with real eigenvalues have been given in terms of Weyl concomitants. In order to impose the Ricci tensor to take the form (40) we can use the algebraic Rainich conditions.[12] But if the Weyl tensor is of type D with real eigenvalues, a part of these Rainich conditions hold identically when we impose the aligned restriction. From these considerations and lemma 10 we have:

Theorem 3: *The A, B, and C Einstein–Maxwell solutions can be characterized by conditions*

$$\alpha\neq 0; \quad S^2+S=0; \quad Ric(x,x)\geqslant 0,$$

$$\mathrm{Tr}\ Ric=0, \quad S[Ric]+Ric=0; \quad (3\alpha)^2-(2\chi)^2\neq 0.$$

$W\equiv W(g)$ *and* $Ric\equiv Ric(g)$ *being the Weyl and Ricci tensors of the metric* g, *and where* $\alpha=\alpha(g)\equiv-(\frac{1}{12}\,\mathrm{Tr}W^3)^{1/3}$, $\chi=\chi(g)\equiv-\frac{1}{2}(\mathrm{Tr}Ric^2)^{1/2}$, $S=S(g)\equiv\frac{1}{3}(\alpha^{-1}W-\frac{1}{2}g\owedge g)$, $S[Ric]_{\alpha\beta}=S_{\alpha\mu\beta\nu}R^{\mu\nu}$ *and* x *is an arbitrary time-like vector*.

This theorem offers an intrinsic and explicit description of the aligned Einstein–Maxwell solutions of type $\mathrm{D}^{0\cdot 0}_{0\cdot 0}$. Now we look for an intrinsic and explicit way to identify every metric of this family, that is, to distinguish the A_i, B_i, and C charged metrics. In a first step we must discriminate between the classes D^{0p0}_{0m0} and, as a consequence of proposition 3, this depends on the nullity of the vectors $v(d\Omega)$ and $h(d\Omega)$. But the expression (29) for the Weyl eigenvalue and lemma 9 imply that, equivalently, the vectors $v(d\alpha)$ and $h(d\alpha)$ determine these properties. So, the same scheme as in the vacuum case[18] can be used to distinguish between the classes.

The last step to obtain the intrinsic and explicit characterization of the solutions is to get an invariant that provides the sign of the bidimensional curvature when this is constant. A straightforward calculation shows that if X_ϵ is constant, then

$$X_\epsilon\Omega^2=\omega_\epsilon\equiv\tfrac{1}{9}(\mathrm{d}\ln(\alpha+\chi))^2-2\alpha-\epsilon\chi. \tag{43}$$

So, we have a characterization of the Einstein–Maxwell A, B, and C-metrics, and we recover the type D static vacuum solutions making $\chi=0$.

Theorem 4: *Let g be an aligned Einstein–Maxwell solution of type $D^{0\cdot 0}_{0\cdot 0}$ (characterized in theorem 3). Let us take the metric concomitants*

$$M\equiv *W(d\alpha,\cdot,d\alpha,\cdot) \quad N\equiv S(d\alpha,\cdot,d\alpha,\cdot),$$

and let x be an arbitrary unitary timelike vector. Then,

(i) *g is a charged C-metric if, and only if, $M\neq 0$;*
(ii) *g is a charged A-metric if, and only if, $M=0$ and $2N(x,x)+trN>0$. Furthermore, it is of type A_1, A_2 or A_3 if $\omega_+>0$, $\omega_+<0$ or $\omega_+=0$, respectively, where $\omega_+\equiv\frac{1}{9}(\mathrm{d}\ln(\alpha+\chi))^2-2\alpha-\chi$;*
(iii) *g is a charged B-metric if, and only if, $M=0$ and $2N(x,x)+trN<0$. Furthermore, it is of type B_1, B_2 or B_3 if $\omega_->0$, $\omega_-<0$ or $\omega_-=0$, respectively, where $\omega_-\equiv\frac{1}{9}(\mathrm{d}\ln(\alpha+\chi))^2-2\alpha+\chi$.*

This theorem provides an algorithm to identify, in the set of all metrics, the charged counterpart of the Ehlers and Kundt[2] vacuum solutions. The particular case of the A_1 metrics corresponds to a charged spherically symmetric spacetime, that is, to the Reissner–Nordström solution. In this case the metric takes the form (38) with $X=1$, and the mass and the charge are related with the constants C and D, respectively. Moreover, these constants can be given in terms of Weyl and Ricci invariants. Then, from the last theorem and previous subsection it follows:

Theorem 5: *Let $Ric\equiv Ric(g)$ and $W\equiv W(g)$ be the Ricci and the Weyl tensors of a spacetime metric g, and let us take the metric concomitants*:

$$\alpha\equiv-(\tfrac{1}{12}\mathrm{Tr}\ W^3)^{1/3},\quad \chi\equiv-\tfrac{1}{2}(\mathrm{Tr}\ Ric^2)^{1/2},\quad \omega\equiv\tfrac{1}{9}g(d\ln\alpha,d\ln\alpha)-2\alpha-\chi, \tag{44}$$

$$S\equiv\frac{1}{3\alpha}(W-\tfrac{1}{2}\alpha g\owedge g),\quad M\equiv *W(d\alpha,\cdot,d\alpha,\cdot),\quad N\equiv S(d\alpha,\cdot,d\alpha,\cdot). \tag{45}$$

The necessary and sufficient conditions for g to be the Reissner–Nordström metric are

$$\alpha\neq 0,\quad S^2+S=0,\quad Ric(x,x)\geqslant 0,$$

$$\mathrm{Tr}\ Ric=0,\quad S[Ric]+Ric=0,\quad (3\alpha)^2-(2\chi)^2\neq 0,$$

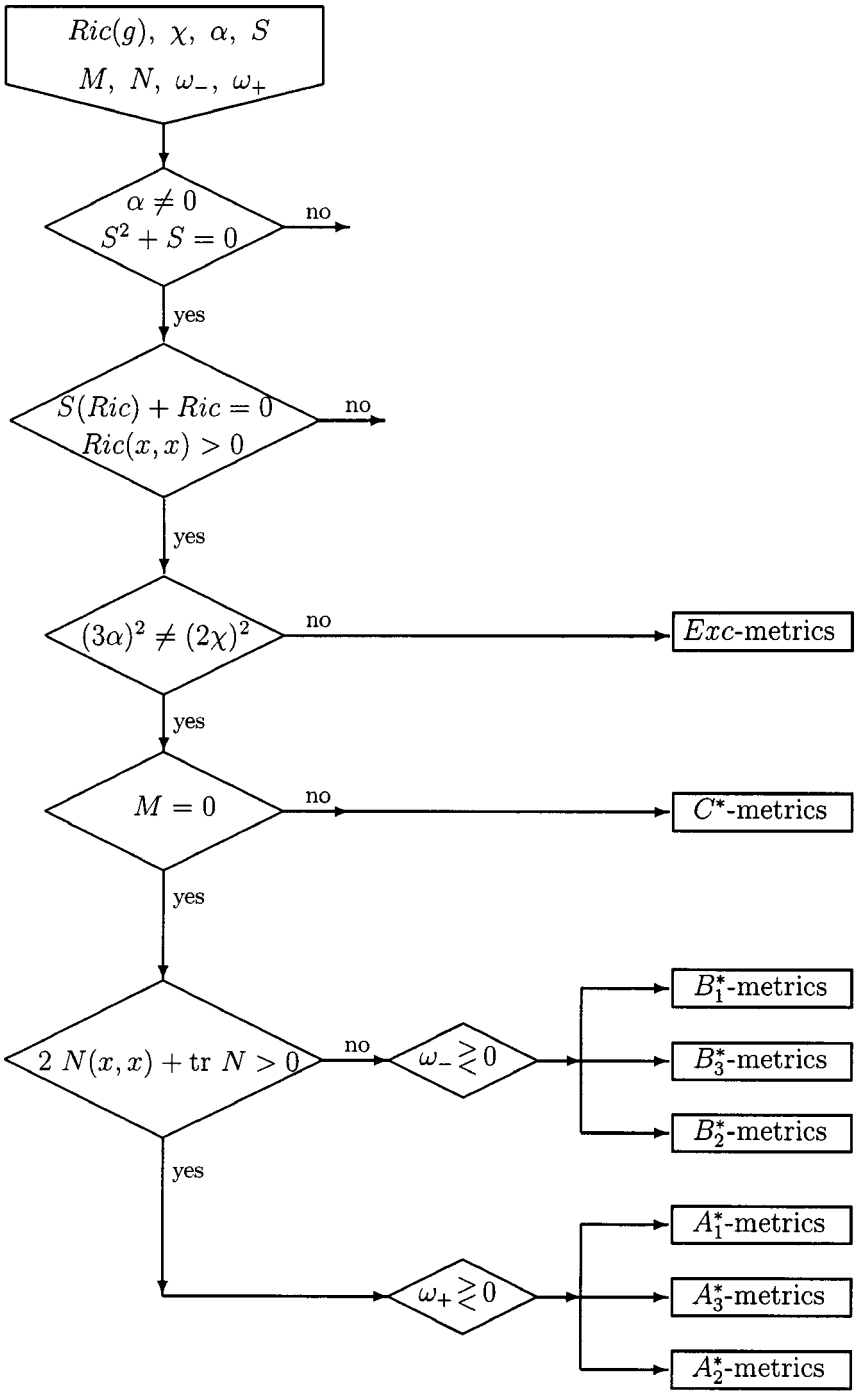
$$M=0,\quad 2N(x,x)+trN>0,\quad \omega>0,$$

where x is an arbitrary unitary time-like vector. Moreover, the mass m and the electric charge e are given, respectively, by $m=(\alpha+\chi)/\omega^{3/2}$ and $e^2=-\chi/\omega^2$, and the timelike Killing vector by $\xi=[\sqrt{\omega}(3\alpha+2\chi)]^{-1}[N(x)/\sqrt{N(x,x)}]$.

C. A summary in algorithmic form

Finally, in order to emphasize the algorithmic nature of our results, we present them as a flow diagram that identifies, among all metrics, every A, B, or C Einstein–Maxwell solution (in the following flow chart we denote them A^*, B^*, and C^*-metrics). The exceptional metrics studied by Plebański are also identified and they are denoted Exc-metrics. This operational algorithm involves an arbitrary unitary timelike vector, x, and some metric concomitants that may be obtained from the components of the metric tensor g in arbitrary local coordinates: The invariants α,

χ, ω_ϵ, S, M, and N are given in (43)–(45) in terms of the Ricci and Weyl tensors. Making $\chi = 0$, we recover the vacuum solutions[18]



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Existence of initial data satisfying the constraints for the spherically symmetric Einstein–Vlasov–Maxwell system

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Using ODE techniques we prove the existence of large classes of initial data satisfying the constraints for the spherically symmetric Einstein–Vlasov–Maxwell system. These include data for which the ratio of total charge to total mass is arbitrarily large. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The global dynamical behavior of self-gravitating matter is a subject of central importance in general relativity. A form of matter which has particularly nice mathematical properties is collisionless matter, described by the Vlasov equation. It has the advantage that it lacks the tendency observed in certain other models, such as perfect fluids, that solutions of the equations of motion of the matter lose differentiability after a finite time. These singularities of the mathematical model form an obstacle to further analysis and prevent the study of the global dynamical properties of the solutions. Collisionless matter is free from these difficulties and there is a growing literature on global properties of solutions of the Einstein–Vlasov system.[1,9]

In Ref. 8, the authors prove the global existence of asymptotically flat solutions of the spherically symmetric Einstein–Vlasov system, with small initial data. That study concerns uncharged particles. We consider, under the same assumption of spherical symmetry, the case where the particles are charged. To describe the full physical situation, we must then couple the previous system to the Maxwell equations that determine the electromagnetic field created by the fast moving charged particles. As will be seen below, that reduces, in the spherically symmetric case, to its electric part.

It is appropriate at this point to examine the motivation for considering this particular problem. We are not aware that it has any direct astrophysical applications. There are, however, two reasons why the problem is interesting. The first is that it extends the knowledge of the Cauchy problem for systems involving the Vlasov equation and it will be seen that it gives rise to new mathematical features compared to those cases studied up to now. The second is connected with the fact that it would be desirable to extend the work of Ref. 8 beyond spherical symmetry. In particular, it would be desirable from a physical point of view to include the phenomenon of rotation. Unfortunately, presently available techniques do not suffice to get away from spherical symmetry. In this situation it is possible to attempt to obtain further intuition by using the analogy between angular momentum and charge, summed up in John Wheeler's statement, ''Charge is a poor man's angular momentum.'' Thus we study spherical systems with charge in the hope that this will give us insight into nonspherical systems without charge. This strategy has recently been

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pursued in the case of a scalar field as matter model, with interesting results.[3,4]

Concerning the Cauchy problem in general relativity, it is well known that in addition to the Einstein evolution equations there are constraint equations which have to be solved. (See, e.g., Ref. 5.) It is only of interest to consider the problem of evolution, if the problem of constraints on the initial data can be solved. In our specific case, we are led to a difficulty in solving the constraints on the initial data, that has not previously been considered in the literature. Let us first recall the situation in Ref. 8 before seeing how it changes in the case of charged particles. In Ref. 8, using the assumption of spherical symmetry, the authors look for two metric functions λ and μ, that depend only on the time coordinate t and on the radial coordinate r, and for the distribution function f of the uncharged particles that depends on t, r and on the 3-velocity v of the particles; the metric functions λ, μ are subject to the Einstein equations with sources generated by the distribution function f of the collisionless uncharged particles which is itself subject to the Vlasov equation. They show that the Einstein equations to determine the unknown metric functions λ and μ, turn out to be two first order ordinary differential equations (ODE) in the radial variable r, coupled to the Vlasov equation in f. Setting $t=0$ in the Einstein equations yields two constraint equations that link the three initial data that are the two initial data for $\lambda(t,r)$ and $\mu(t,r)$ denoted $\mathring{\lambda}(r)$ and $\mathring{\mu}(r)$, respectively, and the initial datum for $f(t,r,v)$ denoted by $\mathring{f}(r,v)$. The equations to be solved are two first order ODE for $\mathring{\lambda}$, $\mathring{\mu}$. The mass function $m(t,r)$ is defined as an integral of f over the hypersurfaces of constant t. The exact definition is given in the next section. Provided the initial mass function $\mathring{m}(r)=m(0,r)$ is everywhere less than $r/2$ the function $\mathring{\lambda}$ can be determined from the relation $1-2m/r=e^{-2\lambda}$. Once this has been done μ can be determined by integration. In this way functions $\mathring{\lambda}$ and $\mathring{\mu}$ can be determined in a straightforward way when $\mathring{f}$ is given, provided the inequality $2m/r<1$ is satisfied on the initial hypersurface. Thus a simple parametrization of the set of initial data satisfying the constraints is obtained. They can be constructed from a non-negative function $\mathring{f}$ which is required to satisfy one inequality.

In the case of charged particles, the problem of constraints on the initial data is not so easy. We consider the case of a spherically symmetric electric field $\vec{E}$ of the form $\vec{E}(t,r)=e(t,r)\,(\vec{r}/r)$, where $e(t,r)$ is an unknown scalar function and $\vec{r}$ the position vector in $\mathbb{R}^3$. We denote by $\mathring{e}$ the initial data for $e(t,r)$. The Maxwell equations imply a constraint equation on the initial data, that is a first order ODE in the radial variable r. We now have to face the problem of constraints between the four initial data $\mathring{\lambda}$, $\mathring{\mu}$, $\mathring{f}$, $\mathring{e}$. If the equations for $\mathring{\lambda}$, $\mathring{f}$, and $\mathring{e}$ can be solved then $\mathring{\mu}$ can be determined by a simple integration as in the case of uncharged particles. On the other hand, the problem of determining the first three quantities is more difficult in the charged case due to the coupling of the gravitational and electromagnetic constraints. Any solution of the constraints must satisfy the condition $2m/r<1$ on the initial hypersurface. However, in the charged case m includes a contribution due to the energy density of the electric field and this depends on e and λ. As a consequence, in contrast to the uncharged case, this condition cannot be expressed as an inequality on f alone. Moreover, the equation for e also contains λ and so it is not possible to solve the electromagnetic constraint separately from the gravitational one. There is no alternative but to solve the two constraints together. When $\mathring{f}$ is prescribed the constraints define a system of two coupled nonlinear ordinary differential equations for $\mathring{\lambda}$ and $\mathring{e}$. These equations are singular at $r=0$.

Solving the ordinary differential equations arising from the constraints is a task which must necessarily be mastered before undertaking the study of the problem of evolution for the Einstein–Vlasov–Maxwell system. Since the equations are singular they cannot be handled by standard results of ODE theory alone. In this paper, we prove, using statements developed in Ref. 10 on singular ODE, that, under smallness assumptions on the prescribed initial data function $\mathring{f}$, a corresponding global solution of the constraints exists. This provides a way of showing the existence of initial data $\mathring{\lambda}$, $\mathring{\mu}$, $\mathring{e}$, in the case of an asymptotically flat space–time with a regular center. In other words, we prove that the results obtained for the constraint equations in Ref. 8 that focuses on the case of uncharged particles, extend to the case of charged particles, in the sense that

the initial datum $\mathring{f}$ can still be considered as the only arbitrary initial datum.

Given the complicated nature of the constraint equations it seems impractible to describe the most general class of functions $\mathring{f}$ for which the constraints can be solved. What we have been able to do is to describe two large classes of functions $\mathring{f}$ for which it is possible. The first case treated is a rather obvious one to try. The charge q of a particle is a free parameter in the equations. In the case $q=0$ the equations reduce to the uncharged situation analyzed in Ref. 8. A perturbation argument then allows the case with fixed $\mathring{f}$ and small q to be treated. A more exotic class of initial data is obtained by a rigorous perturbation argument in a regime where the density of particles tends to zero and the charge per particle tends to infinity. This allows the construction of initial data which coincide outside a compact set with data for the Reissner–Nordström solution with arbitrarily large charge to mass ratio. The restriction of these data to the region outside a large radius does not allow an electrovacuum interior which has a regular center or corresponds to a black hole but, as this construction shows, does allow a regular (dynamical) interior with charged matter.

Note that there is a local in time existence theorem available for the Einstein–Vlasov–Maxwell system without symmetry. This can be obtained as the special case of the results of Ref. 2 on the Einstein–Maxwell–Boltzmann system by setting the collision term to zero. There is no discussion of the existence of solutions of the constraints in that paper.

The paper is organized as follows. In Sec. II, we recall the spherically symmetric Einstein–Vlasov–Maxwell system, from which we deduce the constraint equations. In Sec. III, we recall the main result of Ref. 10 which we use and we prove the existence of large classes of solutions of the constraint equations for the Einstein–Vlasov–Maxwell system. The derivation of some facts required in Sec. III concerning regions where there are no particles is contained in the Appendix.

II. FORMULATION OF THE PROBLEM

We consider fast moving collisionless particles with unit mass and charge q. The basic space–time is $(\mathbb{R}^4,g)$, with g a Lorentzian metric with signature $(-,+,+,+)$. In what follows, we assume that greek indices run from 0 to 3 and italic indices run from 1 to 3, unless otherwise specified. We also adopt the Einstein summation convention. The metric g reads locally, in Cartesian coordinates $(x^\alpha)=(x^0,x^i)\equiv(t,\tilde{x})$,

$$ds^2=g_{\alpha\beta}\,dx^\alpha\otimes dx^\beta. \tag{2.1}$$

The assumption of spherical symmetry means that we can take g of the following form (Schwarzschild coordinates):

$$ds^2=-e^{2\mu}\,dt^2+e^{2\lambda}\,dr^2+r^2(d\theta^2+\sin^2\theta d\varphi^2), \tag{2.2}$$

where $\mu=\mu(t,r)$; $\lambda=\lambda(t,r)$; $t\in\mathbb{R}$; $r\in[0,+\infty[$; $\theta\in[0,\pi]$; $\varphi\in[0,2\pi]$. The Einstein–Vlasov–Maxwell system reads

$$R_{\alpha\beta}-\tfrac{1}{2}g_{\alpha\beta}R=8\pi(T_{\alpha\beta}(f)+\tau_{\alpha\beta}(F)), \tag{2.3}$$

$$\mathcal{L}_{X(F)}f=0, \tag{2.4}$$

$$\nabla_\alpha F^{\alpha\beta}=J^\beta,\quad \nabla_\alpha F_{\beta\gamma}+\nabla_\beta F_{\gamma\alpha}+\nabla_\gamma F_{\alpha\beta}=0 \tag{2.5}$$

with

$$T_{\alpha\beta}(f)=-\int_{\mathbb{R}^3}p_\alpha p_\beta f\omega_p,\quad \tau_{\alpha\beta}(F)=-\frac{g_{\alpha\beta}}{4}F_{\gamma\nu}F^{\gamma\nu}+F_{\beta\gamma}F_\alpha{}^\gamma,$$

$$J^{\beta}(f)(x)=q\int_{\mathbb{R}^3}p^{\beta}f(x,p)\omega_p,\quad \omega_p=|g|^{1/2}\frac{\mathrm{d}p^1\,\mathrm{d}p^2\,\mathrm{d}p^3}{p_0},\quad p_0=g_{00}p^0,$$

$$X^{\alpha}(F)=(p^{\alpha},-\Gamma^{\alpha}_{\beta\gamma}p^{\beta}p^{\gamma}-qp^{\beta}F_{\beta}{}^{\alpha}),$$

where $\Gamma^{\alpha}_{\beta\gamma}$ denote the Christoffel symbols. Here, $x=(x^{\alpha})$ is the position and $p=(p^{\alpha})$ is the 4-momentum of particles. In the expressions above, f stands for the distribution function of the charged particles, F stands for the electromagnetic field created by the charged particles. Here (2.3) are the Einstein equations for the metric tensor $g=(g_{\alpha\beta})$ with sources generated by both f and F, that appear in the stress-energy tensor $T_{\alpha\beta}+\tau_{\alpha\beta}$. Equation (2.4) is the Vlasov equation for the distribution function f of the collisionless particles, with $\mathcal{L}_{X(F)}$ the Lie derivative, and (2.5) are the Maxwell equations for the electromagnetic field F, with source (current) generated by f through $J=J(f)$. One verifies that the conservation laws $\nabla_{\alpha}(T^{\alpha\beta}+\tau^{\alpha\beta})=0$ hold if f satisfies the Vlasov equation.

By the assumption of spherical symmetry, we can take g in the form (2.2). One shows, using the Maxwell equation that F reduces to its electric part. We take it in the form $E=(E^{\alpha})$ with $E^0=0$, $E^i=e(t,r)\,(x^i/r)$ and then, a straightforward calculation shows that

$$\tau_{00}=\tfrac{1}{2}e^{2(\lambda+\mu)}e^2(t,r),\quad \tau_{0i}=0,$$

$$\tau_{ij}=\tfrac{1}{2}e^{2\lambda}e^2(t,r)\left\{\left(\delta_{ij}-\frac{x_ix_j}{r^2}\right)-e^{2\lambda}\frac{x_ix_j}{r^2}\right\},$$

where δ_{ij} is the Kronecker symbol.

These relations and results of Ref. 8 show that the spherically symmetric Einstein–Vlasov–Maxwell system implies the following first order ODE system in λ, μ, f, e:

$$e^{-2\lambda}(2r\lambda'-1)+1=8\pi r^2\rho, \tag{2.6}$$

$$e^{-2\lambda}(2r\mu'+1)-1=8\pi r^2p, \tag{2.7}$$

$$\frac{\partial f}{\partial t}+e^{\mu-\lambda}\frac{v}{\sqrt{1+v^2}}\cdot\frac{\partial f}{\partial\tilde{x}}-\left(e^{\mu-\lambda}\mu'\sqrt{1+v^2}+\dot{\lambda}\frac{\tilde{x}\cdot v}{r}-qe^{\lambda+\mu}e(t,r)\right)\frac{\tilde{x}}{r}\cdot\frac{\partial f}{\partial v}=0, \tag{2.8}$$

$$\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{\lambda}e(t,r))=qr^2e^{\lambda}\int_{\mathbb{R}^3}f(t,\tilde{x},v)\mathrm{d}v, \tag{2.9}$$

where $\lambda'=\partial\lambda/\partial r$, $\dot{\lambda}=\partial\lambda/\partial t$, and

$$\rho(t,\tilde{x})=\int_{\mathbb{R}^3}f(t,\tilde{x},v)\sqrt{1+v^2}\,\mathrm{d}v+\frac{1}{2}e^{2\lambda(t,\tilde{x})}e^2(t,\tilde{x}), \tag{2.10}$$

$$p(t,\tilde{x})=\int_{\mathbb{R}^3}\left(\frac{\tilde{x}\cdot v}{r}\right)^2f(t,\tilde{x},v)\frac{\mathrm{d}v}{\sqrt{1+v^2}}-\frac{1}{2}e^{2\lambda(t,\tilde{x})}e^2(t,\tilde{x}). \tag{2.11}$$

Here (2.6) and (2.7) are the Einstein equations for λ and μ, (2.8) is the Vlasov equation for f and (2.9) is the Maxwell equation for e. Here $\tilde{x}$ and v belong to $\mathbb{R}^3$, $r:=|\tilde{x}|$, $\tilde{x}\cdot v$ denotes the usual scalar product of vectors in $\mathbb{R}^3$, and $v^2:=v\cdot v$. The distribution function f is assumed to be invariant under simultaneous rotations of $\tilde{x}$ and v, hence ρ and p can be regarded as functions of t and r. It is assumed that $f(t)$ has compact support for each fixed t. We are interested in asymptotically flat space–times which leads to imposing the boundary condition that

$$\lim_{r\to\infty}\mu(t,r)=0. \tag{2.12}$$

They should also have a regular center which means that in addition to λ, μ, and e being smooth functions of t and r, including at $r=0$, the boundary condition $\lambda(t,0)=0$ should be satisfied for all t. Note that the condition that $\lambda(t,r)$ tends to zero as $r\to\infty$, which is part of asymptotic flatness, follows from the field equations and the fact that $f(t)$ has compact support. This is because in the region where f vanishes the general solution of (2.6) satisfies the condition $\lambda(r)=O(1/r)$ as $r\to\infty$.

Let $m(r)=4\pi\int_0^r s^2\rho(s)\mathrm{d}s$. This is the mass function referred to in the introduction. Its limit M as $r\to\infty$ is the total or ADM (Arnowitt–Deser–Misner) mass of the system. The function $n=\int_{\mathbb{R}^3} f\,\mathrm{d}v$ is the number density of particles and nq the charge density. The total charge of the system is given by $Q=4\pi q\int_0^\infty s^2 e^{\lambda(s)}n(s)\mathrm{d}s$.

Now, define the initial data by

$$f(0,\tilde{x},v)=\mathring{f}(\tilde{x},v);\ \lambda(0,\tilde{x})=\mathring{\lambda}(\tilde{x})=\mathring{\lambda}(r);\ \ \mathring{e}(0,\tilde{x})=\mathring{e}(\tilde{x})=\mathring{e}(r) \tag{2.13}$$

with $\mathring{f}\in C_0^\infty$ being a C^∞ function with compact support, which is non-negative and spherically symmetric, i.e.,

$$\forall A\in \mathrm{SO}(3),\ \ \forall(\tilde{x},v)\in\mathbb{R}^6,\ \ \mathring{f}(A\tilde{x},Av)=\mathring{f}(\tilde{x},v).$$

We obtain the constraint equations on the initial data by taking (2.6), (2.7), and (2.9) for $t=0$, that give

$$e^{-2\mathring{\lambda}}(2r\mathring{\lambda}'-1)+1=8\pi r^2\int_{\mathbb{R}^3}\sqrt{1+v^2}\,\mathring{f}(r,v)\mathrm{d}v+4\pi r^2 e^{2\mathring{\lambda}}\mathring{e}^2, \tag{2.14}$$

$$\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{\mathring{\lambda}}\mathring{e})=qr^2e^{\mathring{\lambda}}\int_{\mathbb{R}^3}\mathring{f}(r,v)\mathrm{d}v=J(\mathring{f}), \tag{2.15}$$

$$e^{-2\mathring{\lambda}}(2r\mathring{\mu}'+1)-1=8\pi r^2\int_{\mathbb{R}^3}\left(\frac{\tilde{x}\cdot v}{r}\right)^2\mathring{f}(r,v)\frac{\mathrm{d}v}{\sqrt{1+v^2}}-4\pi r^2 e^{2\mathring{\lambda}}\mathring{e}^2. \tag{2.16}$$

We observe that, if $\mathring{f}$ is given and if we can solve (2.14) and (2.15) for $\mathring{\lambda}$ and $\mathring{e}$ then (2.16) determines at once $\mathring{\mu}'$. Using the boundary condition (2.12) then determines $\mathring{\mu}$. So we can concentrate on (2.14) and (2.15). In what follows, we fix $\mathring{f}$ in (2.14) and (2.15) and we look for a unique global asymptotically flat solution $(\mathring{\lambda},\mathring{e})$ of the system (2.14) and (2.15) above with regular center. Note that, using the compact support of $\mathring{f}$ and the equations (2.14) and (2.15), it follows that $\mathring{\lambda}$ and $\mathring{e}$ tend to zero as $r\to\infty$. It also follows from (2.14) and (2.15) and the regularity of the solution that $\mathring{\lambda}'(0)=0$ and $\mathring{e}(0)=0$.

III. EXISTENCE OF GLOBAL SOLUTIONS OF THE CONSTRAINTS

In this section the existence of global solutions of the equations (2.14) and (2.15) will be proved. Let us state first of all the following result of Ref. 10 on which our global existence theorem relies.

Theorem 3.1: *Let V be a finite-dimensional real vector space, $N:V\to V$ a linear mapping, $G:I\times V\to V$ a smooth (i.e., C^∞) mapping and $g:I\to V$ a smooth mapping, where I is an open interval in $\mathbb{R}$ containing zero. Consider the equation*

$$s\frac{\mathrm{d}f}{\mathrm{d}s}+Nf=sG(s,f(s))+g(s) \tag{3.1}$$

for a function f defined on a neighborhood of 0 in I and taking values in V. Suppose that each eigenvalue of N has a positive real part. Then there exists an open interval J with $0 \in J \subset I$ and a unique bounded C^1 function f on $J\backslash\{0\}$ satisfying (3.1). Moreover f extends to a C^∞ solution of (3.1) on J. If N, G, and g depend smoothly on a parameter z and if the eigenvalues of N are distinct then the solution also depends smoothly on z.

Proof: See Theorem 1 in Ref. 10, p.989.

Remark 1: The assumption that N has distinct eigenvalues is to ensure that N can be reduced to diagonal form by a similarity transformation depending smoothly on z. In particular, Theorem 3.1 applies if N is already a diagonal matrix.

Theorem 3.2: *(local existence) Let $\mathring{f} \in C^\infty(\mathbb{R}^6)$ be non-negative, compactly supported and spherically symmetric. Then, the equations (2.14) and (2.15) have a unique local and regular solution $(\mathring{\lambda}, \mathring{e})$ defined on some interval $[0,R]$, $R>0$. The solution depends smoothly on the parameter q.*

Proof: Let $\mathring{f} \in C^\infty(\mathbb{R}^6)$ be non-negative, compactly supported and spherically symmetric. By a regular solution we mean one which is smooth and for which $\mathring{\lambda} = 0$ at $r = 0$. It follows that for any regular solution $\mathring{\lambda}$ can be written in the form:

$$\mathring{\lambda}(r) = rL(r) \tag{3.2}$$

for a smooth function $L(r)$. Equation (3.2) implies $\mathring{\lambda}' = L + rL'$ and (2.14)–(2.15) can be written

$$rL' + L = \frac{1}{2r}(1 - e^{2rL}) + 4\pi r e^{2rL}\left(\int_{\mathbb{R}^3} \sqrt{1+v^2}\,\mathring{f}(r,v)\,\mathrm{d}v + \frac{1}{2}e^{2rL}\mathring{e}^2 \right), \tag{3.3}$$

$$r\mathring{e}' + 2\mathring{e} = -r\mathring{e}(L + rL') + rq\int_{\mathbb{R}^3} \mathring{f}(r,v)\,\mathrm{d}v. \tag{3.4}$$

The function $e^{2x} - 1 - 2x$ vanishes to first order at the origin and hence $e^{2x} - 1 - 2x = x^2 F_0(x)$ for a smooth function F_0. Hence the equation for L can be rewritten in the form

$$rL' + L = -L + \frac{r}{2}L^2 F_0(rL) + 4\pi r e^{2rL}\left(\int_{\mathbb{R}^3} \sqrt{1+v^2}\,\mathring{f}\,\mathrm{d}v + \frac{1}{2}e^{2rL}\mathring{e}^2 \right).$$

Thus

$$rL' + 2L = rG_1(r, L, \mathring{e}, \mathring{f}), \tag{3.5}$$

where

$$G_1(r, L, \mathring{e}, \mathring{f}) = \frac{1}{2}L^2 F_0(rL) + 4\pi e^{2rL}\int_{\mathbb{R}^3} \sqrt{1+v^2}\,\mathring{f}(r,v)\,\mathrm{d}v + 2\pi e^{4rL}\mathring{e}^2$$

and (3.4) reads, given (3.5),

$$r\mathring{e}' + 2\mathring{e} = -r\mathring{e}(-L + rG_1(r, L, \mathring{e}, \mathring{f})) + rq\int_{\mathbb{R}^3} \mathring{f}(r,v)\,\mathrm{d}v.$$

Hence,

$$r\mathring{e}' + 2\mathring{e} = rG_2(r, L, \mathring{e}, \mathring{f}), \tag{3.6}$$

where

$$G_2(r,L,\mathring{e},\mathring{f})=L\mathring{e}-r\mathring{e}G_1(r,L,\mathring{e},\mathring{f})+q\int_{\mathbb{R}^3}\mathring{f}(r,v)\mathrm{d}v.$$

Setting $G=\binom{G_1}{G_2}$ and $\Phi=\binom{L}{\mathring{e}}$ and using (3.5) and (3.6), the equations (2.14) and (2.15) can be written:

$$r\frac{\mathrm{d}\Phi}{\mathrm{d}r}+2\Phi=rG(r,\Phi(r)). \tag{3.7}$$

We apply Theorem 3.1 with $V=\mathbb{R}^2$, $N\Phi=2\Phi$ to (3.7) and, since G clearly depends smoothly on q, obtain the desired result. Thus Theorem 3.2 is proved.

Theorem 3.3 (Global existence, low charge): *Let $\mathring{f}\in C^\infty(\mathbb{R}^6)$ be non-negative, compactly supported and spherically symmetric with*

$$8\pi\int_0^r s^2\left(\int_{\mathbb{R}^3}\sqrt{1+v^2}\mathring{f}(s,v)\mathrm{d}v\right)\mathrm{d}s<r. \tag{3.8}$$

Then, for q small enough, the equations (2.14) and (2.15) have a unique global and regular solution $(\mathring{\lambda},\mathring{e})$ defined on $[0,+\infty[$ that satisfies the boundary condition $\mathring{\lambda}(0)=0$.

Proof: Let $\mathring{f}\in C^\infty(\mathbb{R}^6)$ be non-negative, compactly supported and spherically symmetric. We assume that $\mathring{f}$ is fixed and satisfies (3.8). By Theorem 3.2, the equations (2.14) and (2.15) have a unique local regular solution on some interval $[0,R]$, $R>0$. Again, Theorem 3.1 shows that, for fixed $\mathring{f}$, there exists $E>0$, such that for $q\in[-E,E]$, R can be chosen uniformly and the solution on $[0,R]$ depends continuously on the parameter q. Now, for fixed $\mathring{f}$ and q, the solution has a right maximal interval of existence $[0,R_*[$, $R_*=R_*(\mathring{f},q)$. We have to show that $R_*=+\infty$. In fact, the second term on the right-hand side of (2.14) vanishes for $q=0$, as one can see by integrating (2.15) over $[0,r]$, $r>0$. It follows that for $q=0$, (2.14) and (2.15) have a global solution under the sole assumption (3.8) on $\mathring{f}$. Then by the stability theorem for ODE, for every $R>0$, there exists a number $E>0$, such that, for every $q\in[-E,E]$, the system (3.7) has a solution Φ_E that exists on $[0,R]$ (see Theorem 4, p. 92 in Ref. 7). Thus $R_*>R$. Now, we can choose R large so that $\operatorname{supp}\mathring{f}\subset[0,R]\times\mathbb{R}^3$, i.e., $\mathring{f}(r,v)=0$ for $r\geqslant R$. If R_0 is the radius of the support of the distribution function then R may be chosen to be bigger than $m(R_0)+Q^2/(8\pi R_0)$ for all q in the interval $[E,E]$. Hence by the lemma of the appendix the solution extends to one which is global and regular. This completes the proof of the theorem.

Theorem 3.4 (Global existence, high charge): *Let $\overline{f}\in C^\infty(\mathbb{R}^6)$ be non-negative, compactly supported and spherically symmetric. Then, for q large enough, the equations (2.14) and (2.15) have a global and regular solution $(\mathring{\lambda},\mathring{e})$ defined on $[0,+\infty[$ that satisfies the boundary condition $\mathring{\lambda}(0)=0$ for which $\mathring{f}$ is a constant multiple of $\overline{f}$. Moreover the charge to mass ratio Q/M of the solution can be made as large as desired.*

Proof: We assume that $\overline{f}$ is fixed as in the assumptions of the theorem. We set

$$\alpha=q^{-1},\quad \overline{f}=\alpha^{-k}\mathring{f},\quad \overline{e}=\alpha^{-(k-1)}\mathring{e}$$

for some integer $k\geqslant 2$. Then (2.14) and (2.15) can be written as

$$e^{-2\mathring{\lambda}}(2r\mathring{\lambda}'-1)+1=8\pi r^2\left(\alpha^k\int_{\mathbb{R}^3}\overline{f}(r,v)\mathrm{d}v+\frac{1}{2}e^{2\mathring{\lambda}}\alpha^{2(k-1)}\overline{e}^2\right), \tag{3.9}$$

$$2\overline{e}+r\overline{e}\mathring{\lambda}'+r\overline{e}'=-r\int_{\mathbb{R}^3}\overline{f}(r,v)\mathrm{d}v. \tag{3.10}$$

Introducing a variable L as defined in (3.2) puts these equations into a form closely analogous to that obtained in the proof of the last theorem. In fact the left-hand side has the same form as in that case. All that is changed is the form of the nonlinear terms on the right-hand side. The equations depend on α as a parameter in a way which is smooth in a neighborhood of $\alpha=0$. For $\alpha=0$ the function $\mathring{\lambda}$ vanishes identically while the equation for $\overline{e}$ becomes linear and has a global regular solution. From this point on we can argue just as in the proof of Theorem 3.3 to conclude that for α sufficiently small there is a unique global regular solution of these equations. Here we must use the fact that $m(R_0)+Q^2/(8\pi R_0)$ is bounded independently of α for α small. The assumption that α is small corresponds to q being large. The distribution function belonging to the solution is obtained from $\mathring{f}$ by a constant rescaling. The charge to mass ratio of the solution is proportional to α^{-k} and thus tends to infinity as α tends to zero. This completes the proof.

Remark 2: The solution in the exterior region is part of the Reissner–Nordström solution.[6]

Remark 3: Our motivation in proving these theorems was to construct initial data for the Einstein–Vlasov–Maxwell system. The same arguments apply with other kinds of charged matter such as a charged fluid as sources for the Einstein equations.

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APPENDIX

This appendix contains an analysis of exterior regions free of particles in initial data sets for the Einstein–Vlasov–Maxwell system. Let $\mathring{f}$ be an initial distribution function of compact support. Let R_0 be the radius of its support in space so that $\mathring{f}$ vanishes for all $r\geqslant R_0$. In this appendix we are only concerned with quantities on the initial hypersurface and so we will drop the label zero indicating the restriction of space–time quantities to the initial hypersurface.

Lemma 1: Consider a solution of the constraint equations for the spherically symmetric Einstein–Vlasov–Maxwell system defined for $0\leqslant r\leqslant R_1$ *and having a regular center. Suppose that radius* R_0 *of the support of the distribution function* f *is less than* R_1. *Let* $\tilde{M}=m(R_0)+Q^2/(8\pi R_0)$. *Then if* $R_1>2\tilde{M}$ *the given solution extends to a unique solution of the constraints defined for all* $r\in[0,\infty[$ *which is asymptotically flat and has* $f=0$ *for* $R\geqslant R_0$.

Proof: Integrating the constraint equation (2.15) gives

$$r^2e^{\lambda(r)}e(r)=q\int_0^r s^2e^{\lambda(s)}\int_{\mathbb{R}^3}f(s,v)\,\mathrm{d}v. \tag{A1}$$

For $r\geqslant R_0$ the upper limit r in the integral can be replaced by R_0 or infinity without changing the value of the expression. It is equal to $Q/4\pi$ where Q is the total charge of the system defined in Sec. II. For $r\geqslant R_0$ the function f vanishes and the mass function m defined in Sec. II satisfies

$$m'=\frac{2\pi}{r^2}(Q/4\pi)^2. \tag{A2}$$

It follows that $\tilde{M}(r)=m(r)+Q^2/(8\pi r)$ is independent of r. If the solution exists globally in r and is asymptotically flat then taking the limit $r\to\infty$ shows that $\tilde{M}$ is equal to the ADM mass M. In any case $\tilde{M}$ is positive and it follows that in the exterior region $m=\tilde{M}-Q^2/(8\pi r)$. In order to determine whether a solution can be extended to larger values of the radius it is enough to ensure that $1-2\tilde{M}/r+Q^2/(4\pi r^2)$ remains positive. For in that case we can define λ by means of the relation

$$e^{-2\lambda}=1-2\tilde{M}/r+Q^2/(4\pi r^2). \tag{A3}$$

Note that $\lim_{r\to\infty}\lambda(r)=0$. Once this has been done we can define μ to be equal to $-\lambda$ and $e(r)=r^{-2}e^{-\lambda}(Q/4\pi)$ in the external region and this gives the unique solution satisfying the correct boundary conditions. If $r>2\tilde{M}$ then $1-2\tilde{M}/r+Q^2/(8\pi r^2)$ is automatically positive and the desired result is obtained.

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Relativistic stars in differential rotation: bounds on the dragging rate and on the rotational energy

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For general relativistic equilibrium stellar models (stationary axisymmetric asymptotically flat and convection-free) with differential rotation, it is shown that for a wide class of rotation laws the distribution of angular velocity of the fluid has a sign, say ''positive,'' and then both the dragging rate and the angular momentum density are positive. In addition, the ''mean value'' (with respect to an intrinsic density) of the dragging rate is shown to be less than the mean value of the fluid angular velocity (in full general, without having to restrict the rotation law, nor the uniformity in sign of the fluid angular velocity); this inequality yields the positivity and an upper bound of the total rotational energy. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1636515]

I. INTRODUCTION

One of the most interesting of the relativistic effects produced by the rotation of a star is the dragging of inertial frames (also called Lense-Thirring effect).[1] This has been classically described in terms of its *local* effects on gyroscopes and particles. However, its cumulative effects on the motion of particles give a much simpler description: a locally non-rotating test particle, that is dragged along in the gravitational field of the star, has an angular velocity, as seen from a non-rotating observer at spatial infinity, which is named *angular velocity of cumulative dragging, or rate of rotational dragging*, shortly called *dragging rate*.[2,3] It is physically expected that, for isolated rotating stars in thermodynamic equilibrium, this dragging rate A has the same sign (rotation sense) as the fluid angular velocity Ω, if this one has a ''uniform'' sign throughout the fluid (in the general differentially rotating case). Indeed, Lindblom[4] and, independently, Hansen and Winicour (1977)[5] seem to establish this result, however, without explicitly fulfilling the corresponding requirements when applying the Hopf theorem (a maximum principle) to an elliptic operator in a certain domain, concerning the boundedness of its coefficients on the boundary of the domain, specifically on the axis of rotation, and the C^1 (and not C^2) regularity of the metric functions across the surface of the star.

Also, (assuming in the description above that the test particle does not collide with the star's matter if it goes through the star) one is tempted to conjecture, in principle in the rigidly rotating case with $\Omega=\text{const}=\Omega_*>0$, that the dragging rate is bounded above by the fluid angular velocity, $A\leqslant\Omega_*$. And Hansen and Winicour (1975)[5] offer some proof of this (although with the same objection as above).

In the general differentially rotating case, however, an analogous relation should not be expected to be so simple; first, because different portions of the star's interior could have opposite rotational motion about the same axis (assuming a convection-free fluid), and, second (even if the fluid angular velocity has a sign), because, due to the integrability condition of the equation of motion, the distribution of fluid angular velocity, Ω-profile, cannot be freely prescribed; instead, it is derived (together with the potential functions, integrating the field equations) once an appropriate *rotation law* is given. Most of the literature concerning numerical works on differentially rotating neutron stars make generally the ansatz for a certain rotation law which yields $A\leqslant\Omega$. Nevertheless, for a more general law such a relation is not so obvious. Hansen and Winicour

(1977)[5] have made some attempts to give a result, however they needed the unphysical assumption that the star's matter occupies the whole space.

One of the aims of this work is precisely to find general and physically reasonable assumptions on the rotation law of a differentially rotating stellar model, so that the dragging rate is (at each interior point) less than the fluid angular velocity, and, hence, the *angular momentum density* is positive (vanishing on the axis) provided the weak energy condition is satisfied. For that matter we consider the time-angle field equation's component, which is elliptic and linear in the dragging potential A in coordinates adapted to the symmetries. The approach with the metric in these coordinates is attractive because the field equations become semilinear elliptic. Specially, they reduce to four (coupled) elliptic equations for the four metric functions. One has however to control the coordinate singularities of the equations on the axis of rotation, but these can be treated mathematically using the axial symmetry of the physical problem.[6] So handled, the elliptic equation in A writes in a ''regular'' form and has bounded coefficients; this allows us to apply a maximum principle to several differential inequalities, which, using the C^1-matching on the star's surface and the asymptotic flatness of the metric, will lead to the mentioned and other interesting inequalities.

More generally, as was conjectured by Thorne[2] (p. 245), the *mean value* of A is expected to be less than the *mean value* of Ω. However, to my knowledge, there is in the literature no explicit and so general result in this direction. The other purpose of the present work is then to derive a ''general'' inequality on ''mean values'' with respect to a density function. In addition, related to this question is the concept of *total rotational energy* of the star. Hartle[7] has given bounds for this rotational energy in the slow rotation limit, which we aim here to generalize.

The paper is organized as follows. After reviewing in Sec. II the model for a relativistic star which is rotating differentially, Sec. III is devoted to handle the concerned field equation, elliptic and linear in the dragging potential, with special attention to the regularity and boundedness properties of the involved functions, as a preparation allowing us to apply the maximum principles (reviewed in the Appendixes) in Sec. IV, where inequalities concerning mainly the positivity of the dragging rate and of the angular momentum density are derived. In Sec. V a general ''mean values inequality'' is derived in full general; and the positivity and upper bound of the total rotational energy is established in the general differentially rotating case. Finally, in Sec. VI the relevant results are briefly summarized.

II. MODEL FOR A DIFFERENTIALLY ROTATING RELATIVISTIC STAR

The space–time of an isolated rotating star in thermodynamic equilibrium within general relativity theory is generally represented by an asymptotically flat stationary axisymmetric four-dimensional Lorentzian manifold $(\mathcal{M},\mathbf{g})$, with metric $\mathbf{g}=g_{\alpha\beta}\,\mathrm{d}x^\alpha\,\mathrm{d}x^\beta$ satisfying Einstein's equations,

$$G_{\alpha\beta}:=R_{\alpha\beta}-\tfrac{1}{2}R\,g_{\alpha\beta}=8\pi\,T_{\alpha\beta}\,, \tag{1}$$

for the energy-momentum tensor of a perfect fluid, $T_{\alpha\beta}=(\varepsilon+p)\,u_\alpha u_\beta+p\,g_{\alpha\beta}$, with 4-velocity u^α, energy density ε, and pressure p. Signature of $\mathbf{g}$ is here considered to be $(-+++)$. Since the star is isolated, the matter (perfect fluid) is confined in a compact region in the space (interior), with vacuum, $T_{\alpha\beta}=0$, on the outside.

We denote the two (commuting) global time and axial Killing vector fields[8] by $\boldsymbol{\xi}=\partial_t$ and $\boldsymbol{\eta}=\partial_\phi$, respectively, where $x^0\equiv t$ labels the spacelike hypersurfaces which are invariant under time translations, and $x^1\equiv\phi$ is the axial-angle coordinate around the axis of rotation, given by $\boldsymbol{\eta}\equiv 0$; $(t,\phi)\in\mathbb{R}\times[0,2\pi[$. The metric components will then only depend on the two remaining spatial coordinates, $g_{\alpha\beta}=g_{\alpha\beta}(x^2,x^3)$.

We shall assume that the fluid motion is purely azimuthal (nonconvective), i.e., the fluid 4-velocity is contained in the 2-surface spanned by the two Killing fields, (as one-forms)

$$\mathbf{u}\wedge\boldsymbol{\xi}\wedge\boldsymbol{\eta}=0 \quad \text{(circularity condition)}\,. \tag{2}$$

In that case it can be seen[9] that the 2-surface elements orthogonal to the two-dimensional group orbits of the Killing fields are surface forming (the same holds in the vacuum region); and, consequently, the metric may be written in a form which is explicitly symmetric under the change $(t,\phi)\to(-t,-\phi)$. In the 2-surfaces orthogonal to the orbits we can always introduce *isotropic coordinates* $(x^2,x^3)=(\rho,z)$ without loss of generality, so that the metric can always be reduced to the standard form[3,10]

$$\mathbf{g}=g_{\alpha\beta}\,\mathrm{d}x^{\alpha}\,\mathrm{d}x^{\beta}=-e^{2U}\,\mathrm{d}t^2+e^{-2U}[\rho^2e^{2B}(\mathrm{d}\phi-A\,\mathrm{d}t)^2+e^{2K}(\mathrm{d}\rho^2+\mathrm{d}z^2)]\,, \tag{3}$$

where the metric functions $K,U,B,$ and A depend only on the (ρ,z)- coordinates of the ''meridian plane.'' Here ρ and z are cylindrical coordinates at the asymptotically flat infinity, and, using the remaining freedom of conformal transformations in the meridian plane, we choose these coordinates such that $\rho=0$ represents the axis of rotation and $(\rho,z)\in\mathbb{R}_0^+\times\mathbb{R}$ (denoting $\mathbb{R}_0^+:=\{x\in\mathbb{R}\,|\,x\geqslant 0\}$). The metric functions $\rho\,e^B$, U, and A can be written as invariant combinations of the Killing fields in the form

$$\rho^2e^{2B}=-\det((g_{\mu\nu})_{\mu,\nu=t,\phi})=-\mathbf{g}(\boldsymbol{\xi},\boldsymbol{\xi})\,\mathbf{g}(\boldsymbol{\eta},\boldsymbol{\eta})+\mathbf{g}(\boldsymbol{\xi},\boldsymbol{\eta})^2\,,$$

$$e^{2U}=\frac{\rho^2e^{2B}}{\mathbf{g}(\boldsymbol{\eta},\boldsymbol{\eta})}, \tag{4}$$

$$A=-\frac{\mathbf{g}(\boldsymbol{\xi},\boldsymbol{\eta})}{\mathbf{g}(\boldsymbol{\eta},\boldsymbol{\eta})}\quad,$$

and they can be interpreted physically as follows: $\rho\,e^B$ represents a sort of distance from the rotation axis (and, hence, B is, to some extent, a measure how far is ρ from being that distance); U is a generalization of the gravitational potential; and A is the *angular velocity of cumulative dragging, or dragging rate*. The remaining metric function is K, the conformal factor in the meridian plane.

Throughout the following we shall denote the closure and the boundary of a set X by $\overline{X}$ and ∂X, respectively. We fix the notions

$$I\equiv\text{interior of the star}:=\{(\rho,z)\in\mathbb{R}_0^+\times\mathbb{R}\;\mid\;p(\rho,z)>0\}\subset\mathbb{R}_0^+\times\mathbb{R}\,,$$

$$E\equiv\text{exterior of the star}:=(\mathbb{R}_0^+\times\mathbb{R})\backslash\overline{I}\subset\mathbb{R}_0^+\times\mathbb{R}\,, \tag{5}$$

$$S\equiv\text{star's surface}:=\overline{I}\cap\overline{E}=\partial I\subset\mathbb{R}_0^+\times\mathbb{R}\,,$$

I and E open in the *induced topology in* $\mathbb{R}_0^+\times\mathbb{R}\subset\mathbb{R}^2$; that means, although part of the axis ($\rho=0$) is in I (and part in E), the only points of the axis which are in $\partial I=S$ (and in $\partial E=S\cup\{\infty\}$) are the poles, if they exist. The set $I\subset\mathbb{R}_0^+\times\mathbb{R}$ is supposed to be bounded and connected. Concerning the regularity of $S=\partial I$, we assume it satisfies an exterior sphere condition everywhere (cf. Definition in Appendix A).

Within our star model, the *matching* conditions (from the interior and the exterior solutions) require that the pressure vanishes identically on the star's surface, $p=0$ on S. In the exterior ($T_{\alpha\beta}=0$) we have $\varepsilon=p=0$. Furthermore, ε and p satisfy a barotropic equation of state in the interior,

$$\varepsilon=\varepsilon(p)\quad\text{ in }\ \overline{I}\,. \tag{6}$$

We assume the pressure p to be continuous with respect to the coordinates, and also $p\mapsto\varepsilon(p)$ a continuous function,

$$p \in C^0(\mathbb{R}_0^+ \times \mathbb{R}), \quad p \mapsto \varepsilon(p) \in C^0(\mathbb{R}_0^+), \tag{7}$$

satisfying the *weak energy condition*,[11]

$$\varepsilon + p \geqslant 0 \quad (\text{in} \quad \mathbb{R}_0^+ \times \mathbb{R}). \tag{8}$$

[Notice, by the definition of the interior, (5), if $\varepsilon \geqslant 0$ in $\overline{I}$, as it is generally assumed, we shall have even $\varepsilon + p > 0$ in I, and, hence, condition (8) follows. In addition, since the equation of state is defined only in the interior, (6), requirement (7) does not guarantee the continuity of ε across the star's surface (where $p = 0$), namely, if $\varepsilon(p = 0) > 0$, then a jump discontinuity of ε across the star's surface occurs.]

From the circularity condition (2) on the fluid 4-velocity (in $\overline{I}$), this is of the form

$$\mathbf{u} = u^t(\boldsymbol{\xi} + \Omega\, \boldsymbol{\eta}), \quad \text{where} \quad \Omega \equiv \frac{u^\phi}{u^t} = \frac{\mathrm{d}\phi}{\mathrm{d}t}$$

is the angular velocity of the fluid measured by a distant observer in an asymptotically flat space–time, and the fact that the 4-velocity $\mathbf{u}$ is a unit timelike vector field determines the normalization factor u^t, such that $\mathbf{g}(\mathbf{u},\mathbf{u}) = -1$, i.e.,

$$(u^t)^{-2} = e^{2U} - \rho^2 e^{2(B-U)}(\Omega - A)^2 =: N, \tag{9}$$

from where $N = (u^t)^{-2} > 0$ in $\overline{I}$. Indeed, we do not allow that the velocity of light is approached somewhere, and, hence, even

$$N \geqslant \text{const} > 0 \quad \text{in} \quad \overline{I}. \tag{10}$$

We consider a star rotating differentially with a distribution of angular velocity (*rotation profile*) $\Omega = \Omega(\rho, z)$, a continuously differentiable function,

$$\Omega \in C^1(\overline{I}). \tag{11}$$

However, the Ω-profile of the fluid cannot be freely chosen, this shows up in the following. The integrability conditions of the field equations (1), that is, the equation of hydrostatic equilibrium $T^{\alpha\beta}{}_{;\beta} = 0$ (from $G^{\alpha\beta}{}_{;\beta} = 0$) (where ";" denotes covariant derivative), particularly, its part orthogonal to the fluid 4-velocity $\mathbf{u}$, reduces to the Euler equation,

$$\mathrm{d}p = -(\varepsilon + p)\, \mathbf{a}, \tag{12}$$

where $\mathbf{a}$ is the 4-acceleration of the fluid, $\mathbf{a} = \nabla_{\mathbf{u}}\mathbf{u}$. Specifically,

$$\mathbf{a} = \mathrm{d}V + u^t u_\phi\, \mathrm{d}\Omega, \quad V \equiv \tfrac{1}{2} \ln N, \tag{13}$$

$u^t u_\phi = \rho^2 e^{2(B-U)}(\Omega - A) N^{-1}$. But the integrability condition of Eq. (12) taking into account (6) is $\mathrm{d}\mathbf{a} = 0$; following then, from (13), $d(u^t u_\phi) \wedge \mathrm{d}\Omega = 0$. The special case where $\Omega = \text{const}$ is called *rigid rotation* (or *uniform rotation*). In general we shall have $\Omega \neq \text{const}$, following then,

$$u^t u_\phi = \mathcal{F}(\Omega), \tag{14}$$

for some function $\mathcal{F}$, *rotation law*. By specifying the function $\mathcal{F}(\Omega)$ a specific model of *differential rotation* is obtained. [Note, since in the Newtonian limit $u^t u_\phi \to \rho^2 \Omega$, Eq. (14) expresses the general relativistic generalization of the Newtonian "rotation on cylinders" theorem, $\Omega = \mathcal{G}(\rho^2)$.]

Further requirements on our stellar model are

(a) the metric functions are (at least) two times continuously differentiable in the interior and in the exterior of the star, and continuously differentiable everywhere (cf. note in Sec. III B),

$$K,U,B,A \in C^2(I)\cap C^2(E)\cap C^1(\mathbb{R}_0^+\times\mathbb{R})\,; \tag{15}$$

(b) in order that the metric functions are symmetric with respect to the z-axis ($\rho=0$) (''axisymmetric solutions''), and, hence, the metric (3), defined on $\mathcal{M}$ excluding the axis, can be extended to an at least C^1 axisymmetric tensor field in the whole space–time $\mathcal{M}$, we assume that

$$\text{as } \rho\to 0,\quad \partial_\rho K,\ \partial_\rho U,\ \partial_\rho B,\ \partial_\rho A\to 0\,, \tag{16}$$

and, for completeness, also $\partial_\rho\varepsilon$, $\partial_\rho p\to 0$;

(c) finally, by the asymptotic flatness requirement, denoting $\mathcal{D}:=(\partial_\rho,\partial_z)$,

$$\text{as } R:=(\rho^2+z^2)^{1/2}\to\infty,\quad K,U,B,A\to 0 \text{ and } \mathcal{D}K,\mathcal{D}U,\mathcal{D}B,\mathcal{D}A\to\mathbf{0}\,. \tag{17}$$

Notice, from C^1 regularity, in (15), and asymptotic flatness, (17), it follows, in particular, that the metric functions and their derivatives are bounded,[12]

$$|K|,|U|,|B|,|A|<\infty \quad \text{and} \quad \|\mathcal{D}K\|,\|\mathcal{D}U\|,\|\mathcal{D}B\|,\|\mathcal{D}A\| <\infty \quad \text{in } \mathbb{R}_0^+\times\mathbb{R}\,. \tag{18}$$

III. THE ELLIPTIC EQUATION FOR THE DRAGGING RATE *A*

A. The time-angle field equation component

The $(t\phi)$ component of Einstein's equation (1) in these coordinates takes the form[6]

$$\partial_{\rho\rho}A+\partial_{zz}A+\frac{3}{\rho}\partial_\rho A+\langle 3\mathcal{D}B-4\mathcal{D}U\,,\,\mathcal{D}A\rangle=-\psi^2\cdot(\Omega-A)\,, \tag{19}$$

$$\text{with}\quad \psi^2:=16\pi\frac{e^{2K}}{N}(\varepsilon+p)\quad [\geqslant 0,\ \text{by (8) and (10)}]\,, \tag{20}$$

where $\langle .,.\rangle$ denotes the Euclidean scalar product. Since, from condition (16), $v(\rho,z)=v(-\rho,z)$ for $v=K,U,B,A$, i.e., we are considering only axisymmetric solutions of the field equations, and since only ''axisymmetric operations'' appear in these equations, we consider the following transformation (in the spirit of Ref. 6) in order to avoid the coordinate singularity [of Eq. (19)] on the axis of symmetry (z-axis, i.e., $\rho=0$). To this end we use the 5-*lift* of each function $v\equiv v(\rho,z)$ (on $\mathbb{R}^5$), for the metric functions $v=K,U,B,A$ and also for $v=\Omega,\varepsilon,p$, where the *n-lift* of $v:\mathbb{R}_0^+\times\mathbb{R}\to\mathbb{R}$ on flat $\mathbb{R}^n$, axisymmetric around the x_n-axis, is defined as follows:

$$v\mapsto\tilde{v}\quad \text{such that } \tilde{v}(x)\equiv\tilde{v}(x_1,\ldots,x_n):=v(\rho=({x_1}^2+\cdots+{x_{n-1}}^2)^{1/2},\ z=x_n)\,, \tag{21}$$

and, for every function $\tilde{v}:\mathbb{R}^n\to\mathbb{R}$, the *meridional cut* (*in direction* x_1) *of* $\tilde{v}$,

$$\tilde{v}\mapsto v\quad \text{such that } v(\rho,z):=\tilde{v}(\rho,0,\ldots,0,z)\,. \tag{22}$$

For axisymmetric functions, both operations are isomorphisms and inverse to each other; but the relevant properties of n-lift and meridional cut are that (a) they leave the regularity conditions and the norms invariant, (b) they commute with ''axisymmetric operations,'' in particular, with all operations in Eq. (19), like multiplication and scalar product, yielding especially (for $n=5$)

$$\langle\mathcal{D}v,\mathcal{D}w\rangle=\langle\nabla\tilde{v},\nabla\tilde{w}\rangle\,,\ \text{denoting } \nabla:=(\partial_1,\ldots,\partial_5)\quad (\partial_i\equiv\partial_{x_i},\quad \partial_{ij}\equiv\partial_{x_i}\partial_{x_j})\,,$$

and, remarkably, (c) they transform the operator $\partial_{\rho\rho}+\partial_{zz}+[(n-2)/\rho]\,\partial_\rho$ $(n\geqslant 2)$ into the flat n-dimensional Laplacian, and vice versa; having for $n=5$,

$$\partial_{\rho\rho}v+\partial_{zz}v+\frac{3}{\rho}\partial_{\rho}v=\sum_{i=1}^{5}\partial_{ii}\tilde{v}=:\Delta\tilde{v}\,.$$

Hence, with the 5-lift, Eq. (19) writes in the form

$$\Delta\tilde{A}+\langle 3\nabla\tilde{B}-4\nabla\tilde{U}\,,\nabla\tilde{A}\rangle=-\tilde{\psi}^2\cdot(\tilde{\Omega}-\tilde{A})\,, \tag{23}$$

$\tilde{\psi}^2$ defined like ψ^2, (20), but with 5-*lifted* functions (on $\mathbb{R}^5$).

B. Regularity and boundedness of the metric functions

Let us see how conditions (15)–(18) transmit through the 5-lift. First, from conditions (15) and (16) it follows

$$\tilde{K},\tilde{U},\tilde{B},\tilde{A}\in C^1(\mathbb{R}^5)\,, \tag{24}$$

because (for $v=K,U,B,A$) $v\in C^1(\mathbb{R}_0^+\times\mathbb{R})$ and $\partial_\rho v\to 0$ as $\rho\to 0$ imply $\tilde{v}\in C^1(\mathbb{R}^5)$.

Note: In fact, as seen in Ref. 6, with the use of these mathematical tools (n-lift and meridional cut, for different numbers n), the elliptic system of field equations (1) may be regarded as a set of *Poisson-like equations*, where the nonlinearities (quadratic terms in the first derivatives of the metric functions) are contained in the inhomogeneous terms on the right-hand side. Making the weak requirement that the metric functions and their derivatives are essentially bounded, $\tilde{v},\nabla\tilde{v}\in L^\infty$, since also $\tilde{\varepsilon},\tilde{p}\in L^\infty$ [by condition (7) and $\tilde{\varepsilon}=\tilde{p}=0$ in the exterior], and $\tilde{\Omega}\in L^\infty$ [by (11)], we have that the right-hand side is essentially bounded. Then, by the regularity of Poisson's integral,[13] (at least) $\tilde{v}\in C^{1,\alpha}$ for some $\alpha<1$; in particular, $\tilde{v}\in C^1$, i.e., (24). This justifies requirements (15) and (16) in Sec. II.

Combining (15) and (16) we obtain also that the 5-lifted metric functions are class C^2 in the interior and in the exterior of the star (in $\mathbb{R}^5$). That is, denoting

$$\mathcal{I}:=\{(x_1,\ldots,x_5)\in\mathbb{R}^5\ \ |\ ((x_1{}^2+\cdots+x_4{}^2)^{1/2},x_5)\in I\}\subset\mathbb{R}^5 \tag{25}$$

and, analogously, $\mathcal{E}$ and $\mathcal{S}$, from E and S [cf. (5)], respectively, we have for $\tilde{v}=\tilde{K},\tilde{U},\tilde{B},\tilde{A}$,

$$\tilde{v}\in C^2(\mathcal{I})\cap C^2(\mathcal{E})\cap C^1(\mathbb{R}^5)\,. \tag{26}$$

The asymptotic flatness condition (17) implies, through the 5-lift, that

$$\text{as}\quad R=\|x\|=(x_1{}^2+\cdots+x_5{}^2)^{1/2}\to\infty,\quad \tilde{v}\to 0\ \text{ and }\ \nabla\tilde{v}\to\mathbf{0}\,; \tag{27}$$

but $\tilde{v}\in C^1(\mathbb{R}^5)$, that is, $\tilde{v}\in C^0(\mathbb{R}^5)$ and $\nabla\tilde{v}\in[C^0(\mathbb{R}^5)]^5$, yielding, together with conditions (27), their respective boundedness,

$$|\tilde{v}|<\infty\quad\text{and}\quad\|\nabla\tilde{v}\|<\infty\ \text{ in }\ \mathbb{R}^5\,. \tag{28}$$

C. Notation convention and roundup

We have seen in Sec. III A that Eq. (23) is equivalent to Eq. (19) through the 5-lift and the meridional cut, (21) and (22) for $n=5$. Furthermore, the 5-lift leaves regularity and boundedness properties invariant; see Sec. III B.

Convention: For simplicity in the notation, we omit throughout the following the symbols "$\sim$" for all 5-lifted functions we use. [Once it has been seen how regularity and boundedness properties transmit from the functions defined on $\mathbb{R}_0^+\times\mathbb{R}$ to the lifted ones (on $\mathbb{R}^5$), and since they are equivalent in terms of positivity, and no explicit reference to the first ones will appear throughout the following section, this notation convention seems appropriate.]

Accordingly, we write Eq. (23) in the form

$$L_0 A = -\psi^2 \cdot (\Omega - A)\,, \tag{29}$$

$$\text{with} \quad L_0 A := \Delta A + \langle 3\nabla B - 4\nabla U\,,\, \nabla A\rangle\,, \tag{30}$$

$$\begin{gathered}\psi^2 := 16\pi \frac{e^{2K}}{N}(\varepsilon + p) \;\geqslant 0 \quad (=0 \quad \text{in} \quad \mathcal{E})\,, \\ \text{and} \quad N := e^{2U} - \rho^2 e^{2(B-U)}(\Omega - A)^2 \;\geqslant\; \text{const} > 0 \quad \text{in} \quad \overline{\mathcal{I}},\end{gathered} \tag{31}$$

where $K, U, B, A : \mathbb{R}^5 \to \mathbb{R}$, axisymmetric around the x_5-axis. [Notice, Eq. (29) is so defined in the whole space–time, interior (fluid) and exterior (vacuum), $\overline{\mathcal{I}} \cup \mathcal{E} = \mathbb{R}^5$, but in the exterior $\psi^2 \equiv 0$ ($\varepsilon = p = 0$) and the vacuum field equation is recovered, $L_0 A = 0$ in $\mathcal{E}$.] Also, we have (26)–(28), i.e. (with the notation convention),

$$K, U, B, A \in C^2(\mathcal{I}) \cap C^2(\mathcal{E}) \cap C^1(\mathbb{R}^5)\,, \tag{32}$$

$$\text{as} \quad R = \|x\| = (x_1{}^2 + \cdots + x_5{}^2)^{1/2} \to \infty, \quad K, U, B, A \to 0\,, \tag{33}$$

$$\nabla K, \;\; \nabla U, \;\; \nabla B, \;\; \nabla A \to \mathbf{0}\,; \tag{34}$$

$$|K|, \;\; |U|, \;\; |B|, \;\; |A| \;\; < \infty\,, \tag{35}$$

$$\text{and} \quad \|\nabla K\|, \;\; \|\nabla U\|, \;\; \|\nabla B\|, \;\; \|\nabla A\| \;\; < \infty \;\; \text{in} \;\; \mathbb{R}^5\,. \tag{36}$$

Equation (29), i.e.,

$$L A := L_0 A - \psi^2 \cdot A = -\psi^2 \cdot \Omega\,, \tag{37}$$

writes then

$$L A \equiv a_{ij}(x)\, \partial_{ij} A + b_i(x)\, \partial_i A + c(x)\, A = g(x)$$

with

$$\begin{gathered}a_{ij} \equiv \text{const} = \delta_{ij} \quad (=1 \;\; \text{if} \;\; i=j, \;\; \text{and} \;\; =0 \;\; \text{otherwise})\,, \\ b_i = 3\,\partial_i B - 4\,\partial_i U \quad (\forall\, i,j \in \{1,\ldots,5\}), \quad \text{and} \\ c = -\psi^2 (\leqslant 0)\,, \\ g = c\,\Omega\end{gathered} \tag{38}$$

(where repeated indices indicate summation from 1 to 5). The flat five-dimensional Laplacian Δ, in (30), ($a_{ij} \equiv \delta_{ij}$), and hence L, is obviously strictly and uniformly elliptic everywhere. The coefficients b_i are measurable and bounded functions everywhere, because B and U are C^1, (32), and have bounded derivatives, (36). On the other hand, for the coefficient c [cf. (31)], since (i) the metric functions are continuous, (32), and bounded, (35); (ii) p is continuous everywhere, (7), and has compact support; (iii) ε is continuous in the (closed) interior $\overline{\mathcal{I}}$, from (7); (iv) Ω is in particular continuous (in $\overline{\mathcal{I}}$), (11), and, hence, measurable; and (v) $N \geqslant \text{const} > 0$ (also in $\overline{\mathcal{I}}$), (10); it follows that $c \equiv -\psi^2$ is measurable and bounded in the interior $\mathcal{I}$, and, since $\psi^2 \equiv 0$ ($\varepsilon = p = 0$) in the exterior $\mathcal{E}$, and the boundary (the star's surface) $\partial\mathcal{I} = \mathcal{S}$ is a set of measure zero, we have that the coefficient c is measurable and bounded everywhere. This will allow us in the following section to apply maximum principles in the classical and in the generalized sense to the operator L (and L_0); see Appendixes A and B.

IV. BOUNDS ON THE DRAGGING RATE

A. Positivity of the dragging rate

Proposition 1: If the distribution of angular velocity of the fluid is non-negative (and non-trivial), then the dragging rate is positive everywhere,

$$\Omega \geqslant 0, \quad \Omega \not\equiv 0 \Rightarrow \; A > 0 \, .$$

Proof: Consider the domain G defined by a ball in $\mathbb{R}^5$ centered at the origin $x = \mathbf{0}$ and of arbitrarily large radius σ,

$$G := \mathcal{B}_\sigma(\mathbf{0}) \subset \mathbb{R}^5 \, . \tag{39}$$

Since A is continuously differentiable in $\mathbb{R}^5$, cf. (32), so is in particular in G; but A and ∇A continuous in $\mathbb{R}^5$ implies that they are 2-integrable (are in L^2) in G; consequently,

$$A \in W^{1,2}(G) \cap C^1(G) \, . \tag{40}$$

Hence, the strictly elliptic linear partial differential equation (in A) with measurable and bounded coefficients, (37), is satisfied in a generalized sense in G; see Appendix B. Remarkably, whenever $\Omega \geqslant 0$, Eq. (37) yields the differential inequality

$$L\,A \leqslant 0 \quad \text{in } \; G \, , \tag{41}$$

i.e., A is a generalized supersolution relative to the operator L and the domain G. We pay now special attention to the behavior of A on the boundary: since the radius of the ball G, σ, is arbitrary, we can make it sufficiently large ($\sigma \to \infty$) such that, by the asymptotic flatness condition on A [cf. (33)], A is arbitrarily small on ∂G,

$$\lim_{\sigma \to \infty} A\big|_{\partial G} = 0 \, . \tag{42}$$

We first observe that $A \not\equiv \text{const}$ [because, by (42) and $A \in C^0(\mathbb{R}^5)$, would be $A \equiv \text{const} = 0$, which yields, by Eq. (37), $\Omega \equiv 0$, and we are assuming $\Omega \not\equiv 0$]. Hence, by the strong minimum principle, Theorem 4 in Appendix B, applied to the differential inequality (41), A cannot attain a nonpositive minimum at an interior point of G; using (42), we conclude then $A > 0$ in G, i.e., everywhere.□

Remark 1: A result analogous to Proposition 1 holds with the opposite sense of the rotation; that is, if $\Omega \leqslant 0$ $(\Omega \not\equiv 0)$, then $A < 0$. This follows because Eq. (29) is invariant with respect to the simultaneous change of sign $(\Omega, A) \to (-\Omega, -A)$.

B. Upper bound Ω. Positivity of the angular momentum density

Hereafter we discuss the sign of the difference $\Omega - A$. Remarkably, this determines the sign of $u^t u_\phi$, which, with assumption (8), is the sign of the *angular momentum density*, integrand of the total angular momentum, given by the "volume" integral[14] $J = \int_{\mathcal{I}} 2\pi\, T^t_\phi\, (-g)^{1/2}\, \mathrm{d}x$, where $g \equiv \det(\mathbf{g})$ and $T^t_\phi = (\varepsilon + p)\, u^t u_\phi$.

1. In the rigidly rotating case

Proposition 2: In the particular case of rigid rotation, with $\Omega \equiv \text{const} =: \Omega_* > 0$,

$$0 < A < \Omega_*$$

holds everywhere. As a consequence, in this case, $u^t u_\phi$, *and, hence, the angular momentum density, is non-negative.*

Proof: We consider Eq. (29) for $\Omega \not\equiv \text{const} = \Omega_* > 0$, i.e., $L_0\, A = -\psi^2 \cdot (\Omega_* - A)$, which, since the differential operator L_0, (30), is free from linear term, can be rewritten in the form

$$L_0(A-\Omega_*)=-\psi^2\cdot(\Omega_*-A)\,,$$

or, denoting again the differential operator $L:=L_0-\psi^2$ and defining

$$w(x):=A(x)-\Omega_* \tag{43}$$

in the whole space–time, $x\in\overline{\mathcal{I}}\cup\mathcal{E}=\mathbb{R}^5$ (as already 5-lifted function; cf. Sec. III A),

$$Lw=L(A-\Omega_*)=L_0(A-\Omega_*)-\psi^2\cdot(A-\Omega_*)=0 \quad \text{in } \mathbb{R}^5\,.$$

We have then the strictly elliptic linear (in w) equation

$$Lw=0 \quad (\text{in particular}) \text{ in } G\equiv\mathcal{B}_\sigma(\mathbf{0})\subset\mathbb{R}^5\,, \tag{44}$$

where the radius σ is arbitrary, with $w\in W^{1,2}(G)\cap C^1(G)$, by (40) and (43). On the other hand, by the condition of asymptotic flatness on A [in (33)], A is arbitrarily small on ∂G, provided that σ is sufficiently large, i.e., (42); consequently,

$$\lim_{\sigma\to\infty} w|_{\partial G}=-\Omega_*<0\,. \tag{45}$$

Since $w\not\equiv$const [because, by (45) and continuity, would be $w\equiv$const$=-\Omega_*$ in G, that is, $A\equiv$const$=0$ in G, which is not allowed, by Eq. (37), since here $\Omega\equiv\Omega_*>0$], applying the strong maximum principle, Theorem 4 in Appendix B, to Eq. (44), we get that w cannot attain a nonnegative maximum at an interior point of G; hence, using (45), $w<0$ in G (everywhere), i.e., $A<\Omega_*$ everywhere. Moreover, $A>0$ everywhere, by Proposition 1. This establishes the conclusion of the proposition. □

Observe, in the static case, $\Omega_*=0$, we would have $Lw=0$ and $\lim_{\sigma\to\infty}w|_{\partial G}=0$, following, by the strong maximum and minimum principles, $w\equiv0$, i.e., $A\equiv\Omega_*=0$; as expected, $A\equiv0$.

Remark 2: Likewise, if $\Omega\equiv$const$\equiv\Omega_*<0$, then $0>A>\Omega_*$ everywhere, and, hence, the angular momentum density is nonpositive. We obtain this by applying Proposition 2 to the function $\hat{A}:=-A$, solution of Eq. (29) for $\hat{\Omega}_*:=-\Omega_*>0$ (cf. Remark 1). More explicitly, the angular momentum density of a rigidly rotating stellar model has the same sign as the angular velocity of the fluid. Also, as a result, we have for a fluid rotating rigidly with $\Omega\equiv$const$\equiv\Omega_*\neq0$,

$$0<|A|<|\Omega_*|\,.$$

2. In the general (differentially rotating) case

In the following we shall assume that a function $\mathcal{F}$ (to be specified) has been given, and we have a solution of the problem, that is, (four) metric functions, K, U, B, and A, and a fluid angular velocity distribution, Ω, satisfying the (four) field equations (1) [in particular, the elliptic equation for A, Eq. (29)] and Eq. (14), $u^t u_\phi=\mathcal{F}(\Omega)$. [Notice, in the interior, where the matter terms do not vanish ($p>0,\varepsilon\geqslant0$), substituting into the equation of motion (12) [with (13)] its integrability condition, i.e., Eq. (14), and the equation of state, Eq. (6), we obtain the pressure, p, and the energy density, ε, as functions of ρ, U, B, A, and Ω.]

Remarkably, $u^t u_\phi$ may be written

$$u^t u_\phi\equiv\frac{\rho^2 e^{2(B-U)}(\Omega-A)}{e^{2U}-\rho^2 e^{2(B-U)}(\Omega-A)^2}=\frac{\varrho^2(\Omega-A)}{1-\varrho^2(\Omega-A)^2}=:\Phi(\varrho\,,\Omega-A)\quad\text{with}\quad\varrho:=\rho\,e^{B-2U}\,, \tag{46}$$

where, from (10), $1-\varrho^2(\Omega-A)^2=Ne^{-2U}\geqslant$const$>0$ in $\overline{\mathcal{I}}$. With the defined function (46), Eq. (14) writes

$$\Phi(\varrho\,,\Omega-A)=\mathcal{F}(\Omega)\,. \tag{47}$$

Lemma: Assume

(i) *the function* $\mathcal{F}:\mathbb{R}\to\mathbb{R}$ *is strictly decreasing, and*
(ii) $\exists$ *a constant* Ω_c $(|\Omega_c|<\infty)$ *such that* $\mathcal{F}(\Omega_c)=0$,

then, at each interior point (in $\overline{\mathcal{I}}$*), where Eq.* (47), $\Phi=\mathcal{F}$, *is satisfied, the following holds:*

$$\begin{aligned} &A<\Omega \Leftrightarrow A<\Omega\leqslant\Omega_c \quad (A<\Omega_c),\\ &A>\Omega \Leftrightarrow A>\Omega\geqslant\Omega_c \quad (A>\Omega_c),\\ &A=\Omega \Leftrightarrow A=\Omega=\Omega_c \quad (A=\Omega_c)\,. \end{aligned} \tag{48}$$

Note 1: Due to (i), Ω_c [defined in (ii)] is unique. Also, observe, Ω_c exists and coincides with the (constant) value of Ω on the rotation axis, provided that part of the axis, $\varrho=0$, is in the interior, $\mathcal{I}$, (i.e., if the rotating fluid does not have toroidal topology). This is because at points in $\{\varrho=0\}\cap\mathcal{I}\neq\varnothing$, since $\Phi|_{\varrho=0}=0$ and $\Phi=\mathcal{F}$ in $\mathcal{I}$, we have $\mathcal{F}(\Omega)|_{\varrho=0}=0$; and $\mathcal{F}$ is, by requirement (i), invertible; yielding $\Omega|_{\varrho=0}=\text{const}=\Omega_c$.

Note 2: Observe, if $\mathcal{F}\in C^1$ and $\mathcal{F}'<0$, then, since $\partial_\Omega\Phi\geqslant 0$, Eq. (47) can be solved for Ω, by virtue of the implicit function theorem, yielding $\Omega=\Omega(\rho,U,B,A)$; and, by the regularity of the metric functions, (32), it follows in particular $\Omega\in C^1(\overline{\mathcal{I}})$, requirement (11).

Note 3: It should be stressed that, since Φ is an *increasing* function in Ω, choosing the function $\mathcal{F}$ strictly *decreasing* [requirement (i)], Eq. (47) has a unique solution in Ω (''curve'' solution with ϱ variable). Specially, this makes likely the existence of functions Ω, K, U, B, and A, solutions of the field equations and Eq. (14). Indeed, in numerical works concerning differential rotation the ansatz for the $\mathcal{F}$-law $\mathcal{F}(\Omega)=R_0^2(\Omega_c-\Omega)$, where R_0 is a free parameter describing the length of scale over which Ω changes, is generally used, and they claim they have a solution. (See, e.g., Refs. 15–17.)

Proof: We consider a point $x\in\overline{\mathcal{I}}$ where the metric functions and the fluid angular velocity are solution, in particular, with reference to Eq. (47), the functions Φ and $\mathcal{F}$ valued at this point ''intersect'' each other, i.e.,

$$\Phi(\varrho(x)\,,\,\Omega(x)-A(x))=\mathcal{F}(\Omega(x))\quad(\forall x\in\overline{\mathcal{I}})\,.$$

From requirements (i) and (ii), it follows (at each interior point) $\text{sign}(\mathcal{F})=\text{sign}(\Omega_c-\Omega)$. As regards Φ (at the interior point), on the axis $(\varrho=0)$ it obviously vanishes, cf. (46); following, from the relation $\Phi=\mathcal{F}$ (in $\overline{\mathcal{I}}$), $\Phi=\mathcal{F}=0$ and, thus, $\Omega=\Omega_c$ on the axis. Outside the axis $(\varrho\neq 0)$ we have $\text{sign}(\Phi)=\text{sign}(\Omega-A)$; and, hence (outside the axis)

$$\begin{aligned} &\Phi=\mathcal{F}>0\Leftrightarrow A<\Omega<\Omega_c\,,\\ &\Phi=\mathcal{F}<0\Leftrightarrow A>\Omega>\Omega_c\,,\\ &\Phi=\mathcal{F}=0\Leftrightarrow A=\Omega=\Omega_c\,. \end{aligned}$$

But also,

$$\forall x\in\overline{\mathcal{I}}\ \ /\ \ A(x)<\Omega(x),\quad \begin{cases} A(x)<\Omega(x)<\Omega_c & \text{if } \varrho(x)\neq 0,\\ A(x)<\Omega(x)=\Omega_c & \text{if } \varrho(x)=0, \end{cases}$$

$$\forall x\in\overline{\mathcal{I}}\ \ /\ \ A(x)>\Omega(x),\quad \begin{cases} A(x)>\Omega(x)>\Omega_c & \text{if } \varrho(x)\neq 0,\\ A(x)>\Omega(x)=\Omega_c & \text{if } \varrho(x)=0, \end{cases}$$

$$\text{and}\ \ \forall x\in\overline{\mathcal{I}}\ \ /\ \ A(x)=\Omega(x),\quad A(x)=\Omega(x)=\Omega_c\,.$$

This yields (48). □

We are now in a position to get one of the main results of this work in the general differentially rotating case, namely, the following proposition.

Proposition 3: If the $\mathcal{F}$-law [in Eq. (14)] specifying the model of differential rotation is chosen such that

(i) $\mathcal{F}:\mathbb{R}\to\mathbb{R}$ *strictly decreasing,*
(ii) $\exists$ *a constant* Ω_c $(|\Omega_c|<\infty)$ *such that* $\mathcal{F}(\Omega_c)=0$, *and*
(iii) $\Omega_c>0$,

then

$$0<A<\Omega\leqslant\Omega_c \quad in\ \ \overline{\mathcal{I}}; \tag{49}$$

in particular, $u^t u_\phi\geqslant 0$, *and, hence, the angular momentum density is non-negative. Moreover,*

$$0<A<\max_{\mathcal{S}}\Omega\leqslant\Omega_c \quad in\ \ \mathcal{E}. \tag{50}$$

Note: As remarked above, if the interior (fluid) contains points of the axis, then condition (ii) is already guaranteed, and Ω_c is the constant value of Ω on the axis; cf. Note 1 in the previous lemma. See also Notes 2 and 3. And observe, requirement (iii) is in principle much weaker than $\Omega>0$, but, as seen in the conclusion of this proposition, $\Omega>0$ already follows. Furthermore, the fact that $\Omega\leqslant\Omega_c$ in $\overline{\mathcal{I}}$ shows that in differentially rotating stars the core may rotate faster than the envelope, so that the core can be supported by rapid rotation before mass shedding is reached at the equator.[18]

Proof: We divide the proof in four steps.

First step: Let us see first $A\leqslant\Omega$ in $\overline{\mathcal{I}}$. Suppose (to get a contradiction) $A(x_0)>\Omega(x_0)$ for some $x_0\in\overline{\mathcal{I}}$. We have seen, in the previous lemma, cf. (48), that this is equivalent to $A(x_0)>\Omega(x_0)\geqslant\Omega_c$; and, hence, using hypothesis (iii), $A(x_0)>\Omega_c>0$. Therefore, by the continuity of A [indeed $A\in C^1$, cf. (32)] and the asymptotic flatness [$\lim_{\|x\|\to\infty}A=0$, cf. (33)], we infer that there exists an open and connected neighborhood of x_0, $\mathcal{N}_{x_0}\subset\mathbb{R}^5$, such that

$$\begin{aligned} &A>\Omega_c \quad \text{in}\ \ \mathcal{N}_{x_0},\\ &\text{and}\ \ A=\Omega_c \quad \text{on}\ \ \partial\mathcal{N}_{x_0}. \end{aligned} \tag{51}$$

We distinguish two cases.

Case 1: $\mathcal{N}_{x_0}\cap\mathcal{E}=\varnothing$, that is, the neighborhood is contained in the interior, $\mathcal{N}_{x_0}\subseteq\mathcal{I}$. Thus we have, again using the previous lemma, $A>\Omega\geqslant\Omega_c>0$ in $\mathcal{N}_{x_0}$; particularly, $\Omega-A<0$ in $\mathcal{N}_{x_0}$, and, therefore, by Eq. (29),

$$L_0 A>0 \quad \text{in}\ \ \mathcal{N}_{x_0}\subseteq\mathcal{I}.$$

From (32), in particular, $A\in C^2(\mathcal{I})\cap C^0(\overline{\mathcal{I}})$, and, hence, $A\in C^2(\mathcal{N}_{x_0})\cap C^0(\overline{\mathcal{N}}_{x_0})$. And applying the weak maximum principle, Theorem 1 in Appendix A, to the operator L_0 (on A) in $\mathcal{N}_{x_0}$, we obtain that the maximum of A is reached on the boundary, i.e.,

$$\max_{\overline{\mathcal{N}}_{x_0}} A=\max_{\partial\mathcal{N}_{x_0}} A,$$

contradicting (51).

Case 2: $\mathcal{N}_{x_0}\cap\mathcal{E}\neq\varnothing$. (Notice, here is included the case where $x_0\in\partial\mathcal{I}=\mathcal{S}$.) We denote

$$\mathcal{I}_{x_0} \equiv \mathcal{N}_{x_0} \cap \mathcal{I} \quad \subseteq \mathcal{I},$$

$$\mathcal{E}_{x_0} \equiv \mathcal{N}_{x_0} \cap \mathcal{E} \quad \subset \mathcal{E},$$

and

$$\Gamma \equiv \mathcal{N}_{x_0} \cap \mathcal{S}.$$

Observe, $\Gamma \neq \varnothing$, because $\mathcal{N}_{x_0}$ is connected, $x_0 \in \mathcal{N}_{x_0} \cap \overline{\mathcal{I}} \neq \varnothing$, and, by assumption in this case, $\mathcal{N}_{x_0} \cap \mathcal{E} \neq \varnothing$. Moreover, $\Gamma = \overline{\mathcal{I}}_{x_0} \cap \overline{\mathcal{E}}_{x_0} = \partial\mathcal{I}_{x_0} \cap \partial\mathcal{E}_{x_0}$. Thus, we have in the interior, from (51),

$$A > \Omega_c \quad \text{in} \quad \mathcal{I}_{x_0} \cup \Gamma \quad \subset \mathcal{N}_{x_0} \quad (\Gamma \subset \partial\mathcal{I}_{x_0}),$$

$$A = \Omega_c \quad \text{on} \quad \partial\mathcal{I}_{x_0} \backslash \Gamma \quad \subset \partial\mathcal{N}_{x_0};$$

and, applying the weak maximum principle (Theorem 1 in Appendix A) to the differential inequality [cf. (29)]

$$L_0 A > 0 \quad \text{in} \quad \mathcal{I}_{x_0} \subset \mathcal{I}$$

[again using (48), $A > \Omega \geqslant \Omega_c$ in $\mathcal{I}_{x_0}$], with $A \in C^2(\mathcal{I}_{x_0}) \cap C^0(\overline{\mathcal{I}}_{x_0})$, it follows

$$\max_{\overline{\mathcal{I}}_{x_0}} A = \max_{\partial\mathcal{I}_{x_0}} A = \max_{\Gamma} A;$$

in the exterior, we have analogously, from (51),

$$A > \Omega_c \quad \text{in} \quad \mathcal{E}_{x_0} \cup \Gamma \quad \subset \mathcal{N}_{x_0} \quad (\Gamma \subset \partial\mathcal{E}_{x_0}),$$

$$A = \Omega_c \quad \text{on} \quad \partial\mathcal{E}_{x_0} \backslash \Gamma \quad \subset \partial\mathcal{N}_{x_0}.$$

(Note, the point ∞ is not included in $\partial\mathcal{E}_{x_0}$, because $\Omega_c > 0$ and A is asymptotically flat, $A|_\infty = 0$.) But, in the exterior, $\mathcal{E}$, $\psi^2 \equiv 0$, and we have the elliptic equation for A

$$L_0 A = 0 \quad \text{in} \quad \mathcal{E}_{x_0} \subset \mathcal{E};$$

as a consequence, again by virtue of the maximum principle (Theorem 1 in Appendix A) now in $\mathcal{E}_{x_0}$

$$\max_{\overline{\mathcal{E}}_{x_0}} A = \max_{\partial\mathcal{E}_{x_0}} A = \max_{\Gamma} A.$$

We therefore have

$$\max_{\overline{\mathcal{I}}_{x_0}} A = \max_{\overline{\mathcal{E}}_{x_0}} A = \max_{\Gamma} A =: A(x_1), \quad \text{for some} \quad x_1 \in \Gamma.$$

Thus ($\overline{\mathcal{N}}_{x_0} = \overline{\mathcal{I}}_{x_0} \cup \overline{\mathcal{E}}_{x_0}$)

$$\max_{\overline{\mathcal{N}}_{x_0}} A = A(x_1), \quad \text{for some} \quad x_1 \in \Gamma \subset \mathcal{N}_{x_0} \quad (x_1 \text{ interior point});$$

and, since $A \in C^1(\mathbb{R}^5)$, in particular, $A \in C^1(\mathcal{N}_{x_0})$, it follows

$$\nabla A|_{x_1} = \mathbf{0}. \tag{52}$$

However, this is not possible, because, on the other hand, x_1 is a point of the star's surface $x_1 \in \Gamma \subset \mathcal{S}$, and, from the assumptions on the stellar model, $\partial\mathcal{I} = \mathcal{S}$ satisfies an exterior sphere condition everywhere, i.e., $\partial\mathcal{E} = \mathcal{S} \cup \{\infty\}$ satisfies at each point of $\mathcal{S}$ (in particular, at x_1) an interior sphere condition (cf. Definition in Appendix A). This allows us to apply the called boundary-point lemma, Theorem 2 in Appendix A, for the operator L_0 in the exterior domain $\mathcal{E}_{x_0}$, with respect to the point $x_1 \in \Gamma \subset \partial\mathcal{E}_{x_0}$, being $A(x_1) = \max A$ in $\overline{\mathcal{E}_{x_0}}$. And, since $A \not\equiv \text{const}$ [because $A > \Omega_c > 0$ in $\mathcal{E}_{x_0} \cup \Gamma, A = \Omega_c$ or $2\mathcal{E}_{x_0} \setminus \Gamma$, and A is continuous], this yields

$$\langle \boldsymbol{\nu}, \nabla A \rangle|_{x_1} = \partial_{\boldsymbol{\nu}} A|_{x_1} \neq 0, \quad \boldsymbol{\nu} \equiv \text{ outward pointing unit normal to } \mathcal{S} \text{ at } x_1;$$

contradicting (52). Consequently,

$$A \leqslant \Omega \quad \text{in } \overline{\mathcal{I}}. \tag{53}$$

Second step: $A < \Omega \leqslant \Omega_c$ in $\overline{\mathcal{I}}$. This can be seen as follows. From inequality (53) and using (48) we also have

$$\Omega \leqslant \Omega_c \quad \text{in } \overline{\mathcal{I}}, \tag{54}$$

and, combining (53) and (54),

$$A \leqslant \Omega_c \quad \text{in } \overline{\mathcal{I}}. \tag{55}$$

On the other hand, we have Eq. (29), i.e., $L_0 A = -\psi^2 \cdot (\Omega - A)$, satisfied everywhere, in particular, in the interior (in a classical sense). Let

$$u(x) := A(x) - \Omega_c \quad \forall x \in \overline{\mathcal{I}}.$$

Since Ω_c is constant, we can rewrite Eq. (29),

$$Lu := L_0 u - \psi^2 \cdot u = +\psi^2 \cdot (\Omega_c - \Omega) \geqslant 0 \quad [\text{by } (54)].$$

Hence, we have

$$Lu \geqslant 0 \quad \text{in } \mathcal{I}, \tag{56}$$

where, like A, $u \in C^2(\mathcal{I}) \cap C^0(\overline{\mathcal{I}})$, and

$$u \leqslant 0 \quad \text{in } \overline{\mathcal{I}}, \tag{57}$$

by inequality (55). We want to see $u < 0$. Suppose (to get a contradiction) that $u(\hat{x}) = 0$ for some $\hat{x} \in \mathcal{I}$; then, by (57), $0 = u(\hat{x}) = \max_{\overline{\mathcal{I}}} u$, $\hat{x} \in \mathcal{I}$ (interior point). However, by the strong maximum principle, Theorem 3 in Appendix A, for (56), u cannot reach a non-negative maximum at an interior point of $\mathcal{I}$, unless u is a constant in $\mathcal{I}$. That means, in our case, u cannot vanish somewhere in $\mathcal{I}$ unless it vanishes identically in $\mathcal{I}$. But $u \equiv \text{const} = u(\hat{x}) = 0$ in $\mathcal{I}$, i.e.,

$$A \equiv \text{const} = \Omega_c > 0 \quad \text{in } \mathcal{I}, \quad A \in C^1 \text{ everywhere}, \tag{58}$$

yields, in particular,

$$\nabla A = \mathbf{0} \quad \text{on } \partial\mathcal{I} = \mathcal{S}. \tag{59}$$

On the other hand, in the exterior, $\mathcal{E}$, we have $L_0 A=0$, with $A\in C^2(\mathcal{E})\cap C^0(\overline{\mathcal{E}})$, and, by the weak maximum principle (Theorem 1 in Appendix A)

$$\max_{\overline{\mathcal{E}}} A = \max_{\partial\mathcal{E}=\mathcal{S}\cup\{\infty\}} A\,,$$

but, using asymptotic flatness ($A|_\infty=0$) and (58), actually,

$$\max_{\overline{\mathcal{E}}} A = \max_{\mathcal{S}} A =: A(x_1) \quad \text{for some } x_1\in\mathcal{S}\subset\partial\mathcal{E}\,.$$

In particular, since $A\not\equiv$const, the boundary-point lemma, Theorem 2 in Appendix A, applied to the operator L_0 in the exterior domain $\mathcal{E}$ (where, by assumption, an interior sphere condition is satisfied in particular at $x_1\in\mathcal{S}\subset\partial\mathcal{E}$) yields a nonvanishing outward normal derivative

$$\langle \boldsymbol{\nu}, \nabla A\rangle|_{x_1} = \partial_{\boldsymbol{\nu}} A|_{x_1} \neq 0\,,$$

in contradiction to (59). Therefore, $u<0$ everywhere in $\mathcal{I}$, i.e., $A<\Omega_c$ in $\mathcal{I}$; and, hence, also on $\partial\mathcal{I}$, because, by the weak minimum principle, Theorem 1 in Appendix A, applied to $L_0 A=-\psi^2\cdot(\Omega-A)\leqslant 0$ in $\mathcal{I}$ [by (53)], we get $\min_{\overline{\mathcal{I}}} A=\min_{\partial\mathcal{I}} A$. Therefore, $A<\Omega_c$ in $\overline{\mathcal{I}}$, or, equivalently [cf. (48)],

$$A<\Omega\leqslant\Omega_c \quad \text{in } \overline{\mathcal{I}}\,.$$

Third step: $A>0$ everywhere (i.e., the same conclusion of Proposition 1, but now using different hypotheses). We have seen in the first step $A\leqslant\Omega$ in $\overline{\mathcal{I}}$; which yields, $L_0 A\leqslant 0$ in $\overline{\mathcal{I}}$. On the other hand, $L_0 A=0$ in $\mathcal{E}$. Accordingly,

$$L_0 A\leqslant 0 \quad \text{everywhere in } \overline{\mathcal{I}}\cup\mathcal{E}=\mathbb{R}^5\,.$$

Applying now the strong minimum principle for generalized supersolutions, Theorem 4 in Appendix B, and using asymptotic flatness, as was argued in the proof of Proposition 1, it follows $A>0$ everywhere. [Notice, here $A\not\equiv$const, because, by asymptotic flatness and continuity, $A\equiv$const is equivalent to $A\equiv 0$; by Eq. (37), also $\Omega\equiv 0$, and, hence, from $\Omega-A\equiv 0$, we would have [cf. (46)] $0\equiv\Phi=\mathcal{F}(0)$; but this is not possible, since requirements (i) and (ii) imply $\mathcal{F}(0)>\mathcal{F}(\Omega_c)=0$.] Thus, $A>0$ everywhere, in particular, in the interior; using now the result of the second step, we finally get (49), $0<A<\Omega\leqslant\Omega_c$ in $\overline{\mathcal{I}}$. Notice, hence, $\Omega>0$ (in $\overline{\mathcal{I}}$).

Fourth step: $A<\max_{\mathcal{S}}\Omega\leqslant\Omega_c$ in $\mathcal{E}$. The elliptic equation holding in the exterior,

$$L_0 A=0 \quad \text{in } \mathcal{E}\,,$$

yields, by virtue of the weak maximum principle (Theorem 1 in Appendix A),

$$\max_{\overline{\mathcal{E}}} A = \max_{\partial\mathcal{E}=\mathcal{S}\cup\{\infty\}} A\,;$$

but, using asymptotic flatness ($A|_\infty=0$), we actually have $\max_{\mathcal{S}\cup\{\infty\}} A=\max_{\mathcal{S}} A$. On the other hand, we have seen $A<\Omega\leqslant\Omega_c$ in particular in $\partial\mathcal{I}=\mathcal{S}$, and $\mathcal{S}$ is compact. Hence,

$$\text{in } \mathcal{E}, \quad 0<A\leqslant\max_{\overline{\mathcal{E}}} A = \max_{\mathcal{S}=\partial\mathcal{I}} A < \max_{\mathcal{S}}\Omega\leqslant\Omega_c\,,$$

establishing also (50). □

Remark 3: Analogously as argued in Remarks 1 and 2, it is possible to ''reflect'' Proposition 3. As a consequence, in particular, in a model for a star which is rotating differentially with the

function $\mathcal{F}$ either strictly decreasing with $\Omega_c>0$ or strictly increasing with $\Omega_c<0$, $\mathcal{F}(\Omega_c)=0$, the angular momentum density has the same sign as Ω_c, and, hence, as the angular velocity of the fluid. Also, accordingly, the following holds:

$$0<|A|<|\Omega|\leqslant|\Omega_c| \quad \text{in } \overline{\mathcal{I}},$$

$$0<|A|<|\max_{\mathcal{S}}\Omega|\leqslant|\Omega_c| \quad \text{in } \mathcal{E}.$$

V. GENERAL BOUNDS. ROTATIONAL ENERGY

A. Preliminary observation

Let $u:\mathbb{R}^n\to\mathbb{R}$ be a differentiable function, $V:\mathbb{R}^n\to\mathbb{R}^n$ be a vector field, and $G\subset\mathbb{R}^n$ a domain where Gauss' theorem can be applied. Then, due to

$$\operatorname{div}(uV)=\sum_i \partial_i(uV_i)=\langle \mathcal{D}u,V\rangle+u\operatorname{div}V$$

[where $\langle .,.\rangle$ is the Euclidean scalar product, $\mathcal{D}$ is the gradient operator, and $\operatorname{div}V:=\Sigma_i\partial_i(V_i)$, the divergence], we get, integrating over G and applying the Gauss theorem,

$$\int_G u\operatorname{div}V=-\int_G\langle \mathcal{D}u,V\rangle+\int_{\partial G}u\,\langle V,\boldsymbol{\nu}\rangle\,, \tag{60}$$

where $\boldsymbol{\nu}$ is the outer unit normal of ∂G (and, for simplicity in the notation, volume- and surface elements have been dropped).

B. Appropriate form of the field equation

The general (elliptic) field equation for A, Eq. (19), may be rewritten as follows:

$$\operatorname{div}(\rho^3e^{3B}e^{-4U}\mathcal{D}A)=-f^2\cdot(\Omega-A)\,, \tag{61}$$

where $\mathcal{D}:=(\partial_\rho,\partial_z)$ and div are the flat expressions in $\mathbb{R}^2$, and

$$f^2(\rho,z)\equiv f^2:=\rho^3e^{3B-4U}\psi^2=16\pi\,(\varepsilon+p)\,\frac{\rho^3e^{3B}e^{2(K-2U)}}{e^{2U}-\rho^2e^{2(B-U)}(\Omega-A)^2}\geqslant 0\,.$$

Especially we have $f^2\equiv 0$ in the exterior E of the star [cf. (5)].

Note, in this section (independent of Sec. IV) we go back to the field equation in the meridian plane coordinates, $(\rho,z)\in\mathbb{R}_0^+\times\mathbb{R}$, instead of the 5-*lifted* one (on $\mathbb{R}^5$) (cf. Sec. III A).

C. Main observation

Multiplying Eq. (61) by A, and using Eq. (60), by setting $u=A$, $V=\rho^3e^{3B}e^{-4U}\mathcal{D}A$, and $G=\mathbb{R}_0^+\times\mathbb{R}\subset\mathbb{R}^2$ [actually, we consider a ball in $\mathbb{R}^2$ centered at the origin of the coordinate system with arbitrarily large radius, $\mathcal{B}_\sigma(\mathbf{0})\subset\mathbb{R}^2$, and take $G=\mathcal{B}_\sigma(\mathbf{0})\cap(\mathbb{R}_0^+\times\mathbb{R})\subset\mathbb{R}^2$, $\sigma\to\infty$], we obtain

$$-\int_I f^2A(\Omega-A)=-\int_{\mathbb{R}_0^+\times\mathbb{R}}\rho^3e^{3B}e^{-4U}\|\mathcal{D}A\|^2+\int_{\partial(\mathbb{R}_0^+\times\mathbb{R})}A\,\rho^3e^{3B}e^{-4U}\langle\mathcal{D}A,\nu\rangle\,,$$

where $I\subset\mathbb{R}_0^+\times\mathbb{R}\subset\mathbb{R}^2$ represents the (ρ,z)-coordinates of the interior of the star (note, f^2 vanishes in the exterior E). The first term on the right-hand side (which converges, since $\|\mathcal{D}A\|$ falls off rapidly enough at the spacelike "infinity" [19]) is obviously nonpositive. And the second term

vanishes, because of the asymptotic behavior of A at spatial infinity,[19] and because the integrand, due to the factor ρ^3, vanishes on the axis of rotation $\rho=0$, which is the other part of $\partial(\mathbb{R}_0^+\times\mathbb{R})=\{R=(\rho^2+z^2)^{1/2}\to\infty\}\cup\{\rho=0\}$. Hence, we have found

$$\int_I f^2 A\,(\Omega-A)\geqslant 0\,. \tag{62}$$

D. Consequences

In order to see more the linear algebra behind, we introduce now the bilinear form

$$\langle u,v\rangle_f := \int_I f^2(\rho,z)\,u(\rho,z)\,v(\rho,z)\,\mathrm{d}\rho\,\mathrm{d}z\,,\quad u,v:I\to\mathbb{R}\quad \text{in } L^2(I)\,,$$

and the induced seminorm $\|.\|_f := (\langle .\,,.\rangle_f)^{1/2}$. With this definition we can write inequality (62) as

$$\langle A,\Omega\rangle_f \geqslant \|A\|_f^2\,,$$

and immediately see that especially

$$\langle \Omega,A\rangle_f = \langle A,\Omega\rangle_f \geqslant 0\,. \tag{63}$$

Furthermore, using the Cauchy–Schwarz inequality, we have $\|A\|_f\|\Omega\|_f\geqslant\langle A,\Omega\rangle_f\geqslant\|A\|_f^2$, and hence (since $A\equiv 0\Leftrightarrow\ \Omega\equiv 0$) we get (in full general) the main result of these sections, namely,

$$0\leqslant\|A\|_f\leqslant\|\Omega\|_f\,. \tag{64}$$

Proposition 4:

$$0\leqslant\int_I f^2 A^2\leqslant\int_I f^2\ \ \Omega^2 \tag{65}$$

[without any restriction concerning the rotation law, $\Omega\mapsto\mathcal{F}(\Omega)$ in (14), in the differentially rotating case, nor the regularity and sign uniformity of Ω]. These integrals can be regarded as some kind of "mean value" with respect to the "density" f^2, thus, (65) fulfilling the physical expectations.[2]

In addition, multiplying inequality (64) by $\|\Omega\|_f$, we find (again using the Cauchy–Schwarz inequality) $\|\Omega\|_f^2\geqslant\|\Omega\|_f\|A\|_f\geqslant\langle\Omega,A\rangle_f$, i.e.,

$$\langle\Omega,\Omega-A\rangle_f\geqslant 0\,. \tag{66}$$

Remarkably, the integral given in (66) has an important physical meaning; it is, up to a constant factor, the so-called *total rotational energy* (see, e.g., Refs. 15, 16, 18, and 20),

$$T\equiv\frac{1}{2}\int_I\Omega\,\mathrm{d}J\ \ =\ \ \frac{1}{2}\int_I 2\pi\,\Omega\,T_\phi{}^t\,(-g)^{1/2}\,\mathrm{d}\rho\,\mathrm{d}z\ \ =\ \ \frac{1}{16}\langle\Omega,\Omega-A\rangle_f$$

(also denoted E_{rot} or M_{rot}). Thus, (66) shows $T\geqslant 0$. Furthermore,

$$16\ \ T=\langle\Omega,\Omega-A\rangle_f=\|\Omega\|_f^2-\langle\Omega,A\rangle_f\leqslant\|\Omega\|_f^2\,,$$

by (63). Hence, we have the following proposition.

Proposition 5:

$$0 \leqslant T \equiv \frac{1}{16}\int_I f^2 \ \Omega\,(\Omega - A) \leqslant \frac{1}{16}\int_I f^2 \ \Omega^2\,. \tag{67}$$

This generalizes the result given by Hartle (cf. Ref. 7, Sec. IV) in the limit of slow (differential) rotation to the general differentially rotating case.

VI. CONCLUSIONS

Aiming to derive general properties of equilibrium nonsingular stellar models with differential rotation, we have established that for a wide class of rotation laws the distribution of angular velocity of the fluid has a sign, and then both the dragging rate (angular velocity of locally nonrotating observers) and the angular momentum density have the sign of the fluid angular velocity (Sec. IV). In addition, the mean value (with respect to a density function) of the dragging rate is shown to be less than the mean value of the fluid angular velocity; and this is proved in full general, without having to restrict the rotation law, nor the uniformity in sign of the fluid angular velocity. A further simple calculation of linear algebra on this inequality yields a generalization of the result given by Hartle[7] concerning positivity and upper bound of the total rotational energy in the limit of slow (differential) rotation to the general differentially rotating case (Sec. V).

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APPENDIX A: MAXIMUM (MINIMUM) PRINCIPLES FOR CLASSICAL SUB-(SUPER-) SOLUTIONS

By G we denote an open and connected set, i.e., a domain, in $\mathbb{R}^n$, $n \geqslant 2$. The boundary is denoted by $\partial G \equiv \overline{G} \cap (\mathbb{R}^n \backslash G)$. We define the differential operators

$$L_0 u := a_{ij}(x) \ \partial_{ij} u + b_i(x)\, \partial_i u\,, \quad a_{ij} = a_{ji}\,,$$

and

$$L u := L_0 u + c(x) \cdot u$$

(where the summation convention that repeated indices indicate summation from 1 to n is followed), such that[21]

(1) L (and, hence, L_0) is uniformly elliptic in G in the special form

$$0 < \lambda\,|y|^2 \leqslant a_{ij}(x)\, y_i y_j \leqslant \Lambda\,|y|^2, \quad \forall y \in \mathbb{R}^n \backslash \{0\}, \quad \forall x \in G \quad \left(|y|^2 := \sum_i \ y_i{}^2 \right), \tag{A1}$$

where λ and Λ are constants such that $0 < \lambda \leqslant \Lambda < \infty$;

(2) all coefficients in L (and in L_0), a_{ij}, b_i (for all i and j), and c, are measurable and bounded functions in G,

$$|a_{ij}| < \infty, \quad |b_i| < \infty, \quad |c| < \infty \ \text{ in } \ G \quad (i,j \in \{1,\ldots,n\})\,. \tag{A2}$$

Theorem 1: [the weak maximum (minimum) principle for L_0 $(c = 0)$] *Suppose that* $L_0 u \geqslant 0$ $(\leqslant 0)$ *in a bounded domain* G, *with* $u \in C^2(G) \cap C^0(\overline{G})$. *Then the maximum (minimum) of* u *is attained on the boundary, that is,*

$$\max_{\overline{G}} u = \max_{\partial G} u \quad \left(\min_{\overline{G}} u = \min_{\partial G} u \right).$$

(A proof of that theorem can be found, e.g., in Ref. 22, Theorem 3.1.)

Definition: For a set $G \subset \mathbb{R}^n$, the boundary ∂G is said to satisfy an interior (exterior) sphere condition *at a point $x_1 \in \partial G$ iff there exists a ball $B \subset G$ ($B \subset \mathbb{R}^n \backslash \overline{G}$) with $x_1 \in \partial B$.*

Theorem 2 (the boundary-point lemma): *Suppose that $L_0 u \geqslant 0$ ($c = 0$) in a domain G not necessarily bounded. Let $x_1 \in \partial G$ be such that*

(i) *u is continuous at x_1,*
(ii) *$u(x_1) \geqslant u(x)$ for all $x \in G$, and*
(iii) *∂G satisfies an interior sphere condition at x_1.*

Then the outer normal derivative of u at x_1, if it exists, satisfies the strict inequality

$$\partial_{\boldsymbol{\nu}} u(x_1) > 0,$$

unless $u \equiv \text{const} = u(x_1)$. (A proof of that result can be found, e.g., in Ref. 23, Theorem 7, Chap. 2.) *If $c \leqslant 0$ (in $Lu \geqslant 0$), the same conclusion holds provided $u(x_1) \geqslant 0$.* (See Ref. 23, Theorem 8, Chap. 2. Also Ref. 22, Lemma 3.4.)

Theorem 3 [the strong maximum (minimum) principle for *L*]: *Let $Lu \geqslant 0$ ($\leqslant 0$) in a domain G not necessarily bounded, with $u \in C^2(G) \cap C^0(\overline{G})$, and the operator L satisfying*

$$c \leqslant 0 \quad \text{in } G \tag{A3}$$

apart from conditions (A1) and (A2) above. Then u cannot attain a non-negative maximum (non-positive minimum) at an interior point of G, unless $u \equiv \text{const}$ in G. For $c = 0$, i.e., $L = L_0$, the same conclusion holds without the requirement non-negative (nonpositive). (For the proof we refer again to Ref. 22, Theorem 3.5; or Ref. 23, Theorems 5 and 6, Chap. 2.)

APPENDIX B: MAXIMUM (MINIMUM) PRINCIPLE FOR GENERALIZED SUB-(SUPER-) SOLUTIONS

Consider in a domain (open and connected set) $G \subset \mathbb{R}^n$ ($n \geqslant 2$) the differential operator with principal part of divergence form, defined by

$$Lu = \partial_i [a_{ij}(x) \partial_j u + a_i(x)\, u] + b_i(x)\, \partial_i u + c(x)\, u\,,$$

with $a_{ij} = a_{ji}$. Notice, an operator L of the general form $Lu = \tilde{a}_{ij}(x) \partial_{ij} u + \tilde{b}_i(x) \partial_i u + \tilde{c}(x) u$ may be written in divergence form provided its principal coefficients $\tilde{a}_{ij}$ are differentiable. If furthermore the $\tilde{a}_{ij}$ are constants, then even with coinciding coefficients ($a_{ij} = \tilde{a}_{ij}$, $b_i = \tilde{b}_i$, $c = \tilde{c}$) and $a_i \equiv 0$. Let us assume that

(1) L is strictly elliptic in G, i.e., $\exists$ a constant $\lambda > 0$ such that $\lambda \leqslant$ the minimum eigenvalue of the principal coefficient matrix $[a_{ij}(x)]$,

$$\lambda |y|^2 \leqslant a_{ij}(x)\, y_i y_j \quad \forall y \in \mathbb{R}^n, \quad \forall x \in G\,; \tag{B1}$$

(2) a_{ij}, a_i, b_i, and c are measurable and bounded functions in G,

$$|a_{ij}| < \infty, \quad |a_i| < \infty, \quad |b_i| < \infty, \quad |c| < \infty \text{ in } G \quad (i,j \in \{1,\ldots,n\})\,. \tag{B2}$$

By definition, for a function u which is only assumed to be *weakly differentiable* and such that the functions $a_{ij} \partial_j u + a_i u$ and $b_i \partial_i u + cu$, $i = 1,\ldots,n$ are locally integrable [in particular, for u belonging to the Sobolev space $W^{1,2}(G)$], u is said to satisfy $Lu = g$ in G *in a generalized (or weak) sense* (g also a locally integrable function in G) if it satisfies

$$\mathcal{L}(u,\varphi;G) := \int_G \{(a_{ij}\partial_j u + a_i u)\partial_i\varphi - (b_i\partial_i u + cu)\varphi\}\mathrm{d}x = -\int_G g\,\varphi\,\mathrm{d}x, \quad \forall\varphi \geqslant 0 \quad \varphi \in C_c^1(G)$$

[where $C_c^1(G)$ is the set of functions in $C^1(G)$ with compact support in G].

Notice, u is *generalized sub-(super-)solution* relative to a differential operator L and the domain G [i.e., satisfies $Lu \geqslant 0$ ($\leqslant 0$) in G in a generalized sense] if it satisfies $\mathcal{L}(u,\varphi;G) \leqslant 0$ ($\geqslant 0$), $\forall\varphi \geqslant 0$ $\varphi \in C_c^1(G)$.

Theorem 4 [strong maximum (minimum) principle]: *Let $u \in W^{1,2}(G) \cap C^0(G)$ satisfy $Lu \geqslant 0$ ($\leqslant 0$) in G in a generalized sense, with*

$$\int_G (c\varphi - a_i\partial_i\varphi)\,\mathrm{d}x \leqslant 0, \quad \forall\varphi \geqslant 0\ \varphi \in C_c^1(G) \tag{B3}$$

[equivalent to requirement (A3) in the classical case] and conditions (B1) and (B2) above. Then u cannot achieve a non-negative maximum (nonpositive minimum) in the interior of G, unless u $\equiv$const. (A proof of this theorem can be found in Ref. 22, Theorem 8.19.)

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Elliptic solitons and Gröbner bases

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We consider the solution of spectral problems with elliptic coefficients in the framework of the Hermite *Ansatz*. We show that the search for exactly solvable potentials and their spectral characteristics is reduced to a system of polynomial equations solvable by the Gröbner bases method and others. New integrable potentials and corresponding solutions of the Sawada-Kotera, Kaup-Kupershmidt, Boussinesq equations and others are found. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1633353]

I. INTRODUCTION

The article is devoted to the algorithmic problems associated with integrating the spectral problems

$$\hat{L}\Psi \equiv \frac{d^n}{dx^n}\Psi(x;\lambda)+u_1(x,\lambda)\frac{d^{n-1}}{dx^{n-1}}\Psi(x;\lambda)+\cdots+u_n(x,\lambda)\,\Psi(x;\lambda)=0, \tag{1}$$

where u_j are elliptic functions of x and arbitrary (rational or transcendental) functions of λ. We shall restrict our consideration to the Schrödinger equation

$$\Psi''-u(x)\,\Psi=\lambda\,\Psi, \tag{2}$$

the equation

$$\Psi'''-u(x)\,\Psi'=\lambda\,\Psi, \tag{3}$$

and the generalization of the Halphen equation

$$\Psi'''-u(x)\,\Psi'-v(x)\,\Psi=\lambda\,\Psi. \tag{4}$$

We use the term *potential* for the $u(x), v(x)$-functions. Until the 1970/80s, few exactly solvable potentials were known. Earlier, in 1872, Hermite[28] developed an approach for the integration of the Lamé equation

$$\Psi''-n(n+1)\,\wp(x)\,\Psi=\lambda\,\Psi, \tag{5}$$

and, later, Halphen extended it to the third order equation

$$\Psi'''-(n^2-1)\,\wp(x)\,\Psi'-\tfrac{1}{2}(n^2-1)\,\wp'(x)\,\Psi=\lambda\,\Psi. \tag{6}$$

Here and below $\sigma, \zeta, \wp, \wp'$ denote the standard Weierstrassian functions. See Refs. 25, 19, and 29 for an extensive discussion of these classical examples. According to modern terminology, the set of exactly solvable elliptic potentials is a particular case of finite-gap potentials in elliptic func-

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tions. An intense investigation of elliptic potentials was initiated by Ref. 30, and in 1987 Verdier and Treibich[41,38] unexpectedly found new potentials for the equation (2) in elliptic functions

$$u(x)=6\,\wp(x)+2\,\wp(x-\omega_j) \tag{7}$$

and gave the term *elliptic solitons* to them. Recently V. Matveev drew attention to the fact that such potentials, in Jacobian form, were already considered by Darboux in a short note[12] in 1882. The following year, two comprehensive mémoires by Sparre[36] appeared on this topic.

The development of a theory led to the current result that elliptic solitons are the widest class of finite-gap *explicit* solutions. See, for example, Refs. 34 and 17, recent results in Refs. 35 and 37 and references therein. Reference 1 reviews work in finite-gap theory up to the beginning of the 1990s and Refs. 22 and 24 contain a wide bibliography on that score.

One feature of elliptic solitons is the potential, and the Ψ-function can be found by the Hermite *Ansatz* method.[28] In the case of the potentials with the only pole in a parallelogram of periods, the derivation of the algebraic curve and other characteristics is not difficult. For this purpose it is enough to take a few resultants,[15,1] but in the general case the elimination technique is insufficient. Section II contains a pure algebraic interpretation of Hermite's method. In Sec. III, we show that the general scheme for solving the problem under consideration (1) is reduced to the computation of the Gröbner basis for some polynomial system. After Buchberger's discovery in the 1960s of an algorithm for finding the polynomial ideal bases, this area of algorithmic mathematics has rapidly developed. See Ref. 32 with regard to the modern achievements in this area. Section IV contains a relation between the method and traditional objects in finite-gap integration theory: the canonical form of an algebraic curve $\tilde{F}(\mu,\lambda)=0$ and reduction of one of the holomorphic differentials to the elliptic. Some new examples of elliptic solitons and their applications to the integrable partial differential equations (PDEs) are presented in Secs. V and VI and development of the theory is discussed in Sec. VII.

II. ALGEBRAIC CHARACTERIZATION OF THE HERMITE METHOD

Based on the Φ-function

$$\Phi(x;\alpha)=\frac{\sigma(\alpha-x)}{\sigma(\alpha)\,\sigma(x)}e^{\zeta(\alpha)\,x}, \tag{8}$$

or more precisely *l'élément simple*

$$\mathbf{\Phi}(x;\alpha,k)=\frac{\sigma(\alpha-x)}{\sigma(\alpha)\,\sigma(x)}e^{(\zeta(\alpha)+k)\,x}$$

by Halphen,[26,27] Hermite and Halphen[28,25] considered the following *Ansatz* for the Ψ-function:

$$\Psi=\mathbf{\Phi}(x;\alpha,k)+a_1\mathbf{\Phi}'(x;\alpha,k)+\cdots+a_n\mathbf{\Phi}^{(n)}(x;\alpha,k). \tag{9}$$

The function $\mathbf{\Phi}(x;\alpha,k)$ as well its x-derivatives $\mathbf{\Phi}'(x;\alpha,k)$, …, $\mathbf{\Phi}^{(n)}(x;\alpha,k)$ are doubly-periodic functions of x of the second kind. According to (1), (8) and (9), the expression $\hat{L}\Psi/\mathbf{\Phi}(x-x_0;\alpha,k)$ is a two-periodic meromorphic function with only one simple pole at the point x_0. It must be a constant function. Setting it to be equal to zero, we have $\hat{L}\Psi=0$ under the corresponding choice of additional parameters k, α and a_j. As the $\mathbf{\Phi}(x;\alpha,k)$-function has the first order pole at $x=0$ (Ref. 26, p. 231),

$$\mathbf{\Phi}(x;\alpha,k)=\frac{1}{x}+k+\frac{k^2-\wp(\alpha)}{2}x+\frac{k^3-3\,\wp(\alpha)\,k+\wp'(\alpha)}{6}x^2+\cdots,$$

to solve the problem, it is sufficient to equate to zero only the principal part(s) of the Laurent's expansion(s) of the expression $\hat{L}\Psi$, where Ψ is the *Ansatz* (9) or its multi-pole generalizations (see Examples 1–3 and 7 in Sec. V).

As a nontrivial example we shall consider the five-gap Lamé potential with $n=5$ in (5). It has been studied in Ref. 15, but we give a more simple solution. Note that the cases $n=2, 3, 4$ and partially 5 were considered already in Ref. 27, pp. 527–531. In the same place one can find mention of eliminations.

By Frobenius theory, Ψ must have a fifth order pole at $x=0$ and therefore the *Ansatz* for the Ψ-function should be the following:

$$\Psi=\mathbf{\Phi}+a_1\mathbf{\Phi}'+\cdots+a_4\mathbf{\Phi}^{(\mathrm{IV})}. \tag{10}$$

Substituting (10) in (5) and expanding the result at $x=0$, we obtain a system of equations in the variables k, α, a_j. This system is linear with respect to a_j. We do not write expressions for the a_j [Ref. 15, formula (3.7)]. The remaining equations have the form

$$\begin{aligned} w_1 &\equiv -6k^5+\tfrac{20}{3}(9\wp+\lambda)k^3-60\wp' k^2+(90\wp^2-20\lambda\wp-\tfrac{10}{7}\lambda^2+\tfrac{144}{7}g_2)k-\tfrac{4}{3}(9\wp-5\lambda)\wp', \\ w_2 &\equiv -5k^6+(75\wp+5\lambda)k^4-100\wp' k^3+(225\wp^2-30\lambda\wp-\tfrac{5}{7}\lambda^2+\tfrac{180}{7}g_2)k^2 \\ &\quad -20(3\wp-\lambda)\wp' k+25\wp^3-15\lambda\wp^2+\tfrac{5}{7}(\lambda^2-20g_2)\wp-40g_3-\tfrac{1}{21}\lambda^3+\tfrac{44}{7}g_2\lambda, \end{aligned} \tag{11}$$

which are understood to be equal to zero. The argument α in the $\wp, \wp'$-functions is omitted for brevity. The system (11) has to be considered as algebraic with respect to k and *transcendental* in α. We emphasize that everywhere in the article λ is a parameter, but not variable in polynomial bases. Insomuch as functions $\wp(\alpha)$ and $\wp'(\alpha)$ are related by the Weierstrass equation (torus)

$$w_3\equiv\wp'(\alpha)^2-4\wp(\alpha)^3+g_2\wp(\alpha)+g_3, \tag{12}$$

we supplement (11) by (12) and consider (11) and (12) as a *polynomial* system with respect to independent variables $(k, \wp, \wp')$. The simplest method of solution consists of the elimination of the variable $\wp$ followed by $\wp'$. As a result, we find that k must be a root of the polynomial

$$k^4(5103k^4-945\lambda k^2+40\lambda^2+54g_2)^4(225(27g_2-\lambda^2)P_6^2(\lambda)k^2+P_9(\lambda)P_3^2(\lambda)),$$

where $P_{6,9,3}(\lambda)$ are some polynomials in λ with degrees 6, 9, 3, respectively. It is not difficult to guess that the correct result requires that k and λ are related by the following equation,

$$F(k,\lambda): 225(27g_2-\lambda^2)P_6^2(\lambda)k^2+P_9(\lambda)P_3^2(\lambda)=0, \tag{13}$$

since the differential equation (5) is of second order and we must have not more than two solutions for k with fixed λ. Curve (13) can be brought into the canonical hyperelliptic form

$$\tilde{F}(\mu,\lambda): \mu^2=(27g_2-\lambda^2)P_9(\lambda)$$

by an obvious birational transformation [note a misprint $27g_2^2$ in this formula in Ref. 15, formula (3.8)]. The variables $\wp, \wp'$ as functions of k can be found in the same way: by the sequential reduction of exponents of $\wp, \wp'$ in (11) and (12).

Obviously, the resultant technique is almost impossible if the potential has several poles,[17,34] as the number of variables increases. Another approach consists of finding an equivalent system with the following criterion. It is advisable for the new system to contain linear equations in $\wp, \wp'$. These equations define α as a function of (k, λ):

$$\wp(\alpha)=R_1(k;\lambda), \quad \wp'(\alpha)=R_2(k;\lambda), \tag{14}$$

and we call (14) a cover of torus (12) in *algebraic* form. Suppose one of the new equations does not contain $\wp, \wp'$ (i.e., be a univariate polynomial in k) if the nontrivial solution for k exists. We interpret such a polynomial as *the algebraic curve* $F(k,\lambda)=0$ corresponding to given an elliptic potential. If $F(k,\lambda)$ has a factorized form, then each of the factors is investigated separately. The curve is one of them. It is clear that its degree in k has to be equal to the order n of the equation (1). The canonical form $\tilde{F}(\mu,\lambda)=0$ of the curve is obtained with the help of a birational transformation between variables $(k,\lambda)\leftrightarrow(\mu,\lambda)$ (see an explanation in Sec. IV). Note, there are specialized algorithms for the computation of the univariate polynomial in an ideal without solving the system as a whole.

III. GRÖBNER BASES, CURVES AND COVERS

We clarify the main idea using the previous example. Let us consider three polynomials $w_{1,2,3}(\wp',\wp,k)$ as a system generating an ideal in a polynomial ring $\mathbb{Q}(\lambda,g_2,g_3)[\wp',\wp,k]$,

$$\langle I\rangle = h_1 w_1 + h_2 w_2 + h_3 w_3,$$

where $h_j=h_j(\wp',\wp,k)$ are arbitrary elements of the ring. As is well known, the structure of the solution of the polynomial systems depends on the monomial ordering in a ring.[32] The arguments at the end of Sec. II (see also the elimination theorem in Ref. 11) lead to the choice of pure lexicographic ordering $\wp'\succ\wp\succ k$. Reference 11 contains a good exposition of details of this subject. The main property of the Gröbner base is expressed in the following.

Definition:[11] *Let* $\{w_1, w_2, \ldots\}$ *be a basis of ideal* $I=\langle w_1, w_2, \ldots\rangle$. *Let* $\succ$ *be a monomial ordering on the ring* $\mathbb{Q}[\ldots]$ *and* $\mathrm{LT}(f)$ *denote the leading term (monomial) of a polynomial* $f \in \mathbb{Q}[\ldots]$. *The set* $G=\{f_1, f_2, \ldots, f_N\}$ *is said to be a standard basis (Gröbner basis) if the monomial ideal generated by*

$$\langle \mathrm{LT}(f_1), \mathrm{LT}(f_2), \ldots, \mathrm{LT}(f_N)\rangle$$

is coincident with an ideal $\langle \mathrm{LT}(I)\rangle$ *generated by all the leading terms of* I.

In other words, the leading term of any polynomial in I is divisible by one of the $\mathrm{LT}(f_j)$. According to the definition at the end of Sec. II, the polynomial $F(k;\lambda)$, determining the algebraic curve

$$F(k;\lambda)=0, \tag{15}$$

is a generator of the intersection of the ideal I and the ring of all polynomials in k:

$$\langle F(k;\lambda)\rangle = I \cap \mathbb{Q}(\lambda)[k].$$

Thus we arrive at a general recipe for the solution of the spectral problem (1).

Proposition: Let $\{w_1, w_2, \ldots\}$ *be polynomials in* $\wp'(\alpha), \wp(\alpha), k, \ldots$ *appearing in the Hermite method and determining the solution of the spectral problem (1): the cover of torus (14) and the curve (15). Then we have the following.*

(1) Algorithmically, the method of solution is reduced to the computation of a standard basis for the ideal $I=\langle w_1, w_2, \ldots\rangle$ *with respect to pure lexicographic ordering* $\wp'(\alpha)\succ\wp(\alpha)\succ k \succ\cdots$. (*For example, by Buchberger's syzygy polynomials algorithm.*[7])

(2) Let $G=\{f_1, f_2, \ldots, f_N\}$ *be this basis. The algebraic curve (15) and its projection on the torus (12) in algebraic form (14) are contained in G if the univariate polynomial in k and polynomials (14) exist.*

(3) If G contains a polynomial free from variables $k, \wp'(\alpha), \wp(\alpha)$, *then the spectral problem (1) is* **not integrable** *in the framework of Hermite's Ansatz.*

Proof:

(1) The standard basis always exists and Buchberger's algorithm terminates.[11]

(2) Taking the resultants of $w_1, w_2, \ldots$ we eliminate variables $\wp, \wp'$ and get polynomial(s) $R(k)$. It is obvious that $R(k) \in I$. Using the divisibility

$$\langle \mathrm{LT}(f_1), \mathrm{LT}(f_2), \ldots, \mathrm{LT}(f_N)\rangle = \langle \mathrm{LT}(I)\rangle$$

and lexicographic ordering, the equality $R(k) = h(k)\,\hat{f}$ has to occur for some $\hat{f} \in G$ and $h(k) \in \mathbb{Q}(\lambda)[k]$ (possibly equal to 1). Therefore there exists a polynomial $\hat{f}$ depending only on k. Designating $\hat{f}(k) \equiv F(k;\lambda)$, we obtain the curve (15). If $F(k;\lambda)$ has a factorized form, then the algebraic curve is one of its factors. Analogously, if the polynomials (14) exist, then they necessarily belong to G. In the same way, an important formula, the curve as a cover of the torus (12) in a *transcendental* form (an equation in α)

$$R(\wp'(\alpha), \wp(\alpha); \lambda) = 0, \tag{16}$$

necessarily must be contained in G computed with the ordering $k \succ (\wp'(\alpha) \succ \wp(\alpha) \succ \cdots)$, where permutations inside the brackets are allowed. Note the order of elliptic function (16) in α is equal to the order n of the equation (1).

(3) An existence of such a polynomial implies a restriction on the spectral parameter λ (see an illustrative Example 5). ■

Note a direct link of the point (3) to a treatment of finite-gap potentials as Picard's potentials.[21]

There are numerous algorithmic methods to solve this problem. Among them are the Gröbner basis method,[7,10] the method of characteristic sets, and an effective method of elimination based on the Seidenberg theory.[43] We do not discuss all the modern achievements in this area. See Ref. 32 and references therein for details. Note that the reduction of the holomorphic differential $d\alpha$ to the elliptic one is derived from (14) by the formula

$$d\alpha = \frac{d\wp(\alpha)}{\wp'(\alpha)} = \frac{F_k R_{1\lambda} - F_\lambda R_{1k}}{R_2 F_k} d\lambda, \tag{17}$$

where subscripts k, λ denote the derivatives with respect to k and λ.

IV. CANONICAL FORM OF CURVES AND HOLOMORPHIC DIFFERENTIAL

Formulas (15)–(17) give a noncanonical form of the curve and holomorphic differential, i.e., expressions in the variables (k, λ). The canonical variables (μ, λ) in the algebraic curve $\tilde{F}(\mu, \lambda) = 0$ we call variables λ in (1) and eigenvalue μ of a commuting operator pencil

$$\hat{P}(\lambda)\,\Psi = \mu\,\Psi. \tag{18}$$

Supplementing the polar expansion of the equation (1) by the polar expansion of (18), we get the algebraic equations in variables $(\wp, \wp', k, \mu, \ldots)$. Again, based on the above properties of the Gröbner base, a canonical representation of the solution and all the spectral characteristics are extracted by computing the base with the ordering $(\wp \succ \wp' \succ \cdots) \succ k \succ \mu$. Such a base contains a birational transformation between the (k, μ)-variables in one direction:

$$\mu \to k: \quad k = R_3(\mu; \lambda). \tag{19}$$

An inverse transformation

$$k \to \mu: \quad \mu = R_4(k; \lambda), \tag{20}$$

where $R_{3,4}$ are rational functions of its arguments, is computed by the ordering $(\wp \succ \wp' \succ \cdots) \succ \mu \succ k$.

We add a few words about the efficiency of computations. The solution of a spectral problem itself does not require the inclusion of a commuting operator (18). So, among of its polar expansions one may take (and supplement) those containing only the μ-variable. Evidently, it will enter into the polar expansion with first degree:

$$\mu = w(k, \wp, \wp'; \lambda). \tag{21}$$

After the computation of the base [not including (18)], we will have the curve (15) and cover in algebraic form (14). Substituting it into the equation (21), the pair of equations for the determination of the above transformation (19) and (20) becomes

$$\mu = w(k, R_1(k;\lambda), R_2(k;\lambda); \lambda), \quad F(k;\lambda) = 0. \tag{22}$$

Formulas (19) and (20) are obtained by computation of the bases for (22) with ordering $(k \succ \mu)$ and $(\mu \succ k)$, respectively. See Example 6 for details.

V. EXAMPLES

In this section we demonstrate the ideology of Secs. III and IV on examples. The generality of the technique allows us to make further proofs. Let us prove that the well known potential of Treibich and Verdier (7)[41] for the equation (2) is the only possible integrable two-pole potential in the class

$$u(x) = 6\,\wp(x) + 2\,\wp(x-\Omega), \quad \Omega \neq 0. \tag{23}$$

Example 1. The Treibich–Verdier potential: Parameters λ, g_2, g_3 are fixed and Ω is an unknown constant. The *Ansatz* for the Ψ-function must be the following:

$$\Psi = a_0 \mathbf{\Phi}(x;\alpha,k) + a_1 \mathbf{\Phi}'(x;\alpha,k) + a_2 \mathbf{\Phi}(x-\Omega;\alpha,k). \tag{24}$$

Substituting (23) and (24) into (2) and equating the poles to zero, we obtain Ψ-function

$$\Psi = 6\,\mathbf{\Phi}(-\Omega;\alpha,k)\,\mathbf{\Phi}'(x;\alpha,k) - (3\,k^2 - 3\,\wp_\alpha - 2\,\wp_\Omega - \lambda)\,\mathbf{\Phi}(x-\Omega;\alpha,k)$$

and a system of five polynomials:

$$\begin{aligned}
w_1 &= 2\,(\wp_\alpha - \wp_\Omega)\,k^3 + 3\,(\wp'_\Omega - \wp'_\alpha)\,k^2 + 2\,(\wp_\alpha - \wp_\Omega)(3\,\wp_\alpha - \lambda - 2\,\wp_\Omega)\,k \\
&\quad + (6\,\wp_\Omega - \wp_\alpha)\,\wp'_\alpha - (\wp'_\Omega - \wp'_\alpha)\,\lambda - (7\,\wp_\alpha - 2\,\wp_\Omega)\,\wp'_\Omega, \\
w_2 &= 3\,k^3 - (9\,\wp_\alpha - 4\,\wp_\Omega + \lambda)\,k + 3\,\wp'_\alpha + 3\,\wp'_\Omega, \\
w_3 &= 3\,k^4 - 2\,(9\,\wp_\alpha - 14\,\wp_\Omega - \lambda)\,k^2 + 12\,(\wp'_\Omega + \wp'_\alpha)\,k - 9\,\wp_\alpha^2 \\
&\quad - 2\,(14\,\wp_\Omega + \lambda)\,\wp_\alpha + 12\,\wp_\Omega^2 - 8\,\lambda\,\wp_\Omega - \lambda^2, \\
w_4 &= \wp'^2_\alpha - 4\,\wp^3_\alpha + g_2\,\wp_\alpha + g_3, \\
w_5 &= \wp'^2_\Omega - 4\,\wp^3_\Omega + g_2\,\wp_\Omega + g_3,
\end{aligned} \tag{25}$$

where we used the addition theorems for elliptic functions, the important equality

$$\mathbf{\Phi}(\Omega;\alpha,k)\,\mathbf{\Phi}(-\Omega;\alpha,k) = \wp_\alpha - \wp_\Omega,$$

and designated $\wp_\alpha \equiv \wp(\alpha)$, $\wp_\Omega \equiv \wp(\Omega)$, etc. A common factor $\wp_\alpha - \wp_\Omega$ was removed in polynomial w_3 because it leads to the contradiction: $\alpha = \Omega$ $(a_2 = \infty)$. The system (25) generates the ideal

$$\langle w_1, w_2, w_3, w_4, w_5 \rangle \in \mathbb{Q}(\lambda, g_2, g_3)[k, \wp'_\alpha, \wp_\alpha, \wp'_\Omega, \wp_\Omega]. \tag{26}$$

Note, the same ideal $\langle w_1, \ldots, w_5 \rangle$ in the ring $\mathbb{Q}(\lambda, g_2, g_3, \wp_\Omega)[k, \wp'_\alpha, \wp_\alpha, \wp'_\Omega]$ leads to the just mentioned condition $\wp_\alpha - \wp_\Omega = 0$. Therefore Ω is not arbitrary. Computing the minimal reduced Gröbner basis for (26) with pure lexicographic ordering $\wp'_\alpha \succ \wp_\alpha \succ k \succ \wp'_\Omega \succ \wp_\Omega$, we obtain eight polynomials, some of them having a factorized form. If some of the factors do not depend on λ, we obtain restrictions on $\wp'_\Omega$ and $\wp_\Omega$ equating these factors to zero. There are four such polynomials:

$$G_1 = \wp'_\Omega((\lambda^3 - 4\, g_2 \lambda - 16\, g_3)\, k + (3\, \lambda^2 - 4\, g_2)\, \wp'_\Omega) M,$$

$$G_2 = \wp'_\Omega(16\, \wp'_\Omega\, k + 3\, \lambda^2 - 4\, g_2) M,$$

$$G_3 = (4\, \wp_\Omega^3 - g_2\, \wp_\Omega - g_3)\, (4\, \wp_\Omega - \lambda)\, M,$$

$$G_4 = \wp'_\Omega\, (4\, \wp_\Omega - \lambda)\, M,$$

where the multiplier M denotes $3\, k^2 - \lambda - 5\, \wp_\Omega$. The equation $M = 0$ yields the trivial result $\wp(\alpha) = \wp(\Omega)$. It is checked by recomputing the base (25) with an additional polynomial M. Further, Ω must not depend on λ (!). Therefore, the only solution for Ω is defined by the equation

$$\wp'(\Omega) = 0 \Rightarrow \Omega = \omega_1, \omega_2, \omega_3,$$

where ω_j are the half-periods of elliptic functions. Substituting $\wp'_\Omega = 0, \wp_\Omega = e_1$, $g_2 = 4\,(e_1^2 + e_1 e_2 + e_2^2)$, $g_3 = -4\, e_1 e_2 (e_1 + e_2)$ into (25) and recomputing the basis with respect to the ordering $\wp'_\alpha \succ \wp_\alpha \succ k$, we obtain the well known algebraic curve of genus 2 and all algebraic-geometric objects.[2,34]. For classification results of the Treibich–Verdier potentials and other elliptic ones, see Ref. 34, the appendix in Ref. 16 and the most recent results in Ref. 37.

Example 2: As a preliminary, we shall consider Eq. (3) with potential

$$u(x) = 6\, \wp(x) + 6\, \wp(x - \Omega) \tag{27}$$

and the restriction $g_2 = 0$. As before, we have the *Ansatz* for the Ψ-function

$$\Psi = \mathbf{\Phi}(x; \alpha, k) + a_1 \mathbf{\Phi}(x - \Omega; \alpha, k)$$

and the original basis of the ideal is generated by five polynomials. Computing the Gröbner basis G, we obtain a system of eight polynomials. Only two of them have a factorized form:

$$G_1 = (64\, \lambda^3 k^3 - 27\, (\lambda^2 + 16\, g_3)^2)(\wp'_\Omega\, k - 3\, \wp_\Omega^2),$$

$$G_2 = (64\, \lambda^3 k^3 - 27\, (\lambda^2 + 16\, g_3)^2)((4\, \wp_\Omega^3 - g_3) k - 3\, \wp'_\Omega \wp_\Omega^2).$$

The nontrivial solution will take place if and only if (k, λ) are coordinates of the algebraic curve which is the first factor in G_1, G_2. In the next example we rule out the condition $g_2 = 0$.

Example 3: If g_2 is free, the straightforward computing of the basis is unsuccessful. Indeed, the Gröbner base method is universal and therefore it can be ineffective in some special cases. But our interest is only with the *zero structure* of the polynomial system. Thus, the characteristic sets method[42] is the best approach in this case. Under the ordering $\wp_\Omega \prec \wp'_\Omega \prec k \prec \wp_\alpha \prec \wp'_\alpha$, the characteristic set has the form

$$f_1 = (64\, (k\, \lambda + g_2)(k\, \lambda - 2\, g_2)^2 - 27\, (\lambda^2 + 16\, g_3)^2)\, k\, M,$$

$$
\begin{aligned}
f_2 &= (8\,(k\lambda - 2\,g_2)\,\wp_\alpha - 8\,k^3\lambda + 16\,g_2\,k^2 + 3\,\lambda^2 + 48\,g_3)\cdot(4\,\wp'_\Omega k + g_2 - 12\,\wp_\Omega^2)\,k,\\
f_3 &= (32\,(k\lambda - 2\,g_2)\,\lambda^3\,\wp'_\alpha - 192\,g_2^2\,k^2\,\lambda^2 + (\lambda^4 - 288\,g_3\,\lambda^2 - 6912\,g_3^2 + 2^8\,g_2^3)\,k\,\lambda\\
&\quad - g_2\,(11\,\lambda^4 + 864\,g_3\,\lambda^2 + 6912\,g_3^2 - 2^8\,g_2^3))\,k\,M,\\
f_4 &= \wp'^2_\Omega - 4\,\wp^3_\Omega + g_2\,\wp_\Omega + g_3,
\end{aligned}
\tag{28}
$$

where

$$
M \equiv 64\,\wp'_\Omega\,\wp_\Omega\,k^2 - 4\,(3\,\wp'_\Omega\,\lambda - 16\,g_2\,\wp_\Omega - 12\,g_3 + 96\,\wp^3_\Omega)\,k + 3\,(12\,\wp^2_\Omega - g_2)(\lambda + 4\,\wp'_\Omega).
$$

Factorization shows that the variable Ω is separated in polynomials $f_{1,2,3}$. Therefore f_1 gives an algebraic curve independent of Ω:

$$
64\,(k\,\lambda + g_2)(k\,\lambda - 2\,g_2)^2 = 27\,(\lambda^2 + 16\,g_3)^2. \tag{29}
$$

The polynomials $\{f_2, f_3\}$ are an algebraic form of the cover (14). However, the genus of the curve (29) is unity and we have a cover of a torus by a torus. Hence, if moduli of both tori are equal, then there is a one-to-one correspondence between the global parameter α of the torus (12) and the global parameter τ of the torus (29). The next step is to find it. After the birational change of variables $(k,\lambda)\leftrightarrow(y,x)$,

$$
k = \frac{3\,y^2 + 2\,g_2\,x + 3\,g_3}{4\,y\,x}, \quad \lambda = 4\,y,
$$

we obtain the canonical form of the curve (29) as $y^2 = 4\,x^3 - g_2\,x - g_3$ with an obvious uniformization and the equality $\alpha = 2\,\tau$. The final solution of the problem (3) and (27) is as follows:

$$
\begin{aligned}
\Psi(x;\lambda) &= a\,\mathbf{\Phi}(x;2\,\tau,k) + \mathbf{\Phi}(\Omega;2\,\tau,k)\,\mathbf{\Phi}(x-\Omega;2\,\tau,k), \quad \lambda = -4\,\wp'(\tau),\\
a &= \zeta(2\,\tau + \Omega) - 2\,\zeta(\tau) - \zeta(\Omega), \quad k = 2\,\zeta(\tau) - \zeta(2\,\tau).
\end{aligned}
\tag{30}
$$

The passage to the limit $\tau \to \omega_j$ in (30) leads to the solution under the condition $\lambda = 0$:

$$
\Psi(x;\lambda = 0) = C_1\,(\zeta(x) - \zeta(x-\Omega)) + C_2.
$$

An attempt to integrate the more general potential

$$
u(x) = 6\,\wp(x - \Omega_1) + 6\,\wp(x - \Omega_2) + A
$$

with a nonzero constant A failed. However, this point has an explanation in the theory of nonlinear partial differential equations. Indeed, the spectral problem (3) is associated with the Sawada–Kotera (SK) equation[33]

$$
u_t = u_{xxxxx} - 5\,u\,u_{xxx} - 5\,u_x\,u_{xx} + 5\,u^2\,u_x. \tag{31}
$$

By assuming that the poles $\Omega_{1,2}$ depend on time t, one obtains an isospectral deformation of this potential. This simple calculation yields the stationary solution of (31)

$$
u(x,t) = 6\,\wp(x - c\,t) + 6\,\wp(x - c\,t - \Omega) + A
$$

with the conditions

$$
c + 12\,g_2 + 5\,A^2 + 60\,A\,\wp(\Omega) = 0, \quad A\,\wp'(\Omega) = 0.
$$

Therefore ($\Omega=\omega_j$ and A is free) or ($A=0$ and Ω is free). In the both cases we obtain a restriction on a velocity c of two canoidal waves. See an example in Ref. 40 for the case $A=0$. Recently, Conte and Musette obtained a similar result [Ref. 31 formula (84)] and revealed a remarkable more general solution in an old paper by Chazy[8] in the context of the Painlevé analysis:

$$u(x,t)=6\,\wp(x-c\,t-\Omega;\,g_2,g_3)+6\,\wp(x-\tilde{c}\,t-\tilde{\Omega};\,\tilde{g}_2,\tilde{g}_3),$$
$$c=3\,g_2-15\,\tilde{g}_2,\quad \tilde{c}=3\,\tilde{g}_2-15\,g_2. \tag{32}$$

Strictly speaking, Chazy's solution (Ref. 8 p. 380) corresponds to the stationary equation (31) and therefore to the case $\tilde{g}_2=g_2$ ($\tilde{c}=c$) in (32). One can show that the potential (32) is the stationary solution of a linear combination of the equation (31) and higher SK–equation of the seventh order

$$u_t=u_{7x}-\ -7(u\,u_{5x}+2\,u_x\,u_{4x}+3\,u_{xx}u_{xxx}-2\,u^2\,u_{xxx}-6\,u\,u_x\,u_{xx}-u_x^3+\tfrac{4}{3}u^3\,u_x). \tag{33}$$

Section VII contains additional information for this potential. We do not enumerate other one-pole elliptic potentials $u(x)=A\,\wp(x)+B$ for the equation (3). For example, one of them is $u=30\,\wp(x)\pm 3\,\sqrt{3\,g_2}$ (see also Ref. 5).

Example 4: Let us consider a general one-pole elliptic potential for the equation (4),

$$\Psi'''-(a\,\wp(x)+d)\,\Psi'-(b\,\wp'(x)+c\,\wp(x))\,\Psi=\lambda\,\Psi, \tag{34}$$

in the framework of the *Ansatz*

$$\Psi=\mathbf{\Phi}(x;\alpha,k).$$

Using the above techniques in the ring $\mathbb{Q}(a,b,c,d)[\wp_\alpha,\wp'_\alpha,k]$ we do not get the solution: $I=\langle 1\rangle$. Therefore (a,b,c,d) have to depend on each other. After calculations in the ring $\mathbb{Q}(a,b,c)[\wp_\alpha,\wp'_\alpha,k,d]$ we determine step by step the constants $(a,\,b,\,c,\,d)$ and get the following. The first polynomial in a base is

$$-8\,b^3\,(2\,b-3)^3\,\lambda^2-4\,c\,(2\,b-3)^2\,(4\,d\,b^3-12\,b^2\,d-b\,c^2+6\,c^2)\,\lambda+\cdots=0.$$

Equating to zero the coefficients in front of $\lambda^2,\,\lambda$ we obtain

$$b=\tfrac{3}{2}\quad\text{or}\quad b=0.$$

In these cases we will have, respectively,

$$3\,d-c^2=0,\quad (216\,\lambda+c^3-36\,c\,d)\,c^3=0.$$

Therefore $(b=\frac{3}{2}, d=c^2/3)$ or $b=c=0$. In the first case, we have

$$\Psi'''-3\,(\wp(x)+c^2)\,\Psi'-(\tfrac{3}{2}\wp'(x)+3\,c\,\wp(x))\Psi=\lambda\,\Psi,\qquad \Psi(x;\lambda)=\mathbf{\Phi}(x;\alpha,c).$$

The nonramified cover of the torus (16) of genus $g=1$ is

$$\wp'(\alpha)-6\,c\,\wp(\alpha)+2\,\lambda+4\,c^3=0.$$

c is an arbitrary constant and the condition $g_2=0$ (Ref. 29, example 3.10) does not appear. Note, there is no such restriction in the Halphen equation (6) with $n=5$ as in Ref. 15. It appears only for $n=4$.[17] The second case is known:[29]

$$\Psi'''-(6\,\wp(x)+d)\,\Psi'=\lambda\,\Psi,$$
$$108\,\lambda\,\wp'(\alpha)+36\,(d^2-3\,g_2)\,\wp(\alpha)+27\,\lambda^2-108\,g_3-4\,d^3=0 \quad (\text{genus } g=2). \tag{35}$$

See Ref. 3 for an application of this potential.

Note that both cases can be found in Ref. 28 t. III, pp. 372, 522, in Jacobian functions and Ref. 19, III/IV, pp. 460, 462, in Weierstrassian functions. No other possibilities exist. The same technique is applicable to other *Ansätze*. The next one is a nontrivial example along these lines.

Example 5: The equation (34) in the framework of the *Ansatz*

$$\Psi=a_0\mathbf{\Phi}(x;\alpha,k)+\mathbf{\Phi}'(x;\alpha,k). \tag{36}$$

As a consequence of corresponding indicial equation (38) with $\nu=2$, without loss of generality we set $b=12-a$ in (34). Solutions for a,c,d must not depend on λ and k. One solution suggests itself. Indeed, the first polynomial in the original base has the form

$$(a-12)\,((a-18)\,(k^2-\wp_\alpha)+2\,c\,k)+2\,(a-18)\,d+c^2=0.$$

With $a=12$, this polynomial does not depend on k,α and we get (after the replacement $c\to 12\,c$)

$$a=12,\quad b=0,\quad d=12\,c^2,\quad a_0=k-2\,c.$$

Moreover, the ideal in the ring $\mathbb{Q}(\lambda,c,g_2,g_3)[\wp_\alpha,\wp'_\alpha,k]$ is not equal to $\langle 1\rangle$ and, therefore, c is an arbitrary constant. Thus, the equation (34) and its solution take the form

$$\Psi'''-12\,(\wp(x)+c^2)\,\Psi'-12\,c\,\wp(x)\,\Psi=\lambda\,\Psi,$$
$$\Psi(x;\lambda)=\mathbf{\Phi}'(x;\alpha,k)-2\,c\,\mathbf{\Phi}(x;\alpha,k). \tag{37}$$

We do not give here the large formulas for the cover (14), or the four-sheet cover in the form (16) and write only a skeleton of the nonhyperelliptic trigonal algebraic curve (15) of genus $g=3$,

$$64\,(\lambda^2+32\,c^3\,\lambda+2^8\,c^6-108\,g_2\,c^2)(\lambda-11\,c^3)\,k^3+(\cdots)\,k^2+(\cdots)\,k+(\cdots)=0,$$

where $(\cdots)$ designate some polynomials in λ,c,g_2,g_3 with integer coefficients.[5] Under $c=0$ we arrive at the case (27) with $\Omega=0$.

The higher *Ansätze* (9) are investigated in a similar manner. Indeed, by Fuchs–Frobenius theory, if Ψ has the expansion $\Psi=x^{-\nu}+\cdots$, then a,b satisfy the determining equation

$$-\nu(\nu+1)(\nu+2)+a\,\nu+2\,b=0. \tag{38}$$

A natural question appears: under what parameters (a,b) does the equation (38) have integral solutions for ν? One of solutions is Halphen's equation (6). It corresponds to $2\,b=a$ and (38) reduces to

$$a=n^2-1 \quad (n\equiv\nu+1).$$

As in the previous example we can list all the possible cases for the *Ansatz* (36). Indeed, assuming $b=12-a$ and (a,d,c) to be arbitrary, the origin base contains three polynomials.[5] The first and second of them are linear in $\wp$, $\wp'$. Solving them and substituting into the base again, we obtain the remaining polynomial in (λ,k):

$$-4\,(a-12)^2\,(a-18)^2\,((a-6)\,(a-18)\,k+c\,(a-9))\,\lambda+(\cdots)\,k+(\cdots)=0,$$

where dots denote a polynomial in (a,c,d,g_2,g_3). It must be zero for all values of λ. Splitting it in λ we get two linear polynomials in k. Their compatibility condition is the polynomial

$$(a-6)(a-8)(108\,c^4-72\,(a-18)^2\,d\,c^2+(a-18)^4\,(12\,d^2-(a-12)^2\,g_2))=0$$

and solution for k

$$k=-\frac{(a-9)\,c}{(a-6)\,(a-18)}.$$

The verifying of Weierstrass's relation (12) yields a polynomial in λ:

$$(a-6)^3(a-12)^3(a-18)^6\,\lambda^2+(\cdots)\,\lambda+(\cdots)=0.$$

Under $a\neq 6,12,18$ we arrive at the point (3) of the Proposition. Therefore, only three possibilities exist: $a=6,12,18$. The corresponding final solutions for the variables $(\wp',\wp,k)$ are obtained separately: by recomputing the base. Thus, besides (37), we have the following integrable potentials [note a misprint $\wp(x)$ instead of $\wp'(x)$ in one of the formulas in Ref. 5]:

$$\Psi'''-(18\,\wp(x)+d)\,\Psi'+6\,\wp'(x)\,\Psi=\lambda\,\Psi,\quad \Psi'''-(6\,\wp(x)+d)\,\Psi'-6\,\wp'(x)\,\Psi=\lambda\,\Psi.$$

See Ref. 39 for solutions of the generalized Halphen equation (6) and Ref. 5 for details of Example 5.

It should perhaps be noted here that the example (37) is the generalization $c\neq 0$ of the first nontrivial case $n=-3$ in a series of other Halphen's equations (Ref. 27, p. 554),

$$w'''-\frac{4}{3}n^2\,w'\,\wp(z)-\frac{2}{27}n\,(n+3)\,(4\,n-3)\,w\,\wp'(z)=0 \tag{39}$$

without a spectral parameter. [The example (39) was revealed by E. Previato.] Notation as in Ref. 19 III/IV: Ex. 15, p. 464. Indicial equation (38) for the example (39) becomes

$$(3\,\nu+2\,n)(3\,\nu+2\,n+6)(3\,\nu-4\,n+3)=0$$

and $(n+3)(n+6)(4\,n-9)=0$ for the *Ansatz* (36) $(\nu=2)$.

Example 6: Halphen's equation (6) with $n=5$. Here we display only the final formulas in the context of Sec. IV:

(i) the commuting operator pencil (18):

$$\lambda\,\Psi''-14\,(4\,\wp(x)^2-g_2)\,\Psi'+16\,(7\,\wp'(x)-\lambda)\,\wp(x)\,\Psi=\mu\,\Psi;$$

(ii) the polynomial (21):

$$6\,\mu-56\,k^5+560\,\wp_\alpha\,k^3-20\,(28\,\wp'_\alpha-\lambda)\,k^2+168\,(5\,\wp_\alpha^2-g_2)\,k-4\,(28\,\wp'_\alpha+5\,\lambda)\,\wp_\alpha=0;$$

(iii) the birational transformation (19, 20), which is quadratic in (k,μ):

$$\mu=\frac{32}{49}\,\frac{(2\,(\lambda^2-392\,g_3)\,k\,\lambda+7\,(5\,\lambda^2-784\,g_3)\,g_2)\,((\lambda^2-392\,g_3)\,k-21\,g_2\,\lambda)}{\lambda^4-208\,g_3\lambda^2+3136\,(g_2^3+4\,g_3^2)},$$

$$k=\frac{7}{8}\,\frac{\mu^2-4\,g_2\,(5\,\lambda^2-784\,g_3)}{(\lambda^2-392\,g_3)\,\lambda};$$

(iv) the canonical form of the algebraic curve of genus 4 (see also Ref. 39):

$$\tilde{F}(\mu,\lambda):\mu^3-4\,g_2\,(11\,\lambda^2-784\,g_3)\,\mu-\lambda^5+208\,g_3\,\lambda^3-3136\,(g_2^3+4\,g_3^2)\,\lambda=0;$$

(v) the eight-sheet cover in the form (16):

$$2^8\,(\lambda^2-392\,g_3)^3\,\lambda\,\wp'(\alpha)-2^8 49\,g_2\,(\lambda^2+112\,g_3)\,(\lambda^2-392\,g_3)^2\,\wp(\alpha)+\lambda^8-\cdots=0.$$

Note that both this cover and its algebraic form (14) are the expansive expressions, whereas the reduced holomorphic differential (17) in the variables (k,λ) and (μ,λ) is given by the simple formulas:

$$\frac{d\wp(\alpha)}{\wp'(\alpha)}=\frac{-8\,(\lambda^2-56\,g_3)}{3\,\mu^2-4\,g_2\,(11\,\lambda^2-784\,g_3)}\,d\lambda=\frac{-7\,(\lambda^2-56\,g_3)}{(\lambda^2-392\,g_3)\,(3\,\lambda\,k+14\,g_2)}\,d\lambda.$$

Analogs of the above formulas are derived for all other examples in the article.

Example 7: The two-pole potential for the equation (4) with *Ansatz*

$$\Psi=\mathbf{\Phi}(x;\alpha,k)+a_1\,\mathbf{\Phi}(x-\Omega;\alpha,k).$$

The general two-pole elliptic potentials contain many parameters—multipliers before the $\wp'$, $\wp$, ζ-functions. We do not give their exhaustive classification and consider only the most interesting case

$$\Psi'''-3\,(\wp(x)+\wp(x-\Omega)-\wp(A))\,\Psi'-\tfrac{3}{2}(\wp'(x)+\wp'(x-\Omega)+B\,\wp(x)-B\,\wp(x-\Omega))\Psi=\lambda\,\Psi. \tag{40}$$

By virtue of the Proposition, the Gröbner base contains all the information about the solution, i.e., all the following formulas. As before we obtain that Ω, A are arbitrary constants and

$$B=2\,\sqrt{\wp(\Omega)-\wp(A)}.$$

The parameters k and λ as meromorphic functions are connected by an algebraic equation of the genus 2 independent of Ω (compare with Ref. 35):

$$2\,\lambda\,k^3+(3\,\wp_A^2-g_2)\,k^2-3\,\wp_A\,\lambda\,k-\tfrac{1}{4}\lambda^2+\wp_A'^2=0. \tag{41}$$

The equation (41) can be realized as a two-sheet cover of a torus in the form (16),

$$\lambda\,\wp'(\alpha)+(3\,\wp_A^2-g_2)\,\wp(\alpha)+\tfrac{1}{4}\lambda^2+\wp_A^3-g_3=0.$$

The algebraic form of cover (14) has the form

$$\wp(\alpha)=k^2+\wp_A,\quad \wp'(\alpha)=(g_2-3\,\wp_A^2)\,\frac{k^2}{\lambda}-\frac{\wp_A'^2}{\lambda}-\frac{\lambda}{4}.$$

VI. SOLUTIONS OF INTEGRABLE PDEs

The spectral problem (4) and (40) corresponds to the Boussinesq equation

$$3\,u_{tt}=(2\,u^2-u_{xx})_{xx}, \tag{42}$$

and the arbitrariness of Ω means the existence of an isospectral deformation of the potential

$$u(x,t)=3\,\wp(x-\Omega_1(t))+3\,\wp(x-\Omega_2(t))-3\,\wp_A. \tag{43}$$

Substituting the two-gap *Ansatz* (43) in (42), we get the well known system of pairwise-interacting particles $\Omega_{1,2}(t)$ of the Calogero–Moser system type[30] with a repulsion potential and immovable center of mass. Integration leads to an equation for $\Omega_1(t)$:

$$\dot{\Omega}_1^2 = 4\,\wp(2\,\Omega_1 - c) - 4\,\wp_A, \quad \Omega_2 = c - \Omega_1.$$

Using the uniformization of the corresponding elliptic curve, we obtain the explicit solution

$$\Omega_1(t) = \frac{1}{2}\wp^{-1}\left(\widetilde{\zeta}(\tau+\nu) - \widetilde{\zeta}(\tau-\nu) - \widetilde{\zeta}(2\,\nu) + \frac{1}{4}\wp_A\right) + \frac{c}{2},$$
$$\nu = \pm\frac{1}{2}\widetilde{\wp}^{-1}\left(\frac{\wp_A^2}{16} + \frac{g_2}{24}\right), \quad \widetilde{\wp}'(2\,\nu) = -\frac{1}{32}(\wp_A^3 - g_2\,\wp_A + 2\,g_3), \tag{44}$$

where $\tau = 8\,(t - t_0)$ and c, t_0 are arbitrary constants. An implicit form of this solution with $c = 0$ in terms of Jacobi's sn, cn, dn-functions is given in Ref. 20 and in the earlier citation[9] in the context of solutions of the Kadomtsev–Petviashvili equation. In (44), the elliptic integral $\wp^{-1}$ is calculated with invariants g_2, g_3, and the $\widetilde{\zeta}$, $\widetilde{\wp}^{-1}$-functions with invariants

$$\widetilde{g}_2 = \frac{1}{16}\left(g_2\,\wp_A^2 + 3\,g_3\,\wp_A + \frac{g_2^2}{12}\right), \quad \widetilde{g}_3 = -\frac{g_3}{2^8}(\wp'^2_A + 2g_3) + \frac{g_2^3}{2^7 3^3} - \frac{g_2\,\widetilde{g}_2}{24}.$$

The reduction case $B = 0$ in (40) corresponds to the Kaup–Kupershmidt (KK) equation

$$u_t = u_{xxxxx} - 5\,u\,u_{xxx} - \tfrac{25}{2}u_x\,u_{xx} + 5\,u^2\,u_x \tag{45}$$

and its stationary solution

$$u(x,t) = 3\,\wp(x - c\,t) + 3\,\wp(x - c\,t - \Omega) - 3\,\wp(\Omega), \tag{46}$$

but the velocity c depends on the distance between poles:

$$c = 3g_2 - 45\,\wp^2(\Omega).$$

The generalization of (46) in a similar way as the solution (32) is

$$u(x,t) = -12\,(\wp_1 + \wp_2) + 3\left(\frac{\wp_1' - \wp_2'}{\wp_1 - \wp_2}\right)^2, \tag{47}$$

where

$$\wp_1 \equiv \wp(x - c\,t - \Omega; g_2, g_3), \quad \wp_2 \equiv \wp(x - c\,t - \hat{\Omega}; g_2, \hat{g}_3), \quad c = -12\,g_2.$$

Here Ω, $\hat{\Omega}$, g_2, g_3, $\hat{g}_3$ are five arbitrary constants. Using a connection between the SK(u)- and KK(w)-equations and the Tzitzeica equation

$$\phi_{xt} = e^{\phi} - e^{-2\,\phi} \tag{48}$$

with the Fordy–Gibbons equation[18]

$$v_t = v_{xxxxx} - 5\,(v_x\,v_{xxx} + v^2\,v_{xxx} + v_{xx}^2 + v_x^3 + 4\,v\,v_x\,v_{xx} - v^4\,v_x)$$

via the Miura transformations

$$u=v^2-v_x, \quad w=v^2+2\,v_x, \quad u=\phi_{xx}+\phi_x^2,$$

we obtain stationary solutions for the v-function

$$v(x,t)=\frac{\wp_1'-\wp_2'}{\wp_1-\wp_2}.$$

Nonstationary solution of the equation (48) has the form

$$\phi(x,t)=\ln 2\,c+\ln(\wp(x+c\,t-\Omega;g_2,g_3)-\wp(x-c\,t-\hat{\Omega};g_2,\hat{g}_3))$$

with the restriction: $4\,(\hat{g}_3-g_3)\,c^3=1$. The details of calculations (44) are expounded in Ref. 5 and the formula (47), and the Ψ-function for the potentials (32) and (47) in Refs. 5, 4, and 40.

VII. CONCLUDING REMARKS AND DISCUSSION

The investigation of elliptic solitons can be automated by polynomial techniques. The Gröbner base method provides a unified approach to the solution of related problems. The technique suggested with minor modifications is extended to matrix spectral problems.

As the Examples 2, 3 and 5 show, the algebraic curves can be degenerate (multiply roots of discriminant).

The general case in Example 7 for the equation (4),

$$\begin{gathered}u(x)=a\,\wp(x)+b\,\wp(x-\Omega)+c\,\zeta(x)-c\,\zeta(x-\Omega),\\ v(x)=d\,\wp'(x)+e\,\wp'(x-\Omega)+f\,\wp(x)+g\,\wp(x-\Omega)+h\,\zeta(x)-h\,\zeta(x-\Omega),\end{gathered} \tag{49}$$

requires additional research.

To all appearances, the example (37) has to fit into the hierarchy of higher Boussinesq equations, studied in full in Refs. 13 and 14. Multi-pole potentials are investigated by involving the addition theorem for the $\mathbf{\Phi}$-function:

$$\mathbf{\Phi}(x+z;\alpha,k)=\frac{1}{2}\,\frac{\mathbf{\Phi}(x;\alpha,k)\,\mathbf{\Phi}(z;\alpha,k)}{\wp_x-\wp_z}\left(\frac{\wp_\alpha'+\wp'_x}{\wp_\alpha-\wp_x}-\frac{\wp_\alpha'+\wp'_z}{\wp_\alpha-\wp_z}\right).$$

A natural assumption suggests itself: *all the potentials, obtained by the above method, are finite-gap ones*. At least, by construction, all such potentials belong to the set of exact integrable (explicit Ψ[40]) and the Ψ-function is a single-value function on a Riemann surface of the algebraic curve $F(k,\lambda)=0$ and meromorphic function (in x) for all values of λ (Picard's theorem[21,23]). Since our Ψ is expressible in terms of Weierstrassian σ, all the corresponding spectral problems become quadrature integrable. See Ref. 6 for further explanations of this concept of integrability in the example of the Schrödinger equation and see Ref. 40 and the example below for other spectral problems. Note that all linear independent solutions for the Ψ-function are obtained by choosing the k-branch of algebraic equation (15).

If the assumption is valid, then the potentials for the spectral problems (2)–(4) are free of residues (a consequence of Θ-formulas), and therefore *Ansätze* for the multi-pole potentials [say (49)] do not have to involve the ζ-functions. This strongly decreases the number of parameters and the computational task.

The potential (32)

$$u=6\,\wp(x-\Omega;g_2,g_3)+6\,\wp(x-\tilde{\Omega};\tilde{g}_2,\tilde{g}_3) \tag{50}$$

with arbitrary invariants $g_2, g_3, \tilde{g}_2, \tilde{g}_3$ is a finite-gap one for the equation (3), but its spectral characteristics can not be obtained in the framework of elliptic soliton theory. The corresponding commuting operator pencil is derived with the help of the equation (33) and takes the form

$$(9\,(u-c_1)\,\lambda-3\,u'''+6\,u\,u'+c_1\,u')\,\Psi''-(27\,\lambda^2+9\,u'\,\lambda-u^{(\mathrm{IV})}-3\,u'^2+\tfrac{4}{3}u^3-c_1\,u''-c_1\,u^2$$
$$+27\,c_2)\,\Psi'+6\,\lambda\,(u''-u^2+c_1\,u)\,\Psi=\mu\,\Psi.$$

Hence, the canonical form $\widetilde{F}(\mu,\lambda)=0$ of the associated trigonal curve of genus $g=4$ is obtained by elimination of Ψ:

$$a^3\,\mu^3+3^5(36\,a^2\,b\,\lambda^4-(a^5-16\,g_2\,a^4+16\,g_2^2\,a^3+192\,(b-3\,g_3)\,a^2\,b+192\,g_2\,a\,b^2)\,\lambda^2$$
$$+48\,(g_3\,a^5-g_2\,a^4\,b+4\,a^2\,b^3))\,\mu+3^6\,(27\,a^3\,\lambda^7-216\,(a^3b-4\,g_3\,a^3+2\,g_2\,a^2\,b+8\,b^3)\,\lambda^5$$
$$-2\,(a^6+30\,g_2\,a^5-96\,g_2^2\,a^4-8\,(45\,b^2-216\,g_3\,b-8\,g_2^3+432\,g_3^2)\,a^3+576\,(b$$
$$+6\,g_3)\,g_2\,a^2\,b-2^8 9\,g_2^2\,a\,b^2-2^8 3^3\,(b^4-2\,g_3\,b^3)\,\lambda^3-288\,(a^3-2\,g_2\,a^2+24\,b^2)(g_3\,a^3$$
$$-g_2\,a^2\,b+4\,b^3)\,\lambda=0,\quad a\equiv g_2-\tilde{g}_2,\quad b\equiv g_3-\tilde{g}_3,$$

and the corresponding Ψ-function is given by the expression

$$\Psi(x;\lambda)=\exp\int\frac{\lambda\,F^2-G\,H+F\,H'-F'\,H}{G^2-u\,F^2-F\,H+F'\,G-F\,G'}\,dx,$$

where prime denotes a derivation in x and

$$F\equiv-3\,u'''+6\,u\,u'-3\,c_1\,u'+9\,(u-c_1)\,\lambda,\quad H\equiv6\,(u''-u^2+c_1\,u)\,\lambda-\mu,$$

$$G\equiv u^{(\mathrm{IV})}+c_1\,(u''+u^2)-3\,u'^2-9\,u'\,\lambda-\frac{4}{3}u^3-27\,(\lambda^2+c_2),$$

$$c_1\equiv-12\,\frac{g_3-\tilde{g}_3}{g_2-\tilde{g}_2},\quad c_2\equiv\frac{8\,(3\,\tilde{g}_3+g_3)\,g_2-(3\,g_3+\tilde{g}_3)\,\tilde{g}_2}{3\,g_2-\tilde{g}_2}.$$

One particular case of the potential (50) and the more general property of finite-gap potentials are discussed in Ref. 40.

The natural generalization of Hermite's method is to consider nonlinear homogeneous *Ansätze* for the Ψ-function. For instance, the quadratic *Ansatz*

$$\Psi=e^{kx}\sum_{j,\,n}A_{jn}\,\Phi(x-\Omega_j;\,\alpha)\,\Phi(x-\Omega_n;\,\alpha).$$

However, this does not fit into the framework of finite-gap integration theory, because the poles of the potential can depend on the spectral parameter. The following example with the transcendental dependence on spectral parameter elucidates this:

$$\Psi''=(6\,\wp(x)+2\,\wp(x-\lambda)+4\,\wp(\lambda))\,\Psi,\quad \Psi(x;\lambda)=\Phi^2(x;\,\lambda).$$

Actually, the quadratic (and higher) *Ansätze* will not give an advantage due to the relation

$$\Phi(x;\alpha)^2=-\boldsymbol{\Phi}'(x;2\,\alpha,\zeta(2\,\alpha)-2\,\zeta(\alpha))$$

and we again arrive at the framework of Hermite's method.

Note that the nonintegrability of equation (1) in context of the point (3) of the Proposition, nevertheless, can be useful for its integrability with special values of λ or for more complex operator pencils with a dependence of the potential (say parameters a,b,c,d in Examples 4 and 5) on λ. The availability of additional constants in the potentials may be considered as a family of spectral pencils, and under fixed values of λ, as new spectral problems. For instance, the two-gap

Lamé potential $u=6\,\wp(x)$ for Eq. (5) is obtained from example (35) with $\lambda=0$ and $d\to\lambda$, $\Psi'\to\Psi$. A less simple example is to swap the parameters $\lambda\leftrightarrow c$ in Eq. (37), whereupon one finds the finite-gap operator λ-pencil

$$\Psi'''-12\,(\wp(x)+\lambda^2)\,\Psi'-(c+12\,\lambda\,\wp(x))\,\Psi=0$$

with the algebraic curve $F(k,\lambda)=0$ of genus $g=8$ [Ref. 5, formula (15)].

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A class of nonautonomous coupled KdV systems

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A class of nonautonomous coupled Korteweg–de Vries (KdV) systems in $(1+1)$ dimensions are considered for integrability classification. Integrability of the systems is associated with the existence of a certain recursion operator. Some new integrable nonautonomous two-component KdV systems are found. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1628838]

I. INTRODUCTION

There has been a constant interest in finding new scalar and multicomponent integrable nonlinear equations because of both the rich mathematical structures they possess and the wide variety of physical systems having interesting properties that are described by such equations. For this purpose, many classes of scalar and multicomponent KdV type equations are classified based on different aspects of integrability such as existence of infinitely many symmetries and/or conservation laws, bi-Hamiltonian structure, master symmetries, recursion operator, formal symmetry of infinite rank, Lax representation, Painlevé property, etc.[1–13]

Despite their frequent appearance in applications where inhomogeneous properties of physical media are taken into account, nonautonomous versions of KdV type equations are only investigated for scalar equations. These investigations gave negative results for existence of original nonautonomous scalar KdV type equations.[5,14,15] All the known equations that are apparently nonautonomous were also found to be transformable to the usual KdV or to its well-known modifications. On the other hand, due to their importance in applications, systematic derivation of nonautonomous versions of KdV and other integrable equations are considered in Ref. 16.

Most of the systematic integrability classifications of multicomponent equations are performed only for nondegenerate systems,[1–4,9,12,13] usually having the identity matrix as the coefficient of highest order (derivative) terms. Degenerate systems are relatively less interested. Systems of this latter type are usually introduced on their own.[17,18] There are also systematic works to obtain such systems.[6,8,10] However, the most generic degenerate systems known so far are obtained in a physical problem,[7] where a class of degenerate KdV type extended two-component equations are introduced with their bi-Hamiltonian structure in the context of asymptotic integrability of water waves.

Recently, we have started classification of nonautonomous multicomponent KdV systems based on the existence of a certain recursion operator.[13] We obtained the nonautonomous versions of autonomous Svinolupov Jordan KdV systems[4] therein. In the present work, we proceed with the recursion operator based integrability classification of nonautonomous KdV type multicomponent equations. Motivated by the results of the above-mentioned earlier works and the form of cylindrical KdV equation, here we aim to classify both degenerate and nondegenerate classes of the following N-component nonautonomous KdV type extended equations

$$q_t^i = b_j^i q_{xxx}^j + s_{jk}^i(t) q^j q_x^k + y_j^i(t) q^j, \quad i,j,k = 1,2,\ldots,N, \tag{1}$$

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where $q^i=q^i(x,t)$ are the dependent variables. We associate integrability of system (1) with the existence of a recursion operator whose form we assume to be

$$\mathcal{R}^i_j=z^i_j(t)D^2+a^i_{jk}(t)q^k+h^i_j(x,t)+[c^i_{jk}(t)q^k_x+w^i_j(t)]D^{-1}, \tag{2}$$

where $D=d/dx$ and D^{-1} is the formal inverse operator ($DD^{-1}=D^{-1}D=1$).

Systems admitting a recursion operator are integrable in existence of infinitely many symmetries sense because by definition a recursion operator maps symmetries of a system to other symmetries of it endlessly.[19]

Here, in (1) and (2) except for b^i_j which are assumed to be constants, all the coefficient terms are introduced with their presumed dependence on the independent variables x and t. Sufficient differentiability of these coefficients with respect to their independent variables is also assumed.

System (1) admits recursion operator (2) if they satisfy the integrability criterion[19]

$$\mathcal{R}^i_{j,t}=\mathcal{K}'^i_r\mathcal{R}^r_j-\mathcal{R}^i_r\mathcal{K}'^r_j, \tag{3}$$

where

$$\mathcal{K}'^i_j=b^i_jD^3+s^i_{kj}(t)q^kD+s^i_{jk}(t)q^k_x+y^i_j(t)$$

is the Fréchet derivative of the system (1).

In Sec. II we give the conditions for (1) and (2) to satisfy the integrability criterion (3) for an arbitrary number N of components. In Sec. III we briefly explain our classification algorithm which is based on the Jordan canonical forms of matrices and finally in Sec. IV we give the two-component ($N=2$) systems we found as solutions of the integrability conditions.

II. INTEGRABILITY CONDITIONS

The integrability criterion (3) leads to some algebraic and differential conditions among the coefficient terms of the system (1) and the recursion operator (2). In the following proposition we give these conditions.

Proposition 1: Let $q^i(x,t)$ be functions of x and t satisfying system of equations (1) which admits a recursion operator $\mathcal{R}^i_j$ given in (2). Then the coefficient terms $b^i_j,s^i_{jk}(t),y^i_j(t),z^i_j(t),a^i_{jk}(t),h^i_j(x,t),c^i_{jk}(t),w^i_j(t)$ satisfy the following relations:

$$\begin{gathered}
3b^i_ka^k_{jl}+b^i_kc^k_{jl}+s^i_{kl}z^k_j-2z^i_ks^k_{lj}-z^i_ks^k_{jl}-c^i_{kl}b^k_j=0,s^i_{mk}a^k_{jl}-a^i_{km}s^k_{lj}=0,\\
3b^i_ka^k_{jl}+3b^i_kc^k_{jl}-z^i_ks^k_{lj}-2z^i_ks^k_{jl}=0,a^i_{jk}b^k_l-b^i_ka^k_{jl}-3b^i_kc^k_{jl}+z^i_ks^k_{jl}=0,\\
b^i_kz^k_j-z^i_kb^k_j=0,b^i_kh^k_j-h^i_kb^k_j=0,b^i_kc^k_{jl}-c^i_{jk}b^k_l=0,w^i_k(s^k_{lj}-s^k_{jl})=0,\\
c^i_{km}(s^k_{jl}-s^k_{lj})=0,c^i_{jk}s^k_{ml}-s^i_{km}c^k_{jl}=0,c^i_{jk}s^k_{ml}-s^i_{mk}c^k_{jl}=0,\\
a^i_{jk}s^k_{ml}+a^i_{km}s^k_{jl}+c^i_{kl}s^k_{jm}-s^i_{mk}a^k_{jl}-s^i_{mk}c^k_{jl}-s^i_{kl}a^k_{jm}=0,\\
b^i_ka^k_{jl}+s^i_{lk}z^k_j-z^i_ks^k_{lj}-a^i_{kl}b^k_j=0,s^i_{lk}h^k_j-h^i_ks^k_{lj}=0,s^i_{kl}h^k_j-h^i_ks^k_{jl}=0,\\
z^i_{j,t}-3b^i_kh^k_{j,x}-b^i_kw^k_j-y^i_kz^k_j+z^i_ky^k_j+w^i_kb^k_j=0,w^i_{j,t}-y^i_kw^k_j+w^i_ky^k_j=0,\\
a^i_{jl,t}+a^i_{jk}y^k_l-s^i_{lk}h^k_{j,x}-s^i_{lk}w^k_j-y^i_ka^k_{jl}+a^i_{kl}y^k_j+w^i_ks^k_{jl}=0,b^i_kh^k_{j,xx}=0,\\
c^i_{jl,t}+c^i_{jk}y^k_l-s^i_{kl}w^k_j-y^i_kc^k_{jl}+c^i_{kl}y^k_j=0,h^i_{j,t}-b^i_kh^k_{j,xxx}-y^i_kh^k_j+h^i_ky^k_j=0.
\end{gathered} \tag{4}$$

This proposition is the straightforward result of calculating operator equality (3) together with (1) and (2).

Although we obtained the integrability conditions for systems with any arbitrary number N of components, our focus in the rest of this work is to systematically obtain the solutions of these conditions in the two-component ($N=2$) case.

III. CLASSIFICATION ALGORITHM

Having obtained the integrability conditions and specified the number N, our basic aim is to determine the integrable systems (or classes of systems) with their associated recursion operators by solving the whole set of conditions (4). For this purpose we base our classification on b^i_j and solve conditions (4) for each of the specially chosen different forms of b^i_j matrix. Having chosen a certain b^i_j matrix, we first solve the algebraic part of the equations in (4). Although the number of algebraic equations is quite large even for $N=2$, since the constituent equations are polynomials of order at most two in the unknowns, they can be solved by computer algebra systems conveniently. We used REDUCE[20] and MUPAD[21] software for computations. Each nontrivial solution to the algebraic part is then subjected to the remaining differential conditions.

In general, for a certain b^i_j matrix there exist many solutions to the integrability conditions (4). However, some of these solutions give rise to systems which are not interesting: Decoupled systems, trivially coupled systems like $u_t=F[u,t]$, $v_t=G[u,t]$ or completely linear systems. Besides these, some solutions require the recursion operator to be identity, in case of which (3) is obviously inconclusive for the integrability of the system at hand. We call solutions giving rise to these kind of systems or recursion operators as *trivial solutions*. We discard all such trivial solutions.

For the choice of the form of b^i_j matrix we make use of the Jordan canonical form theorem of matrices which says that under similarity transformations any 2×2 constant matrix, say A, is equivalent to one of the following matrices which are the Jordan canonical forms:

$$J(1)=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad J(2)=\begin{pmatrix}\lambda_1&0\\0&\lambda_2\end{pmatrix},\quad J(3)=\begin{pmatrix}\lambda&1\\0&\lambda\end{pmatrix}, \tag{5}$$

where λ_i are the eigenvalues of original matrix A. Nonautonomous systems associated with the identity matrix $J(1)$ are extensively investigated in Ref. 13. Our present classification concerns the classes associated with the latter two matrices $J(2)$ and $J(3)$. Starting from these matrices and taking equivalence of systems under scale transformations of evolution parameter t into account we conclude that (excluding the null matrix) without loss of generality, it is sufficient to consider

$$b(1)=\begin{pmatrix}1&0\\0&\lambda\end{pmatrix},\quad b(2)=\begin{pmatrix}1&\lambda\\0&1\end{pmatrix},\quad b(3)=\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad b(4)=\begin{pmatrix}0&1\\0&0\end{pmatrix} \tag{6}$$

as 2×2 matrices for b^i_j in our classification. Here, in $b(1)$ $\lambda\neq1$ and $\lambda\neq0$, in $b(2)$ $\lambda\neq0$. Any two-component quasilinear evolution equation, such as (1), whose coefficient matrix b^i_j of leading order terms other than the identity can be put in a form such that its transformed coefficient matrix, say $\tilde{b}^i_j$, is either of $b(1)$, $b(2)$, $b(3)$ or $b(4)$. Therefore, it is natural to say a system is in Jordan canonical form if so is its coefficient matrix b^i_j.

In literature, except for a few systems, most of the integrable systems are given in Jordan canonical form. One of these exceptions is the systems with five arbitrary constants introduced by Fokas and Liu in the context of asymptotic integrability of water waves.[7] As an illustrative example of the above proposal about the Jordan canonical forms of systems, we reconsider the Fokas–Liu systems and give their Jordan canonical forms together with the transformations bringing them to these forms here. These systems are originally given as

$$
\begin{aligned}
&u_t+v_x+\epsilon[(3\beta_1+2\beta_4)\beta_3 uu_x+(2+\beta_1\beta_4)\beta_3(uv)_x+\beta_1\beta_3 vv_x\\
&\quad+(\beta_1+\beta_4)\beta_2 u_{xxx}+(1+\beta_1\beta_4)\beta_2 v_{xxx}]=0,\\
&v_t+u_x+\epsilon[(2+3\beta_1\beta_4)\beta_3 vv_x+(\beta_1+2\beta_4)\beta_3(uv)_x+\beta_1\beta_3\beta_4 uu_x\\
&\quad+(1+\beta_1\beta_4)\beta_2\beta_4 v_{xxx}+(\beta_1+\beta_4)\beta_2\beta_4 u_{xxx}]=0,
\end{aligned}
\tag{7}
$$

where ϵ, β_1, β_2, β_3, β_4 are arbitrary constants and $\beta_1^2\neq 1$. Systems (7) reduce to linear systems for $\epsilon=0$ or $\beta_3=0$ and to first order (hydrodynamic type) systems for $\beta_2=0$. Here, we consider only the third order nonlinear systems by taking $\epsilon\neq 0$, $\beta_2\neq 0$, $\beta_3\neq 0$. Furthermore, we make the following distinction:

(i) $\beta_1\neq -2\beta_4/\beta_4^2+1$, $\beta_1^2\neq 1$,
(ii) $\beta_1=-2\beta_4/\beta_4^2+1$, $\beta_4\neq 0$, $\beta_4^2\neq\pm 1$,
(iii) $\beta_1=-2\beta_4/\beta_4^2+1$, $\beta_4=0$,

in the space of arbitrary parameters.

In case (i), applying the following change of dependent variables

$$
\begin{pmatrix}\tilde{u}\\ \tilde{v}\end{pmatrix}=\frac{\beta_3}{2\beta_2(\beta_1\beta_4^2+\beta_1+2\beta_4)}\begin{pmatrix}\beta_1+\beta_4 & \beta_1\beta_4+1\\ \pm\beta_4\sqrt{\beta_1^2-1} & \mp\sqrt{\beta_1^2-1}\end{pmatrix}\begin{pmatrix}u-A_1\\ v-B_1\end{pmatrix},
\tag{8}
$$

and rescaling of evolution parameter t,

$$
\tau=-\epsilon\beta_2(\beta_1\beta_4^2+\beta_1+2\beta_4)t,
\tag{9}
$$

we arrive at a Jordan canonical form of systems (7) irrespective of the values of constant shifting parameters A_1 and B_1.[10] But let us for the sake of simplicity of final expression take

$$
A_1=\frac{-\beta_1\beta_4^3+3\beta_1\beta_4+2}{\epsilon\beta_3[\beta_1\beta_4^2+\beta_1+2\beta_4]^2},\quad B_1=\frac{3\beta_1\beta_4^2-\beta_1+2\beta_4^3}{\epsilon\beta_3[\beta_1\beta_4^2+\beta_1+2\beta_4]^2}.
$$

After all, we get

$$
\begin{aligned}
\tilde{u}_\tau&=\tilde{u}_{xxx}+3\tilde{u}\tilde{u}_x+2\tilde{v}\tilde{v}_x+\frac{4(\beta_4^2+2\beta_1\beta_4+1)}{\epsilon\beta_2[\beta_1\beta_4^2+\beta_1+2\beta_4]^2}\tilde{u}_x,\\
\tilde{v}_\tau&=2(\tilde{u}\tilde{v})_x,
\end{aligned}
\tag{10}
$$

as a Jordan canonical form of systems (7) in the new variables in the mentioned case of arbitrary parameters ϵ and β_i, $i=1,2,3,4$.

In case (ii), the following transformation:

$$
\begin{pmatrix}\tilde{u}\\ \tilde{v}\end{pmatrix}=\begin{pmatrix}0 & \dfrac{\beta_3}{\beta_2\beta_4}\\ \dfrac{\epsilon\beta_3\beta_4(1-\beta_4^2)}{\beta_4^2+1} & -\dfrac{\epsilon\beta_3(1-\beta_4^2)}{\beta_4^2+1}\end{pmatrix}\begin{pmatrix}u-A_2\\ v-B_2\end{pmatrix},
\tag{11}
$$

where

$$
A_2=\frac{-2\beta_4^4-\beta_4^2+1}{2\epsilon\beta_3\beta_4^2(\beta_4^2-1)^2},\quad B_2=\frac{-\beta_4(\beta_4^2+1)}{2\epsilon\beta_3(\beta_4^2-1)^2},
$$

gives the following Jordan canonical form of systems (7):

$$\begin{aligned}\tilde{u}_t&=\tilde{v}_{xxx}+2(\tilde{u}\tilde{v})_x+\frac{2(\beta_4^2+1)}{\epsilon\beta_2\beta_4(\beta_4^2-1)^2}\tilde{v}\tilde{v}_x,\\ \tilde{v}_t&=2\tilde{v}\tilde{v}_x+\frac{2}{\beta_4}\tilde{v}_x+\frac{\epsilon\beta_2(\beta_4^2-1)^2}{\beta_4^2+1}\tilde{u}_x.\end{aligned}\tag{12}$$

In case (iii), i.e., for $\epsilon\neq 0$, $\beta_2\neq 0$, $\beta_3\neq 0$, $\beta_1=0$, $\beta_4=0$, systems (7) reduce to a system which is already in Jordan canonical form. A simple scaling of t brings it to the form which has $b(4)$ as its b_j^i matrix.

It is apparent and in accordance with the above proposal regarding the Jordan canonical forms that the coefficient matrix b_j^i of systems (10) and (12) are $b(3)$ and $b(4)$, respectively. By including the Jordan matrices into the classification algorithm at the beginning, we restrict ourselves to a convenient base for obtaining the results without any loss of generality. In our classification algorithm each of the matrices $b(i)$, $i=1,2,3,4$ in (6) cause a different set of solutions to the integrability conditions (4). We call a collection of systems obtained under a certain $b(i)$ matrix as a class and naturally identify each class with its $b(i)$ matrix.

IV. CLASSES

In the rest of our work, we present the found two-component nontrivial integrable systems and their associated recursion operators with a slight change $q^1=u$ and $q^2=v$ in notation.

A. Class $b(1)$

Although our main concern is the nonautonomous systems, solutions of integrability conditions (4) give rise to autonomous systems as well. In each class we first give the autonomous systems with their respective recursion operators. In the present class, there is only the following autonomous integrable system:

$$\begin{aligned}u_t&=u_{xxx}+c_1(2vu_x+uv_x),\\ v_t&=\tfrac{1}{4}v_{xxx}+2c_1vv_x,\end{aligned}\tag{13}$$

where c_1 is an arbitrary constant.[10] The recursion operator admitted by (13) is

$$\mathcal{R}=\begin{pmatrix} D^2+\frac{4}{3}c_1v & c_1u+\frac{2}{3}c_1u_xD^{-1}\\ 0 & \frac{1}{4}D^2+\frac{4}{3}c_1v+\frac{2}{3}c_1v_xD^{-1}\end{pmatrix}.$$

The only nonautonomous system in the present class is

$$\begin{aligned}u_t&=u_{xxx}+\frac{c_1}{\sqrt{t}}(2vu_x+uv_x),\\ v_t&=\frac{1}{4}v_{xxx}+\frac{2c_1}{\sqrt{t}}vv_x,\end{aligned}\tag{14}$$

where c_1 is an arbitrary constant. This system admits the following recursion operator:

$$\mathcal{R}=\begin{pmatrix} tD^2+\frac{1}{3}x+\frac{4}{3}c_1\sqrt{t}v & c_1\sqrt{t}u+\frac{2}{3}c_1\sqrt{t}u_xD^{-1} \\ 0 & \frac{1}{4}tD^2+\frac{1}{3}x+\frac{4}{3}c_1\sqrt{t}v+\frac{1}{3}(2c_1\sqrt{t}v_x+\frac{1}{2})D^{-1} \end{pmatrix}.$$

The above-mentioned systems (13) and (14) are the only nontrivial systems in $b(1)$ class. All other solutions of integrability conditions (4) with $b^i_j=b(1)$ are trivial.

Systems related by invertible transformations are considered equivalent.[13–16] Therefore, we analyzed all the found nonautonomous systems in regard to their transformability to autonomous systems through a certain class of transformations. In the next proposition we present the result relevant to the system (14).

Proposition 2: Nonautonomous system (14) is not transformable to any autonomous system by the invertible change of variables:

$$\begin{aligned} x&=\alpha(\tilde{t})\tilde{x}+\beta(\tilde{t}),\ t=\gamma(\tilde{t}),\\ u(x,t)&=\delta(\tilde{t})\tilde{u}(\tilde{x},\tilde{t})+\phi(\tilde{x},\tilde{t}),\\ v(x,t)&=\rho(\tilde{t})\tilde{v}(\tilde{x},\tilde{t})+\psi(\tilde{x},\tilde{t}). \end{aligned} \tag{15}$$

This proposition can be verified by explicitly transforming system (14) by transformations (15). After the transformation, requirement of the coefficients of new dependent variables to be constants leads to contradiction.

B. Class $b(2)$

In this class there is only the following nontrivial system as solution of integrability conditions (4):

$$\begin{aligned} u_t&=u_{xxx}+\lambda v_{xxx}+\frac{c_1}{\sqrt{t}}(uv)_x+\frac{\lambda c_1}{2\sqrt{t}}vv_x,\\ v_t&=v_{xxx}+\frac{c_1}{\sqrt{t}}vv_x, \end{aligned} \tag{16}$$

which is integrable for arbitrary constants c_1 and $\lambda\neq 0$ introduced in $b(2)$ of (6). This system admits the recursion operator $\mathcal{R}=\left(\begin{smallmatrix}\mathcal{R}^0_0 & \mathcal{R}^0_1\\ \mathcal{R}^1_0 & \mathcal{R}^1_1\end{smallmatrix}\right)$ with

$$\mathcal{R}^0_0=tD^2+\frac{1}{3}x+\frac{2}{3}c_1\sqrt{t}v+\frac{1}{3}(c_1\sqrt{t}v_x+\frac{1}{2})D^{-1},$$

$$\mathcal{R}^0_1=\lambda tD^2+\frac{2}{3}c_1\sqrt{t}u+\frac{1}{3}\lambda c_1\sqrt{t}v+\frac{1}{3}c_1\sqrt{t}\left(u_x+\frac{\lambda}{2}v_x\right)D^{-1},$$

$$\mathcal{R}^1_0=0,$$

$$\mathcal{R}^1_1=tD^2+\frac{1}{3}x+\frac{2}{3}c_1\sqrt{t}v+\frac{1}{3}(c_1\sqrt{t}v_x+\frac{1}{2})D^{-1}.$$

A straightforward calculation proves the following statement about system (16).

Proposition 3: System (16) is not transformable to any autonomous system by transformations (15).

C. Class $b(3)$

For $b_j^i = b(3)$ in (6), solutions of integrability conditions (4) give rise to the following list of autonomous systems and their associated recursion operators:

(i)

$$\begin{matrix} u_t = u_{xxx} + 3c_1 u u_x, \\ v_t = c_1 u v_x + c_2 v u_x, \end{matrix} \quad \mathcal{R} = \begin{pmatrix} D^2 + 2c_1 u + c_1 u_x D^{-1} & 0 \\ c_2 v + c_1 v_x D^{-1} & 0 \end{pmatrix}, \tag{17}$$

where c_1 and c_2 are arbitrary constants.[6,17]

(ii)

$$\begin{matrix} u_t = u_{xxx} + 3c_1 u u_x + c_2 v v_x, \\ v_t = c_1 (uv)_x, \end{matrix} \quad \mathcal{R} = \begin{pmatrix} D^2 + 2c_1 u + c_1 u_x D^{-1} & c_2 v \\ c_1 v + c_1 v_x D^{-1} & 0 \end{pmatrix}, \tag{18}$$

where c_1 and c_2 are arbitrary constants. For $c_1 \neq 0$ and $c_2 \neq 0$ this system is equivalent to the Ito system[18] through $u \to (2/c_1)\, u$, $v \to (2/\sqrt{c_1 c_2})\, v$. It is also possible to obtain the Ito system as $\beta_1 = -(\beta_4^2 + 1)/2\beta_4$ $(\beta_4 \neq 0)$, reduction of system (10). Therefore, Fokas–Liu system[7] includes the Ito system as a special case.

(iii)

$$\begin{matrix} u_t = u_{xxx} + 3c_1 u u_x, \\ v_t = (c_1 u + c_2 v) v_x, \end{matrix} \quad \mathcal{R} = \begin{pmatrix} D^2 + 2c_1 u + c_1 u_x D^{-1} & 0 \\ c_1 v_x D^{-1} & c_2 v \end{pmatrix}, \tag{19}$$

where c_1 and c_2 are arbitrary constants.[8]

The followings are the nonautonomous systems with their respective recursion operators in the $b(3)$ class.

(iv)

$$\begin{gathered} u_t = u_{xxx} + c_1 t^{-(\alpha + 2/3)} v v_x + c_2 t^{-(\alpha+1)} v, \\ v_t = t^{-2/3} v v_x, \end{gathered} \tag{20}$$

where c_1, c_2, and α are arbitrary constants. This system admits the recursion operator

$$\mathcal{R} = \begin{pmatrix} tD^2 + \dfrac{x}{3} + \alpha D^{-1} & t^{-\alpha}(c_1 t^{1/3} v + c_2 D^{-1}) \\ 0 & t^{1/3} v + \dfrac{x}{3} \end{pmatrix}. \tag{21}$$

(v)

$$\begin{gathered} u_t = u_{xxx} + e^{-\alpha t}(c_1 v v_x + c_2 v), \\ v_t = v v_x, \end{gathered} \tag{22}$$

where c_1, c_2, and α are arbitrary constants. The recursion operator is

$$\mathcal{R} = \begin{pmatrix} D^2 + \alpha D^{-1} & e^{-\alpha t}(c_1 v + c_2 D^{-1}) \\ 0 & v \end{pmatrix}. \tag{23}$$

(vi)

$$u_t = u_{xxx} + c_1 c_2 t^{-1/2} u u_x,$$
$$v_t = \tfrac{1}{3}(c_1 c_2 t^{-1/2} u v_x + c_1 t^{-2/3} v v_x + c_2 t^{-5/6} u), \tag{24}$$

where c_1 and c_2 are arbitrary constants. This system admits the recursion operator

$$\mathcal{R}_0^0 = tD^2 + \frac{x}{3} + \frac{2}{3} c_1 c_2 t^{1/2} u + \frac{1}{3}\left(c_1 c_2 t^{1/2} u_x + \frac{1}{2} \right) D^{-1},$$
$$\mathcal{R}_1^0 = 0,$$
$$\mathcal{R}_0^1 = \tfrac{1}{3} c_2 (c_1 t^{1/2} v_x + t^{1/6}) D^{-1}, \tag{25}$$
$$\mathcal{R}_1^1 = \tfrac{1}{3}(c_1 t^{1/3} v + x).$$

Solutions of integrability conditions (4) other than those giving the above list of systems are trivial. Therefore, the above list of systems is the complete list of nontrivial systems in the $b(1)$ class.

The following proposition is about the transformability of nonautonomous systems found in the present class.

Proposition 4: None of the nonautonomous systems (20), (22), and (24) is transformable to any autonomous system by transformations (15).

The $\alpha = 0$ special case of system (22) is the only exception. In this case system (22) is apparently autonomous. This proposition can be verified by direct calculation for each of the mentioned systems.

D. Class $b(4)$

Solutions of integrability conditions (4) with $b_j^i = b(4)$ in (6) give rise to the following list of nontrivial, integrable subclasses of systems:

(i)

$$u_t = v_{xxx} + v u_x + c_1 u v_x + s v v_x + y v,$$
$$v_t = v v_x, \tag{26}$$

where c_1 is an arbitrary constant, is integrable if the undetermined functions $s = s(t)$ and $y = y(t)$ satisfy the differential constraint

$$\frac{ds}{dt} + c_1 y = 0. \tag{27}$$

These systems admit the recursion operator

$$\mathcal{R} = \begin{pmatrix} \left(1 - \dfrac{c_1}{2}\right) v & D^2 + c_1 u + s v + \dfrac{c_1}{2} u_x D^{-1} \\ 0 & \left(1 - \dfrac{c_1}{2}\right) v + \dfrac{c_1}{2} v_x D^{-1} \end{pmatrix}. \tag{28}$$

(ii)

$$u_t = v_{xxx} + c_1(vu_x + 2uv_x) + svv_x + yv,$$
$$v_t = vv_x, \tag{29}$$

where c_1 is an arbitrary constant, is integrable if the undetermined functions $s=s(t)$ and $y=y(t)$ satisfy the differential constraint

$$\frac{ds}{dt} + (3c_1 - 1)y = 0. \tag{30}$$

The recursion operator is

$$\mathcal{R} = \begin{pmatrix} 0 & D^2 + 2c_1u + sv + c_1u_xD^{-1} \\ 0 & (1-c_1)v + c_1v_xD^{-1} \end{pmatrix}. \tag{31}$$

In this subclass we observed that the $c_1=1$ particular case of system (29) with (30) admits two recursion operators $\mathcal{R}(1)$ and $\mathcal{R}(2)$. The first one is (31) with $c_1=1$. The second recursion operator is

$$\mathcal{R}(2) = \begin{pmatrix} 0 & tD^2 + 2tu + tsv + (tu_x - \frac{1}{2}s)D^{-1} \\ 0 & (tv_x + 1)D^{-1} \end{pmatrix}. \tag{32}$$

(iii)

$$u_t = v_{xxx} + t^{-2/3}(vu_x + c_1vv_x) + yv,$$
$$v_t = t^{-2/3}vv_x, \tag{33}$$

where c_1 is an arbitrary constant, is integrable for any arbitrary function $y=y(t)$. The recursion operators of this system are

$$\mathcal{R}(1) = \begin{pmatrix} \frac{x}{3} + t^{1/3}v & tD^2 + c_1t^{1/3}v \\ 0 & \frac{x}{3} + t^{1/3}v \end{pmatrix}, \quad \mathcal{R}(2) = \begin{pmatrix} 0 & D^{-1} \\ 0 & 0 \end{pmatrix}. \tag{34}$$

The second operator $\mathcal{R}(2)$ is not a proper recursion operator because of its nilpotent character. Even though $\mathcal{R}(2)$ solely is not sufficient for integrability, any linear combination of it with $\mathcal{R}(1)$ is a recursion operator for system (33).

(iv)

$$u_t = v_{xxx} + t^{\alpha}\left(uv_x + \frac{\alpha+1}{3\alpha+2}vu_x + svv_x\right) + yv,$$
$$v_t = \frac{\alpha+1}{3\alpha+2}t^{\alpha}vv_x, \tag{35}$$

where $\alpha \neq -2/3$ is an arbitrary constant, is integrable if the undetermined functions $s=s(t)$ and $y=y(t)$ satisfy the differential constraint

$$\frac{ds}{dt} + y = 0. \tag{36}$$

These systems admit the recursion operator

$$\mathcal{R}_0^0=-\frac{\alpha}{2}\left(x+\frac{t^{\alpha+1}}{3\alpha+2}v\right),$$

$$\mathcal{R}_1^0=tD^2+t^{\alpha+1}u+t^{\alpha+1}sv+\tfrac{1}{2}[t^{\alpha+1}u_x-(3\alpha+2)s]D^{-1},$$

$$\mathcal{R}_0^1=0, \tag{37}$$

$$\mathcal{R}_1^1=-\frac{\alpha}{2}\left(x+\frac{t^{\alpha+1}}{3\alpha+2}v\right)+\frac{1}{2}[t^{\alpha+1}v_x+3\alpha+2]D^{-1}.$$

(v)

$$u_t=v_{xxx}+e^{t/\alpha}(vu_x+3uv_x+svv_x)+yv,$$

$$v_t=e^{t/\alpha}vv_x, \tag{38}$$

where $\alpha\neq 0$ is an arbitrary constant, is integrable if the undetermined functions $s=s(t)$ and $y=y(t)$ satisfy the differential constraint

$$\frac{\mathrm{d}s}{\mathrm{d}t}+3y=0. \tag{39}$$

The recursion operator is

$$\mathcal{R}_0^0=-\tfrac{1}{2}(x+\alpha e^{t/\alpha}v),$$

$$\mathcal{R}_1^0=\alpha\left[D^2+3e^{t/\alpha}u+e^{t/\alpha}sv+\frac{1}{2}\left(3e^{t/\alpha}u_x-\frac{1}{\alpha}s\right)D^{-1}\right],$$

$$\mathcal{R}_0^1=0, \tag{40}$$

$$\mathcal{R}_1^1=-\tfrac{1}{2}(x+\alpha e^{t/\alpha}v)+\tfrac{3}{2}(\alpha e^{t/\alpha}v_x+1)D^{-1}.$$

(vi)

$$u_t=v_{xxx}+(uv)_x+svv_x+yv,$$

$$v_t=vv_x, \tag{41}$$

is integrable for any arbitrary functions $s=s(t)$ and $y=y(t)$. These systems admit the recursion operators $\mathcal{R}(1)$, $\mathcal{R}(2)$, and $\mathcal{R}(3)$, where

$$\mathcal{R}(1)_0^0=-v_xD^{-1},$$

$$\mathcal{R}(1)_1^0=D^2+2u-2\left(\int y\,\mathrm{d}t\right)v+\left[u_x+\left(\int y\,\mathrm{d}t\right)v_x\right]D^{-1},$$

$$\mathcal{R}(1)_0^1=0, \tag{42}$$

$$\mathcal{R}(1)_1^1=v_xD^{-1},$$

$$\mathcal{R}(2)_0^0=-x-tv-2(tv_x+1)D^{-1},$$

$$\mathcal{R}(2)_1^0=2tu+2\left(\int (s-ty)\mathrm{d}t\right)v+\left[tu_x+\left(\int\left(s+2ty+3\int y\,\mathrm{d}t\right)\mathrm{d}t\right)v_x+3\int y\,\mathrm{d}t\right]D^{-1},$$

$$\mathcal{R}(2)_0^1=0,$$

$$\mathcal{R}(2)_1^1=-x-tv+(tv_x+1)D^{-1},$$

$$\mathcal{R}(3)=\begin{pmatrix}0 & x+tv\\ 0 & 0\end{pmatrix}. \tag{43}$$

(vii)

$$u_t=v_{xxx}+\frac{1}{\sqrt{t}}(uv)_x+svv_x+yv,$$

$$v_t=\frac{1}{\sqrt{t}}vv_x, \tag{44}$$

is integrable for any arbitrary functions $s=s(t)$ and $y=y(t)$. These systems admit the recursion operators $\mathcal{R}(1)$, $\mathcal{R}(2)$, and $\mathcal{R}(3)$ where

$$\mathcal{R}(1)_0^0=x+2\sqrt{t}v+(2\sqrt{t}v_x+1)D^{-1},$$

$$\mathcal{R}(1)_1^0=2tD^2-\left[\left(\int\left(2\sqrt{t}y+\frac{1}{\sqrt{t}}\int y\,\mathrm{d}t\right)\mathrm{d}t\right)v_x+\int y\,\mathrm{d}t\right]D^{-1},$$

$$\mathcal{R}(1)_0^1=0,$$

$$\mathcal{R}(1)_1^1=x+2\sqrt{t}v, \tag{45}$$

$$\mathcal{R}(2)_0^0=x+2\sqrt{t}v,$$

$$\mathcal{R}(2)_1^0=4tD^2+4\sqrt{t}u+2\left(\int(s-2\sqrt{t}y)\mathrm{d}t\right)v+\left[2\sqrt{t}u_x+\left(\int\left(s+\frac{1}{\sqrt{t}}\int y\,\mathrm{d}t\right)\mathrm{d}t\right)v_x+\int y\,\mathrm{d}t\right]D^{-1},$$

$$\mathcal{R}(2)_0^1=0,$$

$$\mathcal{R}(2)_1^1=x+2\sqrt{t}v+(2\sqrt{t}v_x+1)D^{-1},$$

$$\mathcal{R}(3)=\begin{pmatrix}0 & x+2\sqrt{t}v\\ 0 & 0\end{pmatrix}. \tag{46}$$

Solutions of integrability conditions (4) with $b_j^i=b(4)$ other than those giving the above list of systems are trivial.

We have the following proposition on the transformability of nonautonomous systems of the above subclasses found in the present class.

Proposition 5: None of the nonautonomous systems in each of the subclasses (26), (29), (33), (35), (38), (41) and (45) of class $b(4)$ *is transformable to any autonomous system by transformations (15).*

In the above subclasses, some choice of undetermined functions or arbitrary constants, like, for example, $y(t)=0$ in (30), can lead to autonomous systems. Such autonomous systems are out of the scope of Proposition 5.

It has been recently observed that some recursion operators, which are called weak, do not always generate symmetry hierarchies correctly.[22] Some of the operators we found in this work are of this type. The source of this weakness and possible solutions which relies on the found weak recursion operators are extensively investigated in Ref. 23.

We would like to remark that our classification is a partial classification which gives only systems (1) admitting recursion operator of form (2). As it is shown in a recent work,[24] even an autonomous coupled KdV system may admit a strange recursion operator which is not of form (2).

Systems whose recursion operators are bi-Hamilton factorizable, are of special interest from a physical point of view. Our knowledge on whether the recursion operators we obtained in this work are factorizable in this way is very limited at the moment. We have only some negative results about the bi-Hamilton factorizability of some of the found recursion operators up to the Hamilton operators, which are a multicomponent generalization of the Hamilton operators of the usual KdV equation.

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2-geometries and the Hamilton–Jacobi equation

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By using two different procedures we show that on the space of solutions of a certain class of second-order ordinary differential equations, $u''=\Lambda(s,u,u')$, a two-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the two-dimensional Hamilton–Jacobi equation, $g^{ab}u_{,a}u_{,b}=1$ holds. Furthermore, we show that this structure is invariant under a certain subset of contact transformations (canonical transformations). Two examples are given. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1639957]

I. INTRODUCTION

In the early years of the 20th century, while studying the structure and transformation properties of second- and third-order ordinary differential equations (ODEs), Lie, Tresse, Wünschmann,[1–4] among others, discovered that there was a rich differential geometry induced on the solution spaces of the differential equations. This work was greatly developed and generalized by Cartan and Chern[5–9] in the 1930s–1940s. Bryant,[10] in more recent years, studied the geometry associated with fourth-order ODEs. Tod[11] showed how third-order ODEs could generate three-dimensional Einstein–Weyl metrics.

With a totally different motivation and from a different point of view originating with general relativity, Frittelli, Kozameh and Newman, in a series of papers,[12–17] came to the same set of issues and problems. Rather than starting with given differential equations, the point of view of these authors began with three- and four-dimensional conformal Lorentzian manifolds, already containing a metric. They then studied families of complete solutions to the eikonal equation on these manifolds. From these solutions, by the elimination of the space–time coordinates, the differential equations of Cartan and Chern were reobtained. However, from this point of view, unwittingly, the Cartan/Chern work was generalized from ODEs to pairs of second-order partial differential equations (PDEs) whose solution spaces could be identified with any four-dimensional manifold with a conformal Lorentzian metric. In particular, they showed that the Einstein equations could be reformulated in terms of pairs of second-order PDEs.

Later, with Kamran and Nurowski,[18–22] this work was connected with the Cartan/Chern work for both the equivalence problem for differential equations under a variety of transformations and with the theory of Cartan normal conformal connections. With this consideration one saw how the differential equations (both the third-order equation and the pair of second-order equations) had to lie in a restricted class defined by the vanishing of the so-called Wünschmann (or generalized Wünschmann) equation.

An underlying unifying theme in many of the discussions was the existence of the eikonal

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equation and families of complete solutions. These solutions could be obtained either via the given third-order ODE or pair of second-order PDEs or alternatively from the solutions to the eikonal equation on the given conformal background space.

In the present work, we return to the geometry associated with a new class of second-order ODEs. The connecting link with the earlier work is that now we use the time-independent Hamilton–Jacobi equation rather than the eikonal equation to obtain this new class. We show (via two different procedures) that, in the solution spaces of the ODEs, either a two-dimensional Riemannian or Lorentzian metric can be constructed in a natural way. Furthermore all 2-metrics can be found by this procedure. The metric structure associated with each differential equation is preserved when the equation is transformed by a subset of contact transformations (namely canonical transformations).

In Sec. II we begin with a two-dimensional manifold, $\mathcal{M}$, with no further structure and then investigate arbitrary families of curves on $\mathcal{M}$ given by $u=\text{constant}=Z(x^a,s)$. (The x^a are local coordinates on $\mathcal{M}$ and s parametrizes the families and takes values on $\mathcal{S}^1$ or on $\mathcal{R}$.) More specifically, we ask when do such families of curves define a two-dimensional metric, $g_{ab}(x^a)$, such that

$$g^{ab}\nabla_a Z(x^a,s)\nabla_b Z(x^a,s)=1. \tag{1}$$

We will show that the $u=Z(x^a,s)$ must also satisfy a second-order ODE,

$$u''=\Lambda(u,u',s), \tag{2}$$

that lies in a special class of equations that we will refer to as ''Wünschmann-like,'' defined by the restriction of Λ to solutions of

$$\Lambda_{us}+\Lambda_{uu}u'+\Lambda_{uu'}\Lambda-2\Lambda_u\Lambda_{u'}=0. \tag{3}$$

The prime denotes ''s'' derivatives. Note that in the solutions $u=Z(x^a,s)$, the x^a are a pair of integration constants for Eq. (2) while the ''s'' is an integration constant for Eq. (1).

Before proceeding we make the following important remark:

Remark 1: The time independent Hamilton–Jacobi equation for a particle, with mass m and energy E, in a two-dimensional Riemannian space under the influence of a potential and the eikonal equation describing the evolution of the light rays in a two-dimensional isotropic optical medium characterized by its index of refraction, i.e., either of

$$g^{*ab}\nabla_a S(x^a,s)\nabla_b S(x^a,s)=E-V(x^a),$$

$$g^{*ab}\nabla_a S(x^a,s)\nabla_b S(x^a,s)=n(x^a),$$

can be rewritten in the form of Eq. (1) by dividing the equations by either $E-V(x^a)$ or by $n(x^a)$ and simultaneously rescaling the metric by the same factors.

This action has the effect of changing certain properties of solutions to the Hamilton–Jacobi (HJ) equation. Normally for the two-dimensional (HJ) equation a complete solution contains two constants of integration, where one of them is E. In our case, after the conformal rescaling, the E is hidden as a *fixed* constant in the metric g^{ab} and the solution will depend now on only one parameter, ''s.'' With an abuse of language, we will refer to $u=Z(x^a,s)$ as a ''restricted complete'' solution to the (HJ) equation. This change, in turn, leads to modifications in certain transformation properties of the solutions; contact transformations become canonical transformations. This issue is discussed in Sec. III.

In Sec. III we begin with a general second-order ODE (prime denotes s derivatives)

$$u''=\Lambda(s,u,u'), \tag{4}$$

whose solution space is parametrized by two independent constants of integration $x^a=(x^1,x^2)$. Then by studying the two-parameter family of curves in the (u,s) space defined as solutions to Eq. (2), namely,

$$u=Z(x^a,s), \tag{5}$$

and their generalized Jacobi fields, $(\delta u,\ \delta u')$ obtained by the independent variation of the two constants of integration x^a and one s derivative of Eq. (5) we show how a simple condition leads to the Wünschmann-like condition and the associated two-dimensional metric. In this section it is also remarked that this structure is invariant under a certain subclass of contact transformations. Finally, two particular examples are presented.

II. TWO-DIMENSIONAL METRICS AND THE WÜNSCHMANN-LIKE CONDITION

We begin with a two-dimensional manifold $\mathcal{M}$ (with local coordinates $x^a=(x^1,x^2)$) and assume we are given a one-parameter set of functions $u=Z(x^a,s)$, the parameter s can take values on $\mathcal{S}^1$ or on $\mathcal{R}$. We also assume that for a fixed value of the parameter s, the level curves

$$u=\text{const}=Z(x^a,s), \tag{6}$$

locally foliate the manifold $\mathcal{M}$ and that $u=Z(x^a,s)$ satisfies the (HJ) equation, Eq. (1),

$$g^{ab}\nabla_a Z(x^a,s)\nabla_b Z(x^a,s)=1, \tag{7}$$

for some unknown metric $g_{ab}(x^a)$.

Remark 2: The statement that for any fixed value of s, $u=Z(x^a,s)$ is a solution of Eq. (1), in the case of the eikonal equation, means that the level curves of u are wave fronts. That is, in this case we are looking for the conditions on the one-parameter family of functions u such that its associated level curves are the wave fronts associated with an optical metric (see Torres del Castillo[23] for a definition of the optical metric). In this case, it can be shown that in order to construct an arbitrary wave front in the two-dimensional isotropic optical medium, via the envelope construction, we require that $-\pi\leqslant s\leqslant\pi$.

The basic idea now is to solve Eq. (1) for the three components of the metric in terms of $\nabla_a Z(x^a,s)$. To do so, we will consider a number of parameter derivatives of the condition (1), and then by manipulation of these derivatives, obtain both the two-dimensional metric and the equation defining the curves and the conditions it must satisfy, which we will refer to as the Wünschmann-like condition.

Remark 3: The notation is as follows: there will be two types of differentiation, one is with respect to the local coordinates, x^a, of the manifold $\mathcal{M}$, denoted by ∇_a or "comma a," the other is with respect to the parameter s, denoted by a prime.

We first note that the one-parameter family of ''level'' curves, Eq. (6), can be obtained as solutions to the second-order ODE

$$u''=\Lambda(u,u',s). \tag{8}$$

It can be found by first calculating

$$u''(x^a,s)\equiv\Lambda^*(x^a,s). \tag{9}$$

Then by inverting the pair

$$u=Z(x^a,s),$$

$$u'=Z'(x^a,s)$$

obtaining

$$x^a = x^a(u,u',s) \tag{10}$$

the two x^a can be eliminated in Λ^* yielding Eq. (8).

Remark 4: Equation (10) can be thought of as an "s" dependent coordinate transformation between x^a and (u,u').

We define two parametrized scalars,

$$\theta^i = \{\theta^0, \theta^1\} \equiv \{u,u'\} = \{Z(x^a,s), Z'(x^a,s)\}, \tag{11}$$

which for each value of s forms a coordinate system intrinsically adapted to the curves.

From the two scalars, θ^i, we have their associated gradient basis $\theta^i{}_a$ given by

$$\theta^i{}_a = \nabla_a \theta^i = \{Z_{,a}, \partial Z_{,a}\}, \tag{12}$$

and its dual vector basis $\theta_i{}^a$, so that

$$\theta_i{}^a \theta^j{}_{,a} = \delta_i^j, \quad \theta_i{}^a \theta^i{}_{,b} = \delta_b{}^a. \tag{13}$$

Remark 5: The total s derivative of a function $F = F(s,u,u')$ is defined by

$$DF \equiv F_s + F_u u' + F_{u'} \Lambda. \tag{14}$$

It is easier to search for the components of the two-dimensional metric in the gradient basis rather than in the original coordinate basis. Furthermore, it is preferable to use the contravariant components rather than the covariant components of the metric; that is, we are interested in

$$g^{ij}(x^a,s) = g^{ab}(x^a)\, \theta^i{}_{,a}\, \theta^j{}_{,b}. \tag{15}$$

The metric components and the Wünschmann-like condition, for this case, are obtained by repeatedly operating with ∂_s on Eq. (7), that is on

$$g^{00} = g^{ab} Z_{,a} Z_{,b} = 1. \tag{16}$$

Applying ∂_s on Eq. (16) yields

$$\partial_s (g^{ab} Z_{,a} Z_{,b}) = 2 g^{ab} Z'_{,a} Z_{,b} = 2 g^{10} = 0, \tag{17}$$

where we have used that $\partial_s g^{ab} = 0$. Applying ∂_s on Eq. (17) we obtain, using Eq. (8),

$$g^{ab} (\Lambda_{,a} Z_{,b} + Z'_{,a} Z'_{,b}) = 0. \tag{18}$$

Since

$$\Lambda_{,a} = \Lambda_u Z_{,a} + \Lambda_{u'} Z'_{,a}, \tag{19}$$

then Eq. (18) is equivalent to

$$g^{11} = g^{ab} Z'_{,a} Z'_{,b} = -\Lambda_u.$$

Therefore, the final result is

$$(g^{ij}) = \begin{pmatrix} 1 & 0 \\ 0 & -\Lambda_u \end{pmatrix}. \tag{20}$$

Remark 6: Since $\det(g^{ij}) \neq 0$ *then* Λ_u *cannot be zero.*

Finally taking the ∂_s of Eq. (18), we obtain the Wünschmann-like condition, for $\Lambda(u,u',s)$; namely,

$$D\Lambda_u = 2\Lambda_u \Lambda_{u'}. \tag{21}$$

Since

$$D\Lambda_u = \Lambda_{us} + \Lambda_{uu} u' + \Lambda_{uu'} \Lambda, \tag{22}$$

then Eq. (21) is equivalent to

$$\Lambda_{us} + \Lambda_{uu} u' + \Lambda_{uu'} \Lambda - 2\Lambda_u \Lambda_{u'} = 0. \tag{23}$$

Summarizing: We have the result that given a second-order ODE, $u'' = \Lambda(u, u', s)$, where Λ satisfies Eq. (23), then in its space of solutions there exists a natural two-dimensional metric given by

$$g = g_{ab} \mathrm{d}x^a \, \mathrm{d}x^b = \left[Z_{,a} Z_{,b} - \left(\frac{1}{\Lambda_u} \right) \partial Z_{,a} \partial Z_{,b} \right] \mathrm{d}x^a \, \mathrm{d}x^b. \tag{24}$$

Furthermore, the solutions $u = Z(x^a, s)$ satisfy the (HJ) equation

$$g^{ab} \nabla_a Z(x^a, s) \nabla_b Z(x^a, s) = 1$$

with the just determined metric, Eq. (24). (See the examples to follow.)

III. AN ALTERNATIVE DERIVATION OF THE METRICS AND THE WÜNSCHMANN-LIKE CONDITION

We begin with the general second-order ODE

$$u'' = \Lambda(u, u', s) \tag{25}$$

and its two-parameter family of solution

$$u = Z(x^a, s). \tag{26}$$

We define the varied solution by

$$\delta u = Z_{,a}(x^a, s) \mathrm{d}x^a, \tag{27}$$

$$\delta u' = Z'_{,a}(x^a, s) \mathrm{d}x^a \tag{28}$$

which, in turn, satisfies the deviation equation [or linearized Eq. (25)]

$$\delta u'' = \delta\Lambda(u, u', s) \equiv \Lambda_u \delta u + \Lambda_{u'} \delta u'. \tag{29}$$

In the two-dimensional (u, s) space, for fixed x^a, Eqs. (27) and (28) define, via the two $\mathrm{d}x^a$, a two-parameter family of neighboring curves. Rather than treating the variation to be associated with the independent $\mathrm{d}x^a$, we will treat the two $(\delta u, \delta u')$ as independent variations (the s behavior is subjected to the deviation equation). On this two-dimensional space of independent curves we define an infinitesimal quadratic distance; that is a metric distance between nearby curves. At the beginning of the discussion this distance will depend on the value of s; that is, will depend on a point on the first curve for the comparison with the neighboring one. As conditions are imposed this distance is completely determined.

To begin with, we define a metric distance (the g_{AB} to be determined) between nearby curves, at the point s, by

$$g(x^a, s) = g_{AB} \delta u^A \delta u^B = g_{00} \delta u \, \delta u + 2 g_{01} \delta u \, \delta u' + g_{11} \delta u' \, \delta u'. \tag{30}$$

The following conditions are imposed on the metric:

(1) The first condition is that $g_{00}=1$.

Remark 7: Actually g_{00} can be taken as an arbitrary function of x^a, e.g., $E-V(x^a)$ or $n(x^a)$ which can then be used to conformally rescale the metric. (See Remark 1.)

(2) The second condition is that

$$Dg=0, \tag{31}$$

where D, the total "s" derivative, is defined by Eq. (14).

Remark 8: This is simply the condition that the metric distance between the two curves is independent of the point on the curves.

Theorem 1: *Given a second-order ODE [Eq. (25)] and its deviation equation, Eq. (29), if the metric defined by Eq. (30) with $g_{00}=1$ satisfies Eq. (31), then the metric is uniquely determined as a function of $\Lambda(u,u',s)$ when $\Lambda(u,u',s)$ satisfies the differential equation (the Wünschmann-like condition) given by Eq. (23).*

Proof: By directly applying the two conditions to Eq. (30), we obtain

$$g_{00}=1, \tag{32}$$

$$g_{01}=0,$$

$$g_{11}=-\left(\frac{1}{\Lambda_u}\right), \tag{33}$$

and

$$Dg_{11}=-2\Lambda_{u'}g_{11}. \tag{34}$$

From Eqs. (33) and (34), the Wünschmann-like condition, Eq. (23) immediately follows. Since $\delta u(x^a,s)=Z_{,a}\mathrm{d}x^a$ and $\delta u'(x^a,s)=Z'_{,a}\mathrm{d}x^a$, then by using Eqs. (32)–(34), we find that the metric Eq. (30) can be written as

$$g(x^a,s)=\left[Z_{,a}Z_{,b}-\frac{1}{\Lambda_u}Z'_{,a}Z'_{,b}\right]\mathrm{d}x^a\,\mathrm{d}x^b. \tag{35}$$

That is, we have obtained Eq. (24) by another procedure. Observe that the condition $g_{00}=1$ is equivalent to Eq. (1).

In some of the earlier mentioned work on the eikonal equation in three- and four-dimensional Lorentzian spaces, it was proved that the conformal Lorentzian metrics associated with third-order ODEs and pairs of second-order PDEs satisfying the Wünschmann condition and generalized Wünschmann condition is preserved when the differential equation is transformed by a contact transformation. For our case, there is an analogous result given by the following:

Theorem 2: *Let Eq. (25) be a second-order ODE, with Λ satisfying condition (23) and let*

$$\overline{u''}=\overline{\Lambda}(\overline{u},\overline{u'},\overline{s}) \tag{36}$$

be a second-order ODE locally equivalent to Eq. (25) under the subset of contact transformations generated by the generating function

$$H(s,u,\overline{s},\overline{u})=\overline{u}-u-G(s,\overline{s}). \tag{37}$$

Then under this subset of contact transformations the metric (30) is preserved.

The proof is exactly as that presented in Ref. 18 for the third-order ODE case. Here we only justify the form of the generating function (37). To this end, we review the definition of a general contact transformation.

Theorem 3: *Every contact transformation which is not a prolonged point transformation is determined in terms of a generating function* $H(s,u,\overline{s},\overline{u})$ *by solving the following three implicit equations for* $\overline{s}$, $\overline{u}$, $\overline{u}'$:

$$H(s,u,\overline{s},\overline{u})=0, \quad H_s+u'H_u=0, \quad H_{\overline{s}}+\overline{u}'H_{\overline{u}}=0. \tag{38}$$

The generating function $H(s,u,\overline{s},\overline{u})$ *is an arbitrary smooth function, subject only to the solubility of Eq. (38) for* $\overline{s}$, $\overline{u}$, $\overline{u}'$.

For a proof of this theorem see, for example, Olver.[24]

Without loss of generality one can take

$$H=\overline{u}-\overline{V}(u,s,\overline{s}), \tag{39}$$

so that the contact transformation has the form

$$\begin{aligned}\overline{u}&=\overline{V}(u,s,I(s,u,u')),\\ \overline{s}&=I(s,u,u'),\\ \overline{u}'&=\overline{V}_{\overline{s}}(u,s,I(s,u,u')),\end{aligned} \tag{40}$$

where $I(s,u,u')$ is obtained by solving

$$\overline{V}_s+u'\overline{V}_u=0, \tag{41}$$

for $\overline{s}$ in terms of s, u and u'.

As we pointed out earlier, for each value of s, the two-parameter family of solutions

$$u=Z(x^a,s) \tag{42}$$

of (25) is also a one-parameter family of solutions of Eq. (1), i.e., are ''restricted complete'' integrals of Eq. (1). We now invoke the envelope construction (slightly changed by our modification of the complete integral) to take one ''restricted complete'' integral of Eq. (1) into another such solution.

Consider the function $\overline{u}=\overline{Z}(x^a,\overline{s})$ defined by

$$\overline{u}=\overline{V}(u,s,\overline{s}), \tag{43}$$

where u is defined by Eq. (42) and s is defined implicitly as a function of x^a and $\overline{s}$ by the envelope condition[18,25]

$$\overline{V}_u u'+\overline{V}_s=0. \tag{44}$$

Note that although (44) has the same form as (41), it involves the variables x^a and s. Using both Eqs. (43) and (44), we have that

$$\overline{u}_{,a}=\overline{V}_u u_{,a}\,. \tag{45}$$

By direct substitution of $\overline{u}_{,a}$ into the (HJ) equation, Eq. (1), we see that it is a new ''restricted complete'' integral if and only if $\overline{V}_u^2=1$. That is, $\overline{u}=\overline{V}(u,s,\overline{s})$ has the form $\overline{u}=\pm u+G(s,\overline{s})$. For simplicity, taking the positive sign, we have that if $u(x^a,s)$ is a ''restricted complete'' integral of Eq. (1) then

$$\overline{u}=u+G(s,\overline{s}), \tag{46}$$

where s is defined implicitly as a function of x^a and $\bar{s}$ by the envelope condition

$$u' + G_s = 0, \tag{47}$$

which is a new "restricted complete" integral of Eq. (1). Equations (46) and (47) define a particular subset of the contact transformations given by contact transformations

$$\bar{u} = u + G(s, \bar{s}), \tag{48}$$

$$u' = -G_s, \tag{49}$$

$$\bar{u}' = G_{\bar{s}}. \tag{50}$$

The generating function for this set of contact transformation is given by

$$H(s, u, \bar{s}, \bar{u}) = \bar{u} - u - G(s, \bar{s}) = 0. \tag{51}$$

Remark 9: The transformations Eqs. (48), (49), and (50) have a rather strange or perhaps unconventional interpretation as a canonical transformation. If we have a two-dimensional phase space (q,p) *and a canonical transformation to* (P,Q) *given by*

$$p = \partial_q G,$$

$$P = -\partial_Q G,$$

with generating function $G(q,Q)$*, we see that this is identical to Eqs. (49) and (50) if we identify* $(q,Q) \Leftrightarrow (s,\bar{s})$ and $(p,P) \Leftrightarrow (u', \bar{u}')$ *and ignore the* $u \Leftrightarrow \bar{u}$ *transformation.*

IV. TWO EXAMPLES

Observe that the trivial solutions to Eq. (23) under the condition that $\Lambda_u \neq 0$ are: $\Lambda = \pm u$. Here we discuss these two cases.

(a) *The case* $\Lambda = -u$. From Eq. (25) we obtain that u is such that

$$u'' + u = 0. \tag{52}$$

That is, $u(x^a, s)$, satisfies the harmonic oscillator equation with unit frequency. The general solution to Eq. (52) is given by

$$u = Z(x^a, s) = x^a l_a \equiv x \cos s + y \sin s, \tag{53}$$

where $-\pi \leqslant s \leqslant \pi$, $l_a = (\cos s, \sin s)$ and $x^a = (x,y)$ are two constants of integration, which define locally the space of solutions of Eq. (52). From Eq. (53), we have

$$u' = Z'(x^a, s) = x^a m_a \equiv -x \sin s + y \cos s. \tag{54}$$

That is, $m_a = (-\sin s, \cos s)$. We thus obtain that for this case

$$\begin{aligned} \theta^0{}_{,a} &= Z_{,a} = l_a, \\ \theta^1{}_{,a} &= Z'_{,a} = m_a. \end{aligned} \tag{55}$$

From Eq. (24) and the definitions of l_a and m_b, we find that the two-dimensional metric living on the space of solutions of Eq. (52) is given by

$$g = g_{ab} \mathrm{d}x^a \, \mathrm{d}x^b = (l_a l_b + m_a m_b) \mathrm{d}x^a \, \mathrm{d}x^b = \mathrm{d}x^2 + \mathrm{d}y^2, \tag{56}$$

i.e., the two-dimensional Euclidean metric. In this case the eikonal equation reduces to

$$Z_{,x}^{2}+Z_{,y}^{2}=1. \tag{57}$$

From theorem 2, we know that there is a large family of second-order ODEs such that their solutions also yield two-dimensional Euclidean metrics on the solution space. The entire family is connected by a contact transformation given by the generating function (51), with u given by Eq. (53). We give a particular example, obtained with

$$G(s,\overline{s})=\overline{s}(\cos s+\sin s).$$

After a straightforward calculation one obtains the new solution

$$\overline{u}^{2}=(x+\overline{s})^{2}+(y+\overline{s})^{2} \tag{58}$$

and the new second-order ODE

$$\overline{u}''=\overline{\Lambda}(\overline{s},\overline{u},\overline{u}')=\left(\frac{2-(\overline{u}')^{2}}{\overline{u}}\right). \tag{59}$$

A direct computation shows that, $\overline{u}$, given by Eq. (58), is a new family of solutions of the (HJ) equation (57). The explicit contact transformations yielding these results are

$$\overline{u}=u+u'\left(\frac{\cos s+\sin s}{\sin s-\cos s}\right),\quad \overline{s}=\left(\frac{u'}{\sin s-\cos s}\right),\quad \overline{u}'=\cos s+\sin s. \tag{60}$$

(b) The case $\Lambda=u$. In this case, our ODE, Eq. (25) is

$$u''-u=0, \tag{61}$$

with general solution

$$u=Z(x^{a},s)=x^{a}\tilde{l}_{a}\equiv x\cosh s+y\sinh s, \tag{62}$$

where $s\in\mathcal{R}$, $\tilde{l}_{a}=(\cosh s,\sinh s)$ and $x^{a}=(x,y)$ are two constants of integration defining the space of solutions. By differentiating, we have

$$u'=Z'(x^{a},s)=x^{a}\tilde{m}_{a}\equiv x\sinh s+y\cosh s, \tag{63}$$

with $\tilde{m}_{a}=(\sinh s,\cosh s)$. From Eq. (12) we see that

$$\begin{aligned}\theta^{0}{}_{,a}&=Z_{,a}=\tilde{l}_{a},\\ \theta^{1}{}_{,a}&=Z'_{,a}=\tilde{m}_{a},\end{aligned} \tag{64}$$

and the two-dimensional metric living on the solution space is given by

$$g=g_{ab}\mathrm{d}x^{a}\,\mathrm{d}x^{b}=(\tilde{l}_{a}\tilde{l}_{b}-\tilde{m}_{a}\tilde{m}_{b})\mathrm{d}x^{a}\,\mathrm{d}x^{b}=\mathrm{d}x^{2}-\mathrm{d}y^{2}, \tag{65}$$

i.e., the two-dimensional Minkowski metric. Equation (1) reduces to

$$u_{,x}^{2}-u_{,y}^{2}=1. \tag{66}$$

As in the previous example, there is a further family of second-order ODEs producing two-dimensional Lorentzian metrics on their solution spaces obtained by the special contact transformations. A particular example, obtained when

$$G(s,\overline{s})=\overline{s}(\cosh s+\sinh s),$$

is

$$\overline{u}^2=(x+\overline{s})^2-(y+\overline{s})^2, \tag{67}$$

which satisfies the ODE

$$\overline{u}''=\overline{\Lambda}(\overline{s},\overline{u},\overline{u}')=-\left(\frac{(\overline{u}')^2}{\overline{u}}\right). \tag{68}$$

The contact transformation is explicitly given by

$$\overline{u}=u-u',\quad \overline{s}=-\left(\frac{u'}{\sinh s+\cosh s}\right),\quad \overline{u}'=\sinh s+\cosh s. \tag{69}$$

V. CONCLUSIONS

In this work, we have shown that the ideas and procedures developed earlier that related certain ODEs and PDEs to the eikonal equation and conformal metrics on their solution spaces can be generalized to the Hamilton–Jacobi equation. In the earlier treatment of the eikonal equation we had complete solutions of the equation which led to ODEs and sets of PDEs. These, in turn, led to the transformation groups, connecting the ODEs and PDEs, being the contact group. Here the ''restricted complete'' solutions yielded a special class (Wünschmann-like) of ODEs and, in addition, limited the allowed transformations to a restricted set of contact transformations.

We point out that, though we have used, in the present work, only the two-dimensional, time independent HJ equation, this can be generalized. In a future paper we will present the results for the three-dimensional HJ equation.

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Analogies between colored Lévy noise and random channel approach to disordered kinetics

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We point out some interesting analogies between colored Lévy noise and the random channel approach to disordered kinetics. These analogies are due to the fact that the probability density of the Lévy noise source plays a similar role as the probability density of rate coefficients in disordered kinetics. Although the equations for the two approaches are not identical, the analogies can be used for deriving new, useful results for both problems. The random channel approach makes it possible to generalize the fractional Uhlenbeck–Ornstein processes (FUO) for space- and time-dependent colored noise. We describe the properties of colored noise in terms of characteristic functionals, which are evaluated by using a generalization of Huber's approach to complex relaxation [Phys. Rev. B **31**, 6070 (1985)]. We start out by investigating the properties of symmetrical white noise and then define the Lévy colored noise in terms of a Langevin equation with a Lévy white noise source. We derive exact analytical expressions for the various characteristic functionals, which characterize the noise, and a functional fractional Fokker–Planck equation for the probability density functional of the noise at a given moment in time. Second, by making an analogy between the theory of colored noise and the random channel approach to disordered kinetics, we derive fractional equations for the evolution of the probability densities of the random rate coefficients in disordered kinetics. These equations serve as a basis for developing methods for the evaluation of the statistical properties of the random rate coefficients from experimental data. Special attention is paid to the analysis of systems for which the observed kinetic curves can be described by linear or nonlinear stretched exponential kinetics.
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I. INTRODUCTION

In this article we show that there are some useful analogies between the theory of colored Lévy noise and the random channel approach for rate processes in disordered systems. Even though the evolution equations for the two problems are different, they share some common features, which may be used for deriving new results in both fields. We show that the theory of colored Lévy noise can be formulated in a simple way by applying the random channel approach from disordered kinetics; moreover, it is possible to introduce a more complex type of Lévy noise, which is both space and time dependent. Conversely, by analogy with the theory of colored Lévy

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noise, it is possible to derive equations for the probability density of rate coefficients in disordered kinetics. These equations serve as a basis for proposing methods for extracting statistical informations about the fluctuations of the rate coefficients from experimental data.

The study of Lévy stochastic processes is a major subject of topical interest in statistical physics; its development is of importance in connection with a broad class of phenomena from physics, chemistry and biology and even economics. Examples include the dispersive transport in solid-state physics,[1] the study of vortex motion in high-temperature superconductors, moving interfaces in porous media, random field magnets, spin glasses, the propagation of electromagnetic or acoustic waves in random media,[2–4] random phase modulation in spectroscopy,[5] reaction kinetics in disordered systems,[6,7] the structure of biological organs,[8] the growth of a population in a random environment,[9] and the fluctuation of prices in the stock market.[10]

For the study of these types of processes most classical approaches cannot be used, due to the presence of the diverging moments of the Lévy distribution; new theoretical methods are needed, such as the development of path integrals for Lévy-type stochastic processes.[11] The study of Lévy stochastic processes is an active area of research. In this context the fractional Uhlenbeck–Ornstein processes (FUO), with a long history, play an important role. A first stochastic process of this type was introduced in 1942 by Doob[12] by starting out from the classical Uhlenbeck–Ornstein (CUO) process[13] and by replacing the standard Wiener noise by a (symmetric) Lévy stable noise. In 1982 West and Shesadri studied a harmonic oscillator with a fluctuating Lévy noise source.[14] In 2000 Garbaczewski and Olkiewicz[15] introduced an Ornstein–Uhlenbeck–Cauchy process, where the noise source obeys a probability law of the Cauchy (Lorentz) type.

A second type of fractal generalization of the Uhlenbeck–Ornstein process is based on the use of fractional evolution equations. Metzler, Barkai, and Klafter introduced a fractional Fokker–Planck equation describing the stochastic evolution of a particle under the combined influence of an external, nonlinear force and a thermal heat bath.[16] It seems plausible that there is a connection between their Fokker–Planck equation and a fractional generalization of the Uhlenbeck–Ornstein process. This type of connection is apparent in other studies of Lévy diffusion in external force fields, which make use both of Langevin equations with Lévy noise sources and fractional evolution equations.[17,18]

A third type of FUO was introduced by Koyama and Hara[19] in connection with earthquake dynamics. They started out from an overdamped harmonic oscillatior with a random noise source and applied a succession of renormalization processes of the type introduced by Shlesinger, Hughes, Montroll, and West[8,20,21] in stochastic dynamics. The result is a FUO process characterized by temporal correlation functions with long tails, which seems to have different properties from the first two types mentioned above.

The relaxation and reaction processes occurring in disordered systems have been studied both from the experimental and theoretical points of view.[6,7,22–28] In this field most papers focus on the experimental and theoretical study of processes with linear kinetics described by stretched exponential survival functions. There are also some attempts of extending this research to the case of nonlinear processes.[24] Many theoretical developments are based on the idea that the rate coefficients are random variables, which are the result of the additive contribution of a random number of reaction channels which obey certain probability laws. This idea was introduced in 1948 in a seminal paper by Foerster[25] dealing with the extinction of fluorescence in spectroscopical experiments. The description of the fluctuations of rate coefficients in terms of the contribution of a random number of reaction channels is referred to the as random channel approach (RCA). Various developments of the RCA for linear kinetics have been reported.[6,22–24,26] In this paper we are especially interested in the RCA approach suggested by Huber[22] in 1985 and in an alternative approach for systems with dynamic disorder developed by Allinger and Blumen.[26] Recently it has been shown that Huber's theory is exact for a Poissonian distribution of independent channels.[23] Moreover, this equation also holds beyond the range of validity of the Poissonian distribution: it emerges as a universal scaling law for a uniform random distribution of reaction channels characterized by nonintermittent fluctuations.[23] These universal scaling laws have been extended to systems with dynamical disorder.[23] A major problem in disordered kinetics is the evaluation of the

statistical properties of rate coefficients from experimental data. The field of chemical kinetics dealing with this problem is referred to as "spectral kinetic analysis."[29] Though this field is in an early stage of development, a few methods of spectral kinetic analysis are available.

In this article we aim to bridge the gap between these two area of research. The structure of the article is the following. In Secs. II–IV we show that with suitable changes Huber's approach to RCA in disordered kinetics can be used for describing white and colored Lévy noise. We study space- and time-dependent colored Lévy noise and introduce a space-dependent generalization of the fractional Uhlenbeck–Ornstein processes. In Sec. V we use the analogies between the random-channel approach to disordered kinetics and the theory of Lévy colored noise, by deriving equations for the probability densities of the random rate coefficients. In Sec. VI we use these equations for deriving methods of evaluation of the statistical properties of rate coefficients from experimental data.

II. HUBER STOCHASTIC PROCESSES AND LÉVY NOISE

In this section we make a connection between Huber stochastic processes and Lévy noise and extend the theory of Gaussian colored noise to the more complicated case of Lévy fluctuations. The Gaussian colored noise is assumed to be generated by the exponential damping of a random variable subject to the action of Gaussian white noise.[30] Consider a scalar noise source $F(\mathbf{r},t)$ at position $\mathbf{r}$ and time t: the properties of colored noise can be described by the Langevin equation

$$\frac{\partial F(\mathbf{r},t)}{\partial t}=\mathbb{L}F(\mathbf{r},t)+\omega F_0(\mathbf{r},t), \tag{1}$$

where $\mathbb{L}$ is a time-independent, but generally space-dependent, linear transport operator, ω is a characteristic frequency, and $F_0(\mathbf{r},t)$ is a Gaussian noise source with an average value equal to zero and with delta correlated cumulants of the second order:

$$\langle F_0(\mathbf{r},t)\rangle=0, \quad \langle\langle F_0(\mathbf{r}_1,t_1)F_0(\mathbf{r}_2,t_2)\rangle\rangle=A\,\delta(t_1-t_2)\,\delta(\mathbf{r}_1-\mathbf{r}_2). \tag{2}$$

A suitable choice for the transport operator is

$$\mathbb{L}\ldots=-\omega+\cdots+\omega\lambda^2\nabla_r^2+\cdots, \tag{3}$$

where λ is a characteristic diffusion length.

The classical analysis of the colored Gaussian noise characterized by Eqs. (1)–(3) is usually done by performing a Fourier analysis of the moments and the cumulants of the noise source $F(\mathbf{r},t)$. This method cannot be extended to the Lévy noise, because in this case the moments and cumulants of $F(\mathbf{r},t)$ diverge. To overcome this difficulty we generalize a method recently used by us[18] for the analysis of one-dimensional Lévy diffusion in a force field. We focus our efforts on the evaluation of characteristic functionals of the noise which can be evaluated even if the moments and cumulants are divergent. Such an approach is useful because many experimental observables can be evaluated if the characteristic functional is known. Our analysis proceeds in two steps. We first consider the noise source $F_0(\mathbf{r},t)$ to establish a suitable physical model for Lévy white noise and evaluate the characteristic functionals, which describe its stochastic properties. The next step is to study the colored Lévy noise as characterized by the Langevin equation (1) where the fluctuation of the random force $F_0(\mathbf{r},t)$ is described by Lévy white noise.

The fluctuations of the random force $F_0(\mathbf{r},t)$ are described by using a generalized Huber approach.[22,23] The random force $F_0(\mathbf{r},t)$ is made up of the additive contribution of a large number N of individual components $g_m(\mathbf{r},t)$, each of which is a random function corresponding to a given relaxation channel

$$F_0(\mathbf{r},t)=\sum_{m=1}^{N} g_m(\mathbf{r},t). \tag{4}$$

This physical model of white Lévy noise is essentially a model of Brownian motion for which the contribution of an individual event (a collision) to the random force is a stochastic function, which obeys fractal statistics. The statistics of individual events can be conveniently expressed in terms of Huber's theory of complex relaxation.[22] In this context we formally attach a channel to each individual (collision) event. Both the number N of channels and the contributions $g_1(\mathbf{r},t),\ldots,g_N(\mathbf{r},t)$ of the different channels are random; their stochastic properties can be described by a Poissonian random point process characterized by a density of channels which obeys a scaling law of the negative power law type. The space–time characteristic functional of white noise can be expressed as a dynamic average

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\left\langle \exp\left\{ i\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\mathcal{K}(\mathbf{r}',t')\sum_{m=1}^{N} g_m(\mathbf{r}',t')d\mathbf{r}'\,dt'\right\}\right\rangle. \tag{5}$$

where $\mathcal{K}(\mathbf{r}',t')$ is a suitable test function attached to the random force $F_0(\mathbf{r},t)$ and the dynamic average $\langle\cdots\rangle$ is taken over all possible values of the number N of channels and over all possible values of the random functions $g_1(\mathbf{r}',t'),\ldots,g_N(\mathbf{r}',t')$. The detailed computation of the average in Eq. (5) is presented in Sec. III.

The second step of our analysis consists in expressing the random force $F(\mathbf{r},t)$ of the colored noise as a functional of the noise source of the white noise $F_0(\mathbf{r},t)$ and in evaluating the characteristic functional of the colored noise

$$\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\left\langle \exp\left\{ i\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\mathcal{K}(\mathbf{r}',t')F(\mathbf{r}',t')d\mathbf{r}'\,dt'\right\}\right\rangle, \tag{6}$$

in terms of the characteristic functional $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ of the white noise. The computations are presented in Sec. IV.

III. TIME- AND SPACE-DEPENDENT LÉVY WHITE NOISE

The dynamic average in Eq. (5) can be expressed by using two different sets of probability density functionals, either in terms of the probability density functional attached to the components $g_1(\mathbf{r}',t'),\ldots,g_N(\mathbf{r}',t')$ or of the probability density functional of the random force $F_0(\mathbf{r},t)$, respectively. The stochastic properties of the number N of channels and of the components $g_1(\mathbf{r}',t'),\ldots,g_N(\mathbf{r}',t')$ attached to the different channels can be expressed in terms of a set of grand canonical probability density functionals

$$Q_0,Q_N[g_1(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)]\mathcal{D}[g_1(\mathbf{r};t)]\cdots\mathcal{D}[g_N(\mathbf{r};t)],\quad N=1,2,..., \tag{7}$$

which obey a normalization condition which includes an $1/N!$ Gibbs factor

$$Q_0+\sum_{N=1}^{\infty}\frac{1}{N!}\overline{\int\int}\cdots\overline{\int\int}\,Q_N[g_1(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)]\mathcal{D}[g_1(\mathbf{r};t)]\cdots\mathcal{D}[g_N(\mathbf{r};t)]=1. \tag{8}$$

Here $\mathcal{D}[g_1(\mathbf{r};t)],\ldots,\mathcal{D}[g_M(\mathbf{r};t)]$ are suitable integration measures over the space of functions $g_1(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)$ and $\overline{\int\int}$ stands for the operation of path integration. Similarly, the stochastic properties of the total random force $F_0(\mathbf{r},t)$ attached to the Lévy white noise can be expressed in terms of the probability density functional:

$$\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\ \text{ with }\ \overline{\int\int}_{\mathbf{r},t}\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]=1. \tag{9}$$

In this article we assume that the different channels are independent and thus the grand canonical probability density functionals (6) obey Poissonian statistics:

$$Q_0=\exp\left\{-\overline{\int\int}\rho_g[g(\mathbf{r}';t')]\mathcal{D}[g(\mathbf{r}';t')]\right\}, \tag{10}$$

$$Q_N[g_1(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)]\mathcal{D}[g_1(\mathbf{r};t)]\cdots\mathcal{D}[g_N(\mathbf{r};t)]$$
$$=\exp\left\{-\overline{\int\int}\rho_g[g(\mathbf{r}';t')]\mathcal{D}[g(\mathbf{r}';t')]\right\}\rho_g[g_1(\mathbf{r};t)]\mathcal{D}[g_1(\mathbf{r};t)]\cdots\rho_g[g_N(\mathbf{r};t)]\mathcal{D}[g_N(\mathbf{r};t)]. \tag{11}$$

For Lévy white noise the functional average density of states $\rho_g[g(\mathbf{r};t)]\mathcal{D}[g(\mathbf{r};t)]$ obeys a scaling condition of the negative power law type. By generalizing the approach from Ref. 23 for space-dependent systems we can give the following discrete representation for $\rho_g[g(\mathbf{r};t)]\mathcal{D}[g(\mathbf{r};t)]$:

$$\rho_g(g;\Delta\mathbf{r},\Delta t)dg=\kappa_0(\alpha)(\Delta t\Delta\mathbf{r})^{(1-\alpha)}|g|^{-(1+\alpha)}dg,\quad \Delta\mathbf{r}=\prod_{=1}^{m}\Delta r,\ \ \kappa_0(\alpha)>0,\ \ 2>\alpha>0, \tag{12}$$

and

$$g_n^{(u,\mathbf{v})}=g_n(t_0+u\Delta t,r_1+v_1\Delta r_1,\ldots,r_m+v_m\Delta r_m),\quad n=1,...,N, \tag{13}$$

where m is the space dimension, $\kappa_0>0$ is a positive proportionality factor, u,v are current labels, and $2>\alpha>0$ is a dimensionless fractal exponent. By using this discrete representation we can formally express the Poissonian grand canonical probability density functionals $Q_0,\ldots,Q_N[g_t(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)]\mathcal{D}[g_t(\mathbf{r};t)]\cdots\mathcal{D}[g_N(\mathbf{r};t)],\ldots,$ (10) and (11) with the following limits:

$$Q_0=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\prod_{u,\mathbf{v}}\left[\exp\left(-\int_{-\infty}^{+\infty}\rho_g(g^{(u,\mathbf{v})};\Delta\mathbf{r},\Delta t)dg^{(u,\mathbf{v})}\right)\right], \tag{14}$$

$$Q_N[g_1(\mathbf{r};t),\ldots,g_N(\mathbf{r};t)]\mathcal{D}[g_1(\mathbf{r};t)]\cdots\mathcal{D}[g_N(\mathbf{r};t)]$$
$$=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\left\{\prod_{u,\mathbf{v}}\left[\exp\left(-\int_{-\infty}^{+\infty}\rho_g(g^{(u,\mathbf{v})};\Delta\mathbf{r},\Delta t)dg^{(u,\mathbf{v})}\right)\prod_{w=1}^{N}\rho_g(g_w^{(u,\mathbf{v})})dg_w^{(u,\mathbf{v})}\right]\right\}. \tag{15}$$

By using the discrete representation (14) and (15) the ensemble average in Eq. (5) can be easily evaluated. After some calculations we come to a closed expression for the characteristic functional $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ of Lévy white noise

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\left\langle\prod_{w=1}^{N}\prod_{u,\mathbf{v}}\exp\{i\mathcal{K}^{(u,\mathbf{v})}g_w^{(u,\mathbf{v})}\Delta\mathbf{r}\Delta t\}\right\rangle$$
$$=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\prod_{u,\mathbf{v}}\exp\left(-\int_{-\infty}^{+\infty}\rho_g(g^{(u,\mathbf{v})};\Delta\mathbf{r},\Delta t)dg^{(u,\mathbf{v})}\right)$$
$$\times\sum_{N}\frac{1}{N!}\left[\prod_{w=1}^{N}\int_{-\infty}^{+\infty}\exp\{i,\mathcal{K}^{(u,\mathbf{v})}g_w^{(u,\mathbf{v})}\Delta\mathbf{r}\Delta t\}\rho_g(g_w^{(u,\mathbf{v})})dg_w^{(u,\mathbf{v})}\right]$$
$$=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\prod_{u,\mathbf{v}}\exp\left(-\kappa_0(\Delta t\Delta\mathbf{r})^{-(1-\alpha)}2\int_0^{+\infty}|g|^{-(1+\alpha)}\right.$$

$$\times(1-\cos\{\mathcal{K}^{(u,\mathbf{v})}g\Delta t\Delta\mathbf{r}\})dg\Bigg)$$

$$=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\prod_{u,\mathbf{v}}\exp\left(-\kappa_0(\Delta t\Delta\mathbf{r})^{1-\alpha}2\frac{\Gamma(1-\alpha)}{\alpha}|\mathcal{K}^{(u,\mathbf{v})}\Delta t\Delta\mathbf{r}|^{\alpha}\cos\left(\frac{\pi\alpha}{2}\right)\right). \tag{16}$$

By passing to the continuous limit in Eq. (16) we have

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\exp\left(-c\int_{-\infty}^{+\infty}\cdots\int\int_{-\infty}^{+\infty}|\mathcal{K}(\mathbf{r}',t')|^{\alpha}\,d\mathbf{r}'\,dt'\right), \tag{17}$$

where

$$c=2\kappa_0(\alpha)\frac{\Gamma(1-\alpha)}{\alpha}\cos\left(\frac{\pi\alpha}{2}\right), \tag{18}$$

and $\Gamma(x)$ is the complete gamma function. Equation (17) is the main result of this section. The characteristic functional $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ expresses all stochastic properties of Lévy white noise. By evaluating the functional derivatives of $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ and $\ln\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ with respect to the test function $\mathcal{K}(\mathbf{r}',t')$ we can check that for $2>\alpha>0$ all positive moments as well as all cumulants attached to the Lévy white noise are divergent. The probability density functional of white Lévy noise, $\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]$, can be formally expressed as an inverse Fourier transform of the characteristic functional $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$. We rewrite the definition (5) of the characteristic functional $\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ of the Lévy white noise in terms of the probability functional $\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]$

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\overline{\int\int_{\mathbf{r},t}}\exp\left\{i\int_{-\infty}^{+\infty}\cdots\int\int_{-\infty}^{+\infty}\mathcal{K}(\mathbf{r}',t')F_0(\mathbf{r}',t')d\mathbf{r}'\,dt'\right\}$$
$$\times\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]. \tag{19}$$

Now we use a discrete representation for Eq. (19):

$$G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]=\int\cdots\int\exp\left\{i\sum_{u,\mathbf{v}}\mathcal{K}^{(u,\mathbf{v})}F_0^{(u,\mathbf{v})}\Delta t\Delta\mathbf{r}\right\}P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]\prod_{u,\mathbf{v}}dF_0^{(u,\mathbf{v})}, \tag{20}$$

where $P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]\Pi_{u,\mathbf{v}}dF_0^{(u,\mathbf{v})}$ is a joint probability which is a discrete representation of the probability functional $\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]$ and $G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]$ is the Fourier transform of $P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]$. We have

$$\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]\prod_{u,\mathbf{v}}dF_0^{(u,\mathbf{v})}, \tag{21}$$

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]. \tag{22}$$

By applying an inverse Fourier transformation to Eq. (20) we come to

$$P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]\prod_{u,\mathbf{v}} dF_0^{(u,\mathbf{v})}=\prod_{u,\mathbf{v}} dF_0^{(u,\mathbf{v})}\int\cdots\int \exp\left\{-i\sum_{u,\mathbf{v}} \mathcal{K}^{(u,\mathbf{v})}F_0^{(u,\mathbf{v})}\Delta t\Delta\mathbf{r}\right\}$$
$$\times G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]\prod_{u,\mathbf{v}}\left(\frac{d\mathcal{K}^{(u,\mathbf{v})}}{2\pi}\right). \tag{23}$$

In the continuous limit Eq. (23) becomes

$$\mathcal{P}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')]$$
$$=\left\{\overline{\int\int}_{\mathbf{r},t}\exp\left[-\int_{-\infty}^{+\infty}\cdots\int\int_{-\infty}^{+\infty}[i\mathcal{K}(\mathbf{r}',t')F_0(\mathbf{r}',t')\right.\right.$$
$$\left.\left.+c|\mathcal{K}(\mathbf{r}',t')|^{\alpha}]d\mathbf{r}'\,dt'\right]\right\}\mathcal{D}^{\mathrm{inv}}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]\,\mathcal{D}^0_{\mathbf{r},t}[F_0(\mathbf{r}',t')], \tag{24}$$

where

$$\mathcal{D}^{\mathrm{inv}}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\lim_{\Delta\mathbf{r}\to\mathbf{0},\Delta t\to 0}\prod_{u,\mathbf{v}}\left(\frac{d\mathcal{K}^{(u,\mathbf{v})}}{2\pi}\right) \tag{25}$$

is an integration measure over the space of functions $\mathcal{K}(\mathbf{r}',t')$.

From Eqs. (21)–(25) we notice that the Lévy white noise is described by an independent stochastic process, that is, the fluctuations of the noise source at a given time and position are independent of the fluctuations of the noise source at other times and positions. For this reason, the expressions for the characteristic functional and for the probability density functional are separable, that is, they can be expressed as products of factors corresponding to different points in the space–time continuum. This can be easily seen from the discrete representations $G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]$ and $P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]$. We have

$$G^0_{\mathbf{r},t}[\mathcal{K}^{(u,\mathbf{v})}]=\prod_{u,\mathbf{v}}\exp\{-c(\Delta t\Delta\mathbf{r})|\mathcal{K}^{(u,\mathbf{v})}|^{\alpha}\}, \tag{26}$$

$$P^0_{\mathbf{r},t}[\|F_0^{(u,\mathbf{v})}\|]=\prod_{u,\mathbf{v}}\left\{\frac{1}{[c(\Delta t\Delta\mathbf{r})]^{1/\alpha}}\Psi_{\alpha}\left\{\frac{F_0^{(u,\mathbf{v})}}{[c(\Delta t\Delta\mathbf{r})]^{1/\alpha}}\right\}\right\}, \tag{27}$$

where

$$\Psi_{\alpha}(x)=(2\pi)^{-1}\int_{-\infty}^{+\infty}\exp(-ikx-|k|^{\alpha})dk \tag{28}$$

is the one-variable symmetrical Lévy probability density.[8]

In various physical, chemical, and biological problems the observables of physical interest are linked averages of the type

$$\Phi(t)=\left\langle\exp\left[-\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{t}\zeta(\mathbf{r}',t')F_0(\mathbf{r}',t')d\mathbf{r}'\,dt'\right]\right\rangle. \tag{29}$$

By using Eq. (17) such linked averages can be easily evaluated with our approach. We have

$$\Phi(t)=\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')=\zeta(\mathbf{r}',t')[h(t'-t_0)-h(t'-t)]]$$
$$=\exp\left(-c\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{t}|\zeta(\mathbf{r}',t')|^{\alpha}\,d\mathbf{r}'\,dt'\right), \tag{30}$$

where $h(x)$ is the Heaviside step function.

It is easy to check that in the limit $\alpha\to 2$ the white Lévy noise studied in this section reduces to the usual Gaussian white noise. The characteristic functional and the probability density functional of the noise become Gaussian. We pass in Eq. (17) to the limit $\alpha\to 2$ and assume that the limit

$$\lim_{\alpha\to 2}\left[2k_0(\alpha)\frac{\Gamma(1-\alpha)}{\alpha}\cos\left(\frac{\pi\alpha}{2}\right)\right]=c_2 \tag{31}$$

exists and is finite. We come to

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\exp\left(-c_2\int_{-\infty}^{+\infty}\cdots\int\int_{-\infty}^{+\infty}|\mathcal{K}(\mathbf{r}',t')|^2\,d\mathbf{r}'\,dt'\right), \tag{32}$$

which corresponds to an independent, space- and time-dependent Gaussian stochastic process with finite cumulants:

$$\langle\langle F_0(\mathbf{r},t)\rangle\rangle=0, \tag{33}$$

$$\langle\langle F_0(\mathbf{r}_1,t_1)F_0(\mathbf{r}_2,t_2)\rangle\rangle=2c_2\delta(t_1-t_2)\,\delta(\mathbf{r}_1-\mathbf{r}_2), \tag{34}$$

$$\langle\langle F_0(\mathbf{r}_1,t_1)\cdots F_0(\mathbf{r}_m,t_m)\rangle\rangle=0,\quad m>2. \tag{35}$$

In conclusion, in this section we have used the Huber approach for studying the stochastic properties of the space- and time-dependent Lévy white noise. The type of Lévy white noise introduced by using the Huber approach is a space-dependent generalization of the Lévy noises introduced by Doob,[12] West and Shesadri,[14] and Garbaczewski and Olkiewicz.[15] We have derived expressions for the characteristic functional and the probability functional of the noise source and have indicated that the positive moments and the cumulants of the noise source are infinite. We have shown that the Gaussian white noise can be recovered as a limit case of Lévy white noise, which corresponds to a fractal exponent α equal to two.

IV. TIME- AND SPACE-DEPENDENT LÉVY COLORED NOISE

In the case of the white Lévy noise studied in the preceding section the values of the noise source at different positions in the space–time continuum are independent random variables selected from the same probability density, which is of the Lévy type. For this reason the stochastic process which describes the white Lévy noise is stationary. In the case of colored noise, however, it makes sense to consider the broader case where the noise is generally nonstationary. In this section we study Lévy colored noise which obeys a Langevin equation of the type (1), where $F_0(\mathbf{r},t)$ is a Lévy white noise described by Eq. (17); however the white noise does not act from any time value between $-\infty$ and $+\infty$, but rather in a time window, limited by a lower value $t=t_0$. Under these circumstances we should introduce a lower time cutoff in Eq. (17), resulting in

$$\mathfrak{G}^0_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\exp\left(-c\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{+\infty}|\mathcal{K}(\mathbf{r}',t')|^{\alpha}\,d\mathbf{r}'\,dt'\right). \tag{36}$$

Then the colored noise is generally nonstationsary and the stationary colored noise corresponds to the limit $t_0\to-\infty$.

The next step is to express the properties of colored noise in terms of the properties of white noise. We express the general solution of the evolution equation (1) in terms of a Green function, which is the solution of

$$\frac{\partial \mathcal{G}(\mathbf{r};\mathbf{r}'',t-t'')}{\partial t}=\mathbb{L}\mathcal{G}(\mathbf{r};\mathbf{r}'',t-t''), \tag{37}$$

with the initial condition

$$\mathcal{G}(\mathbf{r};\mathbf{r}'',0)=\delta(\mathbf{r}-\mathbf{r}''); \tag{38}$$

in particular, if the linear transport operator $\mathbb{L}...$ is translationally invariant, so is the Green function, that is, $\mathcal{G}(\mathbf{r};\mathbf{r}'',t-t'')=\mathcal{G}(\mathbf{r}-\mathbf{r}'',t-t'')$. The solution of Eq. (1), corresponding to the initial condition $F(\mathbf{r},t=t_0)=F(\mathbf{r},t_0)$, is

$$F(\mathbf{r},t)=\int_{-\infty}^{+\infty}\cdots\int \mathcal{G}(\mathbf{r};\mathbf{r}_0,t-t_0)F(\mathbf{r}_0,t_0)d\mathbf{r}_0+\omega\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{t}\mathcal{G}(\mathbf{r};\mathbf{r}'',t-t'')F_0(\mathbf{r}'',t'')d\mathbf{r}''\,dt''. \tag{39}$$

The characteristic functional of the noise source $F(\mathbf{r},t)$ can be easily evaluated. By assuming that the distribution of the initial value $F(\mathbf{r},t=t_0)=F(\mathbf{r},t_0)$ is independent of the noise source $F_0(\mathbf{r},t)$ from Eq. (6) we come to

$$\begin{aligned}\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]&=\left\langle \exp\left\{ i\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{+\infty}\mathcal{K}(\mathbf{r}',t')\int_{-\infty}^{+\infty}\cdots\int\mathcal{G}(\mathbf{r}';\mathbf{r}_0,t'-t_0)F(\mathbf{r}_0,t_0)d\mathbf{r}_0\,d\mathbf{r}'\,dt'\right\}\right\rangle\\&\times\left\langle \exp\left\{ i\omega\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{+\infty}\mathcal{K}(\mathbf{r}',t')\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{t}\mathcal{G}(\mathbf{r}';\mathbf{r}'',t'-t'')F_0(\mathbf{r}'',t'')d\mathbf{r}''\,dt''\,d\mathbf{r}'\,dt'\right\}\right\rangle.\end{aligned} \tag{40}$$

Now we introduce the probability functional of the random force field $F(\mathbf{r},t_0)$ at the initial time $t=t_0$,

$$\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t_0]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t_0]\ \text{ with }\ =\overline{\int\int_{\mathbf{r}}}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t_0]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t_0]=1, \tag{41}$$

and the corresponding characteristic functional

$$\begin{aligned}\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t_0]&=\left\langle \exp\left\{ i\int_{-\infty}^{+\infty}\cdots\int F(\mathbf{r}')K(\mathbf{r}')d\mathbf{r}'\right\}\right\rangle\\&=\overline{\int\int_{\mathbf{r}}}\exp\left[i\int K(\mathbf{r}')F(\mathbf{r}')d\mathbf{r}'\right]\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t_0]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t_0].\end{aligned} \tag{42}$$

By combining Eqs. (40) and (42) we obtain

$$\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]=\mathfrak{G}_{\mathbf{r},t}^{\text{transient}(t_0)}[\mathcal{K}(\mathbf{r}',t')]\mathfrak{G}_{\mathbf{r},t}^{\text{normal}(t_0)}[\mathcal{K}(\mathbf{r}',t')], \tag{43}$$

where

$$\mathfrak{G}_{\mathbf{r},t}^{\text{transient}(t_0)}[\mathcal{K}(\mathbf{r}',t')]=\mathfrak{G}_{\mathbf{r}}\left[K(\mathbf{r}')=\int_{t_0}^{\infty}\mathcal{K}(\mathbf{r}'',t'')\int_{-\infty}^{+\infty}\cdots\int\mathcal{G}(\mathbf{r}'';\mathbf{r}',t''-t_0)d\mathbf{r}''\,dt''\right] \tag{44}$$

is a transient component and

$$\mathfrak{G}_{\mathbf{r},t}^{\text{normal}(t_0)}[\mathcal{K}(\mathbf{r}',t')] = \exp\left(-D_{\text{fract.}} \int_{-\infty}^{+\infty} \cdots \int \int_{t'=t_0}^{+\infty} \left| \int_{-\infty}^{+\infty} \cdots \int \int_{t''-t'}^{\infty} \mathcal{G}(\mathbf{r}''-\mathbf{r}',t''-t')\mathcal{K}(\mathbf{r}'',t'')d\mathbf{r}''\,dt'' \right|^{\alpha} d\mathbf{r}'\,dt' \right) \tag{45}$$

is a normal component;

$$D_{\text{fract.}} = \frac{2\kappa_0(\alpha)\omega^{\alpha}}{\alpha}\Gamma(1-\alpha)\cos\left(\frac{\pi\alpha}{2}\right) = c\,\omega^{\alpha} \tag{46}$$

is a fractional diffusion coefficient.

Equations (43)–(45) are the main results of this section. The characteristic functional $\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ expresses all stochastic properties of the Lévy colored noise. In particular, by computing the functional derivatives of $\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ and $\ln \mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$ we can show that for $2>\alpha>0$ all positive moments and cumulants of the noise source are infinite. The probability functional of the colored noise

$$\mathcal{P}_{\mathbf{r},t}[F(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}[F(\mathbf{r}',t')] \quad \text{with} \quad \overline{\int\int}_{\mathbf{r},t} \mathcal{P}_{\mathbf{r},t}[F(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}[F(\mathbf{r}',t')] = 1 \tag{47}$$

can be formally expressed as an inverse Fourier transform of $\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]$. By using a discrete representation for $\mathcal{P}_{\mathbf{r},t}[F(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}[F(\mathbf{r}',t')]$ similar to the one used in the preceding section we can show that

$$\begin{aligned}\mathcal{P}_{\mathbf{r},t}[F(\mathbf{r}',t')]&\mathcal{D}_{\mathbf{r},t}[F(\mathbf{r}',t')] \\ &= \left\{ \overline{\int\int}_{\mathbf{r},t} \exp\left[-i \int_{-\infty}^{+\infty} \cdots \int \int_{-\infty}^{+\infty} \mathcal{K}(\mathbf{r}',t')F_0(\mathbf{r}',t')d\mathbf{r}'\,dt' \right] \right. \\ &\quad \left. \times \mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}^{\text{inv}}[\mathcal{K}(\mathbf{r}',t')] \right\} \mathcal{D}_{\mathbf{r},t}[F_0(\mathbf{r}',t')].\end{aligned} \tag{48}$$

For the study of many problems it is enough if we know the stochastic properties of the noise source at a given moment in time, $t'=t$. In this case we can use the marginal probability density functional

$$\begin{aligned}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t]&\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t] \\ &= \overline{\int\int}_{\mathbf{r},t} \{\delta[F(\mathbf{r}',t')-F(\mathbf{r}',t)]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}'),t]\}\mathcal{P}_{\mathbf{r},t}[F(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}[F(\mathbf{r}',t')]\end{aligned} \tag{49}$$

and the corresponding characteristic functional

$$\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t] = \overline{\int\int}_{\mathbf{r}} \exp\left\{ i \int_{-\infty}^{+\infty} \cdots \int K(\mathbf{r}')F(\mathbf{r}')d\mathbf{r}' \right\} \mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t]. \tag{50}$$

This characteristic functional can be easily evaluated from Eqs. (43)–(45). We have

$$\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]=\mathfrak{G}_{\mathbf{r},t}[\mathcal{K}(\mathbf{r}',t')=K(\mathbf{r}')\,\delta(t-t')]$$
$$=\mathfrak{G}_{\mathbf{r}}\left[\int_{-\infty}^{+\infty}\cdots\int K(\mathbf{r}'')\mathcal{G}(\mathbf{r}'';\mathbf{r}',t-t_0)d\mathbf{r}'';t_0\right]$$
$$\times\exp\left(-D_{\text{fract.}}\int_{-\infty}^{+\infty}\cdots\int\int_{t_0}^{t}\left|\int_{-\infty}^{+\infty}\cdots\int\mathcal{G}(\mathbf{r}'';\mathbf{r}',t-t')K(\mathbf{r}'')d\mathbf{r}''\right|^{\alpha}d\mathbf{r}'\,dt'\right). \tag{51}$$

We notice that the $\mathfrak{G}_{\mathbf{r}}$ term can be viewed as an integration constant and thus Eq. (51) has the structure of a solution of a linear evolution equation. Such an evolution equation can be easily built by evaluating the time derivative $\partial\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]/\partial t$ and the functional derivative $\delta\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]/\delta K(\mathbf{r}'')$ and by eliminating the initial condition $\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t_0]$ from the resulting equations. After some computations we come to

$$\frac{\partial}{\partial t}\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]=\int\left\{iK(\mathbf{r}'')\mathbb{L}\left[\mathbf{r}'',-i\frac{\delta}{\delta K(\mathbf{r}')}\right]\right\}\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]\,d\mathbf{r}''$$
$$-D_{\text{fract.}}\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]\int|K(\mathbf{r}'')|^{\alpha}\,d\mathbf{r}''. \tag{52}$$

We recall that the symmetric fractional derivative of order α of a function $\varphi(\lambda)$ can be defined as an inverse Fourier transform:[17,31]

$$\frac{\partial^{\alpha}}{\partial\lambda^{\alpha}}\varphi(\lambda)=-\mathcal{F}^{-1}[\overline{\varphi}(q)|q|^{\alpha}]=\frac{-1}{2\pi}\int_{-\infty}^{+\infty}\overline{\varphi}(q)|q|^{\alpha}\exp(-iq\lambda)dq, \tag{53}$$

where

$$\overline{\varphi}(q)=\int_{-\infty}^{+\infty}\varphi(\lambda)\exp(iq\lambda)d\lambda \tag{54}$$

is the Fourier transform of $\varphi(\lambda)$. By using Eqs. (53) and (54) we can introduce the following heuristic definition for the fractional functional derivative of order α, evaluated at a single position $\mathbf{r}=\mathbf{r}''$,

$$\frac{\delta^{\alpha}}{\delta[F(\mathbf{r}'',t)]^{\alpha}}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)]=\frac{\partial^{\alpha}}{\partial\lambda^{\alpha}}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)+\lambda\,\delta(\mathbf{r}'-\mathbf{r}'')]|_{\lambda=0}. \tag{55}$$

In Appendix A we show that, by means of an inverse Fourier transformation, Eq. (52) leads to a fractional functional Fokker–Planck equation for the probability density functional $\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)]$, which contains the fractional derivative (55). We obtain

$$\frac{\partial}{\partial t}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)]=\int\frac{\delta}{\delta F(\mathbf{r}'',t)}\{[\mathbb{L}F(\mathbf{r}',t)]\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)]\}d\mathbf{r}''$$
$$+D_{\text{fract.}}\int\frac{\delta^{\alpha}}{\delta[F(\mathbf{r}'',t)]^{\alpha}}\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}',t)]d\mathbf{r}''. \tag{56}$$

Equation (56) has an important consequence: it can be used for deriving evolution equations for joint probability density functionals of dynamical systems subject to colored noise by means of Van Kampen's method of compound master equations. A simple example is a nonlinear reaction-diffusion system subject to environmental fluctuations, described in terms of a one-variable multiplicative noise, such as fluctuations of the temperature.

An important type of colored noise corresponds to the case where the linear Langevin equation (1) is an equation of the reaction-diffusion type in unlimited space and the evolution operator $\mathbb{L}...$ has the standard form (3). In this case the Green function is translationally invariant. We have

$$\mathcal{G}(\mathbf{r}-\mathbf{r}'',t-t'')=[4\pi\omega\lambda^2(t-t'')]^{-m/2}\exp\left[-\omega(t-t'')-\frac{(\mathbf{r}-\mathbf{r}'')^2}{4\omega\lambda^2(t-t'')}\right], \tag{57}$$

with

$$\int_{-\infty}^{+\infty}\cdots\int\int_{t=t''}^{+\infty}\omega\mathcal{G}(\mathbf{r}-\mathbf{r}'',t-t'')d\mathbf{r}\,dt=1, \tag{58}$$

where m is the space dimension. It is easy to check that in the limit $\mathfrak{G}_t[\mathcal{K}(t')]$ with the constraint (31) the colored noise corresponding to Eq. (57) reduces to the standard Gaussian colored noise introduced by Lam and Bagayoko[30] and studied by Vlad, Ross, and Mackey.[32]

In conclusion, in this section we have derived analytic expressions for the characteristic functional and probability density functional of space- and time-dependent colored Lévy noise [Eqs. (48)–(51)]. In Appendix B we show that our general expression describes as a particular case the main properties of space-independent colored Lévy noise studied in the literature. By using a heuristic definition of the fractional functional derivative introduced in Appendix A, we have derived a fractional functional Fokker–Planck equation, which describes the properties of Lévy colored noise at a given moment in time, Eq. (58). This fractional functional Fokker–Planck equation can be used as a basis for deriving evolution equations for dynamical systems subjected to Lévy colored noise.

V. RATE PROCESSES IN DISORDERED SYSTEMS. EQUATIONS FOR THE RATE COEFFICIENTS

In this section we make an analogy between the theory of Lévy noise developed in this paper and the theory of rate processes in disordered systems. Our purpose is to use this analogy for deriving equations for the stochastic properties of the rate coefficients of a rate process in disordered systems. The results derived in this section are used in Sec. VI for suggesting methods for extracting kinetic information from experimental data.

For simplicity, in this section we limit ourselves to the study of rate processes with static disorder. We assume the validity of the random channel model in its simplest form. We consider a rate process described by a system of deterministic kinetic evolutions with random parameters of the type

$$d\mathbf{x}/dt=\mathcal{R}(\mathbf{x},\mathbf{W}), \tag{59}$$

where $\mathbf{x}=(x_1,x_2,\ldots)$ is the composition vector of the system, $\mathbf{W}=(W_1,W_2,\ldots)$ is the vector of the total rate coefficients and $\mathcal{R}=(\mathcal{R}_1,\mathcal{R}_2,\ldots)$ is the vector of the reaction rates. In Eq. (59) the intrinsic chemical fluctuations of the composition vector $\mathbf{x}$ are neglected and the only source of randomness are the random values of the vector of rate coefficients $\mathbf{W}$. We assume that the random variations of the different total rate coefficients $W_1,W_2,\ldots$ are independent of each other and that each total rate W_v can be represented by a linear superposition of various contributions of different reaction channels

$$W_v=\sum_u k_{vu}, \quad v=1,...,m, \tag{60}$$

where v is the channel label and m is the number of total rate coefficients.

We assume that the number N_v and the magnitudes $k_{v1},\ldots,k_{vN_v}$ obey Poissonian statistics. For processes with static disorder we can introduce the grand canonical probability densities

$$Q_{vN_v}(k_{v1},\ldots,k_{vN_v})dk_{v1}\cdots dk_{vN_v},\ \ Q_{1v}(k_{1v})dk_{1v},\ldots, \tag{61}$$

which obey the normalization conditions

$$Q_{v0}+\sum_{N_v=1}^{\infty}\frac{1}{N_v!}\int\cdots\int Q_{vN_v}(k_{v1},\ldots,k_{vN_v})dk_{v1}\cdots dk_{vN_v}=1. \tag{62}$$

For Poissonian statistics we have

$$Q_{v0}=\exp\left[-\int\rho_v(k_v)dk_v\right], \tag{63}$$

$$Q_{vN_v}(k_{v1},\ldots,k_{vN_v})dk_{v1}\cdots dk_{vN_v}=\exp\left[-\int\rho_v(k_v)dk_v\right]\rho_v(k_{v1})dk_{v1}\cdots\rho_v(k_{vN_v})dk_{vN_v}, \tag{64}$$

where $\rho_v(k_v)dk_v$, $v=1,2,...$, are average numbers of channels with contributions to the total rates between k_v and k_v+dk_v.

Now we introduce the probability density $\mathcal{P}(\mathbf{W})$ of the total rate coefficients, which obeys the normalization condition $\int\mathcal{P}(\mathbf{W})d\mathbf{W}=1$, and the corresponding characteristic function:

$$\mathcal{G}(\boldsymbol{\theta})=\int_0^{\infty}\cdots\int_0^{\infty}\exp\left(-\sum_v\theta_vW_v\right)\mathcal{P}(\mathbf{W})d\mathbf{W}, \tag{65}$$

where θ_v are the Laplace variables conjugated to the total rate coefficients W_v. We notice that, since the total rate coefficients are non-negative, the generating function $\mathcal{G}(\boldsymbol{\theta})$ of the probability density $\mathcal{P}(\mathbf{W})$ of the total rate coefficients can be defined as a multiple Laplace transform of $\mathcal{P}(\mathbf{W})$ with respect to the random variables W_v.

The probability density $\mathcal{P}(\mathbf{W})$ of the total rate coefficients W_v can be expressed as a multiple grand canonical average of a product of delta functions:

$$\begin{aligned}\mathcal{P}(\mathbf{W})&=\left\langle\prod_v\delta\left(W_v-\sum_u k_{vu}\right)\right\rangle\\&=\sum_{N_1}^{\infty}\cdots\sum_{N_m}^{\infty}\int\cdots\int\prod_{v=1}^{m}\left[\frac{1}{N_v!}\delta\left(W_v-\sum_u k_{vu}\right)Q_{vN_v}(k_{v1},\ldots,k_{vN_v})dk_{v1},\ldots,dk_{vN_v}\right].\end{aligned} \tag{66}$$

In general the grand canonical averages in Eq. (66) are hard to evaluate directly. However, if we take the multiple Laplace transform of Eq. (66) the generating function $\mathcal{G}(\boldsymbol{\theta})$ can be easily computed. By using the Poissonian laws (63) and (64) we come to

$$\begin{aligned}\mathcal{G}(\boldsymbol{\theta})&=\int_0^{\infty}\cdots\int_0^{\infty}\exp\left(-\sum_v\theta_vW_v\right)\sum_{N_1}^{\infty}\cdots\sum_{N_m}^{\infty}\int_0^{\infty}\cdots\int_0^{\infty}\prod_{v=1}^{m}\left[\frac{1}{N_v!}\delta\left(W_v-\sum_u k_{vu}\right)\right.\\&\quad\left.\times Q_{vN_v}(k_{v1},\ldots,k_{vN_v})dk_{v1},\ldots,dk_{vN_v}\right]d\mathbf{W}\\&=\prod_{v=1}^{m}\left\{\sum_{N_v=0}^{\infty}\frac{1}{N_v!}\left[\int\rho_v(k_v)\exp(-\theta_vk_v)dk_v\right]^{N_v}\exp\left[-\int\rho_v(k_v)dk_v\right]\right\},\end{aligned} \tag{67}$$

from which, by evaluating the sum over N_v, we come to

$$\mathcal{G}(\boldsymbol{\theta})=\exp\left[-\sum_{v=1}^{m}\int_0^{\infty}(1-\exp(\theta_v k_v))\rho_v(k_v)dk_v\right]=\prod_{v=1}^{m}\mathcal{G}_v(\theta_v) \tag{68}$$

with

$$\mathcal{G}_v(\theta_v)=\exp\left[-\int_0^{\infty}(1-\exp(-\theta_v k_v))\rho_v(k_v)dk_v\right]. \tag{69}$$

By taking the inverse Laplace transform of Eq. (68) we come to

$$\mathcal{P}(\mathbf{W})d\mathbf{W}=\prod_{v=1}^{m}[\mathcal{P}_v(W_v)dW_v], \tag{70}$$

where

$$\mathcal{P}_v(W_v)dW_v=\mathcal{L}^{-1}[\mathcal{G}_v(\theta_v)]dW_v \tag{71}$$

is the probability that the vth total rate has a value between W_v and W_v+dW_v; the functions $\mathcal{G}_v(\theta_v)$ are the characteristic functions of the probability densities $\mathcal{P}_v(W_v)$ and $\mathcal{L}^{-1}$ denotes the inverse Laplace transformation. As expected for independent random variables the probability density of the vector of the total rate coefficients, $\mathbf{W}$, is the product of the probability densities of different rate coefficients.

An important particular case is that for which the average densities of channels $\rho_v(k_v)$, $v=1,...,m$, attached to the different rate coefficients W_v, $v=1,...,m$, obey self-similar power scaling laws, similar to Eq. (12) introduced in Sec. III for Lévy noise

$$\rho_v(k_v)=\kappa_v\alpha_v(k_v)^{-(1+\alpha_v)},\quad 1>\alpha_v>0;\quad v=1,...,m, \tag{72}$$

where κ_v and α_v are scaling factors and fractal exponents attached to the different total rate coefficients, respectively. By using the scaling laws (72) the integrals in Eqs. (69) and (70) can be easily evaluated, resulting in

$$\mathcal{G}_v(\theta_v)=\exp[-(\Omega_v\theta_v)^{\alpha_v}], \tag{73}$$

where

$$\Omega_v=[(\alpha_v)^{-1}\kappa_v(\alpha_v)\Gamma(1-\alpha_v)]^{1/\alpha_v}. \tag{74}$$

The probability densities $\mathcal{P}_v(W_v)$ can be easily evaluated, resulting in

$$\mathcal{P}_v(W_v)=(\Omega_v)^{-1}\varphi_{\alpha_v}(W_v/\Omega_v), \tag{75}$$

where

$$\varphi_\alpha(x)=\mathcal{L}^{-1}[\exp(-s^\alpha)],\quad 1>\alpha>0, \tag{76}$$

is a Lévy probability density of a non-negative variable x, s is the Laplace variable conjugated to x, and α is a dimensionless fractal exponent.

Since the probability densities $\mathcal{P}_v(W_v)$ of the total rate are of the Lévy type we expect that they obey fractional evolution equations similar to Eqs. (56) and (B18) from Sec. IV and Appendix B. By differentiating Eqs. (73) with respect to Ω_v we come to

$$\Omega_v\frac{\partial}{\partial\Omega_v}\mathcal{G}_v+\alpha_v(\Omega_v\theta_v)^{\alpha_v}\mathcal{G}_v=0,\quad v=1,...,m. \tag{77}$$

Now we recall the definition of the asymmetric fractional derivative of order $\alpha, 1>\alpha>0$ of a function $f(x)$ of a non-negative variable[31] x,

$$\frac{d^{\alpha}}{dx^{\alpha}} f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x \frac{f(y)dy}{(x-y)^{\alpha}}, \quad 1>\alpha>0, \tag{78}$$

and apply the inverse Laplace transformation to Eqs. (77), resulting in

$$\frac{\partial}{\partial \Omega_v} \mathcal{P}_v + \alpha_v (\Omega_v)^{\alpha_v - 1} \frac{\partial^{\alpha_v}}{\partial (W_v)^{\alpha_v}} \mathcal{P}_v = 0. \tag{79}$$

The fractional Fokker–Planck equation (79) can be easily extended to the more general case where the state densities $\rho_v(k_v)$, $v=1,...,m$, are arbitrary. Since $\rho_v(k_v)dk_v$, $v=1,...,m$, are pure numbers, it follows that the state densities $\rho_v(k_v)$, $v=1,...,m$, have the physical dimension $[k_v]^{-1}$. Dimensional analysis requires that $\rho_v(k_v)$, $v=1,...,m$, must depend on m constants Ω_v, $v=1,...,m$ with physical dimension $[k_v]$. We have

$$\rho_v(k_v) = (\Omega_v)^{-1} \chi_v(k_v/\Omega_v), \quad v=1,...,m, \tag{80}$$

where $\chi_v(x_v)$, $v=1,...,m$, are dimensionless densities of channels and $x_v = k_v/\Omega_v$. By using Eqs. (80) we can express Eqs. (69) in the following form,

$$\mathcal{G}_v(\theta_v) = \exp[-\eta_v(\theta_v \Omega_v)], \tag{81}$$

where

$$\eta_v(y) = \int_0^{\infty} (1-\exp(-xy)) \chi_v(x) dx. \tag{82}$$

By differentiating Eq. (81) with respect to Ω_v we come to

$$\frac{\partial}{\partial \Omega_v} \mathcal{G}_v + \theta_v \xi_v(\Omega_v \theta_v) \mathcal{G}_v = 0, \tag{83}$$

with

$$\xi_v(y) = \frac{\partial}{\partial y} \eta_v(y) = \int_0^{\infty} \exp(-xy) x \chi_v(x) dx = \mathcal{L}[x \chi_v(x)], \tag{84}$$

where $\mathcal{L}$ denotes the direct Laplace transformation. Now we apply the inverse Laplace transformation to Eqs. (83), resulting in a set of integrodifferential equations which are generalizations of the Fokker Planck equations (79)

$$\frac{\partial}{\partial \Omega_v} \mathcal{P}_v + (\Omega_v)^{-2} \frac{\partial}{\partial (W_v)} \int_0^{W_v} (W_v - W') \chi_v \left(\frac{W_v - W'}{\Omega_v} \right) \mathcal{P}_v(W') dW' = 0. \tag{85}$$

If the self-similar scaling laws (72) hold, then

$$\chi_v(x) = \frac{\alpha_v}{\Gamma(1-\alpha_v)} x^{-(1+\alpha_v)}, \tag{86}$$

and Eqs. (85) reduces to the fractional equations (79).

In conclusion in this section we have studied the statistical properties of the total rate coefficients for a nonlinear disordered system obeying independent random channel statistics. We have

derived relations for the probability densities of the total rate coefficients and their characteristic functions, and have shown that if the average densities of channels obey self-similar power scaling laws, then the probability densities of the total rate coefficients are of the Lévy type. In this particular case we have derived stationary fractional Fokker–Planck equations for the probability densities of the total rate coefficients. In the general case where the average densities of channels are arbitrary we have derived integrodifferential equations for the probability densities of the total rate coefficients; as expected, for self-similar distributions of channels these integrodifferential equations reduce to fractional Fokker–Planck equations. In the next section we use these results for suggesting methods for the extraction of kinetic information from experimental data.

VI. RATE PROCESSES IN DISORDERED SYSTEMS. EXTRACTION OF INFORMATION FROM EXPERIMENTAL DATA

In disordered kinetics the experimental observables are usually average concentrations. We denote by

$$\mathbf{x}(t)=\mathbf{\Theta}(\mathbf{x}_0,\mathbf{W};t) \tag{87}$$

the solution of the evolution equations (59) with the initial condition. We need to evaluate the average concentration vector

$$\langle \mathbf{x}(t)\rangle=\int_0^\infty\cdots\int_0^\infty \mathbf{\Theta}(\mathbf{x}_0,\mathbf{W};t)\mathcal{P}(\mathbf{W})d\mathbf{W}. \tag{88}$$

We express $\mathbf{\Theta}(\mathbf{x}_o,\mathbf{W};t)$ as an inverse Fourier transform,

$$\mathbf{\Theta}(\mathbf{x}_o,\mathbf{W};t)=\frac{1}{(2\pi)^m}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\overline{\mathbf{\Theta}}(\mathbf{x}_o,\mathbf{q};t)\exp(-i\mathbf{q}\cdot\mathbf{W})d\mathbf{q}, \tag{89}$$

where

$$\overline{\mathbf{\Theta}}(\mathbf{x}_o,\mathbf{q};t)=\int_0^\infty\cdots\int_0^\infty \mathbf{\Theta}(\mathbf{x}_o,\mathbf{W};t)\exp(i\mathbf{q}\cdot\mathbf{W})d\mathbf{W}, \tag{90}$$

and where $\mathbf{q}$ is the vector of Fourier variables attached to the vector of total rate coefficients $\mathbf{W}$. In Eq. (90) we have taken into account that the total rate coefficients cannot be negative. By inserting Eqs. (89) and (90) into Eq. (88) and making use of Eq. (65) we come to

$$\begin{aligned}\langle \mathbf{x}(t)\rangle&=\frac{1}{(2\pi)^m}\int_0^\infty\cdots\int_0^\infty\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\mathbf{\Theta}(\mathbf{x}_o,\mathbf{W}';t)\exp(i\mathbf{q}\cdot\mathbf{W}')\\&\quad\times d\mathbf{W}'d\mathbf{q}\int_0^\infty\cdots\int_0^\infty\exp(-i\mathbf{q}\cdot\mathbf{W})\mathcal{P}(\mathbf{W})d\mathbf{W}\\&=\frac{1}{(2\pi)^m}\int_0^\infty\cdots\int_0^\infty\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\mathcal{G}(i\mathbf{q})\mathbf{\Theta}(\mathbf{x}_o,\mathbf{W}';t)\exp(i\mathbf{q}\cdot\mathbf{W}')d\mathbf{W}'\,d\mathbf{q}.\end{aligned} \tag{91}$$

Now we insert Eq. (68) into Eq. (91) resulting in

$$\langle \mathbf{x}(t)\rangle = \frac{1}{(2\pi)^m}\int_0^\infty\cdots\int_0^\infty\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\exp\left(i\mathbf{q}\cdot\mathbf{W}' - \sum_{v=1}^{m}\int_0^\infty (1-\exp(-iq_vk_v))\rho_v(k_v)dk_v\right)$$
$$\times\Theta(\mathbf{x}_o,\mathbf{W}';t)d\mathbf{W}'\,d\mathbf{q}$$
$$= \pi^{-m}\int_0^\infty\cdots\int_0^\infty\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\Theta(\mathbf{x}_o,\mathbf{W}';t)\exp\left(-\sum_{v=1}^{m}\int_0^\infty (1-\cos(q_vk_v))\rho_v(k_v)dk_v\right)$$
$$\times\prod_{v=1}^{m}\left\{\cos\left[q_vW_v' + \int_0^\infty \sin(q_vk_v)\rho_v(k_v)dk_v\right]\right\}d\mathbf{W}'\,d\mathbf{q}. \tag{92}$$

In particular, if the average densities of channels obey the self-similar scaling laws (72), we have

$$\langle \mathbf{x}(t)\rangle = \pi^{-m}\int_0^\infty\cdots\int_0^\infty\int_0^\infty\cdots\int_0^\infty\Theta(\mathbf{x}_o,\mathbf{W}';t)\exp\left(-\sum_{v=1}^{m}(q_v\Omega_v)^{\alpha_v}\cos\left(\frac{\pi\alpha_v}{2}\right)\right)$$
$$\times\prod_{v=1}^{m}\left\{\cos\left[q_vW_v' + (q_v\Omega_v)^{\alpha_v}\sin\left(\frac{\pi\alpha_v}{2}\right)\right]\right\}d\mathbf{W}'\,d\mathbf{q}. \tag{93}$$

Equation (92) expresses the experimental observables, the average concentrations, in terms of the average densities of channels for a general nonlinear kinetic system with static disorder described by the independent random channel model. In particular, Eq. (93) gives the average concentration vector for scale-independent, self-similar distributions of reaction channels. From this point of view Eq. (93) can be considered as a nonlinear generalization of the stretched exponential kinetic law, for multi-species nonlinear chemical processes.

The experimental evaluation of kinetic parameters for the rate processes in disordered systems usually proceeds in two steps. The analysis starts with the extraction from experimental data of the statistical properties of the rate coefficients, that is, with the evaluation of the probability densities $\mathcal{P}_v(W_v)$ or of the moments or cumulants of the total rate coefficients, followed by the evaluation of the average densities of channels $\rho_v(k_v)$ from the probability densities $\mathcal{P}_v(W_v)$ of the total rate coefficients. We think that there are at least two different methods for evaluating the functions $\rho_v(k_v)$ in terms of the probability densities $\mathcal{P}_v(W_v)$. One first method is based on the use of the generalized fractional equations (85). By taking the inverse Laplace transform of Eqs. (81) we notice that the total probability densities of the total rates can be expressed as $\mathcal{P}_v(W_v) = (\Omega_v)^{-1}\mathfrak{G}_N(W_v/\Omega_v)$ where $\mathfrak{G}_v(w_v)$ are the probability densities of the dimensionless total rates $w_v = W_v/\Omega_v$. By expressing Eqs. (85) in terms of $\mathfrak{G}_v(w_v)$, after lengthy manipulations we get a set of integral equations for the average densities of channels $\rho_v(k_v)$. A second method is based on the derivation, from Eqs. (69), of a set of differential equations for the generating functions $\mathcal{G}_v(\theta_v)$. Since both methods lead to the same integral equations, in the following we present only the second method, which is shorter.

We differentiate Eqs. (69) with respect to θ_v, resulting in

$$-\frac{\partial}{\partial\theta_v}\mathcal{G}_v(\theta_v) = \mathcal{G}_v(\theta_v)\frac{\partial}{\partial\theta_v}\int_0^\infty (1-\exp(-\theta_vk_v))\rho_v(k_v)dk_v = \mathcal{G}_v(\theta_v)\mathcal{L}\{k_v\rho_v(k_v)\}, \tag{94}$$

from which we come to

$$\mathcal{L}\{W_v\mathcal{P}_v(W_v)\} = \mathcal{L}\{\mathcal{P}_v(W_v)\}\mathcal{L}\{k_v\rho_v(k_v)\}. \tag{95}$$

By applying the inverse Laplace transformation to Eqs. (95) we obtain a set of convolution equations for the densities of channels, which can be solved numerically:

$$W_v \mathcal{P}_v(W_v) = \int_0^{W_v} \mathcal{P}_v(W_v - k_v) k_v \rho_v(k_v) dk_v . \tag{96}$$

Equations (92), (93), (95), and (96) are general theoretical results. In order to apply them for the analysis of experimental data more detailed kinetic information is necessary. In this section we consider three single and two species chemical systems for which a detailed analysis is possible.

The first example is the first order, irreversible reaction

$$\mathrm{X} \rightarrow \text{Products}. \tag{97}$$

In this case the solution of the evolution equation (59) is

$$x(t) = x_0 \exp(-Wt), \tag{98}$$

and the average concentration is described by Huber's equation[22]

$$\langle x(t) \rangle / x_0 = \mathcal{G}(t) = \exp\left\{ -\int_0^{\infty} [1 - \exp(-kt)] \rho(k) dk \right\}, \tag{99}$$

where $\mathcal{G}(t)$ is the characteristic function of the probability density of the total rate coefficient. In this case the ratio between the average concentration at time t and the initial concentration is simply the Laplace transform of the probability density $\mathcal{P}(W)$ of the total rate coefficient:

$$\langle x(t) \rangle / x_0 = \int_0^{\infty} \exp(-Wt) \mathcal{P}(W) dW. \tag{100}$$

It follows that for first order kinetics the probability density $\mathcal{P}(W)$ of the total rate coefficient can be obtained from Eq. (100) by means of inverse numerical Laplace transformation. If $\mathcal{P}(W)$ is known, then the average density of channels $\rho(k)$ can be evaluated from Eqs. (95) and (96). We note that for stretched exponential kinetics the moments and the cumulants of the total rate coefficient are divergent. However, if the average density of channels $\rho(k)$ does not obey a self-similar scaling law the moments and cumulants of the total rate coefficients may be finite. If numerical data are not precise, inverse numerical Laplace transformation is not possible. However, the first few moments and cumulants can be evaluated from the time derivatives of the average concentration. We have

$$\langle W^m \rangle = (-1)^m \frac{d^m}{dt^m} \left[\frac{\langle x(t) \rangle}{x_0} \right] \Bigg|_{t=0} \tag{101}$$

for the moments and

$$\langle\langle W^m \rangle\rangle = (-1)^m \frac{d^m}{dt^m} \ln \left[\frac{\langle x(t) \rangle}{x_0} \right] \Bigg|_{t=0} \tag{102}$$

for the cumulants.

The second example is a first order, irreversible reaction, with a single equilibrium state:

$$\mathrm{X} \rightleftarrows \mathrm{Y}. \tag{103}$$

The solution of the kinetic equations (59) for a closed system is given by

$$\frac{x(t)}{x_0 + y_0} = \frac{1}{K_{\mathrm{eq}} + 1} + \left[\frac{x_0}{x_0 + y_0} - \frac{1}{K_{\mathrm{eq}} + 1} \right] \exp(-W_{\Sigma} t), \tag{104}$$

and a similar equation for the concentration $y(t)$ of the species Y. Here x_0 and y_0 are the initial concentrations of the species X and Y, respectively, $W_\Sigma = W_+ + W_-$ is the total rate coefficient of the process; W_+ and W_- are rate coefficients of the forward and backward processes (103), respectively, and $K_{\rm eq} = W_-/W_-$ is the equilibrium constant of the process. For a process with a single equilibrium state, although the rate coefficients W_+ and W_- are random, their ratio $K_{\rm eq} = W_+/W_-$ is constant and equal to the equilibrium constant of the process. Under these circumstances it can be shown[24] that the random channel model can be expressed in terms of a single density of channels, $\rho_\Sigma(k_\Sigma)$ corresponding to the total rate coefficient $W_\Sigma = W_+ + W_-$. We have

$$\frac{\langle x(t)\rangle}{x_0+y_0} = \frac{1}{K_{\rm eq}+1} + \left[\frac{x_0}{x_0+y_0} - \frac{1}{K_{\rm eq}+1}\right]\int_0^\infty \mathcal{P}_\Sigma(W_\Sigma)\exp(-W_\Sigma t)\,dW_\Sigma$$
$$= \frac{1}{K_{\rm eq}+1} + \left[\frac{x_0}{x_0+y_0} - \frac{1}{K_{\rm eq}+1}\right]\exp\left\{-\int_0^\infty \rho_\Sigma(k_\Sigma)[1-\exp(-k_\Sigma t)]\,dk_\Sigma\right\}. \quad (105)$$

and a similar equation for the average concentration $\langle y(t)\rangle$ of the Y species. It follows that the probability density of the rate coefficients can be expressed as

$$\mathcal{P}_\Sigma(W_\Sigma) = \mathcal{L}^{-1}\left\{\frac{\langle x(t)\rangle(K_{\rm eq}+1)-(x_0+y_0)}{x_0(K_{\rm eq}+1)-(x_0+y_0)}\right\} \quad (106)$$

and the moments and cumulants of the total rate coefficient can be computed from

$$\langle W^m\rangle = (-1)^m \frac{d^m}{dt^m}\left[\frac{\langle x(t)\rangle(K_{\rm eq}+1)-(x_0+y_0)}{x_0(K_{\rm eq}+1)-(x_0+y_0)}\right]\Bigg|_{t=0}, \quad (107)$$

$$\langle\langle W^m\rangle\rangle = (-1)^m \frac{d^m}{dt^m}\ln\left[\frac{\langle x(t)\rangle(K_{\rm eq}+1)-(x_0+y_0)}{x_0(K_{\rm eq}+1)-(x_0+y_0)}\right]\Bigg|_{t=0}. \quad (108)$$

The average density of channels can be determined from Eqs. (95) and (96).

The third example is a nonlinear, irreversible reaction,

$$\nu \mathrm{X} \rightarrow \text{Products}, \quad (109)$$

where ν is a stoichiometric coefficient bigger than one. The solution of the kinetic equation for a given realization of the total rate coefficient W is given by

$$x(t)/x_0 = \{1+(\nu-1)(x_0)^{\nu-1}Wt\}^{-1/(\nu-1)}, \quad (110)$$

where W is the total rate coefficient of the process. The application of Eq. (92) leads to the following expression for the average concentration $\langle x(t)\rangle$ of species X:

$$\frac{\langle x(t)\rangle}{x_0} = \frac{1}{\Gamma((\nu-1)^{-1})}\int_0^\infty \lambda^{1/(\nu-1)}\exp\left\{-z-\int_0^\infty \rho(k)[1-\exp(-\lambda(\nu-1)(x_0)^{\nu-1}kt)]\,dk\right\}d\lambda$$
$$= \int_0^\infty \frac{\mathcal{P}(W)\,dW}{\{1+(\nu-1)(x_0)^{\nu-1}Wt\}^{1/(\nu-1)}}. \quad (111)$$

Equation (111) is a linear integral equation for the probability density $\mathcal{P}(W)$ of the total rate coefficient. This integral equation can be transformed, through discretization, into a linear matrix equation which can be solved numerically. If the probability density $\mathcal{P}(W)$ is known, then the average density $\rho(k)$ of channels can be evaluated from Eqs. (95) and (96).

The positive moments of the total rate coefficient can be evaluated from a relation similar to Eqs. (101) and (107):

$$\langle W^m\rangle=[-(\nu-1)(x_0)^{\nu-1}]^{-m}\frac{\Gamma(m+(\nu-1)^{-1})}{\Gamma((\nu-1)^{-1})}\frac{d^m}{dt^m}\left[\frac{\langle x(t)\rangle}{x_0}\right]\Bigg|_{t=0}. \tag{112}$$

We do not have direct expressions for the cumulants of the total rate coefficient; they can, however, be computed step by step from the moments.

In conclusion, in this section we have made, a connection between the probability densities of the total rate coefficients, the average densities of channels, and the average concentrations, which are experimental observables in disordered chemical kinetics. We have developed methods for extracting statistical information about the fluctuations of the rate coefficients from experimental data. We have illustrated our approach by considering three simple chemical reactions.

VII. CONCLUSIONS

In this article we have pointed out some useful analogies between colored Lévy noise and the random channel approach in disordered kinetics. The exploitation of these analogies produces interesting results in both areas of research. By using Huber's stochastic approach for disordered kinetics we have managed to come up with a space- and time-dependent generalization of Lévy colored noise. In disordered kinetics, by using the analogies with Lévy colored noise, we have managed to develop a general theory of nonlinear chemical kinetics with static disorder. We have studied the statistical properties of the rate coefficients and developed methods for extracting information about rate statistics from experimental data.

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APPENDIX A: FRACTIONAL, FUNCTIONAL FOKKER–PLANCK EQUATION FOR COLORED LÉVY NOISE

We consider a discrete representation $P_{\mathbf{r}}[\|F_0^{(u,\mathbf{v})}\|;t]\Pi_{\mathbf{v}}dF^{(\mathbf{v})}$ of the probability $\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t]$. We have

$$\mathcal{P}_{\mathbf{r}}[F(\mathbf{r}');t]\mathcal{D}_{\mathbf{r}}[F(\mathbf{r}');t]=\lim_{\Delta\mathbf{r}\to 0}P_{\mathbf{r}}[\|F_0^{(\mathbf{v})}\|;t]\prod_{\mathbf{v}}dF^{(\mathbf{v})}, \tag{A1}$$

$$\mathfrak{G}_{\mathbf{r}}[K(\mathbf{r}');t]=\lim_{\Delta\mathbf{r}\to\mathbf{0}}G_{\mathbf{r}}[K^{(\mathbf{v})};t], \tag{A2}$$

where

$$G_{\mathbf{r}}[K^{(\mathbf{v})};t]=\int_{-\infty}^{+\infty}\cdots\int\exp\left\{i\sum_{\mathbf{v}}K^{(\mathbf{v})}F^{(\mathbf{v})}\Delta\mathbf{r}\right\}P_{\mathbf{r}}[\|F^{(\mathbf{v})}\|;t]\prod_{\mathbf{v}}dF_0^{(\mathbf{v})} \tag{A3}$$

is the Fourier transform of the discrete probability $P_{\mathbf{r}}[\|F_0^{(u,\mathbf{v})}\|;t]\Pi_{\mathbf{v}}dF^{(\mathbf{v})}$. We use a discrete representation of Eq. (52), in terms of $G_{\mathbf{r}}[K^{(\mathbf{v})};t]$, and evaluate the inverse Fourier transform with respect to $K^{(\mathbf{v})}$. The evaluation of the inverse Fourier transform of the first two terms is trivial. In order to evaluate the inverse Fourier transform of the third term,

$$\mathcal{J}_3=D_{\text{fract.}}\int_{-\infty}^{+\infty}\cdots\int\exp\left\{-i\sum_{\mathbf{v}}K^{(\mathbf{v})}F^{(\mathbf{v})}\Delta\mathbf{r}\right\}\left[\sum_{\mathbf{v}}\Delta\mathbf{r}|K^{(\mathbf{v})}|^{\alpha}\right]G_{\mathbf{r}}[K^{(\mathbf{v})};t]\prod_{\mathbf{v}}\left(\frac{dK^{(\mathbf{v})}\Delta\mathbf{r}}{2\pi}\right), \tag{A4}$$

we use the definition (57) of the symmetric fractional derivative of order α, resulting in

$$\mathcal{J}_3 = D_{\text{fract.}} \sum_{\mathbf{v}} (\Delta \mathbf{r})^{1-\alpha} \frac{\partial^\alpha}{\partial [F^{(\mathbf{v})}]^\alpha} P_{\mathbf{r}}[\|F_0^{(u,\mathbf{v})}\|;t]. \tag{A5}$$

By passing to the continuous notations and using the heuristic definition (55) of the fractional functional derivative of order α we come to Eq. (56).

APPENDIX B: SPACE-INDEPENDENT COLORED LÉVY NOISE

In this appendix we apply our approach for studying the particular case of space-independent Lévy colored noise. The space independent white noise can be characterized by the probability functional

$$\mathcal{P}_t^0[F_0(t')]\mathcal{D}_t^0[F_0(t')] \quad \text{with} \quad \overline{\int\int_t} \mathcal{P}_t^0[F_0(t')]\mathcal{D}_t^0[F_0(t')] = 1 \tag{B1}$$

or by the characteristic functional

$$\mathfrak{G}_t^0[\mathcal{K}(t')] = \overline{\int\int_t} \exp\left\{ i \int_{-\infty}^{+\infty} \mathcal{K}(t') F_0(t') dt' \right\} \mathcal{P}_t^0[F_0(t')]\mathcal{D}_t^0[F_0(t')]. \tag{B2}$$

The random force $F_0(t')$ can be expressed as the sum of the contributions of different individual events (channels):

$$F_0(t') = \sum_{m=1}^{N} g_m(t'). \tag{B3}$$

We assume that the fluctuations of the components $g_m(t')$ can be described by a Poissonian point process characterized by an average functional density of states $\rho_g[g(t)]\mathcal{D}[g(t)]$ which obeys a scaling condition of the negative power law type similar to Eq. (12). By considering a discrete representation of the average functional density of states $\rho_g[g(t)]\mathcal{D}[g(t)]$ we have

$$\rho_g(g;\Delta t)dg = \chi_0(\alpha)(\Delta t)^{(1-\alpha)}|g|^{-(1+\alpha)}dg, \quad \chi_0(\alpha) > 0, \quad 2 > \alpha > 0. \tag{B4}$$

The scaling law (B4) leads to the following expression for the characteristic functional of the white noise:

$$\mathfrak{G}_t^0[\mathcal{K}(t')] = \exp\left(-c \int_{-\infty}^{+\infty} |\mathcal{K}(t')|^\alpha dt' \right), \quad \text{where} \quad c = 2\chi_0(\alpha) \frac{\Gamma(1-\alpha)}{\alpha} \cos\left(\frac{\pi\alpha}{2}\right). \tag{B5}$$

The probability functional corresponding to the characteristic functional (B5) can be expressed as the continuous limit of a product of symmetric Lévy probability densities:

$$\mathcal{P}_{\mathbf{r},t}^0[F_0(\mathbf{r}',t')]\mathcal{D}_{\mathbf{r},t}^0[F_0(\mathbf{r}',t')] = \lim_{\Delta t \to 0} \prod_u \left\{ \frac{dF_0^{(u)}}{[c(\Delta t)]^{1/\alpha}} \Psi_\alpha \left\{ \frac{F_0^{(u,\mathbf{v})}}{[c(\Delta t)]^{1/\alpha}} \right\} \right\}, \tag{B6}$$

where $\Psi_\alpha(x)$ is the one-variable symmetrical Lévy probability density given by Eq. (28).

A given realization $F(t)$ of space-independent colored noise obeys the Langevin equation

$$\partial F(t)/\partial t = \omega[-F(t) + F_0(t)]. \tag{B7}$$

We start out by considering the case of nonstationary colored noise and for this reason we introduce a cutoff value t_0 in the expression (B5) for the characteristic functional $\mathfrak{G}_t^0[\mathcal{K}(t')]$ of the white noise, resulting in

$$\mathfrak{G}_t^0[\mathcal{K}(t')]=\exp\left(-c\int_{t_0}^{+\infty}|\mathcal{K}(t')|^{\alpha}\,dt'\right). \tag{B8}$$

From Eqs. (B7) and (B8) we get the following expression for the characteristic functional of colored noise:

$$\mathfrak{G}_t[\mathcal{K}(t')]=\mathfrak{G}_t^{\text{transient}(t_0)}[\mathcal{K}(t')]\mathfrak{G}_t^{\text{normal}(t_0)}[\mathcal{K}(t')], \tag{B9}$$

where the transient component $\mathfrak{G}_t^{\text{transient}(t_0)}[\mathcal{K}(t')]$ and the normal component $\mathfrak{G}_t^{\text{normal}(t_0)}[\mathcal{K}(t')]$ are given by

$$\mathfrak{G}_t^{\text{transient}(t_0)}[\mathcal{K}(t')]=\mathfrak{G}_r\left[K=\int_{t_0}^{\infty}\mathcal{K}(t'')\exp[-\omega(t''-t_0)dt'';t_0\right], \tag{B10}$$

$$\mathfrak{G}_t^{\text{normal}(t_0)}[\mathcal{K}(t')]=\exp\left(-c\int_{t_0}^{+\infty}\left|\int_{t''=t'}^{\infty}\mathcal{K}(t'')\,\omega\exp[-\omega(t''-t')]dt''\right|^{\alpha}dt'\right) \tag{B11}$$

and where

$$\mathfrak{G}[K;t_0]=\int_{-\infty}^{+\infty}P(F;t_0)\exp(iKF)dF \tag{B12}$$

is the Fourier transform of the probability density $P(F;t_0)$ of the colored noise at time t_0.

In particular, the characteristic function

$$\mathfrak{G}[K;t]=\int_{-\infty}^{+\infty}P(F;t)\exp(iKF)dF \tag{B13}$$

of the colored noise at time t is given by

$$\mathfrak{G}[K;t]=\mathfrak{G}[K\exp[-\omega(t-t_0)];t_0]\exp\left\{-\frac{D_{\text{fract.}}}{\alpha\omega}|K|^{\alpha}[1-\exp[-\alpha\omega(t-t_0)]]\right\}, \tag{B14}$$

where

$$D_{\text{fract.}}=c\,\omega^{\alpha}=2\,\omega^{\alpha}\chi_0(\alpha)\frac{\Gamma(1-\alpha)}{\alpha}\cos\left(\frac{\pi\alpha}{2}\right) \tag{B15}$$

is a space-independent fractional diffusion coefficient similar to the one defined in the space-dependent case by Eq. (46).

The probability density $P(F;t)$ of the colored noise at time t can be easily evaluated by taking the inverse Fourier transform of Eq. (B14). We have

$$P(F;t)=\left(\frac{\alpha\omega}{D_{\text{fract.}}}\right)^{1/\alpha}\frac{\exp[\omega(t-t_0)]}{[\exp[\alpha\omega(t-t_0)]-1]^{1/\alpha}}\int_{-\infty}^{+\infty}P(F_0;t_0)$$
$$\times\Psi_{\alpha}\left\{\left(\frac{\alpha\omega}{D_{\text{fract.}}}\right)^{1/\alpha}\frac{F\exp[\omega(t-t_0)]-F_0}{[\exp[\alpha\omega(t-t_0)]-1]^{1/\alpha}}\right\}dF_0. \tag{B16}$$

From Eq. (B16) we notice that as $t\to\infty$ the probability density $P(F;t)$ of the colored noise tends towards a Lévy stable form which is independent of the initial condition $P(F_0;t_0)$:

$$P(F;t)\to P_{st}(F)=(\alpha\omega/D_{\text{fract.}})^{1/\alpha}\Psi_\alpha[F(\alpha\omega/D_{\text{fract.}})^{1/\alpha}],\ \text{independent of}\ P(F_0;t_0),\ \text{as}\ t\to\infty. \tag{B17}$$

It is easy to check that the probability density $P(F;t)$ of the colored noise given by Eq. (B16) is the solution of a fractional Fokker–Planck equation:

$$\frac{\partial}{\partial t}P(F;t)=\frac{\partial}{\partial F}[\omega FP(F;t)]+D_{\text{fract.}}\frac{\partial^\alpha}{\partial F^\alpha}P(F;t). \tag{B18}$$

We notice that the fractional Fokker–Planck equation (B18) is the same as the fractional Fokker–Planck equation introduced by Metzler, Barkai, and Klafter for describing the stochastic evolution of a particle under the combined influence of an external, nonlinear force and a thermal heat bath.[16] It follows that the fractional Lévy noise introduced by using the Huber approach is equivalent to the fractional Lévy noise described by the fractional Fokker–Planck equation of Metzler, Barkai, and Klafter.[16] We also point out that our fractional functional Fokker–Planck equation (56) is a generalization of the Metzler, Barkai, and Klafter equation (B18) to the case of space and time dependent Lévy colored noise.

In particular, if $t_0\to-\infty$ or if the initial probability density $P(F_0;t_0)$ is the same as the stationary probability density $P_{st}(F)$, then the colored noise is stationary and the characteristic functional (B14) becomes

$$\mathfrak{G}_t[\mathcal{K}(t')]=\exp\left(-D_{\text{fract.}}\int_{-\infty}^{+\infty}\left|\int_{t''=t'}^{\infty}\mathcal{K}(t'')\exp[-\omega(t''-t')]dt''\right|^\alpha dt'\right). \tag{B19}$$

The stochastic process described by the characteristic functional (B19) is a statistical fractal generalization of the Uhlenbeck–Ornstein process. In the particular case where the fractal exponent α tends towards 2, $\alpha\to2$, and the limit

$$\lim_{\alpha\to2}D_{\text{fract.}}=\lim_{\alpha\to2}\left[2\omega^\alpha\chi_0(\alpha)\frac{\Gamma(1-\alpha)}{\alpha}\cos\left(\frac{\pi\alpha}{2}\right)\right]=D \tag{B20}$$

exists and is finite, we recover the classical Uhlenbeck–Ornstein process.

A linked average depending on the colored noise,

$$\Phi(t)=\left\langle\exp\left[-\int_{t_0}^{t}\zeta(t')F(t')dt'\right]\right\rangle, \tag{B21}$$

can be easily evaluated from the expression (B19) for the characteristic functional $\mathfrak{G}_t[\mathcal{K}(t')]$. We have

$$\Phi(t)=\mathfrak{G}_t^0[\mathcal{K}(t')=\zeta(t')[h(t'-t_0)-h(t'-t)]]. \tag{B22}$$

The fractional Fokker–Planck equation (B18) can be used for deriving evolution equations for joint probability density functions of dynamical systems subject to colored noise by means of Van Kampen's method of compound master equations. For example, we consider a nonlinear system subjected to environmental fluctuations, described in terms of a one-variable multiplicative noise. We express the evolution equations of the system in the following form:

$$\frac{\partial}{\partial t}\mathbf{x}(t)=\mathfrak{F}[\mathbf{x}(t);F(t);t], \tag{B23}$$

where $\mathbf{x}(t)$ is a state vector, and $\mathfrak{F}[\mathbf{x}(t);F(t);t]$ is a nonlinear vectorial function which depends on the state vector $\mathbf{x}(t)$, the noise $F(t)$ and the time t. By using the method of compound master equations we can derive a fractional stochastic Liouville equation for the joint probability density $P(\mathbf{x},F;t)$:

$$\frac{\partial}{\partial t}P(\mathbf{x},F;t)=-\nabla_{\mathbf{x}}\cdot[\mathfrak{F}[\mathbf{x};F;t]P(\mathbf{x},F;t)]+\frac{\partial}{\partial F}[\omega F P(\mathbf{x},F;t)]+D_{\text{fract.}}\frac{\partial^{\alpha}}{\partial F^{\alpha}}P(\mathbf{x},F;t). \tag{B24}$$

The probability density $P(\mathbf{x};t)$ of the state vector $\mathbf{x}$ at time t can be evaluated by solving Eq. (B24) with suitable initial and boundary conditions and by integrating the solution over all possible values of the random noise source F:

$$P(\mathbf{x},t)=\int_{-\infty}^{\infty}P(\mathbf{x},F;t)dF. \tag{B25}$$

In summary, in this appendix we studied the particular case of space-independent colored Lévy noise. We have derived expressions for the characteristic functional and probability density functional of space-independent colored Lévy noise. We have shown that the probability density of Lévy noise at a given time obeys a fractional Fokker–Planck equation. The colored Lévy noise derived by using the Huber approach is equivalent to the colored Lévy noise described by the fractional Fokker–Planck equation (B18), which is the same as the fractional Fokker–Planck equation derived by Metzler, Barkai and Klafter[16] by using a different approach.

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On the integration of products of Whittaker functions with respect to the second index

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Several new formulas are developed that enable the evaluation of a family of definite integrals containing the product of two Whittaker $W_{\kappa,\mu}(x)$-functions. The integration is performed with respect to the second index μ, and the first index κ is permitted to have any complex value, within certain restrictions required for convergence. The method utilizes complex contour integration along with various symmetry relations satisfied by the Whittaker functions. The new results derived in this article are complementary to the previously known integrals of products of Whittaker functions, which generally treat integration with respect to either the first index κ or the primary argument x. A physical application involving radiative transport is discussed. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Many problems in mathematical physics involve differential equations with solutions that can be expressed in terms of Whittaker's functions $W_{\kappa,\mu}(x)$ and $M_{\kappa,\mu}(x)$. Examples of the diverse applications include studies of the spectral evolution resulting from the Compton scattering of radiation by hot electrons,[1–3] modeling of the structure of the hydrogen atom,[4] analysis of the Schrödinger equation,[5] studies of the Coulomb Green's function,[6] and analysis of fluctuations in financial markets.[7]

In a number of applications, it is necessary to evaluate integrals of Whittaker functions. This need may arise out of the requirement to satisfy normalization or orthogonality conditions. In particular, in the analysis of time-dependent Compton scattering, it is necessary to evaluate integrals containing the product of two Whittaker $W_{\kappa,\mu}(x)$-functions, where the variable of integration is the second index μ. This is an unusual situation that is not covered by any of the previously known formulas for integrals of products of Whittaker functions. The required integrals in the Compton scattering application are members of the general family

$$I(s)\equiv\int_0^\infty \frac{u\sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{s+u^2}W_{\kappa,iu}(x)W_{\kappa,iu}(x_0)\,du, \tag{1}$$

where x and x_0 are real and positive, and s and κ are complex. This integral converges for all values of s in the complex plane, with the exclusion of the negative real semiaxis, provided that $\mathcal{R}e\,\kappa\neq 1/2,3/2,5/2,...$, if $\mathcal{I}m\,\kappa\neq 0$. It also converges in the special case $s=0$, provided $\mathcal{R}e\,\kappa\neq 1/2,3/2,5/2,...$. In this article we derive several exact formulas for the evaluation of the integral $I(s)$ that fully describe all of the convergent cases.

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II. FUNDAMENTAL EQUATIONS

We shall begin by briefly reviewing some of the basic properties of the Whittaker functions that will be useful in our later work. The Whittaker functions $W_{\kappa,\mu}(z)$ and $M_{\kappa,\mu}(z)$ are confluent hypergeometric functions that are related to the Kummer functions $\Phi(a,b,z)$ and $\Psi(a,b,z)$ by[8,9]

$$\begin{aligned} M_{\kappa,\mu}(z) &= z^{\mu+1/2}e^{-z/2}\Phi(\tfrac{1}{2}+\mu-\kappa,1+2\mu;z), \\ W_{\kappa,\mu}(z) &= z^{\mu+1/2}e^{-z/2}\Psi(\tfrac{1}{2}+\mu-\kappa,1+2\mu;z). \end{aligned} \tag{2}$$

For small values of $|z|$, the function $M_{\kappa,\mu}(z)$ is given by the power series

$$M_{\kappa,\mu}(z) = e^{-z/2}z^{\mu+1/2}\sum_{n=0}^{\infty}\frac{(\frac{1}{2}-\kappa+\mu)_n}{(1+2\mu)_n}\frac{z^n}{n!}, \tag{3}$$

where $(a)_n$ denotes the Pochhammer symbol, defined by[9]

$$(a)_n \equiv \frac{\Gamma(a+n)}{\Gamma(a)}. \tag{4}$$

The function $W_{\kappa,\mu}(z)$ can be expressed in terms of $M_{\kappa,\mu}(z)$ using[8]

$$W_{\kappa,\mu}(z) = \frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa)}M_{\kappa,\mu}(z) + \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa)}M_{\kappa,-\mu}(z). \tag{5}$$

The integrand in Eq. (1) for $I(s)$ is an even function of u, and therefore we can write

$$I(s) = \frac{1}{2}\int_{-\infty}^{\infty}\frac{u\sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{s+u^2}W_{\kappa,iu}(x)W_{\kappa,iu}(x_0)du. \tag{6}$$

Next we utilize (5) to express $W_{\kappa,iu}(x_0)$ as

$$W_{\kappa,iu}(x_0) = \frac{\Gamma(-2iu)}{\Gamma(\frac{1}{2}-\kappa-iu)}M_{\kappa,iu}(x_0) + \frac{\Gamma(2iu)}{\Gamma(\frac{1}{2}-\kappa+iu)}M_{\kappa,-iu}(x_0), \tag{7}$$

which can be rewritten as

$$W_{\kappa,iu}(x_0) = \frac{\Gamma(-2iu)\Gamma(2iu)}{\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}\left[\frac{\Gamma(\frac{1}{2}-\kappa+iu)}{\Gamma(2iu)}M_{\kappa,iu}(x_0) + \frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(-2iu)}M_{\kappa,-iu}(x_0)\right]. \tag{8}$$

By employing the recurrence formula for the gamma function, $z\Gamma(z)=\Gamma(z+1)$, we can obtain the alternative form

$$W_{\kappa,iu}(x_0) = \frac{\Gamma(-2iu)\Gamma(1+2iu)}{\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}\left[\frac{\Gamma(\frac{1}{2}-\kappa+iu)}{\Gamma(1+2iu)}M_{\kappa,iu}(x_0) - \frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(1-2iu)}M_{\kappa,-iu}(x_0)\right]. \tag{9}$$

Using this result to substitute for $W_{\kappa,iu}(x_0)$ in (6) now yields

$$I(s)=\frac{1}{2}\int_{-\infty}^{\infty}\frac{u\sinh(2\pi u)}{s+u^2}\Gamma(-2iu)\Gamma(1+2iu)W_{\kappa,iu}(x)$$
$$\times\left[\frac{\Gamma(\frac{1}{2}-\kappa+iu)}{\Gamma(1+2iu)}M_{\kappa,iu}(x_0)-\frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(1-2iu)}M_{\kappa,-iu}(x_0)\right]du. \tag{10}$$

By utilizing the reflection formula for the gamma function,

$$\Gamma(1+2iu)\Gamma(-2iu)=\frac{\pi i}{\sinh(2\pi u)}, \tag{11}$$

along with the symmetry relation [see Eq. (5)]

$$W_{\kappa,iu}(x)=W_{\kappa,-iu}(x), \tag{12}$$

we can rewrite (10) as

$$I(s)=\frac{\pi i}{2}\int_{-\infty}^{\infty}\frac{u}{s+u^2}\left[\frac{\Gamma(\frac{1}{2}-\kappa+iu)}{\Gamma(1+2iu)}W_{\kappa,iu}(x)M_{\kappa,iu}(x_0)\right.$$
$$\left.-\frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(1-2iu)}W_{\kappa,-iu}(x)M_{\kappa,-iu}(x_0)\right]du. \tag{13}$$

This relation can be split into two identical integrals, and consequently our expression for $I(s)$ can be reduced to

$$I(s)=-\pi i\int_{-\infty}^{\infty}\frac{u}{s+u^2}\frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(1-2iu)}W_{\kappa,-iu}(x)M_{\kappa,-iu}(x_0)du. \tag{14}$$

III. CONTOUR INTEGRATION

The fundamental expression for the integral $I(s)$ given by (1) is clearly symmetrical with respect to the interchange of x and x_0. We can use this flexibility to select the arguments of the W and M functions in such a way that the integration along the curved portion of the closed contour C in Fig. 1 vanishes in the limit $r\to\infty$. By employing asymptotic analysis, we find that this occurs if $x_{\max}$ is the argument of the W function and $x_{\min}$ is the argument of the M function, where

$$x_{\min}\equiv\min(x,x_0),\quad x_{\max}\equiv\max(x,x_0). \tag{15}$$

Equation (14) for $I(s)$ can therefore be recast as the complex contour integral

$$I(s)=\oint_C L(u)du, \tag{16}$$

where

$$L(u)\equiv-\pi i\frac{u}{s+u^2}\frac{\Gamma(\frac{1}{2}-\kappa-iu)}{\Gamma(1-2iu)}W_{\kappa,-iu}(x_{\max})M_{\kappa,-iu}(x_{\min}). \tag{17}$$

We shall proceed to obtain an exact, closed form expression for $I(s)$ by utilizing the residue theorem to evaluate the integral in (16).

The integrand $L(u)$ has a simple pole located at $u=i\sqrt{s}$, where $\sqrt{s}$ denotes the principle branch of the square root function. This pole is located in quadrant II of the complex u plane if

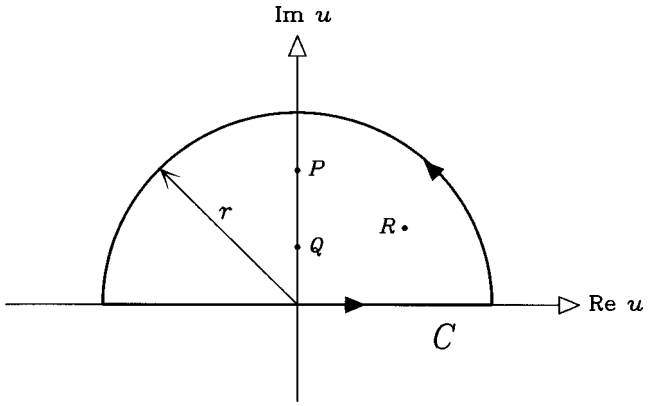

FIG. 1. Integration around the closed contour C yields $I(s)$ in the limit $r\to\infty$ [see Eq. (16)]. In this example, κ is a real number in the range $\frac{3}{2}<\kappa<\frac{5}{2}$, and consequently there are two simple poles (P and Q) located inside the contour on the imaginary axis [see Eq. (18)]. The imaginary part of s is less than zero in this instance, and consequently there is also a simple pole, R, located at $u=i\sqrt{s}$ in quadrant I.

$\mathcal{I}ms\geqslant 0$, and otherwise it is located in quadrant I. In either case, the pole is contained within the closed integration contour C. Additional simple poles are located at the singularities of the function $\Gamma(\frac{1}{2}-\kappa-iu)$, which occur where the quantity $\frac{1}{2}-\kappa-iu$ is equal to zero or a negative integer. At least one of the poles falls in the upper half-plane if $\mathcal{R}e\kappa>\frac{1}{2}$. The poles are located at $u=u_n$, where

$$u_n\equiv i(\kappa-\tfrac{1}{2}-n),\quad n=0,1,...,[\mathcal{R}e\kappa-\tfrac{1}{2}], \tag{18}$$

and $[a]$ indicates the integer part of a. Note that if $\mathcal{R}e\kappa<\frac{1}{2}$, then only the pole at $u=i\sqrt{s}$ is contained within the contour C.

We can now use the residue theorem to write

$$I(s)=2\pi i\sum_{n=0}^{[\mathcal{R}e\kappa-1/2]}\mathrm{Res}(u_n)+2\pi i\,\mathrm{Res}(i\sqrt{s}), \tag{19}$$

where $\mathrm{Res}(u_*)$ denotes the residue associated with the simple pole located at $u=u_*$.

IV. EVALUATION OF THE RESIDUES

The residue corresponding to the simple pole at $u=i\sqrt{s}$ is easily computed using the formula

$$\mathrm{Res}(i\sqrt{s})=\lim_{u\to i\sqrt{s}}(u-i\sqrt{s})L(u), \tag{20}$$

which can be immediately evaluated to obtain

$$\mathrm{Res}(i\sqrt{s})=-\frac{\pi i}{2}\frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})}W_{\kappa,\sqrt{s}}(x_{\max})M_{\kappa,\sqrt{s}}(x_{\min}). \tag{21}$$

Similarly, the residues associated with the simple poles located at $u=u_n$ are evaluated using

$$\mathrm{Res}(u_n)=\lim_{u\to u_n}(u-u_n)L(u). \tag{22}$$

Because the poles in this case correspond to the singularities of the function $\Gamma(\frac{1}{2}-\kappa-iu)$, we will require evaluation of the quantity

$$\lim_{u\to u_n}(u-u_n)\Gamma(\tfrac{1}{2}-\kappa-iu). \tag{23}$$

By combining (4) and (18) with the recurrence relation $z\Gamma(z)=\Gamma(z+1)$, we obtain

$$\Gamma\left(\frac{1}{2}-\kappa-iu\right)=\frac{\Gamma(\frac{1}{2}-\kappa-iu+n)}{(\frac{1}{2}-\kappa-iu)_n}=\frac{i\Gamma(1+iu_n-iu)}{(iu_n-iu-n)_n(u-u_n)}, \tag{24}$$

and therefore

$$\lim_{u\to u_n}(u-u_n)\Gamma\left(\frac{1}{2}-\kappa-iu\right)=\frac{i(-1)^n}{n!}, \tag{25}$$

where we have used the fact that $(-n)_n=(-1)^n n!$ Next we need to evaluate the Whittaker functions appearing on the right-hand side of (17) in the limit $u\to u_n$. Using (2) and (18), we find that

$$\begin{aligned} M_{\kappa,-iu_n}(z)&=e^{-z/2}z^{\kappa-n}\Phi(-n,2\kappa-2n;z),\\ W_{\kappa,-iu_n}(z)&=e^{-z/2}z^{\kappa-n}\Psi(-n,2\kappa-2n;z). \end{aligned} \tag{26}$$

By employing Eqs. (13.6.9) and (13.6.27) from Abramowitz and Stegun,[9] we can rewrite these expressions as

$$\begin{aligned} M_{\kappa,-iu_n}(z)&=\frac{n!}{(\alpha+1)_n}e^{-z/2}z^{(\alpha+1)/2}P_n^{(\alpha)}(z),\\ W_{\kappa,-iu_n}(z)&=(-1)^n n!e^{-z/2}z^{(\alpha+1)/2}P_n^{(\alpha)}(z), \end{aligned} \tag{27}$$

where $P_n^{(\alpha)}(z)$ denotes the Laguerre polynomial, and

$$\alpha\equiv 2\kappa-2n-1=-2iu_n. \tag{28}$$

Combining (17), (22), (25), and (27), we obtain for the residue

$$\mathrm{Res}(u_n)=\frac{2\pi i\alpha}{4s-\alpha^2}\frac{n!}{\Gamma(\alpha+n+1)}e^{-(x+x_0)/2}(xx_0)^{(\alpha+1)/2}P_n^{(\alpha)}(x)P_n^{(\alpha)}(x_0). \tag{29}$$

Utilizing this result along with (19) and (21), we conclude that

$$\begin{aligned} I(s)&=\int_0^\infty \frac{u\sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{s+u^2}W_{\kappa,iu}(x)W_{\kappa,iu}(x_0)du\\ &=\pi^2\frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})}W_{\kappa,\sqrt{s}}(x_{\max})M_{\kappa,\sqrt{s}}(x_{\min})\\ &\quad-4\pi^2e^{-(x+x_0)/2}\sum_{n=0}^{[\mathcal{R}e\,\kappa-1/2]}\frac{\alpha n!}{\Gamma(\alpha+n+1)}\frac{(xx_0)^{(\alpha+1)/2}}{4s-\alpha^2}P_n^{(\alpha)}(x)P_n^{(\alpha)}(x_0), \end{aligned} \tag{30}$$

where $\alpha=2\kappa-2n-1$. This previously unknown integral formula is one of the main results of the article. Note that the summation is carried out only if $\mathcal{R}e\,\kappa\geqslant\frac{1}{2}$. The integral on the left-hand side

of (30) converges for all complex values of s with the exception of the negative real semiaxis, provided that $\mathcal{R}e\,\kappa \neq 1/2,3/2,5/2,...$, if $\mathcal{I}m\,\kappa \neq 0$. When $s=0$, the integral converges provided $\mathcal{R}e\,\kappa$ is not a positive half-integer.

A case of special interest can be generated by setting $x_0 = x$ in (30). The result obtained is the *quadratic normalization integral*,

$$\int_0^\infty \frac{u \sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{s+u^2} W^2_{\kappa,iu}(x)\,du$$
$$= \pi^2 \frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})} W_{\kappa,\sqrt{s}}(x) M_{\kappa,\sqrt{s}}(x) - 4\pi^2 e^{-x} \sum_{n=0}^{[\mathcal{R}e\,\kappa - 1/2]} \frac{\alpha n!}{\Gamma(\alpha+n+1)} \frac{x^{\alpha+1}}{4s-\alpha^2} [P_n^{(\alpha)}(x)]^2, \tag{31}$$

which is useful in situations involving the development of a series expansion in terms of a set of normalized basis functions. In the following sections, we shall proceed to discuss the limiting behavior of (30) observed when two of the poles coincide, as well as its relation to formulas appearing in the previous literature.

V. LIMITING BEHAVIOR

An interesting situation arises if the quantity $\frac{1}{2}-\kappa+\sqrt{s}$ is equal to zero or a negative integer, because in this case the integral $I(s)$ converges, although the first term on the right-hand side of (30) formally *diverges* due to the appearance of the factor $\Gamma(\frac{1}{2}-\kappa+\sqrt{s})$. This occurs when

$$\sqrt{s} = \sqrt{s_m} \equiv \kappa - \tfrac{1}{2} - m, \tag{32}$$

where m is a positive integer or zero. Since $\sqrt{s}$ denotes the principle branch of the square root function, it follows that $\sqrt{s}$ is located in either quadrants I or IV of the complex s plane, depending on whether $\mathcal{I}m\,s$ is positive or negative. Hence $\mathcal{R}e\,\sqrt{s} \geqslant 0$ in general, and therefore the function $\Gamma(1/2-\kappa+\sqrt{s})$ has no singularities unless $\mathcal{R}e\,\kappa \geqslant \frac{1}{2}$. The values of m yielding singularities for a given value of κ are

$$m = 0,1,...,[\mathcal{R}e\,\kappa - \tfrac{1}{2}]. \tag{33}$$

When $s = s_m$, the divergence of the first term on the right-hand side of (30), containing the factor $\Gamma(\frac{1}{2}-\kappa+\sqrt{s})$, is exactly balanced by the divergence of the $n=m$ term in the sum, leaving a finite residual quantity. This situation corresponds to a coincidence of the pole located at $u = i\sqrt{s}$ with the pole located at $u = u_m = i(\kappa - \frac{1}{2} - m)$ [see Eq. (18)]. In this case the resulting pole has order two. The associated residue can be computed by using the standard formula for a second-order pole, but it is more efficient to approach the calculation by evaluating Eq. (30) for $I(s)$ in the limit $s \to s_m$. The limiting value of the sum of the two divergent terms is given by

$$K \equiv \lim_{s \to s_m} \pi^2 \frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})} W_{\kappa,\sqrt{s}}(x_{\max}) M_{\kappa,\sqrt{s}}(x_{\min})$$
$$- 4\pi^2 e^{-(x+x_0)/2} \frac{\lambda m!}{\Gamma(\lambda+m+1)} \frac{(x x_0)^{(\lambda+1)/2}}{4s-\lambda^2} P_m^{(\lambda)}(x) P_m^{(\lambda)}(x_0), \tag{34}$$

where

$$\lambda \equiv 2\kappa - 2m - 1 = 2\sqrt{s_m}. \tag{35}$$

Equation (34) can be rewritten as

$$K=\lim_{s\to s_m}\frac{N}{D}, \tag{36}$$

where

$$N\equiv\pi^2(s-s_m)\frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})}W_{\kappa,\sqrt{s}}(x_{\max})M_{\kappa,\sqrt{s}}(x_{\min})$$
$$-\pi^2e^{-(x+x_0)/2}\frac{\lambda m!}{\Gamma(\lambda+m+1)}(xx_0)^{(\lambda+1)/2}P_m^{(\lambda)}(x)P_m^{(\lambda)}(x_0), \tag{37}$$

and

$$D\equiv s-s_m. \tag{38}$$

We can demonstrate that the numerator N vanishes in the limit $s\to s_m$ as follows. First we use (4) and (32) along with the recurrence relation for the gamma function to write

$$\Gamma\left(\frac{1}{2}-\kappa+\sqrt{s}\right)=\frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s}+m)}{(\frac{1}{2}-\kappa+\sqrt{s})_m}=\frac{(\sqrt{s}+\sqrt{s_m})\Gamma(1+\sqrt{s}-\sqrt{s_m})}{(s-s_m)(\sqrt{s}-\sqrt{s_m}-m)_m}, \tag{39}$$

and therefore [cf. Eq. (25)]

$$\lim_{s\to s_m}(s-s_m)\Gamma\left(\frac{1}{2}-\kappa+\sqrt{s}\right)=\frac{(-1)^m}{m!}2\sqrt{s_m}. \tag{40}$$

Furthermore, based on (27), (28), and (35), we note that

$$M_{\kappa,\sqrt{s_m}}(z)=\frac{m!}{(\lambda+1)_m}e^{-z/2}z^{(\lambda+1)/2}P_m^{(\lambda)}(z),$$
$$W_{\kappa,\sqrt{s_m}}(z)=m!(-1)^me^{-z/2}z^{(\lambda+1)/2}P_m^{(\lambda)}(z). \tag{41}$$

Taken together, (37), (40), and (41) indicate that the numerator N vanishes in the limit $s\to s_m$. The denominator D also vanishes in this limit, and therefore we can employ L'Hôpital's rule to evaluate K by writing

$$K=\lim_{s\to s_m}\frac{\partial N}{\partial s}\Big/\lim_{s\to s_m}\frac{\partial D}{\partial s}. \tag{42}$$

Since $\partial D/\partial s=1$ and the second term on the right-hand side of (37) is independent of s, we obtain

$$K=\lim_{s\to s_m}\frac{\partial}{\partial s}\pi^2(s-s_m)\frac{\Gamma(\frac{1}{2}-\kappa+\sqrt{s})}{\Gamma(1+2\sqrt{s})}W_{\kappa,\sqrt{s}}(x_{\max})M_{\kappa,\sqrt{s}}(x_{\min}). \tag{43}$$

Upon differentiation, we obtain after a fairly lengthy calculation

$$K=\frac{\pi^2e^{-(x+x_0)/2}(xx_0)^{(\lambda+1)/2}m!P_m^{(\lambda)}(x)P_m^{(\lambda)}(x_0)}{\Gamma(\lambda+m+1)}\left[-\gamma_E+\frac{1}{\lambda}+H-2\psi(\lambda+1)-\frac{1}{m+1}+\sum_{n=1}^{m+1}\frac{1}{n}\right], \tag{44}$$

where $\gamma_E\approx-0.577$ is Euler's constant, $\lambda=2\kappa-2m-1$,

$$H \equiv \frac{\partial}{\partial \beta} \ln[\, W_{\kappa,\beta}(x_{\max}) M_{\kappa,\beta}(x_{\min})\,] \Big|_{\beta=\sqrt{s_m}}, \tag{45}$$

and

$$\psi(z) \equiv \frac{d}{dz} \ln \Gamma(z). \tag{46}$$

Combining results, we find that in the special case $s = s_m = (\kappa - m - \frac{1}{2})^2$ the integral $I(s)$ is given by

$$\begin{aligned} I(s) &= \int_0^\infty \frac{u \sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{(\kappa-m-1/2)^2+u^2} W_{\kappa,iu}(x) W_{\kappa,iu}(x_0)\, du \\ &= K - 4\pi^2 e^{-(x+x_0)/2} \sum_{\substack{n=0 \\ n\neq m}}^{[\mathcal{R}e\,\kappa - 1/2]} \frac{\alpha n!}{\Gamma(\alpha+n+1)} \frac{(x x_0)^{(\alpha+1)/2}}{4s-\alpha^2} P_n^{(\alpha)}(x) P_n^{(\alpha)}(x_0), \end{aligned} \tag{47}$$

where $\alpha = 2\kappa - 2n - 1$. The allowed range of values for m is given by (33), which indicates that we must have $\mathcal{R}e\,\kappa \geqslant \frac{1}{2}$ in order for any of these special cases to occur. Note that the singular term with $n = m$ is not included in the sum, since that term is contained within K. Equations (30) and (47) cover all of the convergent cases of the fundamental integral $I(s)$. In Sec. VI we present simplified results obtained for certain values of the parameters.

VI. SPECIAL CASES

The general nature of the expression for $I(s)$ given by (30) encompasses many interesting special cases involving particular values for the parameters κ, s, x, and x_0. In this section, we shall briefly discuss a few illustrative examples obtained when the first index κ is equal to an integer, in which case the general solution for $I(s)$ simplifies considerably. For brevity, we shall focus here on situations with $s \neq s_m$. However, we emphasize that formulas similar to those discussed below that are applicable to the case $s = s_m$ can also be obtained in a straightforward manner by starting with (47) rather than (30).

A. $\kappa = 0$

When $\kappa = 0$, the summation in (30) is not performed at all. Making use of the identities[9]

$$\Gamma\left(\frac{1}{2} - iu\right)\Gamma\left(\frac{1}{2} + iu\right) = \frac{\pi}{\cosh(\pi u)} \tag{48}$$

and

$$\sinh(2\pi u) = 2 \sinh(\pi u)\cosh(\pi u), \tag{49}$$

we find that (30) reduces to

$$\int_0^\infty \frac{u \sinh(\pi u)}{s+u^2} W_{0,iu}(x) W_{0,iu}(x_0)\, du = \frac{\pi}{2} \frac{\Gamma(1/2+\sqrt{s})}{\Gamma(1+2\sqrt{s})} W_{0,\sqrt{s}}(x_{\max}) M_{0,\sqrt{s}}(x_{\min}). \tag{50}$$

This result is convergent for all complex values of s, excluding the negative real semiaxis. Hence the point $s = 0$ is convergent in this case.

B. $\kappa=1$

When $\kappa=1$, there is one simple pole located at $s_0=\frac{1}{4}$, and we can make use of the identity

$$\Gamma\left(-\frac{1}{2}-iu\right)\Gamma\left(-\frac{1}{2}+iu\right)=\frac{4\pi}{\cosh(\pi u)(1+4u^2)}, \tag{51}$$

along with (49) to reduce (30) to the form

$$\int_0^\infty \frac{u\sinh(\pi u)}{(1+4u^2)(s+u^2)}W_{1,iu}(x)W_{1,iu}(x_0)du=\frac{\pi}{8}\frac{\Gamma(\sqrt{s}-\frac{1}{2})}{\Gamma(1+2\sqrt{s})}W_{1,\sqrt{s}}(x_{\max})M_{1,\sqrt{s}}(x_{\min}) - \frac{\pi}{2}\frac{xx_0e^{-(x+x_0)/2}}{4s-1}. \tag{52}$$

The right-hand side converges for all complex values of s with the exception of the point $s=\frac{1}{4}$ [which must be treated using (47)] and the negative real semiaxis. The point $s=0$ is convergent.

C. $\kappa=2$

In this case there are two simple poles, located at $s_0=\frac{9}{4}$ and $s_1=\frac{1}{4}$. Utilizing the identity

$$\Gamma\left(-\frac{3}{2}-iu\right)\Gamma\left(-\frac{3}{2}+iu\right)=\frac{16\pi}{\cosh(\pi u)(9+4u^2)(1+4u^2)}, \tag{53}$$

along with (49), we can simplify (30) to obtain

$$\int_0^\infty \frac{u\sinh(\pi u)}{(9+4u^2)(1+4u^2)(s+u^2)}W_{2,iu}(x)W_{2,iu}(x_0)du = \frac{\pi}{32}\frac{\Gamma(\sqrt{s}-\frac{3}{2})}{\Gamma(1+2\sqrt{s})}W_{2,\sqrt{s}}(x_{\max})M_{2,\sqrt{s}}(x_{\min})-\frac{\pi}{8}e^{-(x+x_0)/2} \times\sum_{n=0}^{1}\frac{(3-2n)n!}{\Gamma(4-n)}\frac{(xx_0)^{2-n}}{4s-(3-2n)^2}P_n^{(3-2n)}(x)P_n^{(3-2n)}(x_0). \tag{54}$$

Evaluation of the Laguerre polynomials yields

$$\int_0^\infty \frac{u\sinh(\pi u)}{(9+4u^2)(1+4u^2)(s+u^2)}W_{2,iu}(x)W_{2,iu}(x_0)du = \frac{\pi}{32}\frac{\Gamma(\sqrt{s}-\frac{3}{2})}{\Gamma(1+2\sqrt{s})}W_{2,\sqrt{s}}(x_{\max})M_{2,\sqrt{s}}(x_{\min})-\frac{\pi}{16}xx_0e^{-(x+x_0)/2}\left[\frac{xx_0}{4s-9}+\frac{(2-x)(2-x_0)}{4s-1}\right], \tag{55}$$

which is convergent for all complex values of s, excluding the negative real semiaxis and the points $s=\frac{1}{4}$, $s=\frac{9}{4}$. These two points must be treated using (47). Note that the point $s=0$ is convergent in this case. Similar results can be obtained for any positive or negative integer value of κ. The integral formula given by (55) is of particular significance in treating the scattering of radiation in an ionized plasma with a constant temperature, as discussed in Sec. VII.

VII. APPLICATION TO THERMAL COMPTONIZATION

One of the most important physical applications of the results developed in this article involves the repeated Compton scattering of photons by a hot Maxwellian distribution of electrons with temperature T_e and number density n_e in an ionized plasma. This process, referred to as "thermal Comptonization," is the primary mechanism responsible for the production of the radiation spectra observed from celestial x-ray sources such as active galaxies, black holes, and neutron

stars.[2] When the electron temperature T_e is constant, the Green's function, $f_{\rm G}$, describing the temporal evolution of an initially monoenergetic radiation distribution satisfies the Kompaneets partial differential equation[1]

$$\frac{\partial f_{\rm G}}{\partial y}=\frac{1}{x^2}\frac{\partial}{\partial x}\left[x^4\left(f_{\rm G}+\frac{\partial f_{\rm G}}{\partial x}\right)\right], \tag{56}$$

where the dimensionless photon energy and the dimensionless time are denoted by

$$x(\epsilon)\equiv\frac{\epsilon}{kT_e},\quad y(t)\equiv n_e\sigma_{\rm T}c\,\frac{kT_e}{m_ec^2}(t-t_0), \tag{57}$$

respectively, and the quantities ϵ, t_0, t, $\sigma_{\rm T}$, m_e, c, and k represent the photon energy, the initial time, the current time, the Thomson cross section, the electron mass, the speed of light, and Boltzmann's constant, respectively. The terms proportional to $f_{\rm G}$ and $\partial f_{\rm G}/\partial x$ inside the parentheses on the right-hand side of (56) express in turn the effects of electron recoil and stochastic (second-order Fermi) photon energization. At the initial time $t=t_0$, the radiation distribution is monoenergetic, and the Green's function satisfies the initial condition

$$f_{\rm G}(x,x_0,y)\big|_{y=0}=x_0^{-2}\delta(x-x_0), \tag{58}$$

where the dimensionless initial energy is given by

$$x_0\equiv\frac{\epsilon_0}{kT_e}. \tag{59}$$

By operating on (56) with $\int_0^\infty x^2\,dx$, we can establish that $f_{\rm G}$ has the convenient normalization

$$\int_0^\infty x^2 f_{\rm G}(x,x_0,y)\,dx=\text{const}=1, \tag{60}$$

where the final result follows from the initial condition [Eq. (58)]. Note that this normalization is maintained for all values of y, which reflects the fact that Compton scattering conserves photons. It can be shown based on (56) that the Laplace transform of the Green's function,

$$F(x,x_0,s)\equiv\int_0^\infty e^{-sy}f_{\rm G}(x,x_0,y)\,dy, \tag{61}$$

is given by[3]

$$F(x,x_0,s)=x_0^{-2}x^{-2}e^{(x_0-x)/2}\frac{\Gamma(\mu-\frac{3}{2})}{\Gamma(1+2\mu)}M_{2,\mu}(x_{\rm min})W_{2,\mu}(x_{\rm max}), \tag{62}$$

where the quantity μ is a function of the transform variable s, defined by

$$\mu(s)\equiv(s+\tfrac{9}{4})^{1/2} \tag{63}$$

and

$$x_{\rm min}\equiv\min(x,x_0),\quad x_{\rm max}\equiv\max(x,x_0). \tag{64}$$

The solution for the Green's function is obtained by performing the inverse Laplace transformation using the Mellin integral,

$$f_G(x,x_0,y)=\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{sy}F(x,x_0,s)ds, \tag{65}$$

where the real constant γ is chosen so that the line $\mathcal{R}es=\gamma$ lies to the right of the singularities in the integrand. By transforming the variable of integration from s to

$$s'\equiv s+\tfrac{9}{4}, \tag{66}$$

we can obtain the equivalent expression

$$f_G(x,x_0,y)=\frac{e^{-9y/4}}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{s'y}\tilde{F}(x,x_0,s')ds', \tag{67}$$

where

$$\tilde{F}(x,x_0,s')\equiv x_0^{-2}x^{-2}e^{(x_0-x)/2}\frac{\Gamma(\sqrt{s'}-\frac{3}{2})}{\Gamma(1+2\sqrt{s'})}M_{2,\sqrt{s'}}(x_{\min})W_{2,\sqrt{s'}}(x_{\max}). \tag{68}$$

The exact solution for the Green's function $f_G(x,x_0,y)$ can be obtained by taking the inverse Laplace transformation of (55), which yields

$$\begin{aligned}&\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{sy}\frac{\Gamma(\sqrt{s}-\frac{3}{2})}{\Gamma(1+2\sqrt{s})}W_{2,\sqrt{s}}(x_{\max})M_{2,\sqrt{s}}(x_{\min})ds\\&\quad=\frac{32}{\pi}\int_0^\infty\frac{u\sinh(\pi u)}{(9+4u^2)(1+4u^2)}W_{2,iu}(x)W_{2,iu}(x_0)\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{e^{sy}}{s+u^2}ds\,du\\&\qquad+\frac{xx_0}{2}e^{-(x+x_0)/2}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{sy}\left[\frac{xx_0}{s-9/4}+\frac{(2-x)(2-x_0)}{s-1/4}\right]ds,\end{aligned} \tag{69}$$

where we have interchanged the order of integration in the double integral. The inverse Laplace transformations on the right-hand side of (69) are elementary in nature and can be evaluated using the formula

$$\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{e^{sy}}{s+k}ds=e^{-ky}. \tag{70}$$

By utilizing this result in (69), we obtain

$$\begin{aligned}&\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{sy}\frac{\Gamma(\sqrt{s}-\frac{3}{2})}{\Gamma(1+2\sqrt{s})}W_{2,\sqrt{s}}(x_{\max})M_{2,\sqrt{s}}(x_{\min})ds\\&\quad=\frac{32}{\pi}\int_0^\infty e^{-u^2y}\frac{u\sinh(\pi u)}{(9+4u^2)(1+4u^2)}W_{2,iu}(x)W_{2,iu}(x_0)du\\&\qquad+\frac{xx_0}{2}e^{-(x+x_0)/2}[xx_0e^{9y/4}+(2-x)(2-x_0)e^{y/4}].\end{aligned} \tag{71}$$

We can now combine (67), (68), and (71) to show that the exact solution for the time-dependent Green's function is given by[3]

$$f_G(x,x_0,y)=\frac{32}{\pi}e^{-9y/4}x_0^{-2}x^{-2}e^{(x_0-x)/2}\int_0^\infty e^{-u^2y}\frac{u\sinh(\pi u)}{(1+4u^2)(9+4u^2)}W_{2,iu}(x_0)W_{2,iu}(x)du+\frac{e^{-x}}{2}$$
$$+\frac{e^{-x-2y}}{2}\frac{(2-x)(2-x_0)}{x_0x}. \tag{72}$$

Since the fundamental partial differential equation (56) is linear, the particular solution for the radiation distribution corresponding to an *arbitrary* initial spectrum can be found via convolution using the Green's function. The result given by (72) is therefore of central importance in the field of theoretical x-ray astronomy.

VIII. CONCLUSION

In this article, we have developed several new formulas for the evaluation of a family of integrals containing the product of two Whittaker $W_{\kappa,\mu}(x)$-functions, when the integration occurs with respect to the second index μ, and that index is imaginary. The fundamental integral we have focused on is

$$I(s)\equiv\int_0^\infty\frac{u\sinh(2\pi u)\Gamma(\frac{1}{2}-\kappa-iu)\Gamma(\frac{1}{2}-\kappa+iu)}{s+u^2}W_{\kappa,iu}(x)W_{\kappa,iu}(x_0)du. \tag{73}$$

This is related to the Whittaker function index transformation discussed in Refs. 10 and 11. An expression of particular interest is the quadratic normalization integral given by (31). The results presented in (30) and (47) for $I(s)$ allow the exact evaluation of all of the convergent cases of this integral without the need to resort to numerical integration. We also point out that by utilizing Eqs. (2), one can easily obtain a set of analogous integration formulas applicable to the Kummer functions $\Phi(a,b,z)$ and $\Psi(a,b,z)$. While integrals of this precise type have not been considered before, it is worth noting that $I(s)$ is a member of a wider group of integrals containing the product of two Whittaker *W*-functions. In general, the other integrals in this group involve integration with respect to one of the other parameters, rather than the second index as we have considered here. We briefly review a few of these related integrals below.

Several formulas are available in the previous literature for evaluating the integral of the product of two Whittaker $W_{\kappa,\mu}(x)$-functions with respect to the primary argument *x*. For example, based upon Eq. (9.12) from Buchholz[12] or Eq. (20.3.40) from Erdélyi *et al.*[13] or Eq. (7.611.3) from Gradshteyn and Ryzhik,[8] we have

$$\int_0^\infty W_{\kappa,\mu}(x)W_{\sigma,\mu}(x)\frac{dx}{x}=\frac{1}{\kappa-\sigma}\frac{\pi}{\sin(2\pi\mu)}\left[\frac{1}{\Gamma(\frac{1}{2}-\kappa+\mu)\Gamma(\frac{1}{2}-\sigma-\mu)}\right.$$
$$\left.-\frac{1}{\Gamma(\frac{1}{2}-\kappa-\mu)\Gamma(\frac{1}{2}-\sigma+\mu)}\right], \tag{74}$$

which is valid provided $|\mathcal{R}e\,\mu|<\frac{1}{2}$. We note that the formulas in Refs. 8 and 13 are missing a factor of π, and the formula in Ref. 12 contains two incorrect signs. Another closely related example is given by Eq. (7.611.6) from Gradshteyn and Ryzhik[8] or Eq. (20.3.41) from Ref. 13,

$$\int_0^\infty x^{\sigma-1}W_{\kappa,\mu}(x)W_{-\kappa,\mu}(x)dx=\frac{\Gamma(\sigma+1)\Gamma(\sigma/2+\frac{1}{2}+\mu)\Gamma(\sigma/2+\frac{1}{2}-\mu)}{2\Gamma(\sigma/2+1+\kappa)\Gamma(\sigma/2+1-\kappa)}, \tag{75}$$

which is valid provided $\mathcal{R}e\,\sigma>2|\mathcal{R}e\,\mu|-1$.

A few formulas that treat the integration of a product of two Whittaker $W_{\kappa,\mu}(x)$-functions with respect to the first index κ have also been known for some time. The most general expression is Eq. (15.10b) from Buchholz,[12] which can be written as

$$\int_0^\infty \Gamma(k-iu)\Gamma(k+iu)W_{iu,k-1/2}(x)W_{-iu,k-1/2}(x_0)du$$

$$=\sqrt{\pi}\Gamma(2k)(xx_0)^k(x+x_0)^{-2k+1/2}K_{2k-1/2}\left(\frac{x+x_0}{2}\right), \tag{76}$$

where $K_{2k-1/2}(z)$ denotes the modified Bessel function. When $k=\frac{1}{2}$, this formula reduces to Eq. (7.691) from Ref. 8, which states that

$$\int_0^\infty \mathrm{sech}(\pi u)W_{iu,0}(x)W_{-iu,0}(x_0)du=\frac{\sqrt{xx_0}}{x+x_0}e^{-(x+x_0)/2}. \tag{77}$$

The new results for $I(s)$ obtained in this article [Eqs. (30) and (47)] are in some sense complementary to these previously known formulas. We emphasize that the expressions developed here are of significance in a variety of applications, including the problem of the Comptonization of radiation in an isothermal plasma, discussed in Sec. VII. Our general approach may also allow the determination of the Green's function solution for the one-dimensional Schrödinger equation with the Morse potential.[14] We plan to pursue this question in future work.

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Topologically nontrivial quantum layers

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Given a complete noncompact surface Σ embedded in $\mathbb{R}^3$, we consider the Dirichlet Laplacian in the layer Ω that is defined as a tubular neighborhood of constant width about Σ. Using an intrinsic approach to the geometry of Ω, we generalize the spectral results of the original paper by Duclos *et al.* [Commun. Math. Phys. **223**, 13 (2001)] to the situation when Σ does not possess poles. This enables us to consider topologically more complicated layers and state new spectral results. In particular, we are interested in layers built over surfaces with handles or several cylindrically symmetric ends. We also discuss more general regions obtained by compact deformations of certain Ω. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The spectral properties of the Dirichlet Laplacian in infinitely stretched regions have attracted a lot of attention since the existence of geometrically induced discrete spectrum for certain strips in the plane was proved in Ref. 1. The study was motivated by mesoscopic physics where a reasonable model for the dynamics of a particle in quantum waveguides is given by the Laplacian in hard-wall tubular neighborhoods of infinite curves in $\mathbb{R}^d$, $d=2,3$ (quantum strips, tubes), or surfaces in $\mathbb{R}^3$ (quantum layers); see Refs. 2 and 3 for the physical background and references. Nowadays, it is well known that any nontrivial curvature of the reference curve, that is asymptotically straight, produces bound states below the essential spectrum in the strips and tubes.[2,4,5]

The analogous problem in curved layers is much more complicated and it was investigated quite recently in Refs. 6–8. Let Σ be a complete noncompact surface embedded in $\mathbb{R}^3$, Ω be a tube of radius $a>0$ about Σ, i.e. (see Fig. 1),

$$\Omega := \{z \in \mathbb{R}^3 \mid \text{distance}\,(z,\Sigma) < a\}, \tag{1}$$

and $-\Delta_D^{\Omega}$ denote the Dirichlet Laplacian in $L^2(\Omega)$. If the surface is a locally deformed plane, the existence of bound states below the essential spectrum of the Laplacian was demonstrated in Ref. 7. A more general situation was treated in Ref. 6; assuming that Σ is nontrivially curved, it has asymptotically vanishing curvatures and possesses a pole, several sufficient conditions are found

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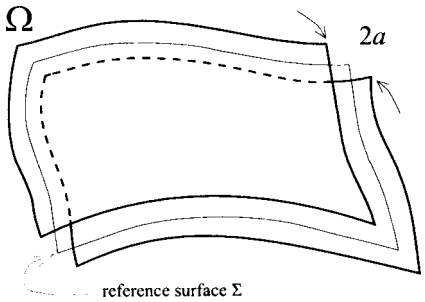

FIG. 1. The configuration space Ω defined by (1) as the space delimited by two parallel surfaces at the distance a from Σ.

which guarantee the existence of discrete spectrum. Finally, let us mention that an asymptotic expansion of the ground-state eigenvalue in layers built over mildly curved planes was found in Ref. 8.

While Ref. 6 covers a wide class of layers, the technical requirement about the existence of a pole on Σ (i.e., the exponential map is a diffeomorphism) restricted substantially the topological structure of the reference surface. In particular, Σ was necessarily diffeomorphic to $\mathbb{R}^2$ and as such it was simply connected. The main goal of this paper is to extend the sufficient conditions established in Ref. 6 without assuming the existence of poles on Σ and without making any other (unnatural) topological and geometrical assumptions. In addition to this substantial generalization, we will derive particularly interesting spectral results for quantum layers built over surfaces with handles or several cylindrically symmetric ends (see Figs. 2–4).

Let us recall the reason why the existence of a pole on Σ was required in Ref. 6. According to the usual strategy used in the spectral theory of quantum waveguides, one expresses the Laplacian $-\Delta_D^\Omega$ in the pair of coordinates (x,u), where x parametrizes the reference surface Σ and $u \in (-a,a)$ its normal bundle. Assuming the existence of a pole, Σ could be parametrized globally by means of geodesic polar coordinates, which were well suited for the construction of explicit mollifiers on Σ needed to regularize generalized trial functions establishing the existence of bound states below the essential spectrum.

There are several possibilities how to treat surfaces without poles. Since the above-mentioned regularization is needed out of a compact part of Σ only, one way is to replace the polar coordinates by geodesic coordinates based on a curve enclosing the interior part. This approach is well suited for surfaces of one end (see the definition below), however, it has to be modified in more general situations. In this paper, we introduce a different strategy which does not require any special choice of coordinates on Σ. We employ substantially a consequence of Ref. 9 that if the Gauss curvature is integrable then there always exists a sequence of functions on Σ having the properties of the mollifiers mentioned earlier.

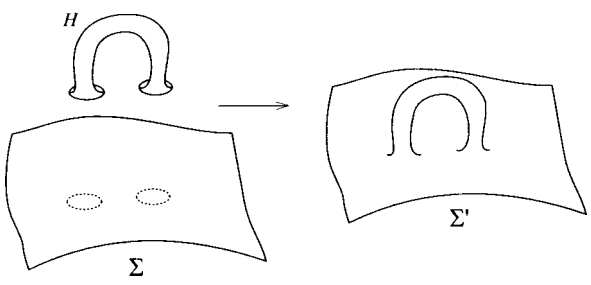

FIG. 2. Surface with a handle Σ' is constructed from Σ by attaching smoothly to it a curved cylindrical surface H. By virtue of Corollary 1, one handle is sufficient to achieve the condition (a) of Theorem 1.

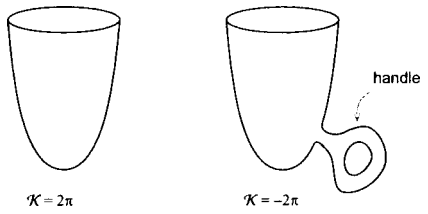

FIG. 3. Elliptic paraboloid (without or with one handle attached, respectively) of Example 1.

II. STATEMENT OF RESULTS

To state here the main results we need to introduce some notation and basic assumptions. Let κ_1^2 denote the spectral threshold of the planar layer of width $2a$, i.e., $\kappa_1 := \pi/(2a)$. The induced metric on Σ and the corresponding covariant derivative will be denoted by g and ∇_g, respectively. Let K, M, and $k_\pm$ denote, respectively, the Gauss curvature, the mean curvature, and the principal curvatures of Σ. Denoting by $\mathrm{d}\Sigma$ the surface area-element, we may define the total Gauss curvature $\mathcal{K}$ and the total mean curvature $\mathcal{M}$, respectively, by the integrals

$$\mathcal{K} := \int_\Sigma K \, \mathrm{d}\Sigma, \quad \mathcal{M}^2 := \int_\Sigma M^2 \, \mathrm{d}\Sigma. \tag{2}$$

The latter always exists (it may be $+\infty$), while the former is well defined provided

$$\langle \mathrm{H1} \rangle \quad K \in L^1(\Sigma),$$

which will be a characteristic assumption of this work. Henceforth, we shall also assume that $k_\pm$ are bounded and

$$\langle \mathrm{H2} \rangle \quad a < \rho_m := (\max\{\|k_+\|_\infty, \|k_-\|_\infty\})^{-1} \quad \text{and } \Omega \text{ does not overlap,}$$

which we need in order to ensure that the layer Ω is a submanifold of $\mathbb{R}^3$. An open set $E \subseteq \Sigma$ is called an *end* of Σ if it is connected, unbounded and if its boundary ∂E is compact (see Fig. 4); its total curvatures are defined by means of (2) with the domain of integration being the subset E only. We say that a manifold embedded in $\mathbb{R}^3$ is cylindrically symmetric if it is invariant under rotations about a fixed axis in $\mathbb{R}^3$. Our main result reads as follows.

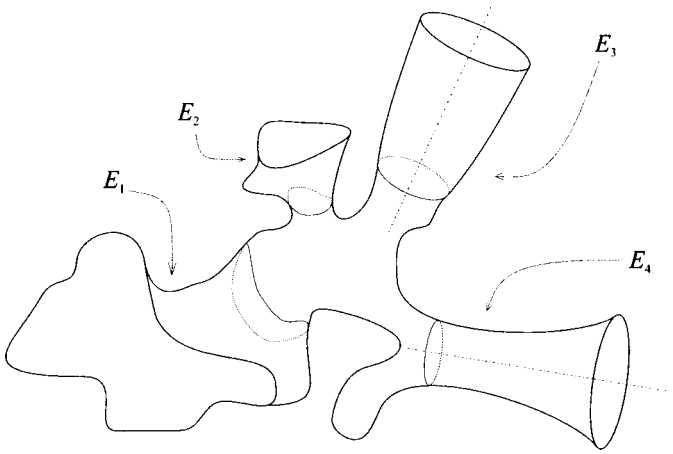

FIG. 4. Surface with four ends $(E_1, \ldots, E_4)$. By virtue of Theorem 2, each cylindrically symmetric end (E_3, E_4) with a positive total Gauss curvature and curvatures vanishing at infinity produces at least one discrete eigenvalue.

Theorem 1: *Let Σ be a complete noncompact connected surface of class C^2 embedded in $\mathbb{R}^3$ and satisfying $\langle$H1$\rangle$. Let the layer Ω defined by (1) as the tube of radius $a>0$ about Σ satisfy $\langle$H2$\rangle$.*

(i) If the curvatures K and M vanish at infinity of Σ, then

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) = \kappa_1^2 .$$

(ii) If the surface Σ is not a plane, then any of the conditions

(a) $\mathcal{K} \leqslant 0$,
(b) *a is small enough and* $\nabla_g M \in L^2_{\mathrm{loc}}(\Sigma)$,
(c) $\mathcal{M} = +\infty$ *and* $\nabla_g M \in L^2(\Sigma)$,
(d) *Σ contains a cylindrically symmetric end with a positive total Gauss curvature*

is sufficient to guarantee that

$$\inf \sigma(-\Delta_D^{\Omega}) < \kappa_1^2 .$$

Consequently, if the surface Σ is not a plane but its curvatures vanish at infinity, then any of the conditions (a)–(d) is sufficient to guarantee that $-\Delta_D^{\Omega}$ has at least one eigenvalue of finite multiplicity below the threshold of its essential spectrum, i.e., $\sigma_{\mathrm{disc}}(-\Delta_D^{\Omega}) \neq \varnothing$.

Let us compare this theorem with the results obtained in Ref. 6. An improvement concerns the essential spectrum. While only a lower bound on the threshold was found in Ref. 6, here we shall use known results about the spectral threshold of complete surfaces in order to show that the essential spectrum starts just at κ_1^2. Conditions (a)–(d) are adopted from Ref. 6, however, we do not assume that Σ is of class C^3 in (b) and (c) of Theorem 1, which was required in Ref. 6 in order to give a meaning to $\nabla_g M$. Indeed, only the integrability conditions on the gradient are needed.

The most significant generalization concerning all the results is that we have gotten rid of the strong assumption about the existence of a pole on Σ. Actually, Theorem 1 involves quantum layers built over general surfaces without any additional hypotheses about the existence of a special global parametrization, the number of ends, and other topological and geometrical restrictions.

An interesting new spectral result then follows from the observation that making the topology of Σ more complicated than that of the plane, one always achieves that the basic condition (a) is satisfied.

Corollary 1: Under the assumptions of Theorem 1, one has $\inf \sigma(-\Delta_D^{\Omega}) < \kappa_1^2$ *whenever Σ is not conformally equivalent to the plane.*

Indeed, the Cohn–Vossen inequality[10] yields

$$\mathcal{K} \leqslant 2\pi\,(2-2h-e), \tag{3}$$

where h is the genus of Σ, i.e., the number of handles, and e is the number of ends. In particular, the condition (a) of Theorem 1 is always fulfilled whenever the surface is not simply connected.

Example 1: Let Σ be the elliptic paraboloid. It is easy to check that it has curvatures vanishing at infinity and that the condition (c) of Theorem 1 is always fulfilled. On the other hand, it violates the condition (d) whenever it is not a paraboloid of revolution, and the condition (a) does not hold because the total Gauss curvature is always equal to 2π. Attaching a handle to Σ, the total curvature becomes equal to -2π (see Fig. 3).

It was proven in Ref. 6 that any layer built over a cylindrically symmetric surface diffeomorphic to $\mathbb{R}^2$ has a spectrum below the energy κ_1^2. Since this class of reference surfaces may only have a non-negative total Gauss curvature, it gave an important alternative condition to (a) in the case $\mathcal{K}>0$. In Theorem 1, an interesting generalization to Ref. 6 is introduced by virtue of the condition (d), where it is supposed now that only an unbounded subset of Σ admits a cylindrical symmetry at infinity (see Fig. 4). This extension is possible due to the fact that the sequence of trial functions establishing the existence of spectrum below κ_1^2 for surfaces of revolution with $\mathcal{K}>0$ is ''localized at infinity'' (i.e., for any compact set of Ω, there is an element from the

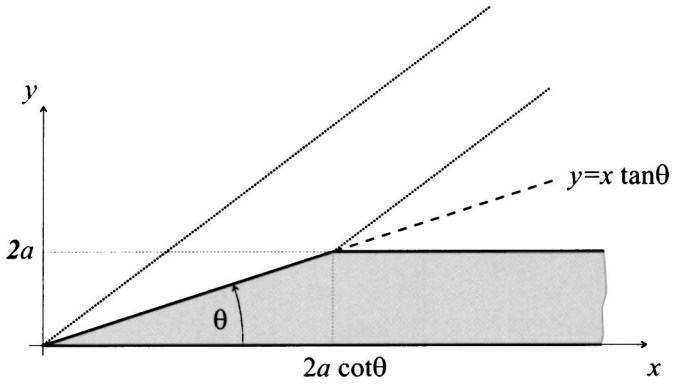

FIG. 5. The planar region of Example 2.

sequence supported out of the compact). Consequently, it may be localized just at the end satisfying condition (d) of Theorem 1. Since any deformation of a bounded part of Ω does not affect this spectral result, we may consider more general regions than tubes (1). What is important is that such local deformations do not include only bends and protrusions which are traditionally a source of binding, but constrictions as well. Moreover, since such trial functions localized at different ends will be orthogonal as elements of $L^2(\Omega)$, we may produce an arbitrary number of bound states by attaching to Ω a sufficient number of suitable outlets. Finally, since the essential spectrum is stable under compact deformation of Ω, we arrive at the following result.

Theorem 2: *Let Ω be a layer (1) satisfying $\langle$H1$\rangle$, $\langle$H2$\rangle$ and the condition (i) of Theorem 1. Assume that the reference surface Σ contains $N\geqslant 1$ cylindrically symmetric ends, each of them having a positive total Gauss curvature. Let Ω' be an unbounded region without boundary in $\mathbb{R}^3$ obtained by any compact deformation of Ω. Then*

(i) $\inf\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega'})=\kappa_1^2$,
(ii) there will be at least N eigenvalues in $(0,\kappa_1^2)$, with the multiplicity taken into account.

Example 2: Fix $\theta\in(0,\pi/2)$ and consider the conical region Ω' in $\mathbb{R}^3$ given by rotating the planar region (see Fig. 5):

$$\{(x,y)\in\mathbb{R}^2\,|\;\;(x,y)\in((0,2a\cot\theta)\times(0,x\tan\theta])\cup([2a\cot\theta,\infty)\times(0,2a))\}$$

along the axis $y=x\tan\theta$ in $\mathbb{R}^3$. Note that Ω' is not a layer (1) because of the singularity of the conical surface. Nevertheless, it may be considered as a compact deformation of the layer built over a smoothed cone whose total Gauss curvature is equal to $2\pi(1-\sin\theta)\in(0,2\pi)$. Consequently, we know that $-\Delta_D^{\Omega'}$ possesses at least one discrete eigenvalue below κ_1^2 due to Theorem 2. This is a nontrivial result for flat enough conical layers only, since using a trick analogous to that of Ref. 11 one can check that the cardinality of $\sigma_{\mathrm{disc}}(-\Delta_D^{\Omega'})$ can exceed any fixed integer for θ small enough.

III. PRELIMINARIES

Let Σ be a connected orientable surface of class C^2 embedded in $\mathbb{R}^3$. The orientation can be specified by the choice of a globally defined unit normal vector field, $n:\Sigma\to S^2$, which is a function of class C^1. For any $x\in\Sigma$, the Weingarten map

$$L_x:\; T_x\Sigma\to T_x\Sigma:\{\xi\mapsto-\mathrm{d}n_x(\xi)\} \tag{4}$$

defines the principal curvatures $k_\pm$ of Σ as its eigenvalues with respect to the induced metric g. The Gauss curvature and the mean curvature are defined by $K:=k_+k_-$ and $M:=\frac{1}{2}(k_++k_-)$, respectively, and are continuous functions on Σ.

Put $a>0$. We define a layer Ω of width $2a$ as the image of the mapping

$$\mathcal{L}:\ \Sigma\times(-a,a)\to\mathbb{R}^3:\{(x,u)\mapsto x+u\,n(x)\}. \tag{5}$$

Henceforth, we shall always assume ⟨H2⟩. Then $\mathcal{L}$ induces a diffeomorphism and Ω is a submanifold of $\mathbb{R}^3$ corresponding to the set of points squeezed between two parallel surfaces at the distance a from Σ (see Fig. 1), i.e., if Σ does not have a boundary then the definition of Ω via (5) and (1) are equivalent. We shall identify it with the Riemannian manifold $\Sigma\times(-a,a)$ endowed with the metric G induced by the immersion (5). One has

$$G=g\circ(I_x-u\,L_x)^2+\mathrm{d}u^2,\quad \mathrm{d}\Omega=(1-2Mu+Ku^2)\mathrm{d}\Sigma\,\mathrm{d}u, \tag{6}$$

where I_x denotes the identity map on $T_x\Sigma$ and $\mathrm{d}\Omega$ stands for the volume element of Ω. It is worth noticing that (6) together with ⟨H2⟩ yields that G can be estimated by the surface metric,

$$C_-g+\mathrm{d}u^2\leqslant G\leqslant C_+g+\mathrm{d}u^2,\quad \text{where}\quad C_\pm:=(1\pm a\rho_m^{-1})^2. \tag{7}$$

Remark 1: Formally, it is possible to consider $(\Sigma\times(-a,a),G)$ as an abstract Riemannian manifold where only the surface Σ is embedded in $\mathbb{R}^3$. Then we do not need to assume the second part of ⟨H2⟩, i.e., "Ω does not overlap."

We denote by $-\Delta_D^\Omega$, or simply $-\Delta$, the Dirichlet Laplacian on $L^2(\Omega)$. We shall consider it in a generalized sense as the operator associated with the Dirichlet form

$$Q(\psi,\phi):=\int_\Omega\langle\nabla\psi,\nabla\phi\rangle\,\mathrm{d}\Omega\quad\text{with}\quad \mathrm{Dom}\,Q:=W_0^{1,2}(\Omega). \tag{8}$$

Here ∇ is the gradient corresponding to the metric G and $\langle\cdot,\cdot\rangle$ denotes the inner product in the manifold Ω induced by G; the associated norm will be denoted by $|\cdot|$. Similarly, the inner product and the norm in the Hilbert space $L^2(\Omega)$ will be denoted by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively. We shall sometimes abuse the notation slightly by writing $(\cdot,\cdot)\equiv\int_\Omega\langle\cdot,\cdot\rangle\mathrm{d}\Omega$ and $\|\cdot\|\equiv\int_\Omega|\cdot|\mathrm{d}\Omega$ for vector fields. The subscript "g" will be used in order to distinguish similar objects associated to the surface Σ.

Since the quadratic form Q is densely defined, symmetric, positive, and closed on its domain, the corresponding Laplacian $-\Delta$ is a positive self-adjoint operator. Denoting by $(x^\mu)\equiv(x^1,x^2)$ local coordinates for Σ and by G^{ij} the coefficients of the inverse of G in the coordinates $(x^i)\equiv(x^\mu,u)$ for Ω, we can write

$$-\Delta\ =\ -|G|^{-1/2}\partial_i|G|^{1/2}G^{ij}\partial_j\ =\ -|G|^{-1/2}\partial_\mu|G|^{1/2}G^{\mu\nu}\partial_\nu-\partial_u^2+2M_u\,\partial_u \tag{9}$$

in the form sense, where $|G|:=\det G$ and

$$M_u:=\frac{M-Ku}{1-2Mu+Ku^2}, \tag{10}$$

which is the mean curvature of the parallel surface $\mathcal{L}(\Sigma\times\{u\})$.

The above definitions of Ω and the corresponding Dirichlet Laplacian are valid for any orientable surface Σ of class C^2 provided ⟨H2⟩ (or its first part only in view of Remark 1) holds true. Nevertheless, since we are interested in the existence of discrete spectrum of $-\Delta_D^\Omega$, and it always exists whenever Ω is bounded, in the sequel we shall assume that Σ is *complete* and *noncompact*.

It is easy to see that the spectrum of the planar layer $\Omega_0 := \mathbb{R}^2 \times (-a,a)$ is purely continuous and coincides with the interval $[\kappa_1^2, \infty)$, where the threshold is the first eigenvalue of the Dirichlet Laplacian on the transverse section, i.e., $\kappa_1 := \pi/(2a)$. In what follows we shall use the corresponding normalized eigenfunction given explicitly by

$$\chi_1(u) := \sqrt{\frac{1}{a}} \cos \kappa_1 u. \tag{11}$$

Using the identities $|\nabla u| = 1$ and $-\Delta u = 2M_u$, we get

$$-\Delta \chi_1(u) = 2M_u \chi_1'(u) + \kappa_1^2 \chi_1(u)\,. \tag{12}$$

IV. ESSENTIAL SPECTRUM

We shall localize the essential spectrum of $-\Delta_D^\Omega$ for *asymptotically planar* layers, i.e., the curvatures of Σ vanish at infinity which we abbreviate by

$$K, M \overset{\infty}{\to} 0. \tag{13}$$

Recall that a function f, defined on a noncompact manifold Σ, is said to vanish at infinity if

$$\forall \epsilon > 0 \quad \exists R_\epsilon > 0, x_\epsilon \in \Sigma \quad \forall x \in \Sigma \setminus \overline{B(x_\epsilon, R_\epsilon)} : \quad |f(x)| < \epsilon\,,$$

where $B(x_\epsilon, R_\epsilon)$ denotes the open ball of center x_ϵ and radius R_ϵ. The property (13) is equivalent to the vanishing of the principal curvatures, i.e., $k_\pm \overset{\infty}{\to} 0$.

The proof of statement (i) of Theorem 1 is achieved in two steps. If the layer is asymptotically planar, then it was shown in Ref. 6 that the essential spectrum of $-\Delta_D^\Omega$ is bounded from below by κ_1^2 provided the surface possesses a pole. Here we adapt this proof (based on a Neumann bracketing argument) to the case of any complete surface with asymptotically vanishing curvatures. In the second part of this section, we establish the opposite bound on the threshold by means of a different method.

A. Lower bound, $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \geqslant \kappa_1^2$

Fix an $\epsilon > 0$ and consider an open precompact region $\mathcal{B} \supseteq B(x_\epsilon, R_\epsilon)$ with C^1-smooth boundary such that

$$\forall (x,u) \in \Omega_{\mathrm{ext}} : (1 - a\epsilon)^2 \leqslant 1 - 2M(x)\, u + K(x)\, u^2 \leqslant (1 + a\epsilon)^2, \tag{14}$$

where $\Omega_{\mathrm{ext}} := \Omega \setminus \overline{\Omega}_{\mathrm{int}}$ with $\Omega_{\mathrm{int}} := \mathcal{B} \times (-a,a)$. Denote by $-\Delta_N$ the Laplacian $-\Delta_D^\Omega$ with a supplementary Neumann boundary condition on $\partial\mathcal{B} \times (-a,a)$, that is, the operator associated with the form $Q_N := Q_N^{\mathrm{int}} \oplus Q_N^{\mathrm{ext}}$, where

$$Q_N^\omega(\psi, \phi) := \int_{\Omega_\omega} \langle \nabla \psi, \nabla \phi \rangle \, \mathrm{d}\Omega, \quad \mathrm{Dom}\, Q_N^\omega := \{ \psi \in W^{1,2}(\Omega_\omega) \,|\, \psi(\cdot, \pm a) = 0 \}$$

for $\omega \in \{\mathrm{int}, \mathrm{ext}\}$. Since $-\Delta_D^\Omega \geqslant -\Delta_N$ and the spectrum of the operator associated to Q_N^{int} is purely discrete, cf. Ref. 12, Chap. 7, the minimax principle gives the estimate

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \geqslant \inf \sigma_{\mathrm{ess}}(-\Delta_N^{\mathrm{ext}}) \geqslant \inf \ \sigma(-\Delta_N^{\mathrm{ext}}),$$

where $-\Delta_N^{\mathrm{ext}}$ denotes the operator associated to Q_N^{ext}. Neglecting the non-negative "longitudinal" part of the Laplacian [i.e., the first term at the right-hand side of (9)] and using the estimates (14), we arrive easily at the following lower bound:

$$-\Delta_N^{\mathrm{ext}} \geqslant \left(\frac{1-a\epsilon}{1+a\epsilon}\right)^2 \kappa_1^2 \quad \text{in} \quad L^2(\Omega_{\mathrm{ext}}),$$

which holds in the form sense (see also proof of Theorem 4.1 in Ref. 6). The claim then follows by the fact that ϵ can be chosen arbitrarily small.

B. Upper bound, $\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) \leqslant \kappa_1^2$

It follows from Ref. 13 that if $K \overset{\infty}{\to} 0$ then the threshold of the (essential) spectrum of the Laplacian on Σ, $-\Delta_g$, equals 0. This is equivalent to the statement that for any $\varepsilon > 0$ there exists an infinite-dimensional subspace $\mathcal{D}_g \subseteq C_0^\infty(\Sigma)$ such that

$$\forall \varphi \in \mathcal{D}_g: \quad \|\nabla_g \varphi\|_g \leqslant \varepsilon \|\varphi\|_g . \tag{15}$$

It is easy to see that the following identity holds true:

$$\forall \varphi \in C_0^\infty(\Sigma): \quad \|\nabla \varphi \chi_1\|^2 = \||\nabla \varphi|\, \chi_1\|^2 - (\varphi \chi_1, \varphi \Delta \chi_1). \tag{16}$$

Using the estimates (7) and (15), we have

$$\||\nabla \varphi|\, \chi_1\|^2 \leqslant (C_+ / C_-^2)\, \varepsilon^2 \|\varphi\, \chi_1\|^2,$$

while the second term at the right-hand side of (16) can be rewritten by means of (12) as follows:

$$-(\varphi \Delta \chi_1, \varphi \chi_1) = \kappa_1^2 \|\varphi\, \chi_1\|^2 + (\varphi \chi_1', 2M_u \varphi \chi_1).$$

Integrating by parts with respect to u in the second term at the right-hand side of the last equality, we conclude from (16) that for any $\varepsilon > 0$ there exists $\mathcal{D} := \mathcal{D}_g \otimes \{\chi_1\} \subset C_0^\infty(\Omega)$ such that

$$\forall \psi \in \mathcal{D}: \quad \|\nabla \psi\|^2 - (\psi, K_u \psi) \leqslant (\kappa_1^2 + (C_+ / C_-^2)\, \varepsilon^2) \|\psi\|^2,$$

where

$$K_u := \frac{K}{1 - 2Mu + Ku^2}$$

is the Gauss curvature of the parallel surface $\mathcal{L}(\Sigma \times \{u\})$. This proves that $\inf \sigma_{\mathrm{ess}}(-\Delta - K_u) \leqslant \kappa_1^2$. Since K_u vanishes at infinity by the assumption (13), i.e., the operator $K_u(-\Delta + 1)^{-1}$ is compact in $L^2(\Omega)$, the same spectral result holds for the operator $-\Delta$.

Remark 2: Notice that only $K \overset{\infty}{\to} 0$ is needed in order to establish the upper bound.

V. GEOMETRICALLY INDUCED SPECTRUM

It was shown in Sec. IV that the threshold of the essential spectrum is stable under any deformation of the planar layer such that the deformed layer is still planar asymptotically in the sense of (13). The aim of this section is to prove the sufficient conditions (a)–(d) of the second part of Theorem 1, which guarantee the existence of spectrum below the energy κ_1^2. Since the spectral threshold of the planar layer is just κ_1^2, the spectrum below this value is induced by the curved geometry and it consists of discrete eigenvalues if the layer is asymptotically planar.

All the proofs here are based on the variational idea of finding a trial function Ψ from the form domain of $-\Delta_D^{\Omega}$ such that

$$Q_1[\Psi] := Q[\Psi] - \kappa_1^2 \|\Psi\|^2 < 0. \tag{17}$$

The important technical tool needed to establish conditions (a)–(c) is the existence of appropriate mollifiers on Σ which is ensured by the following lemma.

Lemma 1: Assume $\langle$H1$\rangle$. *Then there exists a sequence* $\{\varphi_n\}_{n\in\mathbb{N}}$ *of smooth functions with compact supports in* Σ *such that*

(1) $\forall n\in\mathbb{N}$: $0\leqslant\varphi_n\leqslant 1$,
(2) $\|\nabla_g\varphi_n\|_g \underset{n\to\infty}{\to} 0$,
(3) $\varphi_n \underset{n\to\infty}{\to} 1$ *uniformly on compacts of* Σ.

Proof: If $\langle$H1$\rangle$ holds true then it follows from Ref. 9 that (Σ,g) is conformally equivalent to a closed surface from which a finite number of points have been removed. However, the integral $\|\nabla_g\varphi_n\|_g$ is a conformal invariant and it is easy to find a sequence having the required properties on the ''pierced'' closed surface. □

This sequence enables us to regularize a generalized trial function which would give formally a negative value of the functional (17), however, it is not integrable in $L^2(\Sigma)$. Since the trial functions used below are adopted from Ref. 6 and the proofs using different mollifiers of Lemma 1 require just slight modifications, we will not go into great details in the proofs of conditions (a)–(c). The sufficient condition (d) does not use the mollifiers of Lemma 1. This condition is established by means of the fact that the sequence of trial functions employed in Ref. 6 for cylindrically symmetric layers was localized only at infinity of the layer.

A. Condition (a)

Using the first transverse mode (11) as the generalized trial function, one gets

$$Q_1[\varphi_n\chi_1]=\||\nabla\varphi_n|\,\chi_1\|^2+(\varphi_n,K\varphi_n)_g\,.$$

Since $|\nabla\varphi_n|$ can be estimated by $|\nabla_g\varphi_n|_g$ by means of (7), the first term at the right-hand side tends to zero as $n\to\infty$ due to Lemma 1. The second one tends to the total Gauss curvature $\mathcal{K}$ because of Lemma 1 and the dominated convergence theorem. Hence, if $\mathcal{K}<0$, we can find a finite n_0 such that $Q_1[\varphi_{n_0}\chi_1]<0$.

In the critical case, i.e., $\mathcal{K}=0$, one adds to $\varphi_n\chi_1$ a small deformation term. Let ε be a real number, which will be specified later, and let j be an infinitely smooth positive function on Σ with a compact support in a region where the mean curvature M is nonzero and does not change sign. Defining $\theta(x,u):=j(x)u\chi_1(u)$, one can write

$$Q_1[\varphi_n\chi_1+\varepsilon\theta]=Q_1[\varphi_n\chi_1]+2\varepsilon\,Q_1(\theta,\varphi_n\chi_1)+\varepsilon^2Q_1[\theta].$$

Since $\mathcal{K}=0$, the first term at the right-hand side of this identity tends to zero as $n\to\infty$. The shifted quadratic form in the second term can be written as a sum of three terms:

$$Q_1(\theta,\varphi_n\chi_1)=(\theta,2M_u\,\varphi_n\chi_1')+(\nabla\theta\chi_1,\nabla\varphi_n)-2(\theta\nabla\chi_1,\nabla\varphi_n),$$

where the last two terms tend to zero as $n\to\infty$ by means of the Schwarz inequality, the estimates (7) and Lemma 1, while an explicit calculation gives that the first integral is equal to $-(j,M\varphi_n)_g$ which tends to a *nonzero* number $-(j,M)_g$. Since θ does not depend on n, one gets

$$Q_1[\varphi_n\chi_1+\varepsilon\theta]\underset{n\to\infty}{\to}-2\varepsilon\,(j,M)_g+\varepsilon^2Q_1[\theta],$$

which may be made negative by choosing ε sufficiently small and of an appropriate sign. □

B. Conditions (b) and (c)

Here we use the trial function $\psi_n(x,u):=(1+M(x)u)\,\varphi_n(x)\chi_1(u)$. Since

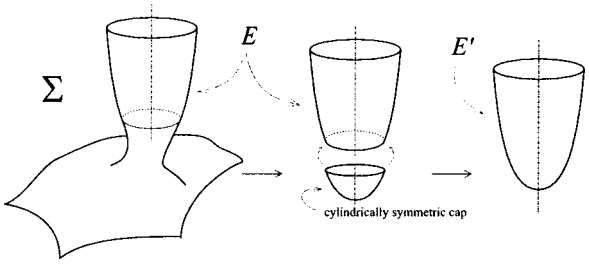

FIG. 6. Construction of a simply connected surface of revolution E' from a cylindrically symmetric end $E\subset\Sigma$.

$$\nabla\psi_n(\cdot,u)=(1+Mu)(\nabla\varphi_n)\chi_1(u)+(\nabla M)u\,\varphi_n\chi_1(u)$$
$$+\,((1+Mu)\kappa_1\,\varphi_n\chi_1'(u)+M\varphi_n\chi_1(u))\nabla u, \tag{18}$$

it is easy to see that $\psi_n\in\mathrm{Dom}\,Q$ provided $\nabla_g M\in L^2_{\mathrm{loc}}(\Sigma)$. In this context and for further considerations, we recall that the curvatures K and M are uniformly bounded, cf. ⟨H2⟩. One has

$$Q_1[\psi_n]\leqslant 2((1+a\|M\|_\infty)^2\||\nabla\varphi_n|\,\chi_1\|^2+a^2\||\nabla M|\,\varphi_n\chi_1\|^2)$$
$$+(\varphi_n,(K-M^2)\varphi_n)_g+\frac{\pi^2-6}{12\kappa_1^2}(\varphi_n,KM^2\varphi_n)_g\,. \tag{19}$$

The inequality giving the factor 2 comes from the first line at the right-hand side of (18) and is established by means of Minkovski's inequality and evident estimates. The second line of (19) is the result of a direct calculation and concerns the terms of the second line of (18).

We start by checking the sufficient condition (c) of Theorem 1. If $\nabla_g M$ is L^2-integrable and ⟨H1⟩ holds true, then all the terms at the right-hand side of (19) tend to finite values as $n\to\infty$, except for the first integral at the second line which tends to $-\infty$ due to the assumption $\mathcal{M}=+\infty$. Hence we can find a finite n_0 such that $Q_1[\psi_{n_0}]<0$.

There are two observations which lead to the condition (b). First, the integral containing $K-M^2$ in (19) is always negative for any nonplanar and noncompact surface, which can be seen by rewriting the difference of curvatures by means of the principal curvatures, i.e., $K-M^2=-\frac{1}{4}(k_+-k_-)^2$. Second, the first term at the right-hand side of (19) tends to zero as $n\to\infty$ because of (7) and Lemma 1, and the remaining ones vanish for n fixed as $a\to 0$. (For the latter we recall that κ_1^{-2} is proportional to a^2.) Hence we can find a sufficiently large n_0 such that the sum of the first term at the right-hand side of (19) and the first integral at the second line of (19) is negative, and then choose the layer half-width a so small that $Q_1[\psi_{n_0}]<0$. □

C. Condition (d)

Let Σ contain a cylindrically symmetric end E with a positive total Gauss curvature, $\mathcal{K}_E>0$.

Let us recall first the strategy employed in Ref. 6 to prove the existence of bound states in layers built over surfaces of revolution diffeomorphic to $\mathbb{R}^2$ with a positive total Gauss curvature, i.e., $E=\Sigma$. The essential ingredient is supplied by an information about the behavior of the mean curvature M at infinity. In particular, if $\mathcal{K}>0$, then $|M|(\det g)^{1/2}$ is bounded but does not vanish at infinity of Σ and neither M nor M^2 are integrable in $L^1(\Sigma)$. On the other hand, the Gauss curvature is supposed to be integrable, cf. ⟨H1⟩. Constructing an appropriate family of trial functions $\{\Psi_n\}_{n\in\mathbb{N}}$ that is localized at infinity (i.e., $\forall$ compact $\Omega_c\subset\Omega\,\exists n\in\mathbb{N}$: supp $\Psi_n\cap\Omega_c=\varnothing$) one succeeds to eliminate the contribution of the Gauss curvature and, at the same time, to ensure that $Q_1[\Psi_n]$ remains negative as $n\to\infty$. We refer to the proof of Theorem 6.1 in Ref. 6 for more details and an explicit form of $\{\Psi_n\}_{n\in\mathbb{N}}$.

The fact that the family of trial functions was localized at infinity makes it possible to extend the proof to our more general situation. If $E \neq \Sigma$, we construct from E a new cylindrically symmetric surface E' diffeomorphic to $\mathbb{R}^2$ by attaching smoothly to it a cylindrically symmetric *cap*, i.e., a simply connected surface with a compact boundary (see Fig. 6). Since the attached surface is cylindrically symmetric and simply connected, its total Gauss curvature cannot be negative, which can be seen by the Gauss–Bonnet theorem and a natural parametrization, cf. Ref. 6, Sec. 6. Consequently, the total Gauss curvature of E' will not be less than the value $\mathcal{K}_E$. Since the latter is positive by assumption, the mean curvature of E' behaves at infinity like required for the use of $\{\Psi_n\}_{n\in\mathbb{N}}$, which proves the existence of spectrum below κ_1^2 for the layer about E'. However, the identical asymptotic behavior holds for the mean curvature of E as well. Hence, in order to establish the desired spectral result for the initial Ω, it is sufficient to construct the sequence $\{\Psi_n\}_{n\in\mathbb{N}}$ only at the infinity of the cylindrically symmetric layer built over the end E.

VI. CONCLUDING REMARKS

The main interest of this paper was the Dirichlet Laplacian, $-\Delta_D^\Omega$, in the layer region Ω defined as a tubular neighborhood of a complete noncompact surface embedded in $\mathbb{R}^3$. Using an intrinsic approach to the geometry of Ω, the conditions of the original paper,[6] sufficient to guarantee the existence of bound states below the essential spectrum of $-\Delta_D^\Omega$, were significantly extended to layers built over general surfaces without any strong topological restrictions; see Theorem 1 for the summary of the main results.

An important open problem is to decide whether the discrete spectrum exists also for layers over surfaces with $\mathcal{K}>0$ such that none of the conditions (b)–(d) of Theorem 1 is satisfied. (We remind that, due to Corollary 1, it concerns surfaces diffeomorphic to $\mathbb{R}^2$ only.) In view of the condition (c), it would be very desirable to prove the following conjecture:

$$\mathcal{K}>0 \;\Rightarrow\; \mathcal{M}=+\infty. \tag{20}$$

Taking into account the definition of K and M by means of the principal curvatures, it may seem that there is no reason to expect this property. However, the principal curvatures cannot be regarded as arbitrary functions because the first and second fundamental forms of Σ have to satisfy some integrability conditions (the Gauss and Codazzi–Mainardi equations). Note that we have proved the conjecture (20) for cylindrically symmetric surfaces in Ref. 6.

Finally, interesting spectral results are expected if the ambient space $\mathbb{R}^3$ is replaced by an Euclidean space of higher dimension (more complicated normal bundle of Σ) or even by a general Riemannian manifold (nontrivial structure of the ambient curvature tensor).

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Star exponentials for any ordering of the elements of the inhomogeneous symplectic Lie algebra

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We compute for any ordering the star exponentials of all polynomials of degree not greater than two on the 2ℓ-dimensional phase space of a quantum system with ℓ degrees of freedom, and we show in the particular case of the Moyal star product that the Weyl transform of the Moyal star exponential of the one-dimensional harmonic oscillator Hamiltonian is the evolution operator of this quantum system.
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I. INTRODUCTION

A general method of quantization, known under the name of star products method, was proposed in Ref. 1 for an arbitrary symplectic manifold, by Bayen *et al.* In the case of the symplectic phase space $\mathbb{R}^{2\ell}$ of a nonrelativistic quantum system with ℓ degrees of freedom, the Weyl transform[2,3] of the Moyal star product of two admissible symbols (which are functions or distributions on this space) is the product of the corresponding operators on the Hilbert space $L^2(\mathbb{R}^\ell)$. The Moyal star exponentials were introduced and computed in Refs. 1 and 2 for specific homogeneous polynomials, in order to determine the spectrum of the corresponding observables. Later, the Moyal star exponentials of all polynomials of degree not greater than two on $\mathbb{R}^{2\ell}$ were obtained in Ref. 4 and were used to show the existence of classical trajectories for quantum systems whose Hamiltonian belongs to the space of these polynomials.

However, it was noticed in Ref. 5 that the Moyal star product, which corresponds to the completely symmetric ordering, is not appropriate in field theory for the quantization of the free scalar field Hamiltonian. So, a new star product, called the normal star product, which corresponds to the normal ordering, was introduced in this paper and the normal star exponential of this Hamiltonian was computed in this paper, in order to determine (in the context of the star product method) the spectrum of this Hamiltonian. More recently, the normal star exponentials of all quadratic forms on the space $\mathbb{R}^2$ were obtained in Ref. 6.

The purpose of this article is to compute for any ordering, including the normal ordering, the star exponentials of all polynomials of degree not greater than two on the symplectic space $\mathbb{R}^{2\ell}$, $\ell \geqslant 1$. Furthermore, it was proved in Ref. 3 that the Weyl transforms of the Moyal star exponentials of the real homogeneous polynomials of degree two on $\mathbb{R}^{2\ell}$ are one-parameter groups of unitary operators. In the last section of this article, we prove in the particular case of the (real) Hamiltonian H of the one-dimensional harmonic oscillator that the one-parameter group $\mathrm{op}(\mathrm{Exp}_*^{M} tH)$, $t \in \mathbb{R}$, is generated by the essentially skew self-adjoint operator $\mathrm{op}(H/i\hbar)$, and then that this one-parameter group is the evolution operator of this quantum system.

II. GENERAL RESULTS AND NOTATIONS

Let $\mathbb{R}^{2\ell}$ be the phase space of a nonrelativistic quantum system with ℓ degrees of freedom, whose points are denoted by $x=\Sigma_{j=1}^{\ell} q^j e_j + \Sigma_{j=1}^{\ell} p^j e_j^-$ or $x=\Sigma_{j=1}^{2\ell} x^j e_j$, where $e_j^- = e_{j+\ell}$ if $1 \leqslant j \leqslant \ell$. Let $\omega = \Sigma_{j=1}^{\ell} dq^j \wedge dp^j$ be the canonical symplectic form on $\mathbb{R}^{2\ell}$. The Poisson bracket of two elements f and g of $\mathcal{C}^\infty(\mathbb{R}^{2\ell})$ is given by the formula

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$$P(f,g)=\sum_{j,k=1}^{2\ell}\Lambda^{jk}\frac{\partial f}{\partial x^j}\frac{\partial g}{\partial x^k}$$

with $\Lambda^{j,j+\ell}=-\Lambda^{j+\ell,j}=1$ if $1\leqslant j\leqslant \ell$, the other coefficients being equal to zero.

A general star product of f and g is given by the formal expansion[1]

$$f*g=fg+\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{i\hbar}{2}\right)^n C_n(f,g),$$

where the two-cochains C_n are given by the formula

$$C_n(f,g)=\sum_{j_r,k_s=1}^{2\ell}\Gamma^{j_1k_1}\cdots\Gamma^{j_nk_n}D_{j_1\cdots j_n}fD_{k_1\cdots k_n}g,$$

where the coefficients Γ^{jk} are arbitrary constant numbers and where

$$D_{j_1\cdots j_n}\ f=\frac{\partial^n f}{\partial x^{j_1}\cdots\partial x^{j_n}}.$$

Furthermore, we suppose that these two-cochains satisfy the following formulas:[1,7]

$$\sum_{r+s=n}\frac{1}{r!s!}C_r(C_s(f,g),h)=\sum_{r+s=n}\frac{1}{r!s!}C_r(f,C_s(g,h)), \tag{1a}$$

$$C_1(f,g)-C_1(g,f)=2P(f,g). \tag{1b}$$

Formula (1a), which implies the associativity of the star product, is automatically satisfied if the coefficients Γ^{jk} are arbitrary constant numbers (Theorem 3, p. 69 of Ref. 1, and note that the proof of this theorem remains valid for arbitrary constant coefficients). We denote by Λ and Γ, respectively, the matrices (Λ^{jk}) and (Γ^{jk}), $1\leqslant j,\ k\leqslant 2\ell$. Then, formula (1b), which implies the relation $q_j*p_k-p_k*q_j=i\hbar\,\delta_{jk}$, is equivalent to the following formula:

$$\Gamma-{}^T\Gamma=2\Lambda, \tag{2}$$

where ${}^T\Gamma$ denotes the transpose of the matrix Γ. We have on the precedently chosen basis of $\mathbb{R}^{2\ell}$

$$\Lambda=\begin{pmatrix}0 & I_\ell\\ -I_\ell & 0\end{pmatrix}\quad (I_\ell \text{ is the unit } \ell\times\ell \text{ matrix}).$$

We have $\Gamma_M=\Lambda$ for the Moyal star product,

$$\Gamma_N=2\begin{pmatrix}0 & I_\ell\\ 0 & 0\end{pmatrix}$$

for the normal star product, and $\Gamma_{aN}=-{}^T\Gamma_N$ for the antinormal star product. In this article, the symbols M, N, and aN will, respectively, refer to the Moyal, normal, and antinormal star products. Let us note that we have the same (as the last two one) matrices of coefficients for respectively the antistandard and standard orderings.[8]

The star exponential (for a general star product) of $f\in\mathcal{C}^\infty(\mathbb{R}^{2\ell})$ is defined by the formal expansion:[1,2]

$$\mathrm{Exp}_*tf=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n f^{*n}$$

with $f^{*n}=f*\cdots*f$ (n factors).

In the following, we consider the star exponentials of functions for a general ordering, that is for star products whose associated matrix Γ with constant entries satisfies formula (2).

III. STAR EXPONENTIALS FOR ANY ORDERING OF THE ELEMENTS OF THE HOMOGENEOUS SYMPLECTIC LIE ALGEBRA

Let us consider the case of the homogeneous polynomials of degree two on $\mathbb{R}^{2\ell}$ of the form $X(x)=\Sigma_{j,k=1}^{2\ell}a_{jk}x^jx^k$, where the matrix $A=(a_{jk})$ is symmetric with complex entries. Let us write $X(x)=(Ax|x)$, where $(-|-)$ denotes the usual inner product on $\mathbb{R}^{2\ell}$ that we extend in a natural way to a symmetric bilinear product on $\mathbb{C}^{2\ell}$. Let us note that if X is a polynomial of degree not greater than 2 and if $f\in C^\infty(\mathbb{R}^{2\ell})$, then $C_n(X,f)=0$ for $n\geqslant 3$.

Let us write $f_n=X^{*n}$ with $X=(Ax|x)$ and denote by $\tilde{A}=(\tilde{a}_{jk})$ the symmetric matrix $\tilde{A}={}^T\Gamma A\Gamma$. We have the following lemma.

Lemma 1: The functions f_n are polynomials of degree $2n$ on $\mathbb{R}^{2\ell}$ which satisfy the following recursion relation:

$$f_{n+1}=Xf_n+i\hbar\sum_{j,k,r=1}^{2\ell}\Gamma^{jk}a_{jr}x^rD_kf_n-\frac{\hbar^2}{4}\sum_{j,k=1}^{2\ell}\tilde{a}_{jk}D_{jk}f_n \tag{3}$$

with $f_0(x)=1$.

Remark: The analogs of Lemma 1 of Ref. 4 and of its corollary are not true for a general ordering.

To obtain the expression of Exp_*tX, we first look for a solution of the partial differential equation:

$$i\hbar\frac{\partial F}{\partial t}(t,x)=XF+i\hbar\sum_{j,k,r=1}^{2\ell}\Gamma^{jk}a_{jr}x^rD_kF-\frac{\hbar^2}{4}\sum_{j,k=1}^{2\ell}\tilde{a}_{jk}D_{jk}F \tag{4}$$

with $F(0,x)=1$, in the form

$$F(t,x)=f(t)^{-1}\exp i(g(t)x|x), \tag{5}$$

where $f(t)$ and $g(t)$ are holomorphic functions with values, respectively, in the complex field and in the space of the symmetric $2\ell\times 2\ell$ matrices with complex entries. We are led to the following differential system:

$$g'(t)=-\frac{1}{\hbar}A+A\Gamma g(t)+g(t)^T\Gamma A-\hbar g(t)\tilde{A}g(t), \tag{6}$$

$$\frac{f'(t)}{f(t)}=\frac{\hbar}{2}\mathrm{tr}(\tilde{A}g(t)), \tag{7}$$

with $g(0)=0$, $f(0)=1$, and where $\mathrm{tr}\,A$ denotes the trace of the matrix A. [Let us note that we have used the formula $(A\Gamma g(t)x|x)=(g(t)^T\Gamma Ax|x)$ in this computation, in order to obtain a symmetric matrix $g(t)$.]

Let us note that Eq. (6) is a Riccati matrix differential equation. So, following Ref. 9, p. 11, we look for a solution of this differential equation in the form $g(t)=V(t)U(t)^{-1}$, where $U(t)$ is a nonsingular matrix. We then obtain the following linear matrix differential system:

$$U'(t)=-{}^T\Gamma AU(t)+\hbar\tilde{A}V(t), \tag{8a}$$

$$V'(t)=-\frac{1}{\hbar}AU(t)+A\Gamma V(t), \tag{8b}$$

with $U(0)=I_{2\ell}$ and $V(0)=0$. The solution of this system can be written in the form

$$\begin{pmatrix} U(t) \\ V(t) \end{pmatrix} = (\exp t\Phi)\begin{pmatrix} I_{2\ell} \\ 0_{2\ell} \end{pmatrix},$$

and if we consider the $4\ell\times 4\ell$ matrices Φ^n, $n\geqslant 1$, as 2×2 block matrices (Φ^n_{jk}), $1\leqslant j,\ k\leqslant 2$, we obtain with the aid of formula (2): $\Phi^n_{11}=-2^{n-1}\,{}^T\Gamma A(\Lambda A)^{n-1}$ and $\Phi^n_{21}=-(2^{n-1}/\hbar)\times A(\Lambda A)^{n-1}$. We deduce from these formulas that

$$U(t)=I-(1/2)\sum_{n=1}^{\infty}((2t)^n/n!)^T\Gamma A(\Lambda A)^{n-1}, \tag{9a}$$

$$V(t)=-(1/2\hbar)\sum_{n=1}^{\infty}((2t)^n/n!)A(\Lambda A)^{n-1}. \tag{9b}$$

If we introduce the relation $\Lambda^2=-I$ in the preceding formulas and if we set $\Pi_1=-(\frac{1}{2})\Gamma\Lambda$, $\Pi_2=(\frac{1}{2})\,{}^T\Gamma\Lambda$, $\Pi=\Pi_1-\Pi_2$, and if we note [with the aid of formula (2)] that $\Pi_1+\Pi_2=I$, we obtain

$$U(t)=(\cosh t\Lambda A-\Pi\sinh t\Lambda A)\exp t\Lambda A, \tag{9a$'$}$$

$$V(t)=(1/\hbar)\Lambda(\sinh t\Lambda A)\exp t\Lambda A. \tag{9b$'$}$$

We thus obtain

$$g(t)=(1/\hbar)\Lambda\sinh t\Lambda A(\cosh t\Lambda A-\Pi\sinh t\Lambda A)^{-1}. \tag{10}$$

To solve Eq. (7), let us first note that if $u_{jk}(t)$ are the entries of the nonsingular matrix $U(t)$, and if $U_{jk}(t)$ are the corresponding cofactors, we have

$$\mathrm{tr}(U'(t)U(t)^{-1})=(\det U(t))^{-1}\sum_{j,k=1}^{2\ell}u'_{jk}(t)U_{jk}(t).$$

We then obtain, with the aid of the derivative property of determinants, the following lemma:

Lemma 2: If $U(t)$ is a nonsingular matrix with differentiable or holomorphic entries, we have

$$\mathrm{tr}(U'(t)U(t)^{-1})=(\det U(t))^{-1}(\det U(t))'.$$

With the aid of this lemma and of formulas (7) and (8a), we obtain

$$\frac{f'(t)}{f(t)}=\frac{1}{2}(\det U(t))^{-1}(\det U(t))'+\frac{1}{2}\mathrm{tr}({}^T\Gamma A),$$

and if we use the relation $\det(\exp t\Lambda A)=1$ (due to $\mathrm{tr}\,\Lambda A=0$, since ${}^T\Lambda=-\Lambda$) in formula (9a$'$), we obtain

$$f(t)=\exp\left(\frac{t}{2}\mathrm{tr}\,A\Gamma\right)(\det(\cosh t\Lambda A-\Pi\sinh t\Lambda A))^{1/2}. \tag{11}$$

If we consider now the power series expansion in t of the holomorphic function $F(t,x)$ [of formula (5)] around the origin,

$$F(t,x)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n C_n(x)$$

with $C_n(x)=(i\hbar)^n\partial^n F(t,x)/\partial t^n|_{t=0}$, and if we keep in mind that the function $F(t,x)$ is a solution of the partial differential equation (4), it is easy to show that the functions $C_n(x)$ satisfy the recursion relation (3) with $C_0(x)=1$. We thus have $C_n(x)=f_n(x)$ for all $n\in\mathbb{N}$.

Finally, let us note that formula (10) can be written in the form

$$g(t)=(1/\hbar)\Lambda\tanh t\Lambda A(I-\Pi\tanh t\Lambda A)^{-1},$$

and let us note that if we denote by $\|A\|$ the operator norm of the matrix A in the 2ℓ-dimensional Hilbert space $\mathbb{C}^{2\ell}$, the function $F(t,x)$ is analytic if $\|tA\|<\pi/2$ and $\|\Pi\tanh t\Lambda A\|\leqslant\|\Pi\|\tan\|tA\|<1$. We can now formulate the main result of this paper.

Theorem 1: *Let $X=(Ax|x)$ for $x\in\mathbb{R}^{2\ell}$, where A is a symmetric matrix with complex entries. Then the power series in t,*

$$\mathrm{Exp}_*tX=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n X^{*n},\tag{12}$$

has a radius of convergence $\rho\geqslant(1/\|A\|)\mathrm{Arc}\tan(1/\|\Pi\|)$ [we set Arc tan $(1/0)=\pi/2$*], and we have for any $t\in\mathbb{C}$, $|t|<\rho$ and any $x\in\mathbb{R}^{2\ell}$,*

$$\mathrm{Exp}_*tX=f(t)^{-1}\exp i(g(t)x|x)$$

with

$$f(t)=\exp\left(\frac{t}{2}\mathrm{tr}\,A\Gamma\right)(\det(\cosh t\Lambda A-\Pi\sinh t\Lambda A))^{1/2},$$

$$g(t)=\frac{1}{\hbar}\Lambda(\tanh t\Lambda A)(I-\Pi\tanh t\Lambda A)^{-1},$$

$$\Pi=-\tfrac{1}{2}(\Gamma+{}^T\Gamma)\Lambda.$$

We choose for $(\det(\cosh t\Lambda A-\Pi\sinh t\Lambda A))^{1/2}$ *the principal value.*

Remark: We have $\|A\|=\sup|\mu_i|$ where μ_i are the eigenvalues of the matrix A if A is a real (and symmetric) matrix or if A is a normal (complex) matrix.

Since the function $F(t,x)$ is analytic for $|t|<\rho$ and $x\in\mathbb{R}^{2\ell}$, then for each $t\in\mathbb{C}$, $|t|<\rho$, the series (12) converges uniformly on compact sets of $\mathbb{R}^{2\ell}$. We have the following theorem.

Theorem 2: *For any $t\in\mathbb{C}$, $|t|<\rho$, the series (12) converges weakly in $\mathcal{D}'(\mathbb{R}^{2\ell})$.*

Remarks:

(1) The symmetry of the matrix $g(t)$ follows from the formula ${}^T\Pi=\Lambda\Pi\Lambda$ and is easily checked by using the power series expansion of the function $(1-x)^{-1}$. We have

$$g(t)={}^Tg(t)=(1/\hbar)\Lambda(I-(\tanh t\Lambda A)\Pi)^{-1}\tanh t\Lambda A.$$

(2) We have $\Pi_M=0$, and we can note that, in this particular case of the Moyal star product, Theorem 1 was previously obtained in Ref. 4. We have

$$\Pi_N=\begin{pmatrix}I_\ell & 0\\ 0 & -I_\ell\end{pmatrix}$$

(Π_N is the projection operator on the q-space minus the projection operator on the p-space), and we have $\Pi_{aN}=-\Pi_N$.

(3) In the case of the space $\mathbb{R}^2$, it is easy to show by using the Hamilton–Cayley theorem that $(\Lambda A)^2=dI_2$ [since $\mathrm{tr}(\Lambda A)=0$] with $d=-\det A$. We then have $\cosh t\Lambda A=(\cosh t\sqrt{d})I_2$ and

$\sinh t\Lambda A=((\sinh t\sqrt{d})/\sqrt{d})\Lambda A$ where $\sqrt{d}$ is one of the square roots of d and an easy calculation using the preceding formulas shows that we have, for $X(q,p)=aq^2+2bqp+cp^2$ and $\varepsilon=+1$ for the normal star product and $\varepsilon=-1$ for the antinormal star product,

$$\mathrm{Exp}_*^{\varepsilon} tX=(f_\varepsilon(t))^{-1}\exp i(\alpha_\varepsilon(t)X(q,p)+\beta_\varepsilon(t)qp)$$

with

$$f_\varepsilon(t)=e^{\varepsilon tb}(\varphi_\varepsilon(t))^{1/2}$$

[we choose for $(\varphi_\varepsilon(t))^{1/2}$ the principal value],

$$\varphi_\varepsilon(t)=\cosh 2t\sqrt{d}-\varepsilon b(\sinh 2t\sqrt{d})/\sqrt{d},$$

$$\alpha_\varepsilon(t)=-(2\hbar\varphi_\varepsilon(t))^{-1}(\sinh 2t\sqrt{d})/\sqrt{d},$$

$$\beta_\varepsilon(t)=\varepsilon(\hbar\varphi_\varepsilon(t))^{-1}(\cosh 2t\sqrt{d}-1),$$

$d=b^2-ac$, where $\sqrt{d}$ is one of the square root of d. Let us note that this result does not depend on the choice of the square root of d. This result was previously obtained in Ref. 6 for the case $\varepsilon=+1$ with a minor difference due to a minor difference of the definition of star exponentials.

(4) In the case of a homogeneous polynomial of degree two on $\mathbb{R}^{2\ell}$, $\ell>1$, of the form $X(q,p)=\Sigma_{j=1}^{\ell}X_j(q,p)$ with $X_j(q,p)=a_jq_j^2+2b_jq_jp_j+c_jp_j^2$ and if we choose the basis e_1, $e_{\overline{1}},\ldots,e_\ell$, $e_{\overline{\ell}}$ of $\mathbb{R}^{2\ell}$, the matrices A, Λ, Γ, and Π are block diagonal matrices with 2×2 blocks, we then have for most orderings, including the completely symmetric (Moyal), normal and antinormal orderings

$$\mathrm{Exp}_* tX=\prod_{j=1}^{\ell}\mathrm{Exp}_* tX_j.$$

($\Pi_{j=1}^{\ell}$ denotes the ordinary product of the preceding functions.) We have for the Moyal star product

$$\mathrm{Exp}_*^M tX=\prod_{j=1}^{\ell}(\cosh t\sqrt{d_j})^{-1}\exp\left(-\frac{i}{\hbar}\frac{\tanh t\sqrt{d_j}}{\sqrt{d_j}}X_j\right),$$

which is a generalization of formula (6–11) of Ref. 2.

(5) If we consider the matrix A as a 2×2 block matrix (A_{jk}), $1\leqslant j,k\leqslant2$, we have $\tilde{A}_N=0$ if $A_{11}=0$ and $\tilde{A}_{aN}=0$ if $A_{22}=0$. We have $f(t)=1$ in both cases. We have in particular

$$\mathrm{Exp}_*^{\varepsilon}\left(t\sum_{j=1}^{\ell}\omega_jq_jp_j\right)=\exp\frac{\varepsilon i}{\hbar}\left(\sum_{j=1}^{\ell}(1-e^{\varepsilon t\omega_j})q_jp_j\right).$$

Let us note that to connect this result in the case $\varepsilon=+1$ with formula 3.5 of Ref. 5, and since the deformation parameter in Ref. 5 is $\hbar$ instead of $i\hbar$, we must replace Λ and Γ_N by $(1/i)\Lambda$ and $(1/i)\Gamma_N$, respectively. Formulas (2), (9a), (9b), and (11) remain valid when expressed with these new matrices, but we must introduce the relation $(-i\Lambda)^2=I$ in (9a), (9b) and set $\Pi=(\frac{1}{2})(-i\Gamma_N-i^T\Gamma_N)(-i\Lambda)=\Pi_N$. The right-hand side of (10) is then multiplied by -1. Hence we have

$$f(t)=f_N(-it)\quad\text{and}\quad g(t)=ig_N(-it).$$

IV. STAR EXPONENTIALS FOR ANY ORDERING OF THE ELEMENTS OF THE INHOMOGENEOUS SYMPLECTIC LIE ALGEBRA

Let us now consider the case of the inhomogeneous polynomials of degree not greater than 2 on $\mathbb{R}^{2\ell}$. We obtain in the same way as in the homogeneous case the following theorem.

Theorem 3: *Let $X=(Ax|x)+(b|x)+c$ where $A=(a_{jk})$ is a symmetric matrix with complex entries, $b=(b_j)\in\mathbb{C}^{2\ell}$ and $c\in\mathbb{C}$. Then the power series*

$$\mathrm{Exp}_*tX=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n X^{*n}$$

has a radius of convergence $\rho\geqslant(1/\|A\|)\,\mathrm{Arc\,tan}(1/\|\Pi\|)$ and we have for $t\in\mathbb{C}$, $|t|<\rho$ and $x\in\mathbb{R}^{2\ell}$

$$\mathrm{Exp}_*tX=f(t)^{-1}\exp i[(g(t)x|x)+(k(t)|x)-ct/\hbar]$$

with

$$g(t)=\frac{1}{\hbar}\Lambda(I-(\tanh t\Lambda A)\Pi)^{-1}\tanh t\Lambda A,$$

$$k(t)=\frac{1}{\hbar}\Lambda(I-(\tanh t\Lambda A)\Pi)^{-1}\frac{\tanh t\Lambda A}{\Lambda A}\Lambda b,$$

$$f(t)=\exp\left(\frac{t}{2}\mathrm{tr}\,A\Gamma\right)\exp\left(\frac{i}{4}(\varphi(t)|b)\right)(\det(\cosh t\Lambda A-\Pi\sinh t\Lambda A))^{1/2},$$

$$\varphi(t)=\frac{1}{\hbar}\,\frac{\tanh t\Lambda A-t\Lambda A}{(\Lambda A)^2}\Lambda b-\frac{\tanh t\Lambda A}{\Lambda A}\Pi\Lambda k(t).$$

For the proof of this theorem, we first look for a solution of the partial differential equation:

$$i\hbar\,\frac{\partial F(t,x)}{\partial t}=XF+i\hbar\sum_{j,k=1}^{2\ell}\Gamma^{jk}\left(\frac{bj}{2}+\sum_{r=1}^{2\ell}a_{jr}x^r\right)D_kF-\frac{\hbar^2}{4}\sum_{j,k=1}^{2\ell}\tilde{a}_{jk}D_{jk}F$$

such that $F(0,x)=1$, in the form

$$F(t,x)=f(t)^{-1}\exp i((g(t)x|x)+(k(t)|x)+\ell(t)),$$

where $g(t)$, $k(t)$, $\ell(t)$, and $f(t)$ are holomorphic functions with values in the space of the symmetric $2\ell\times2\ell$ matrices with complex entries, in $\mathbb{C}^{2\ell}$ and in $\mathbb{C}$ for the last two functions, respectively. We are led to the differential system

$$g'(t)=-\frac{1}{\hbar}A+A\Gamma g(t)+g(t)^{T}\Gamma A-\hbar g(t)\tilde{A}g(t), \tag{13}$$

$$k'(t)=-\frac{b}{\hbar}+A\Gamma k(t)+g(t)^{T}\Gamma b-\hbar g(t)\tilde{A}k(t), \tag{14}$$

$$\frac{f'(t)}{f(t)}=\frac{\hbar}{2}\mathrm{tr}(\tilde{A}g(t))+i\left(\frac{c}{\hbar}+\ell'(t)\right)-\frac{i}{2}(b|\Gamma k(t))+i\frac{\hbar}{4}(\tilde{A}k(t)|k(t)), \tag{15}$$

with $g(0)=0$, $k(0)=0$ and $f(0)=1$.

Let us note that Eq. (13) was already solved in Sec. III (see Remark 1 following Theorem 2). To solve Eq. (14), let us consider the analytic function

$$g_1(t)=\frac{1}{\hbar}\Lambda(I-(\tanh t\Lambda A)\Pi)^{-1}\frac{\tanh t\Lambda A}{\Lambda A},$$

which satisfies the relation $g_1'(t)=g'(t)/\Lambda A$.

We deduce from Eq. (13) that the function $g_1(t)$ satisfies the following equation:

$$g_1'(t)=-\frac{1}{\hbar}\Lambda^{-1}+A\Gamma g_1(t)+g(t)^{T}\Gamma\Lambda^{-1}-\hbar g(t)\tilde{A}g_1(t). \tag{16}$$

It is then obvious that the function $k(t)=g_1(t)\Lambda b$ is the solution of Eq. (14). To solve Eq. (15), let us set $\ell(t)=-ct/\hbar$ and let us note that the first part of the right-hand side of this equation was already integrated in Sec. III. The last part of this right-hand side is equal to $(i/4)(h(t)\Lambda b|b)$ with

$$h(t)=-\Gamma g_1(t)-\Lambda^{T}g_1(t)^{T}\Gamma\Lambda-\hbar\Lambda^{T}g_1(t)\tilde{A}g_1(t).$$

Let us note that the matrix $g_1(t)$ is not symmetric. Introducing the relation $g(t)=-A\Lambda^{T}g_1(t)$ in formula (16), we deduce that $(\Lambda g_1(t)+t/\hbar I)'=-\Lambda Ah(t)$. Now, if we set

$$g_2(t)=\frac{1}{\hbar}\frac{\tanh t\Lambda A-t\Lambda A}{(\Lambda A)^2}-\frac{\tanh t\Lambda A}{\Lambda A}\Pi\Lambda g_1(t),$$

and if we use the power series expansion of the function $(1-x)^{-1}$, we obtain

$$\Lambda g_1(t)+\frac{t}{\hbar}I=-\Lambda Ag_2(t).$$

We then deduce from the analytic properties of these functions that $h(t)=g_2'(t)$ and it suffices to set $\varphi(t)=g_2(t)\Lambda b$ to obtain the solution of Eq. (15).

V. MOYAL STAR EXPONENTIAL OF THE HAMILTONIAN OF THE ONE-DIMENSIONAL HARMONIC OSCILLATOR AND EVOLUTION OPERATOR OF THIS QUANTUM SYSTEM

Let us consider the homogeneous polynomials of degree 2 on $\mathbb{R}^{2\ell}$ written in the form $X=(Ax|x)$ where A is a real and symmetric matrix. Then the Weyl transforms $\mathrm{op}(\mathrm{Exp}_*^M tX)$ of the Moyal star exponentials of these polynomials form groups of unitary operators of the Hilbert space $L^2(\mathbb{R}^\ell)$ (propositions 13 and 14 of Ref. 3). In this section, we prove in the particular case of the Hamiltonian $H=\frac{1}{2}(p^2+q^2)$ of the one-dimensional harmonic oscillator that the group of unitary operators $\mathrm{op}\,(\mathrm{Exp}_*^M tH)$ is the evolution operator of this quantum system. We have the following proposition:

Proposition 1: Let $H=\frac{1}{2}(q^2+p^2)$ be the Hamiltonian of the one-dimensional harmonic oscillator. Then the Weyl transform $\mathrm{op}(H)$ of the function H is an essentially self-adjoint operator on $L^2(\mathbb{R})$ and we have for t real and sufficiently small

$$\mathrm{op}(\mathrm{Exp}_*^M tH)=\exp\frac{t}{i\hbar}\overline{\mathrm{op}(H)},$$

where $\overline{\mathrm{op}(H)}$ is the closure of the operator $\mathrm{op}(H)$.

Proof: We have for $u,\ v\in\mathscr{S}(\mathbb{R})$: $(\mathrm{op}(H)u|v)=\langle\hat{H}(\alpha),\chi_{u,v}(\alpha)\rangle=\langle H(x),\hat{\chi}_{u,v}(x)\rangle$ where $(u|v)=\int u(q)\overline{v(q)}\,dq$ is the scalar product on $L^2(\mathbb{R})$, $\hat{f}(\alpha)=\int e^{-i\langle\alpha,x\rangle}f(x)\,d\mu(x)$ with $f\in\mathscr{S}(\mathbb{R}^2)$, $x=(q,p)$, $\alpha=(a,b)$, $\langle\alpha,x\rangle=aq+bp$, $d\mu(x)=dqdp/2\pi$ and

$$\chi_{u,v}(a,b)=\exp\left(i\frac{\hbar}{2}ab\right)\int e^{iaq'}u(q'+\hbar b)\overline{v(q')}\,dq'.$$

(Let us note that an apparently different but equivalent definition is given in Ref. 3 with the use of the symplectic Fourier transformation.) We must prove for t real and sufficiently small that

$$\langle \mathrm{Exp}_*^M tH,\quad \hat{\chi}_{u,v}\rangle=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n\langle H^{*n},\ \hat{\chi}_{u,v}\rangle \tag{17}$$

with

$$\hat{\chi}_{u,v}(q,p)=\frac{2}{|\hbar|}\int \exp\left(2\frac{i}{\hbar}pb\right)u(q-b)\overline{v(q+b)}\,db. \tag{18}$$

The convergence of the expansion (17) does not hold automatically, since the series (12) (with $X=H$) converges in $\mathcal{D}'(\mathbb{R}^2)$ but $\hat{\chi}_{u,v}$ belongs to $\mathcal{S}(\mathbb{R}^2)$.

We shall estimate the functions $\hat{X}_{u,v}$ in order to apply Lebesgue's dominated convergence theorem. For this purpose, we consider the complete system of eigenvectors (then of analytic vectors) of the operator $\mathrm{op}(H)$:

$$u_n(q)=(2^n n!\sqrt{\pi|\hbar|})^{-1/2}e^{-q^2/2|h|}H_n(q/\sqrt{|\hbar|}),\quad n\in\mathbb{N},$$

where H_n denotes the Hermite polynomial of degree n (cf. Ref. 10). The operator $\mathrm{op}(H)$ is then essentially self-adjoint and we obtain by using formula (18)

$$\hat{\chi}_{u_r,u_s}(q,p)=e^{-(q^2+p^2)/|\hbar|}P_{r,s}(q,p),\quad r,\quad s\in\mathbb{N},$$

where $P_{r,s}$ is a polynomial of degree not greater than $r+s$ in p and q. On the other hand, we know that we have $H^{*n}=K_n(H)$ for the Moyal star product on the phase space $\mathbb{R}^2$, where the functions $K_n(x)$ are polynomials of degree n which satisfy the recursion relation [formula (6.2) of Ref. 2, or remark 2 at the end of this section]

$$K_{n+1}(x)=xK_n(x)-\frac{\hbar^2}{4}K_n'(x)-\frac{\hbar^2}{4}xK_n''(x),\quad K_0(x)=1.$$

Let us now consider the polynomials $C_n(x)$ with non-negative coefficients, defined by the recursion relation

$$C_{n+1}(x)=xC_n(x)+\frac{|\hbar|^2}{4}C_n'(x)+\frac{|\hbar|^2}{4}xC_n''(x),\quad C_0(x)=1. \tag{19}$$

It is then obvious that we have

$$|H^{*n}|=|K_n(H)|\leqslant C_n(|H|),$$

hence

$$\sum_{n=0}^{\infty}\frac{1}{n!}\left|\frac{t}{i\hbar}\right|^n|H^{*n}(q,p)|\leqslant\sum_{n=0}^{\infty}\frac{1}{n!}\left|\frac{t}{\hbar}\right|^n C_n\left(\frac{q^2+p^2}{2}\right). \tag{20}$$

Let us now consider the Moyal star product with the deformation parameter $-i|\hbar|$ instead of $\hbar$ (let us note that this parameter does not need to be real in the definition of star products and in the computation of star exponentials), and let us note that the recursion relation (19) is the relation

giving $H^{*n}=C_n(H)$ for this new deformation parameter. Then by using (for this new parameter) Theorem 1 and Remark 4 following Theorem 2 for $|t|$ instead of t, it is easy to show that the right-hand side of inequality (20) is equal to

$$\left(\cos\frac{|t|}{2}\right)^{-1}\exp\left(\frac{p^2+q^2}{|\hbar|}\tan\frac{|t|}{2}\right),$$

and the convergence of the series (17) is then established with $u=u_r$ and $v=u_s$ for $|t|$ sufficiently small.

Remarks:

(1) The property that X^{*n}, for the Moyal star product, is a function $K_n(X)$ of X if X is a homogeneous polynomial of degree two on $\mathbb{R}^2$ does not remain valid on $\mathbb{R}^{2\ell}$ with $\ell>1$. This property does not remain valid for a general ordering, even for $\ell=1$.

(2) If $X=(Ax|x)$ is a homogeneous polynomial of degree two on $\mathbb{R}^2$, where A is a symmetric 2×2 matrix with complex entries, and if we set $X^{*n}=K_n(X)$ for the Moyal star product, then it is easy to show by using Remark 3 following Theorem 2 that the recursion relation (3) can be written in the form

$$K_{n+1}(X)=XK_n(X)+d\hbar^2K_n'(X)+d\hbar^2XK_n''(X)$$

with $d=-\det A$.

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A system of nonlinear algebraic equations connected with the multisoliton solution of the Benjamin–Ono equation

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The multisoliton solution of the Benjamin–Ono equation is derived from the system of nonlinear algebraic equations. This finding is unexpected from the scheme of the inverse scattering transform method, which constructs the multisoliton solution through the system of linear algebraic equations. The anlaysis developed here is also applied to the rational multisoliton solution of the Kadomtsev–Petviashvili equation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1641153]

I. INTRODUCTION

The Benjamin–Ono (BO) equation describes the unidirectional prepagation of weakly nonlinear internal waves in a stratified fluid of great depth.[1–3] It can be written in an appropriate dimensionless form as

$$u_t+2uu_x+Hu_{xx}=0, \tag{1.1a}$$

where $u=u(x,t)$ is a real function representing the amplitude of the wave, the operator H is the Hilbert transform defined by

$$Hu(x,t)=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{u(y,t)}{y-x}dy, \tag{1.1b}$$

and the subscripts t and x appended to u denote partial differentiation.

A large number of studies have been done for the mathematical structure of the BO equation.[4] In particular, the initial value problem under vanishing boundary conditions has been solved by means of the inverse scattering transform (IST) method.[5,6] The IST provides a procedure to construct solutions explicitly for a certain class of initial data. A typical example is the reflectionless potential (or multisoliton potential) for which the solution is obtained simply by solving the system of *linear* algebraic equations. This remarkable feature is common to the completely integrable nonlinear evolution equations solvable by the IST.

The purpose of this paper is to show that the multisoliton solution of the BO equation can also be derived from a system of *nonlinear* algebraic equations. Since the IST reduces the nonlinear problem to the linear one characterized by a system of linear integral equations, the novel result presented here will not be predicted from the scheme of the IST. An alternative derivation of the multisoliton solution described here will give a new insight into the structure of the solution.

In Sec. II, we first describe the N-soliton (N: positive integer) solution of the BO equation constructed by the IST. Then, we introduce a system of nonlinear algebraic equations and show that it leads to the N-soliton solution as well. This fact is verified based only on an elementary theory of determinants. Section III is devoted to concluding remarks where the analysis, similar to

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that developed here, is aplied to the rational N-soliton solution of the Kadomtsev–Petviashvili (KP) equation. In the Appendix, we summarize the Lagrange interpolation formula and related formulas which will be used in Sec. II.

II. SYSTEM OF NONLINEAR ALGEBRAIC EQUATIONS

A. Notation

Before entering into the detailed analysis, we introduce the notation which will be used throughout this paper.

1. Matrices

The $N\times N$ matrices $M,V,\tilde{V},W,Z,F,$ and $\tilde{F}$ are defined by the relations

$$M=(m_{jk})=(\zeta_j\delta_{jk}-2i(1-\delta_{jk})(a_j-a_k)^{-1}),\quad \zeta_j=x-a_jt-x_{j0}+\frac{i}{a_j}, \tag{2.1a}$$

$$V=(v_{jk})=(\alpha_j^{k-1}), \tag{2.1b}$$

$$\tilde{V}=(\tilde{v}_{jk})=\left(\frac{\partial|V|}{\partial v_{jk}}\right),\quad |V|=\det V, \tag{2.1c}$$

$$W=(w_{jk})=((k-1)\alpha_j^{k-2}), \tag{2.1d}$$

$$Z=(z_{jk})=(z_j\delta_{jk}),\quad z_j=\zeta_j+\sum_{\substack{k=1\\(k\neq j)}}^{N}\frac{1}{\alpha_j-\alpha_k}, \tag{2.1e}$$

$$F=Z-WV^{-1}=(f_{jk}), \tag{2.1f}$$

$$\tilde{F}=(\tilde{f}_{jk})=\left(\frac{\partial|F|}{\partial f_{jk}}\right),\quad |F|=\det F, \tag{2.1g}$$

where δ_{jk} is Kronecker's delta, a_j and x_{j0} are real constants satisfying the conditions $a_j>0$,$a_j\neq a_k$ for $j\neq k$ $(j,k=1,2,\ldots,N)$ and $\alpha_j=ia_j/2$ $(j=1,2,\ldots,N)$. Note that V is the Vandermonde matrix and $\tilde{v}_{jk}$ is the cofactor of v_{jk}. We use the convention that a term like $(1-\delta_{jk})(a_j-a_k)^{-1}$ is taken to be zero if $j=k$.

2. Vectors

The column vectors $\mathbf{x}$ and $\mathbf{b}$ with N elements are defined as follows:

$$\mathbf{x}={}^t(x_j)={}^t(s_{N-j+1}), \tag{2.2a}$$

$$\mathbf{b}={}^t(b_j)={}^t(-z_j\alpha_j^N+N\alpha_j^{N-1}), \tag{2.2b}$$

where the superscript t denotes the transpose and the elements s_{N-j+1} will be defined later.

3. Polynomials

The polynomials $g(x)$ and $g_k(x)$ are defined by the relations

$$g(x)=\prod_{j=1}^{N}(x-\alpha_j)=\sum_{s=0}^{N}(-1)^s\sigma_s x^{N-s},\quad (\sigma_0=1), \tag{2.3a}$$

$$g_k(x)=\prod_{\substack{j=1\\(j\neq k)}}^{N}(x-\alpha_j)=\sum_{s=0}^{N-1}(-1)^s\sigma_{s,k}x^{N-1-s},\ \ (k=1,2,\ldots,N), \tag{2.3b}$$

where σ_s are fundamental symmetric polynomials constructed from α_j according to the relations

$$\sigma_1=\sum_{j=1}^{N}\alpha_j,\ \ \sigma_2=\sum_{\substack{j,k=1\\(j<k)}}^{N}\alpha_j\alpha_k,\ldots,\ \ \sigma_N=\prod_{j=1}^{N}\sigma_j, \tag{2.3c}$$

and $\sigma_{k,s}$ in (2.3b) is expressed in terms of σ_p and α_k as[7]

$$\sigma_{k,s}=\sum_{p=0}^{s}\sigma_p(-\alpha_k)^{s-p}. \tag{2.3d}$$

It follows from the definition (2.3) that $g'(\alpha_j)=g_j(\alpha_j)$ where $g'(x)=dg(x)/dx$.

B. *N*-soliton solution of the BO equation

Let ϕ_j be the solution of the following system of *linear* algebraic equations

$$\zeta_j\phi_j-2i\sum_{\substack{k=1\\(k\neq j)}}^{N}\frac{\phi_k}{a_j-a_k}=1,\ \ (j=1,2,\ldots,N). \tag{2.4}$$

Then, the N-soliton solution of the BO equation is given by[5,6,8]

$$u=i\sum_{j=1}^{N}(\phi_j-\phi_j^*)=i\frac{\partial}{\partial x}\ln\frac{f}{f^*}, \tag{2.5}$$

where $f=|M|$ and ϕ_j^* denotes the complex conjugate of ϕ_j. We note that a direct proof of the N-soliton solution, without recourse to the IST, has been performed on the basis of Eq. (2.4).[8] The last expression in (2.5) is very important in the present analysis. It stems from the relation[8]

$$\sum_{j=1}^{N}\phi_j=\frac{f_x}{f}. \tag{2.6}$$

To show (2.6), we note the relation

$$f_x=\begin{vmatrix} m_{11} & \cdots & m_{1N} & 1\\ \vdots & \ddots & \vdots & \vdots\\ m_{N1} & \cdots & m_{NN} & 1\\ -1 & \cdots & -1 & 0\end{vmatrix}, \tag{2.7}$$

which is derived with use of the formula

$$\begin{vmatrix} m_{11} & \cdots & m_{1N} & x_1\\ \vdots & \ddots & \vdots & \vdots\\ m_{N1} & \cdots & m_{NN} & x_N\\ y_1 & \cdots & y_N & z\end{vmatrix}=|M|z-\sum_{j,k=1}^{N}\tilde{m}_{jk}x_jy_k, \tag{2.8}$$

combined with the relation $\sum_{\substack{j,k=1\\(j\neq k)}}^{N}\tilde{m}_{jk}=0$ ($\tilde{m}_{jk}$: cofactor of m_{jk}).

C. System of nonlinear algebraic equations

Let ψ_k be the solution of the following system of *nonlinear* algebraic equations:

$$\sum_{k=1}^{N} \frac{1}{\alpha_j-\alpha_k+\psi_k}=\zeta_j+\sum_{\substack{k=1\\(k\neq j)}}^{N} \frac{1}{\alpha_j-\alpha_k}\equiv z_j \quad (j=1,2,\ldots,N). \tag{2.9}$$

Now, we show that the above system of equations yields the N-soliton solution (2.5) of the BO equation. The basic idea in performing the analysis is to transform the nonlinear system (2.9) into the linear system by introducing the nonlinear transformation

$$s_1=\sum_{j=1}^{N}(\psi_j-\alpha_j),\quad s_2=\sum_{\substack{j,k=1\\(j<k)}}^{N}(\psi_j-\alpha_j)(\psi_k-\alpha_k),\ldots,s_N=\prod_{j=1}^{N}(\psi_j-\alpha_j). \tag{2.10}$$

It then follows that the system (2.9) can be transformed into the system of linear algebraic equations for the new variables s_j

$$\sum_{k=1}^{N}\{z_j\alpha_j^{k-1}-(k-1)\alpha_j^{k-2}\}s_{N-k+1}=-z_j\alpha_j^N+N\alpha_j^{N-1} \quad (j=1,2,\ldots,N). \tag{2.11}$$

If we use the notations (2.1) and (2.2), we can write (2.11) compactly in the matrix form

$$(ZV-W)\mathbf{x}=FV\mathbf{x}=\mathbf{b}. \tag{2.12}$$

D. Solution

To solve Eq. (2.12), we first observe that $|F|\neq 0$ and $|V|\neq 0$. The former relation follows from $|F|=|M|$ [see (2.25) later] together with a fact $|M|\neq 0$ for real x and t which is derived from (2.4). The latter relation is obvious since $|V|=\Pi_{\substack{j,k=1\\(j>k)}}^{N}(\alpha_j-\alpha_k)$ (:Vandermonde determinant) and $\alpha_j\neq\alpha_k$ for $j\neq k$. With these facts in mind, the solution of Eq. (2.12) is readily obtained by using Cramer's rule as

$$\mathbf{x}=\frac{{}^t(\tilde{F}\tilde{V})\mathbf{b}}{|F||V|}. \tag{2.13}$$

Hence, the jth element of $\mathbf{x}$ is given by

$$x_j=\frac{1}{|F||V|}\sum_{m,n=1}^{N} b_m\tilde{f}_{mn}\tilde{v}_{nj} \quad (j=1,2,\ldots,N), \tag{2.14}$$

where $\tilde{v}_{nj}$ is the cofactor of v_{nj}. In terms of (2.3b) and (2.3d), the explicit expression of $\tilde{v}_{nj}$ reads as[7]

$$\tilde{v}_{nj}=\frac{(-1)^{N-j}\sigma_{n,N-j}}{g_n(\alpha_n)}|V|. \tag{2.15}$$

Using the formula (2.8), we can put (2.14) into the form of the bordered determinant

$$x_j=-\frac{1}{|F||V|}\begin{vmatrix} f_{11} & \cdots & f_{1N} & b_1\\ \vdots & \ddots & \vdots & \vdots\\ f_{N1} & \cdots & f_{NN} & b_N\\ \tilde{v}_{1j} & \cdots & \tilde{v}_{Nj} & 0\end{vmatrix}. \tag{2.16}$$

The next step is to modify (2.16) by employing the properties of the determinant. Since $V^{-1}={}^t\tilde{V}/|V|$, one sees that $F=Z-WV^{-1}=Z-W{}^t\tilde{V}/|V|$. In view of (2.1d), (2.1e), and (2.3b), the (j,k) element of F takes the form

$$f_{jk}=z_j\delta_{jk}-\frac{1}{|V|}\sum_{l=1}^{N} w_{jl}\tilde{v}_{kl}=z_j\delta_{jk}-\frac{g_k'(\alpha_j)}{g_k(\alpha_k)}, \tag{2.17}$$

where $g_k'(\alpha_j)=dg_k(x)/dx|_{x=\alpha_j}$. The relations

$$\frac{g_j'(\alpha_j)}{g_j(\alpha_j)}=\sum_{\substack{k=1\\(k\neq j)}}^{N}\frac{1}{\alpha_j-\alpha_k},\quad g_k'(\alpha_j)=\frac{g_j(\alpha_j)}{\alpha_j-\alpha_k}\quad (j\neq k), \tag{2.18}$$

follow immediately from the definition (2.3b) of $g_k(x)$. Substituting (2.18) into (2.17), we arrive at the expression

$$f_{jk}=\zeta_j\delta_{jk}-(1-\delta_{jk})\frac{1}{\alpha_j-\alpha_k}\frac{g_j(\alpha_j)}{g_k(\alpha_k)}. \tag{2.19}$$

Let $|B|$ be the $(N+1)\times(N+1)$ bordered determinant which appears on the right-hand side of (2.16). We modify $|B|$ in a sequence of steps. First, we add the kth column multiplied by α_k^N to the $(N+1)$th column $(k=1,2,\ldots,N)$. Then, after some calculations, the $(n,N+1)$ element of $|B|$ which is referred to as $b_{n,N+1}$ is found to be as

$$\begin{aligned} b_{n,N+1}&=-\sum_{\substack{k=1\\(k\neq n)}}^{N}\frac{\alpha_k^n}{\alpha_n-\alpha_k}\frac{g_n(\alpha_n)}{g_k(\alpha_k)}-\sum_{\substack{k=1\\(k\neq n)}}^{N}\frac{\alpha_n^N}{\alpha_n-\alpha_k}+N\alpha_n^{N-1}\\ &=g_n(\alpha_n)\sum_{s=1}^{N}\alpha_n^{s-1}\sum_{k=1}^{N}\frac{\alpha_k^{N-s}}{g_k(\alpha_k)}-\alpha_n^N\sum_{\substack{k=1\\(k\neq n)}}^{N}\frac{1}{\alpha_n-\alpha_k}\left(\frac{g_n(\alpha_n)}{g_k(\alpha_k)}+1\right). \end{aligned} \tag{2.20}$$

If we use the formulas (A2) and (A3), this expression simplifies to

$$b_{n,N+1}=g_n(\alpha_n)\quad (n=1,2,\ldots,N). \tag{2.21}$$

On the other hand, the $(N+1,N+1)$ element of $|B|$ which is referred to as $b_{N+1,N+1}$ is given by

$$b_{N+1,N+1}=(-1)^{N-j}|V|\sum_{k=1}^{N}\frac{\sigma_{k,N-j}\alpha_k^N}{g_k(\alpha_k)}=(-1)^{N-j}|V|\sigma_{N-j+1}, \tag{2.22}$$

where the formula (A7) has been used in deriving the last expression of (2.22). Thus, $|B|$ is modified into the form

$$|B|=\begin{vmatrix} f_{11} & \cdots & f_{1N} & g_1(\alpha_1)\\ \vdots & \ddots & \vdots & \vdots\\ f_{N1} & \cdots & f_{NN} & g_N(\alpha_N)\\ \tilde{v}_{1j} & \cdots & \tilde{v}_{Nj} & b_{N+1,N+1}\end{vmatrix}. \tag{2.23}$$

Next, we extract the factor $g_j(\alpha_j)$ from the jth row of $|B|$ $(j=1,2,\ldots,N)$ and the factor $g_j^{-1}(\alpha_j)$ from the jth column of $|B|$ $(j=1,2,\ldots,N)$, respectively, and see that these factors cancel out completely. If we combine this result with (2.15), (2.19), and (2.22) and note the relations $\alpha_j=ia_j/2(j=1,2,\ldots,N)$, $|B|$ is transformed into the form

$$|B|=(-1)^{N-j}|V|\begin{vmatrix} m_{11} & \cdots & m_{N1} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ m_{1N} & \cdots & m_{NN} & 1 \\ \sigma_{1,N-j} & \cdots & \sigma_{N,N-j} & \sigma_{N-j+1} \end{vmatrix}. \tag{2.24}$$

The relation

$$|F|=|M| \tag{2.25}$$

follows from (2.1a) and (2.19) by a similar calculation. Substititing (2.24) and (2.25) into (2.16) and using the formula $|{}^tM|=|M|$, we finally obtain

$$x_j=-\frac{(-1)^{N-j}}{|M|}\begin{vmatrix} m_{11} & \cdots & m_{1N} & \sigma_{1,N-j} \\ \vdots & \ddots & \vdots & \vdots \\ m_{N1} & \cdots & m_{NN} & \sigma_{N,N-j} \\ 1 & \cdots & 1 & \sigma_{N-j+1} \end{vmatrix} \quad (j=1,2,\ldots,N). \tag{2.26}$$

In the above solution, the case $j=N$ yields the particularly interesting result since $\sigma_{k,0}=1$ ($k=1,2,\ldots,N$) by virtue of (2.3d). Applying the formula (2.8) into (2.26) with $j=N$, we find that

$$s_1=x_N=-\sigma_1+\frac{1}{|M|}\begin{vmatrix} m_{11} & \cdots & m_{1N} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ m_{N1} & \cdots & m_{NN} & 1 \\ -1 & \cdots & -1 & 0 \end{vmatrix}. \tag{2.27}$$

It then turns out from (2.3c), (2.6), (2.7), (2.10), and (2.27) that

$$\sum_{j=1}^{N}\psi_j=s_1+\sigma_1=\frac{f_x}{f}=\sum_{j=1}^{N}\phi_j. \tag{2.28}$$

If we combine (2.5) with (2.28), we obtain the expression of the BO N-soliton solution in terms of the solution of the nonlinear system (2.9) as

$$u=i\sum_{j=1}^{N}(\psi_j-\psi_j^*). \tag{2.29}$$

III. CONCLUDING REMARK

The analysis developed in this paper can be applied to soliton solutions with the structure similar to that of the N-soliton solution of the BO equation. An example is the rational N-soliton solution of the following KP equation:[9]

$$(u_t+6uu_x+u_{xxx})_x+3\alpha^2u_{yy}=0,\ \ u=u(x,y,t), \tag{3.1}$$

where α is a complex parameter. Consider the system of linear algebraic equations for Φ_j

$$\xi_j\Phi_j+2\sum_{\substack{k=1\\(k\neq j)}}^{N}\frac{\Phi_k}{\nu_j-\nu_k}=1 \quad (j=1,2,\ldots,N), \tag{3.2a}$$

with

$$\xi_j = x + \alpha^{-1}\nu_j y - 3\nu_j^2 t - \xi_{j0}, \tag{3.2b}$$

where ν_j and ξ_{j0} are complex constants satisfying the conditions $\nu_j \neq \nu_k$ for $j \neq k$ $(j,k = 1,2,\ldots,N)$. Then, the N-soliton solution of Eq. (3.1) can be expressed in terms of Φ_j as[10,11]

$$u = 2\frac{\partial}{\partial x}\left[\sum_{j=1}^{N} \Phi_j\right]. \tag{3.3}$$

Suppose that Ψ_j satisfy the following system of nonlinear algebraic equations:

$$\sum_{k=1}^{N} \frac{2}{\nu_j - \nu_k + 2\Psi_k} = \xi_j + \sum_{\substack{k=1 \\ (k\neq j)}}^{N} \frac{2}{\nu_j - \nu_k} \quad (j = 1,2,\ldots,N). \tag{3.4}$$

Then, one finds that

$$\sum_{j=1}^{N} \Phi_j = \sum_{j=1}^{N} \Psi_j. \tag{3.5}$$

In conclusion, it will be worthwhile to comment on an application of the result presented in this paper. We first point out that the analog of the nonlinear system (2.9) has been proposed for providing an alternative way to construct the N-soliton solution of the Korteweg–de Vries (KdV) equation.[12] It has played a central role in the study of the initial value problem of the KdV equation with small dispersion.[12] While the corresponding initial value problem is still unsolved for the BO equation, the nonlinear system (2.9) may be employed to elucidate asymptotic solution of the BO equation in the limit of small dispersion.

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APPENDIX: LAGRANGE INTERPOLATION AND RELATED FORMULAS

In this appendix, we summarize the Lagrange interpolation formula and related formulas which are used in Sec. II.

The Lagrange interpolation formula is given by the relation

$$\frac{f(z)}{g(z)} = \sum_{j=1}^{N} \frac{f(\alpha_j)}{g'(\alpha_j)} \frac{1}{z - \alpha_j}, \tag{A1}$$

where $g(z)$ is defined by (2.3a), $f(z)$ is a polynomial of order $N-1$ at most and $g'(\alpha_j) = dg(x)/dx|_{x=\alpha_j} = g_j(\alpha_j)$.

If we put $f(z) = z^m$ $(m = 1,2,\ldots,N-1)$ and integrate (A1) with respect to z along the large circle $|z| = R$ within which all the α_j locate, we obtain $\int_{|z|=R} f(z)/g(z)dz = 2\pi i \delta_{m,N-1}$ in the limit of $R \to \infty$. On the other hand, we can use the Cauchy residue theorem to evaluate the integral of the right-hand side of (A1). This gives the result $2\pi i \Sigma_{j=1}^{N} \alpha_j^N / g'(\alpha_j)$. Equating the two expressions, one obtains

$$\sum_{j=1}^{N} \frac{\alpha_j^m}{g'(\alpha_j)} = \delta_{m,N-1} \quad (m = 1,2,\ldots,N-1). \tag{A2}$$

Applying the same procedure to the integral $\int_{|z|=R} [(z-\alpha_n)g(z)]^{-1} dz$ yields the formula

$$\sum_{\substack{k=1\\(k\neq n)}}^{N} \frac{1}{\alpha_k-\alpha_n}\left(\frac{g_n(\alpha_n)}{g_k(\alpha_k)}+1\right)=0 \quad (n=1,2,\ldots,N). \tag{A3}$$

If we put $f(z)=z^{N-1}, z=x^{-1}$ in (A1), expand it in powers of x and note (2.3a), (A1) can be written in the form

$$1=\left\{\sum_{m=0}^{N}(-1)^m\sigma_m x^m\right\}\sum_{n=0}^{\infty}J_n x^n, \quad J_n\equiv\sum_{j=1}^{N}\frac{\alpha_j^{N-1+n}}{g'(\alpha_j)}. \tag{A4}$$

Comparing the same power of x on both-sides of (A4), one obtains the recurrence relation that determines J_n:

$$J_0=1, \quad \sum_{m=0}^{p}(-1)^m\sigma_m J_{p-m}=0 \quad (p=1,2,\ldots). \tag{A5}$$

The first four of J_n read as

$$J_1=\sigma_1, \quad J_2=-\sigma_2+\sigma_1^2, \quad J_3=\sigma_3-2\sigma_1\sigma_2+\sigma_1^3,$$

$$J_4=-\sigma_4+2\sigma_1\sigma_3+\sigma_2^2-3\sigma_1^2\sigma_2+\sigma_1^4.$$

It follows from (A5) with $p=n+1$ that

$$\sigma_{n+1}=\sum_{m=0}^{n}(-1)^{n-m}\sigma_m J_{n+1-m}. \tag{A6}$$

The following relation is a consequence of (2.3d) and (A6):

$$\sum_{k=1}^{N}\frac{\sigma_{k,j-1}\alpha_k^N}{g'(\alpha_k)}=\sigma_j \quad (j=1,2,\ldots,N). \tag{A7}$$

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On the reduction and the existence of approximate analytic solutions of some basic nonlinear ODEs in mathematical physics and nonlinear mechanics

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Using series of admissible functional transformations we reduce the one-dimensional axisymmetric nonlinear Schrödinger (NLS) equation, as well as the forced damped nonlinear Duffing (NLD) equation to equivalent nonlinear first-order integrodifferential equations. The forced undamped (NLD) equation results as a special case. The reduced integrodifferential equations are exact. In the limits of small or large values of the parameters characterizing these nonlinear problems, we prove that further reductions lead to first-order nonlinear ordinary differential equations which, except in case of the (NLS) equation, are of the Abel classes. The approximate reduced (NLS) equation admits exact analytic solutions. On the other hand, taking into account the known exact analytic solutions of the equivalent Abel classes of equations we show that there do not exist analytic solutions of the above two nonlinear Duffing oscillators. However, if further asymptotic approximations take place, new approximate analytic solutions concerning the (NLD) equations are constructed. [DOI: 10.1063/1.1635065]

I. INTRODUCTION

Standing and traveling waves in one-dimensional lattices[1–3] and in systems described by nonlinear partial differential equations[4] have been extensively studied in the literature. In Refs. 5 and 6 the existence and properties of standing wave solutions of the nonlinear Schrödinger (NLS) equation were investigated. Also, the study of two-dimensional axisymmetric breathers using Padé approximants was developed in Ref. 7. This problem is governed by a one-dimensional (NLS) equation with cubic nonlinearities. On the other hand, whereas weakly nonlinear oscillators with weak damping can be approximately solved using techniques such as averaging,[8] or multiple-scale,[9] exact solutions of undamped or damped forced oscillators with strong nonlinearities are still leaking. Perturbation problems addressing approximately damped nonlinear free oscillations include Refs. 10–12. Also, the unforced Van der Pol oscillator was studied extensively as the prototypical system possessing a limit cycle and as a model for relaxation oscillation of large values of its parameter. Representative works include Refs. 13 and 14. Additional works focused on the forced response, the resulting bifurcations as parameters change, and on chaotic response of the oscillator (see Refs. 15 and 16).

Recently, it was proved that there are not analytic solutions of the unforced damped Duffing oscillator in terms of known (tabulated) functions.[17] It followed that in order to solve this free damped problem a set of new analytic functions must be defined. The same holds true also for the Van der Pol free oscillator.[18] However, in this last case and for large values of the characteristic parameter (relaxation oscillations) it was proved that there exists an approximate analytic solution.

In this work we deal with the possibility of constructing exact analytic solutions for the one-dimensional axisymmetric (NLS) equation, as well as for the forced damped and undamped (NLD) equations. Using series of admissible functional transformations we succeed in reducing

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the examined nonlinear ODEs to equivalent first-order nonlinear integrodifferential equations, constituting the corresponding intermediate integrals in the phase plane. The reduced equations are exact. In the limits of small or large values of the parameters characterizing these nonlinear problems, we prove that the reduced equations assume approximate asymptotic forms that are amenable to perturbation analysis. These approximations also change the NLS to a solvable nonlinear first-order ODE, and the NLD equations to nonlinear ODEs of the Abel classes. Taking into account the existing known exact analytic solutions of these classes of equations, we show that there do not exist exact analytic solutions of the above two (NLD) problems in terms of known (tabulated) analytic functions. However, if further asymptotic approximations take place, new approximate analytic solutions concerning the two nonlinear Duffing oscillators are constructed.

The solution methodology introduced in the paper is general and can be applied to some of the most interesting second- and third-order nonlinear ODEs of mathematical physics and nonlinear mechanics, including the forced Van der Pol nonlinear oscillator; the Thomas–Fermi equation; the simplified Blasius equation; the Langmuir equation; the Kidder equation,[19] as well the plastic spin equations in simple shear.[20]

II. THE REDUCTION PROCEDURE

We shall investigate three kinds of strongly nonlinear ODEs appearing in the fields of nonlinear mechanics and mathematical physics. The first is the one-dimensional axisymmetric NLS equation, deriving in the ''continuum approximation'' of the equations of motion governing the antiphase vibrations of a two-dimensional array of weakly coupled nonlinear oscillators. The other two are the forced damped and undamped Duffing equations with no linear stiffness terms [(NLD) equations], produced in 1918 by Duffing and describing strongly nonlinear oscillations.

Before we address the issue of the reduction of the above-mentioned equations, we will provide an admissible functional transformation that can reduce a class of nonlinear ODEs to a different class. Consider the nonlinear ODE of the second order of the type

$$\left[f\left(\frac{1}{y'_x} \right) + g(y) \right]'_x - H(x) y'_x = 0, \tag{2.1}$$

where y, f, g, and H are known smooth and continuously differentiable functions. Here the notation $y'_x = dy/dx$, $y''_{xx} = d^2y/dx^2, \ldots$ is used for the derivatives.

The functional transformation

$$w'_\xi = F(x)y(x), \quad \xi = \pm |G(x)| \tag{2.2}$$

in which w and ξ are also smooth and continuously differentiable functions, while F and G are to be determined, furnishes the expressions

$$y'_x = \left(\frac{w'_\xi}{F} \right)'_x = \frac{\pm |G'_x|}{F} w''_{\xi\xi} - \frac{F'_x}{F^2} w'_\xi, \quad \xi'_x = \pm |G'_x|. \tag{2.3}$$

Introducing these results into (2.1) we obtain

$$\left[f\left(\frac{1}{\dfrac{\pm |G'_x|}{F} w''_{\xi\xi} - \dfrac{F'_x}{F^2} w'_\xi} \right) + g\left(\frac{w'_\xi}{F} \right) \right]'_\xi (\pm |G'_x|) - H(x) \left(\frac{\pm |G'_x|}{F} w''_{\xi\xi} - \frac{F'_x}{F^2} w'_\xi \right) = 0. \tag{2.4}$$

We define functions F and G such that

$$\frac{\pm|G_x'|}{F}=\frac{F_x'}{F^2},\quad \pm|G_x'|=H\frac{\pm|G_x'|}{F}, \tag{2.5}$$

that is to say such that

$$F(x)=H(x),\quad (\ln|F|)_x'=\pm|G_x'|=\xi_x'.$$

Thus, the above-mentioned functional transformation takes the following concrete form:

$$w_\xi'=e^\xi y(x),\quad F(x)=H(x)=e^\xi\quad (\ln F=\pm G), \tag{2.6}$$

and the ODE (2.1) is transformed to the equivalent one

$$\left[f\left(\frac{e^{2\xi}}{H_x'}\frac{1}{w_{\xi\xi}''-w_\xi'}\right)+g(e^{-\xi}w_\xi')\right]_\xi'=w_{\xi\xi}''-w_\xi'. \tag{2.7}$$

Note that H_x' can be expressed in terms of the function $\exp(\xi)$ by way of the second of (2.6). Integration of the last equation results in

$$f\left(\frac{e^{2\xi}}{H_x'}\frac{1}{w_{\xi\xi}''-w_\xi'}\right)+g(e^{-\xi}w_\xi')=w_\xi'-w, \tag{2.8}$$

where the constant of integration is missing since both second-order equations (2.1) and (2.8) are equivalent between them.

Let us now analyze the three kinds of prescribed equations.

A. The one-dimensional axisymmetric Schrödinger equation

The type of the equation is

$$\begin{gathered}y_{xx}''+\frac{1}{x}y_x'-\lambda_1 y+\lambda_2 y^k=0,\quad k=\text{integer},\\ \lambda_1>0,\quad \lambda_2>0,\quad -\infty<x<+\infty\quad (x\neq 0).\end{gathered} \tag{2.9}$$

By the first transformation,

$$y(x)=\eta(\xi),\quad \xi=\xi(x)\Rightarrow y_x'=\eta_\xi'\xi_x',\quad y_{xx}''=\eta_{\xi\xi}''\xi_x'^2+\eta_\xi'\xi_{xx}'', \tag{2.10}$$

we reduce (2.9) in the form

$$\xi_x'^2\eta_{\xi\xi}''+\xi_{xx}''\eta_\xi'+\frac{1}{x}\xi_x'\eta_\xi'-\lambda_1\eta+\lambda_2\eta^k=0$$

and we define $\xi(x)$ such that $\xi_{xx}''=-(1/x)\xi_x'$. Thus, the transformation (2.10) becomes

$$y(x)=\eta(\xi),\quad \xi=\pm\ln|x|,\quad -\infty<\xi<+\infty \tag{2.11}$$

and (2.9) is transformed to the following second-order ODE:

$$\begin{gathered}\eta_{\xi\xi}''-(\lambda_1\eta-\lambda_2\eta^k)e^{\pm 2\xi}=0,\\ -\infty<\xi<+\infty,\quad -\infty<\eta<+\infty.\end{gathered} \tag{2.12}$$

The additional substitution

$$\eta(\xi)=\omega(t), \quad t=e^{\pm 2\xi} \tag{2.13}$$

converts (2.12) in

$$\begin{gathered}(t\omega_t')_t'-\tfrac{1}{4}(\lambda_1\omega-\lambda_2\omega^k)=0,\\ 0<t<+\infty, \quad -\infty<\omega<+\infty,\end{gathered} \tag{2.14}$$

while, changing the variables in the last equation, we extract a second-order nonlinear ODE of the type (2.1), that is

$$\left(\frac{t}{t_\omega'}\right)_\omega'-\frac{1}{4}(\lambda_1\omega-\lambda_2\omega^k)t_\omega'=0. \tag{2.15}$$

Thus, referring to the transformation (2.3), that is to say setting

$$w_{\bar\xi}'=g(\omega)t(\omega), \quad \bar\xi=\pm|f(\omega)| \tag{2.16a}$$

with concrete form

$$g(\omega)=\tfrac{1}{4}(\lambda_1\omega-\lambda_2\omega^k), \quad \bar\xi=\pm|f(\omega)|=\pm\ln|g(\omega)|\Rightarrow g(\omega)=e^{\bar\xi}, \tag{2.16b}$$

we succeed in reducing (2.15) in

$$\left[\frac{w_{\bar\xi}'}{\bar\xi_\omega'(w_{\bar\xi\bar\xi}''-w_{\bar\xi}')}\right]_{\bar\xi}'=w_{\bar\xi\bar\xi}''-w_{\bar\xi}', \tag{2.17a}$$

where

$$\begin{gathered}w_{\bar\xi}'=e^{\bar\xi}t(\omega), \quad \lambda_1\omega-\lambda_2\omega^k=4e^{\bar\xi},\\ -\infty<\bar\xi<+\infty, \quad -\infty<\omega<+\infty, \quad 0<t<+\infty.\end{gathered} \tag{2.17b}$$

Integrating (2.17a) we extract the following second-order nonlinear ODE:

$$\frac{w_{\bar\xi}'}{\bar\xi_\omega'}=(w_{\bar\xi}'-w)(w_{\bar\xi}'-w)_{\bar\xi}', \tag{2.18}$$

similar to Eq. (2.8).

By way of the second of (2.17b) we have $\bar\xi=\ln|\frac{1}{4}(\lambda_1\omega-\lambda_2\omega^k)|$ and thus one evaluates

$$\bar\xi_\omega'=\frac{(\lambda_1-k\lambda_2\omega^{k-1})}{(\lambda_1\omega-\lambda_2\omega^k)}.$$

Therefore, (2.18) can be rewritten as

$$\begin{gathered}(w_{\bar\xi}'-w)(w_{\bar\xi}'-w)_{\bar\xi}'=\tfrac{1}{4}e^{-\bar\xi}h(e^{\bar\xi}),\\ h(e^{\bar\xi})=\lambda_1-k\lambda_2\omega^{k-1}.\end{gathered} \tag{2.19}$$

Integration of (2.19) results in

$$\frac{1}{2}(w'_{\bar{\xi}}-w)^2-4\int \frac{e^{\bar{\xi}}}{h(e^{\bar{\xi}})}w'_{\bar{\xi}}d\bar{\xi}=C_1, \tag{2.20a}$$

or, equivalently, in

$$\frac{1}{2}(w'_{\bar{\xi}}-w)^2-4\frac{e^{\bar{\xi}}}{h(e^{\bar{\xi}})}w+4\int \frac{h(e^{\bar{\xi}})e^{\bar{\xi}}-h'_{e^{\bar{\xi}}}(e^{\bar{\xi}})e^{2\bar{\xi}}}{h^2(e^{\bar{\xi}})}wd\bar{\xi}=C_1,$$
$$0<w<+\infty, \quad -\infty<\bar{\xi}<+\infty, \tag{2.20b}$$

where C_1 is a constant of integration.

The nonlinear integrodifferential equation of the first-order (2.20a) constitutes the intermediate integral in the phase plane of the one-dimensional axisymmetric (NLS) equation (2.9).

B. The forced damped nonlinear Duffing equation

The equation under consideration is of the type

$$y''_{xx}+\lambda_3 y'_x-\lambda_1 y+\lambda_2 y^3=A\sin(\Omega x),$$
$$\lambda_1>0, \quad \lambda_2>0, \quad \lambda_3>0, \quad A>0, \tag{2.21}$$
$$-\infty<x<+\infty.$$

By a transformation similar to (2.10), that is to say by the transformation

$$y(x)=z(s), \quad s=\sqrt{\lambda_1}x \tag{2.22}$$

we reduce (2.21) in the form

$$z''_{ss}+\mu z'_s-z+\lambda z^3=\Lambda\sin(\overset{*}{\Omega}s),$$
$$\mu=\frac{\lambda_3}{\sqrt{\lambda_1}}>0, \quad \lambda=\frac{\lambda_2}{\lambda_1}>0, \quad \Lambda=\frac{A}{\lambda_1}>0, \quad \overset{*}{\Omega}=\frac{\Omega}{\sqrt{\lambda_1}}, \tag{2.23}$$
$$-\infty<s<+\infty.$$

Changing the variables and setting simultaneously

$$\omega(z)=\overset{*}{\Omega}s(z), \tag{2.24}$$

we transform (2.24) to the following null nonlinear ODE of the second order:

$$\omega''_{zz}-\overset{*}{\mu}\omega'^2_z+(az-bz^3)\omega'^3_z+c\sin\omega\omega'^3_z=0, \tag{2.25a}$$

$$\overset{*}{\mu}=\frac{\mu}{\overset{*}{\Omega}}=\frac{\lambda_3}{\overset{*}{\Omega}\sqrt{\lambda_1}}>0, \quad a=\frac{1}{\overset{*}{\Omega}^2}>0, \quad b=\frac{\lambda}{\overset{*}{\Omega}^2}>, \quad c=\frac{\Lambda}{\overset{*}{\Omega}^2}=\frac{A}{\overset{*}{\Omega}^2\lambda_1}>0, \quad \overset{*}{\Omega}=\frac{\Omega}{\sqrt{\lambda_1}}>0,$$
$$-\infty<\omega<+\infty, \quad -\infty<z<+\infty. \tag{2.25b}$$

For $\omega_z' \neq 0$ the last equation can be rewritten as follows:

$$\left(\frac{1}{\omega_z'} + c\cos\omega + \overset{*}{\mu} z\right)_z' - (\mathrm{a}z - bz^3)\omega_z' = 0, \tag{2.26}$$

which is of the type (2.1). Introducing transformation (2.2) with concrete form

$$\begin{gathered} w_\xi' = e^\xi \omega(z), \quad az - bz^3 = e^\xi, \\ -\infty < \xi < +\infty, \end{gathered} \tag{2.27}$$

(2.26) becomes

$$\left[\frac{e^{2\xi}}{h(e^\xi)}\frac{1}{w_{\xi\xi}'' - w_\xi'} + c\cos(e^{-\xi}w_\xi') + \overset{*}{\mu} f(e^\xi)\right]_\xi' = w_{\xi\xi}'' - w_\xi', \tag{2.28a}$$

$$h(e^\xi) = \mathrm{a} - 3bz^2, \quad f(e^\xi) = z, \quad \mathrm{a}z - bz^3 = e^\xi,$$

$$\mathrm{a},\ b,\ c,\ \text{and}\ \overset{*}{\mu}\ \text{as in Eq. (2.25b)}, \tag{2.28b}$$

$$-\infty < \xi < +\infty, \quad -\infty < w < +\infty.$$

Setting again

$$e^{-\xi}w(\xi) = p(\xi) \Rightarrow e^{-\xi}(w_\xi' - w) = p_\xi', \quad e^{-\xi}(w_{\xi\xi}'' - w_\xi') = p_{\xi\xi}'' + p_\xi' \tag{2.29}$$

and integrating (2.28a), we extract the following second-order nonlinear ODE:

$$\frac{e^\xi}{h(e^\xi)} + c\cos(p + p_\xi')(p + p_\xi')_\xi' + \overset{*}{\mu} f(e^\xi)(p + p_\xi')_\xi' - e^\xi p_\xi'(p + p_\xi')_\xi' = 0, \tag{2.30}$$

which is similar to Eq. (2.8).

Noting that

$$\int e^\xi p_\xi' p_{\xi\xi}'' \mathrm{d}\xi = \frac{1}{2}e^\xi p_\xi'^2 - \frac{1}{2}\int e^\xi p_\xi'^2 \mathrm{d}\xi,$$

$$\int f(e^\xi)(p + p_\xi')_\xi' \mathrm{d}\xi = f(e^\xi)(p + p_\xi') - \int (p + p_\xi') f_{e^\xi}' e^\xi \mathrm{d}\xi = f(p + p_\xi') - p f_{e^\xi}' e^\xi + \int p f_{e^\xi e^\xi}'' e^{2\xi} \mathrm{d}\xi,$$

the integration of (2.30) results in

$$\begin{aligned} &\frac{1}{2}e^\xi p_\xi'^2 + \frac{1}{2}\int e^\xi p_\xi'^2 d\xi - c\sin(p + p_\xi') - \overset{*}{\mu} f(e^\xi)(p + p_\xi') + \overset{*}{\mu} p f_{e^\xi}' e^\xi - \overset{*}{\mu}\int p f_{e^\xi e^\xi}'' e^{2\xi} \mathrm{d}\xi \\ &\quad - \int \frac{e^\xi}{h(e^\xi)} \mathrm{d}\xi = C_1, \end{aligned} \tag{2.31}$$

where C_1 is an integration constant.

The nonlinear integrodifferential equation of the first-order (2.31) constitutes the intermediate integral in the phase plane of the forced damped (NLD) oscillator (2.21).

C. The forced undamped nonlinear Duffing equation

This equation has the following restricted form in comparison with (2.21):

$$y''_{xx}-\lambda_1 y+\lambda_2 y^3=A\sin(\Omega x),$$
$$\lambda_1>0,\quad \lambda_2>0,\quad A>0, \tag{2.32}$$
$$-\infty<x<+\infty.$$

In other words it is a special case of (2.21). Thus, according to the same procedure as previously developed, the intermediate integral corresponding to (2.31) in the case of the forced undamped (NLD) oscillator becomes through (2.31) by setting $\overset{*}{\mu}=0$ $(\lambda_3=0)$, that is

$$\frac{1}{2}e^{\xi}p'^{2}_{\xi}+\frac{1}{2}\int e^{\xi}p'^{2}_{\xi}\mathrm{d}\xi-c\sin(p+p'_{\xi})-\int\frac{e^{\xi}}{h(e^{\xi})}\mathrm{d}\xi=C_1. \tag{2.33}$$

Here, C_1 is an integration constant, while $p(\xi)$ and $h(e^{\xi})$ are as in Eqs. (2.29) and (2.28b), respectively.

The three nonlinear integrodifferential equations (2.20a), (2.31), and (2.33), constitute the intermediate integrals in the phase plane of the corresponding one-dimensional axisymmetric (NLS) equation, and the forced damped and undamped (NLD) oscillators. They are exact since no approximations were made in the already introduced admissible functional transformations. As these equations do not admit exact analytic solutions, as a result one must resort to asymptotic approximations by considering specific ranges of the parameters being introduced. In Sec. III we focus on the limits of small or large values of the parameter $\lambda=\lambda_2/\lambda_1$, $(1/\lambda=\lambda_1/\lambda_2)$, and derive simplified approximations for the reduced three equations.

III. APPROXIMATIONS: EXISTENCE AND NONEXISTENCE OF EXACT ANALYTIC SOLUTIONS

We now consider the three types of equations examined in Sec. II and investigate their reductions to equivalent nonlinear differential equations of the first order. Our study of the reduced equations indicates the absence of exact analytic solutions of the original (NLS) equation and the (NLD) oscillators, e.g., the absence of exact solutions in terms of known (tabulated) functions.

A. The one-dimensional axisymmetric (NLS) equation with cubic nonlinearities

In Ref. 7 it was proved that the study of two-dimensional axisymmetric breathers using Padé approximants leads to the solution of a one-dimensional (NLS) equation with cubic nonlinearities. Thus, according to the results of this reference and in order to have the same order of nonlinearities for the three types of equations being examined, we prefer to investigate the NLS equation with cubic nonlinearities.

In this case the function $h(e^{\bar{\xi}})$ of the intermediate integral (2.20a) becomes

$$h(e^{\bar{\xi}})=\lambda_1-3\lambda_2\omega^2,\quad \lambda_1\omega-\lambda_2\omega^3=4e^{\bar{\xi}}. \tag{3.1}$$

We express the cubic (Cardan) equation $\lambda_1\omega-\lambda_2\omega^3=4e^{\bar{\xi}}$ in the form

$$\omega^3+\overset{*}{p}\omega+\overset{*}{q}=0, \tag{3.2a}$$

with

$$\overset{*}{p}=-\lambda,\quad \overset{*}{q}=\frac{4}{\lambda_2}e^{\bar{\xi}},\quad \lambda=\frac{\lambda_1}{\lambda_2} \tag{3.2b}$$

and discriminant $\overset{*}{Q}$ given by the well-known formula

$$\overset{*}{Q}=\left(\frac{\overset{*}{p}}{3}\right)^3+\left(\frac{\overset{*}{q}}{2}\right)^2=-\frac{\lambda^3}{27}+\left(\frac{2e^{\overline{\xi}}}{\lambda_2}\right)^2. \tag{3.2c}$$

When $\overset{*}{Q}<0$, Eq. (3.2a) possesses three real, distinct roots, whereas when $\overset{*}{Q}>0$ there exist a single real root and a complex conjugate pair of roots. The case $\overset{*}{Q}=0$ must be rejected since, if $\overset{*}{Q}$ vanishes, the variable $\overline{\xi}$, and therefore the variable y, become constants. Based on these observations we now distinguish the following cases.

Case 1: $\overset{*}{Q}<0$. The distinct real roots of the cubic equation (3.2a) are ($\overset{*}{q}<0$)

$$\omega_1=2\sqrt{-\frac{\overset{*}{p}}{3}}\cos\frac{\alpha}{3}>0,\quad \omega_2=-2\sqrt{-\frac{\overset{*}{p}}{3}}\cos\frac{\alpha-\pi}{3}<0,$$

$$\omega_3=-2\sqrt{-\frac{\overset{*}{p}}{3}}\cos\frac{\alpha+\pi}{3}<0,\quad \cos\alpha=-\frac{\overset{*}{q}}{2\sqrt{-\left(\frac{\overset{*}{p}}{3}\right)^3}},\quad -\frac{\pi}{2}<\alpha<\pi. \tag{3.3}$$

Case 2: $\overset{*}{Q}>0$. The one real root of the cubic equation (3.2a) is given by

$$\omega=A+B,\quad A=\sqrt[3]{-\frac{\overset{*}{q}}{2}+\sqrt{\overset{*}{Q}}},\quad B=\sqrt[3]{-\frac{\overset{*}{q}}{2}-\sqrt{\overset{*}{Q}}}. \tag{3.4}$$

By now, we focus on the limits of small or large values of the parameter $\lambda=\lambda_1/\lambda_2>0$, and derive simplified approximations for the nonlinear integrodifferential equation (2.20a).

The limit $0<\lambda=\lambda_1/\lambda_2\ll 1$. We develop an analytic approximation to the reduced equation (2.20a) in the limit of small values of the parameter $\lambda=\lambda_1/\lambda_2$. Recalling formula (3.2c) giving the discriminant $\overset{*}{Q}$ of the cubic equation (3.2a) we observe that, if $\lambda\ll 1$, then $\overset{*}{Q}$; is positive, e.g., $\overset{*}{Q}=(2e^{\overline{\xi}}/\lambda_2)^2+\mathbf{O}(\lambda^3)>0$, and the real root of Eq. (3.2a) becomes

$$\omega=-\left(\frac{4e^{\overline{\xi}}}{\lambda_2}\right)^{1/3}\Rightarrow e^{\overline{\xi}/3}=-\left(\frac{\lambda_2\omega^3}{4}\right)^{1/3}. \tag{3.5}$$

This approximation permits us to write the following:

(i)

$$\overline{\xi}=\ln\left|\frac{\lambda_2\omega^3}{4}\right|=\ln\left|\frac{\lambda_2}{4}\right|+\ln|\omega|^3=\ln\left|\frac{\lambda_2}{4}\right|+3\ln|\omega|=\ln\left|\frac{\lambda_2}{4}\right|+3\ln\left|\frac{4\lambda_1 e^{\overline{\xi}}}{\lambda_1\lambda_2}\right|=\ln\left|\frac{\lambda_2}{4}\right|+\ln\left|\frac{4}{\lambda_1}\right|+\ln|\lambda e^{\overline{\xi}}|$$

$$=\ln\left|\frac{\lambda_2}{\lambda_1}\right|+n\lambda e^{\overline{\xi}}-1-C_0+\mathbf{O}(\lambda^2),\quad C_0=\sum_{m=2,3,\ldots}^{n}\frac{1}{m}.$$

For simplicity and without loss of generality one neglects the constant C_0 and takes $n=1$. Thus one obtains

$$\lambda e^{\bar{\xi}}=\bar{\xi}+1-\ln\left|\frac{1}{\lambda}\right|\Rightarrow e^{\bar{\xi}}=\frac{\bar{\xi}+1-\ln\left|\frac{1}{\lambda}\right|}{\lambda}. \tag{3.6}$$

(ii)

$$\frac{\bar{\xi}}{3}=\frac{1}{3}\ln\left|\frac{\lambda_2\omega^3}{4}\right|=\frac{1}{3}\ln\left|\frac{\lambda_2}{4}\right|+\ln|\omega|=\frac{1}{3}\ln\left|\frac{\lambda_2}{4}\right|+\ln\left|\frac{4e^{\bar{\xi}}}{\lambda_2}\right|^{1/3}=\frac{1}{3}\ln\left|\frac{\lambda_2}{4}\right|+\frac{1}{3}\ln\left|\frac{4}{\lambda_1}\right|+\ln|\lambda e^{\bar{\xi}}|^{1/3}$$

$$=\frac{1}{3}\ln\left|\frac{1}{\lambda}\right|+[(\lambda e^{\bar{\xi}})^{1/3}-1].$$

Thus, we obtain

$$(\lambda e^{\bar{\xi}})^{1/3}=\frac{\bar{\xi}}{3}+1-\frac{1}{3}\ln\left|\frac{1}{\lambda}\right|\Rightarrow e^{\bar{\xi}/3}=\frac{\bar{\xi}+3-\ln\left|\frac{1}{\lambda}\right|}{3\lambda^{1/3}}. \tag{3.7}$$

Recalling the intermediate integral (2.20a) we evaluate

$$\frac{e^{\bar{\xi}}}{h(e^{\xi})}=\frac{e^{\bar{\xi}}}{\lambda_1-3\lambda_2\omega^2}=\frac{1}{\lambda_1}\frac{e^{\bar{\xi}}}{1-3\frac{1}{\lambda}\omega^2}=\frac{1}{\lambda_1}\frac{e^{\bar{\xi}}}{1-\frac{3}{\lambda}\left(\frac{4e^{\xi}}{\lambda_2}\right)^2},$$

which, since $1/\lambda\gg 1$, and based on the previous results, it can be approximately written as

$$\frac{e^{\bar{\xi}}}{h(e^{\xi})}\cong\sim-\frac{e^{\bar{\xi}}}{3\lambda_2\left(\frac{4e^{\xi}}{\lambda_2}\right)^{2/3}}=-\frac{e^{\bar{\xi}/3}}{6\sqrt[3]{2}\lambda_2^{1/3}}=-\frac{1}{18\sqrt[3]{2}}\frac{\bar{\xi}+3-\ln\left|\frac{1}{\lambda}\right|}{\sqrt[3]{\lambda_1}}.$$

We estimate now the integral appearing in (2.20a) as follows:

$$4\int\frac{e^{\bar{\xi}}}{h(e^{\xi})}w'_{\bar{\xi}}d\bar{\xi}=-\frac{2}{3\sqrt[3]{2}\sqrt[3]{\lambda_2}}\int w'_{\bar{\xi}}e^{\bar{\xi}/3}d\bar{\xi}=-\frac{2}{\sqrt[3]{2}\sqrt[3]{\lambda_2}}\int w'_{\bar{\xi}}d(e^{\bar{\xi}/3})$$

$$=-\frac{\sqrt[3]{4}}{\sqrt[3]{\lambda_2}}\int w'_{\bar{\xi}}d\left(\frac{\bar{\xi}+3-\ln\left|\frac{1}{\lambda}\right|}{3\sqrt[3]{\lambda}}\right)=-\frac{\sqrt[3]{4}}{3\sqrt[3]{\lambda_1}}w.$$

Thus, the integrodifferential equation (2.20a), constituting the exact intermediate integral of the (NLS) equation (2.9) with cubic nonlinearities, can be approximated in case $0<\lambda\ll 1$ by the following first-order nonlinear ODE:

$$\frac{1}{2}(w'_{\bar{\xi}}-w)^2+\frac{\sqrt[3]{4}}{3\sqrt[3]{\lambda_1}}w=C_1. \tag{3.8}$$

The limit $+\infty>\lambda=\lambda_1/\lambda_2\gg 1$. In this case the discriminant $\overset{*}{Q}$ of the cubic equation (3.2c) becomes negative. In fact, since $0<1/\lambda\ll 1$, we have

$$\overset{*}{Q}=\left(\frac{\overset{*}{p}}{3}\right)^3+\left(\frac{\overset{*}{q}}{2}\right)^2=-\frac{\lambda^3}{27}+\left(\frac{2\lambda e^{\bar{\xi}}}{\lambda_1}\right)^2=-\left(\frac{\lambda}{3}\right)^3\left[1-\left(\frac{3}{\lambda}\right)^3\left(\frac{2\lambda e^{\bar{\xi}}}{\lambda_1}\right)^2\right]$$

$$=-\left(\frac{\lambda}{3}\right)^3\left[1-\frac{1}{\lambda}\left(\frac{6\sqrt{3}e^{\bar{\xi}}}{\lambda_1}\right)^2\right]=-\left(\frac{\lambda}{3}\right)^3+\mathbf{O}(\lambda^{-1})<0.$$

Then, the positive real root ω of (3.2a) is given by the first of equations (3.3) and it can be asymptotically approximated by expanding the general form of the variable α in terms of large parameter. Indeed, taking into account the fourth of equations (3.3) we find

$$\alpha=\arccos\left(-\frac{2e^{\bar{\xi}}}{\lambda_2}\frac{1}{\sqrt{\left(\frac{\lambda}{3}\right)^3}}\right)$$

$$=\frac{\pi}{2}-\left[-\frac{2e^{\bar{\xi}}}{\lambda_2}\frac{1}{\sqrt{\left(\frac{\lambda}{3}\right)^3}}-\frac{1}{6}\left(\frac{2e^{\bar{\xi}}}{\lambda_2}\frac{1}{\sqrt{\left(\frac{\lambda}{3}\right)^3}}\right)^3-\cdots\right]$$

$$=\frac{\pi}{2}+\frac{2e^{\bar{\xi}}}{\lambda_2}\frac{1}{\sqrt{\left(\frac{\lambda}{3}\right)^3}}+\mathbf{O}(\lambda^{-9/2}),$$

and thus we evaluate

$$\frac{\alpha}{3}=\frac{\pi}{6}+\frac{2\sqrt{3}e^{\bar{\xi}}}{\lambda_2\lambda^{3/2}}+\mathbf{O}(\lambda^{-9/2}).$$

Therefore we obtain

$$\cos\frac{\alpha}{3}=\cos\left(\frac{\pi}{6}+\frac{2\sqrt{3}e^{\bar{\xi}}}{\lambda_2\lambda^{3/2}}\right)=\frac{\sqrt{3}}{2}(1+\mathbf{O}(\lambda^{-3}))-\frac{1}{2}\left(\frac{2\sqrt{3}e^{\bar{\xi}}}{\lambda_2\lambda^{3/2}}+\mathbf{O}(\lambda^{-9/2})\right)$$

$$=\frac{\sqrt{3}}{2}-\frac{\sqrt{3}e^{\bar{\xi}}}{\lambda_2\lambda^{3/2}}+\mathbf{O}(\lambda^{-3}),$$

and the above-mentioned real root ω is asymptotically approximated in terms of large parameter as

$$\omega=\sqrt{\lambda}-\frac{\sqrt{3}e^{\bar{\xi}}}{\lambda_2\lambda}+\mathbf{O}(\lambda^{-3}). \tag{3.9}$$

The above-given approximations enable us to also write the following approximations:

(i)

$$\bar{\xi}=\ln\left|\frac{\lambda\lambda_2}{2}(\sqrt{\lambda}-\omega)\right|=\ln\left|\frac{\lambda_1}{2}\right|+\ln|\sqrt{\lambda}-\omega|=\ln\left|\frac{\lambda_1}{2}\right|+\ln\left|\sqrt{\lambda}-\sqrt{\lambda}+\frac{2e^{\bar{\xi}}}{\lambda\lambda_2}\right|$$

$$=\ln\left|\frac{\lambda_1}{2}\right|+\ln\left|\frac{2e^{\bar{\xi}}}{\lambda\lambda_2}\right|=\ln\left|\frac{\lambda_1}{2}\right|+n\frac{2e^{\bar{\xi}}}{\lambda\lambda_2}-1-C_0+\mathbf{O}(\lambda^{-2}),\quad C_0=\sum_{m=2,3,\ldots.}^{n}\frac{1}{m}.$$

Neglecting the constant C_0 and taking $n=1$, one obtains

$$\frac{2e^{\bar{\xi}}}{\lambda_2}=\lambda(\bar{\xi}+1-K),\quad K=\ln\left|\frac{\lambda_1}{2}\right|. \tag{3.10}$$

(ii)

$$\begin{aligned}\frac{e^{\bar{\xi}}}{h(e^{\bar{\xi}})}&=\frac{e^{\bar{\xi}}}{\lambda_1-3\lambda_2\left(\sqrt{\lambda}-\dfrac{2e^{\bar{\xi}}}{\lambda\lambda_2}\right)^2}=\frac{e^{\bar{\xi}}}{\lambda_1-3\lambda_2\lambda-3\lambda_2\left(\dfrac{2e^{\bar{\xi}}}{\lambda\lambda_2}\right)^2+6\lambda_2\sqrt{\lambda}\dfrac{2e^{\bar{\xi}}}{\lambda\lambda_2}}\\&=-\frac{1}{2\lambda_1}\frac{e^{\bar{\xi}}}{\dfrac{3}{2\lambda^3}\left(\dfrac{2e^{\bar{\xi}}}{\lambda_2}\right)^2-\dfrac{3}{\lambda^{3/2}}\left(\dfrac{2e^{\bar{\xi}}}{\lambda_2}\right)}=\frac{1}{6\lambda_1}\frac{\lambda^2e^{\bar{\xi}}}{\sqrt{\lambda}\left(\dfrac{2e^{\bar{\xi}}}{\lambda_2}\right)\left[1-\dfrac{1}{2\lambda^{3/2}}\left(\dfrac{2e^{\bar{\xi}}}{\lambda_2}\right)\right]}\\&=\frac{1}{6\lambda_1}\frac{\lambda_2\lambda^{3/2}}{2}\frac{1}{1-\dfrac{1}{2\lambda^{3/2}}\left(\dfrac{2e^{\bar{\xi}}}{\lambda_2}\right)}=\frac{\lambda^{1/2}}{12}\left(1+\frac{1}{2\lambda^{3/2}}\frac{2e^{\bar{\xi}}}{\lambda_2}\right)+\mathbf{O}(\lambda^{-3}).\end{aligned}$$

Thus, we write

$$\frac{e^{\bar{\xi}}}{h(e^{\bar{\xi}})}=\frac{1}{12}\left[\lambda^{1/2}+\frac{1}{2}(\bar{\xi}+1-K)\right]+\mathbf{O}(\lambda^{-3})=\frac{1}{12}\left(\lambda^{1/2}+\frac{e^{\bar{\xi}}}{\lambda\lambda_2}\right)+\mathbf{O}(\lambda^{-3}).$$

After the above abbreviations the integrodifferential equation (2.20a) with cubic nonlinearities can be asymptotically approximated as follows:

$$\frac{1}{2}(w'_{\bar{\xi}}-w)^2-\frac{1}{3}\sqrt{\lambda}w-\frac{1}{3\lambda\lambda_2}\int w'_{\bar{\xi}}de^{\bar{\xi}}=C_1$$

or equivalently

$$\frac{1}{2}(w'_{\bar{\xi}}-w)^2-\frac{1}{3}\left(\sqrt{\lambda}+\frac{1}{2}\right)w=C_1. \tag{3.11}$$

In the next section we will show that both reduced equations (3.8) and (3.11) of the (NLS) equation (2.9) with cubic nonlinearities admit exact analytic solutions.

B. The forced damped (NLD) equation

In the case of the forced damped (NLD) equation the corresponding reduced nonlinear first-order integrodifferential equation is given by (2.31), while the cubic equation (2.27) becomes

$$\begin{gathered}z^3+\overset{*}{p}z+\overset{*}{q}=0,\quad \overset{*}{p}=-\frac{1}{\lambda},\quad \overset{*}{q}=\frac{e^{\xi}}{b}=\frac{\overset{*}{\Omega}{}^2}{\lambda}e^{\xi},\\ b=\frac{\lambda}{\overset{*}{\Omega}{}^2}>0,\quad \lambda=\frac{\lambda_2}{\lambda_1}>0,\quad \overset{*}{\Omega}{}^2=\frac{\Omega^2}{\lambda_1},\end{gathered} \tag{3.12}$$

with the following discriminant $\overset{*}{Q}$:

$$\overset{*}{Q}=\left(\frac{\overset{*}{p}}{3}\right)^3+\left(\frac{\overset{*}{q}}{2}\right)^2=-\frac{1}{27\lambda^3}+\frac{1}{4}\left(\frac{\overset{*}{\Omega}^2}{\lambda}e^{\xi}\right)^2. \tag{3.13}$$

Thus, according to the previously developed in Sec. III A, we distinguish the cases $\overset{*}{Q}<0$ and $\overset{*}{Q}>0$, where the real distinct roots corresponding to the cubic equation (3.12) are given by (3.3) and (3.4), respectively.

The limit $0<\lambda\ll 1$. We approximate $\overset{*}{Q}$ as

$$\overset{*}{Q}=-\frac{1}{27\lambda^3}+\mathbf{O}\left(\frac{1}{\lambda^2}\right)<0, \tag{3.14}$$

and the positive real root of the cubic equation (3.12) becomes

$$z=2\sqrt{\frac{1}{3\lambda}}\cos\frac{\alpha}{3},\quad \alpha=\arccos\left(-\frac{\sqrt{27\lambda}}{2}\,\overset{*}{\Omega}^2e^{\xi}\right). \tag{3.15}$$

This real root can be asymptotically approximated by expanding the general form of α in terms of the small parameter. Indeed, taking into account the expansion

$$\alpha=\arccos\left(-\frac{\sqrt{27\lambda}}{2}\,\overset{*}{\Omega}^2e^{\xi}\right)=\frac{\pi}{2}+\frac{\sqrt{27\lambda}}{2}\,\overset{*}{\Omega}^2e^{\xi}+\mathbf{O}(\lambda^{3/2}),$$

we extract

$$\cos\frac{\alpha}{3}=\cos\left(\frac{\pi}{6}+\frac{\sqrt{27\lambda}}{6}\,\overset{*}{\Omega}^2e^{\xi}\right)=\frac{\sqrt{3}}{2}-\frac{\sqrt{3\lambda}}{4}\,\overset{*}{\Omega}^2e^{\xi}+\mathbf{O}(\lambda).$$

Thus, the real root z becomes

$$z=\frac{1}{\sqrt{\lambda}}-\frac{1}{2}\,\overset{*}{\Omega}^2e^{\xi}+\mathbf{O}(\lambda). \tag{3.16}$$

According to Eq. (2.31), the above-given approximations enable us to also write the following approximations:

(i)

$$\frac{e^{\xi}}{h(e^{\xi})}=\frac{e^{\xi}}{a-3bz^2}=\overset{*}{\Omega}^2e^{\xi}\frac{1}{1-3\lambda\left(\frac{1}{\sqrt{\lambda}}-\frac{\overset{*}{\Omega}^2e^{\xi}}{2}\right)^2}=\overset{*}{\Omega}^2e^{\xi}\frac{1}{1-3+3\sqrt{\lambda}\,\overset{*}{\Omega}^2e^{\xi}-\frac{3\lambda}{4}(\overset{*}{\Omega}^2e^{\xi})^2}$$

$$=-\frac{\overset{*}{\Omega}^2e^{\xi}}{2}e^{\xi}\left[1+\frac{3\sqrt{\lambda}}{2}(\overset{*}{\Omega}^2e^{\xi})\right]+\mathbf{O}(\lambda). \tag{3.17a}$$

(ii)

$$e^{\xi}=(\sqrt{\lambda_1}-\sqrt{\lambda_2}z)\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\Rightarrow\xi=\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|+\ln|\sqrt{\lambda_1}-\sqrt{\lambda_2}z|$$

$$=\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|+\ln\left|\frac{\sqrt{\lambda}\sqrt{\lambda_1}\,\overset{*}{\Omega}{}^2}{2}e^{\xi}\right|=n\frac{\sqrt{\lambda}\sqrt{\lambda_1}\,\overset{*}{\Omega}{}^2}{2}e^{\xi}-1+\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|-C_0+\mathbf{O}(\lambda),$$

$$C_0=\sum_{m=2,3,\ldots}^{n}\frac{1}{m}.$$

Neglecting the constant C_0 and taking $n=1$ we evaluate

$$e^{\xi}=\frac{2}{\sqrt{\lambda}\sqrt{\lambda_1}\,\overset{*}{\Omega}{}^2}(\xi+1-K),\quad K=\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|. \tag{3.17b}$$

(iii)

$$\sin(p+p'_{\xi})=\sin(e^{-\xi}w'_{\xi})=\sin\left[\frac{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}{2}\frac{1}{1+\xi-K}w'_{\xi}\right]=\frac{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}{2}\frac{1}{1+\xi-K}w'_{\xi}+\mathbf{O}(\lambda^{3/2}). \tag{3.17c}$$

Furthermore, by means of Eq. (2.28b), we evaluate

$$f(e^{\xi})=z=\frac{1}{\sqrt{\lambda}}-\frac{1}{2}\,\overset{*}{\Omega}{}^2e^{\xi},\quad f'_{e^{\xi}}=-\frac{1}{2}\,\overset{*}{\Omega}{}^2,\quad f''_{e^{\xi}e^{\xi}}=0, \tag{3.17d}$$

while using transformation (2.29), as well as Eqs. (3.17a)–(3.17d), the nonlinear integrodifferential equation (2.31) can be approximated in case $0<\lambda\ll 1$ by the following first-order nonlinear ODE:

$$\left(1-\frac{1}{2\xi}\right)(w'_{\xi}-w)^2-cw'_{\xi}-\overset{*}{\mu}\left(\frac{1}{\sqrt{\lambda}}-\frac{1}{\sqrt{\lambda}\sqrt{\lambda_1}}\overline{\xi}\right)w'_{\xi}-\frac{\overset{*}{\mu}}{\sqrt{\lambda}\sqrt{\lambda_1}}\overline{\xi}w+\frac{2}{\overset{*}{\Omega}{}^2\lambda\lambda_1}\overline{\xi^2}+\frac{3}{\overset{*}{\Omega}{}^2\lambda\lambda_1\sqrt{\lambda_1}}\overline{\xi^3}$$

$$-\frac{2C_1}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\overline{\xi}=0, \tag{3.18}$$

$$\overline{\xi}=\xi+1-K,\quad K=\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|.$$

Through Eq. (3.17b) we finally evaluate

$$1-\frac{1}{2\bar{\xi}}=1-\frac{1}{2[\ln|\sqrt{\lambda_2}z-\sqrt{\lambda_1}|+K+1-K]}=1-\frac{1}{2[\ln|1-\sqrt{\lambda}z|+\ln|\sqrt{\lambda_1}|+1]}$$

$$=1-\frac{1}{2[1+\ln|\sqrt{\lambda_1}|-\sqrt{\lambda z}]+\mathbf{O}(\lambda)}. \tag{3.19}$$

Setting for simplicity

$$1-\frac{1}{2\bar{\xi}}\cong 1-\frac{1}{2(1+\ln|\sqrt{\lambda_1}|)}=\frac{1+2\ln|\sqrt{\lambda_1}|}{2(1+\ln|\sqrt{\lambda_1}|)},$$

and taking into account that $\overset{*}{\Omega}=\Omega/\sqrt{\lambda_1}$, Eq. (3.18) becomes of the following nonlinear form:

$$(w'_{\bar{\xi}}-w)^2+k\bar{\xi}(w'_{\bar{\xi}}-w)+aw'_{\bar{\xi}}-\beta\bar{\xi}^2+\gamma\bar{\xi}^3-\delta\bar{\xi}=0, \tag{3.20}$$

where

$$k=\frac{\lambda_3}{\Omega\sqrt{\lambda}\sqrt{\lambda_1}}\frac{2(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|},\quad a=-\frac{A\sqrt{\lambda}+\Omega\lambda_3}{\Omega^2\sqrt{\lambda}}\frac{2(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|}, \tag{3.20a}$$

$$\beta=-\frac{4(1+\ln|\sqrt{\lambda_1}|)}{\Omega^2\lambda(1+2\ln|\sqrt{\lambda_1}|)},\quad \gamma=\frac{3(1+\ln|\sqrt{\lambda_1}|)}{\Omega^2\lambda\sqrt{\lambda_1}(1+2\ln|\sqrt{\lambda_1}|)},\quad \delta=\frac{4C_1\sqrt{\lambda_1}(1+\ln|\sqrt{\lambda_1}|)}{\Omega^2\sqrt{\lambda}(1+2\ln|\sqrt{\lambda_1}|)}.$$

We shall prove now that Eq. (3.20) can be further reduced to a first-order Abel nonlinear ODE of the form $yy'_x-y=f(x)$. In fact, we introduce the parameter $\tau=w'_{\bar{\xi}}$ and by differentiation we obtain the well-known equations

$$\frac{d\bar{\xi}}{d\tau}=-\frac{F_{,\tau}}{F_{,\bar{\xi}}+\tau F_{,w}},\quad \frac{dw}{d\tau}=-\frac{\tau F_{,\tau}}{F_{,\bar{\xi}}+\tau F_{,w}} \tag{3.21}$$

in which

$$F\equiv F(\tau,w,\bar{\xi})=(\tau-w)^2+k\bar{\xi}(\tau-w)+a\tau-\beta\bar{\xi}^2+\gamma\bar{\xi}^3-\delta\bar{\xi}=0. \tag{3.22}$$

Here the notation $F_{,x}=\partial F/\partial x$, $F_{,y}=\partial F/\partial y,\ldots$ is used for the partial derivatives.

We compute

$$F_{,\tau}=2(\tau-w)+k\bar{\xi}+a,\quad F_{,w}=-2(\tau-w)-k\bar{\xi},\quad F_{,\bar{\xi}}=k(\tau-w)-2\beta\bar{\xi}+3\gamma\bar{\xi}^2-\delta$$

and the first of (3.21a) becomes

$$\frac{d\bar{\xi}}{d\tau}=-\frac{2(\tau-w)+k\bar{\xi}+a}{-2\beta\bar{\xi}+3\gamma\bar{\xi}^2-\delta+k(\tau-w)-2\tau\left[(\tau-w)+\dfrac{k\bar{\xi}}{2}\right]}. \tag{3.23}$$

Solving also (3.22) for $(\tau-w)$, we evaluate

$$t-w=\frac{-k\bar{\xi}\pm\sqrt{-4a\tau+(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi}}}{2},\quad -4a\tau+(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi}>0, \tag{3.24}$$

while combining the results (3.23) and (3.24) we extract the following:

$$\frac{1}{\tau'_{\bar{\xi}}}=\frac{\pm 2\sqrt{-4a\tau+(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi}}+2a}{-6\gamma\bar{\xi}^2+(4\beta+k^2)\bar{\xi}+2\delta\pm\sqrt{-4a\tau+(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi}}}. \tag{3.25}$$

By the substitution

$$\sqrt{-4a\tau+(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi}}=\sqrt{-4a\tau+\omega(\bar{\xi})}=\sqrt{Q(\bar{\xi})}, \tag{3.26a}$$

$$\begin{aligned}\omega(\bar{\xi})&=(4\beta+k^2)\bar{\xi}^2-4\gamma\bar{\xi}^3+4\delta\bar{\xi},\\ \omega'_{\bar{\xi}}&=2(4\beta+k^2)\bar{\xi}-12\gamma\bar{\xi}^2+4\delta,\end{aligned} \tag{3.26b}$$

which furnishes $1/\tau'_{\bar{\xi}}=4a/(\omega'_{\bar{\xi}}-Q'_{\bar{\xi}})$, Eq. (3.25) results in

$$2\omega\sqrt{Q}-2Q\sqrt{Q}-4ak\sqrt{Q}=2\omega'_{\bar{\xi}}\sqrt{Q}-2\sqrt{Q}Q'_{\bar{\xi}}+2aQ'_{\bar{\xi}}. \tag{3.27}$$

By the new substitution

$$\sqrt{Q}=Z\Rightarrow Q=Z^2\Rightarrow Q'_{\bar{\xi}}=2ZZ'_{\bar{\xi}}, \tag{3.28}$$

we transform (3.27) into the following Abel equation of the second kind:

$$(Z\pm a)Z'_{\bar{\xi}}=\tfrac{1}{2}Z^2+\tfrac{1}{2}(\omega'_{\bar{\xi}}-\omega)+ak, \tag{3.29}$$

while by the well-known transformation (Ref. 21, p. 50)

$$v=(Z\pm a)\exp\left(-\frac{1}{2}\int d\bar{\xi}\right)=(Z\pm a)\exp\left(-\frac{\bar{\xi}}{2}\right), \tag{3.30}$$

we reduce (3.29) in

$$vv'_{\bar{\xi}}\pm ae^{-\bar{\xi}/2}v=\tfrac{1}{2}(\omega'_{\bar{\xi}}-\omega+2ak+a^2)e^{\bar{\xi}}. \tag{3.31}$$

In the sequel, through the general transformation

$$v(\bar{\xi})=q(s),\quad s=s(\bar{\xi})\Rightarrow v'_{\bar{\xi}}=q'_s s'_{\bar{\xi}}$$

with concrete form

$$v(\bar{\xi})=q(s),\quad s=\pm 2ae^{-\bar{\xi}/2}\ (e^{\bar{\xi}/2}=\pm 2a/s), \tag{3.32}$$

(3.31) results in the following Abel equation of the normal form:

$$\begin{aligned}qq'_s-q&=(a+k)\frac{s}{4a^2}-(\omega'_{\bar{\xi}}-\omega)\frac{s}{4a^2},\\ \omega'_{\bar{\xi}}-\omega&=4\gamma\bar{\xi}^3-(12\gamma+4\beta+k^2)\bar{\xi}^2+2(4\beta+k^2-2\delta)\bar{\xi}+4\delta.\end{aligned} \tag{3.33}$$

Also, (3.32) and (3.17b) enable us to write the approximation

$$\left|\frac{2a}{s}\right|=e^{\bar{\xi}/2}\Rightarrow\ln\left|\frac{2a}{s}\right|=\frac{\bar{\xi}}{2}=\frac{\xi+2-K}{2}-\frac{1}{2}=\sqrt{\frac{\sqrt{\lambda}\sqrt{\lambda_1}\overset{*}{\Omega}^2}{2}}e^{(1-K)/2}\left|\frac{2a}{s}\right|-\frac{1}{2},$$

that is to say the approximation

$$\ln\left|\frac{2a}{s}\right|=M\left|\frac{2a}{s}\right|-\frac{1}{2}=Me^{\bar{\xi}/2}-\frac{1}{2},\quad M=\sqrt{\frac{\sqrt{\lambda}\sqrt{\lambda_1}\overset{*}{\Omega}^2}{2}}e^{(1-K)/2}=\frac{1}{\sqrt{e}}. \tag{3.34}$$

Therefore, we evaluate

$$\begin{aligned}\bar{\xi}&=2\ln\left|\frac{2a}{s}\right|=\pm 2M\left(\frac{2a}{s}\right)-1,\\ \bar{\xi}^2&=4M^2\left(\frac{2a}{s}\right)^2+\frac{1}{4}\mp 4M\left(\frac{2a}{s}\right),\\ \bar{\xi}^3&=\pm 8M^3\left(\frac{2a}{s}\right)^3-12M^2\left(\frac{2a}{s}\right)^2\pm 6M\left(\frac{2a}{s}\right)-1,\end{aligned} \tag{3.35}$$

and the Abel equation (3.33) becomes

$$qq_s'-q=p_1s^{-2}+p_2s^{-1}+p_3s+p_4, \tag{3.36a}$$

where

$$\begin{aligned}&p_1=\mp 64a\gamma M^3,\quad p_2=4(24\gamma+4\beta+k^2)M^2,\\ &p_3=\frac{-(-16\gamma-12\beta-3k^2+8\delta+2k+\alpha)}{4\alpha^2},\quad p_4=\pm\frac{4(-9\gamma-4\beta+k^2+\delta)}{a}M,\\ &\alpha,\beta,\gamma,\delta,\quad\text{and } k \text{ as in (3.20a).}\end{aligned} \tag{3.36b}$$

The limit $+\infty>\lambda\gg 1$. We develop new analytic approximations of the reduced integrodifferential equation (2.31) in the limit of large values of the parameter $\lambda=\lambda_2/\lambda_1$, that is to say in case of strongly nonlinear damped oscillations. In terms of the before mentioned analysis, in this case the discriminant $\overset{*}{Q}$ of the cubic equation (3.12) becomes positive, e.g.,

$$\overset{*}{Q}=\frac{1}{4}\left(\frac{\overset{*}{\Omega}^2e^{\xi}}{\lambda}\right)^2+\mathbf{O}(\lambda^{-3})>0 \tag{3.37}$$

and the only one real root z can be asymptotically approximated by expanding the general form (3.4) in terms of the large parameter. This furnishes

$$z=-\left(\frac{\overset{*}{\Omega}^2e^{\xi}}{\lambda}\right)^{1/3}+\mathbf{O}(\lambda^{-1}). \tag{3.38}$$

Thus, according to (2.31), we write the following:

(i)

$$e^{\xi}=-\frac{\lambda}{\overset{*}{\Omega}{}^2}z^3=\frac{\lambda}{\overset{*}{\Omega}{}^2}|z|^3\Rightarrow\xi=\ln\left|\frac{\lambda}{\overset{*}{\Omega}{}^2}\right|+\ln\left|\frac{\overset{*}{\Omega}{}^2e^{\xi}}{\lambda}\right|=\ln\left|\frac{\lambda}{\overset{*}{\Omega}{}^2}\right|+n\frac{\overset{*}{\Omega}{}^2e^{\xi}}{\lambda}-1-C_0+\mathbf{O}(\lambda^{-2}),$$

$$C_0=\sum_{m=2,3,\ldots}^{n}\frac{1}{m}.$$

For simplicity and without loss of generality one neglects C_0 and takes $n=1$. Thus, one obtains

$$e^{\xi}=(\xi+1-K)\frac{\lambda}{\overset{*}{\Omega}{}^2},\quad K=\ln\left|\frac{\lambda}{\overset{*}{\Omega}{}^2}\right|. \tag{3.39a}$$

(ii)

$$\frac{e^{\xi}}{h(e^{\xi})}=\frac{e^{\xi}}{\mathrm{a}-3bz^2}=\frac{\overset{*}{\Omega}{}^2e^{\xi}}{1-3\lambda^{1/3}(\overset{*}{\Omega}{}^2e^{\xi})^{2/3}}. \tag{3.39b}$$

(iii)

$$\sin(p+p'_{\xi})=\sin(e^{-\xi}w'_{\xi})=\sin\left(\frac{\overset{*}{\Omega}{}^2}{\lambda(\xi+1-K)}w'_{\xi}\right)=\frac{\overset{*}{\Omega}{}^2}{\lambda(\xi+1-K)}w'_{\xi}+\mathbf{O}(\lambda^{-3}). \tag{3.39c}$$

(iv)

$$f(e^{\xi})=z=-\left(\frac{\overset{*}{\Omega}{}^2e^{\xi}}{\lambda}\right)^{1/3},\quad f'_{e^{\xi}}=-\frac{1}{3}\left(\frac{\overset{*}{\Omega}{}^2}{\lambda}\right)^{1/3}e^{-2\xi/3},$$

$$f''_{e^{\xi}e^{\xi}}=\frac{2}{9}\left(\frac{\overset{*}{\Omega}{}^2}{\lambda}\right)^{1/3}e^{-5\xi/3}. \tag{3.39d}$$

Using now transformation (2.29), as well as Eqs. (3.39a)–(3.39d), the nonlinear integrodifferential equation (2.31) can be approximated for $+\infty>\lambda\gg1$ by the following first-order nonlinear ODE:

$$\begin{aligned}&\left[1-\frac{1}{2(\xi+1-K)}\right](w'_{\xi}-w)^2-cw'_{\xi}+\overset{*}{\mu}\rho e^{\xi/3}\left(w'_{\xi}-\frac{1}{3}w\right)+\frac{\overset{*}{\mu}\rho}{3}\xi(w'_{\xi}-w)\\&\quad+\frac{\overset{*}{\mu}\rho}{2}e^{-2\xi/3}\left(w'_{\xi}-\frac{5}{3}w\right)-\frac{\overset{*}{\mu}\rho}{2}\left(w'_{\xi}-\frac{1}{3}w\right)+\frac{1}{4}\rho^4e^{7\xi/3}=C_1e^{\xi},\\&\rho=\left(\frac{\overset{*}{\Omega}{}^2}{\lambda}\right)^{1/3}.\end{aligned} \tag{3.40}$$

Setting

$$\bar{\xi}=\xi+1-K \quad \left(\bar{\xi}=\frac{\overset{*}{\Omega}^2}{\lambda}e^{\xi}\right) \tag{3.41a}$$

and writing

$$(\rho e^{\xi})\ll 1\Rightarrow(\rho e^{\xi})^{1/3}\ll(\rho e^{\xi})^{-2/3},\quad \bar{\xi}\ll 1\Rightarrow\xi\ll K=\ln\left|\frac{\lambda}{\overset{*}{\Omega}^2}\right|,$$
$$e^{-2\xi/3}=\rho^2\bar{\xi}^{-2/3}, \tag{3.41b}$$

the above equation can be further simplified as follows:

$$-\frac{1}{2\xi}(w'_{\bar{\xi}}-w)^2-cw'_{\bar{\xi}}+\frac{\overset{*}{\mu}\rho^3}{2}\bar{\xi}^{-2/3}\left(w'_{\bar{\xi}}-\frac{5}{3}w\right)-\frac{\overset{*}{\mu}\rho}{2}\left(w'_{\bar{\xi}}-\frac{1}{3}w\right)+\frac{1}{4}\frac{1}{\rho^3}\bar{\xi}^{7/3}=C_1\frac{1}{\rho^3}\bar{\xi},$$

or equivalently as follows:

$$(w'_{\bar{\xi}}-w)^2+2c\bar{\xi}w'_{\bar{\xi}}-\overset{*}{\mu}\rho^3\bar{\xi}^{1/3}\left(w'_{\bar{\xi}}-\frac{5}{3}w\right)+\overset{*}{\mu}\rho\bar{\xi}\left(w'_{\bar{\xi}}-\frac{1}{3}w\right)-\frac{1}{2}\frac{1}{\rho^3}\bar{\xi}^{10/3}+\frac{2C_1}{\rho^3}\bar{\xi}^2=0. \tag{3.42}$$

We rewrite the third and the fourth terms of (3.42) in the form

$$-\overset{*}{\mu}\rho^3\bar{\xi}^{1/3}(w'_{\bar{\xi}}-w)+\frac{2}{3}\overset{*}{\mu}\rho^3\bar{\xi}^{1/3}w,\quad \frac{\overset{*}{\mu}\rho}{3}\bar{\xi}(w'_{\bar{\xi}}-w)+\frac{2}{3}\overset{*}{\mu}\rho\bar{\xi}w'_{\bar{\xi}}$$

and since it is valid $\rho^3\ll 1$ and $\rho\bar{\xi}\ll\bar{\xi}$, comparison of $2/3\,\overset{*}{\mu}\rho\bar{\xi}w'_{\bar{\xi}}$ with $2c\bar{\xi}w'_{\bar{\xi}}$, as well as of $2/3\,\overset{*}{\mu}\rho^3\bar{\xi}^{1/3}w$ with w^2, results in the following further simplification for the nonlinear ODE (3.42):

$$(w'_{\bar{\xi}}-w)^2+F(\bar{\xi})(w'_{\bar{\xi}}-w)+a\bar{\xi}w'_{\bar{\xi}}+G(\bar{\xi})=0, \tag{3.43a}$$

where

$$a=2c,\quad F(\bar{\xi})=-\overset{*}{\mu}\rho^3\bar{\xi}^{1/3}+\frac{\overset{*}{\mu}\rho}{3}\bar{\xi},\quad G(\bar{\xi})=-\frac{1}{2\rho^3}\bar{\xi}^{10/3}+\frac{2C_1}{\rho^3}\bar{\xi}^2. \tag{3.43b}$$

Both Eqs. (3.20) and (3.43a) are of the same type. Thus, introducing the parameter $\tau=w'_{\bar{\xi}}$ and following the already developed methodology on Eq. (3.43a), we obtain

$$\frac{1}{\tau'_{\bar{\xi}}}=\frac{\pm 2\sqrt{-4a\bar{\xi}\tau+F^2-4G}+2a\bar{\xi}}{F'_{\bar{\xi}}F\mp F'_{\bar{\xi}}\sqrt{-4a\bar{\xi}\tau+F^2-4G}-2G'_{\bar{\xi}}-2a\tau\pm 2\tau\sqrt{-4a\bar{\xi}\tau+F^2-4G}}. \tag{3.44}$$

By the substitution

$$\sqrt{-4a\xi\tau+F^2-4G}=\sqrt{-4a\xi\tau+H(\xi)}=\sqrt{Q(\xi)},$$
$$H(\bar{\xi})=F^2-4G, \tag{3.45}$$

(3.44) becomes

$$\mp 4a\overline{\xi^2}F'_{\overline{\xi}}\sqrt{Q}\pm 2\overline{\xi}F^2\sqrt{Q}\mp 8\overline{\xi}G\sqrt{Q}\mp 2\overline{\xi}Q\sqrt{Q}=\pm 4\overline{\xi}FF'_{\overline{\xi}}\sqrt{Q}\mp 8\overline{\xi}G'_{\overline{\xi}}\sqrt{Q}\mp 2\overline{\xi}\sqrt{Q}Q'_{\overline{\xi}}\mp 2F^2\sqrt{Q}$$
$$\pm 8G\sqrt{Q}\pm 2Q\sqrt{Q}-2a\overline{\xi^2}Q'_{\overline{\xi}},$$

which, further, by the new substitution

$$\sqrt{Q}=Z\Rightarrow Q=Z^2,\quad Q'_{\overline{\xi}}=2ZZ'_{\overline{\xi}} \tag{3.46}$$

results in the following Abel equation of the second kind:

$$(\overline{\xi}Z\pm a\overline{\xi^2})Z'_{\overline{\xi}}=\tfrac{1}{2}(\overline{\xi}+1)Z^2+P(\overline{\xi}),$$
$$P(\overline{\xi})=a\overline{\xi^2}F'_{\overline{\xi}}-\tfrac{1}{2}\overline{\xi}F^2+2\overline{\xi}\gamma+\overline{\xi}FF'_{\overline{\xi}}-2\overline{\xi}G'_{\overline{\xi}}-\tfrac{1}{2}F^2+2G. \tag{3.47}$$

As in the case $0<\lambda\ll 1$, the well-known transformation

$$\omega(\overline{\xi})=(z+a\overline{\xi})\overline{\xi}^{-1/2}\exp\left(-\frac{1}{2}\overline{\xi}\right), \tag{3.48}$$

reduces Eq. (3.47) into the modified Abel form

$$\omega\omega'_{\overline{\xi}}-F_1(\overline{\xi})\omega=F_0(\overline{\xi}),$$
$$F_1(\overline{\xi})=\mp ae^{-\overline{\xi}/2}\overline{\xi}^{1/2},\quad F_0(\overline{\xi})=\left[\frac{P(\overline{\xi})}{\overline{\xi^2}}+\frac{1}{2}(1+\overline{\xi})\right]e^{-\overline{\xi}}. \tag{3.49}$$

In order to reduce Eq. (3.49) to the normal Abel form, we introduce the final general transformation

$$\omega(\overline{\xi})=q(s),\quad s=s(\overline{\xi}) \tag{3.50a}$$

with concrete form

$$\omega(\overline{\xi})=q(s),\quad s=\int F_1(\overline{\xi})\mathrm{d}\overline{\xi}=\mp a\int\overline{\xi}^{1/2}e^{-\overline{\xi}/2}\mathrm{d}\overline{\xi}=-2\overline{\xi}^{1/2}e^{-\overline{\xi}/2}+2\sqrt{\pi}\,\mathrm{erf}\left(\frac{\sqrt{2}}{2}\overline{\xi}^{1/2}\right), \tag{3.50b}$$

where

$$\mathrm{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\mathrm{d}t$$

is the probability integral.

Thus, (3.49) becomes

$$qq'_s-q=\frac{F_0(\overline{\xi})}{F_1(\overline{\xi})},$$
$$s=\int F_1(\overline{\xi})d\overline{\xi}=-2\overline{\xi}^{1/2}e^{-\overline{\xi}/2}+2\sqrt{\pi}\,\mathrm{erf}\left(\frac{\sqrt{2}}{2}\overline{\xi}^{1/2}\right). \tag{3.51}$$

This equation corresponds to (3.33) and it is valid in case of the limit $0<\lambda\ll 1$. Further approximations, concerning the second member of (3.51), are beyond the scope of this investigation.

We have already proved that in the limit of weakly ($0<\lambda\ll 1$) or strongly ($+\infty>\lambda\gg 1$) nonlinear oscillations the forced damped (NLD) equation leads to Abel's equations of the second kind of the normal form [types (3.33) and (3.51)]. It was recently proved by Panayotounakos, Panayotounakou, and Vakakis,[17] that these types of nonlinear ODEs do not admit exact analytic solutions in terms of known (tabulated) functions. Thus, the general conclusion from the above-presented discussion of the forced damped (NLD) equation is that in both limits of weakly or strongly nonlinear oscillations the equivalent equations of the Abel normal form do not admit exact analytic solutions in terms of known functions. For major reason this holds true for the original forced damped problem.

C. The forced undamped (NLD) equation

The forced undamped (NLD) equation is a special case of the damped (NLD) equation, since the governing nonlinear ODE (2.32) arises form (2.21) by setting $\lambda_3=0$. Thus, the procedure of reduction in this case is the same as that of the damped problem. The new results are the following.

The limit $0<\lambda\ll 1$. The approximate ODE (3.30) becomes

$$(w'_{\bar{\xi}}-w)^2+aw'_{\bar{\xi}}-\beta\bar{\xi}^2+\gamma\bar{\xi}-\delta\bar{\xi}=0, \tag{3.52a}$$

where

$$a=-\frac{2(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|}\frac{A}{\Omega^2},\quad \beta=-\frac{2(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|}\frac{2}{\lambda\Omega^2},$$

$$\gamma=\frac{2(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|}\frac{3}{\lambda\sqrt{\lambda_1}\Omega^2},\quad \delta=\frac{4C_1(1+\ln|\sqrt{\lambda_1}|)}{1+2\ln|\sqrt{\lambda_1}|}\frac{\sqrt{\lambda_1}}{\sqrt{\lambda}\Omega^2}, \tag{3.52b}$$

$$\bar{\xi}=1+\xi-K,\quad K=\ln\left|\frac{2}{\overset{*}{\Omega}{}^2\sqrt{\lambda}\sqrt{\lambda_1}}\right|,\quad \overset{*}{\Omega}=\frac{\Omega}{\sqrt{\lambda_1}}.$$

Further reduction of (3.52a) follows the corresponding steps of (3.20) and thus, the equivalent to (3.36a) The Abel equation of the normal form becomes

$$qq'_s-q=p_1s^{-2}+p_2s^{-1}+p_3s+p_4, \tag{3.53a}$$

in which

$$p_1=\mp 8a\gamma M^3,\quad p_2=4(\beta+6\gamma)M^2,\quad p_3=-\frac{a^2+4(3\beta+4\gamma-2\delta)}{4a^2},$$

$$p_4=\mp\frac{2(9\gamma+4\beta-\delta)}{a}M. \tag{3.53b}$$

The limit $1\ll\lambda<+\infty$. In this case the corresponding to (3.40) reduced equation becomes by setting in (3.40) $\overset{*}{\mu}=0$, and thus, the approximate nonlinear ODE (3.42) takes the simplified form

$$(w'_{\bar{\xi}}-w)^2+2c\bar{\xi}w'_{\bar{\xi}}-\frac{1}{2\rho^3}\bar{\xi}^{10/3}+\frac{2C_1}{\rho^3}\bar{\xi}^2=0. \tag{3.54}$$

Therefore the final approximate Abel equation of the normal form, in which the nonlinear exact integrodifferential equation (2.33) reduces, becomes

$$qq_s'-q=\frac{F_0(\bar{\xi})}{F_1(\bar{\xi})}, \tag{3.55a}$$

where

$$\frac{F_0(\bar{\xi})}{F_1(\bar{\xi})}=\mp\frac{1}{a}\left\{[\bar{\xi}F_{\bar{\xi}}'-(1+\bar{\xi})F]\bar{\xi}^{-5/2}+\frac{a^2}{4}(1+\bar{\xi})\bar{\xi}^{-1/2}\right\}e^{-\bar{\xi}/2},$$

$$F(\bar{\xi})=-(\beta\bar{\xi}^{10/3}+\gamma\bar{\xi}^2), \tag{3.55b}$$

$$s=\int F_1(\bar{\xi})\mathrm{d}\bar{\xi}=\mp\frac{a}{2}\int\bar{\xi}^{1/2}e^{-\bar{\xi}/2}\mathrm{d}\bar{\xi}=\pm 2\bar{\xi}^{1/2}e^{-\bar{\xi}/2}+2\sqrt{\pi}\,\mathrm{erf}\left(\frac{\sqrt{2}}{2}\bar{\xi}^{1/2}\right),$$

$$\mathrm{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\mathrm{d}t=\text{probability integral.}$$

The solvability of both approximated reduced Eqs. (3.53a) and (3.55a) in the present case of the limit $1\ll\lambda<+\infty$ follows the general conclusion of the forced damped (NLD) problem.

In the following we provide approximate analytic solutions of the already examined three nonlinear ODEs. In some cases such solutions are indispensable to making use of further assumptions and approximations. These assumptions and approximations are realistic and usual for deriving exact solutions for these strongly nonlinear problems.

IV. APPROXIMATE ANALYTIC SOLUTIONS

We shall present new approximate analytic solutions of the three kinds of equations being examined.

A. The one-dimensional axisymmetric (NLS) equation with cubic nonlinearities

It is was already proved that for the NLS equation and for the limits $0<\lambda=\lambda_1/\lambda_2\ll 1$, and $1\ll\lambda=\lambda_1/\lambda_2<+\infty$, the equivalent nonlinear first-order integrodifferential equation (2.20a) can be asymptotically approximated by the following two nonlinear first-order ODEs.

(i) For $0<\lambda=\lambda_1/\lambda_2\ll 1$ [Eq. (3.8)],

$$\frac{1}{2}(w_{\bar{\xi}}'-w)^2+w=C_1,\quad A=\frac{1}{3}\sqrt[3]{\frac{4}{\lambda_2\lambda}}. \tag{4.1a}$$

(ii) For $1\ll\lambda=\lambda_1/\lambda_2<+\infty$ [Eq. (3.11)],

$$\tfrac{1}{2}(w_{\bar{\xi}}'-w)^2-Bw=C_1,\quad B=\tfrac{1}{3}(\sqrt{\lambda}+\tfrac{1}{2}). \tag{4.1b}$$

Both these equations are of the same type, that is to say of the type

$$(w_{\bar{\xi}}'-w)^2+2aw-2\beta=0, \tag{4.2a}$$

where

$$a=\frac{2}{3}\sqrt[3]{\frac{4}{\lambda_2\lambda}}\quad\text{or}\quad a=-\frac{2}{3}\left(\sqrt{\lambda}+\frac{1}{2}\right),\quad 2\beta=2C_1, \tag{4.2b}$$

and they can be analytically solved. In fact, solving (4.2a) for $(w'_{\bar{\xi}}-w)$ and setting $\sqrt{2(\beta-aw)}=\omega$, we obtain

$$\frac{\omega d\omega}{\omega^2\mp a\omega-2\beta}=-d\bar{\xi},$$

the integration which furnishes (see Ref. 22, p. 69)

$$-\frac{1}{4\beta}\ln\left|\frac{\omega^2}{\omega^2\mp a\omega-2\beta}\right|\mp\frac{a}{4\beta}\int\frac{d\omega}{\omega^2\mp a\omega-2\beta}=-\bar{\xi}+C_2.$$

This integral depends on the sign of the quantity $\Delta=(8C_1+a^2)$. Thus, we distinguish the following three possible solutions in terms of w:

$$\begin{aligned}
&-\frac{1}{4\beta}\ln\left|\frac{2(\beta-aw)}{2(\beta-aw)\mp a\sqrt{\beta-aw}-2\beta}\right|\mp\frac{a}{4\beta\sqrt{-(8C_1+a^2)}}\\
&\quad-\ln\left|\frac{\mp a+2\sqrt{2(\beta-aw)}-\sqrt{-(8C_1+a^2)}}{\mp a+2\sqrt{2(\beta-aw)}+\sqrt{-(8C_1+a^2)}}\right|\\
&\quad=-\bar{\xi}+C_2 \quad \text{if } (8C_1+a^2)<0,\\
&-\frac{1}{4\beta}\ln\left|\frac{2(\beta-aw)}{2(\beta-aw)\mp a\sqrt{\beta-aw}-2\beta}\right|\pm\frac{2a}{4\beta(\mp a+2\sqrt{\beta-aw})}=-\bar{\xi}+C_2 \quad \text{if } -(8C_1+a^2)=0,\\
&-\frac{1}{4\beta}\ln\left|\frac{2(\beta-aw)}{2(\beta-aw)\mp a\sqrt{\beta-aw}-2\beta}\right|\pm\frac{2}{4\beta\sqrt{8C_1+a^2}}\arctan\left(\frac{\mp a+2\sqrt{\beta-aw}}{\sqrt{8C_1+a^2}}\right)\\
&\quad=-\bar{\xi}+C_2 \quad \text{if } (8C_1+a^2)>0,
\end{aligned} \tag{4.3}$$

where C_2 is a second constant of integration.

B. The forced damped (NLD) equation

We shall try to construct approximate analytic solutions of the reduced equation (3.36a) holding in case of the parameter $(0<\lambda\ll 1)$. First one observes that Eq. (3.36a) does not admit exact solutions in terms of known (tabulated) functions (see Ref. 21, pp. 29–32). Thus, new approximations are indispensable. Now combining Eqs. (3.17b) and (3.34) we extract the following:

$$\begin{aligned}
&e^{-\xi}=\frac{1}{1-\sqrt{\lambda}z}\,\frac{1}{\sqrt{\lambda_1}}e^{-K}, \quad \xi=\bar{\xi}-1+K,\\
&s=\pm 2ae^{-\bar{\xi}/2}=\pm 2ae^{(1+\xi-K)/2}=\pm\frac{2a}{\sqrt{e}}\,\frac{1}{\lambda^{1/4}}\,\frac{1}{\sqrt{1-\sqrt{\lambda_1}z}}=\pm\frac{2a}{\sqrt{e}}\,\frac{1}{\lambda^{1/4}}\left(1+\frac{1}{2}\sqrt{\lambda}z\right)+\mathbf{O}(\lambda).
\end{aligned} \tag{4.4}$$

Rewriting the second of the above equations as

$$s=\pm\frac{a}{\sqrt{e}}\,\frac{1}{\lambda^{1/4}}(3-1+\sqrt{\lambda}z)=\pm\frac{3a}{\sqrt{e}\lambda^{1/4}}\mp\frac{a}{\sqrt{e}\lambda^{1/4}}(1-\sqrt{\lambda}z)$$

and introducing the quantity $(1-\sqrt{\lambda}z)$ by way of the first of (4.4), we find

$$s=\pm\frac{3a}{\sqrt{e}\lambda^{1/4}}\mp\frac{a}{e\lambda^{3/4}}e^{\bar{\xi}}=\pm\frac{3a}{\sqrt{e}\lambda^{1/2}}\mp\frac{4a^3}{e\lambda_1^{3/4}}\frac{1}{s^2}.$$

Thus, since $\lambda_1=\lambda_2/\lambda$, one produces the following approximation:

$$\frac{1}{s^2}=\frac{c_1}{\lambda^{1/2}}\mp\frac{c_2}{\lambda^{3/4}}s+\mathbf{O}(\lambda),\quad c_1=\frac{3a^2(e\lambda_2)^{1/2}}{4},\quad c_2=\frac{e\lambda_2^{3/4}}{4a^3}. \tag{4.5}$$

On the other hand, solving this last equation for s we deduce

$$s=\mp\frac{\frac{1}{s^2}-\frac{c_1}{\lambda^{1/2}}}{\frac{c_2}{\lambda^{3/4}}}=\mp\frac{1-\frac{c_1}{\lambda^{1/2}}s^2}{\frac{c_2}{\lambda^{3/4}}s^2},$$

a fact that permits us to write

$$\frac{1}{s}=\mp\frac{1}{\frac{1}{c_2s^2/\lambda^{3/4}}-\frac{c_1/\lambda^{1/2}}{c_2/\lambda^{3/4}}}=\pm\frac{1}{\frac{c_1\lambda^{1/2}}{c_2}-\frac{\lambda^{3/4}}{c_2s^2}}=\pm\frac{1}{\left(1-\frac{\lambda^{1/4}}{c_1s^2}\right)\frac{c_1\lambda^{1/2}}{c_2}}.$$

We approximate again and we obtain

$$\frac{1}{s}=\pm\frac{c_2}{c_1\lambda^{1/2}}\left(1+\frac{\lambda^{1/4}}{c_1}\frac{1}{s^2}\right)+\mathbf{O}(\lambda^{1/2}). \tag{4.6}$$

Until now we succeeded in expressing $1/s^2$ and $1/s$ in terms of s up to $\mathbf{O}(\lambda)$ and $\mathbf{O}(\lambda^{1/2})$, respectively.

Introducing the above-given results into (3.36a) we extract the following Abel nonlinear ODE of the normal form:

$$qq_s'-q=As+B,$$

$$A=p_3\mp\frac{c_2}{\lambda^{3/4}}p_1-\frac{c_2^2}{c_1\lambda^{1/4}}p_2,\quad B=p_4\pm\frac{c_1}{\lambda^{1/2}}p_1\pm\frac{c_2}{c_1}\left(\frac{1}{\lambda^{1/2}}+\frac{1}{\lambda^{3/4}}\right)p_2, \tag{4.7}$$

$$p_1,\ p_2,\ p_3,\ p_4 \text{ as in Eq. (3.36a)};\quad c_1,\ c_2 \text{ as in Eq. (4.5)}.$$

The Abel equation (3.7) admits an exact parametric solution given by the restored formula (see Ref. 21, p. 29, type 1.3.2)

$$s=C_2\exp\left(-\int\frac{v\mathrm{d}v}{v^2-v-A}\right),$$

$$q=C_2\frac{v-1}{A}\exp\left(-\int\frac{v\,dv}{v^2-v-A}\right)-\frac{B}{A}, \tag{4.8}$$

$$v=q_s'=\text{parameter}.$$

Note that for the forced undamped (NLD) equation a similar approximate analytic solution to (4.8) holds true with different factors p_i (i=1,2,3,4) given by Eq. (3.53b).

V. CONCLUSIONS

By a series of admissible functional transformations we reduced the one-dimensional axisymmetric (NLS) equation, and the forced damped or undamped (NLD) equations to equivalent nonlinear integrodifferential equations of the first order. These equations are exact and constitute the intermediate integrals in the phase plane. In the limits of small or large values of the parameters characterizing these nonlinear problems, we expand the reduced integrodifferential equations asymptotically to nonlinear ODEs of the first order. The (NLS) equation changes to solvable first-order form, while the (NLD) equations change to nonlinear ODEs of the Abel classes. Taking into account the existing known exact analytic solutions of these classes of equations, we show that both (NLD) equations do not admit exact analytic solutions in terms of known (tabulated) functions. For further asymptotic approximations we succeed in constructing exact analytic solutions for (NLD) oscillators. The reduction methodology introduced in the paper is general and can be applied to some of the most interesting ODEs of mathematical physics and nonlinear mechanics, including the forced Van der Pol nonlinear oscillator; the Thomas–Fermi equation; the Blasius equation $y'''_{xxx}+\lambda_1 y y''_{xx}=0$; the Langmuir equation $3yy''_{xx}+y'^2_x+4yy'_x+y^2-1=0$; the Kidder equation $\sqrt{1-ayy''_{xx}}+2xy'_x=0$, $0<a<1$, as well as the plastic spin equations in simple shear.[20]

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ERRATUM

Erratum: "Hall effect in noncommutative coordinates" [J. Math. Phys. 43, 4592 (2002)]

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The Hall conductivity on noncommutative plane is given as in (30) if the current defined in (28) is rescaled with a γ factor:

$$\hat{\vec{J}} = \frac{e\gamma^2\rho}{m}\left(\gamma\hat{\vec{p}} + \frac{e}{c}\vec{A} + \vec{a}\right).$$

However, this is not a very natural definition. If one retains the more natural definition (28), the noncommutative Hall conductivity σ_H^{nc} will be independent of the noncommutativity parameter θ and the comments given in Ref. 1 should be taken into account.

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"Squashed entanglement": An additive entanglement measure

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In this paper, we present a new entanglement monotone for bipartite quantum states. Its definition is inspired by the so-called intrinsic information of classical cryptography and is given by the halved minimum quantum conditional mutual information over all tripartite state extensions. We derive certain properties of the new measure which we call "squashed entanglement": it is a lower bound on entanglement of formation and an upper bound on distillable entanglement. Furthermore, it is convex, additive on tensor products, and superadditive in general. Continuity in the state is the only property of our entanglement measure which we cannot provide a proof for. We present some evidence, however, that our quantity has this property, the strongest indication being a conjectured Fannes-type inequality for the conditional von Neumann entropy. This inequality is proved in the classical case. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1643788]

I. INTRODUCTION

Ever since Bennett *et al.*[1,2] introduced the entanglement measures of *distillable entanglement* and *entanglement of formation* in order to measure the amount of nonclassical correlation in a bipartite quantum state, there has been an interest in an axiomatic approach to entanglement measures. One natural axiom is LOCC-monotonicity, which means that an entanglement measure should not increase under *Local Operations and Classical Communication*. Furthermore, every entanglement measure should vanish on the set of separable quantum states; it should be convex, additive, and a continuous function in the state. Though several entanglement measures have been proposed, it turns out to be difficult to find measures that satisfy all of the above axioms. One unresolved question is whether or not entanglement of formation is additive. This is an important question and has recently been connected to many other additivity problems in quantum information theory.[24] Other examples are distillable entanglement, which shows evidence of being neither additive nor convex,[25] and *relative entropy of entanglement*,[28] which can be proven to be nonadditive.[30]

In this paper we present a functional called "squashed entanglement" which has many of these desirable properties: it is convex, additive on tensor products and superadditive in general. It is upper bound by entanglement cost, lower bound by distillable entanglement, and we are able to present some evidence of continuity.

The remaining sections are organized as follows: in Sec. II we will define squashed entanglement and prove its most important properties. In Sec. III we will explain its analogy to a quantity called *intrinsic information*, known from classical cryptography. This constitutes the motivation for our definition.

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The only property that we could not find proof for is continuity. A detailed discussion of this problem follows in Sec. IV, where we show that squashed entanglement is continuous on the interior of the set of states and where we provide evidence in favor of continuity in general. This evidence is based on a Fannes-type inequality for the conditional von Neumann entropy. It is conjectured in general and is true in the classical case, which we will prove in the Appendix.

II. SQUASHED ENTANGLEMENT

In this paper all Hilbert spaces are assumed to be finite dimensional, even though some of the following definitions and statements make sense also in infinite dimension.

Definition 1: Let ρ^{AB} be a quantum state on a bipartite Hilbert space $\mathcal{H}=\mathcal{H}_A\otimes\mathcal{H}_B$. We define the *squashed entanglement* of ρ^{AB} by

$$E_{\mathrm{sq}}(\rho^{AB}) := \inf\{\tfrac{1}{2} I(A;B|E) : \rho^{ABE} \text{ extension of } \rho^{AB}\}.$$

The infimum is taken over all extensions of ρ^{AB}, i.e., over all quantum states ρ^{ABE} with $\rho^{AB}=\mathrm{Tr}_E\rho^{ABE}$. $I(A;B|E) := S(AE)+S(BE)-S(ABE)-S(E)$ is the quantum conditional mutual information of ρ^{ABE}.[3] ρ^A stands for the restriction of the state ρ^{ABE} to subsystem A, and $S(A)=S(\rho^A)$ is the von Neumann entropy of the underlying state, if it is clear from the context. If not, we emphasize the state in subscript, $S(A)_\rho$. Note that the dimension of E is *a priori* unbounded.

Tucci[26] has previously defined the same functional (without the factor $\frac{1}{2}$) in connection with his investigations into the relationship between quantum conditional mutual information and entanglement measures, in particular entanglement of formation.

Our name for this functional comes from the idea that the right choice of a conditioning system reduces the quantum mutual information between A and B, thus "squashing out" the nonquantum correlations. See Sec. III for a similar idea in classical cryptography, which motivated the above definition.

Example 2: Let $\rho^{AB}=|\psi\rangle\langle\psi|^{AB}$ be a pure state. All extensions of ρ^{AB} are of the form $\rho^{ABE}=\rho^{AB}\otimes\rho^E$; therefore

$$\tfrac{1}{2} I(A;B|E) = S(\rho^A) = E(|\psi\rangle),$$

which implies $E_{\mathrm{sq}}(|\psi\rangle\langle\psi|)=E(|\psi\rangle)$.

Proposition 3: E_{sq} *is an* entanglement monotone, *i.e., it does not increase under local quantum operations and classical communication (LOCC) and it is convex.*

Proof: According to Ref. 29 it suffices to verify that E_{sq} satisfies the following two criteria:

(1) For any quantum state ρ^{AB} and any unilocal quantum instrument $(\mathcal{E}_k)$—the $\mathcal{E}_k$ are completely positive maps and their sum is trace preserving[6]—performed on either subsystem,

$$E_{\mathrm{sq}}(\rho^{AB}) \geq \sum_k p_k E_{\mathrm{sq}}(\tilde{\rho}_k^{AB}),$$

where

$$p_k = \mathrm{Tr}\,\mathcal{E}_k(\rho^{AB}) \quad \text{and} \quad \tilde{\rho}_k^{AB} = \frac{1}{p_k}\mathcal{E}_k(\rho^{AB}).$$

(2) E_{sq} is convex, i.e., for all $0\leq\lambda\leq 1$,

$$E_{\mathrm{sq}}(\lambda\rho^{AB}+(1-\lambda)\sigma^{AB}) \leq \lambda E_{\mathrm{sq}}(\rho^{AB})+(1-\lambda)E_{\mathrm{sq}}(\sigma^{AB}).$$

In order to prove 1, we modify the proof of theorem 11.15 in Ref. 19 for our purpose. By symmetry we may assume that the instrument $(\mathcal{E}_k)$ acts unilocally on A. Now, attach two ancilla systems A' and A'' in states $|0\rangle^{A'}$ and $|0\rangle^{A''}$ to the system ABE (i). To implement the quantum operation

$$\rho^{ABE} \to \tilde{\rho}^{AA'BE} := \sum_k (\mathcal{E}_k \otimes \mathrm{id}_E)(\rho^{ABE}) \otimes |k\rangle\langle k|^{A'},$$

with $(|k\rangle^{A'})_k$ being an orthonormal basis on A', we perform (ii) a unitary transformation U on $AA'A''$ followed by (iii) tracing out the system A''. Here, $\tilde{i}$ denotes the system $i \in \{A,B,AB\}$ after the unitary evolution U. Then, for any extension of ρ^{AB},

$$\begin{aligned} I(A;B|E) &\overset{\text{(i)}}{=} I(AA'A'';B|E) \\ &\overset{\text{(ii)}}{=} I(\tilde{A}\tilde{A}'\tilde{A}'';\tilde{B}|\tilde{E}) \\ &\overset{\text{(iii)}}{\geq} I(\tilde{A}\tilde{A}';\tilde{B}|\tilde{E}) \\ &\overset{\text{(iv)}}{=} I(\tilde{A}';\tilde{B}|\tilde{E}) + I(\tilde{A};\tilde{B}|\tilde{E}\tilde{A}') \\ &\overset{\text{(v)}}{\geq} \sum_k p_k I(\tilde{A};\tilde{B}|\tilde{E})_{\rho_k} \\ &\overset{\text{(vi)}}{\geq} \sum_k 2 p_k E_{\mathrm{sq}}(\rho_k). \end{aligned}$$

The justification of these steps is as follows: attaching auxiliary pure systems does not change the entropy of a system, step (i). The unitary evolution affects only the systems $AA'A''$ and therefore does not affect the quantum conditional mutual information in step (ii). To show that discarding quantum systems cannot increase the quantum conditional mutual information

$$I(\tilde{A}\tilde{A}';\tilde{B}|\tilde{E}) \leq I(\tilde{A}\tilde{A}'\tilde{A}'';\tilde{B}|\tilde{E})$$

we expand it into

$$S(AA'E) + S(BE) - S(AA'BE) - S(E) \leq S(AA'A''E) + S(BE) - S(AA'A''BE) - S(E),$$

which is equivalent to

$$S(AA'E) - S(AA'BE) \leq S(AA'A''E) - S(AA'A''BE),$$

the strong subadditivity;[17] this shows step (iii), and for step (iv) we use the *chain rule*,

$$I(XY;Z|U) = I(X;Z|U) + I(Y;Z|UX).$$

For step (v), note that the first term, $I(\tilde{A}';\tilde{B}|\tilde{E})$, is non-negative and that the second term, $I(\tilde{A};\tilde{B}|\tilde{E}\tilde{A}')$, is identical to the expression in the next line. Finally, we have (vi) since $\rho_k^{\tilde{A}\tilde{B}\tilde{E}}$ is a valid extension of ρ_k. As the original extension of ρ^{AB} was arbitrary, the claim follows.

To prove convexity, property 2, consider any extensions ρ^{ABE} and σ^{ABE} of the states ρ^{AB} and σ^{AB}, respectively. It is clear that we can assume, without loss of generality, that the extensions are defined on identical systems E. Combined, ρ^{ABE} and σ^{ABE} form an extension

$$\tau^{ABEE'} := \lambda \rho^{ABE} \otimes |0\rangle\langle 0|^{E'} + (1-\lambda)\sigma^{ABE} \otimes |1\rangle\langle 1|^{E'}$$

of the state $\tau^{AB} = \lambda\rho^{AB} + (1-\lambda)\sigma^{AB}$. The convexity of squashed entanglement then follows from the observation

$$\lambda I(A;B|E)_\rho + (1-\lambda) I(A;B|E)_\sigma = I(A;B|EE')_\tau \geq 2E_{\mathrm{sq}}(\tau^{AB}).$$

Proposition 4: E_{sq} is superadditive in general, and additive on tensor products, i.e.,

$$E_{\mathrm{sq}}(\rho^{AA'BB'}) \geq E_{\mathrm{sq}}(\rho^{AB}) + E_{\mathrm{sq}}(\rho^{A'B'})$$

is true for every density operator $\rho^{AA'BB'}$ on $\mathcal{H}_A \otimes \mathcal{H}_{A'} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B'}$, $\rho^{AB} = \mathrm{Tr}_{A'B'}\rho^{AA'BB'}$, and $\rho^{A'B'} = \mathrm{Tr}_{AB}\rho^{AA'BB'}$,

$$E_{\mathrm{sq}}(\rho^{AA'BB'}) = E_{\mathrm{sq}}(\rho^{AB}) + E_{\mathrm{sq}}(\rho^{A'B'})$$

for $\rho^{AA'BB'}=\rho^{AB}\otimes\rho^{A'B'}$.

Proof: We start with superadditivity and assume that $\rho^{AA'BB'E}$ on $\mathcal{H}_A\otimes\mathcal{H}_{A'}\otimes\mathcal{H}_B\otimes\mathcal{H}_{B'}\otimes\mathcal{H}_E$ is an extension of $\rho^{AA'BB'}$, i.e., $\rho^{AA'BB'}=\mathrm{Tr}_E\rho^{AA'BB'E}$. Then,

$$\begin{aligned}I(AA';BB'|E)&=I(A;BB'|E)+I(A';BB'|EA)\\&=I(A;B|E)+I(A;B'|EB)+I(A';B'|EA)+I(A';B|EAB')\\&\geqslant I(A;B|E)+I(A';B'|EA)\geqslant 2E_{\mathrm{sq}}(\rho^{AB})+2E_{\mathrm{sq}}(\rho^{A'B'}).\end{aligned}$$

The first inequality is due to strong subadditivity of the von Neumann entropy. Note that E is an extension for system AB and EA extends system $A'B'$. Hence, the last inequality is true since squashed entanglement is defined via the infimum over all extensions of the respective states. The calculation is independent of the choice of the extension, which proves superadditivity.

A special case of the above is superadditivity on product states $\rho^{AA'BB'}:=\rho^{AB}\otimes\rho^{A'B'}$. To conclude that E_{sq} is indeed additive on tensor products, it therefore suffices to prove subadditivity on tensor products.

Let ρ^{ABE} on $\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_E$ be an extension of ρ^{AB} and let $\rho^{A'B'E'}$ on $\mathcal{H}_{A'}\otimes\mathcal{H}_{B'}\otimes\mathcal{H}_{E'}$ be an extension for $\rho^{A'B'}$. It is evident that $\rho^{ABE}\otimes\rho^{A'B'E'}$ is a valid extension for $\rho^{AA'BB'}=\rho^{AB}\otimes\rho^{A'B'}$, hence

$$\begin{aligned}2E_{\mathrm{sq}}(\rho^{AA'BB'})&\leqslant I(AA';BB'|EE')\\&=I(A;B|EE')+\underbrace{I(A;B'|EE'B)}_{=0}+I(A';B'|EE'A)+\underbrace{I(A';B|EE'AB')}_{=0}\\&=I(A;B|E)+I(A';B'|EE'A)\\&=I(A;B|E)+I(A';B'|E').\end{aligned}$$

This inequality holds for arbitrary extensions of ρ^{AB} and $\rho^{A'B'}$. We therefore conclude that E_{sq} is subadditive on tensor products. □

Proposition 5: E_{sq} *is upper bounded by* entanglement of formation[1,2]

$$E_{\mathrm{sq}}(\rho^{AB})\leqslant E_F(\rho^{AB}).$$

Proof: Let $\{p_k,|\Psi_k\rangle\}$ be a pure state ensemble for ρ^{AB},

$$\sum_k p_k|\Psi_k\rangle\langle\Psi_k|^{AB}=\rho^{AB}.$$

The purity of the ensemble implies

$$\sum_k p_k S(A)_{\Psi_k}=\tfrac{1}{2}\sum_k p_k I(A;B)_{\Psi_k}.$$

Consider the following extension ρ^{ABE} of ρ^{AB}:

$$\rho^{ABE}:=\sum_k p_k|\Psi_k\rangle\langle\Psi_k|^{AB}\otimes|k\rangle\langle k|^E.$$

It is elementary to compute

$$\sum_k p_k S(A)_{\Psi_k}=\tfrac{1}{2}\sum_k p_k I(A;B)_{\Psi_k}=\tfrac{1}{2}I(A;B|E).$$

Thus, it is clear that entanglement of formation can be regarded as an infimum over a certain class of extensions of ρ^{AB}. Squashed entanglement is an infimum over *all* extensions of ρ^{AB}, evaluated on the same quantity $\frac{1}{2}I(A;B|E)$ and therefore smaller or equal to entanglement of formation. □

Corollary 6: E_{sq} *is upper bounded by* entanglement cost,

$$E_{\mathrm{sq}}(\rho^{AB}) \leqslant E_C(\rho^{AB}).$$

Proof: Entanglement cost is equal to the regularized entanglement of formation,[12]

$$E_C(\rho^{AB}) = \lim_{n\to\infty} \frac{1}{n} E_F((\rho^{AB})^{\otimes n}).$$

This, together with proposition 5, and the additivity of the squashed entanglement (proposition 4) implies

$$E_C(\rho^{AB}) = \lim_{n\to\infty} \frac{1}{n} E_F((\rho^{AB})^{\otimes n}) \geqslant \lim_{n\to\infty} \frac{1}{n} E_{\mathrm{sq}}((\rho^{AB})^{\otimes n}) = E_{\mathrm{sq}}(\rho^{AB}).$$

□

Theorem 7: *Squashed entanglement vanishes for every separable density matrix* ρ^{AB}*, i.e.,*

$$\rho^{AB} \textit{separable} \Rightarrow E_{\mathrm{sq}}(\rho^{AB}) = 0.$$

Conversely, if there exists a finite extension ρ^{ABE} *of* ρ^{AB} *with vanishing quantum conditional mutual information, then* ρ^{AB} *is separable, i.e.,*

$$I(A;B|E) = 0 \quad \textit{and} \quad \dim \mathcal{H}_E < \infty \Rightarrow \rho^{AB} \quad \textit{separable}.$$

Proof: Every separable ρ^{AB} can be written as a convex combination of separable pure states,

$$\rho^{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|^A \otimes |\phi_i\rangle\langle\phi_i|^B.$$

The quantum conditional mutual information of the extension

$$\rho^{ABE} := \sum_i p_i |\psi_i\rangle\langle\psi_i|^A \otimes |\phi_i\rangle\langle\phi_i|^B \otimes |i\rangle\langle i|^E,$$

with orthonormal states ($|i\rangle^E$), is zero. Squashed entanglement thus vanishes on the set of separable states.

To prove the second assertion assume that there exists an extension ρ^{ABE} of ρ^{AB} with $I(A;B|E)=0$ and $\dim \mathcal{H}_E < \infty$. Now, a recently obtained result[13] on the structure of such states ρ^{ABE} applies: there it was shown that in this case the system E can be written as a direct sum of tensor products, such that with a suitable basis transformation $E \to EE'E''$ the state can be rewritten

$$\rho^{ABE} = \sum_i p_i \rho_i^{AE'} \otimes \rho_i^{E''B} \otimes |i\rangle\langle i|^E.$$

Then $\rho^{AB} = \Sigma_i p_i (\mathrm{Tr}_{E'} \rho_i^{AE'}) \otimes (\mathrm{Tr}_{E''} \rho_i^{E''B})$ is separable.

Remark 8: The minimization in squashed entanglement ranges over extensions of ρ^{AB} *with a priori unbounded size.* $E_{\mathrm{sq}}(\rho)=0$ *is thus possible, even if any finite extension has strictly positive quantum conditional mutual information. Therefore, without a bound on the dimension of the extending system, the second part of theorem 7 does not suffice to conclude that* $E_{\mathrm{sq}}(\rho^{AB})$ *implies separability of* ρ^{AB}*. A different approach to this question could be provided by a possible approximate version of the main result of Ref. 13: if there is an extension* ρ^{ABE} *with small quantum conditional mutual information, then the* ρ^{AB} *is close to a separable state. For further discussion on this question, see Secs. III and IV.*

Note that the strict positivity of squashed entanglement for entangled states would, via corollary 6, imply strict positivity of entanglement cost for all entangled states. This is not yet proven, but conjectured as a consequence of the additivity conjecture of entanglement of formation.

Example 9: It is worth noting that in general E_{sq} is strictly smaller than E_F and E_C: consider the totally antisymmetric state σ^{AB} in a two-qutrit system

$$\sigma^{AB}=\tfrac{1}{3}(|\mathrm{I}\rangle\langle\mathrm{I}|+|\mathrm{II}\rangle\langle\mathrm{II}|+|\mathrm{III}\rangle\langle\mathrm{III}|),$$

with

$$|\mathrm{I}\rangle=\frac{1}{\sqrt{2}}(|2\rangle^A|3\rangle^B-|3\rangle^A|2\rangle^B),$$

$$|\mathrm{II}\rangle=\frac{1}{\sqrt{2}}(|3\rangle^A|1\rangle^B-|1\rangle^A|3\rangle^B),$$

$$|\mathrm{III}\rangle=\frac{1}{\sqrt{2}}(|1\rangle^A|2\rangle^B-|2\rangle^A|1\rangle^B).$$

On the one hand, it is known from Ref. 31 that $E_F(\sigma^{AB})=E_C(\sigma^{AB})=1$, though, on the other hand, we may consider the trivial extension,

$$E_{\mathrm{sq}}(\sigma^{AB})\leqslant\tfrac{1}{2}I(A;B)=\tfrac{1}{2}\log 3\approx 0.792.$$

The best known upper bound on E_D for this state, the *Rains bound*,[21] gives the only slightly smaller value $\log\frac{5}{3}\approx 0.737$. It remains open if there exist states for which squashed entanglement is smaller than the Rains bound.

Proposition 10: E_{sq} is lower bounded by distillable entanglement[1,2]

$$E_D(\rho^{AB})\leqslant E_{\mathrm{sq}}(\rho^{AB}).$$

Proof: Consider any entanglement distillation protocol by LOCC, taking n copies of the state $(\rho^{AB})^{\otimes n}$ to a state σ^{AB} such that

$$\|\sigma^{AB}-|s\rangle\langle s|^{AB}\|_1\leqslant\delta, \tag{1}$$

with $|s\rangle$ being a maximally entangled state of Schmidt rank s. We may assume without loss of generality that the support of σ^A and σ^B is contained in the s-dimensional support of $\mathrm{Tr}_B|s\rangle\langle s|$ and $\mathrm{Tr}_A|s\rangle\langle s|$, respectively. Using propositions 4 and 3, we have

$$nE_{\mathrm{sq}}(\rho^{AB})=E_{\mathrm{sq}}((\rho^{AB})^{\otimes n})\geqslant E_{\mathrm{sq}}(\sigma^{AB}), \tag{2}$$

so that it is only necessary to estimate $E_{\mathrm{sq}}(\sigma^{AB})$ vs $E_{\mathrm{sq}}(|s\rangle\langle s|^{AB})=\log s$ (see example 2). For this, let σ^{ABE} be an arbitrary extension of σ^{AB} and consider a purification of it, $|\Psi\rangle\in\mathcal{H}_{ABEE'}$. Chain rule and monotonicity of the quantum mutual information allow us to estimate

$$I(A;B|E)=I(AE;B)-I(E;B)\geqslant I(A;B)-I(EE';AB)=I(A;B)-2S(AB).$$

Further applications of Fannes inequality,[9] lemma 13, give $I(A;B)\geqslant 2\log s-f(\delta)\log s$ and $2S(AB)\leqslant f(\delta)\log s$, with a function f of δ vanishing as δ approaches 0. Hence

$$\tfrac{1}{2}I(A;B|E)\geqslant\log s-f(\delta)\log s.$$

Since this is true for all extensions, we can put this together with Eq. (2), and obtain

$$E_{\mathrm{sq}}(\rho^{AB}) \geqslant \frac{1}{n}(1-f(\delta))\log s,$$

which, with $n\to\infty$ and $\delta\to 0$, concludes the proof, because we considered an arbitrary distillation protocol. □

Remark 11: In the proof of proposition 10 we made use of the continuity of E_{sq} in the vicinity of maximally entangled states. Similarly, E_{sq} can be shown to be continuous in the vicinity of any pure state. This, together with proposition 3, the additivity on tensor products (second part of proposition 4), and the normalization on Bell states, suffices to prove corollary 6 and proposition 10.[15]

Corollary 12:

$$\tfrac{1}{2}(I(A;B)-S(AB)) \leqslant E_{\mathrm{sq}}(\rho^{AB}).$$

Proof: The recently established *hashing inequality*[7] provides a lower bound for the *one-way distillable entanglement* $E_{\mathbf{D}}(\rho^{AB})$,

$$S(B)-S(AB) \leqslant E_{\mathbf{D}}(\rho^{AB}).$$

Interchanging the roles of A and B, we have

$$\tfrac{1}{2}(I(A;B)-S(AB)) \leqslant E_{D}(\rho^{AB}),$$

where we use the fact that one-way distillable entanglement is smaller or equal to distillable entanglement. This, together with the bound from proposition 10, implies the assertion. □

III. ANALOGY TO INTRINSIC INFORMATION

Intrinsic information is a quantity that serves as a measure for the correlations between random variables in information-theoretical secret-key agreement.[18] The *intrinsic (conditional mutual) information* between two discrete random variables X and Y, given a third discrete random variable Z, is defined as

$$I(X;Y\downarrow Z) = \inf\{I(X;Y|\overline{Z}):\overline{Z} \text{ with } XY\to Z\to\overline{Z} \text{ a Markov chain}\}.$$

The infimum extends over all discrete channels Z to $\overline{Z}$ that are specified by a conditional probability distribution $P_{\overline{Z}|Z}$.

A first idea to utilize intrinsic information for measuring quantum correlations was mentioned in Ref. 11. This inspired the proposal of a *quantum analog to intrinsic information*[4] in which the Shannon conditional mutual information plays a role similar to the quantum conditional mutual information in squashed entanglement. This proposal possesses certain good properties demanded of an entanglement measure, and it opened the discussion that has resulted in the current work.

Before we state some similarities in the properties that the *intrinsic information* and *squashed entanglement* have in common, we would like to stress their obvious relation in terms of the definitions. Let $|\Psi\rangle^{ABC}$ be a purification of ρ^{AB} and let ρ^{ABE} be an extension of ρ^{AB} with purification $|\Phi\rangle^{ABEE'}$. Remark that all purifications of ρ^{AB} are equivalent in the sense that there is a suitable unitary transformation on the purifying system with

$$\mathbb{1}^{AB}\otimes U:|\Psi\rangle^{ABC}\mapsto|\Phi\rangle^{ABEE'}.$$

Applying a partial trace operation over system E' then results in the completely positive map

$$\Lambda:\mathcal{B}(\mathcal{H}_C)\to\mathcal{B}(\mathcal{H}_E),$$

$$\mathrm{id}\otimes\Lambda:|\Psi\rangle\langle\Psi|^{ABC}\mapsto\rho^{ABE}.$$

Conversely, every state ρ^{ABE} constructed in this manner is an extension of ρ^{AB}.

This shows that the squashed entanglement equals

$$E_{\mathrm{sq}}(\rho^{AB}) = \inf\{\tfrac{1}{2} I(A;B|E) : \rho^{ABE} = (\mathrm{id}\otimes\Lambda)|\Psi\rangle\langle\Psi|^{ABC}\}, \tag{3}$$

where the infimum includes all quantum operations $\Lambda : \mathcal{B}(\mathcal{H}_C) \to \mathcal{B}(\mathcal{H}_E)$.

In Ref. 5 it is shown that the minimization in $I(X;Y\downarrow Z)$ can be restricted to random variables $\overline{Z}$ with a domain equal to that of Z. This shows that the infimum in the definition is in effect a minimum and that the intrinsic information is a continuous function of the distribution P_{XYZ}. It is interesting to note that the technique used there (and, for that matter, also in the proof that entanglement of formation is achieved as a minimum over pure state ensembles $\rho^{AB} = \Sigma_k p_k |\Psi_k\rangle\langle\Psi_k|^{AB}$ of size $(\mathrm{rank}\ \rho^{AB})^2$), does not work for our problem, and so, we do not have an easy proof of the continuity of squashed entanglement. In the following section this issue will be discussed in some more detail.

In the cryptographic context in which it appears, intrinsic information serves as an upper bound for the secret-key rate $S = S(X;Y||Z)$.[18] S is the rate at which two parties, having access to repeated realizations of X and Y, can distill secret correlations about which a third party, holding realizations of Z, is almost ignorant. This distillation procedure includes all protocols in which the two parties communicate via a public authenticated classical channel to which the eavesdropper has access but cannot alter the transmitted messages. Clearly, one can interpret distillable entanglement as the quantum analog to the secret-key rate. On the one hand, *secret quantum correlations*, i.e., maximally entangled states of qubits, are distilled from a number of copies of ρ^{AB}. In the classical cryptographic setting, on the other hand, one aims at distilling *secret classical correlations*, i.e., secret classical bits, from a number of realizations of a triple of random variables X, Y, and Z.

We proved in proposition 10 that squashed entanglement is an upper bound for distillable entanglement. Hence, it provides a bound in entanglement theory which is analogous to the one in information-theoretic secure key agreement, where intrinsic information bounds the secret-key rate from above.

This analogy extends further to the bound on the formation of quantum states (proposition 5 and corollary 6), where we know of a recently proven classical counterpart, namely, that the intrinsic information is a lower bound on the formation cost of correlations of a triple of random variables X, Y, and Z from secret correlations.[22]

IV. THE QUESTION OF CONTINUITY

Intrinsic information, discussed in the previous section, and entanglement of formation are continuous functions of the probability distribution and state, respectively. This is so, because in both cases we are able to restrict the minimization to a compact domain; in the case of intrinsic information to bounded range $\overline{Z}$ and in entanglment of formation to bounded size decompositions, noting that the functions to be minimized are continuous.

Thus, by the same general principle, we could show continuity if we had a universal bound d on the dimension of E in definition 1, in the sense that every value of $I(A;B|E)$ obtainable by general extensions can be reproduced or beaten by an extension with a d-dimensional system E. Note that if this were true, then (just as for intrinsic information and entanglement of formation) the infimum would actually be a minimum: in remark 7 we have explained that then $E_{\mathrm{sq}}(\rho^{AB}) = 0$ would imply, using the result of,[13] that ρ^{AB} is separable.

As it is, we cannot yet decide on this question, but we would like to present a reasonable conjecture, an inequality of the Fannes-type[9] for the conditional von Neumann entropy, which we can show to imply continuity of E_{sq}. Let us first revisit Fannes' inequality in a slightly nonstandard form:

Lemma 13: For density operators ρ, σ on the same d-dimensional Hilbert space, with $\|\rho-\sigma\|_1\leqslant\epsilon$,

$$|S(\rho)-S(\sigma)|\leqslant\eta(\epsilon)+\epsilon\log d,$$

with the universal function

$$\eta(\epsilon)=\begin{cases}-\epsilon\log\epsilon & \epsilon\leqslant\frac{1}{2},\\ \frac{1}{2} & \text{otherwise.}\end{cases}$$

Observe that η is a concave function. □

Now we can state the conjecture, recalling that for a density operator ρ^{AB} on a bipartite system $\mathcal{H}_A\otimes\mathcal{H}_B$, the conditional von Neumann entropy[3] is defined as

$$S(A|B):=S(\rho^{AB})-S(\rho^B).$$

Conjecture 14: For density operators ρ, σ on the bipartite system $\mathcal{H}_A\otimes\mathcal{H}_B$, with $\|\rho-\sigma\|_1\leqslant\epsilon$,

$$|S(A|B)_\rho-S(A|B)_\sigma|\leqslant\eta(2\epsilon)+3\epsilon\log d_A,$$

with $d_A=\dim\mathcal{H}_A$, or some other universal function $f(\epsilon,d_A)$ vanishing at $\epsilon=0$ on the right-hand side.

Note that the essential feature of the conjectured inequality is that it only makes reference to the dimension of system A. If we were to use Fannes inequality directly with the definition of the conditional von Neumann entropy, we would pick up additional terms containing the logarithm of $d_B=\dim\mathcal{H}_B$. In the Appendix we show that this conjecture is true in the classical case, or more precisely, in the more general case where the states are classical on system B.

In order to show that the truth of this conjecture implies continuity of E_{sq}, consider two states ρ^{AB} and σ^{AB} with $\|\rho^{AB}-\sigma^{AB}\|_1\leqslant\epsilon$. By well-known relations between fidelity and trace distance[10] this means that $F(\rho^{AB},\sigma^{AB})\geqslant1-\epsilon$, hence[16,27] we can find purifications $|\Psi\rangle^{ABC}$ and $|\Phi\rangle^{ABC}$ of ρ^{AB} and σ^{AB}, respectively, such that $F(|\Psi\rangle^{ABC},|\Phi\rangle^{ABC})\geqslant1-\epsilon$. Using Ref. 10 once more, we get

$$\||\Psi\rangle\langle\Psi|^{ABC}-|\Phi\rangle\langle\Phi|^{ABC}\|_1\leqslant2\sqrt{\epsilon}.$$

Now, let Λ be any quantum operation as in Eq. (3): it creates extensions of ρ^{AB} and σ^{AB},

$$\rho^{ABE}=(\mathrm{id}\otimes\Lambda)|\Psi\rangle\langle\Psi|^{ABC},$$

$$\sigma^{ABE}=(\mathrm{id}\otimes\Lambda)|\Phi\rangle\langle\Phi|^{ABC},$$

with

$$\|\rho^{ABE}-\sigma^{ABE}\|_1\leqslant2\sqrt{\epsilon}.$$

Hence, using $I(A;B|E)=S(A|E)+S(B|E)-S(AB|E)$, we can estimate

$$\begin{aligned}|I(A;B|E)_\rho-I(A;B|E)_\sigma|\leqslant{}&|S(A|E)_\rho-S(A|E)_\sigma|+|S(B|E)_\rho-S(B|E)_\sigma|+|S(AB|E)_\rho\\&-S(AB|E)_\sigma|\leqslant3\,\eta(2\sqrt{\epsilon})+6\sqrt{\epsilon}\log(d_Ad_B)=:\epsilon'.\end{aligned}$$

Since this applies to any quantum operation Λ and thus to every state extension of ρ^{AB} and σ^{AB}, respectively, we obtain

$$|E_{\mathrm{sq}}(\rho^{AB})-E_{\mathrm{sq}}(\sigma^{AB})|\leqslant\epsilon',$$

with ϵ' universally dependent on ϵ and vanishing with $\epsilon \to 0$. □

Remark 15: Since E_{sq} is convex it is trivially upper semicontinuous. This also follows from the fact that squashed entanglement is an infimum of continuous functions obtained by bounding the size of the dimension of system E.

This observation, together with results from the general theory of convex functions, implies that squashed entanglement is continuous ''almost everywhere.'' Specifically, with theorem 10.1 in Ref. 23, we have:

Proposition 16: E_{sq} is continuous on the interior of the set of states (i.e., on the faithful states), and more generally, it is continuous when restricted to the relative interior of all faces of the state set.

Continuity near pure states (see remark 11) thus implies continuity of E_{sq} on the set of all rank-2 density operators. □

V. CONCLUSION

In this paper we have presented a new measure of entanglement, which by its very definition allows for rather simple proofs of monotonicity under LOCC, convexity, additivity for tensor products and superadditivity in general, all by application of the strong subadditivity property of quantum entropy. We showed the functional, which we call ''squashed entanglement,'' to be lower bounded by the distillable entanglement and upper bounded by the entanglement cost. Thus, it has most of the ''good'' properties demanded by the axiomatic approaches[14,20,29] without suffering from the disadvantages of other superadditive entanglement monotones. The one proposed in Ref. 8, for example, diverges on the set of pure states.

The one desirable property from the wish list of axiomatic entanglement theory that we could not yet prove is continuity. We have shown, however, that squashed entanglement is continuous near pure states and in the relative interior of the faces of state space. Continuity in general would follow from a conjectured Fannes-type inequality for the conditional von Neumann entropy. The proof of this conjecture thus remains the great challenge of the present work. It might well be of wider applicability in quantum information theory and certainly deserves further study.

Another question to be asked is whether or not there exist states that are nonseparable but, nonetheless, have zero squashed entanglement. We expect this not to be the case: if not by means of proving that the infimum in squashed entanglement is achieved, then by means of an approximate version of the result of Ref. 13. The relation to entanglement measures other than entanglement of formation, entanglement cost and distillable entanglment remains open in general. If $E_{sq}=0$ would imply separability, however, it would follow that for the class of PPT states, squashed entanglement is larger than entanglement measures based on the partial transpose operation, like relative entropy of entanglement, the logarithmic negativity and the Rains bound.

Note added in proof. Alicki and Fannes (quant-ph/0312081) have recently proven our Conjecture 14, with the upper bound $4\epsilon \log d_A + 2\eta(\epsilon) + 2\eta(1-\epsilon)$. Thus, squashed entanglement is now known to be continuous.

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APPENDIX: THE CLASSICAL CASE OF THE CONDITIONAL FANNES INEQUALITY

In this appendix we prove the conjecture 14 for states

$$\rho^{AB} = \sum_k p_k \rho_k^A \otimes |k\rangle\langle k|^B, \tag{A1}$$

$$\sigma^{AB}=\sum_k q_k \sigma_k^A \otimes |k\rangle\langle k|^B, \tag{A2}$$

with an orthogonal basis $(|k\rangle)_k$ and of $\mathcal{H}_B$, probability distributions (p_k) and (q_k), and states ρ_k^A and σ_k^A on A. Note that this includes the case of a pair of classical random variables. In this case, the states ρ_k^A and σ_k^A are all diagonal in the same basis $(|j\rangle)_j$ of $\mathcal{H}_A$ and thus ρ^{AB} and σ^{AB} describe joint probability distributions on a Cartesian product.

The key to the proof is that for states of the form (A1),

$$S(A|B)_\rho=\sum_k p_k S(\rho_k^A),$$

and similarly for the states given in Eq. (A2).

First of all, the assumption implies that

$$\epsilon \geqslant \|\rho^B-\sigma^B\|_1=\sum_k |p_k-q_k|.$$

Hence, we can successively estimate,

$$|S(A|B)_\rho-S(A|B)_\sigma| \leqslant \sum_k |p_k S(\rho_k^A)-q_k S(\sigma_k^A)| \leqslant \sum_k p_k |S(\rho_k^A)-S(\sigma_k^A)|+\sum_k |p_k-q_k| S(\sigma_k^A)$$

$$\leqslant \sum_k p_k(\eta(\epsilon_k)+\epsilon_k \log d_A)+\epsilon \log d_A \leqslant \eta(2\epsilon)+3\epsilon \log d_A,$$

using the triangle inequality twice in the first line, then using $S(\sigma_k^A)\leqslant \log d_A$, applying the Fannes inequality, lemma 13 (with $\epsilon_k := \|\rho_k^A-\sigma_k^A\|_1$), and finally making use of the concavity of its upper bound. To complete this step, we have to show $\Sigma_k p_k \epsilon_k \leqslant 2\epsilon$, which is done as follows:

$$\epsilon \geqslant \|\rho^{AB}-\sigma^{AB}\|_1=\sum_k \|p_k\rho_k^A-q_k\sigma_k^A\|_1 \geqslant \sum_k (\|p_k\rho_k^A-p_k\sigma_k^A\|_1-\|p_k\sigma_k^A-q_k\sigma_k^A\|_1) \geqslant \sum_k p_k\epsilon_k-\epsilon,$$

where we have used the triangle inequality. □

Note that in the case of pure states the conjecture is directly implied by Fannes inequality, lemma 13, since $S(AB)=0$ and $S(A)=S(B)$. Clearly, a proof of the general case cannot proceed along these lines as they do not have the possibility to present the conditional von Neumann entropy as an average of entropies on A.

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Quantum mechanics of damped systems. II. Damping and parabolic potential barrier

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We investigate the resonant states for the parabolic potential barrier known also as inverted or reversed oscillator. They correspond to the poles of meromorphic continuation of the resolvent operator to the complex energy plane. As a by-product we establish an interesting relation between parabolic cylinder functions (representing energy eigenfunctions of our system) and a class of Gel'fand distributions used in our recent paper. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In a recent paper[1] we have investigated a quantization of the simple damped system[1]

$$\dot{u} = -\gamma u. \tag{1.1}$$

To quantize this system we double the number of degrees of freedom, i.e., together with (1.1) we consider $\dot{v} = +\gamma v$. We slightly change the notation: the coordinates (x,p) used in Ref. 1 are replaced by (u,v) in the present paper. The enlarged system is a Hamiltonian one and its quantization leads to the following quantum Hamiltonian:

$$\hat{H} = -\frac{\gamma}{2}(\hat{u}\hat{v} + \hat{v}\hat{u}). \tag{1.2}$$

This Hamiltonian, apart from the continuous spectrum $\sigma(\hat{H}) = (-\infty, \infty)$, displays two families of generalized eigenvectors $f_n^{\pm}$ corresponding to purely imaginary eigenvalues $\hat{H} f_n^{\pm} = \pm E_n f_n^{\pm}$. Clearly, these eigenvectors are not elements from the Hilbert space $\mathcal{H} = L^2(\mathbb{R}_u)$. To describe the quantum-mechanical system defined by (1.2) it is convenient to go beyond the standard Hilbert space formulation of quantum mechanics and to consider a rigged Hilbert space (or so-called Gel'fand triplet)[2,3]

$$\Phi \subset L^2(\mathbb{R}_u) \subset \Phi', \tag{1.3}$$

where Φ is a dense nuclear subspace of $L^2(\mathbb{R}_u)$ and Φ' denotes its dual, i.e., the space of continuous functionals on Φ. The rigged Hilbert space version of quantum mechanics was developed by Böhm,[4] Roberts,[5] and Antoine,[6] and further investigated by Brussels/Austin groups, see, e.g., Refs. 7–10 and the recent review.[11] The primary application of the rigged Hilbert space quantum mechanics is the description of resonances in scattering theory. The conventional definition [see, e.g., Refs. 12–14 and the review (Ref. 15)] states that a resonance corresponds to a pair of conjugated poles of the S-matrix analytically continued to the complex energy plane

$$z_R = E_R - i\frac{\Gamma}{2}, \quad \overline{z_R} = E_R + i\frac{\Gamma}{2}, \tag{1.4}$$

where E_R is the resonant energy and Γ is the width of the resonance. The corresponding generalized eigenvectors $|z_R\rangle$ are called resonant states (or Gamow vectors; see Ref. 11). Other definitions locate resonances as poles of generalized energy eigenfunctions when continued to the complex energy plane or as poles of meromorphic continuation of the resolvent operator. It is argued that resonant states are responsible for the irreversible behavior of quantum systems.

It was shown in Ref. 1 that generalized eigenvectors of the Hamiltonian (1.2) may be interpreted as resonant states, i.e., they correspond to the poles of energy eigenfunctions when continued to the complex energy plane. It turns out that resonant states are responsible for the irreversible behavior. Indeed, we showed that there are two dense subspaces $\Phi_\pm \in L^2(\mathbb{R}_u)$ such that restriction of the unitary group $U(t)=e^{-i\hat{H}t}$ to $\Phi_\pm$ no longer defines a group but gives rise to two semigroups: $U_-(t)=U(t)|_{\Phi_-}$ defined for $t\geqslant 0$ and $U_+(t)=U(t)|_{\Phi_+}$ defined for $t\leqslant 0$. In the framework of Gel'fand triplets it means that the quantum version of the damped system (1.1) corresponds to the Gel'fand triplet $\Phi_-\subset L^2(\mathbb{R}_u)\subset\Phi_-'$ together with the Hamiltonian $\hat{H}|_{\Phi_-}$. Another triplet $\Phi_+\subset L^2(\mathbb{R}_v)\subset\Phi_+'$ together with $\hat{H}|_{\Phi_+}$ corresponds to the quantum pumped system $\dot{v}=+\gamma v$. This way, the fashionable ''arrow of time'' is introduced by restricting the time evolution either to Φ_- or to Φ_+.

In the present paper we continue to study this system but in a different representation. Moreover, we are going to relate the resonant states to the poles of the corresponding S-matrix. Let us observe that performing the linear canonical transformation $(u,v)\to(x,p)$

$$u=\frac{\gamma x-p}{\sqrt{2\gamma}}\,,\quad v=\frac{\gamma x+p}{\sqrt{2\gamma}}\,, \tag{1.5}$$

one obtains for the Hamiltonian

$$\hat{H}=\tfrac{1}{2}(\hat{p}^2-\gamma^2\hat{x}^2). \tag{1.6}$$

It represents the parabolic potential barrier $V(x)=-\gamma^2x^2/2$ and it was studied by several authors in various contexts.[16–22] For obvious reasons it is also called an inverted or reversed oscillator. It is well known that this system gives rise to the generalized complex eigenvalues—the physical reason for that is the potential unbounded from below. We find the corresponding energy eigenstates for (1.6). They are given in terms of parabolic cylinder functions $D_\nu(x)$. Using the Gel'fand–Maurin spectral decomposition we find the resolvent operator $R(z,\hat{H})=(\hat{H}-z)^{-1}$ and relate its poles to the resonant states. Finally, we investigate the scattering problem and derive the relation between resonant and scattering states. It is shown that resonant states have the standard Breit–Wigner energy distribution.

As a by-product we established an interesting relation between the Gel'fand distributions $u_\pm^\lambda$ [23,24] (used in Ref. 1) and parabolic cylinder functions $D_\nu(x)$. The details are included in the Appendix.

II. INVERTED OSCILLATOR AND COMPLEX EIGENVALUES

Let us note that $\hat{H}$ defined in (1.6) corresponds to the Hamiltonian of the harmonic oscillator with purely imaginary frequency $\omega=\pm i\gamma$ (in the literature it is also called an inverted or reversed oscillator). The connection with a harmonic oscillator may be established by the following scaling operator:[25]

$$\hat{V}_\lambda:=\exp\left(\frac{\lambda}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})\right), \tag{2.1}$$

with $\lambda\in\mathbb{R}$. Using commutation relation $[\hat{x},\hat{p}]=i$, this operator may be rewritten as follows:

$$\hat{V}_\lambda = e^{-i(\lambda/2)}\, e^{\lambda \hat{x}\hat{p}} = e^{-i(\lambda/2)}\, e^{-i\lambda x \partial_x}, \tag{2.2}$$

and therefore it defines a complex dilation, i.e., the action of $\hat{V}_\lambda$ on a function $\varphi = \varphi(x)$ is given by

$$\hat{V}_\lambda\, \varphi(x) = e^{-i(\lambda/2)}\, \varphi(e^{-i\lambda} x). \tag{2.3}$$

In particular, one easily finds

$$\hat{V}_\lambda\, \hat{x}\, \hat{V}_\lambda^{-1} = e^{-i\lambda}\hat{x} \quad , \quad \hat{V}_\lambda\, \hat{p}\, \hat{V}_\lambda^{-1} = e^{i\lambda}\hat{p}, \tag{2.4}$$

and hence

$$\hat{V}_\lambda\, (\hat{p}^2 - \gamma^2 \hat{x}^2)\, \hat{V}_\lambda^{-1} = e^{2i\lambda}\, (\hat{p}^2 - e^{-4i\lambda}\, \gamma^2 \hat{x}^2). \tag{2.5}$$

Therefore, for $e^{4i\lambda} = -1$, i.e., $\lambda = \pm \pi/4$, one has

$$\hat{V}_{\pm \pi/4}\, \hat{H}\, \hat{V}_{\pm \pi/4}^{-1} = \pm i \hat{H}_{\rm ho}, \tag{2.6}$$

where

$$\hat{H}_{\rm ho} = \tfrac{1}{2}(\hat{p}^2 + \gamma^2 \hat{x}^2), \tag{2.7}$$

stands for the oscillator Hamiltonian. In particular, if $E_n^{\rm ho} = \gamma(n + \frac{1}{2})$ is an oscillator spectrum

$$\hat{H}_{\rm ho} \psi_n^{\rm ho} = E_n^{\rm ho} \psi_n^{\rm ho}, \tag{2.8}$$

then

$$\hat{H} \mathfrak{f}_n^{\pm} = \pm E_n \mathfrak{f}_n^{\pm}, \tag{2.9}$$

with

$$E_n = i E_n^{\rm ho} = i\, \gamma(n + \tfrac{1}{2}), \tag{2.10}$$

and

$$\mathfrak{f}_n^{\pm}(x) = \hat{V}_{\mp \pi/4}\, \psi_n^{\rm ho}(x) = e^{\pm i \pi/8}\, \psi_n^{\rm ho}(e^{\pm i \pi/4} x). \tag{2.11}$$

Now, recalling that (see, e.g., Ref. 26)

$$\psi_n^{\rm ho}(x) = N_n\, e^{-(\gamma/2) x^2} H_n(\sqrt{\gamma} x), \tag{2.12}$$

where H_n stands for the nth Hermite polynomial and the normalization constant

$$N_n = \left(\frac{\sqrt{\gamma}}{2^n n! \sqrt{\pi}} \right)^{1/2}, \tag{2.13}$$

one obtains the following formulas for the generalized eigenvectors of $\hat{H}$:

$$\mathfrak{f}_n^{\pm}(x) = N_n^{\pm}\, e^{\mp i (\gamma/2) x^2} H_n(\sqrt{\pm i \gamma} x), \tag{2.14}$$

with

$$N_n^{\pm}=e^{\pm i\pi/8}N_n=\left(\frac{\sqrt{\pm i\gamma}}{2^n n!\sqrt{\pi}}\right)^{1/2}. \tag{2.15}$$

Clearly, $\mathfrak{f}_n^{\pm}$ are not elements from $L^2(\mathbb{R})$ but they do belong to the dual of the Schwartz space $\mathcal{S}(\mathbb{R}_x)'$, i.e., they are tempered distributions.

Proposition 1: Two families of generalized eigenvectors $\mathfrak{f}_n^{\pm}$ satisfy the following properties:

1. They are conjugated to each other:

$$\overline{\mathfrak{f}_n^{+}(x)}=\mathfrak{f}_n^{-}(x). \tag{2.16}$$

2. They are orthonormal

$$\langle \mathfrak{f}_n^{\pm}|\mathfrak{f}_m^{\mp}\rangle=\delta_{nm}. \tag{2.17}$$

3. They are complete

$$\sum_{n=0}^{\infty}\overline{\mathfrak{f}_n^{\pm}(x)}\,\mathfrak{f}_n^{\mp}(x')=\delta(x-x'). \tag{2.18}$$

The proof follows immediately from orthonormality and completeness of oscillator eigenfunctions ψ_n^{ho}. Formula (2.16) implies that $\mathfrak{f}_n^{+}$ and $\mathfrak{f}_n^{-}$ are related by the time-reversal operator $\mathbf{T}$: $\mathbf{T}\psi:=\overline{\psi}$.

III. CHANGE OF REPRESENTATION

It should be clear that there exists a relation between generalized eigenvectors $\mathfrak{f}_n^{\pm}(x)$ and $f_n^{\pm}(u)$ found in Ref. 1,

$$f_n^{+}(u)\sim u^n,\quad f_n^{-}(u)\sim\delta^{(n)}(u). \tag{3.1}$$

They define the same eigenvectors $|\pm n\rangle$ but in different representations

$$\mathfrak{f}_n^{\pm}(x)=\langle x|\pm n\rangle,\quad f_n^{\pm}(u)=\langle u|\pm n\rangle.$$

To find this relation, let us observe that the canonical transformation (1.5) is generated by the following generating function:

$$S(x,u)=\frac{\gamma}{2}x^2-\sqrt{2\gamma}xu+\frac{1}{2}u^2, \tag{3.2}$$

that is

$$p=\frac{\partial S}{\partial x},\quad v=-\frac{\partial S}{\partial u}. \tag{3.3}$$

Let us define a unitary operator

$$\mathcal{U}:L^2(\mathbb{R}_u)\to L^2(\mathbb{R}_x)$$

by

$$f\quad\to(\mathcal{U}f)(x)=C\int_{-\infty}^{\infty}f(u)e^{iS(x,u)}\,du, \tag{3.4}$$

where the constant "C" is determined by

$$|C|^2 \int_{-\infty}^{\infty} e^{iS(x,u)}\, e^{-iS(x',u)}\, du = \delta(x-x'). \tag{3.5}$$

It implies $C = e^{i\alpha} C_0$, where α is an arbitrary phase and

$$C_0 = \left(\frac{\gamma}{2\pi^2}\right)^{1/4}. \tag{3.6}$$

In the next section it would be clear that a natural choice for the phase is $\alpha = -\pi/8$. Clearly, $\mathcal{U}$ may be extended to act on $\mathcal{S}(\mathbb{R}_u)'$. It is easy to show that

$$\mathcal{U}(\mathcal{S}(\mathbb{R}_u)') \subset \mathcal{S}(\mathbb{R}_x)'. \tag{3.7}$$

Proposition 2: The generalized eigenvectors $\mathfrak{f}_n^{\pm} \in \mathcal{S}(\mathbb{R}_x)'$ and $f_n^{\pm} \in \mathcal{S}(\mathbb{R}_u)'$ are related by:

$$\mathfrak{f}_n^{\pm} = \mathcal{U} f_n^{\pm}. \tag{3.8}$$

Proof. Let us show that $\mathfrak{f}_n^{+} = \mathcal{U} f_n^{+}$, that is

$$\mathfrak{f}_n^{+}(x) \sim \int u^n e^{iS(x,u)} du. \tag{3.9}$$

Using the definition of $S(x,u)$, one has

$$\begin{aligned} \int u^n e^{iS(x,u)} du &= (-i\sqrt{2\pi\gamma})^{-n} e^{i\gamma x^2/2} \frac{d^n}{dx^n} \int e^{iu^2/2 - i\sqrt{2\gamma}xu} du \\ &= \sqrt{-2\pi i}(-i\sqrt{2\pi\gamma})^{-n} e^{-i\gamma x^2/2} \left(e^{i\gamma x^2} \frac{d^n}{dx^n} e^{-i\gamma x^2} \right). \end{aligned} \tag{3.10}$$

Now, due to the well-known formula for the Hermite polynomials

$$e^{iz^2} \frac{d^n}{dz^n} e^{-iz^2} = (-1)^n H_n(z), \tag{3.11}$$

one obtains

$$\int u^n e^{iS(x,u)} du = \sqrt{-2\pi i} \left(\frac{i}{2}\right)^{-n/2} e^{-i\gamma(x^2/2)} H_n(\sqrt{i\gamma}x) \sim \mathfrak{f}_n^{+}(x). \tag{3.12}$$

To prove that $\mathfrak{f}_n^{-} = \mathcal{U} f_n^{-}$, let us note that

$$\mathfrak{f}_n^{-}(x) = \overline{\mathfrak{f}_n^{+}(x)} \sim \int u^n e^{-iS(x,u)} du. \tag{3.13}$$

It turns out that a function

$$\tilde{S}(x,v) = -S(x,v) = -\frac{\gamma}{2}x^2 + \sqrt{2\gamma}xv - \frac{1}{2}v^2,$$

serves as a generating function for the canonical transformation (1.5)

$$p=\frac{\partial\widetilde{S}}{\partial x},\qquad u=-\frac{\partial\widetilde{S}}{\partial v}.$$

Now, taking into account that f_n^+ and f_n^- are related by the Fourier transformation

$$u^n=\sqrt{2\pi}(-i)^n F^{-1}[\delta^{(n)}(k)](u), \tag{3.14}$$

one obtains

$$\int u^n e^{-iS(x,u)}du=\sqrt{2\pi}(-i)^n\int \delta^{(n)}(u)F^{-1}[e^{-iS}](u)\,du. \tag{3.15}$$

Finally,

$$F^{-1}[e^{-iS}](u)=\frac{1}{\sqrt{2\pi}}\int e^{-iku}\,e^{-iS(x,k)}dk=\sqrt{-i}\,e^{iS(x,u)}, \tag{3.16}$$

and hence

$$\mathfrak{f}_n^-(x)\sim\int \delta^{(n)}(u)e^{iS(x,u)}du, \tag{3.17}$$

which ends the proof. □

IV. ENERGY EIGENSTATES

The spectrum of the self-adjoint operator (1.2) reads $\sigma(\hat{H})=(-\infty,\infty)$ and the corresponding energy eigenstates (in u-representation) are given by (cf. Sec. 6 in Ref. 1)

$$\psi_\pm^E(u)=\frac{1}{\sqrt{2\pi\gamma}}u_\pm^{-(iE/\gamma+1/2)}, \tag{4.1}$$

with $E\in\mathbb{R}$. For the basic properties of the tempered distributions $u_\pm^\lambda\in\mathcal{S}(\mathbb{R}_u)'$, we refer the reader to Refs. 23, 24 (see also the Appendix in Ref. 1). Now, using (x,p) coordinates, the corresponding eigenvalue problem $\frac{1}{2}(\hat{p}^2-\gamma^2\hat{x}^2)\chi^E=E\chi^E$ reads

$$\partial_x^2\chi^E(x)+(\gamma^2x^2+2E)\chi^E(x)=0. \tag{4.2}$$

Introducing a new variable

$$z=\sqrt{2i\gamma}\,x, \tag{4.3}$$

the above equation may be rewritten as follows:

$$\partial_z^2\chi^E+\left(\nu+\frac{1}{2}-\frac{z^2}{4}\right)\chi^E=0, \tag{4.4}$$

with

$$\nu=-\left(i\frac{E}{\gamma}+\frac{1}{2}\right), \tag{4.5}$$

which is the defining equation for the parabolic cylinder functions.[27–29] Its solution $\chi^E(z)$ is a linear combination of $D_\nu(z)$, $D_\nu(-z)$, $D_{-\nu-1}(iz)$, and $D_{-\nu-1}(-iz)$. [These four functions are linearly dependent. For the linear relation see, e.g., formula 9.248 in Ref. 27.] On the other hand,

the energy eigenstates in x-representation $\chi^E(x)$ may be obtained by applying the operator $\mathcal{U}$ defined in (3.4) to the corresponding eigenstates in u-representation $\psi^E_\pm(u)$

$$\chi^E_\pm(x)=(\mathcal{U}\psi^E_\pm)(x)=C\int_{-\infty}^{\infty}\psi^E_\pm(u)\,e^{iS(x,u)}\,du. \tag{4.6}$$

Hence

$$\chi^E_+(x)=\frac{C}{\sqrt{2\pi\gamma}}e^{i\gamma/2\,x^2}\int_0^\infty u^\nu\,e^{-i\sqrt{2\gamma}xu+iu^2/2}\,du=\frac{C}{\sqrt{2\pi\gamma}}\sqrt{i}^{\nu+1}\,e^{-y^2/4}\int_0^\infty\xi^\nu\,e^{y\xi-\xi^2/2}\,d\xi, \tag{4.7}$$

with $y=\sqrt{-2i\gamma}\,x$, and using an integral representation for $D_p(y)$ [formula 9.241(2) in Ref. 27]

$$D_p(y)=\frac{e^{-y^2/4}}{\Gamma(-p)}\int_0^\infty\xi^{-p-1}\,e^{-y\xi-\xi^2/2}\,d\xi, \tag{4.8}$$

one finds

$$\chi^E_+(x)=\frac{C_0}{\sqrt{2\pi\gamma}}\sqrt{i}^{\nu+1/2}\,\Gamma(\nu+1)D_{-\nu-1}(-\sqrt{-2i\gamma}x), \tag{4.9}$$

with ν given in (4.5). The validity of this formula is restricted in Ref. 27 for $\mathrm{Re}\,p<0$. However, as we shall show (see the proof of Proposition 4), it is valid for all $p\in\mathbb{C}$. Similarly, using an obvious relation $(-u)^\lambda_+=u^\lambda_-$, one obtains

$$\chi^E_-(x)=\frac{C_0}{\sqrt{2\pi\gamma}}\sqrt{i}^{\,\nu+1/2}\,\Gamma(\nu+1)D_{-\nu-1}(\sqrt{-2i\gamma}x), \tag{4.10}$$

that is, $\chi^E_-(x)=\chi^E_+(-x)$. Actually, instead of $\chi^E_\pm$ one may use energy eigenstates with the definite parity

$$\chi^E_{\mathrm{even}}=\frac{1}{\sqrt{2}}(\chi^E_+ +\chi^E_-), \tag{4.11}$$

$$\chi^E_{\mathrm{odd}}=\frac{1}{\sqrt{2}}(\chi^E_+ -\chi^E_-), \tag{4.12}$$

that is

$$\mathbf{P}\,\chi^E_{\mathrm{even}}=\chi^E_{\mathrm{even}},\quad \mathbf{P}\,\chi^E_{\mathrm{odd}}=-\chi^E_{\mathrm{odd}}, \tag{4.13}$$

where **P** stands for the parity operator.

Proposition 3: Energy eigenstates $\chi^E_\pm$ satisfy

$$\int_{-\infty}^{\infty}\overline{\chi^E_\pm(x)}\chi^{E'}_\pm(x)\,dx=\delta(E-E') \tag{4.14}$$

and

$$\int_{-\infty}^{\infty}\overline{\chi^E_\pm(x)}\chi^E_\pm(x')\,dE=\delta(x-x'). \tag{4.15}$$

The proof follows immediately from the analogous properties satisfied by energy eigenstates $\psi_{\pm}^{E}$ in u-representation.[1]

In Ref. 1 we have also used another generalized basis $F[\psi_{\pm}^{-E}](u)$. Now, we find its $\mathcal{U}$ image in $\mathcal{S}(\mathbb{R}_x)'$. Recalling the Fourier transformation of $x_{\pm}^{\lambda}$ (see Ref. 23 and Appendix in Ref. 1)

$$F[x_{\pm}^{\lambda}](u)=\frac{\pm i}{\sqrt{2\pi}}e^{\pm i\lambda\pi/2}\Gamma(\lambda+1)(u+i0)^{-\lambda-1}, \tag{4.16}$$

one has

$$F[\psi_{+}^{-E}](u)=\frac{1}{\sqrt{2\pi\gamma}}\frac{(-i)^{\nu}}{\sqrt{2\pi}}\Gamma(-\nu)(u+i0)^{\nu}. \tag{4.17}$$

Therefore, the corresponding x-representation

$$\eta_{+}^{E}(x)=(\mathcal{U}F[\psi_{+}^{-E}])(x) \tag{4.18}$$

is given by

$$\begin{aligned}\eta_{+}^{E}(x)&=\frac{C}{\sqrt{2\pi\gamma}}\frac{(-i)^{\nu}}{\sqrt{2\pi}}\Gamma(-\nu)\int_{-\infty}^{\infty}(u+i0)^{\nu}e^{iS(x,u)}du\\&=\frac{C}{\sqrt{2\pi\gamma}}\frac{(-i)^{\nu}}{\sqrt{2\pi}}(2\sqrt{i})^{\nu+1}\Gamma(-\nu)\,e^{y^2/4}\int_{-\infty}^{\infty}(\xi+i0)^{\nu}e^{-2\xi^2-2iy\xi}d\xi,\end{aligned} \tag{4.19}$$

with $y=\sqrt{2i\gamma}x$. Now, using the following integral representation [formula 9.241(1) in Ref. 27]:

$$D_{\nu}(y)=\frac{1}{\sqrt{\pi}}2^{\nu+1/2}(-i)^{\nu}e^{(y^2/4)}\int_{-\infty}^{\infty}(\xi+i0)^{\nu}e^{-2\xi^2+2iy\xi}d\xi, \tag{4.20}$$

one obtains

$$\eta_{+}^{E}(x)=\frac{C_0}{\sqrt{2\pi\gamma}}\sqrt{i}^{\nu+1/2}\Gamma(-\nu)D_{\nu}(-\sqrt{2i\gamma}x). \tag{4.21}$$

Similarly, one shows that

$$\eta_{-}^{E}(x)=(\mathcal{U}F[\psi_{-}^{-E}])(x) \tag{4.22}$$

is given by

$$\eta_{-}^{E}(x)=\frac{C_0}{\sqrt{2\pi\gamma}}\sqrt{i}^{\nu+1/2}\Gamma(-\nu)D_{\nu}(\sqrt{2i\gamma}x). \tag{4.23}$$

Let us note that

$$\overline{\nu+1}=-\nu \tag{4.24}$$

and

$$\overline{\sqrt{i}^{\nu+1/2}}=\sqrt{i}^{\nu+1/2}. \tag{4.25}$$

Clearly, the transition $\nu+1\to-\nu$ is equivalent to $E\to-E$ and it corresponds to the fact that $\hat{H}\eta_+^E=-E\eta_+^E$, while $\hat{H}\chi_+^E=+E\chi_+^E$. The symmetry between $\chi_\pm^E$ and $\eta_\pm^E$ fully justifies the specific choice of the phase factor in the constant C. One has

$$\eta_\pm^E(x)=\overline{\chi_\pm^E(x)}, \tag{4.26}$$

that is, they are related by the time-reversal operator $\mathbf{T}$: $\eta_\pm^E=\mathbf{T}\chi_\pm^E$. Thus energy eigenstates $\eta_\pm^E$ correspond to the time-reversed system. This way, all four solutions of (4.4) were used to construct four families of energy eigenstates: χ_+^E, χ_-^E, η_+^E, and η_-^E.

V. ANALYTIC CONTINUATION, RESOLVENT, AND RESONANCES

Now, let us continue the energy eigenfunctions $\chi_\pm^E$ and $\eta_\pm^E$ into the energy complex plane $E\in\mathbb{C}$ and let us study its analyticity as functions of E.

Proposition 4: The parabolic cylinder function $D_\lambda(z)$ is an analytic function of $\lambda\in\mathbb{C}$.

For the proof see the Appendix. Due to the above proposition the analytic properties of the energy eigenfunctions are entirely governed by the analytic properties of the Γ function which is present in the definition of $\chi_\pm^E$ and $\eta_\pm^E$. Since $\Gamma(\lambda)$ has simple poles at $\lambda=-n$, with $n=0,1,2,\ldots$, functions $\chi_\pm^E$ have poles at $E=-E_n$, whereas functions $\eta_\pm^E$ have poles at $E=E_n$, where E_n is defined in (2.10). Using a well-known formula for a residue of the Γ function

$$\mathrm{Res}(\Gamma(\lambda);\lambda=-n)=\frac{(-1)^n}{n!}, \tag{5.1}$$

one has

$$\mathrm{Res}(\chi_\pm^E(x);-E_n)=\frac{C_0}{\sqrt{2\pi\gamma}}\frac{(-1)^n}{n!}\sqrt{i}^{-n-1/2}D_n(\mp\sqrt{-2i\gamma}x), \tag{5.2}$$

and

$$\mathrm{Res}(\eta_\pm^E(x);+E_n)=\frac{C_0}{\sqrt{2\pi\gamma}}\frac{(-1)^n}{n!}\sqrt{i}^{n+1/2}D_n(\mp\sqrt{2i\gamma}x). \tag{5.3}$$

Hence, using the relation[27–29] (in Ref. 27 the corresponding equation 9.253 has a wrong sign)

$$D_n(z)=2^{-(n/2)}e^{-z^2/4}H_n\left(\frac{z}{\sqrt{2}}\right),\quad n=0,1,2,\ldots, \tag{5.4}$$

together with

$$H_n(-z)=(-1)^nH_n(z), \tag{5.5}$$

one obtains

$$\mathrm{Res}(\chi_\pm^E(x);-E_n)\sim\mathfrak{f}_n^+(x), \tag{5.6}$$

and

$$\mathrm{Res}(\eta_\pm^E(x);+E_n)\sim\mathfrak{f}_n^-(x). \tag{5.7}$$

Now, it is natural to introduce two Hardy classes of functions.[30,31] Recall that a smooth function $f=f(E)$ is in the Hardy class from above $\mathcal{H}_+^2$ (from below $\mathcal{H}_-^2$) if $f(E)$ is a boundary

value of an analytic function in the upper, i.e., $\mathrm{Im}\,E\geqslant 0$ (lower, i.e., $\mathrm{Im}\,E\leqslant 0$) half complex E-plane vanishing faster than any power of E at the upper (lower) semi-circle $|E|\to\infty$. Define

$$\Phi_- := \{\phi\in\mathcal{S}(\mathbb{R}_x)\mid f(E):=\langle\,\chi_\pm^E|\phi\,\rangle\in\mathcal{S}(\mathbb{R}_E)\cap\mathcal{H}_-^2(\mathbb{R}_E)\}, \tag{5.8}$$

and

$$\Phi_+ := \{\phi\in\mathcal{S}(\mathbb{R}_x)\mid f(E):=\langle\,\eta_\pm^E|\phi\,\rangle\in\mathcal{S}(\mathbb{R}_E)\cap\mathcal{H}_+^2(\mathbb{R}_E)\}. \tag{5.9}$$

It is evident from (4.26) that $\Phi_+=\overline{\Phi_-}$, that is

$$\Phi_+=\mathbf{T}(\Phi_-). \tag{5.10}$$

This construction enables one to define two Gel'fand triplets,

$$\Phi_\pm\subset L^2(\mathbb{R}_x)\subset\Phi_\pm'. \tag{5.11}$$

Note, that $\mathcal{H}_\pm^2(\mathbb{R}_E)$ are Hilbert spaces and the Fourier transform define an isometry between $L^2(-\infty,0)$ [respectively, $L^2(0,\infty)$] and $\mathcal{H}_+^2(\mathbb{R}_E)$ [respectively, $\mathcal{H}_-^2(\mathbb{R}_E)$]. Defining $\Psi_\pm := \mathcal{S}(\mathbb{R}_E)\cap\mathcal{H}_\pm^2(\mathbb{R}_E)$ one obtains the following rigged Hilbert spaces of Hardy class functions:

$$\Psi_\pm\subset\mathcal{H}_\pm^2(\mathbb{R}_E)\subset\Psi_\pm',$$

introduced by Gadella.[13]

Due to the Gel'fand–Maurin spectral theorem,[2,3] any function $\phi^-\in\Phi_-$ may be decomposed with respect to $\chi_\pm^E$ family

$$\phi^-(x)=\sum_\pm\int_{-\infty}^{\infty}dE\,\chi_\pm^E(x)\langle\,\chi_\pm^E|\phi^-\,\rangle, \tag{5.12}$$

and any function $\phi^+\in\Phi_+$ may be decomposed with respect to $\eta_\pm^E$ family

$$\phi^+(x)=\sum_\pm\int_{-\infty}^{\infty}dE\,\eta_\pm^E(x)\langle\,\eta_\pm^E|\phi^+\,\rangle. \tag{5.13}$$

Applying the residue theorem, one easily proves the following.

Theorem 1: *For any function $\phi^\pm\in\Phi_\pm$, one has*

$$\phi^-(x)=\sum_{n=0}^{\infty}\mathfrak{f}_n^-(x)\langle\,\mathfrak{f}_n^+|\phi^-\,\rangle, \tag{5.14}$$

and

$$\phi^+(x)=\sum_{n=0}^{\infty}\mathfrak{f}_n^+(x)\langle\,\mathfrak{f}_n^-|\phi^+\,\rangle. \tag{5.15}$$

The proof goes along the same lines as the corresponding proof of Theorem 2 in Ref. 1. The above theorem implies the following spectral resolutions of the Hamiltonian:

$$\hat{H}=\sum_\pm\int_{-\infty}^{\infty}dE\,E|\chi_\pm^E\,\rangle\langle\,\chi_\pm^E|=-\sum_{n=0}^{\infty}E_n|\mathfrak{f}_n^-\,\rangle\langle\,\mathfrak{f}_n^+|, \tag{5.16}$$

on Φ_-, and

$$\hat{H}=\sum_{\pm}\int_{-\infty}^{\infty}dE\,E|\,\eta_{\pm}^{E}\rangle\langle\,\eta_{\pm}^{E}|=\sum_{n=0}^{\infty}E_n|\mathfrak{f}_n^{+}\rangle\langle\,\mathfrak{f}_n^{-}|, \tag{5.17}$$

on Φ_+. The same techniques may be applied for the resolvent operator

$$R(z,\hat{H})=\frac{1}{\hat{H}-z}\ . \tag{5.18}$$

One obtains

$$R(z,\hat{H})=\sum_{\pm}\int_{-\infty}^{\infty}\frac{dE}{E-z}|\chi_{\pm}^{E}\rangle\langle\,\chi_{\pm}^{E}|=\sum_{n=0}^{\infty}\frac{1}{-E_n-z}|\mathfrak{f}_n^{-}\rangle\langle\,\mathfrak{f}_n^{+}|, \tag{5.19}$$

on Φ_-, and

$$R(z,\hat{H})=\sum_{\pm}\int_{-\infty}^{\infty}\frac{dE}{E-z}|\,\eta_{\pm}^{E}\rangle\langle\,\eta_{\pm}^{E}|=\sum_{n=0}^{\infty}\frac{1}{E_n-z}|\mathfrak{f}_n^{+}\rangle\langle\,\mathfrak{f}_n^{-}|, \tag{5.20}$$

on Φ_+. Hence, $R(z,\hat{H})|_{\Phi_-}$ has poles at $z=-E_n$, and $R(z,\hat{H})|_{\Phi_+}$ has poles at $z=E_n$. As usual, eigenvectors $\mathfrak{f}_n^{-}$ and $\mathfrak{f}_n^{+}$ corresponding to poles of the resolvent are interpreted as resonant states. Note that

$$-\frac{1}{2\pi i}\oint_{\gamma_n}R(z,\hat{H})dz=|\mathfrak{f}_n^{+}\rangle\langle\,\mathfrak{f}_n^{-}|:=\hat{P}_n, \tag{5.21}$$

where γ_n is a closed curve that encircles the singularity $z=E_n$. Clearly

$$\hat{P}_n\cdot\hat{P}_m=\delta_{nm}\hat{P}_n, \tag{5.22}$$

and the spectral decomposition of $\hat{H}$ may be written as follows:

$$\hat{H}=\sum_{n=0}^{\infty}E_n\hat{P}_n=-\sum_{n=0}^{\infty}E_n\hat{P}_n^{\dagger}. \tag{5.23}$$

Finally, let us note, that restriction of the unitary group $U(t)=e^{-i\hat{H}t}$ defined on the Hilbert space $L^2(\mathbb{R})$ to $\Phi_\pm$ no longer defines a group. It gives rise to two semigroups

$$U_-(t):\Phi_-\to\Phi_- \qquad \text{for} \qquad t\geqslant 0, \tag{5.24}$$

and

$$U_+(t):\Phi_+\to\Phi_+ \qquad \text{for} \qquad t\leqslant 0. \tag{5.25}$$

These semigroups frequently appear in the literature on the rigged Hilbert space approach to scattering phenomena, see, e.g., an article by Böhm and Harshman in Ref. 11. We stress that the Hardy classes $\Phi_\pm$ used in our paper have slightly different meaning. Böhm's spaces describe the prepared *in* and *out* states. In our case they are not directly related to the scattering experiment and serve as subspaces of initial conditions.

Using (5.16), (5.17), and the formula for $E_n=i\gamma(n+1/2)$, one finds

$$\phi^{-}(t)=U_-(t)\phi^{-}=\sum_{n=0}^{\infty}e^{-\gamma(n+1/2)t}\,\hat{P}_n^{\dagger}\phi^{-}, \tag{5.26}$$

for $t \geqslant 0$, and

$$\phi^+(t) = U_+(t)\phi^+ = \sum_{n=0}^{\infty} e^{\gamma(n+1/2)t} \hat{P}_n \phi^+, \tag{5.27}$$

for $t \leqslant 0$. We stress that ϕ_t^- (ϕ_t^+) does belong to $L^2(\mathbb{R})$ also for $t<0$ ($t>0$). However, $\phi_t^- \in \Phi_-$ ($\phi_t^+ \in \Phi_+$) only for $t \geqslant 0$ ($t \leqslant 0$). This way the irreversibility enters the dynamics of the reversed oscillator by restricting it to the dense subspace $\Phi_\pm$ of $L^2(\mathbb{R})$.

VI. SCATTERING VS RESONANT STATES

To compare the physical properties of energy eigenstates $\chi_\pm^E$ and $\eta_\pm^E$ and resonant states $\mathfrak{f}_n^\pm$, let us investigate its asymptotic behavior at $x \to \pm\infty$. Following Ref. 29 (see also Refs. 19, 20) one finds

$$\chi_-^E(x \to +\infty) \sim \sqrt{\frac{1}{x}} \exp\left[i\left(\frac{\gamma}{2}x^2 + \frac{E}{\gamma}\log(\sqrt{2\gamma}x) + \frac{\pi}{4}\frac{E}{\gamma} + \frac{\pi}{8} \right) \right], \tag{6.1}$$

and

$$\chi_-^E(x \to -\infty) \sim i\sqrt{\frac{1}{x}} \Bigg\{ (1 + e^{-2\pi(E/\gamma)}) \exp\left[-i\left(\frac{\gamma}{2}x^2 + \frac{E}{\gamma}\log(\sqrt{2\gamma}x) - \frac{\pi}{4}\frac{E}{\gamma} + \frac{3\pi}{8} + \phi \right) \right]$$
$$- e^{-\pi(E/\gamma)} \exp\left[i\left(\frac{\gamma}{2}x^2 - \frac{E}{\gamma}\log(\sqrt{2\gamma}x) - \frac{\pi}{4}\frac{E}{\gamma} + \frac{\pi}{8} \right) \right] \Bigg\}, \tag{6.2}$$

where $\phi = \arg\Gamma(-iE/\gamma + 1/2) = \Gamma(\nu+1)$. Putting $a = -E/\gamma$ in Eq. 19.17.9 in Ref. 29 and using relation 19.3.1

$$U(a,x) = D_{-a-1/2}(x),$$

one finds

$$U\left(-i\frac{E}{\gamma}, \sqrt{2\gamma}x e^{-(1/4)i\pi} \right) = D_{-\nu-1}(\sqrt{-2i\gamma}x) \sim \chi_-^E(x).$$

Hence, energy eigenstates χ_-^E represent scattering states (see Ref. 19 for more details). The same is true for χ_+^E and $\eta_\pm^E$. In particular, one finds for the reflection and transmission amplitudes R and T for $\chi_\pm^E$ scattering states:[17,19]

$$R(\chi_\pm^E) = -\frac{i}{\sqrt{2\pi}} e^{-\pi E/2\gamma} \Gamma\left(\frac{1}{2} - i\frac{E}{\gamma} \right), \tag{6.3}$$

$$T(\chi_\pm^E) = \frac{1}{\sqrt{2\pi}} e^{\pi E/2\gamma} \Gamma\left(\frac{1}{2} - i\frac{E}{\gamma} \right). \tag{6.4}$$

Clearly, computing R and T for time-reversed $\eta_\pm^E$ scattering states, one finds

$$R(\eta_\pm^E) = \overline{R(\chi_\pm^E)}, \qquad T(\eta_\pm^E) = \overline{T(\chi_\pm^E)}. \tag{6.5}$$

Note that $R(\chi_\pm^E)$ and $T(\chi_\pm^E)$ have poles at $E = -E_n$, whereas $R(\eta_\pm^E)$ and $T(\eta_\pm^E)$ have poles at $E = +E_n$. Obviously, the corresponding reflection and transition coefficients $|R|^2$ and $|T|^2$ are time-reversal invariant.

On the other hand, the eigenstates $\mathfrak{f}_n^\pm$ behave as follows:

$$\mathfrak{f}_n^+(x\to\pm\infty)\sim(\pm\sqrt{i\gamma}x)^n\,e^{-i(\gamma/2)x^2}, \tag{6.6}$$

and

$$\mathfrak{f}_n^-(x\to\pm\infty)\sim(\pm\sqrt{-i\gamma}x)^n\,e^{i(\gamma/2)x^2}. \tag{6.7}$$

Note that $\mathfrak{f}_n^-$ are purely outgoing states, whereas $\mathfrak{f}_n^+$ are purely ingoing states. Moreover, resonant states have Breit–Wigner energy distribution. Indeed

$$\langle\chi_-^E|\mathfrak{f}_n^+\rangle\sim\Gamma(-\nu)\int_{-\infty}^{\infty}D_\nu(\sqrt{2\gamma i}x)\,\mathfrak{f}_n^+(x)\,dx. \tag{6.8}$$

Now, D_ν is an entire function of ν and $\Gamma(-\nu)$ has poles at $\nu=k\in\mathbb{N}$. In the domain where $n+1>\mathrm{Re}\,\nu\geqslant 1$, one has

$$\Gamma(-\nu)=\text{analytical part}+\sum_{k=0}^{n}\frac{(-1)^k}{k!(k-\nu)^k}. \tag{6.9}$$

Hence

$$\langle\chi_-^E|\mathfrak{f}_n^+\rangle\sim\text{analytical function of } E+\sum_{k=0}^{n}\frac{(-1)^k}{k!\left(k+i\dfrac{E}{\gamma}+\dfrac{1}{2}\right)}\langle\mathfrak{f}_k^-|\mathfrak{f}_n^+\rangle$$

$$\sim\text{analytical function of } E+\frac{\gamma}{E-E_n}, \tag{6.10}$$

which is consistent with the Breit–Wigner formula.

APPENDIX

The integral formula 9.241(2) in Ref. 27

$$D_\lambda(y)=\frac{e^{-y^2/4}}{\Gamma(-\lambda)}\int_{-\infty}^{\infty}\xi_+^{-\lambda-1}\,e^{-y\xi-\xi^2/2}\,d\xi, \tag{A1}$$

contains two objects: $\Gamma(-\lambda)$ and a distribution $\xi^{-\lambda-1}$ which are singular for $\lambda=0,1,2,\ldots$. However, it is easy to see[23] that

$$\left.\frac{\xi_+^{-\lambda-1}}{\Gamma(-\lambda)}\right|_{p=n}=\delta^{(n)}(\xi), \tag{A2}$$

which shows that (A1) defines an entire function of $\lambda\in\mathbb{C}$. The same is true for

$$D_\lambda(y)=\frac{e^{-y^2/4}}{\Gamma(-\lambda)}\int_{-\infty}^{\infty}\xi_-^{-\lambda-1}\,e^{y\xi-\xi^2/2}\,d\xi, \tag{A3}$$

due to

$$\left.\frac{\xi_-^{-\lambda-1}}{\Gamma(-\lambda)}\right|_{\lambda=n}=(-1)^n\delta^{(n)}(\xi). \tag{A4}$$

The second integral representation given by 9.241(1) in Ref. 27

$$D_\lambda(y)=\frac{1}{\sqrt{\pi}}2^{\lambda+1/2}(-i)^\lambda e^{y^2/4}\int_{-\infty}^{\infty}(\xi+i0)^\lambda\, e^{-2\xi^2+2iy\xi}\,d\xi, \tag{A5}$$

where $(\xi+i0)^\lambda=\xi_+^\lambda+e^{i\pi\lambda}\xi_-^\lambda$, seems to have poles at $\lambda=-1,-2,\ldots$. However, the limit $\lim_{\lambda\to -n}(\xi+i0)^\lambda$ is well defined[23]

$$(\xi+i0)^{-n}=\xi^{-n}-\frac{i\pi(-1)^{n-1}}{(n-1)!}\,\delta^{(n-1)}(\xi). \tag{A6}$$

Thus, formula (A5) also defines an entire function of λ.

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Galerkin analysis for Schrödinger equation by wavelets

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We consider the perturbed Schrödinger equation, which is an elliptic operator with unbounded coefficients. We use wavelets adapted to the Schrödinger operator to deal with problems on the unbounded domain. The wavelets are constructed from Hermite functions, which characterizes the space generated by the Schrödinger operator. We show that the Galerkin matrix can be pre-conditioned by a diagonal matrix so that its condition number is uniformly bounded. Moreover, we introduce a periodic pseudo-differential operator and show that its discrete Galerkin matrix under periodic wavelet system is equal to the Galerkin matrix for the equation with unbounded coefficients under the Hermite system. The convergence is proved in the L^2 topology. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Wavelets have been applied to differential and integral operators in recent years.[5] The main advantage of the wavelet numerical scheme compared with the finite element method and the multilevel method is that for the resulting system of algebraic equations its condition number is uniformly bounded after a simple preconditioning (see, e.g., Jaffard[12] and Dahmen[5]). Moreover, its stiffness matrix can be approximated by a sparse matrix.[2,4,5]

With wavelets constructed through the usual multiresolution analysis method,[7] they cannot be readily applied to operators with unbounded coefficients such as the Schrödinger equation appeared in quantum mechanics

$$-u''(x)+x^2u(x)=f(x), \quad -\infty<x<\infty,$$

as well as operators with singular coefficients. This kind of (partial) differential equations appears in mathematics and physics.

Our purpose in this paper is to use a wavelet basis of the space $L^2(\mathbb{R})$ of the square-integrable functions on the real line $\mathbb{R}$ so that we can apply a Galerkin scheme to the numerical analysis of the following perturbed Schrödinger equation,

$$-(a(x)u'(x))'+b(x)u(x)=f(x), \quad -\infty<x<\infty,$$

which can be viewed as a model of second-order elliptic operators with unbounded coefficients.

The wavelets $\{\psi_{j,k}\}_{j,k\in\mathbb{Z}}$ generated from a mother wavelet ψ are the time–frequency localization of the Fourier kernel $\{e^{ix\xi}\}$, which forms a set of eigenfunctions of the second-order differential operator $-d^2/dx^2$. Jaffard[12] successfully adapted wavelets on the finite domain to the analysis of the general second-order elliptic operator $-d/dx(A(x)d/dx)+B(x)$ with regular coefficients.

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Frazier and Zhang[8] studied the Bessel operator $-g''(x)+(\nu^2-1/4)/x^2\,g(x)$ with singular coefficients. They used the Bessel function $J_\nu(x)$ and the Hankel transform. Their basis functions were obtained through the Hankel transform of the Meyer wavelets. These basis functions have explicit expressions in the Hankel domain just as the Meyer wavelets do in the Fourier domain.

In this paper we shall use eigenfunctions of the Schrödinger operator, namely the Hermite functions, to construct a wavelet-like basis and then adapt them to the analysis of the perturbed Schrödinger equation with unbounded coefficients.

Our basis is adapted to a Schrödinger operator and can be explicitly expressed using the Hermite functions and a known wavelet function from an MRA. These functions are obtained through a similarity between the Hermite functions and the orthonormal system $\{e^{in2\pi x}\}_{n\in\mathbb{Z}}$ instead of the continuous version $\{e^{ix\xi}\}$. Moreover, this construction can be easily generalized to any operators with a complete eigenfunction system.

Hermite functions have been utilized to approximate solutions of partial differential equations on unbounded domains in the context of the spectral method (Refs. 9, 11, 14). When dealing with problems on unbounded domain with a finite difference method or finite element method numerically, one often restricts calculations to some bounded domains and imposes certain conditions on artificial boundaries, which causes numerical errors. The Hermite functions defined on the whole real line can be used to avoid such difficulty. Meanwhile, with the spectral method, solutions can be approximated with accuracy adapted up to its smoothness. Wavelet bases have been applied to numerical solutions of partial differential equations since for its discrete stiffness matrix, the pre-conditioner can be easily constructed and its entries can be compressed.[5,12] Our method will take advantage from both the eigenfunctions and the wavelet functions. We use the former to deal with the geometry of differential operators and regularities of their coefficients so that we can deal with differential equations defined on unbounded domain with unbounded coefficients, and the latter to obtain a simple diagonal pre-conditioner.

The organization of this paper is as follows. In Sec. II, we shall present the construction of our basis functions. We shall introduce a space H associated with the Schrödinger operator and give a characterization of its functions in terms of their coefficients. We notice that the second-order Schrödinger operator acts like a first-order differential operator according to Theorem 3 which is the main result of Sec. II. In Sec. III, we shall use the Galerkin method to approximate solutions of the perturbed Schrödinger equations. Then, we shall estimate the condition number for the discrete Galerkin matrix and establish the convergence of the Galerkin scheme in the $L^2(\mathbb{R})$ space. Finally, we shall introduce a periodic pseudo-differential operator and show that its discrete Galerkin matrix under a periodic wavelet system is equal to the Galerkin matrix for the equation with unbounded coefficients under the Hermite system.

II. HERMITE WAVELETS

We shall use Hermite functions to construct wavelets, for the background on their applications to numerical solutions of partial differential equations; the reader is referred to Refs. 9–11, 15. The Hermite polynomials are defined by

$$h_n(x)=(-1)^n e^{x^2}\frac{d^n}{dx^n}(e^{-x^2}),\quad n=0,1,\ldots.$$

These polynomials are orthogonal in the weighted sense,

$$\int_{-\infty}^{\infty} h_n(x)h_m(x)e^{-x^2}dx=2^n n!\sqrt{\pi}\,\delta_{m,n},$$

where $\delta_{m,n}$ is the Kronecker symbol such that $\delta_{m,n}=1$ when $m=n$ and $\delta_{m,n}=0$, otherwise. It is possible to start with these polynomials, but since the corresponding approximation results are

measured in a weighted sense, their performance might become poor for large x due to the presence of the negative power of the exponential e^{-x^2}. We therefore use Hermite functions instead.

The normalized Hermite function under the norm of $L^2(\mathbb{R})$ is defined to be

$$e_n(x)=\frac{e^{-x^2/2}h_n(x)}{\sqrt{2^n n!\sqrt{\pi}}},\quad \text{with}\quad \|e_n\|_{L^2(\mathbb{R})}=1,\quad n=0,1,\ldots, \tag{1}$$

which satisfies the Schrödinger equation,

$$-e_n''(x)+x^2e_n(x)=(2n+1)e_n(x),\quad n=0,1,\ldots .$$

For fixed n, the function e_n is well-localized in the spatial domain. Moreover, it has the following asymptotic behavior:[10]

$$e_{2n}(x)=\frac{(-1)^n(2n-1)!!}{\sqrt{(2n)!\sqrt{\pi}}}\left[\cos(\sqrt{4n+1}x)+O\left(\frac{1}{\sqrt[4]{n}}\right)\right],\quad \text{as}\quad n\to\infty,$$

$$e_{2n+1}(x)=\frac{(-1)^n(2n-1)!!}{\sqrt{(2n+1)!\sqrt{\pi}}}\left[\sin(\sqrt{4n+3}x)+O\left(\frac{1}{\sqrt[4]{n}}\right)\right],\quad \text{as}\quad n\to\infty.$$

We consider the Schrödinger operator L defined on $C_0^\infty(\mathbb{R})$ by

$$(Lu)(x)=-u''(x)+x^2u(x),\quad u\in C_0^\infty(\mathbb{R}), \tag{2}$$

where $C_0^\infty(\mathbb{R})$ consists of compactly supported C^∞ functions on $\mathbb{R}$.

For the positive operator L, we introduce a norm by

$$\|u\|_{\mathrm{H}}=\langle Lu,u\rangle^{1/2}.$$

The domain of the operator L can be extended to the Hilbert space H defined by

$$H=\overline{\{u\ :\ u\in C_0^\infty(\mathbb{R})\text{such that}\ \|u\|_{\mathrm{H}}<\infty\}},$$

which is the completion of $C_0^\infty(\mathbb{R})$ under the norm $\|\cdot\|_{\mathrm{H}}$.

Functions in the space H can be characterized by the expansion coefficients under the basis $\{e_n\}_{n\in\mathbb{Z}}$. For a proof, the reader is referred to Ref. 13.

Lemma 1: Let $u\in L^2(\mathbb{R})$ with $u=\Sigma_{n=0}^\infty\langle u,e_n\rangle e_n$. Then $u\in H$ if and only if

$$\sum_{n=0}^{\infty}(2n+1)|\langle u,e_n\rangle|^2<\infty. \tag{3}$$

The Fourier transform $\hat{\varphi}$ of φ is defined to be

$$\hat{\varphi}(\xi)=\int_{-\infty}^{\infty}\varphi(x)e^{-i2\pi x\xi}dx.$$

Let φ be a function in $L^2(\mathbb{R})$ such that the following occurs.

(1) φ is a father wavelet; that is, $\hat{\varphi}(2\xi)=m(\xi)\hat{\varphi}(\xi)$ for some 1-periodic measurable function m.
(2) The shifts of φ are orthonormal; that is,

$$\langle\varphi(\cdot-k),\varphi(\cdot-k')\rangle=\delta_{k,k'},\quad \forall\ k,k'\in\mathbb{Z}.$$

(1) φ is normalized by $\hat{\varphi}(0)=1$ and there exist two positive constants C and $\sigma>1$ such that

$$|\hat{\varphi}(\xi)| \leqslant C(1+|\xi|)^{-\sigma}, \quad \forall \quad \xi \in \mathbb{R}. \tag{4}$$

Throughout the paper, C always denotes a general constant.

For example, the father wavelets in the Meyer wavelets and all of the Daubechies wavelets (except the Haar wavelet) satisfy all the above three conditions in (1), (2) and (3).

Now we define a mother wavelet function ψ (see Ref. 7) by

$$\hat{\psi}(\xi) = e^{-i\xi/2}\overline{m(\xi/2+1/2)}\,\hat{\varphi}(\xi/2).$$

We use $\mathbb{Z}_+$ to denote the set of non-negative integers. Denote $\varphi_{j,k} = 2^{j/2}\varphi(2^j \cdot - k)$ and $\psi_{j,k} = 2^{j/2}\psi(2^j \cdot - k)$. It is well known that for any $j_0 \in \mathbb{Z}_+$,

$$\{\varphi_{j_0,k} \ : \ k \in \mathbb{Z}\} \cup \{\psi_{j,k} \ : \ j \geqslant j_0, k \in \mathbb{Z}\} \tag{5}$$

is an orthonormal basis for $L^2(\mathbb{R})$. It follows from (4) that $|\hat{\psi}(\xi)| \leqslant C(1+|\xi|)^{-\sigma}$ for all $\xi \in \mathbb{R}$ since $|m(\xi)| \leqslant 1$.

Let $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ be the torus. Throughout the paper, we shall use the following notation. For any $u \in L^2(\mathbb{R})$, we define a function $u^{\mathrm{per}} \in L^2(\mathbb{T})$ as follows:

$$u^{\mathrm{per}}(x) := \sum_{l \in \mathbb{Z}} u(x+l), \quad x \in \mathbb{T}. \tag{6}$$

Using the Poisson summation formula, for $u \in L^2(\mathbb{R})$ satisfying $|\hat{u}(\xi)| \leqslant C(1+|\xi|)^{-\sigma}$, $\forall$ $\xi \in \mathbb{R}$ for some C and $\sigma > 1$, we have

$$u^{\mathrm{per}}(x) = \sum_{l \in \mathbb{Z}} u(x+l) = \sum_{n \in \mathbb{Z}} \hat{u}(n) e^{i2\pi nx}. \tag{7}$$

Using the Hermite functions $\{e_n\}_{n=0}^{\infty}$ and the wavelet basis in (5), we can construct a wavelet-like system in $L^2(\mathbb{R})$ as follows.

Theorem 1: Let φ and ψ be given above such that the system in (5) is an orthonormal basis for $L^2(\mathbb{R})$. Let e_n be the Hermite functions defined in (1). For $j \in \mathbb{Z}_+$ and $k = 0,1,\ldots,2^j - 1$, we define

$$\Phi_{j,k} = 2^{-j/2} e_0 + \sum_{n=1}^{\infty} [\widehat{\varphi_{j,k}}(n) e_{2n} + \widehat{\varphi_{j,k}}(-n) e_{2n-1}], \tag{8}$$

$$\Psi_{j,k} = \sum_{n=1}^{\infty} [\widehat{\psi_{j,k}}(n) e_{2n} + \widehat{\psi_{j,k}}(-n) e_{2n-1}]. \tag{9}$$

Then for any $j_0 \in \mathbb{Z}_+$,

$$\{\Phi_{j_0,k} \ : \ k = 0,1,\ldots,2^{j_0} - 1\} \cup \{\Psi_{j,k} \ : \ j \geqslant j_0, k = 0,1,\ldots,2^j - 1\} \tag{10}$$

is an orthonormal basis for $L^2(\mathbb{R})$.

Proof: When the functions φ and ψ are the Meyer wavelets, the assertion was proved in Dai.[6] For completeness, here we present a sketch of the proof.

Note that the system in (5) is an orthonormal basis for $L^2(\mathbb{R})$. By a simple argument, it can be easily shown that

$$\{(\varphi_{j_0,k})^{\mathrm{per}} \ : \ k = 0,1,\ldots,2^{j_0} - 1\} \cup \{(\psi_{j,k})^{\mathrm{per}} \ : \ j \geqslant j_0, k = 0,1,\ldots,2^j - 1\} \tag{11}$$

is an orthonormal basis for $L^2(\mathbb{T})$. Since $\widehat{\varphi_{j,k}}(0) = 2^{-j/2}$ and $\widehat{\psi_{j,k}}(0) = 0$, it follows from (7) that

$$(\varphi_{j_0,k})^{\mathrm{per}}(x)=\sum_{n\in\mathbb{Z}}\widehat{\varphi_{j_0,k}}(n)e^{i2\pi nx}=2^{-j_0/2}+\sum_{n=1}^{\infty}[\widehat{\varphi_{j_0,k}}(n)e^{i2\pi nx}+\widehat{\varphi_{j_0,k}}(-n)e^{-i2\pi nx}],$$
$$(\psi_{j,k})^{\mathrm{per}}(x)=\sum_{n\in\mathbb{Z}}\widehat{\psi_{j,k}}(n)e^{i2\pi nx}=\sum_{n=1}^{\infty}[\widehat{\psi_{j,k}}(n)e^{i2\pi nx}+\widehat{\psi_{j,k}}(-n)e^{-i2\pi nx}]. \tag{12}$$

Replacing 1, $e^{i2\pi n\cdot}$ and $e^{-i2\pi n\cdot}$ by e_0, e_{2n} and e_{2n-1} in (12), we obtain (8) and (9). Note that $\{e_n\}_{n=1}^{\infty}$ is an orthonormal basis for $L^2(\mathbb{R})$ and $\{e^{i2\pi n\cdot}\}_{n=-\infty}^{\infty}$ is an orthonormal basis for $L^2(\mathbb{T})$. Now one can easily show that the system in (10) is an orthonormal basis for $L^2(\mathbb{R})$ since the system (11) is an orthonormal basis for $L^2(\mathbb{T})$.

The advantage of replacing the orthonormal basis $\{e_n\}_{n=0}^{\infty}$ by the wavelet-like orthonormal basis in (10) lies in the fact that the new system preserves many desirable features of a wavelet system.

As a direct consequence of Theorem 1, we have the following result.

Theorem 2: Let $u\in L^2(\mathbb{R})$. Then for any $j_0\in\mathbb{Z}_+$, we have

$$u=\sum_{k=0}^{2^{j_0}-1}\langle u,\Phi_{j_0,k}\rangle\Phi_{j_0,k}+\sum_{j=j_0}^{\infty}\sum_{k=0}^{2^j-1}\langle u,\Psi_{j,k}\rangle\Psi_{j,k},\quad \text{in}\quad L^2(\mathbb{R}).$$

Lemma 2: The functions $\Phi_{j,k}$ and $\Psi_{j,k}$ belong to H for all $j\in\mathbb{Z}_+$ and $k=0,1,\ldots,2^j-1$.

Proof: We only prove $\Phi_{j,k}\in H$. The proof for $\Psi_{j,k}$ is similar. Since $\{e_n\}_{n=0}^{\infty}$ is orthonormal, it follows from the definition of $\Phi_{j,k}$ in (8) that

$$\langle\Phi_{j,k},e_n\rangle=\begin{cases}\widehat{\varphi_{j,k}}(n/2), & n \text{ even},\\ \widehat{\varphi_{j,k}}(-(n+1)/2), & n \text{ odd}.\end{cases}$$

Hence, by (4) and $\sigma>1$, we have

$$\begin{aligned}\sum_{n=0}^{\infty}(2n+1)|\langle\Phi_{j,k},e_n\rangle|^2&=(2^{-j/2})^2+\sum_{n=1}^{\infty}[(4n+1)|\widehat{\varphi_{j,k}}(n)|^2+(4n-1)|\widehat{\varphi_{j,k}}(-n)|^2]\\&=2^{-j}+2^{-j}\sum_{n=1}^{\infty}[(4n+1)|\hat{\varphi}(n/2^j)|^2+(4n-1)|\hat{\varphi}(-n/2^j)|^2]\\&\leqslant 2^{-j}+2^{-j}C\sum_{n=1}^{\infty}[(4n+1)(1+n/2^j)^{-2\sigma}+(4n-1)(1+n/2^j)^{-2\sigma}]\\&<\infty.\end{aligned}$$

By Lemma 1, we conclude that $\Phi_{j,k}\in H$.

Let $V_j=\mathrm{span}\{\Phi_{j,k}\}_{k=0}^{2^j-1}$. The subspace V_j will serve as our Galerkin approximation space. By Lemma 2, we have the following result.

Lemma 3: For each $j\in\mathbb{Z}_+$, V_j is a subspace of the Hilbert space H.

We shall use the Sobolev space $H^s(\mathbb{T})$ which consists of all functions $f\in L^2(\mathbb{T})$ such that

$$\|f\|_s=\left(\sum_{n\in\mathbb{Z}}(1+n^2)^s|\hat{f}(n)|^2\right)^{1/2}<\infty,$$

where the discrete Fourier transform $\hat{f}(n)$ of $f\in L^2(\mathbb{T})$ is defined to be

$$\hat{f}(n)=\int_{\mathbb{T}}f(x)e^{-i2\pi nx}\,dx,\quad n\in\mathbb{Z}.$$

Throughout this paper, we use the notation $A \approx B$, which means that there exist positive constants C_1 and C_2, independent of A, B, such that $C_2 B \leqslant A \leqslant C_1 B$.

A periodic function $u \in H^s(\mathbb{T})$ can be characterized in terms of wavelet coefficients in the periodic wavelet system in (11). For a proof of the following result, the reader is referred to Refs. 3, 7.

Lemma 4: Let $u \in H^s(\mathbb{T})(s>0)$ be decomposed into

$$u(x) = c_{0,0}(\varphi_{0,0})^{\mathrm{per}}(x) + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k}(\psi_{j,k})^{\mathrm{per}}(x), \quad x \in \mathbb{T}.$$

Then we have the following norm equivalence:

$$\|u\|_s \approx \left(|c_{0,0}|^2 + \sum_{j=0}^{\infty} 2^{2js} \sum_{k=0}^{2^j-1} |d_{j,k}|^2 \right)^{1/2}.$$

To prove our main results of this section, it is convenient to use pseudo-differential operators. For a background on pseudo-differential operators, see Taylor.[15,16] Let $p: \mathbb{Z} \to \mathbb{C}$ be a symbol. The pseudo-differential operator $P(D)$ with the symbol p is defined to be

$$[P(D)u](x) = \sum_{n \in \mathbb{Z}} e^{i2\pi nx} p(n) \hat{u}(n), \quad u \in C^{\infty}(\mathbb{T}). \tag{13}$$

Lemma 5: Suppose that the symbol p satisfies

$$p(n) \approx (1+n^2)^{r/2},$$

for some $r>0$. Then for $u \in H^{r/2}(\mathbb{T})$, we have

$$\langle P(D)u, u \rangle \approx \|u\|_{r/2}^2.$$

Proof: For $u \in C^{\infty}(\mathbb{T})$, we have the Fourier expansion

$$u(x) = \sum_{n \in \mathbb{Z}} \hat{u}(n) e^{i2\pi nx}.$$

From the orthogonality of $\{e^{i2\pi n \cdot}\}_{n \in \mathbb{Z}}$ in $L^2(\mathbb{T})$, we have

$$\langle P(D)u, u \rangle = \sum_{n \in \mathbb{Z}} p(n) |\hat{u}(n)|^2.$$

Since $p(n) \approx (1+n^2)^{r/2}$, we have

$$\langle P(D)u, u \rangle \approx \sum_{n \in \mathbb{Z}} (1+n^2)^{r/2} |\hat{u}(n)|^2 = \|u\|_{r/2}^2.$$

This completes the proof.

We now characterize the space H via our wavelet system $\{\Phi_{0,0}\} \cup \{\Psi_{j,k} : j \in \mathbb{Z}_+, k = 0,1,\ldots,2^j-1\}$.

Theorem 3: Suppose that $u \in H$ is decomposed as

$$u = c_{0,0}\Phi_{0,0} + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k}\Psi_{j,k}. \tag{14}$$

Then for the Schrödinger operator L, we have

$$\langle Lu,u\rangle \approx |c_{0,0}|^2 + \sum_{j=0}^{\infty} 2^j \sum_{k=0}^{2^j-1} |d_{j,k}|^2. \tag{15}$$

Proof: From the definition of $\Phi_{j,k}$ and $\Psi_{j,k}$, by Theorem 1, we have

$$u = c_{0,0}e_0 + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k} \sum_{n=1}^{\infty} [\widehat{\psi_{j,k}}(n)e_{2n} + \widehat{\psi_{j,k}}(-n)e_{2n-1}].$$

Hence, by applying the operator L, we have

$$Lu = c_{0,0}e_0 + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k} \sum_{n=1}^{\infty} [\widehat{\psi_{j,k}}(n)(4n+1)e_{2n} + \widehat{\psi_{j,k}}(-n)(4n-1)e_{2n-1}].$$

By the orthogonality of the Hermite system $\{e_n\}_{n=0}^{\infty}$, we get

$$\begin{aligned}\langle Lu,u\rangle = |c_{0,0}|^2 + \sum_{j,j'=0}^{\infty} \sum_{k=0}^{2^j-1} \sum_{k'=0}^{2^{j'}-1} d_{j,k}\overline{d_{j',k'}} \sum_{n=1}^{\infty} [(4n+1)\widehat{\psi_{j,k}}(n)\overline{\widehat{\psi_{j',k'}}(n)} \\ + (4n-1)\widehat{\psi_{j,k}}(-n)\overline{\widehat{\psi_{j',k'}}(-n)}].\end{aligned} \tag{16}$$

Consider the pseudo-differential operator $P(D)$ with the symbol p given by

$$p(n) = \begin{cases} 4n+1, & n \geqslant 0, \\ 4|n|-1, & n < 0. \end{cases} \tag{17}$$

Then we have $p(n) \approx (1+n^2)^{1/2}$.

From (7) we deduce that

$$u^{\mathrm{per}} = c_{0,0} + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k} \sum_{n\in\mathbb{Z}} \widehat{\psi_{j,k}}(n)e^{i2\pi n\cdot}. \tag{18}$$

Hence, the application of the pseudo-differential operator $P(D)$ with symbol p defined in (17) can be written as

$$P(D)u^{\mathrm{per}} = c_{0,0} + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k} \sum_{n\in\mathbb{Z}} p(n)\widehat{\psi_{j,k}}(n)e^{i2\pi n\cdot}. \tag{19}$$

From (18) and (19) we get

$$\begin{aligned}\langle P(D)u^{\mathrm{per}},u^{\mathrm{per}}\rangle = |c_{0,0}|^2 + \sum_{j,j'=0}^{\infty} \sum_{k=0}^{2^j-1} \sum_{k'=0}^{2^{j'}-1} d_{j,k}\overline{d_{j',k'}} \sum_{n=1}^{\infty} [(4n+1)\widehat{\psi_{j,k}}(n) \\ \times \overline{\widehat{\psi_{j',k'}}(n)} + (4n-1)\widehat{\psi_{j,k}}(-n)\overline{\widehat{\psi_{j',k'}}(-n)}].\end{aligned} \tag{20}$$

By (17) and Lemma 5 we conclude that

$$\langle P(D)u^{\mathrm{per}},u^{\mathrm{per}}\rangle \approx \|u^{\mathrm{per}}\|_{1/2}^2. \tag{21}$$

On the other hand, by Lemma 4,

$$\|u^{\mathrm{per}}\|_{1/2}^2 \approx |c_{0,0}|^2 + \sum_{j=0}^{\infty} 2^j \sum_{k=0}^{2^j-1} |d_{j,k}|^2. \tag{22}$$

Combining (16), (20)–(22), we conclude that (15) holds.

We point out that in (15) the exponent of 2^j is 1 instead of 2 for the second-order differential operator L, as compared to Lemma 4.

III. GALERKIN ANALYSIS

In this section, we consider the perturbed Schrödinger operator,

$$(Su)(x) = -\frac{d}{dx}\left(a(x)\frac{du(x)}{dx}\right) + b(x)u(x), \quad x \in \mathbb{R}, \tag{23}$$

where the functions a and b are measurable and satisfy

$$0 < a_1 \leqslant a(x) \leqslant a_2, \quad 0 < b_1 \leqslant b(x)/x^2 \leqslant b_2, \quad \forall \ x \in \mathbb{R}, \tag{24}$$

for some positive constants a_1, a_2, b_1 and b_2. In this section, we are interested in the perturbed Schrödinger equation $Su = f$.

We shall use the wavelet system $\{\Phi_{0,0}\} \cup \{\Psi_{j,k} : j \in \mathbb{Z}_+, k = 0,1,\ldots,2^j - 1\}$ to construct a Galerkin approximation scheme for the Schrödinger equation $Su = f$ with a given function $f \in L^2(\mathbb{R})$. We shall first show that the resulting system of algebraic linear equations can be preconditioned by a diagonal matrix. We then show that the Galerkin solution converges. Next we shall show that the discrete Galerkin scheme for the differential equation with unbounded coefficients is equivalent to a discrete Galerkin scheme of a periodic pseudo-differential operator. The latter equation is naturally related to the spectral Galerkin approximation using Hermite functions to solve the equation (23).

A. Galerkin scheme

We use the subspace $V_J \subset H$, which is defined by

$$V_J = \mathrm{span}\{\Phi_{J,k}\}_{k=0}^{2^J-1}$$

to be the Galerkin space. Since the space $\{V_j\}_{j \in \mathbb{Z}_+}$ forms a multi-resolution analysis,[6] the subspace V_J can be also spanned by

$$V_J = \mathrm{span}\{\Phi_{0,0}, \Psi_{j,k} \ : \ 0 \leqslant j < J, 0 \leqslant k < 2^j\}. \tag{25}$$

For convenience of notation, we denote

$$\Psi^0 = \Phi_{0,0} \quad \text{and} \quad \Psi^m = \Psi_{j,k}, \quad m = 1,2,\ldots, \tag{26}$$

where j,k are the unique non-negative integers such that $m = 2^j + k$ and $0 \leqslant k < 2^j$.

The Galerkin scheme for the Schrödinger equation $Su = f$ with $f \in L^2(\mathbb{R})$ is to find $u_J \in V_J$ such that

$$\langle Su_J, v \rangle = \langle f, v \rangle, \quad \forall \ v \in V_J. \tag{27}$$

In view of (25), (27) is equivalent to

$$\langle Su_J, \Psi^m \rangle = \langle f, \Psi^m \rangle, \quad m = 0,1,\ldots,2^J - 1. \tag{28}$$

Since $u_J \in V_J$, there exist $c_{0,0}$ and $d_{j,k}, j = 0,\ldots,J-1, k = 0,\ldots,2^j - 1$ such that

$$u_J = c_{0,0}\Phi_{0,0} + \sum_{j=0}^{J-1}\sum_{k=0}^{2^j-1} d_{j,k}\Psi_{j,k} = \sum_{m=0}^{2^J-1} d^m\Psi^m,$$

where we denote $d^0 = c_{0,0}, d^m = d_{j,k}$ for $m = 2^j + k$ and $0 \leqslant k < 2^j$.

Using matrix notation, the system of equations (28) takes the following form:

$$M_J d = F_J, \tag{29}$$

where M_J is a $2^J \times 2^J$ matrix with entries $M_{m,m'}$ given by

$$M_{m,m'} = \langle S\Psi^m, \Psi^{m'}\rangle,$$

and $F = (\langle f, \Psi^{m'}\rangle)^T$ is a column vector, and $d = (d^0, d^1, \ldots, d^{2^J-1})^T$ is the unknown vector.

B. Pre-conditioning

We now estimate the condition number of the matrix M_J in terms of the scale J. Let D_J be the $2^J \times 2^J$ diagonal matrix with diagonal elements,

$$d_{0,0} = 1, \quad d_{(2^j+k),(2^j+k)} = 2^{j/2}, \quad j = 0,1,\ldots,J-1,\ k = 0,1,\ldots,2^j - 1.$$

Then the equation $M_J d = F_J$ can be rewritten as

$$D_J^{-1} M_J D_J^{-1} D_J d = D_J^{-1} F_J. \tag{30}$$

Let $A_J = D_J^{-1} M_J D_J^{-1}, x_J = D_J d$ and $b_J = D_J^{-1} F_J$. Then the system of equations (30) becomes

$$A_J x_J = b_J. \tag{31}$$

We show that as a function of J, the condition number of the matrix A_J is uniformly bounded.

Lemma 6: Assume that (24) holds. Let A_J be defined as in (31). Then for any J, we have

$$\langle A_J v, v\rangle \approx \langle v, v\rangle, \quad \forall\ v \in \mathbb{C}^{2^J}, \tag{32}$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{C}^{2^J}$. Hence, the system of equations (31) is uniquely solvable.

Proof: For the vector v, we define $g = v_0\Psi_{0,0} + \Sigma_{j=0}^{J-1}\Sigma_{k=0}^{2^j-1} v_{2^j+k} 2^{-j/2}\Psi_{j,k}$. Then by Lemma 3, $g \in H$. Integrating by parts gives

$$\langle Sg, g\rangle = \langle -(ag')' + bg, g\rangle = \langle ag', g'\rangle + \langle bg, g\rangle \approx \langle Lg, g\rangle,$$

where (24) has been used in the last step. Furthermore, by Theorem 3, we have

$$\langle Lg, g\rangle \approx |v_0|^2 + \sum_{j=0}^{J-1} 2^j \sum_{k=0}^{2^j-1} |v_{2^j+k} 2^{-j/2}|^2 = |v_0|^2 + \sum_{j=0}^{J-1}\sum_{k=0}^{2^j-1} |v_{2^j+k}|^2 = \sum_{m=0}^{2^J-1} |v_m|^2 = \langle v, v\rangle.$$

On the other hand, from (26) we have $g = \Sigma_{m=0}^{2^J-1} v_m 2^{-j/2}\Psi^m$ and

$$\langle Sg, g\rangle = \sum_{m,m'=0}^{2^J-1} v_m \overline{v_{m'}} 2^{-(j+j')/2} \langle S\Psi^m, \Psi^{m'}\rangle = \langle A_J v, v\rangle.$$

Therefore, $\langle A_J v, v\rangle \approx \langle v, v\rangle$, as desired.

By Lemma 6 we now estimate the condition number of the matrix A_J in Eq. (31). We have the following result.

Theorem 4: Under the assumption in (24), the condition numbers of the matrices A_J ($J \in \mathbb{Z}_+$) are uniformly bounded (independent of J).

Proof: By Lemma 6, the ratio of the largest eigenvalue and the smallest eigenvalue of the matrix A_J is uniformly bounded. Since the condition number of a matrix can be estimated as the ratio of its largest eigenvalue and smallest eigenvalue, we conclude that the condition numbers of the matrices A_J are uniformly bounded.

C. Convergence of the Galerkin scheme

In this subsection we show that the approximate solution u_J in (27) converges to the solution u of (23) when $J \to +\infty$. The convergence is not in the weighted norm but directly in the $L^2(\mathbb{R})$ sense. We have the following result.

Theorem 5: For $J>0$, let u and u_J be solutions of (23) and (27), respectively. Then we have the estimate

$$\|u-u_J\|_{\mathrm{H}} \leqslant C \inf_{v_J \in V_J} \|u-v_J\|_{\mathrm{H}}, \tag{33}$$

where C is a constant independent of J. In particular, we have

$$u_J \to u, \quad \text{in} \quad L^2(\mathbb{R}).$$

Proof: For $w \in V_J$, from (23) and (27) we have

$$\langle S(u-u_J), w\rangle = 0.$$

Since S is self-adjoint and positive, as in the proof Lemma 6, we have

$$\|u-u_J\|_{\mathrm{H}}^2 \approx \langle S(u-u_J), u-u_J\rangle = \langle S(u-u_J), u-v_J\rangle \leqslant C\|u-u_J\|_{\mathrm{H}} \cdot \|u-v_J\|_{\mathrm{H}}.$$

Hence, we have

$$\|u-u_J\|_{\mathrm{H}} \leqslant C\|u-v_J\|_{\mathrm{H}}, \qquad \forall \ \ v_J \in V_J,$$

which proves (33). Moreover, by virtue of Theorem 3 we have

$$\|u-u_J\|_{L^2(\mathbb{R})} \leqslant \|u-u_J\|_{\mathrm{H}}.$$

Hence, $u_J \to u$ in $L^2(\mathbb{R})$. The proof of Theorem 5 is complete.

D. Spectral approximation

Hermite functions are eigenfunctions of the Schrödinger operator. We can use them to approximate solutions of the equation (23) in the context of the spectral method.

We introduce the notation

$$\tilde{n} = \begin{cases} 2n, & \text{if } \ n \geqslant 0, \\ 2|n|-1, & \text{if } \ n < 0. \end{cases}$$

For the differential operator S defined in (23), let q be a function from $\mathbb{Z}\times\mathbb{Z}$ to $\mathbb{R}$ defined by

$$q(n,n') = \langle S e_{\tilde{n}}, e_{\tilde{n}'}\rangle, \quad n,n' \in \mathbb{Z}. \tag{34}$$

Then the truncated matrix $(q(n,n'))_{|n|,|n'|\leqslant N} (N \in \mathbb{Z}_+)$ is the Galerkin matrix of the spectral approximation of the operator S by Hermite functions.

When S is the Schrödinger operator L in (2), we have $q(n,n') = (2\tilde{n}+1)\delta_{n,n'}$, which is a diagonal matrix. In general, the matrix q is a full matrix.

E. A pseudo-differential operator

We introduce a periodic pseudo-differential operator connected to the Schrödinger equation $Su=f$. This also suggests the necessity to study numerical solutions for pseudo-differential equations.[3,4]

Lemma 7: Let q be defined as in (23) and assume that (24) holds. Then for every $n\in\mathbb{Z}$, $\{q(n,\cdot)\}$ is square summable, that is, $\Sigma_{n'\in\mathbb{Z}}|q(n,n')|^2<\infty$.

Proof: Let $n\in\mathbb{Z}$. Then we have

$$\begin{aligned}\sum_{n'\in\mathbb{Z}}|q(n,n')|^2&=\sum_{n'\in\mathbb{Z}}|\langle Se_{\tilde{n}},e_{\tilde{n}'}\rangle|^2\\&=|\langle Se_{\tilde{n}},e_0\rangle|^2+\sum_{n=1}^{\infty}\left(|\langle Se_{\tilde{n}},e_{2n'}\rangle|^2+|\langle Se_{\tilde{n}},e_{2n'-1}\rangle|^2\right)\\&=\sum_{n'=0}^{\infty}|\langle Se_{\tilde{n}},e_{n'}\rangle|^2\\&=\|Se_{\tilde{n}}\|^2\\&<\infty,\end{aligned}$$

since $\{e_{n'}\}_{n'\in\mathbb{Z}}$ is an orthonormal basis for $L^2(\mathbb{R})$.

Lemma 8: Suppose that the functions a and b satisfy the condition (24). Then we have

$$\sum_{n,n'\in\mathbb{Z}}c_n\overline{c_{n'}}q(n,n')\approx\sum_{n\in\mathbb{Z}}(2|n|+1)|c_n|^2.$$

Proof: Let $u=\Sigma_{n\in\mathbb{Z}}c_ne_{\tilde{n}}$. Then by Lemma 1 we have

$$\sum_{n,n'\in\mathbb{Z}}c_n\overline{c_{n'}}q(n,n')=\sum_{n,n'\in\mathbb{Z}}\langle Sc_ne_{\tilde{n}},c_{n'}e_{\tilde{n}'}\rangle=\langle Su,u\rangle\approx\langle Lu,u\rangle\approx\sum_{n\in\mathbb{Z}}(2|n|+1)|c_n|^2,$$

which completes the proof.

For $(x,n)\in\mathbb{T}\times\mathbb{Z}$, we use the symbol

$$p(x,n)=\sum_{l\in\mathbb{Z}}q(n,n+l)e^{i2\pi lx}.$$

It follows that

$$q(n,n')=\int_0^1 p(x,n)e^{i2\pi(n-n')x}\,dx.$$

Consider the periodic pseudo-differential operator $P(\cdot,D)$ with symbol $p(x,n)$

$$[P(x,D)u](x)=\sum_{n\in\mathbb{Z}}e^{i2\pi nx}p(x,n)\hat{u}(n),\quad u\in C^{\infty}(\mathbb{T}).\tag{35}$$

Theorem 6: Suppose that the assumption (24) holds. Then the pseudo-differential operator defined in (35) can be extended to $H^1(\mathbb{T})$. Moreover, the operator $P(\cdot,D)$ is positive and there is a positive constant C such that

$$P(\cdot,D):H^1(\mathbb{T})\mapsto L^2(\mathbb{T})\quad\text{and}\quad\langle P(\cdot,D)u,u\rangle\geqslant C\|u\|_{1/2}^2,\quad\forall u\in H^{1/2}(\mathbb{T}).$$

Proof: For $u,v\in C^\infty(\mathbb{T})$, we have

$$\begin{aligned}\langle P(\cdot,D)u,v\rangle &= \int_0^1 [P(x,D)u](x)\overline{v(x)}dx\\ &= \int_0^1 \left(\sum_{n\in\mathbb{Z}} e^{i2\pi nx}p(x,n)\hat{u}(n)\right)\overline{\left(\sum_{n'\in\mathbb{Z}} e^{i2\pi n'x}\hat{v}(n')\right)}dx\\ &= \sum_{n,n'\in\mathbb{Z}} \hat{u}(n)\overline{\hat{v}(n')}\int_0^1 e^{i2\pi(n-n')x}p(x,n)dx = \sum_{n,n'\in\mathbb{Z}} \hat{u}(n)\overline{\hat{v}(n')}q(n,n').\end{aligned}$$

Hence, by Lemma 8, we have

$$\begin{aligned}|\langle P(\cdot,D)u,v\rangle| &\leqslant \left|\sum_{n,n'\in\mathbb{Z}} \hat{u}(n)\overline{\hat{v}(n')}q(n,n')\right|\\ &\leqslant C\left(\sum_{n\in\mathbb{Z}}(1+n^2)|\hat{u}(n)|^2\right)^{1/2}\left(\sum_{n'\in\mathbb{Z}}|\hat{v}(n')|^2\right)^{1/2} = C\|u\|_1\|v\|_0, \quad \forall\ v\in C^\infty(\mathbb{T}).\end{aligned}$$

It follows that $\|P(\cdot,D)u\|\leqslant C\|u\|_1$. Moreover, we have

$$\langle P(\cdot,D)u,u\rangle = \sum_{n,n'\in\mathbb{Z}} \hat{u}(n)\overline{\hat{u}(n')}q(n,n') \approx \sum_{n\in\mathbb{Z}}(1+|n|^2)^{1/2}|\hat{u}(n)|^2 = \|u\|_{1/2}^2.$$

Since $C^\infty(\mathbb{T})$ is dense in $H^{1/2}(\mathbb{T})$ and $H^1(\mathbb{T})$, the proof of Theorem 6 is complete.

F. Galerkin scheme for the pseudo-differential operator $P(\cdot,D)$

For a pseudo-differential operator $P(\cdot,D)$ which is defined in (35) and for any given periodic function $f^{\mathrm{per}}\in L^2(\mathbb{T})$, we consider the periodic problem on $\mathbb{T}$,

$$[P(x,D)u^{\mathrm{per}}](x) = f^{\mathrm{per}}(x), \quad x\in\mathbb{T}. \tag{36}$$

We use two bases on $\mathbb{T}$ to approximate solutions of (36). The first basis is the standard Fourier basis $\{e^{i2\pi nx}\}_{n\in\mathbb{Z}}$ and the second one is the periodic wavelet basis.

The Galerkin scheme for the periodic pseudo-differential equation (36) with a Fourier basis is to find

$$u_N^{\mathrm{per}}(x) = \sum_{|n|\leqslant N} u_n e^{i2\pi nx},$$

so that

$$\langle P(\cdot,D)u_N^{\mathrm{per}},v\rangle = \langle f^{\mathrm{per}},v\rangle \quad \forall\ v\in \mathrm{span}\{e^{i2\pi nx}\ :\ n=-N,-N+1,\ldots,N\}. \tag{37}$$

The system of algebraic equations in (37) can be rewritten as

$$F_N u^N = f_N,$$

where $F_N=\{\langle P(\cdot,D)(e^{i2\pi n\cdot}),e^{i2\pi n'\cdot}\rangle\}$ is a $(2N+1)\times(2N+1)$ matrix, $f_N=\{\langle f^{\mathrm{per}},e^{i2\pi n\cdot}\rangle\}^T$ and $u^N=(u_{-N},u_{-N+1},\ldots,u_N)^T$. It can be easily verified that the discrete Galerkin matrix F_N is equal to the Galerkin matrix (34), that is, we have

$$F_N=(q(n,n'))_{|n|,|n'|\leqslant N}.$$

The Galerkin scheme for the periodic pseudo-differential equation (36) with periodic wavelets is to find

$$u^{\mathrm{per}}=d_0+\sum_{j=0}^{J-1}\sum_{k=0}^{2^j-1} d_{2^j+k}(\psi_{j,k})^{\mathrm{per}}$$

such that

$$\langle P(\cdot,D)u^{\mathrm{per}},v\rangle=\langle f^{\mathrm{per}},v\rangle \quad \forall \quad v\in \mathrm{span}\{(\varphi_{J,k})^{\mathrm{per}}(x):\ k=0,\ldots,2^J-1\}. \tag{38}$$

Rewriting the system of equations (38) in terms of $\{d_m\}_{m=0}^{2^J-1}$, we get the matrix equation

$$P_J d=f_J, \tag{39}$$

where $P_J=\{\langle P(\cdot,D)\Psi_{m'}^{\mathrm{per}},\Psi_m^{\mathrm{per}}\rangle\}$ is a $2^J\times 2^J$ matrix, $f_J=\{\langle f^{\mathrm{per}},\Psi_m^{\mathrm{per}}\rangle\}^T$ is a $2^J\times 1$ vector, and $d=\{(d_0,d_1,\ldots,d_{2^J-1})^T\}$. Here we have used the notation $\Psi_0^{\mathrm{per}}=(\varphi_{0,0})^{\mathrm{per}}=1$ and $\Psi_m^{\mathrm{per}}=(\psi_{j,k})^{\mathrm{per}}$, where j,k are the unique non-negative integers such that $m=2^j+k$ and $0\leqslant k<2^j$.

G. Equivalence of the Galerkin matrix M_J and P_J

In this subsection we show that the Galerkin equation (27) for the operator S can be realized by the pseudo-differential operator $P(\cdot,D)$.

We show that the matrix M_J defined in (29) is equal to the matrix defined in (39). To this end, we introduce an isomorphism between $L^2(\mathbb{R})$ and $L^2(\mathbb{T})$. Suppose that $f\in L^2(\mathbb{R})$ has an expansion,

$$f(x)=\sum_{n=0}^{\infty} f_n e_n(x), \quad x\in\mathbb{R},$$

we define a one-periodic function $\underline{f}(x)$ by

$$\underline{f}(x)=f_0+\sum_{n=1}^{\infty}[f_{2n}e^{i2\pi nx}+f_{2n-1}e^{-i2\pi nx}], \quad x\in\mathbb{T}. \tag{40}$$

It is easy to show that $\underline{f}\in L^2(\mathbb{T})$ and in fact $\|f\|_{L^2(\mathbb{R})}=\|\underline{f}\|_{L^2(\mathbb{T})}$. Moreover, we have the following result connecting the differential operator S with the pseudo-differential operator $P(\cdot,D)$.

Lemma 9: For any $f\in H$ and $g\in L^2(\mathbb{R})$, if $\underline{f}$ and $\underline{g}$ are defined in (40), then we have

$$\langle Sf,g\rangle=\langle P(\cdot,D)\underline{f},\underline{g}\rangle. \tag{41}$$

Proof: By (40), it suffices to prove (41) for $g(x)=e_n(x), n\in\mathbb{Z}_+$. First we consider the case $g=e_{2n}, n\in\mathbb{Z}_+$. For $f(x)=\Sigma_{n=0}^{\infty}f_n e_n(x)$ such that all but finitely many f_n are zeros, by definition the periodic function $\underline{g}(x)=e^{i2\pi nx}$. Hence, we have

$$\langle Sf,e_{2n}\rangle=\sum_{n'=0}^{\infty} f_{n'}\langle Se_{n'},e_{2n}\rangle,$$

and for the pseudo-differential operator,

$$\begin{aligned}\langle P(\cdot,D)\underline{f},\underline{g}\rangle &= f_0\langle P(\cdot,D)(1),e^{i2\pi n\cdot}\rangle+\sum_{n'=1}^{\infty}\left[f_{2n'}\langle P(\cdot,D)(e^{i2\pi n'\cdot}),e^{i2\pi n\cdot}\rangle\right.\\ &\quad\left.+f_{2n'-1}\langle P(\cdot,D)(e^{-i2\pi n'\cdot}),e^{i2\pi n\cdot}\rangle\right]\\ &= f_0\int_0^1 p(x,0)e^{-i2\pi nx}\,dx+\sum_{n'=1}^{\infty}\left[f_{2n'}\int_0^1 p(x,n')e^{i2\pi(n'-n)x}\,dx\right.\\ &\quad\left.+f_{2n'-1}\int_0^1 p(x,n')e^{i2\pi(-n'-n)x}\,dx\right]\\ &= f_0 q(0,n)+\sum_{n'=1}^{\infty}\left[f_{2n'}q(n',n)+f_{2n'-1}q(-n',n)\right]\\ &= f_0\langle Se_0,e_{2n}\rangle+\sum_{n'=1}^{\infty}\left[f_{2n'}\langle Se_{2n'},e_{2n}\rangle+f_{2n'-1}\langle Se_{2n'-1},e_{2n}\rangle\right].\end{aligned}$$

The proof for $g=e_{2n+1}$ is similar. The proof of Lemma 9 is complete by the facts that $\mathrm{span}\{e_n : n\in\mathbb{Z}_+\}$ is dense in H and $\{e_n : n\in\mathbb{Z}_+\}$ is an orthonormal basis for $L^2(\mathbb{R})$.

Lemma 10: For $k=0,1,\ldots,2^j-1$, $j,j'=0,1,\ldots,J-1$ and $k'=0,1,\ldots,2^{j'}-1$, for the differential operator S and the pseudo-differential operator P, we have

$$\langle S\Phi_{j,k},\Psi_{j',k'}\rangle=\langle P(\cdot,D)((\varphi_{j,k})^{\mathrm{per}}),(\psi_{j',k'})^{\mathrm{per}}\rangle,$$

$$\langle S\Psi_{j,k},\Psi_{j',k'}\rangle=\langle P(\cdot,D)((\psi_{j,k})^{\mathrm{per}}),(\psi_{j',k'})^{\mathrm{per}}\rangle,$$

$$\langle S\Phi_{j,k},\Phi_{j',k'}\rangle=\langle P(\cdot,D)((\varphi_{j,k})^{\mathrm{per}}),(\varphi_{j',k'})^{\mathrm{per}}\rangle.$$

Proof: From the definition of the functions $\Phi_{j,k}$ and $\Psi_{j,k}$, according to (40), it is easy to verify that $\Phi_{j,k}=(\varphi_{j,k})^{\mathrm{per}}$ and $\Psi_{j,k}=(\psi_{j,k})^{\mathrm{per}}$. Hence, Lemma 10 follows directly from Lemma 9.

The following result is a direct consequence of Lemma 10:

Theorem 7: Let the matrices M_J and P_J be defined, respectively, in (29) and (39). Then we have $M_J=P_J$.

Numerical solutions of pseudo-differential equations by means of wavelets have been studied in several papers such as Refs. 2–4. By Theorem 7 and some results in the literature, the stiffness matrix P_J could be compressed and be approximated by a sparse matrix.

IV. CONCLUSION

We have presented an approximation method to deal with second order elliptic equations with unbounded coefficients on an unbounded domain. The combination of Hermite functions and wavelet functions have the advantages from both the wavelet approximation method and the spectral method.

Note added in the revised version: After submitting this paper, we became aware that multiresolution norm equivalences in weighted spaces $L^2_w((0,1))$ with a weight function w in (0,1) have been obtained in Ref. 1. The Galerkin scheme proposed in this paper deals with the perturbed Schrödinger equations with unbounded coefficients on the unbounded domain $\mathbb{R}$. Our approximation results are measured directly in the $L^2(\mathbb{R})$ and $H^s(\mathbb{R})$ spaces instead of in a weighted sense as in Ref. 1 which deals with the bounded domain (0,1).

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A random matrix approach to the crossover of energy-level statistics from Wigner to Poisson

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We analyze a class of parametrized random matrix models, introduced by Rosenzweig and Porter, which is expected to describe the energy level statistics of quantum systems whose classical dynamics varies from regular to chaotic as a function of a parameter. We compute the generating function for the correlations of energy levels, in the limit of infinite matrix size. The crossover between Poisson and Wigner statistics is measured by a renormalized coupling constant. The model is exactly solved in the sense that, in the limit of infinite matrix size, the energy-level correlation functions and their generating function are given in terms of a finite set of integrals. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1644752]

I. INTRODUCTION

Random Matrix Theory (RMT),[1] originally introduced by Wigner to characterize the statistical behavior of the energy levels of nuclei, has found many successful applications in various fields of physics in recent years. Originally, it was thought that RMT was applicable only to complex systems with many degrees of freedom. Hence, it came as a surprise when it was found that it could equally well describe simple quantum systems, with very few degrees of freedom, as long as their classical dynamics were chaotic. The first evidence of this fact was provided in the seminal paper by Bohigas *et al.*[2] in which the energy level fluctuations of the quantum Sinai billiard were analyzed and shown to be consistent with the predictions of the Gaussian orthogonal ensemble of RMT. Since this pioneering work, it has been checked numerically on a wide variety of systems, that the local statistical properties of the energy levels of a quantum system, whose classical counterpart is chaotic, are well-described by RMT. In particular, the nearest neighbor spacing distribution was found to be in excellent agreement with the spacing distribution between adjacent eigenvalues of random matrices.

In contrast, Berry and Tabor[3] had given strong arguments to justify that, for integrable systems with more than one degree of freedom, the nearest neighbor spacing distribution of the quantum energy levels should have a Poisson distribution, characteristic of uncorrelated levels. This has been confirmed by many numerical studies. There now exist excellent reviews on this topic.[4,5]

However, it is well-known in classical mechanics that purely integrable or purely chaotic systems are rare (at least for systems with a few degrees of freedom). For most systems, the phase space is partitioned into regular and chaotic regions and hence these systems can be referred to as *mixed systems*.

An important physical system illustrating these different behaviors, is the hydrogen atom in a magnetic field. The classical system is essentially integrable (chaotic) at weak (strong) fields but appears to be mixed at intermediate values of the field. This classical behavior has its counterpart in the energy level statistics of the corresponding quantum system, which exhibits a crossover from Poisson to Wigner-type, when the magnetic field is increased.[6] It is, therefore, important to find models of random matrices which could describe the statistics of the energy levels of such mixed systems. Qualitatively, such a model should be governed by a Hamiltonian matrix which is

essentially a sum of two parts, one describing the chaotic part of phase space and hence belonging to the Wigner–Dyson ensemble of the relevant symmetry, and the other corresponding to the regular part of phase space. A number of authors have studied models in which block-diagonal GOE matrices are weakly coupled by matrix elements also belonging to a GOE ensemble.[7,8] In this paper, we consider another class of models, first introduced by Rosenzweig and Porter[9] to describe the observed deviations from the Wigner and Poisson statistics in the spectra of some transition metal atoms.

This class of models is governed by an ensemble of $N\times N$ matrices of the form,

$$H=A+\frac{\lambda}{N^{\alpha}}G, \tag{1}$$

where A and G are either real symmetric matrices (in the orthogonal case) or complex self-adjoint ones (in the unitary case). The matrix elements of G are chosen to be independent random variables with a Gaussian distribution of unit variance. In the context of quantum chaos, G is supposed to correspond to the chaotic region of the classical phase space and hence its eigenvalue distribution should obey the Wigner–Dyson statistics. In contrast, A should correspond to the classically regular region and hence its eigenvalues should exhibit Poisson statistics. It is easily seen that the statistics of the energy levels of H depend only on the eigenvalues of A. Hence, without loss of generality, the matrix A can be chosen to be diagonal. The simplest type of model which can be considered is, therefore, the following one: A is a diagonal matrix, whose elements are independent random variables with a probability distribution $\nu(\cdot)$. Different behaviors can be expected by varying the exponent α in (1). the The case $\alpha=1/2$, corresponds to a perturbed Wigner–Dyson ensemble. It was recently analyzed by Brezin and Hikami.[10] They considered the case in which G belongs to the Gaussian Unitary ensemble (GUE) and A is a *fixed* diagonal matrix. They showed that the energy level statistics for such a matrix ensemble was the same as that of G, i.e., the statistics relevant to the GUE. If $\alpha>1$, the energy level statistics is expected to be Poissonian. The value $\alpha=1$ corresponds to the *crossover regime* and for it one expects new statistics. In fact, by making a numerical study of this model, Rosenzweig and Porter showed that if one chooses the exponent α to be unity, then one obtains energy level statistics which is intermediate between Wigner and Poisson statistics.

Analytical studies of the model for $\alpha=1$, has been done only in the unitary case. These studies made use of certain special features of unitary matrices. However, the case of the GOE, which one encounters more often, and is technically more challenging, had remained virtually unsolved thus far. The only results for this case were perturbative ones in the small λ limit.[11]

In this article, we develop a technique which can be used to study the spectral correlations for the case in which G belongs to the GOE as well as to the one in which it belongs to the GUE. We compute the generating function for the average value of the product of traces of advanced Green's functions, and the mixed product of traces of advanced and retarded Green's functions. All the correlation functions of energy levels can be obtained from it, in the limit where N goes to infinity.

In the case $\alpha=1$, our result for the generating function (in the infinite N limit) is in the form of a finite set of ordinary integrals. Quite generally, we show that the density of states at an energy e is given by $\nu(e)$, and that all the correlation functions are universal functions depending only on the ''renormalized'' coupling constant $\Lambda=\lambda\nu(e)$. This suggests that in order to make a comparison of the results of the model with a given quantum system, it might be plausible to take Λ to be the ratio of $\rho(e)$ and $\rho_{\mathrm{reg}}(e)$, where $\rho(e)$ is the classsical Louiville measure of the energy surface and $\rho_{\mathrm{reg}}(e)$ is the measure corresponding to the regular part of the phase space.

In order to obtain more concrete results, one needs to evaluate the integrals appearing in the expression for the generating functions. This explicit computation, which turns out to be a rather lengthy one, has been done in this paper for the generating function for the two-point correlation function, in the unitary case. From it we can recover the two-point correlation function itself, in

the form of certain integrals over modified Bessel functions. In the orthogonal case, the generating function, even for the two-point correlation function, appears in the form of integrals over elliptic functions and we postpone the study of it to a future paper.

Recently, there has been a certain interest in the computation of the generating function itself.[12–14] In the case of the standard Wigner unitary ensemble this has been motivated by the connection between such a RMT and the statistics of the zeroes of the Riemann zeta function. We think therefore that it is worth reporting the expression we get for the two-point generating function in the unitary case, for the Rosenzweig–Porter ensemble. In the unitary case, in some approaches the formula of Harish-Chandra and Itzykson–Zuber[15,16] proved to be very useful. Recently, Guhr and Kohler[17,18] have extended it to the orthogonal and symplectic cases and, using this approach, have obtained an expression for the two-point correlation function in the orthogonal case for the Rosenzweig–Porter model. However, it is not possible to compare their results with those of this paper due to the difference in the two approaches and the complexity of the formulas.

We would like to make a few remarks about the technique used in this paper. We basically use integrals over auxiliary Grassmannian variables to compute the average over the distribution of the Hamiltonian. However, finally, we evaluate these Grassmannian integrals so as to arrive at a representation in terms of ordinary integrals, in the large N limit. Such an approach for the average Green's function and density of states of a random matrix model was made by Ziegler[20] and Brezin.[21] It is similar, of course in spirit, to the familiar supersymmetric approach, introduced by Efetov[19] in this kind of problem. Note, however, that in the articles using the supersymmetric technique, the supersymmetry plays a crucial role for the computation of the saddlepoint of the action, and of the fluctuations around it. In contrast, in the case considered in this paper, we never have to compute a saddlepoint and Grassmannian variables are only used as an intermediate step in the computation, for purposes of simplification. In this case, no further simplication can be achieved by the use of supersymmetry.

II. GENERATING FUNCTION

We want to calculate the correlation functions $\rho^{(n)}(e_1,\ldots,e_n)$ of the eigenvalues λ_j of an $N \times N$ self-adjoint matrix H. They are defined as

$$\rho^{(n)}(e_1,\ldots,e_n)=\left\langle \prod_{\alpha=1}^{n} \hat{\rho}(e_\alpha) \right\rangle, \tag{2}$$

where

$$\hat{\rho}(e)=\frac{1}{N}\sum_j \delta(e-\lambda_j)$$

is the local density of eigenvalues at the energy e. The angular brackets will henceforth indicate an average over the probability distribution of H.

If $G^s(e)$ denotes the advanced $(s=+1)$ and retarded $(s=-1)$ Green's function

$$G^s(e)=\frac{1}{e-H-is\varepsilon},$$

then

$$\hat{\rho}(e)=\lim_{\varepsilon\uparrow 0^+}\left\{\frac{1}{2\pi i N}\operatorname{tr}[G^+(e)-G^-(e))\right\}.$$

We will use the following identity to compute $[\operatorname{tr} G^s(e)]/N$:

$$\frac{\partial}{\partial\varepsilon_{\pm}}\frac{\det[(\varepsilon_{-}/N)\mathbb{1}_N+is\,(e\mathbb{1}_N-H)]}{\det[(\varepsilon_{+}/N)\mathbb{1}_N+is\,(e\mathbb{1}_N-H)]}\bigg|_{\varepsilon_{-}=\varepsilon_{+}}=\mp\frac{1}{isN}\operatorname{tr}G^{s}(e).$$

The symbol $\mathbb{1}_N$ is used to denote the $N\times N$ identity matrix. Hence, it is evident that the correlation functions of energy levels can be obtained from the *generating function*

$$J_n^S=\left\langle\prod_{\alpha=1}^{n}\frac{\det[\varepsilon_{-}(\alpha)/N+is_{\alpha}(e_{\alpha}-H)]}{\det[\varepsilon_{+}(\alpha)/N+is_{\alpha}(e_{\alpha}-H)]}\right\rangle, \tag{3}$$

where $S=\{s_{\alpha}\}_{\alpha=1}^{n}$, $s_{\alpha}\in\{1,-1\}$, and $\varepsilon_{\pm}(\alpha)>0$, by taking suitable derivatives of it with respect to the variables $\varepsilon_{-}(\alpha)$ or $\varepsilon_{+}(\alpha)$.

In particular, the density of states is given by

$$\rho(e)=\rho^{(1)}(e)=\lim_{\varepsilon_{-}\uparrow 0^{+}}\operatorname{Re}\left\{\frac{1}{\pi}\frac{\partial}{\partial\varepsilon_{-}}J_1^{+}\bigg|_{\varepsilon_{-}=\varepsilon_{+}}\right\}$$

and the two-point correlation function by

$$\rho^{(2)}(e_1,e_2)=\lim_{\varepsilon_{-}\uparrow 0^{+}}\operatorname{Re}\left\{\frac{1}{2\pi^2}\frac{\partial^2[J_2^{+-}+J_2^{++}]}{\partial\varepsilon_{-}(1)\,\partial\varepsilon_{-}(2)}\bigg|_{\varepsilon_{-}=\varepsilon_{+}}\right\}.$$

In this paper, we will consider Hamiltonians H of the form

$$H=A+\frac{\lambda}{N}G, \tag{4}$$

where G is an $N\times N$ matrix whose elements are independent random variables with a Gaussian distribution of unit variance and zero mean. When the matrix elements of G are real (complex), the matrix G belongs to the Gaussian orthogonal (unitary) ensemble of standard RMT. Since the probability distribution of G is independent of the basis, the correlations of the energy levels of H depend only on the eigenvalues $\{a_j\}$ of A. Hence, without loss of generality, we can choose A to be a diagonal matrix whose elements are independent random variables with a probability distribution $\nu(a_j)$.

A. The orthogonal case for finite matrix size

Consider a mixed system governed by a Hamiltonian matrix of the form (4), with the matrix G belonging to the Gaussian orthogonal ensemble (GOE). In this case, it is convenient to express the generating function J^S as the ratio of the *square roots* of the determinants of an antisymmetric matrix and a symmetric one. This is because one can cast such a ratio as a product of integrals over real and Grassmannian variables. In this way the average over the matrix G and a can be easily done. After some standard manipulations, the generating function can be written as follows:

$$J^S=(\det\mathcal{S})^{N/2}\,e^{(1/2\lambda^2)[\operatorname{tr}(\rho_{+}\mathcal{S})^2-\operatorname{tr}\rho_{-}^2]}\int D\nu(A)\int D\varphi_{+}\int D\varphi_{-}\,e^{-(\lambda^2/2N^2)\operatorname{tr}[L_{+}^{t}\mathcal{S})^2+(\rho_{+}\mathcal{S}N/\lambda^2)]^2}$$
$$\times\,e^{(\lambda^2/2N^2)\operatorname{tr}[L_{-}^{t}\Upsilon-(\rho_{-}N/\lambda^2)]^2}\,e^{-(\varphi_{+},(i\mathcal{S}\otimes(e\mathbb{1}_N-A)\varphi_{+})}\,e^{-(\varphi_{-},(i\Upsilon\otimes(\lambda^2/N^2)\,T)\varphi_{-})}. \tag{5}$$

The integration is carried over the vectors φ_{+}, whose components are real, and φ_{-}, whose components are Grassmanian variables, as well as over the variables denoted by a_j. We have used the notation

$$D\nu(A) := \prod_{j=1}^{N} da_j\, \nu(a_j), \tag{6}$$

where the $\nu(a_j)$'s denote the probability distributions of the variables a_js. The $2n\times 2n$ matrices L_σ, with $\sigma = +,-$, and the $N\times N$ matrix T are given by

$$L_\sigma(p\alpha|p'\alpha') = \sum_{i=1}^{n} \varphi_{\sigma i}(p\alpha)\, \varphi_{\sigma i}(p'\alpha')$$

and

$$T_{ij} = \sum_{p=1}^{2} \sum_{\alpha=1}^{n} \varphi_{+i}(p\alpha)\, \varphi_{+j}(p\alpha) s_\alpha. \tag{7}$$

The $2n\times 2n$ matrices $\mathcal{S}$ and Υ are given by

$$\mathcal{S}(p\alpha|p'\alpha') = \delta_{\alpha\alpha'}\, \delta_{pp'} s_\alpha, \tag{8}$$

$$\Upsilon(p\alpha|p'\alpha') = \delta_{\alpha\alpha'}\, \gamma(pp'), \tag{9}$$

where

$$\gamma(pp) = 0, \quad \gamma(12) = -\gamma(21) = 1. \tag{10}$$

Since we consider correlation functions between energy levels around some energy e, on the scale of the mean level spacing, we have decomposed the energies e_α into

$$e_\alpha = e + \frac{r_\alpha}{N}, \tag{11}$$

so that we have introduced the matrices ρ_+ and ρ_- of elements

$$\rho_+(p\alpha|p'\alpha') = \delta_{\alpha\alpha'}\delta_{pp'}[\varepsilon_+(\alpha) + i r_\alpha s_\alpha], \tag{12}$$

$$\rho_-(p\alpha|p'\alpha') = \delta_{\alpha\alpha'}\delta_{pp'}[\varepsilon_-(\alpha) s_\alpha + i r_\alpha]. \tag{13}$$

With the help of Gaussian integrations over auxiliary $n\times n$ matrices Q_+ and Q_-, the exponents in the integrands [on the RHS of (5)] can be reduced to quadratic forms in φ_+ and φ_-. This procedure, which is analogous to the Hubbard Stratonovich transformation, yields the following identities:

$$e^{-(\lambda^2/2N^2)\mathrm{tr}(L_+^t \mathcal{S} + (N/\lambda^2)\mathcal{S}\rho_+)^2} = \frac{1}{d_+} \int DQ_+\, e^{-(1/2)\mathrm{tr}\, Q_+^2}\, e^{-(i\lambda/N)\mathrm{tr}[Q_+(L_+^t \mathcal{S} + N/\lambda^2 \mathcal{S}\rho_+)]},$$

and

$$e^{(\lambda^2/2N^2)\mathrm{tr}(L_-^t \Upsilon - (N/\lambda^2)\rho_-)^2} = \frac{1}{d_-} \int DQ_-\, e^{-(1/2)\mathrm{tr}\, Q_-^2}\, e^{-(\lambda/N)\mathrm{tr}[Q_-(L_-^t \Upsilon - (N/\lambda^2)\rho_-)]}, \tag{14}$$

with

$$d_\pm = \int DQ_\pm\, e^{-(1/2)\mathrm{tr}\, Q_\pm^2}. \tag{15}$$

Following Schäfer and Wegner[22] we choose the matrix Q_+ to be of the form

$$Q_+ = \begin{pmatrix} Q_{11} - i\sqrt{\delta^2 + Q_{12}Q_{21}} & Q_{12} \\ Q_{21} & Q_{22} + i\sqrt{\delta^2 + Q_{21}Q_{12}} \end{pmatrix}. \tag{16}$$

If $s_\alpha = -1$ for $\alpha = 1,\ldots,q$ and $s_\alpha = 1$ for $\alpha = q+1,\ldots,n$, then Q_{11} is a $2(n-q)\times 2(n-q)$ real symmetric matrix, Q_{22} is a $2q\times 2q$ real symmetric matrix, Q_{12} is a $2q\times 2(n-q)$ real matrix, and Q_{21} is a $2(n-q)\times 2q$ real matrix, such that

$$Q_{21}^t = Q_{12}.$$

Here the superscript t denotes the transpose of the matrix.

We consider Q_- to be Hermitian: $Q_-^\dagger = Q_-$, so for $n=1$ it reduces to a real number. In addition, we require Q_- to satisfy the following relation:

$$(Q_- \Upsilon)^t = -(Q_- \Upsilon). \tag{17}$$

The constraint (17) on the matrix Q_- is imposed so as to ensure the validity of the identity (14). Indeed the latter identity, involving such a matrix Q_-, uses the fact that the linear term in Q_-, appearing in the exponential, is of the form $\mathrm{tr}(Q_- E \Upsilon)$, with E being an antisymmetric matrix. We can therefore write the generating function in the form

$$J^S = \frac{(\det \mathcal{S})^{N/2}}{d_+ d_-} \int DQ_+ \int DQ_- \exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_+ + i\frac{\mathcal{S}\rho_+}{\lambda} \right] \right)^2 \times \exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_- - \frac{\rho_-}{\lambda} \right] \right)^2 \hat{K}(Q_+, Q_-) \tag{18}$$

with

$$\hat{K}(Q_+, Q_-) = \int D\nu(a) \int D\varphi_+ \, e^{-(\varphi_+, (i\mathcal{S}\otimes(e\mathbb{1}_N - A)\varphi_+)} \, e^{-(\varphi_+, (i\lambda/N)\mathcal{S}Q_+ \otimes \mathbb{1}_N)\varphi_+)} \times \mathbb{I}_-, \tag{19}$$

where $\mathbb{I}_-$ is the integral over the Grassmannian variables $\{\varphi_{-j}\}$ and is given by

$$\mathbb{I}_- = \int \mathcal{D}\varphi_- \exp[-(\varphi_-, R\varphi_-)], \tag{20}$$

with

$$R := \frac{\lambda}{N}(\Upsilon Q_-) \otimes \mathbb{1}_N + \Upsilon \otimes \left(i(e\mathbb{1}_N - A) + \frac{\lambda^2}{N^2} T \right). \tag{21}$$

The matrix T is defined by (7). In the following section we evaluate the integral $\mathbb{I}_-$ and show that $\hat{K}(Q_+, Q_-)$ depends only on the eigenvalues of the matrices Q_+ and Q_-.

Evaluation of the integral $\mathbb{I}_-$*:* Due to the constraint (17) on the matrix Q_-, the matrix R, defined by (21) is antisymmetric, and we obtain

$$\mathbb{I}_- = \sqrt{\det R}. \tag{22}$$

Moreover, we can show, as follows, that the matrix R depends only on the *eigenvalues* of the matrix Q_-: Defining an $N\times N$ matrix A_1,

$$A_1 := i(e\mathbb{1}_N - A) + \frac{\lambda^2}{N^2} T, \tag{23}$$

we write

$$\det R = \det(\Upsilon \otimes \mathbb{1}_N) \det\left[\frac{\lambda}{N} Q_- \otimes \mathbb{1}_N + \mathbb{1}_{2n} \otimes A_1\right] = \det(\Upsilon \otimes \mathbb{1}_N) \det\left[\frac{\lambda}{N} q_- \otimes \mathbb{1}_N + \mathbb{1}_{2n} \otimes A_1\right] =: \det C, \tag{24}$$

where q_- is the diagonal matrix whose diagonal elements are the eigenvalues of Q_-.

The elements of the matrix C, (24), are given by

$$C(p\alpha, j | p'\alpha', j') = \Upsilon(pp')\left[\frac{\lambda}{N} q_-(\alpha)\delta_{\alpha\alpha'}\,\delta_{jj'} + \delta_{\alpha\alpha'} A_1(jj')\right],$$

where $q_-(\alpha) \equiv q_-(p\alpha)$. This follows from the fact that the eigenvalues of Q_- are doubly degenerate. Hence, the matrix C is *antisymmetric in the label p* and has the form

$$C = \begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix},$$

where D is an $nN \times nN$ matrix defined as follows:

$$D := \frac{\lambda}{N} \tilde{q}_- \otimes \mathbb{1}_N + \mathbb{1}_n \otimes A_1. \tag{25}$$

In (25), $\tilde{q}_-$ denotes an $n \times n$ diagonal matrix with diagonal elements $\tilde{q}_{-\alpha} = q_{1\alpha}$. This leads to the result

$$\mathbb{I}_- = \det D.$$

From (23) and (25) it follows that

$$\det D = \prod_{\alpha=1}^{n} \det\left(\tilde{q}_{-\alpha} \frac{\lambda}{N} \mathbb{1}_N + i(e\mathbb{1}_N - A) + \frac{\lambda^2}{N^2} T\right).$$

For each $\alpha \in \{1, \ldots, n\}$, let us define an $N \times N$ diagonal matrix

$$b_\alpha := \tilde{q}_{-\alpha} \frac{\lambda}{N} \mathbb{1}_N + i(e\mathbb{1}_N - A). \tag{26}$$

In terms of this matrix, we can write

$$\mathbb{I}_- \equiv \det D = \prod_{\alpha} \det b_\alpha \det\left(\mathbb{1}_N + \frac{\lambda^2}{N^2} b_\alpha^{-1} T\right). \tag{27}$$

For each α, let F_α denote a $2n \times 2n$ matrix whose elements are given by

$$F_\alpha(p\gamma | p'\gamma') := \sum_{j=1}^{N} (b_\alpha^{-1})_j \, \varphi_{+j}(p\gamma)\, \varphi_{+j}(p'\gamma').$$

If $\operatorname{tr} A^j = \operatorname{tr} B^j$ for any arbitrary integer j, then

$$\det(\mathbb{1}_n + A) = \det(\mathbb{1}_m + B). \tag{28}$$

Using (28) we have the identity

$$\det\left(\mathbb{1}_N + \frac{\lambda^2}{N^2} b_\alpha^{-1} T\right) = \det\left(\mathbb{1}_{2n} + \frac{\lambda^2}{N^2} \mathcal{S} F_\alpha\right). \tag{29}$$

Hence from (27), (26), and (29) it follows that

$$\mathbb{I}_- = \prod_{j=1}^{N} \det\left(\frac{\lambda}{N}\tilde{q}_- + i(e-a_j)\mathbb{I}_n\right) \prod_{\alpha=1}^{n} \det\left(\mathbb{I}_{2n} + \frac{\lambda^2}{N^2}\mathcal{S}F_\alpha\right), \tag{30}$$

where a_j denotes a diagonal element of the diagonal matrix A. Using the representation of a determinant in terms of a Grassmannian integral, we can write

$$\prod_{\alpha} \det\left(\mathbb{I}_{2n} + \frac{\lambda^2}{N^2}\mathcal{S}F_\alpha\right) = \int D\overline{\Psi}\, D\Psi\, e^{-(\overline{\Psi},\Psi)}\, e^{-(\overline{\Psi},B\Psi)}, \tag{31}$$

where Ψ $(\overline{\Psi})$ is a column (row) vector of length $2n^2$, and

$$(\overline{\Psi},B\Psi) = \sum_{\alpha=1}^{n} \sum_{\beta,\beta'=1}^{2n} \overline{\Psi}_\alpha(\beta) B_\alpha(\beta\beta') \Psi_\alpha(\beta'),$$

where β now refers to the double index $(p\,\gamma)$ and B_α denotes a $2n\times 2n$ matrix whose elements are given by

$$B_\alpha(\beta\beta') = \frac{\lambda^2}{N^2}\mathcal{S}(\beta)\, F_\alpha(\beta\beta'),$$

with $\mathcal{S}(\beta) = s_\gamma$. The relations (30) and (31) yield the following expression for the integral $\mathbb{I}_-$:

$$\mathbb{I}_- = \int D\overline{\Psi}\, D\Psi\, e^{-(\overline{\Psi},\Psi)} \prod_{j=1}^{N} \det\left(\frac{\lambda}{N}\tilde{q}_- + i(e-a_j)\mathbb{I}_n\right)$$
$$\times \exp\left(-\left[\frac{\lambda^2}{N^2}\sum_{j=1}^{N} \sum_{\beta,\beta'=1}^{2n} \varphi_{+j}(\beta)\, \varphi_{+j}(\beta')\, \mathcal{S}_\beta \sum_{\alpha=1}^{n} [b_\alpha^{-1}]_j\, \overline{\Psi}_a(\beta)\, \Psi_a(\beta')\right]\right). \tag{32}$$

We can now insert the representation of $\mathbb{I}_-$, given by (32), in the expression (19) for $\hat{K}$, and perform the integration over φ_+. This yields

$$\hat{K}(Q_+,Q_-) = \int D\overline{\Psi}\, D\Psi\, e^{-(\overline{\Psi},\Psi)} \int D\nu(a) \left[\prod_{j'=1}^{N} \det\left(\frac{\lambda}{N}\tilde{q}_- + i(e-a_{j'})\mathbb{I}_n\right)\right]$$
$$\times \prod_{j=1}^{N} \det\left[\mathcal{S}\left(i(e-a_j)\mathbb{I}_{2n} + i\frac{\lambda}{N}Q_+ + \frac{\lambda^2}{N^2}\mathcal{R}_j\right)\right]^{-(1/2)}, \tag{33}$$

where each R_j is a $2n\times 2n$ matrix with elements

$$\mathcal{R}_j(\beta\beta') = \sum_{\alpha=1}^{n} (b_\alpha^{-1})_j \overline{\Psi}_\alpha(\beta)\, \Psi_\alpha(\beta') = \sum_{\alpha=1}^{n} \left(\frac{\lambda}{N}\tilde{q}_{-\alpha}\mathbb{I}_N + i(e\mathbb{I}_N - A)\right)^{-1}_j \overline{\Psi}_\alpha(\beta)\, \Psi_\alpha(\beta'). \tag{34}$$

From the definition (6) of the measure $D\nu(a)$, it follows that the expression for $\hat{K}(Q_+,Q_-)$ involves a product of N identical integrals and hence can be written in the form

$$\hat{K} = (\det\mathcal{S})^{-N/2} \int D\overline{\chi} D\chi e^{-(\overline{\chi},\chi)} P^N, \tag{35}$$

where

$$P := \int da\ \nu(a) \det\left(\frac{\lambda}{N}\tilde{q}_- + i(e-a)\mathbb{1}_n\right) \det\left[i(e-a)\mathbb{1}_{2n} + i\frac{\lambda}{N}q_+ + \frac{\lambda^2}{N^2}\mathcal{R}\right]^{-1/2}, \tag{36}$$

with

$$\mathcal{R}(\beta\beta') = \sum_{\alpha=1}^{n}\left(\frac{\lambda}{N}\tilde{q}_{-\alpha} + i(e-a)\right)^{-1} \overline{\chi}_\alpha(\beta)\,\chi_\alpha(\beta'). \tag{37}$$

Using the degeneracy of the eigenvalues of α_- we can rewrite P as

$$P = \int da\ \nu(a)\left[\frac{\det X_-}{\det X_+}\right]^{1/2} \det\left(\mathbb{1}_n + \frac{\lambda^2}{N^2}\frac{M(X_+)}{x_-}\right)^{1/2}, \tag{38}$$

where M is the

$$M_{\alpha_1\alpha_2}(q_+) = \sum_{p=1}^{2}\sum_{\gamma=1}^{n}\frac{\chi_{\alpha_1}(p\gamma)\,\overline{\chi}_{\alpha_2}(p\gamma)}{X_+(p\gamma)},$$

and x_- is a diagonal $n\times n$ matrix of elements $x_-(\gamma)$.

Hence, the generating function in the orthogonal case, for finite matrix size, is given by

$$J^S = \frac{(\det\mathcal{S})^{N/2}}{d_+\,d_-}\int DQ_+ \int DQ_- \exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_+ + i\frac{\mathcal{S}\rho_+}{\lambda}\right]\right)^2 \times \exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_- - \frac{\rho_-}{\lambda}\right]\right)^2 \hat{K}(Q_+, Q_-), \tag{39}$$

where

$$\hat{K} = (\det\mathcal{S})^{-N/2}\int D\overline{\chi}D\chi e^{-(\overline{\chi},\chi)}P^N,$$

and P is given by (38).

B. The unitary case for finite matrix size

When the Hamiltonian matrix (4),

$$H = A + \frac{\lambda}{N}G,$$

is such that G belongs to the Gaussian unitary ensemble (GUE), we arrive at an analogous expression for the generating function. There is now no necessity to double the dimension of the matrices so as to accommodate the real variables as we did in the GOE case. Proceeding exactly as before, we arrive at the following expression of the generating function:

$$J^S = \frac{1}{d_+\,d_-}\int DQ_+ \int DQ_- \exp\left(-\frac{1}{2}\mathrm{tr}\left(Q_+ + \frac{iS\rho_+}{\lambda}\right)^2\right) \quad \exp\left(-\frac{1}{2}\mathrm{tr}\left(Q_- - \frac{\rho_-}{\lambda}\right)^2\right)\tilde{K}(q_+, q_-), \tag{40}$$

where

$$\tilde{K} = \int D\overline{\chi}D\chi e^{-(\overline{\chi},\chi)}P^N.$$

Q_- is now simply an $n\times n$ self-adjoint matrix. The $n\times n$ matrix Q_+ has the same block structure as before, but now Q_{ii} with $i=1,2$ are self-adjoint matrices and $Q_{12}=Q_{21}^{\dagger}$. Here $\overline{\chi},\chi$ are Grassmannian vectors of length n, and P is given by

$$P:=\int da\ \nu(a)\left[\frac{\det X_-}{\det X_+}\right]\det\left(\mathbb{1}_n+\frac{\lambda^2}{N^2}\frac{M(X_+)}{X_-}\right), \tag{41}$$

where

$$M_{\alpha_1\alpha_2}=\sum_{\gamma=1}^{n}\frac{\chi_{\alpha_1}(\gamma)\,\overline{\chi}_{\alpha_2}(\gamma')}{X_+(\gamma)},$$

and $X_\pm$ are diagonal $n\times n$ matrices with diagonal elements

$$x_+(\gamma):=i(e-a)+i\frac{\lambda}{N}q_+(\gamma), \tag{42}$$

$$x_-(\gamma):=i(e-a)+\frac{\lambda}{N}q_-(\gamma), \tag{43}$$

respectively.

The above relations, (40)–(41), for the GUE, are found to be very similar in form to the corresponding relations (18)–(38) for the GOE. The only difference lies in the fact that the expression for P involves *square roots* of determinants for the GOE [see (38)], whereas there is no square root appearing in the corresponding relation (41), in the case of the GUE.

C. The orthogonal and unitary case in the limit of infinite matrix size

We will now evaluate the generating function in the limit $N\to\infty$, from which the correlation functions can be obtained by taking various derivatives with respect to the variables $\varepsilon_-(\alpha)$. It can be easily shown that there is no problem in the interchange of the limit $N\to\infty$, with the derivation with respect to ε_-, and the subsequent limit $\varepsilon_-=\varepsilon_+\to 0$.

The result for the generating function both in the orthogonal ($\beta=1$) and the unitary case ($\beta=2$) can be put in the following form:

$$J^S=\frac{\exp\left(\frac{ip\beta}{2}\mathrm{tr}(\varepsilon_--\varepsilon_+)S\right)}{d_+d_-}\int DQ_+Dq_-D\overline{\chi}D\chi\exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_++\frac{i\rho_+S}{\lambda}-\frac{\beta\lambda p}{2}\right]^2\right)$$
$$\times\exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_--\frac{\rho_-}{\lambda}-\frac{i\beta\lambda p}{2}\right]^2-(\overline{\chi},\chi)\right)\exp\left(\lambda\nu(e)\left[\frac{\beta A_o}{2}+A_1^\beta+A_2^\beta\right]\right). \tag{44}$$

Here $\varepsilon_\pm$ are $n\times n$ matrices with diagonal elements $\varepsilon_\pm(\alpha)$, and

$$p=p(e)=\mathbb{P}\int da\frac{\nu(a)}{a-e},$$

with the symbol $\mathbb{P}$ denoting the principal value of the integral. The matrix A_0 is given by

$$A_0=i\pi\,\mathrm{tr}(q_++iq_-)\sigma(q_+),$$

where $\sigma(q_+)$ is the diagonal matrix whose elements are the signs of the imaginary parts of the eigenvalues $q_+(p\gamma)$ of the matrix Q_+,

$$A_1^\beta = \int_{-\infty}^{+\infty} dt \left\{ \left(\frac{\det(t - iq_-)}{\det(t + q_+)} \right)^{\beta/2} - \left[1 - \frac{\beta}{2} \operatorname{tr} \frac{q_+ + iq_-}{t + q_+} \right] \right\}$$

and

$$A_2^\beta = \int_{-\infty}^{+\infty} dt \left(\frac{\det(t - iq_-)}{\det(t + q_+)} \right)^{\beta/2} [\det(1 - R^\beta)^{\beta/2} - 1], \tag{45}$$

where

$$R^1_{\alpha\alpha'} = \frac{1}{t - iq_-(\alpha)} \sum_{p=1}^{2} \sum_{\gamma=1}^{n} \frac{\overline{\chi}_\alpha(p\gamma)\chi_{\alpha'}(p\gamma)}{t + q_+(p\gamma)}$$

and

$$R^2_{\alpha\alpha'} = \frac{1}{t - iq_-(\alpha)} \sum_{\gamma=1}^{n} \frac{\overline{\chi}_\alpha(\gamma)\chi_{\alpha'}(\gamma)}{t + q_+(\gamma)}.$$

This is the main result of this paper. We have expressed the generating function for the correlation functions in terms of a finite set of integrals. Hence we have reduced the problem of the computation of the generating function, in the limit of infinite matrix size, to that of the evaluation of a finite set of integrals. This was our main purpose, since, starting from this explicit expression, we can proceed to evaluate the physically relevant correlation functions. However, as we shall see, the task of evaluating these integrals is nontrivial. Nevertheless, a general conclusion can be drawn from this expression by noting that the generating function has the following structure:

$$J^S = \exp\left(\frac{ip\beta}{2} \operatorname{tr}[(\varepsilon_- - \varepsilon_+)S] \right) K^S\left(\nu\varepsilon_-, \nu\varepsilon_+, \left\{ \nu r_\alpha + \frac{\lambda^2 \beta \nu p}{2} \right\}, \Lambda \right),$$

where $\Lambda = \lambda\, \nu(e)$, can be called the *renormalized coupling constant*.

Since the correlation functions can be computed from the generating function by using the formula

$$\left(\frac{1}{2\pi} \right)^n \prod_{\alpha=1}^{n} \frac{\partial}{\partial \varepsilon_-(\alpha)} J^{(1_n, -1_n)} \Big|_{\varepsilon_- = \varepsilon_+ = 0} = \rho^{(n)}(r_1, \ldots, r_n),$$

where

$$J^{(1_n, -1_n)} = \left\langle \prod_{\alpha=1}^{n} \frac{\det[\varepsilon_-^2(\alpha) + (e_\alpha - H)^2]}{\det[\varepsilon_+^2(\alpha) + (e_\alpha - H)^2]} \right\rangle,$$

is positive, it follows that

$$J^{(1_n, -1_n)} = |K^{(1_n, -1_n)}|,$$

and therefore $\rho^{(n)}$ has the structure

$$\rho^{(n)}(r_1, \ldots, r_n) = \nu^n f_\beta^{(n)}(r_1\nu + a, r_2\nu + a, \ldots, r_n\nu + a; \Lambda), \tag{46}$$

with $a = \lambda^2\beta/2$. However, since the correlation functions are translation invariant, the RHS of (46) does not depend on a.

We shall prove that the density of states $\rho(e)$ is equal to $\nu(e)$. We can therefore conclude that, *on the scale of energy where the mean level spacing is equal to unity*, the correlation functions are *universal*, i.e., they depend only on β and Λ. More precisely,

$$\left[\frac{1}{\rho(e)}\right]^n \rho^{(n)}\left(\frac{r_1}{\rho(e)},\ldots,\frac{r_n}{\rho(e)}\right)=f_\beta^{(n)}(r_1,r_2,\ldots,r_n;\Lambda).$$

Let us now derive Eq. (44). We start with the expressions for the generating functions J^S for the orthogonal [(39)] and unitary [(40)] cases. The integrals (38) and (41) which occur in these expressions can be written in the form of a single integral:

$$P=\int da\ \nu(a)\left(\frac{\det X_-}{\det X_+}\right)^{\beta/2}\left(\det\left[\mathbb{1}+\frac{\lambda^2 M(X_+)}{N^2 X_-}\right]\right)^{\beta/2}.$$

We decompose this into three terms, i.e., $P=P_0+P_1+P_2$, where

$$P_0:=1+\frac{\beta}{2}\int da\ \nu(a)\ \mathrm{tr}\frac{X_- - X_+}{X_+},$$

$$P_1:=\int da\ \nu(a)\left\{\left(\frac{\det X_-}{\det X_+}\right)^{\beta/2}-\left[1+\frac{\beta}{2}\mathrm{tr}\frac{X_- - X_+}{X_+}\right]\right\}$$

and

$$P_2:=\int da\ \nu(a)\left(\frac{\det X_-}{\det X_+}\right)^{\beta/2}\left\{\left[\det\left(1+\frac{\lambda^2 M(X_+)}{N^2 X_-}\right)\right]^{\beta/2}-1\right\}.$$

Let us first evaluate P_0 in the large-N limit,

$$\int da\ \nu(a)\mathrm{tr}\frac{X_- - X_+}{X_+}=-\frac{\lambda}{N}\int da\ \nu(a)\mathrm{tr}\left[(q_+ + iq_-)\left((e-a)\mathbb{1}_{2n}+\frac{\lambda}{N}q_+\right)^{-1}\right]. \tag{47}$$

Since $\mathrm{Im}\, q_+(\gamma)\neq 0$, the integral on the RHS of (47) tends to the expression

$$-p(e)-i\pi\nu(e)\sigma_+(p\gamma)$$

as $N\to\infty$, where $\sigma_+(p\gamma)$ denotes the sign of the imaginary part of the eigenvalue $q_+(p\gamma)$.

Hence, for large N,

$$P_0=1+\frac{\lambda}{N}\frac{\beta}{2}[p\ \mathrm{tr}(q_+ + iq_-)+i\pi\nu\ \mathrm{tr}(q_+ + iq_-)\sigma(q_+)],$$

where $\sigma(q_+)$ is the diagonal matrix with elements $\sigma_+(p\gamma)$. In the second term, P_1, we make the change of variables $e-a=t\lambda/N$, so that it reads

$$P_1=\frac{\lambda}{N}\int_{-\infty}^{+\infty}dt\ \nu(e-t\lambda/N)\left\{\left(\frac{\det(t-iq_-)}{\det(t+q_+)}\right)^{\beta/2}-\left[1-\frac{\beta}{2}\mathrm{tr}\frac{q_+ + iq_-}{t+q_+}\right]\right\}.$$

The term in parentheses is bounded in t and decays like $1/t^2$ when t is large, since $\mathrm{Im}\, q_+(\gamma)\neq 0$. Hence, we can use the dominated convergence theorem[23] to show that if

$$\sup_t \nu(t)<\infty,$$

and $\nu(t)$ is continuous, then for large N,

$$P_1=\frac{\lambda\nu(e)}{N}A_1^\beta.$$

The term P_2 is treated in exactly the same way as P_1, so that asymptotically,

$$P_2=\frac{\lambda\nu(e)}{N}A_2^\beta.$$

Finally,

$$\lim_{N\to\infty}P^N=\exp\left(\frac{\lambda\beta p}{2}\mathrm{tr}(Q_+ + iQ_-)+\lambda\nu\left[\frac{\beta}{2}A_0+A_1^\beta+A_2^\beta\right]\right). \tag{48}$$

Here and henceforth, we write ν for $\nu(e)$. Expression (44) for the generating function, J^S, in the limit of infinite matrix size, is obtained by substituting (48) in expressions (39) and (40) and completing the squares in Q_+ and Q_-.

III. THE DENSITY OF STATES AND THE AVERAGE OF THE PRODUCT OF TRACES OF ADVANCED GREEN'S FUNCTIONS

The only computation which is easy in the general case, is that of the generating function for traces of advanced Green's functions. This corresponds to the choice $s_\alpha=1$ for all $\alpha\in\{1,...,n\}$.

Let $q_\pm(j)$ denote the eigenvalues of the matrices $Q_\pm$. For the above-mentioned choice of the matrix S, we know that $q_+(j)=q'_+(j)-i\delta$, where $q'_+(j)$ is real and δ is positive. Since $q_-(j)$ is also real (and doubly degenerate in the $\beta=1$ case) we see that the integrands in the expressions for A_1^β and A_2^β are analytic in the variable t in the lower half-plane, and decay like $1/t^2$. We can therefore apply Cauchy's theorem to simply conclude that $A_1^\beta=A_2^\beta=0$. In contrast, if we computed these quantities for the case of a mixed product of advanced and retarded Green's functions ($s_\alpha=1, \alpha=1,...,p, s_\alpha=-1, \alpha=p+1,\ldots,n$), there would be $n-p$ singularities in the lower half-plane, and, therefore, A_1^β and A_2^β would be nonzero.

Hence, it follows easily from (44) that the generating function factorizes as follows:

$$J^{1_n}=\exp\left(i(p+i\pi\nu)\sum_{\alpha=1}^{n}[\varepsilon_-(\alpha)-\varepsilon_+(\alpha)]\right)J_+J_-,$$

where

$$J_+=\frac{1}{d_+}\int DQ_+\exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_+ + \frac{i\rho_+ S}{\lambda}-\frac{\beta\lambda}{2}(p+i\pi\nu)\right]^2\right),$$

and

$$J_-=\frac{1}{d_-}\int DQ_-\exp\left(-\frac{1}{2}\mathrm{tr}\left[Q_- - \frac{\rho_-}{\lambda}-\frac{i\beta\lambda}{2}(p+i\pi\nu)\right]^2\right).$$

Hence, we see from the definitions of $d_\pm$ [(15)] that $J_\pm=1$ and

$$J^{1_n}=\exp\left(i(p+i\pi\nu)\sum_{\alpha=1}^{n}[\varepsilon_-(\alpha)-\varepsilon_+(\alpha)]\right).$$

This implies that

$$\lim_{N\to\infty}\left\langle \prod_{\alpha=1}^{n}\frac{1}{N}\operatorname{tr} G^{+}_{e_\alpha}\right\rangle = [-p-i\pi\nu]^n,$$

which in turn shows that average of a product of the traces of advanced (or retarded) Green's functions factorize. In particular, we see that the density of states, $\rho(e)$, is simply given by

$$\rho(e)=\nu(e).$$

IV. UNITARY CASE: THE TWO-POINT GENERATING FUNCTION

There is one major simplification in the unitary case. The integral defining A_2 [(45)] can be explicitly evaluated and gives a *meromorphic* function of the eigenvalues $\{q_{-j}\}$ and $\{q_{+j}\}$ of the matrices Q_- and Q_+, respectively. We first integrate over the Grassmannian variables $\{\chi_j^\alpha, \overline{\chi}_j^\alpha\}$, then over Q_- and finally over Q_+. After a rather lengthy computation we find that the generating function can be expressed as

$$J^{+-}=\frac{4i}{\pi v t}\exp\left[uy+\frac{1}{2\lambda^2}\operatorname{tr}(\rho_+^2-\rho_-^2)\right]\partial_t R, \tag{49}$$

where R is

$$R=\sum_{j=-1}^{4}\alpha_j B_j, \tag{50}$$

$$u=\frac{1}{2i\lambda}\operatorname{tr}(\rho_- -\rho_+ s), \tag{51}$$

$$y=-2\lambda p-\frac{1}{2i\lambda}[\operatorname{tr}\rho_- +\operatorname{tr}(\rho_+ s)], \tag{52}$$

$$t=\frac{1}{\lambda}\operatorname{tr}(\rho_- s), \tag{53}$$

$$v=\frac{\operatorname{tr}\rho_+}{\lambda}, \tag{54}$$

and

$$B_n=\int_{\operatorname{Im} w=-c} dw\, w^{-n}\exp\left[-w^2-iw(v+\Lambda)-\frac{i\Lambda u^2}{w}\right]\int_{-\infty}^{+\infty}dz\exp\left[-z^2\left(1+\frac{i\Lambda}{w}\right)-tz\right], \tag{55}$$

with c being an arbitrary constant larger than Λ. The coefficients α_j are given by

$$\alpha_{-1}==1,\ \alpha_0=2i\Lambda,\ \alpha_1=-\frac{13}{4}\Lambda^2-\frac{v\Lambda}{2},$$

$$\alpha_2=-\frac{3}{2}i\Lambda^3+\frac{i\Lambda}{2}-\frac{3}{4}v\Lambda^2,\ \alpha_3=\frac{\Lambda^4}{4}-\frac{7}{8}\Lambda^2+\frac{v\Lambda^3}{4}+\frac{v^2}{16}\Lambda^2+u^2\Lambda^2,$$

$$\alpha_4=iu^2\Lambda^3-\frac{3}{8}i\Lambda^3,\ \alpha_5=-\frac{u^2}{4}\Lambda^4. \tag{56}$$

Using the recursion formula

$$\partial_t B_n = \frac{t}{2} B_n - i\Lambda \partial_t B_{n+1} \tag{57}$$

we can express the generating function in terms of the B_n for $n \in \{-1,4\}$ and $\partial_t B_5$. One can also show that the B_n can be represented as an integral over the modified Bessel functions.

Once we have this expression for the generating function, we can also compute the two-point correlation function. One finds that it is given [as in Ref. 24] by a sum of integrals over modified Bessel functions. Details of this computation can be found in Ref. 25.

V. ORTHOGONAL CASE: THE TWO-POINT GENERATING FUNCTION

We start from the equation

$$\rho^{(2)}(r_1,r_2) = \frac{1}{2\pi^2} \mathrm{Re}\left\{ \frac{\partial^2 [J_2^{+-} + J_2^{++}]}{\partial \varepsilon_-(1)\, \partial \varepsilon_-(2)} \bigg|_{\varepsilon_- = \varepsilon_+ = 0} \right\}, \tag{58}$$

in order to compute the correlation function $\rho^{(2)}(e_1,e_2)$. Using the fact (established in Sec. III) that

$$J^{+-}|_{\varepsilon_- = \varepsilon_+} = 1, \tag{59}$$

$$\frac{\partial J^{+-}}{\partial \varepsilon_-(1)} = \pi\nu + ip, \tag{60}$$

$$\frac{\partial J^{+-}}{\partial \varepsilon_-(2)} = \pi\nu - ip, \tag{61}$$

$$\frac{\partial^2 J^{++}}{\partial \varepsilon_-(1)\varepsilon_-(2)} \bigg|_{\varepsilon_- = \varepsilon_+ = 0} = (\pi\nu + ip)^2, \tag{62}$$

we can express $\rho^{(2)}(r_1,r_2)$ as

$$\begin{aligned} \rho^{(2)}(r_1,r_2) = &- \frac{1}{\lambda^2\pi^2} p(r_1+r_2) - \frac{2}{\pi^2\lambda^4} r_1 r_2 + \frac{1}{2}\nu^2 - \frac{p^2}{2\pi^2} \\ &- \frac{1}{2d_+ d_- \lambda^2 \pi^2} \int DQ_+ DQ_- \prod_{\alpha=1}^{2} [Q_-(1\alpha|1\alpha) + Q_-(2\alpha|2\alpha)] \\ &\times \exp\left(-\frac{1}{2} \mathrm{tr} \left[\left(Q_- - \frac{\rho_-}{\lambda} - i\beta p \lambda \right)^2 + \left(Q_+ + \frac{i\rho_+ S}{\lambda} - \frac{\beta p \lambda}{2} \right)^2 \right] \right) \times K(q_+,q_-), \end{aligned} \tag{63}$$

where

$$K(q_+,q_-) = \int D\overline{\chi} D\chi \exp(-(\overline{\chi},\chi)) \exp\left(\lambda \nu(e) \left[\frac{1}{2} A_0 + A_1 + A_2 \right] \right);$$

with

$$A_0 = i\pi \,\mathrm{tr}[(q_+ + iq_-)\sigma(q_+)],$$

$$A_1 = \int_{-\infty}^{+\infty} dt\,[\Delta(t)]^{1/2}\left[1 - \frac{1}{2}\sum_{p=1}^{2}\sum_{\gamma=1}^{2}\frac{q_+(p\gamma)+iq_-(\gamma)}{t+q_+(p\gamma)}\right],$$

$$A_2 = \int_{-\infty}^{+\infty} dt\,[\Delta(t)]^{1/2}[\det(\mathbb{1}_2 - R)^{1/2} - 1],$$

and

$$\Delta(t) = \frac{(t-iq_-(1))^2\,(t-iq_-(2))^2}{\prod_{p=1}^{2}\prod_{\gamma=1}^{2}(t+q_+(p\gamma))}.$$

The 2×2 matrix R is given by

$$R_{\alpha\alpha'} = \frac{1}{t-iq_-(\alpha)}\sum_{p=1}^{2}\sum_{\gamma=1}^{2}\frac{\overline{\chi}_\alpha(p\gamma)\chi_{\alpha'}(p\gamma)}{t+q_+(p\gamma)}.$$

We recall that $q_+(p\gamma)$ and $q_-(\gamma)$ are the eigenvalues of Q_+ and Q_-. Two eigenvalues of Q_+ have a positive imaginary part. The other two have a negative imaginary part.

A_1 can be expressed in terms of elliptic integrals. The same is true for A_2, once we note that

$$\det(\mathbb{1}_2 - R) = 1 - X \quad \text{with} \quad X = \mathrm{tr}\,R - \det R,$$

so that

$$\det(\mathbb{1}_2 - R)^{1/2} - 1 = \sum_{n=1}^{8} X^n c_n,$$

since the X are Grassmannian variables [c_n are constants]. One can then integrate over the Grassmannian variables, to compute K. We will not reproduce this computation here, since we have not analyzed the resulting expression for the correlation function. It can finally be noted that for higher order correlation functions, hyperelliptic integrals appear.

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Time dependent transformations in deformation quantization

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We study the action of time dependent canonical and coordinate transformations in phase space quantum mechanics. We extend the covariant formulation of the theory by providing a formalism that is fully invariant under both standard and time dependent coordinate transformations. This result considerably enlarges the set of possible phase space representations of quantum mechanics and makes it possible to construct a causal representation for the distributional sector of Wigner quantum mechanics. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1641152]

I. INTRODUCTION

The phase space formulation of quantum mechanics was originally introduced by Weyl[1] and Wigner[2] and further developed by Moyal.[3] The theory lives on the classical phase space and its key algebraic structures (the star-product and the Moyal bracket) are both $\hbar$-deformations of the standard algebraic structures of classical mechanics.[4–11] Because of this its mathematical formalism is remarkably similar to that of classical statistical mechanics, a property that has been perceived by many as a conceptual and technical advantage when addressing a wide range of specific problems.[11–17] This relative success, together with the fact that the deformed algebraic structures play a key part in some current developments in M-theory,[18–21] led to an intense research on applications of the deformation quantization approach as well as on the further development of its mathematical structure.

The Wigner theory uses the symmetric ordering prescription (the Weyl order) to find a particular phase space representation of quantum mechanics. Different representations provide different points of view and may suggest new solutions for both technical and conceptual problems. They may even suggest new interpretations for the entire quantum theory, as in the case of the de Broglie Bohm formulation. For its importance, the topic of finding new, more general phase space representations of quantum mechanics has been studied in depth. Cohen[22] introduced a generalization of the Weyl map, providing in an unified fashion all phase space representations that correspond to different ordering prescriptions of operator quantum mechanics. The resulting theory of quasidistributions includes as particular cases the Wigner and the de Broglie Bohm[23,24] formulations. Vey[25] and several others,[8,11,26–30] developed the covariant generalization of Wigner's theory. The new formulation renders phase space quantum mechanics fully invariant under the action of phase space coordinate transformations. By doing so it provides a general formula for the $\hbar$-deformations of the Poisson bracket and makes it possible to apply deformation quantization methods to a larger set of dynamical systems including those displaying the structure of a curved phase space manifold.

The aim of this article is to extend the covariant formulation further by admitting the possibility of time dependent coordinate transformations. We will study the action of these transformations in phase space quantum mechanics and rewrite the covariant Wigner theory in a fully invariant form under their action. We derive the time dependent covariant form of the starproduct,

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Moyal bracket, Moyal dynamical equation and stargenvalue equation as well as the covariant probabilistic functionals, providing all key ingredients of the time dependent covariant formulation of Wigner quantum mechanics. This result enlarges the set of possible phase space representations of quantum mechanics and provides a more general formula for the $\hbar$-deformations of the Poisson bracket, which may now include an explicit time dependence.

The new set of representations provides new possible formulations for a generic quantum mechanical problem. In some cases this may considerably simplify the technical resolution of the problem. In Sec. VI a simple example illustrates how a suitable time dependent representation leads to a far simpler description of the dynamics of the quasidistribution. More relevant is the fact that the new formalism makes it possible to construct a phase space representation of quantum mechanics where the quasidistribution displays a classical causal structure, i.e., the Wigner function evolves according to the Liouville equation. A formulation displaying this set of properties cannot be (easily) accomplished using the standard methods of quantum mechanics (not even within the standard covariant Wigner formalism) and it proves that the de Broglie Bohm theory is not the unique possible causal formulation of quantum mechanics. In the new causal representation the quantum dynamical behavior is completely removed from the distributional sector of the theory and is exclusively placed on the observables' sector. In particular, if the quasidistribution is positive defined at the initial time, it will remain so for all times. These properties reinforce the formal analogy between phase space quantum mechanics and classical statistical mechanics and make the causal formulation especially suitable to study the semiclassical limit of quantum mechanics.

This article is organized as follows: in Sec. II we review the main topics of the covariant formulation of the Wigner theory. In Sec. III we study the action of time dependent canonical transformations in standard operator quantum mechanics. Particular attention is devoted to the behavior of the density matrix. In Sec. IV we derive the time dependent covariant formulation of Wigner quantum mechanics. In Sec. V a particular set of coordinates is used to obtain the causal phase space representation. In Sec. VI a simple example illustrates some of the former results and in Sec. VII we present the conclusions.

II. COVARIANT WIGNER QUANTUM MECHANICS

Let us consider an N dimensional dynamical system. Its classical formulation lives on the phase space T^*M which, to make it simple, we assume to be flat. A global Darboux chart can then be naturally defined on T^*M, for which the symplectic structure reads $w=dq_i\wedge dp_i$, where $\{q_i,p_i,i=1,...,N\}$ is a set of canonical variables.

Upon quantization the set $\{\hat{q}_i\}$ yields a complete set of commuting observables. Let then $\hat{A}(\hat{\vec{q}},\hat{\vec{p}})$ be a generic operator acting on the physical Hilbert space $\mathcal{H}$. The Weyl map

$$W_{(q,p)}(\hat{A})=\hbar^N\int d^N\vec{y}e^{-i\vec{p}\cdot\vec{y}}\left\langle \vec{q}+\frac{\hbar}{2}\vec{y}\left|\hat{A}\right|\vec{q}-\frac{\hbar}{2}\vec{y}\right\rangle, \tag{1}$$

where we introduced the vector notation $\vec{y}\equiv(y_1,\ldots,y_N)$ and $|\vec{q}\pm\hbar/2\vec{y}\rangle$ are eigenstates of $\hat{\vec{q}}$, provides a Lie algebra isomorphism between the algebra $\hat{\mathcal{A}}(\mathcal{H})$ of linear operators acting on the Hilbert space $\mathcal{H}$ and the algebra of phase space functions $\mathcal{A}(T^*M)$ endowed with a $*$-product and Moyal bracket [let $A,B\in\mathcal{A}(T^*M)$]:

$$A*_{(q,p)}B=Ae^{(i\hbar/2)\overleftarrow{\partial}_k J^{kl}_{(q,p)}\overrightarrow{\partial}_l}B,\quad [A,B]_{M_{(q,p)}}=\frac{2}{\hbar}A\sin\left(\frac{\hbar}{2}\overleftarrow{\partial}_k J^{kl}_{(q,p)}\overrightarrow{\partial}_l\right)B, \tag{2}$$

where the derivatives $\overleftarrow{\partial}$ and $\overrightarrow{\partial}$ act on A and B, respectively, and $J^{kl}_{(q,p)}$ is the klth element of the symplectic matrix in the variables $(\vec{q},\vec{p})$:

$$J_{(q,p)}=\begin{pmatrix} 0_{N\times N} & -1_{N\times N} \\ 1_{N\times N} & 0_{N\times N} \end{pmatrix}. \tag{3}$$

We also introduced the compact notation: $O^k=p_k, k=1,\ldots,N$; $O^k=q_{k-N}, k=N+1,\ldots,2N$; $\partial/\partial O^k=\partial_k$ and sum over repeated indices is understood.

We now consider a second set of fundamental operators $(\hat{\vec{Q}},\hat{\vec{P}})$ unitarily related to $(\hat{\vec{q}},\hat{\vec{p}})$, i.e., $\hat{\vec{q}}=\hat{U}\hat{\vec{Q}}\hat{U}^{-1}$ and $\hat{\vec{p}}=\hat{U}\hat{\vec{P}}\hat{U}^{-1}$ where $\hat{U}$ is some unitary operator. The new operators satisfy the Heisenberg commutation relations, yield a new Weyl map $W_{(Q,P)}$ and induce a phase space transformation $(\vec{q},\vec{p})\rightarrow(\vec{Q},\vec{P})$ acting on a generic observable through the procedure (let $U=W_{(Q,P)}(\hat{U})$):

$$A(\vec{q},\vec{p})=W_{(q,p)}(\hat{A})\rightarrow A'(\vec{Q},\vec{P})=W_{(Q,P)}(\hat{A})=U*_{(Q,P)}A(\vec{Q},\vec{P})*_{(Q,P)}U^{-1}\quad . \tag{4}$$

The phase space implementation of the unitary transformation preserves the starproduct and the Moyal bracket but, as is well known, it does not act as a coordinate transformation (the exceptions are the linear transformations): let $\vec{q}(\vec{Q},\vec{P})=W_{(Q,P)}(\hat{q})$ and $\vec{p}(\vec{Q},\vec{P})=W_{(Q,P)}(\hat{p})$ and we find that in general $A'(\vec{Q},\vec{P})\neq A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))$. We conclude that the standard Wigner formulation is non-covariant.

We now introduce the generalized Weyl map.[8] Let the transformation $(\vec{q},\vec{p})\rightarrow(\vec{Q},\vec{P})$ be a phase space diffeomorphism defined, in general terms, by $\vec{q}=\vec{q}(\vec{Q},\vec{P})$ and $\vec{p}=\vec{p}(\vec{Q},\vec{P})$. In particular, the transformation of the canonical variables $(\vec{q},\vec{p})$ might be given by the unitary transformation above, but this is not required. The generalized Weyl map is then defined by[8]

$$W^{(q,p)}_{(Q,P)}(\hat{A})=\hbar^N\int d^N\vec{x}\int d^N\vec{y}\, e^{-i\vec{p}(\vec{Q},\vec{P})\cdot\vec{y}}\delta(\vec{x}-\vec{q}(\vec{Q},\vec{P}))\left\langle \vec{x}+\frac{\hbar}{2}\vec{y}\right|\hat{A}\left|\vec{x}-\frac{\hbar}{2}\vec{y}\right\rangle, \tag{5}$$

where $|\vec{x}\pm\hbar/2\vec{y}\rangle$ are eigenstates of $\hat{\vec{q}}$. The new map implements the transformation $(\vec{q},\vec{p})\rightarrow(\vec{Q},\vec{P})$ as a coordinate transformation in quantum phase space; let $A'(\vec{Q},\vec{P})=W^{(q,p)}_{(Q,P)}(\hat{A})$ and $A(\vec{q},\vec{p})=W_{(q,p)}(\hat{A})$ and we have $A'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))$, though in general it does not preserve the functional form of the star-product and Moyal bracket. Instead it yields the more general covariant star-product and Moyal bracket:[8,11]

$$\begin{aligned} A'(\vec{Q},\vec{P})*'_{(Q,P)}B'(\vec{Q},\vec{P})&=A'(\vec{Q},\vec{P})e^{(i\hbar/2)\vec{\nabla}'_iJ'^{ij}_{(Q,P)}\vec{\nabla}'_j}B'(\vec{Q},\vec{P}),\\ [A'(\vec{Q},\vec{P}),B'(\vec{Q},\vec{P})]_{M'_{(Q,P)}}&=\frac{2}{\hbar}A'(\vec{Q},\vec{P})\sin\left(\frac{\hbar}{2}\vec{\nabla}'_iJ'^{ij}_{(Q,P)}\vec{\nabla}'_j\right)B'(\vec{Q},\vec{P}), \end{aligned} \tag{6}$$

where the covariant derivative is given by (let $O'^i=P_i, i=1,\ldots,N$; $O'^i=Q_{i-N}, i=N+1,\ldots,2N$)

$$\nabla'_iA'=\partial'_iA',\quad \nabla'_i\nabla'_jA'=\partial'_i\partial'_jA'-\Gamma'^k_{ij}\partial'_kA',\quad \partial'_i=\partial/\partial O'^i,\quad i,j,k=1,\ldots,2N, \tag{7}$$

and

$$J'^{ij}_{(Q,P)}(\vec{Q},\vec{P})=\frac{\partial O'^i}{\partial O^k}\frac{\partial O'^j}{\partial O^l}J^{kl}_{(q,p)},\quad \Gamma'^i_{jk}(\vec{Q},\vec{P})=\frac{\partial O'^i}{\partial O^b}\frac{\partial^2O^b}{\partial O'^j\partial O'^k} \tag{8}$$

are the new symplectic structure and Poisson connection associated to the coordinates $(\vec{Q},\vec{P})$. Notice that in Eq. (8) we explicitly took into account the phase space flat structure.

When formulated in terms of these structures Wigner mechanics becomes invariant under the action of general coordinate transformations:

$$A'(\vec{Q},\vec{P})*'_{(Q,P)}B'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))*_{(q,p)}B(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) \quad \forall_{A,B\in\mathcal{A}(T*M)}, \tag{9}$$

the covariant generalization of the Moyal and stargenvalue equations reading

$$\begin{gathered}\dot{f}'_W=[H',f'_W]_{M'_{(Q,P)}},\\ A'*'_{(Q,P)}g'_a=g'_a*'_{(Q,P)}A'=ag'_a,\end{gathered} \tag{10}$$

where $f'_W(\vec{Q},\vec{P};t)=(1/(2\pi\hbar)^N)\,W^{(q,p)}_{(Q,P)}(|\psi(t)\rangle\langle\psi(t)|)$ is the covariant Wigner function and g'_a is the left- and right-stargenfunction associated to the eigenvalue a.

These equations transform covariantly under arbitrary phase space diffeomorphisms yielding, in any coordinates, identical mathematical solutions and thus identical physical predictions:

$$P(A'(\vec{Q},\vec{P};t)=a)=\int d^N\vec{Q}\int d^N\vec{P}(\det J'^{ij}_{(Q,P)})^{-1/2}\delta_{*'_{(Q,P)}}(A'(\vec{Q},\vec{P})-a)f'_W(\vec{Q},\vec{P};t), \tag{11}$$

where $\delta_{*'_{(Q,P)}}(A'-a)$ is a particular solution of (10), displaying the following explicit form:[9,11]

$$\delta_{*'_{(Q,P)}}(A'(\vec{Q},\vec{P})-a)=\frac{1}{2\pi}\int dk\ \ e^{ik(A'(\vec{Q},\vec{P})-a)}_{*'_{(Q,P)}}, \tag{12}$$

the $*$-exponential being given by $e^{A'}_{*'_{(Q,P)}}=\Sigma_{n=0}^{\infty}(1/n!)\,\Omega_n$ where $\Omega_0=1$ and $\Omega_{n+1}=\Omega_n*'_{(Q,P)}A'$.

This concludes our review of the main topics of the covariant formulation of Wigner quantum mechanics. The reader should refer to Refs. 8 and 11 for more detailed presentations of the theory.

III. TIME DEPENDENT CANONICAL TRANSFORMATIONS

The aim of this section is to succinctly review some aspects of time dependent canonical transformations in standard operator quantum mechanics. Let $\hat{\vec{A}}=\hat{\vec{A}}(\hat{\vec{q}},\hat{\vec{p}},t)$ and $\hat{\vec{B}}=\hat{\vec{B}}(\hat{\vec{q}},\hat{\vec{p}},t)$ be a new set of fundamental operators $[\hat{A}_i,\hat{B}_j]=i\hbar\,\delta_{ij},\forall t$. Let $\hat{T}$ be the generator of the canonical transformation,

$$\frac{\partial}{\partial t}\hat{\vec{A}}=\frac{1}{i\hbar}[\hat{\vec{A}},\hat{T}] \quad \text{and} \quad \frac{\partial}{\partial t}\hat{\vec{B}}=\frac{1}{i\hbar}[\hat{\vec{B}},\hat{T}], \tag{13}$$

and to make it simple let us also impose the initial conditions $\hat{\vec{A}}(0)=\hat{\vec{q}}$ and $\hat{\vec{B}}(0)=\hat{\vec{p}}$. Then, the unitary transformation reads

$$\hat{\vec{A}}=\hat{V}(t)\hat{\vec{q}}\,\hat{V}^{-1}(t)=\hat{\vec{A}}(\hat{\vec{q}},\hat{\vec{p}},t) \quad \text{and} \quad \hat{\vec{B}}=\hat{V}(t)\hat{\vec{p}}\,\hat{V}^{-1}(t)=\hat{\vec{B}}(\hat{\vec{q}},\hat{\vec{p}},t), \tag{14}$$

where $\hat{V}(t)=\exp((i/\hbar)\hat{T}t)$. The former relations can be immediately inverted, $\hat{\vec{q}}=\hat{V}^{-1}(t)\hat{\vec{A}}\hat{V}(t)$ and $\hat{\vec{p}}=\hat{V}^{-1}(t)\hat{\vec{B}}\hat{V}(t)$, and lead straightforwardly to the dynamical equation for a generic observable:

$$\frac{d}{dt}\hat{F}(\hat{\vec{A}},\hat{\vec{B}},t)=\frac{1}{i\hbar}[\hat{F},\hat{H}+\hat{T}]+\frac{\partial}{\partial t}\hat{F}(\hat{\vec{A}},\hat{\vec{B}},t). \tag{15}$$

We now consider the density matrix of the system: $\hat{\rho}(t)=|\psi(t)\rangle\langle\psi(t)|$ where $|\psi(t)\rangle$ is the corresponding quantum state at the time t. In the $\hat{q}$ representation we have[9]

$$\hat{\rho}(t)=\int d^N\vec{q}\,'\,d^N\vec{q}\,''\langle\vec{q}\,''|\psi(t)\rangle\langle\psi(t)|\vec{q}\,'\rangle|\vec{q}\,''\rangle\langle\vec{q}\,'|$$
$$=\int d^N\vec{q}\,'\,d^N\vec{q}\,''\;\;\psi(\vec{q}\,'',t)\psi^*(\vec{q}\,',t)e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\hat{\vec{p}}}\hat{\Delta}(\hat{\vec{q}}-\vec{q}\,')$$
$$=\int d^N\vec{q}\,'\,d^N\vec{q}\,''\;\;\psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0)e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\hat{\vec{p}}(\hat{\vec{q}},\hat{\vec{p}},-t)}\hat{\Delta}(\hat{\vec{q}}(\hat{\vec{q}},\hat{\vec{p}},-t)-\vec{q}\,')=\hat{\rho}(\hat{\vec{q}},\hat{\vec{p}},t), \tag{16}$$

where $\hat{\Delta}(\hat{\vec{q}}-\vec{q}\,')=\hat{\Delta}(\hat{q}_1-q_1')\cdots\hat{\Delta}(\hat{q}_N-q_N')$ and $\hat{\Delta}(\hat{q}_i-q_i')=(1/2\pi)\int dk e^{ik(\hat{q}_i-q_i')}$. Moreover, $\hat{\vec{q}}(\hat{\vec{q}},\hat{\vec{p}},t)$ and $\hat{\vec{p}}(\hat{\vec{q}},\hat{\vec{p}},t)$ are the Heisenberg time evolutions of the fundamental operators $\hat{\vec{q}}$ and $\hat{\vec{p}}$. The action of the time dependent canonical transformation on the density matrix is now easily implemented, $\hat{\rho}(t)=\hat{\rho}(\hat{\vec{q}}(\hat{\vec{A}},\hat{\vec{B}},t),\hat{\vec{p}}(\hat{\vec{A}},\hat{\vec{B}},t),t)=\hat{V}^{-1}(t)\hat{\rho}(\hat{\vec{A}},\hat{\vec{B}},t)\hat{V}(t)=\hat{\rho}'(\hat{\vec{A}},\hat{\vec{B}},t)$, from where it follows that in the $\hat{A}$ representation

$$\frac{\partial}{\partial t}\hat{\rho}'(\hat{\vec{A}},\hat{\vec{B}},t)=\frac{\partial\hat{V}^{-1}(t)}{\partial t}\hat{\rho}\hat{V}(t)+\hat{V}^{-1}(t)\left(\frac{\partial}{\partial t}\hat{\rho}(\hat{\vec{A}},\hat{\vec{B}},t)\right)\hat{V}(t)+\hat{V}^{-1}(t)\hat{\rho}\frac{\partial\hat{V}(t)}{\partial t}$$
$$=\frac{1}{i\hbar}[\hat{T},\hat{\rho}']+\frac{1}{i\hbar}\hat{V}^{-1}[\hat{H},\hat{\rho}]\hat{V}=\frac{1}{i\hbar}[\hat{T}+\hat{H}',\hat{\rho}'], \tag{17}$$

where $\hat{H}'(\hat{\vec{A}},\hat{\vec{B}},t)=\hat{H}(\hat{\vec{q}}(\hat{\vec{A}},\hat{\vec{B}},t),\hat{\vec{p}}(\hat{\vec{A}},\hat{\vec{B}},t))=\hat{V}^{-1}(t)\hat{H}(\hat{\vec{A}},\hat{\vec{B}})\hat{V}(t)$.

IV. TIME DEPENDENT TRANSFORMATIONS IN PHASE SPACE QUANTUM MECHANICS

In this section we study the action of time dependent transformations in phase space quantum mechanics. We consider an arbitrary N dimensional quantum system with Hamiltonian $\hat{H}$ and described by the wave function $\psi(t)$. As we have seen, the original Weyl transform $W_{(q,p)}$ yields the standard Wigner formulation of the system. The time evolution of the Wigner function $f_W(\vec{q},\vec{p},t)=(1/(2\pi\hbar)^N)\,W_{(q,p)}(|\psi(t)\rangle\langle\psi(t)|)$ is dictated by the standard Moyal equation where the Moyal bracket and the starproduct are given by Eq. (2). We then consider two different phase space implementations of a time dependent operator transformation.

(1) *Unitary time dependent transformations and the map* $W_{(A,B)}$. At the quantum operator level we introduce the unitary transformation $(\hat{\vec{q}},\hat{\vec{p}})\rightarrow(\hat{\vec{A}},\hat{\vec{B}})$ defined by Eqs. (13) and (14). The new variables $(\hat{\vec{A}},\hat{\vec{B}})$ satisfy the Heisenberg commutation relations and thus a new Weyl map $W_{(A,B)}$ can be constructed. It displays the standard functional structure given by Eq. (1) and yields a starproduct $*_{(A,B)}$ and Moyal bracket $[,]_{M_{(A,B)}}$ also displaying the non-covariant functional form Eq. (2). The time evolution of the new Wigner function,

$$f_W'(\vec{A},\vec{B},t)=\frac{1}{(2\pi\hbar)^N}W_{(A,B)}(\hat{\rho}'(\hat{\vec{A}},\hat{\vec{B}},t))=V^{-1}(t)*_{(A,B)}f_W(\vec{A},\vec{B},t)*_{(A,B)}V(t), \tag{18}$$

where $V(t)=W_{(A,B)}(\hat{V})$, reads

$$\frac{\partial}{\partial t}f_W'(\vec{A},\vec{B},t)=[H'+T,f_W']_{M_{(A,B)}}, \tag{19}$$

and is just the (A,B)-Weyl transform of Eq. (17). Notice that just like in the time independent case the unitary transformation $(\vec{q},\vec{p})\rightarrow(\vec{A},\vec{B})$ does not, in general, act as a coordinate transformation: $f_W'(\vec{A},\vec{B},t)\neq f_W(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)$.

(2) *Coordinate transformations and the map* $W^{(q,p)}_{(A,B)}$. We follow the steps of the time independent case and introduce a time dependent phase space diffeomorphism $(\vec{q},\vec{p})\to(\vec{A},\vec{B})$ defined in generic terms by $\vec{q}=\vec{q}(\vec{A},\vec{B},t)$; $\vec{p}=\vec{p}(\vec{A},\vec{B},t)$. This coordinate transformation is not required to be a symplectomorphism (i.e., to preserve the Poisson bracket) nor to preserve the Moyal bracket between the fundamental variables (i.e., to satisfy $[q_i(\vec{A},\vec{B},t),p_j(\vec{A},\vec{B},t)]_{M_{(A,B)}}=\delta_{ij}$ and $[q_i(\vec{A},\vec{B},t),q_j(\vec{A},\vec{B},t)]_{M_{(A,B)}}=[p_i(\vec{A},\vec{B},t),p_j(\vec{A},\vec{B},t)]_{M_{(A,B)}}=0$ for all $i,j=1,\ldots,N$).

We then define the time dependent generalized Weyl transform in the variables $(\vec{A},\vec{B})$:

$$W^{(q,p)}_{(A,B)}:\hat{\mathcal{A}}(\mathcal{H})\to\mathcal{A}(T^*M);\quad \hat{F}\to F'(\vec{A},\vec{B},t)=W^{(q,p)}_{(A,B)}(\hat{F})=W_{(q,p)}(\hat{F})\big|_{\vec{q}=\vec{q}(\vec{A},\vec{B},t)\wedge\vec{p}=\vec{p}(\vec{A},\vec{B},t)}. \tag{20}$$

The explicit form of $W^{(q,p)}_{(A,B)}$ is given by the trivial time dependent generalization of Eq. (5):

$$W^{(q,p)}_{(A,B)}(\hat{F})=\hbar^N\int d^N\vec{x}\int d^N\vec{y}\;\; e^{-i\vec{p}(\vec{A},\vec{B},t)\cdot\vec{y}}\,\delta(\vec{x}-\vec{q}(\vec{A},\vec{B},t))\left\langle \vec{x}+\frac{\hbar}{2}\vec{y}\left|\hat{F}\right|\vec{x}-\frac{\hbar}{2}\vec{y}\right\rangle, \tag{21}$$

from which follows the covariant *time dependent* $*$-product and Moyal bracket:

$$W^{(q,p)}_{(A,B)}(\hat{F}\hat{G})=F'(\vec{A},\vec{B},t)*'_{(A,B)}G'(\vec{A},\vec{B},t)=F(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t))*_{(q,p)}G(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t)), \tag{22}$$

and $[F',G']_{M'_{(A,B)}}=(1/i\hbar)\,(F'*'_{(A,B)}G'-G'*'_{(A,B)}F')$ where $F'(\vec{A},\vec{B},t)=W^{(q,p)}_{(A,B)}(\hat{F})$, $F(\vec{q},\vec{p},t)=W_{(q,p)}(\hat{F})$ and likewise for G and G'. The two algebraic structures display the functional form given by Eqs. (6)–(8) with the obvious inclusion of an explicit time dependence.

The dynamical structure of the theory displays more significant corrections. Let $f'_W(\vec{A},\vec{B},t)=(1/(2\pi\hbar)^N)\,W^{(q,p)}_{(A,B)}(|\psi(t)\rangle\langle\psi(t)|)$ be the covariant Wigner function. It satisfies $f'_W(\vec{A},\vec{B},t)=f_W(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)$ and thus

$$\begin{aligned}
\frac{\partial}{\partial t}f'_W(\vec{A},\vec{B},t)&=\left(\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_2}\right)f_W(\vec{q}(\vec{A},\vec{B},t_1),\vec{p}(\vec{A},\vec{B},t_1),t_2)\Big|_{t_1=t_2=t}\\
&=[H(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t),f_W(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)]_{M_{(q,p)}}+\frac{\partial f_W}{\partial\vec{q}}\cdot\frac{\partial\vec{q}}{\partial t_1}+\frac{\partial f_W}{\partial\vec{p}}\\
&\quad\cdot\frac{\partial\vec{p}}{\partial t_1}\Big|_{t_1=t}=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}+\left(\frac{\partial f'_W}{\partial A_i}\frac{\partial A_i}{\partial q_j}+\frac{\partial f'_W}{\partial B_i}\frac{\partial B_i}{\partial q_j}\right)\frac{\partial q_j}{\partial t}\\
&\quad+\left(\frac{\partial f'_W}{\partial A_i}\frac{\partial A_i}{\partial p_j}+\frac{\partial f'_W}{\partial B_i}\frac{\partial B_i}{\partial p_j}\right)\frac{\partial p_j}{\partial t}=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}+\frac{\partial f'_W}{\partial A_i}\left(\frac{\partial A_i}{\partial q_j}\frac{\partial q_j}{\partial t}\right.\\
&\quad\left.+\frac{\partial A_i}{\partial p_j}\frac{\partial p_j}{\partial t}\right)+\frac{\partial f'_W}{\partial B_i}\left(\frac{\partial B_i}{\partial q_j}\frac{\partial q_j}{\partial t}+\frac{\partial B_i}{\partial p_j}\frac{\partial p_j}{\partial t}\right)=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}-\frac{\partial f'_W}{\partial\vec{A}}\\
&\quad\cdot\frac{\partial\vec{A}}{\partial t}-\frac{\partial f'_W}{\partial\vec{B}}\cdot\frac{\partial\vec{B}}{\partial t},
\end{aligned} \tag{23}$$

where in the last step we used the fact that $\vec{A}=\vec{A}(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)$ and likewise for $\vec{B}$. Further, contraction over repeated indices is understood, i.e.,

$$\frac{\partial f_W}{\partial q_i}\frac{\partial q_i}{\partial t_1}=\frac{\partial f_W}{\partial \vec{q}}\cdot\frac{\partial \vec{q}}{\partial t_1}=\sum_{i=1}^{N}\frac{\partial f_W}{\partial q_i}\frac{\partial q_i}{\partial t_1}.$$

Equation (23) constitutes a generalization of the Moyal covariant equation (10) and renders the dynamics of the Wigner function fully invariant under the action of general time dependent phase space diffeomorphisms.

Let us then consider several particular cases in more detail:

(a) If the transformation $(\vec{q},\vec{p})\rightarrow(\vec{A},\vec{B})$ is time independent, then Eq. (23) reduces to the standard covariant Moyal equation (10).

(b) If, on the other hand, it is unitary, i.e., if $\vec{A}(\vec{q},\vec{p},t)=V(t)*_{(q,p)}\vec{q}*_{(q,p)}V^{-1}(t)$ and $\vec{B}(\vec{q},\vec{p},t)=V(t)*_{(q,p)}\vec{p}*_{(q,p)}V^{-1}(t)$ satisfying $\partial\vec{A}/\partial t=[\vec{A},T]_{M_{(q,p)}}$ and $\partial\vec{B}/\partial t=[\vec{B},T]_{M_{(q,p)}}$ with initial conditions $\vec{A}(\vec{q},\vec{p},0)=\vec{q}$ and $\vec{B}(\vec{q},\vec{p},0)=\vec{p}$, then in Eq. (23) we have

$$\begin{aligned}\frac{\partial\vec{A}}{\partial t}=\frac{\partial}{\partial t}\vec{A}(\vec{q},\vec{p},t)\Big|_{\vec{q}=\vec{q}(\vec{A},\vec{B},t)\wedge\vec{p}=\vec{p}(\vec{A},\vec{B},t)}&=[\vec{A}(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t),T(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t))]_{M_{(q,p)}}\\&=[\vec{A},T'(\vec{A},\vec{B},t)]_{M'_{(A,B)}},\end{aligned}\tag{24}$$

where $T'(\vec{A},\vec{B},t)=W^{(q,p)}_{(A,B)}(\hat{T})$. An equivalent result is valid for $\partial\vec{B}/\partial t$. Substituting these results in Eq. (23) we get

$$\frac{\partial}{\partial t}f'_W(\vec{A},\vec{B},t)=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}+\frac{\partial f'_W}{\partial\vec{A}}\cdot[T',\vec{A}]_{M'_{(A,B)}}+\frac{\partial f'_W}{\partial\vec{B}}\cdot[T',\vec{B}]_{M'_{(A,B)}}.\tag{25}$$

(c) Finally, we consider the case where the transformation $(\vec{q},\vec{p})\rightarrow(\vec{A},\vec{B})$ is a symplectomorphism. Let T be the generator. Then $\vec{A}(\vec{q},\vec{p},t)$ satisfies $\partial\vec{A}/\partial t=\{\vec{A},T\}_{(q,p)}=\{\vec{A},T\}_{(A,B)}$ and likewise for $\vec{B}$. Hence, Eq. (23) reduces to

$$\begin{aligned}\frac{\partial}{\partial t}f'_W(\vec{A},\vec{B},t)&=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}-\frac{\partial f'_W}{\partial\vec{A}}\cdot\{\vec{A},T\}_{(A,B)}-\frac{\partial f'_W}{\partial\vec{B}}\cdot\{\vec{B},T\}_{(A,B)}\\&=[H'(\vec{A},\vec{B},t),f'_W(\vec{A},\vec{B},t)]_{M'_{(A,B)}}+\{T,f'_W\}_{(A,B)}.\end{aligned}\tag{26}$$

To finish this section let us study the $^{(q,p)}_{(A,B)}$-representation of a general stargenfunction. Let $\hat{F}$ be a generic operator and $F'(\vec{A},\vec{B},t)=W^{(q,p)}_{(A,B)}(\hat{F})$. The $*$-genvalue equation in the $^{(q,p)}_{(A,B)}$-representation is then written

$$F'(\vec{A},\vec{B},t)*'_{(A,B)}g'_a(\vec{A},\vec{B},t)=g'_a(\vec{A},\vec{B},t)*'_{(A,B)}F'(\vec{A},\vec{B},t)=ag'_a(\vec{A},\vec{B},t)\tag{27}$$

and displays the solution

$$\begin{aligned}g'_a(\vec{A},\vec{B},t)=\delta_{*'_{(A,B)}}[F'(\vec{A},\vec{B},t)-a]&=\frac{1}{2\pi}\int dk e^{ik[F'(\vec{A},\vec{B},t)-a]}_{*'_{(A,B)}}\\&=\frac{1}{2\pi}\int dk e^{ik[F(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)-a]}_{*_{(q,p)}},\end{aligned}\tag{28}$$

where $F(\vec{q},\vec{p},t)=W_{(q,p)}(\hat{F})$. Further, if $g_a(\vec{q},\vec{p},t)$ is such that $F*_{(q,p)}g_a=g_a*_{(q,p)}F=ag_a$ then $g'_a(\vec{A},\vec{B},t)=g_a(\vec{q}(\vec{A},\vec{B},t),\vec{p}(\vec{A},\vec{B},t),t)$, a result that follows immediately from Eqs. (22) and (28). Therefore the stargenvalue equation transforms covariantly under the action of general time dependent coordinate transformations.

As an illustrative example let us consider the one-dimensional simple case $\hat{F}=\hat{q}\Rightarrow W^{(q,p)}_{(A,B)}(\hat{q})=q(A,B,t)$. The solution of the $*$-genvalue equation (27) is then

$$g'_a(A,B,t)=\frac{1}{2\pi}\int dk e^{ik[q(A,B,t)-a]}_{*'_{(A,B)}}=\frac{1}{2\pi}\int dk e^{ik[q(A,B,t)-a]}_{*_{(q,p)}}=\frac{1}{2\pi}\int dk e^{ik[q(A,B,t)-a]}$$
$$=\delta[q(A,B,t)-a], \tag{29}$$

and displays the time evolution

$$\frac{\partial}{\partial t}g'_a(A,B,t)=\frac{\partial\delta}{\partial q}[q(A,B,t)-a]\frac{\partial q}{\partial t}(A,B,t). \tag{30}$$

Furthermore, if the transformation $(q,p)\rightarrow(A,B)$ is symplectic with generator T, then $\partial q/\partial t=\{q,-T\}_{(A,B)}$ and

$$\frac{\partial}{\partial t}g'_a(A,B,t)=-\{g'_a,T\}_{(A,B)}. \tag{31}$$

V. THE CAUSAL REPRESENTATION

As an application of the formalism let us consider a finite dimensional dynamical system described by a generic Hamiltonian $\hat{H}$ and use the generalized time dependent Weyl map to derive in a systematic way (1) the Schrödinger and (2) the Heisenberg phase space pictures and (3) a new phase space representation where the Wigner function displays a fully classical time evolution.

To begin with, we introduce the time dependent unitary transformation generated by $\hat{T}=-\hat{H}$. A new set of fundamental operators is given by $\hat{\vec{A}}=\hat{\vec{A}}(\hat{\vec{q}},\hat{\vec{p}},t)$ and $\hat{\vec{B}}=\hat{\vec{B}}(\hat{\vec{q}},\hat{\vec{p}},t)$, solutions of Eq. (13) and satisfying the initial conditions $\hat{\vec{A}}(0)=\hat{\vec{q}}$ and $\hat{\vec{B}}(0)=\hat{\vec{p}}$. Given the relation between $\hat{H}$ and $\hat{T}$ they also satisfy

$$\hat{\vec{A}}=\hat{\vec{A}}(\hat{\vec{q}},\hat{\vec{p}},t)=\hat{\vec{q}}(\hat{\vec{q}},\hat{\vec{p}},-t)\quad\text{and}\quad\hat{\vec{B}}=\hat{\vec{B}}(\hat{\vec{q}},\hat{\vec{p}},t)=\hat{\vec{p}}(\hat{\vec{q}},\hat{\vec{p}},-t), \tag{32}$$

where $\hat{\vec{q}}(\hat{\vec{q}},\hat{\vec{p}},t)$ and $\hat{\vec{p}}(\hat{\vec{q}},\hat{\vec{p}},t)$ are the Heisenberg time evolution of the fundamental operators $\hat{\vec{q}}$ and $\hat{\vec{p}}$. From (32) we define a new set of phase space coordinates $\vec{A}=\vec{A}_M(\vec{q},\vec{p},t)=W_{(q,p)}(\hat{A})$ and $\vec{B}=\vec{B}_M(\vec{q},\vec{p},t)=W_{(q,p)}(\hat{B})$ satisfying the Moyal equations,

$$\frac{\partial\vec{A}_M}{\partial t}=[\vec{A}_M,T]_{M_{(q,p)}},\quad\frac{\partial\vec{B}_M}{\partial t}=[\vec{B}_M,T]_{M_{(q,p)}},\quad T=W_{(q,p)}(\hat{T}), \tag{33}$$

and the initial conditions $\vec{A}_M(\vec{q},\vec{p},0)=\vec{q}$ and $\vec{B}_M(\vec{q},\vec{p},0)=\vec{p}$. The subscript M indicates that the *functions* A_M and B_M obey the Moyal equations. Intuitively, they can be seen as the quantum phase space histories of the system.

A second set of (purely classical) phase space coordinates will also be required: $\vec{Q},\vec{P}$ are given by $\vec{Q}=\vec{Q}(\vec{A},\vec{B},t)$ and $\vec{P}=\vec{P}(\vec{A},\vec{B},t)$ and satisfy the classical Hamiltonian equations,

$$\frac{\partial\vec{Q}}{\partial t}=\{\vec{Q},-T(\vec{A},\vec{B})\}_{(A,B)},\quad\frac{\partial\vec{P}}{\partial t}=\{\vec{P},-T(\vec{A},\vec{B})\}_{(A,B)},\quad T(\vec{A},\vec{B})=W_{(A,B)}(\hat{T}), \tag{34}$$

and the initial conditions $\vec{Q}(\vec{A},\vec{B},0)=\vec{A}$, $\vec{P}(\vec{A},\vec{B},0)=\vec{B}$. Notice that $T(\vec{A},\vec{B})$ displays the same functional form as $T(\vec{q},\vec{p})=W_{(q,p)}(\hat{T})$. Solving the algebraic equations $\vec{Q}=\vec{Q}(\vec{A},\vec{B},t)$, $\vec{P}=\vec{P}(\vec{A},\vec{B},t)$ with respect to $\vec{A},\vec{B}$ we get $\vec{A}=\vec{A}_C(\vec{Q},\vec{P},t)$ and $\vec{B}=\vec{B}_C(\vec{Q},\vec{P},t)$ where the subscript C indicates that $\vec{A}_C$ and $\vec{B}_C$ are the solutions of the classical Hamilton's equations,

$$\frac{\partial\vec{A}_C}{\partial t}=\{\vec{A}_C,T(\vec{Q},\vec{P})\}_{(Q,P)},\quad \frac{\partial\vec{B}_C}{\partial t}=\{\vec{B}_C,T(\vec{Q},\vec{P})\}_{(Q,P)}, \tag{35}$$

where $T(\vec{Q},\vec{P})=T(\vec{A}_C(\vec{Q},\vec{P},t),\vec{B}_C(\vec{Q},\vec{P},t))$ displays the same functional form as $T(\vec{A},\vec{B})$ (notice that T is the generator of the canonical transformation). Also notice that in general $\vec{q}(\vec{A},\vec{B},t)\neq\vec{Q}(\vec{A},\vec{B},t)$ and $\vec{p}(\vec{A},\vec{B},t)\neq\vec{P}(\vec{A},\vec{B},t)$ (the exceptions happen for T quadratic in the phase space variables). While the variables $(\vec{q},\vec{p})$ describe the *quantum* phase space time evolution, the variables $(\vec{Q},\vec{P})$ describe the *classical* phase space trajectories. The transformation $(\vec{A},\vec{B})\rightarrow(\vec{Q},\vec{P})$ is a phase space symplectomorphism exclusively defined at the classical level, i.e., it is not [and unlike $(\vec{q},\vec{p})\rightarrow(\vec{A},\vec{B})$ it could not be] inherited from a quantum operator transformation.

Finally, from Eqs. (16) and (32) the density matrix $\hat{\rho}(t)=|\psi(t)\rangle\langle\psi(t)|$ admits the expansions

$$\hat{\rho}(t)=\int d^N\vec{q}\,'d^N\vec{q}\,''\psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0)e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\hat{\vec{p}}(\hat{\vec{q}},\hat{\vec{p}},-t)}\hat{\Delta}[\hat{\vec{q}}(\hat{\vec{q}},\hat{\vec{p}},-t)-\vec{q}\,']=\hat{\rho}(\hat{\vec{q}},\hat{\vec{p}},t),$$
$$\hat{\rho}(t)=\int d^N\vec{q}\,'d^N\vec{q}\,''\psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0)e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\hat{\vec{B}}}\hat{\Delta}(\hat{\vec{A}}-\vec{q}\,')=\hat{\rho}(\hat{\vec{A}},\hat{\vec{B}},0). \tag{36}$$

With these preliminaries settled down we address the derivation of the three phase space pictures:

(1) *Schrödinger picture and the map* $W_{(q,p)}$. From the first expansion for the density matrix (36) we immediately get

$$\begin{aligned}f_W(\vec{q},\vec{p},t)&=\frac{1}{(2\pi\hbar)^N}W_{(q,p)}[\hat{\rho}(t)]\\&=\frac{1}{(2\pi\hbar)^N}\int d^N\vec{q}\,'d^N\vec{q}\,''\psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0)e_{*(q,p)}^{(-i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{p}(\vec{q},\vec{p},-t)}*_{(q,p)}\\&\quad\times\delta_{*(q,p)}[\vec{q}(\vec{q},\vec{p},-t)-\vec{q}\,']\end{aligned} \tag{37}$$

and the time evolution of the Wigner function obeys the standard Moyal equation: $(\partial/\partial t)f_W=[H,f_W]_{M_{(q,p)}}$. We also have $W_{(q,p)}(|\vec{q}_0\rangle\langle\vec{q}_0|)=\delta_*(\vec{q}-\vec{q}_0)=\delta(\vec{q}-\vec{q}_0)$ and so $(\partial/\partial t)\,\delta(\vec{q}-\vec{q}_0)=0$ and likewise for $\vec{p}$, i.e., the dynamics is cast in the Schrödinger picture.

(2) *Heisenberg picture and the map* $W_{(A,B)}$. From the second expansion in (36) we get

$$\begin{aligned}\frac{1}{(2\pi\hbar)^N}W_{(A,B)}[\hat{\rho}(t)]&=\frac{1}{(2\pi\hbar)^N}W_{(A,B)}[\hat{\rho}(\vec{A},\vec{B},0)]\\&=\frac{1}{(2\pi\hbar)^N}\int d^N\vec{q}\,'d^N\vec{q}\,''\psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0)e_{*(A,B)}^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}}*_{(A,B)}\\&\quad\times\delta^N{}_{*(A,B)}(\vec{A}-\vec{q}\,').\end{aligned} \tag{38}$$

Let us check explicit that the previous formula yields the standard (in this case time independent) expression of the Wigner function. The same derivation would also apply to Eq. (37). We start by considering the term evolving starproducts in more detail:

$$
\begin{aligned}
e^{-i/\hbar(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}}_{*(A,B)} *_{(A,B)} \delta^N *_{(A,B)} (\vec{A}-\vec{q}\,') &= e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}} *_{(A,B)} \delta^N(\vec{A}-\vec{q}\,') \\
&= \frac{1}{(2\pi)^N} \sum_{n=0}^{+\infty} \frac{1}{n!} \left(-\frac{i\hbar}{2} \right)^n e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}} \left[-\frac{i}{\hbar}(\vec{q}\,'' \right. \\
&\quad \left. -\vec{q}\,')\cdot\frac{\partial}{\partial\vec{A}} \right]^n \int d^N\vec{k}\, e^{i\vec{k}\cdot(\vec{A}-\vec{q}\,')} \\
&= \frac{1}{(2\pi)^N} e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}} \int d^N\vec{k} \sum_{n=0}^{+\infty} \frac{1}{n!} \left(-\frac{i}{2}\vec{k}\cdot(\vec{q}\,'' \right. \\
&\quad \left. -\vec{q}\,') \right)^n e^{i\vec{k}\cdot(\vec{A}-\vec{q}\,')} \\
&= e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}} \frac{1}{(2\pi)^N} \int d^N\vec{k}\, e^{i\vec{k}\cdot(\vec{A}-\vec{q}\,'+\vec{q}\,'/2-\vec{q}\,''/2)} \\
&= e^{-i/\hbar(\vec{q}\,''-\vec{q}\,')\cdot\vec{B}} \delta^N\left(\vec{A}-\frac{\vec{q}\,'}{2}-\frac{\vec{q}\,''}{2} \right). \qquad (39)
\end{aligned}
$$

Substituting this expression in (38) we get

$$
\begin{aligned}
\frac{1}{(2\pi\hbar)^N} W_{(A,B)}[\hat{\rho}(t)] &= \frac{1}{(2\pi\hbar)^N} \int d^N\vec{q}\,' d^N\vec{q}\,'' \psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0) 2^N \delta^N(2\vec{A}-\vec{q}\,' \\
&\quad -\vec{q}\,'') e^{-(2i/\hbar)(\vec{A}-\vec{q}\,')\cdot\vec{B}} = \frac{1}{(\pi\hbar)^N} \int d^N\vec{q}\,' \psi(2\vec{A} \\
&\quad -\vec{q}\,',0)\psi^*(\vec{q}\,',0) e^{-(2i/\hbar)(\vec{A}-\vec{q}\,')\cdot\vec{B}} = \frac{1}{(\pi\hbar)^N} \int d^N\vec{y}\, \psi(\vec{A}+\vec{y},0)\psi^*(\vec{A} \\
&\quad -\vec{y},0) e^{-(2i/\hbar)\vec{y}\cdot\vec{B}} = f_W(\vec{A},\vec{B},0), \qquad (40)
\end{aligned}
$$

where in the last step we made $\vec{y}=\vec{A}-\vec{q}\,'$. We indeed recovered the standard definition of the Wigner function. Moreover we see that $(\partial/\partial t) f_W = 0$, as it should and in perfect agreement with Eq. (19) taking into account that $T=-H$. On the other hand, we also have

$$
g_{\vec{q}_0}(\vec{A},\vec{B},t) = W_{(A,B)}(|\vec{q}_0\rangle\langle\vec{q}_0|) = \delta^N_{*(A,B)}[\vec{q}(\vec{A},\vec{B},t)-\vec{q}_0] = \frac{1}{(2\pi)^N} \int d^N\vec{k}\, e^{i\vec{k}\cdot(\vec{q}(\vec{A},\vec{B},t)-\vec{q}_0)}_{*(A,B)}, \qquad (41)
$$

where $\vec{q}=\vec{q}(\vec{A},\vec{B},t)$ is the solution with respect to $\vec{q}$ of the algebraic equations $\vec{A}=\vec{A}_M(\vec{q},\vec{p},t)$, $\vec{B}=\vec{B}_M(\vec{q},\vec{p},t)$ defined in Eq. (33). It also follows from Eq. (33) that $\vec{q}(\vec{A},\vec{B},t)$ satisfies $\partial\vec{q}/\partial t = [\vec{q},-T]_{M_{(A,B)}}$. Therefore,

$$
\frac{\partial}{\partial t} g_{\vec{q}_0}(\vec{A},\vec{B},t) = [g_{\vec{q}_0}(\vec{A},\vec{B},t),H]_{M_{(A,B)}}, \qquad (42)
$$

and we obtained the phase space Heisenberg picture.

(3) *Causal picture and the map* $W^{(A,B)}_{(Q,P)}$. We finally consider the action of the map $W^{(A,B)}_{(Q,P)}$ on the second expansion for the density matrix (36). From Eq. (40) it follows that (notice that $W^{(A,B)}_{(Q,P)} = W_{(A,B)}$)

$$
\begin{aligned}
f'_W(\vec{Q},\vec{P},t) &= \frac{1}{(2\pi\hbar)^N} W^{(A,B)}_{(Q,P)}[\hat{\rho}(t)] \\
&= \frac{1}{(2\pi\hbar)^N} \int d^N\vec{q}\,' d^N\vec{q}\,'' \psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0) e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot \vec{B}_C(\vec{Q},\vec{P},t)}_{*'(Q,P)} *'_{(Q,P)} \delta^N_{*'(Q,P)} \\
&\quad [\vec{A}_C(\vec{Q},\vec{P},t)-\vec{q}\,'] \\
&= \frac{1}{(2\pi\hbar)^N} \int d^N\vec{q}\,' d^N\vec{q}\,'' \psi(\vec{q}\,'',0)\psi^*(\vec{q}\,',0) e^{-(i/\hbar)(\vec{q}\,''-\vec{q}\,')\cdot \vec{B}_C(\vec{Q},\vec{P},t)}_{*(A,B)} *_{(A,B)} \delta^N_{*(A,B)} \\
&\quad [\vec{A}_C(\vec{Q},\vec{P},t)-\vec{q}\,'] \\
&= f_W(\vec{A}_C(\vec{Q},\vec{P},t),\vec{B}_C(\vec{Q},\vec{P},t),0) = f_W(\vec{Q}(\vec{Q},\vec{P},-t),\vec{P}(\vec{Q},\vec{P},-t),0),
\end{aligned} \tag{43}
$$

where $\vec{Q}(\vec{Q},\vec{P},t)=\vec{A}_C(\vec{Q},\vec{P},-t)$ and $\vec{P}(\vec{Q},\vec{P},t)=\vec{B}_C(\vec{Q},\vec{P},-t)$ are the classical time evolution of the canonical variables $(\vec{Q},\vec{P})$ [cf. (35)]

$$
\dot{\vec{Q}}=\{\vec{Q},-T(\vec{Q},\vec{P})\}_{(Q,P)} \quad \text{and} \quad \dot{\vec{P}}=\{\vec{P},-T(\vec{Q},\vec{P})\}_{(Q,P)} \tag{44}
$$

associated with the Hamiltonian $H(\vec{Q},\vec{P})=-T(\vec{Q},\vec{P})=W_{(A,B)}(\hat{H})|_{\vec{A}=\vec{Q}\wedge\vec{B}=\vec{P}}$. Hence, the time evolution of the Wigner function is given by

$$
\frac{\partial}{\partial t} f'_W(\vec{Q},\vec{P},t)=\{f'_W,T\}_{(Q,P)}=\{H,f'_W\}_{(Q,P)}. \tag{45}
$$

On the other hand, for the $*$-genfunctions $W^{(A,B)}_{(Q,P)}(|\vec{q}_0\rangle\langle\vec{q}_0|)$ we have from Eq. (41)

$$
\begin{aligned}
g'_{\vec{q}_0}(\vec{Q},\vec{P},t) &= \delta^N_{*'_{(Q,P)}}(\vec{q}-\vec{q}_0) = \delta^N_{*_{(A,B)}}(\vec{q}(\vec{A},\vec{B},t)-\vec{q}_0)|_{\vec{A}=\vec{A}_C(\vec{Q},\vec{P},t)\wedge\vec{B}=\vec{B}_C(\vec{Q},\vec{P},t)} \\
&= g_{\vec{q}_0}(\vec{A}_C(\vec{Q},\vec{P},t),\vec{B}_C(\vec{Q},\vec{P},t),t),
\end{aligned} \tag{46}
$$

and so [cf. (35) and (42)]

$$
\begin{aligned}
\frac{\partial}{\partial t} g'_{\vec{q}_0}(\vec{Q},\vec{P},t) &= \left\{ \frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_2} \right\} g_{\vec{q}_0}(\vec{A}_C(\vec{Q},\vec{P},t_2),\vec{B}_C(\vec{Q},\vec{P},t_2),t_1)\Big|_{t_1=t_2=t} \\
&= [g'_{\vec{q}_0},H]_{M'_{(Q,P)}} - \{g'_{\vec{q}_0},H\}_{(Q,P)}.
\end{aligned} \tag{47}
$$

In this representation both the Wigner function and the stargenfunctions evolve in time, the Wigner function displaying a fully classical evolution. In particular, if the Wigner function is positive defined at the initial time, it will remain so for all times. We conclude that the source of the quantum behavior has been completely removed from the distributional sector of the theory and is now exclusively placed on the observables (stargenfunctions) sector.

VI. EXAMPLE

To illustrate our previous results let us consider a two particle system described by the Hamiltonian,

$$
\hat{H}=\frac{\hat{p}_1^2}{2M}+\frac{\hat{p}_2^2}{2m}+k\hat{q}_1\hat{p}_2^2, \tag{48}
$$

where $(\hat{q}_1,\hat{p}_1)$ are the canonical variables of the particle of mass M and $(\hat{q}_2,\hat{p}_2)$ are those of the particle of mass m and k is a coupling constant.

The Weyl map $W_{(q,p)}$ yields the (q,p)-Hamiltonian symbol,

$$H=W_{(q,p)}(\hat{H})=\frac{p_1^2}{2M}+\frac{p_2^2}{2m}+kq_1p_2^2, \tag{49}$$

and the Moyal equations $\dot{z}=[z,H]_{M_{(q,p)}}$ for the fundamental variables $z=q_1,q_2,p_1$ or p_2. These display the solutions

$$\begin{aligned} q_1(t)&=q_1(0)+\frac{p_1(0)}{M}t-\frac{k}{2M}p_2(0)^2t^2,\\ p_1(t)&=p_1(0)-kp_2(0)^2t,\\ q_2(t)&=q_2(0)+\left\{\frac{p_2(0)}{m}+2kq_1(0)p_2(0)\right\}t+\frac{k}{M}p_1(0)p_2(0)t^2-\frac{k^2}{3M}p_2(0)^3t^3,\\ p_2(t)&=p_2(0), \end{aligned} \tag{50}$$

which coincide exactly with the classical time evolution, i.e., with the solutions of the classical Hamiltonian equations for the classical Hamiltonian (49). This property is not shared by the Wigner function, its time evolution satisfying the equation

$$\frac{\partial f_W}{\partial t}=[H,f_W]_{M_{(q,p)}}\Leftrightarrow\frac{\partial f_W}{\partial t}=\{H,f_W\}_{(q,p)}+\frac{\hbar^2}{24}\left[2\left\{2kp_2,\frac{\partial^2 f_W}{\partial q_2\partial p_1}\right\}_{(q,p)}-\left\{2kq_1,\frac{\partial^2 f_W}{\partial q_2^2}\right\}_{(q,p)}\right], \tag{51}$$

which is obviously not of the form of the Liouville equation. Consequently, the Wigner function does not satisfy $f_W(\vec{q},\vec{p},t)=f_W(\vec{q}(-t),\vec{p}(-t),0)$ with $\vec{q}(t),\vec{p}(t)$ given by Eq. (50), and $\vec{q}=(q_1,q_2)$, $\vec{p}=(p_1,p_2)$, i.e., it does not display a classical causal structure.

We now introduce a new set of fundamental operators,

$$\begin{aligned} \hat{A}_1&=\hat{q}_1-\frac{\hat{p}_1}{M}t-\frac{k}{2M}\hat{p}_2^2t^2,\\ \hat{B}_1&=\hat{p}_1+k\hat{p}_2^2t,\\ \hat{A}_2&=\hat{q}_2-\left\{\frac{\hat{p}_2}{m}+2k\hat{q}_1\hat{p}_2\right\}t+\frac{k}{M}\hat{p}_1\hat{p}_2t^2+\frac{k^2}{3M}\hat{p}_2^3t^3,\\ \hat{B}_2&=\hat{p}_2, \end{aligned} \tag{52}$$

satisfying the Heisenberg algebra $[\hat{A}_1,\hat{B}_1]=[\hat{A}_2,\hat{B}_2]=i\hbar$, all other commutators being zero. The transformation (52) is unitary and generated by $\hat{T}=-\hat{H}$. Applying the Weyl map $W_{(q,p)}$ to Eq. (52) and comparing the result with (50) we get

$$\left.\begin{array}{l} A_1(\vec{q},\vec{p},t)=q_1(-t) \\ B_1(\vec{q},\vec{p},t)=p_1(-t) \\ A_2(\vec{q},\vec{p},t)=q_2(-t) \\ B_2(\vec{q},\vec{p},t)=p_2(-t) \end{array}\right. \Leftrightarrow \left\{\begin{array}{c} q_1(\vec{A},\vec{B},t)=A_1+\dfrac{B_1}{M}t-\dfrac{k}{2M}B_2^2t^2 \\ p_1(\vec{A},\vec{B},t)=B_1-kB_2^2t \\ q_2(\vec{A},\vec{B},t)=A_2+\left\{\dfrac{B_2}{m}+2kA_1B_2\right\}t+\dfrac{k}{M}B_1B_2t^2-\dfrac{k^2}{3M}B_2^3t^3 \\ p_2(\vec{A},\vec{B},t)=B_2\,. \end{array}\right. \tag{53}$$

The density matrix satisfies $\hat{\rho}(\hat{\vec{q}},\hat{\vec{p}},t)=\hat{\rho}(\hat{\vec{A}}(\hat{\vec{q}},\hat{\vec{p}},t),\hat{\vec{B}}(\hat{\vec{q}},\hat{\vec{p}},t),0)$ [cf. (36)] and thus the Wigner function $f_W(\vec{A},\vec{B},t)=W_{(A,B)}(\hat{\rho})=f_W(\vec{A},\vec{B},0)$ is static. On the other hand, in this representation, the fundamental stargenfunctions do evolve in time. For instance, (let $|x\rangle$ be the general eigenket of $\hat{q}_1$ with associated eigenvalue x),

$$g_x(\vec{A},\vec{B},t)=W_{(A,B)}(|x\rangle\langle x|)=\delta_{*_{(A,B)}}[q_1(\vec{A},\vec{B},t)-x]=\frac{1}{2\pi}\int dk\, e^{ik(q_1(\vec{A},\vec{B},t)-x)}_{*_{(A,B)}}$$

$$=\frac{1}{2\pi}\int dk\, e^{ik(q_1(\vec{A},\vec{B},t)-x)}=\delta[q_1(\vec{A},\vec{B},t)-x] \tag{54}$$

satisfies

$$\frac{\partial}{\partial t}g_x(\vec{A},\vec{B},t)=[g_x(\vec{A},\vec{B},t),H]_{M_{(A,B)}}=\{g_x(\vec{A},\vec{B},t),H\}_{(A,B)}\,. \tag{55}$$

Hence, the Weyl transform $W_{(A,B)}$ casts the phase space dynamics in the Heisenberg picture. Accordingly, the time dependence is exclusively displayed by the observable (stargenfunction) sector of the theory.

We now consider the action of the generalized Weyl map $W^{(A,B)}_{(q,p)}$. The associated time dependent covariant starproduct $*'_{(q,p)}$ and Moyal bracket $[\ ,\ ]_{M_{(q,p)}}$ are characterized by [using the time dependent version of Eqs. (6)–(8) and making $O'^1=p_1$, $O'^2=p_2$, $O'^3=q_1$, $O'^4=q_2$, $O^1=B_1$, $O^2=B_2$, $O^3=A_1$, $O^4=A_2$ and $i,j=1,...,4$]

$$\begin{gathered} J'^{ij}_{(q,p)}=J^{ij}_{(q,p)}\,, \\ \Gamma'^1_{22}=2kt,\quad \Gamma'^3_{22}=\frac{k}{M}t^2,\quad \Gamma'^4_{12}=\Gamma'^4_{21}=\frac{k}{M}t^2,\quad \Gamma'^4_{22}=\frac{2k^2}{M}p_2t^3,\quad \Gamma'^4_{32}=\Gamma'^4_{23}=-2kt, \end{gathered} \tag{56}$$

all other Christoffel symbols being zero. Notice that the connection is time dependent.

The new Wigner function [cf. (53)]

$$f'_W(\vec{q},\vec{p},t)=W^{(A,B)}_{(q,p)}(\hat{\rho})=f_W(\vec{A}(\vec{q},\vec{p},t),\vec{B}(\vec{q},\vec{p},t),0)=f_W(\vec{q}(\vec{q},\vec{p},-t),\vec{p}(\vec{q},\vec{p},-t),0) \tag{57}$$

satisfies the Liouville equation

$$\frac{\partial f'_W}{\partial t}=\frac{\partial f_W}{\partial\vec{A}}\cdot\frac{\partial\vec{A}}{\partial t}+\frac{\partial f_W}{\partial\vec{B}}\cdot\frac{\partial\vec{B}}{\partial t}=\frac{\partial f_W}{\partial\vec{q}}\cdot\{H,\vec{q}\}_{(q,p)}+\frac{\partial f_W}{\partial\vec{p}}\cdot\{H,\vec{p}\}_{(q,p)}=\{H,f_W\}_{(q,p)}=\{H,f'_W\}_{(q,p)}\,. \tag{58}$$

The quantum behavior is displayed by the stargenfunction sector alone. However, for this system, we also have (let $z=q_1,p_1\vee p_2$ and $|z_0\rangle$ be a generic eigenket of $\hat{z}$ with associated eigenvalue z_0)

$$W^{(A,B)}_{(q,p)}(|z_0\rangle\langle z_0|)=\delta_{*'(q,p)}(z-z_0)=\delta_{*(A,B)}(z(\vec{A},\vec{B},t)-z_0)|_{\vec{A}=\vec{A}(\vec{q},\vec{p},t)\wedge\vec{B}=\vec{B}(\vec{q},\vec{p},t)}$$
$$=\delta(z(\vec{A},\vec{B},t)-z_0)|_{\vec{A}=\vec{A}(\vec{q},\vec{p},t)\wedge\vec{B}=\vec{B}(\vec{q},\vec{p},t)}=\delta(z-z_0), \quad (59)$$

where in the third step we used the fact that $e^{ik(z(\vec{A},\vec{B},t)-z_0)}_{*_{(A,B)}}=e^{ik(z(\vec{A},\vec{B},t)-z_0)}$. Hence, the former three fundamental stargenfunctions display a classical structure and satisfy $\{\delta_{*'(q,p)}(z-z_0),H\}=0$. We conclude that for this system, in this representation, the nontrivial (quantum) behavior is displayed by the stargenfunction $z=q_2$ alone.

A final remark is in order: in this example we were not required to use the most general formalism of Sec. V (3) (causal picture and the map $W^{(A,B)}_{(Q,P)}$) to derive the causal phase space representation of the system. This is so because the dynamical structure of the system is exceptionally simple: the quantum and the classical trajectories [which in the most general case have to be described by two different sets of coordinates, $(\vec{q},\vec{p})$ and $(\vec{Q},\vec{P})$, respectively] are identical. Indeed, Eq. (50) solves both the Moyal and the Hamiltonian equations of motion and thus we were not required to introduce a second set of ''classical'' coordinates $(\vec{Q},\vec{P})$.

VII. CONCLUSIONS

Using a time dependent extension of the generalized Weyl map we enlarged the set of possible phase space representations of quantum mechanics, derived a more general formula for the $\hbar$-deformations of the Poisson bracket and proved that there is a phase space representation where the quantum quasidistribution displays a causal dynamical structure. In this formulation the quantum behavior is displayed by the $*$-genfunctions (observables) sector alone. Such a property may lead to interesting applications in the field of the semiclassical limit of quantum mechanics given the fact that in the causal representation the quantum behavior has become, in fact, independent from the state of the system.

The comparison with the de Broglie Bohm formulation seems inevitable. In the de Broglie Bohm theory the source of quantum behavior is the quantum potential together with a modification of the momentum $*$-genvalue equation. The theory admits an interpretation in terms of causal (but not classical) trajectories. In the Wigner causal formulation the effect of the quantum potential has been replaced by further corrections in the observables ($*$-genfunctions) sector of the theory and the achievement was that the particle trajectories became fully classical. It is quite remarkable that this shift of the source of the quantum behavior (from the distributional to the observables sector) could be fully performed and it may lead to an alternative causal interpretation for quantum mechanics.

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Contextual approach to quantum mechanics and the theory of the fundamental prespace

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We constructed a Hilbert space representation of a contextual Kolmogorov model. This representation is based on two fundamental observables—in the standard quantum model these are the position and momentum observables. This representation has all distinguishing features of the quantum model. Our representation is not standard model with hidden variables. In particular, this is not a reduction of the quantum model to the classical one. © *2004 American Institute of Physics.*
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I. INTRODUCTION

We construct a representation of a Kolmogorovian contextual model in a Hilbert space. Complexes of physical conditions—contexts—are represented by complex amplitudes (or in the abstract framework by normalized vectors of a Hilbert space).

In the papers of Refs. 1–3 there was shown that by using non-Kolmogorovian probabilistic models (see Accardi[4–8] on the role of non-Kolmogorovian models in foundations of QM) such a representation can be constructed on the basis of a so called *contextual formula of total probability* for observables b and a:

$$p_C^b(x)=\sum_y \quad p_C^a(y) \quad p^{b/a}(x/y)$$

$$+2\sum_{y_1<y_2}\sqrt{p_C^a(y_1) \quad p_C^a(y_2) \quad p^{b/a}(x/y_1) \quad p^{b/a}(x/y_2)} \quad \cos\theta_C^{(y_1y_2)}(x), \tag{1}$$

where $p_C^a(y)=\mathbf{P}(a=y/C), p_C^b(x)=\mathbf{P}(b=x/C)$ are probabilities to observe values $a=y$ and $b=x$ under the complex of physical conditions—*context*—C and $p^{b/a}(x/y)=\mathbf{P}(b=x/a=y)$ are transition probabilities. A complex amplitude $\varphi_C^{b/a}(x)$ corresponding to the representation (1) gives the QM-representation of context C. Recently in the preprints[9] it was shown that we can do the same even in the conventional Kolmogorov framework by using the *contextual interpretation* of his measure-theoretical probabilistic model. This paper contains an extended presentation of ideas from Ref. 9.

We shall show that for a Kolmogorov probability space $\mathcal{K}=(\Omega,\mathcal{F},\mathbf{P})$ and a pair of *incompatible Kolmogorovian random variables* b and a we can construct a natural quantum representation. This representation is rigidly based on a pair of variables b and a—fundamental (for that concrete representation of physical reality) observables. In particular, the standard quantum representation is based on the *position and momentum observables*. There exists a map $J^{b/a}$ which maps contexts (represented by subsets of Ω) into quantum states≡complex b/a-transition amplitudes of probability. In some sense we came back to the original Hilbert's viewpoint to a wave function as a transition amplitude; see Ref. 10; see also Lande,[11] Accardi,[4] Ballentine,[12] and Gudder.[13]

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Points of Ω are interpreted as *fundamental physical parameters*. If you like HV... But the general HV-approach was so discredited by former investigations (since people wanted too much for such a HV-description) that we would not like even to refer to HV. We call Ω *prespace* and fundamental parameters—prepoints.

The main distinguishing feature of the representation map $J^{b/a}$ is the huge *compression of information*. In particular, every point represented in the conventional mathematical model of physical space by a vector $x \in \mathbf{R}^3$ is the image of a subset

$$B_x = \{\omega \in \Omega : b(\omega) = x\},$$

of Ω which can contain millions of prepoints. In the conventional quantum the representation of the prespace the fundamental variable $b = q$ is the position observable. We have a similar picture for the momentum observable. In the quantum model we consider "classical physical points" $x \in \mathbf{R}^3$ as represented by eigenvectors of the position operator. Thus by going from the "classical physical space" $\mathbf{R}^3$ to the quantum physical (Hilbert) space H and then to the prespace Ω we obtain finer and finer descriptions of reality.

Another distinguishing feature of the $J^{b/a}$-representation of the prespace Ω in the Hilbert space H is the creation of superpositions of "classical states." The origin of the quantum superposition can be very easily explained by our prespace model. For example, let us consider a context $C \subset \Omega$ such that $C \subset B_{x_1} \cup B_{x_2}, x_1, x_2 \in \mathbf{R}^3, x_1 \neq x_2$, but neither $C \subset B_{x_1}$ nor $C \subset B_{x_2}$. The image $\varphi_C = J^{b/a}(C) \in H$ is a quantum state describing a quantum system which is "in a superposition of the positions" x_1 and x_2.

In this model (as it was wanted by Einstein) *the Heisenberg uncertainty relation can be violated* for fundamental observables (e.g., the position and momentum) which are used for our classical and quantum representations of reality. Points ($\omega \in \Omega$) of the prespace are *dispersion free states*.

In our model only the two fundamental observables correspond to random variables on the prespace. Other quantum and classical observables have only some indirect relation to random variables on the prespace. So we could not consider such, e.g., quantum observables as real observables–functions of fundamental parameters. Nevertheless, for a wide class of quantum observables (including QM-Hamiltonians) we have the coincidence of averages with averages of corresponding random variables on Ω. Here we speak about averages with respect to the state $\varphi_C = J^{b/a}(C)$ and context C, respectively. In our model only quantum observables belonging to a special class [class $\mathcal{O}_+(a,b)$] have a realist interpretation.

We underline that our investigations have nothing to do with attempts to find some general probabilistic model which would contain Kolmogorov as well as quantum probabilities as particular cases, cf., e.g., Mackey,[14] Gudder,[13] Ludwig,[15] Devies and Lewis,[16] Ballentine,[12] and Hardy.[17] For us the main distinguishing feature of quantum theory is not a new ("quantum") behavior of probabilities, but a special way of the representation of (ordinary) probability.

By our model dispersion free states (e.g., position and momentum observables) can exist and *the Heisenberg's uncertainty principle can be violated*.

II. CONTEXTUAL FORMULA OF TOTAL PROBABILITY

Let $(\Omega, \mathcal{F}, \mathbf{P})$ be a Kolmogorov probability space.[18]

By the standard Kolmogorov axiomatics sets $A \in \mathcal{F}$ represent *events*. In our simplest model of *contextual probability* (Kolmogorovian contextual model) the same system of sets, $\mathcal{F}$, is used to represent complexes of experimental physical conditions—*contexts*. We can consider a set $C \in \mathcal{F}$ as a collection of physical parameters ω describing a complex of physical conditions. This is a context–interpretation of sets $C \in \mathcal{F}$.

By the event–interpretation of sets $A \in \mathcal{F}$ such a set A is a collection of physical parameters inducing the corresponding event (denoted by the same symbol A).

In principle, in a mathematical model events and contexts can be represented by different families of sets, see, e.g., Renye's model. We will not do this from the beginning. But later we will fix a proper subfamily of contexts $\mathcal{C}\subset\mathcal{F}$.

The conditional probability is mathematically defined by the Bayes' formula:

$$\mathbf{P}(A/C)=\frac{\mathbf{P}(AC)}{\mathbf{P}(C)},\quad \mathbf{P}(C)\neq 0.$$

In our contextual model this probability has the meaning of the probability of occurrence of the event A under the complex of physical conditions C. Thus it is not the probability of occurrence of the event A under the condition that the event C has occurred (as it is assumed in the Kolmogorov theory). (The reader might think that the difference in interpretations is negligible. But I would like to underline that this is the crucial point of all our considerations.)

Thus it would be more natural to call $\mathbf{P}(A/C)$ a *contextual probability* and not *conditional probability*. Roughly speaking, to find $\mathbf{P}(A/C)$ we should find parameters ω^A favoring the occurrence of the event A among parameters ω^C describing the complex of physical conditions C.

Let $\mathcal{A}=\{A_n\}$ be finite or countable complete group of inconsistent contexts:

$$A_iA_j=\varnothing,\quad i\neq j,\qquad \cup_i A_i=\Omega.$$

Let $B\in\mathcal{F}$ be an event and $C\in\mathcal{F}$ be a context and let $\mathbf{P}(C)>0$. We have the standard formula of total probability:

$$\mathbf{P}(B/C)=\frac{\mathbf{P}(BC)}{\mathbf{P}(C)}=\sum_n \frac{\mathbf{P}(BA_nC)\mathbf{P}(A_nC)}{\mathbf{P}(C)\mathbf{P}(A_nC)}$$

[if $\mathbf{P}(A_nC)>0$ for all n], and hence

$$\mathbf{P}(B/C)=\sum_n \mathbf{P}(A_n/C)\mathbf{P}(B/A_nC). \tag{2}$$

Of course, in the conventional Kolmogorov model we operate only with events. Thus, in spite of using the standard Kolmogorov measure-theoretical probabilistic formalism, from the very beginning we use a new interpretation of conditioning in this formalism. Instead of the conventional even-conditioning, we use *context-conditioning*. Thus there is nothing new from the mathematical viewpoint and the reader may be curious: Is it possible to find something new by using the same mathematical apparatus and by changing only the interpretation? Yes, we shall construct a totally new representation of the Kolmogorov model in a Hilbert space. This representation is nontrivial—Kolmogorovian (but contextual) random variables are represented by in general noncommutative operators.

In particular, let a and b be discrete random variables taking values $a_i, i=1,\ldots,k_a$ and $b_j, j=1,\ldots,k_b$, where $k_a, k_b<\infty$. We have

$$\mathbf{P}(b=b_i/C)=\sum_n \mathbf{P}(a=a_n/C)\mathbf{P}(b=b_i/a=a_n,C)\quad .$$

Let a measurement of the variable a disturb essentially physical systems $\omega\in\Omega$. Let us fix some complex of conditions (*context*) C. One cannot measure b and a simultaneously in the context C. Thus the probabilities $\mathbf{P}(b=b_i/a=a_n,C)$ are "hidden" (or ontic) probabilities. (We are not able to select parameters ω^{A_n} favouring to the realization of $a=a_n$ without to disturb context C.) However, we can measure the variable b in the context $A_n=\{\omega: a(\omega)=a_n\}$. Thus we cannot prepare for the context C systems ω such that we know that simultaneously $b(\omega)$

$=b_i, a(\omega)=a_n$, but we can prepare systems ω such that $a(\omega)=a_n$ and in this context we can perform the b-measurement. Hence the probabilities $\mathbf{P}(b=b_i/a=a_n)=\mathbf{P}(B_i/A_n)$ are well defined. Here

$$B_i=\{\omega\in\Omega: b(\omega)=b_i\} \quad \text{and} \quad A_n=\{\omega\in\Omega: a(\omega)=a_n\}.$$

I would like to modify the formula of total probability (2) by eliminating hidden probabilities $\mathbf{P}(b=b_i/a=a_n, C)$ and using only observable probabilities $\mathbf{P}(b=b_i/a=a_n)$.

Definition 1: (Context) *A set C belonging to $\mathcal{F}$ is said to be a context with respect to a complete group of inconsistent contexts $\mathcal{A}=\{A_n\}$ if $\mathbf{P}(A_nC)\neq 0$ for all n.*

We denote the set of all $\mathcal{A}$-contexts by the symbol $\mathcal{C}_{\mathcal{A}}$.

Definition 2: Let $\mathcal{A}=\{A_n\}$ and $\mathcal{B}=\{B_n\}$ be two complete groups of inconsistent contexts. They are said to be incompatible if $\mathbf{P}(B_nA_k)\neq 0$ for all n and k.

Thus $\mathcal{B}$ and $\mathcal{A}$ are incompatible iff every B_n is a context with respect to $\mathcal{A}$ and *vice versa*; see Appendix 1 for details.

Random variables a and b inducing incompatible complete groups $\mathcal{A}=\{A_n\}$ and $\mathcal{B}=\{B_k\}$ of inconsistent contexts are said to be *incompatible random variables*.

Theorem 1 (Interference formula of total probability): *Let $\mathcal{A}$ and $\mathcal{B}$ be incompatible and let C be a context with respect to $\mathcal{A}$. Then the following "interference formula of total probability" holds true for any $B\in\mathcal{B}$:*

$$\mathbf{P}(B/C)=\sum \mathbf{P}(A_n/C)\mathbf{P}(B/A_n)+2\sum_{n<m}\lambda_{nm}(B/\mathcal{A},C)\sqrt{\mathbf{P}(A_n/C)\mathbf{P}(A_m/C)\mathbf{P}(B/A_n)\mathbf{P}(B/A_m)}, \tag{3}$$

where

$$\lambda_{nm}(B/\mathcal{A};C)=\frac{\delta_{nm}(B/\mathcal{A};C)}{2\sqrt{\mathbf{P}(A_n/C)\mathbf{P}(B/A_n)\mathbf{P}(A_m/C)\mathbf{P}(B/A_m)}}$$

and

$$\delta_{nm}(B/\mathcal{A};C)=\frac{[\mathbf{P}(A_n/C)(\mathbf{P}(B/A_nC)-\mathbf{P}(B/A_n))+\mathbf{P}(A_m/C)(\mathbf{P}(B/A_mC)-\mathbf{P}(B/A_m))]}{k_a-1} \tag{4}$$

Proof: We have

$$\mathbf{P}(B/C)=\sum_n \mathbf{P}(A_n/C)(\mathbf{P}(B/A_nC)+\mathbf{P}(B/A_n)-\mathbf{P}(B/A_n))=\sum_n \mathbf{P}(A_n/C)\mathbf{P}(B/A_n)+\delta(B/\mathcal{A},C),$$

where

$$\delta(B/\mathcal{A},C)=\sum_n \mathbf{P}(A_n/C)(\mathbf{P}(B/A_nC)-\mathbf{P}(B/A_n)). \tag{5}$$

Finally, we remark that we can represent the perturbation term as the sum of perturbation terms corresponding to pairs of (A_n, A_m):

$$\delta(B/\mathcal{A},C)=\sum_{n<m}\delta_{nm}(B/\mathcal{A};C),$$

where $\delta_{nm}(B/\mathcal{A};C)$ is given by (4).

The $\lambda_{nm}(B/\mathcal{A},C)$ are called *coefficients of statistical disturbance*. Coefficients $\lambda_{nm}(B/\mathcal{A},C)$ describe disturbances of probabilities induced by filtrations with respect to values $a=a_n$ in the

context C. Depending on magnitudes of these coefficients we can rewrite the nonconventional formula of total probability in various forms that are useful for representing (3) as a transformation in a complex linear space or a Clifford modular; see Ref. 19 for details.

In our further investigations we will use the following result.

Lemma 1: Let conditions of Corollary 1 hold true. Then

$$\sum_k \delta(B_k/\mathcal{A},C)=0. \tag{6}$$

Proof: We have $1=\Sigma_k \mathbf{P}(B_k/C)=\Sigma_k\Sigma_n \mathbf{P}(A_n/C)\mathbf{P}(B_k/A_n)+\Sigma_k\delta(B_k/\mathcal{A},C)$. But $\Sigma_n(\Sigma_k \mathbf{P}(B_k/A_n))\mathbf{P}(A_n/C)=1$.

As a consequence of this lemma we have

$$\sum_k \sum_{l<m} \lambda_{lm}(B_k/\mathcal{A},C)\sqrt{\mathbf{P}(A_l/C)\mathbf{P}(A_m/C)\mathbf{P}(B_k/A_l)\mathbf{P}(B_k/A_m)}=0. \tag{7}$$

(1) Suppose that $a=a_n$ filtrations (in the context C) induce statistical disturbances having relatively small coefficients $\lambda_{nm}(B/\mathcal{A},C)$, namely, for every $B\in\mathcal{B}$,

$$|\lambda_{nm}(B/\mathcal{A},C)|\leqslant 1 \ .$$

[First we prepare a statistical ensemble O_C of physical systems ω under the complex of (e.g., physical) conditions C. Then we perform a measurement of the random variable a for elements of the ensemble O_C. Finally, we select all systems for which we obtained the value $a=a_n$.]

In this case we can introduce new statistical parameters $\theta_{nm}(B/\mathcal{A},C)\in[0,\pi]$ and represent the coefficients of statistical disturbance in the trigonometric form:

$$\lambda_{nm}(B/\mathcal{A},C)=\cos\theta_{nm}(B/\mathcal{A},C).$$

Parameters $\theta_{nm}(B/\mathcal{A},C)$ are said to be *relative phases* of an event B with respect to a complete group of inconsistent events $\mathcal{A}$ (in the context C).

In this case we obtain the following interference formula of total probability:

$$\mathbf{P}(B/C)=\sum_n \mathbf{P}(A_n/C)\mathbf{P}(B/A_n)+2\sum_{n<m}\cos\theta_{nm}(B/\mathcal{A},C)$$
$$\times\sqrt{\mathbf{P}(A_n/C)\mathbf{P}(A_m/C)\mathbf{P}(B/A_n)\mathbf{P}(B/A_m)}. \tag{8}$$

This is nothing other than the famous *formula of interference of probabilities*. [Typically this formula is derived by using the Hilbert space (unitary) transformation corresponding to the transition from one orthonormal basis to another and Born's probability postulate. The orthonormal basis under quantum consideration consist of eigenvectors of operators (noncommutative) corresponding to quantum physical observables a and b.] We demonstrated that in the opposite of the common (especially in quantum physics) opinion nontrivial interference of probabilities need not be related to some non-Kolmogorovian features of a probabilistic model. In our considerations everything is Kolmogorovian. The interference of probabilities is a consequence of the impossibility of using conditioning with respect to $\{a=a_n,C\}$ (to combine two contexts—C and a) for random variables a which measurement disturbs essentially physical systems $\omega\in\Omega$.

Starting from (8) we shall derive (for dichotomous random variables) Born's rule, construct for any context C a complex probability amplitude, introduce a Hilbert space structure on the space of complex amplitudes and represent random variables on the Kolmogorov probability space by (in general noncommutative) operators in the Hilbert space.

(2) Suppose that $a=a_n$ filtrations induce statistical disturbances having relatively large coefficients $\lambda_{nm}(B/\mathcal{A},C)$, namely, for every $B\in\mathcal{B}$,

$$|\lambda_{nm}(B/\mathcal{A},C)|\geqslant 1\ .$$

In this case we can introduce new statistical parameters $\theta_{nm}(B/\mathcal{A},C)\in[0,+\infty]$ and represent the coefficients of statistical disturbance in the trigonometric form

$$\lambda_{nm}(B/\mathcal{A},C)=\pm\cosh\theta_{nm}(B/\mathcal{A},C).$$

Parameters $\theta_{nm}(B/\mathcal{A},C)$ are said to be hyperbolic *relative phases* of an event B with respect to a complete group of inconsistent events $\mathcal{A}$ (in the context C).

In this case we obtain the following interference formula of total probability:

$$\mathbf{P}(B/C)=\sum_n \mathbf{P}(A_n/C)\mathbf{P}(B/A_n)\pm 2\sum_{n<m}\cosh\theta_{nm}(B/\mathcal{A},C)$$
$$\times\sqrt{\mathbf{P}(A_n/C)\mathbf{P}(A_m/C)\mathbf{P}(B/A_n)\mathbf{P}(B/A_m)}. \tag{9}$$

(3) Suppose that $a=a_n$ filtrations induce for some n statistical disturbances having relatively small coefficients $\lambda_{nm}(B/\mathcal{A},C)$ and for other n statistical disturbances having relatively large coefficients $\lambda_{nm}(B/\mathcal{A},C)$. Here we have the interference formula of total probability containing trigonometric as well as hyperbolic interference terms.

III. DICHOTOMOUS RANDOM VARIABLES

We study only models with *trigonometric interference*. We set

$$\mathcal{C}=\{C\in\mathcal{C}_{\mathcal{A}}:|\lambda(B_j/\mathcal{A},C)|\leqslant 1\}.$$

We call elements of $\mathcal{C}$ trigonometric contexts. We shall see that QM can be interpreted as a representation of trigonometric contexts. We can also introduce hyperbolic contexts which can be represented in a hyperbolic Hilbert space; see Ref. 19.

A. Interference and complex probability amplitude, Born's rule

Let us study in more detail the case of incompatible dichotomous random variables $a=a_1,a_2,b=b_1,b_2$. We set $Y=\{a_1,a_2\},X=\{b_1,b_2\}$ ("spectra" of random variables a and b). Let $C\in\mathcal{C}$ be a context for both random variables a and b. We set

$$p_C^a(y)=\mathbf{P}(a=y/C),p_C^b(x)=\mathbf{P}(b=x/C),p(x/y)=\mathbf{P}(b=x/a=y),$$

$x\in X,y\in Y$. The interference formula of total probability (8) can be written in the following form:

$$p_c^b(x)=\sum_{y\in Y}p_C^a(y)p(x/y)+2\cos\theta_C(x)\sqrt{\prod_{y\in Y}p_C^a(y)p(x/y)}\ , \tag{10}$$

where $\theta_C(x)=\theta(b=x/\mathcal{A},C)=\arccos\lambda(b=x/\mathcal{A},C),x\in X,C\in\mathcal{C}$. We remark that in the case of dichotomous random variables:

$$\delta(b=x/\mathcal{A},C)=p_c^b(x)-\sum_{y\in Y}p_C^a(y)p(x/y)$$

and

$$\lambda(b=x/\mathcal{A},C)=\frac{\delta(b=x/\mathcal{A},C)}{2\sqrt{\prod_{y\in Y}p_C^a(y)p(x/y)}}.$$

By using the elementary formula:

$$D=A+B+2\sqrt{AB}\cos\theta=|\sqrt{A}+e^{i\epsilon\theta}\sqrt{B}|^2,$$

for $A,B>0,\epsilon=\pm 1,\theta\in[0,\pi]$. we can represent the probability $p_C^b(x)$ as the square of the complex amplitude:

$$p_C^b(x)=|\varphi_C(x)|^2 \quad . \tag{11}$$

We fix some pair of signs $\epsilon(x),x\in X$ [e.g., $\epsilon(b_1)=-1$ and $\epsilon(b_2)=+1$]. We set

$$\varphi(x)\equiv\varphi_C(x)=\sqrt{p_C^a(a_1)p(x/a_1)}+e^{\epsilon(x)\theta_C(x)}\sqrt{p_C^a(a_2)p(x/a_2)} \quad . \tag{12}$$

We denote the space of functions: $\varphi:X\to\mathbf{C}$ by the symbol $E=\Phi(X,\mathbf{C})$. Since $X=\{b_1,b_2\}$, the E is the two dimensional complex linear space. Dirac's δ-functions $\{\delta(b_1-x),\delta(b_2-x)\}$ form the canonical basis in this space. For each $\varphi\in E$ we have

$$\varphi(x)=\varphi(b_1)\,\delta(b_1-x)+\varphi(b_2)\,\delta(b_2-x).$$

By using the representation (12) we construct the map

$$J^{b/a}:\mathcal{C}\to\Phi(X,\mathbf{C}). \tag{13}$$

The $J^{b/a}$ maps contexts (complexes of, e.g., physical conditions) into complex amplitudes. The representation (11) of probability as the square of the absolute value of the complex (b/a)-amplitude is nothing other than the famous *Born rule*.

Remark 1: We underline that the complex linear space representation (12) of the set of contexts $\mathcal{C}$ is based on a pair (a,b) of incompatible (Kolmogorovian) random variables. Here $\varphi_C=\varphi_C^{b/a}$.

The complex amplitude $\varphi_C(x)$ can be called a *wave function* of the complex of physical conditions, context C; cf. Refs. 1–3, or a *pure state*.

We recall that we obtained complex probability amplitudes in the conventional Kolmogorov framework without appealing to the standard wave or Hilbert space arguments. As we shall see, the map $J^{b/a}$ gives a *quantum-like representation* of the conventional Kolmogorov probability model.

In principle, we can represent each context $C\in\mathcal{C}$ by a family of complex amplitudes:

$$\varphi(x)\equiv\varphi_C(x)=\sum_{y\in Y}\sqrt{p_C^a(y)p(x/y)}e^{i\xi_C(x/y)}, \tag{14}$$

such that

$$\xi_C(x/a_1)-\xi_C(x/a_2)=\theta_C(x).$$

For such complex amplitudes we also have Born's rule (11). However, to simplify considerations we shall consider only the representation (12) and the map (13) induced by this representation.

B. Hilbert space representation of Born's rule

We set

$$e_x^b(\cdot)=\delta(x-\cdot).$$

The representation (11) can be rewritten in the following form:

$$p_C^b(x)=|(\varphi_C,e_x^b)|^2 \quad , \tag{15}$$

where the scalar product in the space $E=\Phi(X,C)$ is defined by the standard formula:

$$(\varphi,\psi)=\sum_{x\in X}\varphi(x)\overline{\psi}(x).$$

The system of functions $\{e_x^b\}_{x\in X}$ is an orthonormal basis in the Hilbert space $H=(E,(\cdot,\cdot))$.

Let $X\subset R$. By using the Hilbert space representation of Born's rule (15) we obtain the Hilbert space representation of the expectation of the (Kolmogorovian) random variable b:

$$E(b/C)=\sum_{x\in X}xp_C^b(x)=\sum_{x\in X}x|\varphi_C(x)|^2=(\hat{b}\varphi_C,\varphi_C)\quad, \tag{16}$$

where $\hat{b}:\Phi(X,\mathbf{C})\to\Phi(X,\mathbf{C})$ is the multiplication operator. This operator can also be determined by its eigenvectors: $\hat{b}e_x^b=xe_x^b, x\in X$.

We set

$$u_j^a=\sqrt{p_C^a(a_j)},u_j^b=\sqrt{p_C^b(b_j)},p_{ij}=p(b_j/a_i),u_{ij}=\sqrt{p_{ij}},\theta_j=\theta_C(b_j),\epsilon_j=\epsilon(b_j)\quad.$$

We remark that the coefficients u_j^a,u_j^b depend on a context C; so $u_j^a=u_j^a(C),u_j^b=u_j^b(C)$. We also consider the *matrix of transition probabilities* $\mathbf{P}^{b/a}=(p_{ij})$. It is always a *stochastic matrix*. (So $p_{i1}+p_{i2}=1,i=1,2.$) We have, see (14), that

$$\varphi_C=v_1^be_1^b+v_2^be_2^b,\quad\text{where}\quad v_j^b=u_1^au_{1j}+u_2^au_{2j}e^{i\epsilon_j\theta_j}\quad.$$

So

$$p_C^b(b_j)=|v_j^b|^2=|u_1^au_{1j}+u_2^au_{2j}e^{i\epsilon_j\theta_j}|^2. \tag{17}$$

This is the *interference representation of probabilities* that is used, e.g., in quantum formalism. [By starting with the general representation (14) we obtain $v_j^b=u_1^au_{1j}e^{i\xi_{1j}}+u_2^au_{2j}e^{i\xi_{2j}}$ and the interference representation $p_C^b(b_j)=|v_j^b|^2=|u_1^au_{1j}e^{i\xi_{1j}}+u_2^au_{2j}e^{i\xi_{2j}}|^2$.] We recall that we obtained (17) starting with the interference formula of total probability (10).

C. Born's rule and Hilbert space representations

We would like to obtain (17) by using the standard quantum procedure, namely, transition from the orthonormal basis $\{e_j^b\}$ corresponding the b-variable to a new basis $\{e_j^a\}$ which corresponds to the a-variable. Thus we would like to have Born's rule not only in the b-representation, but also in the a-representation. As we shall see, we cannot be lucky in the general case. Starting from two arbitrary incompatible (Kolmogorovian) random variables a and b we obtained a complex linear space representation of the probabilistic model which is essentially more general than the standard quantum representation. In our (more general) linear representation the "dual variable" a need not be represented by a symmetric operator (matrix) in the Hilbert space H generated by the b.

For any context C_0, we can represent the $\varphi=\varphi_{C_0}$ in the form

$$\varphi=u_1^ae_1^a+u_2^ae_2^a, \tag{18}$$

where

$$e_1^a=(u_{11},\quad u_{12})\quad e_2^a=(e^{i\epsilon_1\theta_1}u_{21},\quad e^{i\epsilon_2\theta_2}u_{22}). \tag{19}$$

Here $\{e_i^a\}$ is a system of vectors in E corresponding to the a-observable. We suppose that vectors $\{e_i^a\}$ are linearily independent, so $\{e_i^a\}$ is a basis in E. We have

$$e_1^a = v_{11}e_1^b + v_{12}e_2^b, \qquad e_2^a = v_{21}e_1^b + v_{22}e_2^b.$$

Here $V=(v_{ij})$ is the matrix corresponding to the transformation of complex amplitudes: $v_{11}=u_{11}, v_{21}=u_{21}$ and $v_{12}=e^{i\epsilon_1\theta_1}u_{21}, v_{22}=e^{ii\epsilon_2\theta_2}u_{22}$.

We would like to find a class of matrixes V such that Born's rule (in the Hilbert space form), see (15), holds true also in the a-basis:

$$p_C^a(a_j) = |(\varphi, e_j^a)|^2 \quad .$$

By (18) we have Born's rule iff $\{e_i^a\}$ was an *orthonormal basis*, i.e., the V is a *unitary* matrix. Since we study the two-dimensional case (i.e., dichotomous random variables), $V \equiv V^{b/a}$ is unitary iff the matrix of transition probabilities $\mathbf{P}^{b/a}$ is *double stochastic*. (So it is stochastic and, moreover, $p_{1j}+p_{2j}=1, j=1,2$.)

However, there is some difficulty. In fact, we constructed the a-basis starting with one fixed context C_0. The basis e_j^a depends on C_0 [via the phases $\theta_{C_0}(x)$]: $e_j^a = e_j^a(C_0)$. In principle, the validity of Born's rule for the context C_0 in the basis $e_j^a(C_0)$ need not imply this rule for any context C in the same basis $e_j^a(C_0)$. We shall see that for double stochastic matrices of transition probabilities (and only such matrices) we can really construct the a-representation starting with some fixed C_0. However, we should choose signs $\epsilon(x)$ in the representation (12) in a special way. We recall that the map $J^{b/a}$ was constructed for fixed signs ϵ_1 and ϵ_2; so $J^{b/a}=J^{b/a}(\epsilon_1,\epsilon_2)$.

We now investigate this problem. We remind the reader that we constructed the matrix V by using the fixed context C_0, so $V=V(C_0)$. For any $C \in \mathcal{C}$, we would like to represent the wave function as

$$\phi_C = v_1^a(C)e_1^a(C_0) + v_2^a(C)e_2^a(C_0), \quad \text{where} \quad |v_j^a(C)|^2 = p_C^a(a_j). \tag{20}$$

It is clear that, for any $C \in \mathcal{C}$, we can represent the wave function as

$$\phi_C(b_1) = u_1^a(C)v_{11}(C_0) + e^{i\epsilon_1[\theta_C(b_1)-\theta_{C_0}(b_1)]}u_2^a(C)v_{12}(C_0),$$

$$\phi_C(b_2) = u_1^a(C)v_{21}(C_0) + e^{i\epsilon_1[\theta_C(b_2)-\theta_{C_0}(b_2)]}u_2^a(C)v_{22}(C_0).$$

Thus to obtain (20) we should have

$$\epsilon_1[\theta_C(b_1)-\theta_{C_0}(b_1)] = \epsilon_2[\theta_C(b_2)-\theta_{C_0}(b_2] \pmod{2\pi}, \tag{21}$$

for any pair of contexts C_0 and C_1. Thus

$$\Delta(C) = \epsilon_1\theta_C(b_1) - \epsilon_2\theta_C(b_2) = \Delta \tag{22}$$

should be a constant (mod 2π) on $\mathcal{C}$.

D. The role of the condition of double stochasticity

Lemma 2: Let a and b be incompatible random variables and let the matrix of transition probabilities $\mathbf{P}^{b/a}$ *be double stochastic. Then*

$$\cos\theta_C(b_1) = -\cos\theta_C(b_2), \tag{23}$$

for any context $C \in \mathcal{C}$.

Proof: By Lemma 1 we have

$$\sum_{x\in X} \cos\theta_C(x)\sqrt{\prod_{y\in Y} p_c^a(y)p(x/y)} = 0.$$

But for a double stochastic matrix $(p(x/y))$ we have

$$\prod_{y\in Y} p_c^a(a_1)p(b_1/y)=\prod_{y\in Y} p_c^a(a_2)p(b_2/y).$$

Since random variables a and b are incompatible, we have $p(x/y)\neq 0, x\in X, y\in Y$. Since $C\in\mathcal{C}_{\mathcal{A}}$, we have $p_C^a(y)\neq 0, y\in Y$. We obtain (23).

Thus for a double stochastic matrix $\mathbf{P}^{b/a}$ we can choose

$$\theta_C(b_2)=\pi-\theta_C(b_1). \tag{24}$$

Proposition 1: Let the conditions of Lemma 2 hold true. Then the condition (22) holds true for any Kolmogorov model iff $\epsilon_1=-\epsilon_2$.

Proof: By (24) we obtain

$$\Delta(C)=(\epsilon_1+\epsilon_2)\theta_C(b_1)-\epsilon_2\pi.$$

Let us denote the unit sphere in the Hilbert space $E=\Phi(X,\mathbf{C})$ by the symbol S. The map $J^{b/a}:\mathcal{C}\to S$ need not be a surjection (injection); see the examples in Sec. VI. In general the set of pure states corresponding to a Kolmogorovian model,

$$S_{\mathcal{C}}\equiv S_{\mathcal{C}}^{b/a}=J^{b/a}(\mathcal{C}),$$

is just a proper subset of the sphere S. The structure of the set of pure states $S_{\mathcal{C}}$ is determined by the Kolmogorov model.

We remark that for a double stochastic matrix $\mathbf{P}^{b/a}$ (and $\epsilon_1=-\epsilon_2$) the condition (22) does not depend on the set $\mathcal{C}$ (i.e., a Kolmogorov model). Here always $\Delta=\pi$. We also remark that, in fact, only double stochastic matrices $\mathbf{P}^{b/a}$ has such a property. By using calculations which have been done in the proof of Lemma 1 we obtain the following more general result.

Lemma 2a: Let a and b be incompatible random variables. Then for any context $C\in\mathcal{C}$ *the following equality holds true*:

$$\cos\theta_C(b_1)=-k\cos\theta_C(b_2), \tag{25}$$

where

$$k\equiv k^{b/a}=\sqrt{\frac{p_{12}p_{22}}{p_{11}p_{21}}}.$$

Proposition 2: Let $k>0$ *be a real number and let angles* $\theta_1,\theta_2\in[0,\pi]$ *be connected by (22). If for all* $\theta_2\in[0,\pi]$,

$$\cos\theta_1=-k\cos\theta_2,$$

then $k=1$ *and* $\Delta=\pi$.

Proof: By (22) we have $\theta_1=\epsilon_1\Delta+\epsilon_1\epsilon_2\theta_2$. Thus $\cos(\epsilon_1\Delta+\epsilon_1\epsilon_2\theta_2)=-k\cos\theta_2$ for all $\theta_2\in[0,\pi]$. So $\cos(\Delta+\epsilon_2\theta_2)=-k\cos\theta_2$. Let $\theta_2=\epsilon_2(-\Delta+\pi/2)$. So $\cos(-\Delta+\pi/2)=0$. Thus $\Delta=0$ or $\Delta=\pi$. Let $\Delta=0$. Then $\cos\theta=-k\cos\theta$ for any $\theta\in[0,\pi]$. This contradicts the positivity of k. So $\Delta=\pi$ and $k=1$. To get both $\theta_1,\theta_2\in[0,\pi]$ we should choose $\epsilon_1=-\epsilon_2$.

We also remark that $k^{b/a}=1$ iff $\mathbf{P}^{b/a}$ is double stochastic.

E. Extension of the Hilbert space representation map

The sets A_i are not contexts with respect to $\mathcal{A}$, since $\mathbf{P}(A_1A_2)=0$. Thus $J^{b/a}(A_i)$ cannot be defined by (12). It is natural to extend the map $J^{b/a}$ to sets A_i by setting

$$J^{b/a}(A_i)=e_i^a,\quad i=1,2.$$

We set

$$\overline{\mathcal{C}}=\mathcal{C}\cup\mathcal{A}.$$

Thus we have constructed the Hilbert space representation:

$$J^{b/a}:\overline{\mathcal{C}}\to S.$$

We set $S_{\overline{\mathcal{C}}}=J^{b/a}\overline{\mathcal{C}}$.

F. Nonsensitive contexts

Let $\delta(B_i/\mathcal{A},C)=0,i=1,2$. So $\lambda(B_i/\mathcal{A},C)=0$ and, hence, $\theta(B_i/\mathcal{A},C)=\pi/2$. Here (for $x\in X$)

$$\varphi_C(x)=J^{b/a}(C)(x)=\sqrt{p_C^a(a_1)p(x/a_1)}+e^{i\epsilon(x)(\pi/2)}\sqrt{p_C^a(a_2)p(x/a_2)}. \tag{26}$$

Thus

$$\varphi_C(x)=\sqrt{p_C^a(a_1)p(x/a_1)}+\epsilon(x)i\sqrt{p_C^a(a_2)p(x/a_2)}. \tag{27}$$

We set

$$\mathcal{C}_0=\{C\in\mathcal{C}:\delta(B_j/\mathcal{A},C)=0\}.$$

Contexts $C\in\mathcal{C}_0$ are said to be b/a-nonsensitive contexts. These are complexes of physical (or, e.g., social) conditions C such that a measurement of a under C does not disturb the probability distribution of b. We remark that Ω always belong to $\mathcal{C}_0$. However, in general $\mathcal{C}_0\neq\{\Omega\}$; see Sec. VI.

G. Noninjectivity of the Hilbert space representation map

Let $C_1,C_2\in\mathcal{C}$ be contexts such that probability distributions of random variables a and b under C_1 and C_2, respectively, coincide:

$$p_{C_1}^a(y)=p_{C_2}^a(y),y\in Y,\quad p_{C_1}^b(x)=p_{C_2}^b(x),x\in X.$$

In such a case $\delta(b=x/\mathcal{A},C_1)=\delta(b=x/\mathcal{A},C_2)$. Thus corresponding phases also coincide: $\theta(b=x/\mathcal{A},C_1)=\theta(b=x/\mathcal{A},C_2)$. Hence $\phi_{C_1}(x)=\phi_{C_2}(x),x\in X$, and $J^{b/a}(C_1)=J^{b/a}(C_2)$; see Sec. VI for examples.

H. Nonquantum Hilbert space representations of Kolmogorovian models

Of course, for arbitrary random variables a and b the matrix $\mathbf{P}^{b/a}$ need not be double stochastic. Thus a representation of probabilities by vectors in a *single Hilbert space* we can obtain for a very restricted class of random variables. In particular, such random variables are considered in quantum theory (in the formalism of Dirac–von Neumann). In general, for each random variable we should introduce its own scalar product and corresponding Hilbert space:

$H_b=(E,(\cdot,\cdot)_b)$, $H_a=(E,(\cdot,\cdot)_a),\ldots$, where

$$(\varphi,\psi)_b=\sum_j v_j^b\overline{w}_j^b,\quad \text{for}\quad \varphi=\sum_j v_j^b e_j^b,\psi=\sum_j w_j e_j^b$$

and

$$(\varphi,\psi)_a=\sum_j v_j^a\overline{w_j^a},\quad \text{for}\quad \varphi=\sum_j v_j^a e_j^a,\psi=\sum_j w_j^a e_j^a.$$

The Hilbert spaces $H_b,H_a,\ldots,$ give the b-representation, the a-representation, ... Thus $p_C^b(b_j)=|(\varphi,e_j^b)_b|^2$ and $p_C^a(a_j)=|(\varphi,e_j^a)_a|^2$ and so on. In the H_a we have

$$E(a/C)=\sum_{y\in Y} yp_C^a(y)=a_1|(\varphi_C,e_1^a)_a|^2+a_2|(\varphi_C,e_2^a)_a|^2=(\hat{a}\varphi_C,\varphi_C)_a\ ,$$

where the operator $\hat{a}:E\to E$ is determined by its eigenvectors: $\hat{a}e_j^a=a_je_j^a$.

Of course, the representation of random variables by linear operators is just a convenient mathematical tool to represent the average of a random variable by using only the Hilbert space structure. We recall that we started with purely ''classical'' Kolmogorovian random variables.

As in the conventional quantum formalism we can also consider the map

$$\tilde{J}^{b/a}:\overline{\mathcal{C}}\to\tilde{\Phi}(X,\mathbf{C}).\tag{28}$$

Here $\tilde{\Phi}(X,\mathbf{C})$ is the space of equivalent classes of functions under the equivalence relation: φ equivalent ψ iff $\varphi=t\psi$, $t\in\mathbf{C}$, $|t|=1$, and $\tilde{J}^{b/a}(C)=t\phi_C$, $t\in\mathbf{C}$, $|t|=1$, where $C\in\overline{\mathcal{C}}$.

Conclusion: In the contextual probabilistic approach we can construct a natural map from the set of contexts into the unit sphere of the complex Hilbert space. Such a map is determined by a pair a,b of incompatible random variables. Unitarity of the matrix $V^{b/a}$ of transition from the basis $\{e_i^a\}$ to the basic $\{e_i^b\}$ (these basis correspond to random variables a and b, respectively) is equivalent to the possibility of using Born's rule both in the a and b representations. In general (i.e., for an arbitrary set of contexts) such a construction can be realized only for a **double stochastic matrix** *of transition probabilities*.

Everywhere below we restrict our considerations to the case in which the matrix of transition probabilities $\mathbf{P}^{b/a}$ is *double stochastic*.

IV. NONCOMMUTATIVITY OF OPERATORS REPRESENTING KOLMOGOROVIAN RANDOM VARIABLES

We consider in this section the case of real valued random variables. Here the spectra of random variables b and a are subsets of $\mathbf{R}$.

We set $q_1=\sqrt{p_{11}}=\sqrt{p_{22}}$ and $q_2=\sqrt{p_{12}}=\sqrt{p_{21}}$.

Thus the vectors of the a-basis, see (19), have the following form:

$$e_1^a=(q_1,q_2),\quad e_2^a=(e^{i\epsilon_1\theta_1}q_2,e^{i\epsilon_2\theta_2}q_1)\ .$$

Since $\theta_1+\theta_2=\pi$, we get $e_2^a=e^{i\epsilon_2\theta_2}(-q_2,q_1)$. The factor $e^{i\epsilon_2\theta_2}$ does not play any role in probabilistic considerations. Hence we can work in the new basis:

$$e_1^a=(q_1,q_2),\quad e_2^a=(-q_2,q_1).$$

We now find matrices of operators $\hat{a}$ and $\hat{b}$ in the b-representation. The latter one is diagonal. For $\hat{a}$ we have $\hat{a}=V\,\mathrm{diag}(a_1,a_2)V^\star$, where $v_{11}=v_{22}=q_1,v_{21}=-v_{12}=q_2$. Thus

$$a_{11}=a_1q_1^2+a_2q_2^2,\ \ a_{22}=a_1q_2^2+a_2q_1^2,\ \ a_{12}=a_{21}=(a_1-a_2)q_1q_2.$$

Hence

$$[\hat{b},\hat{a}]=\hat{m},$$

where $m_{11}=m_{22}=0$ and $m_{12}=-m_{21}=(a_1-a_2)(b_2-b_1)q_1q_2$. Since $a_1\neq a_2, b_1\neq b_2$ and $q_j\neq 0$, we have $\hat{m}\neq 0$.

V. THE ROLE OF SIMULTANEOUS DOUBLE STOCHASTICITY OF $P^{b/a}$ AND $P^{a/b}$

Starting with the b-representation—complex amplitudes $\phi_C(x)$ defined on the spectrum (range of values) of a random variable b—we constructed the a-representation. This construction is natural (i.e., reproduce Born's probability rule) only in the case in which $\mathbf{P}^{b/a}$ is double stochastic. We would like to have a symmetric model. So by starting with the a-representation—complex amplitudes $\phi_C(y)$ defined on the spectrum (range of values) of a random variable a—we would like to construct the natural b-representation. Thus both matrices of transition probabilities $\mathbf{P}^{b/a}$ and $\mathbf{P}^{a/b}$ should be double stochastic.

Theorem 2: *Let the matrix* $\mathbf{P}^{b/a}$ *be double stochastic. The contexts* B_1, B_2 *belong to* $\mathcal{C}$ *iff the matrix* $\mathbf{P}^{a/b}$ *is double stochastic.*

Proof: We have

$$\lambda(B_2/\mathcal{A},B_1)=-\frac{\mu_1^2+\mu_2^2}{2\mu_1\mu_2},$$

where $\mu_j=\sqrt{p^a_{B_1}(a_j)p(b_2/a_j)}$. So $\lambda(B_2/\mathcal{A},B_1)\geqslant 1$ and we have the trigonometric behavior only in the case $\mu_1=\mu_2$. Thus $p^a_{B_1}(a_1)p(b_2/a_1)=p^a_{B_1}(a_2)p(b_2/a_2)$. In this case $\lambda(B_2/\mathcal{A},B_1)=-1$, so $\theta(B_2/\mathcal{A},B_1)=\pi$, and consequently $\theta(B_1/\mathcal{A},B_1)=0$. We pay attention to the fact that $p^a_{B_i}(a_j)=p^{a/b}(a_j/b_i)\equiv p(a_j/b_i)$. Thus we have

$$p(a_1/b_1)p(b_2/a_1)=p(a_2/b_1)p(b_2/a_2). \tag{29}$$

In the same way by using conditioning with respect to B_2 we obtain

$$p(a_1/b_2)p(b_1/a_1)=p(a_2/b_2)p(b_1/a_2).$$

By using the double stochasticity of $\mathbf{P}^{b/a}$ we can rewrite the last equality as

$$p(a_1/b_2)p(b_2/a_2)=p(a_2/b_2)p(b_2/a_1). \tag{30}$$

Thus by (29) and (30) we have

$$\frac{p(a_1/b_2)}{p(a_2/b_1)}=\frac{p(a_2/b_2)}{p(a_1/b_1)}.$$

Hence $p(a_1/b_2)=tp(a_2/b_1)$ and $p(a_2/b_2)=tp(a_1/b_1), t>0$. But $1=p(a_1/b_2)+p(a_2/b_2)=t[p(a_2/b_1)+p(a_1/b_1)]=t$.

To finish the proof we need the following well known result.

Lemma 3: Both matrices of transition probabilities $\mathbf{P}^{b/a}$ *and* $\mathbf{P}^{a/b}$ *are double stochastic iff the transition probabilities are symmetric, i.e.,*

$$p(b_i/a_j)=p(a_j/b_i), \quad i,j=1,2. \tag{31}$$

This is equivalent that random variables a and b have the uniform probability distribution: $p^a(a_i)=p^b(b_i)=1/2$, $i=1,2$.

This lemma has important physical consequences. A natural (Bornian) Hilbert space representation of contexts can be constructed only on the basis of a pair of (incompatible) uniformly distributed random variables.

Lemma 4: Let both matrices $\mathbf{P}^{b/a}$ *and* $\mathbf{P}^{a/b}$ *be double stochastic. Then*

$$\lambda(B_i/\mathcal{A},B_i)=1. \tag{32}$$

Proof: Here $\delta(B_i/\mathcal{A},B_i)=1-p(b_i/a_1)p(a_1/b_i)-p(b_i/a_2)p(a_2/b_i)=1-p(a_1/b_i)^2-p(a_2/b_i)^2=2p(a_1/b_i)p(a_2/b_i)$. Thus $\lambda(B_i/\mathcal{A},B_i)=1$.

By (32) we have

$$\lambda(B_i/\mathcal{A},B_j)=-1, i\neq j.$$

Thus

$$\theta(B_i/\mathcal{A},B_i)=0 \text{ and } \theta(B_i/\mathcal{A},B_j)=\pi, i\neq j.$$

Proposition 2: Let both matrices of transition probabilities $\mathbf{P}^{b/a}$ *and* $\mathbf{P}^{a/b}$ *be double stochastic. Then*

$$J^{b/a}(B_j)(x)=\delta(b_j-x), x\in X, \quad \text{and} \quad J^{a/b}(A_j)(y)=\delta(a_j-y), y\in Y.$$

Proof: Because $\theta(B_1/\mathcal{A},B_1)=0$ we have

$$J^{b/a}(B_1)(b_1)=\sqrt{p(a_1/b_1)p(b_1/a_1)}+e^{i0}\sqrt{p(a_2/b_1)p(b_1/a_2)}=p(a_1/b_1)+p(a_2/b_1)=1.$$

Because $\theta(B_2/\mathcal{A},B_1)=\pi$ we have

$$\begin{aligned} J^{b/a}(B_1)(b_2)&=\sqrt{p(a_1/b_1)p(b_2/a_1)}+e^{i\pi}\sqrt{p(a_2/b_1)p(b_2/a_2)}\\ &=\sqrt{p(a_1/b_1)}(\sqrt{p(b_2/a_1)}-\sqrt{p(a_2/b_1)})=0. \end{aligned}$$

Thus in this case,

$$J^{b/a}(B_i)=e_i^b, \quad i=1,2.$$

VI. EXAMPLE OF THE HILBERT SPACE REPRESENTATION OF THE CONTEXTUAL KOLMOGOROVIAN MODEL

We consider an example of a Kolmogorov probability space and a pair of dichotomous random variables a,b which are incompatible. In this example the set of contexts with nontrivial disturbance term $\delta, \delta\neq 0$, is nonempty, so $\mathcal{C}_0\neq\mathcal{C}$.

A. Kolmogorov probability space and incompatible random variables

We find the image $S_{\mathcal{C}}$ of the set of contexts $\mathcal{C}$ in the Hilbert sphere $S\subset E=\Phi(X,C)$. In this example $S_{\mathcal{C}}$ is a proper subset of the sphere S. The Hilbert space representation map $J^{b/a}$ is not injective. Random variables a and b are represented by symmetric operators in the Hilbert space E. They do not commute.

Let $\Omega=\{\omega_1,\omega_2,\omega_3,\omega_4\}$ and $\mathbf{P}(\omega_j)=p_j>0, \Sigma_{j=1}^4 p_j=1$. Let

$$A_1=\{\omega_1,\omega_2\}, A_2=\{\omega_3,\omega_4\},$$

$$B_1=\{\omega_1,\omega_4\}, B_2=\{\omega_2,\omega_3\}.$$

Let $p_1=p_3=q<\frac{1}{2}$ and $p_2=p_4=(1-2q)/2$. We denote this Kolmogorov probability space by the symbol $\mathcal{K}(q)$.

Here $\mathbf{P}(A_1)=\mathbf{P}(A_2)=\mathbf{P}(B_1)=\mathbf{P}(B_2)=\frac{1}{2}$. So the random variables a and b are uniformly distributed. Thus both matrices of transition probabilities $\mathbf{P}^{b/a}$ and $\mathbf{P}^{a/b}$ are double stochastic. Here

$$\mathbf{P}^{b/a}=\mathbf{P}^{a/b}=\begin{pmatrix} 2q & 1-2q \\ 1-2q & 2q \end{pmatrix}.$$

We have the symmetry condition $\mathbf{P}(B_i/A_j)=\mathbf{P}(A_j/B_i)$.

B. Hilbert space representation of contexts

We choose $\epsilon_1=-1$ and $\epsilon_2=+1$ to fix the map $J^{b/a}$. We start with two point contexts.

(a) Let $C=C_{24}=\{\omega_2,\omega_4\}$. Here $\mathbf{P}(C)=1-2q$, $\mathbf{P}(B_j/C)=\mathbf{P}(A_j/C)=\frac{1}{2}$. Thus $\delta=0$. By using the representation (27), we obtain

$$\varphi_{C_{24}}(x)=\begin{cases}\sqrt{q}-i\sqrt{\dfrac{1-2q}{2}}, & x=b_1;\\ \sqrt{\dfrac{1-2q}{2}}+i\sqrt{q}, & x=b_2.\end{cases} \tag{33}$$

(b) Let $C=C_{13}=\{\omega_1,\omega_3\}$. Here everything is as in (a). So we have $\varphi_{C_{13}}=\varphi_{C_{24}}$ Thus $J^{b/a}$ is not injective: $J^{b/a}(C_{24})=J^{b/a}(C_{13})$.

(c) Let $C=C_{14}=\{\omega_1,\omega_4\}=B_1$. By general theory we have $\varphi_{C_{14}}(x)=\delta(b_1-x)=e_1^b$. In the same way, $\varphi_{C_{23}}=\delta(b_2-x)=e_2^b$.

To find the Hilbert space representation of sets $C=C_{12}=\{\omega_1,\omega_2\}=A_1$ and $C=C_{34}=\{\omega_3,\omega_4\}=A_2$ we have to construct the basis $\{e_j^a\}$. We can choose

$$e_1^a=\begin{pmatrix}\sqrt{2q}\\ \sqrt{1-2q}\end{pmatrix},\quad e_2^a=\begin{pmatrix}-\sqrt{1-2q}\\ \sqrt{2q}\end{pmatrix}.$$

(d) Let $C=C_{123}=\{\omega_1,\omega_2,\omega_3\}$. Here $\mathbf{P}(C)=(2q+1)/2$, $\mathbf{P}(A_1/C)=\mathbf{P}(B_2/C)=1/(2q+1)$, $\mathbf{P}(A_2/C)=\mathbf{P}(B_1/C)=2q/(2q+1)$. Thus $\delta(B_1/\mathcal{A},C)=2q(2q-1)/(2q+1)$ and, hence, $\lambda(B_1/\mathcal{A},C)=-\sqrt{1-2q}/2$. This context is trigonometric, i.e., the measurement of the random variable a under the complex of physical conditions C induces nontrivial, but a relatively small statistical disturbance of the "b-property;" so $C_{123}\in\mathcal{C}$. We remark that $\lambda(B_2/\mathcal{A},C)=\sqrt{1-2q}/2$ (since $\mathbf{P}^{b/a}$ is double stochastic). [We pay attention on the dependence of $\theta=\arccos\sqrt{1-2q}/2$ on the parameter q: $\theta(q)$ increases from $\pi/3$ to $\pi/2$, when q increases from 0 to 1/2.] We have

$$\varphi_{C_{123}}(x)=\begin{cases}\sqrt{\dfrac{2q}{2q+1}}-e^{i\arccos\sqrt{1-2q}/2}\sqrt{\dfrac{2q(1-2q)}{2q+1}}, & x=b_1,\\ \sqrt{\dfrac{1-2q}{2q+1}}+e^{i\arccos\sqrt{1-2q}/2}\dfrac{2q}{\sqrt{2q+1}}, & x=b_2.\end{cases}$$

Remark: In principle, we could choose, e.g.,

$$e_2^a=\begin{pmatrix}-e^{i\theta}\sqrt{1-2q}\\ e^{i\theta}\sqrt{2q}\end{pmatrix},\quad \theta=\arccos\frac{\sqrt{1-2q}}{2}.$$

Thus

$$\varphi_{C_{123}}=\frac{1}{\sqrt{2q+1}}e_1^a+e^{i\arccos\sqrt{1-2q}/2}\sqrt{\frac{2q}{2q+1}}e_2^a\ .$$

(e) Let $C=C_{124}=\{\omega_1,\omega_2,\omega_4\}$. Here $\mathbf{P}(C)=1-q$, $\mathbf{P}(A_1/C)=\mathbf{P}(B_1/C)=1/2(1-q)$, $\mathbf{P}(A_2/C)=\mathbf{P}(B_2/C)=(1-2q)/2(1-q)$. Thus $\delta(B_1/\mathcal{A},C)=q(1-2q)/(1-q)$ and, hence, $\lambda(B_1/\mathcal{A},C)=\sqrt{q/2}<1$, and the context $C_{124}\in\mathcal{C}$. Thus

$$\varphi_{C_{124}}(x)=\begin{cases}\sqrt{\dfrac{q}{1-q}}+e^{-i\arccos\sqrt{q/2}}\dfrac{1-2q}{\sqrt{2(1-q)}}, & x=b_1,\\ \sqrt{\dfrac{1-2q}{2(1-q)}}-e^{-i\arccos\sqrt{q/2}}\sqrt{\dfrac{q(1-2q)}{1-q}}, & x=b_2;\end{cases}$$

$$\varphi_{C_{124}}(x)=\frac{1}{\sqrt{2(1-q)}}\ e_1^a-e^{-i\arccos\sqrt{q/2}}\sqrt{\frac{1-2q}{2(1-q)}}\ e_2^a.$$

(f) Let $C=C_{234}=\{\omega_2,\omega_3,\omega_4\}$. Here $\mathbf{P}(C)=1-q$, $\mathbf{P}(A_1/C)=\mathbf{P}(B_1/C)=(1-2q)/2(1-q)$, $\mathbf{P}(A_2/C)=\mathbf{P}(B_2/C)=1/2(1-q)$. Thus $\delta(B_1/\mathcal{A},C)=q(2q-1)/(1-q)$ and, hence, $\lambda(B_1/\mathcal{A},C)=-\sqrt{q/2}$, $\lambda(B_2/\mathcal{A},C)=\sqrt{q/2}$. Here

$$\varphi_{C_{234}}(x)=\begin{cases}\sqrt{\dfrac{q(1-2q)}{1-q}}-e^{i\arccos\sqrt{q/2}}\sqrt{\dfrac{1-2q}{2(1-q)}}, & x=b_1,\\ \dfrac{1-2q}{\sqrt{2(1-q)}}+e^{i\arccos\sqrt{q/2}}\sqrt{\dfrac{q}{1-q}}, & x=b_2;\end{cases}$$

$$\varphi_{C_{234}}(x)=\sqrt{\frac{1-2q}{2(1-q)}}\ e_1^a+e^{i\arccos\sqrt{q/2}}\frac{1}{\sqrt{2(1-q)}}\ e_2^a\ .$$

(g) Let $C=C_{134}=\{\omega_1,\omega_3,\omega_4\}$. Here $\mathbf{P}(C)=(2q+1)/2$, $\mathbf{P}(A_1/C)=\mathbf{P}(B_2/C)=2q/(2q+1)$, $\mathbf{P}(A_2/C)=\mathbf{P}(B_1/C)=1/(2q+1)$. Thus $\delta(B_1/\mathcal{A},C)=2q(1-2q)/(2q+1)$ and, hence, $\lambda(B_1/\mathcal{A},C)=\sqrt{1-2q}/2$. Thus

$$\varphi_{C_{134}}(x)=\begin{cases}\dfrac{2q}{\sqrt{2q+1}}+e^{-i\arccos\sqrt{1-2q}/2}\sqrt{\dfrac{1-2q}{2q+1}}, & x=b_1,\\ \sqrt{\dfrac{2q(1-2q)}{2q+1}}-e^{-i\arccos\sqrt{1-2q}/2}\sqrt{\dfrac{2q}{2q+1}}, & x=b_2;\end{cases}$$

$$\varphi_{C_{134}}=\sqrt{\frac{2q}{2q+1}}\ e_1^a-e^{-i\arccos\sqrt{1-q}/2}\frac{1}{\sqrt{2q+1}}\ e_2^a.$$

(h) Let $C=\Omega$. Here we know from the beginning that $\delta(B_j/\mathcal{A},C)=0$. Here $\mathbf{P}(A_i/C)=\mathbf{P}(A_i)=1/2$ and $\mathbf{P}(B_i/C)=\mathbf{P}(B_i)=1/2$. Thus $J^{b/a}(\Omega)=J^{b/a}(C_{24})=J^{b/a}(C_{13})=(33)$.

In this example the set of nonsensitive contexts contains three contexts: $\mathcal{C}_0=\{\Omega,C_{24},C_{13}\}$. We have

$$S_{\mathcal{C}}=\{\varphi_\Omega,\varphi_{C_{14}}=e_1^b,\varphi_{C_{23}}=e_2^b,\varphi_{C_{12}}=e_1^a,\varphi_{C_{23}}=e_2^a,\varphi_{C_{124}},\varphi_{C_{234}},\varphi_{C_{123}},\varphi_{C_{134}}\}.$$

So the set of pure states $S_{\mathcal{C}}$ is a finite, nine-point, subset of the unit sphere in the two-dimensional Hilbert space.

We remark that there is a parameter $q\in(0,1/2)$ determining a Kolmogorov probability model $\mathcal{K}(q)$. For each value of q we have a finite set of pure states. However, a family $\mathcal{K}(q)$, $q\in(0,1/2)$, of Kolmogorov probability spaces generates a "continuous" set $\cup_q S_{\mathcal{C}}(q)$ of pure states.

VII. CONTEXTUAL CORRESPONDENCE BETWEEN KOLMOGOROVIAN RANDOM VARIABLES AND QUANTUM OBSERVABLES

We begin with the following standard definition:

Definition 3: For a self-adjoint operator $\hat{d}$ the quantum mean value in the state φ is defined by

$$\langle\hat{d}\rangle_\varphi=(\hat{d}\varphi,\varphi).$$

Theorem 3: *For any map $f:\mathbf{R}\to\mathbf{R}$ we have*

$$\langle f(\hat{a})\rangle_{\varphi_C}=E(f(a)/C), \qquad \langle f(\hat{b})\rangle_{\varphi_C}=E(f(b)/C),$$

for any context $C\in\overline{\mathcal{C}}$.

Proof: By using Borness of the b-representation we obtain

$$E(f(b/C))=\sum_{x\in X} f(x)p_c^b(x)=\sum_{x\in X} f(x)|(\varphi_C,e_x^b)|^2=\langle f(\hat{b})\rangle_{\varphi_C}.$$

The same result we have for the $f(\hat{a})$ since (as $\mathbf{P}^{b/a}$ is double stochastic) we have Born's probability rule both for b and a.

Theorem 4: *Let $f,g:\mathbf{R}\to\mathbf{R}$ be two arbitrary functions. Then*

$$E(f(a)+g(b)/C)=\langle f(\hat{a})+g(\hat{b})\rangle_{\varphi_C},$$

for any context $C\in\overline{\mathcal{C}}$.

Proof: By using linearity of the Kolmogorov mathematical expectation, Theorem 3, and linearity of the Hilbert space scalar product we obtain

$$\begin{aligned}E(f(a(\omega))+g(b(\omega))/C)&=E(f(a(\omega)/C)+E(g(b(\omega))/C))\\&=\langle f(\hat{a})\rangle_{\varphi_C}+\langle g(\hat{b})\rangle_{\varphi_C}=\langle f(\hat{a})+g(\hat{b})\rangle_{\varphi_C}.\end{aligned}$$

Denote the linear space of all random variables of the form $d(\omega)=f(a(\omega))+g(b(\omega))$ by the symbol $\mathcal{O}_+(a,b)$ and the linear space of operators of the form $\hat{d}=f(\hat{a})+g(\hat{b})$ by $\mathcal{O}_+(\hat{a},\hat{b})$.

Theorem 5: *The map $T=T^{a/b}:\mathcal{O}_+(a,b)\to\mathcal{O}_+(\hat{a},\hat{b}), d=f(a)+g(b)\to\hat{d}=f(\hat{a})+g(\hat{b})$, preserves the conditional expectation*

$$\langle T(d)\rangle_{\varphi_C}=(T(d)J(C),J(C))=E(d/C). \tag{34}$$

The transformation T preserves the conditional expectation for random variables $d\in\mathcal{O}_+(a,b)$. But in general we cannot expect anything more, since in general T does not preserve probability distributions. The important problem is to extend the map T for a larger class (linear space?) of Kolmogorovian random variables with preserving (34). It is natural to define (as we always do in the conventional quantum formalism):

$$T(f)(\hat{a},\hat{b})=f(\hat{a},\hat{b}),$$

where $f(\hat{a},\hat{b})$ is the pseudo differential operator with the Weyl symbol $f(a,b)$. We shall see that already for $f(a,b)=ab$ [so $f(\hat{a},\hat{b})=(\hat{a}\hat{b}+\hat{b}\hat{a})/2$] the equality (34) is violated.

We can consider the b and the a as discrete analogs of the position and momentum observables. The operators $\hat{b}$ and $\hat{a}$ give the Hilbert space (quantum) representation of these observables.

We also introduce an analog of the energy observable:

$$\mathcal{H}(\omega)=\frac{h}{2}[a^2(\omega)+V(b(\omega))],$$

where $h>0$ is a constant and $V:\mathbf{R}\to\mathbf{R}$ is a map. The Hilbert space representation of this observable is given by the operator of energy (Hamiltonian),

$$\hat{\mathcal{H}}=\frac{h}{2}(\hat{a}^2+V(\hat{b})).$$

By Theorem 5 for contexts $C \in \overline{\mathcal{C}}$ the averages of the observables $\mathcal{H}(\omega)$ (Kolmogorovian) and $\hat{\mathcal{H}}$ (quantum) coincide:

$$E(\mathcal{H}(\omega)/C) = \langle \mathcal{H} \rangle_{\varphi_C}.$$

However, as we shall see, probability distributions do not coincide.

Proposition 3: There exists context C such that the probability distribution of the random variable $d(\omega) = a(\omega) + b(\omega)$ with respect to C does not coincide with the probability distribution of the corresponding quantum observable $\hat{d} = \hat{a} + \hat{b}$ with respect to the state φ_C.

Proof: It suffices to present an example of such a context C. Take the context $C = C_{234}$ from Sec. VI. We consider the case: $a(\omega) = \pm\gamma, b(\omega) = \pm\gamma, \gamma > 0$; so $d(\omega) = -2\gamma, 0, 2\gamma$. Corresponding Kolmogorovian probabilities can easily be found:

$$p_C^d(-2\gamma) = q/(1-q), \quad p_C^d(0) = (1-2q)/(1-q), \quad p_C^d(2\gamma) = 0.$$

We now find the probability distribution of $\hat{d}$. To do this, we find eigenvalues and eigenvectors of the self-adjoint operator $\hat{d}$. We find the matrix of the operator $\hat{d}$ in the basis $\{e_j^b\}$: $d_{11} = -d_{22} = 4q\gamma$ and $d_{12} = d_{21} = 2\gamma\sqrt{2q(1-2q)}$. We have $k_{1,2} = \pm 2\sqrt{2q}\,\gamma$. Of course, the range of values of the quantum observable $\hat{d}$ differs from the range of values of the random variable d. However, this difference of ranges of values is not so large a problem in this case. The random variable d takes only two values, $-2\gamma, 0$, with the probability one. Moreover, we can represent values of the quantum observable $\hat{d}$ as just an affine transform of values of the random variable d:

$$d_{\text{quantum}} = 2\sqrt{2q}\ \ d - \gamma.$$

In principle we can interpret such a transformation as representing some special measurement procedure. Thus in this example the problem with the spectrum is not crucial. The crucial problem is that d and $\hat{d}$ have different probability distributions.

The corresponding eigenvectors are

$$e_1^d = \frac{1}{\sqrt{2(1-\sqrt{2q})}}(-\sqrt{1-2q}, \sqrt{2q}-1),$$

$$e_2^d = \frac{1}{\sqrt{2(1+\sqrt{2q})}}(-\sqrt{1-2q}, \sqrt{2q}+1).$$

Finally, we find (by using the expression for $\varphi_{C_{234}}$ which was found in Sec. VI):

$$p_c^{\hat{d}}(k_1) = |(\varphi_C, e_1^d)|^2 = \frac{(1-\sqrt{2q})(2+\sqrt{2q})}{4(1-q)},$$

$$p_c^{\hat{d}}(k_2) = |(\varphi_C, e_2^d)|^2 = \frac{(1+\sqrt{2q})(2-\sqrt{2q})}{4(1-q)}.$$

Thus d and $\hat{d}$ have essentially different probability distributions.

VIII. DISPERSION-FREE STATES

As originally stated by von Neumann,[20] the problem of hidden variables is to find whether *dispersion free states exist* in QM. He answered the question in the negative. The problem of the

existence of dispersion free states as well as von Neumann's solution were the subject of great debates. We do not want to go into detail; see, e.g., Ref. 21. In our contextual approach an analog of this problem can be formulated as follows.

Do dispersion free contexts exist? The answer is the positive. In the example of Sec. VI. We can take any atom of the Kolmogorov probability space $\mathcal{K}_q$, e.g., $C=\{\omega_1\}$. Since, for any random variable ξ on the Kolmogorov space $\mathcal{K}_q$, it has a constant value on such a C the dispersion of ξ under the context C is equal to zero:

$$D(\xi/C)=E[(\xi-E(\xi/C))^2/C]=0.$$

However, dispersion free contexts do not belong to the system $\overline{\mathcal{C}}$ of contexts which can be mapped by $J^{a/b}$ into the Hilbert space H. On the one hand, our contextual approach gives the possibility to have the realist viewpoint to QM. On the other hand, it does not contradict to the von Neumann as well as other ''no-go'' theorems. The mathematical representation of contexts (complexes of physical conditions) given by the quantum formalism it too rough to represent dispersion free contexts.

IX. CLASSICAL AND QUANTUM SPACES AS ROUGH IMAGES OF FUNDAMENTAL PRESPACE

Our contextual probabilistic model induces the following picture of physical reality.

A. Prespace and classical space

There exists a prespace Ω which points corresponds to primary (irreducible) states of physical systems, *prestates or fundamental physical parameters*. Functions $d:\Omega\to\mathbf{R}^m$ are said to be *preobservables*. The set of all preobservables is denoted by the symbol $\mathcal{O}_p\equiv\mathcal{O}_p(\Omega)$. We are not able (at least at the moment) to measure an arbitrary preobservable $d\in\mathcal{O}_p$.

Nevertheless, some preobservables can be measured. Suppose that there exists a preobservable b such that all measurements can be reduced to some measurements of b; cf. De Broglie[10] on the possibility of reducing any measurement to a position measurement. Let $X\subset\mathbf{R}^m$ be the range of values of b. The X is said to be a classical space Set $B_x=\{\omega\in\Omega:b(\omega)=x\}=b^{-1}(x),x\in X$.

In principle a set B_x could contain millions of points. Dynamics in X is classical dynamics. In our model, classical dynamics is a rough image of dynamics in the prespace Ω.

B. Quantum mechanics and the Hilbert space representation of prespace contexts

By our *contextual interpretation* the wave function has a realist prespace interpretation. A complex amplitude is nothing than an image (induced by the contextual formula of total probability) of a set of fundamental parameters—context. Thus the Hilbert state space H is not less real than the classical real space $\mathbf{R}^3$.

Observables which probability distributions can be found by using the representation by self-adjoint operators in the Hilbert space are called quantum observables. The set of quantum observables is denoted by the symbol $\mathcal{O}_q(H)$. Neither classical statistical nor quantum mechanics can provide knowledge about the probability distribution of an arbitrary preobservable. Nevertheless, the quantum theory gives some information about some preobservables, namely fundamental preobservable b and a and preobservables d belonging to the class $\mathcal{O}_+(a,b)$.

Neither classical nor quantum mechanics are fundamental theories. They could not give information about the pointwise structure of the prespace Ω. But the quantum formalism represents some complexes of physical conditions—domains in the prespace—which are not represented in the classical space or phase space. Of course, the quantum formalism also represents classical position states $x\in X$ by wave functions φ_{B_x} (Hilbert states e_x^b). Classical states $x\in X$ are images of prespace contexts B_x. But the quantum formalism represents also some sets $C\subset\Omega$ which have no classical images (namely, images in X or Π).

Example: In the example of Sec. VI we take the set $C=C_{123}=\{\omega_1,\omega_2,\omega_3\}$. Neither $C\subset B_1$ nor $C\subset B_2$. This prespace domain C can be described neither by the position $x=b_1$ nor $x=b_2$.

The quantum state $\varphi_C \in S \subset H$ representing this domain of the prespace describes the superposition of the two classical states $x = b_1$ and $x = b_2$. Hence a physical system prepared under the complex physical conditions $C = C_{123}$ is (from the classical viewpoint) in the superposition of two different positions.

Finally, we remark that we have investigated only the case of dichotomous random variables. The general case is essentially more complicated from the mathematical viewpoint. In particular, not every double stochastic matrix can be represented as the square of a unitary matrix and so on... . But I think that from the phemenological viewpoint the case of dichotomous observables is the most important; cf., e.g., Mackey[14] and the general quantum logic approach.

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Bound states in two spatial dimensions in the noncentral case

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We derive a bound on the total number of negative energy bound states in a potential in two spatial dimensions by using an adaptation of the Schwinger method to derive the Birman–Schwinger bound in three dimensions. Specifically, counting the number of bound states in a potential gV for $g=1$ is replaced by counting the number of g_i's for which zero energy bound states exist, and then the kernel of the integral equation for the zero-energy wave functon is symmetrized. One of the keys of the solution is the replacement of an inhomogeneous integral equation by a homogeneous integral equation. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In a previous paper,[1] Chadan, Khuri, and the present authors obtained a bound on the number of bound states in a two-dimensional central potential. This bound has the merit that, for a potential gV, the coupling constant dependence for large g is optimal, i.e., the same as the one of the semiclassical estimate.[2] Previous work on the subject was done by Newton[3] and Seto.[4] We also obtained a bound for the noncentral case, but only by using a rather brutal method which consists of replacing the potential by a central potential which is defined, after choosing a certain origin, by

$$V_c(r)=\mathrm{Inf}\, V(\vec{x}),\qquad |\vec{x}|=r. \tag{1}$$

Because of the monotonicity of the energy levels with respect to the potential, putting V_c in our formulas will give a bound for the potential V. However, for potentials with singularities outside the given origin, this may lead to no bound at all. Our attention has been attracted by the fact that in condensed matter physics problems exist, where counting the bound states on a surface may be useful,[5] but where it is very unlikely that the potential will be central, even approximately.

In the present paper, we obtain a bound on the number of bound states in a noncentral two-dimensional potential, using an adaptation of the Schwinger method to derive the Birman–Schwinger bound[6] in the three-dimensional case. The condition under which we obtain a bound is

$$\int\int \mathrm{d}^2x\,\mathrm{d}^2y\,|V(x)|(\ln|x-y|)^2|V(y)|<\infty. \tag{2}$$

This condition is *nonlinear*, just like that of Birman and Schwinger, but we show in the Appendix that it follows from the linear conditions

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$$\int d^2x\,(\ln(2+|x|))^2\,|V(x)|<\infty,$$
$$\int d^2x\,V_R(|\vec{x}|)\,\ln^-|x|<\infty, \tag{3}$$

where V_R is the circular decreasing rearrangement of $|V|$ (for the definition of V_R, see the Appendix).

Condition (2) has already been proposed by Sabatier.[7] Condition (3) appears in a forthcoming work by Khuri *et al.* dealing with the scattering problem. It has the advantage of showing more clearly what kind of behavior the potential is allowed to have at short and large distances.

The strategy of Schwinger consists of counting the number of zero-energy bound states for a potential gV for $0<g<1$ instead of the actual number of negative energy bound states for $g=1$. In three dimensions these two numbers are equal. Indeed, let $0<g_1,g_2,\ldots,g_n<1$ be the coupling constants for which we have zero-energy bound states. Each g_i is the origin of a bound state trajectory in the $E-g$ plane, $E_i(g)$, with $E_i(g_i)=0$. These trajectories are monotonous decreasing:

$$\frac{dE_i}{dg}=\int V\psi^2 d^nx, \tag{4}$$

by the Feynman–Hellmann theorem, but

$$g_i\int V\psi^2 d^nx=E-\int |\nabla\psi|^2\,d^nx<0 \quad \text{for } E<0. \tag{5}$$

This shows that the number of negative-energy bound states is exactly the same as the number of g_i's<1. At the crossing of any pair of trajectories there is no problem because of their monotonicity.

The same result holds in two dimensions with one modification: any attractive potential (i.e., $\int d^2x\,V<0$) has a bound state for arbitrarily small g, with a binding energy going to zero for $g\to 0$ like $-\exp-(C/g)$.[1] At $E=0$ it disappears and is not included in Schwinger's accounting, so we have to add one unit.

Since we only want a *bound* on the number of bound states, we can always replace $V(y)$ by $-V^-(y)$:

$$V^-(y)=0 \quad \text{for } V>0,$$
$$V^-(y)=-V(y) \quad \text{for } V\leqslant 0. \tag{6}$$

Using $-|V(y)|$ instead of $-V^-(y)$ gives a more crude bound.

It can be shown that the general solution of the zero-energy Schrödinger equation

$$-\Delta\psi-V^-\psi=0 \tag{7}$$

in the equivalent integral form

$$\psi(x)=C-\frac{1}{2\pi}\int \ln k_0|x-y|V^-(y)\psi(y)d^2y \tag{8}$$

has a general asymptotic behavior for $|x|\to\infty$,

$$\psi(x)-C\sim-\ln k_0|x|\;\frac{1}{2\pi}\int V^-(y)\psi(y)d^2y+o(1) \tag{9}$$

under the condition

$$\int V^-(y)\,(\ln(2+|y|))^2\,\mathrm{d}^2y<\infty, \tag{10}$$

which follows from condition (1) as shown in the Appendix. In fact, the proof is easier if one assumes that the potential is lower bounded for large x. One can always cut off the potential and use a limiting procedure at the end.

Zero-energy bound states are characterized by the fact that ψ is *bounded*. Hence we get the necessary condition:

$$\int V^-(y)\psi(y)\mathrm{d}^2y=0. \tag{11}$$

Now we have two possibilities:

I. At infinity $\psi(\vec{x})\to 0$ and hence $C=0$ and those bound state wave functions satisfy a *homogeneous* integral equation

$$\psi_i(x)=-\frac{g_i}{2\pi}\int \mathrm{d}^2y\,\ln(k_0|x-y|)\,V^-(y)\psi_i(y) \tag{12}$$

[notice that the scale factor k_0 disappears because of condition (11)].

This is what happens in the case of a central potential for a nonzero azimuthal angular momentum m.

II. At infinity, $\psi(\vec{x})\to C$, with $C\neq 0$. In this case, the bound state wave functions satisfy an inhomogeneous integral equation. This case has been described in Ref. 8, where it is shown that for a central potential in two dimensions, the $m=0$ phase shift has the universal behavior

$$\delta(k)\sim\frac{\pi}{2\ln k}\quad \text{for } k\to 0, \tag{13}$$

except if there is a zero-energy bound state of type II. Then

$$\delta(k)\ln k\to 0. \tag{14}$$

In Ref. 8, a much stronger result is stated. This much stronger result, however, holds only for a very rapidly decreasing potential.

II. COUNTING BOUND STATES IN CASE I

Following Schwinger, we symmetrize the kernel of the integral equation:

$$\phi_i(x)=g_i\int K(x,y)\,\phi_i(y)\mathrm{d}^2y \tag{15}$$

with

$$\begin{aligned}\phi_i(x)&=\sqrt{V^-(x)}\;\;\psi_i(x),\\ K(x,y)&=-\frac{1}{2\pi}\sqrt{V^-(x)}\,\ln k_0|x-y|\;\;\sqrt{V^-(y)}.\end{aligned} \tag{16}$$

If $V^-(x)$ vanishes in some regions, it seems impossible to go back from ϕ_i to ψ_i. However, this can be remedied by defining

$$V_\epsilon^-(x)=V^-(x)+\epsilon\exp-\mu|x|. \tag{17}$$

Since the bounds we shall get are continuous in V, we can take the limit $\epsilon\to 0$ at the end.

K can be written as

$$K=\Sigma\frac{1}{g_i}|\phi_i\rangle\langle\phi_i|+R. \tag{18}$$

R is a sum over states which do not satisfy (11). The ϕ_i's in themselves do not form a complete set. If we define a by

$$a(x)=\frac{\sqrt{V^-(x)}}{\sqrt{\int V^-(y)\mathrm{d}^2y}} \tag{19}$$

we have

$$\langle a|\phi_i\rangle=0 \tag{20}$$

from property (11), and naturally $\langle a|a\rangle=1$.

If we define $\widehat{\mathrm{Tr}}$, a trace restricted to the ϕ_i's, we have

$$\widehat{\mathrm{Tr}}\,K=\Sigma\frac{1}{g_i}>\sum_{g_i\leqslant 1}\frac{1}{g_i}>N_\mathrm{I},$$

N_I being the number of bound states of type I. However, this trace turns out to be divergent because of the logarithmic singularity of the kernel (the same happened in Schwinger's original work!), and we follow Schwinger to iterate the integral equation (15):

$$\phi_i(x)=g_i^2\int K(x,y)K(y,z)\,\phi_i(z)\mathrm{d}^2y\mathrm{d}^2z$$

and then

$$\widehat{\mathrm{Tr}}\,K^2=\Sigma\frac{1}{g_i^2}>N_\mathrm{I}. \tag{21}$$

Forgetting the caret on the trace still gives a bound because K^2 is a positive operator (contrary to K!), but this bound depends on the scale parameter k_0 entering in the logarithm. Among the missing states in $\widehat{\mathrm{Tr}}$ is the state $|a\rangle$, orthogonal to the ϕ_i's, and this one should be removed from the complete trace. In this way, we get

$$N_\mathrm{I}<\mathrm{Tr}\,K^2-\langle a|K^2|a\rangle,$$

or more explicitly

$$N_\mathrm{I}<\frac{1}{(2\pi)^2}\int V^-(x)(\ln k_0|x-y|)^2V^-(y)\mathrm{d}^2x\mathrm{d}^2y-\frac{1}{(2\pi)^2}$$
$$\times\frac{1}{\int V^-(x)\mathrm{d}^2x}\int V^-(x)(\ln k_0|x-z|)\quad V^-(z)(\ln k_0|z-y|)V^-(y)\,\mathrm{d}^2x\mathrm{d}^2y\mathrm{d}^2z. \tag{22}$$

It is visible that the second term is negative as we announced.

Rewriting N_{I} as

$$\frac{1}{(2\pi)^2}\frac{1}{\int V^-(z)\mathrm{d}^2z}\int \mathrm{d}^2x\mathrm{d}^2y\mathrm{d}^2z\, V^-(x)V^-(y)V^-(z)\ \ [(\ln k_0|x-y|)^2-\ln k_0|x-z|\ln k_0|y-z|],$$

we see that (22) is manifestly *independent* of the scale factor k_0.

III. COUNTING BOUND STATES IN CASE II

At first it would seem that Schwinger's technique will not work because, in Eq. (8), the constant is not zero and therefore we deal with an *inhomogeneous* integral equation which can be written, after the same changes of variables as in Sec. II, given by (16) and (19):

$$\phi_i = C_i a + g_i K\phi_i, \tag{23}$$

with, again,

$$\langle a|\phi_i\rangle = 0, \quad \langle a|a\rangle = 1. \tag{24}$$

Equation (24) is precisely the key property which will make it possible to replace (23) by a *homogeneous equation*.

Again, the ϕ_i's corresponding to different g_i's are orthogonal because

$$\langle\phi_i|\phi_j\rangle = C_j\langle\phi_i|a\rangle + g_j\langle\phi_i|K\phi_j\rangle$$

$$= C_i\langle\phi_j|a\rangle + g_i\langle\phi_j|K\phi_i\rangle.$$

Hence, from (24):

$$\left(\frac{1}{g_i}-\frac{1}{g_j}\right)\langle\phi_i|\phi_j\rangle = 0. \tag{25}$$

Let us call $\mathcal{S}$ the Hilbert space associated with the integral equation (23), and construct a new Hilbert space by removing the element a:

$$\mathcal{S} = \mathcal{S}' \oplus \{a\}. \tag{26}$$

We want to define a new operator K' acting in $\mathcal{S}'$. Let

$$b = Ka. \tag{27}$$

Notice that

$$\langle b|\phi_i\rangle = -\frac{C_i}{g_i}\langle a|a\rangle = -\frac{C_i}{g_i}. \tag{28}$$

We try

$$K' = K - |b\rangle\langle a| - |a\rangle\langle b| + C|a\rangle\langle a|$$

where C will be chosen so that

$$K'a = 0. \tag{29}$$

We have

$$K'|a\rangle = |b\rangle - |b\rangle - \langle b|a\rangle|a\rangle + C|a\rangle,$$

and hence we take

$$C = \langle b|a\rangle = \langle a|K|a\rangle. \tag{30}$$

K' is Hermitian like K, and we get

$$g_i K'|\phi_i\rangle = g_i|K|\phi_i\rangle - g_i\langle b|\phi_i\rangle|a\rangle$$

$$= g_i|K|\phi_i\rangle + C_i|a\rangle.$$

Hence

$$g_i K'|\phi_i\rangle = |\phi_i\rangle, \tag{31}$$

which is *homogeneous*.

To get a bound on the number of bound states of type II, we have to get a bound on trace K'^2 (not surprisingly, trace K' is divergent). It is a lengthy but straightforward exercise to calculate that trace, which gives

$$N_{\mathrm{II}} < \mathrm{tr}\, K^2 - 2\langle a|K^2|a\rangle + (\langle a|K|a\rangle)^2. \tag{32}$$

The last two terms give an overall negative contribution. The first term is the same as the one appearing in N_{I}. It is easy to see that the right-hand side of (32) is independent of the scale parameter k_0 entering into the kernel K. Finally, let us notice that the treatment of case II *contains* case I because, in the argument, it has never been said that $C_i \neq 0$. Equation (31) holds irrespective of whether $C_i = 0$ or $C_i \neq 0$. Notice that the bound on N_{I} is larger than the bound on N_{II}. Therefore the bound on N_{I} becomes completely obsolete.

IV. CONCLUDING REMARKS

If we include the bound state with evanescent energy for zero coupling constant, we get the bound

$$N < 1 + \mathrm{tr}\, K^2 - 2\langle a|K^2|a\rangle + (\langle a|K|a\rangle)^2.$$

Dropping the last two terms still gives a scale-dependent bound—which can be minimized with respect to the scale—which precisely appears in condition (2), itself following from the linear condition (3) as shown in the Appendix.

Conditions (2) and (3) both allow a potential behaving like

$$\frac{1}{r^2(\ln r)^{3+\epsilon}}$$

at infinity, with local singularities not worse than

$$-\frac{1}{|r-r_0|^2(|\ln|r-r_0||)^{2+\epsilon}},$$

ϵ positive, arbitrarily small. Both conditions are violated for $\epsilon < 0$. However, we shall see in the Appendix that (2) is definitely weaker than (3).

Our bound has the merit of being valid for the noncentral case, which, as we said in Sec. I, is important for solid-state physics. However, for a potential gV, it behaves like g^2 for large g, while in Ref. 1, in the central case, we get a bound behaving like g. In Ref. 1 we make a conjecture

which is very far from being proved, but clever mathematical physicists might prove it or something similar. The present work should be considered only as a first step which could possibly give reasonable results for not too large g.

Note added in proof. Our attention has been drawn to the related work by Stoiciu.[10] In this work, which uses a different method, the same integral (2) appears to control the number of bound states. However, there are no counterterms like in Eq. (32), and, as a consequence, the result is scale dependent.

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APPENDIX: COMPARISON OF CONDITIONS (2) AND (3)

Condition (2) is

$$I=\int \mathrm{d}^2x\mathrm{d}^2y\, V^-(x)(\ln|x-y|)^2\, V^-(y)<\infty. \tag{A1}$$

Condition (3) is a set of two conditions:

$$\int \mathrm{d}^2x\,(\ln(2+|x|))^2\, V^-(x)<\infty, \tag{A2}$$

$$\int \mathrm{d}^2x\, V_R(|x|)\ln^-(|x|)<\infty. \tag{A3}$$

In (A3) we use

$$-\ln^-(|x|)=\begin{cases}0 & \text{if } |x|>1\\ -\ln|x| & \text{if } |x|<1.\end{cases}$$

$-V_R(|x|)$, the circular decreasing rearrangement of $V^-(x)$. Since this notion is not very well known among physicists, let us remind the reader that $V_R(|x|)$ is a decreasing function of $|x|$, such that

$$\mu(V_R(|x|)>A)=\mu(V^-(x)>A),\ \forall A,$$

where μ is the Lebesque measure. In more familiar terms, the rearranged Mont Blanc would be a mountain with axial symmetry, with a single peak, such that the surface between the level lines would be the same as the surface between the level lines of the original Mont Blanc (rather awfully dull!).

We shall prove first that the convergence of I in (A1) follows from the convergence of (A2) and (A3). More exactly, we shall get an explicit bound on (A1) in terms of (A2) and (A3). We write

$$I=I_+ + I_- \tag{A4}$$

with

$$I_+ = \int \mathrm{d}^2x \mathrm{d}^2y\, V^-(x)\, (\ln^+|x-y|)^2\, V^-(y), \tag{A5}$$

$$I_- = \int \mathrm{d}^2x \mathrm{d}^2y\, V^-(x)\, (\ln^-|x-y|)^2\, V^-(y). \tag{A6}$$

$\ln^-$ has already been defined. $\ln^+(a)=\ln a$ for $a\geqslant 1, =0$ for $a<1$. It is elementary to get a bound on I_+ from (A2) only. Indeed,

$$0<\ln^+|x-y|<\ln^+(|x|+|y|)<\ln(2+|x|)+\ln(2+|y|)$$

and thus

$$(\ln^+|x-y|)^2<2[(\ln 2+|x|)^2+(\ln(2+|y|))^2]. \tag{A7}$$

Hence

$$I_+<4\int \mathrm{d}^2x\, V^-(x) \quad \int \mathrm{d}^2y\, V^-(y)\, (\ln(2+|y|))^2. \tag{A8}$$

The convergence of the right-hand side of (A8) follows directly from (A2).

Concerning I_-, we use a rearrangement inequality due to Luttinger and Friedberg,[9] which says

$$\int\int \; A(x)\, B(|x-y|)\, C(y)\mathrm{d}^2x\mathrm{d}^2y \leqslant \int \; A_R(|x|)\, B_R(|x-y|)\, C_R(|y|)\, \mathrm{d}^2x\mathrm{d}^2y, \tag{A9}$$

where A,B,C are non-negative functions and A_R, B_R, C_R are their decreasing rearrangements. Since $\ln^-$ and $(\ln^-)^2$ are decreasing functions of their argument they are their own rearrangement. Hence

$$I_-<\int \; \mathrm{d}^2x\mathrm{d}^2y \quad V_R(|x|)(\ln^-(|x-y|))^2\, V_R(|y|). \tag{A10}$$

In (A10), we can carry out first the angular integration, the angle $(\vec{x},\vec{y})$ appearing only in $\ln^-$. However, to be able to do that easily we have to sacrifice some information, i.e., use $(\ln^-|x-y|)^2\leqslant(\ln(|x-y|))^2$. We have to calculate

$$\int \; \frac{\mathrm{d}\theta}{2\pi}(\ln(|x|^2+|y|^2-2|x||y|\cos\theta))^2.$$

We have

$$\ln(|x|^2+|y|^2-2|x||y|\cos\theta)=\ln(|x|-|y|e^{i\theta})+\ln(|x|-|y|e^{-i\theta}).$$

Assume $|x|>|y|$. Then we get

$$\ln(|x|^2+|y|^2-2|x||y|\cos\theta)=2\left[\ln|x|-\Sigma\left(\frac{|y|}{|x|}\right)^n\frac{\cos n\theta}{n}\right]. \tag{A11}$$

Hence, if $|x|>|y|$, using the orthogonality of the $\cos n\theta$:

$$\int \; \frac{\mathrm{d}\theta}{2\pi}(\ln(|x|^2+|y|^2-2|x||y|\cos\theta))^2=4(\ln|x|)^2+2\sum_{n=1}^{\infty}\left(\frac{|y|}{|x|}\right)^{2n}\frac{1}{n^2}.$$

We see a dilogarithm, or Spence function, appearing on the right-hand side. However, we only need to notice that

$$\sup_{|y|\leqslant|x|} \int \frac{\mathrm{d}\theta}{2\pi}(\ln|x|^2+|y|^2-2|y||x|\cos\theta)^2=4(\ln|x|)^2+2\sum_{n=1}^{\infty}\frac{1}{n^2}=4(\ln|x|)^2+\frac{\pi^2}{3}. \tag{A12}$$

In this way we get

$$I_-<(2\pi)^2\times 2\int_{|x|>|y|}|x|\mathrm{d}|x|\,|y|\mathrm{d}|y|\,V_R(|x|)V_R(|y|)\ \left[4(\ln|x|)^2+\frac{\pi^2}{3}\right].$$

Again, we split the integral into

$$\begin{aligned}&32\pi^2\int_{|x|>|y|}|x|\mathrm{d}|x|\,|y|\mathrm{d}|y|\,V_R(|x|)V_R(|y|)(\ln^-|x|)^2\\&\quad+32\pi^2\int_{|x|>|y|}|x|\mathrm{d}|x|\,|y|\mathrm{d}|y|\,V_R(|x|)V_R(|y|)(\ln^+|x|)^2+\frac{4\pi^4}{3}\left[\int|x|\mathrm{d}|x|\,V_R(|x|)\right]^2.\end{aligned} \tag{A13}$$

In the first term of (A13) we can replace $(\ln^-(|x|))^2$ by $\ln^-|x|\ln^-|y|$, since $|x|>|y|$ and since $\ln^-$ is decreasing.

In the second term, we can drop the restriction $|x|>|y|$ and notice that

$$\int \mathrm{d}^2x V_R(|x|)\,(\ln^+(|x|))^2<\int \mathrm{d}^2x V_-(x)(\ln^+(|x|))^2.$$

Indeed, $\int \mathrm{d}^2x A_R(x)\phi(|x|)$, where $\phi(|x|)$ is *increasing*, is less than $\int \mathrm{d}^2x\,A(x)\,\phi(|x|)$. Suppose that $\phi(|x|)\to L$. Then

$$\int \mathrm{d}^2x A_R(x)\phi(|x|)=\int \mathrm{d}^2x A_R(x)L-\int \mathrm{d}^2x A_R(x)(L-\phi(|x|)).$$

$L-\phi(|x|)$ is its own decreasing rearrangement and following the well-known properties

$$\int A_R B_R \mathrm{d}^2x\geqslant\int A(x)B(x)\mathrm{d}^2x$$

and

$$\int A_R(|x|)\mathrm{d}^2x=\int A(x)\mathrm{d}^2x,$$

we get the desired property. If L is infinite, we can use a limiting procedure. Finally, we get

$$\begin{aligned}I_-<16\pi^2\left[\int \mathrm{d}^2x\,V_R(|x|)\ln^-\left|x\right|\right]^2+32\pi^2\int \mathrm{d}^2x\,V_-(x)\int \mathrm{d}^2y\,V_-(y)(\ln(2+|y|))^2\\+\frac{4\pi^4}{3}\left[\int \mathrm{d}^2x\,V_-(x)\right]^2.\end{aligned} \tag{A14}$$

From (A2) and (A3) we see that I_- is bounded. This concludes the proof.

One question is: can we go in the opposite direction? Assume that we know that (A1) holds. There exists certainly a region $|x-x_0|<R$ where $\mathrm{Inf}\, V^- = m > 0$. If such a region did not exist, V^- would be zero almost everywhere! So

$$I > \pi R^2 m \int_{|x|>|x_0|+R+2} V^-(x) \ln[2+|x|]^2 \mathrm{d}^2x. \tag{A15}$$

Now we choose $y_0 > 4+|x_0|+R+2$ and R such that

$$\mathrm{Inf}_{|y-y_0|<R'}\, V_-(y) = m' > 0,$$

then

$$I > \pi R'^2 m' \int_{|x|<|x_0|+R+2} V^-(x)(\ln(4-R'))^2 \mathrm{d}^2x. \tag{A16}$$

This proves that the convergence of (A1) implies the convergence of (A2).

It is not possible to deduce (A3) from (A1) because (A3) involves V_R and (A1) does not. However, in practice the conditions are very similar. Nevertheless, the following example shows that (A3) is stronger than (A1), even for a potential which does not need rearrangement: take the central potential

$$V(|x|) = \begin{cases} -\dfrac{1}{|x|^2 |\ln x|^2 (\ln|\ln|x||)^\gamma} & \text{for } |x| < \dfrac{1}{2e} \\ 0 \quad \text{for } |x| \geqslant \dfrac{1}{2e}. \end{cases} \tag{A17}$$

For $\gamma \leqslant \frac{1}{2}$ (A1) and (A3) are divergent, for $\frac{1}{2} < \gamma \leqslant 1$ (A1) is convergent and (A3) is divergent, for $\gamma > 1$ (A1) and (A3) are convergent.

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Pseudounitary operators and pseudounitary quantum dynamics

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We consider pseudounitary quantum systems and discuss various properties of pseudounitary operators. In particular we prove a characterization theorem for block-diagonalizable pseudounitary operators with finite-dimensional diagonal blocks. Furthermore, we show that every pseudounitary matrix is the exponential of $i=\sqrt{-1}$ times a pseudo-Hermitian matrix, and determine the structure of the Lie groups consisting of pseudounitary matrices. In particular, we present a thorough treatment of 2×2 pseudounitary matrices and discuss an example of a quantum system with a 2×2 pseudounitary dynamical group. As other applications of our general results we give a proof of the spectral theorem for symplectic transformations of classical mechanics, demonstrate the coincidence of the symplectic group $\mathrm{Sp}(2n)$ with the real subgroup of a matrix group that is isomorphic to the pseudounitary group $\mathrm{U}(n,n)$, and elaborate on an approach to second quantization that makes use of the underlying pseudounitary dynamical groups. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1646448]

I. INTRODUCTION

For the past 2 years we have witnessed a growing interest in pseudo-Hermitian Hamiltonians.[1–13] Initially, the concept of a pseudo-Hermitian operator was developed to describe the mathematical structure of (the possibly nonunitary) PT-symmetric quantum systems.[1,2] Then it became clear that any diagonalizable Hamiltonian that admitted a symmetry generated by an invertible antilinear operator was necessarily pseudo-Hermitian.[3,9] The intriguing spectral properties of pseudo-Hermitian Hamiltonians generalize to the class of block-diagonalizable Hamiltonians with finite-dimensional blocks,[6] so does the connection with antilinear symmetries.[10] Among the most important outcomes of the study of pseudo-Hermitian Hamiltonians is the recent solution of the old problem of constructing invariant positive–definite inner products on the solution space of the Klein–Gordon-type equations.[14,15]

A quantum system with a (time-independent) pseudo-Hermitian Hamiltonian has necessarily a pseudounitary evolution. Pseudounitary quantum systems with a two-dimensional Hilbert space provide the simplest nontrivial examples of such systems. As shown in Ref. 14, a classical simple harmonic oscillator is equivalent to a pseudounitary quantum system with a two-dimensional Hilbert space. Recently Ahmed and Jain[11,12] and Ahmed[13] have considered the application of certain 2×2 pseudo-Hermitian matrices in statistical mechanics and elaborated on the fact that they form a Lie algebra.

The purpose of this paper is threefold. First, we use the method of Ref. 6 to obtain a characterization of the block-diagonalizable pseudounitary operators having finite-dimensional diagonal blocks. Next, we confine our attention to pseudounitary matrices and show that they are obtained by exponentiating pseudo-Hermitian matrices. This is a nontrivial result, because, for a fixed η, not every η-pseudounitary matrix is the exponential of $i=\sqrt{-1}$ times an η-pseudo-Hermitian matrix. Finally, we emphasize that unlike the set of η-pseudounitary operators (with a fixed η), the

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set of all pseudounitary operators does not form a group. If the Hilbert space in which these operators act is finite dimensional, then the group of η-pseudounitary operators is isomorphic to one of the groups $\mathrm{U}(n)$ or $\mathrm{U}(n,m)$ for some $m,n\in\mathbb{Z}^+$. For example, the Lie algebra of the pseudounitary matrices constructed in Ref. 11 is isomorphic to u(1,1). This follows from the fact that the corresponding inner product is indefinite; there is no need to go through the calculation of the structure constants as done in Ref. 11.

The paper is organized as follows. In Sec. II we present a brief discussion of some basic properties of pseudounitary operators and their relevance to symplectic transformations. In Sec. III we explore block-diagonalizable pseudounitary operators with finite-dimensional diagonal blocks. In Sec. IV we use the results of Secs. II and III to study pseudounitary matrices. In Sec. V we offer a thorough discussion of the 2×2 pseudounitary matrices. In Sec. VI we study an application of our general results for a quantum system with a pseudounitary dynamical group and elaborate on the relation between the choice of the dynamical group and the issue of second quantization. Finally, in Sec. VII we provide a survey of our main results and present our concluding remarks.

II. PSEUDO-HERMITIAN AND PSEUDOUNITARY OPERATORS

By definition,[1] a linear operator $H:\mathcal{H}\to\mathcal{H}$ acting in a Hilbert space $\mathcal{H}$ is said to be pseudo-Hermitian if there exists a linear, invertible, Hermitian operator $\eta:\mathcal{H}\to\mathcal{H}$ such that

$$H^\dagger=\eta H\eta^{-1}. \tag{1}$$

For a given pseudo-Hermitian operator H, the operator η satisfying (1) is not unique.[7,14] Each choice of η determines a possibly indefinite inner product (a pseudoinner product) on $\mathcal{H}$, namely,

$$\langle\!\langle\psi,\phi\rangle\!\rangle_\eta:=\langle\psi|\,\eta\phi\rangle, \tag{2}$$

where $\psi,\phi\in\mathcal{H}$, and $\langle\,|\,\rangle$ is the original inner product of $\mathcal{H}$. Conversely, every pseudoinner product on $\mathcal{H}$ has the form (2). As a result, η is sometimes called a metric operator.

If we make a particular choice for η, we say that H is η-pseudo-Hermitian. In this case, it is Hermitian with respect to the inner product $\langle\!\langle\,,\rangle\!\rangle_\eta$. Therefore, the study of η-pseudo-Hermitian operators is equivalent to the study of Hermitian operators in a vector space with an indefinite metric.[16] The application of the latter in quantum physics dates back to the 1940s.[17] See also Refs. 18 and 19. As emphasized in Ref. 19, there is an important distinction between the concept of pseudo-Hermiticity, where one does not fix the inner product and has the freedom of choosing it, and the well-studied notion of η-pseudo-Hermiticity.

We can express the defining condition (1) in the form $H^\#=H$ where $H^\#:=\eta^{-1}H^\dagger\eta$ is the η-pseudoadjoint of H. Using the latter one can also define the notion of an η-pseudounitary operator $U:\mathcal{H}\to\mathcal{H}$ by requiring that U satisfies $U^\#=U^{-1}$.

Definition: A linear invertible operator $U:\mathcal{H}\to\mathcal{H}$ is said to be pseudounitary if there exists a linear, invertible, Hermitian operator $\eta:\mathcal{H}\to\mathcal{H}$ such that U is η-pseudounitary, i.e.,

$$U^\dagger=\eta U^{-1}\eta^{-1}. \tag{3}$$

Similarly to the case of pseudo-Hermitian operators, η is not unique. If we make a choice for η, we say that U is η-pseudounitary. In this case it is not difficult to show that U leaves the pseudoinner product $\langle\!\langle\,,\rangle\!\rangle_\eta$ invariant. This is easily seen by writing (3) in the form

$$U^\dagger\eta U=\eta, \tag{4}$$

and using (2) and (4) to check that

$$\langle\!\langle U\psi,U\phi\rangle\!\rangle_\eta=\langle\!\langle\psi,\phi\rangle\!\rangle_\eta,\quad \forall\,\psi,\phi\in\mathcal{H}. \tag{5}$$

Given an η-pseudo-Hermitian operator H one can construct a one-parameter family of η-pseudounitary operators, namely $U(t)=e^{-itH}$ with $t\in\mathbb{R}$.

Proposition 1: Let $\epsilon\in\mathbb{R}^+$, $t\in(-\epsilon,\epsilon)$, $H:\mathcal{H}\to\mathcal{H}$ be a t-independent linear operator acting in a Hilbert space $\mathcal{H}$, $U(t):=e^{-itH}$, and $\eta:\mathcal{H}\to\mathcal{H}$ be a t-independent Hermitian, invertible, linear operator. Then H is η-pseudo-Hermitian if and only if $U(t)$ is η-pseudounitary for all $t\in(-\epsilon,\epsilon)$.

Proof: Suppose that H is η-pseudo-Hermitian, then a direct application of Eq. (1), $U(t)^\dagger=e^{itH^\dagger}$ and $U(t)^{-1}=e^{itH}$, shows that $U(t)$ satisfies (3), i.e., it is η-pseudounitary. Conversely, let $U(t)$ be η-pseudounitary for all $t\in(-\epsilon,\epsilon)$. Then substituting $U(t)$ for U in Eq. (3), taking the derivative of both sides with respect to t, and setting $t=0$ in the resulting expression, we find that H satisfies (1), i.e., it is η-pseudo-Hermitian. □

Because $U(t)$ may be identified with the evolution operator for a quantum system having H as its Hamiltonian, a quantum system with a time-independent Hamiltonian has a pseudounitary evolution if and only if the Hamiltonian is pseudo-Hermitian.[14]

The one-parameter family $U(t)$ clearly forms an Abelian Lie group under composition. This is indeed a subgroup of the group $\mathcal{U}_\eta(\mathcal{H})$ of all η-pseudounitary operators. The latter forms a group because for any pair U_1, $U_2:\mathcal{H}\to\mathcal{H}$ of η-pseudounitary operators,

$$(U_1^{-1}U_2)^\dagger=U_2^\dagger(U_1^\dagger)^{-1}=\eta U_2^{-1}\eta^{-1}(\eta U_1^{-1}\eta^{-1})^{-1}=\eta U_2^{-1}\eta^{-1}\eta U_1\eta^{-1}=\eta(U_1^{-1}U_2)^{-1}\eta^{-1}.$$

Therefore $\mathcal{U}_\eta(\mathcal{H})$ is a subgroup of the group $\mathrm{GL}(\mathcal{H})$ of all invertible linear transformations acting in $\mathcal{H}$. In Ref. 11, the authors considered this group for the case $\mathcal{H}=\mathbb{C}^n$. They call it the pseudounitary group. This terminology is rather misleading as it does not reflect the important fact that a particular choice for η has been made. In fact, it is not true that the product of any two pseudounitary operators V_1 and V_2 is pseudounitary. This is because they may belong to $\mathcal{U}_\eta(\mathcal{H})$ with different η. This observation calls for a more careful study of the structure of the set $\mathcal{U}(\mathcal{H})$ $:=\cup_\eta\mathcal{U}_\eta(\mathcal{H})$ of all pseudounitary operators acting in $\mathcal{H}$.

In the remainder of this section we discuss two simple properties of pseudounitary operators that will be of future use.

Proposition 2: Let η_1 be a Hermitian, invertible, linear operator acting in a Hilbert space $\mathcal{H}$, $A:\mathcal{H}\to\mathcal{H}$, $U_1:\mathcal{H}\to\mathcal{H}$ be invertible linear operators, $U_2:=A^{-1}U_1A$ and $\eta_2:=A^\dagger\eta_1A$. Then U_1 is η_1-pseudounitary if and only if U_2 is η_2-pseudo-Hermitian.

Proof: First note that the defining condition (3) may be written in the form $U\eta^{-1}U^\dagger\eta=I$, where I is the identity operator. Then a simple calculation shows that

$$U_2\eta_2^{-1}U_2^\dagger\eta_2=A^{-1}U_1AA^{-1}\eta_1^{-1}A^{-1\dagger}A^\dagger U_1A^{-1\dagger}A^\dagger\eta_1A=A^{-1}(U_1\eta_1^{-1}U_1^\dagger\eta_1)A.$$

Therefore, $U_1\eta_1^{-1}U_1^\dagger\eta_1=I$ if and only if $U_2\eta_2^{-1}U_2^\dagger\eta_2=I$. □

Proposition 3: Let $U_1:\mathcal{H}\to\mathcal{H}$ be a pseudounitary operator acting in a Hilbert space $\mathcal{H}$ and u be an eigenvalue of U. Then $1/u^*$ is also an eigenvalue of U. In other words, eigenvalues of U are either unimodular ($|u|=1$) or they come in inverse-complex-conjugate pairs $(u,1/u^*)$.

Proof: Let $|u\rangle$ be an eigenvector of U with eigenvalue u, i.e., $U|u\rangle=u|u\rangle$. Acting out both sides of (4) on $u^{-1}|u\rangle$, we find $U^\dagger\eta|u\rangle=u^{-1}\eta|u\rangle$. Because η is invertible, $\eta|u\rangle\neq0$. This in turn means that u^{-1} is an eigenvalue of $U^\dagger$. But the eigenvalues of $U^\dagger$ are complex conjugates of those of U. Therefore, $u^{-1*}=1/u^*$ is an eigenvalue of U. If $u=1/u^*$, u is unimodular; otherwise $(u,1/u^*)$ is a pair of distinct inverse-complex-conjugate eigenvalues. □

As a straightforward application of Proposition 3, consider the case that $\mathcal{H}=\mathbb{C}^{2m}$, for some $m\in\mathbb{Z}^+$, and endow $\mathbb{C}^{2m}$ with the metric operator

$$\eta_J:=iJ, \tag{6}$$

where $J:\mathbb{C}^{2m}\to\mathbb{C}^{2m}$ has the following matrix representation in the standard orthonormal basis of $\mathbb{C}^{2m}$:

$$J=\begin{pmatrix}0_m & -1_m\\ 1_m & 0_m\end{pmatrix}. \tag{7}$$

Here 0_m and 1_m are, respectively, the $m\times m$ zero and identity matrices, respectively. According to (6) and (7), the operator η_J has a Hermitian matrix representation in an orthonormal basis, and $\eta_J^2=1$. Hence η_J is indeed a Hermitian invertible (metric) operator acting in $\mathbb{C}^{2m}$.

Next, observe that the operator J restricted to $\mathbb{R}^{2m}$ yields the usual symplectic form[20] on $\mathbb{R}^{2m}$. The associated symplectic transformations coincide with real $2m\times 2m$ matrices S satisfying[20]

$$S^tJS=J, \tag{8}$$

where S^t stands for the transpose of S. We can view the symplectic transformations S as linear operators acting in $\mathbb{C}^{2p}$. Then the condition that they admit real matrix representations (in the standard basis) takes the form

$$TST=S, \tag{9}$$

where T is the (time-reversal) operator defined by $\forall\vec{z}\in\mathbb{C}^{2p}$, $T\vec{z}=\vec{z}^*$. Making use of (6) and the fact that $T^{-1}=T$ and $S^\dagger=S^t$, we can, respectively, express the defining relations (8) and (9) of the symplectic transformations S as

$$S^\dagger\eta_JS=\eta_J, \tag{10}$$

$$[S,T]=0. \tag{11}$$

Because T is an antilinear Hermitian invertible operator, according to Theorem 2 of Ref. 3, Eq. (11) implies that S is a pseudo-Hermitian operator. Furthermore, Eq. (10) means that S is in addition a pseudounitary operator.

In view of Proposition 3 and the spectral characterization theorem for pseudo-Hermitian operators (Ref. 1, Theorem 2), the fact that symplectic transformations are both pseudo-Hermitian and pseudounitary leads to the following well-known spectral theorem for symplectic transformations.[20]

Theorem 1: Let λ be an eigenvalue of a symplectic transformation S, then so are λ^*, $1/\lambda$, and $1/\lambda^*$.

Proof: Because S is pseudounitary $1/\lambda^*$ is an eigenvalue. Because it is pseudo-Hermitian λ^* and $(1/\lambda^*)^*=1/\lambda$ are eigenvalues. □

III. BLOCK-DIAGONALIZABLE PSEUDOUNITARY OPERATORS WITH FINITE-DIMENSIONAL DIAGONAL BLOCKS

Consider an operator $U:\mathcal{H}\to\mathcal{H}$ acting in a Hilbert space $\mathcal{H}$ and having a discrete spectrum. Then U is said to be block diagonalizable with finite-dimensional diagonal blocks[6] if it can be expressed in the form

$$U=\sum_n\sum_{a=1}^{d_n}\left(u_n\sum_{i=1}^{p_{n,a}}|\psi_n,a,i\rangle\langle\phi_n,a,i|+\sum_{i=1}^{p_{n,a}-1}|\psi_n,a,i\rangle\langle\phi_n,a,i+1|\right), \tag{12}$$

where n is the spectral label, u_n are the eigenvalues of U, d_n is the geometric multiplicity of u_n, $a\in\{1,2,...,d_n\}$ is a degeneracy label, $p_{n,a}$ is the dimension of the Jordan block associated with the labels n and a (these are called the Jordan dimensions[6]), and $\{|\psi_n,a,i\rangle,|\phi_n,a,i\rangle\}$ is a complete biorthonormal system satisfying

$$\langle\psi_n,a,i|\phi_m,b,j\rangle=\delta_{mn}\delta_{ab}\delta_{ij},\quad \sum_n\sum_{a=1}^{d_n}\sum_{i=1}^{p_{n,a}}|\psi_n,a,i\rangle\langle\phi_m,a,i|=1. \tag{13}$$

In view of (12) and (13),

$$U|\psi_n,a,1\rangle=u_n|\psi_n,a,1\rangle,\quad U^\dagger|\phi_n,a,p_{n,a}\rangle=u_n^*|\phi_n,a,p_{n,a}\rangle, \tag{14}$$

i.e., $|\psi_n,a,1\rangle$ are the eigenvectors of U and $|\phi_n,a,p_{n,a}\rangle$ are the eigenvectors of $U^\dagger$. Clearly, the eigenvalues of $U^\dagger$ are complex conjugates of those of U, and if U is invertible the eigenvalues u_n do not vanish.

Lemma 1: Let $U:\mathcal{H}\to\mathcal{H}$ be an invertible operator acting in a Hilbert space $\mathcal{H}$ and $z\in\mathbb{C}-\{0\}$. Then for all $\ell\in\mathbb{Z}^+$,

$$\text{kernel}[(U^{-1}-z^{-1})^\ell]=\text{kernel}[(U-z)^\ell]. \tag{15}$$

Proof: This identity follows by induction over ℓ. For $\ell=1$, we have

$$\begin{aligned}|\xi\rangle\in\text{kernel}[U^{-1}-z^{-1}]&\Leftrightarrow(U^{-1}-z^{-1})|\xi\rangle=0\\ &\Leftrightarrow zU(U^{-1}-z^{-1})|\xi\rangle=0\Leftrightarrow(z-U)|\xi\rangle=0\Leftrightarrow|\xi\rangle\in\text{kernel}[U-z],\end{aligned} \tag{16}$$

where we have used the fact that zU is an invertible operator. Relations (16) show that (15) holds for $\ell=1$. Now, suppose (15) holds for some $\ell=k\in\mathbb{Z}^+$. Then

$$\begin{aligned}|\xi\rangle\in\text{kernel}[(U^{-1}-z^{-1})^{k+1}]&\Leftrightarrow(U^{-1}-z^{-1})^k(U^{-1}-z^{-1})|\xi\rangle=0\\ &\Leftrightarrow(U^{-1}-z^{-1})|\xi\rangle\in\text{kernel}[(U^{-1}-z^{-1})^k]\\ &\Leftrightarrow(U^{-1}-z^{-1})|\xi\rangle\in\text{kernel}[(U-z)^k]\\ &\Leftrightarrow(U-z)^k(U^{-1}-z^{-1})|\xi\rangle=0\\ &\Leftrightarrow zU(U-z)^k(U^{-1}-z^{-1})|\xi\rangle=0\\ &\Leftrightarrow(U-z)^k(z-U)|\xi\rangle=0\Leftrightarrow|\xi\rangle\in\text{kernel}[(U-z)^{k+1}].\end{aligned}$$

Therefore, (15) holds for $\ell=k+1$; by induction, it holds for all $\ell\in\mathbb{Z}^+$. □

Theorem 2: Let $U:\mathcal{H}\to\mathcal{H}$ be an operator acting in a Hilbert space $\mathcal{H}$ and having a discrete spectrum. Suppose that U is block diagonalizable with finite-dimensional diagonal blocks so that (12) holds. Then U is pseudounitary if and only if the eigenvalues u_n of U are either unimodular (i.e., $|u_n|=1$) or they come in inverse-complex-conjugate pairs $(u_n,1/u_n^*)$ and that the geometric multiplicity and the Jordan dimensions for the inverse-complex-conjugate eigenvalues coincide.

Proof: Suppose that U is pseudounitary. Then, according to Proposition 3 the eigenvalues of U are either unimodular or they come in inverse-complex-conjugate pairs. Suppose that u_n and $1/u_n^*$ form a pair of distinct inverse-complex-conjugate eigenvalues. In order to show that they have the same geometric multiplicity and Jordan dimensions we prove that for all $\ell\in\mathbb{Z}^+$, $\text{kernel}(U-u_n)^\ell$ and $\text{kernel}(U-1/u_n^*)^\ell$ have the same (finite) dimension. To see this, first note that U and $U^\dagger$ have the same Jordan block structure; in view of (12), for all $\ell\in\mathbb{Z}^+$, $\text{kernel}(U-u_n)^\ell$ and $\text{kernel}(U^\dagger-u_n^*)^\ell$ have the same (finite) dimension. Hence they are isomorphic as vector spaces. Next, we use the fact that η is an invertible operator to establish the isomorphism between $\text{kernel}(U^\dagger-u_n^*)^\ell$ and

$$\begin{aligned}\text{kernel}[\eta^{-1}(U^\dagger-u_n^*)^\ell\eta]=\text{kernel}[(\eta^{-1}U^\dagger\eta-u_n^*)^\ell]&=\text{kernel}[(U^{-1}-u_n^*)^\ell]\\ &=\text{kernel}[(U-1/u_n^*)^\ell].\end{aligned}$$

Here we have made use of the defining relation (3) and the identity (15) of Lemma 1. This completes the proof that for all $\ell\in\mathbb{Z}^+$, $\text{kernel}(U-u_n)^\ell$ is isomorphic to $\text{kernel}(U-1/u_n^*)^\ell$. Therefore, they have the same (finite) dimension.

Next, suppose that U has unimodular and/or inverse-complex-conjugate pairs of eigenvalues with identical geometric multiplicity and Jordan dimensions. Then U may be expressed as

$$U=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\left(u_{\nu_0}\sum_{i=1}^{p_{\nu_0,a}}|\psi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,i|+\sum_{i=1}^{p_{\nu_0,a}-1}|\psi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,i+1|\right)$$
$$+\sum_{\nu}\sum_{a=1}^{d_\nu}\left[\sum_{i=1}^{p_{\nu,a}}\left(u_\nu|\psi_{\nu+},a,i\rangle\langle\phi_{\nu+},a,i|+\frac{1}{u_\nu^*}|\psi_{\nu-},a,i\rangle\langle\phi_{\nu-},a,i|\right)\right.$$
$$\left.+\sum_{i=1}^{p_{\nu,a}-1}(|\psi_{\nu+},a,i\rangle\langle\phi_{\nu+},a,i+1|+|\psi_{\nu-},a,i\rangle\langle\phi_{\nu-},a,i+1|)\right], \tag{17}$$

where we have set $n=\nu_0$, $\nu+$, or $\nu-$ depending on whether $|u_n|=1$, $|u_n|>1$, or $|u_n|<1$, respectively, and used ν to denote the common value of $\nu+$ and $\nu-$. In order to show that U, as given by (17), is pseudounitary we construct a Hermitian, invertible, linear operator η satisfying (3) or equivalently (4). Consider the ansatz

$$\eta=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\sum_{i,j=1}^{p_{\nu_0,a}}z_{\nu_0,a,i,j}|\phi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,j|+\sum_{\nu}\sum_{a=1}^{d_\nu}\sum_{i,j=1}^{p_{\nu,a}}(\zeta_{\nu,a,i,j}|\phi_{\nu-},a,j\rangle\langle\phi_{\nu+},a,i|$$
$$+\zeta^*_{\nu,a,i,j}|\phi_{\nu+},a,i\rangle\langle\phi_{\nu-},a,j|), \tag{18}$$

where $z_{\nu_0,a,i,j}$ and $\zeta_{\nu,a,i,j}$ are complex coefficients and

$$z^*_{\nu_0,a,i,j}=z_{\nu_0,a,j,i}. \tag{19}$$

The latter relation ensures that η is Hermitian. Now, impose the condition (4). Substituting (17) and (18) in (4) and using the biorthonormality and completeness relations (13), we find after a quite lengthy calculation that $z_{\nu_0,a,i,j}$ and $\zeta_{\nu,a,i,j}$ are solutions of the following equations for $u=u_{\nu_0}$, $p=p_{\nu_0,a}$ and $u=u_\nu$, $p=p_{\nu,a}$, respectively,

$$x_{1,i}=x_{i,1}=0,\quad \forall i\in\{1,2,...,p-1\}, \tag{20}$$

$$ux_{i-1,j}+u^{-1}x_{i,j-1}+x_{i-1,j-1}=0,\quad \forall i,j\in\{2,...,p\}. \tag{21}$$

It turns out that these equations have the following exact solution:

$$x_{i,j}=\begin{cases}0 & \text{for } i+j\leqslant p,\\ \displaystyle\sum_{k=1}^{i+j-p}\binom{i-k-1}{p-j-1}(-1)^{i-k}u^{p+i-j-k}x_{k,p} & \text{for } j<p<i+j,\end{cases} \tag{22}$$

where for all $r,s\in\mathbb{Z}^+$ with $r\leqslant s$

$$\binom{s}{r}:=\frac{s!}{r!(s-r)!},$$

and $x_{k,p}$ with $k\in\{1,2,...,p\}$ are arbitrary complex numbers. We have obtained the solution (22) by a tedious inspection scheme and checked its validity by direct substitution in (21); it clearly satisfies (20). It is important to note that according to (22), $x_{i,j}$ form a $p\times p$ matrix x of the form

$$x=\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & x_{1,p} \\ 0 & 0 & 0 & \cdots & 0 & x_{2,p-1} & x_{2,p} \\ 0 & 0 & 0 & \cdots & x_{3,p-2} & x_{3,p-1} & x_{3,p} \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x_{p-2,3} & \cdots & x_{p-2,p-2} & x_{p-2,p-1} & x_{p-2,p} \\ 0 & x_{p-1,2} & x_{p-1,3} & \cdots & x_{p-1,p-2} & x_{p-1,p-1} & x_{p-1,p} \\ x_{p,1} & x_{p,2} & x_{p,3} & \cdots & x_{p,p-2} & x_{p,p-1} & x_{p,p} \end{pmatrix}. \tag{23}$$

In view of (22) all the entries of x are determined in terms of the entries in the last column. For example, we have

$$x_{i,p-i+1}=(-1)^{i-1}u^{2(i-1)}x_{1,p}, \quad \forall i\in\{1,2,...,p\}. \tag{24}$$

Moreover note that the determinant of x is up to a sign the product of the entries (24). Therefore, x is an invertible matrix provided that $x_{1,p}\neq 0$ and $u\neq 0$. Next, consider the case that u is unimodular and seek for the solutions (22) that make x Hermitian, i.e., find solutions for (20) and (21) subject to the condition

$$x^*_{i,j}=x_{j,i}. \tag{25}$$

Imposing this condition on the solution (22) restricts the choice of the initially free entries, namely $x_{i,p}$. For example, setting $i=p$ and $j=1$ in (22) or alternatively setting $i=p$ in (24), we find $x_{p,1}=(-1)^{p-1}u^{2(p-1)}x_{1,p}$. Now, using (25) which implies $x_{p,1}=x^*_{1,p}$, we find

$$x_{1,p}=\pm\sqrt{(-1)^{p-1}}u^{1-p}\rho, \tag{26}$$

where $\rho=|x_{1,p}|$ is an arbitrary non-negative real number. A similar analysis shows that the condition (25) leads to similar restrictions on the choices of $x_{i,p}$ with $i>1$. But these restrictions do not lead to any contradictions, i.e., (25) can always be satisfied. Indeed there are infinitely many solutions of the form (22) that fulfill (25). In particular, if we choose $|u|=1$ and $\rho\neq 0$, the matrix x is an invertible Hermitian matrix. Setting $u=u_{\nu_0}$, we have a set of solutions $z_{\nu_0,a,i,j}$ of (20) and (21) that respect the condition (19) and that the matrices $z_{\nu_0,a}$ formed out of $z_{\nu_0,a,i,j}$ are invertible. Similarly, setting $u=u_\nu$ we have a set of solutions $\zeta_{\nu,a,i,j}$ of (20) and (21) such that the matrices $\zeta_{\nu,a}$ formed out of $\zeta_{\nu,a,i,j}$ are also invertible. The existence of these solutions is equivalent to the existence of a linear operator η of the form (18) that satisfies (4) and is Hermitian and invertible. The inverse of η is given by

$$\eta^{-1}=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\sum_{i,j=1}^{p_{\nu_0,a}}\widetilde{z}_{\nu_0,a,i,j}|\psi_{\nu_0},a,i\rangle\langle\psi_{\nu_0},a,j|+\sum_{\nu}\sum_{a=1}^{d_\nu}\sum_{i,j=1}^{p_{\nu,a}}(\widetilde{\zeta}_{\nu,a,i,j}|\psi_{\nu-},a,j\rangle\langle\psi_{\nu+},a,i|$$
$$+\widetilde{\zeta}^*_{\nu,a,i,j}|\psi_{\nu+},a,i\rangle\langle\psi_{\nu-},a,j|), \tag{27}$$

where $\widetilde{z}_{\nu_0,a,i,j}$ are the entries of the matrix $z^{-1}_{\nu_0,a}$, and $\widetilde{\zeta}_{\nu,a,i,j}$ are those of $\zeta^{-1\dagger}_{\nu,a}$. One can check by direct calculation that $\eta^{-1}\eta=1$. This completes the proof of the pseudounitarity of U. □

IV. PSEUDOUNITARY MATRICES

According to Theorem 2, a square matrix U is pseudounitary if its eigenvalues are either unimodular or they come in inverse-complex-pairs and that geometric multiplicity and the Jordan dimensions of the latter are identical. A direct consequence of this observation is the following.

Proposition 4: Every pseudounitary matrix U has a unimodular determinant, i.e., $|\det U|=1$.

Proof: This follows from the fact that in the Jordan canonical form of U the nonunimodular entries come is inverse-complex-conjugate pairs $(u_n, 1/u_n^*)$. Hence their product which yields $\det U$ is unimodular. □

According to this proposition the set $\mathcal{U}(\mathbb{C}^n)$ of all $n\times n$ pseudounitary matrices is a subset of the group

$$\Sigma L(n,\mathbb{C}) := \{g \in \mathrm{GL}(n,\mathbb{C}) \mid \ |\det g| = 1\}, \tag{28}$$

of $n\times n$ matrices with unimodular determinant. We shall call $\Sigma L(n,\mathbb{C})$ the *pseudospecial groups*. As a subset of $\mathrm{GL}(n,\mathbb{C})$, $\Sigma L(n,\mathbb{C})$ is the inverse image of the group $\mathrm{U}(1)$ under the homomorphism $\det:\mathrm{GL}(n,\mathbb{C})\to\mathrm{GL}(1,\mathbb{C})$. Therefore, $\Sigma L(n,\mathbb{C})$ is a subgroup of $\mathrm{GL}(n,C)$. In fact, it is not difficult to show that $\Sigma L(n,\mathbb{C})$ is isomorphic to the product group $\mathrm{U}(1)\times\mathrm{SL}(n,\mathbb{C})$. Note however that not every element of the pseudospecial groups is pseudounitary. For example let g be a 2×2 diagonal matrix with diagonal entries $2i$ and $-i/2$. Clearly, $\det g = 1 \in \mathrm{U}(1)$, so $g \in \Sigma L(2,\mathbb{C})$. But, $(2i)^{-1*} = i/2 \neq -i/2$. Hence the eigenvalues $2i$ and $-i/2$ are not inverse-complex-conjugates, and g is not pseudounitary. In general, $\mathcal{U}(\mathbb{C}^n)$ is a proper subset of $\Sigma L(n,\mathbb{C})$.

Next, consider the group $\mathcal{U}_\eta(\mathbb{C}^n)$ for a fixed Hermitian invertible $n\times n$ matrix η. We recall Sylvester's law of inertia according to which η satisfies

$$\eta = A^\dagger \eta_{p,q} A, \tag{29}$$

where A is some invertible $n\times n$ matrix and $\eta_{p,q}$ is a diagonal matrix of the form

$$\eta_{p,q} = \mathrm{diag}(-1,-1,\ldots,-1,1,1,\ldots,1), \tag{30}$$

which has p negative and $q := n-p$ positive entries.

Proposition 5: Let η be an $n\times n$ Hermitian and invertible matrix. Then the group $\mathcal{U}_\eta(\mathbb{C}^n)$ is isomorphic to the pseudounitary group

$$\mathrm{U}(p,q) := \{g \in \mathrm{GL}(n,\mathbb{C}) \mid g^\dagger \eta_{p,q} g = \eta_{p,q}\} = \mathcal{U}_{\eta_{p,q}}(\mathbb{C}^n),$$

for some $p \in \{0,1,\ldots,n\}$ and $q := n-p$. [Note that $\mathrm{U}(0,n) = \mathrm{U}(n)$.]

Proof: Setting $U_2 = U$, $\eta_2 = \eta$, and $\eta_1 = \eta_{p,q}$ in Proposition 2, we see that $U \in \mathcal{U}_\eta(\mathbb{C}^n)$ if and only if $U_1 := AUA^{-1} \in U(p,q)$. Hence, $\mathcal{U}_\eta(\mathbb{C}^n) = A^{-1}U(p,q)A$. Because the conjugation $i_A:\mathrm{GL}(n,\mathbb{C})\to\mathrm{GL}(n,\mathbb{C})$ defined by $i_A(g) := A^{-1}gA$ is an automorphism of the group $\mathrm{GL}(n,\mathbb{C})$ that maps $\mathcal{U}_\eta(\mathbb{C}^n)$ onto $\mathrm{U}(p,q)$, the subgroups $\mathcal{U}_\eta(\mathbb{C}^n)$ and $\mathrm{U}(p,q)$ are isomorphic. □

According to Proposition 5, the pseudounitary groups $\mathcal{U}_\eta(\mathbb{C}^n)$ are isomorphic to and obtained from the classical groups $\mathrm{U}(p,q)$ [or $\mathrm{U}(n)$] by conjugation; $\mathcal{U}_\eta(\mathbb{C}^n) = A^{-1}U(p,q)A$ for some $A \in \mathrm{GL}(n,\mathbb{C})$. Therefore, the set $\mathcal{U}(\mathbb{C}^n)$ may be viewed as the union of the orbits of the subgroups $\mathrm{U}(p,q)$ under conjugation in $\mathrm{GL}(n,\mathbb{C})$. Obviously these orbits, which according to Proposition 4 lie in the pseudospecial group $\Sigma L(n,\mathbb{C})$, are not disjoint. For example, $e^{iH} \in \mathcal{U}(\mathbb{C}^n)$ belongs to both $\mathcal{U}_{\eta_1}(\mathbb{C}^n)$ and $\mathcal{U}_{\eta_2}(\mathbb{C}^n)$, if H is both η_1- and η_2-pseudo-Hermitian. The latter holds if and only if $\eta_2 = A^\dagger \eta_1 A$ for some $A \in \mathrm{GL}(n,\mathbb{C})$ commuting with H.[7]

Another simple consequence of Proposition 5 is the following.

Corollary: Let $m \in \mathbb{Z}^+$. Then the group $\mathrm{Sp}(2m)$ of symplectic transformations of $\mathbb{R}^{2m}$ is isomorphic to the real subgroup of (a matrix group that is isomorphic to) the pseudounitary group $\mathrm{U}(m,m)$.

Proof: According to the argument given above Theorem 1, $\mathrm{Sp}(2m)$ may be identified with the subgroup of $\mathcal{U}_{\eta_J}(\mathbb{C}^{2m})$ consisting of real matrices. It is not difficult to show that the spectrum of η_J consists of -1 and 1 each with multiplicity m. Hence according to Proposition 5, $\mathcal{U}_{\eta_J}(\mathbb{C}^{2m})$ is isomorphic to $\mathrm{U}(m,m)$, and $\mathrm{Sp}(2m)$ is isomorphic to the real subgroup of $\mathcal{U}_{\eta_J}(\mathbb{C}^{2m})$. □

Note also that according to the argument used in the above proof of Theorem 1 and the spectral characterization theorems for pseudo-Hermitian and pseudounitary operators (i.e., Theorem 1 of Ref. 6 and Theorem 2 above), given an eigenvalue λ of a symplectic transformation $S \in \mathrm{Sp}(2m)$, the eigenvalues λ^*, $1/\lambda$, and $1/\lambda^*$ have the same geometric multiplicity and Jordan

dimensions as λ. This in particular proves the well-known fact that S has a unit determinant. In particular, $\mathrm{Sp}(2m)$ may be identified with the real subgroup of (a matrix group that is isomorphic to) $\mathrm{SU}(m,m)$.

Next, we state and prove the following lemma.

Lemma 2: Let $p\in\mathbb{Z}^+$, $E\in\mathbb{C}$, and h be a $p\times p$ matrix of the Jordan form

$$h=E1_p+a_p, \tag{31}$$

where 1_p is the $p\times p$ identity matrix and a_p is the $p\times p$ matrix

$$a_p:=\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0\\ 0 & 0 & 1 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & 0 & 1 & 0\\ 0 & 0 & 0 & \cdots & 0 & 0 & 1\\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix} \tag{32}$$

(a_p provides an irreducible representation of the annihilation operator for a para-Fermion of order $p-1$[21]). Then e^{ih} has the following canonical Jordan form:

$$e^{iE}1_p+a_p. \tag{33}$$

Equivalently, e^{iE} is the unique eigenvalue of e^{ih} with geometric multiplicity 1 and algebraic multiplicity p.

Proof: Using the fact that $a_p^p=0$, we can easily compute

$$e^{ih}=e^{iE}\sum_{\ell=0}^{p-1}\frac{i^\ell a^\ell}{\ell!}.$$

This is an upper triangular matrix with a single eigenvalue (namely e^{iE}) and a single (linearly independent) eigenvector. Therefore its geometric multiplicity is 1 and its algebraic multiplicity is p. □

Theorem 3: Every pseudounitary matrix U may be expressed as e^{iH} for some pseudo-Hermitian matrix H.

Proof: Let U be an $n\times n$ pseudounitary matrix. Clearly, $U\in\mathrm{GL}(n,\mathbb{C})$. Now, because the exponential map for the group $\mathrm{GL}(n,\mathbb{C})$ is onto,[22] there is a square matrix H such that $U=e^{iH}$. We can perform a similarity transformation $H\to\tilde{H}:=A^{-1}HA$ that maps H into its Jordan canonical form $\tilde{H}$. We then have

$$U=Ae^{i\tilde{H}}A^{-1}. \tag{34}$$

In view of Proposition 2 and Lemma 2, $e^{i\tilde{H}}$ is pseudounitary, and its eigenvalues are of the form e^{iE_n} where E_n are the eigenvalues of $\tilde{H}$. Moreover, the geometric multiplicity and the Jordan dimensions of (the canonical Jordan form of) $e^{i\tilde{H}}$ coincide with those of $\tilde{H}$. Now, because $e^{i\tilde{H}}$ is pseudounitary, Theorem 2 implies that the eigenvalues e^{iE_n} of $e^{i\tilde{H}}$ are either unimodular or they come in inverse-complex-conjugate pairs with identical geometric multiplicity and Jordan dimensions. First we consider the unimodular eigenvalues which we denote by $e^{iE_{\nu_0}}$. Because $1=|e^{iE_{\nu_0}}|^2=e^{iE_{\nu_0}}e^{-iE^*_{\nu_0}}$, we have $E_{\nu_0}-E^*_{\nu_0}=2\pi k_{\nu_0}$ for some $k_{\nu_0}\in\mathbb{Z}$. But the left-hand side of this equation is imaginary while its right-hand side is real. This implies $k_{\nu_0}=0$. Hence E_{ν_0} is real. Next, consider the eigenvalues e^{iE_ν} that are not unimodular. These are paired with their inverse-

complex-conjugate, namely, $e^{iE_\nu^*}$. e^{iE_ν} and $e^{iE_\nu^*}$ have the same geometric multiplicity d_ν and Jordan dimensions $p_{\nu,a}$. Because $e^{iE_\nu^*}$ is an eigenvalue of $e^{i\tilde{H}}$, according to Lemma 2 there is an eigenvalue E'_ν of $\tilde{H}$ such that

$$e^{iE_\nu^*}=e^{iE'_\nu}, \tag{35}$$

and that E'_ν has the same geometric multiplicity and Jordan dimensions as $e^{iE_\nu^*}$. Hence the geometric multiplicity and Jordan dimensions of E'_ν are, respectively, d_ν and $p_{\nu,a}$. Furthermore, Eq. (35) implies $E'_\nu=E_\nu^*+2\pi k_\nu$ for some $k_\nu\in\mathbb{Z}$. Now, let $E_{\nu+}$ and $E_{\nu-}$, respectively, denote the eigenvalues of $\tilde{H}$ with positive and negative imaginary part. In view of the preceding argument, for each $E_{\nu+}$ there is an eigenvalue $E_{\nu-}=E_{\nu+}^*+2\pi k_{\nu+}$. Furthermore all the eigenvalues with negative imaginary part may be obtained from the eigenvalues with positive imaginary part in this way. Now, let $\tilde{H}'$ be the matrix obtained from $\tilde{H}$ by replacing the eigenvalues $E_{\nu-}$ with $E'_{\nu-}$ $:=E_{\nu-}-2\pi k_{\nu+}=E_{\nu+}^*$. Then, by construction, $\tilde{H}'$ has real and/or complex-conjugate pairs of eigenvalues, the latter having identical geometric multiplicity and Jordan dimensions. In light of Theorem 1 of Ref. 6, this implies that $\tilde{H}'$ is pseudo-Hermitian. One can also check that

$$e^{i\tilde{H}'}=e^{i\tilde{H}}. \tag{36}$$

Next, let

$$H':=A\tilde{H}'A^{-1}. \tag{37}$$

Clearly, $\tilde{H}'$ is the Jordan canonical form of H'. In particular, H' is also pseudo-Hermitian. Combining Eqs. (34), (36), and (37), we finally have

$$U=Ae^{i\tilde{H}}A^{-1}=Ae^{i\tilde{H}'}A^{-1}=e^{iA\tilde{H}'A^{-1}}=e^{iH'}.$$

This completes the proof of the fact that U is the exponential of i times a pseudo-Hermitian matrix. □

Corollary 1: A square matrix U is pseudounitary if and only if $-i\ln U$ is pseudo-Hermitian, i.e., $U=e^{iH}$ for a pseudo-Hermitian matrix H.

Proof: If U is pseudounitary, then according to Theorem 3 it is of the form e^{iH} for some pseudo-Hermitian matrix. If $U=e^{iH}$ for a pseudo-Hermitian matrix H, then setting $\epsilon=2$, $t=-1$ in Proposition 1 we find that $U=\mathrm{U}(-1)$ is pseudounitary. □

Corollary 1 is rather surprising, for it is well known that the exponential map is not onto for pseudounitary groups such as U(1,1).[22] This does not however contradict the statement of Corollary 1, because when one speaks of a pseudounitary group one fixes the operator η. What has been done in the proof of Theorem 3 is to show that for a given pseudounitary operator U there is an η such that U is η-pseudounitary and $H:=-\ln U$ is η-pseudo-Hermitian. This is not equivalent to the erroneous statement that given an η, $-i\ln U$ is η-pseudo-Hermitian for every η-pseudounitary matrix U. The exponential map for the pseudounitary group $\mathcal{U}_\eta(\mathbb{C}^n)$ is generally not onto, but the exponential map for the set of all pseudounitary matrices is onto. This is another demonstration of the importance of the difference between the notions of η-pseudo-Hermiticity (respectively, η-pseudounitarity) and pseudo-Hermiticity (respectively, pseudounitarity).[19]

V. 2×2 PSEUDOUNITARY MATRICES

In this section we shall study the case $n=2$ in more detail. The following corollary of Theorem 3 yields the general form of 2×2 pseudounitary matrices.

Corollary 2: A 2×2 matrix U is pseudo-Hermitian if and only if $U=A^{-1}DA$ where A is an invertible 2×2 matrix and D is a matrix assuming one of the following three forms:

$$D_1=\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{i(\varphi-\theta)} \end{pmatrix}, \quad \theta,\varphi\in\mathbb{R}, \tag{38}$$

$$D_2=\begin{pmatrix} re^{i\theta} & 0 \\ 0 & e^{i\theta}/r \end{pmatrix}, \quad r\in\mathbb{R}^+, \quad \theta\in\mathbb{R}, \tag{39}$$

$$D_3=\begin{pmatrix} e^{i\theta} & 1 \\ 0 & e^{i\theta} \end{pmatrix}, \quad \theta\in\mathbb{R}. \tag{40}$$

Proof: Block diagonalizing U we find a matrix D which is either diagonal or has the form

$$D=\begin{pmatrix} u & 1 \\ 0 & u \end{pmatrix}, \tag{41}$$

where $u\in\mathbb{C}$. According to Proposition 2, D is also pseudounitary. This together with Theorem 3 imply that

(i) if D is diagonal, its eigenvalues are either both unimodular, i.e., D is of the form (38), or they are inverse-complex-conjugate, i.e., D is of the form (39);
(ii) if D has the form (41), then it has a single eigenvalue u which is necessarily unimodular. That is D is of the form (40). □

In order to demonstrate the utility of Theorem 3, here we include a direct proof of Corollary 2. This proof involves the calculation of the matrices η whose general form is given in the proof of Theorem 2.

A direct proof of corollary 2: First consider the case that U is diagonalizable, then the canonical Jordan form $D=AUA^{-1}$ of U is diagonal. Clearly $\det D=\det U$ and according to Proposition 4 $\det U\in\mathrm{U}(1)$. Hence $|\det D|=1$. This implies that D must have the form

$$D=\begin{pmatrix} \zeta & 0 \\ 0 & e^{i\varphi}/\zeta \end{pmatrix}, \tag{42}$$

where $\zeta:=re^{i\theta}\in\mathbb{C}-\{0\}$ and $e^{i\varphi}\in U(1)$, i.e., $r\in\mathbb{R}^+$ and $\theta,\varphi\in\mathbb{R}$. Next, note that in view of Proposition 2, U is η-pseudounitary if and only if D is $A^{-1\dagger}\eta A^{-1}$-pseudounitary. This reduces the problem to finding the necessary and sufficient conditions on ζ (alternatively r, θ) and φ that make D pseudounitary. Using the general form

$$\eta=\begin{pmatrix} a & \xi \\ \xi^* & b \end{pmatrix}, \quad a,b\in\mathbb{R}, \quad \xi\in\mathbb{C}, \quad ab\neq|\xi|^2, \tag{43}$$

of the Hermitian matrix η and the fact that D is η-pseudounitary for some η of the form (43), i.e., $D^\dagger=\eta D^{-1}\eta^{-1}$ or $D^\dagger\eta D=\eta$, we find that for $\xi=0$: $r=1$ and $D=D_1$, and for $\xi\neq0$: $e^{i\varphi}=e^{i\theta}$ and $D=D_2$. Next, consider the case that U is not diagonalizable. Then D has the form (41). Again because D is pseudounitary, $\det D\in\mathrm{U}(1)$. This implies $u\in\mathrm{U}(1)$, i.e., $u=e^{i\theta}$ for some $\theta\in\mathbb{R}$. Substituting this expression and the general form (43) of η in $D^\dagger\eta D=\eta$, we find that this equation can always be satisfied without restricting θ. Therefore, in this case $D=D_3$. □

The above analysis also yields the form of η for each of the cases considered.

(1) For $D=D_1$, there are two possibilities.
(1a) $e^{i\varphi}\neq e^{2i\theta}$: In this case, $\xi=0$ and η has the diagonal form

$$\eta=\eta_1:=\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \quad a,b\in\mathbb{R}-\{0\}. \tag{44}$$

TABLE I. Operators H_D and η for $D=D_1$, D_2, D_3.

i	D_i	H_{D_i}	η_i
1	$\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{i(\varphi-\theta)} \end{pmatrix}$	$\begin{pmatrix} \theta & 0 \\ 0 & \varphi-\theta \end{pmatrix}$	$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$
2	$\begin{pmatrix} re^{i\theta} & 0 \\ 0 & e^{i\theta}/r \end{pmatrix}$	$\begin{pmatrix} \theta-i\ln r & 0 \\ 0 & \theta+i\ln r \end{pmatrix}$	$\begin{pmatrix} 0 & \xi \\ \xi^* & 0 \end{pmatrix}$
3	$\begin{pmatrix} e^{i\theta} & 1 \\ 0 & e^{i\theta} \end{pmatrix}$	$\begin{pmatrix} \theta & \theta(e^{i\theta}-1)^{-1} \\ 0 & \theta \end{pmatrix}$	$\begin{pmatrix} 0 & \pm ire^{-i\theta} \\ \mp ire^{i\theta} & 0 \end{pmatrix}$

Because a and b may have arbitrary sign, the group $\mathcal{U}_{\eta_1}(\mathbb{C}^2)$ is isomorphic to either U(2) or U(1,1).

(1b) $e^{i\varphi}=e^{2i\theta}$: In this case, $D=e^{i\theta}I$ where I is the 2×2 unit matrix. Hence, there is no restriction on η; it has the general form (43), and $\mathcal{U}_\eta(\mathbb{C}^2)$ is isomorphic to either U(2) or U(1,1). (2) If $D=D_2$ with $r=1$ we recover the case (1b). If $D=D_2$ and $r\neq1$, then $a=b=0$ and η has the off-diagonal form

$$\eta=\eta_2:=\begin{pmatrix} 0 & \xi \\ \xi^* & 0 \end{pmatrix}, \quad \xi\in\mathbb{C}-\{0\}. \tag{45}$$

Because η_2 is an indefinite matrix, $\mathcal{U}_{\eta_2}(\mathbb{C}^2)$ is isomorphic to U(1,1). (3)

(3) If $D=D_3$. Then η has the general form

$$\eta=\eta_3:=\begin{pmatrix} 0 & \pm ire^{-i\theta} \\ \mp ire^{i\theta} & 0 \end{pmatrix}, \quad r\in\mathbb{R}^+, \quad \theta\in\mathbb{R}, \tag{46}$$

and $\mathcal{U}_{\eta_3}(\mathbb{C}^2)$ is isomorphic to U(1,1).

We can check that the above expressions for η are consistent with the general form of η as given in the proof of Theorem 2. Furthermore, we can obtain the explicit form of the operator $H:=-i\ln U$. In view of the identity $U=A^{-1}DA$, it is not difficult to see that if we obtain an operator H_D satisfying $D=e^{iH_D}$, then $H=A^{-1}H_DA$ will satisfy $U=e^{iH}$. Table I gives the operators H_D and η for $D=D_1$, D_2, D_3. Note that in this table $\theta,\varphi\in\mathbb{R}$, $r\in\mathbb{R}^+$, $a,b\in\mathbb{R}-\{0\}$, $\xi\in\mathbb{C}-\{0\}$, and that the trivial case where D is proportional to the unit matrix is omitted.

VI. PSEUDOUNITARY DYNAMICAL GROUPS AND THE HARMONIC OSCILLATOR

Suppose that H is a 2×2 pseudo-Hermitian matrix serving as the (time-independent) Hamiltonian for a quantum system, $U(t):=e^{-itH}$ is the corresponding evolution operator, $\mathcal{E}_H$ is the set of all invertible Hermitian 2×2 matrices η satisfying (1), and

$$\mathcal{U}_H:=\bigcup_{\eta\in\mathcal{E}_H}\mathcal{U}_\eta(\mathbb{C}^2), \quad \mathcal{GU}_H:=\bigcup_{\eta\in\mathcal{E}_H}\mathcal{GU}_\eta(\mathbb{C}^2),$$

where $\mathcal{GU}_\eta(\mathbb{C}^2)$ denotes the Lie algebra of $\mathcal{U}_\eta(\mathbb{C}^2)$. Then clearly $iH\in\mathcal{GU}_H$ and for all $t\in\mathbb{R}$ $U(t)\in\mathcal{U}_H$. This in particular means that for each $\eta\in\mathcal{E}_H$, $\mathcal{U}_\eta(\mathbb{C}^2)$ serves as a dynamical group for the quantum system.[23] If H is diagonalizable with a real spectrum then the dynamical group may be taken to be (isomorphic to) either U(2) or U(1,1) (or one of their subgroups). If H has (nonreal) complex eigenvalues or if it is not diagonalizable, then the dynamical group is necessarily (isomorphic to a subgroup of) U(1,1). [The generalization of this statement to arbitrary block-

diagonalizable pseudo-Hermitian Hamiltonians with finite-dimensional blocks is immediate. If the Hamiltonian is not diagonalizable or has complex eigenvalues, then the dynamical groups that the system admits are necessarily (isomorphic to a subgroup of) $\mathrm{U}(p,q)$ with $p\neq 0\neq q$.]

A concrete example is provided by the classical equation of motion for a simple harmonic oscillator of frequency ω,

$$\ddot{x}+\omega^2 x=0. \tag{47}$$

As explained in Refs. 4 and 14, this equation is equivalent to the Schrödinger equation,

$$i\hbar\frac{d}{dt}\Psi=H\Psi, \tag{48}$$

where

$$\Psi=\begin{pmatrix} x+i\lambda\dot{x} \\ x-i\lambda\dot{x}\end{pmatrix},\quad H=\frac{\hbar}{2}\begin{pmatrix} \lambda\omega^2+\lambda^{-1} & \lambda\omega^2-\lambda^{-1} \\ -\lambda\omega^2+\lambda^{-1} & -\lambda\omega^2-\lambda^{-1}\end{pmatrix}, \tag{49}$$

and $\lambda\in\mathbb{R}^+$ is a time scale. Clearly H is a traceless matrix. It is also easy to check that $\det H\in\mathbb{R}$ if and only if $\omega^2\in\mathbb{R}$. Therefore, according to Theorem 3 of Ref. 6, H is a pseudo-Hermitian matrix provided that $\omega^2\in\mathbb{R}$. Furthermore, H is diagonalizable unless $\omega=0$.

In the following we shall only consider the case $\omega^2\in\mathbb{R}$.

For $\omega\neq 0$, we can easily solve the eigenvalue problem and diagonalize H. The corresponding diagonal matrix has the form $H_D=\hbar\omega\sigma_3$ where σ_3 is the diagonal Pauli matrix $\mathrm{diag}(1,-1)$. Comparing the expression for H_D with the results given in the above table, we see that H_D is η-pseudo-Hermitian with respect to a diagonal metric operator η of the form (44) provided that $\omega^2>0$. In this case the system admits both the dynamical groups U(2) and U(1,1). If $\omega^2<0$, H is η-pseudo-Hermitian with respect to an off-diagonal metric operator η of the form (45) and the system only admits the dynamical group U(1,1). Finally for $\omega=0$, H is not diagonalizable; $U=e^{iH}$ has the Jordan canonical form D_3; it is η-pseudounitary for a metric operator η of the form (46) and the system admits the dynamical group U(1,1). [It is interesting to observe that the noncompact dynamical group U(1,1) arises for the case that $\omega^2<0$ where Eq. (47) admits unbounded solutions.]

For the case $\omega^2>0$, the freedom in the choice of the dynamical group is equivalent to the choice of a positive–definite or an indefinite inner product on the space of solutions of Eq. (47).[14] This freedom does not exist if $\omega^2\leqslant 0$.

Now, consider changing the parameter ω^2 from a positive value down to a negative value. If one adopts an indefinite (but possibly ω^2-dependent) inner product, one can keep H Hermitian with respect to this inner product and view the evolution operator as tracing a curve in the dynamical group U(1,1). The best-known example is the Klein–Gordon inner product that corresponds to the choice $\eta=\sigma_3$, and therefore is independent of the value of the parameter ω^2. However, if one initially adopts a (possibly ω^2-dependent) positive–definite inner product, one cannot maintain the Hermiticity of H with respect to this inner product once ω^2 crosses zero. The dynamical group undergoes an abrupt transition from the group U(2) to the group U(1,1). This transition may be identified with the change of the signature of the metric (operator).

For $\omega^2>0$, one may endow the Hilbert space ($\mathbb{C}^2$) with a positive–definite invariant inner product. In this case the system has a U(2) dynamical group and is physically equivalent to the two-level spin system,[23] i.e., a spin-1/2 particle interacting with a fixed magnetic field. The time evolution is clearly unitary. This equivalence is destroyed once ω^2 becomes nonpositive. In this case the dynamical group is U(1,1) and the system does not admit a unitary evolution with respect to any positive–definite inner product on $\mathbb{C}^2$. For the case that $\omega^2>0$ one could as well choose an indefinite invariant inner product (this is precisely what was done historically). But such a choice leads to a nonunitary quantum system with a two-dimensional Hilbert space and a U(1,1) dynamical group. As is well known the corresponding quantum harmonic oscillator also has a U(1,1) [or

rather SU(1,1)] dynamical group.[23] Therefore, as far as the dynamics is concerned the nonunitary system describing the dynamics of the classical oscillator is equivalent to the unitary quantum harmonic oscillator.

For the case $\omega^2>0$ there are therefore two alternatives. One is to choose a positive–definite invariant inner product which corresponds to the dynamical group U(2). The other is to choose an indefinite invariant inner product which leads to the dynamical group U(1,1).

Now, suppose that one wishes to keep the same dynamical group but insists on being able to describe the dynamics using a unitary quantum system. In the first alternative this is already the case. But in the second alternative one needs to use an infinite-dimensional Hilbert space, because being a noncompact Lie group U(1,1) does not admit a finite-dimensional unitary representation. Therefore *it is the demand for unitarity that leads to the quantization of the oscillator*. The latter is however not unique because U(1,1) has inequivalent unitary irreducible representations. This does not lead to any problems, because the dynamics always takes place in the dynamical group.[23] As a result the dynamical aspects of all possible quantum systems associated with the classical harmonic oscillator are equivalent. [Note that here quantization does not mean the canonical quantization which is unique in the sense that the Weyl–Heisenberg algebra has a unique irreducible (projective) representation. It means defining the Hilbert space as the representation space of a unitary irreducible projective representation of the dynamical group, and representing the Hamiltonian as an element of the Lie algebra of the dynamical group.]

The above two alternatives are also available in describing free Klein–Gordon fields (or more generally Klein–Gordon fields interacting with a stationary magnetic field). The second alternative applies more generally even to the cases of interacting fields. It corresponds to Dirac's method of second quantization that forms the foundations of quantum field theories. The first alternative was noticed quite recently.[14,15,24] (See however Ref. 25 that were brought to the author's attention after the completion of this project.) Its advantage is to provide a genuine probability interpretation for first quantized Klein–Gordon fields.[26] Its main application is in quantum cosmology.[15]

VII. CONCLUSION

In this paper, we explored various properties of pseudounitary operators and proved a spectral characterization theorem for the class of block-diagonalizable pseudounitary operators with finite-dimensional blocks. We applied our results to clarify the structure of pseudounitary matrices paying attention to the role of the inner product and the fact that it is not unique. We showed that the relationship between Hermitian and unitary matrices generalize to the pseudo-Hermitian and pseudounitary matrices. Specifically every pseudounitary matrix is the exponential of i times a pseudo-Hermitian matrix.

We showed that the symplectic transformations of classical mechanics are certain pseudounitary and pseudo-Hermitian operators. This led to a proof of the spectral theorem for symplectic matrices and to the identification of the symplectic groups $\mathrm{Sp}(2n)$ with the real subgroups of certain pseudounitary matrix groups that are isomorphic to $\mathrm{U}(n,n)$. The description of the symplectic transformations in terms of pseudounitary and pseudo-Hermitian operators suggests the possibility of the application of the latter in classical mechanics. (For a related discussion see Ref. 27.)

Furthermore, we derived the canonical forms of arbitrary 2×2 pseudounitary matrices, and studied the pseudounitary system describing a classical harmonic oscillator. For real nonzero frequencies, this system admits both the dynamical groups U(2) or U(1,1). If one imposes the condition of the unitarity of the evolution, then the choice U(2) identifies the dynamics of the oscillator with that of a two-level quantum system, and the choice U(1,1) leads to a quantization of the oscillator. This picture provides a rather interesting link between the demand for unitarity and the need for (second) quantization.

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Equal rank embedding and its related construction to superconformal field theories

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The lowest lines of Euler multiplets corresponding to massless and massive supersymmetric representations are classified. At the level of representation theory, the Euler multiplets constructed by the GKRS method of equal rank embedding of semisimple complex Lie algebras are found to be the intrinsic ground states of superconformal field theories according to the Kazama–Suzuki construction. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1645975]

I. INTRODUCTION

Although a Dirac operator with a cubic term and its square appeared as supercurrent and energy-momentum tensor, respectively, in studies of the superconformal field theories and the supersymmetric Wess–Zumino–Witten action many years ago,[1–3] there has not been much progress on understanding their spectrum. It still needs to determine the explicit representations of these superconformal models.

Recently, a study of equal rank embedding of semisimple complex Lie algebras[4] led Kostant to determine an Euler multiplet as the kernel of the cubic Dirac operator and its square in general.[5] By accident, it was observed that some of the lowest lines of the Euler multiplets match exactly with the known massless and massive supermultiplets[6] and the higher lines of them possibly involve higher spin massless and massive fields. It was also observed that the Kostant operator and its square are the zero mode of the supercurrent and the energy-momentum tensor.[7] In this paper, we will observe these relations from the representation-theoretic viewpoint of Lie algebras and of affine Lie algebras. Understanding a method to obtain the Euler multiplets may help to obtain what the spectrum of the superconformal models really are level by level.

The contents of this paper are organized as follows. In Sec. II, the Kostant operator is reviewed and an eigenvalue of its square is alternatively derived from the representation-theoretic viewpoint including a condition for getting an Euler multiplet. In Sec. III, Euler multiplets that give the massless and massive supermultiplets are classified. Sections IV and V are devoted to a super-Kac–Moody algebras and the Kazama–Suzuki construction of superconformal models. In the last section, the Euler multiplet is shown to be inherent in a ground state of the Kazama–Suzuki superconformal models.

II. KOSTANT OPERATOR AND EULER MULTIPLET

Let J's be generators of a semisimple complex Lie algebra g such that

$$[J_A, J_B] = i f_{[ABC]} J_C, \tag{1}$$

where indices $A,B,C = 1 \cdots \dim g$. A basis of the generators is chosen so that these generators are orthonormal with respect to an inner product on g that is invariant under the adjoint action. In the case that g is semisimple, the inner product on g is the Killing form. Let Λ be in the positive Weyl chamber of g and let J_A^Λ be the image of J_A under the irreducible representation of g with highest

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weight Λ. Kostant's cubic Dirac operator of the pair (g,Λ) is the operator on $V_\Lambda \otimes S$, where V_Λ is a vector space of the representation with the highest weight Λ and S is a spinor module of the complexified Clifford algebra which can be decomposed into the direct sum of the positive spinor representation S^+ and the negative spinor representation S^- when the dimension of the complexified Clifford algebra is even, given by

$$\mathcal{K}_g(\Lambda) = \gamma_A J_A^\Lambda - \frac{i}{2} f_{[ABC]} \gamma_{[A} \gamma_B \gamma_{C]}. \tag{2}$$

The Dirac γ-matrices satisfy the Clifford algebra,

$$\{\gamma_A, \gamma_B\} = 2\delta_{AB}. \tag{3}$$

Squaring (2) gives us

$$\mathcal{K}_g^2(\Lambda) = (J_A^\Lambda)^2 + \left(\frac{i}{2} f_{[ABC]} \gamma_{[A} \gamma_B \gamma_{C]}\right)^2 = C_2(\Lambda) + |\rho_g|^2, \tag{4}$$

where $C_2(\Lambda) = (\Lambda, \Lambda + \rho_g)$ is the quadratic Casimir eigenvalue of the irreducible representation Λ and ρ_g is one-half the sum of positive roots of g. Both $C_2(\Lambda)$ and $|\rho_g|^2$ are calculated in the orthornormal basis $\{e_i\}$ where $(e_i, e_j) = \delta_{ij}$. The eigenvalue of (4) is always positive definite. Therefore, $\mathcal{K}_g^2$ is a positive eigenvalue operator.

In the case of the quotient g/h, the generators $J_i, i = 1 \cdots \dim h$, lie in g and the generators $J_a, a = h+1 \cdots \dim g$, are a basis of the orthogonal complement of h with respect to the Killing form on g. Both J_i and J_a satisfy the following commutation relations:

$$[J_i, J_j] = i f_{[ijk]} J_k, \tag{5}$$

$$[J_i, J_a] = i f_{[iab]} J_b, \tag{6}$$

$$[J_a, J_b] = i f_{[abj]} J_j + i f_{[abc]} J_c. \tag{7}$$

The twisted Dirac operator on $h \subset g$ acting on $V_\Lambda \otimes S$ is

$$\mathcal{K}_h(\Lambda) = \gamma_i \left(J_i^\Lambda - \frac{i}{2} f_{[iab]} \gamma_{[a} \gamma_{b]} \right) - \frac{i}{2} f_{[ijk]} \gamma_{[i} \gamma_j \gamma_{k]}, \tag{8}$$

and the Kostant operator of the quotient g/h is

$$\mathcal{K}_{g/h}(\Lambda) = \mathcal{K}_g(\Lambda) - \mathcal{K}_h(\Lambda) = \gamma_a J_a^\Lambda - \frac{i}{2} f_{[abc]} \gamma_{[a} \gamma_b \gamma_{c]}. \tag{9}$$

(This operator first appeared in the Kazama and Suzuki paper.[2]) Decompose $V_\Lambda \otimes S$ into irreducible representations of h and let V_μ be one of these h-representations, where μ is its highest weight. Restricting (9) to V_μ and squaring gives a scalar operator:

$$(\mathcal{K}_{g/h}(\Lambda)|_{V_\mu})^2 = (J_A^\Lambda)^2 - (J_i^\Lambda + S_i)^2 + S_i^2 = C_2(\Lambda) - C_2(\mu) + |\rho_g|^2 - |\rho_h|^2, \tag{10}$$

where $S_i = -(i/2) f_{[iab]} \gamma_{[a} \gamma_{b]}$. In the last line of (10), $C_2(\Lambda)$ is the quadratic Casimir eigenvalue for g and $C_2(\mu)$ for h. The rhs of Eq. (10) gives the eigenvalues of $(\mathcal{K}_{g/h}(\Lambda)|_{V_\mu})^2$ acting on $V_\Lambda \otimes S$. Since the Kostant operator is self-adjoint, all eigenvalues of (10) are non-negative.

From the representation-theoretic viewpoint of Lie algebras, the eigenvalue of (10) can be naively derived by considering the following inequality:

$$\Lambda + \rho_g \geqslant w^{-1}(\mu + \rho_h), \tag{11}$$

where μ is a weight of h appearing in the decomposition of $V_\Lambda \otimes S$ into irreducible representations of h and w is an element in the Weyl group of g such that $w^{-1}(\mu+\rho_h)$ is a dominant weight. Since the Weyl group preserves scalar product, squaring (11) yields

$$|\Lambda+\rho_g|^2 \geqslant |\mu+\rho_h|^2. \tag{12}$$

The equation (12) gives rise to

$$(\Lambda,\Lambda+2\rho_g)+|\rho_g|^2 \geqslant (\mu,\mu+2\rho_h)+|\rho_h|^2, \tag{13}$$

i.e.,

$$C_2(\Lambda)-C_2(\mu)+|\rho_g|^2-|\rho_h|^2 \geqslant 0. \tag{14}$$

Let c be an element in C, the quotient set of the Weyl group $W(g)/W(h)$. When $\mu = c\cdot\Lambda \equiv c(\Lambda+\rho_g)-\rho_h$, (14) is minimum and equal to zero:

$$C_2(\Lambda)-C_2(\mu)+|\rho_g|^2-|\rho_h|^2 = \begin{cases} 0, & \text{if } \mu = c\cdot\Lambda; \\ \text{positive} & \text{otherwise.} \end{cases}$$

A set of all highest weights $c\cdot\Lambda$ is called the Euler multiplet.

III. CLASSIFICATION OF THE LOWEST LINES OF THE EULER MULTIPLETS

Alternatively, the Euler multiplet can be simply obtained by using the GKRS index,[4]

$$V_\Lambda \otimes S^+ - V_\Lambda \otimes S^- = \sum_{c\in C} \operatorname{sgn}(c) V_{c\cdot\Lambda}, \tag{15}$$

when V_Λ is the one-dimensional irreducible representation of g and it is trivially branched into a one-dimensional representation of h. The lowest line of the Euler multiplets of h is equal to a decomposition of the two spinor representations of $SO(\dim g/h)$ into irreducible representations of h. In the case that an Euler number **C**, the number of c elements in $W(g)/W(h)$, is a small integer, one can compute the Euler multiplet from $\lambda \equiv c(\Lambda+\rho_g)-\rho_h$ as shown in Ref. 6. In the case that the Euler number is a high integer, e.g., $\mathbf{C}>10$, the Euler multiplet can be obtained by branching the irreducible representation V_Λ and the spinor representations of SO(dim g/h) into the representations of h, tensoring them together, and taking the difference between positive and negative spin spaces.

It is observed that when dim $g/h = 4$, 8, 16, and 32, the lowest lines of the Euler multiplets have the right degrees of freedom of the massless and massive supersymmetric representations of the supersymmetric gauge field theories.[6] So, it is convenient to classify the lowest lines of the Euler multipets according to SO(dim g/h). (The Euler multiplets in this section are written in terms of dimensions of the irreducible representations of h.)

(1) SO(4):

$$S^+ = 2_s \text{ and } S^- = 2_c.$$

- $\mathrm{Sp}(4) \supset \mathrm{Sp}(2)\times\mathrm{Sp}(2)$,

$$S^+ = (1,2),$$
$$S^- = (2,1).$$

[In this paper, $\mathrm{Sp}(2n) \equiv U(2n)\cap \mathrm{Sp}(2n,C)$ is a unitary symplectic group.] Since the group Sp(2), a simply-connected double covering group of SO(3), is locally isomorphic to the group SO(3), i.e. $\mathrm{Sp}(2)\sim\mathrm{SO}(3)$, this Euler multiplet corresponds to the $N=1$ smallest massive representation in $3+1$ space–time dimensions when one of the Sp(2) is interpreted as the little group of the inhomogenous Lorentz group $ISO(3,1)$ and to the $N=1$ shortest

massless representation in $5+1$ space–time dimensions when one of the $\mathrm{Sp}(2)\sim\mathrm{SU}(2)$ algebras is interpreted as a chirality group in $\mathrm{SO}(4)\sim\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$, the light-cone little group of $ISO(5,1)$.

- $\mathrm{SU}(3)\supset\mathrm{SU}(2)\times\mathrm{U}(1)$,

$$S^+=2_0,$$
$$S^-=1_{1/2}\oplus 1_{-1/2}.$$

This Euler multiplet corresponds to the $N=2$ massless representation in $3+1$ dimensions when the $\mathrm{U}(1)\sim\mathrm{SO}(2)$ algebra is interpreted as the little group of $ISO(3,1)$ and to the massless representation in $4+1$ when the $\mathrm{SU}(2)\sim\mathrm{SO}(3)$ algebra is interpreted as the little group of $ISO(4,1)$. The $N=2$ supersymmetric multiplet with the highest helicity equal to 1/2 is sometimes called a hypermultiplet.

It is noticed that the $N=2$ massless representation in $3+1$ dimensions which is the lowest line of the Euler multiplets of $\mathrm{SU}(3)\supset\mathrm{SU}(2)\times\mathrm{U}(1)$ can be assembled into an $N=1$ massive representation in $3+1$ dimensions which is the lowest line of the Euler multiplets of $\mathrm{Sp}(4)\supset\mathrm{Sp}(2)\times\mathrm{Sp}(2)$. On the 4-dimensional coset space, the $N=2$ massless representation, considered as a fundamental state of one theory at weak (strong) coupling limit, possibly has a duality with an $N=1$ massive representation, considered as a solitonic state of the other theory at a strong (weak) coupling limit.

(2) $\mathrm{SO}(8)$:

$$S^+=8_s \text{ and } S^-=8_c.$$

- $\mathrm{Sp}(6)\supset\mathrm{Sp}(4)\times\mathrm{Sp}(2)$ and $G_2\supset\mathrm{SU}(2)\times\mathrm{SU}(2)$,

$$S^+=(5,1)\oplus(1,3),$$
$$S^-=(4,2).$$

This Euler multiplet corresponds to the $N=2$ smallest massive representation in $3+1$ dimensions and the $N=2$ shortest massless representation in $5+1$ dimensions.

- $\mathrm{SU}(5)\supset\mathrm{SU}(4)\times\mathrm{U}(1)$,

$$S^+=1_1\oplus 6_0\oplus 1_{-1},$$
$$S^-=4_{1/2}\oplus\overline{4}_{-1/2}.$$

This Euler multiplet corresponds to the $N=4$ Yang–Mills massless representation in $3+1$ dimensions and, since $\mathrm{SU}(4)\sim\mathrm{SO}(6)$, a massless representation in $7+1$ dimensions. However, there are two more possibilities to interpret this Euler multiplet, one as a massless representation on the anti–de Sitter space when the $\mathrm{SU}(4)\times\mathrm{U}(1)\sim\mathrm{SO}(6)\times\mathrm{SO}(2)$ algebra is interpreted as the subgroup of $\mathrm{SO}(6,2)$, the anti-de Sitter group in $6+1$ dimensions, and the other as a massless representation of a conformal theory when interpreted as the conformal group in $5+1$ dimensions.

- $\mathrm{SO}(6)\supset\mathrm{SO}(4)\times\mathrm{SO}(2)$ and $\mathrm{SU}(4)\supset\mathrm{SU}(2)\times\mathrm{SU}(2)\times\mathrm{U}(1)$,

$$S^+=(1,1)_1\oplus(3,1)_0\oplus(1,3)_0\oplus(1,1)_{-1},$$
$$S^-=(2,2)_{1/2}\oplus(2,2)_{-1/2}.$$

There are many possibilities to view this Euler multiplet. It corresponds to the $N=4$ Yang–Mills supermultiplet in $3+1$ dimensions and to a massless multiplet in either $4+1$ or $5+1$ dimensions.

Note that $N=4$ massless representation in $3+1$ dimensions which is the lowest line of the Euler multiplets of $SU(5)\supset SU(4)\times U(1)$, $SO(6)\supset SO(4)\times SO(2)$ and $SU(4)\supset SU(2)\times SU(2)\times U(1)$ can also be assembled into an $N=2$ massive representation in $3+1$ dimensions which is the lowest line of the Euler multiplets of $Sp(6)\supset Sp(4)\times Sp(2)$ and $G_2\supset SU(2)\times SU(2)$. On the 8-dimensional coset space, the $N=2$ massless representations, considered as the fundamental states of one theory at the weak (strong) coupling limit, possibly have a duality with $N=1$ massive representations, considered as the solitonic states of the other theory at the strong (weak) coupling limit.

(3) $SO(16)$:

$$S^+=128_s \text{ and } S^-=128_c.$$

- $F_4\supset SO(9)$,

$$S^+=44\oplus 84,$$
$$S^-=128.$$

This multiplet can be viewed as the $N=1$ massive soliton representation in $9+1$ dimensions and as the $N=1$ massless representation in $10+1$ dimensions. In the later case, it is called the supergravity triplet where the 44-dimensional representation is the degrees of freedom of the spin-2 graviton, the 84-dimensional is the degrees of freedom of the third-rank antisymmetric tensor field and the 128-dimensional is the degrees of freedom of the Rarita–Schwinger spinor-vector called the gravitino.

- $Sp(10)\supset Sp(8)\times Sp(2)$,

$$S^+=(42,1)\oplus(27,3)\oplus(1,5),$$
$$S^-=(48,2)\oplus(8,4).$$

This Euler multiplet corresponds to the $N=4$ smallest massive representation in $3+1$ dimensions and the $N=4$ short massless representation in $5+1$ dimensions.

- $SO(8)\supset SO(4)\times SO(4)\sim SU(2)\times SU(2)\times SU(2)\times SU(2)$,

$$S^+=(5,1,1,1)\oplus(1,5,1,1)\oplus(1,1,5,1)\oplus(1,1,1,5)\oplus(1,3,3,3)\oplus(3,1,3,3)\oplus(3,3,1,3)\oplus(3,3,3,1),$$
$$S^-=(4,2,2,2)\oplus(2,4,2,2)\oplus(2,2,4,2)\oplus(2,2,2,4).$$

This Euler multiplet corresponds to the $N=4$ smallest massive representation in $3+1$ dimensions and $N=2$ massless representaton in $5+1$ dimensions.

- $SU(9)\supset SU(8)\times U(1)$,

$$S^+=1_2\oplus 28_1\oplus 70_0\oplus\overline{28}_{-1}\oplus 1_{-2},$$
$$S^-=8_{3/2}\oplus 56_{1/2}\oplus\overline{56}_{-1/2}\oplus\overline{8}_{-3/2}.$$

Since the highest value of $SO(2)$ is 2, the helicity of graviton in $3+1$ dimensions, this Euler multiplet corresponds to the $N=8$ supergravity representation.

- $SO(10)\supset SO(8)\times SO(2)$,

$$S^+=1_2\oplus 28_1\oplus(35_s)_0\oplus(35_c)_0\oplus 28_{-1}\oplus 1_{-2},$$
$$S^-=8_{3/2}\oplus(56_v)_{1/2}\oplus(56_v)_{-1/2}\oplus 8_{-3/2}.$$

This Euler multiplet corresponds to the $N=8$ supergravity representation in $3+1$ dimensions. After using $SO(8)$ triality, it also corresponds to the chiral $N=4$ supermultiplet of type IIB string theory in $9+1$ dimensions.

- $SU(6)\supset SU(4)\times SU(2)\times U(1)\sim SO(6)\times SO(3)\times SO(2)$,

$$S^+=(1,1)_2\oplus(10,1)_1\oplus(6,3)_1\oplus(20',1)_0\oplus(15,3)_0\oplus(1,5)_0\oplus(\overline{10},1)_{-1}\oplus(6,3)_{-1}\oplus(1,1)_{-2},$$
$$S^-=(4,2)_{3/2}\oplus(20,2)_{1/2}\oplus(\overline{4},4)_{1/2}\oplus(\overline{20},2)_{-1/2}\oplus(4,4)_{-1/2}\oplus(\overline{4},2)_{-3/2}.$$

This Euler multiplet also corresponds to the $N=8$ supergravity representation in $3+1$ dimensions and to a massless representation in $4+1$ and $7+1$ dimensions.

Note that the $N=8$ supergravity multiplet in $3+1$ dimensions which is the lowest line of the Euler multiplets of $SU(9)\supset SU(8)\times U(1)$ and $SO(10)\supset SO(8)\times SO(2)$ can also be assembled into an $N=2$ massive representation in $3+1$ dimensions which is the lowest line of the Euler multiplets of $Sp(10)\supset Sp(8)\times Sp(2)$. On the 16-dimensional coset space, the $N=8$ massless representations, considered the fundamental states of one theory at weak (strong) coupling limit, possibly have a duality with $N=4$ massive representations, considered as the solitonic states of the other theory at the strong (weak) coupling limit.

(4) SO(32):

- $E_6\supset SO(10)\times SO(2)$,

$$S^+=1_4\oplus120_3\oplus770_2\oplus1050_2\oplus3696_1\oplus4312_1\oplus660_0\oplus4125_0\oplus8085_0\oplus4312_{-1}\oplus3696_{-1}$$
$$\oplus1050_{-2}\oplus770_{-2}\oplus120_{-3}\oplus1_{-4},$$
$$S^-=(16_s)_{7/2}\oplus(560_c)_{5/2}\oplus(672_c)_{3/2}\oplus(3696_c)_{3/2}\oplus(2640_s)_{1/2}\oplus(8800_c)_{1/2}\oplus(8800_s)_{-1/2}$$
$$\oplus(2640_c)_{-1/2}\oplus(672_s)_{-3/2}\oplus(3696_s)_{-3/2}\oplus(560_c)_{-5/2}\oplus(16_c)_{-7/2}.$$

This Euler multiplet possibly corresponds to a massive supermultiplet with spin >2 in $10+1$ dimensions.

There also exist the lowest lines of the Euler multiplets that are of SO(6), SO(10), SO(12), etc. and not all of them can be interpreted as the degrees of freedom of the supersymmetric gauge field theories except $Sp(8)\supset Sp(6)\times Sp(2)$ that its lowest line emerges as $N=3$ massive (massless) representation in $3+1$ $(5+1)$ dimensions.

In conclusion, from the facts of group theory, there are different coset spaces. For the 4-, 8-, and 16-dimensional coset spaces, there exist the lowest lines of the Euler multiplets corresponding to the massive and massless supermultiplets.

IV. SUPER-KAC–MOODY ALGEBRAS

By relaxing a positivity condition of determinant of the Cartan matrices, one can get Kac–Moody algebras, of which a subclass constitutes the finite-dimensional (semi)simple Lie algebras. Another subclass of Kac–Moody algebras is affine Lie algebras having the corresponding structure and representation theory in analogy to those of the Lie algebras.[8]

A super-Kac–Moody algebra $\hat{g}$ associated with the Lie algebra g and Lie group G is a Kac–Moody algebra over superspace (z,θ). With the supersymmetrized current decomposition over ordinary space z,

$$J_A(z,\theta)=j_A(z)+\theta J_A(z), \tag{16}$$

the fermions $j_A(z)$ in the adjoint representation of g and $J_A(z)$ are not independent and satisfy the OPEs,

$$j_A(z)j_B(0)\sim\frac{\delta_{AB}}{z}, \tag{17}$$

$$J_A(z)j_B(0)\sim j_A(z)J_B(0)\sim\frac{if_{[ABC]}j_C(0)}{z}, \tag{18}$$

$$J_A(z)J_B(0)\sim\frac{if_{[ABC]}J_C(0)}{z}+\frac{k\delta_{AB}}{z^2}. \tag{19}$$

The level k in (17) is absorbed into the fermion bilinear. To make the fermion and boson current generators independent, Kazama and Suzuki[2] introduced the level $k=\hat{k}+g^\vee$ current decomposition,

$$J_A^k(z)=\hat{J}_A^{\hat{k}}(z)+S_A=\hat{J}_A^{\hat{k}}(z)-\frac{i}{2}f_{[ABC]}j_{[B}j_{C]}(z), \tag{20}$$

so that $\hat{J}_A^{\hat{k}}(z)$ and $S_A(z)$ are mutually independent and, respectively, generate the level $\hat{k}$ and $g^\vee$ ordinary Kac–Moody algebras $\hat{g}$. The level $g^\vee$ Kac–Moody algebra $\hat{g}$ that is constructed by a bilinear form of the fermions in the adjoint representation of g turns out to be isomorphic to the level 1 ordinary Kac–Moody algebra $\widehat{so}(\dim g)$. Therefore, the level k super-Kac–Moody algebra can be regarded as a direct sum of two mutually independent ordinary Kac–Moody algebras,

$$\hat{g}_k=\hat{g}_{\hat{k}}\oplus\widehat{so}(\dim g)_1. \tag{21}$$

In terms of oscillators, (20) is

$$\sum_n (J_n)_A z^{-n-1}=\sum_n (\hat{J}_n)_A z^{-n-1}-\frac{i}{2}f_{[ABC]}\sum_n (b_{-n})_B(b_n)_C z^{-1}. \tag{22}$$

In the representation theory of the ordinary Kac–Moody algebra, (22) corresponds to an affine weight decomposition,

$$(\Lambda+\rho_g;\hat{k}+g^\vee;-n)=(\Lambda;\hat{k};-n)+(\rho_g;g^\vee;0), \tag{23}$$

where n is called a grade. When $n=0$, the affine weight $(\Lambda;\hat{k};0)$ is called the highest weight. From the decomposition (21) of the super-Kac–Moody algebra, there exists the associated $N=1$ superconformal model with the superconformal generators,

$$G(z)=(2/k)^{1/2}\left(j_A(z)\hat{J}_A(z)-\frac{i}{2}f_{[ABC]}j_{[A}j_Bj_{C]}(z)\right), \tag{24}$$

and

$$T(z)=\frac{1}{k}(\hat{J}_A(z)\hat{J}_A(z)-j_A(z)\partial_z j_A(z)). \tag{25}$$

On the rhs of the holomorphic energy-momentum tensor $T(z)$, the first term commutes with the second term. Thus, the central charge of this superconformal model is the sum of the central charges of $\hat{g}_{\hat{k}}$ and $\widehat{so}(\dim g)_1$,

$$c=\frac{\hat{k}\dim \mathrm{G}}{\hat{k}+g^\vee}+\frac{1}{2}\dim \mathrm{G}. \tag{26}$$

The superconformal generators $T(z)$ and $G(z)$ satisfy the OPEs,

$$T(z)T(0)\sim\frac{c}{2z^4}+\frac{2T(0)}{z^2}+\frac{\partial_z T(0)}{z}, \tag{27}$$

$$T(z)G(0)\sim G(z)T(0)\sim \frac{3G(0)/2}{z^2}+\frac{\partial_z G(0)}{z}, \tag{28}$$

$$G(z)G(0)\sim \frac{2c/3}{z^3}+\frac{2T(0)}{z}. \tag{29}$$

The underlying supersymmetric Wess–Zumino–Witten Lagrangian in two dimensions that posseses the super-Kac–Moody algebra $\hat{g}_k$ and the $N=1$ superconformal symmetry was constructed in Ref. 1. The supersymmetric WZW Lagrangian was shown to be equal to the original WZW Lagrangian of $\hat{g}_{\hat{k}}$ plus the Lagrangian of free fermions in the adjoint representation of $\hat{g}_k$. By applying Witten's non-Abelian bosonization rules to the WZW Lagrangian, the supersymmetric WZW theory is equivalent to two free fermion theories.

V. KAZAMA–SUZUKI CONSTRUCTION OF $N=1$ AND $N=2$ SUPERCONFORMAL MODELS

Instead of using Wick's theorem to calculate the OPEs to get the superconformal generators on the coset space, one can simply follow Brink and Ramond's canonical method.[7] The construction of superconformal generators from the coset space method applied to a super-Kac–Moody algebra can be done in analogy to Sec. II.

On the world-sheet, there exists a natural generalization of γ-matrices and generators of a Lie algebra,

$$\gamma_A\rightarrow j_A(z), \tag{30}$$

$$J_A\rightarrow \hat{J}_A(z). \tag{31}$$

The fermions $j_A(z)$ satisfy the anticommutator

$$\{j_A(z),j_B(0)\}=2\delta_{AB}, \tag{32}$$

and the bosonic current generators $\hat{J}_A(z)$ satisfy the level $\hat{k}$ Kac–Moody commutator,

$$[\hat{J}_i(z),\hat{J}_j(0)]=if_{[ijk]}\hat{J}_k(0)+\hat{k}\delta_{ij}\partial_z\delta(z), \tag{33}$$

$$[\hat{J}_i(z),\hat{J}_a(0)]=if_{[iab]}\hat{J}_b(0), \tag{34}$$

$$[\hat{J}_a(z),\hat{J}_b(0)]=if_{[abc]}\hat{J}_c(0)+if_{[abj]}\hat{J}_j(0)+\hat{k}\delta_{ab}\partial_z\delta(z). \tag{35}$$

All indices are the same as in Sec. II.

The supercurrent of $\hat{h}$ that lies in $\hat{g}$ is

$$G_{\hat{h}}(z)=\left(\frac{2}{k}\right)^{1/2}\left(j_i\left(\hat{J}_i-\frac{i}{2}f_{[iab]}j_{[a}j_{b]}\right)-\frac{i}{2}f_{[ijk]}j_{[i}j_jj_{k]}\right)(z), \tag{36}$$

and that of $\hat{g}/\hat{h}$ is

$$G_{\hat{g}/\hat{h}}(z)=G_{\hat{g}}(z)-G_{\hat{h}}(z)=\left(\frac{2}{k}\right)^{1/2}\left(j_a\hat{J}_a-\frac{i}{2}f_{[abc]}j_{[a}j_bj_{c]}\right)(z). \tag{37}$$

By squaring (37) and then using OPEs as in (17)–(19), one yields the energy-momentum tensor,

$$T_{\hat{g}/\hat{h}}(z)=\frac{1}{k}(\hat{J}_a\hat{J}_a-if_{[iab]}\hat{J}_{[i}j_aj_{b]}-\hat{k}j_a\partial_z j_a-f_{[acd]}f_{[acd]}j_{[a}\partial j_{b]}-f_{[abc]}f_{[ade]}j_{[b}j_cj_{[d}j_{e]})(z). \tag{38}$$

In the case that the coset space is symmetric, i.e., the torsion terms $f_{[abc]}$ vanish, (38) reduces to

$$T_{\hat{g}/\hat{h}}(z)=\frac{1}{k}(\hat{J}_A^2-(\hat{J}_i+S_i)^2-\hat{k}j_a\partial_z j_a+S_i^2)(z), \tag{39}$$

where $S_i(z)=-i/2\,f_{[iab]}j_{[a}j_{b]}(z)$. In comparison to (10), the energy-momentum tensor $T_{\hat{g}/\hat{h}}(z)$ is a generalization of Kostant operator $\mathcal{K}^2_{g/h}$. One can also see that OPEs,

$$T_{\hat{g}/\hat{h}}(z)\hat{J}_i(0)\sim T_{\hat{g}/\hat{h}}(z)j_i(0)\sim 0, \tag{40}$$

imply the orthogonal decomposition of the superconformal generators,

$$T_{\hat{g}/\hat{h}}(z)G_{\hat{h}}(0)\sim T_{\hat{g}/\hat{h}}(z)T_{\hat{h}}(0)\sim 0. \tag{41}$$

From (39), one can regard the Kazama–Suzuki construction of the equal rank embedding of super-Kac–Moody algebra as an extension of the GKO construction[9] of ordinary Kac–Moody algebra,

$$(\hat{g}_k/\hat{h}_k)\sim(\hat{g}_{\hat{k}}/\hat{h}_{\hat{k}+g^\vee-h^\vee})\oplus\widehat{so}(\dim\, g/h)_1, \tag{42}$$

with central charge

$$c_{\hat{g}/\hat{h}}=\frac{\hat{k}}{\hat{k}+g^\vee}\dim\, g+\frac{1}{2}\dim\, g/h-\frac{\hat{k}+g^\vee-h^\vee}{\hat{k}+g^\vee}\dim\, h=\frac{3}{2}(\dim\, g/h)-\frac{12}{(\hat{k}+g^\vee)}(|\rho_g|^2-|\rho_h|^2). \tag{43}$$

The equal rank embeddings in Sec. III that can be used to construct the $N=1$ super-conformal models are as follows:

- $\hat{F}_4/\widehat{so}(9)$ with central charge $c_{\hat{g}/\hat{h}}=24\hat{k}/(\hat{k}+9)$;
- $\widehat{Sp}(2n+2)/\widehat{Sp}(2n)\times\widehat{Sp}(2)$ with central charge $c_{\hat{g}/\hat{h}}=6\hat{k}n/(\hat{k}+n+2)$.

In the case that the subalgebra has a $u(1)$ factor, there exists a class of $N=2$ superconformal theories. The $N=2$ superconformal theories have a $u(1)$ current $U(z)$, two supercurrent $G_\pm(z)$ with $u(1)$ charges ±1, and energy-momentum tensor $T(z)$ as their generators. These generators satisfy the OPEs,

$$T(z)T(0)\sim\frac{c/2}{z^4}+\frac{2T(0)}{z^2}+\frac{\partial_z T(0)}{z}, \tag{44}$$

$$T(z)U(0)\sim\frac{\mathrm{U}(0)}{z^2}+\frac{\partial_z \mathrm{U}(0)}{z}, \tag{45}$$

$$T(z)G_\pm(0)\sim\frac{3G_\pm(0)/2}{z^2}+\frac{\partial_z G_\pm(0)}{z}, \tag{46}$$

$$\mathrm{U}(z)\mathrm{U}(0)\sim\frac{c/3}{z^2}, \tag{47}$$

$$\mathrm{U}(z)G_{\pm}(0)\sim\frac{\pm G_{\pm}(0)}{z}, \tag{48}$$

$$G_{+}(z)G_{-}(0)\sim\frac{2c/3}{z^3}+\frac{2\mathrm{U}(0)}{z^2}+\frac{2T(0)+\partial_z\mathrm{U}(0)}{z}, \tag{49}$$

$$G_{+}(z)G_{+}(0)\sim G_{-}(z)G_{-}(0)\sim 0. \tag{50}$$

The simplest representation of the $N=2$ superconformal theories is the $\widehat{su}(2)/\hat{u}(1)$ minimal model with superconformal generators as follows:

$$G_1(z)=\left(\frac{2}{k}\right)^{1/2}(j_1\hat{J}_1+j_2\hat{J}_2)(z), \tag{51}$$

$$G_2(z)=\left(\frac{2}{k}\right)^{1/2}(j_2\hat{J}_1-j_1\hat{J}_2)(z), \tag{52}$$

$$U(z)=\frac{2}{k}\left(\hat{J}_3+\frac{i\hat{k}}{k}\epsilon_{123}j_1j_2\right)(z), \tag{53}$$

$$T(z)=\frac{1}{k}((\hat{J}_1)^2+(\hat{J}_2)^2-ij_1j_2\hat{J}_3-\hat{k}(j_1\partial_z j_1+j_2\partial_z j_2))(z). \tag{54}$$

The superconformal generators (51) and (54) are the generalization of the Kostant operator and its square of the $\mathrm{su}(2)/u(1)$ model. The equal rank embeddings in Sec. III that are extented to construct the $N=2$ superconformal models are as follows:

- $\widehat{\mathrm{su}}(n+1)/\widehat{\mathrm{su}}(n)\times\hat{u}(1)$ with central charge $c_{\hat{g}/\hat{h}}=3\hat{k}n/(\hat{k}+n+1)$;
- $\widehat{\mathrm{so}}(n+2)/\widehat{\mathrm{so}}(n)\times\widehat{\mathrm{so}}(2)$ with central charge $c_{\hat{g}/\hat{h}}=3\hat{k}n/(\hat{k}+n)$, $n\geqslant 2$;
- $\widehat{\mathrm{su}}(m+n)/\widehat{\mathrm{su}}(m)\times\widehat{\mathrm{su}}(n)\times\hat{u}(1)$ with central charge $c_{\hat{g}/\hat{h}}=3\hat{k}mn/(\hat{k}+m+n)$;
- $\hat{E}_6/\widehat{\mathrm{so}}(10)\times\hat{u}(1)$ with central charge $c_{\hat{g}/\hat{h}}=48\hat{k}/(\hat{k}+12)$.

VI. GROUND STATES OF SUPERCONFORMAL THEORIES

As discussed in the previous sections, the decomposition of $\hat{g}$ and $\hat{h}$ at level k are, respectively,

$$\begin{aligned}\hat{g}_k&=\hat{g}_{\hat{k}}\oplus\widehat{\mathrm{so}}(\dim g)_1,\\ \hat{h}_k&=\hat{h}_{\hat{k}+g^\vee-h^\vee}\oplus\widehat{\mathrm{so}}(\dim h)_1,\end{aligned} \tag{55}$$

and in terms of generators are, respectively,

$$\begin{aligned}J^k_A(z)&=\hat{J}^{\hat{k}}_A(z)\underbrace{-\frac{i}{2}f_{[ABC]}j_{[B}j_{C]}(z)}_{g^\vee},\\ J^k_i(z)&=\hat{J}^{\hat{k}}_i(z)\underbrace{-\frac{i}{2}f_{[iab]}j_{[a}j_{b]}(z)}_{g^\vee-h^\vee}\underbrace{-\frac{i}{2}f_{[ijk]}j_{[j}j_{k]}(z)}_{h^\vee}.\end{aligned} \tag{56}$$

From the viewpoint of representation theory, the affine weights of $\hat{g}_k$ and $\hat{h}_k$ corresponding to (55) and (56) are, respectively,

$$\hat{\Lambda}+\hat{\rho}_g=(\Lambda;\hat{k};-m)+(\rho_g;g^\vee;0), \tag{57}$$

$$\hat{\lambda}+\hat{\rho}_h=(\lambda;\hat{k}+g^\vee-h^\vee;-n)+(\rho_h;h^\vee;0). \tag{58}$$

Recall that an affine Weyl group of $\hat{g}$ is a semidirect product of the Weyl group of g by the group of translations by coroots. The affine Weyl group still preserves the affine scalar product.[8] This allows us to define an Euler multiplet of $\hat{g}/\hat{h}$ as a set of the affine weights of $\hat{h}$ in accordance with that of g/h, i.e.,

$$\{c\cdot\hat{\Lambda}\equiv c(\hat{\Lambda}+\hat{\rho}_g)-\hat{\rho}_h\}. \tag{59}$$

Now let us suppose that

$$\hat{\Lambda}+\hat{\rho}_g\geqslant\hat{w}^{-1}(\hat{\mu}+\hat{\rho}_h), \tag{60}$$

where $\hat{\mu}$ is an affine weight of $\hat{h}$ in the decomposition of $V_{\hat{\Lambda}}\otimes\hat{S}$ into irreducible representations of $\hat{h}$ and $\hat{w}$ is an element of the affine Weyl group such that $\hat{w}^{-1}(\hat{\mu}+\hat{\rho}_h)$ is a dominant weight. Squaring (60) yields

$$\frac{1}{2(\hat{k}+g^\vee)}(C_2(\Lambda)-C_2(\mu)+|\rho_g|^2-|\rho_h|^2)-m+n\geqslant 0. \tag{61}$$

From (14), in case of $\mu=c\cdot\Lambda$, one yields a condition $m=n$. This means that in the Kazama–Suzuki construction if $\hat{\mu}=c\cdot\hat{\Lambda}$, the affine weight of $\hat{g}_{\hat{k}}$ at grade m always gives the affine weights of $\hat{h}_{\hat{k}+g^\vee-h^\vee}$ at the same grade m as the Euler multiplet. Adding and subtracting by the eigenvalue of the spinor highest weight of $\widehat{so}(\dim g/h)_1$ to (61), one obtains

$$\underbrace{\frac{1}{2(\hat{k}+g^\vee)}(C_2(\Lambda)-C_2(\mu))+\frac{1}{2}\tilde{\Lambda}^2}_{\Delta\ (=\ \text{conformal dimension})}\underbrace{-\frac{1}{16}(\dim\ g/h)+\frac{1}{2(\hat{k}+g^\vee)}(|\rho_g|^2-|\rho_h|^2)}_{-c_{\hat{g}/\hat{h}}/24}\geqslant 0. \tag{62}$$

The minimum of (62) corresponds to the vanishing of the modular anomaly of the Kazama–Suzuki coset model and is the eigenvalue of zero mode of energy-momentum tensor (39). It also implies that the Euler multiplets are the intrinsic ground states of the superconformal theories.

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On linearity of separating multiparticle differential Schrödinger operators for identical particles

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We show that hierarchies of differential Schrödinger operators for identical particles which are separating for the usual (anti-)symmetric tensor product, are necessarily linear, and offer some speculations on the source of quantum linearity. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1646449]

I. INTRODUCTION

One of the properties considered in speculations about possible fundamental nonlinearities in quantum mechanics is *separation*, that is, product functions evolve as product functions. Separation is considered a nonlinear version of the notion of noninteraction, as then uncorrelated states remain uncorrelated under time evolution. We show here that if separation is combined with either Fermi or Bose statistics embodied in the usual (anti-)symmetrized tensor product states, and if all the multiparticle Shrödinger operators are differential, then they are necessarily linear.

The motivation for studying hierarchies of multiparticle nonlinear Schrödinger equations comes from two sources: (1) intellectual speculation about possible nonlinearities in quantum mechanics,[1] and (2) examples arising in representations of current algebras (diffeomorphism groups).[2] We consider the second motivation compelling as current algebra representations were found to include many known linear quantum systems and to predict new ones, anyons in particular.[3]

The nonlinear theories considered still maintain that states are represented by rays in a Hilbert space, that evolution is given by a (nonlinear) Schrödinger-type equation for the wave function, and that the modulus of the (normalized) wave function gives the probability density of detection. Though these assumptions can all be questioned, an important class of theories do satisfy them.

A complete analysis of separating hierarchies of Schrödinger-type equations for nonidentical particles was given in Ref. 4, however as the world is made up of bosons and fermions, the identical particle case has to be addressed. In Ref. 5 we explored the possibility of formulating a nonlinear relativistic theory based on a nonlinear version of the consistent histories approach to quantum mechanics. A toy model led to a set of equation among which there were instances of a weakened form of the separation property for scalar bosons. This showed once more that such a property is fundamental for understanding any nonlinear extension of ordinary quantum mechanics.

In Ref. 6 we showed that separating second-order differential hierarchies for identical particles are necessarily linear under various simplifying assumptions. We here prove linearity under fewer assumptions and in a more transparent fashion.

The present result should not be taken as an argument against nonlinear quantum mechanics. As such, it would be a much weaker physical argument than the causality violation objections already raised by various authors.[7,8] Though a degree of separability is necessary to be able to isolate and observe an independent physical system, it need not be exact. Another possibility is that in nonlinear theories one could conceivably form multiparticle states from states of fewer number of particles in a way other than by the usual (anti-)symmetric tensor product. In fact by

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using the nonlinear gauge transformations of Doebner, Goldin, and Nattermann[9] one can deform a linear separating hierarchy of differential Schrödinger operators to a nonlinear hierarchy of differential Schrödinger separating with respect to a deformed tensor product. Whether differential hierarchies that are not equivalent to linear ones and separating with respect to deformed tensor products exist, is still to be determined. Last, our results are strictly nonrelativistic. Causal relativistic nonlinear theories are seemingly hard to formulate, though they probably do exist.[5,10] What separation implies in such a context is still to be explored. What the present result hints at is the origin of linearity about which we comment in the final section.

II. SEPARATION

At time t an n-particle wave function Ψ depends on the positions $x_1,\ldots,x_n$ of each particle, where each $x_i \in \mathbb{R}^d$, d being the dimension of space, and on $A_1,\ldots,A_n$ where each A_i is an index denoting the internal degrees of freedom of each particle. Initially we assume the n particles to always belong to different species and so no permutation symmetry property is assumed of the wave function. We use the symbol $s=(s_1,\ldots,s_n)$ as labelling the species of the particle. For initial notational ease we shall combine the internal degrees of freedom index A_i with the position x_i into a single symbol $\xi_i=(x_i,A_i)$ and denote the n-tuple of such by ξ. Thus we denote an n-particle wave function at time t by $\Psi(\xi,t)$.

We assume that the evolution from time t_1 to time t_2 of the state corresponding to the ray with representative wave function $\Psi(\xi,t_1)$ can be expressed by a not necessarily linear evolution operator $E_s(t_2,t_1)$ applied to the wave function, that is

$$\Psi(\xi,t_2)=(E_s(t_2,t_1)\Psi)(\xi,t_1).$$

The simple tensor product of an n- and an m-particle wave function is defined as

$$(\phi\otimes\psi)(\xi_1,\ldots,\xi_n,\xi_{n+1},\ldots,\xi_{n+m})=\phi(\xi_1,\ldots,\xi_n)\psi(\xi_{n+1},\ldots,\xi_{n+m}). \tag{1}$$

The separation property for the simple tensor product now reads

$$E_s(t_2,t_1)(\Psi_1\otimes\Psi_2)=E_{s_1}(t_2,t_1)(\Psi_1)\otimes E_{s_2}(t_2,t_1)(\Psi_2), \tag{2}$$

where the species index s of Ψ is the concatenation of the species indices s_i of the Ψ_i. Strictly speaking, since states correspond to rays and not vectors, the right-hand side should be multiplied by a complex number $\gamma(t_2,t_1,s_1,s_2,\Psi_1,\Psi_2)$. To our knowledge, a full analysis of the possibility of such a factor has not been carried out. For the rest of this paper we shall assume that $\gamma=1$, the general assumption in the literature.

Now, the world is made of bosons and fermions and one should reconsider the separation property when one is dealing with a single species of identical particles. The separation property (2) must then be reformulated with respect to the symmetric or antisymmetric tensor product $\phi\,\hat{\otimes}\,\psi$ which is the right-hand side of (1) symmetrized or antisymmetrized according to either Bose or Fermi statistics:

$$(\phi\hat{\otimes}\psi)(\xi_1,\ldots,\xi_n,\xi_{n+1},\ldots,\xi_{n+m})=\frac{n!m!}{(n+m)!}\sum_{\mathcal{I}}(-1)^{fp(\mathcal{I})}\phi(\xi_{i_1},\ldots,\xi_{i_n})\psi(\xi_{j_1},\ldots,\xi_{j_m}), \tag{3}$$

where $\mathcal{I}=(i_1,\ldots,i_n)$ are n numbers from $\{1,\ldots,n+m\}$, in ascending order, $(j_1,\ldots,j_m)$ the complementary numbers, also in ascending order, f is the Fermi number 0 for bosons and 1 for fermions, and $p(\mathcal{I})$ is the parity (0 for even and 1 for odd) of the permutation $(1,\ldots,n+m)\mapsto(i_1,\ldots,i_n,j_1,\ldots,j_m)$. We have taken into account that both ϕ and ψ are either symmetric or antisymmetric with respect to permutations of their arguments. The normalizing factor

makes the product associative and the map $\phi\otimes\psi\mapsto\phi\hat{\otimes}\psi$ into a projection. For the identical particle case, the species symbol s reduces just to the particle number n.

If we pass to the generators of the evolution operators

$$H_s(t)=\frac{1}{i}\frac{\partial}{\partial t_2}E_s(t_2,t_1)\bigg|_{t_2=t_1=t},$$

then the separation property (2) (under the assumption that $\gamma=1$) becomes

$$H_s(\Psi_1\otimes\Psi_2)=H_{s_1}(\Psi_1)\otimes\Psi_2+\Psi_1\otimes H_{s_2}(\Psi_2), \tag{4}$$

where for notational simplicity we have suppressed indicating the t dependence of the H's. This relation (which we called tensor derivation) was fully analyzed in Ref. 4. Canonical decompositions and constructions were also presented.

An (anti-)symmetric tensor derivation would be a hierarchy of operators H_n that satisfies (4) with $\hat{\otimes}$ instead of $\otimes$. One does not have a classification of these as one has for ordinary tensor derivations as given in Ref. 4. It seems that the conditions to be a tensor derivation in the (anti-)symmetric case is rather stringent, and as we shall now see, in the case of differential operators, implies linearity.

It now becomes convenient to disentangle the space-coordinate x and the internal degree of freedom index A. Our one-particle wave function will thus be denoted by $\psi^A(x)$ with the index as a superscript for convenience. Multiparticle wave function will carry multiple indices in the usual way. The possibly nonlinear operators of the tensor derivation will be assumed to depend on the real and imaginary parts of the wave function in an independent fashion, though, to simplify notation, this is not denoted explicitly. Likewise, for notational ease, internal degree of freedom indices will be suppressed when no confusion can arise.

We shall use a multi-index notation for partial derivatives. Given a function $u(x_1,\ldots,x_n)$ and $I=(i_1,\ldots,i_n)$ an n-tuple of non-negative integers, we denote by $|I|$ the sum $i_1+\cdots+i_n$ and by u_I the partial derivative

$$\partial_I u=\frac{\partial^{|I|}u}{\partial x_1^{i_1}\cdots\partial x_n^{i_n}}.$$

For the case of a function $u(x,y)$ of two variables we write $u_{I,J}$ for I differentiations with respect to x, and J with respect to y.

Let us consider possibly nonlinear differential operators of any order (dependence on time can be construed as simply dependence on a parameter). Such a two-particle operator has the form $H(x,y,\phi^{AB}_{I,J}(x,y))$. Introducing variable names for the arguments of H, we write $H(x,y,a^{AB}_{I,J})$. When ϕ is constrained to be an (anti-)symmetrized product

$$\phi^{AB}(x,y)=\tfrac{1}{2}(\alpha^A(x)\beta^B(y)+(-1)^f\beta^A(x)\alpha^B(y)),$$

then the arguments of H are constrained to take on values of the form

$$a^{AB}_{I,J}=\tfrac{1}{2}(\alpha^A_I\tilde{\beta}^B_J+(-1)^f\beta^A_I\tilde{\alpha}^B_J). \tag{5}$$

Here quantities without the tilde are derivatives evaluated at x and those with, at y. The quantities on the right-hand sides: $\alpha^A_I,\beta^A_I,\tilde{\alpha}^B_J,\tilde{\beta}^B_J$, which we shall call the $\alpha\beta$ quantities, can be given, by Borel's lemma, arbitrary complex values by an appropriate choice of the points x and y and functions α and β. Denote the right-hand sides of the above equations by $\hat{a}^{AB}_{I,J}$.

The separability condition for the symmetrized tensor product now reads

$$2H_2^{AB}(x,y,\hat{a}_{I,J}) = H_1^A(x,\alpha_I)\tilde{\beta}_0^B + \alpha_0^A H_1^B(y,\tilde{\beta}_J) + (-1)^f H_1^A(x,\beta_I)\tilde{\alpha}_0^B + (-1)^f \beta_0^A H_1^B(y,\tilde{\alpha}_J). \tag{6}$$

Now we come to the main point: in the space of the $\alpha\beta$ quantities there are flows that leave $\hat{a}_{I,J}$ invariant, and so must leave the right-hand side of (6) invariant. This leads to linearity.

III. PROOF OF LINEARITY

One easily sees that the following transformations leave the $\alpha\beta$-quantities invariant:

$$\alpha_I^A \mapsto s\alpha_I^A, \quad \tilde{\beta}_J^B \mapsto s^{-1}\tilde{\beta}_J^B;$$

$$\alpha_I^A \mapsto \alpha_I^A + s\beta_I^A, \quad \tilde{\alpha}_J^B \mapsto \tilde{\alpha}_J^B - s(-1)^f \tilde{\beta}_J^B; \tag{7}$$

and the same with α and β interchanged. Symmetry (7) is enough to force linearity.

Note that s is a *complex* parameter, which means that the real and imaginary parts of the quantities undergo separate transformations. As a result, the right-hand side of (6) has to be annihilated by the vector field corresponding to (7):

$$\sum_{C,I} \left(\beta_I^C \frac{\partial}{\partial \alpha_I^C} - (-1)^f \tilde{\beta}_I^C \frac{\partial}{\partial \tilde{\alpha}_I^C} \right), \tag{8}$$

where by $\partial/\partial\alpha_I^C$ we mean the usual convention $(1/2)(\partial/\partial \operatorname{Re}\alpha_I^C - i\partial/\partial \operatorname{Im}\alpha_I^C)$ and similarly for the other partial derivative.

Applying now (8) to the right-hand side of (6), we get

$$\left[\sum_{C,I} \beta_I^C \frac{\partial H_1^A}{\partial \alpha_I^C}(x,\alpha) - H_1^A(x,\beta) \right] \tilde{\beta}_0^B - \beta_0^A \left[\sum_{C,I} \tilde{\beta}_I^C \frac{\partial H_1^B}{\partial \tilde{\alpha}_I^C}(y,\tilde{\alpha}) - H_1(y,\tilde{\beta}) \right] = 0.$$

Now the $\alpha\beta$ quantities can be chosen arbitrarily and generically we have $\beta_0^A \neq 0$ and $\tilde{\beta}_0^B \neq 0$ for all A and B and so generically

$$\frac{1}{\beta_0^A} \left[\sum_{C,I} \beta_I^C \frac{\partial H_1^A}{\partial \alpha_I^C}(x,\alpha) - H_1^A(x,\beta) \right] = \frac{1}{\tilde{\beta}_0^B} \left[\sum_{C,I} \tilde{\beta}_I^C \frac{\partial H_1^B}{\partial \tilde{\alpha}_I^C}(y,\tilde{\alpha}) - H_1(y,\tilde{\beta}) \right].$$

Since both sides depend on different sets of variables, each side is a constant k and we now have

$$\sum_{C,I} \beta_I^C \frac{\partial H_1^A}{\partial \alpha_I^C}(x,\alpha) - H_1^A(x,\beta) = k\beta_0^A.$$

Fixing α this equation states that $H_1(x,\beta)$ is a linear function of β with coefficients depending on x. We have thus shown the following.

Lemma: In an (anti-)symmetric tensor derivation in which the one-particle and two-particle operators are differential, the one-particle operator is necessarily linear.

To show the whole hierarchy is linear we proceed as in Ref. 6. An N-particle wave function for particles in $\mathbb{R}^d$ can be viewed as a one-particle wave function for particles (call them *conglomerate* particles) in $\mathbb{R}^{Nd}$. Consider the separating property for a $2N$-particle operator acting on an (anti-)symmetrized tensor product of two N-particle wave functions, reinterpreted now as a separating property for operators acting on the wave functions of two and one conglomerate particles. The only difference in relation to what we have already done, is the permutation symmetry of conglomerate particles. Let $\phi(x_1,\ldots,x_N)$ and $\psi(y_1,\ldots,y_N)$ be two properly (anti-)symmetric N-particle wave functions. One has using the conventions of (3),

$$(\phi\hat{\otimes}\psi)^{\mathcal{A}}(x_1,\ldots,x_{2N})=\frac{N!^2}{(2N)!}\sum_{\mathcal{I}}(-1)^{fp(I)}\phi^{\mathcal{A}_I}(x_{i_1},\ldots,x_{i_N})\psi^{\mathcal{A}_J}(x_{j_1},\ldots,x_{j_N}),\tag{9}$$

where $\mathcal{A}=(A_1,\ldots,A_{2N})$, $\mathcal{A}_I=(A_{i_1},\ldots,A_{i_N})$, and $\mathcal{A}_J=(A_{j_1},\ldots,A_{j_N})$ are internal degree of freedom indices. For (9) the possible values that one can attribute to the wave function and its derivatives at a point is now more complicated than that given by (5), but since by an appropriate choice of coordinates and an appeal to Borel's lemma we can again use (5) as a particular case for two conglomerate particles, the only differences being the change of the combinatorial factor 1/2 to $N!^2/(2N)!$ and the possibility that the factor $(-1)^f$ may be absent even in the Fermi case. These differences are nonessential to the derivation, and repeating the argument presented above for the two-particle case we see that the operator for one conglomerate particle must be linear and so the N-particle operator must be linear. With this the whole hierarchy must be linear. We thus have the following.

Theorem: *An (anti-)symmetric tensor derivation in which all multiparticle operators are differential, is necessarily linear*.

IV. COMMENTS ON THE ORIGIN OF QUANTUM LINEARITY

Our view on quantum-mechanical linearity is that it is an emergent feature of the world that arises along with the manifold structure of space–time from some more fundamental pregeometric reality. Thus questions of (non)linearity should be joined with the general quantum gravity program. Previous clues in this direction are provided by (1) the apparent connections between linearity and the causal structure of space–time[8,11] and by (2) the difficulty of incorporating internal degrees of freedom, such as spin, in separating nonlinear theories, requiring new multiparticle effects at every particle number.[12] We consider the present result as another such clue, linking linearity to the statistics of identical particles and the possibility of independently evolving systems.

The emergent view of linearity is also supported by the present extremely small experimental bounds on possible nonlinear effects, the suppression factor being about 10^{-20}.[13] If linearity is emergent, experimental evidence would be hard to come by. There is however the possibility that ultra-high-energy cosmic rays actually do probe the hypothetically nonlinear pregeometric regime.[14] The possible role of nonlinearities on the Planck scale has also been considered by Singh,[15] and by Mavromatos and Szabo.[16]

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Casimir energy inside a cavity with triangular cross section

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For a certain class of triangles (with angles proportional to π/N, $N\geqslant 3$) we formulate an image method by making use of the group G_N generated by reflections with respect to the three lines which form the triangle under consideration. We formulate the regularization procedure by classification of subgroups of G_N and corresponding fixed points in the triangle. We then also calculate Casimir energy for a cavity of infinite height with triangular cross section for scalar massless fields. More detailed calculation is given for odd N. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1643196]

I. INTRODUCTION

There is a rather restricted class of geometries, for which we have Casimir energies in explicit forms. On the other hand, to have calculations for larger sets of geometries in hand will certainly help the better understanding of the phenomena and, may also offer new experimental realizations especially in light of the rapid progress in the nanotechnologies.[1] To calculate the energy momentum tensor one has to solve the boundary problem, that is one has to obtain eigenvalues and eigenfunctions for the field which is confined into the given region. The eigenvalues usually correspond to the roots of some special functions. For example for the three-dimensional ball[2] or cylindrical regions[3] to impose the required radial boundary conditions; one has to deal with Bessel functions and with the roots of them.

For some geometries with plane boundaries the Casimir problem is easier, especially if we can employ the method of images. The original parallel plate geometry, and in general rectangular prisms[4] are of that type. For parallel plates the Dirichlet Green function is computed as an infinite sum of the ''free'' propagators to the image points. The images are due to infinite reflections between the planes, a fact that is best visualized in the path integral formulation of the quantum mechanics.[5] Similarly for multiply connected geometries (i.e., for Aharonov–Bohm case) one sums over all homotopically nonequivalent paths. As we see in the next sections the groups generated by the reflections too provide useful guides in the construction of the Green functions. For the parallel plate the group is isomorphic to Z, for the three-dimensional rectangular prism for example, it is Z^3. However if the rectangularity condition is dropped, the groups generated by reflections becomes noncommutative which is the case for the present work.

We calculate the Casimir energy for the massless scalar field for a certain class of triangular regions. We restrict our attention on the triangles whose angles are proportional to π/N, where N is a natural number greater than 2. Namely one of the angles is π/N and another is $\pi/2$ for even N and $\pi[(N-1)/2N]$ for odd N. We also develop a regularization technique by reducing the problem of finding divergences to the classification of points of the region and their stability subgroups.

In Sec. II we investigate the structure of the group G_N generated by the reflections with respect to the three lines which form the triangle. This group will play central role in the con-

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struction of the Green function satisfying the Dirichlet boundary condition, and in the regularization procedure.

We show that this group is isomorphic to the semidirect product of the dihedral group D_N and finite dimensional lattices.

Section III is devoted to the construction of the Green function for the massless scalar field which vanishes on the boundary of the triangle.

In Sec. IV we formulate the regularization procedure for the Green function in the triangle by classification of points in the triangle and their stability groups. The trivial group consisting of the identity element is the stability group for any points in the triangle. The corresponding term in the Green function is the free Green function in Minkowski space which makes an infinite contribution to the energy momentum tensor. Stability group of the points on a side of the triangle is generated by the reflection operator with respect to this side. In this way terms with surface divergences is found. Since at the vertices of the triangle the smoothness condition is violated we also have line divergences (vertex of the triangle in the plane corresponds to the line in three dimensions, that is why we call it line divergence). We find stability groups of these points and corresponding singular terms in the Green function.

In Sec. V we give the general expression for the energy momentum tensor in terms of the sum over elementary power functions. We also see that the energy density per unit length in the direction perpendicular to the triangle under consideration can be represented as the integral over the boundary of this triangle and the integrand is the elementary power functions. We presented the calculation for odd N in detail.

II. REFLECTIONS IN A CLASS OF TRIANGLES

For $N=3,4,5,\ldots$ and $k=1,2,\ldots,N-2$ consider the triangles Δ_k^N in x^1x^2-plane formed by the lines

$$L_1=\{\mathbf{x}\in R^2: x^2=0\}, \tag{1}$$

$$L_2=\{\mathbf{x}\in R^2: x^2=x^1\tan\upsilon\}, \tag{2}$$

$$L_3=\{\mathbf{x}\in R^2: x^2=(b-x^1)\tan(k\upsilon)\}, \tag{3}$$

where b is the length of the side laying on the line L_1 and $\upsilon=\pi/N$ is the angle between L_1 and L_2. (Note that in calculating the Casimir energy for the wedge geometry one also starts with angle π/N, then makes analytic continuation.[6])

The actions of the reflections Q_j with respect to the lines L_j, $j=1,2,3$ on the vector

$$\mathbf{x}=\begin{pmatrix} x^1 \\ x^2 \end{pmatrix} \tag{4}$$

are given by

$$Q_1\mathbf{x}=p\mathbf{x},\quad Q_2\mathbf{x}=rp\mathbf{x},\quad Q_3\mathbf{x}=pr^k\mathbf{x}+\mathbf{x}_0, \tag{5}$$

where

$$r=\begin{pmatrix} \cos 2\upsilon & -\sin 2\upsilon \\ \sin 2\upsilon & \cos 2\upsilon \end{pmatrix},\quad p=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\quad \mathbf{x}_0=(1-pr^k)\begin{pmatrix} b \\ 0 \end{pmatrix}. \tag{6}$$

Denote by G_N the group generated by the these reflections. G_N is one free group with relations. Relations between the elements Q_1, Q_2, and Q_3 can be obtained from the formulas (5), and from the properties of the rotation r and reflection p operators

$$r^N=1,\quad p^2=1,\quad pr=r^{N-1}p,\quad r^k\mathbf{x}_0=-p\mathbf{x}_0. \tag{7}$$

Some of the obvious relations are

$$Q_j^2=1,\ (Q_1Q_2)^N=1, \tag{8}$$

from which we conclude that the reflections Q_1 and Q_2 generate the finite subgroup

$$D_N=\{r^s,pr^s,s=0,1,\ldots,N-1\}, \tag{9}$$

which is the dihedral group of dimension $2N$. Consider the linear space V_N which consists of the vectors

$$\boldsymbol{\xi}=\sum_{s=0}^{N-1} n_s\mathbf{x}_s, \tag{10}$$

where n_s are integers and

$$\mathbf{x}_s=r^s\mathbf{x}_0. \tag{11}$$

The equalities

$$r\mathbf{x}_s=\mathbf{x}_{s+1},\ \ p\mathbf{x}_s=\mathbf{x}_{N-s+k} \tag{12}$$

imply that D_N is the automorphism group of the linear space V_N. The action of D_N is given in the natural way

$$\pi(q)\boldsymbol{\xi}=q\boldsymbol{\xi};\ \ q\in D_N. \tag{13}$$

Since V_N is a vector space over the integer numbers, unlike the spaces over the real numbers, the dimension $|V_N|$ is not necessarily equal to the dimension of the vectors $\mathbf{x}_s$. It may be larger, that is in our case may be greater than two. For example the dimensions of V_5, V_8 are four; while the dimensions of V_3, V_6, and V_4 are two (the vector spaces $V_3\equiv V_6$ and V_4 are known as the hexagonal and square lattices[7]). (For a detailed discussion of this problem, see Appendix A.)

The group G_N is the subgroup of the semidirect product group $D_N\star V_N$. In fact for any element $g\in G_N$ one can find the pair of elements $q\in D_N$ and $\boldsymbol{\xi}\in V_N$ as

$$g\mathbf{x}=q\mathbf{x}+\boldsymbol{\xi}\equiv(q,\boldsymbol{\xi})\mathbf{x};\ \ \mathbf{x}\in R^2. \tag{14}$$

In particular,

$$Q_1=(p,0),\quad Q_2=(rp,0),\ \ Q_3=(pr^k,\mathbf{x}_0). \tag{15}$$

G_N contains two subgroups: D_N and the one generated by Q_3. Since V_N does not contain invariant subspaces with respect to (13) we conclude that there is no subgroup in the semidirect product group which contains D_N and the group generated by Q_3 simultaneously. This fact implies that G_N is isomorphic to $D_N\star V_N$. In the special case of $|V_N|=2$ this group is called the wallpaper group.[7]

III. CONSTRUCTION OF THE GREEN FUNCTION IN THE TRIANGLES WITHOUT OBTUSE ANGLES

Consider the representation of the group G_N in the space of functions on the four-dimensional Minkowski space

$$T(g)f(x)=f(gx). \tag{16}$$

Here the action of the group G_N is given by substitution $\mathbf{x}\to x$, $\boldsymbol{\xi}\to\xi$, $p\to P$, $r\to R$ where

$$R=\begin{pmatrix}1&0&0\\0&r&0\\0&0&1\end{pmatrix},\quad P=\begin{pmatrix}1&0&0\\0&p&0\\0&0&1\end{pmatrix},\tag{17}$$

which are 4×4 matrices and

$$\xi=\begin{pmatrix}0\\ \boldsymbol{\xi}\\0\end{pmatrix},\quad x=\begin{pmatrix}x^0\\ \mathbf{x}\\x^3\end{pmatrix},\tag{18}$$

which are four-dimensional column vectors.

Using (15) one can verify that the operator

$$\mathbf{O}=\sum_{n\in Z}\sum_{s=0}^{N-1}\left(T((R^s,\xi))-T((PR^s,\xi))\right)\tag{19}$$

satisfies the following property:

$$T(Q_j)\mathbf{O}=-\mathbf{O}.\tag{20}$$

In (19), $n=(n_0,n_1,\ldots,n_{|V_N|-1})$ is multi-index and

$$\xi=\sum_{t=0}^{|V_N|-1}n_t x_t,\tag{21}$$

where

$$x_s=\begin{pmatrix}x^0\\ \mathbf{x}_s\\x^3\end{pmatrix}\tag{22}$$

and $\mathbf{x}_s$ are the base vectors described in the previous section.

It is obvious that if we define a function $\mathbf{O}f(x)$, it must vanish on the lines L_j of reflections Q_j; the fact that we make use in the construction of the Green function inside the triangle Δ_k^N, satisfying the Dirichlet boundary conditions. Since the operator $\mathbf{O}$ commutes with the Klein–Gordon operator (which is invariant under translations, rotations and reflections) the function

$$K(x,x')\equiv\mathbf{O}G(x,x')=\sum_{n\in Z}\sum_{s=0}^{N-1}\left(G(R^sx+\xi,x')-G(PR^sx+\xi,x')\right),\tag{23}$$

satisfies the equation

$$\eta^{\mu\nu}\frac{\partial^2}{\partial x^\mu\partial x^\nu}K(x,x')=\mathbf{O}\delta(x-x')\tag{24}$$

for any $x,x'\in M^2\times\Delta_k^N$, $M^2=\{(x_0,x_3)\}$; i.e., the two-dimensional Minkowski space, and the boundary condition

$$K(x,x')\big|_{x\in M^2\times\partial\Delta_k^N}=0,\tag{25}$$

where $\partial\Delta_k^N$ is the boundary of the triangle Δ_k^N. G is is the Green function in the Minkowski space with the metric $\eta=\mathrm{diag}(1,-1,-1,-1)$,

$$G(x,x')=-\frac{1}{4\pi^2}\frac{1}{|x-x'|^2}. \tag{26}$$

The function $K(x,x')$ is the Green function if the right-hand side of (24) is a delta function

$$\mathbf{O}\delta(x-x')=\delta(x-x') \tag{27}$$

for any $x,x'\in M^2\times\Delta_k^N$. The above condition implies that for any $(q,\boldsymbol{\xi})\neq(1,0)$ and for any $\mathbf{x},\mathbf{x}'\in\Delta_k^N$,

$$\delta(q\mathbf{x}+\boldsymbol{\xi}-\mathbf{x}')=0 \tag{28}$$

must be satisfied. In other words any points inside the triangle should be the representative of different orbits of the coset space R^2/G_N. The orbits of the coset space R^2/D_N are

$$[\mathbf{x}]=\{r^s\mathbf{x},pr^s\mathbf{x}:\ s=0,\ldots,N-1\}. \tag{29}$$

It is clear that we can identify this coset space with region X between two lines L_1 and L_2 including the boundaries. For any orbit in R^2/D_N there exists a unique representative in X. Since the group G_N is generated by the elements of D_N and Q_3 the problem of constructing the coset space R^2/G_N reduces to finding the subspaces Y of X such that the reflection Q_3 maps Y into X. Consider the area between three lines L_j, which is the triangle under consideration. The previous condition implies that the two angles $k\upsilon$ and $s\upsilon$ of the triangle between the lines L_1, L_3 and L_2, L_3 must be less than or equal to $\pi/2$. The restrictions

$$k\upsilon\leqslant\frac{\pi}{2},\quad s\upsilon\equiv\pi-(k+1)\upsilon\leqslant\frac{\pi}{2} \tag{30}$$

with solutions

$$k=\begin{cases}\dfrac{N}{2}, & \text{for even } N\\[2ex] \dfrac{N-1}{2}, & \text{for odd } N\end{cases} \tag{31}$$

imply that for triangles without obtuse angle the function $K(x,x')$ in (23) is indeed the Green function. Note that Eqs. (30) have also been solved by $k=(N-2)/2$ for even N. In this case $s=N/2$. For $k=N/2$ we have $s=(N-2)/2$. Therefore this solution is congruent to the previous one; that is $\Delta_{N/2}^N$ goes to $\Delta_{(N-2)/2}^N$ when the length b goes to $b\cos\upsilon$.

Finally we like to remark that, for massive fields, instead of $G(x,x')$ one has to put the Green function for the massive scalar fields in the Minkowski space in (23).

IV. REGULARIZATION OF THE GREEN FUNCTION

In polygonal regions there are three types of singular terms that to be subtracted to obtain the regularized Green function: Free space term, surface, and vertex terms.

Inspecting (23) we observe that the term

$$T(g)G(x,x')=G(gx,x') \tag{32}$$

leads to singularity whenever $gx=x$; that is, the singularities arise at the elements of the group G_N which leave the points fixed. The regularization problem is then reduced to the classification of the points of the region and their stability subgroups:

(i) The identity element (which is the trivial subgroup) leaves all points fixed. The term $T((1,0))G(x,x')$ in (23) therefore gives the volume singularity and is the free Green function.

(ii) The points on the line L_j are left fixed by the reflection Q_j. The group generated by Q_j is then the stability subgroup for the line L_j. Since the identity element of the two-dimensional reflection group is already employed in the volume regularization, the surface singularity terms in (23) are

$$K_S(x,x')=\sum_{j=1}^{3} T(Q_j)G(x,x'). \tag{33}$$

(iii) To discuss the vertex singularities, let us first consider the vertex at the intersection point of the lines L_1 and L_2. The N-dimensional subgroup generated by the element Q_1Q_2 is the stability subgroup of this vertex. The divergence term at the vertex we consider is

$$K_{L_1L_2}(x,x')=\sum_{j=1}^{N-1} T((Q_1Q_2)^j)G(x,x'). \tag{34}$$

The element Q_1Q_3 generates the stability subgroup of the vertex at the intersection point of the lines L_1 and L_3. Due to restriction (31) and $Q_1Q_3=(r^k,-r^k\mathbf{x}_0)$ we conclude that the dimension of this group is 2 for even N and N for odd N. Therefore we have

$$K_{L_1L_3}(x,x')=\sum_{j=1}^{L-1} T((Q_1Q_3)^j)G(x,x'), \tag{35}$$

where L is the dimension of the stability group, that is $L=2$ if N is even and $L=N$ if N is odd.

Finally let us consider the third vertex which is the intersection point of the lines L_2 and L_3. The stability group of this point is generated by the element Q_2Q_3. One can verify that the dimension D of this group is

$$D=\begin{cases} N & \text{for even } \dfrac{N}{2} \\ \dfrac{N}{2} & \text{for odd } \dfrac{N}{2} \\ N & \text{for odd } N, \end{cases} \tag{36}$$

and the corresponding singular line terms are

$$K_{L_2L_3}(x,x')=\sum_{j=1}^{D-1} T((Q_2Q_3)^j)G(x,x'). \tag{37}$$

Collecting all the above terms we arrive at

$$K_L(x,x')=\sum_{j=1}^{N-1} (T((Q_1Q_2)^j)+T((Q_1Q_3)^j)+T((Q_2Q_3)^j))G(x,x') \tag{38}$$

for odd N, and

$$K_L(x,x')=\left(T(Q_1Q_3)+\sum_{j=1}^{N-1} (T((Q_1Q_2)^j)+T((Q_2Q_3)^j))\right)G(x,x') \tag{39}$$

for even $N/2$, and

$$K_L(x,x')=\left(T(Q_1Q_3)+\sum_{j=1}^{N-1}T((Q_1Q_2)^j)+\sum_{j=1}^{(N/2)-1}T((Q_2Q_3)^j)\right)G(x,x') \tag{40}$$

for odd $N/2$. Subtracting all divergences from (23) we obtain the regularized Green function

$$K_r(x,x')=K(x,x')-G(x,x')-K_S(x,x')-K_L(x,x'). \tag{41}$$

Before closing this section we would like to emphasize that if the method of images is applicable to a geometry, the stability group classification is quite a reliable approach to the regularization.

V. ENERGY MOMENTUM TENSOR

The energy momentum tensor for conformally coupled massless scalar field is given by[8]

$$T_{\mu\nu}=\tfrac{2}{3}\partial_\mu\phi\partial_\nu\phi-\tfrac{1}{6}\eta_{\mu\nu}\partial_\rho\phi\partial^\rho\phi-\tfrac{1}{3}\phi\partial_\mu\partial_\nu\phi+\tfrac{1}{12}\eta_{\mu\nu}\phi\partial_\rho\partial^\rho\phi. \tag{42}$$

Since the vacuum expectation value of the product of two scalar fields is the Green function, we can express the energy momentum tensor in the region we study as

$$T_{\mu\nu}=\lim_{x\to x'}\left[\frac{1}{3}(\partial_\mu\partial'_\nu+\partial'_\mu\partial_\nu)-\frac{\eta_{\mu\nu}}{6}\eta^{\sigma\rho}\partial_\sigma\partial'^{\rho}-\frac{1}{6}(\partial_\mu\partial_\nu+\partial'_\mu\partial'_\nu)\right]K_r(x,x'), \tag{43}$$

where $\partial_\mu\equiv\partial/\partial x^\mu$, and $K_r(x,x')$ is given by (41).

The vacuum energy density in particular is given by the following expression (for details, see Appendix B):

$$T_{00}=\frac{1}{6\pi^2}\sum_{(n,s)}\left[\frac{|(pr^s+1)\boldsymbol{\xi}|^2}{|(pr^s-1)\mathbf{x}+\boldsymbol{\xi}|^6}-\frac{2+\cos(2s\upsilon)}{|(r^s-1)\mathbf{x}+\boldsymbol{\xi}|^4}\right]. \tag{44}$$

The summation runs over the indices $n=(n_0,n_1,\ldots,n_{|V_N|-1})\in Z^{|V_N|}$, and $s=0,1,\ldots,N-1$. The terms corresponding to the singularities described in the previous section should be dropped in (44). The term in the second summation in (44) with $(n=0,s=0)$ is the energy of the free vacuum. The terms with $(n=0,s=0)$, $(n=0,s=1)$, and $(n=(1,0,\ldots,0),s=k)$ in the first summation of (44) are surface divergence terms. Note that due to the $|(pr^s+1)\boldsymbol{\xi}|^2$ factor they are automatically zero. This is not surprising since it is known that the energy momentum tensor for comformally coupled scalar field is finite on flat surfaces.[9] Terms $(n=0,s=1,2,\ldots,N-1)$ in the second summation of (44) are line divergent ones in the vertex which is the intersection point of the lines L_1 and L_2. Using the results of the previous section one may also find the vertex divergence terms for other two vertices.

Integrating the above energy density over the triangle Δ_k^N we arrive at the energy density E per unit length in x^3 direction. First we observe the existence of two exact forms

$$\omega_1^s=\frac{2+\cos(2s\upsilon)}{2|(r^s-1)\mathbf{x}+\boldsymbol{\xi}|^4}dx^1\wedge dx^2, \tag{45}$$

$$\omega_2^s=\frac{|(pr^s+1)\boldsymbol{\xi}|^2}{|\mathbf{v}(pr^s)|^6}dx^1\wedge dx^2. \tag{46}$$

They can be rewritten as $\omega_j^s=d\Omega_j^s$, where

$$\Omega_1^s=D_s\frac{((r^s-1)\mathbf{x}+\boldsymbol{\xi})^2dx^1-((r^s-1)\mathbf{x}+\boldsymbol{\xi})^1dx^2}{|(r^s-1)\mathbf{x}+\boldsymbol{\xi}|^4},\quad s\neq 0, \tag{47}$$

$$\Omega_2^s=\frac{|(pr^s+1)\boldsymbol{\xi}|^2}{|(pr^s-1)\mathbf{x}+\boldsymbol{\xi}|^6}(r^{s/2}\mathbf{x})^1 d(r^{s/2}\mathbf{x})^2, \tag{48}$$

where

$$D_s=\frac{2+\cos(2sv)}{6(1-\cos(2sv))}.$$

By making use of the Stokes theorem one can convert the integration over the triangle Δ_k^N into the integral over its boundary $\partial\Delta_k^N$. The energy density per unit length in x^3 direction is then

$$E=-\frac{1}{6\pi^2}\langle J_0+J_1-J_2\rangle, \tag{49}$$

where S_k^N is the area of the triangle Δ_k^N and

$$J_0=\sum_{n\in Z^{|V_N|}}\frac{3S_k^N}{|\boldsymbol{\xi}|^4}, \tag{50}$$

$$J_1=\sum_{n\in Z^{|V_N|}}\sum_{s=1}^{N-1}\int_{\partial\Delta_k^N}\Omega_s^1, \tag{51}$$

$$J_2=\sum_{n\in Z^{|V_N|}}\sum_{s=0}^{N-1}\int_{\partial\Delta_k^N}\Omega_s^2. \tag{52}$$

In J_j we take summation over all values of n and s. The brackets $\langle\ \rangle$ in (49) means that we have to drop the singularity terms. J_j may be divergent if $|V_N|$ is greater than 3. However their difference should be finite. We have to treat each term as formal series. Then collecting them together we obtain the final result.

A. N=odd case as an example

Let us restrict our attention to the case of odd N, for which the vector space V_N appears to be invariant under the half angle rotations $r^{s/2}$. This can be shown from the identity

$$r^{N/2}\boldsymbol{\xi}=-\boldsymbol{\xi}. \tag{53}$$

Using the relations

$$(pr^s\pm 1)=r^{-(s/2)}(p\pm 1)r^{(s/2)},\quad (r^s-1)=-a_s r^{(s/2)+(N/4)} \tag{54}$$

with $a_s=2\sin(sv)$ and making the reparametrization in the multi-index n which is equivalent to the change of variable $r^{s/2}\boldsymbol{\xi}\to\boldsymbol{\xi}$ we arrive at

$$J_1=-\sum_{n\in Z^{|V_N|}}\sum_{s=1}^{(N-1)/2} D_s\int_{\partial\Delta_{N/2}}\frac{(a_s\mathbf{z}-\boldsymbol{\xi})^2dz^1-(a_s\mathbf{z}-\boldsymbol{\xi})^1dz^2}{|a_s\mathbf{z}-\boldsymbol{\xi}|^4}, \tag{55}$$

$$J_2=\sum_{n\in Z^{|V_N|}}\sum_{s=0}^{N-1}\int_{\partial\Delta_s}\frac{|(p+1)\boldsymbol{\xi}|^2}{|(p-1)\mathbf{y}+\boldsymbol{\xi}|^6}y^1dy^2. \tag{56}$$

Here we have used the short notation $\Delta_0\equiv\Delta_k^N$ and $\Delta_s=r^{s/2}\Delta_0$, that is, the triangle Δ_s is Δ_0 rotated by the angle sv. We also used the symmetry $s\to N-s$ in (55) to reduce the summation over s. Denote by a_0, a_1, and c_0 the sides of the triangle Δ_0 laying on the lines L_1, L_2, and L_3.

Then a_s, a_{s+1}, and c_s will be the sides of the triangle Δ_s, that is, $a_{s+1}=r^{s/2}a_s$ and $c_{s+1}=r^{s/2}c_s$. Since the orientation on the side a_{s+1} of the triangle Δ_s is opposite to the one on the side a_{s+1} of Δ_{s+1} we have

$$J_2=\sum_{n\in Z^{|V_N|}}\int_U\frac{|(p+1)\boldsymbol{\xi}|^2}{|(p-1)\mathbf{y}+\boldsymbol{\xi}|^6}y^1dy^2, \tag{57}$$

where the integration contour $U=a_0\cup b_0\cup b_1\cup\cdots\cup b_{N-1}\cup a_N$ oriented anticlockwise. On the sides a_0, a_N, and $c_{(N-1)/2}$ we have $y^2=\text{const}$, that is, these sides do not make contribution in J_2. We also observe that reflection operator $-p$ with respect to the y^2 axis send c_j to c_{N-j-1} with opposite orientation. Since the one form in the integral changes sign under reflection $\mathbf{y}\to-p\mathbf{y}$ one can rewrite the above expression as

$$J_2=2\sum_{n\in Z^{|V_N|}}\sum_{j=0}^{(N-3)/2}\int_{c_j}\frac{|(p+1)\boldsymbol{\xi}|^2}{|(p-1)\mathbf{y}+\boldsymbol{\xi}|^6}y^1dy^2. \tag{58}$$

For given c_j we construct closed contour in the following way. From the end points of c_j draw lines which are parallel to the y^1-axis. They intersect y^2 axis at the points $b\sin j\upsilon$ and $b\sin(j+1)\upsilon$. The interval between these two points, c_j and two intervals between them, which are parallel to the y^1-axes form the desired contour which we denote by C_j. Since at $y^1=0$ and $y^2=\text{const}$ the one form in the above integral is zero. We then have

$$J_2=2\sum_{n\in Z^{|V_N|}}\sum_{j=0}^{(N-3)/2}\int_{C_j}\frac{|(p+1)\boldsymbol{\xi}|^2}{|(p-1)\mathbf{y}+\boldsymbol{\xi}|^6}(y^1-A_jy^2-B_j)dy^2, \tag{59}$$

where we have added the exact forms, which are the second and third terms in the bracket, for an integral of the exact form over the closed form is zero. We choose the coefficients A_j and B_j to satisfy

$$y^1-A_jy^2-B_j=0, \tag{60}$$

for $\mathbf{y}\in c_j$, that is, to make the value of the one form zero on the side c_j. We have

$$A_j=-\frac{\cos\upsilon(k-j)}{\sin\upsilon(k-j)},\quad B_j=b\frac{\sin\upsilon k}{\sin\upsilon(k-j)}, \tag{61}$$

where $k=(N-1)/2$. Nonzero contribution to the integral comes only from the integration over the interval laying on the y^2 axis:

$$J_2=8\sum_{n\in Z^{|V_N|}}\sum_{j=0}^{(N-3)/2}\int_{b\sin j\upsilon}^{b\sin(j+1)\upsilon}\frac{(\xi^1)^2(A_jt+B_j)dt}{((\xi^1)^2+(2t-\xi^2)^2)^3} \tag{62}$$

or

$$J_2=\frac{1}{2b^2\sin^2k\upsilon}\sum_{n\in Z^{|V_N|}}\sum_{j=0}^{(N-3)/2}\frac{\eta_1^2}{\sin(k-j)\upsilon}\int_{f_j}^{f_{j+1}}dx\,\frac{1-x\cos((k-j)\upsilon)}{(\eta_1^2+(x-\eta_2)^2)^3}, \tag{63}$$

where $f_j=\sin j\upsilon/\sin k\upsilon$ and $\boldsymbol{\xi}=2b\sin k\upsilon\boldsymbol{\eta}$ or

$$\boldsymbol{\eta}=\sum_{t=0}^{|V_N|-1}n_t\mathbf{x}_t',\quad \mathbf{x}_t'=r^{t+1/4}\begin{pmatrix}1\\0\end{pmatrix}. \tag{64}$$

(We also used lower indices for the vector $\boldsymbol{\eta}$.)

Now consider expression (55). Rotation $r^{1/2}$ maps interval $a_{N/2}$ on $a_{(N/2)+1}$ which has the opposite orientations. Since the expression under the integral is invariant under transformation $\mathbf{z} \rightarrow r^{1/2}\mathbf{z}$, the contributions from these intervals cancel each other. J_1 is nonzero on the interval $c_{N/2}$. Let us make the change of variable $\mathbf{y}=r^{-(N+1)/4}\mathbf{z}$. Then $c_{N/2}$ goes to $c_{-1/2}$ on which $y^1 = b\cos\upsilon/2$ and $y^2 \in [-b\sin\upsilon/2, b\sin\upsilon/2]$. Therefore,

$$J_1=\sum_{n\in Z^{|V_N|}}\sum_{s=1}^{(N-1)/2} D_s \int_{-b\sin\upsilon/2}^{b\sin\upsilon/2} \frac{\left(ba_s\cos\frac{\upsilon}{2}-\xi^1\right)dy}{\left(\left(ba_s\cos\frac{\upsilon}{2}-\xi^1\right)^2+(a_s y-\xi^2)^2\right)^2} \tag{65}$$

or

$$J_1=\frac{\sin\frac{\upsilon}{2}}{8b^2\sin^3 k\upsilon}\left\langle \sum_{n\in Z^{|V_N|}}\sum_{s=1}^{(N-3)/2}\frac{D_s}{f_s}\int_{-f_s}^{f_s}\frac{\left(f_s\cos\frac{\upsilon}{2}-\eta_1\right)dx}{\left(\left(f_s\cos\frac{\upsilon}{2}-\eta_1\right)^2+\left(x\sin\frac{\upsilon}{2}-\eta_2\right)^2\right)^2}\right\rangle. \tag{66}$$

Note that in the above expression we have dropped the term $s=(N-1)/2$. Since $f_{(N-1)/2}=1$ by the reparametrization $\boldsymbol{\eta}\rightarrow\boldsymbol{\eta}+\mathbf{x}_0'$ we can rewrite it as

$$-\frac{1}{8b^2\sin^3 k\upsilon}D_{(N-1)/2}\sum_{n\in Z^{|V_N|}}\int_{-1}^{1}\frac{\eta_1 dx}{\eta_1^2+\left((x-1)\sin\frac{\upsilon}{2}-\eta_2\right)^2\Big)^2} \tag{67}$$

which is an odd function in the η_1 variable. Therefore it is zero.

B. A special example: $N=3$

Finally let us consider the special case when $N=3$ and $k=1$. We have $\upsilon=\pi/3$ and $\boldsymbol{\xi}=\sqrt{3}b\,\boldsymbol{\eta}$ with

$$\boldsymbol{\eta}=\frac{n_0}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix}+\frac{n_1}{2}\begin{pmatrix}-\sqrt{3}\\1\end{pmatrix}, \tag{68}$$

that is, $|V_3|=2$. We have $S_1^3=(\sqrt{3}/4)\,b^2$, $J_1=0$, and

$$J_0=\frac{\sqrt{3}}{12b^2}\sum_{n\in Z^2}\frac{1}{|\boldsymbol{\eta}|^4}, \tag{69}$$

$$J_2=\frac{2}{3\sqrt{3}b^2}\sum_{n\in Z^2}\eta_1^2\int_0^1 dx\,\frac{2-x}{(\eta_1^2+(x-\eta_2)^2)^3}. \tag{70}$$

The vacuum energy density per unit length in x^3 direction is then

$$E=\frac{\sqrt{3}}{12b^2}\left\langle\sum_{n\in Z^2}\left(\frac{1}{|\boldsymbol{\eta}|^4}+\frac{8}{3}\eta_1^2\int_0^1 dx\,\frac{2-x}{(\eta_1^2+(x-\eta_2)^2)^3}\right)\right\rangle. \tag{71}$$

VI. DISCUSSION

We have calculated the Casimir energy for a class of triangles without an obtuse angle. We applied the method of images. Unlike the case of parallel plate or rectangular prisms, the group generated by reflections is not Abelian; thus, the employment of the image method for triangles is not trivial.

The regularization procedure is observed to be equivalent to the classification of the points in the triangle and their stability subgroups. To renormalize the Green function we subtract the terms corresponding to these stability subgroups. The identity element is the stability subgroup for the all points, reflections, and bi-product of reflections generate the stability subgroups of points on the planes involving the sides, and of the lines passing through the vertices, respectively.

We hope that the technique we used which essentially is based on the employment of the groups generated by reflections from the surfaces, can be employed for other polygonal regions. We also hope that it may even be possible to study some other geometries with smooth boundaries, as the limiting case of the suitable polygonal regions. For example, for an elliptical region such a process may not be as hopeless as dealing with the roots of the Mathieu functions.

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APPENDIX A

To find the dimension $|V_N|$ of V_N one has to investigate the nonzero independent solutions of the equation

$$\sum_{s=0}^{N-1} n_s \mathbf{x}_s = 0. \tag{A1}$$

Assume that we have found all independent solutions $n^t=(n_0^t, n_1^t, \ldots, n_{N-1}^t)$, $t=1,\ldots,m$, then $|V_N|=N-m$. From (11) we observe that Eq. (A1) can be rewritten in the form

$$\sum_{s=0}^{N-1} n_s r^s = 0. \tag{A2}$$

Let N be a prime number. The periodicity condition $r^N=1$ and the identity

$$\frac{1-x^N}{1-x} = 1 + x + \cdots + x^{N-1} \tag{A3}$$

which is valid for $x \neq 1$ imply the solution $n^0=(1,1,\ldots,1)$ of (A1). Let $N=M^l$, where M is a prime and l is a natural number. Then the operators $R_p = r^{N/M^p}$, $p=1,2,\ldots,l$ satisfy the periodicity condition $R_p^{M^p}=1$. This implies $(N/M) + (N/M^2) + \cdots + (N/M^{l-1}) + 1$ relations of the form

$$r^{s_p}(1 + R_p + \cdots + R_p^{M^p-1}) = 0 \tag{A4}$$

or

$$r^{s_p} + r^{(N/M^p)+s_p} + \cdots + r^{(N/M^p)(M^p-1)+s_p} = 0. \tag{A5}$$

We denote the corresponding solutions by n^{s_p}, where $p=1,2,\ldots,l$ and $s_p=0,1,\ldots,(N/M^p)-1$. The rank of the matrix $(n_s^{s_p})$ appears to be N/M and we choose solutions n^{s_1} as independent set. We demonstrate it for $N=2^3$. We have four relations

$$r^{s_1}+r^{4+s_1}=0, \quad s_1=0,1,2,3, \tag{A6}$$

two relations

$$r^{s_2}+r^{2+s_2}+r^{4+s_2}+r^{6+s_2}=0, \quad s_2=0,1, \tag{A7}$$

and one relation

$$1+r+\cdots+r^7=0. \tag{A8}$$

We see that relations (A7) reduce to

$$r^{s_2}+r^{4+s_2}=0, \quad r^{(2+s_2)}+r^{4+(2+s_2)}=0. \tag{A9}$$

Summation of four relations (A9) leads to relation (A8). Therefore we have four independent solutions. The general case can be proved in a similar fashion. Let now $N=M_1^{l_1}M_2^{l_2}\cdots M_f^{l_f}$, where M_j are prime numbers such that $M_1<M_2<\cdots<M_f$. In this case we have $(N/M_1)+(N/M_2)+\cdots+(N/M_f)$ solutions n^{s^j}:

$$r^{s^j}+r^{(N/M_j)+s^j}+\cdots+r^{(N/M_j)(M_j-1)+s^j}=0, \tag{A10}$$

where $j=1,2,\ldots,f$ and $s^j=0,\ldots,(N/M_j)-1$. The rank of the matrix $A_N=(n_s^{s^j})$ gives the number of independent relations. The matrix A_N which consist of $(N/M_1)+(N/M_2)+\cdots+(N/M_f)$ rows and N columns can be shown to have the following form:

$$A_N=\begin{pmatrix} I_1 & I_1 & \cdots & I_1 \\ I_2 & I_2 & \cdots & I_2 \\ \cdots & \cdots & \cdots & \cdots \\ I_f & I_f & \cdots & I_f \end{pmatrix}, \tag{A11}$$

where I_j is the $(N/M_j)\times(N/M_j)$ unit matrix. Note that the number of I_j matrices in the jth row is M_j. Assume that the relations described above exhaust all relations of the form (A1). Then we have $|V_N|=N-\mathrm{rank}(A_N)$. For example, the vector spaces V_3, V_4, and V_6 has dimension two. We conjecture the following result:

$$|V_N|=N-1, \text{ for a prime } N, \tag{A12}$$

$$|V_N|=N-\frac{N}{M}, \quad \text{for } N=M^l \text{ and a prime } M. \tag{A13}$$

APPENDIX B

Here we give a list of formulas used in the derivation of (44),

$$\frac{\partial}{\partial x^\mu}\frac{1}{|ax-x'+\eta|^2}=-\frac{1}{|ax-x'+\eta|^4}\frac{\partial|ax-x'+\eta|^2}{\partial x^\mu}, \tag{B1}$$

$$\frac{\partial^2}{\partial x^\mu\partial x^\nu}\frac{1}{|ax-x'+\eta|^2}=-\frac{1}{|ax-x'+\eta|^4}\frac{\partial^2|ax-x'+\eta|^2}{\partial x^\mu\partial x^\nu} + \frac{2}{|ax-x'+\eta|^6}\frac{\partial|ax-x'+\eta|^2}{\partial x^\mu}\frac{\partial|ax-x'+\eta|^2}{\partial x^\nu}, \tag{B2}$$

$$\frac{\partial}{|ax-x'+\eta|^2}\partial x^{\mu}=2(a(ax-x'+\eta))_{\mu}, \tag{B3}$$

$$\frac{\partial}{|ax-x'+\eta|^2}\partial x'^{\mu}=-2(ax-x'+\eta)_{\mu}, \tag{B4}$$

$$\frac{\partial^2}{|ax-x'+\eta|^2}\partial x^{\mu}\partial x^{\nu}=2a^2_{\mu\nu}, \tag{B5}$$

$$\frac{\partial^2}{|ax-x'+\eta|^2}\partial x^{\mu}\partial x'^{\nu}=-2a_{\mu\nu}, \tag{B6}$$

$$\frac{\partial^2}{|ax-x'+\eta|^2}\partial x'^{\mu}\partial x'^{\nu}=2\eta_{\mu\nu}. \tag{B7}$$

Here a is the matrix of the form PR^s.

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Soliton solutions on noncommutative orbifold T^2/Z_4

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In this paper, we explicitly construct a series of projectors on integrable noncommutative orbifold T^2/Z_4 by extended *GHS* construction. They include integration of two arbitary functions with Z_4 symmetry. Our expression possesses manifest Z_4 symmetry. It is proven that the expression includes all projectors with minimal trace and in their standard expansions, the eigenvalue functions of coefficient operators are continuous with respect to the arguments k and q. Based on the integral expression, we alternately show the derivative expression in terms of the similar kernal to the integral one. Since projectors correspond to soliton solutions of the field theory on the noncommutative orbifold, we thus present a series of corresponding solitons. © *2004 American Institute of Physics.*
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I. INTRODUCTION

String theory is a very promising candidate for a unified description of the fundamental interactions, including quantum gravity. It may provide a conceptual framework to resolve the clash between two of the greatest achievements of 20th century physics: general relativity and quantum mechanics. Noncommutative geometry is originally an interesting topic in mathematics.[1–3] In the past few years, it has been shown that some noncommutative gauge theories can be embedded in string theories[4–6] and noncommutative geometry can also be applied to condensed matter physics. The currents and density of a system of electrons in a strong magnetic field may be described by a noncommutative quantum field theory.[7–9] The connection between a finite quantum Hall system and a noncommutative Chern–Simon matrix model first proposed in Ref. 8 was further elaborated in subsequent papers.[10,11] Many papers concentrated on the research for the related questions about the quantum Hall effect.[12–18] Since the noncommutative space resembles a quantum phase space, it exhibits an interesting spacetime uncertainty relation, which causes an UV/IR mixing[19,20] and a teleological behavior. Noncommutative field theories can be regarded as highly constrained deformation of local field theory. Thus it may help us to understand nonlocality at short distances in quantum gravity.

Solitons in various noncommutative theories have played a central role in understanding the physics of noncommutative theories and certain situations of string theories. The quantum Hall effect practically provides a good illustration of the combination of the three theories.[13,17,18,21] The existence and form of these classical solutions are fairly independent of the details of the theory, making them useful to probe the string behavior. In fact these solitons are the (lower-dimensional) D-branes of string theory manifested in a field theory limit while still capturing many string features.

Starting from the celebrated paper of Gopakumar, Minwalla, and Strominger,[22] there are many

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works to study soliton solutions of noncommutative field theory and integrable systems in the background of noncommutative spaces.[23–30] Although Derrick's theorem forbids solitons in ordinary $2+1$ dimensional scalar field theory,[31] solitons in noncommutative scalar field theory on the plane were constructed in terms of projection operators in Ref. 22. It was soon realized that noncommutative solitons represent D-branes in string field theory with a background B field, and many of Sen's conjectures[32,33] regarding tachyon condensation in string field theory have been beautifully confirmed using properties of noncommutative solitons. Gopakumar, Minwalla, and Strominger made an important finding that in a noncommutative space, a projector may correspond to a soliton in the field theory,[22] which proves the significance of the study of projection operators in various noncommutative spaces. Reiffel[34] constructed the complete set of projection operators on the noncommutative torus T^2. On the basis Boca studied the projection operators on noncommutative orbifold[35] obtaining many important results and showed the well-known example of the projection operator for T^2/Z_4 in terms of the elliptic function. Soliton solutions in noncommutative gauge theory were introduced by Polychronakos in Ref. 23. Martinec and Moore in their important article deeply studied soliton solutions namely projectors on a wide variety of orbifolds, and the relation between physics and mathematics in this area.[27] Gopakumar, Headrick, and Spradlin have shown a rather apparent method to construct the multisoliton solution on noncommutative integrable torus with generic τ.[24] This approach can be generalized to construct the projection operators on the integrable noncommutative orbifold T^2/Z_N.[30]

In this paper, in the case of integrable noncommutative orbifold T^2/Z_4 generated by u_1 and u_2 with

$$u_1u_2=u_2u_1e^{2\pi i/A}, \qquad A=1,2,3,\ldots . \tag{1}$$

We generalize the GHS construction, presenting the explicit symmetric form of a series of projectors with manifest Z_4 symmetry. It includes all the solutions with minimal trace, and in the standard expansions for the projectors [see Eq. (9)]

$$P=\sum_{s,t} u_1^s u_2^t \Psi_{s,t}(u_1^A,u_2^A), \tag{2}$$

where the eigenvalue function $\Psi_{s,t}(v_1^A,v_2^A)$ is continuous (where v_1^A and v_2^A are eigenvalues of u_1^A and u_2^A). The solutions include two arbitrary complex functions with Z_4 symmetry. The kernels of the integrations are closed analytic functions of u_1 and u_2. In the simplest case, when A is an even number, we reobtain the Boca's classic result[35] and obtain a new result when A is an odd number. Moreover the above construction is also applicable to the integrable $T^2/Z_N(N=3,6)$ cases.

This paper is organized as follows: In Sec. II, we introduce operators on the noncommutative orbifold T^2/Z_N. In Sec. III, we introduce the $|k,q\rangle$ representation and provide the matrix element relation for the projectors and deduce the relation between the eigenvalue functions of coefficients and the matrix elements of operators in the $|k,q\rangle$ representation. In Sec. IV, we study the general projectors with minimal trace when the eigen value functions of coefficients are continuous. In Sec. V, we present two kinds of explicit expressions for the projectors with elliptical functions as kernel.

II. NONCOMMUTATIVE ORBIFOLD T^2/Z_N

In this section, we introduce operators on the noncommutative orbifold T^2/Z_N. First we introduce two Hermitian operators $\hat{y}_1$ and $\hat{y}_2$, which satisfy the following commutation relation:

$$[\hat{y}_1,\hat{y}_2]=i. \tag{3}$$

The operators made up of $\hat{y}_1$ and $\hat{y}_2$

$$\hat{O}=\sum_{m,n} C_{mn}\hat{y}_1^m\hat{y}_2^n \tag{4}$$

form the noncommutative plane R^2. All operators on R^2 which commute with U_1 and U_2

$$U_1=e^{-il\hat{y}_2}, \qquad U_2=e^{il(\tau_2\hat{y}_1-\tau_1\hat{y}_2)}, \tag{5}$$

where l,τ_1,τ_2 are all real numbers and $l,\tau_2>0,\tau=\tau_1+i\tau_2$, constitute the noncommutative torus T^2. We have

$$U_1^{-1}\hat{y}_1U_1=\hat{y}_1+l, \qquad U_2^{-1}\hat{y}_1U_2=\hat{y}_1+l\tau_1,$$
$$U_1^{-1}\hat{y}_2U_1=\hat{y}_2, \qquad U_2^{-1}\hat{y}_2U_2=\hat{y}_2+l\tau_2. \tag{6}$$

The operators U_1 and U_2 are two different wrapping operators around the noncommutative torus and their commutation relation is $U_1U_2=U_2U_1e^{-2\pi i(l^2\tau_2/2\pi)}$. When $A=l^2\tau_2/2\pi$ is an integer, we call the noncommutative torus integrable, and introduce two operators u_1 and u_2:

$$u_1=e^{-il\hat{y}_2/A}, \quad u_2=e^{-il(\tau_2\hat{y}_1-\tau_1\hat{y}_2)/A},$$
$$u_1u_2=u_2u_1e^{2\pi i/A}, \quad u_1^A=U_1, \quad u_2^A=U_2^{-1}. \tag{7}$$

The operators on the noncommutative torus are composed of the Laurant series of u_1 and u_2,

$$\hat{O}_{T^2}=\sum_{m,n} C'_{mn}u_1^mu_2^n, \tag{8}$$

where $m,n\in Z$ and C'_{00} is called the trace of the operators, and Eq. (8) includes all operators on the noncommutative torus T^2, satisfying the relation $U_i^{-1}\hat{O}_{T^2}U_i=\hat{O}_{T^2}$. From (7) we can rewrite Eq. (8) as

$$\hat{O}_{T^2}=\sum_{s,t=0}^{A-1} u_1^su_2^t\Psi_{\mathrm{st}}(u_1^A,u_2^A), \tag{9}$$

where Ψ_{st} is Laurant series of the operators u_1^A and u_2^A. We call this formula the standard expression for the operator on the noncommutative torus T^2. The trace for the operator is the constant term's coefficient of Ψ_{00}. Next we introduce rotation R in noncommutative space R^2

$$R(\theta)=e^{-i\theta[(\hat{y}_1^2+\hat{y}_2^2)/2]+i(\theta/2)} \tag{10}$$

with

$$R^{-1}\hat{y}_1R=\cos\theta\hat{y}_1+\sin\theta\hat{y}_2, \qquad R^{-1}\hat{y}_2R=\cos\theta\hat{y}_2-\sin\theta\hat{y}_1, \tag{11}$$

when $\tau=\tau_1+\tau_2=e^{2\pi i/N}$, setting $\theta=2\pi/N(N\in Z)$. The noncommutative torus T^2 is kept invariant under rotation $R_N\equiv R(2\pi/N)$.[35,27,30] Namely $R_N^{-1}\hat{O}_{T^2}R_N$ is still the operators on the noncommutative torus T^2. Now $U_i'\equiv R_N^{-1}U_iR_N$ can be expressed by the monomial of $\{U_i\}$ and their inverses.[27] In this case, we call the operators invariant under rotation R_N on the noncommutative torus as operators on the noncommutative orbifold T^2/Z_N. We can also realize these operators in Fock space. Introduce

$$a=\frac{\hat{y}_2-i\hat{y}_1}{\sqrt{2}}, \qquad a^+=\frac{\hat{y}_2+i\hat{y}_1}{\sqrt{2}}, \tag{12}$$

then

$$[a,a^+]=1, \tag{13}$$

$$R_N=e^{-i\theta a^+ a}. \tag{14}$$

In this paper, we study the projector P on the orbifold T^2/Z_4:

$$\tau=i, \tag{15}$$

$$P^2=P, \tag{16}$$

$$U_j^{-1}PU_j=P, \quad j=1,2, \tag{17}$$

$$R_4^{-1}PR_4=P. \tag{18}$$

III. THE $|k,q\rangle$ REPRESENTATION, STANDARD FORM, AND EIGENVALUE FUNCTION

From the above discussion, we know that the operators U_1 and U_2 commute with each other on the integrable torus T^2 when A is an integer. So we can introduce a complete set of their common eigenstates, namely $|k,q\rangle$ representation[36,37]

$$|k,q\rangle=\sqrt{\frac{l}{2\pi}}e^{-i\tau_1\hat{y}_2{}^2/2\tau_2}\sum_j e^{ijkl}|q+jl\rangle, \tag{19}$$

where the ket on the right is a $\hat{y}_1$ eigenstate. We have

$$\begin{gathered}U_1|k,q\rangle=e^{-ilk}|k,q\rangle, \qquad U_2|k,q\rangle=e^{il\tau_2 q}|k,q\rangle=e^{2\pi iqA/l}|k,q\rangle,\\ id=\int_0^{2\pi/l}dk\int_0^l dq|k,q\rangle\langle k,q|.\end{gathered} \tag{20}$$

It also satisfies

$$|k,q\rangle=\left|k+\frac{2\pi}{l},q\right\rangle=e^{ilk}|k,q+l\rangle. \tag{21}$$

Consider Eq. (9), namely, the standard expansion of operators on T^2 we have

$$\Psi_{\rm st}(u_1^A,u_2^A)|k,q\rangle=\Psi_{\rm st}(e^{-ilk},e^{-2\pi iqA/l})|k,q\rangle\equiv\psi_{\rm st}(k,q)|k,q\rangle, \tag{22}$$

where $\psi_{\rm st}$ is a function of the independent variables k and q, called the eigenvalue function of $\Psi_{\rm st}(u_1^A,u_2^A)$. From (22), we see that the function $\psi_{\rm st}$ is invariant when $q\to q+l/A$,

$$\psi_{\rm st}\left(k,q+\frac{ln}{A}\right)=\psi_{\rm st}(k,q). \tag{23}$$

As long as the eigenvalue function is obtained, the operator on the noncommutative torus can be completely determined. Introducing the new basis $|k,q_0;n\rangle\equiv|k,q_0+ln/A\rangle, k\in[0,2\pi/l), q_0\in[0,l/A)$, we have from (20)

$$\sum_{n=0}^{A-1}\int_0^{2\pi/l}dk\int_0^{l/A}dq_0\left|k,q_0+\frac{ln}{A}\right\rangle\left\langle k,q_0+\frac{ln}{A}\right|=id, \tag{24}$$

$$u_1|k,q\rangle=\left|k,q+\frac{l}{A}\right\rangle, \tag{25}$$

$$u_2|k,q\rangle=e^{-2\pi i\,(q/l)}|k,q\rangle. \tag{26}$$

From the above equation and (21), we see that when any power of the operators u_1 and u_2 act on the $|k,q_0+ln/A\rangle$, the result can be expanded in the basis $|k,q_0+ln'/A\rangle$ with the same k,q_0. So the operators on the noncommutative torus have the same property, namely do not change k and q_0. Thus, for every k and q_0 we get an $A\times A$ matrix, called reduced matrix for the operator, as well as the projector,

$$P_{T^2}\left|k,q_0+\frac{ln}{A}\right\rangle=\sum_{n'}M(k,q_0)_{n'n}\left|k,q_0+\frac{ln'}{A}\right\rangle. \tag{27}$$

It is easy to find that the sufficient and necessary condition for $P^2=P$ is[30]

$$M(k,q_0)^2=M(k,q_0). \tag{28}$$

When T^2 satisfies Z_N symmetry, since after R_N rotation U_i' can be expressed by the monomial of $\{U_i\}$ and their inverses, the state vector $R_N|k,q_0+ln/A\rangle$ is still the common eigenstate of the operators U_1 and U_2. With the completeness of $\{|k,q+ls/A\rangle\}$ and the A-fold degeneracy eigenvalues of U_i in the kq representation, the state can be expanded in the basis $\{|k',q'+ls'/A\rangle\}$

$$R_N\left|k,q_0+\frac{ln}{A}\right\rangle=\sum_{n'}A(k,q_0)_{n'n}\left|k,q_0+\frac{ln'}{A}\right\rangle \tag{29}$$

(it is necessary to point out that the matrix A defined here is the transposed matrix of A defined in formula (93) in Ref. 30) where $k'\in[0,2\pi/l),q'\in[0,l/A)$ are definite and

$$R_N^{-1}\left|k',q_0'+\frac{ln'}{A}\right\rangle=\sum_{n''}A^{-1}(k,q_0)_{n''n'}\left|k',q_0'+\frac{ln''}{A}\right\rangle. \tag{30}$$

We can get the expression for the relation between k', q_0' and k, q_0, The mapping $W:(k,q_0)\rightarrow(k',q_0'),W^N=id$, is essentially a linear relation, and area-preserving. By this fact and since R_N is unitary, we conclude that the matrix A is a unitary matrix, that is to say

$$A^*(k,q_0)_{nn'}=A^{-1}(k,q_0)_{n'n}. \tag{31}$$

The projector on the noncommutative orbifold T^2/Z_N satisfies $R_N^{-1}PR_N=P$, then from (27), (29), (30) one obtains

$$R_N^{-1}PR_N\left|k,q_0+\frac{ln}{A}\right\rangle=\sum_{n}{}'\,[A^{-1}(k,q_0)M(k',q_0')A(k,q_0)]_{n'n}\left|k,q_0+\frac{ln'}{A}\right\rangle, \tag{32}$$

which should be equal to

$$P\left|k,q_0+\frac{ln}{A}\right\rangle=\sum_{n''}M(k,q_0)_{n''n}\left|k,q_0+\frac{ln''}{A}\right\rangle. \tag{33}$$

So, we have

$$M(k',q_0')=A(k,q_0)M(k,q_0)A^{-1}(k,q_0) \tag{34}$$

and the sufficient and necessary condition for the projector on noncommutative orbifold T^2/Z_N to satisfy is

$$M(k,q_0)^2=M(k,q_0), \tag{35}$$

$$M(k',q_0')=A(k,q_0)M(k,q_0)A^{-1}(k,q_0). \tag{36}$$

Next we will study the relation between coefficient function $\psi_{\mathrm{st}}(k,q)$ and the reduced matrix $M(k,q_0)$. From (23), (25), (26), and (27) we have

$$\begin{aligned} P\left|k,q_0+\frac{ln}{A}\right\rangle &= \sum_{s,t} u_1^s u_2^t \Psi_{\mathrm{st}}(u_1^A,u_2^A)\left|k,q_0+\frac{ln}{A}\right\rangle \\ &= \sum_{s,t} e^{-2\pi i(q_0/l+n/A)t}\psi_{\mathrm{st}}(k,q_0)\left|k,q_0+\frac{l(n+s)}{A}\right\rangle \\ &= \sum_{n'} M(k,q_0)_{n'n}\left|k,q_0+\frac{ln'}{A}\right\rangle. \end{aligned} \tag{37}$$

So for $n+s<A$ case, we have

$$M(k,q_0)_{n+s,n}=\sum_{t=0}^{A-1} e^{-2\pi i(q_0/l+n/A)t}\psi_{\mathrm{st}}(k,q_0) \tag{38}$$

and for $n+s\geqslant A$ case, we have

$$M(k,q_0)_{n+s-A,n}=\sum_{t=0}^{A-1} e^{-2\pi i(q_0/l+n/A)t}\psi_{\mathrm{st}}(k,q_0)e^{-ilk}. \tag{39}$$

Setting

$$M(k,q_0)_{n+s,n}=M(k,q_0)_{n+s-A,n}e^{ilk}, \tag{40}$$

we can uniformly write as

$$M(k,q_0)_{n+s,n}=\sum_{t=0}^{A-1} e^{-2\pi i(q_0/l+n/A)t}\psi_{\mathrm{st}}(k,q_0) \tag{41}$$

and have

$$\psi_{\mathrm{st}}(k,q_0)=\frac{1}{A}\sum_{n=0}^{A-1} M(k,q_0)_{n+s,n}e^{2\pi i(q_0/l+n/A)t}. \tag{42}$$

Equations (41) and (42) are the relation between ψ_{st} and the elements of the reduced matrix M.

IV. CONTINUOUS SOLUTION FOR THE PROJECTOR WITH MINIMAL TRACE

Now one may ask what property the reduced matrix M possesses when the coefficient function ψ_{st} is a continuous function. In this section, we mainly answer this question. First we prove the $A\times A$ matrix satisfying the condition $M^2=M$ is always diagonalizable. For any vector ψ, $M\psi$ is invariant under M, namely,

$$M(M\psi)=M\psi. \tag{43}$$

Assume there are totally B linear independent invariant vectors under transformation M, then

(1) For $A=B$ case, the matrix M is identity of the space expanded by the vectors, namely $A\times A$ unit matrix. Of course it is diagonal.

(2) For $B<A$ case, considering any vector a and setting $b=Ma-a$, we find $Mb=0$. Namely any vector a can be expressed as linear combination of invariant vector $c=Ma$ and null vector b under action of M. So the whole linear space is composed of certain invariant vectors and null vectors under action of M. M can be diagonalized in the representation with these vectors as basis. So we have

$$M(k,q_0)=S^{-1}(k,q_0)\overline{M}(k,q_0)S(k,q_0), \tag{44}$$

where

$$\overline{M}(k,q_0)=\mathrm{diag}(1,1,\ldots,1,0,0,\ldots,0). \tag{45}$$

Due to (41), when $\psi_{\mathrm{st}}(k,q_0)$ is continuous, $M(k,q_0)$ is also continuous. However $\mathrm{tr}\,M(k,q_0)=\mathrm{tr}\,\overline{M}(k,q_0)=0,1,2,\ldots,A$, which is discrete, so when ψ_{st} is continuous, the value of $\mathrm{tr}\,M(k,q_0)=A\psi_{00}(k,q_0)$ is invariant for all k and q_0. The trace of the projector is the zero order term of $\psi_{00}(k,q_0)$ in the Laurant expression of e^{-ilk} and $e^{-2\pi iqA/l}$, so we have

$$\mathrm{tr}\,P=\int_0^{2\pi/l}dk\int_0^{l/A}dq\,\frac{A}{2\pi}\psi_{00}(k,q_0)=\int_0^{2\pi/l}dk\int_0^{l/A}dq\,\frac{1}{2\pi}\mathrm{tr}\,M(k,q_0)=\frac{1}{A}\mathrm{tr}\,M(k,q_0). \tag{46}$$

The projector is trivial for $\mathrm{tr}\,M(k,q_0)=0,A$, indicating $P=0$ and $identity$. The nontrivial $\mathrm{tr}\,P=1/A, 2/A,\ldots,(A-1)/A$. In this paper, we only study the nontrivial projector with minimal trace $(\mathrm{tr}\,M(k,q_0)=1)$. Thus

$$M(k,q_0)=s^{-1}(k,q_0)\begin{pmatrix}1&&&\\&0&&\\&&0&\\&&&\ddots\end{pmatrix}s(k,q_0), \tag{47}$$

$$M(k,q_0)_{nn'}=s^{-1}(k,q_0)_{n0}s(k,q_0)_{0n'}\equiv a(k,q_0)_n b(k,q_0)_{n'}. \tag{48}$$

Explicit calculation about R_N acting on $|k,q;n\rangle$ shows that we can divide the complete area $\Sigma:\{k\in[0,2\pi/l),q_0\in[0,l/A)\}$ into N subarea $\sigma_0,\ldots,\sigma_{N-1}$, making $W:\sigma_i\to\sigma_{i+1},(i=0,1,\ldots,N-2),\sigma_{N-1}\to\sigma_0$. If we construct a reduced matrix $M(k,q_0)$ to satisfy (48) in the area σ_0, then the projector corresponding to continuous ψ_{st} with minimal trace is completely determined. In area σ_0, set

$$a_n=\left\langle k,q_0+\frac{ln}{A}\middle|\,\phi_1\right\rangle,\qquad b_n=\left\langle\phi_2\middle|\,k,q_0+\frac{ln}{A}\right\rangle, \tag{49}$$

where

$$\sum_n a_n b_n=\mathrm{tr}\,M(k,q_0)=1. \tag{50}$$

In the other areas σ_j with $(k,q_0)\to(k_j,q_{0j})$ by mapping W^j, we demand

$$a_n(k_j,q_{0j})=\left\langle k_j,q_{0j}+\frac{ln}{A}\middle|\,\phi_1\right\rangle=A^j(k,q_0)_{nn'}a_{n'}(k,q_0), \tag{51}$$

$$b_n(k_j,q_{0j})=\left\langle\phi_2\middle|\,k_j,q_{0j}+\frac{ln}{A}\right\rangle=b_{n'}(k,q_0)A^{-j}(k,q_0)_{n'n}. \tag{52}$$

We thus have all coefficients of $|\phi_1\rangle,\langle\phi_2|$ in $\sigma_0,\ldots,\sigma_{N-1}$. Owing to the completeness of $|k,q_0+ln/A\rangle$ in the area Σ, $|\phi_1\rangle$ and $\langle\phi_2|$ can be determined by the coefficient (49) of $|\phi_1\rangle$ and $\langle\phi_2|$. Meanwhile, in the area σ_j, we have

$$M(k_j,q_{0j})_{nn'}=a_n(k_j,q_{0j})b_{n'}(k_j,q_{0j})=[A^j(k,q_0)M(k,q_0)A^{-j}(k,q_0)]_{nn'}. \tag{53}$$

The matrix $M(k,q_0)$ really satisfies Eq. (34). Consider the state vector

$$\begin{aligned}|\phi_1\rangle&=\int dkdq_0\sum_n\left|k,q_0+\frac{ln}{A}\right\rangle\left\langle k,q_0+\frac{ln}{A}\right|\phi_1\right\rangle\\&=\sum_{j=0}^{N-1}\int_{\sigma_j}dk_jdq_{0j}\sum_n\left|k_j,q_{0j}+\frac{ln}{A}\right\rangle a_n(k_j,q_{0j})\\&=\sum_{j=0}^{N-1}\int_{\sigma_j}dkdq_0\sum_{nn_1}\left|k,q_0+\frac{ln}{A}\right\rangle A^j_{nn_1(k,q_0)}a_{n_1}(k,q_0)\\&=\sum_{j=0}^{N-1}R_N^j\int_{\sigma_0}dkdq_0\sum_n\left|k,q_0+\frac{ln}{A}\right\rangle a_n(k,q_0).\end{aligned} \tag{54}$$

Thus we have

$$R_N|\phi_1\rangle=|\phi_{1\rangle}. \tag{55}$$

In the same way, we get

$$\langle\phi_2|R_N=\langle\phi_2|. \tag{56}$$

That is to say that the state vectors $|\phi_1\rangle$ and $\langle\phi_2|$ are invariant under the rotation R_N.

More generally, we can take any state vectors $|\phi_1\rangle$ and $\langle\phi_2|$ satisfying

$$R_N|\phi_1\rangle=e^{i\alpha_1}|\phi_1\rangle,\qquad\qquad\langle\phi_2|R_N^{-1}=e^{-i\alpha_2}\langle\phi_2| \tag{57}$$

to construct a projection operator on noncommutative orbifold T^2/Z_N. Let $M(k,q_0)$ be given by (48) with

$$a_n(k,q_0)=\frac{\left\langle k,q_0+\frac{ln}{A}\middle|\phi_1\right\rangle}{\sqrt{\Sigma_{n'}\left\langle k,q_0+\frac{ln'}{A}\middle|\phi_1\right\rangle\left\langle\phi_2\middle|k,q_0+\frac{ln'}{A}\right\rangle}}, \tag{58}$$

$$b_n(k,q_0)=\frac{\left\langle\phi_2\middle|k,q_0+\frac{ln}{A}\right\rangle}{\sqrt{\Sigma_{n'}\left\langle k,q_0+\frac{ln'}{A}\middle|\phi_1\right\rangle\left\langle\phi_2\middle|k,q_0+\frac{ln'}{A}\right\rangle}}. \tag{59}$$

The projector of minimal trace and with continuous coefficient functions is surely of this form. It can be verified that $M^2=M$. And it is also covariant under R_N. From (30) we have

$$\begin{aligned}\left\langle\phi_2\middle|k',q_0'+\frac{n'l}{A}\right\rangle&=\left\langle\phi_2\middle|R_N\sum_{n''}A^{-1}(k,q_0)_{n''n'}\middle|k,q_0+\frac{n''l}{A}\right\rangle\\&=e^{i\alpha_2}\sum_{n''}A^{-1}(k,q_0)_{n''n'}\left\langle\phi_2\middle|k,q_0+\frac{n''l}{A}\right\rangle\end{aligned}$$

and similarly

$$\left\langle k',q_0'+\frac{n'l}{A}\middle|\phi_1\right\rangle = e^{-i\alpha_1}\sum_{n''}\left\langle k,q_0+\frac{n''l}{A}\middle|\phi_1\right\rangle A(k,q_0)_{n'n''},$$

giving

$$\sum_n \left\langle k',q_0'+\frac{ln}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k',q_0'+\frac{ln}{A}\right\rangle = \sum_n \left\langle k,q_0+\frac{ln}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln}{A}\right\rangle e^{-i(\alpha_1-\alpha_2)}. \tag{60}$$

Thus,

$$M(k',q_0')_{nn'} = a_n(k',q_0')b_{n'}(k',q_0') = [AMA^{-1}](k,q_0)_{nn'}, \tag{61}$$

P is invariant under rotation R_N due to (36) and really gives the projection operator on the noncommutative orbifold T^2/Z_N. The form of (58) is a generalization of GHS construction. (The condition $P^\dagger = P$ is not satisfied by P like this, which might represent the solitons in a "complex" field.) From the above result, we have

$$M(k,q_0)_{nn'} = \frac{\left\langle k,q_0+\frac{ln}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln'}{A}\right\rangle}{\sum_{n''}\left\langle k,q_0+\frac{ln''}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln''}{A}\right\rangle}. \tag{62}$$

Noticing that this equation satisfies (40), we have

$$\begin{aligned}\psi_{\mathrm{st}}(k,q_0) &= \frac{1}{A}\sum_{n=0}^{A-1} M(k,q_0)_{n+s,n}e^{2\pi i(q_0/l+n/A)t} \\ &= \frac{\frac{1}{A}\sum_{n=0}^{A-1}\left\langle k,q_0+\frac{l(n+s)}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln}{A}\right\rangle e^{2\pi i(q_0/l+n/A)t}}{\sum_n \left\langle k,q_0+\frac{ln}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln}{A}\right\rangle} = \frac{F_{\mathrm{st}}(k,q_0)}{AF_{00}(k,q_0)},\end{aligned} \tag{63}$$

where

$$F_{\mathrm{st}}(k,q_0) \equiv \sum_{n=0}^{A-1}\left\langle k,q_0+\frac{l(n+s)}{A}\middle|\phi_1\right\rangle\left\langle \phi_2\middle|k,q_0+\frac{ln}{A}\right\rangle e^{2\pi i(q_0/l+n/A)t}, \tag{64}$$

with

$$F_{\mathrm{st}}(k,q_0) = F_{\mathrm{st}}(k,q_0+l/A) = F_{\mathrm{st}}(k+2\pi/l,q_0), \tag{65}$$

$$F_{\mathrm{st}}(k,q_0) = F_{s+A,t}(k,q_0)e^{-ilk} \tag{66}$$

$$= F_{s,t+A}(k,q_0)e^{-2\pi i q_0 A/l}. \tag{67}$$

So the function F_{st} is the function of independent variables $X = e^{-ilk}$ and $Y = e^{-2\pi i q_0 A/l}$, namely $F_{\mathrm{st}}(k,q_0) = \Phi_{\mathrm{st}}(X,Y)$. Similarly,

$$\psi_{\mathrm{st}}(k,q_0) = \Psi_{\mathrm{st}}(X,Y) = \frac{\Phi_{\mathrm{st}}(X,Y)}{A\Phi_{00}(X,Y)}. \tag{68}$$

If we change the variable X and Y into u_1^A and u_2^A, respectively, the standard form (9) of the projection operator can be easily obtained. So the key question is to find out $F_{\rm st}(k,q_0)$.

V. COHERENT STATE REPRESENTATION

Introduce coherent states

$$|z\rangle = e^{-(1/2)z\bar{z}} e^{a^+ z}|0\rangle,$$

where $z=x+iy, \bar{z}=x-iy$, satisfies

$$\frac{1}{\pi}\int_{-\infty}^{\infty} d^2z|z\rangle\langle z| \equiv \frac{1}{\pi}\int_{-\infty}^{\infty} dxdy|z\rangle\langle z| = \text{identity}, \tag{69}$$

$$R_N|z\rangle = |\omega_N z\rangle. \tag{70}$$

We can show[30]

$$\langle k,q|z\rangle = \frac{1}{\sqrt{l}\,\pi^{1/4}}\theta\left(\frac{q+\frac{\tau}{\tau_2}k - i\sqrt{2}z}{l}, \frac{\tau}{A}\right) e^{-(\tau/2i\tau_2)k^2 + ikq + \sqrt{2}kz - (z^2 + z\bar{z})/2}, \tag{71}$$

where

$$\theta(z,\tau) \equiv \theta\begin{bmatrix}0\\0\end{bmatrix}(z,\tau)$$

and

$$\theta\begin{bmatrix}a\\b\end{bmatrix}(z,\tau) = \sum_m e^{\pi i\tau(m+a)^2} e^{2\pi i(m+a)(z+b)}. \tag{72}$$

Thus we can expand the state vectors $|\phi_1\rangle$ and $\langle\phi_2|$ in terms of the coherent state,

$$|\phi_1\rangle = \frac{1}{\pi}\int_{-\infty}^{\infty} dxdy|z\rangle\langle z|\phi_1\rangle \equiv \frac{1}{\pi}\int_{-\infty}^{\infty} dxdy f_1(z)|z\rangle, \tag{73}$$

$$\langle\phi_2| = \frac{1}{\pi}\int_{-\infty}^{\infty} dxdy\langle\phi_2|z\rangle\langle z| = \frac{1}{\pi}\int_{-\infty}^{\infty} dxdy f_2(z)\langle z|. \tag{74}$$

The condition (57) is satisfied if and only if

$$f_1(\omega_N^{-1}z) = f_1(z)e^{i\alpha_1}, \tag{75}$$

$$f_2(\omega_N^{-1}z) = f_2(z)e^{-i\alpha_2}. \tag{76}$$

Here $\omega_N = e^{-i(2\pi/N)}$. We have

$$F_{\rm st}(k,q_0) = \frac{1}{\pi^2}\sum_{n=0}^{A-1}\int\left\langle k, q_0 + \frac{l(n+s)}{A}\middle| z_1\right\rangle f_1(z_1)dx_1dy_1\int\left\langle z_2\middle| k, q_0 + \frac{ln}{A}\right\rangle f_2(z_2)dx_2dy_2$$

$$\times e^{2\pi i(q_0/l + n/A)t} = \frac{1}{\pi^2}\int dx_1dy_1dx_2dy_2 g_{\rm st}(k,q_0,z_1,z_2)f_1(z_1)f_2(z_2), \tag{77}$$

where

$$g_{\mathrm{st}}(k,q_0,z_1,z_2)=\sum_{n=0}^{A-1}\left\langle k,q_0+\frac{l(n+s)}{A}\middle|z_1\right\rangle\left\langle z_2\middle|k,q_0+\frac{ln}{A}\right\rangle e^{2\pi i(q_0/l+n/A)t}. \tag{78}$$

We call the kernel g as generating function in coherent state representation. Next, we study the expression of g for Z_4 case. Through g we can give the integration expression for all the projection operators on the T^2/Z_4 with minimal trace and continuous eigenvalue function. Consider the equation

$$\theta(z,\tau)^*=\theta(z^*,-\tau^*). \tag{79}$$

For the z_4 case, $\tau=i, A=l^2/2\pi$. From (71), (73), and (74) we get

$$\begin{aligned}\left\langle k,q+\frac{ls}{A}\middle|z_1\right\rangle\left\langle z_2\middle|k,q+\frac{ls'}{A}\right\rangle &= \frac{1}{l\sqrt{\pi}}\theta\left(\frac{q}{l}+\frac{i}{l}k+\frac{s}{A}-\frac{i\sqrt{2}z_1}{l},\frac{i}{A}\right)\theta\left(\frac{q}{l}-\frac{i}{l}k+\frac{s'}{A}+\frac{i\sqrt{2}z_2^*}{l},\frac{i}{A}\right)\\ &\quad\times e^{-k^2+(k/2)(z_1+z_2^*)+ik[l(s-s')/A]}e^{-(1/2)(z_1^2+(z_2^*)^2+z_1z_1^*+z_2z_2^*)}\\ &\equiv K_{ss'}.\end{aligned} \tag{80}$$

Let $u=lk/2\pi, v=q/l, \mu=-i(\sqrt{2}A/l)z_1, \nu=i(\sqrt{2}A/l)z_2^*$, then

$$K_{ss'}=\frac{C_1}{l\sqrt{\pi}}\theta\left(v+\frac{iu}{A}+\frac{s+\mu}{A},\frac{i}{A}\right)\theta\left(v-\frac{iu}{A}+\frac{s'+\nu}{A},\frac{i}{A}\right)e^{\pi i\,2i/A\,u^2+2\pi i((s+\mu-s'-\nu)/A))u}, \tag{81}$$

where

$$C_1=e^{2\pi i[(-i/4A)(\mu^2+\nu^2)+(i/4A)(|\mu|^2+|\nu|^2)]}. \tag{82}$$

It can be proven that for integer A,

$$\begin{aligned}&\sum_{r=0}^{A-1}e^{2\pi irt/A}\theta(x+r/A,\tau/A)\,\theta(y+r/A,\tau/A)\\ &\quad=A\sum_{d=0,1}\theta\left(-\frac{\tau}{A}(Ad-t)+x-y,\frac{2\tau}{A}\right)\theta\left(\frac{\tau}{A}(-At+A^2d)+A(x+y),2\tau A\right)e^{\pi i(\tau/A)(Ad-t)^2}\\ &\quad\times e^{2\pi i(Ad-t)y}\end{aligned} \tag{83}$$

and

$$\theta(z,\tau)=\sqrt{\frac{i}{\tau}}e^{-\pi iz^2/\tau}\theta\left(\pm\frac{z}{\tau},-\frac{1}{\tau}\right). \tag{84}$$

Thus we have

$$
\begin{aligned}
G_{\mathrm{st}}(u,v) &\equiv g_{\mathrm{st}}(k,q,z_1,z_2) \\
&= e^{2\pi i v t}\sum_r e^{2\pi i r t/A} K_{s+r,r}(u,v) \\
&= \frac{AC_1}{l\sqrt{\pi}}\sqrt{\frac{A}{2}}\sum_{d=0,1} e^{-(\pi/2A)(Ad-t)^2+2\pi i(Ad-t)(\nu/A)-(\pi/2A)(s+\mu-\nu)^2} \\
&\quad \times e^{(\pi i/A)(s+\mu-\nu)(Ad-t)+2\pi i v Ad}\theta\left(u-\frac{1}{2}(Ad-t)+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right) \\
&\quad \times \theta(2Av+s+\mu+\nu-t\tau+iAd,2Ai). \qquad (85)
\end{aligned}
$$

Due to

$$
\sum_{a=0,1}\theta\left(x+\frac{a}{2},\tau\right)=2\theta(2x,4\tau), \qquad (86)
$$

$$
\sum_{a=0,1}(-1)^a\theta\left(x+\frac{a}{2},\tau\right)=2e^{2\pi i(x+\tau/2)}\theta(2x+2\tau,4\tau), \qquad (87)
$$

when d is equal to 0,1,

$$
\theta(2x+2\tau d,4\tau)=\frac{1}{2}\sum_{a=0,1}(-1)^{ad}e^{2\pi i(x+(\tau/2))d}\theta\left(x+\frac{a}{2},\tau\right), \qquad (88)
$$

the function $G_{\mathrm{st}}(u,v)$ can be rewritten as

$$
\begin{aligned}
G_{\mathrm{st}}(u,v) &= \frac{A}{4\pi}e^{2\pi i\phi}\sum_{a,d=0,1}(-1)^{ad}\theta\left(-u+\frac{1}{2}(Ad+t)+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right) \\
&\quad \times\theta\left(-Av+\frac{1}{2}(s+a-\mu-\nu)+\frac{i}{2}t,\frac{Ai}{2}\right), \qquad (89)
\end{aligned}
$$

where

$$
\phi=\frac{i}{4A}(s^2+t^2)-\frac{\mathrm{st}}{2A}+\frac{i}{2A}s(\mu-\nu)-\frac{t}{2A}(\mu+\nu)+\frac{i}{4A}(|\mu|^2+|\nu|^2-2\mu\nu). \qquad (90)
$$

From the above discussion, we know that when A is an even number, only $a=0$ contributes, so we have

$$
G_{\mathrm{st}}(u,v)=\frac{A}{2\pi}e^{2\pi i\phi}\theta\left(-u+\frac{1}{2}t+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right)\theta\left(-Av+\frac{1}{2}(s-\mu-\nu)+\frac{i}{2}t,\frac{Ai}{2}\right)
$$

and when A is an odd number,

$$
\begin{aligned}
G_{\mathrm{st}}(u,v) &= \frac{A}{4\pi}e^{2\pi i\phi}\sum_{a,d=0,1}(-1)^{ad}\theta\left(-u+\frac{1}{2}(Ad+t)+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right) \\
&\quad \times\theta\left(-Av+\frac{1}{2}(Aa+s-\mu-\nu)+\frac{i}{2}t,\frac{Ai}{2}\right). \qquad (91)
\end{aligned}
$$

They can be uniformly written as

$$G_{\mathrm{st}}(u,v)=\frac{A}{4\pi}e^{2\pi i\phi}\sum_{a,d=0,1}(-1)^{ad}\theta\left(-u+\frac{1}{2}(Ad+t)+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right)$$
$$\times\theta\left(-Av+\frac{1}{2}(Aa+s-\mu-\nu)+\frac{i}{2}t,\frac{Ai}{2}\right),\tag{92}$$

which is Z_4 covariant. So we have from (63), (77), and (85),

$$\psi_{\mathrm{st}}(k,q)=\frac{1}{A}\left\{\frac{\int d^2\mu d^2\nu G_{\mathrm{st}}(u,v)f_1(\mu)f_2(\nu)}{\int d^2\mu d^2\nu G_{00}(u,v)f_1(\mu)f_2(\nu)}\right\},\tag{93}$$

where functions f_i should satisfy

$$f_i(\omega_N\xi)=e^{i\alpha_i}f_i(\xi).\tag{94}$$

Let $\hat{u}=(l/2\pi)\hat{y}_2$ and $A\hat{v}=(l/2\pi)\hat{y}_1$, we may replace u,v by $\hat{u}$ and $\hat{v}$ in (93) and get

$$\Psi_{\mathrm{st}}(u_1^A,u_2^A)=\frac{1}{A}\frac{\int d^2\mu d^2\nu G_{\mathrm{st}}\left(\frac{l}{2\pi}\hat{y}_2,\frac{l}{2A\pi}\hat{y}_1\right)f_1(\mu)f_2(\nu)}{\int d^2\mu d^2\nu G_{00}\left(\frac{l}{2\pi}\hat{y}_2,\frac{l}{2A\pi}\hat{y}_1\right)f_1(\mu)f_2(\nu)}.\tag{95}$$

The operators u_1 and u_2 commute with the operators u_1^A and u_2^A, and from (7)

$$u_1^s=e^{-2\pi i\,s/A\hat{u}},\tag{96}$$

$$u_2^t=e^{-2\pi it\hat{v}}.\tag{97}$$

Further taking u_1^s and u_2^t into account, we can insert them to the corresponding operator form of Eq. (89). This leads to the function of $\hat{u}$ and $\hat{v}$

$$\begin{aligned}h_{ad}&\equiv u_1^s u_2^t G_{\mathrm{st}}(\hat{u},\hat{v})\\&=\frac{A}{4\pi}\sum_{a,d=0}^{1}(-1)^{ad}e^{2\pi i\phi}e^{-2\pi i\,s/A\hat{u}}\theta\left(-\hat{u}+\frac{1}{2}(Ad+t)+\frac{i}{2}(s+\mu-\nu),\frac{Ai}{2}\right)\\&\quad\times e^{-2\pi i\hat{v}t}\theta\left(-A\hat{v}+\frac{1}{2}(Aa+s-\mu-\nu)+\frac{i}{2}t,\frac{Ai}{2}\right)\\&=\frac{A}{4\pi}\sum_{a,d=0}^{1}(-1)^{ad}e^{2\pi i(-(3\mathrm{st}/2A)+(i/4A)(|\mu|^2+|\nu|^2-2\mu\nu))}e^{-2\pi i((sd/2)+(ta/2))}\\&\quad\times\theta\begin{bmatrix}\frac{s}{A}\\ \frac{t}{2}\end{bmatrix}\left(-\hat{u}+\frac{1}{2}Ad+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\theta\begin{bmatrix}\frac{t}{A}\\ \frac{s}{2}\end{bmatrix}\left(-A\hat{v}+\frac{1}{2}Aa-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right).\end{aligned}\tag{98}$$

Due to $|\omega_N\mu|=|\mu|,|\omega_N\nu|=|\nu|$, $e^{2\pi i\,(i/4A)(|\mu|^2+|\nu|^2)}$ in the above formula can be attributed to $f_1(\mu)$ and $f_2(\nu)$. Finally, we have

$$
\begin{aligned}
P=&\sum_{s,t} u_1^s u_2^t \Psi_{\mathrm{st}}(u_1^A,u_2^A)\\
=&\sum_{s,t} e^{2\pi i(-(3\mathrm{st}/2A))}\sum_{a,d=0}^{1}(-1)^{ad}\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}e^{-2\pi i((sd/2)+(ta/2))}\\
&\times\theta\begin{bmatrix}\frac{s}{A}\\ \frac{t}{2}\end{bmatrix}\left(-\frac{l\hat{y}_2}{2\pi}+\frac{1}{2}Ad+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\theta\begin{bmatrix}\frac{t}{A}\\ \frac{s}{2}\end{bmatrix}\left(-\frac{l\hat{y}_1}{2\pi}+\frac{1}{2}Aa-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\\
&\times\left\{A\sum_{a,d=0}^{1}(-1)^{ad}\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}\theta\left(-\frac{l\hat{y}_2}{2\pi}+\frac{1}{2}Ad+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\right.\\
&\left.\times\theta\left(-\frac{l\hat{y}_1}{2\pi}+\frac{1}{2}Aa-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\right\}^{-1}. \qquad (99)
\end{aligned}
$$

In the above equation, the two θ functions can not exchange orders with each other. It holds for any integer number A. In the following, we present some discussion.

(1) A is an even number, so $Ad/2$ and $Aa/2$ are integers, too. Due to (72) we have

$$
\begin{aligned}
P=&\sum_{s,t} e^{-3\pi i(\mathrm{st}/A)}\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}\\
&\times\theta\begin{bmatrix}\frac{s}{A}\\ \frac{t}{2}\end{bmatrix}\left(-\frac{l\hat{y}_2}{2\pi}+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\theta\begin{bmatrix}\frac{t}{A}\\ \frac{s}{2}\end{bmatrix}\left(-\frac{l\hat{y}_1}{2\pi}-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\\
&\times\left\{A\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}\theta\left(-\frac{l\hat{y}_2}{2\pi}+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\right.\\
&\left.\times\theta\left(-\frac{l\hat{y}_1}{2\pi}-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\right\}^{-1}. \qquad (100)
\end{aligned}
$$

The above equation is the generalization of the Boca's formula Proposition 3.1(i).[35]

(2) A is an odd number

$$
\begin{aligned}
P=&\sum_{s,t=0}^{A-1} e^{-3\pi i(\mathrm{st}/A)}\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}\sum_{a,d=0}^{1}(-1)^{ad}e^{-2\pi i((sd/2)+(ta/2))}\\
&\times\theta\begin{bmatrix}\frac{s}{A}\\ \frac{t}{2}\end{bmatrix}\left(-\frac{l\hat{y}_2}{2\pi}+\frac{Ad}{2}+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\theta\begin{bmatrix}\frac{t}{A}\\ \frac{s}{2}\end{bmatrix}\left(-\frac{l\hat{y}_1}{2\pi}+\frac{Aa}{2}-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\\
&\times\left\{A\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i(\mu\nu/A)}\sum_{a,d=0}^{1}(-1)^{ad}\theta\left(-\frac{l\hat{y}_2}{2\pi}+\frac{Ad}{2}+\frac{i}{2}(\mu-\nu),\frac{Ai}{2}\right)\right.\\
&\left.\times\theta\left(-\frac{l\hat{y}_1}{2\pi}+\frac{Aa}{2}-\frac{1}{2}(\mu+\nu),\frac{Ai}{2}\right)\right\}^{-1}. \qquad (101)
\end{aligned}
$$

Due to

$$\theta\begin{bmatrix} \frac{s}{A} \\ \frac{t}{2} \end{bmatrix}\left(x+\frac{Ad}{2},\tau\right)=\theta\begin{bmatrix} \frac{s}{2A} \\ 0 \end{bmatrix}(2x,4\tau)(-1)^{sd}e^{2\pi i\,(\mathrm{st}/2A)}$$

$$+\theta\begin{bmatrix} \frac{s+A}{2A} \\ 0 \end{bmatrix}(2x,4\tau)(-1)^{(s+A)d}e^{2\pi i\,[(s+A)t/2A]}, \tag{102}$$

the numerator of P can be written as

$$2\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i\,(\mu\nu/A)}\sum_{s,t=0}^{A-1}\{\overline{\theta}_0\theta_0++\overline{\theta}_1\theta_0(-1)^s+\overline{\theta}_0\theta_1(-1)^t+\overline{\theta}_1\theta_1(-1)^{s+t-1}\}$$

$$=2\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i\,(\mu\nu/A)}\sum_{s,t=0}^{2A-1}e^{(\pi i/A)\,\mathrm{st}}\overline{\theta}_0\theta_0, \tag{103}$$

where

$$\overline{\theta}_\delta=\theta\begin{bmatrix} \frac{t+A\delta}{2A} \\ 0 \end{bmatrix}(2y,4\tau),$$

$$\theta_\delta=\theta\begin{bmatrix} \frac{t+A\delta}{2A} \\ 0 \end{bmatrix}(2x,4\tau),\delta=0,1$$

with

$$x=-\frac{l\hat{y}_2}{2\pi}+\frac{i}{2}(\mu-\nu)$$

and

$$y=-\frac{l\hat{y}_1}{2\pi}-\frac{1}{2}(\mu+\nu).$$

The denominator of P is $2A\int d^2\mu d^2\nu f_1(\mu)f_2(\nu)e^{\pi i\,(\mu\nu/A)}\Sigma_{\delta_1,\delta_2=0}^{1}e^{\pi i\delta_1\delta_2}\overline{\theta}'_{\delta_1}\theta'_{\delta_2}$, where

$$\theta'_\delta=\theta\begin{bmatrix} \frac{\delta}{2} \\ 0 \end{bmatrix}(2x,4\tau),$$

$$\overline{\theta}'_\delta=\theta\begin{bmatrix} \frac{\delta}{2} \\ 0 \end{bmatrix}(2y,4\tau).$$

This formula gives another result compared with Boca's when $f_1(z)=f_2(z)=\delta^2(z-0)$.

Finally, we will give another explicit form of P in terms of the derivative of elliptic functions. Note that the basis $\{|n\rangle\}$ of Fock space produces a phase ω^n under action of R_N. It is not difficult

to find that $e^{i\alpha_1}$ and $e^{i\alpha_2}$ in (57) are both integral powers of ω_N because of $(R_N)^N=$identity. Therefore $|\phi_1\rangle$ and $\langle\phi_2|$ can, respectively, be expanded in the basis $\{|n\rangle\}$ and $\{\langle n|\}$, where

$$|n\rangle=\frac{(a^+)^n}{\sqrt{n!}}|0\rangle. \tag{104}$$

We have the relation between coherent state and particle number eigenstate as the following:

$$\langle z|n\rangle=e^{-(1/2)z\bar{z}}\frac{z^n}{\sqrt{n!}}. \tag{105}$$

Obviously, the general forms of $|\phi_1\rangle$ and $\langle\phi_2|$ in the expansion in terms of particle number eigenstates are $\Sigma_{m=0}^{\infty}c_m\,|i+4m\rangle$ and $\Sigma_{n=0}^{\infty}d_n\,\langle j+4n|$, where i and j are non-negative integers and c_m and d_n are arbitrary constant coefficients. So

$$|\phi_1\rangle=\sum_m\ c_m|i+4n\rangle=\frac{1}{\pi}\sum_m\ \int_{-\infty}^{\infty}dxdyc_m|z\rangle\langle z|i+4m\rangle, \tag{106}$$

$$\langle\phi_2|=\sum_{m=0}^{\infty}\ d_m\langle j+4m|=\frac{1}{\pi}\sum_{n=0}^{\infty}\ \int_{-\infty}^{\infty}dxdyd_n\langle j+4n|z\rangle\langle z|. \tag{107}$$

We let R_N act on $|\phi_1\rangle$ and $\langle\phi_2|$ and get

$$R_N|\phi_1\rangle=\omega^i|\phi_1\rangle, \tag{108}$$

$$\langle\phi_2|R_N^{-1}=\langle\phi_2|\omega^{-j}. \tag{109}$$

Subsequently, we substitute (105), (106), (107) into (64) and make use of the formula

$$\langle k,q|n\rangle=\frac{1}{\sqrt{n!}}\frac{d^n}{dz^n}(e^{(1/2)z\bar{z}}\langle k,q|z\rangle)\|_{z=0} \tag{110}$$

to obtain

$$\begin{aligned}F_{\mathrm{st}}(k,q_0)&=\sum_{m,n}\sum_{h=0}^{A-1}c_md_n\left\langle k,q_0+\frac{l(h+s)}{A}\middle|i+4m\right\rangle\times\left\langle j+4n\middle|k,q_0+\frac{lh}{A}\right\rangle\times e^{2\pi i(q_0/l+h/A)t}\\&=\sum_{m,n}\sum_{h=0}^{A-1}c_md_n\frac{1}{\sqrt{(i+4m)!(j+4n)!}}\frac{d^{n+m}}{dz_1^m\bar{z}_2^n}\left(e^{(1/2)(z_1\bar{z}_1+z_2\bar{z}_2)}\sum_{h=0}^{A-1}\left\langle k,q_0+\frac{l(h+s)}{A}\middle|z_1\right\rangle\right.\\&\quad\left.\times\left\langle z_2\middle|k,q_0+\frac{lh}{A}\right\rangle\times e^{2\pi i(q_0/l+h/A)t}\right)\Bigg\|_{z_1=\bar{z}_2=0}\\&=\sum_{m,n}\sum_{h=0}^{A-1}c_md_n\frac{1}{\sqrt{(i+4m)!(j+4n)!}}\frac{d^{n+m}}{dz_1^m\bar{z}_2^n}(e^{1/2(z_1\bar{z}_1+z_2\bar{z}_2)}g_{\mathrm{st}}(k,q_0,z_1,z_2))\|_{z_1=\bar{z}_2=0}.\end{aligned} \tag{111}$$

So, we get the projector in the case of z_4

$$P=\sum_{m,n} c_m d_n \frac{1}{\sqrt{(i+4m)!(j+4n)!}} \frac{d^{n+m}}{dz_1^m \bar{z}_2^n} \Bigg(e^{z_1\bar{z}_1+z_2\bar{z}_2} \times e^{2\pi i(-(3st/2A))} \times e^{4\pi^2 i z_1 \bar{z}_2}$$

$$\times e^{-2\pi i((sd/2)+(ta/2))} \sum_{a,d=0}^{1} (-1)^{ad} \theta \begin{bmatrix} \frac{s}{A} \\ \frac{t}{2} \end{bmatrix} \left(-\frac{l\hat{y}_2}{2\pi} + \frac{1}{2}Ad + \frac{\sqrt{2}A}{2l}(z_1+\bar{z}_2), \frac{Ai}{2} \right)$$

$$\times \theta \begin{bmatrix} \frac{t}{A} \\ \frac{s}{2} \end{bmatrix} \left(-\frac{l\hat{y}_1}{2\pi} + \frac{1}{2}Aa + \frac{i\sqrt{2}A}{2l}(z_1-\bar{z}_2), \frac{Ai}{2} \right) \Bigg) \Bigg\|_{z_1=\bar{z}_2=0}$$

$$\times \Bigg\{ A \sum_{m,n} \sum_{a,d=0}^{1} (-1)^{ad} c_m d_n \frac{d^{n+m}}{dz_1^m \bar{z}_2^n} \Bigg(e^{z_1\bar{z}_1+z_2\bar{z}_2} \times e^{4\pi^2 i z_1 \bar{z}_2}$$

$$\times \theta \left(-\frac{l\hat{y}_2}{2\pi} + \frac{1}{2}Ad + \frac{\sqrt{2}A}{2l}(z_1+\bar{z}_2), \frac{Ai}{2} \right)$$

$$\times \theta \left(-\frac{l\hat{y}_1}{2\pi} + \frac{1}{2}Aa + \frac{i\sqrt{2}A}{2l}(z_1-\bar{z}_2), \frac{Ai}{2} \right) \Bigg) \Bigg\}^{-1} \Bigg\|_{z_1=\bar{z}_2=0}. \tag{112}$$

Thus, we derive two forms of explicit expressions of the projector P in terms of the integration and derivative of the classical theta functions.

VI. DISCUSSION

In this paper, P is represented by a form of a fraction which make sense only when the denominator has an inverse. The formula demands

$$D=A\int d^2\mu d^2\nu f_1(\mu) f_2(\nu) G_{00}(u,v) \tag{113}$$

is unequal to zero for any real variables u and v. It is easy to prove that when f_1 is equal to f_2^*, the related denominator

$$D=A\sum_n \left\langle k,q+\frac{ln}{A}\middle|\phi\right\rangle \left\langle \phi\middle|k,q+\frac{ln}{A}\right\rangle = A\sum_n \left|\left\langle k,q+\frac{ln}{A}\middle|\phi\right\rangle\right|^2. \tag{114}$$

Thus if $D=0$, then

$$\left\langle k,q+\frac{ln}{A}\middle|\phi\right\rangle = 0, \qquad n=0,1,\ldots,A-1. \tag{115}$$

The zero points of the state vector $|\phi\rangle$ in $|k,q\rangle$ representation should be points equally spaced along q with an interval of l/A. The mapping from k and q to $\langle k,q+ln/A|\phi\rangle \in C$ is a mapping from plane to plane. In general, $\langle k,q+ln/A|\phi\rangle=0$ are some discrete points, and thus it is casual that D is equal to zero. So in this sense, for most of $f_1=f_2^*$, this still not happens (in some sense, the measure of $D=0$ event is zero). Specially, when the state $|\phi_1\rangle=|\phi_2\rangle=|0\rangle$, it can be proved[35] that D is not equal to zero everywhere. Thus set

$$|\phi_1\rangle=|0\rangle+\epsilon|\psi_1\rangle, \qquad \langle\phi_2|=\langle 0|+\epsilon\langle\psi_2|. \tag{116}$$

D is also not equal to zero everywhere for small enough ϵ. But we do not know the situation for general $f_1\neq f_2^*$.

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The BMS group and generalized gravitational instantons

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The ordinary Bondi–Metzner–Sachs (BMS) group B is the best candidate for the fundamental symmetry group of General Relativity. It has been shown that B admits generalizations to real space–times of any signature, and also to complex space–times. It has been suggested that certain continuous unitary irreducible representations (IRs) of B and of its generalizations correspond to gravitational instantons. Here I make this correspondence more precise and I take this suggestion one step further by arguing that a subclass of IRs of B and of its generalizations correspond to *generalized* gravitational instantons. Some of these *generalized* gravitational instantons involve in their definition certain subgroups of the Cartesian product group $C_n \times C_m$, where C_r is the cyclic group of order r. With this motivation, I give the subgroups of $C_n \times C_m$ explicitly. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1645976]

I. INTRODUCTION

In 1962, an intensive study of asymptotically flat space–times, representing bounded gravitational sources emitting gravitational radiation, was undertaken by Bondi and others[1] and this work was generalized by Sachs.[2] These authors imposed radiation-dictated boundary conditions and found, among other things, that the ''asymptotic symmetries'' of such asymptotically flat space–times formed a group B which was independent of the detailed structure of the particular asymptotically flat space–time in question, hence the universality of B and its importance. This group, the so called Bondi–Metzner–Sachs (BMS) group B, contains the Poincare group P, and, furthermore, is infinite dimensional.

Soon after its discovery, the importance of finding the irreducible representations of B was emphasized.[2–4] The irreducible representations of B were constructed in a series of papers by McCarthy.[5–7] The role of the IRs of B is much less well understood than the role of the IRs of P.[8,9] McCarthy, in order to make this role better understood and in order to make contact with other approaches to quantum gravity, where complexified or Euclidean versions of general relativity are frequently considered, generalized B[9] to real space–times of any signature, and also to complex space–times. A significant input in the attempt to interpret the irreducibles of B and of its generalizations came from Kronheimer's work,[11,12] in which he classified *all* ALE gravitational instantons. McCarthy, using Kronheimer's work, conjectured[9] that there is a correspondence between ALE gravitational instantons and certain IRs of B, of EB, and of CB; the groups EB and CB are correspondingly the Euclidean BMS group and the Complex BMS group and both of them are defined in Ref. 9. The aim of this paper is to state and extend this correspondence, and, furthermore, to give explicitly a class of groups which are expected to be involved in the definition of new solutions to the Einstein equations. First, I make explicit and precise the expected correspondence between ALE spaces and IRs of B, EB, and CB; this correspondence has been stated, at least implicitly, in some cases by McCarthy (Ref. 9). Second, I argue that the representation theory of B and of its variants strongly suggests that in all signatures the aforementioned correspondence is naturally extended to non-self-dual solutions of the Einstein equations. Guided by this extended correspondence I (Ref. 10) put forward the conjecture that there are solutions to the Euclidean,

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Complex and Ultrahyperbolic Einstein equations which are neither self-dual nor anti-self-dual but far more general mixtures of them and which involve in their definition subgroups of the Cartesian product group $C_n \times C_m$, where C_r is the cyclic group of order r. With this motivation, I give the subgroups of $C_n \times C_m$ explicitly.

In Sec. II I make explicit the expected correspondence between BMS IRs and (generalized) gravitational instantons. Finally, in Sec. III I give explicitly the subgroups of $C_n \times C_m$.

II. RELATION OF BMS IRs WITH INSTANTONS AND WITH GENERALIZED INSTANTONS

In 1989 Kronheimer[11,12] gave an implicit description of all ALE gravitational instantons. (For the various types of gravitational instantons and for the role they play in the path integral approach to quantum gravity, see for example Ref. 13 and references therein.) Asymptotically locally Euclidean means that outside some compact region the metric approaches the flat (Euclidean) metric on $(S^3/T)\times R$, where T is a finite group of isometries acting freely on S^3 (S^3 is a 3-sphere and R is the straight line of real numbers). (If T is the identity the instanton is asymptotically Euclidean; in this case, however, according to a theorem of Showen and Yau,[14] the only instanton is the Euclidean four space. Eguchi and Hanson[15] gave an explicit metric in the case which T is a cyclic group Z_2 of order 2. Gibbons and Hawking[16] generalized Eguchi's and Hanson's result and gave explicit metrics in the case where T is a cyclic group C_k of order $k \geqslant 2$. The same result was obtained by Hitchin[17] by the Penrose nonlinear graviton technique, which can be extended to any finite subgroup of $SU(2)$. His approach however gives the solutions only implicitly.) Kronheimer's description of ALE instantons is implicit because he does not give explicit expressions for the metrics of the ALE instantons; the description involves constraints, namely, algebraic equations difficult to solve. He proved that the description of the moduli space of *all* gravitational ALE instantons involves the complex linear irreducible representations of the cyclic, the dihedral groups and the symmetry groups of the tetrahedron, cube and icosahedron. More precisely, the description involves the complex linear irreducible representations of the corresponding binary groups. It is precisely these binary groups which appear in the representation theory of B[6] as little groups. In fact, it is this coincidence which led McCarthy[9] to conjecture that there is a relation between IRs of B induced from finite little groups and ALE instantons. To make contact with other approaches to quantum gravity, where complexified or Euclidean versions of general relativity are considered, McCarthy generalized B to real space–times of any signature and to complex space–times and obtained 42 groups. For the purposes of this paper more relevant among these 42 groups are the Complex BMS group $CB = C^\infty(S^2 \times S^2, R) \circledS_T (SL(2,C) \times SL(2,C))$ and its various real sections: the Euclidean BMS group $EB = C^\infty(S^3, R) \circledS_T (SU(2) \times SU(2))$, the Ultrahyperbolic BMS group $B(2,2) = C^\infty(S^1 \times S^1, R) \circledS_T (SL(2,R) \times SL(2,R))$, and the original BMS group $B = C^\infty(S^2, R) \circledS_T SL(2,C)$ (typically $G = C^\infty(A,R) \circledS_T H$ denotes a semi-direct product, where, $C^\infty(A,R)$ is the normal Abelian subgroup of G. A denotes in all cases a compact space and $C^\infty(A,R)$ consists of the supertranslations; they are real-valued infinitely-differentiable functions defined on A. The space $C^\infty(A,R)$ can be given the structure of a linear vector space (over the field of real numbers) under point-wise addition. The representation "T" of H on the linear vector space $C^\infty(A,R)$ which specifies in each case the semi-direct product is not relevant here).

Now, I will state a number of conjectures which establish the relation of gravitational instantons and BMS IRs. Some of them are contained implicitly in Ref. 9. Here, I make them more explicit. These conjectures provide part of the driving force of the research program expounded here; namely of approaching quantum gravity via the representation theory of the BMS group and of its variants. The conjectures will be stated in order of increasing generality.

Conjecture 1: The Eguchi–Hanson metric[15] corresponds to the irreducible of EB induced from the group $I \times C_2$, where I is the identity and C_2 is the cyclic group of order 2.

It should be noted that there is also[9] a correspondence between the Eguchi–Hanson metric and the irreducible of CB induced from the group $I \times C_2$. It appears though, in a very preliminary consideration of the problem, that this correspondence can be explored and made explicit only in a round-about way by using the results of Hithin[17] and Newman,[18] whereas, it appears that the correspondence between the Eguchi–Hanson metric and the relevant irreducible of EB can be

established in a more straightforward way. This explains the reason I am restricting attention to the Euclidean BMS EB in Conjecture 1. Having said that, it is of paramount importance to try and establish the correspondence between the Eguchi–Hanson metric and the associated irreducible of CB, because this will also offer some clues about the relation of IRs of CB and EB; the interrelationship of the groups in Ref. 9 and of their IRs is an indispensable element of the research program considered here. Now I proceed to give Conjecture 2.

Conjecture 2: The gravitational multi-instantons of Gibbons and Hawking[16] correspond to the irreducibles of EB induced from the groups $I\times C_k$, where I is the identity and C_k is the cyclic group of order k, $k\geqslant 2$.

As in the case of the Eguchi–Hanson metric, there is a correspondence between the gravitational multi-instantons of Gibbons and Hawking and the IRs of CB induced from the groups $I\times C_k$. Making explicit this correspondence, by using the results of Hithin[17] and Newman[18] is an important part of the research program considered here. The following Conjecture proceeds one step further than the previous 2 Conjectures and states that there is a strong link between Kronheimer's work[11,12] and the IRs of EB.

Conjecture 3: The moduli spaces of ALE instantons given by Kronheimer in Refs. 11, 12 are precisely the irreducibles of EB induced from the groups $\Gamma\times I$, where Γ is the binary cyclic, binary dihedral, binary tetrahedral, binary octahedral or binary icosahedral and I is the identity element.

Note that here the IRs of EB are induced from little groups which lie only in the first factor of $SU(2)\times SU(2)$. The moduli spaces associated with instantons arise from only one factor of $SU(2)\times SU(2)$ [$SU(2)\times I$ for anti-instantons and $I\times SU(2)$ for instantons]. In Conjecture 3, the choice $\Gamma\times I$ is made because Kronheimer's work deals with anti-instantons. Kronheimer's description of the ALE moduli spaces is partial since it involves constraints. Kronheimer does not solve the constraint equations but the conjecture is being put forward here that the EB IRs give an unconstrained description of the same moduli spaces. There is also a correspondence between the moduli spaces of ALE instantons described by Kronheimer and the IRs of CB induced from the groups $\Gamma\times I$, where Γ was defined in Conjecture 3. As in the previous cases this correspondence can be explored and made clear by using the results of Hitchin and Newman. Kronheimer's work describes *all* ALE instantons; i.e., self-dual solutions to *Euclidean* Einstein equations. The representation theory of the BMS group and of its variants provide clues about (self-dual) solutions of Einstein equations in all signatures, as well as of Complex Einstein equations. First, I will comment on self-dual solutions. Indeed, the representation theory of the groups CB,[9] $B(2,2)$[19] strongly suggests the following Conjecture.

Conjecture 4: There are self-dual solutions to the complex Einstein equations which involve in their definition the IRs of Γ (where Γ was defined in Conjecture 3). The moduli spaces of these solutions correspond to the IRs of CB which are induced from the groups $I\times\Gamma$. There are also self-dual solutions to the ultrahyperbolic Einstein equations which involve in their definition the IRs of C_n, where C_n is the cyclic group of order n. The moduli spaces of these solutions correspond to the IRs of $B(2,2)$ which are induced from the groups C_n.

More importantly, the representation theory of EB, CB,[9] and $B(2,2)$[19] suggests that there are solutions to Euclidean, complex and ultrahyperbolic Einstein equations which are neither self-dual nor anti-self-dual but far more general mixtures of them. To be more precise, we have the following Conjecture.

Conjecture 5: There are solutions to the Euclidean and Complex Einstein equations which are neither self-dual nor anti-self-dual but more general mixtures of them. The moduli spaces of these solutions involve in their definition IRs of subgroups of the direct product $\Gamma_1\times\Gamma_2$, where Γ_1, Γ_2 are (independently) binary cyclic, binary dihedral, binary tetrahedral, binary octahedral or binary icosahedral. The moduli spaces of these solutions correspond to IRs of the groups EB and CB which are induced from the groups $\Gamma_1\times\Gamma_2$. There are also solutions to the ultrahyperbolic Einstein equations which are neither self-dual nor anti-self-dual but more general mixtures of them. The moduli spaces of these solutions involve in their definition IRs of subgroups of the

direct product $C_n \times C_m$. The moduli spaces of these solutions correspond to the IRs of the group $B(2,2)$ which are induced from the same subgroups of $C_n \times C_m$.

It is to be noted that the IRs of CB, EB, and $B(2,2)$ which correspond to solutions which are neither self-dual nor anti-self-dual but more general mixtures of them are not induced from little groups which lie within only one factor of $SU(2) \times SU(2)$ in the cases of CB and EB, or within only one factor of $SO(2) \times SO(2)$ in the case of $B(2,2)$, but are induced from little groups which "lie across" $SU(2) \times SU(2)$ or across $SO(2) \times SO(2)$. Two remarks are now in order.

(1) The previous conjectures claim that there is a correspondence between certain solutions to complex Einstein equations as well as to Euclidean or ultrahyperbolic Einstein equations and certain IRs of the CB, EB, and $B(2,2)$. In *all cases* the IRs give an *unconstrained* description of the corresponding moduli spaces. In the Euclidean signature, Kronheimer's description of the ALE moduli spaces involves constraints, i.e., algebraic equations which he has not solved. The suggestion is being put forward here that in fact one can attempt to use the relevant IRs of EB in order to solve Kronheimer's constraint equations.
(2) In the correspondence conjectured here the IRs, of the relevant in each case, BMS-group are induced from the, relevant in each case, finite *little groups*.

According to the last conjecture in the ultrahyperbolic case, the little groups of $B(2,2)$ are involved in the description of moduli spaces of solutions of the ultrahyperbolic Einstein equations. These little groups are subgroups of $C_n \times C_m$. The direct product $C_n \times C_m$ also appears in the representation theory of both CB and EB and, according to Conjecture 5, subgroups of them are involved in the description of moduli spaces of solutions to the complex and Euclidean Einstein equations. For this reason I give explicitly the subgroups of $C_n \times C_m$ in the next section.

III. SUBGROUPS OF $C_n \times C_m$

It turns out that the explicit construction of the subgroups of $C_n \times C_m$ is a problem more difficult than it might appear at a first consideration. I constructed the subgroups of $C_n \times C_m$ with two entirely independent methods to assure correctness; full details of the construction will be given elsewhere, here I only give the result of the construction. The result is given in an algorithmic fashion; it can be used to write a program which would construct them automatically. It is an interesting fact that the explicit construction of the subgroups of $C_n \times C_m$ involves the prime decomposition of the numbers n and m. An attempt to find them explicitly without invoking the prime decomposition of n and m failed. A key observation is that the direct product $C_n \times C_m$ is a finite Abelian group, and therefore, its rank, i.e., the number of its independent generators, is greater or equal than the rank of any of its subgroups. Consequently, the subgroups of $C_n \times C_m$ have either one or two generators. First, in the first Theorem, I give the generators of the cyclic subgroups of $C_n \times C_m$, and then, in the second Theorem I give the generators of the noncyclic subgroups of $C_n \times C_m$. It will prove convenient to introduce some notation at this point. $\mathcal{P}$ will denote a permutation of the s pairs of numbers $(p_1^{a_1}, p_1^{\beta_1})$, $(p_2^{a_2}, p_2^{\beta_2}), \ldots, (p_s^{a_s}, p_s^{\beta_s})$. Therefore, if $(p_i^{a_i}, p_i^{\beta_i})$, $i = 1,2,\ldots,s$ is one of these pairs of numbers then, $\mathcal{P}(p_i^{a_i}, p_i^{\beta_i}) = (p_j^{a_j}, p_j^{\beta_j})$, for some $j = 1,2,\ldots,s$. For convenience, we will write

$$\mathcal{P}(p_i^{a_i}, p_i^{\beta_i}) = (p_j^{a_j}, p_j^{\beta_j}) \equiv (p_i^{a_i}, p_i^{b_i}), \quad i = 1,2,\ldots,s.$$

Thus, the integer p_j is written as p_i, the non-negative integer a_j is written as a_i, and the non-negative integer β_j is written as b_i. I proceed now to give the first theorem.

Theorem I: *Let $C_n \times C_m$ be the direct product of the cyclic groups of finite order C_n and C_m. Let $n = p_1^{a_1} \cdot p_2^{a_2} \cdots p_s^{a_s}$ and $m = p_1^{\beta_1} \cdot p_2^{\beta_2} \cdots p_s^{\beta_s}$ be the prime decomposition of the integers n and m, i.e., p_i, $i = 1,2,\ldots,s$, are distinct prime numbers and a_i, β_i are non-negative integers. Then we have the following.*

(1) A group,

$$\mathcal{C}=A_1\times A_2\times A_3\times\cdots\times A_s, \tag{1}$$

where A_i *is a cyclic subgroup, not necessarily different from the identity element, of* $C_{p_i^{a_i}}\times C_{p_i^{\beta_i}}$, $i=1,2,...,s$, *is a cyclic subgroup of* $C_n\times C_m$.

(2) Every cyclic subgroup $\mathcal{C}$ *of* $C_n\times C_m$ *is of the form*

$$\mathcal{C}=A_1\times A_2\times A_3\times\cdots\times A_s,$$

where A_i *is a cyclic subgroup, not necessarily different from the identity element of* $C_{p_i^{a_i}}\times C_{p_i^{\beta_i}}$, $i=1,2,...,s$.

(3) For every cyclic group $\mathcal{C}$ *of* $C_n\times C_m$ *the expression (1) is unique.*

A generator of the cyclic subgroup $\mathcal{C}$ *is given by*

$$(x^{\mathcal{A}},y^{\mathcal{B}}), \tag{2}$$

where, x is a generator of C_n, *y is a generator of* C_m,

$$\mathcal{A}=\sum_{i=1}^{\nu} r_i p_i^{a_i-k_i}(n/p_i^{a_i})+\sum_{i=\nu+1}^{\nu+\chi} p_i^{a_i-k_i}(n/p_i^{a_i})+\sum_{i=\nu+\chi+1}^{\nu+\chi+\tau} j_i(n/p_i^{a_i})+\sum_{i=\nu+\chi+\tau+1}^{\nu+\chi+\tau+\psi} p_i^{a_i-k_i}(n/p_i^{a_i}), \tag{3}$$

and

$$\mathcal{B}=\sum_{i=1}^{\nu} p_i^{b_i-k_i}(m/p_i^{b_i})+\sum_{i=\nu+1}^{\nu+\chi} \rho_i p_i^{b_i-k_i+1}(m/p_i^{b_i})+\sum_{i=\nu+\chi+1}^{\nu+\chi+\tau} p_i^{b_i-k_i}(m/p_i^{b_i}) + \sum_{i=\nu+\chi+\tau+1}^{\nu+\chi+\tau+\psi} j_i(m/p_i^{b_i}). \tag{4}$$

The order $|\mathcal{C}|$ *of the group* $\mathcal{C}$ *is given by*

$$|\mathcal{C}|=\prod_{i=1}^{\nu+\chi+\tau+\psi} p_i^{k_i}. \tag{5}$$

The non-negative integers ν, χ, τ, ψ *are such that* $\nu+\chi+\tau+\psi\leqslant s$. *Moreover,* $(p_i^{a_i},p_i^{b_i})=\mathcal{P}(p_i^{a_i},p_i^{\beta_i})$, $i=1,2,...,s$, *for some permutation* $\mathcal{P}$ *of the s pairs of numbers* $(p_1^{a_1},p_1^{\beta_1})$, $(p_2^{a_2},p_2^{\beta_2}),\ldots,(p_s^{a_s},p_s^{\beta_s})$. *Furthermore, when* $i\in\{1,2,...,\nu\}$, $r_i\in\{0,1,2,...,p_i^{k_i}-1\}$, *and when* $\sigma\in\{\nu+\chi+1,\nu+\chi+2,...,\nu+\chi+\tau\}$, $a_\sigma<k_\sigma\leqslant b_\sigma$ *and* $j_\sigma\in\{0,1,2,...,p_\sigma^{a_\sigma}-1\}$. *Finally, when* $q\in\{\nu+1,\nu+2,...,\nu+\chi\}$, $\rho_q\in\{0,1,2,...,p_q^{k_q-1}-1\}$, *and when* $\theta\in\{\nu+\chi+\tau+1,\nu+\chi+\tau+2,...,\nu+\chi+\tau+\psi\}$, $a_\theta\geqslant k_\theta>b_\theta$ *and* $j_\theta\in\{0,1,2,...,p_\theta^{b_\theta}-1\}$.

I give now the second theorem, where generators of all the noncyclic subgroups of $C_n\times C_m$ are given explicitly.

Theorem II: *Let* $C_n\times C_m$ *be the direct product of the cyclic groups of finite order* C_n *and* C_m. *Let* $n=p_1^{a_1}\cdot p_2^{a_2}\cdots p_s^{a_s}$ *and* $m=p_1^{\beta_1}\cdot p_2^{\beta_2}\cdots p_s^{\beta_s}$ *be the prime decomposition of the integers n and m,* i.e., p_i, $i=1,2,...,s$, *are distinct prime numbers and* a_i, β_i *are non-negative integers. Then we have the following.*

(1) A group,

$$\mathcal{C}=A_1\times A_2\times A_3\times\cdots\times A_s, \tag{6}$$

where A_i is a subgroup, not necessarily different from the identity element, of $C_{p_i^{a_i}} \times C_{p_i^{\beta_i}}$, $i=1,2,...,s$, is a subgroup of $C_n \times C_m$ with two generators if at least one of the A_i, $i=1,2,...,s$, has two generators.

(2) Every subgroup $\mathcal{C}$ of $C_n \times C_m$ with two generators is of the form

$$\mathcal{C}=A_1 \times A_2 \times A_3 \times \cdots \times A_s,$$

where A_i is a subgroup, not necessarily different from the identity element, of $C_{p_i^{a_i}} \times C_{p_i^{\beta_i}}$, $i=1,2,...,s$, and, where at least one of the A_i, $i=1,2,...,s$, has two generators.

(3) For every subgroup $\mathcal{C}$ of $C_n \times C_m$ with two generators the expression (6) is unique.

Two generators of a subgroup $\mathcal{C}$ of $C_n \times C_m$ with two generators are given by the following.
(1)

$$g_1=(x^{\mathcal{A}_1}, y^{\mathcal{B}_1}), \tag{7}$$

where x is a generator of C_n, y is a generator of C_m,

$$\begin{aligned}\mathcal{A}_1=&\sum_{i=1}^{\nu} r_i p_1^{a_i-k_i}(n/p_i^{a_i})+\sum_{i=\nu+1}^{\nu+\chi} p_i^{a_i-k_i}(n/p_i^{a_i})+\sum_{i=\nu+\chi+1}^{\nu+\chi+\tau} j_i(n/p_i^{a_i})+\sum_{i=\nu+\chi+\tau+1}^{\nu+\chi+\tau+\psi} p_i^{a_i-k_i}(n/p_i^{a_i})\\&+\sum_{i=\nu+\chi+\tau+\psi+1}^{\nu+\chi+\tau+\psi+\sigma} r_i p_i^{a_i-k_i}(n/p_i^{a_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+1}^{\nu+\chi+\tau+\psi+\sigma+\theta} p_i^{a_i-k_i}(n/p_i^{a_i})\\&+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi} t_i(n/p_i^{a_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+\phi+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi} p_i^{a_i-k_i}(n/p_i^{a_i})\end{aligned} \tag{8}$$

and

$$\begin{aligned}\mathcal{B}_1=&\sum_{i=1}^{\nu} p_i^{b_i-k_i}(m/p_i^{b_i})+\sum_{i=\nu+1}^{\nu+\chi} \rho_i p_i^{b_i-k_i+1}(m/p_i^{b_i})+\sum_{i=\nu+\chi+1}^{\nu+\chi+\tau} p_i^{b_i-k_i}(m/p_i^{b_i})\\&+\sum_{i=\nu+\chi+\tau+1}^{\nu+\chi+\tau+\psi} j_i(m/p_i^{b_i})+\sum_{i=\nu+\chi+\tau+\psi+1}^{\nu+\chi+\tau+\psi+\sigma} p_i^{b_i-k_i}(m/p_i^{b_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+1}^{\nu+\chi+\tau+\psi+\sigma+\theta} \rho_i p_i^{b_i-k_i+1}(m/p_i^{k_i})\\&+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi} p_i^{b_i-k_i}(m/p_i^{b_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+\phi+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi} t_i(m/p_i^{b_i})\end{aligned} \tag{9}$$

(2)

$$g_2=(x^{\mathcal{A}_2}, y^{\mathcal{B}_2}), \tag{10}$$

where,

$$\mathcal{A}_2=\sum_{i=\nu+\chi+\tau+\psi+1}^{\nu+\chi+\tau+\psi+\sigma} p_i^{a_i-l_i}(n/p_i^{a_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi} p_i^{a_i-l_i}(n/p_i^{a_i}) \tag{11}$$

and

$$\mathcal{B}_2=\sum_{i=\nu+\chi+\tau+\psi+\sigma+1}^{\nu+\chi+\tau+\psi+\sigma+\theta} p_i^{b_i-l_i}(m/p_i^{b_i})+\sum_{i=\nu+\chi+\tau+\psi+\sigma+\theta+\phi+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi} p_i^{b_i-l_i}(m/p_i^{b_i}). \tag{12}$$

The order $|\mathcal{C}|$ of the group $\mathcal{C}$ is given by

$$|\mathcal{C}| = \prod_{i=1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi} p_i^{k_i} \times \prod_{i=\nu+\chi+\tau+\psi+1}^{\nu+\chi+\tau+\psi+\sigma+\theta+\phi} p_i^{l_i}. \tag{13}$$

The non-negative integers ν, χ, τ, ψ, σ, θ, ϕ, ξ are such that $\nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi \leqslant s$. Moreover, $(p_i^{a_i}, p_i^{b_i}) = \mathcal{P}(p_i^{a_i}, p_i^{\beta_i})$, $i=1,2,...,s$, for some permutation $\mathcal{P}$ of the s pairs of numbers $(p_1^{a_1}, p_1^{\beta_1})$, $(p_2^{a_2}, p_2^{\beta_2}), \ldots, (p_s^{a_s}, p_s^{\beta_s})$. Furthermore, when $i \in \{1,2,...,\nu\}$, $k_i \leqslant \min(a_i, b_i)$ and $r_i \in \{0,1,2,...,p_i^{k_i}-1\}$, and when $w \in \{\nu+\chi+1, \nu+\chi+2, ..., \nu+\chi+\tau\}$, $a_w < k_w \leqslant b_w$ and $j_w \in \{0,1,2,...,p_w^{a_w}-1\}$. When $q \in \{\nu+1, \nu+2, ..., \nu+\chi\}$, $k_q \leqslant \min(a_q, b_q)$ and $\rho_q \in \{0,1,2,...,p_q^{k_q-1} - 1\}$, and when $y \in \{\nu+\chi+\tau+1, \nu+\chi+\tau+2, ..., \nu+\chi+\tau+\psi\}$, $a_y \geqslant k_y > b_y$ and $j_y \in \{0,1,2,...,p_y^{b_y}-1\}$. When $i_1 \in \{\nu+\chi+\tau+\psi+1, \nu+\chi+\tau+\psi+2, ..., \nu+\chi+\tau+\psi+\sigma\}$, $1 \leqslant l_{i_1} \leqslant k_{i_1} \leqslant \min(a_{i_1}, b_{i_1})$ and $r_{i_1} \in \{0,1,2,...,p_{i_1}^{k_{i_1}-l_{i_1}}-1\}$, and when $q_1 \in \{\nu+\chi+\tau+\psi+\sigma+1, ..., \nu+\chi+\tau+\psi+\sigma+\theta\}$, $1 \leqslant l_{q_1} < k_{q_1} \leqslant \min(a_{q_1}, b_{q_1})$ and $\rho_{q_1} \in \{0,1,2,...,p_{q_1}^{k_{q_1}-l_{q_1}-1}-1\}$. When $w_1 \in \{\nu+\chi+\tau+\psi+\sigma+\theta+1, \nu+\chi+\tau+\psi+\sigma+\theta+2, ..., \nu+\chi+\tau+\psi+\sigma+\theta+\phi\}$, $1 \leqslant l_{w_1} \leqslant a_{w_1} < k_{w_1} \leqslant b_{w_1}$ and $t_{w_1} \in \{0,1,2,...,p_{w_1}^{a_{w_1}-l_{w_1}}-1\}$. Finally, when $y_1 \in \{\nu+\chi+\tau+\psi+\sigma+\theta+\phi+1, \nu+\chi+\tau+\psi+\sigma+\theta+\phi+2, ..., \nu+\chi+\tau+\psi+\sigma+\theta+\phi+\xi\}$, $1 \leqslant l_{y_1} \leqslant b_{y_1} < k_{y_1} \leqslant a_{y_1}$ and $j_{y_1} \in \{0,1,2,...,p_{y_1}^{b_{y_1}-l_{y_1}}-1\}$.

The previous theorems give the subgroups of $C_n \times C_m$. The large number of subgroups indicates that, in the Euclidean, for example, case, the gravitational multi-instantons of Gibbons and Hawking[16] are only a small class of solutions compared to the more general ones which are parametrized with IRs of subgroups of $C_n \times C_m$.

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Hamiltonians separable in Cartesian coordinates and third-order integrals of motion

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We present in this article all Hamiltonian systems in $E(2)$ that are separable in Cartesian coordinates and that admit a third-order integral, both in quantum and in classical mechanics. Many of these superintegrable systems are new, and it is seen that there exists a relation between quantum superintegrable potentials, invariant solutions of the Korteweg–de Vries equation and the Painlevé transcendents. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1633352]

I. INTRODUCTION

In classical mechanics, an n-dimensional Hamiltonian system is called Liouville integrable if it allows n functionally independent integrals of motion in involution (including the Hamiltonian), that is,

$$\{H,X_i\}=0,$$

$$\{X_i,X_j\}=0,\forall i,j.$$

The Hamiltonian $H=H(x_1,\ldots,x_n,p_1,\ldots,p_n)$ and the integrals of motion $X_i=X_i(x_1,\ldots,x_n,p_1,\ldots,p_n)$ must be well defined functions on phase space.[1,11] The system is superintegrable if it allows more than n functionally independent integrals, n of them in involution. It is called maximally superintegrable if it allows $2n-1$ integrals of motion. The best known superintegrable systems in n dimensions are the harmonic oscillator $V=\omega r^2$ and the Coulomb potential $V=\alpha/r$, and they are indeed maximally superintegrable. This may be closely related to Bertrand's theorem[1,2] which states that these are the only rotationally invariant systems for which all finite trajectories are closed.

In quantum mechanics, a Hamiltonian system is said to be integrable if there exists a set $\{X_i\}$ of n well defined, algebraically independent operators (including the Hamiltonian) that commute pairwise. It is superintegrable if it possesses further independent operators, $\{Y_j\}$ that commute with the Hamiltonian. The Y_j do not necessarily commute with each other, nor with the X_i.

The independence of operators in quantum mechanics remains to be defined rigorously.[13,14,17,29] Since we are dealing here only with polynomial differential operators, we can proceed by analogy with the classical case, keeping in mind that a rigorous definition will be needed as soon as we will want to make some more general statements. This choice of a definition will be used only for discussion purposes, since we will find all potentials that admit third-order integrals and all their integrals. The results obtained will therefore hold for any definition of the independence of operators.

Integrable and superintegrable systems, both in quantum and in classical mechanics, attracted considerable interest in the last years. Extensive literature exists about systems with second-order integrals of motion, either in Euclidian space[7–10,22,30] or in spaces with nonzero constant[19,25] or nonconstant curvature.[20] As long as there was no magnetic field in the Hamiltonian, the quantum and classical integrals of motion obeyed the same determining equations, and therefore quantum

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and classical integrability were very similar. Both properties were related to separation of the Hamilton–Jacobi or Schrödinger equations, and also to exact solvability[27] and generalized symmetries.[26]

Systems with higher-order integrals have been studied and classified as early as 1935 in a well-known paper by Drach.[4] This paper considered classical Hamiltonians in complex Euclidian space.[23,24] Efforts were made recently to understand and classify more completely systems with higher-order integrals in classical[13,28] and quantum mechanics.[13,15,16] In spite of these efforts, still relatively few such systems are known. This article is the logical sequel of a systematic search for superintegrable systems with higher order integrals started in Ref. 13. Here we consider two-dimensional real Euclidian space with a one-particle Hamiltonian:

$$H=\tfrac{1}{2}(p_x^2+p_y^2)+V(x,y).$$

We request the existence of two additional integrals of motion, one of second order in the momenta and the other of third order.

The condition of existence for second-order integral implies, both in classical and quantum mechanics, that the Hamiltonian be separable in Cartesian, polar, parabolic or elliptic coordinates. In this article we consider potentials that are separable in Cartesian coordinates:

$$H=\tfrac{1}{2}(p_x^2+p_y^2)+V_1(x)+V_2(y).$$

We found all such systems which admit third-order integrals. Quantum and classical mechanics will be treated simultaneously, for the conditions of existence of integrals of motion, even though not equivalent, are quite similar in both cases.

II. EXISTENCE OF A THIRD-ORDER INTEGRAL

In quantum and classical mechanics, the general third-order commuting operator

$$X=\sum_{i+j=0}^{3} P_{ij}(x,y)p_x^i p_y^j$$

can be reduced to a much simpler form,

$$X=\sum_{\substack{i,j,k\\ i+j+k=3}} A_{ijk}\{L_3^i,p_x^j p_y^k\}+\{g_1(x,y),p_x\}+\{g_2(x,y),p_y\},$$
$$L_3=xp_y-yp_x, \tag{1}$$

where the A_{ijk} are real constants and the g_i real functions. The bracket is the anticommutator. It is not needed in classical mechanics, but in quantum mechanics it allows us to get rid of terms with even powers of the p_i and to make sure the operator is self-adjoint. Furthermore, its use allows us to see clearly the relations between the quantum and the classical cases. Indeed, it was found in Ref. 13 that the requirement that the operator commutes (or Poisson-commutes) with the Hamiltonian

$$H=\tfrac{1}{2}(p_x^2+p_y^2)+V(x,y)$$

implies equations that behave well in the classical limit. Namely, commutativity implies

$$0=g_1V_x+g_2V_y-\frac{\hbar^2}{4}(f_1V_{xxx}+f_2V_{xxy}+f_3V_{xyy}+f_4V_{yyy}$$
$$+8A_{300}(xV_y-yV_x)+2(A_{210}V_x+A_{201}V_y)), \tag{2}$$

$$(g_1)_x = 3f_1(y)V_x + f_2(x,y)V_y, \tag{3}$$

$$(g_2)_y = f_3(x,y)V_x + 3f_4(x)V_y, \tag{4}$$

$$(g_1)_y + (g_2)_x = 2(f_2(x,y)V_x + f_3(x,y)V_y) \tag{5}$$

in quantum mechanics, where

$$f_1(y) = -A_{300}y^3 + A_{210}y^2 - A_{120}y + A_{030},$$

$$f_2(x,y) = 3A_{300}xy^2 - 2A_{210}xy + A_{201}y^2 + A_{120}x - A_{111}y + A_{021},$$

$$f_3(x,y) = -3A_{300}x^2y + A_{210}x^2 - 2A_{201}xy + A_{111}x - A_{102}y + A_{012},$$

$$f_4(x) = A_{300}x^3 + A_{201}x^2 + A_{102}x + A_{003}.$$

The equations in classical mechanics are obtained by setting $\hbar = 0$. We may notice from the quantum equations, or directly from the condition $[H,X]=0$, that we can express all quantum integrable potentials as $\hbar^2\tilde{V}(x,y)$ where $\tilde{V}$ does not depend on $\hbar$. It is often more natural and interesting though to choose arbitrary parameters contained in $\tilde{V}$ to be depending on $\hbar$, so that the potential V does not vanish in the classical limit. One may always verify, though, that through an appropriate transformation of the arbitrary parameters one can write the potential as being proportional to $\hbar^2$.

The three last equations, identical in the quantum and classical cases, yield a linear compatibility condition for V, which reads

$$\begin{aligned} 0 = &-f_3V_{xxx} + (2f_2 - 3f_4)V_{xxy} + (-3f_1 + 2f_3)V_{xyy} - f_2V_{yyy} + 2(f_{2y} - f_{3x})V_{xx} \\ &+ 2(-3f_{1y} + f_{2x} + f_{3y} - 3f_{4x})V_{xy} + 2(-f_{2y} + f_{3x})V_{yy} + (-3f_{1yy} + 2f_{2xy} - f_{3xx})V_x \\ &+ (-f_{2yy} + 2f_{3xy} - 3f_{4xx})V_y. \end{aligned} \tag{6}$$

Further nonlinear compatibility conditions can be obtained from (2)–(5) for the potential, and these are listed in Ref. 13. They are quite complicated, though, and were not used for the results stated in this article.

III. POTENTIALS SEPARABLE IN CARTESIAN COORDINATES

If we set $V = V_1(x) + V_2(y)$ in Eqs. (2)–(5), we find

$$0 = g_1V_{1x} + g_2V_{2y} - \frac{\hbar^2}{4}(f_1V_{1xxx} + f_4V_{2yyy} + 8A_{300}(xV_{2y} - yV_{1x}) + 2(A_{210}V_{1x} + A_{201}V_{2y})), \tag{7}$$

$$(g_1)_x = 3f_1(y)V_{1x} + f_2(x,y)V_{2y}, \tag{8}$$

$$(g_2)_y = f_3(x,y)V_{1x} + 3f_4(x)V_{2y}, \tag{9}$$

$$(g_1)_y + (g_2)_x = 2(f_2(x,y)V_{1x} + f_3(x,y)V_{2y}), \tag{10}$$

with $\hbar = 0$ in the classical case. Equations (8) and (9) are readily integrated, so in the Cartesian case two equations remain to be solved.

The compatibility condition (6) allows us to find ODEs for V_1 and V_2. If we set alternatively $y=0$ and $x=0$, we find

$$(A_{210}x^2 + A_{111}x + A_{012})V_1^{(3)}(x) + 4(2A_{210}x + A_{111})V_1''(x) + 12A_{210}V_1'(x) = ax + b, \tag{11}$$

$$(A_{201}y^2-A_{111}y+A_{021})V_2^{(3)}(y)+4(2A_{201}y-A_{111})V_2''(y)+12A_{201}V_2'(y)=cy+d. \qquad (12)$$

The solutions to the homogeneous part of these equations are easily found and brought to a simple form by translations in x and y. If we take the first one for definiteness, we have four different types of solution. When $A_{210}\neq 0$, we have two possible solutions,

$$V_{1hom}=\frac{c_1}{(x+\alpha)^2}+\frac{c_2}{(x-\alpha)^2},$$

$$V_{1hom}=\frac{c_1}{x^2}+\frac{c_2}{x^3}.$$

If $A_{210}=0$ and $A_{111}\neq 0$, we get

$$V_{1hom}=\frac{c_1}{x^2}+c_2x.$$

Finally, if only $A_{012}\neq 0$, the solution may be brought to the form

$$V_{1hom}=c_2x^2+c_1x.$$

Special solutions are also simple. If $A_{210}\neq 0$, we have $V_{1part}=\alpha x^2+\beta x$. Otherwise, when $A_{111}\neq 0$, $V_{1part}=\alpha x^3+\beta x^2$, finally, if only $A_{012}\neq 0$, $V_{1part}=\alpha x^4+\beta x^3$. Provided that (11) or (12) does not vanish trivially, we can choose V_1 or V_2, respectively, among the following functions:

$$(\text{A.1})\quad f_1=\frac{c_1}{(x+\alpha)^2}+\frac{c_2}{(x-\alpha)^2}+c_3x^2+c_4x,$$

$$(\text{A.2})\quad f_2=\frac{c_1}{x^2}+\frac{c_2}{x^3}+c_3x^2+c_4x,$$

$$(\text{A.3})\quad f_3=\frac{c_1}{x^2}+c_2x^3+c_3x^2+c_4x,$$

$$(\text{A.4})\quad f_4=c_1x^4+c_2x^2+c_3x,$$

$$(\text{A.5})\quad f_5=c_1x^3+c_2x,$$

$$(\text{A.6})\quad f_6=c_1x^2,$$

$$(\text{A.7})\quad f_7=c_1x,$$

and then solve (7)–(10). These long but rather straightforward calculations yield the 15 superintegrable potentials included in Table I. Some of them are obviously particular cases of others, but we listed them separately to account for their additional integrals. Only the third-order integrals are listed, some of them being trivial consequences of lower-order ones. With the exception of the harmonic oscillator, potentials that have first-order integrals are not listed here for they were already presented in Ref. 13 with all their third-order integrals. The complete integrals of motion can be found in the Appendix.

Many of these potentials were not known. The only classical potentials among these are indicated with a $\star$. These are well-known superintegrable potentials (see, e.g., Ref. 10), and all of them, except V_i, are in fact quadratically superintegrable.

TABLE I. Superintegrable potentials that satisfy linear compatibility conditions for nonzero parameters.

Superintegrable potentials	Leading-order terms of the integrals
$\star V_a = a(x^2+y^2)$	L^3; $\{L,p_xp_y\}$; $\{L,p_y^2\}$; $\{L,p_x^2\}$
$\star V_b = a(x^2+y^2)+\frac{b}{x^2}+\frac{c}{y^2}$	$\{L,p_xp_y\}$
$V_c = a(x^2+y^2)+\frac{\hbar^2}{x^2}+\frac{\hbar^2}{y^2}$	L^3; $\{L,p_xp_y\}$
$V_d = a(x^2+y^2)+\frac{\hbar^2}{y^2}$	L^3; $\{L,p_xp_y\}$; $\{L,p_y^2\}$
$V_e = \frac{\hbar^2}{8\alpha^4}(x^2+y^2)+\frac{\hbar^2}{(x-\alpha)^2}+\frac{\hbar^2}{(x+\alpha)^2}$	$2L^3-3\alpha^2\{L,p_y^2\}$; $\{L,p_x^2\}$
$V_f = \frac{\hbar^2}{8\alpha^4}(x^2+y^2)+\frac{\hbar^2}{y^2}+\frac{\hbar^2}{(x+\alpha)^2}+\frac{\hbar^2}{(x-\alpha)^2}$	$2L^3-3\alpha^2\{L,p_y^2\}$
$V_g = \frac{\hbar^2}{8\alpha^4}(x^2+y^2)+\frac{\hbar^2}{(y-\alpha)^2}+\frac{\hbar^2}{(x-\alpha)^2}+\frac{\hbar^2}{(y+\alpha)^2}+\frac{\hbar^2}{(x+\alpha)^2}$	$2L^3-3\alpha^2(\{L,p_x^2\}+\{L,p_y^2\})$
$\star V_h = a(4x^2+y^2)+\frac{b}{y^2}+cx$	$p_xp_y^2$
$\star\ V_i = a(9x^2+y^2)$	$\{L,p_y^2\}$
$V_j = a(9x^2+y^2)+\frac{\hbar^2}{y^2}$	$\{L,p_y^2\}$
$V_k = \frac{\hbar^2}{8\alpha^4}(9x^2+y^2)+\frac{\hbar^2}{(y+\alpha)^2}+\frac{\hbar^2}{(y-\alpha)^2}$	$\{L,p_y^2\}$
$V_l = \frac{\hbar^2}{x^2}+\frac{a}{y^2}$	$\{L^2,p_x\}$; $\{L,p_xp_y\}$; p_x^3
$V_m = \frac{\hbar^2}{x^2}+\frac{\hbar^2}{y^2}$	L^3; $\{L^2,p_x\}$; $\{L^2,p_y\}$ $\{L,p_xp_y\}$; p_x^3; p_y^3
$V_n = ax+\frac{\hbar^2}{y^2}$	$\{L,p_y^2\}$; p_y^3; $p_xp_y^2$
$V_o = \frac{\hbar^2}{y^2}+V(x)$	p_y^3

All the potentials are superintegrable in the quantum case. We therefore notice that classical nontrivial potentials can have many different quantum equivalents. The classical harmonic oscillator V_a can be seen as a limiting case of the quantum potentials V_a, V_c and V_d, and, also, if we set $\alpha=\sqrt{\hbar}/\omega$, of V_e, V_f and V_g, not to mention the similar potentials that can be obtained by permutations of x and y. The anisotropic harmonic oscillator with ratio 1:3 also admits many quantum deformations, but, interestingly, the anisotropic oscillator with ratio 1:2 does not admit such deformations. Notice also that if we want to deal with real potentials only, α must be either real or purely imaginary in potentials V_e, V_f, V_g and V_k. Therefore, these have as a classical limit harmonic oscillators with $a>0$.

All quantum superintegrable potentials reduce to classical ones when the classical limit is considered, sometimes in more than one way. For example, potentials V_e, V_f and V_g give the free motion potential instead of the harmonic oscillator if α remains constant as $\hbar\to 0$.

These potentials all satisfy the linear equations (11) and (12), and can be expressed as sums of simple superintegrable potentials.

Let us now set $A_{210}=A_{111}=A_{012}=0$ so that (11) vanishes trivially. We may also assume that V_1 does not take one of the forms (A.1)–(A.7), for we have already worked these cases out. This is quite useful, for if we set $y=1$ in (6), we obtain for V_1 an equation of the same form as (11)

with different coefficients. These coefficients must therefore vanish, so $A_{300}=A_{201}=A_{102}=0$. This is a significant simplification that allows us to restrict our attention, when considering Eq. (12), to the following three cases:

(i) $V_2=ay^2$;
(ii) $V_2=ay$;
(iii) $A_{120}=A_{021}=0$.

Before we consider each case separately, it is worth noticing that potentials of the form $V=V_1(x)$ that admit third-order integrals independent of y and p_y should appear as solutions here, for the integral remains if we add a function $V_2(y)$ to these potentials. These potentials were found in Refs. 13 and 17 to satisfy the equation

$$\hbar^2 V_1'^2=4V_1^3-g_2V_1-g_3, \tag{13}$$

and can therefore be written as

$$V_1=\hbar^2\mathcal{P}(x), \tag{14}$$

where $\mathcal{P}(x)$ is the Weierstrass elliptic function. Since the y variable plays no role here and these potentials admit integrals with leading-order terms proportional to p_x^3, these solutions will appear in cases (i)–(iii).

A. Case i: $V=V_1(x)+ay^2$

When $V=V_1(x)+ay^2$ and $a\neq 0$, we find that $A_{300}=0$, and the following two equations must be satisfied:

$$0=A_{030}(\hbar^2V_1^{(3)}-6(V_1^2)')+\gamma_1V_1', \tag{15}$$

$$\begin{aligned}0=&A_{120}(-\hbar^2V_1^{(4)}-24a(xV_1)'+6(V_1^2)''-4ax^2V_1''+8a^2x^2)\\&+8aA_{021}(2ax-(xV_1')'-2V_1')+4\eta(2a-V_1''),\end{aligned} \tag{16}$$

where γ_1 and η are arbitrary constants. When $A_{030}\neq 0$, Eq. (15) is equivalent to (13) (up to a translation of V_1 to get rid of γ_1), hence its solutions are of the form (14). These potentials cannot satisfy simultaneously Eq. (16) for nontrivial parameters. This can be observed by expanding (13) in series around $x=0$ and substituting the result in (16). Therefore solutions given by $A_{030}\neq 0$ are of no special interest here.

Let us now set $A_{030}=\gamma_1=0$. Equation (16) can be greatly simplified. We assume that $A_{120}\neq 0$, for otherwise Eq. (16) can be solved to give potential V_h. Then by an appropriate translation of x and V, we can get rid of the terms involving A_{021} and η and finally divide by A_{120}:

$$0=-\hbar^2V_1^{(4)}-24a(xV_1)'+6(V_1^2)''-4ax^2V_1''+8a^2x^2. \tag{17}$$

This equation admits a first integral, namely,

$$k=\hbar^2(xV_1'''-V_1'')+4x(ax^2-3V_1)V_1'+6V_1^2+12ax^2V_1-2a^2x^4. \tag{18}$$

Both (17) and (18) can be simplified by setting $V_1=W(x)+ax^2/3$. Then

$$\hbar^2W^{(4)}=12WW''+12(W')^2+bxW'+2bW-\tfrac{1}{6}b^2x^2 \tag{19}$$

with $b=-8a\neq 0$ for (17), and

$$k_2=3\hbar^2(xW'''-W'')-18x(W^2)'+2(2ax^2+3W)^2 \tag{20}$$

for the first integral. Equation (19) is well known. It is equivalent to Eqs. (3.16) in Ref. 5 and (2.17) in Ref. 21, which were obtained by nonclassical reduction of the Boussinesq equation. It was also shown in Ref. 3 to be a nonclassical reduction of the Kadomtsev–Petviashvili equation. It has the Painlevé property, and, when $b\neq 0$, its solution, given in Ref. 6 [Eq. (2.88)] may be written in terms of the fourth transcendant function of Painlevé, namely,

$$W=\frac{\hbar}{2}b_1P_4'\left(x,\frac{b}{\hbar^2}\right)-\frac{1}{2}bP_4^2\left(x,\frac{b}{\hbar^2}\right)-\frac{1}{2}bxP_4\left(x,\frac{b}{\hbar^2}\right)-\frac{1}{6}\left(\frac{b}{2}x^2+\hbar^2K_1-\hbar b_1\right), \tag{21}$$

where $b_1\equiv\pm\sqrt{-b}=\pm\sqrt{8a}$ and $P_4(x,b/\hbar^2)=P_4(x,b/\hbar^2,K_1,K_2)$ is the fourth transcendant function of Painlevé, and therefore satisfies the equation

$$P_4''(x,\alpha)=\frac{(P_4'(x,\alpha))^2}{2P_4(x,\alpha)}-\frac{3\alpha}{2}P_4(x,\alpha)^3-2\alpha xP_4(x,\alpha)^2-\left(\frac{\alpha}{2}x^2+K_1\right)P_4(x,\alpha)+\frac{K_2}{P_4(x,\alpha)}. \tag{22}$$

K_1 and K_2 are integration constants. The potential therefore reads

$$\begin{aligned}V(x,y)=a(x^2+y^2)+\frac{\hbar}{2}b_1P_4'\left(x,\frac{-8a}{\hbar^2}\right)+4aP_4^2\left(x,\frac{-8a}{\hbar^2}\right)\\ +4axP_4\left(x,\frac{-8a}{\hbar^2}\right)+\frac{1}{6}(-\hbar^2K_1+\hbar b_1).\end{aligned} \tag{23}$$

This potential admits as special cases two anisotropic harmonic oscillators, $V=a(x^2+y^2)$ when $K_2=0$ (and $P_4=0$), and $V=a(x^2/9+y^2)$ when $K_1=0$ and $K_2=-\frac{1}{18}$ (and $P_4=-x/3$), as well as all their quantum deformations that have the form $V=a(p^2x^2+y^2)+f(x)$, that is, potentials V_d, V_e, V_j and V_k (up to a permutation of x and y).

The constant term in the potential, $(-\hbar^2K_1+\hbar b_1)$, can be set to zero, but we will keep it in order to be able to write the quantum and classical integrals in a unified way.

In classical mechanics, the equation (18) with $\hbar=0$ admits a first integral, which reads

$$c=\frac{(9V_1-ax^2)(V_1-ax^2)^3+k^2/4-k(V_1-ax^2)(3V_1+ax^2)}{x^2}.$$

We may therefore write the solution for V_1 implicitly as

$$cx^2-d^2+2d(V_1-ax^2)(3V_1+ax^2)=(9V_1-ax^2)(V_1-ax^2)^3, \tag{24}$$

where c and d are arbitrary constants. If $c=d=0$, we find either the familiar anisotropic harmonic oscillators, or a potential obtained by joining at $x=0$ two halves of anisotropic harmonic oscillators with different ratios. Even though this potential does not have a continuous second derivative, it can be obtained as a limiting case of the family of smooth superintegrable potentials (26).

In the general case the potential may be expressed as the root of a fourth-order polynomial with three arbitrary parameters (a, c and d), although we can set $a=1$ and one of the other two coefficients to ± 1 by scaling x and V_1.

Since Eq. (24) may describe new two-dimensional potentials with bounded motion, it is worth studying for interesting special cases. Indeed, if we assume $a>0$ and $d\geqslant 0$, we can consider the case $c=128a^4\tilde{d}^3/27^2$ and $d=4a^2\tilde{d}^2/27$. Four solutions exist in that case, two of which are translated harmonic oscillators. The remaining two potentials are

$$V=ay^2+\frac{a}{9}(2\tilde{d}+5x^2\pm 4x\sqrt{(\tilde{d}+x^2)}). \tag{25}$$

Up to an additive constant, potentials (25) are equal to

$$V=ay^2+\frac{a}{9}(x\pm 2\sqrt{\tilde{d}+x^2})^2. \tag{26}$$

Those potentials are smooth interpolations between anisotropic harmonic oscillators with ratio 1:1 and 1:3. When $\tilde{d}=0$ (and therefore $c=d=0$) they are the junctions of the two halves of harmonic oscillators mentioned above.

The integral of motion is similar in quantum and classical mechanics, and reads

$$X=\{L,p_x^2\}+\{ax^2y-3yV_1(x),p_x\}-\frac{1}{2a}\left\{\frac{\hbar^2}{4}V_{1xxx}+(ax^2-3V_1)V_{1x},p_y\right\}, \tag{27}$$

where V_1 is a solution to Eq. (24). Therefore the integral for (26) must be slightly modified to take into account the constant term we removed.

B. Case ii: $V=ay+V_1(x)$

Here we find again two equations:

$$\begin{aligned} 0&=\hbar^2A_{120}V_1^{(3)}-6A_{120}(V_1^2)'+12a^2A_{003}+\gamma_1V_1',\\ 0&=\frac{A_{030}}{4}(-6(V_1^2)'+\hbar^2V_1^{(3)})'-\frac{a}{2}A_{120}(6(xV_1)'+x^2V_1'')-aA_{021}((xV_1')'+2V_1')-\gamma_2V_1''+a\gamma_1. \end{aligned} \tag{28}$$

This time we cannot treat the equations separately, but we can, when $A_{120}\neq 0$, translate V to annihilate γ_1. Then we can substitute the first equation in the second to get rid of A_{030}, and finally translate x to get rid of A_{021}. We can then solve the remaining system, first by solving the second, linear equation, and then by substituting the result in the first one. The only solution remaining is then potential $V_n=ay+\hbar^2/x^2$. Hence we can set $A_{120}=0$, and therefore also $A_{003}=\gamma_1=0$ (as $V_1\neq bx$ and $a\neq 0$). In the second equation we can set $\gamma_2=0$. If then $A_{030}=0$, we find $V_1=a/x^2$ which was already classified. If $A_{030}\neq 0$ and $A_{021}=0$, though, the potential $V_1(x)$ is solution to

$$\hbar^2V_1''=6V_1^2+\lambda x+k. \tag{29}$$

If $\lambda\neq 0$, we can set $k=0$, and we find that V_1 can be expressed in terms of the first Painlevé transcendent:

$$V=ay+\hbar^2\omega^2P_1(\omega x), \tag{30}$$

with $\omega^5=\lambda/\hbar^4$.

The integral of motion is

$$X=2p_x^3+3\{V_2(x),p_x\}+\left\{\frac{\hbar^4\omega^5}{4a},p_y\right\}.$$

Notice that in order to consider the limiting case $a=0$, we can multiply the integral by a, and thus we find a potential that depends only on x with a trivial p_y integral. We can also set $\omega^5=a\omega^{5'}$ first, in which case we find the potentials (14). If we look for the classical limit, we find

$$V=ay+b\sqrt{x} \tag{31}$$

with the integral

$$X=2p_x^3+3b\{\sqrt{x},p_x\}-\left\{\frac{3b^2}{2a},p_y\right\}.$$

Returning to Eq. (29) and assuming $\lambda=0$, we find again that V_1 has the form (14), and the integral depends only on x and p_x.

Finally, if we set $A_{030}A_{021}\neq 0$, we have to solve the equation

$$0=\left(-\frac{3}{2}(V_1^2)'+\frac{\hbar^2}{4}V_1^{(3)}\right)'+b((xV_1')'+2V_1'),\quad b=\frac{-aA_{021}}{A_{030}}\neq 0. \tag{32}$$

It can be integrated once to give

$$C_1=-\frac{3}{2}(V_1^2)'+\frac{\hbar^2}{4}V_1^{(3)}+b((xV_1')+2V_1).$$

We can set $C_1=0$ by translations in x and V. The equation admits a first integral which reads

$$2b\hbar^2(V_1(x)-bx)V_1''(x)+b\hbar^2(2b-V_1'(x))V_1'(x)-8bV_1(x)(V_1(x)-bx)^2=k_1. \tag{33}$$

In the classical case, $\hbar=0$, this is enough to solve. The solution, which can be written implicitly in a more compact form, is given by

$$d=V_1(V_1-bx)^2, \tag{34}$$

where d is an arbitrary constant. When $d=0$ we find the familiar case $V=bx+ay$ which admits a first-order integral. We may notice that the implicit form of the solution is somewhat similar to (24).

In the quantum case, we notice that the transformation $W(x)=V_1(x)-bx$, that preserves the Painlevé property, simplifies Eq. (33) which becomes

$$\hbar^2(2WW''-W'^2)-8(W+bx)W^2=k_2 \tag{35}$$

or

$$W''=\frac{W'^2}{2W}+\frac{4W^2}{\hbar^2}+\frac{4bxW}{\hbar^2}+\frac{k_2}{2\hbar^2W}. \tag{36}$$

We can also substitute $Y(x)=\sqrt{W(x)}$ to find

$$\hbar^2Y''=2(Y^2+bx)Y+\frac{k_2}{4Y^3}.$$

If $k_2=0$, we can set $\hbar=1$ and $b=\frac{1}{2}$ by the change of variables

$$Y=(2\hbar b)^{1/3}Z,\quad x=\left(\frac{\hbar^2}{2b}\right)^{1/3}\xi.$$

The solution for $Z(\xi)$ is then a special case of the second Painlevé transcendant, defined by the equation

$$P_2''(x,\alpha)=2P_2(x,\alpha)^3+xP_2(x,\alpha)+\alpha.$$

The solution for V is

$$V(x,y)=bx+ay+(2\hbar b)^{2/3}P_2^2\left(\left(\frac{2b}{\hbar^2}\right)^{1/3}x,0\right), \tag{37}$$

with the particular case $V=bx+ay$.

Now if $k_2\neq 0$, we use (36), which can be normalized by a change of variables,

$$x=-\left(\frac{\hbar^2}{(4b)}\right)^{1/3}\xi, \quad W=-\frac{\sqrt{-k_2}}{(4\hbar b)^{1/3}}Y.$$

We then find

$$Y''=\frac{Y'^2}{2Y}+4\beta Y^2-\xi Y-\frac{1}{2Y}, \tag{38}$$

where $\beta=-\sqrt{-k_2}/(4\hbar b)\neq 0$ is an arbitrary constant. Equation (38) corresponds to case XXXIV, p. 340, in Ref. 18. The solution for $Y(\xi)$ reads

$$2\beta Y=P_2'\left(\xi,-2\beta-\frac{1}{2}\right)+P_2\left(\xi,-2\beta-\frac{1}{2}\right)^2+\frac{\xi}{2}, \tag{39}$$

where P_2 is once again the second Painlevé transcendant. Since β is an arbitrary constant, we can set $\kappa=-2\beta-\frac{1}{2}$.

Back to the original variables, we get

$$V(x,y)=ay+(2\hbar^2b^2)^{1/3}(P_2'(-(4b/\hbar^2)^{1/3}x,\kappa)+P_2^2(-(4b/\hbar^2)^{1/3}x,\kappa)). \tag{40}$$

This potential admits $V=ay$ and $V=ay+\hbar^2/x^2$ as particular cases.

In all cases with $V=ay+V_1(x)$ and $A_{012}A_{030}\neq 0$ the integral of motion is

$$2ap_x^3-2bp_x^2p_y+a\{3V_1(x)-bx,p_x\}-2b\{V_1(x),p_y\}. \tag{41}$$

Limiting values for a, b and $\hbar$ give either known potentials or trivial integrals.

C. Case iii: $A_{120}=A_{021}=0$

Since we set here $A_{120}=A_{021}=0$, we assume $A_{030}A_{003}\neq 0$ [otherwise we would find potentials of the form (14)]. The conditions for the existence of a third-order operator then read

$$\begin{aligned}\hbar^2V_1''(x)&=6V_1^2(x)+A_{003}\sigma x,\\ \hbar^2V_2''(y)&=6V_2^2(y)-A_{030}\sigma y.\end{aligned} \tag{42}$$

If σ vanishes, we find the potential

$$V=\hbar^2(\mathcal{P}(x)+\mathcal{P}(y)),$$

with two integrals that each depend on only one variable, as could have been predicted from the results of Eq. (13). If σ does not vanish, let us set $b_1=A_{003}\sigma$ and $b_2=-A_{030}\sigma$.

If $\hbar=0$, we find that

$$V=\pm\sqrt{\beta_1x}\pm\sqrt{\beta_2y}$$

is superintegrable, where the $\beta_i=b_i/6$ are arbitrary constants.

This defines similar real potentials on each quadrant of the plane. We can again patchwork the pieces to find real continuous potentials defined everywhere, e.g., $V=c_1\sqrt{|x|}+c_2\sqrt{|y|}$, although in that case neither the Hamiltonian nor the integral are differentiable at the equilibrium point.

Finally, if $\hbar \neq 0$, we find that V_1 and V_2 can be both written using the first Painlevé transcendent,

$$V = \hbar^2 \omega_1^2 P_1(\omega_1 x) + \hbar^2 \omega_2^2 P_1(\omega_2 y), \tag{43}$$

where the $\omega_i = (b_i/\hbar^4)^{1/5}$ are arbitrary constants.

The integral of motion is

$$X = 2b_2 p_x^3 - 2b_1 p_y^3 + 3b_2\{V_1(x,b_1),p_x\} - 3b_1\{V_2(y,b_2),p_y\}, \tag{44}$$

both in quantum and classical mechanics.

IV. CONCLUSION

We have found all systems in two-dimensional Euclidian space that admit separation of variables in Cartesian coordinates and at least one third-order integral, both in quantum and classical mechanics. Many new superintegrable potentials were found, and, interestingly, all the quantum superintegrable potentials are found as solutions of equations having the Painlevé property, and this is probably not accidental. Many of the quantum potentials can in fact be written in terms of different transcendent functions of Painlevé, and many are related to group invariant solutions of the Korteweg–de Vries equation, and to reductions of the Boussinesq and KP equations. All classical integrable potentials were found to be limiting cases of quantum ones. They do not obey equations having the Painlevé property, though, for many classical integrable potentials have movable branch points of the form $\sqrt{x-b}$. Thus, in that respect, quantum integrable potentials behave more regularly than classical ones. A natural question is what does the Painlevé property, in quantum mechanics, tell us about classical integrable potentials. Since this article deals mostly with the classification of superintegrable systems, the consideration of such questions regarding their properties and their solutions will be postponed to a future article.

Our investigation provided interesting new examples of the differences between quantum and classical integrability. A systematic search for systems with higher-order integrals is therefore a useful task since we still know little about such systems, and they are likely to share interesting properties.

Note added: The article mentioned earlier[12] indeed shows that superintegrability of separable systems has important physical implications. Even though the systems considered here can all be separated in two independent one-dimensional systems, two-dimensional superintegrability is useful to understand the one-dimensional properties of those separated systems.

Equations (2)–(5) are the necessary and sufficient conditions for the existence of third-order integrals. The general solution to these equations is highly nontrivial, and it is not likely that a direct approach will lead to such a solution for integrals of order higher than four, without the use of new methods. In order to develop such methods, it would be useful to have a rigorous definition of quantum integrability.

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APPENDIX

Here is the complete list of two-dimensional Hamiltonians separable in Cartesian coordinates that admit at least one third-order integral. We also gave all their third-order integrals. Potentials depending on only one Cartesian coordinate are not listed here, for they were classified in Ref. 13. Many of the potentials listed below were already known to be superintegrable, but we listed them

here for completeness and in some cases to take into account additional third-order integrals. Potentials in boxes are those who do not admit enough first- or second-order integrals to make them superintegrable. Most of them were not known before.

Some potentials (namely, V_p and V_q) are not superintegrable according to the usual definition, for their integrals have simple though nontrivial relations with the Hamiltonian. For definitions of parameters the reader is referred to the body of the article. In order to write the integrals of motion in a compact form we often use the notation $V(x,y)=V_1(x)+V_2(y)=V_1+V_2$.

1. Quantum potentials

$$\text{(Q.1)}\quad V=a(x^2+y^2)$$

$$X_1=L^3$$

$$X_2=\{L,p_xp_y\}+a\{2x^2y,p_y\}-a\{2xy^2,p_x\}$$

$$X_3=\{L,p_y^2\}+2a(\{xy^2,p_y\}-\{y^3,p_x\})$$

$$X_4=\{L,p_x^2\}-2a(\{x^2y,p_x\}-\{x^3,p_y\})$$

$$\text{(Q.2)}\quad V=a(x^2+y^2)+\frac{b}{x^2}+\frac{c}{y^2}$$

$$X_1=\{L,p_xp_y\}+\left\{xy\left(-\frac{2b}{x^3}+2ax\right),p_y\right\}-\left\{xy\left(-\frac{2c}{y^3}+2ay\right),p_x\right\}$$

$$\text{(Q.3)}\quad V=a(x^2+y^2)+\frac{\hbar^2}{x^2}+\frac{\hbar^2}{y^2}$$

$$X_1=2L^3-\hbar^2\left\{\frac{3x^2}{y}+2y+\frac{3y^3}{x^2},p_x\right\}+\hbar^2\left\{\frac{3y^2}{x}+2x+\frac{3x^3}{y^2},p_y\right\}$$

$$X_2=\{L,p_xp_y\}+\left\{xy\left(-\frac{2\hbar^2}{x^3}+2ax\right),p_y\right\}-\left\{xy\left(-\frac{2\hbar^2}{y^3}+2ay\right),p_x\right\}$$

$$\text{(Q.4)}\quad V=a(x^2+y^2)+\frac{\hbar^2}{y^2}$$

$$X_1=2L^3-\hbar^2\left\{2y+\frac{3x^2}{y},p_x\right\}+\hbar^2\left\{\frac{3x^3}{y^2}+2x,p_y\right\}$$

$$X_2=\{L,p_xp_y\}-2\left\{axy^2-\frac{\hbar^2x}{y^2},p_x\right\}+2a\{x^2y,p_y\}$$

$$X_3=\{L,p_y^2\}-\left\{2ay^3+\hbar^2\frac{1}{y},p_x\right\}+\left\{\hbar^2\frac{3x}{y^2}+2axy^2,p_y\right\}$$

$$\text{(Q.5)}\quad \boxed{V=\hbar^2\left(\frac{1}{8\alpha^4}(x^2+y^2)+\frac{1}{(x-\alpha)^2}+\frac{1}{(x+\alpha)^2}\right)}$$

$$X_1=2L^3-3\alpha^2\{L,p_y^2\}+\frac{\hbar^2}{4}\left\{y\left(-8+\frac{3y^2}{\alpha^2}-\frac{24y^2(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2}\right),p_x\right\}$$
$$+\frac{\hbar^2}{4}\left\{x\left(8-\frac{3y^2(x^4-10\alpha^2x^2-24\alpha^4)}{\alpha^2(x-\alpha)^2(x+\alpha)^2}\right),p_y\right\}$$

$$X_2=\{L,p_x^2\}+\hbar^2\left\{y\left(\frac{4\alpha^2-x^2}{4\alpha^4}-\frac{6(x^2+\alpha^2)}{(x^2-\alpha^2)^2}\right),p_x\right\}$$
$$+\hbar^2\left\{\frac{x(x^2-4\alpha^2)}{4\alpha^4}-\frac{2x}{x^2-\alpha^2}+\frac{4x(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2},p_y\right\}$$

$$\text{(Q.6)}\quad \boxed{V=\hbar^2\left(\frac{1}{8\alpha^4}(x^2+y^2)+\frac{1}{y^2}+\frac{1}{(x+\alpha)^2}+\frac{1}{(x-\alpha)^2}\right)}$$

$$X_1=2L^3-3\alpha^2\{L,p_y^2\}+\hbar^2\left\{\frac{3y^3}{4\alpha^2}+\frac{6y^3(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2}-\frac{3(x^2-\alpha^2)}{y}-2y,p_x\right\}$$
$$+3\hbar^2\left\{x\left(\frac{x^2-3\alpha^2}{y^2}-\frac{3y^2-8\alpha^2}{12\alpha^2}-\frac{2y^2}{x^2-\alpha^2}+\frac{4y^2(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2}\right),p_y\right\}$$

$$\text{(Q.7)}\quad \boxed{V=\hbar^2\left(\frac{1}{8\alpha^4}(x^2+y^2)+\frac{1}{(y-\alpha)^2}+\frac{1}{(x-\alpha)^2}+\frac{1}{(y+\alpha)^2}+\frac{1}{(x+\alpha)^2}\right)}$$

$$X_1=2L^3-3\alpha^2(\{L,p_x^2\}+\{L,p_y^2\})+\frac{\hbar^2}{4}\left\{y\left(124+\frac{3(x^2+y^2)}{\alpha^2}+\frac{24(x^2-5y^2)}{y^2-\alpha^2}-\frac{144x^2}{x^2-\alpha^2}\right.\right.$$
$$\left.+\frac{24(3x^2-y^2)(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2}+\frac{48(y^2-x^2)(y^2+\alpha^2)}{(y-\alpha)^2(y+\alpha)^2}\right),p_x\Big\}-\frac{\hbar^2}{4}\left\{x\left(124+\frac{3(x^2+y^2)}{\alpha^2}\right.\right.$$
$$\left.\left.-\frac{24(5x^2-y^2)}{x^2-\alpha^2}-\frac{144x^2}{y^2-\alpha^2}-\frac{24(x^2-3y^2)(y^2+\alpha^2)}{(y-\alpha)^2(y+\alpha)^2}+\frac{48(x^2-y^2)(x^2+\alpha^2)}{(x-\alpha)^2(x+\alpha)^2}\right),p_y\right\}$$

$$\text{(Q.8)}\quad V=a(4x^2+y^2)+\frac{b}{y^2}+cx$$

$$X_1=2p_xp_y^2+\left\{-2ay^2+\frac{2b}{y^2},p_x\right\}+\{8axy+cy,p_y\}$$

$$\text{(Q.9)}\quad \boxed{V=a(9x^2+y^2)}$$

$$X_1=\{L,p_y^2\}+\tfrac{2}{3}a\{y^3,p_x\}-6a\{xy^2,p_y\}$$

$$\text{(Q.10)}\quad \boxed{V=a(9x^2+y^2)+\frac{\hbar^2}{y^2}}$$

$$X_1=\{L,p_y^2\}+\left\{\frac{2ay^3}{3}-\frac{\hbar^2}{y},p_x\right\}+\left\{3x\left(-2ay^2+\frac{\hbar^2}{y^2}\right),p_y\right\}$$

$$(\text{Q.11})\quad \boxed{V=\hbar^2\left(\frac{1}{8\alpha^4}(9x^2+y^2)+\frac{1}{(y+\alpha)^2}+\frac{1}{(y-\alpha)^2}\right)}$$

$$X_1=\{L,p_y^2\}+\hbar^2\left\{y\left(\frac{y^2}{12\alpha^4}-\frac{8\alpha^2}{(y^2-\alpha^2)^2}-\frac{2}{y^2-\alpha^2}\right),p_x\right\}+\frac{3\hbar^2}{4}\left\{x\left(\frac{8(y^2+\alpha^2)}{(y^2-\alpha^2)^2}-\frac{y^2}{\alpha^4}\right),p_y\right\}$$

$$(\text{Q.12})\quad \boxed{V=\frac{\hbar^2}{x^2}+\frac{a}{y^2}}$$

$$X_1=\{L^2,p_x\}-2\hbar^2\left\{\frac{y^2}{x^2},p_y\right\}+\left\{3\hbar^2\frac{y^2}{x^2}+2a\frac{x^2}{y^2}+\frac{\hbar^2}{2},p_x\right\}$$

$$X_2=\{L,p_xp_y\}-2\hbar^2\left\{\frac{y}{x^2},p_y\right\}+2a\left\{\frac{x}{y^2},p_x\right\}$$

$$X_3=2p_x^3+\left\{\frac{3\hbar^2}{x^2},p_x\right\}$$

$$(\text{Q.13})\quad \boxed{V=\frac{\hbar^2}{x^2}+\frac{\hbar^2}{y^2}}$$

$$X_1=2L^3-\hbar^2\left\{2y+\frac{3x^2}{y}+\frac{3y^3}{x^2},p_x\right\}+\hbar^2\left\{2x+\frac{3y^2}{x}+\frac{3x^3}{y^2},p_y\right\}$$

$$X_2=\{L^2,p_x\}-2\hbar^2\left\{\frac{y}{x},p_y\right\}+\left\{3\hbar^2\frac{y^2}{x^2}+2\hbar^2\frac{x^2}{y^2}+\frac{\hbar^2}{2},p_x\right\}$$

$$X_3=\{L^2,p_y\}-2\hbar^2\left\{\frac{x}{y},p_x\right\}+\left\{3\hbar^2\frac{x^2}{y^2}+2\hbar^2\frac{y^2}{x^2}+\frac{\hbar^2}{2},p_x\right\}$$

$$X_4=\{L,p_xp_y\}-2\hbar^2\left\{\frac{y}{x^2},p_y\right\}+2\hbar^2\left\{\frac{x}{y^2},p_x\right\}$$

$$X_5=2p_x^3+\left\{\frac{3\hbar^2}{x^2},p_x\right\}$$

$$X_6=2p_y^3+\left\{\frac{3\hbar^2}{y^2},p_y\right\}$$

$$(\text{Q.14})\quad V=ax+\frac{\hbar^2}{y^2}$$

$$X_1=\{L,p_y^2\}-\left\{\frac{\hbar^2}{y},p_x\right\}+\left\{3\frac{\hbar^2x}{y^2}-a\frac{y^2}{2},p_y\right\}$$

$$X_2=2p_y^3+\left\{3\frac{\hbar^2}{y^2},p_y\right\}$$

$$X_3 = 2p_x p_y^2 + 2\hbar^2\left\{\frac{1}{y^2}, p_x\right\} + a\{y, p_y\}$$

$$\text{(Q.15)}\quad \boxed{V = \hbar^2\mathcal{P}(y) + V(x)}$$

$$X_1 = 2p_y^3 + \{3\hbar^2\mathcal{P}(y), p_y\}$$

$$\text{(Q.16)}\quad \boxed{V = \hbar^2(\mathcal{P}(x) + \mathcal{P}(y))}$$

$$X_1 = 2p_x^3 + \{3\hbar^2\mathcal{P}(x), p_x\}$$

$$X_2 = 2p_y^3 + \{3\hbar^2\mathcal{P}(y), p_y\}$$

$$\text{(Q.17)}\quad \boxed{V = \hbar^2\omega_1^2 P_1(\omega_1 x) + \hbar^2\omega_2^2 P_1(\omega_2 y)}$$

$$X_1 = 2\omega_2^5 p_x^3 - 2\omega_1^5 p_y^3 + 3\omega_2^5\{V_1(x,\omega_1), p_x\} - 3\omega_1^5\{V_2(y,\omega_2), p_y\}$$

$$\text{(Q.18)}\quad \boxed{V = a(x^2+y^2) + \frac{\hbar}{2}b_1 P_4'\left(x, \frac{-8a}{\hbar^2}\right) + 4aP_4^2\left(x, \frac{-8a}{\hbar^2}\right) + 4axP_4\left(x, \frac{-8a}{\hbar^2}\right) + \frac{1}{6}(-\hbar^2 K_1 + \hbar b_1)}$$

$$X_1 = \{L, p_x^2\} + \{ax^2 y - 3yV_1, p_x\} - \frac{1}{2a}\left\{\frac{\hbar^2}{4}V_{1xxx} + (ax^2 - 3V_1)V_{1x}, p_y\right\}$$

$$\text{(Q.19)}\quad \boxed{V = ay + \hbar^2\omega^2 P_1(\omega x)}$$

$$X_1 = 2p_x^3 + 3\hbar^2\omega^2\{P_1(\omega x), p_x\} + \left\{\frac{\omega^5\hbar^4}{4a}, p_y\right\}$$

$$\text{(Q.20)}\quad \boxed{V = bx + ay + (2\hbar b)^{2/3}P_2^2\left(\left(\frac{2b}{\hbar^2}\right)^{1/3}x, 0\right)}$$

$$X_1 = 2ap_x^3 - 2bp_x^2 p_y + a\{3V_1(x) - bx, p_x\} - 2b\{V_1(x), p_y\}$$

$$\text{(Q.21)}\quad \boxed{V = ay + (2\hbar^2 b^2)^{1/3}(P_2'(-(4b/\hbar^2)^{1/3}x, \kappa) + P_2^2(-(4b/\hbar^2)^{1/3}x, \kappa))}$$

$$X_1 = 2ap_x^3 - 2bp_x^2 p_y + a\{3V_1(x) - bx, p_x\} - 2b\{V_1(x), p_y\}$$

2. Classical potentials

$$\text{(C.1)}\quad V = a(x^2+y^2)$$

$$X_1 = L^3$$

$$X_2 = \{L, p_x p_y\} + a\{2x^2 y, p_y\} - a\{2xy^2, p_x\}$$

$$X_3 = \{L, p_y^2\} + 2a(\{xy^2, p_y\} - \{y^3, p_x\})$$

$$X_4 = \{L, p_x^2\} - 2a(\{x^2 y, p_x\} - \{x^3, p_y\})$$

$$(\text{C.2})\quad V=a(x^2+y^2)+\frac{b}{x^2}+\frac{c}{y^2}$$

$$X_1=\{L,p_xp_y\}+\left\{xy\left(-\frac{2b}{x^3}+2ax\right),p_y\right\}-\left\{xy\left(-\frac{2c}{y^3}+2ay\right),p_x\right\}$$

$$(\text{C.3})\quad V=a(4x^2+y^2)+\frac{b}{y^2}+cx$$

$$X_1=2p_xp_y^2+\left\{-2ay^2+\frac{2b}{y^2},p_x\right\}+\{8axy+cy,p_y\}$$

$$(\text{C.4})\quad \boxed{V=a(9x^2+y^2)}$$

$$X_1=\{L,p_y^2\}+\tfrac{2}{3}a\{y^3,p_x\}-6a\{xy^2,p_y\}$$

$$(\text{C.5})\quad \boxed{V=\pm\sqrt{\beta_1 x}\pm\sqrt{\beta_2 y}}$$

$$X_1=2\beta_2p_x^3-2\beta_1p_y^3+3\beta_2\{V_1(x,6\beta_1),p_x\}-3\beta_1\{V_2(y,6\ b_2),p_y\}$$

$$(\text{C.6})\quad \boxed{V=ay^2+V_1}\quad \text{where } V_1 \text{ satisfies Eq. (24)}$$

$$X_1=\{L,p_x^2\}+\{ax^2y-3yV_1,p_x\}-\frac{1}{2a}\{(ax^2-3V_1)V_{1x},p_y\}$$

$$(\text{C.7})\quad \boxed{V=ay+b\sqrt{x}}$$

$$X_1=2p_x^3+3b\{\sqrt{x},p_x\}-\left\{\frac{3b^2}{2a},p_y\right\}$$

$$(\text{C.8})\quad \boxed{V=ay+V_1(x)},\quad \text{where } (V_1-bx)^2V_1=d$$

$$X_1=2ap_x^3-2bp_x^2p_y+a\{3V_1(x)-bx,p_x\}-2b\{V_1(x),p_y\}$$

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Equations of arbitrary order invariant under the Kadomtsev–Petviashvili symmetry group

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By means of a simple new approach, a general Kadomtsev–Petviashvili (KP) family with an arbitrary function of group invariants of arbitrary order is proposed. It is proved that the general KP family possesses a common infinite dimensional Kac–Moody–Virasoro Lie point symmetry algebra. The known fourth order one can be re-obtained as a special example. The finite transformation group is presented in a clearer form. The Kac–Moody–Virasoro group invariant solutions and the Kac–Moody group invariant solutions of the KP family are determined by the Boussinesq and KdV families, respectively. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The symmetry study plays a very important role in the nonlinear science. Especially, in the study of $(2+1)$-dimensional integrable models, it is found that for all the known integrable systems there is an isomorphic centerless Virasoro symmetry algebra (Witt algebra):[1–9]

$$[\sigma(f_1),\ \sigma(f_2)]=\sigma(f_2\dot{f}_1-f_1\dot{f}_2), \tag{1.1}$$

where f_1 and f_2 are arbitrary functions of a single independent variable. The dot over the functions f_1 and f_2 denotes the derivative of the functions with respect to their argument. In Ref. 7, a method was established to obtain the models with centerless Virasoro symmetry algebras. In Ref. 3, Güngör and Winternitz pointed out that the variable coefficient Kadomtsev–Petviashvili (KP) equation,

$$\begin{aligned}&[u_t+p(t)uu_x+q(t)u_{xxx}]_x+\sigma(y,t)u_{yy}+a(y,t)u_y\\&\quad+b(y,t)u_{xy}\ c(y,t)u_{xx}+e(y,t)u_x+f(y,t)u+h(y,t)=0,\end{aligned} \tag{1.2}$$

possesses the Virasoro symmetry algebra (1.1) iff it can be transformed to the usual *integrable* constant coefficient KP equation,

$$(u_t+\tfrac{3}{2}uu_x+u_{xxx})_x+\tfrac{3}{4}\delta u_{yy}=0,\quad \delta=\pm 1. \tag{1.3}$$

By using the standard group approach, David, Levi and Winternitz[4] had proved that

$$(u_t+\tfrac{3}{2}uu_x)_x+\tfrac{3}{4}\delta u_{yy}+u_{xx}^{3/2}H(K_2,\ldots,K_{10})=0, \tag{1.4}$$

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with $H(K_2,\ldots,K_{10})$ being an arbitrary function of $K_2,\ldots,K_{10}$ is the only fourth order KP family with the same Kac–Moody–Virasoro symmetry algebra of the usual KP equation. In (1.4), $K_2,\ldots,K_{10}$ are defined by

$$K_2=u_{xxxx}u_{xx}^{-3/2}, \tag{1.5}$$

$$K_3=u_{xxx}u_{xx}^{-5/4}, \tag{1.6}$$

$$K_4=(u_{xx}u_{xxy}-u_{xxx}u_{xy})u_{xx}^{-5/2}, \tag{1.7}$$

$$K_5=(u_{xxx}u_{xyy}-u_{xxy}^2-2\delta u_x u_{xx}u_{xxx})u_{xx}^{-3}, \tag{1.8}$$

$$K_6=[u_{xxx}^2u_{yyy}+2u_{xxy}^3-3u_{xxx}u_{xyy}u_{xxy}+6\delta u_x u_{xxx}(u_{xx}u_{xxy}-u_{xy}u_{xxx})]u_{xx}^{-9/2}, \tag{1.9}$$

$$K_7=(u_{xx}u_{xxxy}-u_{xxxx}u_{xy})u_{xx}^{-11/4}, \tag{1.10}$$

$$K_8=(u_{xxxx}u_{xxyy}-u_{xxxy}^2-2\delta u_x u_{xxx}u_{xxxx})u_{xx}^{-7/2}, \tag{1.11}$$

$$K_9=[u_{xxxx}^2u_{xyyy}+2u_{xxxy}^3-3u_{xxxx}u_{xxyy}u_{xxxy}+6\delta u_x u_{xxxx}(u_{xxx}u_{xxxy}-u_{xxy}u_{xxxx})]u_{xx}^{-21/4}, \tag{1.12}$$

$$\begin{aligned}K_{10}=[&u_{xxxx}u_{yyyy}+2u_{xxyy}^2-4u_{xyyy}u_{xxxy}+12u_x^2(u_{xx}u_{xxxx}+u_{xxx}^2)\\&-12\delta u_x(u_{xyy}u_{xxxx}-2u_{xxy}u_{xxxy}+u_{xxx}u_{xxyy})]u_{xx}^{-4}.\end{aligned} \tag{1.13}$$

In Ref. 5, it is proved that a special type of arbitrary order equation,

$$\left(u_t+\frac{3}{2}uu_x+u_{xxx}\right)_x+\frac{3}{4}\delta u_{yy}+\sum_{n=2}^{M}C_n u_{nx}^{6/(n+2)}=0\quad(M=2,\ 3,\ldots), \tag{1.14}$$

also possesses the symmetry group of the KP equation. In this paper, by using a simple new method, we concentrate on giving some types of autonomous higher order KP family,

$$(u_t+\tfrac{3}{2}uu_x+u_{xxx})_x+\tfrac{3}{4}\delta u_{yy}+F(u)=0, \tag{1.15}$$

which possess a same infinite dimensional Kac–Moody–Virasoro Lie point symmetry algebra, where

$$F(u)\equiv F(u,\ u_x,\ u_{xx},\ldots,u_{x^ny^mt^l},\ \ldots)\equiv F \tag{1.16}$$

is an undetermined function of the field u and its any order derivatives of x, y and t but not explicitly space–time dependent.

II. REVIEW ON THE LIE POINT SYMMETRIES AND FINITE TRANSFORMATIONS OF THE KP EQUATION

The Lie point symmetries and the related Kac–Moody–Virasoro algebra of the usual KP equation (1.3) have been first given by David, Kamran, Levi, and Winternitz[1] by using the standard classical Lie approach.[10,11] The generalized symmetries and the corresponding generalized w_∞ symmetry algebra is obtained by Lou via the formal series symmetry approach.[12,13]

A symmetry σ of the KP equation is a solution of its linearized equation,

$$(\sigma_t+\tfrac{3}{2}\sigma u_x+\tfrac{3}{2}u\sigma_x+\sigma_{xxx})_x+\tfrac{4}{3}\delta\sigma_{yy}=0, \tag{2.1}$$

which means (1.3) is form invariant under the transformation

$$u \to u + \epsilon\sigma,$$

where ϵ is an infinitesimal parameter.

According to the results of Ref. 1, the full Lie point symmetries of the KP equation (1.3) are the linear combinations of the following generators:

$$\sigma_0(h) = hu_x - \tfrac{2}{3}\dot{h}, \tag{2.2}$$

$$\sigma_1(g) = -2gu_y + \tfrac{4}{3}\delta\dot{g}yu_x - \tfrac{8}{9}\delta y\ddot{g}, \tag{2.3}$$

and

$$\sigma_2(f) = fu_t + \tfrac{1}{3}(x\dot{f} - \tfrac{2}{3}\delta y^2\ddot{f})u_x + \tfrac{2}{3}\dot{f}(yu)_y - \tfrac{4}{27}(\tfrac{3}{2}x\ddot{f} - \delta y^2\dddot{f}), \tag{2.4}$$

where f, g, and h are all arbitrary functions of t.

The Kac–Moody–Virasoro type algebra constituted by $\sigma_0(h), \sigma_1(g)$ and $\sigma_2(f)$ reads as

$$[\sigma_0(h_1),\ \sigma_0(h_2)] = [\sigma_0(h),\ \sigma_1(g)] = 0, \tag{2.5}$$

$$[\sigma_1(g_1),\ \sigma_1(g_2)] = \tfrac{2}{3}\sigma_0(\dot{g}_1 g_2 - \dot{g}_2 g_1), \tag{2.6}$$

$$[\sigma_2(f),\ \sigma_0(h)] = \tfrac{1}{3}\sigma_0(\dot{f}h - 3\dot{h}f), \tag{2.7}$$

$$[\sigma_2(f),\ \sigma_1(g)] = \tfrac{1}{3}\sigma_1(2\dot{f}g - 3\dot{g}f), \tag{2.8}$$

$$[\sigma_2(f_1),\ \sigma_2(f_2)] = \sigma_2(\dot{f}_1 f_2 - \dot{f}_2 f_1), \tag{2.9}$$

while the commutator $[G, H]$ of $G \equiv G(u)$ and $H \equiv H(u)$ is defined by

$$[G,\ H] = \lim_{\epsilon \to 0} \frac{\partial}{\partial \epsilon}(G(u + \epsilon H) - H(u + \epsilon G)) \equiv G'H - H'G. \tag{2.10}$$

From (2.9) we know that the subalgebra constituted by $\sigma_2(f)$ is just the Virasoro algebra (1.1).

The general finite transformations related to the symmetries (2.2)–(2.4) had also been given in Ref. 1. Here we rewrite them down in a much simpler and slightly extended form:

Theorem 1: *If $u = u(x,y,t)$ is a solution of the KP equation (1.3) then so also is u' with*

$$u' = \tau_t^{2/3} u(\xi, \eta, \tau) - \frac{2(\ln \tau_t)_t}{9}x - \frac{4\delta\tau_t^{1/3}}{9}\left[(\tau_t^{-1/3})_t y - \frac{\alpha_t}{\tau_t}\right]_t y - \frac{2\beta_t}{3\tau_t^{1/3}} - \frac{2\delta\alpha_t^2}{9\tau_t^{4/3}}, \tag{2.11}$$

where

$$\xi = \tau_t^{1/3}x - \frac{2\delta}{9}\left(\frac{\tau_{tt}}{\tau_t^{2/3}}y^2 + \frac{3\alpha_t}{\tau_t^{1/3}}y\right) + \beta, \tag{2.12}$$

$$\eta = \tau_t^{2/3}y + \alpha, \tag{2.13}$$

and $\{\tau \equiv \tau(t),\ \alpha \equiv \alpha(t),\ \beta \equiv \beta(t)\}$ are arbitrary functions of t.

III. A KP FAMILY WITH A COMMON KAC–MOODY–VIRASORO SYMMETRY ALGEBRA

In this section, we look for the possible equations which possess the totally same symmetries (2.2)–(2.4) and then the Kac–Moody–Virasoro type symmetry algebra (2.5)–(2.9).

A. Models with the Virasoro symmetry (2.4)

The symmetry equation of (1.15) has the form

$$(\sigma_t+\tfrac{3}{2}\sigma u_x+\tfrac{3}{2}u\sigma_x+\sigma_{xxx})_x+\tfrac{3}{4}\delta\sigma_{yy}+F'\sigma=0, \tag{3.1}$$

where F' is the linearized operator of F defined by

$$F'G=\lim_{\epsilon\to 0}\frac{\partial}{\partial\epsilon}F(u+\epsilon G) \tag{3.2}$$

for arbitrary G.

The substitution (2.4) into (3.1) yields

$$\begin{aligned}&\left[f\partial_t+\frac{1}{3}\dot f(x\partial_x+2y\partial_y+6)-\frac{2\delta}{9}y^2\ddot f\partial_x\right]\left(u_{xt}+\frac{3}{2}uu_{xx}+\frac{3}{2}u_x^2+u_{xxxx}+\frac{3}{4}\delta u_{yy}\right)\\&\quad+F'\left[fu_t+\frac{1}{3}\left(x\dot f-\frac{2\delta}{3}y^2\ddot f\right)u_x+\frac{2}{3}\dot f(yu)_y-\frac{4}{27}\left(\frac{3}{2}x\ddot f-\delta y^2\dddot f\right)\right]=0.\end{aligned} \tag{3.3}$$

The use of (1.15) and the elimination of u_{xt} from (3.3) lead to

$$\begin{aligned}&F'\left[fu_t+\frac{1}{3}\left(x\dot f-\frac{2\delta}{3}y^2\ddot f\right)u_x+\frac{2}{3}\dot f(yu)_y-\frac{4}{27}\left(\frac{3}{2}x\ddot f-\delta y^2\dddot f\right)\right]\\&\quad-\left[fF'u_t+\frac{1}{3}\dot f(xF'u_x+2yF'u_y+6F)-\frac{2\delta}{9}y^2\ddot fF'u_x\right]=0.\end{aligned} \tag{3.4}$$

According to the definitions of the function F (1.16) and its linearized operator F' (3.2), we have

$$F'=\sum_{n,m,l}\frac{\partial F}{\partial u_{x^ny^mt^l}}\frac{\partial^{n+m+l}}{\partial x^n\partial y^m\partial t^l},\quad m,n,l\geqslant 0. \tag{3.5}$$

The substitution (3.5) into (3.4) leads to

$$\begin{aligned}&\sum_{n,m,l}\sum_{i=0}^{l-1}C_l^i\frac{\partial F}{\partial u_{x^ny^mt^l}}\left[f^{(l-i)}\partial_t+\frac{f^{(l-i+1)}}{3}(x\partial_x+2y\partial_y)-\frac{2\delta f^{(l-i+2)}}{9}y^2\partial_x\right]u_{x^ny^mt^i}\\&\quad+\sum_{n,m,l}\sum_{i=0}^{l}C_l^i\frac{\partial F}{\partial u_{x^ny^mt^l}}\left[\frac{n}{3}f^{(l-i+1)}\partial_y^2-\frac{2m\delta}{9}f^{(l-i+2)}(2y\partial_y+m-1)\partial_x\right.\\&\quad\left.+\frac{2}{3}(m+1)f^{(l-i+1)}\partial_y^2\right]u_{x^ny^{m-2}t^i}-\sum_l\left[\frac{2}{9}f^{(l+2)}\left(\frac{\partial F}{\partial u_{xt^l}}+x\frac{\partial F}{\partial u_{t^l}}\right)\right.\\&\quad\left.-\frac{4\delta}{27}f^{(l+3)}\left(2\frac{\partial F}{\partial u_{yyt^l}}+2y\frac{\partial F}{\partial u_{yt^l}}+y^2\frac{\partial F}{\partial u_{t^l}}\right)\right]=2\dot fF,\end{aligned} \tag{3.6}$$

where

$$C_{l'}^i\equiv\frac{l'!}{i!(l'-i)!},\quad u_{x^{-n}y^{-m}t^{-l}}=0,\ \forall n\geqslant 1,\ m\geqslant 1,\ l\geqslant 1. \tag{3.7}$$

If we can find an f-independent solution F from (3.6), then we get a model with a Virasoro symmetry (2.4) for arbitrary f. Under the f-independent requirement and the autonomous condition of F, (3.6) is equivalent to the following equation system:

$$\sum_{n,m,l}(n+3l+2m+2)u_{x^n y^m t^l}\frac{\partial F}{\partial u_{x^n y^m t^l}}=6F, \tag{3.8}$$

$$\sum_{n,m,l}(l+1)\frac{\partial F}{\partial u_{x^n y^m t^{l+1}}}u_{x^{n+1}y^m t^l}-\frac{2}{3}\frac{\partial F}{\partial u}=0, \tag{3.9}$$

$$\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^l}}\left(\frac{3}{2}\delta l\partial_y^2-m\partial_x\partial_t\right)u_{x^n y^{m-1}t^{l-1}}=0, \tag{3.10}$$

$$\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^l}}\left[l(3l+n+2m-4)\partial_y^2-\frac{2m\delta}{3}(m-1)\partial_x\partial_t\right]u_{x^n y^{m-2}t^{l-1}}-\frac{2}{3}\frac{\partial F}{\partial u_x}=0, \tag{3.11}$$

$$\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^{l+2}}}u_{x^{n+1}y^m t^{l-k}}-\frac{2}{9}\frac{\partial F}{\partial u_{t^{k+1}}}=0, \tag{3.12}$$

$$\frac{2}{3}\frac{\partial F}{\partial u_{t^k}}-\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^{l+1}}}C_l^{l-k}u_{x^{n+1}y^m t^{l-k}}=0, \tag{3.13}$$

$$\frac{2}{3}\frac{\partial F}{\partial u_{yt^k}}+\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^{l+2}}}\left[\frac{3}{2}\delta C_l^{l-k}\partial_y^2-mC_l^{l-k+1}\partial_x\partial_t\right]u_{x^n y^{m+1}t^{l-k}}=0, \tag{3.14}$$

$$\begin{aligned}&2\frac{\partial F}{\partial u_{yyt^k}}-\frac{3}{2}\delta\frac{\partial F}{\partial u_{xt^{k+1}}}+\frac{3}{4}\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^{l+3}}}\{3\delta[3C_l^{l-k}+C_l^{l-k+1}(n+2m+2)]\partial_y^2\\&-2m(m-1)C_l^{l-k+2}\partial_x\partial_t\}u_{x^n y^{m-2}t^{l-k+1}}=0,\end{aligned} \tag{3.15}$$

where $k=0,\ 1,\ 2,\ldots,$ for (3.12)–(3.15).

To solve the full equation system (3.8)–(3.15) is still quite difficult. However, if we require that the function F is $u_{x^n y^m t^l}$ independent for $l\geqslant 1$, then (3.8)–(3.15) are reduced to

$$\frac{\partial F}{\partial u}=\frac{\partial F}{\partial u_y}=\frac{\partial F}{\partial u_{yy}}=0, \tag{3.16}$$

$$\sum_{n,m}(n+2m+2)u_{x^n y^m}\frac{\partial F}{\partial u_{x^n y^m}}=6F, \tag{3.17}$$

$$\sum_{n,m}mu_{x^{n+1}y^{m-1}}\frac{\partial F}{\partial u_{x^n y^m}}=0, \tag{3.18}$$

$$\sum_{n,m}m(m-1)u_{x^{n+1}y^{m-2}}\frac{\partial F}{\partial u_{x^n y^m}}+\delta\frac{\partial F}{\partial u_x}=0. \tag{3.19}$$

The general solution of (3.16)–(3.17) reads as

$$F=u_{xx}^{3/2}F_1(v_{nm},n,m=0,\ 1,\ 2,\ \ldots,\ \{n,\ m\}\neq\{0,\ 0\},\ \{0,\ 1\},\ \{0,\ 2\})\equiv u_{xx}^{3/2}F_1, \tag{3.20}$$

$$v_{nm}\equiv v_{n,m}\equiv u_{x^n y^m}u_{xx}^{-(n+2m+2)/4}. \tag{3.21}$$

Substituting (3.20) with (3.21) into (3.18) and (3.19), we have

$$\sum_{n,m} m v_{n+1,m-1}\frac{\partial F_1}{\partial v_{nm}}=0, \tag{3.22}$$

$$\sum_{n,m} m(m-1)v_{n+1,m-2}\frac{\partial F_1}{\partial v_{nm}}+\delta\frac{\partial F_1}{\partial v_{10}}=0. \tag{3.23}$$

The general solution of (3.22) has the form of

$$F_1=F_2(y_{nm},n,m=0,\ 1,\ 2,\ \ldots,\ \{n,\ m\}\neq\{0,\ 0\},\ \{0,\ 1\},\ \{0,\ 2\})\equiv F_2, \tag{3.24}$$

$$y_{nm}\equiv y_{n,m}\equiv\sum_{k=0}^{m}(-1)^{m-k}C_m^k v_{n+m-k,k}v_{11}^{m-k}=\sum_{k=0}^{m}(-1)^{m-k}C_m^k u_{x^{n+m-k}y^k}u_{xy}^{m-k}u_{xx}^{(4k-n-6m-2)/4}. \tag{3.25}$$

After finishing some tedious calculations, we know that the substitution of (3.24) into (3.23) yields

$$\sum_{n,m} m(m-1)y_{n+1,m-2}\frac{\partial F_2}{\partial y_{nm}}+\delta\frac{\partial F_2}{\partial y_{10}}=0. \tag{3.26}$$

The general solution of (3.26) reads as

$$F_2=F_0(K_{n,m},m,\ n=0,\ 1,\ 2,\ \ldots)\equiv F_0, \tag{3.27}$$

where F_0 is an arbitrary function of K_{nm} and K_{nm} is given by the following recursion relation

$$K_{nm}=y_{nm}-\sum_{j=1}^{[m/2]}\frac{m!}{j!(m-2j)!}K_{n+j,m-2j}(\delta y_{10})^j, \tag{3.28}$$

with ($\delta_{ii}=1,\ \delta_{ij}=0,\ i\neq j$)

$$K_{n0}=(1-\delta_{n,0}-\delta_{n,1})y_{n0}=(1-\delta_{n,0}-\delta_{n,1})u_{x^n}u_{xx}^{-(n+2)/4}, \tag{3.29}$$

$$K_{n1}=(1-\delta_{n,0})y_{n1}=(1-\delta_{n,0})(u_{x^n y}u_{xx}-u_{xy}u_{x^{n+1}})u_{xx}^{-(n+8)/4}. \tag{3.30}$$

Some further concrete examples of K_{nm} are

$$K_{n2}=(1-\delta_{n,0})(u_{x^n y^2}u_{xx}^2-2u_{x^{n+1}y}u_{xx}u_{xy}+u_{x^{n+2}}u_{xy}^2-2\delta u_{x^{n+1}}u_x u_{xx}^2)u_{xx}^{-(n+14)/4}, \tag{3.31}$$

$$\begin{aligned}K_{n3}=&(u_{x^n y^3}u_{xx}^3-3u_{x^{n+1}y^2}u_{xx}^2u_{xy}+3u_{x^{n+2}y}u_{xx}u_{xy}^2-u_{x^{n+3}}u_{xy}^3)u_{xx}^{-(n+20)/4}\\&-6\delta u_x(u_{x^{n+1}y}u_{xx}-u_{x^{n+2}}u_{xy})u_{xx}^{-(n+12)/4}.\end{aligned} \tag{3.32}$$

$$\begin{aligned}K_{n4}=&(u_{x^n y^4}u_{xx}^4-4u_{x^{n+1}y^3}u_{xx}^3u_{xy}+6u_{x^{n+2}y^2}u_{xx}^2u_{xy}^2-4u_{x^{n+3}y}u_{xy}^3u_{xx}+u_{x^{n+4}}u_{xy}^4)u_{xx}^{-(n+26)/4}\\&-6\delta u_x u_{xx}^{-(n+18)/4}(u_{x^{n+1}y^2}u_{xx}^2-2u_{x^{n+2}y}u_{xx}u_{xy}+u_{x^{n+3}}u_{xy}^2)+12u_{x^{n+2}}u_x^2u_{xx}^{-(n+10)/4}.\end{aligned} \tag{3.33}$$

In summary, it has been proven that the equation

$$(u_t+\tfrac{3}{2}uu_x+u_{xxx})_x+\tfrac{3}{4}\delta u_{yy}+u_{xx}^{3/2}F_0(K_{n,m},m,\ n=0,\ 1,\ 2,\ldots)=0, \tag{3.34}$$

with an arbitrary function of $K_{n,m}$ possesses a common Virasoro symmetry algebra (2.9).

It is straightforward to see that the result (1.4) with (1.5)–(1.13) obtained by David, Levi, and Winternitz is a special case of (3.34) because

$$K_2=K_{4,0},\quad K_3=K_{3,0},\quad K_4=K_{2,1},\quad K_7=K_{3,1},\quad K_5=K_{1,2}K_{3,0}-K_{2,1}^2,$$

$$K_6=K_{3,0}^2K_{0,3}-3K_{2,1}K_{1,2}K_{3,0}+2K_{2,1}^3,\quad K_9=K_{4,0}^2K_{1,3}-3K_{3,1}K_{2,2}K_{4,0}+2K_{3,1}^3, \tag{3.35}$$

$$K_8=K_{2,2}K_{4,0}-K_{3,1}^2,\quad K_{10}=K_{4,0}K_{0,4}-4K_{1,3}K_{3,1}+3K_{2,2}^2.$$

B. Models with the symmetry (2.2)

The substitution (2.2) into (3.1) yields

$$h(u_{xt}+\tfrac{3}{2}uu_{xx}+\tfrac{3}{2}u_x^2+u_{xxxx}+\tfrac{3}{4}\delta u_{yy})_x+F'(hu_x-\tfrac{2}{3}\dot{h})=0. \tag{3.36}$$

Eliminating u_{xt} from (3.36) with help of (1.15), (3.36) becomes

$$F'\left(hu_x-\frac{2}{3}\dot{h}\right)-hF'u_x=0. \tag{3.37}$$

Substituting (3.5) into (3.37), we have

$$\sum_{n,m,l'}\sum_{i=0}^{l'-1}C_{l'}^i h^{(l'-i)}\frac{\partial F}{\partial u_{x^ny^mt^{l'}}}u_{x^{n+1}y^mt^i}-\frac{2}{3}\sum_l h^{(l+1)}\frac{\partial F}{\partial u_{t^l}}=0,\quad l'\geqslant 1. \tag{3.38}$$

If we can find an h-independent solution F from (3.38), then we get a model with a symmetry (2.2) for arbitrary h.

To find all the h-independent solution of (3.38) is equivalent to solve the following infinitely many linear equation system with infinitely many arbitrary independent variables,

$$\sum_{n,m,l}C_l^{l-k-1}\frac{\partial F}{\partial u_{x^ny^mt^l}}u_{x^{n+1}y^mt^{l-k-1}}-\frac{2}{3}\frac{\partial F}{\partial u_{t^k}}=0,\quad k=0,\ 1,\ 2,\ldots,\infty. \tag{3.39}$$

To find general solution of the over-determined equation system of (3.39) is difficult. However, if we require F is not $u_{x^ny^mt^l}$, $(l\geqslant 1)$ dependent, then the general solution of (3.39) reads as

$$F=f_1\equiv f_1(u_{x^ny^m},\ n,m=0,\ 1,\ 2,\ldots,n^2+m^2\neq 0). \tag{3.40}$$

Obviously, $F=u_{xx}^{3/2}F_0(K_{n,m},m,\ n=0,\ 1,\ 2,\ldots)$ shown by (3.34) is only a special case of f_1 of (3.40).

C. Models with the symmetry (2.3)

The substitution (2.3) into (3.1) results in

$$(-2g\partial_y+\tfrac{4}{3}\delta y\dot{g}\partial_x)(u_{xt}+\tfrac{3}{2}uu_{xx}+\tfrac{3}{2}u_x^2+u_{xxxx}+\tfrac{3}{4}\delta u_{yy})$$
$$+F'(-2gu_y+\tfrac{4}{3}\delta\dot{g}yu_x-\tfrac{8}{9}\delta y\ddot{g})=0. \tag{3.41}$$

Eliminating u_{xt} from (3.41) by means of (1.15), we have

$$2gF'u_y-\tfrac{4}{3}\delta y\dot{g}F'u_x+F'(-2gu_y+\tfrac{4}{3}\delta\dot{g}yu_x-\tfrac{8}{9}\delta y\ddot{g})=0. \tag{3.42}$$

The substitution (3.5) into (3.42) leads to

$$\frac{4}{3}\delta\sum_{n,m,l}\sum_{i=0}^{l}C_l^i g^{(l-i+1)}\frac{\partial F}{\partial u_{x^n y^m t^l}}u_{x^{n+1}y^{m-1}t^i}-\frac{8}{9}\delta\sum_l g^{(l+2)}\left(\frac{\partial F}{\partial u_{yt^l}}+y\frac{\partial F}{\partial u_{t^l}}\right)$$
$$+\sum_{n,m,l'}\sum_{i=0}^{l'-1}C_{l'}^i\frac{\partial F}{\partial u_{x^n y^m t^{l'}}}\left(-2g^{(l'-i)}\partial_y+\frac{4}{3}\delta g^{(l'-i+1)}\partial_x\right)u_{x^n y^m t^i}=0. \tag{3.43}$$

If we can find a g-independent solution F from (3.43), then we get a model with a symmetry (2.3) for arbitrary g.

To find out all the g-independent autonomous solutions of (3.43) is equivalent to solve the following equation system:

$$\sum_{n,m,l}mC_l^{l-k-1}\frac{\partial F}{\partial u_{x^n y^m t^l}}u_{x^{n+1}y^{m-1}t^{l-k-1}}-\frac{2}{3}\frac{\partial F}{\partial u_{t^k}}=0, \tag{3.44}$$

$$\sum_{n,m,l}\frac{\partial F}{\partial u_{x^n y^m t^l}}\left[\left(mC_l^{l-k-1}\partial_x\partial_t-\frac{3}{2}\delta C_l^{l-k-2}\partial_y^2\right)u_{x^n y^{m-1}t^{l-k-2}}\right]-\frac{2}{3}\frac{\partial F}{\partial u_{yt^k}}=0. \tag{3.45}$$

To find the general solutions of (3.44)–(3.45) is very difficult. However, if we require that F is $u_{x^n y^m t^l}$ independent for $l\neq 0$, the equation system (3.44)–(3.45) is reduced to

$$\frac{\partial F}{\partial u}=0,\quad \frac{\partial F}{\partial u_y}=0, \tag{3.46}$$

that means

$$F=f_2\equiv f_2(u_{x^n y^m},\ \{n,\ m\}\neq\{0,\ 0\},\{0,\ 1\}), \tag{3.47}$$

where f_2 is an arbitrary function of the indicated variables.

Obviously, (3.47) is a special case of (3.40) and $F=u_{xx}^{3/2}F_0(K_{n,m},m,\ n=0,\ 1,\ 2,\dots)$ is a special case of (3.47). In other words, the general KP family (3.34) possesses not only the Virasoro symmetry algebra (2.9) but also the full Kac–Moody–Virasoro symmetry algebra (2.5)–(2.9). Then the Theorem 1 can be extended as follows.

Theorem 2: *If $u=u(x,\ y,\ t)$ is a solution of the KP family (3.34), then so is u' shown by (2.11)–(2.13).*

IV. GROUP INVARIANT SOLUTIONS OF THE KP FAMILY (3.34)

To find group invariant solutions of a given system means to find the solutions which are solutions of not only the original model but also the symmetry constrained condition, $\sigma=0$. For the KP family (3.34), if the field u satisfies either the model equation or the symmetry constrained condition,

$$\sigma_0(h)+\sigma_1(g)+\sigma_2(f)=0, \tag{4.1}$$

with $\{\sigma_0(h),\ \sigma_1(g),\ \sigma_2(f)\}$ given by (2.2)–(2.4), then the solution is invariant under the Kac–Moody–Virasoro group transformations.

The symmetry constrained equation (4.1) can be easily solved because it is only a first order linear equation.

For the full Kac–Moody–Virasoro symmetries, $f\neq 0$, the general solution of (4.1) read as

$$u=f^{-2/3}U(\xi,\eta)+\frac{2f_t x}{9f}+\frac{4\delta(2f_t^2-3ff_{tt})y^2}{81f^2}+\frac{8\delta(3g_t f-2f_t g)y}{27f^2}+\frac{8\delta g^2}{9f^2}+\frac{2h}{3f}, \tag{4.2}$$

where

$$\xi=\frac{x}{f^{1/3}}+\frac{2\delta(f_t y^2-6gy)}{9f^{4/3}}-\frac{8}{3}\delta\int\frac{g^2}{f^{7/3}}\mathrm{d}t-\int\frac{h}{f^{4/3}}\mathrm{d}t, \tag{4.3}$$

$$\eta=\frac{y}{f^{2/3}}+2\int\frac{g}{f^{5/3}}\mathrm{d}t, \tag{4.4}$$

while the group invariant function, $U(\xi,\ \eta)\equiv U$, should be determined by the so-called similarity reduction equation (a Boussinesq family),

$$\tfrac{3}{4}\delta U_{\eta\eta}+(U_{\xi\xi\xi}+\tfrac{3}{2}UU_\xi)_\xi+U_{\xi\xi}^{3/2}F_0(K_{n,m}(\xi,\eta),m,\ n=0,\ 1,\ 2,\ \ldots)=0, \tag{4.5}$$

which can be obtained by substituting (4.2) into (3.34), where $K_{n,m}(\xi,\ \eta)$ is just $K_{n,m}$ expressed by (3.28) with the transformations $u_{x^n y^m}\to U_{\xi^n\eta^m}$.

For the Kac–Moody symmetries, $f=0$, the general solution of (4.1) possesses the form

$$u=\frac{1}{g}U(\xi,\ \tau)+\frac{g_t x}{3g}+\frac{2\delta(2g_t^2-gg_{tt})y^2}{9g^2}+\frac{(2g_t h-h_t g)y}{6g^2}-\frac{h^2}{6g^2}, \tag{4.6}$$

where

$$\xi=\frac{1}{\sqrt{g}}\left(x+\frac{\delta g_t y^2}{3g}+\frac{hy}{2g}\right), \tag{4.7}$$

$$\tau=\int g^{-3/2}\,\mathrm{d}t \tag{4.8}$$

while the similarity reduction equation of $U(\xi,\ \tau)\equiv U$ is a KdV family,

$$\left(U_\tau+U_{\xi\xi\xi}+\frac{3}{2}UU_\xi\right)_\xi+U_{\xi\xi}^{3/2}F_0(K_{n,m}(\xi,\tau),m,\ \ n=0,\ \ 1,\ \ 2,\ \ \ldots)=0, \tag{4.9}$$

which is a result of the substitution of (4.6) into (3.34) while $K_{n,m}(\xi,\ \tau)$ is just $K_{n,m}$ expressed by (3.28) with the transformations $u_{x^n}\to U_{\xi^n}$ and $u_{x^n y^m}\to 0$ for $m\neq 0$.

V. SUMMARY AND DISCUSSION

In summary, starting from the Kac–Moody–Virasoro symmetry of the usual KP equation and using a quite simple symmetry approach, a general KP family is found such that the family possesses the same Kac–Moody–Virasoro symmetry algebra as the usual KP equation. An arbitrary function of the higher order group invariants is included in the family. The finite Kac–Moody–Virasoro symmetry transformation group is naturally valid for the whole KP family.

The similarity reduction equation for the full Kac–Moody–Virasoro symmetry algebra is expressed by a Boussinesq family while for the Kac–Moody symmetry algebra [constituted by $\sigma_0(h)$ and $\sigma_1(g)$] can be expressed by a KdV family.

For the usual KP equation (1.3),[12] in addition to the Lie point symmetries, there are infinitely many generalized (higher order nonpoint) symmetries which constitute the generalized w_∞ symmetry algebra. If one makes the similar calculations for the general symmetries of the KP equation, one can find that the general nonpoint symmetries of the KP equation are not symmetries of the KP family (3.34).

To obtain (3.34), we have used not only the autonomous condition (i.e., F is not explicitly $\{x, y, t\}$-dependent), but also the condition

$$F_{u_{x^n y^m t^l}}=0, \quad \forall l\neq 0. \tag{5.1}$$

Generally, F may be both $\{x, y, t\}$ and $u_{x^n y^m t^l}$ dependent. We have not yet had a good idea to find all $u_{x^n y^m t^l}$ and $\{x, y, t\}$ dependent solutions of F. However, these kinds of solutions really exist. For instance, by the direct calculations, one can find that

$$J_{n1}\equiv u_{xx}^{-(n+6)/4}\left[\left(u_t+\frac{3}{2}uu_x\right)_x+\frac{3}{4}\delta u_{yy}\right]_{x^n}, \quad n=0, 1, 2,\ldots, \tag{5.2}$$

are also group invariants related to the symmetry algebra (2.5)–(2.9). That means

$$F=u_{xx}^{3/2}f_0(K_{n,m}, J_{n1}, m, n=0, 1, 2, \ldots), \tag{5.3}$$

with f_0 being an arbitrary function of the indicated variables is a special solution of the equation systems (3.8)–(3.15), (3.39) and (3.44)–(3.45).

From (1.15) [or (5.3)] and (3.28), we know that in addition to the KP equation itself and the dispersion-less KP [the Zabolotskaya–Khokhlov (ZK)] equation, one may obtain various models in the family that are rational in the derivatives, say, by selecting F_0 of (1.15) being a linear function of $K_{4k,2l}$, $K_{4k-2,2l+1}$, $k=1, 2,\ldots,l=0, 1, 2, \ldots$, etc.

Though we have found many arbitrary order equations which possess the same Lie point symmetry group of the KP equation, it is still very difficult to say something about the integrability properties of any equations in the family except for the KP and the ZK equation. In particular, we have not yet found higher symmetries or Painlevé properties of any other equations.

Because all the known $(2+1)$-dimensional integrable systems possesses the Virasoro symmetry algebra, the similar properties obtained in this paper for the KP equation may be valid for other $(2+1)$-dimensional systems.

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Hyperelliptic Nambu flow associated with integrable maps

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We study hyperelliptic Nambu flows associated with some n dimensional maps and show that discrete integrable systems can be reproduced as flows of this class. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1643195]

I. INTRODUCTION

Let us consider an n dimensional rectangular box with edges of length $X_1, X_2, \ldots, X_n$. The box will be rigid if there are n independent relations among X_j's

$$x_j = f_j(X_1, X_2, \ldots, X_n), \quad j = 1,2,\ldots,n. \tag{1}$$

This set of constraints defines a map

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_n) \to \boldsymbol{X} = (X_1, X_2, \ldots, X_n). \tag{2}$$

If we relax one of the constraints, say $x_n = f_n$, the box changes its form as x_n varies. We are interested in how it changes. To make clear the problem let us see the case of $n=3$ and assume, for example, that relations (1) are given by the elementary symmetric polynomials

$$\begin{aligned} x_1 &= X_1 + X_2 + X_3, \\ x_2 &= X_1X_2 + X_1X_3 + X_2X_3, \\ x_3 &= X_1X_2X_3. \end{aligned} \tag{3}$$

When all x_j's are fixed the map is determined algebraically by solving the equation

$$X^3 - x_1X^2 + x_2X - x_3 = 0, \tag{4}$$

up to permutations. Relations (3) amount to fix the total length of edges, the total area of surfaces, and the volume of the box. If the volume of the box x_3 varies while x_1 and x_2 are fixed, we will obtain a circle as an intersection of the sphere $X_1^2 + X_2^2 + X_3^2 = x_1^2 - 2x_2$ and the plane $X_1 + X_2 + X_3 = x_1$ in $\boldsymbol{R}^3$ along which $\boldsymbol{X}$ moves. If we fix x_1 and x_3 but leave x_2 free, we will find another curve in $\boldsymbol{R}^3$. Our problem is to find such a curve in general.

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It will be worthwhile to notice here that relations (1) defines an algebraic manifold in $\boldsymbol{R}^n$ if some of x_j's are fixed and the relations are purely algebraic. To see the properties of the manifold one can leave one of the constraints free and vary the constant to study a response of the variables $X_1, X_2, \ldots, X_n$ to the variation.

In our previous work[1,2] we have shown that there exists a Nambu–Hamiltonian flow[3] corresponding to an arbitrary differentiable map such that one of the initial values of the map plays the role of time of the flow. We can apply this result to see the change of the box when x_n varies.

We will study, in this article, how the problem is transcribed into the problem of solving the Nambu equation and the change of the boxes are described in terms of hyperelliptic curves under certain constraints. We are interested in the appearance of the hyperelliptic functions, since they are known to solve soliton equations in general. The second purpose of this article is to show that the reason of the appearance of the hyperelliptic functions is common in two systems, i.e., the soliton equations and the Nambu equations. In other words the Nambu equations provide a way to describe dynamics of integrable systems. We will show that, once the Nambu equations associated with a soliton equation are solved, solutions to the soliton equation can be given by solving purely algebraic relations.

II. NAMBU–HAMILTONIAN FLOWS

Let us first recall briefly the Nambu equations and review our previous results. For a function $f(\boldsymbol{X})$ of n-dimensional variable $\boldsymbol{X} \in \boldsymbol{R}^n$, the generalized Nambu Hamilton equations[3,4] are given by

$$\frac{df}{dt}(\boldsymbol{X}) = \{H_1, H_2, \ldots, H_{n-1}, f(\boldsymbol{X})\}. \tag{5}$$

We define the Nambu bracket $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$, in this article, by the Jacobian

$$\{\varphi_1, \varphi_2, \ldots, \varphi_n\} := \frac{\partial(\varphi_1, \varphi_2, \ldots, \varphi_n)}{\partial(X_1, X_2, \ldots, X_n)}.$$

$n-1$ Hamiltonians $H_1, H_2, \ldots, H_{n-1}$ satisfy

$$\frac{dH_j}{dt} = 0, \quad j = 1,2,\ldots,n-1$$

by definition of the equations. The equations of motion for the dynamical variables X_j's are

$$\begin{aligned}\frac{dX_j}{dt} &= \{H_1, H_2, \ldots, H_{n-1}, X_j\}, \quad j = 1,2,\ldots,n \\ &= (-1)^{n-j} \frac{\partial(H_1, H_2, \ldots, H_{n-1})}{\partial(X_1, X_2, \ldots, X_n)_j}.\end{aligned} \tag{6}$$

Here $(X_1, X_2, \ldots, X_n)_j$ means that X_j is missing among $(X_1, X_2, \ldots, X_n)$.

In Refs. 1 and 2, we proved the following:

Proposition 1: For a differentiable and invertible map (2), with its Jacobian $\det J$*, there exists a Nambu–Hamiltonian flow described by the equations*

$$\frac{dX_j}{dx_n} = \{H_1, H_2, \ldots, H_{n-1}, X_j\}, \quad j = 1,2,\ldots,n, \tag{7}$$

such that the Hamiltonians are given by

$$H_j = x_j, \quad j = 1,2,\ldots,n-2,$$

$$H_{n-1} = \int^{x_{n-1}} (\det J)\ dx_{n-1}.$$

Note that the initial value x_n of the map plays the role of the time variable in this flow. In addition to this proposition we would like to supply a new one which is more convenient to study our present problems.

Proposition 2: For a differentiable and invertible map (2), with its Jacobian $\det J$*, there exists a Nambu–Hamiltonian flow described by the equations*

$$\frac{dX_j}{dt} = \{H_1, H_2, \ldots, H_{n-1}, X_j\}, \quad j = 1,2,\ldots,n, \tag{8}$$

such that the Hamiltonians are given by

$$H_j = x_j, \quad j = 1,2,\ldots,n-1,$$

and the variable t *satisfies*

$$\frac{dx_k}{dt} = \frac{\delta_{k,n}}{\det J}. \tag{9}$$

Here the time variable t is not the initial value x_n itself but related to it by (9). This formulation has an advantage since the other initial values $x_1, x_2, \ldots, x_{n-1}$ of the map remain constant along the Nambu flow.

The proof of Proposition 2 is straightforward. From (9) it follows that

$$\frac{dX_j}{dt} = \sum_k \frac{\partial X_j}{\partial x_k}\frac{dx_k}{dt} = \frac{\partial X_j}{\partial x_n}\frac{1}{\det J} = \frac{\partial(x_1, x_2, \ldots, x_{n-1}, X_j)}{\partial(x_1, x_2, \ldots, x_{n-1}, x_n)}\frac{1}{\det J} = \frac{\partial(x_1, x_2, \ldots, x_{n-1}, X_j)}{\partial(X_1, X_2, \ldots, X_{n-1}, X_n)}$$

$$= \frac{\partial(H_1, H_2, \ldots, H_{n-1}, X_j)}{\partial(X_1, X_2, \ldots, X_{n-1}, X_n)}.$$

Q.E.D.

Hence (8) is true. Conversely (8) implies $dH_j/dt = 0$, hence (9) follows. We notice that, when the Nambu equation (8) is solved,

$$t = \int^{x_n} (\det J)\ dx_n \tag{10}$$

holds. If the Jacobian $\det J$ of the map $\boldsymbol{x} \to \boldsymbol{X}$ was one, we simply have $t = x_n$.

Now suppose we have solved the Nambu equations (8). We then obtain a map $(x_1, \ldots, x_{n-1}, t) \to \boldsymbol{X}$. We can show that the Jacobian $\det J'$ of this map is unity.

To see that we calculate the Jacobian of the inverse map $\boldsymbol{X} \to (x_1, \ldots, x_{n-1}, t)$ and expand it along the last row

$$\det J'^{-1} = \frac{\partial(x_1, x_2, \ldots, x_{n-1}, t)}{\partial(X_1, X_2, \ldots, X_n)} = \sum_{j=1}^{n} \frac{\partial t}{\partial X_j}\Delta_{nj},$$

where Δ_{nj} is the minor of the (nj) element of J'^{-1}. We notice that the right-hand side of (8) is exactly Δ_{nj}. Therefore we obtain

$$\det J'^{-1} = \sum_{j=1}^{n} \frac{\partial t}{\partial X_j} \frac{dX_j}{dt} = 1$$

as a result of equations of motion. Therefore the Jacobian $\det J'$ of the map $(x_1,\ldots,x_{n-1},t)\to \boldsymbol{X}$ is also one and the map preserves the hypervolume element.

III. STUDY OF SOLUTIONS

Since x_j, $j=1,2,\ldots,n-1$ are constants of the flow (8), they form $n-1$ dimensional hypersurfaces

$$x_j = H_j(\boldsymbol{X}), \quad j=1,2,\ldots,n-1 \tag{11}$$

in $\boldsymbol{R}^n$, while the point $\boldsymbol{X}$ moves along a curve formed by an intersection of the hypersurfaces as t changes. Suppose we can solve the constraints (11) for $X_1, X_2, \ldots, X_{n-1}$ as functions of $W := X_n$ and the constants x_j, $j=1,2,\ldots,n-1$. Substituting the results into the right-hand side of the equation for W in (8), we obtain a first order ordinary differntial equation for W,

$$\frac{dW}{dt} = F(W), \tag{12}$$

where F is a function of W and the constants of the flow. The orbit is determined by solving (12), i.e.,

$$t = \int^{W} \frac{dW}{F(W)}. \tag{13}$$

Combining this result with (10) we find

$$\frac{dW}{dx_n} = F(W)\det J.$$

Similarly we obtain equations for all other variables X_j's which determine the dependence on x_n.

A. Elementary symmetric polynomials

First we study a Nambu flow when the constraints (1) are given by the elementary symmetric polynomials

$$\begin{aligned}
x_1 &= X_1 + X_2 + X_3 + \cdots + X_n, \\
x_2 &= X_1X_2 + X_1X_3 + X_2X_3 + \cdots + X_{n-1}X_n, \\
&\vdots \\
x_j &= \sum_{k_1<k_2<\cdots<k_j} X_{k_1}X_{k_2}\cdots X_{k_j}, \\
&\vdots \\
x_n &= X_1X_2\cdots X_n.
\end{aligned} \tag{14}$$

When all x_j's are fixed the map is determined by solving the algebraic equation

$$X^n - x_1X^{n-1} + \cdots - (-1)^n x_{n-1}X + (-1)^n x_n = 0, \tag{15}$$

up to permutations. The relations (14) amount to fix the total length of edges, the total area of surfaces, ..., the total hypervolume of the box. If the hypervolume of the box x_n varies while other x_j's are fixed, we will obtain a curve in $\boldsymbol{R}^n$ along which $\boldsymbol{X}$ moves. Our problem is to find the curve.

The Nambu equation whose Hamiltonians are $x_1, x_2, \ldots, x_{n-1}$ in (14) is given for $W = X_n$ (Ref. 4) by

$$\frac{dW}{dt} = \prod_{1 \leqslant k < l \leqslant n-1} (X_k - X_l).$$

Therefore our task is to solve this equation explicitly. For this to be done we have to know the W dependence of the right hand side. We first notice that the square of the right-hand side is the discriminant of the equation $P_{n-1}(X) = 0$, where

$$P_{n-1}(X) := (X - X_1)(X - X_2) \cdots (X - X_{n-1}). \tag{16}$$

If we expand the polynomial $P_{n-1}(X)$ as

$$P_{n-1}(X) = h_0 X^{n-1} - h_1 X^{n-2} + h_2 X^{n-3} - \cdots + (-1)^{n-1} h_{n-1} \quad (h_0 = 1)$$

$h_1, h_2, \ldots, h_{n-1}$ are the elementary symmetric polynomials of $X_1, X_2, \ldots, X_{n-1}$. Since the discriminant

$$D_{n-1} := \prod_{1 \leqslant k < l \leqslant n-1} (X_k - X_l)^2$$

of $P_{n-1}(X) = 0$ is a symmetric polynomial it can be expressed in terms of $h_1, h_2, \ldots, h_{n-1}$. In fact it is a homogeneous polynomial of h_j's of degree $2(n-2)$. For example in the cases of $n = 3,4,5$

$$D_2 = h_1^2 - 4h_0 h_2,$$

$$D_3 = h_1^2 h_2^2 - 4h_0 h_2^3 - 4h_1^3 h_3 + 18 h_0 h_1 h_2 h_3 - 27 h_0^2 h_3^2,$$

$$\begin{aligned} D_4 = {} & h_1^2 h_2^2 h_3^2 - 4h_1^2 h_2^3 h_4 - 4h_1^3 h_3^3 + 18 h_1^3 h_2 h_3 h_4 - 27 h_1^4 h_4^2 - 4h_0 h_2^3 h_3^2 + 18 h_0 h_1 h_2 h_3^3 + 16 h_0 h_2^4 h_4 \\ & - 80 h_0 h_1 h_2^2 h_3 h_4 + 144 h_0 h_1^2 h_2 h_4^2 - 6 h_0 h_1^2 h_3^2 h_4 + 144 h_0^2 h_2 h_3^2 h_4 - 128 h_0^2 h_2^2 h_4^2 - 192 h_0^2 h_1 h_3 h_4^2 \\ & - 27 h_0^2 h_3^4 + 256 h_0^3 h_4^3. \end{aligned}$$

On the other hand h_j's are related with x_j's according to

$$x_k = h_k + W h_{k-1}, \quad k = 1,2,\ldots,n-1$$

or, equivalently,

$$h_k = x_k - x_{k-1} W + \cdots + (-1)^k W^k, \quad k = 1,2,\ldots,n-1.$$

Therefore the discriminant D_{n-1} is a polynomial of W of degree $(n-2)(n-1)$.

If we susbstitute $D_{n-1}(W)$ into F of (13), we find

$$t = \int^W \frac{dW}{\sqrt{D_{n-1}(W)}}.$$

The other variables $X_1, X_2, \ldots, X_{n-1}$ will be obtained similarly. Hence the orbits derived from the Nambu equations, whose Hamiltonians are elememtary symmetric polynomials, are given by hyperelliptic functions.

In the case of $n=3$ the motion of three variables X_1, X_2, X_3 are constrained on a circle fixed by the constants x_1 and x_2. We find

$$\begin{aligned} X_1 &= \tfrac{1}{3}(x_1 + 2\sqrt{x_1^2 - 3x_2}\cos(\sqrt{3}\ t)), \\ X_2 &= \frac{1}{3}\left(x_1 + 2\sqrt{x_1^2 - 3x_2}\cos\left(\sqrt{3}\ t - \frac{2\pi}{3}\right)\right), \\ X_3 &= \frac{1}{3}\left(x_1 + 2\sqrt{x_1^2 - 3x_2}\cos\left(\sqrt{3}\ t + \frac{2\pi}{3}\right)\right). \end{aligned} \tag{17}$$

If all x_j's are fixed besides x_i the Nambu equation for $W = X_i$ becomes

$$\frac{dW}{dt} = (-W)^{n-i} \prod_{\substack{1 \leqslant k \leqslant l \leqslant n \\ k,j \neq i}} (X_k - X_l).$$

Note that the right-hand side of this equation is just the square root of discriminant of the equation $P_{n-1,i}(X) = 0$, where

$$P_{n-1,i}(X) = \frac{\prod_{j=1}^{n} (X - X_j)}{X - X_i}.$$

The discriminant $D_{n-1,i}$ can be expressed in terms of $h'_1, h'_2, \ldots, h'_{n-1}$, where h'_j is an elementary symmetric polynomial without X_i. As before, $D_{n-1,i}$ is also a polynomial of W of degree $(n-1)(n-2)$. We find

$$t = (-1)^{n-i} \int^{W} \frac{dW}{W^n \sqrt{D_{n-1,i}(W)}}.$$

In the case of $n=3$ we could leave x_2 free, instead of x_3. Under the constraints

$$x_1 = X_1 + X_2 + X_3,$$

$$x_3 = X_1 X_2 X_3,$$

being constant, we find an elliptic curve parameterized by

$$X_1 = \frac{\alpha\gamma\,\mathrm{sn}^2(u,k)}{\gamma - \alpha\,\mathrm{cn}^2(u,k)},$$

$$X_{2,3} = x_1 - \frac{\alpha\gamma\,\mathrm{sn}^2(u,k)}{\gamma - \alpha\,\mathrm{cn}^2(u,k)} \pm \frac{(\alpha-\gamma)^{3/2}\sqrt{\beta}\,\mathrm{cn}(u,k)\ \mathrm{dn}(u,k)}{2(\gamma - \alpha\,\mathrm{cn}^2(u,k))\ \mathrm{sn}(u,k)},$$

where

$$u = \tfrac{1}{2}\sqrt{(\alpha-\gamma)\beta}\ \ t, \quad k = \sqrt{\frac{\alpha(\beta-\gamma)}{\beta(\alpha-\gamma)}}$$

and α, β, and γ are the roots of

$$x^3 - 2x_1x^2 + x_1^2 x - 4x_3 = 0.$$

B. *n* dimensional generalization of Euler top and Nahm equation

An n dimensional box has $n(n-1)/2$ rectangles which are orthogonal with each other. Among them we choose n independent rectangles. If we fix a relation between edge lengths of each of the n rectangles, all X_j's are determined, hence the box becomes rigid.

For example we can fix the diagonals of n rectangles as follows:

$$x_j = \tfrac{1}{2}(X_j^2 + X_{j+1}^2), \quad j = 1,2,\ldots,n, \tag{18}$$

with $X_{n+1} = X_1$ to make the box rigid. The Jacobian of this map is, when n is odd,

$$\det J = (2X_1X_2\cdots X_n)^{-1}.$$

If $x_n = (X_n^2 + X_1^2)/2$ is varied, all X_j's will be changed simultaneously and $\boldsymbol{X}$ draws a curve in $\boldsymbol{R}^n$. The corresponding Nambu equations are

$$\frac{dX_j}{dt} = (-1)^{n-j}\frac{X_1X_2\cdots X_n}{X_j}, \quad j = 1,2,\ldots,n. \tag{19}$$

We can solve the constraints (18) for X_j's

$$X_j^2 = \alpha_j + (-1)^{n-j}W^2, \quad j = 1,2,\ldots,n-1,$$

where

$$\alpha_j = 2(x_j - x_{j+1} + \cdots - (-1)^{n-j}x_{n-1}).$$

The right-hand side of

$$\frac{dW}{dt} = X_1X_2\cdots X_{n-1}$$

is given by a function of W. In fact we obtain

$$t = \int^W \frac{dW}{\sqrt{\prod_{j=1}^{n-1}(\alpha_j + (-1)^{n-j}W^2)}}.$$

Thus we conclude that the point $\boldsymbol{X}$ moves along a hyperelliptic curve. When $n = 3$, the solutions are given by the Jacobi elliptic functions as

$$X_1 = \sqrt{2(x_1 - x_2)}\,\mathrm{dn}(u,k),$$

$$X_2 = \sqrt{2x_2}\,\mathrm{cn}(u,k),$$

$$X_3 = \sqrt{2x_2}\,\mathrm{sn}(u,k),$$

where

$$u := \sqrt{2(x_1 - x_2)}\;\; t, \quad k := \sqrt{\frac{x_2}{x_2 - x_1}}.$$

The above example can be readily generalized to the cases whose constraints can be reduced into the form

$$x_j=\frac{1}{2}\sum_{k=1}^{n}\ \alpha_{jk}X_k^2,\quad j=1,2,\ldots,n-1. \tag{20}$$

The Nambu equations are

$$\frac{dX_j}{dt}=(-1)^{n-j}\det A_j\frac{X_1X_2\cdots X_n}{X_j},\quad j=1,2,\ldots,n,$$

where the matrix A_j is given by eliminating the jth column from the $(n-1)\times n$ matrix $\{\alpha_{jk}\}$. By solving (20) for X_k as a function of $W=X_n$ and the constants and substituting them into

$$\frac{dW}{dt}=\det A_n\ \ X_1X_2\cdots X_{n-1}$$

we again obtain a hyperelliptic integral.

A simple case, i.e.,

$$A=\begin{pmatrix}1 & -1 & 0\\ 0 & 1 & -1\end{pmatrix},$$

which is called the Nahm equation, was discussed in Ref. 4. Another example is the famous Euler top corresponding to the matrix

$$\begin{pmatrix}1 & 1 & 0\\ 0 & 1 & 1\end{pmatrix},$$

which was discussed by Nambu.[3] We note that our generalization of this top to n dimension is different from either one of Refs. 5 or 6.

IV. COMPLETELY INTEGRABLE MAPS

The hyperelliptic functions have been known to solve soliton equations.[7,8] They appear through the variation of subspectral parameters of Lax operators. We are going to show, in this section, that the hyperelliptic solutions of soliton equations can be obtained equally by solving the Nambu equations, which we discussed in the previous section.

A. Brief review of 3 point Toda lattice

Before going into details of the discussion we will review briefly how the hyperelliptic solutions are derived from soliton equations. In order to make clear the point of our arguments we consider a simple example, i.e., 3-point Toda lattice. The time evolution of the 6-dynamical variables $(a_1,a_2,a_3,b_1,b_2,b_3)$ are determined by means of the Lax equation

$$\frac{dL}{dt}=[B,L], \tag{21}$$

where

$$L=\begin{pmatrix}b_1 & a_1 & a_3\\ a_1 & b_2 & a_2\\ a_3 & a_2 & b_3\end{pmatrix},\quad B=\begin{pmatrix}0 & -a_1 & a_3\\ a_1 & 0 & -a_2\\ -a_3 & a_2 & 0\end{pmatrix}.$$

In addition to the periodicity condition, which imposes to a_1,a_2,a_3 a constraint

$$a_1a_2a_3=1/8, \tag{22}$$

the eigenvalues $\lambda_1,\lambda_2,\lambda_3$ of L are constants of motion. Therefore only two variables out of six remain independent. It is conventional to choose two eigenvalues μ_1,μ_2 of the matrix $\left(\begin{smallmatrix} b_1 & a_1 \\ a_1 & b_2 \end{smallmatrix}\right)$ as new such variables. They are called subspectral parameters. The relations between the dynamical variables $(a_1,a_2,a_3,b_1,b_2,b_3)$ and $(\lambda_1,\lambda_2,\lambda_3,\mu_1,\mu_2)$ are algebraic. For instance we have

$$\mu_1+\mu_2=\lambda_1+\lambda_2+\lambda_3-b_3,$$

$$\mu_1\mu_2=b_1b_2-a_1^2.$$

Hence the time dependence of the dynamical variables can be found if we know how μ_1 and μ_2 vary in time.

Solving these algebraic relations for $(\lambda_1,\lambda_2,\lambda_3,\mu_1,\mu_2)$, the Lax equation (21) can be converted into equations which determine the time evolution of μ_1,μ_2 as

$$\frac{d\mu_j}{dt}=\frac{1}{4}\frac{\sqrt{\Delta^2(\mu_j)-4}}{\mu_2-\mu_1}, \quad j=1,2.$$

Here $\Delta(\lambda)$ is a third order polynomial of λ. Solutions to these equations are given in terms of elliptic functions.

We can summarize this result as follows. For the five dynamical variables, which are constrained by three constants of motion, we introduce two intermediate variables, which are also related with the dynamical variables algebraically. If we can find the dependence of the new variables on time, the time dependence of the five dynamical variables will be found by solving the five algebraic relations.

B. Generalization to integrable maps

Let us generalize this idea of solving 3-point Toda lattice to study larger class of integrable systems. For this purpose we consider a map $M(t)\to M(t+1)$ of an $m\times m$ matrix given by

$$M(t+1)=U^{-1}M(t)U. \tag{23}$$

A large number of integrable maps have been known being represented in this form.[9] For an illustration we present here the discrete time m point Toda lattice,

$$M(t)=\begin{pmatrix} i_1+v_1 & 1 & 0 & \cdots & 0 & i_1v_m \\ i_2v_1 & i_2+v_2 & 1 & 0 & & 0 \\ 0 & i_3v_2 & i_3+v_3 & 1 & & \\ \vdots & & \cdots & & \vdots & \\ 0 & 0 & \cdots & & & 1 \\ 1 & 0 & \cdots & 0 & i_mv_{m-1} & i_m+v_m \end{pmatrix},$$

$$U(t)=\begin{pmatrix} i_1 & 1 & 0 & \cdots & 0 \\ 0 & i_2 & 1 & & 0 \\ & & \vdots & & \\ 0 & & & i_{m-1} & 1 \\ 1 & 0 & \cdots & 0 & i_m \end{pmatrix}. \tag{24}$$

In the continuum limit of time the variables (v_j,i_j) are related with (a_j,b_j) of the Lax form by

$$(v_j,i_j)=(2a_j,1-b_j), \quad j=1,2,\ldots,m.$$

Suppose elements of the matrix M in (23) are determined in terms of $m+n-1$ dynamical variables with $n<m+1$. Since eigenvalues of the matrix, which we denote $\lambda_1,\ldots,\lambda_m$, are constant under the map, m variables can be eliminated by solving algebraic relations between the elements of M and the eigenvalues. The problem of solving the evolution equation (23) is turned to finding proper intermediate n variables. They must be responsible faithfully to a variation of the system under the constraints that the eigenvalues are conserved. We can use the Nambu equations to describe such a system.

In order to make concrete our argument we adopt the elementary symmetric polynomials as m independent constants of the map:

$$\begin{aligned} x_1&=\lambda_1+\lambda_2+\cdots+\lambda_m,\\ x_2&=\lambda_1\lambda_2+\lambda_1\lambda_3+\cdots+\lambda_{m-1}\lambda_m,\\ &\vdots\\ x_j&=\sum_{1\leqslant k_1<k_2<\cdots<k_j\leqslant m}\lambda_{k_1}\lambda_{k_2}\cdots\lambda_{k_j},\\ &\vdots\\ x_m&=\lambda_1\lambda_2\cdots\lambda_m. \end{aligned} \tag{25}$$

Writing them explicitly in terms of the elements M_{jk} of the matrix M, we have

$$\begin{aligned} x_1&=M_{11}+M_{22}+\cdots+M_{mm},\\ x_2&=\sum_{1\leqslant j<k\leqslant m}(M_{jj}M_{kk}-M_{jk}M_{kj}),\\ &\vdots\\ x_m&=\det M. \end{aligned} \tag{26}$$

Now we let $X_1,X_2,\ldots,X_n$ be the new n intermediate variables and $x_1,x_2,\ldots,x_{n-1}$ be $n-1$ Hamiltonians of the system such that the intermediate variables are constrained by

$$\begin{aligned} X_1+X_2+\cdots+X_n&=x_1,\\ X_1X_2+X_1X_3+\cdots+X_{n-1}X_n&=x_2,\\ &\vdots\\ \sum_{1\leqslant k_1<k_2<\cdots<k_{n-1}\leqslant n}X_{k_1}X_{k_2}\cdots X_{k_{n-1}}&=x_{n-1}. \end{aligned} \tag{27}$$

The Nambu equations for the new variables are nothing but (8) with $H_j=x_j$, $j=1,2,\ldots,n-1$ and solutions have been already discussed in Sec. III A.

In order to find the behavior of the matrix M of (23), we first identify (25) and (26) to express m variables of the matrix in terms of the m constants $\lambda_1,\ldots,\lambda_m$. The rest of the $n-1$ independent variables of the matrix M will be determined by $X_1,X_2,\ldots,X_n$ if we identity $x_1,x_2,\ldots,x_{n-1}$ of (27) with those of (26). We would like to emphasize here that these steps will be done by purely algebraic procedures.

To be specific we consider the map (23) with M given by (24). We further restrict to the case of $m=3$, i.e., the 3-point Toda lattice. Corresponding to the condition (22) we may impose a constraint

$$v_1v_2v_3=\text{const}, \tag{28}$$

so that the number of independent dynamical variables is five. Via explicit calculations we have

$$\begin{aligned} x_1&=i_1+i_2+i_3+v_1+v_2+v_3,\\ x_2&=i_1i_2+i_1i_3+i_2i_3+i_1v_2+i_2v_3+i_3v_1+v_1v_2+v_1v_3+v_2v_3,\\ x_3&=(1+i_1i_2i_3)(1+v_1v_2v_3) \end{aligned} \tag{29}$$

in the place of (26). The correspondence between (25) and (26) enables us to write three variables of M, say i_1,i_2,i_3, in terms of v_1,v_2,v_3 and the constants $\lambda_1,\lambda_2,\lambda_3$.

If we further identify x_1,x_2 in (29) with those of (3), they, together with the condition (28), determine v_1,v_2,v_3 as functions of X_1,X_2,X_3. Since X_1,X_2,X_3 have been known as given in (17), the behavior of the matrix M is determined.

V. REMARKS AND DISCUSSIONS

We have developed a method to derive Nambu equations from a given map (2). There exist some ambiguities how to relate the time variable t of the Nambu equations to the initial variables of the map. It could be one of the initial variables of the map as in the case of Proposition 1, or a function of it as it was the case of Proposition 2. They are not independent but are related with each other through a reparametrization of the variable t.

If the functions $f_1,f_2,\ldots,f_n$ of the map defined by (1) are purely algebraic, the map will determine an algebraic manifold. To study the nature of the manifold we change one of the initial variables of the map and see the response. Our propositions claim that the Nambu equations provide a systematic method to investigate such a response. By means of some examples we have shown that the manifolds described by certain types of map are characterized by hyperelliptic curves.

When there are known some number of invariants under time evolution, the Nambu equations determine the change of the dynamical variables. Since any function of the invariants is again an invariant there are many possible sets of Nambu equations. Suppose we can choose a proper set of invariants such that the functions are algebraic and the Nambu equations can be solved explicitly. Then the problem of solving the equations of motion are replaced to solve the algebraic relations among variables. We have demonstrated that the hyperelliptic solutions of soliton equations can be derived in this way.

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Geometric integrators and nonholonomic mechanics

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A geometric derivation of nonholonomic integrators is developed. It is based in the classical technique of generating functions adapted to the special features of nonholonomic systems. The theoretical methodology and the integrators obtained are different from those obtained in Cortés and Martínez ["Nonholonomic integrators," Nonlinearity **14**, 1365–1392 (2001)]. In the case of mechanical systems with linear constraints a family of geometric integrators preserving the nonholonomic constraints is given. © *2004 American Institute of Physics.*
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I. INTRODUCTION

A. Introduction to nonholonomic mechanics

The theory of systems with nonholonomic constrains goes back to the XIX century. D'Alembert's or Lagrange–D'Alembert's principle of virtual work and Gauss principle of least constraint can be considered to be the first solutions to the analysis of systems with constraints, holonomic or not. After a period of decay, many authors have recently shown a new interest in that theory and also in its relation to the new developments in control theory, sub-Riemannian geometry, robotics, etc. (see, for instance, Ref. 45). The main characteristic of this period is that Geometry was used in a systematic way (see L.D. Fadeev and A.M. Vershik[49] as an advanced and fundamental reference, and also, Refs. 3, 4, 7, 10, 13, 24, 25, 28, 29, 30, 38).

As is well known, in most problems of particle mechanics, the motion of the particles is constrained in some way; this is the term used to denote the condition that some motions or configurations are not allowed. First, we shall start with a configuration space Q, which is a n-dimensional differentiable manifold, with local coordinates q^i. General two-side or equality constraints are functions of the form $\phi^a(q^i,\dot{q}^i)=0,1\leqslant a\leqslant m$, depending, in general, on configuration coordinates and their velocities. The various kinds of constraints we are concerned with will roughly come in two types: holonomic and nonholonomic, depending whether the constraint is derived from a constraint in the configuration space or not. Therefore, the dimension of the space of configurations is reduced by holonomic constraints but not by nonholonomic constraints. Thus, holonomic constraints permit a reduction in the number of coordinates of the configuration space needed to formulate a given problem (see Ref. 45).

We will restrict ourselves to the case of nonholonomic constraints, since the case of holonomic constraints, and, in particular, the construction of holonomic integrators, is well established in the existing literature. Geometrically, nonholonomic constraints are globally described by a submanifold $\tilde{M}$ of the velocity phase space TQ, the tangent bundle of the configuration space Q. If case $\tilde{M}$ is a vector subbundle of TQ, we are dealing with linear constraints. We will usually refer to $\tilde{M}$ as D and, in such case, the constraints are alternatively defined by a distribution D on the configuration space Q. If this distribution is integrable, we are precisely in the case of holonomic constraints. In case $\tilde{M}$ is an affine subbundle modeled on a vector bundle D, we are in the

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case of affine constraints. In what follows, we will denote by D the constraint submanifold on the velocity phase space, no matter if they are determined by linear or nonlinear constraints.

Given the constraints, we need to specify the dynamical evolution of the system. The central concepts permitting the extension of mechanics from the Newtonian point of view to the Lagrangian one are the notions of virtual displacements and virtual work; these concepts were formulated in the developments of mechanics, in their application to statics. In nonholonomic dynamics, the procedure is given by Lagrange–D'Alembert's principle. We usually consider nonholonomic constraints of linear type, which are the constraints that we will regard as natural in a mechanical sense (although the extension for general nonholonomic constraint will be straightforward). We now come to the description of the constraint forces; for constraints of that type, Lagrange–D'Alembert's principle allows us to determine the set of possible values of the constraint forces only from the set of admissible kinematic states, that is, from the constraint manifold D determined by the vanishing of the nonholonomic constraints. Therefore, assuming that the dynamical properties of the system are mathematically described by a configuration space Q, by a Lagrangian function L and by a distribution determining the linear constraints D, the equations of motion, following Lagrange–D'Alembert's principle, are

$$\left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right)-\frac{\partial L}{\partial q^i}\right]\delta q^i=0, \tag{1}$$

where δq^i denotes the virtual displacements verifying

$$\mu_i^a \delta q^i=0 \tag{2}$$

and $D^o=\text{span}\{\mu^a=\mu_i^a dq^i\}$ (for the sake of simplicity, we will assume that the system is not subject to nonconservative forces). By using the Lagrange multiplier rule, we obtain that

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right)-\frac{\partial L}{\partial q^i}=\overline{\lambda}_a\mu_i^a. \tag{3}$$

The term on the right-hand side represents the constraint force or reaction force induced by the constraints. The functions $\overline{\lambda}_a$ are Lagrange multipliers to be determined in order to obtain a set of second order differential equations. These Lagrangian multipliers are computed using the constraint equations. An interesting remark, that will be used in what follows, is that whenever the Lagrange multipliers $\overline{\lambda}_a=\overline{\lambda}_a(q^i,\dot{q}^i)$ have been determined, then the system of equations (3) can be considered a Lagrangian system subject to external conservative forces given by the right-hand side term, taking, obviously, an initial condition on the constraint submanifold D. The choice of the Lagrange multipliers $\overline{\lambda}_a$ automatically implies that the solution integral curves also verifies the constraint equations.

B. Introduction to geometric integration and discrete mechanics

Standard methods for simulating the motion of a dynamical system, generically called numerical integrators, usually take an initial condition and move it in the direction specified by the equation of motion or an appropriate discretization. But these standard methods ignore all the geometric features of many dynamical systems, as for instance, for Hamiltonian systems we have preservation of the symplectic form, energy (in the autonomous case) and symmetries, if any. However, new methods have been recently developed, called geometric integrators, which are concerned with some of the extra features of geometric nature of the dynamical systems. Usually, these integrators can run, in simulations, for long times with lower spurious effects (for instance, bad energy behavior for conservative systems) than the traditional ones. As is well known, the typical test example is the simulation of the solar system. Therefore, there is presently a great interest in geometric integration of differential equations as, for instance, symplectic integrators of Hamiltonian systems.[17,48]

Discrete variational integrators appear as a special kind of geometric integrators. These integrators have their roots in the optimal control literature in the 1960s and 1970s (Jordan and Polack,[20] Cadzow,[8] Maeda[36,37]) and in the 1980s by Lee,[26,27] Veselov.[44,50] In these papers, there appear the discrete action sum, discrete Euler–Lagrange equations, discrete Noether theorem,.... Although this kind of symplectic integrators have been considered for conservative systems,[18,21,39,43,51,52] it has been recently shown how discrete variational mechanics can include forced or dissipative systems,[22,43] holonomic constraints,[16,43] time-dependent systems,[31,43] frictional contact,[47] and nonholonomic constraints (see Refs. 10, 12). Moreover, it has also been discussed by reduction theory,[5,6,41,42] extension to field theories,[19,40] and quantum mechanics.[46] All these integrators have demonstrated exceptionally good long time behavior and the research of this topic is interesting for numerical and geometric considerations.

At this point, we will describe the discrete variational calculus, following the approach in Ref. 51 (see also Refs. 2, 15). A discrete Lagrangian is a map $L_d: Q\times Q\to\mathbb{R}$ (this discrete Lagrangian may be considered as an approximation of the continuous Lagrangian $L:TQ\to\mathbb{R}$). Define the action sum $S_d: Q^{N+1}\to\mathbb{R}$ corresponding to the Lagrangian L_d by

$$S_d=\sum_{k=1}^{N} L_d(q_{k-1},q_k),$$

where $q_k\in Q$ for $0\leqslant k\leqslant N$. For any covector $\alpha\in T^*_{(x_1,x_2)}(Q\times Q)$, we have a decomposition $\alpha=\alpha_1+\alpha_2$ where $\alpha_i\in T^*_{x_i}Q$. Therefore,

$$dL_d(q_0,q_1)=D_1L_d(q_0,q_1)+D_2L_d(q_0,q_1).$$

The discrete variational principle or Cadzow's principle states that the solutions of the discrete system determined by L_d must extremize the action sum given fixed points q_0 and q_N. Extremizing S_d over q_k, $1\leqslant k\leqslant N-1$, we obtain the following system of difference equations:

$$D_1L_d(q_k,q_{k+1})+D_2L_d(q_{k-1},q_k)=0.$$

These equations are usually called the *discrete Euler–Lagrange equations*. Under some regularity hypothesis (the matrix $(D_{12}L_d(q_k,q_{k+1}))$ is regular), this implicit system of difference equations defines a discrete flow $\Upsilon: Q\times Q\to Q\times Q$, by $\Upsilon(q_{k-1},q_k)=(q_k,q_{k+1})$.

The geometrical properties corresponding to this numerical method are obtained defining the discrete Legendre transformation associated to L_d by

$$FL_d: Q\times Q\to T^*Q,\quad (q_0,q_1)\mapsto(q_0,-D_1L_d(q_0,q_1)),$$

and the 2-form $\omega_d=FL_d^*\omega_Q$, where ω_Q is the canonical symplectic form on T^*Q. The discrete algorithm determined by Υ preserves the symplectic form ω_d, i.e., $\Upsilon^*\omega_d=\omega_d$. Moreover, if the discrete Lagrangian is invariant under the diagonal action of a Lie group G, then the discrete momentum map $J_d: Q\times Q\to\mathfrak{g}^*$ defined by $\langle J_d(q_k,q_{k+1}),\xi\rangle=\langle D_2L_d(q_k,q_{k+1}),\xi_Q(q_{k+1})\rangle$ is preserved by the discrete flow. Therefore, these integrators are symplectic-momentum preserving integrators. Here, ξ_Q is the fundamental vector field determined by $\xi\in\mathfrak{g}$.

Another alternative approach to discrete variational calculus comes from the classical theory of generating functions (see, for instance, Ref. 1). Since (T^*Q,ω_Q) is an exact symplectic manifold, where ω_Q is the canonical symplectic form of T^*Q and $\omega_Q=-d\theta_Q$, the symplectic flow $F_h: T^*Q\to T^*Q$ of a Hamiltonian vector field X_H consists of canonical transormations, and then Graph(F_h), the graph of F_h, is a Lagrangian submanifold of the symplectic manifold $(T^*Q\times T^*Q,\Omega)$ where $\Omega=\pi_2^*\omega_Q-\pi_1^*\omega_Q$. Here, we denote by $\pi_i: T^*Q\times T^*Q\to T^*Q$, $i=1,2$ the canonical projections. Therefore, denoting $\Theta=\pi_2^*\theta_Q-\pi_1^*\theta_Q$ we have that

$$i_{F_h}^*\Omega=-di_{F_h}^*\Theta=0,$$

where $i_{F_h}:\mathrm{Graph}(F_h)\mapsto T^*Q\times T^*Q$ is the canonical inclusion. Then, at least locally, there exists a function $\mathcal{S}^h:\mathrm{Graph}(F_h)\to\mathbb{R}$ such that $i_{F_h}^*\Theta=d\mathcal{S}^h$. Taking (q^i,p_i) as natural coordinates in $\mathrm{Graph}(F_h)$ and $(q^i,p_i,\mathbf{q}^i,\mathbf{p}_i)$ the coordinates in $T^*Q\times T^*Q$, then, $\mathcal{S}^h$ is locally a function of the (q,p) coordinates. Hence, along $\mathrm{Graph}(F_h)$, we have $\mathbf{q}^i=\mathbf{q}^i(q,p)$ and $\mathbf{p}^i=\mathbf{p}^i(q,p)$ and moreover

$$\mathbf{p}_i\,d\mathbf{q}^i-p_i dq^i=d\mathcal{S}^h(q,p).$$

Assume that in a neighborhood of some point $x\in\mathrm{Graph}(F_h)$, we can change this system of coordinates by new independent coordinates $(q^i,\mathbf{q}^i)$ (the local condition is that $\det(\partial\mathbf{q}/\partial p)\neq 0$). In such a case, the function $\mathcal{S}^h$ can be locally expressed as $\mathcal{S}^h=\mathcal{S}^h(q,p)=S^h(q,\mathbf{q})$. The function $S^h(q,\mathbf{q})$ will be called a *generating function of the first kind* of the canonical transformation F_h. Moreover,

$$\begin{cases} p_i=-\dfrac{\partial S^h}{\partial q^i}, \\ \mathbf{p}_i=\dfrac{\partial S^h}{\partial \mathbf{q}^i}. \end{cases}$$

A nice and useful interpretation of the discrete Euler-Lagrange equations is the following theorem.[23,33]

Theorem 1.1: *Let the function S^{Nh} be defined by*

$$S^{Nh}(q_0,q_N)=\sum_{k=0}^{N-1} S^h(q_k,q_{k+1}),$$

where q_k, $1\leqslant k\leqslant N-1$, are stationary points of the right-hand side, that is

$$0=D_2S^h(q_{k-1},q_k)+D_1S^h(q_k,q_{k+1}),\quad 1\leqslant k\leqslant N-1, \tag{4}$$

then S^{Nh} is a generating function of first class for $F_{Nh}:T^*Q\to T^*Q$, for h sufficiently small and where F_{Nh} denotes the flow of X_H over time Nh.

Moreover, if we start with a regular Lagrangian function $L:TQ\to\mathbb{R}$, and $H:T^*Q\to\mathbb{R}$ is the locally associated Hamiltonian, then we also have the following result (for example, see Ref. 33).

Proposition 1.2: *A generating function of the first kind for F_h is given by*

$$S^h(q_0,q_1)=\int_0^h L(q(t),\dot{q}(t))\,dt,$$

where $q(t)$ is a solution of the Euler–Lagrange equations such that $q(0)=q_0$ and $q(h)=q_1$.

The conclusion is that the discrete variational calculus reduces to taking an approximation of the generating function S^h. From this approximation, we obtain a new Lagrangian submanifold of $T^*Q\times T^*Q$ and the relation between subsequent steps is given by (4) for the new generating function, which are precisely the discrete Euler–Lagrange equations. The symplecticity and preservation of momentum are now direct consequences of this description.

C. Introduction to nonholonomic integrators

In a recent paper, Cortés and Martínez[12] have proposed a construction of nonholonomic integrators which is useful for numerical considerations. Their construction is based on the *discrete Lagrange–D'Alembert's principle*. Assuming that the constraints are given by a distribution D, this principle states that

$$(D_1L_d(q_k,q_{k+1})+D_2L_d(q_{k-1},q_k))_i\delta q_k^i=0,\quad 1\leqslant i\leqslant N-1,$$

where $\delta q_k \in D_{q_k}$ and, in addition $(q_k, q_{k+1}) \in D_d$. Here D_d denotes a discrete constraint space $D_d \subset Q \times Q$. This integrator has a good performance and naturally inherits some geometric properties of the continuous problem. Observe that the method is based on the discretization of the Lagrangian and a coherent discretization of the constraints, and both determine the discrete constraint forces.

Alternatively, we propose a nonholonomic integrator based also on the discretization of the Lagrangian function (in a more precise sense, we discretize the action function) but now we take a coherent discretization of the constraint forces and both determine the discrete constraint submanifold. This method gives us, in general, different integrators from those in Ref. 12. The last considerations of the previous section will be our starting point to study nonholonomic integrators, and our equations will be conceptually equivalent to the proposed for systems with external forces (see Ref. 43). In the particular case of mechanical systems with linear constraint in the velocities, we study a subclass of our family of nonholonomic integrators with the property of preservation of the original nonholonomic constraints.

II. GEOMETRICAL FORMULATION OF NONHOLONOMIC SYSTEMS

Let Q be a n-dimensional differentiable manifold, with local coordinates (q^i). The tangent bundle TQ, with induced coordinates $(q^i, \dot{q}^i)$, is equipped with two fundamental geometrical objects:[34] the Liouville vector field Δ and the vertical endomorphism S. In natural bundle coordinates we have

$$\Delta = \dot{q}^i \frac{\partial}{\partial \dot{q}^i}, \quad S = dq^i \otimes \frac{\partial}{\partial \dot{q}^i}.$$

Consider a Lagrangian system, with Lagrangian $L: TQ \to \mathbb{R}$, subject to nonholonomic constraints, defined by a submanifold D of the velocity phase space TQ. We will assume that $\dim D = 2n - m$ and that D is locally described by the vanishing of m independent functions ϕ^a (the "constraint functions").

In geometrical terms, the D'Alembert's principle (or Chetaev's principle for nonlinear constraints) implies that the constraint forces, regarded as 1-forms on TQ along D, take their values in the subbundle $S^*(TD^o)$ of T^*TQ, where TD^o denotes the annihilator of TD in T^*TQ. In an intrinsic way, the equations of motion can be written as (see Refs. 28, 30)

$$(i_X \omega_L - dE_L)_{|D} \in S^*(TD^o),$$

$$X_{|D} \in TD,$$

where ω_L is the Poincaré–Cartan 2-form defined by $\omega_L = -d(S^*(dL))$ and $E_L = \Delta(L) - L$ is the energy function.

In what follows we will also assume that the following *admissibility condition* holds

$$\dim TD^o = \dim S^*(TD^o).$$

This essentially means that the matrix $(\partial \phi^a / \partial \dot{q}^i)$ has rank m everywhere.

We now turn to the Hamiltonian description of the nonholonomic system on the cotangent bundle T^*Q of Q.[3,25,38] The canonical coordinates on T^*Q are denoted by (q^i, p_i), and the cotangent bundle projection will be $\pi_Q: T^*Q \to Q$. Assuming the regularity of the Lagrangian, we have that the Lagrangian and Hamiltonian formulations are locally equivalent. If we suppose, in addition, that the Lagrangian L is hyperregular, then the Legendre transformation $Leg: TQ \to T^*Q, (q^i, \dot{q}^i) \mapsto (q^i, p_i = \partial L / \partial \dot{q}^i)$, is a global diffeomorphism. The constraint functions on T^*Q become $\Psi^a = \phi^a \circ Leg^{-1}$, i.e.,

$$\Psi^a(q^i,p_i)=\phi^a\left(q^i,\frac{\partial H}{\partial p_i}\right),$$

where the Hamiltonian $H:T^*Q\to\mathbb{R}$ is defined by $H=E_L\circ Leg^{-1}$. Since locally $Leg^{-1}(q^i,p_i)=(q^i,\partial H/\partial p_i)$, then

$$H=p_i\dot{q}^i-L(q^i,\dot{q}^i),$$

where $\dot{q}^i$ is expressed in terms of q^i and p_i using Leg^{-1}.

The equations of motion for the nonholonomic system on T^*Q can now be written as follows:

$$\begin{cases}\dot{q}^i=\dfrac{\partial H}{\partial p_i},\\ \dot{p}_i=-\dfrac{\partial H}{\partial q^i}-\lambda_a\dfrac{\partial\Psi^a}{\partial p_j}\mathcal{H}_{ji},\end{cases}\tag{5}$$

together with the constraint equations $\Psi^a(q,p)=0$, where $\mathcal{H}_{ij}$ are the components of the inverse of the matrix $(\mathcal{H}^{ij})=(\partial^2H/\partial p_i\partial p_j)$. Note that

$$\left(\frac{\partial\Psi^a}{\partial p_j}\mathcal{H}_{ji}\right)(q,p)=\left(\frac{\partial\phi^a}{\partial\dot{q}^i}\circ Leg^{-1}\right)(q,p).$$

The symplectic 2-form ω_L is related, via the Legendre map, with the canonical symplectic form ω_Q on T^*Q. Let M denote the image of the constraint submanifold D under the Legendre transformation, and let F be the distribution on T^*Q along M, whose annihilator is given by

$$F^o=Leg_*(S^*(TD^o)).$$

Observe that F^o is locally generated by the m independent 1-forms

$$\mu^a=\frac{\partial\Psi^a}{\partial p_i}\mathcal{H}_{ij}dq^j,\quad 1\leqslant a\leqslant m.$$

Therefore, the ''Hamilton equations'' for the nonholonomic system can be rewritten in intrinsic form as

$$\begin{aligned}&(i_X\omega_Q-dH)_{|M}\in F^o,\\ &X_{|M}\in TM.\end{aligned}\tag{6}$$

Suppose in addition that the following *compatibility condition* $F^\perp\cap TM=\{0\}$ holds, where ''$\perp$'' denotes the symplectic orthogonal with respect to ω_Q. Observe that, locally, this condition means that the matrix

$$(C^{ab})=\left(\frac{\partial\Psi^a}{\partial p_i}\mathcal{H}_{ij}\frac{\partial\Psi^b}{\partial p_j}\right)\tag{7}$$

is regular. On the Lagrangian side, the compatibility condition is locally written as

$$\det(\tilde{C}^{ab})=\det\left(\frac{\partial\phi^a}{\partial\dot{q}^i}W^{ij}\frac{\partial\phi^b}{\partial\dot{q}^j}\right)\neq 0,\tag{8}$$

where W^{ij} are the entries of the Hessian matrix $(\partial^2L/\partial\dot{q}^i\partial\dot{q}^j)_{1\leqslant i,j\leqslant n}$. The compatibility condition is not too restrictive, since, taking into account the admissibility assumption, it is trivially verified by the usual systems of mechanical type (i.e., with a Lagrangian of the form kinetic minus

potential energy), where the $\mathcal{H}_{ij}$ represent the components of a positive definite Riemannian metric. The compatibility condition guarantees in particular the existence of a unique solution of the constrained equations of motion (6) which, henceforth, will be denoted by $X_{H,M}$ on the Hamiltonian side and $\xi_{L,D}$ on the Lagrangian side.

Moreover, if we denote by X_H the Hamiltonian vector field of H, i.e., $i_{X_H}\omega_Q = dH$ then, using the constraint functions, we may explicitely determine the Lagrange multipliers λ_a as

$$\lambda_a = -\mathcal{C}_{ab} X_H(\Psi^b).$$

Next, writing the 1-form

$$\Lambda = -\mathcal{C}_{ab} X_H(\Psi^b) \frac{\partial \Psi^a}{\partial p_j} \mathcal{H}_{ji} dq^i,$$

the nonholonomic equations are equivalently rewritten as

$$\begin{cases} \dot{q}^i = \dfrac{\partial H}{\partial p_i}, \\ \dot{p}_i = -\dfrac{\partial H}{\partial q^i} - \Lambda_i, \end{cases} \tag{9}$$

for initial conditions $(q_0, p_0) \in M$ and $\Lambda = \Lambda_i\, dq^i$. We also denote by $\tilde{\Lambda} = Leg^*(\Lambda)$ the 1-form on TQ wich represents the constraint force once the Lagrange multipliers have been determined. Now, consider the flow $F_t : M \to M$, $t \in I \subseteq \mathbb{R}$ of the vector field $X_{H,M}$, solution of the nonholonomic problem.

Since (9) is geometrically rewritten as

$$i_{X_{H,M}} \omega_Q = dH + \Lambda,$$

($i_{\xi_{L,D}} \omega_L = dE_L + \tilde{\Lambda}$, with $\tilde{\Lambda} = Leg^* \Lambda$, on the Lagrangian side) then

$$L_{X_{H,M}} \theta_Q = d(i_{X_{H,M}} \theta_Q - H) - \Lambda,$$

or, equivalently,

$$L_{X_{H,M}} \theta_Q = d(L \circ Leg^{-1}) - \Lambda.$$

Now, from the dynamical definition of the Lie derivative, we have

$$F_t^*(L_{X_{H,M}} \theta_Q) = \frac{d}{dt}(F_t^* \theta_Q),$$

and integrating, we obtain the following expression, with some abuse of notation,

$$F_h^* \theta_Q - \theta_Q = d\left(\int_0^h L \circ \tilde{F}_t \, dt \right) - \int_0^h F_t^* \Lambda, \tag{10}$$

where $\tilde{F}_t$ is the flow of the vector field $\xi_{L,D}$. In the following sections, we will study geometric integrators which verify a discrete version of Eq. (10).

III. "GENERATING FUNCTIONS" AND NONHOLONOMIC MECHANICS

At this point, we will follow similar arguments for the construction of generating functions for symplectic or canonical maps.[1] However, because of Eq. (10), we have that the nonholonomic flow is not a canonical transformation, i.e.,

$$F_h^*\omega_Q-\omega_Q=d\left(\int_0^h F_t^*\Lambda\right). \tag{11}$$

This description will allow us to construct a new family of nonholonomic integrators for Eq. (3). Denote by $\pi_i:T^*Q\times T^*Q\to T^*Q$, $i=1,2$, the canonical projections. Consider the following forms:

$$\Theta=\pi_2^*\theta_Q-\pi_1^*\theta_Q,$$

$$\Omega=\pi_2^*\omega_Q-\pi_1^*\omega_Q=-d\Theta.$$

Denote by i_{F_h}:Graph$(F_h)\hookrightarrow T^*Q\times T^*Q$ the inclusion map and observe that Graph$(F_h)\subset M\times M$. Then, from (11)

$$i_{F_h}^*\Omega=(\pi_{1_{|\mathrm{Graph}(F_h)}})^*(F_h^*\omega_Q-\omega_Q)=(\pi_{1_{|\mathrm{Graph}(F_h)}})^*\left[d\left(\int_0^h F_t^*\Lambda\right)\right],$$

or, from (10),

$$i_{F_h}^*\Theta=(\pi_{1_{|\mathrm{Graph}(F_h)}})^*\left[d\left(\int_0^h L\circ\tilde{F}_t\,dt\right)-\int_0^h F_t^*\Lambda\right].$$

Let (q_0,p_0,q_1,p_1) be coordinates in $T^*Q\times T^*Q$ in a neighborhood of some point in Graph(F_h). If $(q_0,p_0,q_1,p_1)\in\mathrm{Graph}(F_h)$ then $\Psi^a(q_0,p_0)=0$ and $\Psi^a(q_1,p_1)=0$. Moreover, along Graph(F_h), $q_1=q_1(q_0,p_0)$ and $p_1=p_1(q_0,p_0)$,

$$p_1\,dq_1-p_0dq_0=d\left(\int_0^h L(q(t),\dot{q}(t))\,dt\right)-\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t)), \tag{12}$$

where $(q(t),\dot{q}(t))=\tilde{F}_t(q_0,\dot{q}_0)$ with $Leg(q_0,\dot{q}_0)=(q_0,p_0)$. Here, $\tilde{F}_t$ denotes the flow of $\xi_{L,D}$. Equation (12) is satisfied along Graph(F_h).

Assume that, in a neighborhood of some point $x\in\mathrm{Graph}(F_h)$, we can change this system of coordinates to a new coordinates (q_0,q_1). Denote by

$$S^h(q_0,q_1)=\int_0^h L(q(t),\dot{q}(t))\,dt,$$

where $q(t)$ is a solution curve of the nonholonomic problem with $q(0)=q$ and $q(h)=q_1$. This solution always exists for adequate values of q_0 and q_1. In fact, observe that

$$q_1=q_0+h\frac{\partial H}{\partial p}(q_0,p_0)+o(h^2),$$

hence, since $\det(\partial^2H/\partial p_i\partial p_j)\neq0$, we locally have that $p_0=p_0(q_0,q_1,h)$. But, in addition, $(q_0,p_0)\in M$; therefore $\varphi^a(q_0,q_1,h)=\Psi^a(q_0,p_0(q_0,q_1,h))=0$. Then, the curve

$$(q(t),\dot{q}(t))=Leg^{-1}(F_t(q_0,p_0(q_0,q_1,h))),$$

verifies the required assumptions if $\varphi^a(q_0,q_1,h)=0$.

Thus, we deduce that

$$\begin{cases} p_0 = -\dfrac{\partial S^h}{\partial q_0} + \displaystyle\int_0^h \tilde{\Lambda}(q(t),\dot{q}(t))\,\frac{\partial q}{\partial q_0}, \\ p_1 = \dfrac{\partial S^h}{\partial q_1} - \displaystyle\int_0^h \tilde{\Lambda}(q(t),\dot{q}(t))\,\frac{\partial q}{\partial q_1}, \end{cases} \tag{13}$$

where (q_0,q_1) verifies the constraint functions $\varphi^a(q_0,q_1,h)=0$, now explicitly defined by

$$\varphi^a(q_0,q_1,h) = \Psi^a\left(q_0, -\frac{\partial S^h}{\partial q_0}(q_0,q_1) + \int_0^h \tilde{\Lambda}(q(t),\dot{q}(t))\,\frac{\partial q}{\partial q_0}\right), \quad 1\leqslant a\leqslant m, \tag{14}$$

with $q(t)$ solution of the nonholonomic problem with $q(0)=q_0$ and $q(h)=q_1$.

Next, we will show how the group composite law of the flow F_h

$$F_{Nh} = \underbrace{F_h \circ \ldots \circ F_h}_{N}$$

is expressed in terms of the corresponding ''generating functions'' S^h. Moreover, the following Theorem will result in a new construction of numerical integrators for nonholonomic mechanics when we change the ''generating function'' and the constraint forces by appropriate approximations. As a generalization of Theorem 1.1 we have the following:

Theorem 3.1: *The function S^{Nh}, the "generating function" for F_{Nh}, is given by*

$$S^{Nh}(q_0,q_N) = \sum_{k=0}^{N-1} S^h(q_k,q_{k+1}),$$

where q_k, $1\leqslant k\leqslant N-1$, are points verifying

$$D_2S^h(q_{k-1},q_k) + D_1S^h(q_k,q_{k+1}) = \int_0^h \tilde{\Lambda}(q(t),\dot{q}(t))\,\frac{\partial q}{\partial q_1} + \int_h^{2h} \tilde{\Lambda}(q(t),\dot{q}(t))\,\frac{\partial q}{\partial q_0}, \tag{15}$$

and $q(t)$ is a solution curve of the nonholonomic problem with $q(0)=q_{k-1}$ and $q(h)=q_k$ (respectively, $q(h)=q_k$ and $q(2h)=q_{k+1}$) for the first integral (resp., second integral) of the right-hand side.

Proof: By a recursion argument, it is suffices to prove the result for $N=2$; that is,

$$S^{2h}(q_0,q_2) = S^h(q_0,q_1) + S^h(q_1,q_2),$$

where q_1 verifies condition (15).

Since

$$p_1\,dq_1 - p_0\,dq_0 = dS^h(q_0,q_1) - \int_0^h \tilde{\Lambda}(q(t),\dot{q}(t)),$$

$$p_2\,dq_2 - p_1\,dq_1 = dS^h(q_1,q_2) - \int_h^{2h} \tilde{\Lambda}(q(t),\dot{q}(t)),$$

then

$$p_2\,dq_2 - p_0\,dq_0 = d(S^h(q_0,q_1) + S^h(q_1,q_2)) - \int_0^h \tilde{\Lambda}(q(t),\dot{q}(t)) - \int_h^{2h} \tilde{\Lambda}(q(t),\dot{q}(t)).$$

Since the variables q_1 do not appear on the left-hand side term, it follows that

$$0=D_2S_1^h(q_0,q_1)+D_1S_2^h(q_1,q_2)-\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}-\int_h^{2h}\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0}, \quad (16)$$

and for a choice of q_1 verifying (16), then

$$S^{2h}(q_0,q_2)=S^h(q_0,q_1)+S^h(q_1,q_2)$$

is a ''generating function of the first kind'' of F_{2h} because

$$p_2\,dq_2-p_0\,dq_0=dS^{2h}(q_0,q_2)-\int_0^{2h}\tilde{\Lambda}(q(t),\dot{q}(t)).$$

■

Equation (15) determines a implicit system of difference equations which permits us to obtain q_2 from the initial data q_0 and q_1. An interesting consequence of this is that these equations preserve the constraint submanifold determined by the constraints $\varphi^a=0$, $1\leqslant a\leqslant m$. In fact, if $\varphi^a(q_0,q_1,h)=0$ (that is $\Psi^a(q_0,p_0)=0$) then

$$\varphi^a(q_1,q_2,h)=\Psi^a\left(q_1,\frac{\partial S^h}{\partial q_1}(q_0,q_1)-\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}\right),$$

and now, applying (13), we obtain that

$$\varphi^a(q_1,q_2,h)=\Psi^a(q_1,p_1)=0,$$

since $F_h(q_0,p_0)=(q_1,p_1)$ and the flow preserves the constraints.

The next remark will be a key result for the construction of nonholonomic integrators.

Remark 3.2: Replace Eq. (13) by

$$\begin{cases} p_0=-\dfrac{\partial\tilde{S}^h}{\partial q_0}+\alpha_0^h(q_0,q_1), \\ p_1=\dfrac{\partial\tilde{S}^h}{\partial q_1}-\alpha_1^h(q_0,q_1), \end{cases} \quad (17)$$

where $\tilde{S}^h$ is a function of (q_0,q_1) coordinates and $\alpha^h=\alpha_0^h\,dq_0+\alpha_1^h\,dq_1$, and replace the constraints functions by

$$\tilde{\varphi}^a(q_0,q_1,h)=\Psi^a\left(q_0,-\frac{\partial\tilde{S}^h}{\partial q^0}+\alpha_0^h(q_0,q_1)\right), \quad (18)$$

that is,

$$p_1\,dq_1-p_0\,dq_0=d\tilde{S}^h-\alpha^h,$$

along $\tilde{\varphi}^a=0$.

Assume that

$$\det\left(\frac{\partial^2\tilde{S}^h}{\partial q_0\partial q_1}-\frac{\partial\alpha_0^h}{\partial q_1}\right)\neq 0, \quad (19)$$

then, applying the implicit function theorem we have that, locally, $q_1=q_1(q_0,p_0)$, and therefore, the mapping

$$G_h(q_0,p_0)=(q_1,p_1)$$

is well-defined.

Consider the mapping G_{Nh} defined by

$$G_{Nh}=\underbrace{G_h\circ\ldots\circ G_h}_{N}.$$

Following a similar argument to Theorem 3.1, Graph(G_{Nh}) is described by

$$\begin{cases} p_0=-\dfrac{\partial\widetilde{S}^{Nh}}{\partial q_0}(q_0,q_N)+\alpha_0^{Nh}(q_0,q_N), \\ p_N=\dfrac{\partial\widetilde{S}^{Nh}}{\partial q_N}(q_0,q_N)-\alpha_1^{Nh}(q_0,q_N), \end{cases} \tag{20}$$

where $\widetilde{S}^{Nh}(q_0,q_N)=\Sigma_{k=0}^{N-1}\widetilde{S}^h(q_k,q_{k+1})$ and $\alpha^{Nh}(q_0,q_N)=\Sigma_{k=0}^{N-1}\alpha^h(q_k,q_{k+1})$. Here, the q_k's, $1\leqslant k\leqslant N-1$, verify

$$D_2\widetilde{S}^h(q_{k-1},q_k)+D_1\widetilde{S}^h(q_k,q_{k+1})=\alpha_1^h(q_{k-1},q_k)+\alpha_0^h(q_k,q_{k+1}),\quad 1\leqslant k\leqslant N-1. \tag{21}$$

A. Constraint error analysis

As we have seen, if our "generating function" is S^h, then we have exact preservation of the constraints φ^a. We now investigate what happens when the "generating function" is an approximation. We follow similar arguments to those in Sec. III C in Ref. 43.

Assume that Q, and also TQ and T^*Q, are finite-dimensional vector spaces with inner product $\langle .,. \rangle$ and corresponding norm $\|\ \|$.

Consider an "approximated generating function" $\widetilde{S}^h$ and an approximated discrete constraint force $\alpha^h=\alpha_i^h\,dq^i$ for the nonholonomic problem, both of order r (all the functions are assumed to be C^2); hence, there exists an open set $U\subset D$ with compact closure and constants $c,d_i>0$, $1\leqslant i\leqslant n$, and $H>0$ such that

$$\widetilde{S}^h(q_0,q_1)=S^h(q_0,q_1)+C(q_0,q_1,h)h^{r+1}, \tag{22}$$

$$\alpha_i^h=\int_0^h\tilde{\Lambda}_i(q(t),\dot{q}(t))\,dt+D_i(q_0,q_1,h)h^{r+1}, \tag{23}$$

for all solution $q(t)$ of the nonholonomic problem with $q(0)=q_0$, $q(h)=q_1$ and initial condition belonging to U and $h\leqslant H$. Here C and D_i, $1\leqslant i\leqslant n$, are smooth functions such that $\|C(q_0,q_1,h)\|\leqslant c$ and $\|D_i(q_0,q_1,h)\|\leqslant d_i$ on U.

Taking derivatives we have that

$$\frac{\partial\widetilde{S}^h}{\partial q_0}(q_0,q_1)=\frac{\partial S^h}{\partial q_0}(q_0,q_1)+\frac{\partial C}{\partial q_0}(q_0,q_1,h)h^{r+1}$$

and also

$$\alpha_0^h(q_0,q_1)=(\alpha_0)_i^h\frac{\partial q^i}{\partial q_0}=\int_0^h\tilde{\Lambda}_i(q(t),\dot{q}(t))\frac{\partial q^i}{\partial q_0}dt+\sum_{i=1}^n\frac{\partial D_i}{\partial q_0}(q_0,q_1,h)h^{r+1},$$

where now $\alpha^h=\alpha_0^h\,dq_0+\alpha_1^h\,dq_1$.

Therefore, we deduce that

$$\begin{aligned}\tilde{\varphi}^a(q_0,q_1,h)&=\Psi^a\left(q_0,-\frac{\partial\tilde{S}}{\partial q^0}+\alpha_0(q_0,q_1)\right)\\&=\Psi^a\left(q_0,-\frac{\partial S^h}{\partial q_0}+\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0}\right)+E^a(q_0,q_1,h)h^{r+1}\\&=\Psi^a(q_0,p_0)+E^a(q_0,q_1,h)h^{r+1}\\&=E^a(q_0,q_1,h)h^{r+1},\end{aligned}$$

where E^a are bounded functions. Thus, the discrete algorithm preserves the constraints up to order r.

B. Local error analysis

Assuming that

$$\det\left(\frac{\partial^2\tilde{S}^h}{\partial q_0\partial q_1}-\frac{\partial\alpha_0^h}{\partial q_1}\right)\neq 0, \tag{24}$$

we obtain a discrete flow $G^h: V\subseteq T^*Q\to T^*Q$. Now, using Eqs. (13), (22), and (23) we deduce that

$$\begin{cases} p_0=-\dfrac{\partial S^h}{\partial q_0}+\displaystyle\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0}=\frac{\partial\tilde{S}^h}{\partial q_0}(q_0,q_1)+\alpha_0^h(q_0,q_1)+E_0(q_0,q_1,h)h^{r+1},\\ p_1=\dfrac{\partial S^h}{\partial q_1}-\displaystyle\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}=\frac{\partial\tilde{S}^h}{\partial q_1}(q_0,q_1)-\alpha_1^h(q_0,q_1)+E_1(q_0,q_1,h)h^{r+1},\end{cases} \tag{25}$$

where E_0 and E_1 are smooth and bounded functions.

Applying the implicit function theorem to (25), it is easy to show, from conditions (22) and (23), that G^h is an integrator of $X_{H,M}$ of order r (see for details Theorem 2.3.1 in Ref. 43).

IV. CONSTRUCTION OF NONHOLONOMIC INTEGRATORS

In what follows and for simplicity assume that Q is a vector space. Since $S^h(q_0,q_1)=\int_0^h L(q(t),\dot{q}(t))\,dt$, where $q(t)$ is a nonholonomic solution with $q(0)=q_0$ and $q(h)=q_1$, using Remark 3.2, we can obtain nonholonomic integrators by taking adequate approximations of the "generating function" S^h and the extra-term $\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))$.

Consider, for instance, the approximation

$$S_\alpha^h(q_0,q_1)=hL\left((1-\alpha)q_0+\alpha q_1,\frac{q_1-q_0}{h}\right), \tag{26}$$

for some parameter $\alpha\in[0,1]$. (In general, we will write $S_\alpha^h(q_0,q_1)\approx S^h(q_0,q_1)$.)

A natural approximation of the constraint forces adapted to our choice of approximation for S^h are

$$\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0}\approx(1-\alpha)h\tilde{\Lambda}\left((1-\alpha)q_0+\alpha q_1,\frac{q_1-q_0}{h}\right),$$

$$\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}\approx\alpha h\tilde{\Lambda}\left((1-\alpha)q_0+\alpha q_1,\frac{q_1-q_0}{h}\right).$$

Consequently, Eqs. (21) give us the following numerical method for nonholonomic systems:

$$D_2S^h_\alpha(q_{k-1},q_k)+D_1S^h_\alpha(q_k,q_{k+1})=\alpha h\tilde{\Lambda}\left((1-\alpha)q_{k-1}+\alpha q_k,\frac{q_k-q_{k-1}}{h}\right)$$
$$+(1-\alpha)h\tilde{\Lambda}\left((1-\alpha)q_k+\alpha q_{k+1},\frac{q_{k+1}-q_k}{h}\right),$$
$$1\leqslant k\leqslant N-1,$$

with initial condition satisfying

$$\tilde{\varphi}^a(q_0,q_1,h)=\Psi^a\left(q_0,-\frac{\partial S^h_\alpha}{\partial q_0}(q_0,q_1)+(1-\alpha)h\tilde{\Lambda}\left((1-\alpha)q_0+\alpha q_1,\frac{q_1-q_0}{h}\right)\right)=0.$$

Remark 4.1: Obviously, it is possible to produce a wider variety of discrete methods. For example,

$$S^h_{\mathrm{sym},\alpha}=\tfrac{1}{2}S^h_\alpha+\tfrac{1}{2}S^h_{1-\alpha},$$

gives a second-order method for any $\alpha\in[0,1]$. Also, higher-order approximations of the function S^h may be considered.

Example 4.2: Nonholonomic particle: Consider the Lagrangian $L:T\mathbb{R}^3\to\mathbb{R}$

$$L=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2)-(x^2+y^2),$$

subject to the constraint

$$\phi=\dot{z}-y\dot{x}=0.$$

It is easy to compute the nonholonomic differential equations

$$\ddot{x}=-\frac{2x+y\dot{x}\dot{y}}{1+y^2},$$

$$\ddot{y}=-2y,$$

$$\ddot{z}=\frac{-2xy+\dot{x}\dot{y}}{1+y^2},$$

where now the constraint 1-form is

$$\tilde{\Lambda}=\frac{2xy-\dot{x}\dot{y}}{1+y^2}(dz-ydx).$$

The system being simulated here is purely conservative and so there should be no loss of energy over time.

Taking

$$S^h_{1/2}(x_0,y_0,z_0,x_1,y_1,z_1)=\frac{h}{2}\left[\left(\frac{x_1-x_0}{h}\right)^2+\left(\frac{y_1-y_0}{h}\right)^2+\left(\frac{z_1-z_0}{h}\right)^2\right]-\left(\frac{x_0+x_1}{2}\right)^2-\left(\frac{y_0+y_1}{2}\right)^2,$$

we obtain the nonholonomic integrator

$$\frac{x_1-x_0}{h}-h\frac{x_1+x_0}{2}-\frac{x_2-x_1}{h}-h\frac{x_2+x_1}{2}=-\frac{h}{2}\left[\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\cdot\frac{y_1+y_0}{2}\right.$$
$$\left.+\frac{\frac{(x_2+x_1)(y_2+y_1)}{2}-\frac{(x_2-x_1)(y_2-y_1)}{h^2}}{1+\left(\frac{y_2+y_1}{2}\right)^2}\cdot\frac{y_2+y_1}{2}\right],$$

$$\frac{y_1-y_0}{h}-h\frac{y_1+y_0}{2}-\frac{y_2-y_1}{h}-h\frac{y_2+y_1}{2}=0,$$

$$\frac{z_1-z_0}{h}-\frac{z_2-z_1}{h}=\frac{h}{2}\left[\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\right.$$
$$\left.+\frac{\frac{(x_2+x_1)(y_2+y_1)}{2}-\frac{(x_2-x_1)(y_2-y_1)}{h^2}}{1+\left(\frac{y_2+y_1}{2}\right)^2}\right].$$

The constraint function on $\mathbb{R}^3\times\mathbb{R}^3$ is

$$\tilde{\varphi}^a(x_0,y_0,z_0,x_1,y_1,z_1,h)$$
$$=-\frac{z_1-z_0}{h}-\frac{h}{2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}$$
$$+y_0\left[\frac{x_1-x_0}{h}+h\frac{x_1+x_0}{2}-\frac{h}{2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\cdot\frac{y_1+y_0}{2}\right].$$

Figures 1 and 2 show the preservation of energy as a key point of comparison of computational implementations of the method exposed above to other methods. In Fig. 3 we show the behavior of the constraint function.

Remark 4.3: Generating function approach and discrete Lagrange–d'Alembert principle: A discussion: As is well known, a remarkable feature of symplectic transformations is that it can be expressed in terms of a single real-valued function S, the generating function of the canonical transformation. Therefore, any symplectic integrator has associated a generating function. Now, taking adequate approximations of the generating function associated to the exact flow of a Hamiltonian system, we generate symplectic integrators (see, for instance, symplectic and symplectic partitioned Runge–Kutta methods in Ref. 17) by using generating functions of the first kind, second kind, and so on. It is also possible to construct symplectic numerical methods of higher order considering better approximations of the generating function in the Hamilton–Jacobi equation (see Ref. 9).

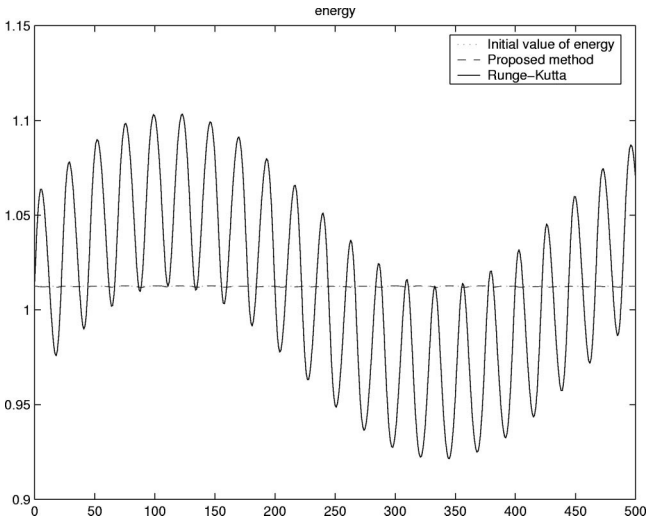

FIG. 1. Comparison of the method introduced here to the traditional Runge–Kutta method of fourth order, showing an improvement in several orders of magnitude. Observe that, in this scale, the value of the energy in each step of our algorithm is practically undistinguishable from the initial value of the energy, therefore our method does not artificially dissipate energy.

As we have said in Sec. I B, the discrete variational approach and the generating function approach are in fact the same on generating function of the first kind. That is, considering the action integral as a function of (q_0,q_1), for the solution $q(t)$ of the Euler–Lagrange equations we have that

$$S^h(q_0,q_1)=\int_0^h L(q(t),\dot{q}(t))\,dt$$

(this is precisely, the exact discrete Lagrangian following the notation in Marsden and West[43]). Therefore, a discrete Lagrangian L_d is a discrete approximation of the above action integral or, in other words, an approximated generating function for S^h.

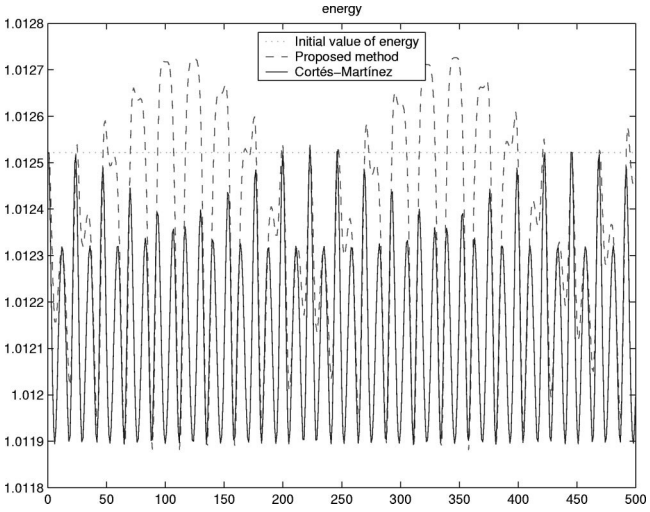

FIG. 2. A comparison between our method and the one that appeared in Refs. 10 and 12. A similar behavior is observed. Nevertheless, a slightly better behavior can also be appreciated, where the proposed algorithm shows on average a better preservation of the original energy.

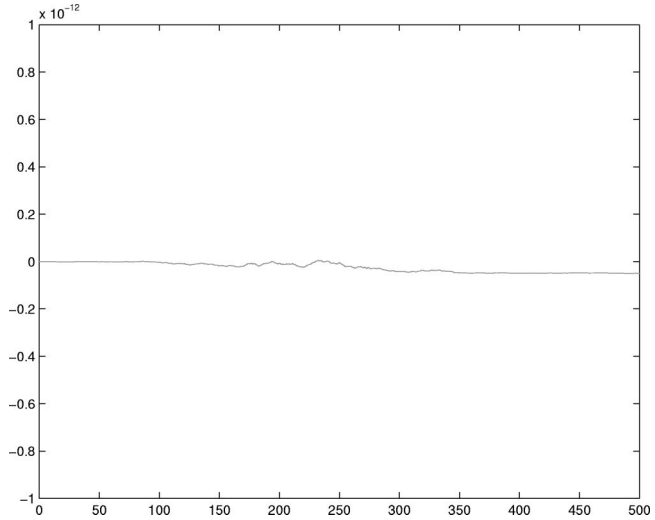

FIG. 3. For the same initial conditions and data, the following graph shows very good behavior of the constraint function evolution with time (notice the small scale).

In Sec. III B of Ref. 43, the authors discuss Discrete variational mechanics with forces and using the so-called *Discrete Lagrange–d'Alembert principle*, they simulate a given forced Lagrangian or Hamiltonian system choosing discrete Lagrangians and discrete forces to approximate the exact quantities.

Formally, the approach followed in Secs. III and IV is equivalent to the approach given in Ref. 43 considering a nonholonomic system as a Lagrangian system with forces determined with the constraint equations. However, a new insight is gained from the generating function approach. First, our theory is ready for the constructions of new numerical integrators for nonholonomic systems using Hamilton–Jacobi theory for nonholonomic systems (see Ref. 14) or even ''generating functions'' for nonholonomic system of different kinds. Observe that, for instance, symplectic Runge–Kutta methods were generated using generating functions of the third kind (see Ref. 48). Second, since symplectic integrators based on generating functions is strongly established in numerical analysis research, we think that our presentation will be clearer than the usual one of discrete Lagrangians frequently used by the geometrical mechanics researchers.

V. MECHANICAL SYSTEMS WITH LINEAR CONSTRAINTS: GEOMETRIC NUMERICAL METHODS PRESERVING CONSTRAINTS

In Secs. III and IV we have constructed a family of numerical integrators for nonholonomic mechanics; these integrators do not preserve the constraint but we show that the violation of the constraint is very small. This answer is not completely satisfactory for a numerical method for a nonholonomic system (as, for instance, rolling constraints in wheeled vehicles), therefore we impose the preservation of the nonholonomic constraints obtaining a subfamily of the above numerical integrators in this section. As we shall show more insight is performed by restricting ourselves to the particular (but general in a mechanical sense) case of Lagrangians of mechanical type ($L=T-V$) and constraints linear on velocities.

Therefore, suppose that the mechanical system, given by the Lagrangian $L:TQ\to\mathbb{R}$

$$L(v_q)=\tfrac{1}{2}g(v_q,v_q)-V(q)$$

is subjected to nonholonomic constraints $\phi^a:TQ\to\mathbb{R}$, $1\leqslant a\leqslant m$. Since the nonholonomic constraints usually found in mechanics are linear in the velocities, we will assume that

$$\phi^a(q,\dot{q}) = \mu_i^a(q)\dot{q}^i, \quad 1 \leqslant a \leqslant m.$$

From a geometric point of view, these linear constraints are determined by prescribing a distribution $\mathcal{D}$ on Q of dimension $n-m$ such that the annihilator of $\mathcal{D}$ is locally given by

$$\mathcal{D}^o = \langle \mu^a = \mu_i^a dq^i; 1 \leqslant a \leqslant m \rangle .$$

In this manner, the solutions of the nonholonomic Lagrangian system satisfy

$$\nabla_{\dot{c}(t)}\dot{c}(t) = -\operatorname{grad} V(c(t)) + \lambda(\dot{c}(t)), \quad \dot{c}(t) \in \mathcal{D}_{c(t)}, \tag{27}$$

where λ is a section of $\mathcal{D}^\perp$ along c, and $\mathcal{D}^\perp$ stands for the orthogonal complement of $\mathcal{D}$ with respect to the metric g.

Since g is a Riemannian metric, the $m \times m$ matrix $(C^{ab}) = (\mu_i^a g^{ij} \mu_j^b)$ is symmetric and regular. Therefore, we can explicitly determine

$$\lambda(q^i(t),\dot{q}^i(t)) = C_{ab}\left(\left(-\Gamma_{jk}^i \dot{q}^j \dot{q}^k - g^{ij}\frac{\partial V}{\partial q^j} \right) \mu_i^a + \dot{q}^i \dot{q}^j \frac{\partial \mu_i^a}{\partial q^j} \right) Z^b, \tag{28}$$

where (C_{ab}) is the inverse matrix of (C^{ab}), Γ_{jk}^i are the Christoffel components and the vector field Z^a is defined by

$$g(Z^a, Y) = \mu^a(Y), \quad \text{for all vector field } Y, \quad 1 \leqslant a \leqslant m,$$

that is, Z^a is the gradient of the 1-form μ^a. Thus, $\mathcal{D}^\perp = \langle Z^a \rangle$, $1 \leqslant a \leqslant m$. In local coordinates, we have

$$Z^a = g^{ij}\mu_i^a \frac{\partial}{\partial q^j}.$$

By using the metric g and the distribution $\mathcal{D}$ we can obtain two complementary projectors

$$\mathcal{P}: TQ \to \mathcal{D},$$

$$\mathcal{Q}: TQ \to \mathcal{D}^\perp,$$

with respect to g. The projector $\mathcal{Q}$ is locally described by

$$\mathcal{Q} = C_{ab} Z^a \otimes \mu^b.$$

Using these projectors we can obtain the equations of motion as follows. A curve $c(t)$ is a motion for the nonholonomic system if it satisfies the constraints, say, $\phi^a(\dot{c}(t)) = 0$, for all a, and, in addition, the "projected equation of motion,"

$$\mathcal{P}(\nabla_{\dot{c}(t)}\ \dot{c}(t)) = -\mathcal{P}(\operatorname{grad} V(c(t))) \tag{29}$$

is fulfilled. But these conditions are equivalent to

$$\dot{c}(t) \in \mathcal{D}_{c(t)}, \quad \overline{\nabla}_{\dot{c}(t)}\dot{c}(t) = -\mathcal{P}(\operatorname{grad} V(c(t))),$$

where $\overline{\nabla}$ is the modified linear connection defined by

$$\overline{\nabla}_X Y = \nabla_X Y + (\nabla_X \mathcal{Q})(Y)$$

for all vector fields X and Y on Q.

Since the constraints are linear then, from (14)

$$-\mu_i^a(q_0)g^{ij}(q_0)\frac{\partial S^h}{\partial q_0^j}(q_0,q_1)+\mu_i^a(q_0)g^{ij}(q_0)\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0^j}=0,\quad 1\leqslant a\leqslant m,\quad (30)$$

or, in terms of projectors,

$$\mathcal{Q}_{|q_0}(D_1S^h(q_0,q_1)))=\mathcal{Q}_{|q_0}\left(D_1\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\right).\quad (31)$$

Moreover, the dynamics preserves the constraints Ψ^a which implies that

$$\Psi^a\left(q_1,\frac{\partial S^h}{\partial q_1}(q_0,q_1)-\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}\right)=0,$$

or, in other words,

$$\mathcal{Q}_{|q_1}(D_2S^h(q_0,q_1))=\mathcal{Q}_{|q_1}\left(D_2\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\right).\quad (32)$$

Therefore, Eqs. (31) and (32) show that the preservation of the exact constraints is equivalent to give a prescription about the relationship between the ''generating function'' and the constraint forces.

Thus, Eq. (15),

$$D_2S^h(q_{k-1},q_k)+D_1S^h(q_k,q_{k+1})=\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}+\int_h^{2h}\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0},$$

can be rewritten using expression (32) as follows:

$$\mathcal{P}_{|q_k}(D_2S^h(q_{k-1},q_k))+D_1S^h(q_k,q_{k+1})=\mathcal{P}_{|q_k}\left(\int_0^h\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_1}\right)+\int_h^{2h}\tilde{\Lambda}(q(t),\dot{q}(t))\frac{\partial q}{\partial q_0}.\quad (33)$$

Now, considering an approximated generating function $\tilde{S}^h$ and an approximate constraint force $\alpha^h=\alpha_0^h(q_0,q_1)\,dq_0+\alpha_1^h(q_0,q_1)\,dq_1$, as in Remark 3.2, from the previous discussion, we now substitute the approximated constraint force by

$$\tilde{\alpha}^h=\alpha_0^h(q_0,q_1)\,dq_0+\mathcal{P}_{|q_1}(\alpha_1^h(q_0,q_1)\,dq_1)+\mathcal{Q}_{|q_1}(D_2\tilde{S}^h(q_0,q_1))).$$

Therefore for $\tilde{S}^h$ and $\tilde{\alpha}^h$, Eqs. (21) are rewritten as

$$\mathcal{P}_{|q_k}(D_2\tilde{S}^h(q_{k-1},q_k))+D_1\tilde{S}^h(q_k,q_{k+1})=\mathcal{P}_{|q_k}(\alpha_1^h(q_{k-1},q_k))+\alpha_0^h(q_k,q_{k+1}),\quad (34)$$

for $1\leqslant k\leqslant N-1$. The importance of Eq. (34) is that they generate an algorithm which automaticaly preserves the exact constraint functions Ψ^a. In fact, if we apply the projector $\mathcal{Q}$ to Eq. (34) we obtain

$$\mathcal{Q}_{|q_k}(D_1S^h(q_k,q_{k+1}))=\mathcal{Q}_{|q_k}(\alpha_0^h(q_k,q_{k+1}))\quad (35)$$

or

$$\tilde{\varphi}^a(q_k,q_{k+1},h)=\Psi^a\left(q_k,-\frac{\partial\tilde{S}^h}{\partial q_0}(q_k,q_{k+1})+\alpha_0^h(q_k,q_{k+1})\right)=0,$$

that is, the constraints are satisfied.

Therefore the geometric algorithm that we have obtained work as follows:

$$\mathcal{P}_{|q_k}(D_2\tilde{S}^h(q_{k-1},q_k))+D_1\tilde{S}^h(q_k,q_{k+1})=\mathcal{P}_{|q_k}(\alpha_1^h(q_{k-1},q_k))+\alpha_0^h(q_k,q_{k+1}),$$

with initial condition satisfying:

$$\tilde{\varphi}^a(q_0,q_1,h)=0.$$

Choosing α_0^h and α_1^h in $\mathcal{D}^0$, we obtain equations for nonholonomic integrators with more geometric flavor:

Geometric nonholonomic integrator:

$$\mathcal{P}_{|q_k}(D_2\tilde{S}^h(q_{k-1},q_k)+D_1\tilde{S}^h(q_k,q_{k+1}))=0 \tag{36}$$

which is interpreted as a discretization of Eq. (29),

$$\overline{\nabla}_{\dot{c}(t)}\dot{c}(t)=-\mathcal{P}(\mathrm{grad}\,(V(c(t)))).$$

In a future work we will study from numerical and geometrical points of view this particular subclass of geometric integrators.

Nonholonomic integrators preserving constraints: For the class of integrators introduced in Sec. IV, we find the following family of nonholonomic integrators preserving constraints:

$$\begin{aligned}\mathcal{P}_{|q_k}(D_2S_\alpha^h(q_{k-1},q_k))+D_1S_\alpha^h(q_k,q_{k+1})=\alpha h\mathcal{P}_{|q_k}&\left(\tilde{\Lambda}\left((1-\alpha)q_{k-1}+\alpha q_k,\frac{q_k-q_{k-1}}{h}\right)\right)\\&+(1-\alpha)h\tilde{\Lambda}\left((1-\alpha)q_k+\alpha q_{k+1},\frac{q_{k+1}-q_k}{h}\right),\\&1\leqslant k\leqslant N-1\ ,\end{aligned}$$

with initial conditions satisfying

$$-\mu_i^a(q_0)g^{ij}(q_0)\frac{\partial S_\alpha^h}{\partial q_0^j}(q_0,q_1)+(1-\alpha)h\mu_i^a(q_0)g^{ij}(q_0)\tilde{\Lambda}_j\left((1-\alpha)q_0+\alpha q_1,\frac{q_1-q_0}{h}\right)=0.$$

Example 5.1 (The nonholonomic particle revisited): Constructing the previous algorithm for the nonholonomic particle, we obtain the following preserving constraint integrator:

$$\frac{1}{1+y_1^2}\left(\frac{x_1-x_0}{h}-h\frac{x_1+x_0}{2}\right)-\frac{x_2-x_1}{h}-h\frac{x_2+x_1}{2}+\frac{y_1}{1+y_1^2}\left(\frac{z_1-z_0}{h}\right)$$

$$=-\frac{h}{2}\left[\frac{\frac{1}{1+y_1^2}\cdot\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\cdot\frac{y_1+y_0}{2}\right.$$

$$+\frac{\frac{(x_2+x_1)(y_2+y_1)}{2}-\frac{(x_2-x_1)(y_2-y_1)}{h^2}}{1+\left(\frac{y_2+y_1}{2}\right)^2}\cdot\frac{y_2+y_1}{2}$$

$$\left.-\frac{y_1}{1+y_1^2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\right]\frac{y_1-y_0}{h}$$

$$-h\frac{y_1+y_0}{2}-\frac{y_2-y_1}{h}-h\frac{y_2+y_1}{2}=0,$$

$$\frac{y_1^2}{1+y_1^2}\left(\frac{z_1-z_0}{h}\right)-\frac{z_2-z_1}{h}+\frac{y_1}{1+y_1^2}\left(\frac{x_1-x_0}{h}-h\frac{x_1+x_0}{2}\right)$$

$$=\frac{h}{2}\left[\frac{y_1^2}{1+y_1^2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}+\frac{\frac{(x_2+x_1)(y_2+y_1)}{2}-\frac{(x_2-x_1)(y_2-y_1)}{h^2}}{1+\left(\frac{y_2+y_1}{2}\right)^2}\right.$$

$$\left.-\frac{y_1}{1+y_1^2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\cdot\frac{y_1+y_0}{2}\right]$$

with initial conditions satisfying (see Fig. 4)

$$\tilde{\varphi}^a(x_0,y_0,z_0,x_1,y_1,z_1,h)$$

$$=-\frac{z_1-z_0}{h}-\frac{h}{2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}$$

$$+y_0\left[\frac{x_1-x_0}{h}+h\frac{x_1+x_0}{2}-\frac{h}{2}\frac{\frac{(x_1+x_0)(y_1+y_0)}{2}-\frac{(x_1-x_0)(y_1-y_0)}{h^2}}{1+\left(\frac{y_1+y_0}{2}\right)^2}\cdot\frac{y_1+y_0}{2}\right].$$

Remark 5.2: In numerical analysis, an approach to the numerical solution of differential equations is by projecting into a subset of invariants. These projection techniques do not deteriorate the convergence order of the method but they can, in some cases, destroy the good long-time behavior of the solution. However a different behavior arises in the projection techniques that we have constructed in this section.

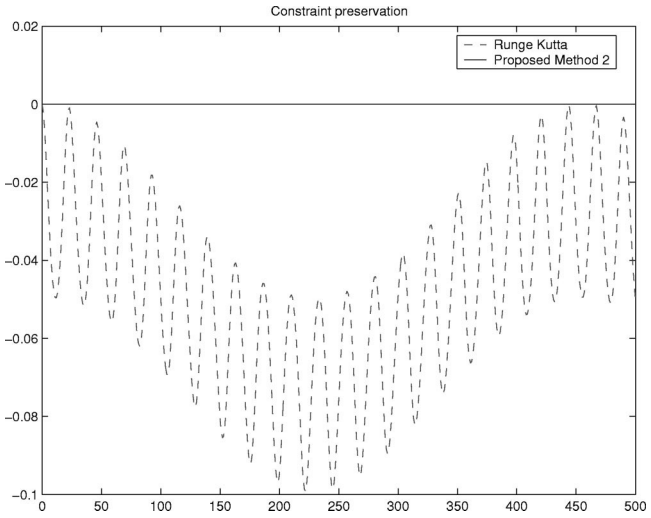

FIG. 4. For the same initial conditions and data, the graph shows the exact preservation of the constraint function evolution with time of our algorithm.

Observe that a remarkable feature of nonholonomic systems is the nonpreservation of the symplectic form, therefore its flow does not act as symplectic transformations; in a geometric way

$$L_{X_{H,M}}\omega_Q = d\Lambda \neq 0.$$

In Sec. III, we have generated integrators verifying a discrete version of the previous equation. The use of projection techniques are adequate in this case, since we *recover* the geometrical properties of the nonholonomic system.

In the continuous setting it is well known, for instance, in Ref. 30, how to obtain the solution of nonholonomic systems from the free dynamics using projection techniques. Also, projection techniques are used in a Riemannian setting, modifying the Levi–Civita connection to obtain an affine connection which gives as the correct dynamics (see Ref. 11 and references therein). This is the main idea of Sec. V, where we show that projection techniques are useful for nonholonomic systems. Observe, for instance, the integrator proposed in (36). We take a variational integrator and then symplectic (a bad property for a nonholonomic integrator), and projecting orthogonally the discrete Euler–Lagrange equations, we obtain a nonholonomic integrator.

VI. CONCLUSION

A new numerical algorithm has been proposed for nonholonomic mechanics. This algorithm is based in the underlying geometry of nonholonomic systems. For mechanical systems with linear constraints, a geometric integrator preserving constraints is proposed.

In future work, we will explore reduction schemes for discrete systems using the approach of generating functions. It is also interesting to use generating functions of different kinds; in a recent work,[32] we have shown that generating functions of second class generate algorithms which are symplectic (in some sense) for discrete optimal control theory (see also Ref. 33). Moreover, we may easily extend the generating function technique in order to consider variable time stepping and also the time-dependent case and it would be possible to use this formalism for classical field theories.

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Nonintegrability of the Suslov problem

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In this paper we investigate the Suslov problem in the case when the vector of nonholonomic constraint coincides with the third principal axis of the body, and the fixed point of the body lies in the principal plane defined by the third and the first principal axes but is out of these axes. We called this version of the Suslov problem the generalized Kozlov case, and we prove that in this case a third real meromorphic first integral functionally independent together with the energy and geometrical integrals does not exist. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Let us consider the rotational motion of a rigid body around a fixed point O in a constant gravity field. The motion of the body is restricted by one nonholonomic constraint $\langle \mathbf{a},\boldsymbol{\omega}\rangle=0$, where $\boldsymbol{\omega}=(\omega_1,\omega_2,\omega_3)$ is the body angular velocity and $\mathbf{a}$ is a vector fixed in the body. Here and below all vectors are taken with respect to the principal axes reference frame, and $\langle\cdot,\cdot\rangle$ denotes the standard scalar product. This is the formulation of the classical Suslov problem[30] which is one of the most famous problems in nonholonomic mechanics. Equations of motion of the Suslov problem have the following form:

$$\begin{aligned} \mathbb{I}\dot{\boldsymbol{\omega}}&=\mathbb{I}\boldsymbol{\omega}\times\boldsymbol{\omega}+\epsilon\boldsymbol{\gamma}\times\mathbf{b}+\lambda\mathbf{a},\\ \dot{\boldsymbol{\gamma}}&=\boldsymbol{\gamma}\times\boldsymbol{\omega},\quad \langle\mathbf{a},\boldsymbol{\omega}\rangle=0, \end{aligned} \tag{1}$$

where λ is the Lagrange multiplier, $\mathbb{I}=\mathrm{diag}(I_1,I_2,I_3)$ is the matrix of inertia of the body; ϵ is the product of the mass of the body, the gravity constant and the distance between point O and the mass center of the body; vectors $\boldsymbol{\gamma}=(\gamma_1,\gamma_2,\gamma_3)$ and $\mathbf{b}=(b_1,b_2,b_3)$ are the unit vertical vector and the unit vector along the line connecting point O with the center of mass of the body, respectively.

In this paper we assume that vector $\mathbf{a}$ coincides with one of the principal axes, and, without loss of generality, we can choose it as the third axis, i.e., $\mathbf{a}=(0,0,1)$. For such choice equations (1) read

$$\begin{aligned} I_1\dot{\omega}_1&=\epsilon(\gamma_2 b_3-\gamma_3 b_2),\\ I_2\dot{\omega}_2&=\epsilon(\gamma_3 b_1-\gamma_1 b_3),\\ \dot{\gamma}_1&=-\omega_2\gamma_3, \end{aligned} \tag{2}$$

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$$\dot{\gamma}_2 = \omega_1 \gamma_3,$$

$$\dot{\gamma}_3 = \omega_2 \gamma_1 - \omega_1 \gamma_2.$$

The above system has two independent first integrals

$$\mathcal{I}_1 = \tfrac{1}{2}(I_1\omega_1^2 + I_2\omega_2^2) + \epsilon\langle \mathbf{b}, \boldsymbol{\gamma}\rangle, \quad \mathcal{I}_2 = \langle \boldsymbol{\gamma}, \boldsymbol{\gamma}\rangle.$$

Additionally, the above mentioned choice of **a** guarantees that the phase flow of system (2) preserves the standard measure in $\mathbb{R}^5 = \mathbb{R}^2\{\omega_1, \omega_2\} \times \mathbb{R}^3\{\boldsymbol{\gamma}\}$, see Refs. 13 and 14. Thus, by the theorem of Jacobi about the last multiplier,[8] if there exists a third independent first integral $\mathcal{I}_3$ which is functionally independent together with $\mathcal{I}_1$ and $\mathcal{I}_2$, then the Suslov problem is integrable by quadratures.

The known integrable cases of system (2) are the following:

(1) the Suslov case,[30] where $\epsilon = 0$, then $\mathcal{I}_3 = \omega_1$;
(2) the Kharlamova–Zabelina case,[11] where $\langle \mathbf{b}, \mathbf{a}\rangle = 0$. The third first integral is $\mathcal{I}_3 = I_1\omega_1 b_1 + I_2\omega_2 b_2$;
(3) the Kozlov case, where **b** is parallel to **a** and $I_1 = I_2$, then $\mathcal{I}_3 = \omega_1\gamma_1 + \omega_2\gamma_2$.

In what follows we study cases when $\epsilon \neq 0$, and, without loss of generality, we can put $\epsilon = 1$.

For the case when **b** is parallel to **a** Kozlov[13,14] reduced equations (2) to a Hamiltonian system with two degrees of freedom. The Hamiltonian function of this system is the following:

$$H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}\left[h - \frac{1}{2}\left(\frac{q_1^2}{I_1} + \frac{q_2^2}{I_2}\right)\right]^2, \tag{3}$$

where $q_1 = I_1\omega_1$ and $q_2 = I_2\omega_2$. It depends on parameter h which is the fixed energy value of the original problem. The integrability of the Hamiltonian system generated by (3) was investigated by Ziglin in Ref. 37 where he proved the following two theorems.

Theorem 1: *If $h \neq 0$ and $I_1 \neq I_2$, then the Hamiltonian system given by (3) has no additional complex meromorphic first integral in the complexified phase space.*

Theorem 2: *If $h = 0$ and*

(1) $\eta \neq r$, or

(2) $\sqrt{2}\cos(\pi\eta) \neq \cos(\pi r)$, where $\eta = \sqrt{1 + 8\alpha}/4$, $\alpha = I_1/I_2$, and r is rational,

then the system with Hamiltonian (3) has no additional complex meromorphic first integral in the neighborhood of the origin of coordinates.

Using these results, in Ref. 39 Ziglin showed that

Theorem 3: *If $b_1 = b_2 = 0$, then the Suslov system (2) has an additional complex meromorphic first integral only in the case $I_1 = I_2$.*

In the above theorem it is assumed that the complexified phase space of system (2) is $M^4 = \mathbb{C}^2 \times \mathbb{S}^2_{\mathbb{C}}$, where $\mathbb{S}^2_{\mathbb{C}}$ is the complex Poisson sphere

$$\mathbb{S}^2_{\mathbb{C}} = \{(\gamma_1, \gamma_2, \gamma_3) \in \mathbb{C}^3 \,|\, \gamma_1^2 + \gamma_2^2 + \gamma_3^2 = 1\}.$$

In Ref. 16 we proved that in the cases 1 and 2 excluded in Theorem 2 the system is also nonintegrable. Finally, in Ref. 38, Ziglin proved the following:

Theorem 4: *If $b_1 = b_2 = 0$, then the Suslov system (2) has an additional real meromorphic first integral only in the case $I_1 = I_2$.*

Ziglin obtained results formulated in Theorems 1–3 applying his theory formulated in two fundamental papers.[35,36] The main idea of his approach lies in a study of the monodromy group of variational equations for a particular nonequilibrium solution. In our improvement of the Ziglin result given by Theorem 2 we applied the differential Galois extension of the Ziglin theory developed by Morales-Ruiz and Ramis (see Refs. 20, 23, 24). In this approach the monodromy

group is replaced by the differential Galois group of the variational equations. Both the Ziglin and Morales-Ramis theories are specified for Hamiltonian systems. However, the main ideas of both of them are valid for general systems. In fact, Ziglin proved Theorem 2 using this ''non-Hamiltonian'' part of his theory.

In this paper we consider a case when vector **b** is not parallel or perpendicular to vector **a**. More precisely, we assume that $b_2=0$ but $b_1b_3\neq 0$, in other words, the vector of nonholonomic constraint coincides with the third principal axis of the body, and the fixed point of the body lies in the principal plane defined by the third and the first principal axes and is out of them. We called this version of the Suslov problem the generalized Kozlov case and our aim is to prove its nonintegrability. Our main result is the following:

Theorem 5: *If $b_2=0$ and $b_1b_3\neq 0$, then system (2) does not possess a real meromorphic first integral which is functionally independent together with $\mathcal{I}_1$ and $\mathcal{I}_2$.*

Let us notice that in the above theorem, as in Theorem 4, we talk about the nonexistence of a *real* first integral. Using Ziglin or Morales-Ramis theory we are able to prove the nonexistence of a *complex* meromorphic first integral. To show the nonexistence of a real meromorphic first integral we need to investigate variational equations along one parameter family of particular solutions for which the corresponding Riemann surfaces depend on the parameter values in a prescribed way. The key point is to show that in an *arbitrary* complex neighborhood of the real phase space the system does not admit an additional meromorphic first integral, and for this purpose a family of particular solutions is needed. These ideas were applied by Ziglin[38] in his proof of Theorem 4. In this proof the crucial role plays the fact that, in the Kozlov case, the Suslov problem admits *two* families of particular solutions. In the generalized Kozlov case considered in this paper, the system depends on two parameters, and there exists only one family of particular solutions (see Sec. III). This makes the problem difficult. In our proof of Theorem 5 we combine ideas of Ziglin[38] with the differential Galois approach.

Our interest in the Suslov problem is motivated by the fact that, recently, nonholonomic systems attracted attention of many investigators, see, e.g., Refs. 15, 2, 18, 5, 34. The dynamics of nonholonomic systems differs in many respects from the dynamics of the holonomic ones. Let us mention only that for nonholonomic systems we have no widely accepted notion of integrability as it is the case for Hamiltonian systems, see Refs. 13, 7, 19. Investigations of known integrable cases of the generalized Suslov problem[25,1,26] showed that for generic values of first integrals invariant manifolds defined by their common level have genus higher than one. Thus a global view of an integrable nonholonomic system is different from the familiar image of an integrable Hamiltonian system when the phase space is foliated by invariant tori. We also remark that several generalizations of the Suslov problem to higher dimensions were proposed recently, see Refs. 9, 33.

The plan of this paper is following. In the next section we describe basic facts from the Ziglin and differential Galois theory which are needed to understand the proof of our main result. In Sec. III we derive a family of particular solutions of the system and variational equations around them. Finally, in Sec. IV, we present a proof of Theorem 5.

II. THEORY

Below we describe only basic notions and facts concerning the Ziglin theory following[35] in our exposition. A more detailed and formal presentation can be found in Ref. 3. Let M be a complex n-dimensional manifold. We consider a system of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}x=v(x),\quad t\in\mathbb{C},\quad x\in M. \tag{4}$$

If $\varphi(t)$ is a nonequilibrium solution of (4) passing through $p\in M$, i.e., $\varphi(0)=p$, then the maximal analytic continuation of $\varphi(t)$ defines a Riemann surface Γ with t as a local coordinate. More formally it can be described as follows. The map $(t,q)\to\Phi_t(q)$, where $\Phi_t(q)$ is the solution of (4) passing through $q\in M$, is defined in a certain neighborhood $\mathcal{U}\times V$ of $(0,p)\in\mathbb{C}\times M$. Then Γ is the

component of p in the topology on M defined by the basis given by the sets $\{\Phi_t(p)|t\in\mathcal{U}\}$. The natural inclusion $i:\Gamma\to M$ is an immersion but not necessarily a proper map. Thus, using a global language it is necessary to distinguish Γ and $i(\Gamma)\subset M$.

Together with system (4) we also consider variational equations restricted to $T_\Gamma M$, i.e.,

$$\dot{\xi}=T(v)\xi, \quad \xi\in T_\Gamma M. \tag{5}$$

We can reduce the order of this system by one. Let $N:=T_\Gamma M/T\Gamma$ be the normal bundle of Γ, and π: $T_\Gamma M\to N$ be the projection. Then system (5) induces the following system on *N:*

$$\dot{\eta}=\pi_\star(T(v)\pi^{-1}\eta), \quad \eta\in N, \tag{6}$$

which is called the normal variational equations along Γ.

Assume now that f is a holomorphic first integral of Eqs. (4) defined in a neighborhood of Γ. By $[f]_p$ we denote the first nonconstant homogeneous term in the Taylor expansion of f at the point $p\in\Gamma$. We called it the leading part of f. Although to define $[f]_p$ we have to use local coordinates, it is a well defined homogeneous polynomial function on T_pM. Moreover, the degree of $[f]_p$ does not depend on $p\in\Gamma$. Such function $[f]$ defined on $T_\Gamma M$ is a holomorphic first integral of variational equations (5) which is a polynomial with respect to fibers variables. If f is a meromorphic first integral of (4), then we define $[f]_p$ in the following way. As f is meromorphic, we can write $f=a/b$, where a and b are holomorphic, and then we put $[f]_p=[a]_p/[b]_p$. This defines correctly a rational function on T_pM and a rational (with respect to fibers variables) first integral $[f]$ of (5). If $[f]$ is a first integral of (5), then $[f]\circ\pi^{-1}$ is a first integral of (6). For details, see Refs. 36, 20, 3.

If we know that system (4) possesses holomorphic first integrals $H=(H_1,\ldots,H_k)$ in a neighborhood of Γ such that their differentials $\mathrm{d}H_i$, $i=1,...,k$ are linearly independent on Γ, then $\mathrm{d}H_i\circ\pi^{-1}$ for $i=1,...,k$ are independent first integrals of (6). Their common zero level

$$N_0:=\{\eta\in N|\mathrm{d}H_i\circ\pi^{-1}\eta=0,\ i=1,...,k\},$$

defines a m-dimensional linear bundle over Γ, where $m=n-k-1$. Using these integrals we can reduce the order of system (6). Namely, we consider the reduced normal variational equations

$$\dot{\eta}=\pi_\star(T(v)\pi^{-1}\eta), \quad \eta\in N_0. \tag{7}$$

The monodromy group $\mathcal{M}$ of this system is the image of the fundamental group $\pi_1(\Gamma,t_0)$ obtained in the process of continuation of local solutions defined in a neighborhood of t_0 along closed paths with the base point t_0. In our case it is a subgroup of $\mathrm{GL}(m,\mathbb{C})$. If we fix the set of m linearly independent solutions of (7) then group $\mathcal{M}$ is a matrix group acting naturally on m vector space of variables $Z=(z_1,\ldots,z_m)$. Thus, it acts also on the ring of polynomials $\mathbb{C}[Z]$ and on the field of fractions $\mathbb{C}(Z)$. By $L:=\mathbb{C}(Z)^{\mathcal{M}}$ we denote the field of invariants of this action. We can consider $\mathbb{C}\subset L$ as a field extension. For an integer r, $1\leqslant r\leqslant m$, we say that $\mathcal{M}$ is r-Ziglin or exactly r-Ziglin, if the $\mathrm{transdeg}_{\mathbb{C}}L\geqslant r$ or $\mathrm{transdeg}_{\mathbb{C}}L=r$, respectively; here $\mathrm{transdeg}_{\mathbb{C}}L$ denotes the transcendence degree of field extension $\mathbb{C}\subset L$. The following lemma formulated by Ziglin gives the necessary condition for integrability, see Proposition on p. 183 in Ref. 35 and Proposition on p. 4 in Ref. 38.

Lemma 1: If system (4) possesses a meromorphic first integral which is functionally independent together with H and defined in a neighborhood $\mathcal{U}\subset M$ such that the fundamental group of Γ is generated by loops lying in $\mathcal{U}$ then, the monodromy group $\mathcal{M}$ of the reduced normal variational equations (7) is 1-Ziglin.

Thus, under assumptions of the above lemma the monodromy group possesses at least one nonconstant rational invariant function, which in the Ziglin nomenclature is called a first integral of the monodromy group. Here it is important to notice that the existence of the rational invariant mentioned in the above lemma is related to the fact that from the existence of a meromorphic first

integral for system (4) follows the existence of a rational first integral (with respect to fibres variables) of variational equations, and this integral must be constant along an arbitrary continuation of a local solution of variational equations.

Having a linear system (6) we can apply for its study also the differential Galois theory. For a general introduction to this theory, see Refs. 27, 10, 4, 17. Here we only describe basic notions of this theory and we refer the reader to the cited papers for a fully detailed exposition.

Let F be a differential field of characteristic zero, i.e., a field with an additive operation $'$: $F\to F$, called derivation, satisfying the Leibniz rule. For example, $F=\mathbb{C}(z)$ with derivation being the standard differentiating d/dz. The kernel of the derivation is a subfield of F called the subfield of constants and we denote it by F'. We assume that it is algebraically closed. When $F\subset L$ is a field extension, and L is a differential field, then we call it a differential field extension if the derivation on L restricted to F coincides with that of F. An automorphism σ: $L\to L$ is called a differential automorphism if it commutes with the derivation on L. The differential Galois group $\mathcal{G}(L/F)$ of a differential field extension $F\subset L$ is a subgroup of differential automorphisms σ: $L\to L$ for which $\sigma_{|F}=\mathrm{id}_F$.

Let us consider the following system of linear equations

$$x'=Ax, \tag{8}$$

where A is an $n\times n$ matrix with elements in F, and $x=[x_1,\ldots,x_n]^T$ is a vector of length n. If x is a solution of the above system, then usually its components x_i for $i=1,\ldots,n$ are not elements of F and belong to a certain differential extension of F. A differential extension field L of F is called a Picard–Vessiot extension associated with (8) if it is generated by n linearly independent over F' solutions $x^{(i)}\in L^n$, $i=1,\ldots,n$ of (8) and the field of constants of L coincides with F'. It can be shown that a Picard–Vessiot extension exists and it is unique up to the differential isomorphism. The differential Galois group of (8) is the differential Galois group $\mathcal{G}(L/F)$ of the Picard–Vessiot extension $F\subset L$ associated with (8). It can be shown that the differential Galois group of (8) is an algebraic subgroup of $\mathrm{GL}(n,F')$.

Now, we can return to Eq. (7). Let $\mathcal{G}$ denote its differential Galois group. It is an algebraic subgroup of $\mathrm{GL}(n-k-1,\mathbb{C})$. Group $\mathcal{G}$ is "bigger" than the monodromy group and it contains $\mathcal{M}$, see Theorem 2.4 in Ref. 20. For a Fuchsian system the monodromy group is dense in $\mathcal{G}$ (in the Zariski topology), see Theorem 3.16 in Ref. 3.

As we mentioned above, if system (4) possesses a meromorphic first integral, then (7) has a first integral and this fact imposes a restriction on $\mathcal{G}$. In fact, we have a lemma which is analogous to Lemma 1.

Lemma 2: If system (4) possesses a meromorphic first integral which is functionally independent together with H and defined in a neighborhood $\mathcal{U}\subset M$ of Γ, then the differential Galois group $\mathcal{G}$ of the reduced normal variational Eqs. (7) is 1-Ziglin.

The above lemma is a variant of Lemma 4.6 in Ref. 20 adopted for a general situation.

Remark 1: In Refs. 36 and 38 instead of common zero level of first integrals $\mathrm{d}H_i\circ\pi^{-1}$ Ziglin considered an arbitrary level

$$N_p:=\{\eta\in F\,|\,\mathrm{d}H_i\circ\pi^{-1}\eta=p_i,\ \ p_i\in\mathbb{C},\ \ i=1,\ldots,k\}.$$

Then, instead of a linear, we have an affine bundle over Γ, Eqs. (7) are generally not homogeneous ones, and the monodromy group is a subgroup of affine transformations in dimension m. Until now this construction has not been translated to the differential algebra language. In the proof of nonintegrability of the Goryachev–Chaplygin case of the heavy top, it was necessary to consider N_p with $p\neq 0$, see Ref. 38. Thus, it seems that this extension is important in applications.

In our considerations given in the last section we use some facts concerning the differential Galois group of a second order differential equation of the following form:

$$y''=ry,\quad r\in\mathbb{C}(z),\quad '\equiv\frac{\mathrm{d}}{\mathrm{d}z}. \tag{9}$$

For this equation $\mathcal{G}$ is an algebraic subgroup of $\mathrm{SL}(2,\mathbb{C})$. The following lemma describes all possible types of $\mathcal{G}$ and relates these types to forms of solution of (9), see Refs. 12, 20.

Lemma 3: Let $\mathcal{G}$ be the differential Galois group of Eq. (9). Then one of four cases can occur.

(1) $\mathcal{G}$ is triangulizable; in this case Eq. (9) has a solution of the form $y=\exp\int\omega$, where $\omega\in\mathbb{C}(z)$;
(2) $\mathcal{G}$ is conjugated with a subgroup of

$$D^{\dagger}=\left\{\left[\begin{array}{cc} c & 0 \\ 0 & c^{-1}\end{array}\right]\middle| c\in\mathbb{C}^*\right\}\cup\left\{\left[\begin{array}{cc} 0 & c \\ c^{-1} & 0\end{array}\right]\middle| c\in\mathbb{C}^*\right\},$$

in this case Eq. (9) has a solution of the form $y=\exp\int\omega$, where ω is algebraic over $\mathbb{C}(z)$ of degree 2;
(3) $\mathcal{G}$ is primitive and finite; in this case all solutions of Eq. (9) are algebraic;
(4) $\mathcal{G}=\mathrm{SL}(2,\mathbb{C})$ and Eq. (9) has no Liouvillian solution.

For a definition of Liouvillian solution see, e.g., Ref. 12. We need a more precise characterization of case 1 in the above lemma. It is given by the following lemma, see Lemma 4.2 in Ref. 28.

Lemma 4: Let $\mathcal{G}$ be the differential Galois group of Eq. (9) and assume that $\mathcal{G}$ is triangulizable. Then, either

(1) Eq. (9) has a unique solution y such that $y'/y\in\mathbb{C}(z)$, and $\mathcal{G}$ is conjugate to a subgroup of the triangular group

$$\mathcal{T}=\left\{\left[\begin{array}{cc} a & b \\ 0 & a^{-1}\end{array}\right]\middle| a,b\in\mathbb{C},a\neq 0\right\}.$$

Moreover, $\mathcal{G}$ is a proper subgroup of $\mathcal{T}$ if and only if there exists $m\in\mathbb{N}$ such that $y^m\in\mathbb{C}(z)$. In this case $\mathcal{G}$ is conjugate to

$$\mathcal{T}_m=\left\{\left[\begin{array}{cc} a & b \\ 0 & a^{-1}\end{array}\right]\middle| a,b\in\mathbb{C},a^m=1\right\},$$

where m is the smallest positive integer such that $y^m\in\mathbb{C}(z)$, or
(2) Eq. (9) has two linearly independent solutions y_1 and y_2 such that $y_i'/y_i\in\mathbb{C}(z)$, then $\mathcal{G}$ is conjugate to a subgroup of

$$\mathcal{D}=\left\{\left[\begin{array}{cc} a & 0 \\ 0 & a^{-1}\end{array}\right]\middle| a\in\mathbb{C},a\neq 0\right\}.$$

In this case, $y_1y_2\in\mathbb{C}(z)$. Furthermore, $\mathcal{G}$ is conjugate to a proper subgroup of $\mathcal{D}$ if and only if $y_1^m\in\mathbb{C}(z)$ for some $m\in\mathbb{N}$. In this case $\mathcal{G}$ is a cyclic group of order m where m is the smallest positive integer such that $y_1^m\in\mathbb{C}(z)$.

In case 2 of the above lemma we know that $s=y_1y_2\in\mathbb{C}(z)$. Differentiating s three times, and using the fact that y_i satisfies Eq. (9), we obtain

$$s'''=2r's+4rs'. \tag{10}$$

The above equation is called the second symmetric power of Eq. (9). For applications of symmetric powers of differential operators to study the existence of Liouvillian solutions and differential Galois group see, e.g., Refs. 28, 29, 32.

III. PARTICULAR SOLUTIONS AND VARIATIONAL EQUATIONS

We consider now the complexification of system (2), i.e., we assume that $(\omega_1,\omega_2,\gamma_1,\gamma_2,\gamma_3)\in\mathbb{C}^5$ and $t\in\mathbb{C}$. From now on we put $I_2=1$. This can be achieved without loss of generality by a proper choice of units.

First, let us notice that if $b_2=0$, then the following three-dimensional complex hyperplane:

$$\Pi=\{(\omega_1,\omega_2,\gamma_1,\gamma_2,\gamma_3)\in\mathbb{C}^5|\omega_1=\gamma_2=0\},$$

is invariant with respect to the flow generated by (2). System (2) restricted to Π reads

$$\begin{aligned}\dot{\omega}_2&=\gamma_3 b_1-\gamma_1 b_3,\\ \dot{\gamma}_1&=-\omega_2\gamma_3,\\ \dot{\gamma}_3&=\omega_2\gamma_1,\end{aligned}\tag{11}$$

possesses two first integrals

$$\mathcal{I}_1|_\Pi=\tfrac{1}{2}\omega_2^2+b_1\gamma_1+b_3\gamma_3,\quad \mathcal{I}_2|_\Pi=\gamma_1^2+\gamma_3^2,$$

and can be integrated explicitly. Phase curves $i(\Gamma_E)\subset\Pi\subset\mathbb{C}^5$ of system (2) defined by

$$\tfrac{1}{2}\omega_2^2+b_1\gamma_1+b_3\gamma_3=E,\quad \gamma_1^2+\gamma_3^2=1,\quad (\omega_2,\gamma_1,\gamma_2)\in\Pi=\mathbb{C}^3$$

are algebraic and, as an intersection of two quadrics, they are elliptic curves. For further analysis we choose a one parameter family Γ_k which in time parametrization is given by

$$\varphi_k(t)=(0,\omega_2(t),\gamma_1(t),0,\gamma_3(t)),\tag{12}$$

where

$$\begin{aligned}\omega_2(t)&:=-2k\,\mathrm{cn}(t,k),\\ \gamma_1(t)&:=-[1-2k^2\,\mathrm{sn}^2(t,k)]b_1-2k\,\mathrm{sn}(t,k)\mathrm{dn}(t,k)b_3,\\ \gamma_3(t)&:=-[1-2k^2\,\mathrm{sn}^2(t,k)]b_3+2k\,\mathrm{sn}(t,k)\mathrm{dn}(t,k)b_1,\end{aligned}\tag{13}$$

and

$$k=\sqrt{\frac{1+E}{2}},\quad 0<k<1.$$

In the above formulas $\mathrm{sn}(t,k)$, $\mathrm{cn}(t,k)$, and $\mathrm{dn}(t,k)$ denote the Jacobi elliptic functions of argument t and modulus k. Particular solutions defined by (12) and (13) are single-valued, meromorphic, and double periodic with periods

$$T_1(k)=2K(k)+2iK'(k),\quad T_2(k)=2K(k)-2iK'(k),$$

where $K(k)$ is the complete elliptic integral of the first kind with modulus k, $K'(k):=K(k')$, and $k':=\sqrt{1-k^2}$. In each period cell they have two simple poles at

$$s_1(k)=iK'(k),\quad s_2(k)=-iK'(k)\ \mod\ (T_1(k),T_2(k)).$$

Thus, Riemann surfaces Γ_k are tori with two points removed.

The variational equations along a particular solution $\varphi_k(t)$ have the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} o_1 \\ o_2 \\ g_1 \\ g_2 \\ g_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & b_3/I_1 & 0 \\ 0 & 0 & -b_3 & 0 & b_1 \\ 0 & -\gamma_3(t) & 0 & 0 & -\omega_2(t) \\ \gamma_3(t) & 0 & 0 & 0 & 0 \\ 0 & \gamma_1(t) & \omega_2(t) & 0 & 0 \end{bmatrix} \begin{bmatrix} o_1 \\ o_2 \\ g_1 \\ g_2 \\ g_3 \end{bmatrix},$$

and they have two first integrals

$$\mathcal{J}_1 = \omega_2(t)o_2 + b_1 g_1 + b_3 g_3, \quad \mathcal{J}_2 = \gamma_1(t)g_1 + \gamma_3(t)g_3.$$

Let us notice that these first integrals do not depend on o_1 and g_2, and this is why we can choose them as coordinates in the fibre over $\varphi_k(t)$ of the reduced phase space. Thus the reduced normal variational equations read

$$\dot{o}_1 = \frac{b_3}{I_1} g_2, \quad \dot{g}_2 = \gamma_3(t)o_1,$$

or simply

$$\ddot{o} = \frac{b_3}{I_1}\gamma_3(t)o, \quad o = o_1. \tag{14}$$

From the form of this equation, we can see that its monodromy group, as well as its differential Galois group, are contained in SL(2,$\mathbb{C}$). Now, in order to apply the differential Galois approach effectively, the crucial point is to transform (14) to an equation with rational coefficients. In other words, we want to transform (14) from Γ_k to the Riemann sphere $\mathbb{CP}^1$. If we make the following mapping:

$$t \to z = \frac{1 + b_1\gamma_1(t) + b_3\gamma_3(t)}{b_1\gamma_3(t) - b_3\gamma_1(t)}, \tag{15}$$

then (14) transforms to

$$o'' + p(z)o' + q(z)o = 0, \quad ' = \frac{\mathrm{d}}{\mathrm{d}z}, \tag{16}$$

where

$$p(z) = \frac{z(1 - 2k'^2(1+z^2))}{(1+z^2)(k^2 - k'^2 z^2)},$$
$$q(z) = -\frac{\alpha b_3(2b_1 z + b_3(z^2-1))}{(1+z^2)^2(k^2 - k'^2 z^2)}, \quad \alpha = \frac{1}{I_1}. \tag{17}$$

We note here that transformation (15) does not change the identity component of (14).

Equation (16) is Fuchsian and it possesses four regular singular points over $\mathbb{CP}^1$

$$z_1 = i, \quad z_2 = -i, \quad z_3 = \frac{k}{k'}, \quad z_4 = -\frac{k}{k'}.$$

It is more convenient to work with the reduced form of (16) which we obtain introducing a new dependent variable w by the following formula:

$$w = o \exp\left[\frac{1}{2}\int_{z_0}^{z} p(s)\mathrm{d}s\right]. \tag{18}$$

As the result, we obtain the following equation:

$$w'' = r(z)w, \quad r(z) = \tfrac{1}{2}p'(z) + \tfrac{1}{4}p(z)^2 - q(z). \tag{19}$$

The partial fraction decomposition of rational function $r(z)$ can be written as

$$r(z) = \sum_{i=1}^{4}\left[\frac{\alpha_i}{(z-z_i)^2} + \frac{\beta_i}{z-z_i}\right], \tag{20}$$

where

$$\alpha_1 = \alpha_2^* = -\tfrac{3}{16} + \tfrac{1}{2}\alpha b_3(b_3 - ib_1),$$

$$\alpha_3 = \alpha_4 = -\tfrac{3}{16},$$

and

$$\beta_1 = \beta_2^* = -\frac{i}{16}(1+4k'^2) + \alpha(b_1 + ib_3)b_3k'^2,$$

$$\beta_3 = \frac{1}{16}\sqrt{\frac{k'}{k}}[(6k^2-1) - 8\alpha b_3((2k^2-1)b_3 + 2k'kb_1)],$$

$$\beta_4 = -\frac{1}{16}\sqrt{\frac{k'}{k}}[(6k^2-1) - 8\alpha b_3((2k^2-1)b_3 - 2k'kb_1)].$$

In the above formulas the star denotes the complex conjugation. It is important to notice that transformation (18) with $p(z)$ given by (17) does not change the identity component of differential Galois group of (16), see Proposition 4.25 in Ref. 3.

IV. PROOF OF THEOREM 5

For Eq. (19) exponents $\rho_i^{\pm}$ at singular points z_i, $i = 1,...,4$ are the following:

$$\rho_i^{\pm} = \tfrac{1}{2}(1 \pm \Delta_i), \quad \Delta_i = \sqrt{1+4\alpha_i}, \quad i = 1,...,4.$$

Let M_i be the local monodromy matrix corresponding to a small circle around singular point z_i, see, e.g., Ref. 28. Then eigenvalues $\lambda_i^{\pm}$ of matrix M_i are given by the following formula:

$$\lambda_k^{\pm} = \exp[2\pi i\rho_k^{\pm}], \quad k = 1,...,4.$$

Let us notice here that when $b_1b_3 \neq 0$, then $\rho_k^{\pm} \notin \mathbb{Q}$ for $k = 1, 2$. Thus, $\lambda_k^{\pm}$ for $k = 1, 2$ are not roots of unity.

First, we show the following:

Lemma 5: If $b_1b_3 \neq 0$, then for $0 < k < 1$ the identity component $\mathcal{G}^0$ of differential Galois group of Eq. (19) is not Abelian.

Proof: From Lemma 3 it follows that $\mathcal{G}^0$ can be Abelian only in the first three cases given in this lemma. We consider them successively.

Assume that $\mathcal{G}$ is conjugate to a subgroup of triangular group $\mathcal{T}$ and that $\mathcal{G}^0$ is Abelian. By Lemma 4 $\mathcal{G}^0$ is Abelian in two cases: either $\mathcal{G}$ is conjugate to a proper subgroup of $\mathcal{T}$, or it is conjugate to a subgroup of the diagonal group $\mathcal{D}$. The first possibility cannot occur. In fact, if it is

so, then all elements g of $\mathcal{G}$ have eigenvalues a and a^{-1} such that $a^m=1$ for some $m\in\mathbb{N}$. We know that local monodromy matrices around singular points belong to $\mathcal{G}$. But we also know that eigenvalues of M_1 and M_2 are not mth roots of unity. Thus this case is impossible. Let us consider the second possibility. It follows from Lemma 4 that in this case there exist two solutions y_1 and y_2 of (19) such that $y_i'/y_i\in\mathbb{C}(z)$, $i=1$, 2, and $s=y_1y_2\in\mathbb{C}(z)$. As we remarked just after formulation of Lemma 4, s satisfies a third order linear differential Eq. (10). We show that this equation in the case considered does not have a rational solution. For $r=r(z)$ given by (20) Eq. (10) is Fuchsian and has the same singular points z_i, $i=1,...,4$, as (19). The infinity is also a regular singular point for Eq. (10). Exponents at singular points are the following:

$$R_i=\{1,1\pm\Delta_i\},\quad i=1,...,4,$$

and the exponents at infinity are $R_\infty=\{-2,-1,0\}$.

Now, let $s=P/Q$, $P,Q\in\mathbb{C}[z]$ be a rational solution of (10). Without loss of generality we can assume that

$$Q=\prod_{i=1}^{K}(z-r_i)^{n_i},\quad n_i\in\mathbb{N}.$$

Then, as it is well known, $r_i\in\{z_1,\ldots,z_4\}$ and $-n_i$ are exponents at r_i. However, in our case there is no singular point at $\mathbb{C}$ with an exponent which is a negative integer. Thus $Q=1$ and $s=P$. Let $N=\deg P$. Then $\rho=-N$ is an exponent at infinity. Hence $\deg P\leqslant 2$. Assume that $\deg P=2$, then from (10) it follows that

$$2r'(z)P+4r(z)P'=0,$$

and thus $(r(z)P^2)'=0$. Consequently, $r(z)=cP^{-2}$ for some $c\in\mathbb{C}$. However, direct calculations show that when $b_1b_3\neq 0$, and $0<k<1$, it is impossible. This excludes the second possibility in case 1 of Lemma 3.

Let us assume that $\mathcal{G}$ is conjugate to a subgroup of $D^\dagger$ (i.e., we have case 2 from Lemma 3). In this case $\mathcal{G}^0$ is Abelian. We show that for Eq. (19) this cannot occur. To this end, we apply case II of the Kovacic algorithm, see p. 18 of Ref. 12. First, we determine auxiliary sets E_i for each singular point. These sets are defined as follows:

$$E_i=\{2,2\pm 2\Delta_i\}\cap\mathbb{Z},\quad i=1,...,4.$$

Thus we have

$$E_1=E_2=\{2\},\quad E_3=E_4=\{1,2,3\}.$$

Additionally, we define $E_\infty=\{0,2,4\}$. Then, according to the Kovacic algorithm, we check if there exists an element $e=(e_\infty,e_1,\ldots,e_4)$ in Cartesian product $E=E_\infty\times E_1\times\cdots\times E_4$ such that the following number

$$d(e)=\frac{1}{2}\left(e_\infty-\sum_{i=1}^{4}e_i\right),$$

is a non-negative integer. However, in our case $d(e)<0$ for all $e\in E$. Thus, $\mathcal{G}$ is not conjugate to a subgroup of $D^\dagger$.

Finally, let us assume that $\mathcal{G}$ is conjugate to a finite imprimitive subgroup of $\mathrm{SL}(2,\mathbb{C})$ (this is case 3 in Lemma 3). However, a necessary condition for this case is that at each singular point exponents are distinct and rational, see Theorem 3.6 in Ref. 29. As we have already mentioned, in our case when $b_1b_3\neq 0$ then $\rho_k^{\pm}\notin\mathbb{Q}$ for $k=1$, 2. Thus, $\mathcal{G}$ cannot conjugate to a finite imprimitive subgroup of $\mathrm{SL}(2,\mathbb{C})$.

In this way, we eliminate all possibilities when $\mathcal{G}^0$ can be Abelian and this ends the proof.□

Using the above lemma we are able to prove the following:

Lemma 6: If $b_1 b_3 \neq 0$, then for $0<k<1$, in an arbitrary neighborhood $\mathcal{U}\in\mathbb{C}^5$ of phase curve Γ_k, the complexified Suslov system (2) does not possess a meromorphic first integral which is functionally independent together with $\mathcal{I}_1$ and $\mathcal{I}_2$.

Proof: Assume that there exists a meromorphic first integral of (2) which is defined in a neighborhood $\mathcal{U}\subset\mathbb{C}^5$ of phase curve Γ_k, and is functionally independent together with $\mathcal{I}_1$ and $\mathcal{I}_2$. Then, according to Lemma 2, the differential Galois group $\mathcal{G}$ of Eq. (14) has a rational invariant. But $\mathcal{G}$ is an algebraic subgroup of SL(2,C) and such groups possess a rational invariant only if $\mathcal{G}^0$ is Abelian, see Example 2.11(b) in Ref. 3. As the identity components of differential Galois group of Eqs. (14), (16), and (19) are the same, $\mathcal{G}^0$ of (19) is Abelian. However, in Lemma 5 we proved that $\mathcal{G}^0$ for this equation is not Abelian. The contradiction finishes the proof. □

Point $x_0=(0,0,b_1,0,b_3)\in\Pi$ is a hyperbolic equilibrium of system (2). The phase curve Γ_1 corresponds to solution (13) with $k=1$. It contains two real components which are real phase curves corresponding to real solutions homoclinic to x_0. Their union is $\mathrm{Re}\,\Gamma_1$ and we denote its closure by Ω.

Lemma 7: For an arbitrary complex neighborhood $\mathcal{U}\subset\Pi$ of Ω there exists $\epsilon>0$, such that for $0<|k-1|<\epsilon$ the fundamental group $\pi_1(\Gamma_k)$ of phase curve Γ_k is generated by loops lying in $\mathcal{U}$.

Proof: Periods $T_1(k)$ and $T_2(k)$ of solution (13) are primitive. Minimal real and imaginary periods are $T(k)=4K(k)$ and $T'(k)=4iK'(k)$. As a base point $x(k)\in\Gamma_k$ we choose $x(k)=\varphi_k(t_0(k))$ where $t_0(k)=K(k)$. Let us notice that from (13) it follows that

$$\gamma_1(t_0(k))=(2k^2-1)b_1-2kk'b_3,$$
$$\gamma_3(t_0(k))=(2k^2-1)b_3+2kk'b_1,\quad \omega_2(t_0(k))=0. \tag{21}$$

Now, let

$$\lambda_k,\lambda_k':[0,1]\to\Gamma_k,$$

be the loops with base point $x(k)$ corresponding to periods $T(k)$ and $T'(k)$. These loops cross at point

$$x'(k)=\Phi_k(t_0(k)+T(k)/2)=\Phi_k(t_0(k)+T'(k)/2). \tag{22}$$

As a result, we obtain four semiloops with end points $x(k)$ and $x'(k)$. The fundamental group $\pi_1(\Gamma_k)$ of Γ_k is generated by these semiloops, see Fig. 1. Let us analyze what happens when k tends to 1. From (21) it follows that $x(k)$ tends to x_0 and from (13) we deduce that loop λ_k tends to Ω. To see what happens with loop λ_k' when k tends to 1, let us put $t=t_0(k)+i\tau$ in formulas (13). We obtain

$$\omega_2(t)=2ikk'\frac{\mathrm{sn}(\tau,k')}{\mathrm{dn}(\tau,k')},$$

$$\gamma_1(t)=-\left[1-\frac{2k^2}{\mathrm{dn}^2(\tau,k')}\right]b_1-2kk'\frac{\mathrm{cn}(\tau,k')}{\mathrm{dn}^2(\tau,k')}b_3, \tag{23}$$

$$\gamma_3(t)=-\left[1-\frac{2k^2}{\mathrm{dn}^2(\tau,k')}\right]b_3+2kk'\frac{\mathrm{cn}(\tau,k')}{\mathrm{dn}^2(\tau,k')}b_1.$$

Thus, loop λ_k' tends to point x_0 as k tends to 1. □

Now, we are ready to present our proof of Theorem 5.

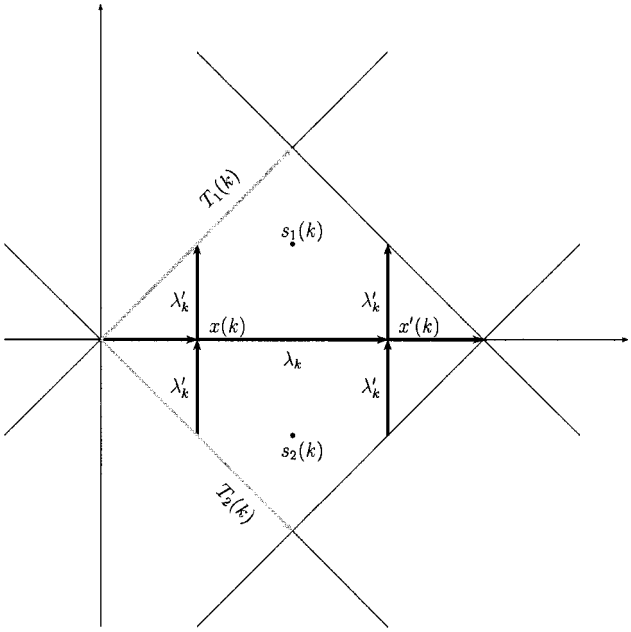

FIG. 1. Parallelogram of period with marked loops.

Proof: Assume that there exists a real meromorphic first integral $\mathcal{I}$ of system (2) which is functionally independent together with $\mathcal{I}_1$ and $\mathcal{I}_2$. We can extend it to a complex meromorphic first integral defined in a complex neighborhood of $\mathbb{R}^5 \subset \mathbb{C}^5$. Thus, there exists a meromorphic first integral defined in a neighborhood $\mathcal{U}$ of Ω. Moreover, by Lemma 7, there exists ϵ such that for $0<|1-k|<\epsilon$ the fundamental group of phase curves Γ_k is generated by loops lying in $\mathcal{U}$. Hence, by Lemma 1, the monodromy group $\mathcal{M}$ of the reduced normal variational equations for the phase curve Γ_k possesses a rational invariant. However, in Lemma 5, we show that the identity component of differential Galois group of (19) is not Abelian. Thus, as (19) is Fuchsian, by Theorem 3.17 of Ref. 3, $\mathcal{M}$ does not possess a rational invariant. Contradiction with Lemma 1 finishes the proof. □

V. REMARKS

Without doubt the Ziglin and Morales-Ramis theories are elegant and, what is more important, powerful tools for proving nonintegrability. However, both of them do not give any information about *dynamical mechanisms* which cause the nonintegrability. For Hamiltonian systems some efforts were done to connect known dynamical phenomena causing the nonintegrability with the properties of the differential Galois group of the variational equations. A nice example is described in Chap. 7 of Ref. 20, see also Ref. 21. It seems that the analysis presented in Ref. 22 gives a new ideas to better understanding of dynamical meaning of the nonintegrability in the sense of the differential Galois theory.

In the generalized Kozlov case the Suslov problem is not a Hamiltonian one, and we can only conjecture what the dynamical mechanism of the nonintegrability is. Restricting system (2) to the level $\mathcal{I}_2=1$ we obtain a four-dimensional system preserving the volume. It possesses a hyperbolic equilibrium of the saddle type. The stable and unstable manifolds of this equilibrium cross transversally along two pendulumlike homoclinic loops. In the case of Hamiltonian systems it is known that a transversal intersection of asymptotic manifolds is not an obstacle for the integrability—an example is the famous C. Neumann system, see Ref. 6. However, as it was shown by Turaev and Shilnikov,[31] if there exists at least three transversal homoclinic orbits that leave and approach the saddle equilibrium tangentially to the leading directions, then the system is not integrable and chaotic. The leading directions correspond to the eigendirections of the minimal positive and

maximal negative characteristic exponents. Four-dimensional systems preserving the volume are ''close'' to the Hamiltonian one. We suspect that for the Suslov system considered in this paper the existence of a large number of orbits homoclinic to the equilibrium causes its nonintegrability.

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An extension of the classical theory of algebraic invariants to pseudo-Riemannian geometry and Hamiltonian mechanics

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We develop a new approach to the study of Killing tensors defined in pseudo-Riemannian spaces of constant curvature that is ideologically close to the classical theory of invariants. The main idea, which provides the foundation of the new approach, is to treat a Killing tensor as an algebraic object determined by a set of parameters of the corresponding vector space of Killing tensors under the action of the isometry group. The spaces of group invariants and conformal group invariants of valence two Killing tensors defined in the Minkowski plane are described. The group invariants, which are the generators of the space of invariants, are applied to the problem of classification of orthogonally separable Hamiltonian systems defined in the Minkowski plane. Transformation formulas to separable coordinates expressed in terms of the parameters of the corresponding space of Killing tensors are presented. The results are applied to the problem of orthogonal separability of the Drach superintegrable potentials. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The classical theory of algebraic invariants has long been recognized as a common branch of commutative algebra, algebraic geometry, representation theory, and algebraic combinatorics. This observation confirms yet again that ''Mathematics is the study of analogies between analogies ....'' [1] With this perspective the main aim of this paper is to establish an apparently new connection between the classical theory of algebraic invariants of vector spaces of homogeneous polynomials and a theory of algebraic invariants of vector spaces of Killing tensors defined in pseudo-Riemannian spaces of constant curvature. A second goal is to apply the results to a classification problem which arises in the theory of separation of variables for the Hamilton–Jacobi equation in classical dynamics. The results obtained provide a framework for the solution of many problems arising in mathematical physics.

Recall that the prime object of study in the classical theory of algebraic invariants[2,3] is the space $V=S^n\mathbb{C}^m$ of homogeneous polynomials of degree n in m variables $x_1,\ldots,x_m$, which has

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dimension $d=\binom{n+m-1}{n}$. As a consequence, the main problem is to describe the set of invariants and covariants (i.e., polynomials of the parameters $a_1,\ldots,a_d$ and $a_1,\ldots,a_d,x_1,\ldots,x_m$, respectively) that remain fixed under the action of the group $GL_m(\mathbb{C})$ acting linearly on V.[2] Consider the following illustrating example:[2]

Example 1.1: Let $f\in S^2\mathbb{C}^2$ be a general quadratic form defined over $\mathbb{C}$

$$f(x_1,x_2)=a_1x_1^2+2a_2x_1x_2+a_3x_2^2. \tag{1.1}$$

Under the action of the corresponding group $GL_2(\mathbb{C})$:

$$T=\begin{bmatrix}\alpha_{11} & \alpha_{12}\\ \alpha_{21} & \alpha_{22}\end{bmatrix}\in GL_2(\mathbb{C}),\quad \begin{matrix}x_1=\alpha_{11}x_1'+\alpha_{12}x_2',\\ x_2=\alpha_{21}x_1'+\alpha_{22}x_2'\end{matrix},\quad \det(T)\neq 0$$

the quadratic form given by (1.1) transforms as follows:

$$f'(x_1',x_2')=a_1'x_1'^{\,2}+2a_2'x_1'x_2'+a_3'x_2'^{\,2},$$

where

$$a_1'=a_1\alpha_{11}^2+2a_2\alpha_{11}\alpha_{21}+a_3\alpha_{21}^2,$$

$$a_2'=a_1\alpha_{11}\alpha_{12}+a_2(\alpha_{11}\alpha_{22}+\alpha_{12}\alpha_{21})+a_3\alpha_{21}\alpha_{22},$$

$$a_3'=a_1\alpha_{12}^2+2a_2\alpha_{12}\alpha_{22}+a_3\alpha_{22}^2.$$

It is easily seen that the quantity $\Delta_{qf}=a_1a_3-a_2^2$ is an *invariant* modulo the factor $\det(T)^2$, since it tansforms under the transformation induced by the groups as follows:

$$\Delta_{qf}'=a_1'a_3'-a_2'^{\,2}=(\det T)^2\Delta_{qf}.$$

We observe that the invariant Δ_{qf} can be immediately applied to the *classification of (centrally symmetric) conic sections* in the Euclidean plane $\mathbb{R}^2$ (the above considerations also hold true for $x_1,x_2\in\mathbb{R}^2$). Indeed, for the conic sections defined by

$$f(x_1,x_2)=a_1x_1^2+2a_2x_1x_2+a_3x_2^2=\text{const} \tag{1.2}$$

we can distinguish, for example, the following cases:

(a) if Δ_{qf}, a_1 and $f(x_1,x_2)$ are of the same sign, then (1.2) defines an ellipse in $\mathbb{R}^2$,
(b) if $\Delta_{qf}<0$, then (1.2) defines a hyperbola in $\mathbb{R}^2$,
(c) if $\Delta_{qf}=0$, and $a_1\neq 0$, then (1.2) defines a pair of straight lines $\mathbb{R}^2$.

The example above illustrates that the invariants are very effective in various classification problems.

In modern mathematical language the main problem of the classical theory of algebraic invariants can be formulated as follows:

Problem 1.1: Determine the linear action of a group G on a K-vector space V. Then in the ring of polynomial functions $K[V]$ describe the subring $K[V]^G$ of all polynomial functions on V which are invariant under the action of G.

In order to create a satisfactory realization of these ideas in pseudo-Riemannian geometry, we need to determine counterparts of the group G and K-vector space V, as well as properly define the action of the group in the corresponding vector space defined in a pseudo-Riemannian manifold $(M,\mathbf{g})$. The natural choice for such a group is the isometry group $I(M)$ if it exists, while the vector space where its action can be determined is the vector space of Killing tensors of a fixed valence defined on $(M,\mathbf{g})$.

Killing tensors of valence two play a pivotal role in the theory of orthogonally separable Hamiltonian systems. Therefore the results of such an extension, by which we mean group invariants of the vector spaces of Killing tensors, can be applied to the problem of classification of orthogonally separable Hamiltonian systems (see Sec. IV) which admit first integrals quadratic in the momenta that, in turn, are determined by the Killing tensors of valence two.

The paper is organized as follows: In Sec. II we describe how the basic ideas of the classical theory of algebraic invariants can be incorporated into the study of Killing tensors defined in pseudo-Riemannian manifolds of constant curvature. In Sec. III we solve the problem of finding all isometry group invariants of the space of Killing tensors of valence two defined in the Minkowski plane $\mathbb{R}^2_1$. Section IV links the theory of group invariants of Killing tensors with the Hamilton–Jacobi theory of separation of variables. In Sec. V we characterize Killing tensors defined in $\mathbb{R}^2_1$ with respect to the Liouville–Morera coordinates. Section VI contains an analogous classification in terms of the pseudo-Cartesian coordinates. We describe all admissible rigid motions of $\mathbb{R}^2_1$ in Sec. VII. Section VIII contains a group invariant classification of Killing tensors defined in $\mathbb{R}^2_1$. In Sec. IX we compare the results of Sec. VIII with analogous classifications obtained by other methods. In Sec. X we present transformation formulas in terms of the parameters of the space of Killing tensors of valence two to separable coordinates for Hamiltonian systems defined in $\mathbb{R}^2_1$. The main algorithm based on the results of Secs. VIII and X is the subject of Sec. XI. In Sec. XII we show how the obtained results can be employed in the study of systems of hydrodynamic type. Section XIII is devoted to applications of the results to the problem of orthogonal separability of the Drach superseparable potentials. In Sec. XIV we make concluding remarks.

II. THE EXTENSION

Using the ideas presented in the Introduction as a motivation, we consider a pseudo-Riemannian space $(M,\mathbf{g})$ of constant curvature, where $\dim M=n$ and $\mathbf{g}$ denotes the metric tensor. We shall assume that the manifold M is complete.

Definition 2.1: A Killing tensor $\mathbf{K}^p$ *of valence* p *defined in* $(M,\mathbf{g})$ *is a symmetric* $(p,0)$ *tensor satisfying the Killing tensor equation:*

$$[\mathbf{K}^p,\mathbf{g}]=0, \tag{2.1}$$

where $[,]$ *denotes the Schouten bracket.*[4] *When* $p=1$, $\mathbf{K}^1$ *is said to be a Killing vector (infinitesimal isometry) and Eq. (2.1) reads*

$$\mathcal{L}_{\mathbf{K}^1}\mathbf{g}=0, \tag{2.2}$$

where $\mathcal{L}$ *denotes the Lie derivative operator*.

Remark 2.1: Throughout this paper, unless otherwise specified, $[,]$ denotes the Schouten bracket, which is a generalization of the usual Lie bracket of vector fields.

The set of all Killing vectors of $(M,\mathbf{g})$, denoted by $i(M)$, is a Lie algebra, which is also a Lie subalgebra of the space $\mathcal{X}(M)$ of all vector fields defined on M. As is well-known, $d=\dim i(M)=\frac{1}{2}n(n+1)$ iff the space $(M,\mathbf{g})$ is of constant curvature.[5,6]

It follows immediately from (2.1) that the Killing tensors of the same valence p constitute a vector space $\mathcal{K}^p(M)$. Moreover, the following properties hold true:

$$[\ ,\ ]:\ \mathcal{K}^p(M)\oplus\mathcal{K}^q(M)\to\mathcal{K}^{p+q-1}(M), \tag{2.3}$$

$$[\mathbf{K}^p,\mathbf{K}^q]=-[\mathbf{K}^q,\mathbf{K}^p]\quad(\text{skew-symmetry}), \tag{2.4}$$

$$[[\mathbf{K}^p,\mathbf{K}^q],\mathbf{K}^r]+(\text{cycle})=0\quad(\text{Jacobi identity}). \tag{2.5}$$

Therefore one can consider a graded Lie algebra of Killing tensors defined on $(M,\mathbf{g})$ with respect to the Schouten bracket $[,]$:

TABLE I. Comparison with the classical theory of algebraic invariants.

	Classical theory of algebraic invariants	Group invariants of Killing tensors
Group	Linear group $GL_m(\mathbb{C})$	Isometry group $I(M)$
Space	Vector space $S^n\mathbb{C}^m$	Space $\Sigma \simeq \mathbb{R}^d$ determined by $\mathcal{K}^p(M)$
Objects preserved by the group	Polynomials of $a_1,\ldots,a_d$ (invariants) and $a_1,\ldots,a_d,x_1,\ldots,x_m$ (covariants), where $d=\dim S^n\mathbb{C}^m$	Functions of $a_1,\ldots,a_d$, where $d=\dim \mathcal{K}^p(M)$

$$\mathcal{K}_{\text{alg}}=\mathcal{K}^0(M)\oplus\mathcal{K}^1(M)\oplus\mathcal{K}^2(M)\oplus\cdots\oplus\mathcal{K}^p(M)\oplus\cdots, \tag{2.6}$$

where $\mathcal{K}^0(M)=\mathbb{R}$, $\mathcal{K}^1(M)=i(M)$ and $p=0,1,2,\ldots$, denotes the valence of the Killing tensors belonging to the corresponding space $\mathcal{K}^p(M)$. The following two fundamental *structural properties* of Killing tensors defined on pseudo-Riemannian spaces of constant curvature are crucial in applications:

SPI: A Killing tensor $\mathbf{K}^p$ defined on $(M,\mathbf{g})$ is a *sum of symmetrized tensor products* of Killing vectors, or infinitesimal generators of the Lie algebra of the corresponding isometry group.

SPII: The set of all Killing tensors of valence $p\geqslant 1$ defined on $(M,\mathbf{g})$, where $\dim(M)=n$, is a *vector space of dimension d* determined by the *Delong–Takeuchi–Thompson (DTT) formula:*[7–9]

$$d=\frac{1}{n}\binom{n+p}{p+1}\binom{n+p-1}{p},\quad p\geqslant 1. \tag{2.7}$$

Accordingly, a Killing tensor of valence p is an *algebraic object* determined by its d parameters, or an element of the corresponding vector space of Killing tensors.

Recall that formula (2.7) was derived first for the cases $p=1$ (see above) and $p=2$.[10,11,13] An extensive study of Killing tensors defined in pseudo-Riemannian spaces of constant curvature was undertaken by Delong in his 1982 Ph.D. thesis,[7] where the author discovered, among many other beautiful results, formula (2.7) for arbitrary $p>2$. This result was obtained independently by Takeuchi[8] and Thompson[9] by making use of SPI. In addition, SPI has been routinely employed to solve classification problems in the Hamilton–Jacobi theory of separation of variables (see, for instance, Refs. 14, 15). Our approach to these problems is based on SPII, which we use to extend the basic ideas of the classical theory of algebraic invariants to pseudo-Riemannian geometry. The results are applied to problems arising in the Hamilton–Jacobi theory of separation of variables. Indeed, in view of SPII, a Killing tensor of valence p can be interpreted as an algebraic object, or an element of the corresponding vector space $\mathcal{K}^p(M)$, determined by d parameters $a_1,\ldots,a_d$, where $d=\dim \mathcal{K}^p(M)$, which makes it natural to consider the induced action of the isometry group $I(M)$ in the space Σ with the coordinates $a_1,\ldots,a_d$ (note Σ is isomorphic to $\mathbb{R}^d$:$\Sigma\simeq\mathbb{R}^d$). Therefore in complete analogy with the main problem of the classical theory of algebraic invariants (see above), we formulate the following problem for the vector spaces of Killing tensors defined in pseudo-Riemannian spaces of constant curvature:

Problem 2.1: Determine the action induced by the group of isometries in the space Σ determined by $a_1,\ldots,a_d$. Then in the space of functions defined on Σ describe the subspace of all functions in Σ which are invariant under the action induced by the isometry group.

To make the exposition clearer, we compare the corresponding main components of the two theories in Table I.

It should be mentioned that Delong[7] made a considerable effort to establish a link between the study of Killing tensors defined in spaces of constant curvature and the classical theory of algebraic invariants. However, his approach appears to be different from the one employed in this work. More specifically, by treating the Killing tensors as functions on the cotangent bundle T^*M, he considered the action of the Hamiltonian flow group in $\mathcal{K}_{\text{alg}}$. This set up prompted him to

consider cotangent bundles of the spaces where the group acted linearly (for instance, $T^*\mathbb{R}^n$). In this view, the algebra $\mathcal{K}_{\text{alg}}$ is itself the algebra of invariants of the Hamiltonian flow group.

In our setting, in order to determine the action of $I(M)$ in Σ, we treat each element of the vector space $\mathcal{K}^p(M)$ as a function of its parameters $a_1^0,\ldots,a_d^0$: $\mathbf{K}_0^p=\mathbf{K}_0^p(a_1^0,\ldots,a_d^0)$, where the number d is given by (2.7). Denote by $\mathrm{Diff}\,\mathcal{K}^p(M)$ all Killing tensors in $\mathcal{K}^p(M)$ whose parameters are smooth functions of $a_1,\ldots,a_d$. It is easy to see that $\mathrm{Diff}\,\mathcal{K}^p(M)$ is generated by $\mathrm{Diff}\,(\mathbb{R}^d)$—the group of all diffeomorphisms of $\Sigma\simeq\mathbb{R}^d$. To determine the action of $I(M)$ we introduce a *map* π: $\mathrm{Diff}\,\mathcal{K}^p(M)\to\mathcal{X}(\Sigma)$ defined as follows:

$$\pi:\ \mathbf{K}^p(a_1^0,\ldots,a_d^0)\to\sum_{i=1}^{d} a_i^0\frac{\partial}{\partial a_i}, \tag{2.8}$$

where $a_1,\ldots,a_d$ are the general parameters that span the space Σ and $\mathcal{X}(\Sigma)$ denotes the space of vector fields on Σ. Note, in general a_i^0, are functions of $a_1,\ldots,a_d$: $a_i^0=a_i^0(a_1,\ldots,a_d)$, $i=1,\ldots,d$. Hence, every element of the vector space $\mathcal{K}^p(M)$ is mapped to a vector field in $\mathcal{X}(\Sigma)$. Moreover, it is clear that $\ker\pi=\{\mathbf{0}\}$, therefore π is an *isomorphism* between the two spaces. A simple interpretation of this construction is the following: With a given Killing vector field $\mathbf{X}$ on M we associate a linear mapping $\mathcal{L}_{\mathbf{X}}:\mathcal{K}^p(M)\to\mathcal{K}^p(M)$, hence, a linear mapping $\tilde{\mathcal{L}}_{\mathbf{X}}:\Sigma\to\Sigma$, since $\mathcal{K}^p(M)$ is identified with Σ. This mapping is represented by d equations:

$$a_i^0=a_i^0(a_1,\ldots,a_d),\quad i=1,\ldots,d.$$

Accordingly, we define a vector field $\mathbf{V}_{\mathbf{X}}$ on Σ by setting

$$\mathbf{V}_{\mathbf{X}}=a_i^0(a_1,\ldots,a_d)\frac{\partial}{\partial a_i}.$$

Remark 2.2: To define the map π according to the formula (2.8) properly, we need an explicit representation of the general Killing tensor $\mathbf{K}^p\in\mathcal{K}^p(M)$ under consideration given in terms of a fixed system of coordinates. Such a representation can be obtained on a case by case basis. For example, consider the case $p=2$, $M=\mathbb{R}^2$: Solving the corresponding Killing tensor equation (2.1) in (say) Cartesian coordinates, one obtains the general form of a Killing tensor in $\mathcal{K}^2(\mathbb{R}^2)$:

$$K^{ij}=\begin{pmatrix} A+2\alpha y+\gamma y^2 & C-\alpha x-\beta y-\gamma xy\\ C-\alpha x-\beta y-\gamma xy & B+2\beta x+\gamma x^2\end{pmatrix}, \tag{2.9}$$

where K^{ij} are the components of the general $\mathbf{K}^2\in\mathcal{K}^2(\mathbb{R}^2)$. The six parameters $A,B,C,\alpha,\beta,\gamma$ are the constants of integration. They also represent the dimension of the space $\mathcal{K}^2(\mathbb{R}^2)$, which alternatively can be calculated by making use of the formula (2.7).

Now for a fixed $\mathbf{K}_0^2\in\mathrm{Diff}\,\mathcal{K}^2(\mathbb{R}^2)$ given in terms of the Cartesian coordinates $(x,y)\in\mathbb{R}^2$ the map π: $\mathrm{Diff}\,\mathcal{K}^2(\mathbb{R}^2)\to\mathcal{X}(\Sigma)$ can be defined[20] as follows:

$$\pi\begin{pmatrix} A_0+2\alpha_0 y+\gamma_0 y^2 & C_0-\alpha_0 x-\beta_0 y-\gamma_0 xy\\ C_0-\alpha_0 x-\beta_0 y-\gamma_0 xy & B_0+2\beta_0 x+\gamma_0 x^2\end{pmatrix}$$
$$=A_0\frac{\partial}{\partial A}+B_0\frac{\partial}{\partial B}+C_0\frac{\partial}{\partial C}+\alpha_0\frac{\partial}{\partial\alpha}+\beta_0\frac{\partial}{\partial\beta}+\gamma_0\frac{\partial}{\partial\gamma},$$

where the parameters $A_0,B_0,C_0,\alpha_0,\beta_0,\gamma_0$ determine a given Killing tensor $\mathbf{K}_0^2\in\mathrm{Diff}\,\mathcal{K}^2(\mathbb{R}^2)$ and are smooth functions of parameters $A,B,C,\alpha,\beta,\gamma$ that span the corresponding space Σ.

Let $\mathbf{X}_1,\ldots,\mathbf{X}_r$, $r=\frac{1}{2}n(n+1)$ be the generators (Killing vectors) of the Lie algebra $i(M)=\mathcal{K}^1(M)$. Define the set of vector fields $\mathbf{V}_1,\ldots,\mathbf{V}_r\in\mathcal{X}(\Sigma)$ via a composition $F_*:=\pi\circ\mathcal{L}$ of π and

the Lie derivative deformation of the general Killing tensor $\mathbf{K}^p=\mathbf{K}^p(a_1,\ldots,a_d)\in\mathcal{K}^p(M)$ (i.e., the general solution of the Killing tensor equation $[\mathbf{K}^p,\mathbf{g}]=0$, with $a_1,\ldots,a_d$ as the constants of integration):

$$\mathbf{V}_i:=\pi\mathcal{L}_{\mathbf{X}_i}\mathbf{K}^p, \quad \text{or} \quad \mathbf{V}_i=F_*(\mathbf{X}_i), \quad i=1,\ldots,r. \tag{2.10}$$

Note $\mathcal{L}_{\mathbf{X}_i}\mathbf{K}^p\in\mathrm{Diff}\,\mathcal{K}^p(M)$, hence π is well-defined.

Remark 2.3: Note that in view of the Jacobi identity (2.5) for any $\mathbf{X}\in\mathcal{K}^1(M)$ and $\mathbf{K}^p\in\mathrm{Diff}\,\mathcal{K}^p(M)$ the deformed tensor $\tilde{\mathbf{K}}^p=\mathcal{L}_{\mathbf{X}}\mathbf{K}^p$ is also a Killing tensor: $\tilde{\mathbf{K}}^p\in\mathcal{K}^p(M)$, $p\geqslant 1$, which confirms that the formula (2.10) is well-defined. In general, a Lie algebra deformation $\mathcal{L}_{\mathbf{Y}}\mathbf{K}^p$, where $\mathbf{Y}\in TM$ is an arbitrary vector field, does not yield a Killing tensor: $\mathcal{L}_{\mathbf{Y}}\mathbf{K}^p\notin\mathcal{K}^p(M)$.

This interesting fact about the Lie derivative deformation of symmetric tensorial quantities is reminiscent of a well-known fact in Poisson geometry, where skew-symmetric tensorial quantities are involved in similar settings. More specifically, recall that for a bi-Hamiltonian system defined by a bi-Hamiltonian vector field $\mathbf{X}_{H_1,H_2}$ satisfying

$$\mathbf{X}_{H_1,H_2}=[\mathbf{P}_1,H_1]=[\mathbf{P}_2,H_2],$$

where $\mathbf{P}_1$, $\mathbf{P}_2$ are compatible Poisson bi-vectors (i.e., $[\mathbf{P}_1,\mathbf{P}_2]=0$) Oevel[16] considered a *scaling symmetry*, namely, a vector field $\mathbf{Z}_0$ satisfying the following scaling properties for $\mathbf{X}_{H_1,H_2}$ and the compatible Poisson pair $\mathbf{P}_1$, $\mathbf{P}_2$:

$$\mathcal{L}_{\mathbf{Z}_0}\mathbf{X}_{H_1,H_2}=\alpha\mathbf{X}_{H_1,H_2}, \quad \mathcal{L}_{\mathbf{Z}_0}\mathbf{P}_1=\beta\mathbf{P}_1, \quad \mathcal{L}_{\mathbf{Z}_0}\mathbf{P}_2=\gamma\mathbf{P}_2,$$

where α, β and $\gamma\in\mathbb{R}$. Recall also that in this situation the scaling symmetry $\mathbf{Z}_0$ is a *master symmetry*, a concept introduced by Fuchssteiner[17] (see also Ref. 18 for more details). Indeed, for the vector field $\mathbf{X}_{H_1,H_2}$ we have $[[Z_0,\mathbf{X}_{H_1,H_2}],\mathbf{X}_{H_1,H_2}]=0$. Therefore Z_0 is a master symmetry of $\mathbf{X}_{H_1,H_2}$. Then the hierarchy of the vector fields $\{\mathbf{Z}_i\}_{i=0}^{\infty}$, where $\mathbf{Z}_i=\mathbf{A}^i\mathbf{Z}_0$ ($\mathbf{A}=\mathbf{P}_2\mathbf{P}_1^{-1}$, provided $\det\mathbf{P}_1\neq 0$) constitute a Virasoro type Lie algebra with the commutator relation $[\mathbf{Z}_i,\mathbf{Z}_j]=(\beta+\gamma)(i-j)\mathbf{Z}_{i+j}$, $i,j=0,1,2,\ldots$. Moreover, the Lie derivative deformations $\mathcal{L}_{\mathbf{Z}_i}\mathbf{P}_1=\tilde{\mathbf{P}}_1^i$, $\mathcal{L}_{\mathbf{Z}_i}\mathbf{P}_2=\tilde{\mathbf{P}}_2^i$, $i=0,1,2,\ldots$. yield Poisson bi-vectors $\tilde{\mathbf{P}}_1^i$ and $\tilde{\mathbf{P}}_2^i$. For more details see Ref. 16. Just like in the case of the Lie derivative deformations of Killing tensors described above, this fact also does not hold true in general for arbitrary vector fields. More specifically, for an arbitrary vector field $\mathbf{X}$ defined on the corresponding manifold, the tensorial quantities $\mathcal{L}_{\mathbf{X}}\mathbf{P}_i$, $i=1,2$ are not necessarily Poisson bi-vectors.

We also note that the parameters $\tilde{a}_1,\ldots,\tilde{a}_d$ of $\tilde{\mathbf{K}}^p\in\mathrm{Diff}\,\mathcal{K}^p(M)$ are functions of the general parameters $a_1,\ldots,a_d$ that span the space $\Sigma:\tilde{\mathbf{K}}^p=\tilde{\mathbf{K}}^p(\tilde{a}_1(a_1,\ldots,a_d),\ldots,\tilde{a}_d(a_1,\ldots,a_d))$. Moreover, each vector field $\mathbf{V}_i\in\mathcal{X}(\Sigma)$, $i=1,\ldots,r$ carries the information about both the corresponding Killing vector $\mathbf{X}_i\in i(M)=\mathcal{K}^1(M)$, $i=1,\ldots,r$ and the general Killing tensor $\mathbf{K}^p\in\mathcal{K}^p(M)$. However, *the action of* $\mathbf{V}_i$ *is determined in the space* Σ *of the parameters* $a_1,\ldots,a_d$.

Conjecture 2.1: Suppose the generators $\mathbf{X}_1,\ldots,\mathbf{X}_r$ *of* $i(M)$ *satisfy the following commutator relations:*

$$[\mathbf{X}_i,\mathbf{X}_j]=c_{ij}^k\mathbf{X}_k, \tag{2.11}$$

where c_{ij}^k, $i,j,k=1,\ldots,r$ *are the structural constants. Then the corresponding vector fields* $\mathbf{V}_i\in\mathcal{X}(\Sigma)$, *defined by (2.10) satisfy the same commutator relations:*

$$[\mathbf{V}_i,\mathbf{V}_j]=c_{ij}^k\mathbf{V}_k. \tag{2.12}$$

Therefore the map $F_*:=\pi\circ\mathcal{L}:i(M)\to i_\Sigma(M)$ *is a Lie algebra isomorphism, where* $i_\Sigma(M)$ *is the Lie algebra generated by* $\mathbf{V}_1,\ldots,\mathbf{V}_r$.

The validity of the formula (2.12) can be confirmed directly on a case by case basis, provided that the general form of a Killing tensor $\mathbf{K}^p \in \mathcal{K}^p(M)$ is available (see Sec. III). Thus, the authors, Robin Deeley and Joshua Horwood have verified in this way that the isomorphism described in Conjecture 2.1 holds true for the following spaces of Killing tensors (vectors): $\mathcal{K}^1(\mathbb{R}^2)$, $\mathcal{K}^1(\mathbb{R}^2_1)$, $\mathcal{K}^1(\mathbb{R}^3)$, $\mathcal{K}^2(\mathbb{R}^2)$, $\mathcal{K}^2(\mathbb{R}^2_1)$ (see below), $\mathcal{K}^2(\mathbb{S}^2)$, $\mathcal{K}^3(\mathbb{R}^2)$, and $\mathcal{K}^2(\mathbb{R}^3)$,[19] where $\mathbb{S}^2$ denotes the two-sphere.

Note that the same procedure can be carried out for any invariant subspace of $\mathcal{K}^p(M)$. Therefore one can determine the action of $I(M)$ on any subspace of $\mathcal{K}^p(M)$ invariant under the action of $I(M)$. Once the isomorphism $i(M) \simeq i_\Sigma(M)$ is established, we can define $I(M)$-*invariants* and *conformal* $I(M)$-*invariants* of a vector space of Killing tensors $\mathcal{K}^p(M)$ as well as its invariant subspaces.

Definition 2.2: Let $(M,\mathbf{g})$ *be an n-dimensional pseudo-Riemannian manifold of constant curvature,* $\mathcal{K}^p(M)$*—the corresponding vector space of Killing tensors of valence p defined on* $(M,\mathbf{g})$ *and* $\mathcal{Q}(M) \subseteq \mathcal{K}^p(M)$*—an invariant subspace of* $\mathcal{K}^p(M)$*. A smooth function* $F:\Sigma \to \mathbb{R}$ *is said to be an* $I(M)$*-invariant of* $\mathcal{Q}(M) \subseteq \mathcal{K}^p(M)$ *iff*

$$\mathbf{V}_i(F) = 0, \tag{2.13}$$

where $\mathbf{V}_i$, $i = 1,\ldots,r$ *are the generators of the Lie algebra* $i_\Sigma(M)$ *defined as above for* $\mathcal{Q}(M)$.

A smooth function $G:\Sigma \to \mathbb{R}$ *is said to be a conformal* $I(M)$*-invariant of* $\mathcal{Q}(M) \subseteq \mathcal{K}^p(M)$ *iff*

$$\mathbf{V}_i(G) = \epsilon_i, \tag{2.14}$$

where $\epsilon_i \in \mathbb{R}$ *for* $i = 1,\ldots,r$.

Definition 2.3: An element $\mathbf{K}^2 \in \mathcal{K}^2(M)$ *is said to be nontrivial if and only if it is not a multiple of the metric* $\mathbf{g}$: $\mathbf{K}^2 \neq \ell\mathbf{g}$, $\ell \in \mathbb{R}$.

Let $\mathcal{Q}(\mathbb{R}^2)$ denote the subspace of all nontrivial Killing tensors in $\mathcal{K}^2(\mathbb{R}^2)$. Without loss of generality we can assume that $\mathcal{Q}(\mathbb{R}^2)$ is defined by the general nontrivial Killing tensor whose components are given by

$$Q^{ij} = \begin{pmatrix} A' + 2\alpha y + \gamma y^2 & C - \alpha x - \beta y - \gamma xy \\ C - \alpha x - \beta y - \gamma xy & 2\beta x + \gamma x^2 \end{pmatrix}, \quad i,j = 1,2, \tag{2.15}$$

where $A' = A - B$, and $A, B, C, \alpha, \beta, \gamma$ are the parameters appearing in (2.9). In view of Definition 2.2, one can determine $I(\mathbb{R}^2)$-invariants of $\mathcal{Q}(\mathbb{R}^2)$. Recall that Problem 2.1 for the vector subspace of nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}^2)$ has been solved by the authors in Ref. 20. The precise result is given in the following theorem:

Theorem 2.1: *Every smooth* $I(\mathbb{R}^2)$*-invariant of the subspace* $\mathcal{Q}(\mathbb{R}^2) \subset \mathcal{K}^2(\mathbb{R}^2)$ *enjoys the following form:*

$$F(\Delta^1_{\mathbb{R}^2}, \Delta^2_{\mathbb{R}^2}), \tag{2.16}$$

where $F: \mathbb{R}^2 \to \mathbb{R}$ *is a smooth function,*

$$\Delta^1_{\mathbb{R}^2} = \gamma, \quad \Delta^2_{\mathbb{R}^2} = (\alpha^2 - \beta^2 - \gamma A')^2 + 4(\gamma C + \alpha\beta)^2, \tag{2.17}$$

and $A, B, C, \alpha, \beta, \gamma$ *are the parameters defined in (2.9).*

Definition 2.4: The quantities $\Delta^i_{\mathbb{R}^2}$, $i = 1,2$ *are called the fundamental* $I(\mathbb{R}^2)$*-invariants of* $\mathcal{K}^2(\mathbb{R}^2)$.

Note that the fundamental $i(\mathbb{R}^2)$-invariants are homogeneous polynomials in $A, B, C, \alpha, \beta, \gamma$. It is important to note that both the number of fundamental invariants and the form of F in this case are in compliance with the following well-known theorem of the theory of invariants.

Theorem 2.2 (Ref. 12): *Let G act semiregularly on the m-dimensional manifold M with s-dimensional orbits. If $x_0 \in M$, then there exist precisely $m-s$ functionally independent local invariants $\zeta^1(x),\ldots,\zeta^{m-s}(x)$ defined in a neighborhood of x_0. Moreover, any other local invariant of the group action defined near x_0 is of the form*

$$\zeta(x)=F(\zeta^1(x),\ldots,\zeta^{m-s}(x)) \tag{2.18}$$

for some smooth function F. If the action of G is regular, then the invariants can be taken to be globally invariant in a neighborhood of x_0.

Indeed, $\dim \Sigma' = 5$, $\dim i_{\Sigma'}(\mathbb{R}^2)=3$. Therefore, according to Theorem 2.2, the number of fundamental invariants comes down to $5-3=2$.

The quantities $\Delta^i_{\mathbb{R}^2}, i=1,2$ to classify families of confocal conics in $\mathbb{R}^2$ which define orthogonally-separable coordinate webs for the Hamiltonian systems with two degrees of freedom defined in $\mathbb{R}^2$ admitting quadratic first integrals of motion. In this case the confocal conics are the integral curves of the eigenvectors of the corresponding Killing tensors $\mathcal{K}^2(\mathbb{R}^2)$. If the eigenvalues λ_1,λ_2 are not everywhere constant, they define the two families of confocal conics: $\lambda_i = \text{const}, i=1,2$. If one or both of the eigenvalues are everywhere constant one also has to consider the eigenvectors. Once an element of $\mathcal{Q}(\mathbb{R}^2)\subset\mathcal{K}^2(\mathbb{R}^2)$ is available, it is easy to determine the type of the corresponding confocal conics (*coordinate webs*), provided the Killing tensor in question is linearly independent of the metric tensor **g**. Thus, we have the following classification (compare with Example 1.1):

(a) if $\Delta^1_{\mathbb{R}^2}=0$, $\Delta^2_{\mathbb{R}^2}=0$, then (2.9) defines the Cartesian web in $\mathbb{R}^2$;

(b) if $\Delta^1_{\mathbb{R}^2}=0$, $\Delta^2_{\mathbb{R}^2}\neq 0$, then (2.9) defines the parabolic web in $\mathbb{R}^2$;

(c) if $\Delta^1_{\mathbb{R}^2}\neq 0$, $\Delta^2_{\mathbb{R}^2}=0$, then (2.9) defines the polar web in $\mathbb{R}^2$;

(d) if $\Delta^1_{\mathbb{R}^2}\neq 0$, $\Delta^2_{\mathbb{R}^2}\neq 0$, then (2.9) defines the elliptic-hyperbolic web in $\mathbb{R}^2$.

The geometrical significance of the invariants is given by the following formula:

$$k^2=\frac{\sqrt{\Delta^2_{\mathbb{R}^2}}}{(\Delta^1_{\mathbb{R}^2})^2}, \tag{2.19}$$

where k is interpretable as half the distance between the foci of the confocal conics in the elliptic–hyperbolic case.

In the following section we describe the vector space of Killing tensors $\mathcal{K}^2(\mathbb{R}^2_1)$ from this viewpoint and derive the corresponding $I(\mathbb{R}^2_1)$-invariants and conformal $I(\mathbb{R}^2_1)$-invariants to be applied in the sequel to a classification problem in the Hamilton–Jacobi theory of separation of variables that is described in Sec. IV.

III. GROUP INVARIANTS OF THE VECTOR SPACE $\mathcal{K}^2(\mathbb{R}^2_1)$

In this section the discussion proceeds from the general to the particular. We apply the concepts introduced in the previous section to the study of the Killing tensors of valence two defined in the Minkowski plane $\mathbb{R}^2_1$ that constitute the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$.

Remark 3.1: Here and below **K** denotes a Killing tensor of valence two.

The analysis presented in this section is parallel to the corresponding study carried out by the authors in Ref. 20 of the Killing tensors of valence two defined the Euclidean plane $\mathbb{R}^2$, i.e., the elements of the vector space $\mathcal{K}^2(\mathbb{R}^2)$. We observe first that in view of the formula (2.7) $\dim \mathcal{K}^2(\mathbb{R}^2_1)=6$. Alternatively, this fact can be verified by solving the corresponding Killing tensor equation $[\mathbf{K},\mathbf{g}]=0$ in, (say) pseudo-Cartesian coordinates $(t,x)\in\mathbb{R}^2_1$ for the Lorentzian metric $\mathbf{g}=\text{diag}(1,-1)$ of $\mathbb{R}^2_1$. As expected, the general solution given by

$$K^{ij}=\begin{pmatrix} A+2\alpha x+\gamma x^2 & C+\alpha t+\beta x+\gamma tx \\ C+\alpha t+\beta x+\gamma xt & B+2\beta t+\gamma t^2 \end{pmatrix}, \tag{3.1}$$

contains six parameters A, B, C, α, β, and γ (constants of integration) that span the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$. Here K^{ij} are the contravariant components of the general Killing tensor $\mathbf{K}\in\mathcal{K}^2(\mathbb{R}^2_1)$. We also note that the form of the general solution (3.1) is analogous to the general solution of the Killing tensor equation in the Euclidean plane (2.9). Next, in order to compute the $I(\mathbb{R}^2_1)$-invariants and conformal $I(\mathbb{R}^2_1)$-invariants of $\mathcal{K}^2(\mathbb{R}^2_1)$ we have to make use, in accordance with the procedure described in the preceding section, of the Lie algebra isomorphism between $i(\mathbb{R}^2_1)=\mathcal{K}^1(\mathbb{R}^2_1)$ and $i_\Sigma(\mathbb{R}^2_1)$, where $i_\Sigma(\mathbb{R}^2_1)$ is the corresponding subspace of $\mathcal{X}(\Sigma)$ generated by the vector fields defined via the formula (2.10) and $\Sigma\simeq\mathbb{R}^6$ is the space spanned by the six parameters A,B,C, α, β, and γ. In what follows, we establish the isomorphism directly by employing the general representation (3.1).

Lemma 3.1: The vector space $i_\Sigma(\mathbb{R}^2_1)$ is a Lie subalgebra of $\mathcal{X}(\Sigma)$ isomorphic to $i(\mathbb{R}^2_1)=\mathcal{K}^1(\mathbb{R}^2_1)$.

Proof: Consider the Lie algebra $i(\mathbb{R}^2_1)$ of the Lie group $I(\mathbb{R}^2_1)$ generated by the three Killing vectors:

$$\mathbf{T}=\frac{\partial}{\partial t},\quad \mathbf{X}=\frac{\partial}{\partial x},\quad \mathbf{H}=x\frac{\partial}{\partial t}+t\frac{\partial}{\partial x}. \tag{3.2}$$

They correspond, respectively, to the translations along t and x and a hyperbolic rotation and satisfy the following commutator relations:

$$[\mathbf{T},\mathbf{X}]=0,\quad [\mathbf{T},\mathbf{H}]=\mathbf{X},\quad [\mathbf{X},\mathbf{H}]=\mathbf{T}. \tag{3.3}$$

The corresponding flows generated by the vector fields (3.2) are given by

$$\begin{aligned} &\sigma_{\mathbf{T}}(a,(t,x))=t+a,\quad a\in\mathbb{R},\\ &\sigma_{\mathbf{X}}(b,(t,x))=x+b,\quad b\in\mathbb{R},\\ &\sigma_{\mathbf{H}}(\phi,(t,x))=(t\cosh\phi+x\sinh\phi,t\sinh\phi+x\cosh\phi), \end{aligned} \tag{3.4}$$

where $\phi\in\mathbb{R}$ is the (oriented) *Lorentz angle*. To define the map $\pi:\mathrm{Diff}\,\mathcal{K}^2(\mathbb{R}^2_1)\to\mathcal{X}(\Sigma)$ we use the generic formula (3.1) and the definition (2.8):

$$\begin{aligned} &\pi\begin{pmatrix} A_0+2\alpha_0 x+\gamma_0 x^2 & C_0+\alpha_0 t+\beta_0 x+\gamma_0 tx \\ C_0+\alpha_0 t+\beta_0 x+\gamma_0 tx & B_0+2\beta_0 t+\gamma_0 t^2 \end{pmatrix}\\ &\quad=A_0\frac{\partial}{\partial A}+B_0\frac{\partial}{\partial B}+C_0\frac{\partial}{\partial C}+\alpha_0\frac{\partial}{\partial\alpha}+\beta_0\frac{\partial}{\partial\beta}+\gamma_0\frac{\partial}{\partial\gamma}, \end{aligned}$$

for a particular element of $\mathrm{Diff}\,\mathcal{K}^2(\mathbb{R}^2_1)$ defined by $A_0,B_0,C_0,\alpha_0,\beta_0,\gamma_0$:

$$\mathbf{K}^2_0=\mathbf{K}^2_0(A_0,B_0,C_0,\alpha_0,\beta_0,\gamma_0)\in\mathcal{K}^2(\mathbb{R}^2_1).$$

Our next step is to define the vector fields $\mathbf{V}_1$, $\mathbf{V}_2$, and $\mathbf{V}_3$ in $\mathcal{X}(\Sigma)$ that correspond to the Killing vectors $\mathbf{T}$, $\mathbf{X}$, and $\mathbf{H}$ in $\mathcal{X}(\mathbb{R}^2_1)$, respectively, via the composition map $\pi\circ\mathcal{L}$ employing the formula (2.10). They are found to be

$$\mathbf{V}_1=\pi(\mathcal{L}_{\mathbf{T}}(\mathbf{K}))=2\beta\frac{\partial}{\partial B}+\alpha\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\beta},$$

$$\mathbf{V}_2=\pi(\mathcal{L}_{\mathbf{X}}(\mathbf{K}))=2\alpha\frac{\partial}{\partial A}+\beta\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\alpha},$$

$$\mathbf{V}_3=\pi(\mathcal{L}_{\mathbf{H}}(\mathbf{K}))=-2C\left(\frac{\partial}{\partial A}+\frac{\partial}{\partial B}\right)-(A+B)\frac{\partial}{\partial C}-\beta\frac{\partial}{\partial\alpha}-\alpha\frac{\partial}{\partial\beta}.$$

Note that the vector fields $\mathbf{V}_1$, $\mathbf{V}_2$, and $\mathbf{V}_3$ satisfy the commutator relations

$$[\mathbf{V}_1,\mathbf{V}_2]=0,\quad [\mathbf{V}_1,\mathbf{V}_3]=-\mathbf{V}_2,\quad [\mathbf{V}_2,\mathbf{V}_3]=-\mathbf{V}_1. \tag{3.5}$$

Choosing $-\mathbf{V}_1$, $-\mathbf{V}_2$, and $-\mathbf{V}_3$ as a basis of the Lie algebra $i_\Sigma(\mathbb{R}_1^2)$ immediately confirms that it is isomorphic to $i(\mathbb{R}_1^2)$ [see (3.3)]. □

Now we can *bring the problem of finding $I(\mathbb{R}_1^2)$-invariants and conformal $I(\mathbb{R}_1^2)$-invariants of $\mathcal{K}^2(\mathbb{R}_1^2)$ to the space Σ spanned by the six parameters $A,B,C,\alpha,\beta,\gamma$ or any $I(\mathbb{R}_1^2)$-invariant subspace of $\mathcal{K}^2(\mathbb{R}_1^2)$*. Indeed, the action of $I(\mathbb{R}_1^2)$ in Σ is equivalent to its action in Σ', where Σ' is the parameter space spanned by the five parameters $A'',C,\alpha,\beta,\gamma$, where $A''=A+B$ and $A,B,C,\alpha,\beta,\gamma$ span Σ and Σ' is the five-parameter space of parameters corresponding on the subspace of nontrivial Killing tensors $\mathcal{Q}(\mathbb{R}_1^2)\subset\mathcal{K}^2(\mathbb{R}_1^2)$. Thus, we can assume without loss of generality that contravariant components of the general nontrivial Killing tensor $\mathbf{Q}\in\mathcal{Q}(\mathbb{R}_1^2)$ are given by

$$Q^{ij}=\begin{pmatrix} A''+2\alpha x+\gamma x^2 & C+\alpha t+\beta x+\gamma tx\\ C+\alpha t+\beta x+\gamma xt & 2\beta t+\gamma t^2\end{pmatrix}, \tag{3.6}$$

where $A,B,C,\alpha,\beta,\gamma$ are as in (3.1).

Remark 3.2: We note that the general form (3.6) can be transformed to the form

$$\tilde{Q}^{ij}=\begin{pmatrix} A'''+2\alpha x+\gamma x^2 & C+\alpha t+\beta x+\gamma tx\\ C+\alpha t+\beta x+\gamma xt & A'''+2\beta t+\gamma t^2\end{pmatrix}, \tag{3.7}$$

where $A'''=(A+B)/2$, by adding a multiple of the metric. Obviously, this transformation does not affect the $I(\mathbb{R}_1^2)$-invariants of the subspace of nontrivial Killing tensors.

Next, using the procedure described above we can employ the composition $F_*=\pi\circ\mathcal{L}$ to determine the vector fields $\mathbf{V}_i'\in\mathcal{X}(\Sigma')$, $i=1,2,3$ that correspond to the generators of $i(\mathbb{R}_1^2)$.

Corollary 3.1: Let $\mathcal{Q}(\mathbb{R}_1^2)\subset\mathcal{K}^2(\mathbb{R}_1^2)$ be the invariant subspace of nontrivial Killing tensors of valence two defined in the Minkowski plane. Then the vector space $i_{\Sigma'}(\mathbb{R}_1^2)$ spanned by $\mathbf{V}_i'$, $i=1,2,3$ is a Lie subalgebra of $\mathcal{X}(\Sigma')$ isomorphic to $i(\mathbb{R}_1^2)=\mathcal{K}^1(\mathbb{R}_1^2)$.

Proof: The proof is identical to that of Lemma 3.1. □

Employing Definition 2.2 and the result of Corollary 3.1 we obtain the following theorem:

Theorem 3.1: *(a) Assume in (3.6) $\gamma\neq 0$. Then a smooth function $G:\Sigma\to\mathbb{R}$ is a conformal $I(\mathbb{R}_1^2)$-invariant of $\mathcal{Q}(\mathbb{R}_1^2)\subset\mathcal{K}^2(\mathbb{R}_1^2)$ iff it has the following form:*

$$G=|Z_+|^{\epsilon}\tilde{F}(\Delta^1_{\mathbb{R}_1^2},\Delta^2_{\mathbb{R}_1^2}), \tag{3.8}$$

where $\tilde{F}:\mathbb{R}^2\to\mathbb{R}$ is a smooth function, $\epsilon\in\mathbb{R}$ and $\Delta^1_{\mathbb{R}_1^2},\Delta^2_{\mathbb{R}_1^2}\in\Sigma'$ are homogeneous polynomials of $A'',C,\alpha,\beta,\gamma$ given by

$$\Delta^1_{\mathbb{R}_1^2}=\gamma,\quad \Delta^2_{\mathbb{R}_1^2}=(\alpha^2+\beta^2-\gamma A'')^2-4(\gamma C+\alpha\beta)^2 \tag{3.9}$$

and

$$Z_+=\gamma(A''+2C)-(\alpha-\beta)^2. \tag{3.10}$$

(b) Assume in (3.6) $\gamma\neq 0$. Then a smooth function $F:\Sigma\to\mathbb{R}$ is a $I(\mathbb{R}^2_1)$-invariant of $\mathcal{Q}(\mathbb{R}^2_1)\subset\mathcal{K}^2(\mathbb{R}^2_1)$ iff it assumes the following form:

$$F=F(\Delta^1_{\mathbb{R}^2_1},\Delta^2_{\mathbb{R}^2_1}), \tag{3.11}$$

where $A'',C,\alpha,\beta,\gamma$ are as in (3.6).

Proof: Recall that invariance of an object under the entire Lie group is equivalent to infinitesimal invariance under the infinitesimal generators of the corresponding Lie algebra. In view of Corollary 3.1 the vector fields $\mathbf{V}'_i$, $i=1,2,3$ given by

$$\mathbf{V}'_1=\pi(\mathcal{L}_{\mathbf{T}}(\mathbf{Q}))=\alpha\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\beta},$$

$$\mathbf{V}'_2=\pi(\mathcal{L}_{\mathbf{X}}(\mathbf{Q}))=2\alpha\frac{\partial}{\partial A''}+\beta\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\alpha},$$

$$\mathbf{V}'_3=\pi(\mathcal{L}_{\mathbf{H}}(\mathbf{Q}))=-2C\frac{\partial}{\partial A''}-A''\frac{\partial}{\partial C}-\beta\frac{\partial}{\partial\alpha}-\alpha\frac{\partial}{\partial\beta}$$

can be chosen as a basis of the Lie algebra $i_{\Sigma'}(\mathbb{R}^2_1)$. Here $\mathbf{Q}$ is given by (3.6).

(a)$\Rightarrow$We solve the system of PDE's

$$\mathbf{V}'_i(G)=\epsilon_i, \tag{3.12}$$

for $i=1,2,3$. We view the system (3.12) as a system of three inhomogeneous linear partial differential equations in five variables that can be conveniently solved by repeated application of the method of characteristics. In the case $\gamma\neq 0$, we obtain solution (3.8). We note that the existence of a solution forces $\epsilon_1=\epsilon_2=0$, while ϵ in (3.8) is ϵ_3.

(a)$\Leftarrow$Straightforward.

(b)$\Rightarrow$The proof is analogous to part (a). This time we solve by the method of characteristics a simpler system of PDE's, namely,

$$\mathbf{V}'_i(F)=0, \tag{3.13}$$

for $i=1,2,3$. The general solution is given by (3.11).

(b)$\Leftarrow$Straightforward. □

Corollary 3.2: $\Delta^i_{\mathbb{R}^2_1}$, $i=1,2$ given by (3.11) are $I(\mathbb{R}^2_1)$-invariants of $\mathcal{K}^2(\mathbb{R}^2_1)$.

Definition 3.1: The quantities $\Delta^i_{\mathbb{R}^2_1}$, $i=1,2$ are called the fundamental $I(\mathbb{R}^2_1)$-invariants of $\mathcal{K}^2(\mathbb{R}^2_1)$.

Remark 3.3: As expected, in view of Theorem 2.2, we have obtained two $I(\mathbb{R}^2_1)$-invariants: $\dim\Sigma'-\dim i(\mathbb{R}^2_1)=5-3=2$.

Remark 3.4: We note that the $I(\mathbb{R}^2_1)$-invariants of the subspace of nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}^2_1)$ have a striking resemblance to the $I(\mathbb{R}^2)$-invariants of the subspace of nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}^2)$ [see (4.18)]. In spite of such a similarity, however, the polynomial $\Delta^2_{\mathbb{R}^2}\geqslant 0$, while $\Delta^2_{\mathbb{R}^2_1}$ factors over the reals.

Corollary 3.3: Let $Z_\pm=\gamma(A''\pm 2C)-(\alpha\mp\beta)^2$. The functions $I_\pm:\Sigma\to\mathbb{R}$ given by

$$I_\pm:=\operatorname{sgn}(Z_\pm) \tag{3.14}$$

are $I(\mathbb{R}^2_1)$-invariants of $\mathcal{Q}(\mathbb{R}^2_1)\subset\mathcal{K}^2(\mathbb{R}^2_1)$.

Proof: We note first that

$$Z_+ Z_- = \Delta^2_{\mathbb{R}^2_1}.$$

Next, using formulas (3.4) for the flows of the generators of $i(\mathbb{R}^2_1)$, we obtain

$$\overline{Z}_\pm = e^{\mp 2\phi} Z_\pm,$$

which implies the result. □

Various additional conformal $I(\mathbb{R}^2_1)$-invariants arise from the solution of the system of PDE's (3.12) used in the proof of part (a) of Theorem 3.1 when $\gamma = 0$. They will be used in the sequel to solve the problem of classification of separable Hamiltonian systems defined in the Minkowski plane $\mathbb{R}^2_1$.

Theorem 3.2: *Let $\gamma = 0$ in (3.7). Then $G: \Sigma \to \mathbb{R}$ is a conformal $I(\mathbb{R}^2_1)$-invariant of $\mathcal{Q}(\mathbb{R}^2_1) \subset \mathcal{K}^2(\mathbb{R}^2_1)$ iff*

(*a*)

$$G = \exp\left(\epsilon_3 \operatorname{arctanh}\left(\frac{-\beta}{\alpha} \right) \right) \tilde{F}(\alpha^2 - \beta^2), \tag{3.15}$$

when $\alpha^2 \neq \beta^2$. In this case $\epsilon_1 = \epsilon_2 = 0$.

(*b*)

$$G = |\alpha|^{-\epsilon_3/2} \exp\left(\frac{\epsilon_1 (A'' - 2C)}{4\alpha} \right) \tilde{F}((A'' + 2C)\alpha), \tag{3.16}$$

when $\alpha^2 = \beta^2 \neq 0$, $\alpha = \beta$. In this case $\epsilon_1 = \epsilon_2$.

(*c*)

$$G = |\alpha|^{\epsilon_3/2} \exp\left(\frac{-\epsilon_1 (A'' + 2C)}{4\alpha} \right) \tilde{F}((A'' - 2C)\alpha), \tag{3.17}$$

when $\alpha^2 = \beta^2 \neq 0$, $\alpha = -\beta$. In this case $\epsilon_1 = -\epsilon_2$.

In each of the above cases, $\tilde{F}$ represents an arbitrary smooth function.

Using the results of Theorem 3.2 we can derive additional $I(\mathbb{R}^2_1)$-invariants that will be used in the forthcoming sections to classify special separable cases of Hamiltonian systems defined in $\mathbb{R}^2_1$.

Corollary 3.4: Let $\gamma = 0$ in (3.6). Then we have
(i) $F = \operatorname{sgn}(\alpha^2 - \beta^2)$ is an $I(\mathbb{R}^2_1)$-invariant of $\mathcal{Q}(\mathbb{R}^2_1) \subset \mathcal{K}^2(\mathbb{R}^2_1)$,
(ii) let $\alpha^2 = \beta^2 \neq 0$. *Define*

$$\mu_\pm := \frac{A'' \pm 2C}{\alpha}. \tag{3.18}$$

Then we have

- *(a) then for $I_+ = 0, I_- = -1$ (i.e., $\alpha = \beta$), $F = \operatorname{sgn}(\mu_+)$ is an $I(\mathbb{R}^2_1)$-invariant of $\mathcal{Q}(\mathbb{R}^2_1) \subset \mathcal{K}^2(\mathbb{R}^2_1)$,*
- *(b) then for $I_+ = -1, I_- = 0$ (i.e., $\alpha = -\beta$), $F = \operatorname{sgn}(\mu_-)$ is an $I(\mathbb{R}^2_1)$-invariant of $\mathcal{Q}(\mathbb{R}^2_1) \subset \mathcal{K}^2(\mathbb{R}^2_1)$.*

IV. HAMILTON–JACOBI THEORY OF SEPARATION OF VARIABLES AND GROUP INVARIANTS OF KILLING TENSORS

Since the time of its inception in the 19th century the problem of integrability of a general Hamiltonian system defined by a natural Hamiltonian has been extensively studied. Its beauty and richness are largely due to a profound connection with the Hamilton–Jacobi theory of separation

of variables.[21–27] To establish the requisite language of the theory to be used throughout this paper, we recall briefly its basic concepts. Let $(M,\mathbf{g})$ be an n-dimensional pseudo-Riemannian manifold. Recall that a Hamiltonian system defined by a natural Hamiltonian function with a scalar potential V, which can be written as

$$H(\mathbf{q},\mathbf{p})=\tfrac{1}{2}g^{ij}(\mathbf{q})p_ip_j+V(\mathbf{q}), \tag{4.1}$$

can in many cases be integrated by quadratures by considering the corresponding Hamilton–Jacobi equation (HJE). Here g^{ij} are the contravariant components of the corresponding metric tensor $\mathbf{g}$ and $(\mathbf{q},\mathbf{p})\in T^*M$ are the canonical position-momenta coordinates. The procedure consists of a canonical coordinate transformation (CT) $T:(\mathbf{q},\mathbf{p})\rightarrow(\mathbf{u},\mathbf{v})$ to *separable coordinates* (SC) $(\mathbf{u},\mathbf{v})$, with respect to which the Hamilton–Jacobi equation

$$\frac{1}{2}g^{ij}(\mathbf{u})\frac{\partial W}{\partial u^i}\frac{\partial W}{\partial u^j}+V(\mathbf{u})=E,\quad v_j=\frac{\partial W}{\partial u^i}, \tag{4.2}$$

admits a *complete integral* (CI) $W(\mathbf{u},\mathbf{c})$, satisfying the nondegeneracy condition: $\det\|\partial^2W/\partial u^i\partial c_j\|_{n\times n}\neq 0$, where $\mathbf{c}=(c_1,\ldots,c_n)$ is a constant vector. The function W is usually sought in the form

$$W(\mathbf{u},\mathbf{c})=\sum_{i=1}^{n}W_i(u^i,\mathbf{c}),$$

which is the essence of the *additive separation ansatz*. In view of Jacobi's theorem, once W has been found, the integral curves of the flow generated by (4.40) can be determined from the equations

$$v_i=\frac{\partial W}{\partial u^i},\quad b_j=\frac{\partial W}{\partial c_j},\quad t-t_0=\frac{\partial W}{\partial E},$$

where $i=1,\ldots,n$, $j=1,\ldots,n-1$. The inverse canonical transformation $(\mathbf{u},\mathbf{v})\rightarrow(\mathbf{q},\mathbf{p})$ yields the solution in terms of the original position-momenta coordinates $(\mathbf{q},\mathbf{p})$. Geometrically, the Hamilton–Jacobi equation and its solution W can be interpreted as follows (see Benenti[22]): In a neighborhood of a regular point Eq. (4.2) determines a hypersurface $\mathcal{H}\subset T^*M$, while the set of equations $v_i=\partial W/\partial u_i$ determine a Lagrangian submanifold $\Lambda\subset T^*M$, as an image of a closed one-form dW. Therefore W is a solution to (4.2) iff $\mathcal{H}\subset\Lambda$.

The principal special cases of the canonical transformations to separable coordinates are the *point transformation*, in which case the separable coordinates are given by $u^i=u^i(\mathbf{q})$, $i=1,\ldots,n$ and the *generic (nonpoint) transformation*, in which case we have: $u^i=u^i(\mathbf{q},\mathbf{p})$, $v^i=v^i(\mathbf{q},\mathbf{p})$, $i=1,\ldots,n$. Moreover, the point transformation in this context is *(non)orthogonal* iff the metric tensor $\mathbf{g}$ of (4.40) is (non)diagonal with respect to the separable coordinates $u^1,\ldots,u^n$.

The existence of separable coordinates $(\mathbf{u},\mathbf{v})$ is usually guaranteed by the existence of an additional geometrical structure associated with the dynamics of the Hamiltonian system defined by (4.1). Thus, in the case of a point transformation to separable coordinates, they can be determined by the geometric properties of a certain Killing tensor (orthogonal separation of variables), or a Killing tensor in conjunction with an abelian Lie algebra of Killing vectors (nonorthogonal separation of variables).[28] These Killing tensors correspond to first integrals quadratic in the momenta of the Hamiltonian system defined by (4.1). When the canonical transformation to the separable coordinates is not a point transformation, the separable coordinates $(\mathbf{u},\mathbf{v})$ can be determined by the existence of either a (quasi-)bi-Hamiltonian structure or a Lax pair or both. A vast literature on the subject has emerged in recent years. Many papers have been devoted to the study

of integrable systems admitting bi-Hamiltonian and/or Lax representations from the point of view of separation of variables (see, for example, Refs. 29–35, as well as the relevant references therein).

Orthogonally separable Hamiltonian systems defined by natural Hamiltonians of the type (4.1) represent the most studied class of systems whose integrability can be asserted within the framework of the Hamilton–Jacobi theory. Examples of the Hamiltonian system belonging to this class include such well-known physical models as the harmonic oscillator, Coulomb–Kepler potential, the two integrable cases of the Hénon–Heiles potential, Yatsun's integrable potentials, the two particle nonperiodic Toda lattice, Calogero–Moser potential, and others. Global properties of the Hamiltonian systems defined on Riemannian manifolds have also been extensively studies by many authors (see Ref. 36 and the references therein). Since the first paper by Liouville[37] (see also Ref. 38 for historical details) devoted to the study of orthogonally separable Hamiltonians, the theoretical background has been developed by many well-known authors, including Morera,[39] Stäckel,[40] Eisenhart,[5] Kalnins and Miller,[13] Benenti,[28] and others (see also the relevant references therein). The compact and refined criterion of orthogonally separability due to Benenti[28] subsumes most of the previous results on orthogonal separability. It reads:

Theorem 4.1: *The Hamiltonian system defined by (4.1) is orthogonally separable if and only if there exists a valence two Killing tensor* $\mathbf{K}$ *with pointwise simple and real eigenvalues, orthogonally integrable eigenvectors such that* $d(\hat{\mathbf{K}}dV)=0$, *where the linear operator* $\hat{\mathbf{K}}$ *is given by* $\hat{\mathbf{K}}:=\mathbf{Kg}$.

The separable coordinates are defined by the integral curves of the eigenvectors of $\mathbf{K}$.[28] When $n=2$ the separable coordinates are also defined by the eigenvalues and/or the eigenvectors of $\mathbf{K}$. The tensor $\mathbf{K}$ satisfies the Killing tensor Eq. (2.1), which in component form can be written as follows:

$$[\mathbf{g},\mathbf{K}]^{ijk}=g^{(ij}{}_{,\ell}K^{k)\ell}-K^{(ij}{}_{,\ell}g^{k)\ell}=0. \tag{4.3}$$

It should be mentioned, however, that in applications involving the Hamiltonian systems defined in higher dimensions often an auxiliary tensor $\mathbf{L}$ is required in order to construct the separable coordinates. It is given by $\mathbf{L}:=1/(n-1)\mathrm{tr}(\mathbf{K})\mathbf{g}-\mathbf{K}$ and called a *conformal Killing tensor* (CKT).[41] The eigenvalues of $\mathbf{L}$ provide the coordinates of separations. Clearly, the Killing tensors $\mathbf{L}$ and $\mathbf{K}$ share the same *integrable* eigenvectors.

An important new facet to the theory of orthogonally separable Hamiltonian systems was added by Ferapontov and Fordy[42,43] in the form of a connection between the theory of orthogonally separable Hamiltonian systems and the theory of partial differential equations of *hydrodynamic type*. It appears that a system satisfying the conditions of Theorem 4.1 can be naturally associated with such a system of PDE's. Moreover, the process of finding separable coordinates in the original Hamiltonian system can then be related to the process of determining Riemann invariants in the corresponding system of hydrodynamic type. This fruitful idea has been extended to the study of Hamiltonian systems with vector potentials (see the review in Ref. 43, and references therein).

As has been previously mentioned, the study of orthogonally separable natural Hamiltonians in the sense described above was initiated by Liouville.[37] He considered the Hamiltonian system with two degrees of freedom modeling the motion of a particle on a curved surface. More specifically, Liouville showed that if there exists a coordinate system (u,v) in which the Hamiltonian enjoys the form

$$H=(A(u)+B(v))^{-1}[\tfrac{1}{2}(\epsilon_1 p_u^2+\epsilon_2 p_v^2)+C(u)+D(v)], \tag{4.4}$$

then the canonical Hamilton equations can be integrated by quadratures. The form of H also implies that the corresponding HJE can be integrated by separation of variables. In (4.4) $A(u)$,

$B(v)$, $C(u)$, $D(v)$ are smooth functions and $(\epsilon_1)^2=(\epsilon_2)^2=1$. Note that the form (4.4) has been derived without making any assumptions about the curvature of the two-dimensional pseudo-Riemannian space $(M,\mathbf{g})$.

In 1881 Morera[39] solved the converse problem. Thus, he showed that if a Hamiltonian system with two degrees of freedom can be solved by separation of variables, then there exists a system of coordinates in which the Hamiltonian (4.1) assumes the *Liouville form* (4.4). He also showed that in the Euclidean plane *orthogonal* separation of variables occurred only in Cartesian, polar, parabolic, and elliptic–hyperbolic coordinates, provided the Hamiltonian assumed the form (4.4) in the separable coordinates. We note that there can exist other systems of coordinates with respect to which the HJE separates, while the Hamiltonian (4.1) is not in the Liouville form (4.4).

This remarkable equivalence can also be reformulated in the form of the celebrated *Bertrand–Darboux–Whittaker theorem*,[47] which states that separability of the HJE corresponding to the Hamiltonian system with two degrees of freedom defined by (4.1) is equivalent to the existence of a second first integral quadratic in the momenta:

$$F=K^{ij}(\mathbf{q})p_ip_j+U(\mathbf{q}),\quad i,j=1,2, \tag{4.5}$$

where K^{ij} are the components of the corresponding Killing tensor $\mathbf{K}$ with pointwise simple and real eigenvalues and $dU=2\hat{\mathbf{K}}dV$. The theorem appears to be a particular case of Theorem IV, since the eigenvectors of $\mathbf{K}$ in this case are automatically integrable. For a long time a procedure based on the Bertrand–Darboux–Whittaker theorem has provided a working method for integrating the Hamiltonian systems with two degrees of freedom defined by (4.1). More specifically, once a second integral quadratic in the momenta has been found, the method consists of solving the second order PDE resulting from the involutiveness of F and H. The solution is used to transform a given Hamiltonian to the form (4.4). The coordinates (u,v), thus determined, provide separable coordinates for the associated HJE, which entails complete integrability of the Hamiltonian system defined by (4.1). However, even in the simplest case, namely when the Hamiltonian system (4.1) is defined in the Euclidean plane, finding the separable coordinates following this scheme involves quite a few steps.[47] The procedure is illustrated by the following example.

Example 4.1 (Method I. Second Integrable Case of Yatsun): Let a Hamiltonian system be defined by the following Hamiltonian function:

$$H_2(q^1,q^2,p_1,p_2) = \tfrac{1}{2}(p_1^2 + p_2^2) + V_2(q^1,q^2), \tag{4.6}$$

where

$$V_2(q^1,q^2) = -2\left((q^1)^4 + 2(q^1)^2(q^2)^2 + \frac{2\lambda}{g^2}(q^2)^4\right) + 4((q^1)^3 + q^1(q^2)^2) - 2((q^1)^2 + (q^2)^2). \tag{4.7}$$

This system describes the equations of motion of an SU(2) Yang–Mills theory after O(4)-symmetry reduction.[44,45] It has been shown[44,45] that the Hamiltonian system is completely integrable if $g^2=2\lambda$ admitting the following additional first integral independent of (4.6):

$$F_2=((q^2)^2+\tfrac{3}{4})p_1^2-(2q^1-1)q^2p_1p_2+(q^1-1)q^1p_2^2-3(q^1)^4-2(q^1)^2(q^2)^2+(q^2)^4 +6(q^1)^3+2(q^1)(q^2)^2-3(q^1)^2. \tag{4.8}$$

Therefore in view of the previous comments the Hamiltonian system in question can be solved by the Hamilton–Jacobi method of separation of variables. To find the separable coordinates, we employ the procedure based on the Bertrand–Darboux–Whittaker theorem, which involves bringing the Hamiltonian function (4.6) to the form (4.4):

(1) Observe that the components of the Killing tensor are given by

$$K^{(1)}=\begin{pmatrix} \frac{3}{4}+(q^2)^2 & \frac{1}{2}q^2-q^1q^2 \\ \frac{1}{2}q^2-q^1q^2 & -q^1+(q^1)^2 \end{pmatrix}. \tag{4.9}$$

(2) Write down the PDE implied by the compatibility condition $d(\hat{\mathbf{K}}dV)=0$:

$$\left(\frac{\partial^2 V}{\partial(q^2)^2}-\frac{\partial^2 V}{\partial(q^1)^2}\right)(-2q^1q^2+q^2)+2\frac{\partial^2 V}{\partial q^1\partial q^2}\left((q^2)^2-(q^1)^2+\frac{3}{4}+q^1\right)+\frac{\partial V}{\partial q^1}6q^2+\frac{\partial V}{\partial q^2}(-6q^1+3)=0. \tag{4.10}$$

(3) Perform the change of the variable $q^1\to z+\frac{1}{2}$, $q^2\to y$, to obtain

$$\left(\frac{\partial^2 V}{\partial z^2}-\frac{\partial^2 V}{\partial y^2}\right)zy+\frac{\partial^2 V}{\partial z\partial y}(y^2-z^2+1)+\frac{\partial V}{\partial z}3y-\frac{\partial V}{\partial y}3z=0. \tag{4.11}$$

(4) Consider (following Darboux!) the differential equation of the characteristics of (4.11):

$$zy(dy^2-dz^2)+(z^2-y^2-1)dzdy=0. \tag{4.12}$$

(5) Introduce the new variables $u:=z^2$ and $v:=y^2$ to transform (4.12) into the following ODE:

$$\left(\frac{dv}{du}\right)^2(u-v)+\frac{dv}{du}(u-v-1)=0, \tag{4.13}$$

which is a *Clairaut's equation,* which has a general solution of the form

$$(m+1)(mz^2-y^2)-m=0 \tag{4.14}$$

in the original variables z,y.

(6) Rewrite (4.14) in terms of a new parameter α to get

$$\frac{z^2}{\alpha^2}+\frac{y^2}{\alpha^2-1}=1.$$

Observe that the characteristic curves of the PDE are two families of confocal conics. Therefore taking the parameters of the confocal hyperbolas and ellipses as coordinates, we have

$$z=\alpha\beta, \quad y=[(\alpha^2-1)(1-\beta)]^{1/2},$$

or

$$z=\cosh(u)\cos(v), \quad y=\sinh(u)\sin(v).$$

(7) Write the PDE (4.11) in terms of new variables α and β to obtain

$$(\beta^2-\alpha^2)\frac{\partial^2 V}{\partial\alpha\partial\beta}+2\beta\frac{\partial V}{\partial\alpha}-2\alpha\frac{\partial V}{\partial\beta}=0,$$

which has a general solution

$$V=\frac{f(\alpha)-\phi(\beta)}{\alpha^2-\beta^2}$$

in the Liouville form.

(8) Finally, transform back to the original coordinates q^1 and q^2 to find

$$\begin{cases} q^1 = \frac{1}{2} + \cosh(u)\cos(v), \\ q^2 = \sinh(u)\sin(v). \end{cases} \tag{4.15}$$

Therefore the separable coordinates are of the shifted elliptic–hyperbolic type.

(9) Transform the momenta and potential accordingly, to obtain the following Liouville form of the Hamiltonian H_2 in the elliptic–hyperbolic coordinates

$$H_2 = \frac{\frac{1}{2}(p_u^2 + p_v^2) + g(\cos^2(v)) - g(\cosh^2(u))}{\cosh^2(u) - \cos^2(v)}, \tag{4.16}$$

where $p_u = \partial W/\partial u$, $p_v = \partial W/\partial v$, and

$$g(\eta) = 2\eta^3 - 3\eta^2 + \tfrac{9}{8}\eta. \tag{4.17}$$

Hence we conclude that the Hamiltonian H_2 is orthogonally separable in the (u,v) coordinates.

For example, this is essentially the procedure used by Rauch–Wojciechowski[48] to integrate the second integrable case of the Hénon–Heiles potential by the Hamilton–Jacobi method of separation of variables and obtain the transformations to the separable coordinates. Recently the method has been generalized to higher dimensions,[49] in which case one has to deal not with a single PDE, but a system of PDE's of the type (4.10) called the *Bertrand–Darboux system of PDE's*.

The above example illustrates that the problem of integrating a Hamiltonian system by the Hamilton–Jacobi method of separation of variables consists essentially of two parts. *First*, one has to determine the type of the system of separable coordinates involved and recall the known coordinate transformations from (q^1,q^2) to (u,v). At this stage the separable coordinates are defined up to the action of the isometry group $I(\mathbb{R}^2)$. *Second*, one has to locate the separable coordinates (u,v) with respect to the given original coordinates (q^1,q^2), that is to take into account any additional translation and/or rotation determined by the action of $I(\mathbb{R}^2)$. Thus, in Example 4.1 the orthogonal separable coordinates have been determined to be shifted elliptic–hyperbolic coordinates. The corresponding coordinate transformation from (q^1,q^2) to (u,v) is given by (4.15).

It is clear that the whole procedure rests on the properties of the Killing tensor (4.9) as well as the action of the isometry group $I(\mathbb{R}^2)$. This observation enabled the present authors to considerably simplify the procedure by making it completely algebraic.[20] To this end, we determined the action of the isometry group $I(\mathbb{R}^2)$ in the space $\mathcal{K}^2(\mathbb{R}^2)$ defined by the general form (2.9) and derived the $I(\mathbb{R}^2)$-*invariants* $\Delta^1_{\mathbb{R}^2}$ and $\Delta^2_{\mathbb{R}^2}$ of (2.9) as polynomial functions of the parameters $A,B,C,\alpha,\beta,\gamma$:

$$\Delta^1_{\mathbb{R}^2} = \gamma, \quad \Delta^2_{\mathbb{R}^2} = (\alpha^2 - \beta^2 + \gamma(B-A))^2 + 4(\gamma C + \alpha\beta)^2. \tag{4.18}$$

The functions $\Delta^i_{\mathbb{R}^2}$, $i=1,2$ can be used to characterize the type of separable coordinate(s), given the Killing tensor defined by a first integral (4.1) quadratic in the momenta. The six parameters $A,B,C,\alpha,\beta,\gamma$ have also been used to determine any translation and/or rotation of the separable coordinates (u,v) with respect to the original coordinates (q^1,q^2). See Table I in Ref. 20 for more details. In order to illustrate the new method and compare it with Method I used above, we reconsider the Hamiltonian system defined by (4.7) from this new viewpoint.

Example 4.2 [Method II (Ref. 20). Second Integrable Case of Yatsun]: To employ the new method based on the $I(\mathbb{R}^2)$-group invariants of the Killing tensors, we again begin by considering the Killing tensor defined by the first integral (4.8).

(1) The corresponding Killing tensor defined by the first integral quadratic in the momenta is found to be

$$K^{(1)}=\begin{pmatrix} \frac{3}{4}+(q^2)^2 & \frac{1}{2}q^2-q^1q^2 \\ \frac{1}{2}q^2-q^1q^2 & -q^1+(q^1)^2 \end{pmatrix}. \tag{4.19}$$

(2) Comparing (4.19) with (2.9), we determine the parameters: $A=\frac{3}{4}$ $B=C=\alpha=0$ $\beta=-\frac{1}{2}$, and $\gamma=1$. Next, we use Table I in Ref. 20 to find after a simple computation that in addition to $\Delta^1_{\mathbb{R}^2}=\gamma=1\neq 0$, the second $I(\mathbb{R}^2)$-invariant $\Delta^2_{\mathbb{R}^2}=1/4\neq 0$. This indicates that the coordinates of separation are of the elliptic–hyperbolic type. Using the corresponding formulas presented in Table I,[20] we find the constants $a=1/2$, $b=0$ (translations along the q^1 and q^2 axes, respectively), $\theta=0$ (rotation angle), $k=1$ (the distance between the foci). This immediately yields the transformation formulas to the separable coordinates:

$$\begin{cases} q^1=\frac{1}{2}+\cosh(u)\cos(v), \\ q^2=\sinh(u)\sin(v), \end{cases} \tag{4.20}$$

which agrees with the results previously obtained.

Clearly, the new method considerably simplifies the process of integration by replacing an *analytical* procedure with an *algebraic* one (compare with Example 4.1). Due to this fact, *it is now easy to incorporate the algorithm into a computer algebra package*. The corresponding programs have been implemented in the computer algebra system MAPLE.

In the present paper we take the next step in developing the algorithm by extending its applicability to the Hamiltonian systems defined in the Minkowski plane $\mathbb{R}^2_1$. The situation in this case is much more complicated than the case of Hamiltonian systems defined in the Euclidean plane $\mathbb{R}^2$ due to the fact that there exist a larger number of separable coordinate systems. It is well known[25,15] that in this setting there exist ten distinct (in a certain sense) types of separable systems of coordinates determined by the corresponding Killing tensors. Therefore one has to find an appropriate set of invariants of the general Killing tensor that can be used to characterize each of the separable coordinate systems and to determine the corresponding transformations to separable coordinates.

V. SEPARABLE KILLING TENSORS IN THE LIOUVILLE–MORERA COORDINATES (u,v)

In this section we extend our study to the Hamiltonian systems defined in the Minkowski plane $\mathbb{R}^2_1$. We shall follow the general procedure based on $I(\mathbb{R}^2)$-invariants devised in Ref. 20 to classify orthogonally separable Hamiltonian systems defined in the Euclidean plane $\mathbb{R}^2$. In order to be able to employ the (conformal) $I(\mathbb{R}^2_1)$-invariants of $\mathcal{K}^2(\mathbb{R}^2_1)$ to the classification problem, we determine first the orthogonally-separable Hamiltonian systems defined in $\mathbb{R}^2_1$ with respect to a special system of coordinates that is introduced below.

Consider a Hamiltonian system with two degrees of freedom defined by

$$H(\mathbf{q},\mathbf{p})=\tfrac{1}{2}g^{ij}p_ip_j+V(\mathbf{q}), \tag{5.1}$$

where g^{ij}, $i,j=1,2$ are the contravariant components of a Lorentzian metric $\mathbf{g}$, which asserts that the underlying manifold $(M,\mathbf{g})$ is pseudo-Riemannian. According to the approach to the study of integrability of Hamiltonian systems with two degrees of freedom defined in Riemannian spaces introduced by Liouville,[37] we claim that if the metric $\mathbf{g}$ as well as the potential function V in (5.1) take on special *separable* forms in some coordinate system (u,v), the Hamiltonian system defined by (5.1) can be integrated by quadratures with respect to (u,v). It has been shown in Ref. 53 that in the coordinates (u,v) the Hamiltonian function takes on the following form:

$$H=(A(u)+B(v))^{-1}[\tfrac{1}{2}(p_u^2-p_v^2)+C(u)+D(v)], \tag{5.2}$$

where $A(u)$, $B(v)$, $C(u)$, and $D(v)$ are arbitrary smooth functions. This setting also implies additive separation of variables in the corresponding HJE (4.2). Note that the metric entering the formula (5.2) enjoys the *Liouville form:*

$$ds^2=(A(u)+B(v))(du^2-dv^2). \tag{5.3}$$

Conversely, following Morera,[39] we can also conclude that if the Hamiltonian system defined by (5.1) can be integrated via additive separation of variables in the associated HJE (4.2), the Hamiltonian function (5.1) can be transformed to the form (5.2) with respect to the separable coordinates. Hence, in view of this classical equivalence, we call (u,v) the *Liouville–Morera (LM) separable coordinates*.

It is easy to see that the Hamiltonian system defined by (5.1) in the LM coordinates admits an additional first integral of motion of the form:

$$F=\frac{B(v)p_u^2+A(u)p_v^2+2(B(v)C(u)-A(u)D(v))}{A(u)+B(v)}. \tag{5.4}$$

Note, the integral of motion (5.4) is quadratic in the momenta with the corresponding (covariant) Killing tensor $\mathbf{K}^{LM}\in\mathcal{K}^2(\mathbb{R}_1^2)$ given by

$$\mathbf{K}^{LM}=(A(u)+B(v))\,\mathrm{diag}(B(v),A(u)). \tag{5.5}$$

Clearly, the functions $A(u)$ and $B(v)$ are the eigenvalues of the linear operator $\hat{\mathbf{K}}=\mathbf{K}^{LM}\mathbf{g}^{-1}$, where $\mathbf{g}$ is the metric of (5.1). Employing the corresponding eigenvectors of $\mathbf{K}^{LM}$, one can show by solving the Killing tensor equation (2.1) in the moving frame of the normalized eigenvectors,[52] that the most general solution has the following form:

$$\mathbf{K}=\ell\mathbf{g}+m\mathbf{K}^{LM}, \tag{5.6}$$

where $\ell,m\in\mathbb{R}$ are arbitrary constants. In this work we are concerned with the case when the Riemann curvature tensor is zero. Solving the resulting differential equation allows us to determine the ten admissible metrics along with the corresponding Killing tensors [corresponding to (5.3) and (5.6), respectively], which we list below (see Ref. 52 for more details). In essence, solving these differential equations yields the explicit formulas for the functions $A(u),B(v),C(u)$, and $D(v)$ in (5.3) and (5.6). Note that the eigenvalues λ_1,λ_2 of the Killing tensor (5.5) determine the *ten orthogonal separable coordinate webs:* $\lambda_i=\mathrm{const}$, $i=1,2$, provided they are not everywhere constant. If one or both of them are everywhere constant, the corresponding eigenvectors have to be also used. The orthogonal separable webs so defined can be employed to solve the associated HJE via additive separation of variables. In summary, the ten *separable cases* (SC) are determined by their respective metrics and Killing tensors:

$$\mathrm{SC1}:\ \begin{cases}\mathrm{d}s^2_{(1)}=\mathrm{d}u^2-\mathrm{d}v^2,\\ \mathbf{K}^{(1)}=\mathrm{diag}(1,0),\end{cases} \tag{5.7}$$

$$\mathrm{SC2}:\ \begin{cases}\mathrm{d}s^2_{(2)}=\mathrm{d}u^2-u^2\mathrm{d}v^2,\\ \mathbf{K}^{(2)}=\mathrm{diag}(0,u^4),\end{cases} \tag{5.8}$$

$$\mathrm{SC3}:\ \begin{cases}\mathrm{d}s^2_{(3)}=(u+v)(\mathrm{d}u^2-\mathrm{d}v^2),\\ \mathbf{K}^{(3)}=(u+v)\mathrm{diag}(v,u),\end{cases} \tag{5.9}$$

$$\mathrm{SC4}:\ \begin{cases}\mathrm{d}s^2_{(4)}=(u^2-v^2)(\mathrm{d}u^2-\mathrm{d}v^2),\\ \mathbf{K}^{(4)}=(u^2-v^2)\mathrm{diag}(v^2,u^2),\end{cases} \tag{5.10}$$

$$\text{SC5:}\quad \begin{cases} ds^2_{(5)} = k^2(\sin u + \sin v)(du^2 - dv^2), \\ \mathbf{K}^{(5)} = k^2(\sin u + \sin v)\,\mathrm{diag}(\sin v, \sin u), \end{cases} \tag{5.11}$$

$$\text{SC6:}\quad \begin{cases} ds^2_{(6)} = (e^u + e^v)(du^2 - dv^2), \\ \mathbf{K}^{(6)} = (e^u + e^v)\,\mathrm{diag}(e^v, e^u), \end{cases} \tag{5.12}$$

$$\text{SC7}\ :\begin{cases} ds^2_{(7)} = (e^u - e^v)(du^2 - dv^2), \\ \mathbf{K}^{(7)} = (e^u - e^v)\,\mathrm{diag}(-e^v, e^u), \end{cases} \tag{5.13}$$

$$\text{SC8:}\quad \begin{cases} ds^2_{(8)} = k^2(\sinh u + \sinh v)(du^2 - dv^2), \\ \mathbf{K}^{(8)} = k^2(\sinh u + \sinh v)\,\mathrm{diag}(\sinh v, \sinh u), \end{cases} \tag{5.14}$$

$$\text{SC9}\ :\begin{cases} ds^2_{(9)} = k^2(\cosh u + \cosh v)(du^2 - dv^2), \\ \mathbf{K}^{(9)} = k^2(\cosh u + \cosh v)\,\mathrm{diag}(\cosh v, \cosh u), \end{cases} \tag{5.15}$$

$$\text{SC10:}\quad \begin{cases} ds^2_{(10)} = k^2(\cosh u - \cosh v)(du^2 - dv^2), \\ \mathbf{K}^{(10)} = k^2(\cosh u - \cosh v)\,\mathrm{diag}(-\cosh v, \cosh u). \end{cases} \tag{5.16}$$

Thus, once the coordinates of separation (u,v) for the Hamiltonian (5.1) and additional first integral (5.4) are available, it is not difficult to determine the type of separation of variables occurring in the associated HJE (4.2). Indeed, one has to simply compare the metric of the Hamiltonian (5.1) and Killing tensor of the additional first integral of motion (5.4) with the list above and select the right SC. Then, the problem is solved. However, it is often the case that a Hamiltonian function is determined initially with respect to the pseudo-Cartesian coordinates, in which case (5.1) takes the form:

$$H(\mathbf{q},\mathbf{p}) = \tfrac{1}{2}(p_1^2 - p_2^2) + V(q^1, q^2). \tag{5.17}$$

Thus, in order to solve the problem of integrability in this case, one needs to answer the following questions.

(1) Is the Hamilton–Jacobi equation of (5.17) orthogonally separable in one or *more* of the above systems of coordinates?
(2) If yes, how does one determine the coordinate transformation(s) to the system(s) of separable coordinates?

The first question can be solved by employing Theorem 4.1, which generalizes the results concerning the geodesic case obtained by Eisenhart[5] (see also Ref. 13). Next, one can make use of the general solution of the Killing tensor equation (2.1) in the coordinates (5.17):

$$K_{ij} = \begin{pmatrix} A + 2\alpha q^2 + \gamma(q^2)^2 & C - \alpha q^1 - \beta q^2 - \gamma q^1 q^2 \\ C - \alpha q^1 - \beta q^2 - \gamma q^1 q^2 & B + 2\beta q^1 + \gamma(q^1)^2 \end{pmatrix}. \tag{5.18}$$

By applying the compatibility condition $d(\hat{\mathbf{K}}dV) = 0$ (see Theorem 4.1) to (5.18) one then obtains all of the admissible Killing tensors defining the first integrals quadratic in momenta. If there is at least one Killing tensor with real and pointwise distinct eigenvalues, the system defined by (4.1) is *orthogonally separable*. The existence of more Killing tensors with the designated properties indicates that the system is *superseparable*.[20,28,51]

Finding the answer to the second problem is much more complex. It is largely due to the fact that the separable coordinates defined by the ten Killing tensors above are defined only up to the action of the isometry group $I(\mathbb{R}^2_1)$, i.e., up to the corresponding *hyperbolic* rotation and/or translations of the Minkowski plane $\mathbb{R}^2_1$. Geometrically, this means that in general (due to the existence of the potential function V in (5.1)) the two systems of coordinates of $\mathbb{R}^2_1$ featured in this

section, namely, (q^1,q^2) and (u,v) are not aligned in $\mathbb{R}^2_1$. It is our main objective therefore to use the (conformal) $I(\mathbb{R}^2_1)$-invariants of the space $\mathbb{R}^2_1$ to develop an effective *algorithmic method* for determining the transformations to separable coordinates for the Hamiltonian system defined by (5.1).

VI. SEPARABLE KILLING TENSORS IN THE CANONICAL PSEUDO-CARTESIAN COORDINATES (t,x)

Consider the geodesic Hamiltonian function defined in $\mathbb{R}^2_1$, which amounts to setting $V(\mathbf{q})=$constant in (5.17):

$$H(t,x,p_t,p_x)=\tfrac{1}{2}(p_t^2-p_x^2), \tag{6.1}$$

where (t,x) are *canonical pseudo-Cartesian coordinates*. Unlike the general case ($V(\mathbf{q})\neq$const) described in the previous section, the corresponding Hamiltonian system is orthogonally separable in all ten of the coordinate systems SC1-10. Moreover, we can choose pseudo-Cartesian coordinates to have a particularly simple relation with the separable web in each of the separable cases SC1-10. We call the pseudo-Cartesian coordinates thus chosen *canonical pseudo-Cartesian coordinates* (t,x). The transformations $(t,x)\to(u,v)$ between the separable coordinates (u,v) defined by each of the separable webs and the canonical pseudo-Cartesian coordinates (t,x) are listed below, together with their corresponding Killing tensors obtained from (5.7) to (5.16) via the tensor transformation laws.

Coordinate transformations:

SC1

$$\begin{aligned} t&=u,\\ x&=v, \end{aligned} \tag{6.2}$$

SC2

$$\begin{aligned} t&=u\cosh v,\\ x&=u\sinh v, \end{aligned} \tag{6.3}$$

SC3

$$\begin{aligned} t&=\tfrac{1}{4}(u+v)^2+\tfrac{1}{2}(u-v),\\ x&=-\tfrac{1}{4}(u+v)^2+\tfrac{1}{2}(u-v), \end{aligned} \tag{6.4}$$

SC4

$$\begin{aligned} t&=\tfrac{1}{2}(u^2+v^2),\\ x&=uv, \end{aligned} \tag{6.5}$$

SC5

$$\begin{aligned} t&=2\sqrt{2}k\cos\left(\frac{u}{2}+\frac{\pi}{4}\right)\cos\left(\frac{v}{2}+\frac{\pi}{4}\right),\\ x&=2\sqrt{2}k\sin\left(\frac{u}{2}+\frac{\pi}{4}\right)\sin\left(\frac{v}{2}+\frac{\pi}{4}\right), \end{aligned} \tag{6.6}$$

SC6

$$t=\sinh(\tfrac{1}{2}(u-v))+2e^{(1/2)(u+v)},$$
$$x=\sinh(\tfrac{1}{2}(u-v))-2e^{(1/2)(u+v)}, \tag{6.7}$$

SC7

$$t=\cosh(\tfrac{1}{2}(u-v))+2e^{(1/2)(u+v)},$$
$$x=\cosh(\tfrac{1}{2}(u-v))-2e^{(1/2)(u+v)}, \tag{6.8}$$

SC8

$$t=k\sqrt{2}(\cosh(\tfrac{1}{2}(u+v))+\sinh(\tfrac{1}{2}(u-v))),$$
$$x=k\sqrt{2}(\cosh(\tfrac{1}{2}(u+v))-\sinh(\tfrac{1}{2}(u-v))), \tag{6.9}$$

SC9

$$t=2k\sqrt{2}\sinh\frac{u}{2}\cosh\frac{v}{2},$$
$$x=2k\sqrt{2}\cosh\frac{u}{2}\sinh\frac{v}{2}, \tag{6.10}$$

SC10

$$t=2k\sqrt{2}\cosh\frac{u}{2}\cosh\frac{v}{2}$$
$$x=2k\sqrt{2}\sinh\frac{u}{2}\sinh\frac{v}{2}. \tag{6.11}$$

Separable Killing tensors in canonical pseudo-Cartesian coordinates:
SC1

$$\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \tag{6.12}$$

SC2

$$\begin{pmatrix}x^2 & -tx\\ -tx & t^2\end{pmatrix}, \tag{6.13}$$

SC3

$$\begin{pmatrix}\frac{1}{4}-x & -\frac{1}{4}+\frac{1}{2}t-\frac{1}{2}x\\ -\frac{1}{4}+\frac{1}{2}t-\frac{1}{2}x & \frac{1}{4}+t\end{pmatrix}, \tag{6.14}$$

SC4

$$\begin{pmatrix} 0 & -x \\ -x & 2t \end{pmatrix}, \tag{6.15}$$

SC5

$$\begin{pmatrix} k^2-\frac{1}{4}x^2 & \frac{1}{4}tx \\ \frac{1}{4}tx & k^2-\frac{1}{4}t^2 \end{pmatrix}, \tag{6.16}$$

SC6

$$\begin{pmatrix} \frac{1}{4}x^2 & -\frac{1}{4}-\frac{1}{4}tx \\ -\frac{1}{4}-\frac{1}{4}tx & \frac{1}{4}+\frac{1}{4}t^2 \end{pmatrix}, \tag{6.17}$$

SC7

$$\begin{pmatrix} -\frac{1}{4}+\frac{1}{4}x^2 & \frac{1}{4}-\frac{1}{4}tx \\ \frac{1}{4}-\frac{1}{4}tx & -\frac{1}{4}+\frac{1}{4}t^2 \end{pmatrix}, \tag{6.18}$$

SC8

$$\begin{pmatrix} \frac{1}{4}x^2 & k^2-\frac{1}{4}tx \\ k^2-\frac{1}{4}tx & \frac{1}{4}t^2 \end{pmatrix}, \tag{6.19}$$

SC9

$$\begin{pmatrix} k^2+\frac{1}{4}x^2 & -\frac{1}{4}tx \\ -\frac{1}{4}tx & k^2+\frac{1}{4}t^2 \end{pmatrix}, \tag{6.20}$$

SC10

$$\begin{pmatrix} -k^2+\frac{1}{4}x^2 & -\frac{1}{4}tx \\ -\frac{1}{4}tx & -k^2+\frac{1}{4}t^2 \end{pmatrix}. \tag{6.21}$$

Remark 6.1: Note that the Killing tensors (6.12)–(6.21) in the coordinates (t,x) are symmetrized sums of (tensor) products of the Killing vectors (3.2). In addition, we observe that the formulas (6.12)–(6.21) are compatible with the general form (5.18).

Figures 1–10 illustrate the ten separable webs defined by the eigenvectors of the respective Killing tensors (6.12)–(6.21) in terms of the corresponding canonical pseudo-Cartesian coordinates (6.2)–(6.11) (see also Refs. 14, 15).

Remark 6.2: We can use the separable Killing tensors in the (t,x) coordinates to solve the problem of classification in terms of the $I(\mathbb{R}^2_1)$-invariants of $\mathcal{K}^2(\mathbb{R}^2_1)$. However, to solve the problem of finding (point) transformations from the noncanonical pseudo-Cartesian coordinates (q^1,q^2) of (5.17) to orthogonally separable coordinates (u,v) a more delicate analysis, which takes into account all the metric-preserving and signature-reversing transformations of $\mathbb{R}^2_1$ including the actions induced by the isometry group $I(\mathbb{R}^2_1)$, has to be undertaken.

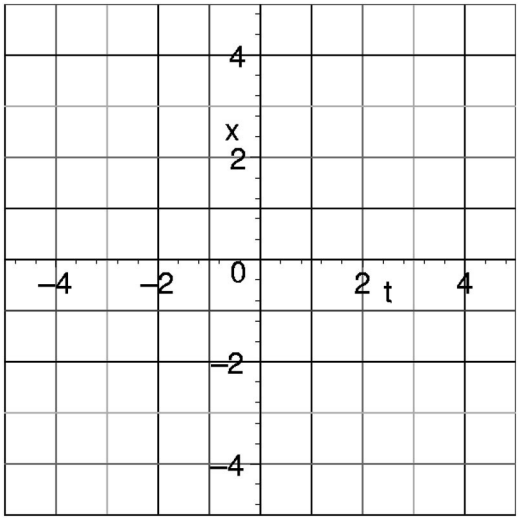

FIG. 1. Separable case 1.

VII. RIGID MOTIONS

As explained in the previous section the canonical pseudo-Cartesian coordinates (t,x) have been chosen to have a simple relation with the separable webs in each of the cases SC1–SC10. These choices are reflected in the coordinate transformations $(t,x)\rightarrow(u,v)$ defined by (6.2)–(6.11). It must be noted that even though the original coordinates (q^1,q^2) are also pseudo-Cartesian, they are equivalent to the coordinates (t,x) only modulo transformations which preserve the Lorentzian metric **g** of the Hamiltonian (4.1) or reverse its signature. The set of such transformations forms a group L (under composition) generated by elements of the discrete group $R=\langle R_1,R_2\rangle$, where

$$R_1:\ \overline{t}=t,\ \overline{x}=-x \quad (\text{spatial reflection } x\leftrightarrow -x),$$

$$R_2:\ \overline{t}=x,\ \overline{x}=t \quad (\text{permutation } t\leftrightarrow x),$$

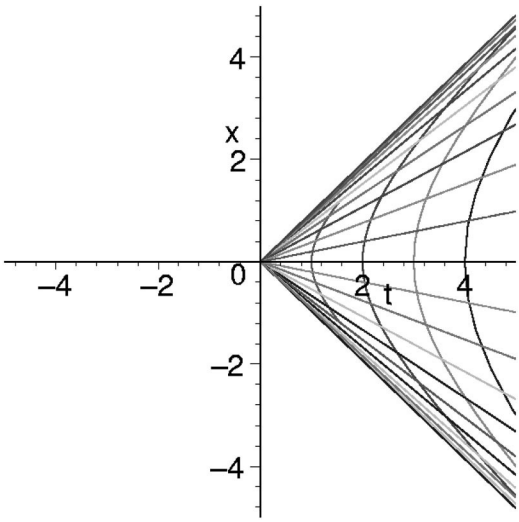

FIG. 2. Separable case 2.

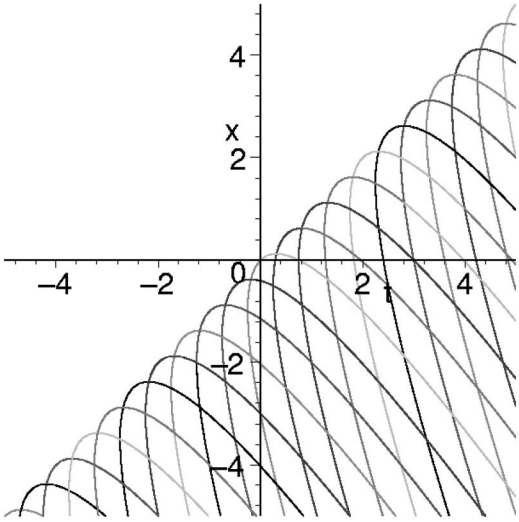

FIG. 3. Separable case 3.

and the continuous group $I(\mathbb{R}_1^2)$. Note that R consists of eight discrete transformations. Recall that the set of isometries $I(\mathbb{R}_1^2)$ constitutes a Lie group that consists of all translations $t_{\mathbf{a}}$ of $\mathbb{R}_1^2$ [which is an abelian subgroup of $I(\mathbb{R}_1^2)$ isomorphic under vector addition to $\mathbb{R}^2$] and the set of linear isometries $\mathrm{O}_1(2)$ [the latter being a closed subgroup of $GL_2(\mathbb{R})$] $I(\mathbb{R}_1^2)$ is commonly known as the *Poincaré group* or *inhomogeneous Lorentz group*. Note that the element of $\mathrm{O}_1(2)$ defined by the semiorthogonal matrix

$$\begin{pmatrix} \cosh\phi & \sinh\phi \\ \sinh\phi & \cosh\phi \end{pmatrix}$$

for the corresponding $\phi \in \mathbb{R}$ is called a *hyperbolic rotation* in $\mathbb{R}_1^2$ through an (oriented) Lorentz angle ϕ. $\mathrm{O}_1(2)$ is not compact [unlike O(2)] and has four components. The canonical pseudo-Cartesian coordinates (t,x) can be related to the given pseudo-Cartesian coordinates (q^1,q^2) through the following parametrization of the group L:

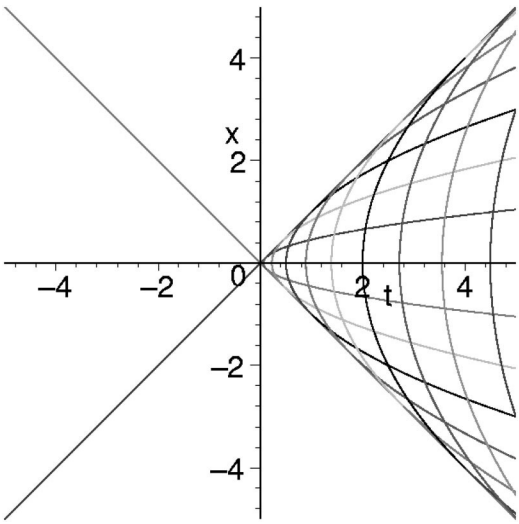

FIG. 4. Separable case 4.

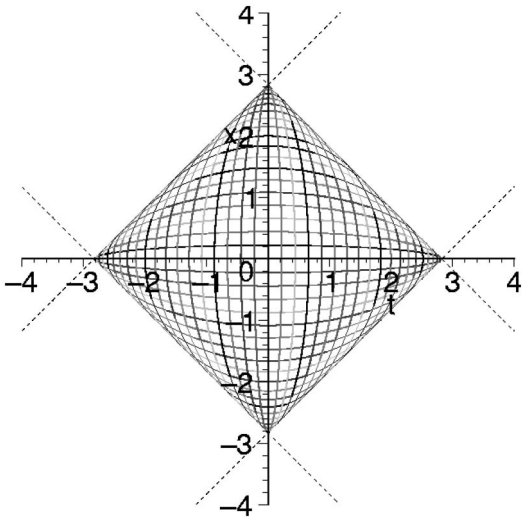

FIG. 5. Separable case 5.

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = t_{\mathbf{a}} \circ \rho_\phi \circ r \begin{pmatrix} t \\ x \end{pmatrix} = \begin{pmatrix} \cosh\phi & \sinh\phi \\ \sinh\phi & \cosh\phi \end{pmatrix} \left[r \begin{pmatrix} t \\ x \end{pmatrix} \right] + \begin{pmatrix} a \\ b \end{pmatrix}, \tag{7.1}$$

where $r \in R$. Hence, once the problem of classifying the separable cases has been accomplished, we can effect the transformation from the given coordinates (q^1,q^2) to the separable coordinates (u,v) according to

$$(q^1,q^2) = t_{\mathbf{a}} \circ \rho_\phi \circ r \circ T_{(i)}(u,v), \tag{7.2}$$

where $T_{(i)}$ is the appropriate standard coordinate transformation [listed in (6.2)–(6.11)] corresponding to the separable case.

Recall that the components of any Killing tensor in Minkowski space have a similar form (2.9) with respect to any system of pseudo-Cartesian coordinates. Following the approach developed in Ref. 20, we note that transformations (7.1) from the (q^1,q^2) pseudo-Cartesian coordinates

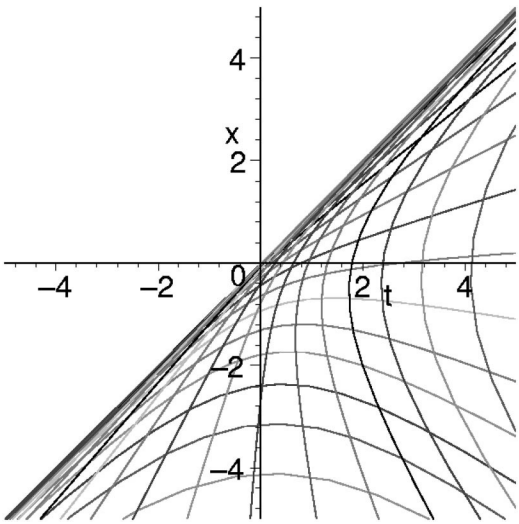

FIG. 6. Separable case 6.

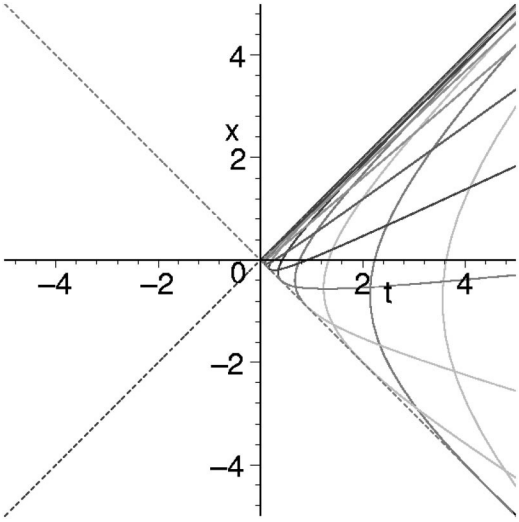

FIG. 7. Separable case 7.

to the (t,x) pseudo-Cartesian coordinates induces (under the tensor transformation laws) a transformation on the parameters A,B,C,α,β and γ of (2.9). In the following, the barred parameters define the components of the Killing tensor of (4.5) in the coordinates (q^1,q^2).

The discrete transformations R_1 and R_2 induce the following transformations:

$$R_1:\ \overline{A}=A,\ \overline{B}=B,\ \overline{C}=-C,\ \overline{\alpha}=-\alpha,\ \overline{\beta}=\beta,\ \overline{\gamma}=\gamma, \tag{7.3}$$

$$R_2:\ \overline{A}=B,\ \overline{B}=A,\ \overline{C}=C,\ \overline{\alpha}=\beta,\ \overline{\beta}=\alpha,\ \overline{\gamma}=\gamma. \tag{7.4}$$

Every continuous transformation of the Lie group $I(\mathbb{R}_1^2)$ can be parametrized according to [see (3.4)]

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = t_{\mathbf{a}} \circ \rho_\phi \begin{pmatrix} t \\ x \end{pmatrix} = \begin{pmatrix} \cosh\phi & \sinh\phi \\ \sinh\phi & \cosh\phi \end{pmatrix} \begin{pmatrix} t \\ x \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix}, \tag{7.5}$$

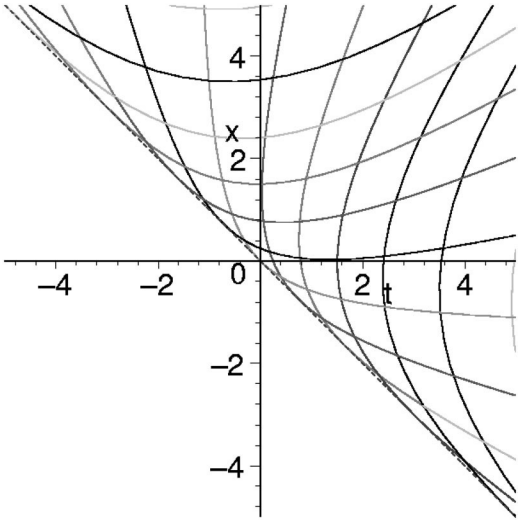

FIG. 8. Separable case 8.

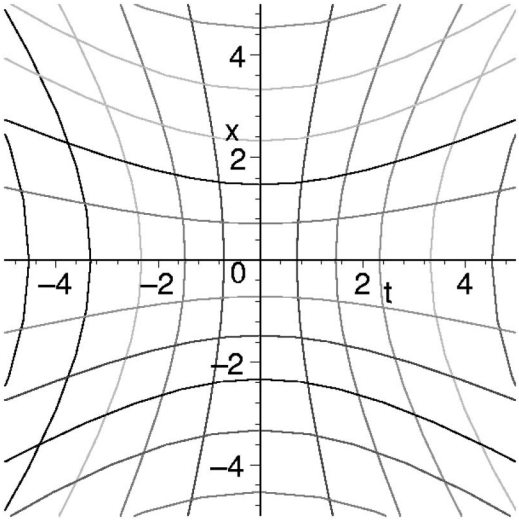

FIG. 9. Separable case 9.

and induces the following transformations on the parameters:

$$\overline{A}=A\cosh^2\phi-2C\cosh\phi\sinh\phi+B\sinh^2\phi+\gamma b^2-2(\alpha\cosh\phi+\beta\sinh\phi)b,$$

$$\overline{B}=A\sinh^2\phi-2C\cosh\phi\sinh\phi+B\cosh^2\phi+\gamma a^2-2(\beta\cosh\phi+\alpha\sinh\phi)a,$$

$$\begin{aligned}\overline{C}=&C(\cosh^2\phi+\sinh^2\phi)-(A+B)\cosh\phi\sinh\phi,\\&+(a\alpha+b\beta)\cosh\phi+(a\beta+b\alpha)\sinh\phi-\gamma ab,\end{aligned}\tag{7.6}$$

$$\overline{\alpha}=\alpha\cosh\phi+\beta\sinh\phi-\gamma b,$$

$$\overline{\beta}=\alpha\sinh\phi+\beta\cosh\phi-\gamma a,$$

$$\overline{\gamma}=\gamma.$$

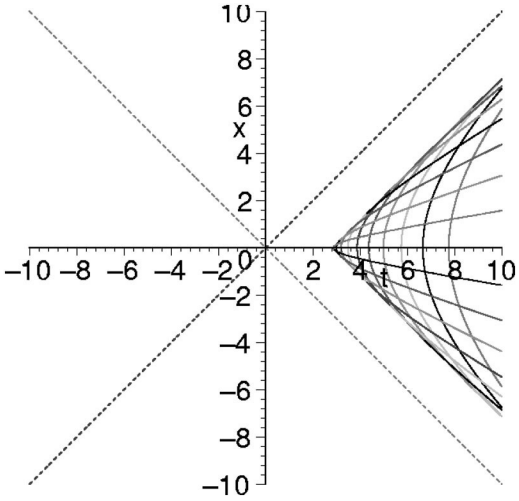

FIG. 10. Separable case 10.

TABLE II. Relevant reflections for the separable cases of Minkowski space.

SC	Type I	Type II	Reflections possibly needed
SC1	R_1, R_2	R_1	none
SC2	R_1	R_1, R_2	none
SC3	none	$(R_1 \circ R_2)^2$	$R_1, R_2, R_1 \circ R_2$
SC4	R_1	R_1	R_2
SC5	R_1	R_1, R_2	none
SC6	none	R_2	R_1
SC7	none	R_2	R_1
SC8	none	R_2	R_1
SC9	R_1, R_2	R_1, R_2	none
SC10	R_1	R_1, R_2	none

Note that for a given separable case, the transformation (7.2) to the separable coordinates need not be unique. In fact, the presence of the discrete group $R = \langle R_1, R_2 \rangle$ of transformations allows for certain redundancies to occur. We formalize these ideas below.

Definition 7.1: $(U,V) = \psi(u,v)$ *is a trivial separable transformation if either:*

(1) $\psi(u,v) = (\psi_1(u), \psi_2(v))$, *or*
(2) $\psi(u,v) = (\psi_1(v), \psi_2(u))$

where $\psi_1, \psi_2 : \mathbb{R} \to \mathbb{R}$ *are invertible maps.*

Remark 7.1: Note that (u,v) are separable coordinates for the Hamilton–Jacobi equation iff (U,V) are.

Definition 7.2: Let $r \in R$ *and* $T_{(n)}$ *be one of the standard coordinate transformations associated with* $SC[n]$ (*i.e.*, $(t,x) = T_{(n)}(u,v)$). *We say that*

(a) r *is a type I trivial reflection if* $r \circ T_{(n)}(u,v) = T_{(n)}(\psi(u,v))$, *where* $\psi(u,v)$ *is a trivial separable transformation.*
(b) r *is a type II trivial reflection if* r *induces a tensor transformation law which leaves invariant the components of the canonical separable Killing tensor associated with* $SC[n]$.

We define r *to be a trivial reflection with respect to* $SC[n]$ *if it is either a type I or type II trivial reflection.*

Type I trivial reflections are redundant in the classification because they can be realized as a composition of the standard coordinate transformation and a trivial separable transformation on (u,v)-space. Trivial reflections of type II are redundant because the components of the separable Killing tensor with respect to given (q^1, q^2) coordinates (i.e., the coordinate system in which we perform the classification) are the same for both (7.1) and (7.5).

To motivate these definitions, we consider the following examples:

Example 7.1: Suppose that we have a Hamiltonian H which admits a separation of variables of SC5 type and the transformation to separable coordinates (u,v) is given by

$$(q^1, q^2) = t_{\mathbf{a}} \circ \rho_\phi (t,x), \tag{7.7}$$

$$(t,x) = T_{(5)}(u,v) \tag{7.8}$$

for some $\mathbf{a}$ and ϕ. Consider the trivial separable transformation $(u,v) = (-U - \pi/2, V)$. Then $R_1 \circ T_{(5)}(U,V) = T_{(5)}(\psi(U,V))$. Thus, R_1 is a type I trivial reflection with respect to SC5.

Example 7.2: Consider SC9. The parameters appearing in the components (6.20) of the corresponding separable Killing tensor with respect to (t,x) coordinates are $A = B = k^2$, $C = \alpha = \beta = 0$, $\gamma = \frac{1}{4}$. These values are invariant under the transformation laws (7.3), (7.4) induced by R_1, R_2. Thus, R_1 and R_2 are type II trivial reflections with respect to SC9.

Examining each separable case, we generate the following list of trivial reflections (see Table II), and hence narrow down the list of discrete transformations which potentially play an role in

TABLE III. Group invariant classification scheme of the ten separable cases of the Minkowski space $\mathbb{R}_1^2$.

Separable case	SC1	SC2	SC3	SC4	SC5
γ	0	$\neq 0$	0	0	$\neq 0$
$\{I_+, I_-\}$	$\{0\}$	$\{0\}$	$\{0,-1\}$	$\{-1\}$	$\{-1\}$
Separable case	SC6	SC7	SC8	SC9	SC10
γ	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$\{I_+, I_-\}$	$\{0,+1\}$	$\{0,-1\}$	$\{-1,+1\}$	$\{+1\}$	$\{-1\}$

the classification to be developed. In effect, we concentrate on developing a classification *up to trivial reflection*.

Note that in SC3, there are no type I trivial reflections, and $(R_1 \circ R_2)^2$ is the only type II trivial reflection. It can be shown that the identity transformation, R_1, R_2, and $(R_1 \circ R_2)^2$ induce different transformations of the components of the separable Killing tensor of SC3. Moreover, every element of R induces a transformation on the components of the SC3 separable Killing tensor which coincides with one of these four transformations.

The strategy for classifying the separable cases in the Minkowski plane is an extension of the ideas presented in Ref. 20. More specifically, we derive invariants under the action of $I(\mathbb{R}_1^2)$ and $R = \langle R_1, R_2 \rangle$ which can be used to distinguish the Killing tensors (6.12)–(6.20). These invariants will lead to an efficient algorithm for constructing the transformation to separable coordinates.

VIII. CLASSIFICATION IN TERMS OF THE ISOMETRY AND REFLECTION GROUPS

Having considered invariants under the action of continuous transformations, we now consider the effect of the discrete transformations on each of the $I(\mathbb{R}_1^2)$-invariants I_+, I_-, γ. Using the transformation laws (7.3) and (7.4), we get

$$R_1: \ \overline{I}_+ = I_-, \ \ \overline{I}_- = I_+, \ \ \overline{\gamma} = \gamma, \tag{8.1}$$

$$R_2: \ \overline{I}_+ = I_+, \ \ \overline{I}_- = I_-, \ \ \overline{\gamma} = \gamma. \tag{8.2}$$

Hence, we can say that the *unordered* list $\{I_+, I_-\}$ is invariant under hyperbolic rotations, translations, and the reflections R_1, R_2.

We now use the three $I(\mathbb{R}_1^2)$-invariants γ, I_+ and I_-, to classify the ten separable cases of the Minkowski space $\mathbb{R}_1^2$. Evaluating these invariants on each of the Killing tensors listed in (6.12)–(6.21) (i.e., representatives of each separable case SC1–SC10), we arrive at the following classification scheme for the separable cases of Minkowski space $\mathbb{R}_1^2$. We summarize these results in Table III.

Remark 8.1: If $\gamma = 0$, $I_\pm = 0$ or -1, whereas if $\gamma \neq 0$, $I_\pm = -1, 0$, or $+1$. Hence, there are nine combinations of γ and $\{I_+, I_-\}$. Note that SC5 and SC10 are characterized by the same values of the group invariants γ, I_-, and I_+. This agrees with the geometrical properties of the corresponding metrics, namely, they give rise to two *distinct* coordinate systems that cover two disjoint areas of the same space (for more details, see Refs. 27, 14, 15).

IX. EQUIVALENT CLASSIFICATIONS

We note that the above *group invariant* scheme allows the classification of the separable cases SC1–SC10 modulo a hyperbolic rotation and translation of the space $\mathbb{R}_1^2$ and as such can be compared with the classification derived by Kalnins[14] for the Laplace equation defined in $\mathbb{R}_1^2$ and

$\mathbb{R}_1^3$. An excellent exposition of these results based on the generators of the Lie symmetry algebra of the Klein–Gordon equation can be found in Ref. 27. Indeed, recall that the product separation of variables in the Helmholtz equation

$$\Delta\psi + K^2\psi = 0 \tag{9.1}$$

is equivalent to orthogonal separation of variables in the corresponding geodesic Hamiltonian.[54,55] In this setting the Laplacian Δ is a Casimir operator of the corresponding group of isometries, which clearly corresponds to the metric of the Hamiltonian (4.1). Thus, the Laplacian acting in the Minkowski space $\mathbb{R}_1^2$ takes the form

$$\Delta = \frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2}.$$

In order to classify the separable systems in this case, Kalnins[14] considered the generators of the Lie algebra $i(\mathbb{R}_1^2)$ (in our notations) **T**, **X**, and **H** to construct inequivalent quadratic operators corresponding to the ten separable cases. In our language these operators are the ten separable Killing tensors exhibited in Sec. VI, viewed, according to SPI, as sums of symmetrized products of **T**, **X**, and **H**.

A different approach to this problem for the geodesic equations in $\mathbb{R}_1^2$ has been developed by Rastelli,[15] who considered it from the point of view of singular points of the orthogonal separable coordinates (which are naturally equivalent to the singular points of the eigenvalues of the separable Killing tensors) and both classified the ten separable cases and found the coordinate transformations to the separable coordinates from the given ones.

The method of classification presented in the previous section is equivalent to the classifications described above.

X. TRANSFORMATION FORMULAS TO SEPARABLE COORDINATES

The $I(\mathbb{R}_1^2)$-invariants γ, I_+ and I_- of a Killing tensor $\mathbf{K}\in\mathcal{K}^2(\mathbb{R}_1^2)$ indicate, according to Table III, which SC it corresponds to. Although being exhaustive, this classification does not tell us where the corresponding separable web is located in $\mathbb{R}_1^2$ with respect to the origin or its orientation with respect to the given coordinate axes. Therefore a more delicate analysis is necessary to formalize the procedure. In this section we analyze each separable case and find the corresponding Lorentz angle ϕ along with the parameters of translation a and b [see (7.2)].

Let **K** be a particular solution of the Killing tensor equation (2.1) and the compatibility condition $d(\hat{\mathbf{K}}dV)=0$. We assume that this particular solution is a nonmetric solution, i.e., **K** is linearly independent of **g**. If multiples of the metric are the only Killing tensors compatible with the potential V, then the Hamiltonian is not separable. Recall from (5.6) that **K** satisfies the tensorial equation $\mathbf{K}=\ell\mathbf{g}+m\mathbf{K}^{(\mathbf{L})}$, where $\mathbf{K}^{(\mathbf{L})}$ is one of the separable Killing tensors. In components,

$$K_{ij} = \ell g_{ij} + m\overline{K}_{ij}^{(L)}, \quad \ell, m \in \mathbb{R}. \tag{10.1}$$

Note that if (10.1) is written with respect to the pseudo-Cartesian coordinates (t,x), then the right-hand side of the equation is determined according to the ten cases listed in Sec. VI. (There are in fact only nine cases since $\mathbf{K}^{(5)}$ and $\mathbf{K}^{(10)}$ are linearly dependent.) The difficulty here is that the left-hand side is not determined since the relation between (t,x) coordinates and given (q^1,q^2) is not known *a priori*. It is known that they are related by a proper or improper rigid motion (7.1). To determine the parameters a,b,ϕ,k,r appearing in (7.1) in terms of the known information (i.e., $A,B,C,\alpha,\beta,\gamma$) appearing in the components of **K** written with respect to (q^1,q^2), we adopt the following approach:

(1) Use the group invariant classification (Table III) to determine which separable Killing tensor $\mathbf{K}^{(\mathbf{L})}$ appears in Eq. (10.1).

(2) Starting with the (t,x) components of the appropriate $\mathbf{K}^{(\mathbf{L})}$ [see (6.12)–(6.21)], use the tensor transformation laws associated with (7.1) to write (10.1) with respect to (q^1,q^2). Here, a,b,ϕ,k,r appearing in (7.1) are the parameters to be determined.
(3) Solve (10.1), expressing a,b,ϕ,k in terms of $A,B,C,\alpha,\beta,\gamma$ and determining which $r\in R$ must be used.

In carrying out step (2) of the above approach, we permit only the relevant reflections listed in Table II to complete the classification of each separable case. The components of the separable Killing tensors with respect to (q^1,q^2) coordinates are given below.

SC1: No reflections used,

$$\overline{K}^{(1)}=\begin{pmatrix}\cosh^2\phi & -\cosh\phi\sinh\phi\\ -\cosh\phi\sinh\phi & \sinh^2\phi\end{pmatrix}. \tag{10.2}$$

SC2: No reflections used,

$$\overline{K}^{(2)}=\begin{pmatrix}(q^2-b)^2 & -(q^1-a)(q^2-b)\\ -(q^1-a)(q^2-b) & (q^1-a)^2\end{pmatrix}. \tag{10.3}$$

SC3.11: No reflections used,

$$\overline{K}^{(3)}=\begin{pmatrix}\frac{1}{4}e^{2\phi}-e^{-\phi}(q^2-b) & -\frac{1}{4}e^{2\phi}+\frac{1}{2}e^{-\phi}(b-a+q^1-q^2)\\ -\frac{1}{4}e^{2\phi}+\frac{1}{2}e^{-\phi}(b-a+q^1-q^2) & \frac{1}{4}e^{2\phi}+e^{-\phi}(q^1-a)\end{pmatrix}. \tag{10.4}$$

SC3.12: Reflection R_2 used,

$$\overline{K}^{(3)}=\begin{pmatrix}\frac{1}{4}e^{2\phi}+e^{-\phi}(q^2-b) & -\frac{1}{4}e^{2\phi}-\frac{1}{2}e^{-\phi}(b-a+q^1-q^2)\\ -\frac{1}{4}e^{2\phi}-\frac{1}{2}e^{-\phi}(b-a+q^1-q^2) & \frac{1}{4}e^{2\phi}-e^{-\phi}(q^1-a)\end{pmatrix}. \tag{10.5}$$

SC3.21: Reflection R_1 used,

$$\overline{K}^{(3)}=\begin{pmatrix}\frac{1}{4}e^{-2\phi}+e^{\phi}(q^2-b) & \frac{1}{4}e^{-2\phi}+\frac{1}{2}e^{\phi}(a+b-q^1-q^2)\\ \frac{1}{4}e^{-2\phi}+\frac{1}{2}e^{\phi}(a+b-q^1-q^2) & \frac{1}{4}e^{-2\phi}+e^{\phi}(q^1-a)\end{pmatrix}. \tag{10.6}$$

SC3.22: Reflection $R_1\circ R_2$ used,

$$\overline{K}^{(3)}=\begin{pmatrix}\frac{1}{4}e^{-2\phi}-e^{\phi}(q^2-b) & \frac{1}{4}e^{-2\phi}-\frac{1}{2}e^{\phi}(a+b-q^1-q^2)\\ \frac{1}{4}e^{-2\phi}-\frac{1}{2}e^{\phi}(a+b-q^1-q^2) & \frac{1}{4}e^{-2\phi}-e^{\phi}(q^1-a)\end{pmatrix}. \tag{10.7}$$

SC4.1: No reflections used,

$$\overline{K}^{(4)}=\begin{pmatrix}2\sinh\phi(q^2-b) & (a-q^1)\sinh\phi+(b-q^2)\cosh\phi\\ (a-q^1)\sinh\phi+(b-q^2)\cosh\phi & 2\cosh\phi(q^1-a)\end{pmatrix}. \tag{10.8}$$

SC4.2: Reflection R_2 used,

$$\overline{K}^{(4)}=\begin{pmatrix}2\cosh\phi(q^2-b) & (a-q^1)\cosh\phi+(b-q^2)\sinh\phi\\ (a-q^1)\cosh\phi+(b-q^2)\sinh\phi & 2\sinh\phi(q^1-a)\end{pmatrix}. \tag{10.9}$$

SC5: No reflections used,

$$\overline{K}^{(5)}=\begin{pmatrix} k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^2-b)^2 & -2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^1-a)(q^2-b) \\ -2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^1-a)(q^2-b) & k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^1-a)^2 \end{pmatrix}. \tag{10.10}$$

SC6.1: No reflections used,

$$\overline{K}^{(6)}=\begin{pmatrix} \frac{1}{4}(e^{2\phi}+(q^2-b)^2) & -\frac{1}{4}(e^{2\phi}+(q^1-a)(q^2-b)) \\ -\frac{1}{4}(e^{2\phi}+(q^1-a)(q^2-b)) & \frac{1}{4}(e^{2\phi}+(q^1-a)^2) \end{pmatrix}. \tag{10.11}$$

SC6.2: Reflection R_1 used,

$$\overline{K}^{(6)}=\begin{pmatrix} \frac{1}{4}(e^{-2\phi}+(q^2-b)^2) & \frac{1}{4}(e^{-2\phi}-(q^1-a)(q^2-b)) \\ \frac{1}{4}(e^{-2\phi}-(q^1-a)(q^2-b)) & \frac{1}{4}(e^{-2\phi}+(q^1-a)^2) \end{pmatrix}. \tag{10.12}$$

SC7.1: No reflections used,

$$\overline{K}^{(7)}=\begin{pmatrix} \frac{1}{4}((q^2-b)^2-e^{2\phi}) & \frac{1}{4}(e^{2\phi}-(q^1-a)(q^2-b)) \\ \frac{1}{4}(e^{2\phi}-(q^1-a)(q^2-b)) & \frac{1}{4}((q^1-a)^2-e^{2\phi}) \end{pmatrix}. \tag{10.13}$$

SC7.2: Reflection R_1 used,

$$\overline{K}^{(7)}=\begin{pmatrix} \frac{1}{4}((q^2-b)^2-e^{-2\phi}) & -\frac{1}{4}(e^{-2\phi}+(q^1-a)(q^2-b)) \\ -\frac{1}{4}(e^{-2\phi}+(q^1-a)(q^2-b)) & \frac{1}{4}((q^1-a)^2-e^{-2\phi}) \end{pmatrix}. \tag{10.14}$$

SC8.1: No reflections used,

$$\overline{K}^{(8)}=\begin{pmatrix} -2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^2-b)^2 & k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^1-a)(q^2-b) \\ k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^1-a)(q^2-b) & -2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^1-a)^2 \end{pmatrix}. \tag{10.15}$$

SC8.2: Reflection R_1 used,

$$\overline{K}^{(8)}=\begin{pmatrix} 2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^2-b)^2 & -k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^1-a)(q^2-b) \\ -k^2(\cosh^2\phi+\sinh^2\phi)-\frac{1}{4}(q^1-a)(q^2-b) & 2k^2\cosh\phi\sinh\phi+\frac{1}{4}(q^1-a)^2 \end{pmatrix}. \tag{10.16}$$

SC9: No reflections used,

$$\overline{K}^{(9)}=\begin{pmatrix} k^2(\cosh^2\phi+\sinh^2\phi)+\frac{1}{4}(q^2-b)^2 & -2k^2\cosh\phi\sinh\phi-\frac{1}{4}(q^1-a)(q^2-b) \\ -2k^2\cosh\phi\sinh\phi-\frac{1}{4}(q^1-a)(q^2-b) & k^2(\cosh^2\phi+\sinh^2\phi)+\frac{1}{4}(q^1-a)^2 \end{pmatrix}. \tag{10.17}$$

SC10: No reflections used,

$$\overline{K}^{(10)}=\begin{pmatrix} -k^2(\cosh^2\phi+\sinh^2\phi)+\frac{1}{4}(q^2-b)^2 & 2k^2\cosh\phi\sinh\phi-\frac{1}{4}(q^1-a)(q^2-b) \\ 2k^2\cosh\phi\sinh\phi-\frac{1}{4}(q^1-a)(q^2-b) & -k^2(\cosh^2\phi+\sinh^2\phi)+\frac{1}{4}(q^1-a)^2 \end{pmatrix}. \tag{10.18}$$

TABLE IV. Invariant classification of subcases.

Separable case	γ	$\{I_+, I_-\}$	Subcase	Invariant classification
SC3	0	$\{0,-1\}$	SC3.11: No reflections.	$\mu_-<0$
			SC3.12: R_2 used.	$\mu_->0$
			SC3.21: R_1 used.	$\mu_+>0$
			SC3.22: $R_1\circ R_2$ used.	$\mu_+<0$
SC4	0	$\{-1\}$	SC4.1: No reflections.	$\alpha^2-\beta^2<0$
			SC4.2: R_2 used.	$\alpha^2-\beta^2>0$
SC6	$\neq 0$	$\{0,+1\}$	SC6.1: No reflections.	$I_+=0$, $I_-=+1$
			SC6.2: R_1 used.	$I_+=+1$, $I_-=0$
SC7	$\neq 0$	$\{0,-1\}$	SC7.1: No reflections.	$I_+=0$, $I_-=-1$
			SC7.2: R_1 used.	$I_+=-1$, $I_-=0$
SC8	$\neq 0$	$\{-1,+1\}$	SC8.1: No reflections.	$I_+=+1$, $I_-=-1$
			SC8.2: R_1 used.	$I_+=-1$, $I_-=+1$

Now take any Killing tensor **K** with pointwise real and simple eigenvalues. With respect to given coordinates (q^1,q^2), it must have components of the form (2.9), and must satisfy Eq. (10.1), where $\overline{K}_{ij}^{(L)}$ has components according to one of the separable cases listed in (10.2)–(10.18). To identify which of these components must be used, we use the invariant classification provided in Table III. However, we refine this classification to distinguish subcases where reflections are required. According to Table II, we have to consider reflections for the separable cases SC3, SC4, SC6, SC7, and SC8. For these cases, we can use derived conformal invariants (which *are* sensitive to certain reflections) to provide a classification of these subcases. We present the invariant classification of subcases in Table IV.

By using the invariant classification of the separable cases listed in Tables III and IV, and Eq. (10.1), we can account for the action of the Lie group $I(\mathbb{R}_1^2)$ and find expressions for the parameters a, b, ϕ and k in terms of the given A, B, C, α, β, and γ. Thus, we have (see also Sec. IV in Ref. 20) the transformation to separable coordinates (u,v):

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = (t_{\mathbf{a}}\circ\rho_{\phi}\circ r\circ T_{(i)})\begin{pmatrix} u \\ v \end{pmatrix}, \tag{10.19}$$

where r is an element of the discrete group of reflections $R=\langle R1,R2\rangle$. Letting $\tilde{T}_{(i)}=r\circ T_{(i)}$ we get

$$\begin{cases} q^1 = t\cosh\phi + x\sinh\phi + a \\ q^1 = t\sinh\phi + x\cosh\phi + b, \end{cases} \quad \begin{pmatrix} t \\ x \end{pmatrix} = \tilde{T}_{(i)}\begin{pmatrix} u \\ v \end{pmatrix}. \tag{10.20}$$

The values of the parameters a,b,ϕ,k and the transformation $\tilde{T}_{(i)}$ are given below for each separable case.

SC1: $\gamma=0, I_\pm=0$ [Note, in this case, real and distinct eigenvalues occur iff $(A+B)^2-4C^2>0$].

$$a,b \text{ arbitrary}, \quad \sinh(2\phi)=\begin{cases} \dfrac{-2C}{\sqrt{(A+B)^2-4C^2}}, & \text{if } A+B>0, \\ \dfrac{2C}{\sqrt{(A+B)^2-4C^2}}, & \text{if } A+B<0. \end{cases} \tag{10.21}$$

$$\tilde{T}_{(1)}: \begin{cases} t=u, \\ x=v. \end{cases} \tag{10.22}$$

SC2: $\gamma\neq 0, I_\pm=0$

$$a=\frac{-\beta}{\gamma},\quad b=\frac{-\alpha}{\gamma},\quad \phi \text{ arbitrary.} \tag{10.23}$$

$$\tilde{T}_{(2)}:\begin{cases} t=u\cosh(v),\\ x=u\sinh(v). \end{cases} \tag{10.24}$$

SC3: $\gamma=0,\{I_+,I_-\}=\{-1,0\}$

Define $\mu_\pm=(A+B\pm 2C)/\alpha$.

Subcase 3.1: If $I_+=-1, I_-=0$, then

$$a-b=\frac{A+B+2C}{4\alpha}\quad \text{(one parameter family)}, \tag{10.25}$$

$$e^{3\phi}=\left|\frac{A+B-2C}{2\alpha}\right|, \tag{10.26}$$

$\mu_-<0$	$\mu_->0$
$\tilde{T}_{(3.11)}:\begin{cases} t=\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v)\\ x=-\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v)\end{cases}$	$\tilde{T}_{(3.12)}:\begin{cases} t=-\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v).\\ x=\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v)\end{cases}$

Subcase 3.2: If $I_+=0, I_-=-1$, then

$$a+b=\frac{2C-A-B}{4\alpha}\quad \text{(one parameter family)}, \tag{10.27}$$

$$e^{3\phi}=\left|\frac{2\alpha}{A+B+2C}\right|, \tag{10.28}$$

$\mu_+>0$	$\mu_+<0$
$\tilde{T}_{(3.21)}:\begin{cases} t=\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v)\\ x=\frac{1}{4}(u+v)^2-\frac{1}{2}(u-v)\end{cases}$	$\tilde{T}_{(3.22)}:\begin{cases} t=-\frac{1}{4}(u+v)^2-\frac{1}{2}(u-v).\\ x=-\frac{1}{4}(u+v)^2+\frac{1}{2}(u-v)\end{cases}$

SC4: $\gamma=0, I_\pm=-1$

$$a=\frac{\beta(A+B)+2\alpha C}{2(\alpha^2-\beta^2)},\quad b=\frac{\alpha(A+B)+2\beta C}{2(\beta^2-\alpha^2)}. \tag{10.29}$$

If $\alpha^2-\beta^2<0$, then $\tanh\phi=\alpha/\beta$ and

$$\tilde{T}_{(4a)}:\begin{cases} t=\frac{1}{2}(u^2+v^2),\\ x=uv. \end{cases} \tag{10.30}$$

If $\alpha^2-\beta^2>0$, then $\tanh\phi=\beta/\alpha$ and

$$\tilde{T}_{(4b)}:\begin{cases} t=uv,\\ x=\frac{1}{2}(u^2+v^2). \end{cases} \tag{10.31}$$

SC5 and SC10: $\gamma\neq 0, I_{\pm}=-1\ (\Rightarrow \Delta^2_{\mathbb{R}^2_1}>0)$

$$a=-\frac{\beta}{\gamma},\quad b=-\frac{\alpha}{\gamma},\quad \sinh(2\phi)=\frac{2(\gamma C+\alpha\beta)}{\sqrt{\Delta^2_{\mathbb{R}^2_1}}},\quad k^2=\frac{\sqrt{\Delta^2_{\mathbb{R}^2_1}}}{8\gamma^2}. \tag{10.32}$$

$$\tilde{T}_{(5)}:\begin{cases} t=2k\sqrt{2}\cos\left(\frac{u}{2}+\frac{\pi}{4}\right)\cos\left(\frac{v}{2}+\frac{\pi}{4}\right),\\ x=2k\sqrt{2}\sin\left(\frac{u}{2}+\frac{\pi}{4}\right)\sin\left(\frac{v}{2}+\frac{\pi}{4}\right),\end{cases} \tag{10.33}$$

or

$$\tilde{T}_{(10)}:\begin{cases} t=2k\sqrt{2}\cosh\left(\frac{u}{2}\right)\cosh\left(\frac{v}{2}\right),\\ x=2k\sqrt{2}\sinh\left(\frac{u}{2}\right)\sinh\left(\frac{v}{2}\right)\end{cases}. \tag{10.34}$$

SC6: $\gamma\neq 0, \{I_+, I_-\}=\{0,+1\}$

$$a=-\frac{\beta}{\gamma},\quad b=-\frac{\alpha}{\gamma}. \tag{10.35}$$

If $I_+=0, I_-=+1\ (\Rightarrow \gamma C+\alpha\beta<0)$, $e^{2\phi}=-(\gamma C+\alpha\beta)/\gamma^2$ and

$$\tilde{T}_{(6a)}:\begin{cases} t=\sinh\left(\frac{u-v}{2}\right)+2\exp\left(\frac{u+v}{2}\right),\\ x=\sinh\left(\frac{u-v}{2}\right)-2\exp\left(\frac{u+v}{2}\right)\end{cases}. \tag{10.36}$$

If $I_+=+1, I_-=0\ (\Rightarrow \gamma C+\alpha\beta>0)$, $e^{2\phi}=\gamma^2/(\gamma C+\alpha\beta)$ and

$$\tilde{T}_{(6b)}:\begin{cases} t=\sinh\left(\frac{u-v}{2}\right)+2\exp\left(\frac{u+v}{2}\right),\\ x=-\sinh\left(\frac{u-v}{2}\right)+2\exp\left(\frac{u+v}{2}\right)\end{cases}. \tag{10.37}$$

SC7: $\gamma\neq 0, \{I_+, I_-\}=\{0,-1\}$

$$a=-\frac{\beta}{\gamma},\quad b=-\frac{\alpha}{\gamma}. \tag{10.38}$$

If $I_+=0, I_-=-1\ (\Rightarrow \gamma C+\alpha\beta>0)$, $e^{2\phi}=(\gamma C+\alpha\beta)/\gamma^2$ and

$$\tilde{T}_{(7a)}:\begin{cases} t=\cosh\left(\frac{u-v}{2}\right)+2\exp\left(\frac{u+v}{2}\right),\\ x=\cosh\left(\frac{u-v}{2}\right)-2\exp\left(\frac{u+v}{2}\right)\end{cases}. \tag{10.39}$$

If $I_+=-1, I_-=0\ (\Rightarrow \gamma C+\alpha\beta<0)$, $e^{2\phi}=\gamma^2/-(\gamma C+\alpha\beta)$ and

$$\tilde{T}_{(7b)}:\begin{cases} t=\cosh\left(\dfrac{u-v}{2}\right)+2\exp\left(\dfrac{u+v}{2}\right), \\ x=-\cosh\left(\dfrac{u-v}{2}\right)+2\exp\left(\dfrac{u+v}{2}\right). \end{cases} \tag{10.40}$$

SC8: $\gamma\neq 0, \{I_+, I_-\}=\{+1,-1\}$ $(\Rightarrow \Delta^2_{\mathbb{R}^2_1}<0)$,

$$a=-\frac{\beta}{\gamma}, \quad b=-\frac{\alpha}{\gamma}, \quad k^2=\frac{\sqrt{-\Delta^2_{\mathbb{R}^2_1}}}{8\gamma^2}. \tag{10.41}$$

If $I_+=+1, I_-=-1$, then

$$\sinh(2\phi)=\frac{\alpha^2+\beta^2-\gamma(A+B)}{\sqrt{-\Delta^2_{\mathbb{R}^2_1}}},$$

and

$$\tilde{T}_{(8a)}:\begin{cases} t=k\sqrt{2}\left(\cosh\left(\dfrac{u+v}{2}\right)+\sinh\left(\dfrac{u-v}{2}\right)\right), \\ x=k\sqrt{2}\left(\cosh\left(\dfrac{u+v}{2}\right)-\sinh\left(\dfrac{u-v}{2}\right)\right). \end{cases} \tag{10.42}$$

If $I_+=-1, I_-=+1$ then

$$\sinh(2\phi)=\frac{\gamma(A+B)-\alpha^2-\beta^2}{\sqrt{-\Delta^2_{\mathbb{R}^2_1}}},$$

and

$$\tilde{T}_{(8b)}:\begin{cases} t=k\sqrt{2}\left(\cosh\left(\dfrac{u+v}{2}\right)+\sinh\left(\dfrac{u-v}{2}\right)\right), \\ x=-k\sqrt{2}\left(\cosh\left(\dfrac{u+v}{2}\right)-\sinh\left(\dfrac{u-v}{2}\right)\right). \end{cases} \tag{10.43}$$

SC9: $\gamma\neq 0, I_\pm=+1$ $(\Rightarrow \Delta^2_{\mathbb{R}^2_1}>0)$,

$$a=-\frac{\beta}{\gamma}, \quad b=-\frac{\alpha}{\gamma}, \quad \sinh(2\phi)=\frac{-2(\gamma C+\alpha\beta)}{\sqrt{\Delta^2_{\mathbb{R}^2_1}}}, \quad k^2=\frac{\sqrt{\Delta^2_{\mathbb{R}^2_1}}}{8\gamma^2}, \tag{10.44}$$

$$\tilde{T}_{(9)}:\begin{cases} t=2k\sqrt{2}\sinh\left(\dfrac{u}{2}\right)\cosh\left(\dfrac{v}{2}\right), \\ x=2k\sqrt{2}\cosh\left(\dfrac{u}{2}\right)\sinh\left(\dfrac{v}{2}\right). \end{cases} \tag{10.45}$$

Remark 10.1: The formulas above indicate that the parameter k that enters the transformation formulas (6.6), (6.9), (6.10), and (6.11) is determined by $\Delta^1_{\mathbb{R}^2_1}=\gamma$ and $\Delta^2_{\mathbb{R}^2_1}$ according to the following formulas for the corresponding separable cases:

$$\text{SC5, SC9, SC10:}\quad k^2=\frac{\sqrt{\Delta^2_{\mathbb{R}^2_1}}}{8\Delta^1_{\mathbb{R}^2_1}},\quad (\Delta^2_{\mathbb{R}^2_1}>0),$$

$$\text{SC8:}\quad k^2=\frac{\sqrt{-\Delta^2_{\mathbb{R}^2_1}}}{8\Delta^1_{\mathbb{R}^2_1}},\quad (\Delta^2_{\mathbb{R}^2_1}<0). \tag{10.46}$$

Note they bear a striking resemblance to the analogous formula (2.19) derived in the study of Killing tensors of valence two defined in the Euclidean plane.

XI. THE ALGORITHM

The algorithm based on the results above for solving the Hamiltonian systems defined in $\mathbb{R}^2_1$ mimics the corresponding algorithm described in Ref. 20 for the Hamiltonian systems defined in $\mathbb{R}^2$ and consists of the following major steps:

(1) For a given natural Hamiltonian defined in the pseudo-Cartesian coordinates (q^1,q^2) by (5.17), use the generic Killing tensor (2.9) and impose the compatibility condition $d(\hat{\mathbf{K}}dV)=0$, to find the restrictions on the coefficients.
(2) Decompose the solution found in step (1) as follows:

$$\mathbf{K}=\ell_0\mathbf{g}+\sum_{i=1}^{n}\ell_i\mathbf{K^{(i)}}, \tag{11.1}$$

where ℓ_i are arbitrary constants and $\{\mathbf{g},\mathbf{K^{(1)}},\ldots,\mathbf{K^{(n)}}\}$ is a pointwise linearly independent set of Killing tensors. Since $\dim\mathcal{K}^2(\mathbb{R}^2_1)=6$, then $n\leqslant 5$. If $n=0$, then H is not orthogonally separable. If $n\geqslant 2$, then H is superseparable.
(3) Each component $\mathbf{K^{(i)}}$ in the decomposition (11.1) represents one of SC1–SC10. They can be determined by evaluating the invariants γ, I_-, I_+ for each $\mathbf{K^{(i)}}$. Then the results of the previous section can be used to find the parameters a,b,k, and ϕ. Finally, employ (7.5) to perform the coordinate transformation from (q^1,q^2) to separable coordinates.

We stress that this algorithm is purely algebraic in the sense that once the parameters a,b,k, and ϕ are determined in each case, the transformation to separable coordinates amounts to algebraic operations presented in the previous section for SC1–SC10.

XII. DIAGONALIZATION OF CERTAIN SYSTEMS OF THE HYDRODYNAMIC TYPE

Recall that a Hamiltonian function (4.1) along with an additional first integral quadratic in momenta (4.5) gives rise to a quasilinear system of the hydrodynamic type in a natural way. This remarkable observation due to Ferapontov and Fordy[42] (see also Ref. 43 for more details) allows us to use the classification above in terms of the group invariants γ, I_-, and I_+ in order to diagonalize the corresponding system of hydrodynamic type and thus find its Riemann invariants. Indeed, the Hamiltonian flows generated by the commuting H and F induce a two-dimensional surface parametrized by the "times" κ and τ:

$$q^i_\kappa=\frac{\partial H}{\partial p_i},\quad q^i_\tau=\frac{\partial F}{\partial p_i},$$

or, taking into account the formulas (5.17) and (2.9), we may write

$$q^1_\kappa=p_1,$$

$$q^2_\kappa=-p_2, \tag{12.1}$$

$$q^1_\tau = 2[(A+2\alpha q^2+\gamma(q^2)^2)p_1+(C-\alpha q^1-\beta q^2-\gamma q^1 q^2)p_2],$$

$$q^2_\tau = 2[(C-\alpha q^1-\beta q^2-\gamma q^1 q^2)p_1+(B+2\beta q^1+\gamma(q^1)^2)p_2].$$

Eliminating p_1 and p_2, we arrive at the following system of hydrodynamic type:

$$\begin{aligned} q^1_\tau &= 2[(A+2\alpha q^2+\gamma(q^2)^2)q^1_\kappa-(C-\alpha q^1-\beta q^2-\gamma q^1 q^2)q^2_\kappa], \\ q^2_\tau &= 2[(C-\alpha q^1-\beta q^2-\gamma q^1 q^2)q^1_\kappa-(B+2\beta q^1+\gamma(q^1)^2)q^2_\kappa]. \end{aligned} \tag{12.2}$$

At this stage we can use the information provided by the parameters A, B, C, α, β, γ to diagonalize the system (12.2). Indeed, computing the $I(\mathbb{R}^2_1)$-invariants γ, I_- and I_+ and then transforming the given coordinates of the original Hamiltonian system to the separable coordinates (u,v) according to the scheme of Sec. VI brings the original Hamiltonian system (i.e., H and F) to the Liouville form (5.2)–(5.4) and thus, the system of PDE's (12.2) to the following diagonal form:

$$\begin{aligned} u_\tau &= B(v)u_\kappa, \\ v_\tau &= A(u)v_\kappa. \end{aligned} \tag{12.3}$$

After a point transformation the system (12.3) can be brought to the form

$$\begin{aligned} \tilde{u}_\tau &= \tilde{v}\tilde{u}_\kappa, \\ \tilde{v}_\tau &= \tilde{u}\tilde{v}_\kappa, \end{aligned} \tag{12.4}$$

with $\tilde{u}$ and $\tilde{v}$ as the Riemann invariants of the associated system of hydrodynamic type. The methods of solving of such systems of PDE's are presented in Ref. 42.

XIII. APPLICATION: THE DRACH SUPERINTEGRABLE POTENTIALS

The method described in the preceding sections provides a systematic and straightforward means of determining separable coordinates for the Hamiltonian systems defined in the Minkowski plane admitting first integrals of motion quadratic in the momenta. For an application of the method, we turn our attention to the well-known Drach potentials.[56] Indeed, recall that in 1935, Drach listed ten scalar potentials $V(x,y)$ for a general Hamiltonian systems defined by a Hamiltonian of the form

$$H(x,y,p_x,p_y)=p_x p_y+V(x,y), \tag{13.1}$$

each of which admits an additional first integral cubic in the momenta. Note that the metric of (13.1) is Lorentzian.

It has been shown recently by Rañada[57] and independently later by Tsiganov[58] that seven out of the ten integrable cases isolated by Drach are in fact superintegrable admitting, in addition quadratic first integrals of motion. More specifically, it has been shown explicitly in Ref. 58 that the seven integrable systems in question are of the Stäckel-type.

It is easy to see that the signature-preserving point transformation

$$x=\frac{1}{\sqrt{2}}(q^1+q^2), \quad y=\frac{1}{\sqrt{2}}(q^1-q^2), \tag{13.2}$$

brings the Hamiltonian system defined by (13.1) to the form (5.17). After this transformation has been performed we can employ the algorithm presented in Sec. XI to determine the transformations to separable coordinates and thus solve the corresponding Hamiltonian systems by quadra-

tures. Indeed, as illustrative examples consider cases (b) and (c) from the Drach list[56] assuming $\mu=1$ and $a=1$, respectively. The transformation (13.2) yields the following potentials with respect to the pseudo-Cartesian coordinates (q^1,q^2):

$$\tilde{V}_1(q^1,q^2)=\frac{c_1\sqrt{2}}{\sqrt{(q^1)^2-(q^2)^2}}+\frac{2c_2}{(q^2)^2}+\frac{2c_3q^1}{\sqrt{(q^1)^2-(q^2)^2}(q^2)^2}, \tag{13.3}$$

$$\tilde{V}_2(q^1,q^2)=\frac{c_1}{2}((q^1)^2-(q^2)^2)+\frac{2c_2}{(q^2)^2}+\frac{2c_3}{(q^1)^2}, \tag{13.4}$$

where $c_1,c_2,c_3\in\mathbb{R}$ are arbitrary constants. Following the algorithm, we use the generic Killing tensor (5.18) and impose the compatibility conditions $d(\hat{\mathbf{K}}d\tilde{V}_1)=0$ and $d(\hat{\mathbf{K}}d\tilde{V}_2)=0$, respectively. These conditions imply the corresponding Killing tensors have the following forms:

$$\mathbf{K}_{\tilde{V}_1}=\begin{pmatrix} A+\gamma(q^2)^2 & -\beta q_2-\gamma q^1q^2 \\ -\beta q^2-\gamma q^1q^2 & -A+2\beta q^1+\gamma(q^1)^2 \end{pmatrix}, \tag{13.5}$$

and

$$\mathbf{K}_{\tilde{V}_2}=\begin{pmatrix} A+\gamma(q^2)^2 & -\gamma q^1q^2 \\ -\gamma q^1q^2 & B+\gamma(q^1)^2 \end{pmatrix}, \tag{13.6}$$

respectively, where A, B, β, $\gamma\in\mathbb{R}$ are arbitrary constants. The presence of the arbitrary constants indicates that the respective Hamiltonian systems are in fact *superintegrable*. Indeed, according to (11.1) the compatible Killing tensors $\mathbf{K}_{\tilde{V}_1}$ and $\mathbf{K}_{\tilde{V}_2}$ decompose as follows:

$$\mathbf{K}_{\tilde{V}_1}=A\mathbf{g}+\beta\mathbf{K}^{(4)}+\gamma\mathbf{K}^{(2)}, \tag{13.7}$$

$$\mathbf{K}_{\tilde{V}_2}=-B\mathbf{g}+(A+B)\mathbf{K}^{(1)}+\gamma\mathbf{K}^{(2)}, \tag{13.8}$$

where $\mathbf{g}$ denotes the metric tensor and the Killing tensors $\mathbf{K}^{(1)}$, $\mathbf{K}^{(2)}$, and $\mathbf{K}^{(4)}$ correspond to SC1, SC2, and SC4, respectively [see (6.12), (6.13), and (6.15)]. This fact can also be independently confirmed by evaluating the invariants γ, $\{I_-,I_+\}$ and the parameters a, b, k, and ϕ for $\mathbf{K}^{(1)}$, $\mathbf{K}^{(2)}$, and $\mathbf{K}^{(4)}$. Indeed, employing the results of Secs. VIII and X, we have

$$\begin{aligned} &\mathbf{K}^{(1)}:\ \ \gamma=0,\{I_-,I_+\}=\{0\},\quad \phi=0,\\ &\mathbf{K}^{(2)}:\ \ \gamma\neq 0,\{I_-,I_+\}=\{0\},\quad a=b=0,\\ &\mathbf{K}^{(4)}:\ \ \gamma=0,\{I_-,I_+\}=\{-1\},\quad a=b=\phi=0. \end{aligned} \tag{13.9}$$

We conclude therefore that the Hamiltonian systems defined by (13.3) and (13.4) are orthogonally s̄uperseparable. More specifically, the Hamiltonian system defined by (13.3) is separable with respect to SC2 and SC4, while the Hamiltonian system defined by (13.4) with respect to SC1 and SC2. The corresponding transformation formulas to separable coordinates are given by the formulas (6.2) (SC1), (6.3) (SC2), and (6.5) (SC4) [see also (13.9) and (10.20)].

XIV. CONCLUSION

We wish to conclude our paper with another quotation from Gian-Carlo Rota:[1]

''The apex of mathematical achievement occurs when two or more fields which were thought to be entirely unrelated turn out to be closely intertwined. Mathematicians have never decided whether they should feel excited or upset by such events.''

We have demonstrated how the ideas of classical invariant theory developed by many notable mathematicians of the 19th century, including Cayley, Gauss, Gordan, Hermite, Hilbert, and Sylvester,[3] can naturally be incorporated into the study of Killing tensors defined in pseudo-Riemannian spaces of constant curvature. A new set of group invariants has been brought to light and applied to the problem of the classification of separable Hamiltonians in the Minkowski plane. The application has enabled us to recognize their geometrical significance. The new method has been also successfully applied by the authors to the study of Hamiltonian systems with two degrees of freedom defined in $\mathbb{R}^2$ admitting first integrals that are cubic in the momenta.[19] More specifically, the corresponding set of $I(\mathbb{R}^2)$-invariants of $\mathcal{K}^3(\mathbb{R}^2)$ has led to a classification of the first integrals up to their leading cubic terms. Analogous programs have been launched to study the group invariants of the Killing tensors of valence two defined in two-dimensional spaces of nonzero constant curvature[59] and in the Euclidean space $\mathbb{R}^3$ (Ref. 60) (see also Refs. 61 and 62).

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The Potts model on $\mathbb{Z}^d$ with countable set of spin values

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The Potts model with countable set Φ of spin values on $\mathbb{Z}^d$ is considered. It is proved that with respect to Poisson distribution on Φ the set of limiting Gibbs measures is not empty. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The Potts model [Potts (1982)] has received an increasing theoretical and experimental interest in recent years, and at present a great many rigorous and approximate results are known. An extended summary of results and bibliography can be found in the review article by Wu (1982) and references therein.

The model can be studied both $\mathbb{Z}^d$ and Cayley tree J^k, i.e., a graph having no cycles, from each vertex of which emanates exactly $(k+1)$ edges. In the Potts model spin variables $\sigma(x)$ which take values on a discrete set $\Phi=\{0,1,2,\ldots,q\}$, $q\geqslant 2$ are associated with each vertex x of the $\mathbb{Z}^d$ or tree J^k. The Potts model on the $\mathbb{Z}^d$ or Cayley tree J^k is defined by the Hamiltonian

$$H(\sigma)=-J\sum_{\langle x,y\rangle}\delta_{\sigma(x)\sigma(y)}-h\sum_{x\in V}\delta_{0\sigma(x)},$$

where V is Z^d or the set of vertices in J^k, the first sum is taken over all nearest neighbors, δ in the first and second sums is the Kroneker's symbol.

In this paper we consider the case when Φ is the set of non-negative integer numbers, i.e., Φ is a countable set. We show that for the Poisson distribution on Φ the set of limiting Gibbs distribution is a nonempty set.

II. THE POISSON GIBBS MEASURES

Let Φ be the set of non-negative integer numbers. In this paper we consider the Potts model on the integer lattice $\mathbb{Z}^d$, $d\geqslant 1$. It is defined by the Hamiltonian

$$H(\sigma)=-J\sum_{\substack{\langle x,y\rangle\\ x,y\in\mathbb{Z}^d}}\delta_{\sigma(x)\sigma(y)}-h\sum_{x\in\mathbb{Z}^d}\delta_{0\sigma(x)},$$

where $\sigma:\mathbb{Z}^d\to\Phi$ is a configuration and the first sum taken over all nearest neighbors, i.e., $\|x-y\|=1$ with $\|x\|=\max|x_i|$.

Let Ω be the set of all configurations and for arbitrary finite subset $\Lambda\subset\mathbb{Z}^d$; $\Omega(\Lambda)$ be a set of all configuration $\sigma(\Lambda)$ *on* Λ. For finite $V_n=\{x\in\mathbb{Z}^d|\ \|x\|=n\}\subset\mathbb{Z}^d$, the full energy of configuration $\sigma(V_n)$ under boundary condition $\overline{\sigma}(\mathbb{Z}^d\backslash V_n)$, i.e., fixed configuration on $\mathbb{Z}^d\backslash V_n$, is defined the following way:

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$$H(\sigma(V_n)|\overline{\sigma}(\mathbb{Z}^d\backslash V_n))=-J\sum_{\substack{\langle x,y\rangle,\\ x\in V_n}}\delta_{\sigma(x)\sigma(y)}-J\sum_{\substack{\langle x,y\rangle\\ x\in V_n,\,y\in\mathbb{Z}^d\backslash V_n}}\delta_{\sigma(x)\sigma(y)}-h\sum_{x\in V_n}\delta_{0\sigma(x)}.$$

Let us consider the partition function on V_n with respect to some measure λ on Φ:

$$Z_n(\overline{\sigma}(\partial V_n))=\int_{\Omega(V_n)}\exp(-H(\sigma(V_n)|\overline{\sigma}(\mathbb{Z}^d\backslash V_n)))\prod_{s\in V_n}d\lambda(\sigma(s)),$$

where $\partial V_n=V_{n+1}\backslash V_n$.

As λ is a discrete measure, then this integral is represented in the form of plurigenus,

$$\begin{aligned}Z_n(\overline{\sigma}(\partial V_n))&=\sum_{x\in V_n}\sum_{\sigma(x)=0}^{\infty}\exp(-H(\sigma(V_n)|\overline{\sigma}(\mathbb{Z}^d\backslash V_n)))\prod_{x\in V_n}\lambda(\sigma(x))\\&=\sum_{x\in V_n}\sum_{\sigma(x)=0}^{\infty}\exp\Bigg(J\sum_{\substack{\langle x,y\rangle\\ x,y\in V_n}}\delta_{\sigma(x)\sigma(y)}+J\sum_{\substack{\langle x,y\rangle\\ x\in V_n,\,y\in\mathbb{Z}^d\backslash V_n}}\delta_{\sigma(x)\sigma(y)}\\&\quad+h\sum_{x\in V_n}\delta_{0\sigma(x)}\Bigg)\prod_{x\in V_n}\lambda(\sigma(x)).\end{aligned}$$

If λ is the counting measure, i.e., $\lambda(\{i\})=1$ for any $i\in\Phi$, then the partition function reduces to infinity for arbitrary boundary condition $\overline{\sigma}(Z\backslash V_n)$.

Let λ be a probabilistic measure on Φ. Then the partition function is a finite under arbitrary boundary condition $\overline{\sigma}(\mathbb{Z}^d\backslash V_n)$ and conditional Gibbs measure on volume V_n has the following form:

$$P_n(\sigma(V_n)|\ \overline{\sigma}(\mathbb{Z}^d\backslash V_n))=\frac{\exp(-H(\sigma(V_n)|\ \overline{\sigma}(\mathbb{Z}^d\backslash V_n)))\prod_{x\in V_n}\lambda(\sigma(x))}{Z_n(\overline{\sigma}(\partial V_n))},$$

that is, P_n is the discrete measure on $\Omega(V_n)$.

The main result is the following.

Theorem: For a Poisson distribution ν on Φ, i.e., $\nu(i)=\exp(-\lambda)(\lambda^i/i!)$, where λ is the arbitrary positive number and the set of all limit Gibbs measure is a nonempty set.

Proof: The proof is based on the Dobrushin theorem about the existence of the limit of Gibbs measures if the set of values of variables $\sigma(x)$, $x\in\mathbb{Z}^d$ is the separable complete metric space [Dobrushin (1968, 1970)].

Evidently, the set Φ of all non-negative integer numbers with discrete metric,

$$d(x,y)=\begin{cases}1, & x\neq y;\\ 0, & x=y,\end{cases}\tag{1}$$

is the complete separable metric space.

Definition [Dobrushin (1968)]: Let M be a complete separable metric space. A continuous function h on M is called a *compact*, if for any $t\in(-\infty,\infty)$ the set $\{m\in M\colon h(m)\leqslant t\}$ is the compact set in M.

As the set of all non-negative integer numbers Φ is complete separable metric space with respect to discrete metric (1), then arbitrary function h on Φ is continuous. Evidently, there are a lot of compact non-negative functions on Φ. For example, the identity map $h(i)=i$ for any $i\in\Phi$ is a compact function.

Theorem of Dobrushin [Dobrushin (1968, 1970)]: Assume that there is a Hamiltonian H, for which is possible to find the following: (1) a compact non-negative function h on the set Φ; (2) the system of numbers $\{c(x,y),\ x\in\mathbb{Z}^d, y\in\mathbb{Z}^d\}$, and a constant $c\in(0,1)$ with $\Sigma_y|c(x,y)|\leqslant c$ for any $x\in\mathbb{Z}^d$, and number $K>0$, such that for finite subset $V\subset\mathbb{Z}^d$ and arbitrary boundary condition $\overline{\sigma}(\mathbb{Z}^d\backslash V)$ with $\max_{x\in V}\Sigma_{y\in\mathbb{Z}^d\backslash V}|c(x,y)|h(\overline{\sigma}(y))<\infty$, the conditional Gibbs measure is defined and

$$\int h(\sigma(x))\ p(\sigma(V))|\sigma(\mathbb{Z}^d\backslash V)\prod_{y\in V} d\chi(\sigma(y))\leqslant K+\sum_{y:y\neq x} c(x,y)h(\overline{\sigma}(y)),$$

where χ is a measure on Φ.

(3) For any $x\in\mathbb{Z}^d$ and for any continuous bounded function $g(\sigma)$ on Φ there is the sequence of finite subset $W_n\subset\mathbb{Z}^d, \cup_n W_n=\mathbb{Z}^d\backslash\{x\}$, the system of non-negative numbers $d^{(n)}(x,y)$, $y\neq x$ with $\Sigma_{y\in\mathbb{Z}^d}d^{(n)}(x,y)\leqslant D^{(n)}\to 0$ and the sequence of continuous boundary functions $f_n(\sigma(W_n))$ such that

$$\left|\int g(\sigma(x))p(\sigma(x)\left|\overline{\sigma}(\mathbb{Z}^d\backslash\{x\}))d\chi(\sigma(x))-f_n(\sigma(W_n))\right|\right|\leqslant D^n+\sum_{y\neq x} d^{(n)}(x,y)h(\sigma(y)),$$

for arbitrary boundary condition $\overline{\sigma}(\mathbb{Z}^d\backslash\{x\})$ with $\Sigma_{y\neq x}c(x,y)h(\overline{\sigma}(y))<\infty$.

Then there exists at least one limit Gibbs measure.

Let us take the function $h(i)=i$ as a compact function. Then [see Sinai (1982)], our problem amounts to the finding of constants K, $c(x,y)$, $c\in(0,1)$ with $\Sigma_y|c(x,y)|\leqslant c<1$ such that

$$\frac{\sum_{\sigma(x)=0}^{\infty}\sigma(x)\exp(-H(\sigma(x)|\overline{\sigma}(\partial x))\nu(\sigma(x)))}{\sum_{\sigma(x)=0}^{\infty}\exp(-H(\sigma(x)|\overline{\sigma}(\partial x))\nu(\sigma(x)))}\leqslant K+\sum_{y\neq x} c(x,y)\sigma(y), \tag{2}$$

where $\partial x=\{y\in\mathbb{Z}^d|\ \|x-y\|=1\}=\{y^1,y^2,\ldots,y^{3^d-1}\}$.

Assume

$$A=\frac{\sum_{\sigma(x)=0}^{\infty}\sigma(x)\exp(-H(\sigma(x)|\overline{\sigma}(\partial x))\nu(\sigma(x)))}{\sum_{\sigma(x)=0}^{\infty}\exp(-H(\sigma(x)|\overline{\sigma}(\partial x))\nu(\sigma(x)))}=\frac{\sum_{j=0}^{\infty} j\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d\text{-}1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j)}{\sum_{j=0}^{\infty}\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d\text{-}1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j)}.$$

As for a Poisson measure ν we have $j\nu(j)=\lambda\nu(j-1)$ *for* $j\geqslant 1$ and for $j=0$ the first term in the numerator is equal to zero; then

$$A=\frac{\lambda\sum_{j=1}^{\infty}\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d-1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j-1)}{\sum_{j=0}^{\infty}\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d-1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j)}.$$

After the change of variable $j-1$ to j in the numerator, we have

$$A=\frac{\lambda\sum_{j=0}^{\infty}\exp\left(h\delta_{j+1,0}+J\sum_{i=1}^{3^d-1}\delta_{j+1,\overline{\sigma}(y^i)}\right)\nu(j)}{\sum_{j=0}^{\infty}\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d-1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j)}$$

$$=\lambda+\lambda\frac{\sum_{j=0}^{\infty}\left[\exp\left(h\delta_{j+1,0}+J\sum_{i=1}^{3^d-1}1\,\delta_{j+1,\overline{\sigma}(y^i)}\right)-\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d-1}\delta_{j\overline{\sigma}(y^i)}\right)\right]\nu(j)}{\sum_{j=0}^{\infty}\exp\left(h\delta_{0j}+J\sum_{i=1}^{3^d-1}\delta_{j\overline{\sigma}(y^i)}\right)\nu(j)}.$$

Assume

$$c(x,y)=\begin{cases}(4d)^{-1}, & \text{if } \|x-y\|=1;\\ 0 & \text{otherwise.}\end{cases}$$

Then inequality (2) is essentially more simple and it is necessary to find a constant K, such that

$$A\leqslant K+\frac{1}{4d}\sum_{i=1}^{3^d-1}\overline{\sigma}(y^i), \tag{3}$$

for all boundary configurations $\overline{\sigma}(\mathbb{Z}^d\backslash\{x\})$.

In order to avoid numerous indices we are restricted to considering the case $d=1$. Then A has the form

$$\lambda+\lambda\frac{\sum_{j=0}^{\infty}(B(j)-B'(j))\nu(j)}{\sum_{j=0}^{\infty}B'(j)\nu(j)},$$

where

$$B(j)=\exp\left(h\delta_{j+1,0}+J(\delta_{j+1,\overline{\sigma}(x-1)}+\delta_{j+1,\overline{\sigma}(x+1)})\right)$$

and

$$B'(j)=\exp\left(h\delta_{0j}+J(\delta_{j,\overline{\sigma}(x-1)}+\delta_{j,\overline{\sigma}(x+1)})\right).$$

Then it is necessary to find a constant K such that

$$A\leqslant K+\frac{\overline{\sigma}(x-1)+\overline{\sigma}(x+1)}{4}, \tag{4}$$

for all boundary configurations $\overline{\sigma}(Z\backslash\{x\})$.

Let us assume for definiteness, that $J>0$. We shall divide the domain $\{\overline{\sigma}(x-1)\geqslant 0,\ \overline{\sigma}(x+1)\geqslant 0\}$ into 4 subsets (Fig. 1).

Let us divide the proof of the inequality (4) into three steps.

(1) If $(\overline{\sigma}(x-1),\overline{\sigma}(x+1))\in F_1$, then we can find a constant K_1, such that

$$A\leqslant K_1+\frac{\overline{\sigma}(x-1)+\overline{\sigma}(x+1)}{4}.$$

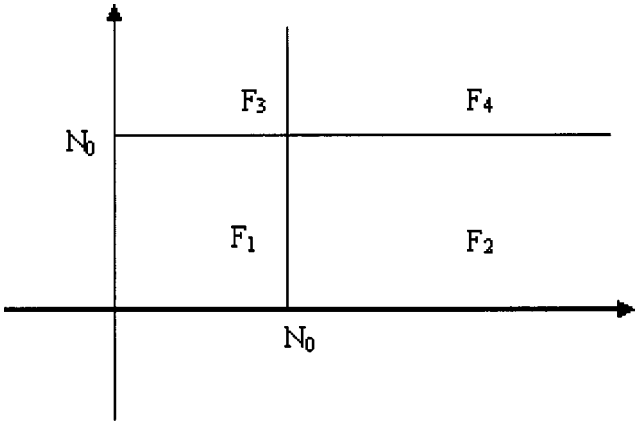

FIG. 1. The partion of the domain into 4 subsets.

It is possible as F_1 is a finite set.

(2) For $(\overline{\sigma}(x-1),\overline{\sigma}(x+1))\in F_4$, we shall consider separately the following cases.

(a) Assume $|\overline{\sigma}(x-1)-\overline{\sigma}(x+1)|\geqslant 2$. Then A has the following form:

$$A=\lambda+\lambda\frac{\alpha\nu(0)+\beta\nu(\overline{\sigma}(x-1)-1)-\beta\nu(\overline{\sigma}(x+1)-1)-\beta\nu(\overline{\sigma}(x+1))}{\exp(h)\nu(0)+\exp(J)(\nu(\overline{\sigma}(x-1))+\nu(\overline{\sigma}(x+1)))+\gamma}$$

$$<\lambda+\lambda\frac{\left(|\alpha|\nu(0)+\beta\left(\frac{\overline{\sigma}(x-1)\nu(\overline{\sigma}(x-1))}{\lambda}-\nu(\overline{\sigma}(x-1))\right)\right.}{\exp(h)\nu(0)}$$

$$+\lambda\frac{\beta\left(\frac{\overline{\sigma}(x+1)\nu(\overline{\sigma}(x+1))}{\lambda}-\nu(\overline{\sigma}(x+1))\right)}{\exp(h)\nu(0)}$$

$$<\lambda+\lambda\frac{|\alpha|}{\exp(h)}+\frac{|\beta|}{\exp(h)\nu(0)}[\overline{\sigma}(x-1)\nu(\overline{\sigma}(x-1))+\overline{\sigma}(x+1)\nu(\overline{\sigma}(x+1))]$$

$$<\lambda\left(1+\frac{|\alpha|}{\exp(h)}\right)+\frac{\beta\nu(N_0)}{\exp(h)\nu(0)}[\overline{\sigma}(x-1)+\overline{\sigma}(x+1)],$$

where $\alpha=1-\exp(h)$, $\beta=\exp(J)-1$ and $\gamma=1-(\nu(0)+\nu(\overline{\sigma}(x-1))+\nu(\overline{\sigma}(x+1)))$.

If we choose N_0^a such that $(\exp(J)-1)\nu(N_0^a)/\exp(h)\nu(0)<1/4$, then

$$K_4^a=\lambda+\lambda\frac{|\exp(h)-1|}{\exp(h)}.$$

(b) Let $|\overline{\sigma}(x-1)+\overline{\sigma}(x+1)|=1$. Then

$$A=\lambda+\lambda\frac{\alpha\nu(0)+(\exp(J)-\exp(h))\nu(\overline{\sigma}(x-1)-1)-\beta\nu(\overline{\sigma}(x+1))}{\exp(h)\nu(0)+\exp(J)(\nu(\overline{\sigma}(x-1))+\nu(\overline{\sigma}(x+1)))+\gamma}$$

$$<\lambda+\lambda\frac{|\alpha|\nu(0)+|\exp(J)-\exp(h)|\cdot\frac{\overline{\sigma}(x-1)\nu(\overline{\sigma}(x-1))}{\lambda}}{\exp(h)\nu(0)}$$

$$=\lambda\left(1+\frac{|\alpha|}{\exp(h)}\right)+\frac{|\exp(J)-\exp(h)|\overline{\sigma}(x-1)\nu(\overline{\sigma}(x-1))}{\exp(h)\nu(0)},$$

where α, β, γ are as above.

If we choose N_0^b such that $(\exp(J)-1)\nu(N_0^b)/\exp(h)\nu(0)<1/2$, then

$$K_4^b=\lambda+\lambda\frac{|\exp(h)-1|}{\exp(h)}=K_4^a.$$

Let $\overline{\sigma}(x-1)=\overline{\sigma}(x+1)$. Then

$$A=\lambda+\lambda\frac{\alpha\nu(0)+\beta'\nu(\overline{\sigma}(x-1)-1)-\beta'\nu(\overline{\sigma}(x-1))}{\exp(h)\nu(0)+\exp(2J)\nu(\overline{\sigma}(x-1))+\gamma'}$$

$$<\lambda\left(1+\frac{|\exp(h)-1|}{\exp(h)}\right)+\frac{\exp(2J)-1}{\exp(h)\nu(0)}\overline{\sigma}(x-1)\nu(\overline{\sigma}(x-1)),$$

where $\alpha=1-\exp(h)$, $\beta'=\exp(2J)-1$ and $\gamma'=1-\nu(0)-\nu(\overline{\sigma}(x-1))$.

If we choose N_0^c such that $(\exp(2J)-1)/\exp(h)\nu(0)\,\nu(N_0^c)<1/2$, then for $N_0=\max(N_0^a,N_0^b,N_0^c)$ will be valid (4) with $K=\lambda(1+|\exp(h)-1|/\exp(h))$ for all $(\overline{\sigma}(x-1),\overline{\sigma}(x-1))\in F_4$.

(3) At last we consider the case $(\overline{\sigma}(x-1),\overline{\sigma}(x+1))\in F_2\cup F_3$.

Let for definiteness $0\leqslant\overline{\sigma}(x-1)\leqslant N_0$ and $\overline{\sigma}(x+1)>N_0$, that is $(\overline{\sigma}(x-1),\overline{\sigma}(x+1))\in F_2$. Here we shall divide the proof of inequality (4) into four steps

(a) Assume $\overline{\sigma}(x-1)=0$. Then

$$A=\lambda+\lambda\frac{(1-\exp(h+J))\nu(0)+\beta\nu(\overline{\sigma}(x+1)-1)-\beta\nu(\overline{\sigma}(x+1))}{\exp(h+J)\nu(0)+\exp(J)\nu(\overline{\sigma}(x+1))+1-\nu(0)-\nu(\overline{\sigma}(x+1))}$$

$$<\lambda\left(1+\frac{|\exp(h+J)-1|}{\exp(h+J)}\right)+\frac{\exp(J)-1}{\exp(h+J)\nu(0)}\nu(\overline{\sigma}(x+1)).$$

As $\exp(J)>1$, then for choosing above N_0 it is evidently

$$\frac{(\exp(J)-1)\nu(N_0)}{\exp(h+J)\nu(0)}<\frac{(\exp(J)-1)\nu(N_0)}{\exp(h)\nu(0)}<\frac{1}{4}.$$

(b) Assume $\overline{\sigma}(x-1)=1$. Then

$$A<\lambda\left(1+\frac{|\exp(h)-\exp(J)|}{\exp(h)}\right)+\frac{\exp(J)-1}{\exp(h)\nu(0)}\nu(\overline{\sigma}(x+1))\overline{\sigma}(x+1),$$

and for choosing N_0, inequality (4) is valid. Here $K=\lambda(1+|\exp(J)-\exp(h)|/\exp(h))$.

(c) Assume $1<\overline{\sigma}(x-1)<N_0$. Then A is defined as case (2)(a) and

$$A<\lambda\left(1+\frac{|\exp(h)-1|}{\exp(h)}\right)+\frac{\exp(J)-1}{\exp(h)\nu(0)}\nu(\overline{\sigma}(x-1))\overline{\sigma}(x-1)+\frac{\exp(J)-1}{\exp(h)\nu(0)}\nu(\overline{\sigma}(x+1))\overline{\sigma}(x+1).$$

As $\overline{\sigma}(x+1)>N_0$, $1<\overline{\sigma}(x-1)<N_0$ and

$$A<\lambda\left(1+\frac{|\exp(h)-1|}{\exp(h)}\right)+\frac{\exp(J)-1}{\exp(h)\nu(0)}\nu(\overline{\sigma}(x-1))\overline{\sigma}(x-1)+\frac{1}{4}\overline{\sigma}(x+1),$$

then at the expense of the extension the constant will be valid (4).

(d) At last let $\overline{\sigma}(x-1)=N_0$. Then it is enough to consider the case $\overline{\sigma}(x+1)=N_0+1$ and again at the expanse of extension of constant will be valid. Thus all conditions of Dobrushin's theorem are valid, so that the set of limiting Gibbs measures is not empty. The same way we can prove inequality (2) for arbitrary positive integer d.

To prove similar theorem for Potts model on Cayley tree, we can use the theory of Markov random fields. This result will be presented in other paper.

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Quasiperiodic functions theory and the superlattice potentials for a two-dimensional electron gas

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We consider Novikov problem of the classification of level curves of quasiperiodic functions on the plane and its connection with the conductivity of two-dimensional electron gas in the presence of both orthogonal magnetic field and the superlattice potentials of a special type. We show that the modulation techniques used in the recent papers on the two-dimensional (2-D) heterostructures permit us to obtain the general quasiperiodic potentials for 2-D electron gas and consider the asymptotic limit of conductivity when $\tau\to\infty$. We use the quasiclassical approach introduced by Beenakker for the modulated electron gas and investigate the level curves of quasiperiodic potentials (Novikov problem) to get the asymptotic behavior of conductivity in this limit. Using the theory of quasiperiodic functions we introduce here the topological characteristics of the quasiperiodic potentials observable in the conductivity. The corresponding characteristics are the direct analog of the ''topological numbers'' introduced recently by Novikov and the present author in the conductivity of normal metals. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In the present paper we consider the modern experimental techniques of potential modulation for the two-dimensional electron gas and show that they permit us to obtain the quasiperiodic potentials on the plane with different numbers of quasiperiods. Then we use the topological results concerning the geometry of the level curves of such potentials (the Novikov problem) to obtain the asymptotic ($\tau\to\infty$) behavior of the conductivity phenomena in these systems. Namely, we consider the quasiclassical approach, where the quasiclassical cyclotron orbits drift along the level curves of potential in the presence of magnetic field B which makes the geometry of such level curves important for transport phenomena. Our approach is based on the topological methods used previously (by Novikov and the author) in the theory of normal metals (Refs. 19, 25, 30) and the quasiclassical description of the transport phenomena in high-mobility 2-D electron gas introduced by Beenakker[36] for the explanation of new oscillations in B-dependence of conductivity found in the periodically modulated 2-D electron gas (Weiss, Klitzing, Ploog, and Weimann).[33]

We will consider here the cases of potentials with 3 and 4 quasiperiods and use the set of rather deep topological theorems concerning the Novikov problem obtained during the last years. Let us say here that these two cases are actually the only cases which were studied seriously in topology and where the very nice results were obtained. Namely, the full classification of the nonclosed level curves was obtained for the case of potentials with 3 quasiperiods on the plane and it was shown[15,26] that only the so-called ''topologically regular'' level curves appear in the case when the nonclosed level curves exist in the nonzero energy interval $\epsilon_1\leqslant V(\mathbf{r})\leqslant\epsilon_2$. The corresponding curves reveal the nice geometrical properties being bounded by the straight strips of the finite width in the plane and passing through them. Moreover, it can be shown that the mean directions of these strips always correspond to some topological numbers characterizing the potential $V(\mathbf{r})$. Thus for the case of 3 quasiperiods these numbers can be represented as the indivis-

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ible integer triples (m_1,m_2,m_3) which can be defined experimentally from the mean directions of potential level curves. For the case of 4 quasiperiods the corresponding numbers are the 4-tuples which can again be defined from the mean directions of the topologically regular open level curves in the transport phenomena. However, in the last case the existence of topologically regular open level curves can be stated only for small perturbations of purely periodic potentials in $\mathbb{R}^2$.[27]

In this paper we show that the special modulations of 2-D electron gas give the quasiperiodic potentials on the plane and introduce the corresponding topological numbers and their connection with the modulation pictures. Let us say that the topological numbers of this kind were introduced already in the theory of normal metals,[19,25,30] where the "geometric strong magnetic field limit" in the galvanomagnetic phenomena was considered. For this case only the situation with 3 quasiperiods was important and the topological numbers had the form of the integer triples (m_1,m_2,m_3). Another feature of the situation in the normal metals is that just the Fermi energy level ϵ_F is important for the asymptotic behavior of conductivity in the "geometric limit."

As we already said, we will use here the "drifting orbits" approximation and consider the case $\tau\to\infty$ which corresponds to the "geometric limit" in the situation of 2-D electron gas. We consider in detail the electrical conductivity tensor σ^{ik} in the asymptotic form for $\tau\to\infty$ when the strong anisotropy of σ^{ik} reveals the mean directions of topologically regular trajectories and gives the corresponding topological numbers.

Let us say also that the cases of chaotic behavior of the potential level curves are also possible for the quasiperiodic potentials $V(\mathbf{r})$.[16,22] The asymptotic behavior of σ^{ik} is more complicated in this case and we will not consider it here in detail. For the case of 3 quasiperiods, however, the generic behavior of conductivity should correspond to a topologically regular situation and the chaotic cases are "exclusive," unlike the cases with big numbers of quasiperiods.

II. BASIC DEFINITIONS AND HISTORICAL NOTES

According to the standard definition the quasiperiodic function $f(\mathbf{r})$, $\mathbf{r}\in\mathbb{R}^n$ with N quasiperiods $(N\geqslant n)$ is a restriction of a periodic function $F(\mathbf{R})$, $\mathbf{R}\in\mathbb{R}^N$ with N linearly independent periods $\mathbf{l}_1,\ldots,\mathbf{l}_N$ in the bigger linear space $\mathbb{R}^N$ to some "plane" $\mathbb{R}^n\subset\mathbb{R}^N$. The corresponding subspace $\mathbb{R}^n$ can then be given by a linear system,

$$a_{11}y^1+a_{12}y^2+\cdots+a_{1N}y^N=b_1,$$

$$\cdots$$

$$a_{N-n,1}y^1+a_{N-n,2}y^2+\cdots+a_{N-n,N}y^N=b_{N-n}.$$

We will say that the plane $\mathbb{R}^n$ has the maximal irrationality if it is not parallel to any vector $\mathbf{l}$ belonging to the lattice L generated by vectors $\mathbf{l}_1,\ldots,\mathbf{l}_N$:

$$L=\{p_1\mathbf{l}_1+\cdots+p_N\mathbf{l}_N,\quad p_1,\ldots,p_N\in\mathbb{Z}\}.$$

We will call the plane $\mathbb{R}^n\subset\mathbb{R}^N$ rational if it contains (i.e., parallel to) exactly n linearly independent vectors belonging to L.

Obviously the generic planes $\mathbb{R}^n$ in $\mathbb{R}^N$ have the maximal irrationality. It is easy to see also that any vector $\mathbf{l}\in L$ parallel to the plane $\mathbb{R}^n$ in the nongeneric situation becomes a period of the function $f(\mathbf{r})$ in $\mathbb{R}^n$. The function $f(\mathbf{r})$ corresponding to the rational plane $\mathbb{R}^n\subset\mathbb{R}^N$ is an n-periodic function in the ordinary sense. It is easy to see also that the generic quasiperiodic function $f(\mathbf{r})$ with N quasiperiods has no periods in $\mathbb{R}^n$ for $N>n$.

We are going to consider the case $n=2$ such that the function $f(\mathbf{r})=f(x,y)$ is a quasiperiodic function on the two-dimensional plane $\mathbb{R}^2$. Namely, we will describe here the important features of the global geometry of the level curves $f(\mathbf{r})=\text{const}$ (Novikov problem) which will play the main role for the phenomena discussed in this paper.

Let us say here that the Novikov problem is still unsolved for the case of arbitrary $N>2$ and we are going to deal here with the cases $N=3$ and $N=4$ where the new topological and physical results were obtained during the last years (see Refs. 10–30). According to the definition the corresponding functions $f(\mathbf{r})$ will be the restrictions of the periodic functions in $\mathbb{R}^3$ and $\mathbb{R}^4$ on some two-dimensional planes $\mathbb{R}^2$. Let us say some words here about this situation.

We will start with the very important case $N=3$ where the full classification of the curves $f(\mathbf{r})=\text{const}$ is constructed now. This case plays an extremely important role for the galvanomagnetic phenomena in normal metals (see Refs. 19, 25, 30) where the function $\hat{f}(\mathbf{p})$, $\mathbf{p}=(p_1,p_2,p_3)$ is defined in the space of quasimomenta of the Bloch electron in the crystal. The function $f(\mathbf{p})$ is a restriction of the three-periodic function $\hat{f}(\mathbf{p})$ on the two-dimensional plane (orthogonal to the magnetic field) embedded in $\mathbb{R}^3$. The level curves of $f(\mathbf{p})$ are the intersections of the corresponding plane $\Pi=\mathbb{R}^2$ with the 3-periodic two-dimensional level surfaces of the (smooth) function $\hat{f}(\mathbf{p})$ (dispersion relation). From the physical point of view the level curves of the function f are the quasiclassical electron trajectories in the **p**-space in the presence of magnetic field **B**. We have in this case the one-parametric family of planes Π orthogonal to **B** and the one-parametric set of the quasiperiodic functions defined in the different planes. The form of trajectory in the coordinate space is defined in this case by its form in the **p**-space, keeping all the main features of global geometry. For instance the projection of orbit on xy-plane in **r**-space coincides precisely with the trajectory in **p**-space rotated by $\pi/2$. We do not discuss here the corresponding foundations in detail and just give a reference on the well-known books (Refs. 6–9) where different points of this approach are considered. Let us give also the reference on the recent papers,[31,32] where the mathematically rigorous approach to a derivation of the corresponding system in **p**-space and the history of the question are represented. We also point out that only the trajectories close to the Fermi level are important for the case of normal metals.

The importance of the geometry of these trajectories for the galvanomagnetic phenomena was pointed out in Refs. 1–3 (see also survey articles[4,5]) where also the first examples of concrete two-dimensional periodic Fermi surfaces in $\mathbb{R}^3$ were considered. The problem of full classification of such trajectories was set by Novikov in Ref. 10 and considered later in his school (Zorich, Dynnikov, and Tsarev).

Let us say here that this problem is rather complicated already for $N=3$ and required the nontrivial methods based on topology and dynamical systems theory to be solved completely. The most important breakthroughs in this problem were made in Refs. 11 and 15, where the very important topological theorems about the nonclosed trajectories were proved.

Based on these methods the ''topological quantum characteristics'' observable in the conductivity of normal metals were introduced in Ref. 19. These characteristics arise from the geometry of the Fermi surface and have the form of the triples of the integer numbers connected with the asymptotic behavior of conductivity for $B\to\infty$ (see also the survey articles[25,30]). For these physical phenomena the additional property pointed out in Ref. 19 and called later the ''topological resonance'' played an important role. We will see here how all these properties can be revealed in the two-dimensional electron gas in the quasiperiodic potential $V(\mathbf{r})$.

Recently the full classification of the different trajectories in this situation was finished by Dynnikov,[22,26] which permits us to describe the total picture of the asymptotic behavior of conductivity for $B\to\infty$ in normal metals with arbitrary complicated dispersion relations.[30]

The case $n=2$, $N=4$ was started by Novikov in Ref. 27 where the deep topological theorem analogous to the result of Ref. 11 for this situation was proved. Let us point out here that the case $N=4$ looks very complicated from topological point of view and this theorem is the only deep topological result in this case up to now.

In this paper, however, we work with the coordinate space rather than with the momenta space and consider the quasiperiodic functions $V(\mathbf{r})$ where $\mathbf{r}=(x,y)$ plays the role of the ordinary coordinate vector on the plane. In this situation only one plane $\mathbb{R}^2$ embedded in $\mathbb{R}^3$ or $\mathbb{R}^4$ will be important. However, also the global characteristics of the total family of potentials corresponding

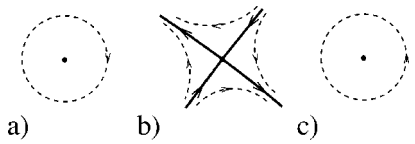

FIG. 1. The level curves of the function $V(\mathbf{r})$ close to the local minimum, the saddle-point and the local maximum of $V(\mathbf{r})$.

to different parallel planes will arise through the action of the ''quasiperiodic group'' as we will see below.

III. THE QUASICLASSICAL TRAJECTORIES AND 2-D ELECTRON GAS

Let us introduce first the notations for the different level curves of potential $V(\mathbf{r})$ according to Refs. 22, 25, 26, 30. We will assume now that the function $V(\mathbf{r})$ is a Morse function on $\mathbb{R}^2$, i.e., all the critical points of $V(\mathbf{r})$ ($\nabla V(\mathbf{r})=0$) are nondegenerate ($\det\|\partial_i\partial_j V\|\neq 0$). All the critical points of $V(\mathbf{r})$ can then be just the nondegenerate local minima, the nondegenerate saddle points or the nondegenerate local maxima. The local geometry of the level curves close to these critical points are shown in Figs. 1(a)–1(c).

Let us call now the level curves of $V(\mathbf{r})$ the quasiclassical drift trajectories according to our further considerations.[62] We will also put formally the arrows on the level curves according to the direction of drift in the magnetic field.

Definition 1: We call the trajectory nonsingular if it is not adjacent to the critical (saddle) point of the function $V(\mathbf{r})$. The trajectories adjacent to the critical points as well as the critical points themselves we call singular trajectories (see Fig. 1).

Definition 2: We call the nonsingular trajectory compact if it is closed on the plane. We call the nonsingular trajectory open if it is unbounded in $\mathbb{R}^2$.

The examples of singular, compact and open nonsingular trajectories are shown in Figs. 2(a)–2(c).

It is easy to see also that the singular trajectories have the measure zero among all the trajectories on the plane.

The geometry of compact trajectories will not be interesting for us here since we are going to consider the ''geometric'' limit corresponding to the long lifetime between the two scattering processes. In this limit we assume that every center of drifting cyclotron orbit belongs to the same trajectory for a rather long time. This means in particular that all compact trajectories will be passed many times before jumping to another trajectory due to the scattering act. This situation corresponds precisely to the ''geometric strong magnetic field limit'' considered in Refs. 1–3, 19, 25, 30 where the conductivity in normal metals was studied. However, in our situation this geometric limit does not correspond to strong magnetic field limit as we will see below.

Definition 3: We call the open trajectory topologically regular (corresponding to ''topologically integrable'' case) if it lies within the straight line of finite width in $\mathbb{R}^2$ and passes through it from $-\infty$ to ∞ [see Fig. 3(a)] All other open trajectories we will call chaotic [Fig. 3(b)].

In the simple case of periodic function $V(\mathbf{r})$ ($N=2$) all open trajectories are periodic and we have only a ''topologically regular'' case according to our classification. However, in the quasiperiodic case the situation is much more complicated and the chaotic trajectories can exist already

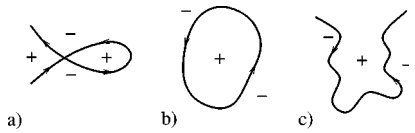

FIG. 2. The singular, compact and open nonsingular quasiclassical trajectories. The signs ''+'' and ''−'' show the regions of larger and smaller values of $V(\mathbf{r})$, respectively.

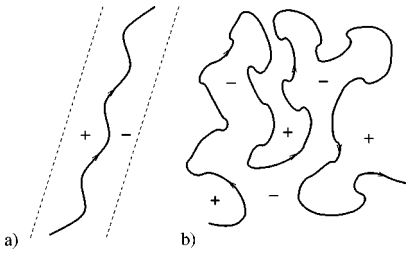

FIG. 3. "Topologically regular" (a) and "chaotic" (b) level curves of the function $V(\mathbf{r})$ in the plane $\mathbb{R}^2$.

for $N=3$.[16,22] These special trajectories can reveal rather complicated stochastic behavior for the general quasiperiodic potentials but fortunately the "generic" open trajectories are still topologically regular for the case $N=3$. Let us point out that this fact was formulated first by Novikov in the form of conjecture and plays now (together with "topological resonance") the crucial role for topological phenomena in normal metals (Refs. 19, 25, 30). Here we are also going to consider mainly the "topologically regular" situation for $N=3$ and $N=4$, and we will show that the same "topological numbers" can be observed also for two-dimensional electron gas in the specific potentials (quasiperiodic superlattices) built by the special experimental techniques in 2-dimensional structures.

Let us describe now the quasiclassical approach for the two-dimensional electron gas that we are going to consider.

The quasiclassical consideration of the 2-D electron gas in the presence of rather strong magnetic field B and a potential $V(\mathbf{r})$ was started in Ref. 36 in connection with the oscillations of conductivity discovered in Ref. 33. The experiment in Ref. 33 (Weiss, Klitzing, Ploog, and Weimann) used the holographic illumination of high mobility AlGaAS–GaAS heterojunctions at the temperatures $T\leqslant 4.2$ K. The expanded laser beam was split into two parts which gave an interference picture with the period a on the two-dimensional sample. The magnetic field $\mathbf{B}$ was directed normally to the sample and the electron behavior was determined by the magnetic field and the additional periodic potential,

$$V(\mathbf{r})=V(x), \quad V(x+a)=V(x),$$

arising after the holographic illumination. The amplitude of $V(x)$ was much smaller than the Fermi energy of the system. Measuring the resistivity in the both directions along and perpendicular to the interference fringes the authors of Ref. 33 found the magnetoresistance oscillations in $1/B$ for magnetic fields smaller than needed for Shubnikov–de Haas oscillations.

This phenomenon was explained by Beenakker in Ref. 36 from the quasiclassical consideration and called the "Commensurability oscillations." According to the quasiclassical approach the potential $V(x)$ should be averaged over the quasiclassical electron cyclotron orbit with radius $r_B=mv_F/eB$ on the Fermi level to get the effective averaged potential $\overline{V}(x,B)=V_B^{\text{eff}}(x)$ depending on the magnetic field B. The condition of weakness of potential $V(x)$ $[eV_{\text{rms}}/\epsilon_F\ll 1$, where V_{rms} is the root mean square of $V(x)]$ should be imposed in this situation. The drift of the center of cyclotron orbit is then given by the equation

$$\frac{d\mathbf{r}_0}{dt}=\frac{e}{B^2}[\nabla V_B^{\text{eff}}(\mathbf{r}_0)\times\mathbf{B}]. \tag{1}$$

According to (1) we have the drift of the centers of cyclotron orbits along the level curves of $V_B^{\text{eff}}(\mathbf{r})=V_B^{\text{eff}}(x)$ with the speed proportional to $\|\nabla V_B^{\text{eff}}(\mathbf{r})\|$ on these curves. As was pointed out in Ref. 36 the drifting motion gives the anisotropic contribution to the conductivity in the plane depending on the potential $V_B^{\text{eff}}(x)$. The crucial role for the magnetoresistance oscillations is then played by the strong dependence of $V_B^{\text{eff}}(\mathbf{r})$ on the value of B connected with the commensurability

of the cyclotron radius r_B (for a given Fermi energy) and the period of potential a. The corresponding contribution to the conductivity was thus the oscillating function of $1/B$ due to the periodic commensurability $2r_B=ka$ with some integer k.

The explicit formulas for the conductivity was obtained in Ref. 36 for the model potential having the form $V(x)=V_x\cos 2\pi x/a$. Obviously the main features of this picture will also be true for many generic periodic potentials $V(x)$. Let us also give here the references on the papers in Refs. 34, 35, 37, 42, 44, 45, 47–52, 54, 57, 60, 61, where different questions connected with this problem were considered (we are sorry for the impossibility to give here the complete list of works in this area).

Let us consider now the works where the situation of potentials $V(\mathbf{r})$ modulated both in the x and y directions was considered. The potential $V(\mathbf{r})=V(x,y)$ was induced in this case by the two independent sets of interference fringes parallel to the x and y axes and the potential $V(x,y)$ was the periodic function in $\mathbb{R}^2$ with two periods given by vectors $(a,0)$ and $(0,a)$.

As was found experimentally,[47,49,50] the additional modulation in the y direction suppresses the commensurability oscillations in this case. The quasiclassical consideration of this situation was made in Ref. 58 where again the drift of electron orbits along the constant energy levels of potential $V(x,y)$ was considered. Two types of the drift trajectories were considered in Ref. 58: (1) the ''pinned orbits'' (corresponding to compact energy level curves); (2) the ''drifting orbits'' (corresponding to unbounded energy level curves in the plane).

As was assumed in Ref. 58 only the contribution of the ''drifting orbits'' was important for the commensurability oscillations in this case and the ''pinned orbits'' were unessential for this phenomenon. According to this assumption the suppression of the commensurability oscillations can be explained by the appearance of the ''pinned orbits'' for the potentials modulated both in the x and y directions. Unlike the case of potentials modulated just in the x direction the new condition that the compact trajectories are passed many times by the centers of cyclotron orbits between two scattering acts appeared in Ref. 58. This requirement is similar to the condition of the ''geometric strong magnetic field limit'' considered in Refs. 1–3 for normal metals. However, the limit $B\to\infty$ does not correspond to the geometric limit in this situation and only $\tau\to\infty$ should be considered as the geometric limit for this case. It is easy to see also that only periodic ''drifting orbits'' can appear for purely periodic potentials $V(x,y)$.

Let us also point out here that the analytic dependence of the resistance on the value of B was also calculated in Ref. 58 in the interesting interval for the model potentials having few harmonics. This dependence is more complicated compared with the case of 1-D modulated potentials but still reveals the effect of commensurability also in this situation. The mean directions of trajectories that appeared in Ref. 58 were parallel to x and y axes and to the diagonal $y=-x$ in the different examples. As was also pointed out in Ref. 58 the ''drifting orbits'' can exist only for potentials with the broken rotational symmetry which explains the maximal suppression of the commensurability oscillations for the case of equal modulation intensity in both the x and y directions.

In this paper we will not consider in detail the B-dependence of conductivity for our more complicated potentials since it should reveal much more complicated behavior in this case. Instead we are going to consider the geometric properties of the conductivity tensor in the limit $\tau\to\infty$ arising from the global geometry of nonsingular open trajectories. Namely, we will show that this type of potential can be considered as the particular case of the quasiperiodic potentials with the fixed number of quasiperiods and use the results obtained for the Novikov problem to get the ''topological characteristics'' of the conductivity in this case. Let us say that this type of ''topological quantities'' arise in the completely different way compared, for example, with the Hall effect and characterize the geometry of the asymptotic of the conductivity tensor (but not its absolute values).

We will not also put any special conditions on potential $V(x,y)$ except the quasiperiodic properties. The formulated results will have the general topological form valid for the generic potentials $V(x,y)$.

Before we start the geometric consideration we want to say also that the holographic illumination is not the unique way to produce the superlattice potentials for the two-dimensional electron

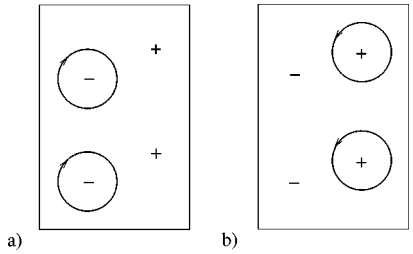

FIG. 4. The level curves of $f(\mathbf{r})$ close to the minimal and maximal values of f.

gas. Let us mention here the works,[38–41,43,46,47,50,53,55,56] where the different techniques using the biasing of the specially made metallic gates and the piezoelectric effect were considered. Both 1-D and 2-D modulated potentials as well as more general periodic potentials with square and hexagonal geometry appeared in this situation. We want to point out that the quasiperiodic potentials can also be made by these techniques in the same way using the superposition of several 1-D modulations. Actually these techniques give even more possibilities to produce the potentials of different types even for the quasiperiodic situation. For example, the superposition of the general periodic potential with the generic 1-D modulation will give the quasiperiodic potentials with 3 quasiperiods which are more general than made just by 3 interference pictures. Also the superpositions of two general periodic potentials on the plane will give the class of the quasiperiodic potentials with 4 quasiperiods more general than those which we will consider in detail here. However, we would like for simplicity to restrict ourselves to the simpler pictures of superpositions of 1-D modulation pictures which give already all the features of general behavior. We will also use everywhere the term ''interference picture'' for the modulation pictures. The general geometrical results will then be true for the other techniques also.

IV. NOVIKOV PROBLEM AND THE GEOMETRIC LIMIT FOR THE CASE OF 3 QUASIPERIODS

Let us come now to the Novikov problem and start the topological consideration of the level curves of quasiperiodic functions.

We will first describe the situation for the arbitrary periodic potential $V(x,y)$ with some periods $\mathbf{l}_1,\mathbf{l}_2 \in \mathbb{R}^2$. This picture is rather simple from the topological point of view but it is convenient to give it here just to introduce the notations and to show the general approach which we are going to use. Let us consider the generic periodic function $f(\mathbf{r})$ on $\mathbb{R}^2$ with the values belonging to some interval $[f_{\min},f_{\max}]$. We are interested in the form of the level curves $f(\mathbf{r})=c$ where $f_{\min}\leqslant c\leqslant f_{\max}$. It is easy to see that for the values of c close to the minimal or maximal value of f all such level curves are just the small closed loops bounding the small regions of lower or higher values of f [see Figs. 4(a) and 4(b)].

It is not difficult to prove also that the extended trajectories (singular or nonsingular) always exist in some closed connected ''energy interval'' $f_1\leqslant c\leqslant f_2$ ($f_{\min}<f_1\leqslant f_2<f_{\max}$). In a generic situation we have $f_1<f_2$, but for special functions $f(\mathbf{r})$ also the case $f_1=f_2$ is possible. This fact is actually true for any quasiperiodic function and does not depend on the number of quasiperiods (the proof in Ref. 22 given for $N=3$, works actually for any N without any change). Every nonsingular open trajectory is periodic for the periodic function $f(\mathbf{r})$ with the mean direction given by some integral vector $\mathbf{l}=m_1\mathbf{l}_1+m_2\mathbf{l}_2$ of lattice generated by periods $\mathbf{l}_1,\mathbf{l}_2$. We can see then that every nonsingular open trajectory for periodic $f(\mathbf{r})$ corresponds to ''topologically regular'' case.

It is easy to see also that there can be only the finite number of energy levels for the periodic Morse function where the singular trajectories can exist. We can claim then that the nonsingular open trajectories always exist in the generic case $f_1<f_2$. The opposite statement is also true since

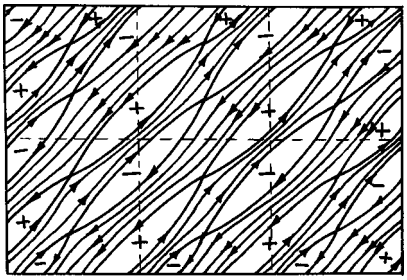

FIG. 5. The layers of open periodic trajectories with the ''nontrivial'' opposite directions [(1,1) and $(-1,-1)$] for the generic periodic function $f(\mathbf{r})$.

the nonsingular open trajectories are stable with respect to the small change of energy level. The typical situation of the generic case with the layers of open trajectories is shown in Fig. 5.

All the open trajectories do not intersect each other and have the common mean direction passing in both the ''direct'' and the ''opposite'' way.

The opposite nongeneric case $f_1=f_2$ corresponds to the absence of the nonsingular open trajectories in the plane. The typical picture for $f_1=f_2$ is a ''singular net'' on the level $f(\mathbf{r})=f_1=f_2$ and the closed trajectories at all the other levels (Fig. 6). Let us pay here special attention to the last fact to compare this situation with the more complicated quasiperiodic case.

It follows also that the case $f_1=f_2$ always takes place for potentials with any kind of rotational symmetry since the nonsingular open trajectories cannot exist in this situation.

Let us give here also the references on the work[59] where the nice quantization picture based on the topology of periodic quasiclassical drift trajectories in the magnetic field was considered.

The generic periodic potentials $V(\mathbf{r})$ arise in the experiments described above when the two independent interference pictures with arbitrary directions of interference fringes are present at the same sample. The potential $V(\mathbf{r})$ is a functional of the total intensity of radiation $I(\mathbf{r})$ and has the same periodicity for any (even nonlocal) translationally invariant dependence of $V(\mathbf{r})$ on the field $I(\mathbf{r}')$. For simplicity we will put the requirement that the functional $V(\mathbf{r})[I]$ has the variational derivative $\delta V(\mathbf{r})/\delta I(\mathbf{r}')$ decreasing for large enough $|\mathbf{r}-\mathbf{r}'|$. We assume also that the functional $V(\mathbf{r})[I]$ is smooth, i.e., gives the smooth function $V(\mathbf{r})$ for any smooth distribution $I(\mathbf{r}')$.

Let us now come to our main purpose and consider the potentials $V(\mathbf{r})$ having the more complicated form. Let us have now three independent interference pictures on the plane with three different generic directions of fringes $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \boldsymbol{\eta}_3$ and periods a_1, a_2, a_3 (see Fig. 7).

The total intensity $I(\mathbf{r})$ will be the sum of intensities,

$$I(\mathbf{r})=I_1(\mathbf{r})+I_2(\mathbf{r})+I_3(\mathbf{r}),$$

of the independent interference pictures.

We assume that there are at least two noncoinciding directions (say $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2$) among the set $(\boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \boldsymbol{\eta}_3)$.

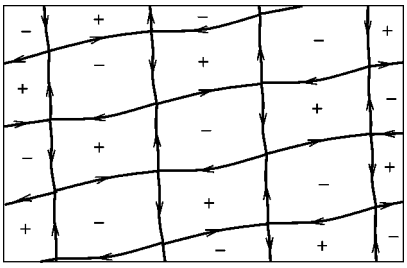

FIG. 6. The singular periodic net on the level $f(\mathbf{r})=f_1=f_2$ for the nongeneric periodic function $f(\mathbf{r})$.

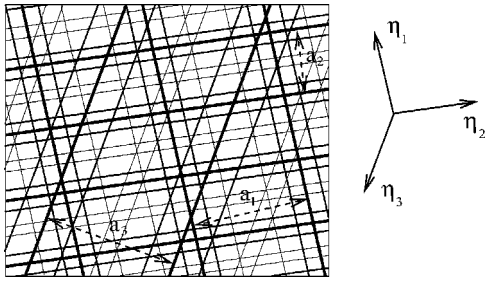

FIG. 7. The schematic sketch of the three independent interference pictures on the plane with different periods and intensities.

Let us draw three straight lines q_1, q_2, q_3 with the directions $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \boldsymbol{\eta}_3$ and choose the "positive" and "negative" half-planes for every line q_i on the plane. Let us consider now three linear functions $X(\mathbf{r})$, $Y(\mathbf{r})$, $Z(\mathbf{r})$ on the plane which are the distances from the point $\mathbf{r}$ to the lines q_1, q_2, q_3 with the signs "+" or "−" depending on the half-plane for the corresponding line q_i (Fig. 8).

The coordinates

$$\mathbf{R}(\mathbf{r}) = (X(\mathbf{r}), Y(\mathbf{r}), Z(\mathbf{r}))$$

now give the parametric representation of our plane $\Pi^2 = \mathbb{R}^2$ in the 3-dimensional space $\mathbb{R}^3$. The total intensity $I(\mathbf{r})$ can be considered then as the restriction to Π^2 of the periodic function $\hat{I}(X,Y,Z)$:

$$\hat{I}(X,Y,Z) = I_1(X) + I_2(Y) + I_3(Z),$$

corresponding to the lattice in $\mathbb{R}^3$ generated by vectors $(a_1,0,0)$, $(0,a_2,0)$, $(0,0,a_3)$. The plane Π^2 passes through the origin according to Fig. 8 (although it is not necessary if the lines q_1, q_2, q_3 do not intersect at one point in $\mathbb{R}^2$).

Let us point out here that the standard inner product on the plane Π^2 does not coincide with the product in $\mathbb{R}^3$ in this construction [from the metric point of view the plane $\mathbb{R}^2$ will be linearly deformed in the embedding $\mathbf{R} = \mathbf{R}(x,y)$]. However, the inner product will not be important at all in our further considerations so we do not pay any attention to this fact. Let us just say that it is possible to introduce the special inner product in $\mathbb{R}^3$ such that it's restriction on Π^2 will give the standard metric in $\mathbb{R}^2$. Nevertheless, all the topological statements will be invariant under the group of all nondegenerate linear transformations and we will not need this construction at all.

We can define now the smooth periodic functions $\hat{V}(X,Y,Z)$ and $\hat{V}_B^{\text{eff}}(X,Y,Z)$ in $\mathbb{R}^3$ such that the functions $V(x,y)$ and $V_B^{\text{eff}}(x,y)$ will be the restrictions of $\hat{V}(X,Y,Z)$ and $\hat{V}_B^{\text{eff}}(X,Y,Z)$ on the plane Π^2. Indeed, consider any point $\mathbf{R} = (X,Y,Z) \in \mathbb{R}^3$. Let us draw the two-dimensional plane

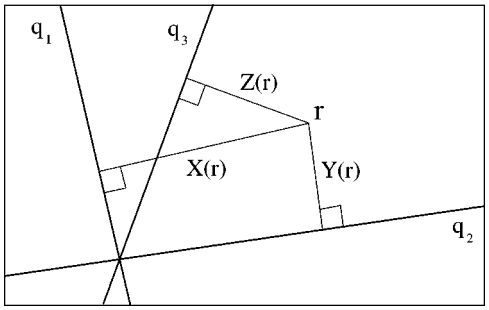

FIG. 8. The coordinates $X(\mathbf{r})$, $Y(\mathbf{r})$ and $Z(\mathbf{r})$ on the plane.

$\Pi^{2\prime}$ through the point $\mathbf{R}$ parallel to the plane Π^2. We have then the total intensity $I'(\mathbf{R})$ in the plane $\Pi^{2\prime}$ defined as the restriction of $\hat{I}(X,Y,Z)$ on $\Pi^{2\prime}$. Let us define now the functions $\hat{V}(X,Y,Z)$ and $\hat{V}_B^{\text{eff}}(X,Y,Z)$ at the point $\mathbf{R}$ as the corresponding functions defined in the plane $\Pi^{2\prime}$ passing through $\mathbf{R}$ using the functional $V(\mathbf{r})[I]$ and the averaging over the cyclotron orbits in $\Pi^{2\prime}$. It is easy to see that the functions $\hat{V}(X,Y,Z)$, $\hat{V}_B^{\text{eff}}(X,Y,Z)$ are the smooth periodic functions in $\mathbb{R}^3$ with periods $(a_1,0,0)$, $(0,a_2,0)$, $(0,0,a_3)$. Obviously the functions $\hat{V}|_{\Pi^2}$ and $\hat{V}_B^{\text{eff}}|_{\Pi^2}$ give the required potential $V(\mathbf{r})$ and the effective potential $V_B^{\text{eff}}(\mathbf{r})$ in the initial two-dimensional plane $\mathbb{R}^2$.

Let us introduce now the important definition of the ''quasiperiodic group'' acting on the potentials described above. As we saw, our construction gives us the embedding Π^2 of the initial plane $\mathbb{R}^2$ in the three-dimensional space $\mathbb{R}^3$. At the same time we get the additional planes $\Pi^{2\prime}$ in $\mathbb{R}^3$ parallel to Π^2 with different $I'(\mathbf{r})$, $V'(\mathbf{r})$, $V_B^{\text{eff}\prime}(\mathbf{r})$ corresponding to the same $\hat{I}(\mathbf{R})$, $\hat{V}(\mathbf{R})$ and $\hat{V}_B^{\text{eff}}(\mathbf{R})$. It is easy to see that the functions $I'(\mathbf{r})$, $V'(\mathbf{r})$, $V_B^{\text{eff}\prime}(\mathbf{r})$ correspond to the case of three interference pictures with the same mean directions of fringes and periods $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ but with shifted positions of maxima and minima for every interference picture.

Definition 4: We will say that all the potentials $V'(\mathbf{r})$ (*as well as* $V_B^{\text{eff}\prime}(\mathbf{r})$ *for every given* B) *are related by a "quasiperiodic group" of transformations.*

According to the Definition 4 we define the action of a ''quasiperiodic group'' in $\mathbb{R}^2$ as the parallel shifts of the plane Π^2 in the space $\mathbb{R}^3$. The ''quasiperiodic group'' is then the 3-parametric Abelian group isomorphic to 3-dimensional torus $\mathbb{T}^3=\mathbb{R}^3/L$,

$$L=m_1(a_1,0,0)+m_2(0,a_2,0)+m_3(0,0,a_3),$$

$$(m_1,m_2,m_3)\in\mathbb{Z}^3,$$

containing the (noncompact) algebraic subgroup of ordinary translations in $\mathbb{R}^2$.

As we will see below, this definition will be very convenient in the consideration of open trajectories for potentials of this type in $\mathbb{R}^2$. Namely, we will see that all the global properties of open trajectories will be the same for all potentials related by the ''quasiperiodic group'' in the case of generic $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$. In other words, for the generic $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ the global geometry of open trajectories will not depend on the positions of minima and maxima of the interference pictures and will be defined just by the set $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ and the intensities I_1, I_2, I_3 [although the potentials $V(\mathbf{r})$, $V_B^{\text{eff}}(\mathbf{r})$ will be different in these cases]. Let us say, however, that this property can be broken for the special $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ corresponding to purely rational directions of Π^2 in $\mathbb{R}^3$.

According to the previous definition we will say that the quasiperiodic potential has irrationality 3 or maximal irrationality if it has no periods in $\mathbb{R}^2$. We will say that the potential $V(\mathbf{r})$ has irrationality 2 if it has only one (up to the integer multiplier) period in $\mathbb{R}^2$. We will say that the potential $V(\mathbf{r})$ has irrationality 1 if it has two linearly independent periods in $\mathbb{R}^2$.[63] As can be easily seen the last case corresponds to the purely periodic potentials $V(\mathbf{r})$. It is easy to see also that the potentials $V(\mathbf{r})$ of irrationality 3, 2 and 1 correspond to the cases when the plane Π^2 contains no vectors belonging to L, just one (up to the integer multiplier) vector belonging to L and two linearly independent vectors belonging to L, respectively. Obviously all the potentials related by the ''quasiperiodic group'' have the same irrationality in the plane.

Let us discuss now briefly the connection of irrationality with the directions and periods of interference pictures in our situation.

We assume as previously that there are at least two different directions of the interference fringes in our picture. The picture given by the two corresponding sets of interference fringes is purely periodic in $\mathbb{R}^2$ with the periods $\mathbf{u}_1$, $\mathbf{u}_2$ parallel to $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$, respectively (see Fig. 9).

We can see then that the total picture has a period in $\mathbb{R}^2$ if some nontrivial integer linear combination,

$$m_1\mathbf{u}_1+m_2\mathbf{u}_2\ ,\quad (m_1,m_2)\in\mathbb{Z}^2/(0,0),$$

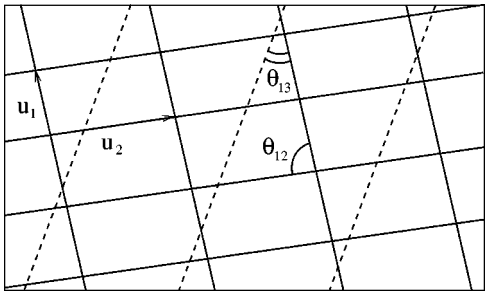

FIG. 9. The periodic picture formed by two sets of parallel interference fringes with common directions $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ and the added third set with direction $\boldsymbol{\eta}_3$.

of periods $\mathbf{u}_1$, $\mathbf{u}_2$ leaves invariant also the third interference picture corresponding to pair $(\boldsymbol{\eta}_3, a_3)$.

The corresponding condition for $m_1\mathbf{u}_1+m_2\mathbf{u}_2$ can then be written in the form

$$(m_1\mathbf{u}_1+m_2\mathbf{u}_2, \boldsymbol{\xi}_3)=ka_3 \quad , \quad k\in\mathbb{Z}, \tag{2}$$

where $\boldsymbol{\xi}_3$ is a unit vector orthogonal to $\boldsymbol{\eta}_3$ in the plane.

The equation (2) has no nontrivial solutions in the generic situation and can be satisfied only for special $\boldsymbol{\eta}_3$ and a_3. It is not difficult to show that for purely rational potentials $V(\mathbf{r})$ [two linearly independent solutions of (2)] the direction $\boldsymbol{\eta}_3$ should also correspond to the integer vector in the lattice L' generated by vectors $\mathbf{u}_1$, $\mathbf{u}_2$:

$$L'=\{m_1\mathbf{u}_1+m_2\mathbf{u}_2 \quad , \quad (m_1,m_2)\in\mathbb{Z}^2\}.$$

We can put for this case $\boldsymbol{\eta}_3 \sim m_1\mathbf{u}_1+m_2\mathbf{u}_2$ for some integer m_1, m_2. Also the corresponding period a_3 should satisfy the special condition in this situation. If we introduce the angles θ_{12}, θ_{13} between the directions $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ and $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_3$, $0<\theta_{12}\leqslant\pi/2$, $0<\theta_{13}\leqslant\pi$ (Fig. 9) we can get the relations for θ_{13} and a_3 which define all the pairs $(\boldsymbol{\eta}_3, a_3)$ corresponding to purely rational potentials $V(\mathbf{r})$:

$$tg\ \theta_{13}=\frac{m_2a_1\sin\theta_{12}}{m_1a_2-m_2a_1\cos\theta_{12}}, \tag{3}$$

$$k_3a_3\sin\theta_{12}=k_1a_1\sin(\theta_{12}+\theta_{13})+k_2a_2\sin\theta_{13}, \tag{4}$$

where $m_1,m_2,k_1,k_2,k_3\in\mathbb{Z}$, $(m_1,m_2)\neq(0,0)$, $(k_1,k_2)\neq(0,0)$, $k_3\neq0$.

For the case of just one period (irrationality 2) we can have either the condition (3) for θ_{13} (''+ rational'' direction of $\boldsymbol{\eta}_3$) but with a_3 not satisfying to (4) or the condition (4) for a_3 but with θ_{13} not satisfying to (3).

It is easy to see that both cases of irrationality 1 and 2 have the measure zero among all potentials constructed by three arbitrary interference pictures.

As we already said above the case of irrationality 1 corresponds to the purely periodic potentials $V(x,y)$. Let us however make here some remark. Namely, for arbitrary periodic potential $V(x,y)$ the corresponding periods $\mathbf{l}_1$, $\mathbf{l}_2$ can be much bigger than the values of a_1, a_2, a_3. We can conclude then that even the ''topologically regular'' periodic open trajectories can have a rather nontrivial structure on the rather long distances since the period of the trajectory is very big. The width of the straight line containing the periodic trajectory can be also compatible with periods of $V(x,y)$ in this case being quite big with respect to the periods of modulations a_1, a_2, a_3. Also the rational mean direction of the periodic trajectories can have a ''rather big denominator'' such that this rationality will not play an essential role in the real picture. Instead, the typical features observable in the generic situation of irrationality 3 will appear on the distances smaller than the

periods $|\mathbf{l}_1|$, $|\mathbf{l}_2|$ of potential $V(x,y)$. According to this remark we can actually try to consider the potentials of irrationality 1 or 2 as the generic potentials of irrationality 3 if the periods of these potentials are rather big. The special features connected with rationality can then be revealed only for very big values of τ such that the free motion length is much larger than $|\mathbf{l}_1|$, $|\mathbf{l}_2|$.

Let us formulate now (in our language) the first theorem about the open trajectories for the quasiperiodic potentials $V(\mathbf{r})$ and $V_B^{\text{eff}}(\mathbf{r})$ with 3 quasiperiods corresponding to the first theorem on the Novikov problem proved in Ref. 11.

Theorem 1: *Consider the purely periodic potential* $V^{(0)}(\mathbf{r})$ *(or* $V_B^{(0)\text{eff}}(\mathbf{r})$*) generated by three independent interference pictures with some parameters* $(\boldsymbol{\eta}_1^{(0)},a_1^{(0)})$, $(\boldsymbol{\eta}_2^{(0)},a_2^{(0)})$, $(\boldsymbol{\eta}_3^{(0)},a_3^{(0)})$ *satisfying to (3), (4). Then for all the potentials* $V(\mathbf{r})$ *(and* $V_B^{\text{eff}}(\mathbf{r})$*) with parameters* $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ *close enough to* $(\boldsymbol{\eta}_1^{(0)},a_1^{(0)})$, $(\boldsymbol{\eta}_2^{(0)},a_2^{(0)})$, $(\boldsymbol{\eta}_3^{(0)},a_3^{(0)})$ *all the open nonsingular electron trajectories will correspond to the topologically regular case only.*

Using the same methods as in Ref. 11 it is possible to prove also that Theorem 1 will be true also for small variations of the intensities $I_1(\mathbf{r})$, $I_2(\mathbf{r})$, $I_3(\mathbf{r})$ of the laser beams and the form of the functional $V(\mathbf{r})[I]$.

Let us say here that Theorem 1 makes a rather strong statement about the generic potentials close to periodic ones. However, the corresponding "stability zones" for parameters $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3)$ (and I_1, I_2, I_3) depend on the initial values of $(\boldsymbol{\eta}_1^{(0)},a_1^{(0)})$, $(\boldsymbol{\eta}_2^{(0)},a_2^{(0)})$, $(\boldsymbol{\eta}_3^{(0)},a_3^{(0)})$ and become very small for the large values of periods $|\mathbf{l}_1|$, $|\mathbf{l}_2|$ of the initial potential. Due to this reason Theorem 1 cannot say anything about arbitrary potential $V(\mathbf{r})$ (with 3 quasiperiods) since we can have the situation when it does not belong to any stability zone corresponding to any rational potential $V^{(0)}(\mathbf{r})$. Nevertheless, this theorem is very important and we will see also that only the result of this type can be formulated for the more complicated case of potentials with 4 quasiperiods.

Let us discuss now the general situation of arbitrary potentials $V(\mathbf{r})$ with 3 quasiperiods. We will start first with the generic situation of potentials of irrationality 3 and then discuss the additional features which can arise in the cases of irrationality 1 and 2. Let us make here the reference on the survey article,[26] where the final theorems in the most complete form were formulated. The development of this problem and the considerations of physical phenomena can be found in Refs. 10–30. Let us say also that all the results in Ref. 26 and in all previous papers were formulated in another language using the 3-dimensional topology terminology. We will not discuss here the topological questions in detail and just claim that the following statements can be derived from the topological theorems formulated in Ref. 26.

Theorem 2: *Let us fix the value of B and consider the generic quasiperiodic potential* $V_B^{\text{eff}}(\mathbf{r})$ *(of irrationality 3) taking the values in some interval* $\epsilon_{\min}(B)\leqslant V_B^{\text{eff}}(\mathbf{r})\leqslant\epsilon_{\max}(B)$*. Then we have the following.*

(1) Open quasiclassical trajectories $V_B^{\text{eff}}(\mathbf{r})=c$ *always exist either in the connected energy interval,*

$$\epsilon_1(B)\leqslant c\leqslant\epsilon_2(B)$$

$[\epsilon_{\min}(B)<\epsilon_1(B)<\epsilon_2(B)<\epsilon_{\max}(B)]$ *or just at one energy value* $c=\epsilon_0(B)$ *[i.e.* $\epsilon_1(B)=\epsilon_2(B)=\epsilon_0(B)$*].*

(2) For the case of the finite interval $[\epsilon_1(B)<\epsilon_2(B)]$ *all the nonsingular open trajectories correspond to the topologically regular case, i.e., lie in the straight strips of the finite width [Fig. 3(a)] and pass through them. All the strips have the same mean directions for all the energy levels* $c\in[\epsilon_1(B),\epsilon_2(B)]$ *such that all the open trajectories are on average parallel to each other for all values of* c*.*

(3) The values $\epsilon_1(B)$, $\epsilon_2(B)$ *or* $\epsilon_0(B)$ *are the same for all the potentials of irrationality 3 connected by the "quasiperiodic group."*

(4) For the case of the finite energy interval $[\epsilon_1(B)<\epsilon_2(B)]$ *all the nonsingular open trajectories also have the same mean direction for all the potentials (of irrationality 3) connected by the "quasiperiodic group."*

We can see from Theorem 2 that the ''topologically integrable'' situation is typical also for the case of quasiperiodic functions with 3 quasiperiods being connected with the generic case $\epsilon_1(B)<\epsilon_2(B)$. Let us say also that for the case of just one energy level $[\epsilon_1(B)=\epsilon_2(B)=\epsilon_0(B)]$ containing the open trajectories both the topologically regular and ''chaotic'' behavior of open trajectories are possible (see Ref. 22). This situation can be compared with the situation of purely periodic potentials where the nonsingular periodic open trajectories always appear in the case of a finite energy interval $[\epsilon_1(B)>\epsilon_2(B)]$ but only the periodic ''singular nets'' are possible for the case $\epsilon_1(B)=\epsilon_2(B)=\epsilon_0(B)$. As we see here the quasiperiodic potentials give another possibility in the last case.

Let us consider now the asymptotic behavior of conductivity in the case of topologically regular open trajectories when $\tau\to\infty$. According to previous papers[36,51,58] we will divide here the conductivity tensor in two parts $\sigma_0^{ik}(B)$ and $\Delta\sigma^{ik}(B)$ corresponding to the conductivity without any potential $V(\mathbf{r})$ and an additional contribution due to potential $V(\mathbf{r})$. We have then

$$\sigma^{ik}(B)=\sigma_0^{ik}(B)+\Delta\sigma^{ik}(B).$$

In the approximation of the drifting cyclotron orbits the parts $\sigma_0^{ik}(B)$ and $\Delta\sigma^{ik}(B)$ can be interpreted as caused, respectively, by the (infinitesimally small) difference in the electron distribution function on the same cyclotron orbit (weak angular dependence) and the (infinitesimally small) difference in the occupation of different trajectories by the centers of cyclotron orbits at different points of $\mathbb{R}^2$ (on the same energy level) as the linear response to the (infinitesimally) small external field $\mathbf{E}$. The asymptotic $\tau\to\infty$ of both parts $\sigma_0^{ik}(B)$ and $\Delta\sigma^{ik}(B)$ can then be written from the same arguments used in Refs. 1–3 with some additional remarks specific for this situation. We will just say here that the first part $\sigma_0^{ik}(B)$ has the standard asymptotic form:

$$\sigma_0^{ik}(B)\sim\frac{ne^2\tau}{m^{\mathrm{eff}}}\begin{pmatrix}(\omega_B\tau)^{-2} & (\omega_B\tau)^{-1}\\ (\omega_B\tau)^{-1} & (\omega_B\tau)^{-2}\end{pmatrix},$$

for $\omega_B\tau\gg 1$ due to the weak angular dependence ($\sim 1/\omega_B\tau$) of the distribution function in the same cyclotron orbit. We have then that the corresponding longitudinal conductivity decreases for $\tau\to\infty$ in all the directions in $\mathbb{R}^2$ and the corresponding condition is just $\omega_B\tau\gg 1$ in this case.

For the part $\Delta\sigma^{ik}(B)$ the limit $\tau\to\infty$ should, however, be considered as the condition that every trajectory is passed for a rather long time by the drifting cyclotron orbits to reveal its global geometry. Thus another parameter τ/τ_0 where τ_0 is the characteristic time of completion of close trajectories should be used in this case and we should put the condition $\tau/\tau_0\gg 1$ to have the asymptotic regime for $\Delta\sigma^{ik}(B)$. In this situation the difference between the open and closed trajectories plays the main role and the asymptotic behavior of conductivity can be calculated in the form analogous to that used in Refs. 1–3 for the case of normal metals. Namely,

$$\Delta\sigma^{ik}(B)\sim\frac{ne^2\tau}{m^{\mathrm{eff}}}\begin{pmatrix}(\tau_0/\tau)^2 & \tau_0/\tau\\ \tau_0/\tau & (\tau_0/\tau)^2\end{pmatrix},$$

in the case of closed trajectories and

$$\Delta\sigma^{ik}(B)\sim\frac{ne^2\tau}{m^{\mathrm{eff}}}\begin{pmatrix}* & \tau_0/\tau\\ \tau_0/\tau & (\tau_0/\tau)^2\end{pmatrix},$$

$(*\sim 1)$ for the case of open topologically regular trajectories if the x-axis coincides with the mean direction of trajectories.

We can see then that only the contribution of open orbits to $\Delta\sigma^{ik}(B)$ remains in (longitudinal) conductivity for $\tau\to\infty$. Let us say that these formulas give just the asymptotic form of conductivity for $\tau\to\infty$. In the more precise form they should include also the multipliers proportional to

the parts of the phase volume filled by the closed and open trajectories and the appropriate definition of m^{eff} in this situation. We will not, however, consider this part in detail since we will need only the anisotropy of the tensor σ^{ik} in the ''geometric limit.''

The condition $\tau/\tau_0 \gg 1$ is much stronger than $\omega_B \tau \gg 1$ in the situation described above just according to the definition of the slow drift of the cyclotron orbits. We can keep then just this condition in our further considerations and assume that the main part of conductivity is given by $\Delta\sigma^{ik}(B)$ in this limit. It is easy to see also that the magnetic field B should not be ''very strong'' in this case.

According to the remarks above we can write now the main part of the conductivity tensor $\sigma^{ik}(B)$ in the limit $\tau \to \infty$ for the case of topologically regular open orbits. Let us take the x axis along the mean direction of open orbits and take the y axis orthogonal to x. The asymptotic form of σ^{ik}, $i,k=1,2$ can then be written as

$$\sigma^{ik} \sim \frac{ne^2\tau}{m^{\text{eff}}} \begin{pmatrix} * & \tau_0/\tau \\ \tau_0/\tau & (\tau_0/\tau)^2 \end{pmatrix}, \quad \tau_0/\tau \to 0, \tag{5}$$

where $*$ is some value of order of 1 (constant as $\tau_0/\tau \to 0$).

The asymptotic form of σ^{ik} makes possible the experimental observation of the mean direction of topologically regular open trajectories if the value τ/τ_0 is rather big.

Let us introduce here the ''topological numbers'' characterizing the regular open trajectories introduced first in Ref. 19 for the case of normal metals. We will give the topological definition of these numbers using the action of the ''quasiperiodic group'' on the quasiperiodic potentials. Let us assume for simplicity that the potential $V_B^{\text{eff}}(\mathbf{r})$ is generic and has irrationality 3. We assume that we have the ''topologically integrable'' situation where the topologically regular open trajectories exist in some finite energy interval $\epsilon_1(B) \leqslant c \leqslant \epsilon_2(B)$. According to Theorem 2 the values $\epsilon_1(B)$, $\epsilon_2(B)$ and the mean directions of open trajectories are the same for all the potentials constructed from our potential with the aid of the ''quasiperiodic group.'' It follows also from the topological picture that all the topologically regular trajectories are absolutely stable under the action of the ''quasiperiodic group'' (for the case of irrationality 3) and can just ''crawl'' in the plane for the continuous action of such transformations.

Let us make now the following transformation.

We take the first interference picture $((\boldsymbol{\eta}_1, a_1))$ and shift continuously the interference fringes in the direction of $X(\mathbf{r})$ (orthogonal to $\boldsymbol{\eta}_1$) to the distance a_1 keeping two other interference pictures unchanged. It is easy to see that we will have at the end the same potentials $V(x,y)$ and $V_B^{\text{eff}}(x,y)$ due to the periodicity of the first interference picture with period a_1. Let us fix now some energy level $c \in (\epsilon_1(B), \epsilon_2(B))$ and look at the evolution of nonsingular open trajectories [for $V_B^{\text{eff}}(x,y)$] while making our transformation. We know that we should have the parallel open trajectories in the plane at every time and the initial picture should coincide with the final picture according to the construction. The form of trajectories can change during the process but their mean direction will be the same according to Theorem 2.[64]

We can claim then that every open trajectory will be ''shifted'' to another open trajectory of the same picture by our continuous transformation. It is not difficult to prove that all the trajectories will then be shifted by the same number of positions n_1 (positive or negative) which depends on the potential $V_B^{\text{eff}}(x,y)$ (Fig. 10).

The number n_1 is always even since all the trajectories appear by pairs with the opposite drift directions.

Let us now do the same with the second and the third sets of the interference fringes and get an integer triple (n_1, n_2, n_3) which is a topological characteristic of potential $V_B^{\text{eff}}(x,y)$ (the ''positive'' direction of the numeration of trajectories should be the same for all these transformations).

The triple (n_1, n_2, n_3) (defined up to the common sign) can be represented as

$$(n_1, n_2, n_3) = M\,(m_1, m_2, m_3),$$

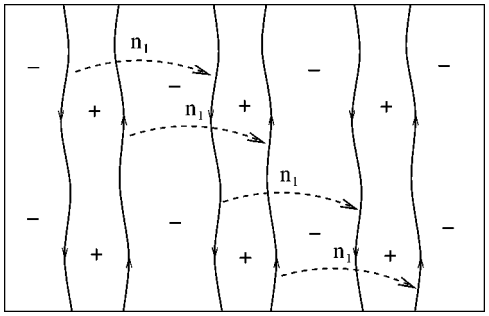

FIG. 10. The shift of "topologically regular" trajectories by a continuous transformation generated by the special path in the "quasiperiodic group."

where $M \in \mathbb{Z}$ and (m_1,m_2,m_3) is the indivisible integer triple. Both M and (m_1,m_2,m_3) have the topological meaning connected with the number of connected components carrying open trajectories in $\mathbb{R}^3$ and the homological class of every component in $\mathbb{T}^3=\mathbb{R}^3/L$ up to the sign.

Let us mention that for periodic potentials $V(x,y)$ made just by two interference pictures with common directions $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ the corresponding transformations are actually equivalent to the shifts along the periods $\mathbf{u}_2$ and $\mathbf{u}_1$, respectively (Fig. 9). It is not difficult to see that the corresponding numbers (m_1,m_2) are equal then (up to the common sign) to $(-i_1,i_2)$ where (i_1,i_2) is the indivisible integer mean direction of periodic open trajectories in the lattice L' generated by vectors $\{\mathbf{u}_1,\mathbf{u}_2\}$. It is easy to see also that the vectors $\{X(\mathbf{r})/a_1, Y(\mathbf{r})/a_2\}$ give the dual basis to the basis $\{\mathbf{u}_2,\mathbf{u}_1\}$ and the mean direction of open orbits can be defined from the linear equation

$$m_1X(\mathbf{r})/a_1+m_2Y(\mathbf{r})/a_2=0$$

on the plane.

It can be proved that the similar situation also takes place for the topologically regular open trajectories in the case of quasiperiodic potentials $V(\mathbf{r})$. Let us omit here the detailed consideration of the topological picture and just say that the common direction of open trajectories in $\mathbb{R}^2$ is defined completely by the triple (m_1,m_2,m_3). Let us formulate here the corresponding statement:

Theorem 3: *Consider the functions*

$$X'(\mathbf{r})=X(\mathbf{r})/a_1\ ,\ \ Y'(\mathbf{r})=Y(\mathbf{r})/a_2\ ,\ \ Z'(\mathbf{r})=Z(\mathbf{r})/a_3,$$

in $\mathbb{R}^2$. *The mean direction of the regular open trajectories is given by the linear equation:*

$$m_1X'(x,y)+m_2Y'(x,y)+m_3Z'(x,y)=0 \tag{6}$$

where (m_1,m_2,m_3) *is the indivisible integer triple introduced above.*

The triples (m_1,m_2,m_3) coincide precisely with the "Topological Quantum Numbers" introduced in Ref. 19 for the conductivity in normal metals. Let us say that the condition (6) determines completely the numbers (m_1,m_2,m_3) (from the mean direction of open trajectories) for potentials of irrationality 3. This fact permits us to extract the values of (m_1,m_2,m_3) from the direct conductivity observations using the anisotropy of tensor $\sigma^{ik}(B)$. [The formula (6) is also true for the case of so-called "stable" open trajectories for potentials of irrationality 1 and 2 (see below). The triple (m_1,m_2,m_3) generally speaking may not be defined uniquely from the mean directions of open trajectories in these cases and the arguments based on quasiperiodic group play then the main role in the definition of (m_1,m_2,m_3). However, it can be measured from the direct conductivity observations also in these cases due to the stability of these numbers with respect to the small change of parameters $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$.]

The very important property of the integer triples (m_1,m_2,m_3) is their stability with respect to the small variations of all the parameters $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, a_1, a_2, a_3, I_1, I_2, I_3 and even of the form of dependence $V(\mathbf{r})[I]$. This means that the space of parameters $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$ where the situation $\epsilon_2(B)>\epsilon_1(B)$ for the energy interval containing the open trajectories takes place can be divided into different ''stability zones'' Γ_α where the relations (6) are valid for generic $V_B^{\mathrm{eff}}(\mathbf{r})$ with the same values of $(m_1^\alpha,m_2^\alpha,m_3^\alpha)$. Let us emphasize here that the mean directions of open trajectories are different for the different values of parameters even within the same stability zone Γ_α and the equation (6) gives the fixed relation of these directions with the directions and periods of the interference fringes for a given stability zone.

The zones Γ_α form an everywhere dense set in the total space of parameters and in general we can have an infinite number of zones parametrized by the numbers $(m_1^\alpha,m_2^\alpha,m_3^\alpha)$. The triples $(m_1^\alpha,m_2^\alpha,m_3^\alpha)$ form some subset of all possible integer triples (m_1,m_2,m_3) (defined up to the common sign) and give an important topological characteristic of the potentials $V_B^{\mathrm{eff}}(\mathbf{r})$ made by 3 interference pictures. The sizes of zones Γ_α decrease for the big numbers $(m_1^\alpha,m_2^\alpha,m_3^\alpha)$ and the total set $\{\cup\Gamma_\alpha\}$ give a rather complicated subset in the space of parameters $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$. Let us say also that the topologically regular open trajectories are also stable with respect to any variation of potential $V_B^{\mathrm{eff}}(\mathbf{r})$ small enough which makes it possible to observe them also for slightly imperfect quasiperiodic potentials $V(\mathbf{r})$.

Before starting with special possibilities for the periodic (irrationality 1) or ''partly periodic'' (irrationality 2) potentials we will say here some words about the ''chaotic'' behavior of open trajectories possible in the case $\epsilon_1(B)=\epsilon_2(B)=\epsilon_0(B)$. Let us say that for $\epsilon_1(B)=\epsilon_2(B)$ both the situations of topologically regular and chaotic behavior of open trajectories are possible in the quasiperiodic case. The first situation always takes place when the corresponding set $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$ belongs to the boundary of some stability zone Γ_α in the space of parameters. In this case all the nonsingular open trajectories are topologically regular and correspond to the same numbers $(m_1^\alpha,m_2^\alpha,m_3^\alpha)$. Another situation arises when the set $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$ is an accumulation point for the zones Γ_α but does not belong to the boundary of any Γ_α. In this situation much more complicated chaotic behavior of open orbits appear at the energy level $V_B^{\mathrm{eff}}(\mathbf{r})=\epsilon_0(B)$. Obviously the ''chaotic'' behavior can be possible only for potentials of irrationality 2 or 3. Let us say also that the cases of irrationality 2 (Tsarev chaotic behavior) and 3 (Dynnikov chaotic behavior) demonstrate completely different types of chaotic behavior in this situation.

The first example of chaotic open trajectory was constructed by Tsarev[16,22] for the case of irrationality 2. The corresponding chaotic trajectory, however, has an asymptotic direction but cannot be bounded by any straight strip of the finite width in $\mathbb{R}^2$. As was later proved by Dynnikov,[22] this situation always takes place for chaotic trajectories in the case of irrationality 2. The asymptotic behavior of the conductivity tensor reveals also the strong anisotropy for large τ in this situation with slightly different from (5) dependence on τ for $\tau\to\infty$.

The more complicated chaotic trajectories were constructed by Dynnikov[22] for the case of irrationality 3 (the approximate form of such kinds of trajectories is shown in Fig. 3(b). The trajectories of this second kind do not have any asymptotic direction in $\mathbb{R}^2$ ''walking everywhere'' in the plane. The form of the conductivity tensor for this type of trajectory was suggested in Ref. 24 and is more complicated, then (5). We will not discuss here all the details and just say that the conductivity decreases in this case in all directions for $\tau\to\infty$ as some noninteger powers of τ.[65] Let us also add here that all the chaotic trajectories are completely unstable with respect to the small variations of parameters $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$ (but remain chaotic with the ''same geometric properties'' under the action of the ''quasiperiodic group'').

Let us discuss also the B-dependence of tensor $\sigma^{ik}(B)$ for the limit $\tau\to\infty$. The value of B belongs here to some interval $B_1\leqslant B\leqslant B_2$ such that both the drifting orbits approximation and the condition $\tau/\tau_0\gg 1$ (as well the absence of quantum oscillations) are true. The effective potential $V_B^{\mathrm{eff}}(\mathbf{r})$ is a function of B in this case and the geometry of trajectories depends on B through the potential $V_B^{\mathrm{eff}}(\mathbf{r})$. Let us just say here that it can also be proved using topological considerations that the topologically regular open orbits are also ''locally stable'' with respect to the small

variations of B. However, for rather big changes of value of B it is possible to have ''jumps'' in this picture and get different mean directions of open trajectories (as well as the chaotic cases) in the different parts of the interval $[B_1,B_2]$. Let us add also that the structure of the B dependence can be rather complicated in this case containing the infinite number of small subintervals with very big numbers (m_1,m_2,m_3) as well as the chaotic cases.

Actually, all the theorems 1–3 can be reformulated in the same form if we add the parameter B to parameters $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, a_1, a_2, a_3, I_1, I_2, I_3 introduced above. The probability of ''jumps'' will then increase for the small stability zones Γ_α corresponding to big numbers (m_1,m_2,m_3) and the B-dependence of $\sigma^{ik}(B)$ will depend strongly on the part of the phase space. The chaotic trajectories will be completely unstable with respect to any small variations of B.

In the same way we can consider the ''stability zones'' $\Gamma_\alpha^{\text{ext}}$ in the extended space of parameters including the value of the magnetic field B. The total set $\{\cup\Gamma_\alpha^{\text{ext}}\}$ will have then the analogous structure containing in general the infinite number of zones $\Gamma_\alpha^{\text{ext}}$ and triples (m_1,m_2,m_3) being everywhere dense in the total set of parameters.

Let us formulate now the general conjecture of Novikov about the chaotic cases for potentials with 3 quasiperiods. In our situation we will assume that potentials are parametrized by parameters,

$$(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3)$$

or

$$(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3,I_1,I_2,I_3,B),$$

and maybe some additional parameters characterizing the functional $V(\mathbf{r})[I]$.

Novikov conjecture: The set of parameters corresponding to the chaotic behavior of open trajectories has measure zero in the total space of parameters.

Let us point out that the Novikov conjecture was strictly proved in the important case when only the quasiclassical trajectories belonging to some fixed energy level are taken into account.[22] This is precisely the situation arising in the conductivity in normal metals where only the trajectories close to the Fermi surface are important. The more general situation was also investigated numerically[29] for the case of the special analytic dispersion relations where the Novikov conjecture was also confirmed. However, the general proof of Novikov conjecture for an arbitrary set of parameters is still unknown.

We will point out now some additional possibilities which can arise in the nongeneric case of potentials of irrationality 1 or 2 (see Ref. 26 for detailed mathematical considerations).

Let us start with the case of irrationality 2 when only one period $\mathbf{l}$ (up to the integer multiplier) exists in $\mathbb{R}^2$. All the parts (1)–(4) of Theorem 2 are also true for potentials of irrationality 2. We need, however, to make one remark about the situation when the mean direction of the ''topologically regular'' open trajectories coincides with the period $\mathbf{l}$ of potential. Easy to see that the open trajectories are actually periodic in $\mathbb{R}^2$ in this case with the same period $\mathbf{l}$. In this situation some ''additional pairs'' of periodic open trajectories can arise and disappear under the action of the ''quasiperiodic group.'' These pairs arise from the periodic sets of closed trajectories under the changing of positions of interference fringes [with the same $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3)$] and disappear in the same way (Fig. 11).

The trajectories of this kind are unstable with respect to the small variations of parameters $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3)$ and will be destroyed after any small variation which does not conserve the period $\mathbf{l}$ of potential. These trajectories always present for all the potentials of irrationality 2 connected by the ''quasiperiodic group'' (on the same energy levels) if they exist at least for one of them. However, these trajectories can ''jump'' over the two-dimensional plane $\mathbb{R}^2$ disappearing in one place and arising in the other under the action of group transformations. We can call these trajectories ''partly stable'' (or also ''jumping'') in contrary to the absolutely stable (''crawling'')

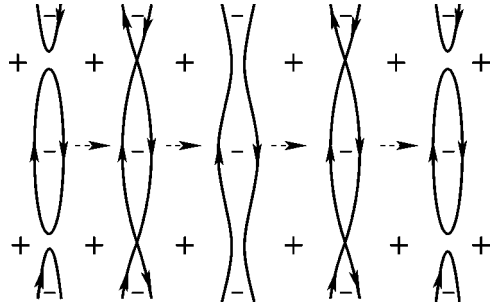

FIG. 11. The arising and the disappearance of the periodic trajectories under the action of the ''quasiperiodic group'' for potentials of irrationality 2 or 1.

trajectories described above. It can be proved also that the phase volume corresponding to both stable and ''jumping'' open trajectories is also the same for potentials connected by the quasiperiodic group in this situation.

The triple of the integer numbers (n_1,n_2,n_3) can be defined here in the same way as in the case of irrationality 3 but these additional pairs of trajectories should be completely ignored when the action of the ''quasiperiodic group'' is considered. The motion of stable open orbits (which always exist in this situation) gives then the same topological numbers M and (m_1,m_2,m_3) as for close generic potentials.

All the trajectories still have the same mean direction in this situation and the asymptotic form (5) for $\tau\to\infty$ is also true in this case. The formula (6) is also valid for the directions of open trajectories with the same (m_1,m_2,m_3). At the end we mention that the situation described above can arise only if the mean directions of stable open orbits coincide with the period $\mathbf{l}$ of potential $V_B^{\text{eff}}(\mathbf{r})$ and is absent if it is not so. As we already mentioned the chaotic behavior is also possible for potentials of irrationality 2 but it is always simpler than for the irrationality 3 potentials.

Let us now say some words about the purely periodic potentials (irrationality 1) which can also appear for special $(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2,\boldsymbol{\eta}_3,a_1,a_2,a_3)$. As we already said all the open trajectories are purely periodic in this case and only a ''topologically integrable'' situation is possible. We also mentioned already that the extended trajectories can exist here either in the continuous energy interval $\epsilon_1(B)\leqslant c\leqslant\epsilon_2(B)$ or just at one energy level $c=\epsilon_0(B)$ (periodic singular nets). All the values $\epsilon_1(B)$, $\epsilon_2(B)$, $\epsilon_0(B)$, however, are not necessarily invariant here with respect to the ''quasiperiodic group'' action and can be different for different potentials connected by the ''quasiperiodic group'' transformations. Also the mean directions of open orbits can be different for two potentials belonging to the same orbit of the ''quasiperiodic group.''

We have then that unlike the cases of irrationality 3 or 2 the positions of interference minima and maxima can be important here for the conductivity behavior and the parameters $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$ do not determine the picture completely. It can be proved, however, that the change of the mean directions of open orbits is possible only if the case of a ''periodic singular net'' takes place at least for one (actually at least for two) potential belonging to the same orbit of the ''quasiperiodic group.'' We can assume then that this situation takes place only if the periodic potential is prepared specially to have this property and it does not take place for potentials with rather big periods $\mathbf{l}_1$, $\mathbf{l}_2$ appearing ''by chance'' in the modulation picture. Thus we can assume that the periodic potentials with rather big $\mathbf{l}_1$, $\mathbf{l}_2$ arising ''by chance'' can be considered actually as the generic potentials on the physical level of strictness and do not give any special features.

V. NOVIKOV PROBLEM FOR THE CASE OF POTENTIALS WITH 4 QUASIPERIODS

Let us consider now a more complicated case when $N=4$ and we have the potential made by 4 independent interference pictures (Fig. 12).

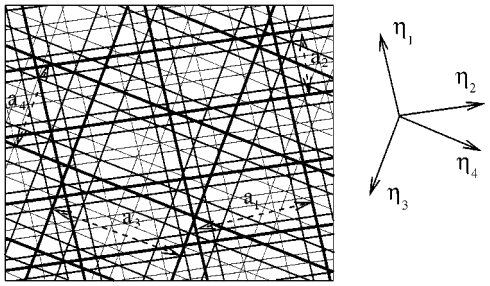

FIG. 12. The potential with 4 quasiperiods made by 4 independent sets of interference fringes with directions $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, $\boldsymbol{\eta}_4$ and periods a_1, a_2, a_3, a_4.

The situation in this case is more complicated than in the case $N=3$ and no general classification of open trajectories exists at the time. We will present here the theorem of Novikov[27] which gives the statement analogous to the Zorich theorem (Theorem 1) in this situation.

Like in the previous case we define here the embedding of the plane $\mathbb{R}^2$ in the four-dimensional space $\mathbb{R}^4$ using the functions $X(\mathbf{r})$, $Y(\mathbf{r})$, $Z(\mathbf{r})$, $W(\mathbf{r})$ defined in the same way for four interference pictures. We will need also the functions $X'(\mathbf{r})$, $Y'(\mathbf{r})$, $Z'(\mathbf{r})$, $W'(\mathbf{r})$ defined as

$$X'(\mathbf{r})=X(\mathbf{r})/a_1\ ,\ Y'(\mathbf{r})=Y(\mathbf{r})/a_2\ ,$$

$$Z'(\mathbf{r})=Z(\mathbf{r})/a_3\ ,\ W'(\mathbf{r})=W(\mathbf{r})/a_4$$

(in the same way as previously for the case $N=3$).

The "total intensity function" $\hat{I}(\mathbf{R})$, $\mathbf{R}\in\mathbb{R}^4$ is defined here as

$$\hat{I}(\mathbf{R})=I_1(X)+I_2(Y)+I_3(Z)+I_4(W),$$

and is a periodic function with periods $(a_1,0,0,0)$, $(0,a_2,0,0)$, $(0,0,a_3,0)$, $(0,0,0,a_4)$ in $\mathbb{R}^4$. The "big potentials" $\hat{V}(\mathbf{R})$ and $\hat{V}_B^{\mathrm{eff}}(\mathbf{R})$ are also defined for every point $\mathbf{R}\in\mathbb{R}^4$ through the functional $V(\mathbf{R})[I]$ and the averaging over the cyclotron orbits in the plane $\Pi^{2\prime}\in\mathbb{R}^4$ passing through the point $\mathbf{R}$ and parallel to the initial plane Π^2. It is easy to see again that the functions $\hat{V}(\mathbf{R})$, $\hat{V}_B^{\mathrm{eff}}(\mathbf{R})$ are the smooth 4-periodic functions in $\mathbb{R}^4$ and the potentials $V(\mathbf{r})$, $V_B^{\mathrm{eff}}(\mathbf{r})$ are the restrictions of $\hat{V}(\mathbf{R})$ and $\hat{V}_B^{\mathrm{eff}}(\mathbf{R})$ on the plane Π^2 embedded in $\mathbb{R}^4$. We can define again the action of the "quasiperiodic group" on the potentials $V(\mathbf{r})$, $V_B^{\mathrm{eff}}(\mathbf{r})$ which is now isomorphic to the four-dimensional torus $\mathbb{T}^4=\mathbb{R}^4/L$, where L is an integer lattice generated by vectors $(a_1,0,0,0)$, $(0,a_2,0,0)$, $(0,0,a_3,0)$, $(0,0,0,a_4)$. Let us mention also that the action of this group can be defined here in the same way as the shifts of positions of minima and maxima of the interference fringes keeping the same the directions $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, $\boldsymbol{\eta}_4$ and periods a_1, a_2, a_3, a_4.

Again the statement that the open trajectories always exist either on the connected energy interval $\epsilon_1(B)\leqslant c\leqslant\epsilon_2(B)$ or just at one energy level $\epsilon_0(B)$ for any $V_B^{\mathrm{eff}}(\mathbf{r})$ is true for the case of 4 quasiperiods. It can be also proved that the values of $\epsilon_1(B)$, $\epsilon_2(B)$ or $\epsilon_0(B)$ are the same for generic potentials belonging to the same orbit of the "quasiperiodic group." Moreover, the global behavior of open trajectories is also the same in this case for all such potentials and the asymptotic behavior of conductivity (which is *a priori* unknown here for the general case) does not depend on the positions of maxima and minima for the fixed generic $(\boldsymbol{\eta}_1,a_1)$, $(\boldsymbol{\eta}_2,a_2)$, $(\boldsymbol{\eta}_3,a_3)$, $(\boldsymbol{\eta}_4,a_4)$. These properties, however, can be destroyed for the specially made periodic potentials $V(\mathbf{r})$ like in the case of 3 quasiperiods.

Let us consider now the purely periodic potential $V(\mathbf{r})$ formed now by four interference pictures. We assume again that at least two (say $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$) directions of interference fringes are not parallel to each other and give a double-periodic picture in the plane like in the case of potentials with 3 quasiperiods. Let us introduce the angles $(\theta_{12},\ \theta_{13},\ \theta_{14})$ between the directions $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$,

$\boldsymbol{\eta}_3$, $\boldsymbol{\eta}_4$ in the same way as in the case of three interference pictures. From the requirement of periodicity we then will have the same requirements (3)–(4) for the angles θ_{13}, θ_{14} and the periods a_3, a_4 with some integer numbers m_1', m_2', k_1', k_2', k_3' (for θ_{13} and a_3) and m_1'', m_2'', k_1'', k_2'', k_3'' (for θ_{14} and a_4). It is easy to prove that these conditions are also sufficient for the periodicity of the resulting potential $V(\mathbf{r})$.

The theorem of Novikov permits us to formulate here the following property of the potentials $V_B^{\text{eff}}(\mathbf{r})$ close enough to purely periodic potentials:

Theorem 4: *Consider the purely periodic potential* $V_B^{(0)\text{eff}}(\mathbf{r})$ *built by four interference pictures with the directions and periods* $(\boldsymbol{\eta}_1^{(0)}, a_1^{(0)})$, $(\boldsymbol{\eta}_2^{(0)}, a_2^{(0)})$, $(\boldsymbol{\eta}_3^{(0)}, a_3^{(0)})$, $(\boldsymbol{\eta}_4^{(0)}, a_4^{(0)})$. *Then there exists such small region* Γ *of parameters* $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, $\boldsymbol{\eta}_4$, a_1, a_2, a_3, a_4, I_1, I_2, I_3, I_4 *containing the initial potential* $V_B^{(0)\text{eff}}(\mathbf{r})$ *that for all the generic potentials* $V_B^{\text{eff}}(\mathbf{r})$ *corresponding to the point of* Γ *the following statements are true.*

(1) All the nonsingular open trajectories lie in the straight strips of finite width and pass through them.

(2) All the regular trajectories have the mean direction in $\mathbb{R}^2$ *given by the equation*

$$m_1 X'(\mathbf{r}) + m_2 Y'(\mathbf{r}) + m_3 Z'(\mathbf{r}) + m_4 W'(\mathbf{r}) = 0,$$

with some integer (indivisible) 4-tuple (m_1, m_2, m_3, m_4) *which is the same for all the (generic) points of "stability zone"* Γ.

(3) The mean direction of open trajectories are the same for generic potentials belonging to the same orbit of the "quasiperiodic group."

Using Novikov theorem it is possible to prove also that the 4-tuples (m_1, m_2, m_3, m_4) can be also defined through the action of the "quasiperiodic group" in the same way as in the case of 3 quasiperiods.

The asymptotic behavior of conductivity tensor σ^{ik} is also the same in this case by the same reasons and the mean directions of the open trajectories [and the integer 4-tuples (m_1, m_2, m_3, m_4)] can be measured experimentally.

According to Novikov theorem the regions with "topologically regular" behavior can be found in any (arbitrarily small) open region of parameters $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$, $\boldsymbol{\eta}_3$, $\boldsymbol{\eta}_4$, a_1, a_2, a_3, a_4, I_1, I_2, I_3, I_4 and B. However, unlike the case $N=3$ there is no theorem here restricting the existence of "chaotic" trajectories only to the case of just one energy level ($\epsilon_1 = \epsilon_2 = \epsilon_0$) containing open trajectories. As we mentioned already, the case $N=4$ is much more complicated from topological point of view and there is no general classification of open trajectories in this case at the time. It is not clear also if the topologically regular behavior corresponds here to the generic situation or not and the probability to find the chaotic behavior is unknown for this situation.

Let us now make some more general remark about the Novikov problem in connection with 2-D potentials $V(\mathbf{r})$. As can be seen, the potentials $V(\mathbf{r})$ with rather many quasiperiods can be considered also as an interesting model of random potentials on the plane. This model is rather different from the standard models of random potentials but still can have common features with them for big N when the chaotic behavior of the open trajectories appears. However, there is no strict theorems now which could connect Novikov problem with the problems of random potentials on the plane.

VI. CONCLUSION

We considered the special type of superlattices modulations giving the quasiperiodic potentials $V(\mathbf{r})$ and $V_B^{\text{eff}}(\mathbf{r})$ on the plane. For this type of potentials we considered the "geometric limit" ($\tau \to \infty$) of conductivity in the presence of a magnetic field based on the global geometry of the level curves of $V_B^{\text{eff}}(\mathbf{r})$. The main attention was paid to the so-called "topologically regular" behavior of nonsingular open level curves for the cases of potentials with 3 and 4 quasiperiods. It was shown that it is possible to introduce the "topological numbers" characterizing the asymptotic

behavior of σ^{ik} similar to the numbers introduced previously in the theory of normal metals. For the case of 3 quasiperiods it was possible to give also the description of the structure of the space of parameters giving potentials $V_B^{\text{eff}}(\mathbf{r})$ according to the topological type of their nonsingular open level curves. For the case of 4 quasiperiods only the part of the space of parameters corresponding to potentials close to ''purely rational'' was considered. It was shown that the corresponding ''topological numbers'' having the form of the integer of 4-tuples can be also introduced in this case.

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[62] Let us use here the word ''orbit'' for the circular cyclotron electron orbit in the magnetic field **B** and ''trajectory'' for the drift of the center of cyclotron orbit in the presence of $V(\mathbf{r})$. We hope that there should be no misunderstanding because of two similar terms.
[63] We are sorry for a little bit unnatural definitions of irrationality. Here we follow the standard definitions arising from the 3-D topology approach.
[64] The last property was first mentioned in Ref. 19 in the case of normal metals and called later the ''Topological Resonance.'' This property plays the important role for the conductivity of normal metals making possible the experimental observation of ''Topological Numbers'' for this case.
[65] The consideration in Ref. 24 is based on the purely geometrical aspects and does not include the quantum corrections due to the jumps from one part of trajectory to another. It can be shown, however, that for chaotic trajectories of the Dynnikov type these jumps should be also important for rather big values of τ. It is possible to show also that the power dependence on τ should then change to rapid exponential decreasing of σ when $\tau \to \infty$ after some characteristic (rather big) value of τ due to these quantum corrections.

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Decomposition of tensor product representations of the unitary matrix quantum group $SU_q(2)$

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Representations of $SU_q(2)$ are labeled by a phase playing the role of a Casimir operator. The coproduct $SU_q(2)$ is used to form direct product representations which can be reduced to irreducible ones. Direct product of two representations with given phases can be reduced to a representation with any given phase. Coefficients necessary for this procedure are calculated. The calculation can also be performed in the Fourier transformed space which replaces the phase by an integer. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1644753]

q-deformations of Lie groups and Lie algebras[1–4] have attracted a lot of attention in recent years and have been intensively studied. These deformations are endowed with a Hopf algebra structure and the coproduct of the Hopf algebra makes the construction of tensor products of representations possible. For the special case of (nondeformed) SU(2) Lie algebra, this procedure is very well known in physics and is called the addition of angular momentum. For q-deformed Lie algebras, this procedure is well investigated and q-Clebsch–Gordan coefficients[5] have been computed. For q-deformed matrix Lie groups, however, this procedure exhibits some new methods and ideas. The irreducible $*$-representations of continuous functions $C(SU_q(2))$ on the quantum group $SU_q(2)$ were classified in the late 1980s and it was found that $C(SU_q(2))$ has two distinct families of irreducible representations, one of which is one dimensional and the other is infinite dimensional.[6,7] The tensor products of the irreducible representation of the algebra of $C(SU_q(2))$ on the quantum group $SU_q(2)$ were studied by Lesniewski and Rinaldi.[8] They proved by using a number of combinatorial identities of q-calculus that the tensor product of two infinite dimensional irreducible representations is equivalent to a direct integral of infinite dimensional irreducible representations. On the other hand, Van der Jeugt[9,10] developed the representation theory for the Jordanian quantum algebra $U_h(sl(2))$ and gave the closed form expressions for the action of the generators of $U_h(sl(2))$ on the basis vectors of finite-dimensional irreducible representations. He also obtained a general formula for the Clebsch–Gordan coefficients.

In this paper, we investigate the decomposition of the tensor product of two irreducible representations of $C(SU_q(2))$ algebra generated by the elements belonging to a 2×2 $SU_q(2)$ quantum matrix group by using the Hopf algebra coproduct and the Fourier transformed space. As has been shown by Vaksman and Soibelman,[7] the representation space has a basis $|n,\alpha\rangle$ when $n \in \mathbb{N}$ is discrete and $\alpha \in [0,2\pi)=S^1$. If the tensor product of representations after reduction is taken, then it is found that

$$|n,\alpha\rangle=\sum_{n_1,n_2} C(n,\alpha|n_1,\alpha_1,n_2,\alpha_2)\ |n_1,\alpha_1\rangle\otimes|n_2,\alpha_2\rangle.$$

Our approach is the same as that of Lesniewski and Rinaldi except that the dependence on α, α_1, and α_2 is handled more carefully. Note that there is no integration over α_1 and/or α_2 in the

formula above since the parameter α denotes the eigenvalue of a central operator and is analogous to the total angular momentum quantum number j of the Lie algebra SU(2) for which the analog formula is given by

$$|j,m\rangle=\sum_{m_1+m_2=m} C(j,m|j_1,m_1,j_2,m_2)|j_1,m_1\rangle\otimes|j_2,m_2\rangle,$$

where m is the magnetic quantum number and

$$j=|j_1-j_2|,|j_1-j_2|+1,\ldots,j_1+j_2.$$

It should be pointed out that for the quantum group $SU_q(2)$ there is no constraint on the summation over n_1 and n_2. It will be shown that all possible values of n_1 and n_2 contribute to a given value of n. A similar remark is also valid for α_1, α_2, and α.

The well-known $SU_q(2)$ quantum matrix group is composed of the matrices[4]

$$U=\begin{pmatrix} a & -qb \\ b^* & a^* \end{pmatrix}.$$

Let A be the Hopf algebra over the complex numbers generated by the elements a, a^*, b, and b^*, satisfying the Hermiticity conditions $(a^*)^*=a$, $(b^*)^*=b$ and the commutation relations

$$aa^*+q^2bb^*=1,$$

$$a^*a+b^*b=1,$$

$$ab=qba,$$

$$ab^*=qb^*a,$$

$$bb^*=b^*b. \tag{1}$$

The coproduct $\Delta:A\mapsto A\otimes A$, the antipode $S:A\mapsto A$ and the co-unit $\varepsilon:A\mapsto\mathbb{C}$ are defined by

$$\Delta(a)=a\otimes a-qb\otimes b^*,\ \ \varepsilon(a)=1,\ \ S(a)=a^*,$$

$$\Delta(b)=a\otimes b+b\otimes a^*,\ \ \varepsilon(b)=0,\ \ S(b)=-q^{-1}b,$$

$$\Delta(a^*)=(\Delta(a))^*,\quad \varepsilon(a^*)=1,\ \ S(a^*)=a,$$

$$\Delta(b^*)=(\Delta(b))^*,\quad \varepsilon(b^*)=0,\ \ S(b^*)=-q(b^*). \tag{2}$$

It can easily be seen that the defining commutation relations in (1) of the algebra A are invariant under $b\leftrightarrow b^*$. Therefore, it turns out to be that under $b\leftrightarrow b^*$ there exists a related second coproduct with

$$\Delta(a)=a\otimes a-qb^*\otimes b,$$

$$\Delta(b^*)=a\otimes b^*+b^*\otimes a^*,$$

$$\Delta(a^*)=(\Delta(a))^*,$$

$$\Delta(b)=(\Delta(b^*))^*. \tag{3}$$

Then one should look for a representation of the Hopf algebra A on a Hilbert space such that b is invertible. If b is not invertible, then its zero eigenvalue subspace is a trivial irreducible

representation where $b=0$ and a is any unitary operator. If b is invertible, then a^*a and the phase of b form a commuting set. It should be noted that a^* and a act as creation and annihilation operators, respectively. In other words, the actions of a, a^*, b, and b^* on $|n,\alpha\rangle$ are

$$a|n,\alpha\rangle=(1-q^{2n})^{1/2}|n-1,\alpha\rangle,$$

$$a^*|n,\alpha\rangle=(1-q^{2n+2})^{1/2}|n+1,\alpha\rangle,$$

$$b|n,\alpha\rangle=q^n e^{i\alpha}|n,\alpha\rangle,$$

$$b^*|n,\alpha\rangle=q^n e^{-i\alpha}|n,\alpha\rangle, \tag{4}$$

where $\alpha,\beta\in[0,2\pi)$ and the normalization is chosen $\langle n,\alpha|m,\beta\rangle=\delta_{nm}\delta(\alpha-\beta)$. For a fixed α, we denote the Hilbert space spanned by $|n,\alpha\rangle$ by H_α. H_α having different values of α are orthogonal.

The coproduct given by (2) is an homomorphism from the Hopf algebra A into $A\otimes A$ and hence it can be used to find a representation of A in $H_{\alpha_1}\otimes H_{\alpha_2}$.

Proposition 1: If $|0,\alpha;\alpha_1,\alpha_2\rangle\in H_{\alpha_1}\otimes H_{\alpha_2}$ is defined such that

$$\Delta(a)|0,\alpha;\alpha_1,\alpha_2\rangle=0,$$

$$\Delta(b)|0,\alpha;\alpha_1,\alpha_2\rangle=e^{i\alpha}\ |0,\alpha;\alpha_1,\alpha_2\rangle, \tag{5}$$

then

$$|0,\alpha;\alpha_1,\alpha_2\rangle=\sum_{n,m=0}^{\infty}\frac{q^{nm}}{\sqrt{f_n(q^2)}\ \sqrt{f_m(q^2)}}e^{i(m\alpha_1-n\alpha_2)}e^{i(n-m)\alpha}|n,\alpha_1\rangle\otimes|m,\alpha_2\rangle, \tag{6}$$

where

$$|n,\alpha\rangle\equiv\frac{(a^*)^n}{\sqrt{f_n(q^2)}}\ |0,\alpha\rangle \tag{7}$$

with

$$f_n(q^2)=(1-q^2)\cdots(1-q^{2n}). \tag{8}$$

Proof 1: Let $|0,\alpha;\alpha_1,\alpha_2\rangle=\Sigma_{n,m=0}^{\infty}C_{n,m}\ |n,\alpha_1\rangle\otimes|m,\alpha_2\rangle$, where $C_{n,m}$ are the coefficients to be determined so that the relations in (5) hold.

If the Hopf algebra coproduct relations given by (2) are taken into consideration together with (5), then one gets the following recursion relations for $C_{n,m}$:

$$C_{n+1,m+1}=\frac{q^{n+m+1}}{\sqrt{1-q^{2(n+1)}}\ \sqrt{1-q^{2(m+1)}}}e^{i(\alpha_1-\alpha_2)}C_{n,m},$$

$$C_{n,m}=q^m\ \sqrt{1-q^{2(n+1)}}\ e^{i(\alpha_2-\alpha)}\ C_{n+1,m}+q^n\ \sqrt{1-q^{2m}}\ e^{i(\alpha_1-\alpha)}C_{n,m-1}. \tag{9}$$

The recursion relations above for $C_{n,m}$ have the unique solution

$$C_{n,m}=\frac{q^{nm}}{\sqrt{f_n(q^2)}\ \sqrt{f_m(q^2)}}e^{i(m\alpha_1-n\alpha_2)}e^{i(n-m)\alpha} \tag{10}$$

for $C_{0,0}=1$. This can easily be verified by putting

$$C_{n,m}=\frac{q^{nm}}{\sqrt{f_n(q^2)}\ \sqrt{f_m(q^2)}}\ e^{in(\alpha-\alpha_2)}\ e^{im(\alpha_1-\alpha)}\ B_{n,m}$$

into (9) which leads to $B_{n,m}$ being independent of n and m.

It should be pointed out that $|n,\alpha;\alpha_1,\alpha_2\rangle$ can be computed as

$$|n,\alpha;\alpha_1,\alpha_2\rangle=\frac{(\Delta(a^*))^n}{\sqrt{f_n(q^2)}}|0,\alpha;\alpha_1,\alpha_2\rangle \tag{11}$$

satisfying

$$\Delta(a)|n,\alpha;\alpha_1,\alpha_2\rangle=\sqrt{1-q^{2n}}|n-1,\alpha;\alpha_1,\alpha_2\rangle,$$

$$\Delta(a^*)|n,\alpha;\alpha_1,\alpha_2\rangle=\sqrt{1-q^{2(n+1)}}|n+1,\alpha;\alpha_1,\alpha_2\rangle,$$

$$\Delta(b)|n,\alpha;\alpha_1,\alpha_2\rangle=q^n e^{i\alpha}|n,\alpha;\alpha_1,\alpha_2\rangle,$$

$$\Delta(b^*)|n,\alpha;\alpha_1,\alpha_2\rangle=q^n e^{-i\alpha}|n,\alpha;\alpha_1,\alpha_2\rangle. \tag{12}$$

It is important to note that the recursion relations in (9) where the coefficients $C_{n,m}$ are given by (10) have the appearance of Fourier series in α_1 and α_2. In the Lesniewski and Rinaldi approach, α_1 and α_2 are taken to be zero. Our approach suggests that the construction being made can also be performed in the Fourier dual space where instead of a phase $0\leqslant\alpha<2\pi$, one can use an integer $k\in\mathbb{Z}$ such that

$$|n,\alpha\rangle=\sum_{k=-\infty}^{\infty} e^{ik\alpha}|n,k\rangle, \tag{13}$$

where the inverse of (13) reads

$$|n,k\rangle=\frac{1}{2\pi}\int_0^{2\pi}|n,\alpha\rangle\ \ e^{-ik\alpha}\ \ d\alpha \tag{14}$$

and $\langle n_1,k_1|n_2,k_2\rangle=\delta_{n_1n_2}\ \delta_{k_1k_2}$.

The actions of a, a^*, b, and b^* on $|n,k\rangle$ are

$$a|n,k\rangle=\sqrt{1-q^{2n}}|n-1,k\rangle,$$

$$a^*|n,k\rangle=\sqrt{1-q^{2n+2}}|n+1,k\rangle,$$

$$b|n,k\rangle=q^n|n,k-1\rangle,$$

$$b^*|n,k\rangle=q^n|n,k+1\rangle, \tag{15}$$

where $n\in\mathbb{N}$ and $k\in\mathbb{Z}$.

Proposition 2: If the analog of (5) in the Fourier dual space H_k of H_α is given by

$$\Delta(a)|0,k;k_1,k_2\rangle=0,$$

$$\Delta(b)|0,k;k_1,k_2\rangle=|0,k-1;k_1,k_2\rangle, \tag{16}$$

then

$$|0,k;k_1,k_2\rangle=\begin{cases}\displaystyle\sum_{n=0}^{\infty}\frac{q^{n(n+k)}}{\sqrt{f_n(q^2)f_{n+k}(q^2)}} & \\ \quad\cdot|n+k,k_1-n\rangle\otimes|n,k_2+k+n\rangle \quad \text{if } k\geqslant 0 & \\ \displaystyle\sum_{n=0}^{\infty}\frac{q^{n(n-k)}}{\sqrt{f_n(q^2)f_{n-k}(q^2)}} & \\ \quad\cdot|n,k_1+k-n\rangle\otimes|n-k,k_2+n\rangle \quad \text{if } k\leqslant 0 & \end{cases} \tag{17}$$

where $|n,k\rangle$ is given by (14) and $f_n(q^2)$ is defined by (8).

Proof 2: Let $|0,k;k_1,k_2\rangle=\Sigma_{n_1,n_2}C^k_{n_1,k_1,n_2,k_2}|n_1,k_1\rangle\otimes|n_2,k_2\rangle$, where $C^k_{n_1,k_1,n_2,k_2}$ are the coefficients to be determined so that the relations in (16) hold. Then, the following recursion relations are found:

$$C^{k-1}_{n_1,k_1,n_2,k_2}=C^k_{n_1+1,k_1,n_2,k_2+1}q^{n_2}\sqrt{1-q^{2(n_1+1)}}+C^k_{n_1,k_1+1,n_2-1,k_2}q^{n_1}\sqrt{1-q^{2n_2}},$$

$$C^k_{n_1,k_1+1,n_2,k_2-1}=\frac{\sqrt{1-q^{2n_1+2}}\ \sqrt{1-q^{2n_2+2}}}{q^{n_1+n_2+1}}C^k_{n_1+1,k_1,n_2+1,k_2}. \tag{18}$$

Even though these recursion relations are rather difficult to handle, their solution can be found by considering the Fourier transform of (6). The analog of (13) for $|0,\alpha;\alpha_1,\alpha_2\rangle$ is

$$|0,\alpha;\alpha_1,\alpha_2\rangle=\sum_{k,k_1,k_2=-\infty}^{\infty}e^{ik\alpha}e^{ik_1\alpha_1}e^{ik_2\alpha_2}|0,k;k_1,k_2\rangle, \tag{19}$$

where $|0,k;k_1,k_2\rangle$ is given by (18).

Inverting (20) and then using (6) together with (13), one obtains

$$|0,k;k_1,k_2\rangle=\frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi}\sum_{n,m=0}^{\infty}\sum_{k_1',k_2'=-\infty}^{\infty}\frac{q^{nm}}{\sqrt{f_n(q^2)}\ \sqrt{f_m(q^2)}}$$
$$\cdot e^{i(m-k_1+k_1')\alpha_1}\ e^{-i(n+k_2-k_2')\alpha_2}\ e^{i(n-m-k)\alpha}\cdot|n,k_1'\rangle\otimes|m,k_2'\rangle\ d\alpha\ d\alpha_1\ d\alpha_2.$$

Considering whether $k\geqslant 0$ or $k\leqslant 0$, $n=m+k$ or $m=n-k$ is chosen, respectively, and hence $|0,k;k_1,k_2\rangle$ is calculated to be the required solution given by (17).

Then $|n,k;k_1,k_2\rangle$ can be computed from $|0,k;k_1,k_2\rangle$ given by (17) by applying $\Delta(a^*)$ n-times; that is

$$|n,k;k_1,k_2\rangle=\frac{(\Delta(a^*))^n}{\sqrt{f_n(q^2)}}|0,k;k_1,k_2\rangle. \tag{20}$$

The algebra defined by (1) for invertible b contains a central element $b^{-1}b^*$ which is represented by $e^{-i\alpha}$. Omitting this element from the algebra yields another consistent algebra whose defining relations are again (1) with one additional equation $b=b^*$. However, this truncated algebra is not endowed with a Hopf algebra structure and thus can not be considered to be a quantum group. Although the representation of this truncated algebra is essentially the same and given by (4) with $\alpha=0$, direct products are not amenable to reduction as there is no coproduct. Hence formulas such as (6) and (17) are direct consequences of the quantum group structure.

The methods of this paper can readily be extended to representations of more general quantum groups. One important point in this regard is the correct handling of the central elements of the algebra. Although these central elements are represented by real or complex numbers in the

representation, their nontrivial coproduct gives a highly nontrivial contribution to the decomposition of the tensor product of two irreducible representations of the quantum group.

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The irreducible unitary representations of the extended Poincaré group in (1+1) dimensions

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We prove that the extended Poincaré group in $(1+1)$ dimensions $\overline{\mathcal{P}}$ is nonnilpotent solvable exponential, and therefore that it belongs to type I. We determine its first and second cohomology groups in order to work out a classification of the two-dimensional relativistic elementary systems. Moreover, all irreducible unitary representations of $\overline{\mathcal{P}}$ are constructed by the orbit method. The most physically interesting class of irreducible representations corresponds to the anomaly-free relativistic particle in $(1+1)$ dimensions, which cannot be fully quantized. However, we show that the corresponding coadjoint orbit of $\overline{\mathcal{P}}$ determines a covariant maximal polynomial quantization by unbounded operators, which is enough to ensure that the associated quantum dynamical problem can be consistently solved, thus providing a physical interpretation for this particular class of representations. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Much of the interest in the extended Poincaré group in $(1+1)$ dimensions $\overline{\mathcal{P}}$ stems from the fact that the Callan–Giddings–Harvey–Strominger (CGHS) model of two-dimensional dilatonic gravity[1] may be formulated as a gauge theory[2] of $\overline{\mathcal{P}}$. The ''string-inspired'' CGHS theory is particularly interesting because it generates an exactly solvable model of quantum gravity, which allows the investigation of several aspects of quantum black hole physics.[3,4] An outstanding problem in this context is the coupling of matter sources in an extended Poincaré gauge-invariant fashion.[5–7]

The main purpose of this paper is to prove that $\overline{\mathcal{P}}$ is solvable exponential, so that the Bernat–Pukanszky theory of exponential groups[8,9] can be strictly applied to work out all its unitary irreducible representations (irrep's). Some of these irrep's were presented in Gadella *et al.*[10] but, although it was mentioned[11] that these irrep's were calculated by the Mackey theory and the orbit method, it was not shown that $\overline{\mathcal{P}}$ has a regular semidirect product structure, nor that $\overline{\mathcal{P}}$ is solvable exponential. These authors adopt the same point of view as that of Cariñena *et al.*,[12] which should be contrasted with ours.

Our approach to the two-dimensional relativistic elementary systems is similar to that which was adopted by Azcárraga and Izquierdo[13] with respect to a nonrelativistic particle of unit charge in a constant magnetic field. Indeed, we show in this paper that the coadjoint orbit corresponding to the anomaly-free relativistic particle in $(1+1)$ dimensions determines a covariant maximal polynomial quantization for it, which provides a physical interpretation for the associated class of irrep's of $\overline{\mathcal{P}}$.

This paper is organized as follows. In Sec. II, we show that $\overline{\mathcal{P}}$ is solvable exponential and calculate its first and second cohomology groups. In Sec. III, we determine the coadjoint orbits of

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$\bar{\mathcal{P}}$ in order to classify the two-dimensional relativistic elementary systems and to work out explicitly all the irrep's of $\bar{\mathcal{P}}$. In Sec. IV, we provide a physical interpretation for a particular class of irrep's of $\bar{\mathcal{P}}$ through a covariant maximal polynomial quantization of the anomaly-free relativistic particle in $(1+1)$ dimensions. Finally, in Sec. V we draw our conclusions and discuss further possible developments. We sketch the method of orbits in the Appendix, in order to provide some supplementary material for the understanding of Sec. III.

II. THE EXTENDED POINCARÉ GROUP IN (1+1) DIMENSIONS $\bar{\mathcal{P}}$

The extended Poincaré algebra $\bar{\mathfrak{i}}_2^1$ is defined by means of an unconventional contraction of a pseudoextension[13] of the anti–de Sitter algebra so(2,1) as

$$[P_a,J]=\sqrt{-h}\varepsilon_a{}^b P_b, \quad [P_a,P_b]=B\varepsilon_{ab}I, \quad \text{and} \quad [P_a,I]=[J,I]=0, \tag{1}$$

where $a,b\in\{0,1\}$, $\varepsilon^{01}=-\varepsilon_{01}=1$, and the indices a and b are raised and lowered by the metric $h_{ab}=\mathrm{diag}(1,-1)$ with $h:=\det h_{ab}=-1$. Throughout this paper, we shall adopt units where $c=1$. The generators of translations are $P_a:=\bar{T}_a$, and their dimensions are L^{-1}. The generator of Lorentz transformations is $J:=\bar{T}_2$, which is dimensionless. The central generator, the dimension of which is $[\hbar]^{-1}$, is $I:=\bar{T}_3$, and the central charge has dimension $[B]=L^{-2}\times[\hbar]$.

The group law $g''(\theta''^a,\alpha'',\beta'')=g'(\theta'^a,\alpha',\beta')g(\theta^a,\alpha,\beta)$ determined by Eq. (1) is given by

$$\theta''^b=\theta'^b+\Lambda(\alpha')^b{}_a\theta^a, \quad \alpha''=\alpha'+\alpha, \quad \text{and} \quad \beta''=\beta'+\beta+\frac{B}{2}\theta'^c\varepsilon_{cb}\Lambda(\alpha')^b{}_a\theta^a, \tag{2}$$

where $\Lambda(\alpha)^a{}_b=\delta^a{}_b\cosh\alpha+\sqrt{-h}\varepsilon^a{}_b\sinh\alpha$, and it corresponds to the coset decomposition $g(\theta^a,\alpha,\beta)=\exp(\theta^a P_a)\exp(\alpha J)\exp(\beta I)$. The adjoint representation of $\bar{\mathcal{P}}$ is given by

$$(\mathrm{Ad}\,g)^A{}_B=\begin{pmatrix} \Lambda^a{}_b & \theta^c\varepsilon_c{}^a\sqrt{-h} & 0 \\ 0 & 1 & 0 \\ B\theta^c\varepsilon_{cd}\Lambda^d{}_b & -\dfrac{B}{2\sqrt{-h}}\theta^a\theta_a & 1 \end{pmatrix},$$

and the invariant Casimir operator determines the metric h_{AB} such that $\langle V,V\rangle=h^{AB}V_AV_B=V^aV_a-2(B/\sqrt{-h})V_2V_3$, for any vector $V=V^A\bar{T}_A$ in $\bar{\mathfrak{i}}_2^1$, with $A,B\in\{0,1,2,3\}$. The dimensions of the metric components are $[h_{ab}]=L^{-2}$, and $[h_{23}]=[h_{32}]=[\hbar]^{-1}$.

The extended Poincaré algebra has the structure of a semidirect product $\bar{\mathfrak{i}}_2^1=\mathrm{so}(1,1)\times_\rho\mathrm{wh}$, where $\mathrm{so}(1,1)=\mathfrak{R}$ is the Abelian subalgebra generated by J, and wh is the maximal nilpotent ideal spanned by $\{P_0,P_1,I\}$, which is isomorphic to the Lie algebra of the Weyl–Heisenberg group WH. The representation ρ of so(1, 1) on wh is given by the restriction of the adjoint representation of $\bar{\mathfrak{i}}_2^1$ to so(1, 1).

It is well-known that $\bar{\mathfrak{i}}_2^1$ is solvable;[5] however, it is also not nilpotent, since its descending central series, $\bar{\mathfrak{i}}_2^{1\,1}=\bar{\mathfrak{i}}_2^1$, $\bar{\mathfrak{i}}_2^{1\,2}=[\bar{\mathfrak{i}}_2^1,\bar{\mathfrak{i}}_2^{1\,1}]=\mathrm{wh}$, …, $\bar{\mathfrak{i}}_2^{1\,k}=[\bar{\mathfrak{i}}_2^1,\bar{\mathfrak{i}}_2^{1\,k-1}]=\mathrm{wh}$ $\forall k\geqslant 2$, does not vanish for any value of k. It is also not difficult to see that the extended Poincaré group $\bar{\mathcal{P}}$ and its Lie algebra $\bar{\mathfrak{i}}_2^1$ are solvable exponential, since for any $X\in\bar{\mathfrak{i}}_2^1$ the eigenvalues of $ad(X)$ are all real.[14]

As a consequence, $\bar{\mathcal{P}}$ is defined as the connected and simply connected image of $\bar{\mathfrak{i}}_2^1$ by the exponential mapping $\bar{\mathcal{P}}=\exp(\bar{\mathfrak{i}}_2^1)$, and every element $g\in\bar{\mathcal{P}}$ belongs to a one-parameter subgroup, so the group law given by Eq. (2) holds globally. Another consequence is that $\bar{\mathcal{P}}$ is homologically trivial; therefore, the Van Est theorem[13] ensures that the cohomology groups on $\bar{\mathcal{P}}$ are canonically isomorphic to the corresponding cohomology groups on $\bar{\mathfrak{i}}_2^1$.

The first cohomology group of $\overline{\mathfrak{i}_2^1}$ can be readily calculated, $H_0^1(\overline{\mathfrak{i}_2^1},\mathfrak{R})=(\overline{\mathfrak{i}_2^1}/[\overline{\mathfrak{i}_2^1},\overline{\mathfrak{i}_2^1}])^*=\mathfrak{R}$. In order to work out the second cohomology group, it is enough to show that the space of two-cocycles $Z_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})\subset\Lambda^2\overline{\mathfrak{i}_2^1}$ has the same dimension of the space of two coboundaries $B_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})$. It turns out that $\dim H_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})=\dim Z_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})-\dim B_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})=0$.

III. CONSTRUCTION OF THE IRREP'S OF $\overline{\mathcal{P}}$ BY ITS COADJOINT ORBITS

It will be shown in Sec. IV that the anomaly-free Lagrangian describing a relativistic particle in flat two-dimensional space–time must be invariant under $\overline{\mathcal{P}}$, consistently with $H_0^2(\overline{\mathcal{P}},\mathfrak{R})=0$. It follows that the relevant dynamical group in two dimensions is $\overline{\mathcal{P}}$, so the adequate statement of the principle of relativity in $(1+1)$ dimensions should require that the equations of motion are covariant under the transformations of $\overline{\mathcal{P}}$.

This means that the elementary particles in $(1+1)$ dimensions must belong to irrep's of $\overline{\mathcal{P}}$ at the quantum level, and constitute relativistic elementary systems in this sense. On the other hand, the group-theoretic approach is concerned about a corresponding notion of elementary system at the classical level, i.e., a system that cannot be decomposed into smaller parts without breaking the symmetry.[15] It turns out that the irreducibility condition is translated naturally into a transitivity one at the classical level; therefore, a classical elementary system is defined as a homogeneous symplectic manifold (HSM). We say that an elementary system (S,Ω) is a Hamiltonian G-space,[16] or a strictly homogeneous symplectic manifold, if further the dynamical group G possesses a Poisson action upon S.

We recall that, due to the Kirillov theorem,[17] every HSM associated with some dynamical group G is locally isomorphic to a coadjoint orbit of G or to a coadjoint orbit of the central extension of G by $\mathfrak{R}$. Then, if further all the coadjoint orbits of G are simply connected and $H_0^2(\mathfrak{g},\mathfrak{R})=0$, then the momentum mapping will be a symplectomorphism between every classical elementary system (S,Ω) upon which the action of $\mathfrak{g}$ is globally Hamiltonian and a certain coadjoint orbit.

Applying this theorem, we discover that every classical relativistic elementary system upon which the action of $\overline{\mathfrak{i}_2^1}$ is globally Hamiltonian is simply connected, and symplectomorphic to one of the coadjoint orbits of $\overline{\mathcal{P}}$ that are calculated below, since it is a connected solvable exponential Lie group with $H_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})=0$ (see Sec. II). Although this classification does not exhaust all the two-dimensional relativistic elementary systems, since $H_0^1(\overline{\mathcal{P}},\mathfrak{R})=\mathfrak{R}$, it is general enough to include the most physically interesting cases, such as the anomaly-free relativistic particle in $(1+1)$ dimensions.

The coadjoint orbit through $\zeta=\zeta_A\overline{\omega}^A$ in $\overline{\mathfrak{i}_2^1}^*$ is formed by the points $\mu=u_A\overline{\omega}^A$ satisfying $u_A=\zeta_B(Adg^{-1})^B{}_A$, where $\{\overline{\omega}^A\}$ is the basis of $\overline{\mathfrak{i}_2^1}^*$ dual to $\{\overline{T}_A\}$. As a consequence, the following identities hold: $u^Au_A=\zeta^A\zeta_A$ and $u_3=\zeta_3$. The stability group of $\zeta\in\overline{\mathfrak{i}_2^1}^*$ is generated by the subalgebra $\overline{\mathfrak{i}_{2\zeta}^1}\subset\overline{\mathfrak{i}_2^1}$, which is the kernel of the Kirillov two-form $B_\zeta(X,Y)$, formed by the vectors $Y\in\overline{\mathfrak{i}_2^1}$ for which $\langle\zeta,[X,Y]\rangle=0$, $\forall X\in\overline{\mathfrak{i}_2^1}$. The dimension of the coadjoint orbit can be deduced from the dimension of the stability group.

As the space of coadjoint orbits of $\overline{\mathcal{P}}$ parametrizes both the set of relativistic elementary systems in two dimensions and the unitary dual of $\overline{\mathcal{P}}$, we will present the coadjoint orbits of $\overline{\mathcal{P}}$ together with their associated irrep's. The problem splits into three cases, and we will follow the methodology sketched in the Appendix for working out all the irrep's of $\overline{\mathcal{P}}$.

Since $ad(X)$ is traceless for all $X\in\overline{\mathfrak{i}_2^1}$, $\overline{\mathcal{P}}$ is unimodular (i.e., $\Delta_{\overline{\mathcal{P}}}=1$). Also, because the real eigenvalues of $ad(X)$ are not all zero for every $X\in\overline{\mathfrak{i}_2^1}$, $\overline{\mathcal{P}}$ is not quasinilpotent (see the Appendix). Consequently, in order to apply the method of orbits to $\overline{\mathcal{P}}$, we must find for any $\zeta\in\overline{\mathfrak{i}_2^1}^*$ a subalgebra $\mathfrak{h}\subset\overline{\mathfrak{i}_2^1}$ of a maximal dimension in the family of the subalgebras subordinate to ζ, further satisfying Pukanszky's condition.

A. Case $\zeta_3 \neq 0$

The coadjoint orbit is the two-dimensional surface diffeomorphic to $\mathfrak{R}^2$ in the three-dimensional hyperplane $u_3=\zeta_3$, defined by the equations

$$u_2=\frac{u^a u_a\sqrt{-h}}{2Bu_3}-\frac{\zeta^A\zeta_A\sqrt{-h}}{2Bu_3} \quad \text{and} \qquad u_3=\zeta_3, \tag{3}$$

and passing through the point $\zeta=(0,0,-[(\zeta^A\zeta_A\sqrt{-h})/2B\zeta_3],\zeta_3)$. These coadjoint orbits are classified by ζ_3 and $\zeta^A\zeta_A$.

Since we may choose any point on the coadjoint orbit (see the Appendix), we pick ζ. Denoting by (J,P_+,I) the subalgebra of $\overline{1_2^1}$ spanned by these vectors, where $P_+=P_0+P_1$, it is clear that $\mathfrak{h}=(J,P_+,I)$ is subordinate to ζ, since its first derived algebra is $[\mathfrak{h},\mathfrak{h}]=(P_+)$, which is orthogonal to ζ or $\langle\zeta,(P_+)\rangle=0$. The subalgebra $\mathfrak{h}$ subordinate to ζ is also admissible, since its codimension is 1, which is half the dimension of the coadjoint orbit, and it satisfies Pukanszky's condition $\zeta+\mathfrak{h}^\perp\subset\mathrm{orb}(\zeta)$. Since any other admissible subalgebra leads to a unitary equivalent representation (see the Appendix), we choose $\mathfrak{h}$.

The typical element of the subgroup H generated by $\mathfrak{h}$ will be denoted by $h(\theta^+,\alpha,\beta)=\exp(\theta^+P_+)\exp(\alpha J)\exp(\beta I)$, so that we can define (see the Appendix) the one-dimensional representation of H by $\chi(\theta^+,\alpha,\beta)=U(h(\theta^+,\alpha,\beta))=\exp(i(-\alpha[(\zeta^A\zeta_A\sqrt{-h})/2B\zeta_3]+\beta\zeta_3))$. The adjoint representation of the subgroup H can be straightforwardly calculated, so that the modulus of H is given by $\Delta_H(h)=|\det(\mathrm{Ad}\,h)|^{-1}=e^{\alpha}$. The space $L(\overline{\mathcal{P}},H,U)$ invariant under right translations on $\overline{\mathcal{P}}$ is formed by the complex functions satisfying the condition (see the Appendix)

$$\begin{aligned}
&F(h(\theta^{+\prime},\alpha',\beta')\cdot g(\theta^a,\alpha,\beta))=e^{-(\alpha'/2)}\chi(\theta^{+\prime},\alpha',\beta')F(g(\theta^a,\alpha,\beta)),\\
&F\left(g\left(\Lambda^a{}_b(\alpha')\theta^b+\theta^{+\prime},\alpha'+\alpha,\beta'+\beta+\frac{B}{2}\theta^{+\prime}e^{\alpha'}(\theta^0-\theta^1)\right)\right)\\
&\quad=e^{-(\alpha'/2)}\exp\left(i\left(-\alpha'\frac{\zeta^A\zeta_A\sqrt{-h}}{2B\zeta_3}+\beta'\zeta_3\right)\right)F(g(\theta^a,\alpha,\beta)).
\end{aligned} \tag{4}$$

This means that the space $L(\overline{\mathcal{P}},H,U)$ is determined by the value of F at $\theta^0=\alpha=\beta=0$.

It is not difficult to see that every element of $\overline{\mathcal{P}}$ can be uniquely written as $g=h\cdot k$, where $h\in H$, $k\in K$, and K is the one-parameter subgroup of $\overline{\mathcal{P}}$ generated by $P_1\in\overline{1_2^1}$. Choosing the Borel mapping $s(x):=k$, where $x\in X=H\backslash\overline{\mathcal{P}}$ and $x=Hg=Hhk=Hk$, we can identify the right-coset space X with the subgroup $K\subset\overline{\mathcal{P}}$, in the sense that $s(X)=K$. The bi-invariant measure on $\overline{\mathcal{P}}$ splits into $d\mu(g)=\Delta_{H,\overline{\mathcal{P}}}(h)d\nu_s(x)d\nu(h)$, where the measure on X is determined by the right Haar measure on $K=\mathfrak{R}$, $d\nu_s(x)=d\nu(s(x))$, which is only $\overline{\mathcal{P}}$-quasi-invariant, because $\Delta_{\overline{\mathcal{P}}}(h)\neq\Delta_H(h)$, and is recognized to be just the Lebesgue measure $d\mu$ on $\mathfrak{R}$. Then, we can construct the Hilbert space $L^2(X,\nu_s,\mathbf{C})=L^2(\mathfrak{R},d\mu)$, formed by the functions defined by $f(x)=F(s(x))$, for every $F\in L^2(\overline{\mathcal{P}},H,U)$ (see the Appendix), which obviously admits a $\overline{\mathcal{P}}$-invariant scalar product.

Solving the equation $s(x)g=hs(xg)$ for $h=h(\theta^+,\alpha',\beta')$, where $k=k(\theta^1)$ and $g=g(\theta''^a,\alpha'',\beta'')$, we can realize the induced representation $\mathrm{ind}(\overline{\mathcal{P}},H,U)$ on the separable Hilbert space $L^2(\mathfrak{R},d\mu)$ of the square-integrable complex functions having compact support on $\mathfrak{R}$ through

$$\begin{aligned}
[T(g)f](\theta^1)=e^{-(\alpha''/2)}\exp\Bigg[i\Bigg(&-\frac{\zeta^A\zeta_A\sqrt{-h}}{2B\zeta_3}\alpha''+\Bigg(\beta''+\frac{B}{2}\theta''^0\theta^1-\frac{B}{4}((\theta''^0)^2-(\theta^1+\theta''^1)^2)\\
&-\frac{B}{4}e^{-2\alpha''}(\theta''^0-\theta^1-\theta''^1)^2\Bigg)\zeta_3\Bigg)\Bigg]f((\theta^1+\theta''^1-\theta''^0)e^{-\alpha''}).
\end{aligned} \tag{5}$$

The corresponding representation of any $X \in \overline{\mathfrak{i}_2^1}$ can be readily calculated, yielding

$$\rho(I) = i\zeta_3, \quad \rho(J) = -\frac{1}{2} + i\left(-\frac{\zeta^A \zeta_A \sqrt{-h}}{2B\zeta_3} + \frac{B}{2}(\theta^1)^2 \zeta_3 \right) - \theta^1 \frac{\partial}{\partial \theta^1},$$

$$\rho(P_0) = iB\theta^1 \zeta_3 - \frac{\partial}{\partial \theta^1}, \quad \text{and} \quad \rho(P_1) = \frac{\partial}{\partial \theta^1}. \tag{6}$$

This representation is anti-Hermitian, and the operator identity $\rho(J) = \sqrt{-h}(\rho(P^a)\rho(P_a) + \zeta^A \zeta_A)/2B\rho(I)$ holds. So, we can write these irrep's simply as $T^{\zeta^A \zeta_A, \zeta_3}(g(\theta^a, \alpha, \beta)) = \exp(\theta^a \rho(P_a))\exp(\alpha\rho(J))\exp(\beta\rho(I))$.

The irrep's $T^{\zeta^A \zeta_A, \zeta_3}$ are faithful, and it can be shown that, in natural units and for $B = 1$, they are unitary equivalent to the irrep's of $\overline{\mathcal{P}}$ presented in Gadella *et al.*,[10] but they are more general than the latter. Since the quantization of the corresponding elementary systems does not look anomalous (see Sec. IV), the irrep's in the form $T^{\zeta^A \zeta_A, \zeta_3}$ are the most physically interesting ones, although they do not correspond to coadjoint orbits of $\overline{\mathcal{P}}$ which are HSM's for $\mathcal{P}$.

B. Case $\zeta_3 = 0$ and $\zeta_a = 0$

The coadjoint orbit is the point $(0,0,\zeta_2,0)$ in the three-dimensional hyperplane $u_3 = 0$. These coadjoint orbits are classified by ζ_2. It is clear that the subalgebra $\mathfrak{h} = \overline{\mathfrak{i}_2^1}$ is subordinate to ζ, since its first derived algebra is $[\mathfrak{h}, \mathfrak{h}] = \mathfrak{wh}$, which is orthogonal to ζ or $\langle \zeta, \mathfrak{wh} \rangle = 0$. The subalgebra $\mathfrak{h}$ subordinate to ζ is also admissible, since $\operatorname{codim} \mathfrak{h} = 0$, which is half the dimension of the coadjoint orbit, and it satisfies Pukanszky's condition $\zeta + \mathfrak{h}^\perp \subset \operatorname{orb}(\zeta)$. It is not difficult to see that there is no other admissible subalgebra subordinate to ζ.

Denoting by $h(\theta^a, \alpha, \beta) = \exp(\theta^a P_a)\exp(\alpha J)\exp(\beta I)$ the typical element of the subgroup H generated by $\mathfrak{h}$, we can (see the Appendix) define the one-dimensional representation of H by $\chi(\theta^a, \alpha, \beta) = U(h(\theta^a, \alpha, \beta)) = \exp(i\alpha\zeta_2)$. Since $H = \overline{\mathcal{P}}$ is unimodular, the space $L(\overline{\mathcal{P}}, H, U)$ invariant under right translations on $\overline{\mathcal{P}}$ is formed by the complex functions satisfying the condition

$$F(h(\theta'^a, \alpha', \beta') \cdot g(\theta^a, \alpha, \beta)) = \chi(\theta'^a, \alpha', \beta') F(g(\theta^a, \alpha, \beta)),$$

$$F\left(g\left(\Lambda^a{}_b(\alpha')\theta^b + \theta'^a, \alpha' + \alpha, \beta' + \beta + \frac{B}{2}\theta'^a \varepsilon_{ab} \Lambda^b{}_c(\alpha')\theta^c \right) \right) = \exp(i\alpha'\zeta_2) F(g(\theta^a, \alpha, \beta)). \tag{7}$$

This means the space $L(\overline{\mathcal{P}}, H, U) = \mathbf{C}$ is determined by the value of F at $\theta^a = \alpha = \beta = 0$, or $F(g(\theta^a, \alpha, \beta)) = \exp(i\alpha\zeta_2)F(e)$, so it is identified with the set of complex numbers.

It follows that the Hilbert space $L^2(\overline{\mathcal{P}}, H, U)$ is one-dimensional and it is formed by the complex functions $F \in L(\overline{\mathcal{P}}, H, U)$ for which $\|F\|^2 < \infty$, where $\|F\|^2 = (F, F)$ and the $\overline{\mathcal{P}}$-invariant scalar product is given by $(F_1, F_2) = \overline{F_1(e)} F_2(e)$. Consequently (see the Appendix), we can realize the induced representation $\operatorname{ind}(\overline{\mathcal{P}}, H, U)$ on the Hilbert space $L^2(\overline{\mathcal{P}}, H, U)$ through $[T(g)F](g') = \exp(i\alpha\zeta_2)F(g')$, where $g = g(\theta^a, \alpha, \beta)$ and $g' = g(\theta'^a, \alpha', \beta')$. The corresponding representation of any $X \in \overline{\mathfrak{i}_2^1}$ is given by $\rho(I) = 0$, $\rho(J) = i\zeta_2$, and $\rho(P_a) = 0$.

The representation of $\overline{\mathfrak{i}_2^1}$ on the Hilbert space $\mathbf{C}$ given above is clearly anti-Hermitian; therefore, the irrep's of $\overline{\mathcal{P}}$ may be simply written as $T^{\zeta_2}(g(\theta^a, \alpha, \beta)) = \exp(\theta^a \rho(P_a))\exp(\alpha\rho(J))\exp(\beta\rho(I))$, and the operator identity $\rho(P^a)\rho(P_a) - 2B/\sqrt{-h}\,\rho(J)\rho(I) = -\zeta^A \zeta_A$ holds. We note that the irrep's T^{ζ_2} are obviously unfaithful and lack physical interest, although they correspond to coadjoint orbits of $\overline{\mathcal{P}}$ which are HSM's for $\mathcal{P}$.

C. Case $\zeta_3=0$ and $\zeta_a\neq 0$

The coadjoint orbit is the two-dimensional surface diffeomorphic to $\Re^2$, immersed in the three-dimensional hyperplane $u_3=0$ and defined by the equation

$$u^a u_a=\zeta^a\zeta_a, \tag{8}$$

which can be a hyperbolic cylinder or a half-plane translationally invariant in the direction of the u_2 axis. These coadjoint orbits are classified by ζ_a and gather into eight distinct families: two families with $\zeta^a\zeta_a<0$, two with $\zeta^a\zeta_a>0$, and the other four with $\zeta^a\zeta_a=0$ (the u_2 axis does not belong to any family).

As we may choose any point on the coadjoint orbit (see the Appendix), we pick $\zeta=(\zeta_a,\zeta_2,0)$. The subalgebra $\mathfrak{h}=\mathrm{wh}$ is subordinate to ζ, since its first derived algebra is $[\mathfrak{h},\mathfrak{h}]=(I)$, which is orthogonal to ζ or $\langle\zeta,(I)\rangle=0$. The subalgebra $\mathfrak{h}$ subordinate to ζ is also admissible, since $\mathrm{codim}\,\mathfrak{h}=1$, which is half the dimension of the coadjoint orbit, and it satisfies Pukanszky's condition $\zeta+\mathfrak{h}^{\perp}\subset\mathrm{orb}(\zeta)$. Since any other admissible subalgebra leads to a unitary equivalent representation (see the Appendix), we choose $\mathfrak{h}$.

Denoting by $h(\theta^a,\beta)=\exp(\theta^a P_a)\exp(\beta I)$ the typical element of the subgroup H generated by $\mathfrak{h}$, we can (see the Appendix) define the one-dimensional representation of H by $\chi(\theta^a,\beta)=U(h(\theta^a,\beta))=\exp(i\theta^a\zeta_a)$. Due to the fact that $H=\mathrm{WH}$ is unimodular, the space $L(\overline{\mathcal{P}},H,U)$ invariant under right translations on $\overline{\mathcal{P}}$ is formed by the complex functions satisfying the condition

$$F(h(\theta'^a,\beta')\cdot g(\theta^a,\alpha,\beta))=\chi(\theta'^a,\beta')F(g(\theta^a,\alpha,\beta)),$$

$$F\left(g\left(\theta^a+\theta'^a,\alpha,\beta'+\beta+\frac{B}{2}\theta'^a\varepsilon_{ab}\theta^b\right)\right)=\exp(i\theta'^a\zeta_a)F(g(\theta^a,\alpha,\beta)). \tag{9}$$

This means that the space $L(\overline{\mathcal{P}},H,U)$ is determined by the value of F at $\theta^a=\beta=0$.

It is not difficult to see that every element of $\overline{\mathcal{P}}$ can be uniquely written as $g=h\cdot k$, where $h\in H$, $k\in K$, and K is the one-parameter subgroup of $\overline{\mathcal{P}}$ generated by $J\in\overline{1}_2^1$. Choosing the Borel mapping $s(x):=k$, where $x\in X=H\backslash\overline{\mathcal{P}}$ and $x=Hg=Hhk=Hk$, we can identify the right-coset space X with the subgroup $K\subset\overline{\mathcal{P}}$, in the sense that $s(X)=K$. The bi-invariant measure on $\overline{\mathcal{P}}$ splits into $d\mu(g)=\Delta_{H,\overline{\mathcal{P}}}(h)d\nu_s(x)d\nu(h)$, where the measure on X is determined by the right Haar measure on $K=\Re$, $d\nu_s(x)=d\nu(s(x))$, which is $\overline{\mathcal{P}}$-invariant, since $\Delta_{\overline{\mathcal{P}}}(h)=\Delta_H(h)$, and is just the Lebesgue measure $d\mu$ on $\Re$. Then, we can construct the Hilbert space $L^2(X,\nu_s,\mathbf{C})=L^2(\Re,d\mu)$, formed by the functions defined by $f(x)=F(s(x))$ for every $F\in L^2(\overline{\mathcal{P}},H,U)$ (see the Appendix), which obviously admits a $\overline{\mathcal{P}}$-invariant scalar product.

Solving the equation $s(x)g=hs(xg)$ for $h=h(\theta'^a,\beta')$, where $k=k(\alpha)$ and $g=g(\theta''^a,\alpha'',\beta'')$, we can realize the induced representation $\mathrm{ind}(\overline{\mathcal{P}},H,U)$ on the separable Hilbert space $L^2(\Re,d\mu)$ of the square-integrable complex functions having compact support on $\Re$ through $[T(g)f](\alpha)=\exp(i\Lambda(\alpha)^a{}_b\theta''^b\zeta_a)f(\alpha+\alpha'')$. The corresponding representation of any $X\in\overline{1}_2^1$ is given by $\rho(I)=0$, $\rho(J)=\partial/\partial\alpha$, and $\rho(P_a)=i\Lambda(\alpha)^b{}_a\zeta_b$.

The operator identity $\rho(P^a)\rho(P_a)-2(B/\sqrt{-h})\rho(J)\rho(I)=-\zeta^A\zeta_A$ holds and the representation of $\overline{1}_2^1$ on the Hilbert space $L^2(\Re,d\mu)$ is clearly anti-Hermitian, so the irrep's of $\overline{\mathcal{P}}$ may be simply written as $T^{\zeta_a}(g(\theta^a,\alpha,\beta))=\exp(\theta^a\rho(P_a))\exp(\alpha\rho(J))\exp(\beta\rho(I))$. It can be shown that the irrep T^{ζ_a} is equivalent to the Wigner representation of the Poincaré group in $(1+1)$ dimensions $\mathcal{P}$ (see Gadella *et al.*[10] and Ali and Antoine[18]). We note that the irrep's T^{ζ_a} are unfaithful and not too interesting physically, since the quantization of the corresponding classical elementary systems looks anomalous, although they correspond to coadjoint orbits of $\overline{\mathcal{P}}$ which are HSM's for $\mathcal{P}$.

IV. THE ANOMALY-FREE RELATIVISTIC PARTICLE IN (1+1) DIMENSIONS

It is known that the dynamics of the relativistic particle in a flat $(1+1)$ dimensional space–time M is described by the Lagrangian $L_B=L_0+L_{WZ}$, where $L_0=-m\sqrt{\dot{q}^2}$ and $L_{WZ}=-(B/2)\,\varepsilon_{ab}\dot{q}^a q^b$. The central charge B is similar to an applied electrical force driving the particle into an uniformly accelerated relativistic motion[5] and it is an additional free parameter (besides the mass m), fixed at the outset, that the relativistic particle theory must allow for, due to the existence of a nontrivial two cocycle in the second cohomology group of the Poincaré group in $(1+1)$ dimensions $\mathcal{P}$. In fact, it was shown by Bargmann that $H_0^2(\mathcal{P},\mathfrak{R})=\mathfrak{R}$ then, as a consequence of the Lévy–Leblond theorem,[13] all the inequivalent Lagrangians L_B quasi-invariant under $\mathcal{P}$ are classified by the central charge B.

However, it must be emphasized that the Lagrangian L_B is classically anomalous, since it is quasi-invariant under the transformations of $\mathcal{P}$, while the three conserved Noether charges together with the identity $\{\mathcal{N}_a,\mathcal{N}_2,1\}$ constitute a Poisson bracket realization of $\overline{\mathfrak{i}_2^1}$, assuming $B\neq 0$ and $m\neq 0$. Since $H_0^2(\overline{\mathcal{P}},\mathfrak{R})=0$ (see Sec. II), we can eliminate the classical anomaly by adding a third term to L_B, depending on an extra degree of freedom χ with dimension of action and transforming as $\chi'=\chi+\beta+(B/2)\,\theta^a\varepsilon_{ab}\Lambda^b{}_c q^c$ under $\overline{\mathcal{P}}$. This addition neutralizes the Wess–Zumino term L_{WZ}, causing the new Lagrangian $\overline{L}=L_B-\dot{\chi}$ to be invariant under the transformations of $\overline{\mathcal{P}}$. Now, there are four conserved Noether charges $\{\mathcal{N}_a,\mathcal{N}_2,\mathcal{N}_3\}$ associated with the anomaly-free Lagrangian $\overline{L}$, which realize $\overline{\mathfrak{i}_2^1}$ with the identically conserved charge $\mathcal{N}_3=-1$ corresponding to the central generator realized by minus the identity.

Performing the Hamiltonian formulation of the system described by $\overline{L}$, we learn that χ is an internal gauge degree of freedom, corresponding to the phase of the particle's wave function at the quantum level. The reduced phase space Γ_R^+ can be determined by observing that the constraint surface Γ^+ is globally diffeomorphic to $\overline{\mathcal{P}}$, such that the action of the dynamical group upon Γ^+ is simply transitive and free.

It is not difficult to see that the generators of the gauge transformations corresponding to the two primary first-class constraints ϕ_m span a subalgebra of $\mathfrak{X}(\Gamma^+)$ which realizes a two-dimensional Abelian subalgebra of $\overline{\mathfrak{i}_2^1}$; therefore, the reduced phase space $\Gamma_R^+\sim\mathfrak{R}^2$ is diffeomorphic to the homogeneous coset space generated by the translations P_a and can be globally parametrized by the space–time coordinates q^a. The space Γ_R^+ is endowed with the symplectic form $\Omega^{+R}=d\Lambda^{+R}=(B/2)\,\varepsilon_{ab}dq^a\wedge dq^b$, the canonical one form of which is given by the Wess–Zumino form $\Lambda^{+R}=(B/2)\,\varepsilon_{ab}q^a dq^b$.

It turns out that the symplectic manifold (Γ_R^+,Ω^{+R}) is a Hamiltonian G-space and hence a classical relativistic elementary system. Indeed (Γ_R^+,Ω^{+R}) is homogeneous under the action of the dynamical group $\overline{\mathcal{P}}$, which has a Poisson action upon Γ_R^+, such that the globally Hamiltonian vector fields at $s\in\Gamma_R^+$ are given by $\overline{T}_a^{\Gamma_R^+}(s)=(\partial/\partial q^a)$, $\overline{T}_2^{\Gamma_R^+}(s)=\sqrt{-h}\varepsilon^a{}_b q^b(\partial/\partial q^a)$, and $\overline{T}_3^{\Gamma_R^+}(s)=0$. The comoments are given by $u_a^{+R}(s)=Bq^b\varepsilon_{ba}$, $u_2^{+R}(s)=(m^2/2B)+[B/(2\sqrt{-h})]\,q_a q^a$, and $u_3^{+R}(s)=-1$. Note that they are not uniquely determined, since u_2^{+R} is defined up to an additive constant, consistently with $H_0^1(\overline{\mathcal{P}},\mathfrak{R})=\mathfrak{R}$.

The identities $u_A^{+R}u^{+RA}(s)=m^2/\sqrt{-h}$ and $u_3^{+R}(s)=-1$ hold, so $u_2^{+R}(s)$ is functionally dependent on the $u_a^{+R}(s)$, which are regarded as the fundamental dynamical variables, and using the fact that the comoments constitute a Poisson bracket realization of $\overline{\mathfrak{i}_2^1}$, it is not difficult to see that $\{q^a,q^b\}=[\varepsilon^{ab}(\sqrt{-h})^2]/B$. The value of the momentum mapping $\mu_R^+(s)=([u_A^{+R}(s)]/\hbar)\overline{\omega}^A$ at the origin $s_0=(0,0)$ in Γ_R^+ shall be denoted by $\zeta=\mu_R^+(s_0)=(0,0,m^2/(2B\hbar),-1/\hbar)$, which satisfies

$$\zeta^A\zeta_A=\frac{m^2}{\sqrt{-h}\hbar^2}\quad\text{and}\quad\zeta_3=-\frac{1}{\hbar}. \tag{10}$$

The second identity in Eq. (10) follows from the value of $u_3^{+R}(s)$ and the definition of the momentum mapping, so the quantization of (Γ_R^+,Ω^{+R}) satisfies Dirac's quantum condition (this will be shown later).

Moreover, a straightforward calculation shows that[19] the momentum mapping $\mu_R^+:\Gamma_R^+ \to \mathrm{orb}(\zeta)$ is a symplectomorphism between the elementary system (Γ_R^+,Ω^{+R}) and the coadjoint orbit $(\mathrm{orb}(\zeta),b)$ through $\zeta \in \overline{\mathfrak{i}_2^1}^*$, with $\mu_R^+ * b = (\Omega^{+R}/\hbar)$. It follows that Eq. (10) provides a physical interpretation for the parameters labeling the irrep $T^{\zeta^A \zeta_A,\zeta_3}$ of $\overline{\mathcal{P}}$, which corresponds to the relativistic elementary system (Γ_R^+,Ω^{+R}).

A. Quantization of the anomaly-free relativistic particle in (1+1) dimensions

Before we address the quantum dynamics of the relativistic particle, though, let us clear up the quantization of the system at the kinematical level. Let $\varphi(\overline{T_A}) := i\rho(\overline{T_A})$ be the Hermitian representation of $\overline{\mathfrak{i}_2^1}$ on the Hilbert space $L^2(\mathfrak{R},dx)$ defined from Eq. (6), for $\zeta=(0,0,-[(\zeta^A\zeta_A\sqrt{-h})/2B\zeta_3],\zeta_3)$ satisfying Eq. (10), and $\mathfrak{j}\cong\overline{\mathfrak{i}_2^1}$ be the finite-dimensional Lie subalgebra of $C^\infty(\Gamma_R^+)$ spanned by the comoments $\{u_A^{+R}\}$. In addition, let $\lambda:\overline{\mathfrak{i}_2^1}\mapsto C^\infty(\Gamma_R^+)$ be the lift of the mapping $\sigma:\overline{\mathfrak{i}_2^1}\mapsto\mathcal{A}(\Gamma_R^+)$ induced by the left action of $\overline{\mathcal{P}}$ on Γ_R^+, where $\mathcal{A}(\Gamma_R^+)$ denotes the set of all the globally Hamiltonian vector fields on Γ_R^+. The mapping $\lambda(\overline{T_A})=u_A^{+R}$ is a Lie algebra homomorphism and it is well-defined, since Γ_R^+ is simply connected and $H_0^2(\overline{\mathfrak{i}_2^1},\mathfrak{R})=0$.

Then, $\mathrm{orb}(\zeta)$ determines the linear map $\mathcal{Q} := (1/\zeta_3)\,\varphi\circ\lambda^{-1}$ from $\mathfrak{j}$ onto the linear space $\mathrm{Op}(D)=\mathrm{span}\{\mathcal{Q}(u_A^{+R})\}$ of (in general) unbounded Hermitian (or symmetric) operators preserving a fixed dense domain D in $L^2(\mathfrak{R},dx)$, which satisfies $\mathcal{Q}(\{u_A^{+R},u_B^{+R}\}) = -i\zeta_3[\mathcal{Q}(u_A^{+R}),\mathcal{Q}(u_B^{+R})]$ and $\mathcal{Q}(u_3^{+R})=-\mathbf{1}$. For the domain D, we can take the Schwartz space $\boldsymbol{\mathcal{S}}(\mathfrak{R},\mathbf{C})\subset L^2(\mathfrak{R},dx)$ of rapidly decreasing smooth complex-valued functions, for instance.

Recalling that $u_3^{+R}=-1$, we can see that Dirac's quantum condition is satisfied if and only if $\zeta_3=-(1/\hbar)$, consistently with Eq. (10). Furthermore, assuming that D is a domain of essential self-adjointness for $\mathrm{Op}(D)$, we can see that the linear map $\mathcal{Q}$ is actually a prequantization of $\mathfrak{j}$ in the sense of Gotay,[20] since the globally Hamiltonian vector fields $\overline{T}_A^{\Gamma_R^+}$ are complete. It is not difficult to see that $\boldsymbol{\mathcal{S}}(\mathfrak{R},\mathbf{C})$ is a domain of essential self-adjointness for the representation of $\mathfrak{j}$ given by $\mathrm{Op}(D)$.

In order to determine the maximal Lie subalgebra $\mathcal{O}$ of $C^\infty(\Gamma_R^+)$ that can consistently be quantized, we will tie to the approach that aims at providing a quantization of the pair $(\mathcal{O},\mathfrak{b})$, i.e., a prequantization of $\mathcal{O}$ which (among other things) irreducibly represents a suitably chosen basic algebra of observables $\mathfrak{b}\subset C^\infty(\Gamma_R^+)$.[20] It turns out that the suitable basic algebra is $\mathfrak{b}=\mathrm{wh}=\mathrm{span}\{u_0^{+R},u_1^{+R},u_3^{+R}\}$, since the restriction of $\mathcal{Q}$ to $\mathrm{wh}\subset\mathfrak{j}=\mathrm{span}\{u_A^{+R}\}$ provides actually a quantization of the pair $(\mathfrak{b},\mathfrak{b})$, which is equivalent to the usual Schrödinger quantization of a one-dimensional nonrelativistic free particle.

In fact, in the coordinates of Γ_R^+ defined by $q := -(u_0^{+R}+u_1^{+R})/B = -q^1+q^0$ and $p := u_1^{+R} = -Bq^0$, the expression of the associated quantization map $\mathcal{Q}$ is exactly given by the Schrödinger representation of wh in the position representation $\{|x\rangle\}$; $\hat{q} := \mathcal{Q}(q)=x$, $\hat{p} := \mathcal{Q}(p) = -i\hbar\,(\partial/\partial x)$, and $\hat{1} := \mathcal{Q}(1)=\mathbf{1}$ on the domain D, such as $D=\boldsymbol{\mathcal{S}}(\mathfrak{R},\mathbf{C})\subset L^2(\mathfrak{R},dx)$. The standard canonical quantization is well-defined; however, there is no full quantization of $(C^\infty(\Gamma_R^+),\mathfrak{b})$ in which a Von Neumann rule is compatible with the Schrödinger quantization.

Indeed, due to the strong Groenewold–Van Hove no-go theorem,[20] there is no quantization of (P,wh) on $\mathfrak{R}^2\sim\Gamma_R^+$, where P denotes the polynomial subalgebra of $C^\infty(\Gamma_R^+)$ generated by $\mathfrak{b}=\mathrm{wh}$. It turns out that the only two distinct isomorphism classes of maximal Lie subalgebras of P which contain wh are those represented by P^2 and by the set of polynomials $S=\{f(q)p+g(q)\}$, where P^2 denotes the subspace of polynomials of degree at most 2, and f,g are polynomials.[20]

The quantization of the pair (P^2,wh) is provided by the well-known extended metaplectic quantization. On the other hand, the only classical observable in this paper that will require it is

the comoment u_2^{+R}, which is in $P^2 \subset P$ but not in wh. For all the other observables that we will consider, such as position, momentum, potential energy, relativistic energy, or the Hamiltonian, the Schrödinger quantization will be enough. In particular, we will not consider any observable in S.

In addition, a straightforward calculation shows that the extended metaplectic quantization $\mathcal{Q}$ of (P^2,wh) is covariant with respect to $\overline{\mathcal{P}}$ in the sense that, for every $f(q,p)$ in $P^2 \subset P \subset C^\infty(\Gamma_R^+)$ and $g=g(\theta^a,\alpha,\beta) \in \overline{\mathcal{P}}$, we have $\mathcal{Q}(f(q',p'))=T^{\zeta^A\zeta_A,\zeta_3}(g^{-1})\mathcal{Q}(f(q,p))T^{\zeta^A\zeta_A,\zeta_3}(g)$, where $(q',p')=l_g(q,p)$ is the left action on Γ_R^+ generated by the globally Hamiltonian vector fields $\overline{T}_A^{\Gamma_R^+}$, and ζ satisfies Eq. (10).

B. Quantum dynamics of the anomaly-free relativistic particle in (1+1) dimensions

As far as the quantum dynamics of the system is concerned, we remark that the total energy of the particle depends explicitly on time, so it does not provide a suitable Hamiltonian. For this reason, we turn to consider the dynamics from the point of view of the reduced phase space Γ_R^+. The volume two form of space–time determines the symplectic form $\Omega^{+R}=-(B/\sqrt{-h})\,\text{vol}$, which is expressed in the coordinates (q,p) of Γ_R^+ by $\Omega^{+R}=-dp\wedge dq$, with the Wess–Zumino form given by minus the Liouville form $\Lambda^{+R}=-pdq$.

Up to gauge equivalence, the dynamics on Γ_R^+ is specified by $q^0(\tau)=\tau$

$$q^1(\tau)=q^1(\tau_0)-\sqrt{m^2+\tilde{p}(\tau_0)^2}/B+\sqrt{m^2+\tilde{p}(\tau)^2}/B,$$

and $\tilde{p}(\tau)=\tilde{p}(\tau_0)+B(\tau-\tau_0)$, for a given $\tilde{p}(\tau_0)$, with $\tau_0 \in \Re$. It follows that the proper time is given by $t'=m/B\,\text{arsinh}[\tilde{p}(\tau)/m]$, and $\tilde{p}(\tau)$ is the kinematical momentum, since $\tilde{p}(\tau)=\gamma(\tau)m\,(dq^1/dt)\,(\tau)$.

Note that the equations for $q^a(\tau)$ are regarded as Hamilton equations, while that for $\tilde{p}(\tau)$ is an identity. Moreover, retaining the space–time meaning of the reduced phase space, the world-line W of the particle is also a Hamiltonian flow in the symplectic manifold Γ_R^+. Calculating the globally Hamiltonian vector field corresponding to this flow, $X_H(\tau)=\overline{T}_0^{\Gamma_R^+}(\tau)+[\tilde{p}(\tau)/\sqrt{m^2+\tilde{p}(\tau)^2}]\overline{T}_1^{\Gamma_R^+}(\tau)$, and applying the antihomomorphism of Lie algebras $\lambda \circ \sigma^{-1}(\overline{T}_a^{\Gamma_R^+})=u_a^{+R}$, we get the Hamiltonian $H(q,p,\tau)$.

The corresponding Hamiltonian operator splits into two parts $\hat{H}(\hat{q},\hat{p},\tau)=\hat{H}_0(\hat{q},\hat{p})+\hat{V}(\hat{p},\tau)$, where $\hat{H}_0(\hat{q},\hat{p})=-B\hat{q}-\hat{p}$ and $\hat{V}(\hat{p},\tau)=[\tilde{p}(\tau)/\sqrt{m^2+\tilde{p}(\tau)^2}]\,\hat{p}$. Solving the eigenvalue problem $\hat{H}_0|E\rangle=E|E\rangle$, we discover that $\hat{H}_0$ has continuous spectrum with the normalized eigenfunctions given by $\langle x|E\rangle=(1/\sqrt{2\pi\hbar})\exp[-(i/\hbar)(Ex+(B/2)x^2)]$, so $\langle E'|E\rangle=\delta(E'-E)$.

Note that classically $H_0=u_0^{+R}=Bq^1=-2\mathcal{E}_{\text{pot}}(q^1)$, so $\hat{H}_0(\hat{q},\hat{p})=-2\hat{\mathcal{E}}_{\text{pot}}(\hat{q},\hat{p})$ has the meaning of a potential energy operator. Besides this fact, the total energy operator $\hat{\mathcal{H}}(\hat{q},\hat{p},\tau)=\mathcal{E}(\tau)-\frac{1}{2}\hat{H}_0(\hat{q},\hat{p})$, where $\mathcal{E}(\tau):=\sqrt{m^2+\tilde{p}(\tau)^2}$ is the relativistic energy of the particle, satisfies $[\hat{\mathcal{H}},\hat{H}_0]=0$; therefore the eigenvectors of $\hat{H}_0$ are simultaneously total energy eigenstates. Then, the eigenvalues of the total energy operator are related with those of $\hat{H}_0$ through $\hat{\mathcal{H}}(\tau)|E\rangle=E_T(\tau)|E\rangle$, where $E_T(\tau)=\mathcal{E}(\tau)-E/2$.

In terms of the base kets $\{|E\rangle\}$, the state ket of the system is given at $\tau=\tau_0$ by $|\alpha\rangle=\int_{-\infty}^{+\infty}dE\,c_E(\tau_0)|E\rangle$, where $c_E(\tau_0)$ is some known complex function of E satisfying $\int_{-\infty}^{+\infty}dE|c_E(\tau_0)|^2=1$. Then, for $\tau>\tau_0$, the state ket will be $|\alpha,\tau_0;\tau\rangle=\int_{-\infty}^{+\infty}dE c_E(\tau)e^{-(iE/\hbar)(\tau-\tau_0)}|E\rangle$, where the $c_E(\tau)$'s satisfy the coupled differential equations

$$i\hbar\frac{dc_E}{d\tau}(\tau)=\int_{-\infty}^{+\infty}dE'\langle E|\hat{V}|E'\rangle e^{[i(E-E')/\hbar](\tau-\tau_0)}c_{E'}(\tau).$$

Solving the resulting linear homogeneous partial differential equations, we get

$$c_E(\tau)=\frac{1}{\sqrt{2\pi\hbar|B|}}\exp\left(-\frac{iE^2}{2B\hbar}\right)\int_{-\infty}^{+\infty}D_\lambda\exp\left[\frac{i\lambda}{\hbar B}(-E-\sqrt{m^2+\tilde{p}(\tau)^2}+\sqrt{m^2+\tilde{p}(\tau_0)^2})\right]d\lambda,$$

$$\text{where}\quad D_\lambda=\frac{1}{\sqrt{2\pi\hbar|B|}}\int_{-\infty}^{+\infty}c_E(\tau_0)\exp\left[\frac{iE}{B\hbar}\left(\frac{E}{2}+\lambda\right)\right]dE.$$

Suppose now that the system is initially prepared in an energy eigenstate $|\alpha\rangle=|E\rangle$, then at a later time $\tau>\tau_0$ the state will be given by

$$|\alpha,\tau_0;\tau\rangle=\exp\left[\frac{i}{2B\hbar}(-(E-\sqrt{m^2+\tilde{p}(\tau)^2}+\sqrt{m^2+\tilde{p}(\tau_0)^2})^2+E^2)\right]\cdot\exp\left[-\frac{i}{\hbar}(E-\sqrt{m^2+\tilde{p}(\tau)^2}\right.$$
$$\left.+\sqrt{m^2+\tilde{p}(\tau_0)^2})(\tau-\tau_0)\right]\cdot|E-\sqrt{m^2+\tilde{p}(\tau)^2}+\sqrt{m^2+\tilde{p}(\tau_0)^2}\rangle. \tag{11}$$

The probability as a function of time for the particle to be found in the state $|E'\rangle$ is given by $|\langle E'|\alpha,\tau_0;\tau\rangle|^2/\langle\alpha,\tau_0;\tau|\alpha,\tau_0;\tau\rangle\,dE'=\delta(E'-E+\sqrt{m^2+\tilde{p}(\tau)^2}-\sqrt{m^2+\tilde{p}(\tau_0)^2})dE'$, which equals 1 if $E'=E-\sqrt{m^2+\tilde{p}(\tau)^2}+\sqrt{m^2+\tilde{p}(\tau_0)^2}$ or zero otherwise. From Eq. (11), we note that the states $|E\rangle$ are not stationary although they are total energy eigenstates, since the τ-dependent part of the Hamiltonian $\hat{V}(\hat{p},\tau)$ causes transitions to eigenstates $|E-\sqrt{m^2+\tilde{p}(\tau)^2}+\sqrt{m^2+\tilde{p}(\tau_0)^2}\rangle$ of different energy.

In fact, the expectation value of the total energy operator, for instance,

$$\langle\hat{\mathcal{H}}\rangle(\tau)=\frac{\langle\alpha,\tau_0;\tau|\hat{\mathcal{H}}|\alpha,\tau_0;\tau\rangle}{\langle\alpha,\tau_0;\tau|\alpha,\tau_0;\tau\rangle}=\frac{3\mathcal{E}(\tau)}{2}-\frac{\mathcal{E}(\tau_0)}{2}-\frac{E}{2}$$

is τ-dependent. It is not difficult to see that the function $\langle\hat{\mathcal{H}}\rangle(\tau)$ attains to a minimum at $\tau=\tau_0-[\tilde{p}(\tau_0)]/B$, when its value is $\langle\hat{\mathcal{H}}\rangle(\tau_0-[\tilde{p}(\tau_0)/B])=3m/2-[\sqrt{m^2+\tilde{p}(\tau_0)^2}/2]-(E/2)$, which only happens after τ_0 if $\tilde{p}(\tau_0)$ satisfies the condition sign $(B)\tilde{p}(\tau_0)<0$; otherwise, $\langle\hat{\mathcal{H}}\rangle(\tau)$ is a monotonically increasing function of $\tau>\tau_0$. For this reason, the presented quantum states are stable, even though there is no true ground state.

V. DISCUSSION

We showed that the extended Poincaré group in $(1+1)$ dimensions $\overline{\mathcal{P}}$ is a connected solvable exponential Lie group, with $H_0^2(\overline{\mathcal{P}},\Re)=0$ and $H_0^1(\overline{\mathcal{P}},\Re)=\Re$ (see Sec. II). These facts were important to apply the Kirillov theorem to perform a classification of the two-dimensional relativistic elementary systems and to work out explicitly all the irrep's of $\overline{\mathcal{P}}$ by the orbit method (see Sec. III). The particular class of irrep's $T^{\zeta^A\zeta_A,\zeta_3}$ with ζ satisfying Eq. (10) turned out to be connected to a covariant maximal polynomial quantization of the anomaly-free relativistic particle in $(1+1)$ dimensions, which provided a quantum-mechanical interpretation for the construction in this most physically interesting case (see Sec. IV).

We remark that the Bohr–Wilson–Sommerfeld condition[21] is trivially satisfied by the anomaly-free relativistic particle in $(1+1)$ dimensions, and it does not yield the quantization of any observable quantity, which is consistent with the fact that the system is not conservative and the world lines are open. It is worth mentioning that $\overline{\mathcal{P}}$ is related to the one-dimensional oscillator group Os(1) by the Weyl unitary trick. However, the group Os(1) is not solvable exponential, and the orbit method gives all its irrep's only through holomorphic induction.[22]

It is remarkable that the extended metaplectic quantization of the anomaly-free relativistic particle is covariant with respect to $\overline{\mathcal{P}}$, inasmuch as a covariant Stratonovich–Weyl kernel for the corresponding coadjoint orbits has not been found yet.[10] However, this difficulty is not directly

related to the fact that there is an obstruction to fully quantizing the system, since there are symplectic manifolds such as $\mathfrak{R}^2$ or S^2 for which the problem of the generalized Weyl–Wigner–Moyal quantization has successfully been solved,[10] although obstructions have been found.[20]

The group $\overline{\mathcal{P}}$ enjoys several properties in common with the groups WH, E(2), and $\mathrm{Aff}_+(1,\mathfrak{R})$, which found applications in fields such as electronics, signal processing, and quantum optics. As all these groups have square-integrable representations, in a subsequent publication it would be interesting to test whether the irrep's $T^{\zeta^A\zeta_A,\zeta_3}$ of $\overline{\mathcal{P}}$ are square integrable with respect to $\mathrm{orb}(\zeta)$. This fact would allow us to work out the associated generalized coherent states, generalized wavelet transforms, and generalized Wigner functions,[23] which would surely be an invaluable mathematical tool in the context of the phase-space formulation of the quantum anomaly-free relativistic particle in $(1+1)$ dimensions.

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APPENDIX: THE METHOD OF ORBITS

Before considering the Bernat–Pukanszky theory of exponential groups,[8,9] let us briefly review the standard procedure to form a unitary induced representation, since the theory of induced representations developed by Mackey[24,25] plays an essential role in the method of orbits.

Let H be a closed subgroup of a locally compact topological group with a countable basis G and U a one-dimensional unitary representation of H on the complex numbers $\mathbf{C}$. We introduce the space $L(G,H,U)$ of complex-valued measurable functions F on G that satisfy the condition $F(hg)=\Delta_{H,G}(h)^{-1/2}U(h)F(g)$, where $\Delta_{H,G}(h)=\Delta_H(h)/\Delta_G(h)$, $h\in H$, $g\in G$, and $g\mapsto\Delta_G(g)$ is the modulus of the group G.

The group G can be identified with $H\times X$, where X is the right G-space $X=H\backslash G$, since every element of $g\in G$ can be written uniquely in the form $g=hs(x)$ with $x\in X$. Under this identification, the right Haar measure on G splits into the product of a quasi-invariant measure ν_s on X, depending upon the choice of a Borel mapping s of X into G having the property that $s(Hg)\in Hg$, by the right Haar measure on H; $d\nu(g)=\Delta_{H,G}(h)d\nu_s(x)d\nu(h)$. The measure ν_s on X is G-invariant if and only if $\Delta_G(h)=\Delta_H(h)$.

The space $L(G,H,U)$ is clearly invariant under right translations on G. Let $L^2(G,H,U)$ denote the Hilbert space generated by the square-integrable functions F in $L(G,H,U)$; then, we call the unitary representation T acting by right translations upon the Hilbert space $L^2(G,H,U)$, according to $[T(g)F](g')=F(g'g)$, the representation induced in the sense of Mackey by the representation U and we will denote it by $\mathrm{ind}(G,H,U)$.

It is not difficult to see that there is an isomorphism $F\mapsto f$ of the Hilbert space $L^2(G,H,U)$ onto the Hilbert space $L^2(X,\nu_s,\mathbf{C})$, generated by the square-integrable complex functions having compact support on X with respect to the measure ν_s, which associates a function $f\in L^2(X,\nu_s,\mathbf{C})$ defined by $f(x)=F(s(x))$ with every $F\in L^2(G,H,U)$. Under this isomorphism, the induced representations in the sense of Mackey can be realized on the Hilbert space $L^2(X,\nu_s,\mathbf{C})$ through $[T(g)f](x)=\Delta_{H,G}(h)^{-1/2}U(h)f(xg)$, where the element $h\in H$ is defined from the relation $s(x)g=hs(xg)$.

Now, we can sketch the orbit method. Let G be an exponential group, $\mathfrak{g}$ its real exponential Lie algebra, and $\mathfrak{g}^*$ its dual. We say that a subalgebra $\mathfrak{h}\subset\mathfrak{g}$ is subordinate to $\zeta\in\mathfrak{g}^*$ if its first derived algebra is orthogonal to ζ, or $\langle\zeta,[\mathfrak{h},\mathfrak{h}]\rangle=0$. Denoting by $H\subset G$ the subgroup corresponding to the subalgebra $\mathfrak{h}$ subordinate to $\zeta\in\mathfrak{g}^*$, we define the unitary one-dimensional representation of H by $U(\exp X)=\exp(i\langle\zeta,X\rangle)$, which is related to the character χ of H simply by $\chi(\exp X)=U(\exp X)$, where $X\in\mathfrak{h}$.

Then a unitary induced representation $\mathrm{ind}(G,H,U)$ of G is irreducible if and only if the subalgebra $\mathfrak{h}$ subordinate to $\zeta \in \mathfrak{g}^*$ is admissible, i.e., if its dimension is maximal in the family of all subalgebras subordinate to ζ and if it satisfies Pukanszky's condition.[9] The maximality condition is equivalent to $\dim \mathfrak{h} = \dim \mathfrak{g} - \frac{1}{2}\dim \mathrm{orb}(\zeta)$, and Pukanszky's condition requires that the linear variety $\zeta + H^{\perp}$ is contained in $\mathrm{orb}(\zeta)$, where $H^{\perp}$ denotes the orthogonal complement of H in $\mathfrak{g}^*$. Bernat[8] showed that the first condition implies the second one if $\mathfrak{g}$ is quasinilpotent (i.e., all the real eigenvalues of $\mathrm{ad}(X)$ are zero, for all $X \in \mathfrak{g}$), otherwise the two conditions are independent. In particular, every nilpotent group is quasi-nilpotent.

It can be shown[26] that, for any given ζ, there is a subordinate subalgebra $\mathfrak{h}$ satisfying the two conditions above. Moreover, if $\mathfrak{h}_1$ and $\mathfrak{h}_2$ are, respectively, maximal dimension subalgebras subordinate to ζ_1 and ζ_2, further obeying Pukanszky's condition, then $\mathrm{ind}(G,H_1,U_1) = \mathrm{ind}(G,H_2,U_2)$ if and only if ζ_1 and ζ_2 belong to the same coadjoint orbit, the equal sign indicating unitary equivalence. Reciprocally, any irrep of G is representable in the form $\mathrm{ind}(G,H,U)$ by specifying $\mathfrak{h}$ and ζ appropriately, thus establishing a canonical bijection between the space $\mathcal{O}(G)$ of coadjoint orbits and the unitary dual $\hat{G}$ of any solvable exponential Lie group. It is worth mentioning that every coadjoint orbit of the connected and simply connected solvable type I Lie groups (and, in particular, of the exponential groups) is integral (i.e., satisfies the integrality condition).

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Multiplicative anomaly and zeta factorization

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Some aspects of the multiplicative anomaly of zeta determinants are investigated. A rather simple approach is adopted and, in particular, the question of zeta function factorization, together with its possible relation with the multiplicative anomaly issue is discussed. We look primordially into the zeta functions instead of the determinants themselves, as was done in previous work. That provides a supplementary view, regarding the appearance of the multiplicative anomaly. Finally, we briefly discuss determinants of zeta functions that are not in the pseudodifferential operator framework. © *2004 American Institute of Physics.*
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I. INTRODUCTION

A pseudodifferential operator (ΨDO) A of order m on a manifold M_n is defined through its symbol $a(x,\xi)$, which is a function belonging to the space $S^m(\mathbf{R}^n\times\mathbf{R}^n)$ of $\mathbf{C}^\infty$ functions such that for any α, β there exists a constant $C_{\alpha,\beta}$ so that $|\partial_\xi^\alpha\partial_x^\beta a(x,\xi)|\leqslant C_{\alpha,\beta}(1+|\xi|)^{m-|\alpha|}$. The definition of A is given (in the distribution sense) by

$$Af(x)=(2\pi)^{-n}\int e^{i\langle x,\xi\rangle}a(x,\xi)\hat{f}(\xi)\,\mathrm{d}\xi, \tag{1}$$

where f is a smooth function ($f\in\mathcal{S}$) and $\hat{f}$ its Fourier transform. When $a(x,\xi)$ is a polynomial in ξ one gets a differential operator but, in general, the order m can be even complex. For A a positive–definite elliptic ΨDO of positive order $m\in\mathbf{R}$, acting on the space of smooth sections of an n-dimensional vector bundle E over a closed, n-dimensional manifold M, the zeta function is defined as

$$\zeta_A(s)=\mathrm{tr}\,A^{-s}=\sum_j \lambda_j^{-s},\quad \mathrm{Re}\,s>\frac{n}{m}\equiv s_0. \tag{2}$$

Here s_0 is called the abscissa of convergence of $\zeta_A(s)$, which is proven to have a meromorphic continuation to the whole complex plane $\mathbf{C}$ (regular at s_0), provided that A admits a spectral cut: $L_\theta=\{\lambda\in\mathbf{C};\mathrm{Arg}\,\lambda=\theta,\theta_1<\theta<\theta_2\}$, $\mathrm{Spec}\,A\cap L_\theta=\varnothing$ (the Agmon–Nirenberg condition).

The Wodzicki (or noncommutative) residue[1] is the only extension of the Dixmier trace to ΨDOs which are not in $\mathcal{L}^{(1,\infty)}$. Even more, it is the only trace one can define in the algebra of ΨDOs up to a multiplicative constant, and is given by the integral

$$\mathrm{res}\,A=\int_{S^*M}\mathrm{tr}\,a_n(x,\xi)\,\mathrm{d}\xi, \tag{3}$$

with $S^*M\subset T^*M$ the co-sphere bundle on M (some authors set a coefficient in front of the integral). If $\dim M=n=-\mathrm{ord}\,A$ (M compact Riemann, A elliptic, $n\in\mathbf{N}$) it coincides with the Dixmier trace, and one has[1]

$$\operatorname{Res}_{s=1}\zeta_A(s)=\frac{1}{n}\operatorname{res}A^{-1}. \tag{4}$$

However, the Wodzicki residue continues to make sense for ΨDOs of arbitrary order and, even if the symbols $a_j(x,\xi)$, $j<m$, are not invariant under coordinate choice, the integral in (3) is, and defines a trace. In particular, the residua of the poles of the extended definition of zeta function to operators of complex order are also given by the noncommutative residue.

It is well known that the study of zeta functions is central—at least at a basic level, the one needed in fact in usual applications to physics[2,3]—for the issue of giving a sense to the definition of determinant of a ΨDO (see Ref. 4 for the actual state of the art of this concept). This definition goes back to Ray and Singer:[5] for an operator A with spectrum $\lambda_i, i\in I$ (here I needs not be discrete, it can be a multi-index made up of parts of different nature), formally

$$\det A=\prod_{i\in I}\lambda_i=\exp\left(\sum_{i\in I}\log\lambda_i\right). \tag{5}$$

But from the definition of the zeta function

$$\zeta_A(s)=\sum_{i\in I}\lambda_i^{-s}, \tag{6}$$

it turns out that

$$\zeta_A'(0)=-\sum_{i\in I}\log\lambda_i. \tag{7}$$

It is most natural then to define (as Ray and Singer did) the determinant of A by means of the zeta function as[5]

$$\det_\zeta A\equiv\exp[-\zeta_A'(0)]. \tag{8}$$

Note that this is a *definition*, since the above manipulations are formal as long as the convergence properties of the expressions at hand are not fully specified, in accordance with the theorem at the beginning of this section. This is taken care of by the analytical continuation provided in the definition of the zeta function of A.

The definition of the determinant $\det_\zeta A$ only depends on the homotopy class of the spectral cut for A (see above). And one has the following (very useful) asymptotic expansion for the heat kernel:

$$\operatorname{tr}e^{-tA}=\sum_{\lambda\in\operatorname{Spec}A}{}'\ e^{-t\lambda}\sim\alpha_n(A)+\sum_{n\neq j\geqslant 0}\alpha_j(A)t^{-s_j}+\sum_{k\geqslant 1}\beta_k(A)t^k\ln t,\quad t\downarrow 0, \tag{9}$$

where

$$\alpha_n(A)=\zeta_A(0),\quad \alpha_j(A)=\Gamma(s_j)\operatorname{Res}_{s=s_j}\zeta_A(s),\quad s_j\notin-\mathbf{N},$$

$$\alpha_j(A)=\frac{(-1)^k}{k!}[PP\zeta_A(-k)+\psi(k+1)\operatorname{Res}_{s=-k}\zeta_A(s)],\quad s_j=-k,\ k\in\mathbf{N}, \tag{10}$$

$$\beta_k(A)=\frac{(-1)^{k+1}}{k!}\operatorname{Res}_{s=-k}\zeta_A(s),\quad k\in\mathbf{N}\backslash\{0\}.$$

This paper is organized as follows: in the next section we give a short but rather self-contained introduction to the appearance of the multiplicative anomaly[6–18] of zeta determinants. In Sec. III, we point out certain particularities of this anomaly by presenting two very different cases: On the one hand, a new and rather general condition that guarantees the absence of anomaly and, in sharp contrast, a quite particular and very simple case where the anomaly is already nonzero. Then, in Sec. IV, extending and complementing previous work on this subject,[7,8] we pay attention to the product of zeta functions rather than its associated determinants. This lead to the consideration of $\det(B\otimes C)$ instead of $\det(BC)$, with B and C two arbitrary operators. Thus, from that point of view, we are able to obtain rather simple new expressions for determinants, mainly thanks to the strong property of factorization of the zeta function. In the last section we present, in a somewhat more qualitative way, the relationship between all the previous concepts, multiplicative anomaly and zeta factorization, with the appearance of complex poles in the zeta function and other zeta functions that do not belong to the pseudodifferential operator framework. In the Appendix, due to the implementation in a regularization context, we investigate further the topic of zeta function factorization, presenting results, mainly from Number Theory, with two opposite points of view: the construction of Dirichlet L functions from multiplication of simple zeta functions on one hand, and the decomposition of a zeta function in terms of simpler factors on the other hand. This leads to some physical interpretation for the associated heat kernel that we briefly discuss.

II. APPEARANCE OF THE MULTIPLICATIVE ANOMALY

Now, it would seem clear that, if we have a product of two commuting operators,

$$\det{}_\zeta(AB)=\exp\left[\sum_{i\in I}\ \log(\lambda_i\mu_i)\right]=\exp\left[\sum_{i\in I}\ (\log\lambda_i+\log\mu_i)\right]=\exp\left[\sum_{i\in I}\ \log\lambda_i+\sum_{i\in I}\ \log\mu_i\right]$$
$$=\exp\left[\sum_{i\in I}\ \log\lambda_i\right]\exp\left[\sum_{i\in I}\ \log\mu_i\right]=\det{}_\zeta A\,\det{}_\zeta B. \tag{11}$$

But this is *not* true, and *only one* of these steps fails to be true. Below we provide some specific examples to help the reader understand where the problem is.

Actually, very much related with this is the fact that the zeta function trace

$$\mathrm{tr}_\zeta A=\sum_{i\in I}\ \lambda_i=\zeta_A(s=-1) \tag{12}$$

fails to satisfy the additive property; in general

$$\mathrm{tr}_\zeta(A+B)\neq\mathrm{tr}_\zeta A+\mathrm{tr}_\zeta B, \tag{13}$$

for, again, this is a regularized trace (involves analytical continuation) which is used with non-trace-class operators (see also Ref. 4 for the general definition of the trace).

As an example, consider the following commuting linear operators in an infinite-dimensional space, given in diagonal form by

$$A_1=\mathrm{diag}\ (1,2,3,4,\ldots),\quad A_2=\mathrm{diag}\ (1,1,1,1,\ldots), \tag{14}$$

and their sum

$$A_1+A_2=\mathrm{diag}\ (2,3,4,5,\ldots). \tag{15}$$

The corresponding ζ-traces are easily obtained,

$$\mathrm{tr}_\zeta A_1=\zeta_R(-1)=-\tfrac{1}{12},\quad \mathrm{tr}_\zeta A_2=\zeta_R(0)=-\tfrac{1}{2}, \tag{16}$$

$$\mathrm{tr}_\zeta(A_1+A_2)=\zeta_R(-1)-1=-\tfrac{13}{12},$$

ζ_R being the Riemann zeta function. The last trace has been calculated according to the rules of infinite series summation (see, e.g., Hardy[9]). We observe that

$$\mathrm{tr}_\zeta(A_1+A_2)-\mathrm{tr}_\zeta A_1-\mathrm{tr}_\zeta A_2=-\tfrac{1}{2}\neq 0. \tag{17}$$

Unlike for ordinary, finite dimensional determinants, for which we have the property: $\det(AB)=\det(A)\det(B)$, for zeta determinants one rather has to consider, in general, an additional piece (called *anomaly* or *defect*). It is usually written as

$$a(A,B)=\ln\frac{\det(AB)}{\det(A)\det(B)} \tag{18}$$

or

$$a(A,B)=\zeta_A'(0)+\zeta_B'(0)-\zeta_{AB}'(0). \tag{19}$$

Thus the anomaly $a(A,B)$ will vanish if the derivatives at $s=0$ of the respective zeta function satisfy the additive property. There is an explicit expression, due to Wodzicki, for $a(A,B)$, that simplifies enormously the calculation of the multiplicative anomaly in many cases.[1]

III. UNDERSTANDING ZETA TRACES AND ZETA DETERMINANTS

There exist many examples of simple cases with and without multiplicative anomaly.[7,8] We give now a condition that guarantees its absence. Consider the two following zeta functions:

$$\zeta_A(s)=\sum_i \lambda_i^{-s}, \tag{20}$$

$$\zeta_B(s)=\sum_i (c\lambda_i^\alpha)^{-s}=c^{-s}\zeta_A(\alpha s) \quad \text{with} \quad c,\alpha\in\mathbf{R}. \tag{21}$$

The zeta function associated with the product of the eigenvalues is

$$\zeta_{AB}(s)=\sum_i (c\lambda_i^{\alpha+1})^{-s}=c^{-s}\zeta_A((\alpha+1)s), \tag{22}$$

and thus

$$\zeta_{AB}(s)=c^{-s}\zeta_A((\alpha+1)s)\neq\zeta_A(s)+c^{-s}\zeta_A(\alpha s). \tag{23}$$

Performing the substitution $s=0$, we have that

$$\zeta_{AB}'(0)=(\alpha+1)\zeta_A'(0)=\zeta_A'(0)+\alpha\zeta_A'(0)=\zeta_A'(0)+\zeta_B'(0). \tag{24}$$

Therefore, in spite of the fact that the two zeta functions are different, their respective derivatives at zero are equal. This is enough to guarantee the absence of the multiplicative anomaly, namely $a(A,B)=0$. This is quite a general situation, since we have not fixed the λ_i at all. We have only played with the relative difference between the spectra.

A rather different thing is to consider two spectra which are related by an *additive* constant,

$$\mu_i=\lambda_i+c. \tag{25}$$

For simplicity, let us restrict our analysis to the specific example

$$\lambda_n = n, \quad \mu_n = n+1, \quad n = 1,2,3,\ldots. \tag{26}$$

Thus

$$\zeta_A(s) = \zeta_R(s), \quad \zeta_B(s) = \zeta_R(s) - 1, \tag{27}$$

while the zeta function of the product is of Epstein type:[7]

$$\zeta_A(s) = \sum_{n=1}^{\infty} (n^2+n)^{-s} = \sum_{n=1}^{\infty} \frac{\Gamma(n+s)\, 2^{-2n}}{n!\, \Gamma(s)} \zeta_H(2(n+s),3/2). \tag{28}$$

Thus

$$\zeta_A'(0) + \zeta_B'(0) = 2\zeta_R'(0) = -\ln(2\pi), \tag{29}$$

while

$$\zeta_{AB}'(0) = \sum_{n=1}^{\infty} \frac{2^{-2n}}{n} \zeta_H(2n,3/2), \tag{30}$$

which are not equal. Numerically

$$\zeta_{AB}'(0) = 0.4417, \quad \zeta_A'(0) + \zeta_B'(0) = -1.8379, \tag{31}$$

even the signs are different and the anomaly, in such a simple case, is larger in absolute value than the individual results themselves,

$$a = \zeta_A'(0) + \zeta_B'(0) - \zeta_{AB}'(0) = -2.2796. \tag{32}$$

Up to now, we have addressed and tried to explain the problem by looking carefully in the various zeta functions involved in the process. Nevertheless, we can gain a new insight into the multiplicative anomaly issue through consideration of the factorizability properties of the corresponding zeta functions, an analysis important by itself in, e.g., number theory.

IV. ZETA FUNCTION FACTORIZATIONS AND THE MULTIPLICATIVE ANOMALY

As explained, the main practical consequence about the existence of the multiplicative anomaly is that, if, e.g., we want to compute

$$\det A = \det(BC), \tag{33}$$

from the (in principle simpler) determinants $\det B$ and $\det C$, we have to take also into account $a(A,B)$. This is specially important when different factorizations of A, say $A = BC$ and $A = B'C'$, are alternatively considered.[8] We begin by introducing the associated zeta functions that we would use in the computation of the factor determinants,

$$\zeta_B(s) = \sum_i \lambda_i^{-s}, \tag{34}$$

$$\zeta_C(s) = \sum_j \mu_j^{-s}. \tag{35}$$

But, instead of applying the usual and direct procedure as before, here we shall deal with the product of these two zeta functions,

$$\zeta_D(s)=\zeta_B(s)\zeta_C(s)=\sum_i \lambda_i^{-s}\sum_j \mu_j^{-s}. \tag{36}$$

Note that this is the zeta function of an operator, D, which is different from the previous A. Actually, $D=B\otimes C$, as is immediate to realize. In fact, from

$$\zeta_{B\otimes C}(s)=\sum_{i,j}(\lambda_i\mu_j)^{-s}=\sum_i \lambda_i^{-s}\sum_j \mu_j^{-s}, \quad \mathrm{Re}\, s>\max\{\alpha,\beta\}, \tag{37}$$

being α, β, the abscissas of convergence of the individual series, and owing to the uniqueness of the asymptotic continuation to the rest of the complex plane, it turns out that

$$\zeta_{B\otimes C}(s)=\zeta_B(s)\zeta_C(s). \tag{38}$$

In particular,

$$\zeta_{B\otimes C}(s=-1)=\zeta_B(s=-1)\zeta_C(s=-1), \tag{39}$$

that is

$$\mathrm{tr}_\zeta(B\otimes C)=\mathrm{tr}_\zeta B\,\mathrm{tr}_\zeta C, \tag{40}$$

which extends the corresponding property known to hold in finite dimensions.

Now, consider the respective determinants. Recall, to begin with, that in the finite case we have

$$\det(B\otimes C)=(\det B)^{\dim C}(\det C)^{\dim B}, \tag{41}$$

where the dimensions refer to the spaces where the respective operators act. We will now prove that this equation is maintained in the infinite dimensional situation (we will drop the ζ label from the determinants, from now on). In fact, we have [recall that $\zeta_B(0)$ is the zeta *regularized dimension* of the space in which B acts, and the same for the rest]:

$$\det B=\exp[-\zeta_B'(0)], \quad \det C=\exp[-\zeta_C'(0)], \tag{42}$$

$$\det D=\exp[-\zeta_D'(0)]=\exp[-\zeta_B'(0)\zeta_C(0)-\zeta_B(0)\zeta_C'(0)], \tag{43}$$

and we thus see, that

$$\det(D)=(\det B)^{\zeta_C(0)}(\det C)^{\zeta_B(0)}. \tag{44}$$

In the particular case when $\zeta_B(s)$ and $\zeta_C(s)$ have the same value at zero (the two operators act on a space of the same dimension),[10] $\zeta_B(0)=\zeta_C(0)\equiv\tilde{\zeta}(0)$, we get

$$\det(D)=(\det B\det C)^{\tilde{\zeta}(0)}. \tag{45}$$

We have thus shown that the computation of $\det B\det C$ is, in a way, as close to that of $\det(B\otimes C)$ as it is to that of $\det(BC)$, provided when both operators act on the same space and can be multiplied. In fact, the determinant of their tensor product is given in terms of the product of the determinants of the individual operators by introducing the regularized dimension of the space where they act. Formally, it is a kind of exponential anomaly. But notice that this is actually no anomaly, since the exponent is constant (e.g., it does not depend on the particular operators B and C chosen) and it is always equal to the regularized dimension of the space (as it should). When $\zeta_B(0)=\zeta_C(0)=\tilde{\zeta}(0)$, let us compare in more detail the two expressions: the one for the multiplicative anomaly

$$\det(BC)=\det B\,\det C\,e^{a(B,C)}, \tag{46}$$

with the other for the exponential anomaly, thus

$$\exp(a(B,C))=\frac{\det(BC)}{\det B\,\det C}=\frac{\det A}{(\det D)^{1/\zeta(0)}}. \tag{47}$$

This equation seems somewhat artificial, no wonder since it links two nondirectly related quantities, as explained above. It can nevertheless be useful in practical determinations of the multiplicative anomaly.

Some consequences and examples: In general, if one is dealing with factorizations of the type

$$\zeta_A(s)=\prod_i \zeta_{A_i}(s), \tag{48}$$

the determinants are related as $\det A=\Pi_i(\det A_i)^{\Pi_{j\neq i}\zeta_j(0)}$. This can be useful for the computation of determinants of multidimensional zeta functions, once its factorization is known. For a general m-dimensional zeta function, we can write its factorization as $\zeta(s)=\Pi_i^m \zeta_i^{d_i}(s)$ where d_i specifies the dimension of the zeta function, with $m=\Sigma_i d_i$.

A number of different examples can be worked out. For instance, if the zeta functions factors are zero at the origin, then the associated multidimensional determinant is one. This is what happens, for example, for the product of harmonic oscillators,

$$\prod_{n_1=0}^{\infty}\cdots\prod_{n_k=0}^{\infty}\left(n_1+\frac{1}{2}\right)\cdots\left(n_k+\frac{1}{2}\right)=1. \tag{49}$$

Actually, with little more effort a more general case can be considered,

$$\lambda_{n_1\cdots n_k}=(n_1+c_1)\cdots(n_k+c_k),\quad n_1,\ldots,n_k=0,1,2,3,\ldots. \tag{50}$$

Here

$$\zeta(s)=\prod_{j=1}^{k}\zeta_j(s),\quad \zeta_j(s)\equiv\zeta_H(s,c_j). \tag{51}$$

Recalling that

$$\zeta_H(0,c_j)=\tfrac{1}{2}-c_j,\quad \zeta_H'(0,c_j)=\ln\Gamma(c_j)-\tfrac{1}{2}\ln(2\pi), \tag{52}$$

we get

$$\det A=\prod_{j=1}^{k}\det(A_j)^{\Pi_{i\neq j}\zeta_H(0,c_j)}=\prod_{j=1}^{k}\left(\frac{\sqrt{2\pi}}{\Gamma(c_j)}\right)^{\Pi_{i\neq j}(1/2-c_i)}, \tag{53}$$

which reduces to the expression above, Eq. (49), in the particular example considered. This is a nice result of the regularization method.

A second example is the case of a multiple factorization, $\zeta^{(N)}(s)=\Pi_{i=1}^{N}\zeta_i(s)$, in which at least one of the zeta functions evaluated at the origin is zero [without losing generality let us choose $\zeta_1(0)=0$]. Then, the determinant associated with $\zeta^{(N)}(s)$ is just

$$(e^{-\zeta_1'(0)})^{\Pi_{i=2}^{\infty}\zeta_i(0)}, \tag{54}$$

that is, the determinant of the zeta function which is zero at the origin, exponentiated with the product of the other zeta functions at zero. Different situations of this type could be discussed.

V. BEYOND ΨDOs: THE CASE OF COMPLEX POLES

In this concluding section, we want to comment on the appearance, in some important situations, of complex poles, and on its relationship with the multiplicative anomaly and with factorizations. We begin by paying some attention to the anomaly free case (20) and (21) studied in Sec. III. This case corresponds to two commuting operators, for which there is a simple expression for the multiplicative anomaly, due to Wodzicki,[1]

$$a(A,B)=\frac{\operatorname{res}[(\ln(A^bB^{-a}))^2]}{2ab(a+b)}, \tag{55}$$

where $a>0$ and $b>0$ are the orders of A and B, respectively.

In spite of the generality of (20) and (21), it is clear that this is not the most general case inside the class of commuting operators. To begin with, the fact that one is a function of the other is a sufficient but not a necessary condition for the commutation of the operators (think of the operators involved in the quantum mechanics of the hydrogen atom, for example). In addition, one may also argue that a more general function than $\mu_n=f(\lambda_n)=c\lambda_n^{\alpha}$ may be considered as well. For example, an exponential function $f(\lambda_n)=\exp(\lambda_n)$. It can be readily seen that with such a choice we are outside the realm of pseudodifferential operators. For instance, just with $\lambda_n=n$, then $\mu_n=\exp(n)$, and then the associated zeta function is a geometric series:

$$\zeta_B(s)=\sum_{n=1}^{\infty} e^{-ns}=\frac{1}{(e^s-1)}, \tag{56}$$

giving rise to infinitely many complex poles. Nevertheless, this spectra is indeed physical, as shown in Ref. 11, and related to q deformations[11] and to fractal geometry[12] as well. Thus, it is also rather reasonable to expect that associated regularized expressions (such as determinants) may be of physical interest as well. In principle, one can proceed identically—depending on the precise meromorphic structure of the corresponding zeta function—with the formal definition. Likewise, note that the case (20) and (21), not only holds for $\alpha\in\mathbf{R}$, but also for $\alpha\in\mathbf{C}$, as can be readily seen from (22)–(24). Therefore, it is still anomaly free but notice that a complex α introduces complex poles (just as a simple example, consider $\mu_n=n$, then the complex α rotates the pole at $s=1$ to $s=\alpha^{-1}$).

There are other circumstances where we are outside the pseudodifferential operator framework, but there is still interest in the short time asymptotics of the heat kernel or in zeta determinants. This is exactly the case, for instance, when considering heat kernels in noncommutative spaces[13] and when studying products of prime numbers,[14] respectively. Indeed, the zeta function associated to the prime numbers is known,[15]

$$\mathcal{P}(s)=\sum_p p^{-s}=\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\log\zeta(ns), \tag{57}$$

where p are the prime numbers and $\mu(n)$ is the Möbius function. Note that this function has a rich pattern of logarithmic singularities in the complex plane but still the associated *determinant* is of interest and actually follows directly from the derivative of $\mathcal{P}(s)$.[14] Additionally, in this type of regularized products, one can look at multiplicative anomalies as well. For example, following Ref. 14 one can consider the Euler product representation of Riemann's zeta function,

$$\zeta(s)=\frac{\prod_p p^s}{\prod_p p^s-1}, \quad \operatorname{Re}s>1. \tag{58}$$

This expression, considered together with $\mathcal{P}(s)$, gives rise to the following result:[14]

$$\prod_p (p-1)=0 \quad \text{and} \quad \prod_p (p^2-1)=48\pi^2, \tag{59}$$

and the appearance of a multiplicative anomaly is manifest.

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APPENDIX: REMARKS ON ZETA FACTORIZATIONS

We have seen how the discussion of the multiplicative anomaly of determinants, has lead us, in a natural way, to the construction of a zeta function from the product of other zeta functions. Generically, and following the previous notation, let us envisage

$$\zeta_D(s)=\zeta_B(s)\zeta_C(s)=\sum_i \lambda_i^{-s}\sum_j \mu_j^{-s}. \tag{A1}$$

This turns out to be an important construction in number theory. Actually, even with the simplest zeta functions as factors, important and sophisticated $\zeta_D(s)$ are obtained. For example, with the Riemann zeta function itself. In fact, from the Euler product of the Riemann zeta function, we know that it has local factors of degree 1 at each prime, while automorphic L functions have local factors of degree 2 at almost all places.[16] This suggests that we can denote such product as

$$L(s)=\zeta_R(s)\zeta_R(s-k+1), \tag{A2}$$

with $k\geqslant 2$. In Ref. 16 it is shown that the L function is actually

$$L(s)=\sum_{n=1}^{\infty} \sigma_{k-1}(n)n^{-s}, \tag{A3}$$

where σ_k is the arithmetic function (the generalized divisor function, or some over all the divisor of n to some power), given by

$$\sigma_k(n)=\sum_{d|n} d^k. \tag{A4}$$

This appears naturally in the Chowla–Selberg formula and its generalizations.[7]

This shows, in close relationship with the preceding section, how the product of even the simplest of the zeta functions lead to an interesting object by the process considered above, often with important arithmetic properties (and some of these L functions are useful in analytical approaches to the study of algorithms[17,18]). Even more, in general, increasingly complex L functions are very often constructed or represented by a generic product of simpler L functions.[16]

Nevertheless, it seems apparent that instead of exploiting the useful idea of constructing zeta functions, it may also be worth to look at this relation from the other side, that is, as a decomposition of the zeta function on the l.h.s. into several factors. To illustrate the approach for zeta functions, let us just take into account the two simple examples considered in detail in Ref. 19. The zeta function

$$\zeta(s)=\sum_{m,n\in\mathbf{Z}^2}{}' \ (m^2+n^2)^{-s}, \tag{A5}$$

with the summation extended over all pairs $(m,n)\neq(0,0)$ in $\mathbf{Z}^2$, can be expressed as

$$\zeta(s)=4\zeta_R(s)\cdot L(\chi_4,s). \tag{A6}$$

where $\zeta_R(s)$ is the Riemann zeta function and $L(\chi_4,s)$ is the Dirichlet zeta function corresponding to the character χ_4. Another interesting factorization is the following one, for a different particular case of the two-dimensional Epstein zeta function:

$$\zeta(s)=\sum_{m,n\in\mathbf{Z}^2}{}' \ (m^2+mn+n^2)^{-s}=6\zeta_R(s)\cdot L(\chi_3,s). \tag{A7}$$

Once again, we see the natural appearance of L functions, whose determinants are of much interest as well (mainly in a number theoretical context; see Ref. 20 for a review).

These factorizations are particular cases of a more general situation coming from algebraic considerations in number theory.[16] Very general statements are not always possible, but let us compare the previous with the classical results (due to Dirichlet) concerning primitive quadratic forms of any determinant,

$$Q(x)=ax_1^2+bx_1x_2+cx_2^2, \quad (a,b,c)=1 \tag{A8}$$

(the parentheses meaning here maximum common divisor), with $D=-\det Q=b^2-4ac<0$ (the discriminant of Q), and

$$\chi_D(d)=\left(\frac{D}{d}\right). \tag{A9}$$

Then, for $n>0$, $(n,D)=1$, the character sum

$$r(n;D)=\omega_D\sum_{d|n}\chi_D(d) \tag{A10}$$

gives the number of all representations of n by representatives of forms of all classes of discriminant D. Here ω_D stands for the number of automorphs,

$$\omega_D=\begin{cases}6 & \text{if } D=-3,\\ 4 & \text{if } D=-4,\\ 2 & \text{if } D<-4.\end{cases} \tag{A11}$$

Notice how the discriminant gives the right character for the L function and the number of automorphs the right prefactor in the previous example of factorization. Nevertheless, we must point out that these previous examples and the posterior discussion looks so simple, due to the fact that the examples correspond to discriminants D for which the class number $h(D)$ (the number of equivalence classes of primitive binary quadratic forms) is one.

Factorization at the level of the heat kernels: Now, we pay attention to the meaning of the zeta factorization at the level of the respective associated heat kernels. Since A^{-s} and $\exp(-tA)$ are related by the following expression:

$$A^{-s}=\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\exp(-tA)\mathrm{d}t, \tag{A12}$$

then the zeta function is, up to a gamma function, the Mellin transform of the heat kernel. The interest of this expression, considered together with the factorization property, is that it allows, in a probabilistic context, the product of random variables to be directly performed in Mellin space (in contrast to the better known case of the addition of variables, where Fourier transform is used).[21] Therefore, the zeta factorization implies also a product for the respective heat kernels, but a product in the sense of probability theory, that is, the heat kernel (or in a number theoretical context, the theta function) denotes the probability distribution function of a random variable X_i, and then we have the product $X=\Pi_{i=1}^{n}X_i$. Nevertheless, for this to be exactly correct we should take into account the gamma function for each factor and for the resulting zeta function. For example, in the case of a zeta function with two factors:

$$\zeta(s)=\zeta_1(s)\zeta_2(s)\rightarrow\Gamma(s)\Gamma(s)\zeta(s)=\Gamma(s)\zeta_1(s)\Gamma(s)\zeta_2(s)\rightarrow K(t)\cdot\exp(-t)=K_1(t)\cdot K_2(t), \tag{A13}$$

where, in the last expressions, the products are in the sense explained above, and we have used the fact that $\Gamma(s)=\int_0^\infty t^{s-1}\exp(-t)\mathrm{d}t$. Thus, the necessary introduction of gamma factors implies that we have to take into account possible products of the main heat kernel with an exponential distribution.

This stochastic point of view seems both interesting from the mathematical point of view, where a probabilistic interpretation of zeta and theta functions is of interest,[22] and also from a physical point of view, where products of random variables very often constitute a role model of what is known with the name of multiplicative or cascade processes.[23]

Last but not least, the factorization is potentially interesting from the practical point of view in the asymptotic study of the trace of the heat kernel (9) and (10). The contributions can be considered separately, with the exception of the possible coincidence of poles or poles and zeros. This fact introduces interesting phenomena that can be seen with the following example. Consider the product of two Riemann zeta functions,

$$\zeta(s)=\zeta_R(s)\zeta_R(s), \tag{A14}$$

which yield the well-known L function,

$$\zeta(s)=L(s)=\sum_{k=1}^{\infty}\frac{d(k)}{k^s}, \tag{A15}$$

with $d(k)$ the divisor function again. Note the consistency with the previous case (A2)–(A4). The idea is now to construct another zeta function from two very similar factors,

$$\zeta_\varepsilon(s)=\zeta_R(s(1+\varepsilon))\zeta_R(s(1-\varepsilon)), \tag{A16}$$

with $\varepsilon>0$ a very small, real positive number. It seems that these two zeta functions should be almost identical in the whole complex plane, except for the fact that, in the first one, we have a double pole at $s=1$, while the second has two simple poles at $s=(1+\varepsilon)^{-1}$ and $s=(1-\varepsilon)^{-1}$, very close one from the other for ε small. Note that the pointlike structure of a pole allows to play that game. Now, from (9) and (10), it is clear how different the $t\rightarrow 0$ expansion of the associated trace of the heat kernel is, in the two cases. In the first case, we have

$$\mathrm{tr}\,e^{-tA_1}\sim-\frac{\log t}{t},\quad t\downarrow 0, \tag{A17}$$

in sharp contrast with the second case, where

$$\mathrm{tr}\,e^{-tA_2}\sim\Gamma\left(\frac{1}{1+\varepsilon}\right)t^{-[1/(1+\varepsilon)]}+\Gamma\left(\frac{1}{1-\varepsilon}\right)t^{-[1/(1-\varepsilon)]},\quad t\downarrow 0. \tag{A18}$$

We see that the case where the poles collide possesses a partition function which is much bigger the smaller the value of t is (the classical limit). Therefore, the associated partition functions differ considerably in the classical limit. A deeper physical understanding of this phenomena seems to be an interesting open question.

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On the Clebsch–Gordan problem for SU(1,1): Coupling nonstandard representations

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The Clebsch–Gordan coefficients coupling two unitary, irreducible, positive discrete series representations of SU(1,1), are constructed. In contrast to the Clebsch–Gordan coefficients obtained a long time ago by Holman and Biedenharn [Ann. Phys. (N.Y.) **39**, 1 (1966)], the derived coefficients are valid even when coupling nonstandard representations such as those for which the corresponding Bargmann indices k may be $k=\frac{1}{4}$ and/or $\frac{3}{4}$, values associated with the ''two-photon'' realization of the su(1,1) Lie algebra, the corresponding representations covering the even and odd number states, respectively, of the single-mode boson system. These nonstandard cases are actually representations associated with the covering group $\overline{\mathrm{SU}}(1,1)$. The results are extended to the coupling of three positive discrete series and the corresponding SU(1,1) Racah coefficients are obtained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1643542]

I. INTRODUCTION

The Lie group SU(1,1) and its associated Lie algebra su(1,1) plays a prominent role in many areas of quantum mechanics. The Lie algebra su(1,1), and those to which it is isomorphic, $\mathrm{su}(1,1)\sim\mathrm{so}(2,1)\sim\mathrm{sp}(2,\mathrm{R})\sim\mathrm{sl}(2,\mathrm{R})$,[1] are known to be spectrum generating algebras (the corresponding Lie groups being spectrum generating groups) for a number of systems, among them being: the harmonic oscillator,[2] the radial part of the Coulomb and the two and three-dimensional harmonic oscillator problems,[3] the singular oscillator,[2,4] the Morse oscillator,[5] and superfluid helium.[6] Beyond its role in generating spectra, it serves as a dynamical group for certain Hamiltonians of importance in quantum optics. Specifically, the single and double boson mode realizations of the su(1,1) Lie algebra appear in the Hamiltonians for nonlinear interactions that generate the single- and two-mode vacuum states.[7] The states generated from the vacuum are specific types of SU(1,1) coherent states and they are associated with specific representations.

There has recently been some interest, particularly in the context of quantum optics, in the coherent states obtained by coupling together different discrete representations of SU(1,1). These are coherent states associated with the representations of the direct product group $\mathrm{SU}(1,1)\otimes\mathrm{SU}(1,1)$ which is locally isomorphic to SO(2,2) much in the same way as $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ is locally isomorphic to SO(4).[8] There are many realizations of the corresponding Lie algebra su(1,1) which in turn determine the allowed positive discrete unitary irreducible representations (UIRs) which we denote as $\mathcal{D}_k^+$, where k is the Bargmann index[9] and where $k>0$. For what we shall call the *standard* UIRs of the positive discrete series one has $k=\frac{1}{2},1,\frac{3}{2},\ldots$. To couple different representations and obtain the states of the direct product representation $\mathcal{D}_{k_1}^+\otimes\mathcal{D}_{k_2}^+$, we need the SU(1,1) Clebsch–Gordan coefficients (CGCs). The CCGs for the coupling $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ are, of course, the familiar coefficients of angular momentum theory. For the higher dimensional groups such as SU(3), de Swart[10] worked out a rather general scheme that can work for any irreducible representation of any Lie algebra. For SU(1,1) the CCGs were derived many years ago by a number of authors, at least for coupling two standard representations.[11] The realization of the su(1,1) Lie algebra in terms of bilinear products of two sets of bose operators is associated with the standard UIRs. Bambah and Agarwal[12] studied the four-mode coherent states of the

Barut–Girardello-type[13] obtained by coupling together two two-mode realizations of the Lie algebra su(1,1), i.e., coherent states of the Lie algebra $su(1,1)\oplus su(1,1)$, or, equivalently, of the direct product group $SU(1,1)\otimes SU(1,1)$, by making use of the tabulated SU(1,1) CGCs as given in Ref. 11. This works well because the relevant representations being coupled are the standard ones. (It is the standard representations that are relevant to the radial Coulomb and harmonic oscillator problems[3] and the superfluid helium problem.[13]) But the representations associated with the single-mode realizations, sometimes known as the ''two-photon'' algebra, are nonstandard in that the Bargmann index is required to take the values $k=\frac{1}{4},\frac{3}{4}$. These representations are actually those associated with representations of the covering group $\overline{SU(1,1)}$ for which any $k\geqslant 0$ is allowed. (The representations associated with the realizations for the singular oscillator[2,4] and the Morse oscillator[5] are also those of the covering group.) In attempting to couple these nonstandard representations, this author and Benmoussa[14] found that the tabulated SU(1,1) CG coefficients gave nonsensical results (see Appendix). Part of the problem may be that many of these older papers adopt a notation for the state labels identical to that used in the case of su(2), the algebra of angular momentum. That notation tends to obscure important differences between the representations of SU(2) and SU(1,1), quite apart from the fact that for the latter, the unitary representations are all infinite dimensional. We say a little more on this below and in the Appendix. In any case, we rederived the relevant SU(1,1) CGCs in such a manner that allows the coupling of both the standard and nonstandard representations. As in the familiar case of SU(2), one can obtain a recursion relation for the SU(1,1) CGCs.[11] But the method we adopted in Ref. 14 seems to be different than any of the previous methods used and therefore we believe it is worthwhile to elaborate on it apart from any specific application. The idea is to first construct a proper ''ground'' state in the coupled representation by first solving a simple recursion relation analytically. The ''excited'' states are then determined by the application of the coupled raising operator an arbitrary number of times on this ground state, along with the use of the binomial expansion. It is straightforward to extend the procedure to the coupling of three representations of SU(1,1) and to obtain the SU(1,1) Racah coefficients. We believe that the methods used here have the virtue of relative simplicity.

The paper is organized as follows: We first review, in Sec. II, the su(1,1) Lie algebra and relevant positive discrete UIRs. In Sec. III we couple two discrete series and derive the SU(1,1) Clebsch–Gordan coefficients. In Sec. IV we use the results of Sec. III to couple three discrete series and obtain the SU(1,1) Racah coefficients. Section V contains some concluding remarks. As mentioned above, an Appendix is included to illustrate what goes wrong with the tabulated SU(1,1) CGCs when attempting to couple nonstandard representations.

II. REVIEW OF SU(1,1) POSITIVE DISCRETE SERIES REPRESENTATIONS

The su(1,1) Lie algebra consists of the operators K_0, $K_\pm$, satisfying the commutation relations

$$[K_0,K_\pm]=\pm K_\pm,\quad [K_+,K_-]=-2K_0. \tag{1}$$

The operator K_0 generates compact (circular) SU(1,1) transformations, whereas the combinations $K_1=(K_++K_-)/2$ and $K_2=(K_+-K_-)/2i$ generate noncompact (hyperbolic) SU(1,1) transformations. The Casimir operator

$$\mathcal{C}=K_0^2-\tfrac{1}{2}(K_+K_-+K_-K_+) \tag{2}$$

commutes with all the elements of the Lie algebra. The relevant unitary irreducible representations (UIRs) are the positive discrete series $\mathcal{D}_k^+$, whose bases, which are eigenstates of K_0 and $\mathcal{C}$, we denote as $|k,m\rangle$, where k is the so-called Bargmann index taking on the values $k=\frac{1}{2},1,\frac{3}{2},2,\ldots$, and where $m=0,1,2,\ldots,\infty$. These states satisfy the relations

$$K_0|k,m\rangle=(m+k)|k,m\rangle, \tag{3}$$

$$\mathcal{C}|k,m\rangle = k(k-1)|k,m\rangle, \tag{4}$$

$$K_+|k,m\rangle = [(m+1)(m+2k)]^{1/2}|k,m+1\rangle, \tag{5}$$

$$K_-|k,m\rangle = [m(m+2k-1)]^{1/2}|k,m-1\rangle. \tag{6}$$

The states $|k,m\rangle$ may be generated from the "ground" state $|k,0\rangle$ according to

$$|k,m\rangle = \left[\frac{\Gamma(2k)}{m!\Gamma(2k+m)}\right]^{1/2}(K_+)^m|k,0\rangle. \tag{7}$$

We avoid the use of the alternative, pseudoangular mometum labeling of the states, $|j,n\rangle$, frequently encountered in the literature,[11,12] where the eigenvalue of $\mathcal{C}$ is now $j(j+1)$ and that of K_0 is n, where $n=-j,-j+1,-j+2,\ldots$. [We use n instead of m to avoid confusion with our labels adopted for the SU(1,1) bases.] The allowed values of j for the standard unitary irreducible representations are $j=-\frac{1}{2},-1,-\frac{3}{2},\ldots$. The CGCs derived in the $|j,n\rangle$ notation are, at best, confusing to use in coupling nonstandard representations, and, as said above, lead to nonsensical results (as discussed in the Appendix) owing to the peculiar fractional nature of j and of n required for these representations. But the notation $|k,m\rangle$ is convenient because m is *always* a positive integer or zero and the Bargmann index k contains the fractional part of the spectrum of K_0. This turns out to be of an advantage in deriving the Clebsch–Gordan coefficients in what follows.

Before proceeding to that, we briefly give examples of realizations of su(1,1) with standard and nonstandard UIRs. The first we consider is the Schwinger-type[15] two-boson realization given as

$$K_0=\tfrac{1}{2}(a^+a+b^+b+1)\ K_+=a^+b^+,\ K_-=ab, \tag{8}$$

where the operators a and b are the bose operators of the two independent modes. The Casimir operator for this realization can be written as

$$\mathcal{C}=\tfrac{1}{4}(\Delta^2-1), \tag{9}$$

where the operator $\Delta=a^+a-b^+b$ is just the difference between the number of particles in the two modes. With the eigenvalue of Δ denoted by q where q is an integer, the Bargmann index is given by $k=(1+|q|)/2$, where $|q|$ is the degeneracy parameter and $|q|=0,1,2,\ldots$. Thus we have $k=\frac{1}{2},1,\frac{3}{2},\ldots$, so we have the standard UIRs. Assuming that the a mode has q more particles than the b mode, the number states of the two modes, $|n_a\rangle\otimes|n_b\rangle=|n_a,n_b\rangle$, organize themselves into $\mathcal{D}_k^+$ representations of su(1,1) given by $|k,m\rangle=|n+q,n\rangle$, $n=0,1,2,\ldots,\infty$, k is given above and from Eqs. (3) and (8) we have $m=n$.

An example of a realization leading to nonstandard UIRs is[3]

$$K_0=\tfrac{1}{2}(a^\dagger a+\tfrac{1}{2}),\ K_+=\tfrac{1}{2}a^{\dagger 2},\ K_-=\tfrac{1}{2}a^2, \tag{10}$$

where a and $a^\dagger$ are Bose operators. The Casimir operator for this realization takes on the value $\mathcal{C}=-3/16$ meaning that the allowed values of the Bargmann index are restricted to $k=1/4$ and $k=3/4$, values clearly not included within the standard series of discrete UIRs. The correspondence between the usual number states of a harmonic oscillator, $|n\rangle$, and the SU(1,1) basis states $|k,m\rangle$ from Eq. (10) is $|n\rangle\Leftrightarrow|k,m\rangle$ for $n=2(m+k)-1/2$. Note that for $k=\frac{1}{4}$ we have $n=0,2,4,\ldots$, while for $k=\frac{3}{4}$ $n=1,3,5,\ldots$. Thus the Hilbert space $\mathcal{H}$ of the single boson mode is split into even and odd subspaces corresponding to the respective UIRs: $\mathcal{H}=\mathcal{D}_{1/4}^+\oplus\mathcal{D}_{3/4}^+$.

There is one other application of the su(1,1) Lie algebra, not related to the realization given in Eq. (10), but for which one may have $k=\frac{1}{4}$ (mod 1) or $\frac{3}{4}$ (mod 1) whose corresponding represen-

tations describe bosons and fermions, respectively, and which for general k describes particles with fractional statistics, e.g., anyons.[16] These representations, along with those for the "two-photon" algebra, are representations of the covering group $\overline{\mathrm{SU}}(1,1)$.

III. COUPLING TWO POSITIVE DISCRETE SERIES REPRESENTATIONS

Now suppose we have two sets of su(1,1) operators that we denote (1) and (2), i.e., $K_{0,\pm}^{(i)}$, $i=1,2$ such that

$$[K_0^{(i)},K_\pm^{(j)}]=\pm K_\pm^{(i)}\delta_{i,j},\ [K_+^{(i)},K_-^{(j)}]=-2K_0^{(i)}\delta_{i,j}. \tag{11}$$

We then define the operators

$$K_0:=K_0^{(1)}+K_0^{(2)},\ K_+:=_+^{(1)}+K_+^{(2)},\ K_-:=K_-^{(1)}+K_-^{(2)}, \tag{12}$$

which, of course, also satisfy the su(1,1) Lie algebra and generate the direct product group $\mathrm{SU}(1,1)\otimes\mathrm{SU}(1,1)$. Each of these algebras has its respective Casimir operator of the form of Eq. (2). Denoting the Bargmann indices of the representations relevant to the realizations of these two algebras as k_1 and k_2, the representations to be coupled we denote as $\mathcal{D}_{k_1}^+:\{|k_1,m_1\rangle\}$ and $\mathcal{D}_{k_2}^+:\{|k_2,m_2\rangle\}$. The basis of the coupled representation we denote as $|K,M;k_1,k_2\rangle$, which we may sometimes abbreviate as $|K,M\rangle$. The eigenvalue of K_0 is $M+K$ and that of the Casimir operator is $K(K-1)$; that is, the coupled states satisfy Eqs. (3)–(6) with the replacements $k\to K$ and $m\to M$. The Kronecker product of the two positive discrete series reduces to a sum over positive discrete series according to the Clebsch–Gordan decomposition

$$\mathcal{D}_{k_1}^+\otimes\mathcal{D}_{k_2}^+=\sum_{K=k_1+k_2}^{\infty}\mathcal{D}_K^+, \tag{13}$$

where the sum proceeds in integer steps. That is, the allowed values of K are $K=k_1+k_2+l$, where $l=0,1,2,...,\infty$.

We now write the basis of the $\mathrm{SU}(1,1)\otimes\mathrm{SU}(1,1)$ states as

$$|K,M;k_1,k_2\rangle=\sum_{m_1,m_2}C(k_1,k_2,K;m_1,m_2,M)|k_1,m_1\rangle|k_2,m_2\rangle, \tag{14}$$

where the numbers $C(k_1,k_2,K;m_1,m_2,M)$ are the SU(1,1) CG coefficients. We first consider the ground state of the coupled representation where $M=0$:

$$|K,0;k_1,k_2\rangle=\sum_{m_1,m_2}C_{m_1,m_2}|k_1,m_1\rangle|k_2,m_2\rangle, \tag{15}$$

where for the moment, and for convenience, we have set $C(k_1,k_2,K;m_1,m_2,0)=C_{m_1,m_2}$. Acting on the state of Eq. (15) with the operator K_- gives us, since we have a ground state,

$$K_-|K,0;k_1,k_2\rangle=0=\sum C_{m_1,m_2}(K_-^{(1)}+K_-^{(2)})|k_1,m_1\rangle|k_2,m_2\rangle \tag{16}$$

or, using Eq. (6), equivalently,

$$\begin{aligned}0=\sum_{m_1,m_2}C_{m_1,m_2}\{&[m_1(m_1+2k_1-1)]^{1/2}|k_1,m_1-1\rangle|k_2,m_2\rangle\\&+[m_2(m_2+2k_2-1)]^{1/2}|k_1,m_1\rangle|k_2,m_2-1\rangle\}.\end{aligned} \tag{17}$$

This last expression we may rewrite as

$$\sum_{m_1,m_2}\{C_{m_1+1,m_2}[(m_1+1)(m_1+2k_1)]^{1/2}+C_{m_1,m_2+1}[(m_2+1)(m_2+2k_2)]^{1/2}\}|k_1,m_1\rangle|k_2,m_2\rangle=0, \tag{18}$$

from which follows the recursion relation

$$C_{m_1+1,m_2}=-C_{m_1,m_2+1}\left[\frac{(m_2+1)(m_2+2k_2)}{(m_1+1)(m_1+2k_1)}\right]^{1/2}. \tag{19}$$

It is evident that only those states are coupled for which $m_1+m_2=\text{const}$. Setting $m_1+m_2=l$, $l=0,1,2,...,\infty$, the recursion relation can be solved to yield

$$C_{q,l-q}=(-1)^q\left[\binom{l}{q}\frac{\Gamma(2k_1)\Gamma(2k_2+l)}{\Gamma(2k_1+q)\Gamma(2k_2+l-q)}\right]^{1/2}C_{0,l}, \tag{20}$$

where $C_{0,l}$ is from normalization

$$C_{0,l}=\left[\sum_{r=0}^{l}\binom{l}{r}\frac{\Gamma(2k_1)\Gamma(2k_2+l)}{\Gamma(2k_1+r)\Gamma(2k_2+l-q)}\right]^{-1/2}. \tag{21}$$

Thus our ground state may now be written as

$$|K,0;k_1,k_2\rangle=\sum_{q=0}^{l}C(k_1,k_2,K;q,l-q,0)|k_1,q\rangle|k_2,l-q\rangle, \tag{22}$$

where $C(k_1,k_2,K;q,l-q,0)=C_{q,l-q}$. Applying the operator $K_0=K_0^{(1)}+K_0^{(2)}$ to this last equation, it is easy to show that the allowed values of K and hence the allowed representations of $SU(1,1)\otimes SU(1,1)$, are given by $K=k_1+k_2+l$, $l=0,1,2,...,\infty$. The result in Eq. (22) is the proper ''ground'' state for the coupling of any two positive discrete UIRs of SU(1,1).

To obtain the states for $M>0$, the ''excited'' states, we now apply to Eq. (22) the raising operator K_+ of Eq. (3.3b) M times. But we first, make use of Eq. (7) and rewrite Eq. (22) as

$$|K,0,k_1,k_2\rangle=\sum_{q=o}^{l}C(k_1,k_2,K;q,l-q,0)\left[\frac{\Gamma(2k_1)\Gamma(2k_2)}{q!(l-q)!\Gamma(2k_1+q)\Gamma(2k_2+l-q)}\right]^{1/2}$$
$$\times(K_+^{(1)})^q(K_+^{(2)})^{l-q}|k_1,0\rangle|k_2,0\rangle. \tag{23}$$

Now, writing

$$K_+^M=(K_+^{(1)}+K_+^{(2)})^M=\sum_{p=0}^{M}\binom{M}{p}(K_+^{(1)})^p(K_+^{(2)})^{M-p}, \tag{24}$$

applying it to Eq. (23), and making multiple uses of Eq. (7), we obtain

$$|K,M;k_1,k_2\rangle=\left[\frac{\Gamma(2K)}{M!\Gamma(2K+M)}\right]^{1/2}\sum_{q=0}^{l}\sum_{p=0}^{M}C(k_1,k_2,K;q,l-q,0)$$
$$\times\left[\frac{(p+q)!(l+M-p-q)!\Gamma(2k_1+p+q)\Gamma(2k_2+l+M-p-q)}{q!(l-q)!\Gamma(2k_1+q)\Gamma(2k_2+l-q)}\right]^{1/2}$$
$$\times|k_1,p+q\rangle|k_2,l+M-p-q\rangle. \tag{25}$$

Note that there is degeneracy with respect to p and q and therefore we need to collect the coefficients of identical $p+q$. We may then write our state as

$$|K,M;k_1,k_2\rangle=\sum_{m_1=0}^{l+M} C(k_1,k_2,K;m_1,l+M-m_1)|k_1,m_1\rangle|k_2,l+M-m_1\rangle, \tag{26}$$

where

$$C(k_1,k_2,K;m_1,l+M-m_1)$$

$$=\sum_{q=0}^{l}\sum_{p=0}^{M}\delta(m_1,p+q)(-1)^q\frac{1}{q!(l-q)!\Gamma(2k_1+q)\Gamma(2k_2+l-q)}$$

$$\times\left\{\frac{l!\Gamma(2K)\Gamma(2k_1)\Gamma(2k_2+l)(p+q)!(l+M-p-q)!\Gamma(2k_1+p+q)\Gamma(2k_2+l+M-p-q)}{M!\Gamma(2K+M)}\right\}^{1/2}$$

$$\times\left[\sum_{r=0}^{l}\binom{l}{r}\frac{\Gamma(2k_1)\Gamma(2k_2+l)}{\Gamma(2k_1+r)\Gamma(2k_2+l-r)}\right]^{-1/2}, \tag{27}$$

and where, of course, it is understood that $K=k_1+k_2+l$. Note that we have dropped the redundant M by setting

$$C(k_1,k_2,K;m_1,l+M-m_1)\equiv C(k_1,k_2,K;m_1,l+M-m_1,M). \tag{28}$$

Finally we can write our coupled state in the ''standard'' form

$$|K,M;k_1,k_2\rangle=\sum_{m_1=0}^{l+M}\sum_{m_2=0}^{\infty} C(k_1,k_2,K;m_1,m_2,M)|k_1,m_1\rangle|k_2,m_2\rangle, \tag{29}$$

where the SU(1,1) CGCs are now

$$C(k_1,k_2,K;m_1,m_2,M)=\delta(m_2,l+M-m_1)C(k_1,k_2,K;m_1,l+M-m_1). \tag{30}$$

The key to the method we used here in deriving the CGCs is the separation of the integer and fractional parts of the spectrum of the K_0 operators, natural in the notation $|k,m\rangle$, as this allows for simple binomial expansions of the form of Eq. (24), i.e., in finite sums.

Because the CGCs are elements of a unitary transformation they must satisfy the orthogonality condition:

$$\begin{aligned}\delta_{K'K}\delta_{M'M}&=\langle K',M';k_1,k_2|K,M;k_1,k_2\rangle\\&=\sum_{m_1}\sum_{m_1'} C(k_1,k_2,K';m_1',l'+M'-m_1')C(k_1,k_2,K;m_1,l+M-m_1)\\&\quad\times\delta_{m_1'm_1}\delta_{l'+M',l+M}\\&=\sum_{m_1} C(k_1,k_2,K';m_1,l'+M'-m_1)C(k_1,k_2,K;m_1,l+M-m_1)\times\delta_{l'+M',l+M}.\end{aligned} \tag{31}$$

The left-hand side vanishes unless $M'=M$ and since $K=k_1+k_2+l$ and $K'=k_1+k_2+l'$ the condition that $l'=l$ implies that $K'=K$. Thus we can write the orthogonality relation as

$$\sum_{m_1=0}^{K-k_1-k_2+M} C(k_1,k_2,K';m_1,K'-k_1-k_2+M-m_1)$$
$$\times C(k_1,k_2,K;m_1,K-k_1-k_2+M-m_1)=\delta_{K'K}. \tag{32}$$

We now list some results from coupling nonstandard representations. We consider only those representations associated with the realization of the ''two-photon'' algebra given in Eq. (10). For $k_1=\frac{1}{4}=k_2$ and for $l=0$ we have

$$|K=\tfrac{1}{2},M=0;\tfrac{1}{4},\tfrac{1}{4}\rangle=|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},0\rangle_2=|0\rangle_1|0\rangle_2,$$

$$|K=\tfrac{1}{2},M=1;\tfrac{1}{4},\tfrac{1}{4}\rangle=\frac{1}{\sqrt{2}}(|\tfrac{1}{4},1\rangle_1|\tfrac{1}{4},0\rangle_2+|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},1\rangle_2)=\frac{1}{\sqrt{2}}(|2\rangle_1|0\rangle_2+|0\rangle_1|2\rangle_2),$$

$$\begin{aligned}|K=\tfrac{1}{2},M=2;\tfrac{1}{4},\tfrac{1}{4}\rangle&=\sqrt{\tfrac{3}{8}}(|\tfrac{1}{4},2\rangle_1|\tfrac{1}{4},0\rangle_2+|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},2\rangle_2)+\tfrac{1}{2}|\tfrac{1}{4},1\rangle_1|\tfrac{1}{4},1\rangle_2\\&=\sqrt{\tfrac{3}{8}}(|4\rangle_1|0\rangle_2+|0\rangle_1|4\rangle_2)+\tfrac{1}{2}|2\rangle_1|2\rangle_2,\end{aligned} \tag{33}$$

the first three states in the coupled representation. For the upper part of the right-hand side we have used the notation $|k_i,m_i\rangle_i$, where the k_i and m_i have been replaced by their numerical values, and for the lower part we have used the oscillator number states as given by the equivalence $|n\rangle_i\Leftrightarrow|k_i,m_i\rangle$ with $n=2(m_i+k_i)-1/2$.

The sequence of states in Eq. (33) is already physically relevant. It is equivalent to the sequence of states

$$|\psi_{2N}\rangle=\left(\frac{1}{2}\right)^N\sum_{p=0}^{N}\left[\binom{2p}{p}\binom{2N-2p}{N-p}\right]^{1/2}|2p\rangle_1|2N-2p\rangle_2, \tag{34}$$

where number states are used on the right-hand side. These states are known as the arcsine states[17] as the associated joint photon number probabilities for finding $2p$ photons in mode 1 and $2N-2p$ photons in mode 2 form the distribution known in probability theory as the fixed-multiplicative arcsine law of order N.[18] In fact, for the case of two-mode light fields, the states $|\psi_{2N}\rangle$ will be generated by a 50:50 beamsplitter with twin input Fock states of the form $|N\rangle_1|N\rangle_2$. That is, $(|N\rangle_1|N\rangle_2)_{\text{in}}\overset{\text{BS}}{\rightarrow}|\psi_{2N}\rangle_{\text{out}}$.[17] The input twin Fock state, actually a superposition of twin Fock states, can be generate from a down-conversion process with initial vacuum states in these modes.[19] The superposition produced is just the two-mode squeezed vacuum state. The state $|\psi_2\rangle=|K=\frac{1}{2},M=1;\frac{1}{4},\frac{1}{4}\rangle$ was observed many years ago in a well known experiment performed by Hong *et al.*[20] In another, more recent experiment, Ou *et al.*[21] have observed the state $|\psi_4\rangle=|K=\frac{1}{2},M=2;\frac{1}{4},\frac{1}{4}\rangle$. Furthermore, these states may have a practical application in ultrahigh resolution interferometry.[22,23]

For $k_1=\frac{1}{4}=k_2$, but now with $l=1$ such that $K=\frac{3}{2}$, we have the sequence of states

$$|K=\tfrac{3}{2},M=0;\tfrac{1}{4},\tfrac{1}{4}\rangle=\frac{1}{\sqrt{2}}(|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},1\rangle_2-|\tfrac{1}{4},1\rangle_1|\tfrac{1}{4},0\rangle_2)=\frac{1}{\sqrt{2}}(|0\rangle_1|2\rangle_2-|2\rangle_1|0\rangle_2),$$

$$|K=\tfrac{3}{2},M=1;\tfrac{1}{4},\tfrac{1}{4}\rangle=\frac{1}{\sqrt{2}}(|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},2\rangle_2-|\tfrac{1}{4},2\rangle_1|\tfrac{1}{4},0\rangle_2)=\frac{1}{\sqrt{2}}(|0\rangle_1|4\rangle_2-|4\rangle_1|0\rangle_2),$$

$$|K=\tfrac{3}{2},M=2;\tfrac{1}{4},\tfrac{1}{4}\rangle=\frac{1}{\sqrt{32}}(|\tfrac{1}{4},1\rangle_1|\tfrac{1}{4},2\rangle_2-|\tfrac{1}{4},2\rangle_1|\tfrac{1}{4},1\rangle_2)+\sqrt{\frac{15}{32}}(|\tfrac{1}{4},0\rangle_1|\tfrac{1}{4},3\rangle_2-|\tfrac{1}{4},3\rangle_1|\tfrac{1}{4},0\rangle_2)$$

$$=\frac{1}{\sqrt{32}}(|2\rangle_1|4\rangle_2-|4\rangle_1|2\rangle_2)+\sqrt{\frac{15}{32}}(|0\rangle_1|6\rangle_2-|6\rangle_1|0\rangle_2). \tag{35}$$

Notice that in these two examples, only even number states appear. Had we coupled representations for $k_1=k_2=\frac{3}{4}$, only odd states would have appeared.

As a final example, we consider the case for $k_1=\frac{1}{4}$ and $k_2=\frac{3}{4}$ and for $l=0$:

$$|K=1,M=0;\tfrac{1}{4},\tfrac{3}{4}\rangle=|\tfrac{1}{4},0\rangle_1|\tfrac{3}{4},0\rangle_2=|0\rangle_1|1\rangle_2,$$

$$|K=1,M=1;\tfrac{1}{4},\tfrac{3}{4}\rangle=\tfrac{1}{2}(|\tfrac{1}{4},1\rangle_1|\tfrac{3}{4},0\rangle_2+\sqrt{3}|\tfrac{1}{4},0\rangle_1|\tfrac{3}{4},1\rangle_2)=\tfrac{1}{2}(|2\rangle_1|1\rangle_2+\sqrt{3}|0\rangle_1|3\rangle_2),$$

$$|K=1,M=2;\tfrac{1}{4},\tfrac{3}{4}\rangle=\frac{1}{2\sqrt{2}}|\tfrac{1}{4},2\rangle_1|\tfrac{3}{4},0\rangle_2+\tfrac{1}{2}|\tfrac{1}{4},1\rangle_1|\tfrac{3}{4},1\rangle_2+\tfrac{1}{2}\sqrt{\frac{5}{2}}|\tfrac{1}{4},0\rangle_1|\tfrac{3}{4},2\rangle_2$$

$$=\frac{1}{2\sqrt{2}}|4\rangle_1|1\rangle_2+\tfrac{1}{2}|2\rangle_1|3\rangle_2+\tfrac{1}{2}\sqrt{\frac{5}{2}}|0\rangle_1|5\rangle_2,$$

$$\vdots, \tag{36}$$

where, of course, we notice the presence of both even and odd states and that the first in the product states is always even and the second odd.

Coherent states of the Perelomov[4] and Barut-Girardello[13] types based on these coupled states, and possible generation methods, have been discussed elsewhere.[14,24]

IV. COUPLING THREE POSITIVE DISCRETE SERIES

For the sake of completeness, we extend our considerations to the coupling of three SU(1,1) positive discrete series bases, i.e., the coupling $\mathcal{D}^+_{k_1}\otimes\mathcal{D}^+_{k_2}\otimes\mathcal{D}^+_{k_3}$. We first consider the grouping $(\mathcal{D}^+_{k_1}\otimes\mathcal{D}^+_{k_2})\otimes\mathcal{D}^+_{k_3}$. Denoting $k'=k_1+k_2+l$ and, using our previous result of Eq. (26) with an obvious change in the notation, we have

$$|k',m'\rangle\equiv|k',m';k_1,k_2\rangle=\sum_{m_1=0}^{l+m'}C(k_1,k_2,K;m_1,l+m'-m_1)|k_1,m_1\rangle|k_2,l+m'-m_1\rangle. \tag{37}$$

Then, coupling to the third basis we have

$$|K,M;k',k_3\rangle=\sum_{m'=0}^{l+M}C(k',k_3,K;m',L+M-m')|k',m'\rangle|k_3,l+M-m'\rangle, \tag{38}$$

where $K=k'+k_3+L=k_1+k_2+k_3+l+L$. Upon substituting Eq. (37) into Eq. (38) we have

$$|K,M;k',k_3\rangle=\sum_{m'=0}^{l+M}\sum_{m_1=0}^{l+m'}C(k_1,k_2,K;m_1,l+m'-m_1)C(k',k_3,K;m',L+M-m')$$
$$\times|k_1,m_1\rangle|k_2,l+m'-m_1\rangle|k_3,l+M-m'\rangle. \tag{39}$$

For the grouping $\mathcal{D}^+_{k_1}\otimes(\mathcal{D}^+_{k_2}\otimes\mathcal{D}^+_{k_3})$ we first have

$$|k'',m''\rangle \equiv |k'',m'';k_2,k_3\rangle = \sum_{m_2=0}^{l+m''} C(k_2,k_3,k'';m_2,l+m'-m_2)|k_2,m_2\rangle|k_3,l+m''-m_2\rangle, \tag{40}$$

where $k''=k_2+k_3+l'$. Then

$$|K,M;k'',k_1\rangle = \sum_{m''=0}^{L'+M} C(k'',k_1,K;m'',L'+M-m'')|k'',m''\rangle|k_1,L'+M-m''\rangle, \tag{41}$$

and substituting Eq. (40) into Eq. (41) we obtain

$$\begin{aligned}|K,M;k'',k_1\rangle = \sum_{m''=0}^{L'+M}\sum_{m_2=0}^{l+m''} & C(k_2,k_3,k'';m_2,l+m'-m_2)C(k'',k_1,K;m'',L'+M-m'') \\ & \times|k_1,L'+M-m''\rangle|k_2,m_2\rangle|k_3,l+m''-m_2\rangle,\end{aligned} \tag{42}$$

where now $K=k_1+k''+L'=k_1+k_2+k_3+l'+L'$. Evidently, we must require that $l+L=l'+L'$ as we must have the same value of K for either coupling scheme. The coupled bases must be related to each other by a unitary transformation of the form

$$|K,M;k',k_3\rangle = \sum_{k''} U(k'',k')|K,M;k_1,k''\rangle. \tag{43}$$

Following the standard procedures as used in the case of SU(2) (angular momentum),[25] it can be shown that

$$\begin{aligned}U(k'',k') = \sum_{\mu_1}\sum_{\mu_2} & C(k_1,k_2,k';\mu_1,\mu_2)C(k',k_3,K;\mu_1+\mu_2-l,\mu_3) \\ & \times C(k_2,k_3,k'';\mu_2,\mu_3)C(k_1,k',K;\mu_1,\mu_2+\mu_3-l').\end{aligned} \tag{44}$$

One can then define the SU(1,1) Racah coefficient W in the standard way according to

$$W(k_1,k_2,K,k_3;k',k'') = [(2k'+1)(2k''+1)]^{-1/2}U(k'',k'). \tag{45}$$

V. CONCLUSIONS

In this paper we have obtained Clebsch–Gordan coefficients allowing for the coupling of two unitary irreducible positive discrete series representations of SU(1,1) where one or both may be nonstandard, e.g., with Bargmann index $k=\frac{1}{4},\frac{3}{4}$, associated with the ''two-photon'' algebra, or of any case where the Bargmann index is not of the standard values $k=\frac{1}{2},1,\frac{3}{2},\ldots$. We have followed this by coupling three representations and have obtained the SU(1,1) Racah coefficients allowing for the transformation between different orders of couplings.

Possible applications, to be considered elsewhere, are to the coupling of, say, three single-mode (two-photon) representations. Such states, and the corresponding coherent states, might be of interest in quantum optics for three mode fields or in the three-dimensional motion of a trapped ion. Other possibilities, such as the coupling of the ''two-photon'' SU(1,1) states with the two-mode SU(1,1) states, are evident and are under investigation. Beyond applications in quantum optics, applications to the problem of coupling states of other systems associated with representations of SU(1,1), such as the case of the singular oscillator[2,4] also of anyons,[16] may be of interest and will be discussed elsewhere.

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APPENDIX: WHEN GOOD CLEBSCH–GORDAN COEFFICIENTS GO BAD

In the work of Holman and Biedenharn,[11] the su(1,1) bases are labeled using angular momentumlike states $|j,n\rangle$ (we are using n as before) such that

$$K_0|j,n\rangle = n|j,n\rangle,\ C|j,n\rangle = j(j+1)|j,n\rangle, \tag{A1}$$

where, by comparison with Eqs. (3) and (4), $n=-j,-j+1,-j+2,...$ and $j=-k$. The coupled states of two UIRs are given by the relation

$$|J,N;j_1,j_2\rangle = \sum_{n_1=-j_1} C^{j_1,j_2,J}_{n_1,N-n_1,N}|j_1,n_1\rangle|j_2,N-n_1\rangle, \tag{A2}$$

where $J=j_1+j_2-s$, $s=0,1,2,...$, and the CG coefficients $C^{j_1,j_2,J}_{n_1,N-n_1,N}$ are given explicitly in the Appendix of Ref. 12. We consider the ''ground state'' of the representation coupled for which $s=0$ and $N=-j_1-j_2$. The corresponding CGCs are given by[11]

$$C^{j_1,j_2,J}_{-j_1,j_1-J,-J} = (-1)^{J-j_1-j_2}\sqrt{-2J-1}\left[\frac{(j_1-j_2-J-1)!(-j_1-j_2-J-2)}{(-2j_1-1)!(-2J-1)!}\right]^{1/2}. \tag{A3}$$

For the case of coupling two standard representations, say for $k_1=-j_1=\frac{1}{2}=k_2=-j_2$ the coupled state is just $|J=-1,M=1\rangle = |j_1=-\frac{1}{2},n_1=\frac{1}{2}\rangle|j_2=-\frac{1}{2},n_2=\frac{1}{2}\rangle$ and the corresponding CGC is unity as is easy to check. But for the case when coupling the nonstandard representations, say, for $k_1=-j_1=\frac{1}{4}=k_2=-j_2$ and for $s=0$ such that $J=-1/2$ we obtain

$$C^{-\frac{1}{4},-\frac{1}{4},-\frac{1}{2}}_{\frac{1}{4},\frac{1}{4},\frac{1}{2}} = \sqrt{0}\left[\frac{\left(-\frac{1}{2}!\right)(-1)!}{\left(-\frac{1}{2}!\right)0!}\right]^{1/2} = \sqrt{\pm\infty\cdot 0}, \tag{A4}$$

a nonsensical result. Further, as displayed in Holman and Biedenharn[11] the CGCs $C^{j_1,j_2,J}_{n_1,n_2,N}$ are all proportional to $C^{j_1,j_2,J}_{-j_1,j_2-J,-J}$ thus rendering all coefficients suspect for the coupling of nonstandard representations within this scheme. In contrast, the coefficients derived above are well behaved for the case in question. For $k_1=\frac{1}{4}=k_2$, with $l=0$ we have $K=\frac{1}{2}$. Then, from Eqs. (20)–(22) we have

$$|K=\tfrac{1}{2},M=0,k_1=\tfrac{1}{4},k_2=\tfrac{1}{4}\rangle = |k_1=\tfrac{1}{4},q=0\rangle|k_2=\tfrac{1}{4},l-q=0\rangle, \tag{A5}$$

where we have, from Eq. (21), $C_{0,0}=1$ as it should. Thus there is no difficulty in coupling the nonstandard cases and getting sensible results within the approach taken in this paper.

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Singularity confinement and algebraic integrability

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Two important notions of integrability for discrete mappings, algebraic integrability and singularity confinement, have been used for discrete mappings. Algebraic integrability is related to the existence of sufficiently many conserved quantities and singularity confinement is associated with the local analysis of singularities. In this article, the relationship between these two notions is explored for birational autonomous mappings. The main result of this article is that algebraically integrable mappings are shown to have the singularity confinement property. Using this result, the proof of the nonexistence of algebraic conserved quantities for a class of discrete systems is given. © *2004 American Institute of Physics.*
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I. INTRODUCTION

One of the first notions of integrability was introduced by Liouville in the 19th century for Hamiltonian systems in classical mechanics. This type of integrability is based on quantities whose values do not change in time, the so-called *constants of the motion* or *first integrals*. For instance, in many mechanical systems the total energy and the linear and angular momenta are conserved through the dynamics and are examples of such constants. Liouville's fundamental contribution was to prove that if a given Hamiltonian systems admits enough first integrals, it can be solved explicitly by quadratures. More precisely, a $2n$-dimensional Hamiltonian system is said to be *Liouville-integrable* if it admits n functionally independent first integrals in involution (that is their Poisson brackets commute) and such systems can be integrated by quadrature and enjoy a particularly simple topology (the flow lives on products of tori and cylinders). For systems of n first-order ordinary differential equations (ODEs) *algebraic integrability* is defined as the existence $(n-1)$ functionally independent first integrals that are algebraic functions of the dependent variables. The existence of such first integrals is important for integrability as they can be used to reduce the dimensionality of the system.

In the particular case of Hamiltonian systems with more than one degree of freedom, algebraic integrability corresponds to the notion of superintegrability (see Refs. 6, 7, and 16 and references therein). For a $2n$-dimensional Hamiltonian system with $n>1$, the $2n-1$ first integrals needed for the property of algebraic integrability are more than the n ones needed for complete Liouville–Arnold integrability.

A different notion of integrability was introduced by Painlevé in the beginning of the 20th century.[8,25] Although Painlevé's goal was not to define a notion of integrability but rather to build new functions, his property is today widely used for the detection of integrable systems. An ODE is said to possess the *Painlevé property*[1,9,21] if its general solution is single-valued in its maximal domain of analytic continuation. The restrictions the Painlevé property impose on the solutions are so strong that an ODE exhibiting it may be considered for all practical purposes integrable. Many formal links between the Painlevé property and other notions of integrability have been established (see, for example, Refs. 9 and 10). Despite the fact that there is no general algorithmic way to obtain sufficient conditions for a given ODE to have the Painlevé property, necessary conditions can be derived. The algorithmic procedure to obtain such conditions is known as the *Painlevé test*

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or singularity analysis and is based on a local analysis of the solutions around movable isolated singularities.

The notions of algebraic integrability and singularity analysis of the solutions can be extended to finite difference equations. One of the most effective ways to perform singularity analysis in this context is given by *singularity confinement*[5,10–15,17,27–29] which, like the Painlevé test for ODEs, imposes conditions on the singularities of the solutions. Although there exist many striking particular examples which indicate that singularity confinement is closely related to other notions of integrability, there is no clear-cut result which establishes this relationship in a formal and general framework. This article explores the relationship between the notion of algebraic integrability and the property of singularity confinement in discrete mappings.

In the case of systems of ODEs, Yoshida[9,32,33] proved that the degree of a rational first integral is closely related to some exponents that can be obtained through the application of the Painlevé test. In this article, we establish an equivalent result for discrete systems by showing that singularity confinement analysis provides necessary conditions for the existence of an algebraic first integral. Moreover, a lower bound on the degree of rational first integrals can be obtained.

The rest of this article is organized as follows. In Sec. II, we define the notion of singularity and singularity confinement for birational autonomous discrete dynamical systems. In Sec. III, we study the local consequences of the existence of an algebraic first integral on the confinement of the singularities in the two-dimensional case. In Sec. IV, we extend the results of Sec. III to arbitrary dimensions. Applications are discussed in Sec. V.

II. FORMULATION OF THE PROBLEM

In this section we introduce and illustrate the notion of singularity confinement by considering a particular class of two-dimensional autonomous dynamical systems. These examples are used to motivate a formal definition valid in arbitrary dimensions.

Throughout the article the following notation will be used: If $\mathbf{g}$ is an analytic function from $\mathbb{C}^p$ to $\mathbb{C}^r$, then $D\mathbf{g}(\mathbf{x})$ is its *Jacobian* matrix evaluated at $\mathbf{x}\in\mathbb{C}^p$. When $p=r$, the *Jacobian* is denoted by $\det(D\mathbf{g}(\mathbf{x}))$. If f is a complex-valued rational function on $\mathbb{C}^p$, then $\mathrm{num}(f)$ and $\mathrm{den}(f)$ respectively denote the numerator and denominator of f.

A. Simple examples

The basic idea of singularity confinement is to consider the properties of solutions close to some singularities. To illustrate this concept, consider the class of two-dimensional complex dynamical systems of the form

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} g(x_n, y_n) \\ x_n \end{pmatrix}, \tag{2.1}$$

where g is a complex-valued rational function on $\mathbb{C}^2$,

$$g(x,y) = \frac{p(x,y)}{q(x,y)},$$

and p, q are relatively prime polynomials. Two types of singularities can be distinguished for such systems. The singularities of *first type* are the roots of q in $\mathbb{C}^2$, that is, the values (x,y) at which the vector field $\mathbf{f}(x,y)$ in (2.1) has a singularity. The singularities of *second type* are the points where the Jacobian of $\mathbf{f}$ is zero (this type of singularity was first considered in Ref. 12). As an example, consider the following discrete dynamical system:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} -x_n - y_n + a + \dfrac{b}{x_n} \\ x_n \end{pmatrix}, \tag{2.2}$$

where a and b are complex numbers. The analysis is performed for generic values of the parameters a and b. Clearly the right-hand-side of (2.2) presents a singularity if $x_n=0$. To study this singularity we study the behavior of nearby solutions by introducing a small complex perturbation ϵ, with $|\epsilon|>0$. We then set y_0 to be any complex number and $x_0=\epsilon$. The iterates x_p and y_p are then determined for any positive nonzero integer p by the discrete dynamical system (2.2). After one iteration, we have

$$x_1=\frac{b}{\epsilon}+a-y_0+\mathcal{O}(\epsilon). \tag{2.3}$$

In the limit $\epsilon\to 0$, $|x_1|\to\infty$ and, using (2.2) again,

$$x_2=-\frac{b}{\epsilon}+y_0+\mathcal{O}(\epsilon), \tag{2.4}$$

$$x_3=-\epsilon+\mathcal{O}(\epsilon^2). \tag{2.5}$$

The limit $\epsilon\to 0$ of the next iterate x_4 is well defined and given by y_0. Despite the fact that the function $\mathbf{f}$ defined by (2.2) is not well defined on any point of $\mathbb{C}^2$ of the form $(0,y)$, the limit $(x,y)\to(0,y)$ of $\mathbf{f}^4(x,y)$ exists and is given by

$$\lim_{(x,y)\to(0,y)}\mathbf{f}^4(x,y)=\begin{pmatrix} y \\ 0 \end{pmatrix}. \tag{2.6}$$

Moreover, since the value of the limit (2.6) depends on y, the same limit applied on the Jacobian of $\mathbf{f}^4$ is nonzero. The singularity is thus ''confined'' between the iterates 0 and 4 and does not propagate further. This property of confinement is very particular and we show in this article that it is closely related to the existence of a first integral for the system. A first integral for a discrete dynamical system of the form (2.1) is defined to be an analytic nonconstant complex-valued function I defined almost everywhere on $\mathbb{C}^2$ which is preserved by $\mathbf{f}$, that is

$$I(\mathbf{f}(\mathbf{x}))=I(\mathbf{x}), \tag{2.7}$$

for every $\mathbf{x}\in\mathbb{C}^2$ for which (2.7) makes sense. It is important to note that if $\mathbf{f}$ is not defined at a point $\mathbf{x}^*$ where I is well-defined, then the value of I at $\mathbf{x}^*$ is still preserved under $\mathbf{f}$ in the limit sense, i.e.,

$$\lim_{\mathbf{x}\to\mathbf{x}^*} I(\mathbf{f}(\mathbf{x}))=I(\mathbf{x}^*). \tag{2.8}$$

This is a consequence of the fact that $\mathbf{f}$ and I are continuous and defined almost everywhere in $\mathbb{C}^2$. In the particular case of system (2.2), one can check that the following polynomial,

$$I(x,y)=xy(x+y-a)-b(x+y), \tag{2.9}$$

is a first integral. Moreover, following (2.8), the first integral I is preserved in the limit sense through the iterations of the singularity of (2.2). That is,

$$-by=I(0,y)=\lim_{(x,y)\to(0,y)} I(\mathbf{f}^i(x,y)), \quad i=1,2,3,4. \tag{2.10}$$

Note that most integrable systems studied in this article are particular cases of the so-called QRT-family of mappings.[15,26]

The confinement property for the solutions of (2.1) does not hold in general. Although there is no formal result establishing how rare this confinement property might be, the fact that it does not hold for most systems of the form (2.1) has been well established in the literature.[11,13,14,27–29]

The following system is an example where singularities are not confined:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} -x_n - y_n + a + \dfrac{b}{x_n^3} \\ x_n \end{pmatrix}. \tag{2.11}$$

Consider the singularity $(x^*, y^*) = (0, y)$ and, as before, introduce $x_0 = \epsilon$ and $y_0 \in \mathbb{C}$ nonvanishing. The next iterates are $x_1 = b/\epsilon^3 + (a - y_0) - \epsilon$, $x_2 = -b/\epsilon^3 + y_0 + \mathcal{O}(\epsilon^5)$, and $x_3 = \epsilon + \mathcal{O}(\epsilon^5)$. Further, we find that, unlike the previous example, the appropriate cancellations allowing for confinement do not occur and the next iterates are also diverging at $\epsilon = 0$, $x_4 = 2b/\epsilon^3 + (a - y_0) - \epsilon + \mathcal{O}(\epsilon^5)$, and $x_5 = -2b/\epsilon^3 + y_0 + \mathcal{O}(\epsilon^5)$. In general, the sequence of limits $\epsilon \to 0$ of the $|x_p|$ for $p > 0$ repeats the formal triplet $(\infty, \infty, 0)$ indefinitely. This assertion is proven by induction based on the equality

$$\mathbf{f}^3 \begin{pmatrix} -nb/\epsilon^3 + y_0 + \mathcal{O}(\epsilon^5) \\ nb/\epsilon^3 + (a - y_0) - \epsilon + \mathcal{O}(\epsilon^5) \end{pmatrix} = \begin{pmatrix} -(n+1)b/\epsilon^3 + y_0 + \mathcal{O}(\epsilon^5) \\ (n+1)b/\epsilon^3 + (a - y_0) - \epsilon + \mathcal{O}(\epsilon^5) \end{pmatrix} \tag{2.12}$$

for any positive integer n. Therefore, the singularity is not confined. It is generally believed that systems which lack the confinement property will not be integrable. However, there is no definite result attached to this belief. We prove in the next sections that the analysis of the dynamics near the singularities can be used to conclude that (2.11) does not admit an algebraic first integral.

The following example illustrates the occurrence of the second type of singularity. Consider

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} \dfrac{x_n - 1}{y_n} + 2x_n \\ x_n \end{pmatrix}. \tag{2.13}$$

At first sight, the point $(x_n, 0)$ seems to be the only singularity. However, the Jacobian of $\mathbf{f}$ in (2.13) vanishes whenever $x_n = 1$. If $x_0 = 1$ and $y_0 \neq 0$, the next iterate as determined by (2.13) is given by $x_1 = 2$. We then have $x_2 = 5$, $x_3 = 12$. It is not difficult to see that x_i grows with respect to i, and that all iterates of $(1, y_0)$ under (2.13) with $y_0 \neq 0$ are independent of y_0. The singularity here only appears in the inverse of the Jacobian matrix and is not confined.

In the light of the previous examples, we can define the confinement property for singularities of discrete dynamical systems of the form (2.1). A general definition will be given in the next section. A *singularity* of the dynamical system (2.1) is defined to be any point (x^*, y^*) in $\mathbb{C}^2$ at which the right-hand-side of (2.1) is undefined or at which the Jacobian of $\mathbf{f}$ is zero. A singularity (x^*, y^*) is said to be *confined* if there exists a positive integer N such that both limits

$$\lim_{(x,y)\to(x^*,y^*)} \mathbf{f}^N(x,y), \qquad \lim_{(x,y)\to(x^*,y^*)} \det(\mathrm{D}\mathbf{f}^N(x,y)) \tag{2.14}$$

exist and the second limit is nonzero. The smallest number N having this property is referred to as the *confinement number*, that is the number of steps necessary for confinement.

The next example illustrates the case when a singularity of the second type is confined,

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} \dfrac{(x_n - 1/a)(x_n - a)}{y_n (x_n - b)(x_n - 1/b)} \\ x_n \end{pmatrix}, \tag{2.15}$$

where a and b are two nonzero distinct complex numbers which are also both distinct from $1/a$ and $1/b$. The right-hand-side (RHS) of (2.15) presents a singularity of the second type if $x_n=a$ because the Jacobian of $\mathbf{f}$ vanishes. If $x_0=a$ and $y_0\neq 0$, the next iterate as determined by (2.15) will be $x_1=0$; then $x_2=1/a$ and x_3 takes an indeterminate form 0/0. Again, we introduce a small complex perturbation ϵ, $|\epsilon|>0$, then set $x_0=\epsilon$ to find that when $\epsilon\to 0$,

$$x_3\to y_0+a-\frac{1}{a}, \tag{2.16}$$

and we conclude that the singularity is confined. The dynamical system (2.15) has singularity of the first type if $x_n=b$. Applying the same procedure as before with a perturbation ϵ, one finds that the limit $\epsilon\to 0$ of $|x_1|$, x_2 and x_3 gives, respectively, ∞, $1/b$ and $by_0/(b+y_0(1-b^2))$. Thus, any singularity of the form (b,y_0) with $y_0\neq b/(b^2-1)$ is confined in three steps. System (2.15) admits the following rational first integral:

$$I(x,y)=\left(b+\frac{1}{b}\right)(x+y)+\left(a+\frac{1}{a}\right)\left(\frac{1}{x}+\frac{1}{y}\right)-\frac{(1+x^2)(1+y^2)}{xy}. \tag{2.17}$$

The following example shows that the existence of a first integral does not imply that all singularities are confined. The system

$$\begin{pmatrix} x_{n+1}\\ y_{n+1}\end{pmatrix}=\mathbf{f}(x_n,y_n)=\begin{pmatrix} x_n^2/y_n\\ x_n\end{pmatrix} \tag{2.18}$$

has the following first integral:

$$I(x,y)=\frac{xy}{x^2+y^2}. \tag{2.19}$$

The RHS of (2.18) has a pole of order 1 at any point of $\mathbb{C}^2$ of the form $(x,0)$ with $x\neq 0$. As before, if we study this singularity by perturbation we conclude that there is no confinement since the Laurent expansions of the iterations of (x,ϵ) under the discrete system (2.18) around $\epsilon=0$ are all divergent. Although this singularity is not confined, one notices that any point of the form $(x,0)$ with $x\neq 0$ does not have a unique preimage under (2.18). Indeed, the expression defining $\mathbf{f}^{-1}$ given by

$$\mathbf{f}^{-1}(x,y)=\begin{pmatrix} y\\ y^2/x\end{pmatrix} \tag{2.20}$$

has a singularity of second type at $(x,0)$ and all the points of this form are mapped to $(0,0)$ under $\mathbf{f}^{-1}$. This example shows that if one wishes to establish a relationship between singularity confinement and first integrals, particular care should be given in distinguishing different singularities.

B. Preliminaries

The notion of singularity confinement will now be defined in a more general setting. We consider p-dimensional autonomous discrete dynamical systems described by birational mappings on $\mathbb{C}^p$. A *birational mapping* on $\mathbb{C}^p$ is a $\mathbb{C}^p$-valued rational function which is one-to-one almost everywhere in $\mathbb{C}^p$ and whose inverse, where it exists, is also represented by a rational function. The corresponding discrete dynamical systems are written

$$\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n),\qquad \mathbf{x}_n\in\mathbb{C}^p,\qquad n\in\mathbb{Z}, \tag{2.21}$$

where $\mathbf{f}$ is a birational mapping on $\mathbb{C}^p$ with no explicit dependence on n. The ith *iterate* of $\mathbf{x}_0\in\mathbb{C}^p$ under (2.21) is said to *exist* if the following limit,

$$\lim_{\mathbf{x}\to\mathbf{x}_0} \mathbf{f}^i(\mathbf{x}), \tag{2.22}$$

exists. The ith iterate is then defined to be that limit and is denoted $\mathbf{F}^i(\mathbf{x}_0)$.

Definition: A **singularity of type I** *for the discrete dynamical system* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is a point* $\mathbf{x}^* \in \mathbb{C}^p$ *at which* $\mathbf{f}$ *is not defined. The set of singularity of type I associated with the mapping* $\mathbf{f}$ *in* $\mathbb{C}^p$ *is denoted* $S_I(\mathbf{f})$.

Definition: A **singularity of type II** *for the discrete dynamical system* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is a point* $\mathbf{x}^* \in \mathbb{C}^p$ *such that* $\det(\mathrm{D}\mathbf{f}(\mathbf{x}^*))=0$. *The set of singularity of type II in* $\mathbb{C}^p$ *is denoted* $S_{II}(\mathbf{f})$.

In the particular case of birational mappings, we have

$$S_I(\mathbf{f})=\{\mathbf{x}^* \in \mathbb{C}^p | \mathrm{den}(f_i)(\mathbf{x}^*)=0, \quad \text{for some} \quad i \in \{1,2,\ldots,p\}\}, \tag{2.23}$$

$$S_{II}(\mathbf{f})=\{\mathbf{x}^* \in \mathbb{C}^p | \det(\mathrm{D}\mathbf{f}(\mathbf{x}^*))=0\}. \tag{2.24}$$

We call the sets $S_I(\mathbf{f})$ and $S_{II}(\mathbf{f})$ the *singular sets of first and second type*, respectively. The *singular set* $S(\mathbf{f})$ is defined as the union of both sets:

$$S(\mathbf{f})=S_I(\mathbf{f}) \cup S_{II}(\mathbf{f}). \tag{2.25}$$

For both types of singularity we can define the property of confinement.

Definition: Let $\mathbf{x}^* \in \mathbb{C}^p$ *be a singularity of type I or II for the system* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$. *The singularity is said to be* **confined** *if, for some* $i_c \in \mathbb{N}^{>0}$, *the iterate* $\mathbf{F}^{i_c}(\mathbf{x}^*)$ *exists and* $\lim_{\mathbf{x}\to\mathbf{x}^*} \det(\mathrm{D}\mathbf{f}^{i_c}(\mathbf{x}))\neq 0$.

The lowest such i_c is referred to as the *confinement number* that is the number of steps necessary for confinement. From now on, we assume that $\mathbf{f}$ is a birational mapping. The following lemma proves to be useful.

Lemma 2.1: *The image of* $S_{II}(\mathbf{f})$ *under the mapping* $\mathbf{f}$ *lies inside an algebraic variety of codimension 2.*

That is, the birational mapping $\mathbf{f}$ is one-to-one only on the subset of $\mathbb{C}^p$ defined by

$$O_{\mathbf{f}} \equiv \mathbb{C}^p \backslash S(\mathbf{f}). \tag{2.26}$$

As a consequence, the function $\mathbf{f}$ restricted to $O_{\mathbf{f}}$ defines a rational diffeomorphism

$$\mathbf{f}: O_{\mathbf{f}} \to O'_{\mathbf{f}} \equiv \mathbf{f}(O_{\mathbf{f}}), \tag{2.27}$$

whose inverse is also a rational function.

Proof: Assume that $S_{II}(\mathbf{f})\neq\varnothing$. Let $\mathbf{x}_0 \in S_{II}(\mathbf{f})$ and let $\mathbf{x}_1=\mathbf{f}(\mathbf{x}_0)$. From the inverse function theorem, it follows that

$$\lim_{\mathbf{x}\to\mathbf{x}_1} \|\det(\mathrm{D}\,\mathbf{f}^{-1}(\mathbf{x}))\|=\infty. \tag{2.28}$$

Thus, for some i's in $\{1,2,\ldots,p\}$, the denominator of $(\mathbf{f}^{-1})_i$ evaluated at $\mathbf{x}_1$ is zero. Denote those i by i_k, $k=1,2,\ldots,r$. We now prove that at least for one i_k, $\mathrm{num}((\mathbf{f}^{-1})_{i_k})$ also vanishes at $\mathbf{x}_1$. By contradiction, suppose that none of these numerators vanishes at $\mathbf{x}_1$. Thus

$$\lim_{\mathbf{x}\to\mathbf{x}_1} \|\mathbf{f}^{-1}(\mathbf{x})\|=\infty. \tag{2.29}$$

On the other hand, we have

$$\lim_{\mathbf{x}\to\mathbf{x}_0} \|\mathbf{f}^{-1}(\mathbf{f}(\mathbf{x}))\|=\mathbf{x}_0, \tag{2.30}$$

which contradicts Eq. (2.29). Thus, $\mathbf{x}_1$ must be in one of the following sets:

$$A_i=\{\mathbf{x}\in\mathbb{C}^p|\mathrm{num}((\mathbf{f}^{-1})_i)(\mathbf{x})=\mathrm{den}((\mathbf{f}^{-1})_i)(\mathbf{x})=0\},\qquad i\in\{1,2,\ldots,p\}. \tag{2.31}$$

This concludes the proof since each set A_i is defined as the intersection of the zero level sets of two relatively prime polynomials. □

As mentioned earlier, the singularity confinement turns out to be closely related to the existence of a first integral. This relationship will be explored in the next section.

Definition: *A* **first integral** *of* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is an analytic function* $I:U\subset\mathbb{C}^p\to\mathbb{C}$ *where* U *is a dense subset of* $\mathbb{C}^p$ *such that*

(a) $\|(\partial I/\partial x_1,\partial I/\partial x_2,\ldots,\partial I/\partial x_p)\|\neq 0$ *almost everywhere in* U, *and*
(b) $I(\mathbf{f}(\mathbf{x}))=I(\mathbf{x})$.

A first integral can exist in several forms.

Definition: A first integral I *of* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is* **polynomial** (*resp.* **rational**) *if the function* $I(\mathbf{x})$ *is a polynomial (resp. rational) function of* $\mathbf{x}\in\mathbb{C}^p$. *A complex-valued function* $f(\mathbf{x})$ *is* **algebraic** *over* $\mathbb{C}$ *if there exist* $s>0$ *and* $q_0,\ldots,q_s$ *rational in* $\mathbf{x}$ *such that*

$$q_0+q_1f+\cdots+q_sf^s=0. \tag{2.32}$$

If s *is the smallest positive integer such that (2.32) holds, the relation (2.32) is referred to as the minimal polynomial of* f. *A first integral* I *is* **algebraic** *if the function* $I(\mathbf{x})$ *is algebraic*.

Many notions of integrability are used in the literature. In this article, we focus on algebraic integrability. We are interested in determining precisely ''how many'' algebraic first integrals a given discrete system must admit to be algebraically integrable. For instance, suppose that the algebraic functions $A_1(\mathbf{x}),A_2(\mathbf{x}),\ldots,A_r(\mathbf{x})$ defined on $\mathbb{C}^p$ are all first integrals for a given system and $F(z_1,z_2,\ldots,z_r)$ is algebraic on $\mathbb{C}^r$. Then, it is clear that $A(\mathbf{x})=F(A_1(\mathbf{x}),A_2(\mathbf{x}),\ldots,A_r(\mathbf{x}))$ is also a first integral. However, this new first integral adds no knowledge to the given problem since it depends on the other first integrals.

Definition: Let $A_1(\mathbf{x}),A_2(\mathbf{x}),\ldots,A_r(\mathbf{x})$ *be smooth complex-valued functions defined on a domain* $D\subset\mathbb{C}^p$. *Then*

(a) $A_1,A_2,\ldots,A_r$ *are* **functionally dependent** *if, for each* $\mathbf{x}\in D$, *there is a neighborhood* U *of* $\mathbf{x}$ *and a smooth complex-valued function* $F(z_1,z_2,\ldots,z_r)$ *not identically zero on any subset of* $\mathbb{C}^p$ *such that*

$$F(A_1(\mathbf{x}),A_2(\mathbf{x}),\ldots,A_r(\mathbf{x}))=0. \tag{2.33}$$

(b) $A_1,A_2,\ldots,A_r$ *are* **functionally independent** *if they are not functionally dependent when restricted to any open subset of* D.

A simple way to determine if a set of functions is functionally independent is given by the following theorem (see, for example, Ref. 24).

Theorem: *Let* $\mathbf{A}=(A_1,A_2,\ldots,A_r)$ *be a smooth function from a domain* $D\subseteq\mathbb{C}^p$ *to* $\mathbb{C}^r$. *Then,* $A_1(\mathbf{x}),A_2(\mathbf{x}),\ldots,A_r(\mathbf{x})$ *are functionally dependent if and only if* $D\mathbf{A}(\mathbf{x}^*)$ *has rank strictly less than* r *for all* $\mathbf{x}^*\in D$.

We introduce the notion of integrability considered in this article.

Definition: *The discrete dynamical system* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is said to be* **algebraically integrable** *if it admits* $(p-1)$ *algebraic functionally independent first integrals*.

The following theorem is a direct extension of Brun's[9,23] theorem to discrete systems and is useful to extend the results we obtain for rational to algebraic first integrals.

Theorem: *If a discrete dynamical system of* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *has* k *functionally independent algebraic first integrals, then it has* k *functionally independent rational first integrals*.

Proof: Let I be an algebraic first integral and let

$$P(I)=q_0+q_1I+\cdots+q_{s-1}I^{s-1}+I^s \tag{2.34}$$

be its minimal polynomial, where q_i is a rational function of $\mathbf{x}$. Since I depends nontrivially on $\mathbf{x}$, there exists i such that q_i is a nonconstant rational function of $\mathbf{x}$. Since $I(\mathbf{f}(\mathbf{x}))=I(\mathbf{x})$, we have

$$q_0(\mathbf{f}(\mathbf{x}))-q_0(\mathbf{x})+(q_1(\mathbf{f}(\mathbf{x}))-q_1(\mathbf{x}))I(\mathbf{x})+\cdots+(q_{s-1}(\mathbf{f}(\mathbf{x}))-q_{s-1}(\mathbf{x}))I^{s-1}(\mathbf{x})=0. \tag{2.35}$$

Since P is minimal, we have $q_i(\mathbf{f}(\mathbf{x})))=q_i(\mathbf{x})$ and each q_i is a first integral. Now, let I' be another independent first integral whose minimal polynomial is

$$P(I')=q'_0+q'_1I'+\cdots+q'_{s'-1}I'^{s'-1}+I'^{s'}. \tag{2.36}$$

The independence between the two first integrals implies that there exist $i<s, i'<s'$ such that q_i, q'_i are two independent nonconstant rational first integrals. By induction, one can build k independent rational first integrals. □

Therefore, algebraic integrability implies rational integrability and it is sufficient to consider discrete dynamical systems of the form (2.21) which admit $(p-1)$ functionally independent rational first integrals $R_i(\mathbf{x})=P_i(\mathbf{x})/Q_i(\mathbf{x})$ where $i=1,2,\ldots,p-1$ and P_i and Q_i are relatively prime polynomials. Let $L_{i,c}$ be the level set of the first integral R_i corresponding to the value $c \in \mathbb{C}$. Since $\mathbf{f}$ is continuous, it leaves invariant the closure of the level set given by

$$\overline{L_{i,c}}=\{\mathbf{x}\in\mathbb{C}^p \,|\, P_i(\mathbf{x})-c\,Q_i(\mathbf{x})=0\}. \tag{2.37}$$

III. THE TWO-DIMENSIONAL CASE

In this section we study the local implications of algebraic integrability on the confinement of singularities for two-dimensional discrete dynamical systems. We consider a discrete dynamical systems of the form (2.21) which is algebraically integrable, that is, it possesses a nontrivial rational first integral $R(\mathbf{x})=P(\mathbf{x})/Q(\mathbf{x})$ where P and Q are some polynomials over $\mathbb{C}^2$. Let L_c be the level set of R corresponding to the value $c\in\mathbb{C}$.

We first focus our attention on singularities of the first type. The singular set of first type $S_I(\mathbf{f})$ is an algebraic variety since it is defined as the set of zeros of polynomials. We consider its irreducible decomposition is

$$S_I(\mathbf{f})=\bigcup_{i=1}^{d} S_I^{(i)}(\mathbf{f}), \tag{3.1}$$

where each irreducible component $S_I^{(i)}(\mathbf{f})$ is defined as the zero set of an irreducible polynomial on $\mathbb{C}^2$.

In example (2.18), we showed that the existence of a rational first integral does not ensure that all singularities are confined. However, in this case it is not possible to ''enter'' the singularity, meaning that it does not have a unique preimage under the mapping. Moreover, we know that confinement is a generic property, that is, it is only concerned with dense subsets of irreducible components of S_I. For instance, in example (2.15) all singularities of type I of the form (b,y_0) confine in three steps except a particular singularity defined by $y_0=b/(b^2-1)$. The next theorem relates the confinement of singularities to the existence of a rational first integral.

Theorem 3.1: *Consider a two-dimensional birational mapping* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *and assume it has a rational first integral* $R(\mathbf{x})=P(\mathbf{x})/Q(\mathbf{x})$. *Then, for each irreducible component* $S_I^{(j)}(\mathbf{f})$, *we have either*

(a) *there exists* $k_j \in \mathbb{N}^{>0}$ *such that*

$$\lim_{\mathbf{x}\to\mathbf{x}^*} \mathbf{f}^{k_j}(\mathbf{x}) \tag{3.2}$$

exists for almost all $\mathbf{x}^* \in S_I^{(j)}(\mathbf{f})$, *or*

(b) *there exists* $l_j \in \mathbb{N}^{>0}$ *such that* $S_I^{(j)}(\mathbf{f})$ *lies inside the singular set of the birational mapping defining* $\mathbf{f}^{-l_j}$.

Proof: Without loss of generality, take $j=1$. Consider two cases:

(1) $S_I^{(1)}(\mathbf{f}) \not\subset \overline{L_c}$ for all $c \in \mathbb{C}$.

Let $\mathbf{x}^* \in S_I^{(1)}(\mathbf{f})$ such that $\lim_{\mathbf{x}\to\mathbf{x}^*} \|f_i(\mathbf{x})\|$ exists or is infinity (as opposed to undefined) for $i=1,2$. Suppose that $\mathbf{x}^* \in \overline{L_{c^*}}$ for only one $c^* \in \mathbb{C}$ and that there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{c^*}}$ whose only intersection with any of the singular sets associated with the mappings $\mathbf{f}^i$, $i=1,2,\ldots,q+1$, (q is defined below) is $\mathbf{x}^*$ itself. The set of points satisfying the above properties is dense in $S_I^{(1)}(\mathbf{f})$. Let $\mathbf{p}_i(\epsilon)$, $i=1,2,..,q$, be the paths in $\mathbb{C}^2$ such that

(*i*) $\mathbf{p}_i(\epsilon) \in \overline{L_{c^*}}$ for ϵ small enough, that is,

$$P(\mathbf{p}_i(\epsilon)) - c^* Q(\mathbf{p}_i(\epsilon)) = 0; \text{ and} \tag{3.3}$$

(*ii*) $\|\mathbf{p}_i(\epsilon)\| \to \infty$ as $\epsilon \to 0$ and at least one of the components of $\mathbf{p}_i(\epsilon)$ is of the form $1/\epsilon$.

Note that the number of paths q can depend on the complex number c^* but the values it can take for different c^* can be bounded above by a number depending only on the degrees of P and Q.

Now, consider another path $\mathbf{x}(\sigma) \in \overline{L_{c^*}}$ $\forall \sigma$ such that

$$\lim_{\sigma\to 0} \mathbf{x}(\sigma) = \mathbf{x}^*. \tag{3.4}$$

Since there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{c^*}}$ whose only intersection with $S(\mathbf{f})$ is $\mathbf{x}^*$, $\mathbf{f}(\mathbf{x}(\sigma))$ is well-defined for σ nonzero and small enough. Moreover, since $\mathbf{f}$ preserves $\overline{L_{c^*}}$, $\mathbf{f}(\mathbf{x}(\sigma))$ also lies in $\overline{L_{c^*}}$, and

$$\lim_{\sigma\to 0} \|\mathbf{f}(\mathbf{x}(\sigma))\| = \infty. \tag{3.5}$$

Therefore, there exists a change of variable $\sigma = \sigma(\epsilon)$ of order $\mathcal{O}(\epsilon^s)$ for some $s>0$, so that $\mathbf{f}(\mathbf{x}(\sigma))$ is one of the paths $\mathbf{p}_i$ defined above:

$$\mathbf{f}(\mathbf{x}(\sigma(\epsilon))) = \mathbf{p}_i(\epsilon), \tag{3.6}$$

for some $1 \leqslant i \leqslant q$. Our claim is that there exists m with $m \leqslant q+1$ such that the limit as $\sigma \to 0$ of $\mathbf{f}^m(\mathbf{x}(\sigma))$ exists and is finite. Suppose, by contradiction, that the iterates $\mathbf{f}^k(\mathbf{x}(\sigma))$, $k=1,2,3,\ldots,q+1$, are all divergent at $\sigma=0$. Each iterate $\mathbf{f}^k(\mathbf{x}(\sigma))$ is associated with a unique path $\mathbf{p}_{i_k}(\epsilon)$. This implies that the kth preimage of $\mathbf{p}_{i_k}(\epsilon)$ is finite in the limit $\epsilon \to 0$ and no other $\mathbf{f}^l(\mathbf{x}(\sigma))$ for $1 \leqslant k < l \leqslant q+1$ corresponds to the same $\mathbf{p}_{i_k}(\epsilon)$. Hence the relation between the $q+1$ iterates that are divergent at $\sigma=0$ and the paths $\mathbf{p}_i(\epsilon)$ is injective. This is a contradiction since there are only q paths $\mathbf{p}_i(\epsilon)$.

(2) There exists $c \in \mathbb{C}$ such that $S_I^{(1)}(\mathbf{f}) \subset \overline{L_c}$. Let

$$\overline{L_c} = \bigcup_{i=1}^{r} \overline{L_c^{(i)}} \tag{3.7}$$

be the irreducible decomposition of $\overline{L_c}$ for any $c \in \mathbb{C}$. If $S_I^{(1)}(\mathbf{f})$ lies inside the singular set of $\mathbf{f}^{-1}$, then the theorem is proved. Otherwise, let $k \in \mathbb{N}^{>0}$ be such that $S_I^{(1)}(\mathbf{f})$ does not lie in a singular set associated with the mappings $\mathbf{f}^{-m}$, $m=1,2,\ldots,k$. Then,

$$\overline{\mathbf{f}^{-m}(S_I^{(1)}(\mathbf{f}))} = \bigcup_{i \in B_m} \overline{L_c^{(i)}}, \qquad 1 \leqslant l \leqslant k, \tag{3.8}$$

where each B_m is a subset of $\{1,2,\ldots,r\}$. The k sets in (3.8) are distinct, otherwise, by contradiction, there exist $m_1, m_2 \in \mathbb{N}^{>0}$ such that

$$\overline{\mathbf{f}^{-m_1}(S_I^{(1)}(\mathbf{f}))} = \overline{\mathbf{f}^{-m_2}(S_I^{(1)}(\mathbf{f}))}, \qquad 1 \leqslant m_1 < m_2 \leqslant k. \tag{3.9}$$

This implies that

$$S_I^{(1)}(\mathbf{f}) = \overline{\mathbf{f}^{-1}(\mathbf{f}^{(m_1-m_2+1)}(S_I^{(1)}(\mathbf{f})))}, \tag{3.10}$$

which is a contradiction since $\mathbf{f}$ is undefined almost everywhere on $S_I^{(1)}(\mathbf{f})$. Hence the k sets in (3.8) are distinct. However, there are only finitely many possibilities for the sets B_m in (3.8). Hence $S_I^{(1)}(\mathbf{f})$ must lie inside the singular set of $\mathbf{f}^{-l_1}$ for some l_1. □

Notice that condition (3.2) does not imply that the singularity is confined since the condition that the Jacobian be nonzero must be satisfied. In order to solve this problem, singularities of type II have to be considered. The singular set of second type is not, in general, an algebraic variety but its closure,

$$\overline{S_{II}(\mathbf{f})} = \{\mathbf{x}^* \in \mathbb{C}^p \,|\, \mathrm{num}(\det(\mathrm{D}\mathbf{f}(\mathbf{x}^*))) = 0\}, \tag{3.11}$$

is. Hence, it is possible to introduce the irreducible decomposition

$$\overline{S_{II}(\mathbf{f})} = \bigcup_{i=1}^{s} \overline{S_{II}^{(i)}(\mathbf{f})}, \tag{3.12}$$

where each $S_{II}^{(i)}(\mathbf{f})$ is a subset of $S_{II}(\mathbf{f})$. It is now possible to state the general theorem for singularities of second type.

Theorem 3.2: *Consider a two-dimensional birational mapping* $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ *and assume it has a rational first integral* $R(\mathbf{x}) = P(\mathbf{x})/Q(\mathbf{x})$. *Then, for each irreducible component* $\overline{S_{II}^{(j)}(\mathbf{f})}$, *we have either*

(*a*) *there exists* $k_j \in \mathbb{N}^{>0}$ *such that*

$$\lim_{\mathbf{x} \to \mathbf{x}^*} \det(\mathrm{D}\mathbf{f}^{k_j}(\mathbf{x})) \tag{3.13}$$

exists and is nonzero for almost all $\mathbf{x} \in S_{II}^{(j)}(\mathbf{f})$, *or*

(*b*) *there exists* $l_j \in \mathbb{N}^{>0}$ *such that* $S_{II}^{(j)}(\mathbf{f})$ *lies inside the singular set of* $\mathbf{f}^{-l_j}$.

Proof: The proof is similar to the proof of Theorem 3.1. Again, without loss of generality, we take $j = 1$ and consider two cases.

(1) $\overline{S_{II}^{(1)}(\mathbf{f})} \not\subset \overline{L_c}$ for all $c \in \mathbb{C}$.

The image of $S_{II}^{(1)}(\mathbf{f})$ under the mapping $\mathbf{f}$ is a finite subset of $\mathbb{C}^2$, thanks to Lemma 2.1. Moreover, $S_{II}^{(1)}(\mathbf{f})$ is not contained inside any level set. For any point in the image of $S_{II}^{(1)}(\mathbf{f})$ it is therefore possible to choose two distinct preimages in $S_{II}^{(1)}(\mathbf{f})$ which lie in two different level sets. Since $\mathbf{f}$ preserves $\overline{L_c}$, every point in the image of $S_{II}^{(1)}(\mathbf{f})$ must lie in the set

$$\bigcap_{c \in \mathbb{C}} \overline{L_c} = \{\mathbf{x} \in \mathbb{C}^2 \,|\, P(\mathbf{x}) = Q(\mathbf{x}) = 0\}. \tag{3.14}$$

The elements of this finite set are denoted $\mathbf{s}_i$, $i = 1,2,\ldots,m$. Note that in the case of a polynomial first integral, $Q(\mathbf{x}) = 1$ and this set is empty.

Now, choose $\mathbf{x}^* \in S_{II}^{(1)}(\mathbf{f})$ such that $\mathbf{x}^* \in \overline{L_{c^*}}$ for only one $c^* \in \mathbb{C}$ and there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{c^*}}$ whose only intersection with any of the singular sets associated with the mappings $\mathbf{f}^i$, $i=1,2,\ldots,q+r+1$, (q and r are defined below) is $\mathbf{x}^*$ itself. The set of points satisfying the above properties is dense in $S_{II}^{(1)}(\mathbf{f})$. Consider the q paths $\mathbf{p}_i(\epsilon)$ described in the proof of Theorem 3.1. Consider also the r paths $\mathbf{w}_i(\epsilon)$, $i=1,2,...,r$, in $\mathbb{C}^2$ satisfying

(i) $\mathbf{w}_i(\epsilon) \in \overline{L_{c^*}}$ for ϵ small enough.
(ii) $\mathbf{w}_i(\epsilon) \to \mathbf{s}_{j_i}$ as $\epsilon \to 0$ and one of the components ($k=1$ or 2) of $\mathbf{w}_i(\epsilon)$ is of the form $(\mathbf{s}_{j_i})_k + \epsilon$ for some $1 \leqslant j_i \leqslant m$.

Now, consider another path $\mathbf{x}(\sigma) \in \overline{L_{c^*}}$ such that

$$\lim_{\sigma \to 0} \mathbf{x}(\sigma) = \mathbf{x}^*. \tag{3.15}$$

Since there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{c^*}}$ whose only intersection with $S(\mathbf{f})$ is $\mathbf{x}^*$, $\mathbf{f}(\mathbf{x}(\sigma))$ is well-defined for σ nonzero and small enough. Moreover, since $\mathbf{f}$ preserves $\overline{L_{c^*}}$, $\mathbf{f}(\mathbf{x}(\sigma)) \in \overline{L_{c^*}}$, and

$$\lim_{\sigma \to 0} \mathbf{f}(\mathbf{x}(\sigma)) = \mathbf{s}_i \tag{3.16}$$

for some i such that $1 \leqslant i \leqslant r$. Following the proof of Theorem 3.1, $\mathbf{f}(\mathbf{x}(\sigma))$ can be associated with a path $\mathbf{w}_j(\epsilon)$ (whose limit as $\sigma \to 0$ is $\mathbf{s}_i$). Suppose by contradiction that the $d+r+1$ iterates $\mathbf{f}^k(\mathbf{x}(\sigma))$, $k=1,2,\ldots,d+r+1$, are either divergent at $\sigma=0$ or have a limit $\sigma \to 0$ equal to one of the $\mathbf{s}_i$. Each iterate $\mathbf{f}^k$ is associated with a path $\mathbf{p}_{i_k}(\epsilon)$ or $\mathbf{w}_{i_k}(\epsilon)$. This implies that the unique kth preimage of $\mathbf{p}_{i_k}(\epsilon)$ or $\mathbf{w}_{i_k}(\epsilon)$ must converge to $\mathbf{x}^*$ as $\epsilon \to 0$. The preimage is unique because there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{c^*}}$ whose only intersection with any of the singular sets associated with the mappings $\mathbf{f}^i$, $i=1,2,\ldots,q+r+1$, (q and r are defined below) is $\mathbf{x}^*$ itself. Since $\mathbf{x}^*$ is not one of the $\mathbf{s}_i$, there cannot be two iterates $\mathbf{f}^{k_1}(\mathbf{x}(\sigma))$ and $\mathbf{f}^{k_2}(\mathbf{x}(\sigma))$, $k_1, k_2 \leqslant q+r+1$, associated with the same path. Since there are only $q+r+1$ paths $\mathbf{p}_i(\epsilon)$ and $\mathbf{w}_i(\epsilon)$, there exists a $k \leqslant q+r+1$ such that the limit $\sigma \to 0$ of the kth iterate of $\mathbf{x}(\sigma)$ must be finite and not equal to one $\mathbf{s}_i$ as $\sigma \to 0$. Therefore, the limit $\sigma \to 0$ of the Jacobian of $\mathbf{f}^{k_1}$ evaluated at $\mathbf{x}(\sigma)$ must be a finite nonvanishing number. This ends the proof in the first case.

(2) There exists $c \in \mathbb{C}$ such that $S_I^{(1)}(\mathbf{f}) \subset \overline{L_c}$. The argument leading to the conclusion that $S_{II}^{(j)}(\mathbf{f})$ lies inside the singular set of $\mathbf{f}^{-l_1}$ for some l_1 is identical to the second case considered in the proof of the preceding theorem. □

With Theorem 3.2, it is now easy to see that singularities of type I satisfying the condition (3.2) are confined. Indeed, suppose k_j is the number considered in the first part of Theorem 3.1. If the Jacobian of $\mathbf{f}^{k_j}$ is zero almost everywhere on $S_I^{(j)}(\mathbf{f})$, then $S_I^{(j)}(\mathbf{f})$ becomes a subset of $\overline{S_{II}(\mathbf{f}^{k_j})}$. According to the proof of Theorem 3.1 we know that $S_I^{(j)}(\mathbf{f}) \not\subset \overline{L_c}$ for all $c \in \mathbb{C}$. Thus, as a consequence of Theorem 3.2, the singularities in $S_I^{(j)}(\mathbf{f})$ must be confined. We can state a general theorem including both types of singularities. To do so, we introduce the irreducible decomposition associated with $S(\mathbf{f})$

$$S(\mathbf{f}) = \bigcup_{i=1}^{d+s} S^{(i)}(\mathbf{f}), \tag{3.17}$$

where d and s are defined in (3.1) and (3.12).

Theorem 3.3: *Consider a two-dimensional birational mapping* $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ *and assume it has a rational first integral* $R(\mathbf{x}) = P(\mathbf{x})/Q(\mathbf{x})$. *Let* $S(\mathbf{f})$ *be its singular set with irreducible components* $S^{(j)}(\mathbf{f})$. *Then, for each* j, *either*

(a) *almost all singularities of* $S^{(j)}(\mathbf{f})$ *are confined in the same number of steps, or*
(b) *there exists* $l_j \in \mathbb{N}^{>0}$ *such that* $S^{(j)}(\mathbf{f})$ *lies inside the singular set of* $\mathbf{f}^{-l_j}$.

IV. ARBITRARY DIMENSIONS

In this section, we extend the results of the previous section to birational mappings of arbitrary dimension p. The mappings are assumed to be algebraically integrable, that is, they admit $(p-1)$ functionally independent first integrals $R_i(\mathbf{x})=P_i(\mathbf{x})/Q_i(\mathbf{x})$, $i=1,2,\ldots,p-1$. Then, the closure of the level sets associated with $\mathbf{c}\in\mathbb{C}^{p-1}$ is given by

$$\overline{L_{\mathbf{c}}}=\{\mathbf{x}\in\mathbb{C}^p \,|\, P_i(\mathbf{x})-c_i\,Q_i(\mathbf{x})=0, \quad \text{for } 1\leqslant i\leqslant p-1\}=\bigcap_{i=1}^{p-1}\overline{L_{i,c_i}}, \tag{4.1}$$

with $\overline{L_{i,c_i}}$ defined in (2.37). A set of constants $\mathbf{c}\in\mathbb{C}^{p-1}$ is said to be *regular* for the first integrals $\mathbf{R}=(R_1,R_2,\ldots,R_{p-1})$ if $\mathrm{D}\mathbf{R}(\mathbf{x})$ has rank equal to $(p-1)$ almost everywhere on $\mathbf{R}^{-1}(\mathbf{c})$. The set $\overline{L_{\mathbf{c}}}$ is then an algebraic variety of codimension $(p-1)$.

Our main Theorems 3.1–3.3 can be readily generalized to arbitrary dimensions and we only give here an outline of the proofs.

Theorem 4.1: *Consider a p-dimensional birational mapping* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *and assume it is algebraically integrable with first integrals* $R_i(\mathbf{x})=P_i(\mathbf{x})/Q_i(\mathbf{x})$, $i=1,2,\ldots,p-1$. *Then for each irreducible component* $S_I^{(j)}(\mathbf{f})$, *we have either*

(*a*) *there exists* $k_j\in\mathbb{N}^{>0}$ *such that*

$$\lim_{\mathbf{x}\to\mathbf{x}^*}\mathbf{f}^{k_j}(\mathbf{x}) \tag{4.2}$$

exists for almost all $\mathbf{x}\in S_I^{(j)}(\mathbf{f})$, or

(*b*) *there exists* $l_j\in\mathbb{N}^{>0}$ *such that* $S_I^{(j)}(\mathbf{f})$ *lies inside the singular set of the birational mapping defining* $\mathbf{f}^{-l_j}$.

Proof: Without loss of generality, take $j=1$. Consider two cases:

(1) $S_I^{(1)}(\mathbf{f})\not\subset\overline{L_{i,c}}$ for all $c\in\mathbb{C}$ and $1\leqslant i\leqslant p-1$.

Let $\mathbf{x}^*\in S_I^{(1)}(\mathbf{f})$ such that $\lim_{\mathbf{x}\to\mathbf{x}^*}\|f_i(\mathbf{x})\|$ exists or is infinite (as opposed to undefined) for $i=1,\ldots,p$. Suppose that $\mathbf{x}^*\in\overline{L_{\mathbf{c}^*}}$ for only one $\mathbf{c}^*\in\mathbb{C}^{p-1}$ which is regular and that there is a neighborhood of $\mathbf{x}^*$ on $\overline{L_{\mathbf{c}^*}}$ whose only intersection with the singular sets associated with the mappings $\mathbf{f}^i$, $i=1,2,\ldots,q+1$, (q is defined below) is $\mathbf{x}^*$ itself. The set of points satisfying the above properties is dense in $S_I^{(1)}(\mathbf{f})$. Let q be the number of paths $\mathbf{p}_i(\epsilon)$, $i=1,2,..,q$, in $\mathbb{C}^p$ such that

(i) $\mathbf{p}_i(\epsilon)\in\overline{L_{\mathbf{c}^*}}$ for ϵ small enough. That is,

$$P_k(\mathbf{p}_i(\epsilon))-c_k^*\,Q_k(\mathbf{p}_i(\epsilon))=0, \quad k=1,2,\ldots,p-1. \tag{4.3}$$

(ii) $\|\mathbf{p}_i(\epsilon)\|\to\infty$ as $\epsilon\to 0$ and at least one of the components of $\mathbf{p}_i(\epsilon)$ is of the form $1/\epsilon$.

Using the fact that $\overline{L_{\mathbf{c}^*}}$ is of codimension $p-1$, the rest of the proof follows exactly the similar case in the proof of Theorem 3.1.

(2) There exists $c\in\mathbb{C}$ and i, $1\leqslant i\leqslant p-1$, such that $S_I^{(1)}(\mathbf{f})\subset\overline{L_{i,c}}$. This part of the proof is identical to the corresponding part in the proof of Theorem 3.1 except that $\overline{L_{i,c}}$ is considered instead of $\overline{L_c}$. □

Theorem 4.2: *Consider a p-dimensional birational mapping* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *and assume it is algebraically integrable with rational first integrals* $R_i(\mathbf{x})=P_i(\mathbf{x})/Q_i(\mathbf{x})$, $i=1,2,\ldots,p-1$. *Then, for each irreducible component* $\overline{S_{II}^{(j)}(\mathbf{f})}$, *we have either*

(*a*) *there exists* $k_j\in\mathbb{N}^{>0}$ *such that*

$$\lim_{\mathbf{x}\to\mathbf{x}^*}\det(D\mathbf{f}^{\mathbf{k_j}}(\mathbf{x})) \tag{4.4}$$

exists and is nonzero for almost all $\mathbf{x}\in S_{II}^{(j)}(\mathbf{f})$, *or*

(*b*) *there exists* $l_j\in\mathbb{N}^{>0}$ *such that* $S_{II}^{(j)}(\mathbf{f})$ *lies inside the singular set of* $\mathbf{f}^{-l_j}$.

Proof: The proof is similar to the proof of Theorem 3.2 and the only difference comes in the first case, when $\overline{S_{II}^{(1)}(\mathbf{f})}\not\subset\overline{L}_{i,c}$ for all $c\in\mathbb{C}$ and $1\leqslant i\leqslant p-1$. Following the proof of Theorem 3.2, for any point in the image of $S_{II}^{(1)}(\mathbf{f})$ it is possible to choose two distinct preimages in $S_{II}^{(1)}(\mathbf{f})$ which lie in two different level sets. Indeed, from Lemma 2.1, the image of $S_{II}^{(1)}(\mathbf{f})$ under the mapping $\mathbf{f}$ lies in a subset of codimension 2 inside $\mathbb{C}^p$. Since $\mathbf{f}$ preserves $\overline{L}_{i,c}$, the points in the image of $S_{II}^{(1)}(\mathbf{f})$ must lie in the set

$$\bigcap_{c\in\mathbb{C},i\leqslant p-1}\overline{L}_{i,c}=\{\mathbf{x}\in\mathbb{C}^2|P_i(\mathbf{x})=Q_i(\mathbf{x})=0\}. \tag{4.5}$$

Since the first integrals are functionally independent, the set defined above is finite. The rest of the proof is similar to the proof of Theorem 3.2 except that one should specify that $\mathbf{c}^*$ has to be regular. □

Theorem 4.3: *Consider a p-dimensional birational mapping* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *and assume it is algebraically integrable. Let* $S(\mathbf{f})$ *be its singular set with irreducible components* $S^{(j)}(\mathbf{f})$. *Then, for each* j, *either*

(a) *almost all singularities of* $S^{(j)}(\mathbf{f})$ *are confined in the same number of steps, or*
(b) *there exists* $l_j\in\mathbb{N}^{>0}$ *such that* $S^{(j)}(\mathbf{f})$ *lies inside the singular set of* $\mathbf{f}^{-l_j}$.

V. COROLLARIES AND APPLICATIONS

In the previous two sections, the existence of first integrals was assumed to obtain local information on the confinement property. Here, the information given by the singularity confinement property is used to obtain global information on the discrete dynamical systems such as the nonexistence of algebraic first integral and the degree of possible rational first integrals. The results of this section can be considered as a discrete analog of Yoshida's theorem[9,32,33] which, for ODEs, relates the Kovalevskaya exponents given by the Painlevé test to the degree of a rational first integral. The first corollary is a direct consequence of Theorem 4.3.

Corollary 5.1: Consider a p-dimensional birational mapping $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *with a nonempty singular set* $S(\mathbf{f})$. *If there exists an irreducible components* $S^{(j)}(\mathbf{f})$ *in which almost all singularities are not confining and such that* $S^{(j)}(\mathbf{f})\not\subset S(\mathbf{f}^{-k})$ *for any positive* k, *then the system is not algebraically integrable.*

As an example of this corollary, we show that system (2.11), defined by

$$\mathbf{f}(x,y)=\begin{pmatrix}-x-y+a+\dfrac{b}{x^3}\\ x\end{pmatrix}, \tag{5.1}$$

is not algebraically integrable. Recall that singularities of the form $(0,y)$ are nonconfining. In order to use Corollary 5.1 and prove that this mapping does not admit an algebraic first integral, one must show that points of the form $(0,y)$ are not generically in the singular set of $\mathbf{f}^{-l}$ for some

$l>0$. The singular set of $\mathbf{f}^{-1}$ consists of points of the form $(x,0)$. Thus, we must prove that generic iterates of $(0,y)$ under $\mathbf{f}^{-1}$ do not belong to the set of points of the form $(x,0)$. The inverse of the mapping (5.1) is given by

$$\mathbf{f}^{-1}(x,y)=\begin{pmatrix} y \\ -x-y+a+\dfrac{b}{y^3} \end{pmatrix}. \tag{5.2}$$

This mapping can be obtained from $\mathbf{f}$ of (5.1) by interchanging x and y. Therefore, we can follow the analysis performed in (2.12) to perform a Laurent expansion in y to show that

$$\mathbf{f}^{-2}(x_0,y_0)=\begin{pmatrix} b/y_0^3+(a-x_0)-y_0+\mathcal{O}(y_0^5) \\ -b/y_0^3+x_0+\mathcal{O}(y_0^5) \end{pmatrix}. \tag{5.3}$$

Moreover, we have

$$\mathbf{f}^{-3}\begin{pmatrix} nb/y_0^3+(a-x_0)-y_0+\mathcal{O}(y_0^5) \\ -nb/y_0^3+x_0+\mathcal{O}(y_0^5) \end{pmatrix}=\begin{pmatrix} (n+1)b/y_0^3+(a-x_0)-y_0+\mathcal{O}(y_0^5) \\ -(n+1)b/y_0^3+x_0+\mathcal{O}(y_0^5) \end{pmatrix}, \tag{5.4}$$

where n is any positive integer. Hence, points of the form $(0,y)$ are not generically sent to points of the form $(x,0)$ by applications of $\mathbf{f}^{-1}$ and, from Corollary 5.1, system (2.11) does not admit an algebraic first integral.

In general, algebraic integrability restricts the possible *local* behavior of singularities. Theorem 4.3 gives two possible local behaviors but, in each case, the singularity can have several different *global* behaviors. Consider an irreducible component of the singular set $S^{(1)}(\mathbf{f})$. In the proofs of Theorems 3.3 and 4.3, we considered two cases: $S^{(1)}(\mathbf{f})\not\subset\overline{L_{\mathbf{c}}}$ and $S^{(1)}(\mathbf{f})\subset\overline{L_{\mathbf{c}}}$. When $S^{(1)}(\mathbf{f})\not\subset\overline{L_{\mathbf{c}}}$ the singularities of $S_I^{(1)}(\mathbf{f})$ are generically confined. In this case, two different types of global behavior can be expected. First, after meeting a finite number singularities, the mapping generically never meets other singularities (note that this must also be true in the backward direction, that is for $\mathbf{f}^{-1}$). We will refer to such a behavior as *global confinement*. Second, the singularities may be confined but not globally. Because, for each dynamical system of the form (2.21), there are only finitely many irreducible parts to $S(\mathbf{f})$, the mapping must, at one point, come back to the initial singularity and take $S_I^{(1)}(\mathbf{f})$ into itself. We say that such singularities are *periodic*. We now define formally these two types of global behavior and illustrate them.

Definition: A singularity $\mathbf{x}^*\in\mathbb{C}^p$ *for a birational mapping* $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *is said to be* **globally confined** *if there exist* $k',k''\in\mathbb{N}^{>0}$ *such that* $\mathbf{x}^*\notin S(\mathbf{f}^k)$ *for any* $k>k'$ *and* $\mathbf{x}^*\notin S(\mathbf{f}^{-k})$ *for any* $k>k''$.

An example of such a behavior is given by system (2.2). For this system, points of the form $(x,0)$ are not sent to points of the form $(0,y)$ through successive applications of $\mathbf{f}$. To prove this, let (x_n,y_n) be the nth iterate of $(x,0)$. If $n=4k$, an expansion of $\mathbf{f}^4(x,0)$ reveals that $(x_{4k},y_{4k})=(kx+\mathcal{O}(x^2),(-k+1)x+\mathcal{O}(x^2))$, $k=1,2,\ldots$. This fact also implies that $x_{4k+3}=-kx+\mathcal{O}(x^2)$ and we conclude that x_{4k+3} and x_{4k} are neither infinite nor vanishing. By contradiction assume that there exists n such that $(x_n,y_n)=(0,y)$. Therefore, either $n=4k+1$ or $n=4k+2$. However, from Eq. (2.4) we know that x_{n+2} is infinite which is a contradiction. We conclude that no iterate of $(x,0)$ falls onto a point of the form $(0,y)$ and singularities of the form $(0,y)$ are globally confined.

Definition: Consider the singular set of a birational mapping $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ *and one of its irreducible component* $S^{(j)}(\mathbf{f})$. *If there is a* $k\in\mathbb{N}^{>0}$ *such that* $\mathbf{f}^k(S^{(j)}(\mathbf{f}))=S^{(j)}(\mathbf{f})$, *then the elements of* $S^{(j)}(\mathbf{f})$ *are said to be* **periodic singularities** *of period* k.

An example of such a behavior is given by a particular case of the Gambier system[13,14]

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} \dfrac{(y_n + (1/a - a - 1))x_n - a + 1}{x_n + y_n} \\ 1 - 1/y_n \end{pmatrix}, \tag{5.5}$$

where a is a nonzero complex constant. The system (5.5) admits a singularity of type II at any point of the form (x,a). Then the first iterate of a point of this form is given by $(1/a-1,1-1/a)$. But the Jacobians of $\mathbf{f}^2$ and $\mathbf{f}^3$ at (x,a) are nonzero and the singularity is confined. It is not globally confined since $\mathbf{f}^4(x,a)=\mathbf{f}(x,a)=(1/a-1,1-1/a)$ and the singularity is periodic. The system admits the following first integral:

$$I(x,y) = \frac{y^3 - 3y + 1}{y(y-1)}. \tag{5.6}$$

Now, consider the second case considered in the proofs of Theorems 3.3 and 4.3: $S^{(1)}(\mathbf{f}) \subset \overline{L_{i,c}}$ for some c. If the singularities of $S^{(1)}(\mathbf{f})$ are generically confined in k steps, then $\mathbf{f}^k(S^{(1)}(\mathbf{f}))$ has to be a set of the form of the RHS of (3.8). Since there are only finitely many of those, the singularities cannot be globally confined. So, either they are periodic, or $S^{(1)}(\mathbf{f})$ lies inside the singular set of $\mathbf{f}^k$ for all k greater than a certain k'. It must also be true in the backward direction and if the singularities are not periodic $S^{(1)}(\mathbf{f})$ lies inside the singular set of $\mathbf{f}^{-k}$ for all k greater than a certain k''. We will refer to these singularities as *ubiquitous singularities*. An example of such a behavior is given by the singularities of Eq. (2.18) of the form $(x,0)$. These singularities are not confined but they are in the singular set of $\mathbf{f}^{-l}$ for any $l>0$ and, therefore, these singularities are ubiquitous. Note that singularities of the form $(0,y)$ are also ubiquitous.

Definition: A singularity $\mathbf{x}^* \in \mathbb{C}^p$ *of a birational mapping is said to be* **ubiquitous** *if there exist a* $k' \in \mathbb{N}^{>0}$ *such that* $\mathbf{x}^* \in S(\mathbf{f}^k)$ *for any* $k > k'$ *and a* $k'' \in \mathbb{N}^{>0}$ *such that* $\mathbf{x}^* \in S(\mathbf{f}^{-k})$ *for any* $k > k''$.

Given a discrete dynamical system of the form (2.21) and an irreducible component $S^{(j)}(\mathbf{f})$ of the singular set, one would like to be able to obtain information on the first integrals. The only way one can know if a given irreducible component of the singular set lies inside a level set is by studying the global behavior of the singularity. If the singularity is globally confined, then $S^{(j)}(\mathbf{f})$ does not lie inside a level set, but if it is ubiquitous, then it does. If the singularities are periodic, no conclusion can be reached.

Information on first integrals can be obtained by studying singularities of type I. Consider the paths $\mathbf{p}_i$ defined in the two-dimensional case in the proof of Theorem 3.1. The number of these paths is bounded above by the maximum of the degrees of P and Q. Moreover, for each $S_I^{(j)}(\mathbf{f}) \not\subset \overline{L_c}$ for all c, consider k_j', the lowest value k_j can take. Then $k_j' - 1$ is the number of different paths $\mathbf{p}_i$ realized by iterating a point close to the singularity under the mapping. Hence, the following corollary holds.

Corollary 5.2: Consider a two-dimensional birational mapping with rational first integral $R = P/Q$. *Consider also the irreducible components of the singular set of the first type* $S_I^{(j)}(\mathbf{f})$ *for which the singularities are globally confined. Then the maximum of the degrees of* P *and* Q *is bounded below by the number*

$$\sum_j (k_j' - 1), \tag{5.7}$$

where k_j' *is given by the lowest value* k_j *of Theorem 3.1.*

In example (2.2), the singular set has a unique component in which singularities are globally confined with $k=4$ and the degree of the first integral is exactly $k-1=3$. Note, however, that the corollary only provides a lower bound as shown in the following example,

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} -y_n + x_n + \dfrac{a}{x_n} \\ x_n \end{pmatrix}, \tag{5.8}$$

where a is a nonvanishing complex number. Here again, one can check that singularities of the form $(0,y)$ are confined in four steps and since confinement is global, the lower bound for the numerator and denominator of a first integral is 3. However, the rational first integral $I=P/Q$ with lowest degree possible on P and Q is given by

$$I=(x_n-y_n)^2(x_n y_n-a)^2, \tag{5.9}$$

which is of degree 6, not 3 (note, however, the rather degenerate nature of the first integral).

Next, we turn our attention to singularities of type II in the case when $S_{II}^{(j)}(\mathbf{f}) \not\subset \overline{L_{i,c}}$ for all c and all i. From the proof of Theorems 3.2 and 4.2, one sees that, as long as the singularities are not confined, the iterates of $S_{II}^{(j)}(\mathbf{f}) \not\subset \overline{L_{\mathbf{c}}}$ must be roots of both P_i and Q_i for all rational first integrals P_i/Q_i. Therefore, we have the following corollary.

Corollary 5.3: Consider an algebraically integrable p-dimensional birational mapping with the rational first integral $R=P/Q$. Consider also an irreducible component of the singular set of the second type $S_{II}^{(j)}(\mathbf{f})$ whose singularities are globally confined. Let k_j be the corresponding confinement number. Then the finite elements of the set

$$\bigcup_{i=1}^{k_j-1} \mathbf{f}^i(S_I^{(j)}(\mathbf{f}))$$

are roots of both P and Q.

This corollary is best illustrated in example (2.15) where $(0,a)$ and $(1/a,0)$ are roots of both the numerator and denominator of the rational function (2.17).

The previous corollary has an immediate consequence for the existence of polynomial first integrals.

Corollary 5.4: Consider an algebraically integrable p-dimensional birational mapping. If this system admits singularities of the second type which are globally confined, then there is no polynomial first integral.

The last result concerns the case when the irreducible component of the singular set lies inside the closure of a level set of the first integral. In Secs. III and IV, it was found that if $\mathbf{f}^k$ (for $k \in \mathbb{N}$) is well-defined on $S^{(j)}(\mathbf{f})$ and its Jacobian is nonzero, then $\mathbf{f}^k(S^{(j)}(\mathbf{f}))$ must be a set of the form of the RHS of (3.8), hence it lies on a level set. This is stated in the following corollary.

Corollary 5.5: Consider a p-dimensional birational mapping $\mathbf{x}_{n+1}=\mathbf{f}(\mathbf{x}_n)$ together with an irreducible component of the singular set $S^{(j)}(\mathbf{f})$ for which the singularities are ubiquitous. If $\mathbf{f}^k$ is well-defined almost everywhere on $S^{(j)}(\mathbf{f})$ and its Jacobian is nonzero, then $\mathbf{f}^k(S^{(j)}(\mathbf{f}))$ lies inside the closure of a level set of the first integrals.

Note that the case $k=0$ should also be included meaning that $S^{(j)}(\mathbf{f})$ itself lies inside the closure of a level set of the first integrals.

This corollary can be applied to example (2.18). Since the two sets of singularities ($(x,0)$ and $(0,y)$) are ubiquitous, they are level sets of the first integral (2.19).

As a final example, consider the system

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \mathbf{f}(x_n, y_n) = \begin{pmatrix} -y_n + x_n + \dfrac{a}{x_n^2} \\ x_n \end{pmatrix}, \tag{5.10}$$

where a is a nonzero complex number. This example was first used in Ref. 17 to show that singularity confinement is not sufficient for integrability. Following example (2.2), it is easy to

show that singularities of the form $(0,y)$ are generically globally confined. However, numerical analysis performed on this system strongly suggests that it exhibits chaotic behavior.[17]

VI. CONCLUSIONS

In this article, we defined different types of singularities and their confinement property for autonomous discrete birational dynamical systems. The theory of singularity confinement was developed more than 10 years ago[11,12,27] and different types of singularities have been implicitly used. Here, in order to relate algebraic integrability to singularity confinement we have found necessary to give a formal definition of different singularities and their confinement property.

In Secs. III and IV, we showed that algebraic integrability for birational mappings implies that singularities are either locally confined or some preimages are not well-defined.

In Sec. V, we studied global properties of birational mappings and showed that there are three types of behavior for singularities compatible with algebraic integrability. Namely, singularities are either globally confined, periodic, or ubiquitous. Remarkably, in the seminal papers describing singularity confinement, similar behaviors were found heuristically to be compatible with integrability.[11–13,15,27,28] However, the classical approach relies mostly on a local analysis of the singularities. An important aspect of the results shown in this article is that global properties have to be satisfied for a system to be algebraically integrable. To unify these different concepts, we define the confinement property for a discrete system in the following way:

Definition: A birational mapping is said to have the **confinement property** *if its singularities are, generically, globally confined, periodic, or ubiquitous*.

Then the most important result of this article can be rephrased as follows.

Theorem: *An algebraically integrable birational mapping has the confinement property*.

In particular, this result shows that every mapping in the QRT-family[15,26] has the confinement property both in the symmetric and asymmetric cases. This fact also holds for the recently discovered class of integrable birational discrete systems discovered in Ref. 22. Moreover, from examples such as system (5.10), we have strong numerical evidence that the confinement property is necessary but not sufficient for algebraic integrability.

In this article, we also found sufficient conditions for nonintegrability. Essentially, if singularities are confined in one direction and not in the other, the system cannot be algebraically integrable.

Finally, the remaining corollaries of Sec. V provide information on the existence and degree of rational first integrals directly from the singularity confinement procedure.

All the examples of integrable discrete systems considered in this article have a first integral of genus 0 or 1. It is not possible to find a birational mapping of infinite order preserving an algebraic curve of genus 2 or higher. The argument proving this fact is due to Veselov (Ref. 31, p. 35). It makes use of the Hurwitz theorem which tells us that the automorphic group of an algebraic curve of genus 2 or higher is finite.

Another important question concerns the relation between the confinement property and other types of integrability for discrete dynamical systems (see, for example, Refs. 2, 4, 5, 17, and 30). In particular, in a work by Bellon,[3] the proof that two-dimensional birational mappings admitting a first integral satisfy the *algebraic entropy*[4,17] integrability condition is given.

Since the only mappings studied here were birational, we could have made use of the projective space in which the point at infinity plays no particular role. Hence only singularities of type II should be studied. However, the ideas presented in this article could not be extended for the case of nonautonomous or discrete dynamical systems that are not birational. For instance, the integrable nonrational mapping derived in Refs. 18–20 could not be studied. It is therefore crucial to give a definition of singularity confinement that can be applied to general discrete systems.

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Mathematical properties of a new Levin-type sequence transformation introduced by Čížek, Zamastil, and Skála. I. Algebraic theory

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Čížek, Zamastil, and Skála [J. Math. Phys. **44**, 962–968 (2003)] introduced in connection with the summation of the divergent perturbation expansion of the hydrogen atom in an external magnetic field a new sequence transformation which uses as input data not only the elements of a sequence $\{s_n\}_{n=0}^{\infty}$ of partial sums, but also explicit estimates $\{\omega_n\}_{n=0}^{\infty}$ for the truncation errors. The explicit incorporation of the information contained in the truncation error estimates makes this and related transformations potentially much more powerful than, for instance, Padé approximants. Special cases of the new transformation are sequence transformations introduced by Levin [Int. J. Comput. Math. B **3**, 371–388 (1973)] and Weniger [Comput. Phys. Rep. **10**, 189–371 (1989), Secs. 7–9; Numer. Algor. **3**, 477–486 (1992)] and also a variant of Richardson extrapolation [Philos. Trans. R. Soc. London, Ser. A **226**, 299–349 (1927)]. The algebraic theory of these transformations—explicit expressions, recurrence formulas, explicit expressions in the case of special remainder estimates, and asymptotic order estimates satisfied by rational approximants to power series—is formulated in terms of hitherto unknown mathematical properties of the new transformation introduced by Čížek, Zamastil, and Skála. This leads to a considerable formal simplification and unification. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1643787]

I. INTRODUCTION

The most important and most versatile systematic approximation method in quantum physics is eigenvalue perturbation theory (see, for example, Ref. 137). Thus, the question, whether perturbation expansions converge or diverge, is of principal importance. Already in 1952, Dyson[56] had argued that perturbation expansions in quantum electrodynamics should diverge. Around 1970, Bender and Wu[10–12] showed in their work on anharmonic oscillators that factorially divergent perturbation expansions occur also in nonrelativistic quantum mechanics. In the following years, many other quantum systems were investigated, and in the overwhelming majority factorially divergent perturbation expansions were found (see, for example, Ref. 65, Table I or the articles reprinted in Ref. 98). Consequently, summation methods are needed to give the divergent perturbation series of quantum physics any meaning beyond mere formal expansions and to extract numerical information from them. A very readable discussion of the usefulness of summation and related techniques from a physicist's point of view can be found in the monograph by Bender and Orszag.[8]

Factorially divergent power series occur also in asymptotic expansions for special functions. However, special functions can normally be computed via a variety of different representations. Accordingly, in mathematics there is usually no compelling need to use divergent series for computational purposes, whereas in quantum physics it is frequently quite difficult or even impossible to find alternatives to divergent perturbation expansions. Consequently, summation tech-

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niques are far more important in physics than in mathematics. Nevertheless, the evaluation of special functions by summing divergent asymptotic expansions can be remarkably effective (see, for example, Refs. 147, 150, 154, 161).

In physics, the best known and most widely used summation techniques are Borel summation,[16,17] which replaces a divergent perturbation expansion by a Laplace-type integral, and the method of Padé approximants,[110] which transforms the partial sums of a power series to a rational function. Both approaches have been remarkably successful, but they have—like all other numerical techniques—certain shortcomings and limitations. For example, the Borel method is very powerful, but conceptually and computationally very demanding. From a technical point of view, Padé approximants can be applied remarkably easily, but they are not necessarily powerful enough to sum all perturbation series of interest. For example, Graffi and Grecchi[70] showed rigorously that Padé approximants are not able to sum the perturbation expansion of the octic anharmonic oscillator whose series coefficients grow roughly like $(3n)!/n^{1/2}$ [Ref. 11, Eq. (3)]. Accordingly, it is worth while to look for alternative techniques which are at least in some cases capable of producing better summation results.

Padé approximants accomplish an acceleration of convergence or a summation by converting the partial sums of a power series to a doubly indexed sequence of rational functions. This is also done by other, albeit less well known nonlinear transformations (see, for example, Refs. 20, 21, 33, 146, 166). It is not so well known among nonspecialists that some of these transformations sum many strongly divergent power series much more effectively than Padé approximants can do it. Particularly suited for the summation of strongly divergent series is a class of sequence transformations introduced by Levin[99] in 1973. These transformations use as input data not only the elements of a slowly convergent or divergent sequence $\{s_n\}_{n=0}^{\infty}$, whose elements may for instance be the partial sums $s_n=\sum_{k=0}^{n}a_k$ of an infinite series, but also explicit remainder estimates $\{\omega_n\}_{n=0}^{\infty}$. Several generalizations and extensions of Levin's transformation were derived later, for instance in Refs. 146, Secs. 7–9 or in Ref. 148. Further details as well as the description of several other Levin-type transformations can be found in a recent review by Homeier.[82]

The explicit incorporation of the information contained in the remainder estimates $\{\omega_n\}_{n=0}^{\infty}$ makes all Levin-type transformation potentially very powerful (see for example the numerical examples in Refs. 140, 141, 146). In the case of divergent alternating series, the so-called delta transformation [Ref. 146, Eq. (8.4-4)] was found to be particularly useful.[18,48–50,85,91,146–153,155,156,158,162,163]

However, sequence transformations in general or the Levin-type transformations mentioned above in particular are not only useful for the summation of divergent perturbation expansions. In recent years, many other successful applications of Levin-type transformations have been reported in the literature (see, for example, Refs. 2, 4–6, 13–15, 19, 39, 48, 49, 54, 55, 57, 63, 66, 71–74, 77–84, 86–90, 92, 94, 95, 97, 100, 103, 108, 109, 111–114, 116–119, 127–130, 132, 138, 139, 142, 144–152, 154, 158, 161, 164, 165). This list does not claim to be complete, but it suffices to show that Levin-type transformations are extremely useful computational tools which deserve to be more widely known.

In connection with the summation of the perturbation series for a hydrogen atom in an external magnetic field, Čížek, Zamastil, and Skála introduced a new sequence transformation [Ref. 50, Eq. (10)], which in the notation of Ref. 146 can be expressed as follows:

$$\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n) = \frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{1}{\omega_{n+j}}}, \quad k,n\in\mathbb{N}_0. \tag{1.1}$$

Here as well as later in the text it is always assumed that $\prod_{k=l}^{n}a_k=1$ holds if it is a so-called empty product with $l>n$.

The sequence transformation (1.1) contains the as yet unspecified parameters q_m with $1\leqslant m\leqslant k-1$. As discussed in Sec. II in more details, several other sequence transformations can be

obtained by specifying the parameters q_m. If we for instance choose $q_m=\beta$ with $\beta>0$, we obtain Levin's transformation $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$ (Ref. 99) in the notation of Ref. 146 [Eq. (7.1-7)], if we choose $q_m=\beta+m-1$, we obtain $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$ [Ref. 146, Eq. (8.2-7)], which is the parent transformation of the so-called delta transformation [Ref. 146, Eq. (8.4-4)] mentioned above, and if we choose $q_m=\xi-m+1$ with $\xi>0$, we obtain $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$ [Ref. 146, Eq. (9.2-6)]. Then, there is a sequence transformation $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ [Ref. 148, Eq. (3.2)] which—depending on the value of the parameter α—interpolates between Levin's transformation $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$ and $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$. It is obtained by choosing $q_m=\beta+[m-1]/\alpha$.

Thus, the transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ introduced by Čížek, Zamastil, and Skála provides a unifying concept for a large and practically important class of sequence transformations, and all results derived for $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ can immediately be translated to the analogous results for its various special cases. However, so far only the explicit expression for this transformation as the ratio of two finite sums according to (1.1) is known [Ref. 50, Eq. (10)], and many other mathematical properties of interest are unknown.

In Sec. II, the explicit expression for $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ is rederived by applying a suitable annihilating difference operator to the model sequence (2.12) according to (2.9). This annihilation operator approach was originally introduced in Ref. 146, Sec. 3.2 in connection with a simplified derivation of the explicit expression for Levin's transformation[99] and the construction of explicit expressions for other, closely related sequence transformations (Ref. 146, Secs. 7–9). This annihilation operator approach does not only produce the explicit expression (1.1), but it also provides a convenient starting point for the derivation of a recursive scheme for the numerators and denominators in (1.1), which is done in Sec. III, and for a theoretical convergence analysis, which will be done in Ref. 160.

In Sec. IV, simple explicit remainder estimates introduced by Levin[99] and Smith and Ford,[140] which in the terminology of Ref. 146 yield the u, t, v, and d variants of Levin's sequence transformation, are used in combination with $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$. The effectiveness of these remainder estimates is motivated and studied via some model sequences. Surprisingly, the v type remainder estimate produces more effective asymptotic estimates for the truncation errors of these model sequences than the other simple remainder estimates. Moreover, it is shown that all t type variants considered in this article are actually analogous d type variants in disguise.

In Sec. V, variants of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ are studied which closely resemble the Richardson extrapolation process.[115] These variants can be used in the case of logarithmic convergence ($\rho=1$ in (4.7)), whose acceleration constitutes a formidable computational problem.

In Sec. VI, the u, t, d, and v variants of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ are applied to the partial sums of a (formal) power series. This produces rational approximants that resemble Padé approximants, which are defined via the accuracy-through-order relationship (6.3). In the case of the u and d variants, the resulting rational expressions are actually Padé-type approximants, which satisfy the modified accuracy-through-order relationship (6.16).[22,23] In the case of the t and v variants, the resulting expressions are slight generalizations of a Padé-type approximant. With the help of the accuracy-through-order relationship (6.16), which defines Padé-type approximants, the accuracy-through-order relationships satisfied by these rational functions can be derived easily. These accuracy-through-order relationships are needed if the rational approximants derived from $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ are to be used for the prediction of unknown power series coefficients.

This article is concluded in Sec. VII by a short summary and a critical assessment of the essential features of the new Levin-type transformation introduced recently by Čížek, Zamastil, and Skála.[50]

Only the mathematical properties of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ and its various special cases are treated in this article, albeit in a relatively detailed way. Anybody interested in other sequence transformations should consult the monograph by Brezinski and Redivo Zaglia.[33] It contains a wealth of material and provides a very readable introduction to a rapidly growing subfield of numerical mathematics. The older history of sequence transformations up to about 1945 is treated in a monograph by Brezinski,[26] and the more recent history is discussed in two articles, also by Brezinski.[27,31]

Finally, one should not forget that the study of sequence transformations remains incomplete without the simultaneous study of Padé approximants. Here, I recommend the book by Baker and Graves-Morris.[3]

II. EXPLICIT EXPRESSIONS VIA ANNIHILATION OPERATORS

Let us assume that $\{s_n\}_{n=0}^{\infty}$ is a slowly convergent or divergent sequence, whose elements may for instance be the partial sums $s_n=\sum_{k=0}^{n}a_k$ of an infinite series. A *sequence transformation* is a rule which maps a sequence $\{s_n\}_{n=0}^{\infty}$ to a new sequence $\{s_n'\}_{n=0}^{\infty}$ with hopefully better numerical properties.

The basic step for the construction of a sequence transformation is the assumption that the elements of a convergent or divergent sequence $\{s_n\}_{n=0}^{\infty}$ can be partitioned into a (generalized) limit s and a remainder r_n according to

$$s_n = s+r_n, \quad n\in\mathbb{N}_0. \tag{2.1}$$

A sequence transformation tries to accomplish an acceleration of convergence or a summation by eliminating the remainders r_n as effectively as possible from the input data s_n with the help of numerical techniques. In realistic problems, a sequence transformation can only eliminate approximations to the remainders. Consequently, the transformed sequence $\{s_n'\}_{n=0}^{\infty}$ will also be of the type of (2.1), which means that s_n' can also be partitioned into the (generalized) limit s and a transformed remainder r_n' according to

$$s_n' = s+r_n', \quad n\in\mathbb{N}_0. \tag{2.2}$$

The transformed remainders $\{r_n'\}_{n=0}^{\infty}$ are in general different from zero for all finite values of n. However, convergence is accelerated if the transformed remainders $\{r_n'\}_{n=0}^{\infty}$ vanish more rapidly than the original remainders $\{r_n\}_{n=0}^{\infty}$ according to

$$\lim_{n\to\infty}\frac{s_n'-s}{s_n-s} = \lim_{n\to\infty}\frac{r_n'}{r_n} = 0, \tag{2.3}$$

and a divergent sequence is summed if the transformed remainders r_n' vanish as $n\to\infty$.

In practice, an in principle unlimited variety of different types of remainders can occur. Therefore, it is essential to make some assumptions—either explicitly or implicitly—which provide the basis for the construction of a sequence transformation.

Let us assume that we have sufficient reason to believe that the elements of a sequence $\{s_n\}_{n=0}^{\infty}$ can for all $n\in\mathbb{N}_0$ be expressed by an expansion of the following type:

$$s_n = s+\sum_{j=0}^{\infty} c_j\,\psi_j(n). \tag{2.4}$$

The $\psi_j(n)$ are assumed to be *known* functions of n, but otherwise essentially arbitrary, and the c_j are unspecified coefficients independent of n. Hence, the ansatz (2.4) incorporates convergent as well as divergent sequences, depending upon the behavior of the functions $\psi_j(n)$ as $n\to\infty$.

If we want to accelerate the convergence of $\{s_n\}_{n=0}^{\infty}$ to its limit s or to sum it in the case of divergence with the help of a sequence transformation, we have to compute approximations to the remainders $\sum_{j=0}^{\infty}c_j\psi_j(n)$ and to eliminate them from the input data. However, the remainders of the sequence (2.4) contain an infinite number of unspecified coefficients c_j. Consequently, a complete determination of the remainders and their subsequent elimination cannot be accomplished by purely numerical means.

Let us also assume that the functions $\{\psi_j(n)\}_{j=0}^{\infty}$ form an asymptotic sequence as $n\to\infty$, i.e., that they satisfy for all $j\in\mathbb{N}_0$,

$$\psi_{j+1}(n) \;=\; o(\psi_j(n)), \quad n\to\infty. \tag{2.5}$$

The best, which a purely numerical process can accomplish, is the elimination of a finite number of the leading terms of (2.4). Obviously, this corresponds to the transformation of the sequence (2.4) to a new sequence $\{s_n'\}_{n=0}^{\infty}$ whose elements satisfy

$$s_n' \;=\; s+\sum_{j=0}^{\infty} c_j'\,\psi_{k+j}(n), \quad n\in\mathbb{N}_0, \quad k\in\mathbb{N}. \tag{2.6}$$

The c_j' are numerical coefficients that depend on k as well as on the coefficients c_j in (2.4).

In (2.6), the original remainders $\Sigma_{j=0}^{\infty}c_j\psi_j(n)$ are not completely eliminated from the elements of the input sequence (2.4). Since, however, the functions $\{\psi_j(n)\}_{j=0}^{\infty}$ are by assumption an asymptotic sequence according to (2.5), the transformed remainders $\Sigma_{j=0}^{\infty}c_j'\psi_{k+j}(n)$ in (2.6) should at least for sufficiently large values of $k\in\mathbb{N}$ have significantly better numerical properties than the original remainders $\Sigma_{j=0}^{\infty}c_j\psi_j(n)$.

Assumptions about the n-dependence of the truncation errors r_n can be incorporated into the transformation process via model sequences. In this approach, a sequence transformation is constructed which produces the (generalized) limit s of the model sequence

$$s_n \;=\; s+r_n \;=\; s+\sum_{j=0}^{k-1} c_j\,\psi_j(n), \quad k\in\mathbb{N}, \quad n\in\mathbb{N}_0, \tag{2.7}$$

if it is applied to $k+1$ consecutive elements $s_n, s_{n+1},\ldots, s_{n+k}$ of this model sequence. Since the $\psi_j(n)$ are assumed to be known functions of n, an element of this model sequence contains $k+1$ unknowns, the (generalized) limit s and the k unspecified coefficients $c_0, c_1,\ldots, c_{k-1}$. Accordingly, it follows from Cramer's rule that a sequence transformation, which is exact for the model sequence (2.7), can be expressed as the ratio of two determinants (see, for example, Ref. 33, Sect. 1.5). However, determinantal representations will not be considered here since they are computationally unattractive. Fortunately, the sequence transformation, which is exact for the general model sequence (2.7), can also be computed recursively, as shown independently by Schneider,[131] Håvie,[75] and Brezinski.[24] An alternative recursive scheme, which is more economical than the original recursive scheme, was later obtained by Ford and Sidi.[67]

A detailed discussion of the construction of sequence transformations via model sequences as well as many examples can for instance be found in the book by Brezinski and Redivo Zaglia[33] or in Ref. 146.

Levin-type sequence transformations try to make the transformation process more efficient by explicitly utilizing the information contained in remainder estimates $\{\omega_n\}_{n=0}^{\infty}$. Thus, a sequence transformation is constructed which is exact for the elements of the model sequence [Ref. 146, Eq. (3.2-9)]

$$s_n \;=\; s+\omega_n z_n, \quad n\in\mathbb{N}_0. \tag{2.8}$$

The remainder estimates ω_n are assumed to be known, and the correction terms z_n should be chosen in such a way that the products $\omega_n z_n$ provide sufficiently accurate and rapidly convergent approximations to actual remainders. The principal advantage of this approach is that only the correction terms $\{z_n\}_{n=0}^{\infty}$ have to be determined. If good remainder estimates can be found, the determination of z_n and the subsequent elimination of $\omega_n z_n$ from s_n often leads to substantially better results than the construction and subsequent elimination of other approximations to r_n.

The model sequence (2.8) has another indisputable advantage: There exists a systematic approach for the construction of a sequence transformation which is exact for this model sequence. Let us assume that a *linear* operator $\hat{T}$ can be found which annihilates for all $n\in\mathbb{N}_0$ the correction term z_n according to $\hat{T}(z_n)=0$. Then, a sequence transformation, which is exact for the model

sequence (2.8), can be obtained by applying $\hat{T}$ to $[s_n - s]/\omega_n = z_n$. Since $\hat{T}$ annihilates z_n and is by assumption linear, the following sequence transformation $\mathcal{T}$ is exact for the model sequence (2.8) [Ref. 146, Eq. (3.2-11)]:

$$\mathcal{T}(s_n, \omega_n) = \frac{\hat{T}(s_n/\omega_n)}{\hat{T}(1/\omega_n)} = s. \tag{2.9}$$

The construction of sequence transformations via annihilation operators was introduced in Ref. 146, Sec. 3.2 in connection with a rederivation of Levin's transformation[99] and the construction of some other, closely related sequence transformations (Refs. 146, Secs. 7–9).

Later, this annihilation operator approach was discussed and extended in books by Brezinski[28] and Brezinski and Redivo Zaglia[33] and in articles by Brezinski,[27,29–31] Brezinski and Matos,[32] Brezinski and Redivo Zaglia,[34–36] Brezinski and Salam,[37] Homeier,[82] Matos,[102] and Weniger.[148]

Simple and yet very powerful sequence transformations result (Ref. 146, Secs. 7–9) if the annihilation operator $\hat{T}$ in (2.9) is based upon the finite difference operator Δ defined by $\Delta f(n) = f(n+1) - f(n)$. In the following text, it will always be tacitly assumed that Δ acts on the variable n only. As is well known, the kth power of the finite difference operator annihilates a polynomial $P_{k-1}(n)$ of degree $k-1$ in n according to $\Delta^k P_{k-1}(n) = 0$. Thus, the correction terms z_n in (2.8) should be chosen in such a way that multiplication of z_n by some suitable quantity $w_k(n)$ yields a polynomial $P_{k-1}(n)$ of degree $k-1$ in n. If such a $w_k(n)$ can be found, then

$$\Delta^k [w_k(n)\, z_n] = \Delta^k P_{k-1}(n) = 0 \tag{2.10}$$

and the weighted difference operator $\hat{T} = \Delta^k w_k(n)$ annihilates z_n. Thus, the corresponding sequence transformation (2.9) is given by the ratio

$$\mathcal{T}_k^{(n)}(w_k(n)|s_n, \omega_n) = \frac{\Delta^k[w_k(n) s_n/\omega_n]}{\Delta^k[w_k(n)/\omega_n]}. \tag{2.11}$$

The sequence transformation (1.1) introduced by Čížek, Zamastil, and Skála can be constructed via the model sequence [Ref. 50, Eq. (9)]

$$s_n = s + \omega_n \sum_{j=0}^{k-1} \frac{c_j}{\prod_{m=1}^{j} (n+q_m)}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0, \tag{2.12}$$

for which it is exact.

It will become clear later (compare (4.5) and the discussion related to it) that in (2.12) as well as in the model sequences (2.16), (2.19), (2.23), and (2.27), which can be derived from (2.12), it makes sense to assume $c_0 \neq 0$.

Both in the model sequence (2.12) as well as in the sequence transformation, which is derived from it, we want to admit $n = 0$. Moreover, this model sequence should have a consistent behavior for all $n \in \mathbb{N}_0$. In particular, the signs of the terms in (2.12) should not depend on n. Thus, we normally require $q_m > 0$ for $1 \leqslant m \leqslant k-1$, but otherwise these parameters are essentially arbitrary.

Multiplication of the sum in (2.12) by $\Pi_{m=1}^{k-1}(n+q_m)$ yields $\Sigma_{j=0}^{k-1} c_j \Pi_{m=j+1}^{k-1}(n+q_m)$, which is a polynomial of degree $k-1$ in n. Thus, $\hat{T} = \Delta^k \Pi_{m=1}^{k-1}(n+q_m)$ is the operator which annihilates the correction term in (2.12), and we obtain from (2.9) the following difference operator representation for the sequence transformation introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)]:

$$\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n) = \frac{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\frac{s_n}{\omega_n}}{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\frac{1}{\omega_n}}, \quad k,n\in\mathbb{N}_0. \tag{2.13}$$

It will become clear later that this difference operator representation is in some sense more fundamental and more important than the explicit expression which can be derived easily from it. We only have to insert the well-known relationship

$$\Delta^k f(n) = (-1)^k\sum_{j=0}^{k}(-1)^j\binom{k}{j}f(n+j) \tag{2.14}$$

into the numerator and denominator of (2.13) to obtain

$$\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n) = \frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}(n+j+q_m)\right\}\frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}(n+j+q_m)\right\}\frac{1}{\omega_{n+j}}}, \quad k,n\in\mathbb{N}_0. \tag{2.15}$$

In the case of large transformation orders k, terms that are large in magnitude occur in the binomial sums in the numerator and denominator of (2.15). The same problem occurs also in explicit expressions for other Levin-type sequence transformation discussed later. In the case of some FORTRAN compilers, this can easily lead to overflow. To decrease the magnitude of the terms, it has become customary to include an additional normalization factor. Thus, we divide numerator and denominator of (2.15) by $\Pi_{m=1}^{k-1}(n+k+q_m)$ and obtain (1.1). Such an approach is always possible since the coefficients of a ratio like (2.15) are only defined up to a common nonzero factor.

If we choose in (2.12) $q_m=\beta$ with $\beta>0$, we obtain the model sequence for Levin's transformation[99] in the notation of Ref. 146, Eq. (7.1-2),

$$s_n = s+\omega_n\sum_{j=0}^{k-1}\frac{c_j}{(\beta+n)^j}, \quad k\in\mathbb{N}, \quad n\in\mathbb{N}_0. \tag{2.16}$$

Thus, the corresponding annihilation operator is given by $\hat{T}=\Delta^k(\beta+n)^{k-1}$ and Levin's transformation[99] can in the notation of Ref. 146, Eq. (7.1-7) be expressed as follows:

$$\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)=\mathcal{G}_k^{(n)}(\beta,s_n,\omega_n)=\frac{\Delta^k[(\beta+n)^{k-1}s_n/\omega_n]}{\Delta^k[(\beta+n)^{k-1}/\omega_n]} \tag{2.17}$$

$$=\frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(\beta+n+j)^{k-1}}{(\beta+n+k)^{k-1}}\frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(\beta+n+j)^{k-1}}{(\beta+n+k)^{k-1}}\frac{1}{\omega_{n+j}}}, \quad k,n\in\mathbb{N}_0. \tag{2.18}$$

If we choose in (2.12) $q_m=\beta+m-1$ with $\beta>0$, we obtain the following model sequence [Ref. 146, Eq. (8.2-1)] for the sequence transformation $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$ which is a truncated factorial series involving Pochhammer symbols $(\beta+n)_j=\Gamma(\beta+n+j)/\Gamma(\beta+n)$:

$$s_n = s+\omega_n\sum_{j=0}^{k-1}\frac{c_j}{(\beta+n)_j}, \quad k\in\mathbb{N}, \quad n\in\mathbb{N}_0. \tag{2.19}$$

The fundamental properties of factorial series are for instance discussed in books by Nielsen[105] and Nörlund.[106,107]

The annihilation operator for the model sequence (2.19) is given by $\hat{T}=\Delta^k(\beta+n)_{k-1}$ and the sequence transformation $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, which is exact for the model sequence (2.19), can be expressed as follows [Ref. 146, Eq. (8.2-7)]:

$$\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)=\mathcal{G}_k^{(n)}(\beta+m-1,s_n,\omega_n)=\frac{\Delta^k[(\beta+n)_{k-1}s_n/\omega_n]}{\Delta^k[(\beta+n)_{k-1}/\omega_n]} \tag{2.20}$$

$$=\frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(\beta+n+j)_{k-1}}{(\beta+n+k)_{k-1}}\frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(\beta+n+j)_{k-1}}{(\beta+n+k)_{k-1}}\frac{1}{\omega_{n+j}}},\quad k,n\in\mathbb{N}_0\,. \tag{2.21}$$

The ratio (2.21) was originally derived by Sidi[134] for the construction of explicit expressions for Padé approximants of some special hypergeometric series. However, Sidi's article[134] provides no evidence that he intended to use this ratio as a sequence transformation. Moreover, I am not aware of any article of Sidi where the properties of the sequence transformation $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$ were discussed or where it was applied. Later, $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$ was used in the Master's thesis of Shelef[133] for the numerical inversion of Laplace transforms, but it seems that this Master's thesis was not published elsewhere. The first refereed and generally accessible article, where an application of (2.21) as a sequence transformation was described, is,[165] where the u-variant (4.13) was employed [Ref. 165, Eq. (9)]. The mathematical properties of (2.21) as a sequence transformation and in particular its connection with factorial series were developed independently of Sidi and Shelef in (Ref. 146, Secs. 8 and 13) (compare also Ref. 8 of Ref. 165).

If we choose in (2.12) $q_m=\xi-m+1$ with $\xi>0$, we obtain the following model sequence [Ref. 146, Eq. (9.2-1)] for the sequence transformation $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$:

$$s_n = s+\omega_n\sum_{j=0}^{k-1}\frac{c_j}{\prod_{m=1}^{j}(\xi+n-m+1)} \tag{2.22}$$

$$= s+\omega_n\sum_{j=0}^{k-1}\frac{(-1)^j c_j}{(-\xi-n)_j} = s+\omega_n\sum_{j=0}^{k-1}\frac{c_j'}{(-\xi-n)_j},\quad k\in\mathbb{N},\quad n\in\mathbb{N}_0\,. \tag{2.23}$$

Thus, the corresponding annihilation operator is given by $\hat{T}=\Delta^k(-\xi-n)_{k-1}$ and the sequence transformation $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$ can be expressed as follows [Ref. 146, Eq. (9.2-6)]:

$$\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)=\mathcal{G}_k^{(n)}(\xi-m+1,s_n,\omega_n)=\frac{\Delta^k[(-\xi-n)_{k-1}s_n/\omega_n]}{\Delta^k[(-\xi-n)_{k-1}/\omega_n]} \tag{2.24}$$

$$=\frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(-\xi-n-j)_{k-1}}{(-\xi-n-k)_{k-1}}\frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(-\xi-n-j)_{k-1}}{(-\xi-n-k)_{k-1}}\frac{1}{\omega_{n+j}}},\quad k,n\in\mathbb{N}_0\,. \tag{2.25}$$

If we choose in (2.12) $q_m=\beta+[m-1]/\alpha$ with $\alpha,\beta>0$, we obtain the following model sequence [Ref. 148, Eq. (3.1)] for the sequence transformation $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$:

$$s_n = s + \omega_n \sum_{j=0}^{k-1} \frac{c_j}{\prod_{m=1}^{j} (\beta+n+[m-1]/\alpha)} \tag{2.26}$$

$$= s + \omega_n \sum_{j=0}^{k-1} \frac{\alpha^j c_j}{(\alpha[\beta+n])_j} = s + \omega_n \sum_{j=0}^{k-1} \frac{c_j'}{(\alpha[\beta+n])_j}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0 . \tag{2.27}$$

Thus, the corresponding annihilation operator is given by $\hat{T}=\Delta^k(\alpha[\beta+n])_{k-1}$ and the sequence transformation $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ can be expressed as follows [Ref. 148, Eq. (3.2)]:

$$\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)=\mathcal{G}_k^{(n)}(\beta+[m-1]/\alpha,s_n,\omega_n)=\frac{\Delta^k[(\alpha[\beta+n])_{k-1}s_n/\omega_n]}{\Delta^k[(\alpha[\beta+n])_{k-1}/\omega_n]} \tag{2.28}$$

$$=\frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(\alpha[\beta+n+j])_{k-1}}{(\alpha[\beta+n+k])_{k-1}} \frac{s_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(\alpha[\beta+n+j])_{k-1}}{(\alpha[\beta+n+k])_{k-1}} \frac{1}{\omega_{n+j}}},$$

$$k,n \in \mathbb{N}_0 . \tag{2.29}$$

Depending upon the value of $\alpha>0$, the sequence transformation $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ interpolates between $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$ and Levin's sequence transformation $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$. If we choose $\alpha=1$ in (2.29) and compare the resulting expression with (2.21), we find

$$\mathcal{C}_k^{(n)}(1,\beta,s_n,\omega_n) = \mathcal{S}_k^{(n)}(\beta,s_n,\omega_n), \tag{2.30}$$

and if we use

$$\lim_{\alpha\to\infty} \frac{(\alpha[\beta+n+j])_{k-1}}{\alpha^{k-1}} = \lim_{\alpha\to\infty} \prod_{m=1}^{k-1} (\beta+n+j+[m-1]/\alpha) = (\beta+n+j)^{k-1} \tag{2.31}$$

in (2.29) and compare the resulting expression with (2.18), we find

$$\lim_{\alpha\to\infty} \mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n) = \mathcal{L}_k^{(n)}(\beta,s_n,\omega_n) . \tag{2.32}$$

Thus, the construction of explicit expressions for the Levin-type sequence transformations $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$, $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ with the help of annihilation operators is almost trivial. However, the annihilation operator approach does not only work in the case of the comparatively simple annihilating difference operators in (2.13), (2.17), (2.20), (2.24), and (2.28). In Ref. 146, Sec. 7.4 it was shown that Richardson extrapolation[115] and Sidi's generalized Richardson extrapolation process[135] can be derived by using divided differences as annihilation operators. Then, it was shown by Brezinski and Redivo Zaglia,[34,35] Brezinski and Matos,[32] and Matos[102] that the majority of the currently known transformations for scalar sequence can be derived via the annihilation operator approach. The generalization of this approach to vector and matrix sequences was discussed by Brezinski and Redivo Zaglia[36] and Brezinski and Salam.[37]

III. RECURRENCE FORMULAS

In the theory of sequence transformations it is relatively uncommon that closed form expressions of the type of (1.1), (2.18), (2.21), (2.25), and (2.29) are known. The majority of the currently known sequence transformations are defined and computed via recursive schemes. From a computational point of view, the lack of an explicit expression is normally no disadvantage. The use of recurrence formulas is in most cases (much) more efficient, in particular if a whole sequence of transforms must be computed simultaneously.

It is an additional advantage of the annihilation operator approach described in Sec. II that it permits a convenient construction of a recursive scheme for the numerators and denominators of $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$. For that purpose, let us define

$$\Gamma_k^{(n)} = \Gamma_k^{(n)}(q_m, u_n) = \Delta^k X_k^{(n)}, \quad k,n \in \mathbb{N}_0, \tag{3.1}$$

$$X_k^{(n)} = X_k^{(n)}(q_m, u_n) = \prod_{m=1}^{k-1} (n+q_m)\, u_n, \quad k,n \in \mathbb{N}_0. \tag{3.2}$$

Comparison with (2.13) shows that $\Gamma_k^{(n)}$ corresponds apart from a missing phase factor $(-1)^k$ to the numerator in (2.15) if we choose $u_n = s_n/\omega_n$, and to the denominator in (2.15) if we choose $u_n = 1/\omega_n$.

The quantities $X_k^{(n)}$ satisfy for $k \geqslant 2$ the two-term recursion

$$X_k^{(n)} = (n+q_{k-1})\, X_{k-1}^{(n)}. \tag{3.3}$$

Next, we use the commutator relationship [see Ref. 64 or Ref. 146, Eq. (7.2-2)]

$$\Delta^k (n+q_{k-1}) - (n+q_{k-1})\, \Delta^k = k\, E\, \Delta^{k-1}, \tag{3.4}$$

which can be proven by complete induction. This commutator can be rewritten as follows:

$$\Delta^k (n+q_{k-1}) = [(n+k+q_{k-1})\, E - (n+q_{k-1})]\, \Delta^{k-1}. \tag{3.5}$$

Here, E is the shift operator defined by $Ef(n) = f(n+1)$.

The combination of (3.1), (3.2), (3.3), and (3.5) yields

$$\Gamma_k^{(n)} = \Delta^k (n+q_{k-1})\, X_{k-1}^{(n)} \tag{3.6}$$

$$= [(n+k+q_{k-1})\, E - (n+q_{k-1})]\, \Delta^{k-1} X_{k-1}^{(n)} \tag{3.7}$$

$$= (n+k+q_{k-1})\, \Gamma_{k-1}^{(n+1)} - (n+q_{k-1})\, \Gamma_{k-1}^{(n)}, \quad k \geqslant 2, \quad n \in \mathbb{N}_0. \tag{3.8}$$

Finally, we rescale $\Gamma_k^{(n)}$ according to

$$G_k^{(n)} = G_k^{(n)}(q_m, u_n) = \frac{\Gamma_k^{(n)}(q_m, u_n)}{\prod_{m=1}^{k-1} (n+k+q_m)}, \quad k,n \in \mathbb{N}_0. \tag{3.9}$$

If we combine (3.8) and (3.9) and take into account that (3.1) and (3.2) imply $\Gamma_0^{(n)} = u_n$ and $\Gamma_1^{(n)} = u_{n+1} - u_n$, respectively, we obtain the following recursive scheme for the numerators and denominators of the sequence transformation (1.1) introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)]:

$$G_0^{(n)} = u_n, \quad n \in \mathbb{N}_0, \tag{3.10a}$$

$$G_1^{(n)} = u_{n+1} - u_n, \quad n \in \mathbb{N}_0, \tag{3.10b}$$

$$G_{k+1}^{(n)} = G_k^{(n+1)} - \frac{n+q_k}{n+k+q_k+1} \prod_{m=1}^{k-1} \frac{n+k+q_m}{n+k+q_m+1} G_k^{(n)}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{3.10c}$$

If we choose $u_n = s_n/\omega_n$, this recursive scheme produces the numerator of (1.1), and if we choose $u_n = 1/\omega_n$, we obtain the denominator of (1.1).

As shown in Ref. 146, Secs. 7.3, 8.3, and 9.3, recursive schemes for the numerator and denominator sums of the sequence transformations $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$. $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, and $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$ can be derived in the same way. The recursive scheme [Ref. 146, Eq. (7.2-8)]

$$L_0^{(n)} = u_n, \quad n\in\mathbb{N}_0, \tag{3.11a}$$

$$L_{k+1}^{(n)} = L_k^{(n+1)} - \frac{(\beta+n)(\beta+n+k)^{k-1}}{(\beta+n+k+1)^k} L_k^{(n)}, \quad k,n\in\mathbb{N}_0, \tag{3.11b}$$

produces the numerator and denominator sums in (2.18) if we choose $u_n=s_n/\omega_n$ and $u_n=1/\omega_n$, respectively. We obtain (3.11) from (3.10) by choosing $q_m=\beta$.

Similarly, the recursive schemes [Ref. 146, Eq. (8.3-7)]

$$S_0^{(n)} = u_n, \quad n\in\mathbb{N}_0, \tag{3.12a}$$

$$S_{k+1}^{(n)} = S_k^{(n+1)} - \frac{(\beta+n+k-1)(\beta+n+k)}{(\beta+n+2k-1)(\beta+n+2k)} S_k^{(n)}, \quad k,n\in\mathbb{N}_0, \tag{3.12b}$$

and [Ref. 146, Eq. (9.3-6))]

$$M_0^{(n)} = u_n, \quad n\in\mathbb{N}_0, \tag{3.13a}$$

$$M_{k+1}^{(n)} = M_k^{(n+1)} - \frac{\xi+n-k+1}{\xi+n+k+1} M_k^{(n)}, \quad k,n\in\mathbb{N}_0, \tag{3.13b}$$

produce the numerator and denominator sums in (2.21) and (2.25), respectively. The recursive schemes (3.12) and (3.13) can be obtained from (3.10) by setting $q_m=\beta+m-1$ and $q_m=\xi-m+1$, respectively.

If we set $q_m=\beta+[m-1]/\alpha$ in (3.10), we obtain the recursive scheme for the interpolating transformation $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$:

$$C_0^{(n)} = u_n, \quad n\in\mathbb{N}_0, \tag{3.14a}$$

$$C_1^{(n)} = u_{n+1}-u_n, \quad n\in\mathbb{N}_0, \tag{3.14b}$$

$$C_{k+1}^{(n)} = C_k^{(n+1)} - \frac{(\alpha[\beta+n]+k-1)(\alpha[\beta+n+k])_{k-1}}{(\alpha[\beta+n+k+1])_k} C_k^{(n)}, \quad k\in\mathbb{N},n\in\mathbb{N}_0. \tag{3.14c}$$

This scheme produces the numerator and denominator sums of (2.29) if we choose $u_n=s_n/\omega_n$ and $u_n=1/\omega_n$, respectively. The recurrence formula published in Ref. 148, Eq. (3.3) contains errors.

IV. LEVIN'S EXPLICIT REMAINDER ESTIMATES

It follows from (2.13), (2.14), (2.17), (2.20), (2.24), and (2.28) that all sequence transformations considered in this article can be expressed as follows:

$$T_k^{(n)}(s_n,\omega_n) = \frac{\Delta^k\{P_{k-1}(n)\, s_n/\omega_n\}}{\Delta^k\{P_{k-1}(n)/\omega_n\}}, \quad k\in\mathbb{N}, \quad n\in\mathbb{N}_0. \tag{4.1}$$

Here, $P_{k-1}(n)$ is a polynomial of degree $k-1$ in n. Obviously, the remainder estimates $\{\omega_n\}_{n=0}^{\infty}$ have to satisfy the minimal requirement that $\Delta^k\{P_{k-1}(n)/\omega_n\}\neq 0$ for all *finite* $k,n\in\mathbb{N}_0$. In the following text, this will always be assumed.

The weighted difference operator $\Delta^k P_{k-1}(n)$ in (4.1) is linear. Accordingly, such a sequence transformation satisfies

$$T_k^{(n)}(s_n,\omega_n) \;=\; s+\frac{\Delta^k\{P_{k-1}(n)\,[s_n-s]/\omega_n\}}{\Delta^k\{P_{k-1}(n)/\omega_n\}},\quad k\in\mathbb{N},\quad n\in\mathbb{N}_0\,. \tag{4.2}$$

This property of Levin-type transformations has some far-reaching consequences. Let us assume that we can find for a given sequence $\{s_n\}_{n=0}^{\infty}$ a sequence $\{\omega_n\}_{n=0}^{\infty}$ of *perfect* remainder estimates such that

$$s_n \;=\; s+r_n \;=\; s+c\,\omega_n,\quad c\neq 0,\quad n\in\mathbb{N}_0\,. \tag{4.3}$$

The polynomial $P_{k-1}(n)$ in (4.1) is of degree $k-1$ in n, which implies that it is annihilated by Δ^k according to $\Delta^k P_{k-1}(n)=0$. Thus, the transformation problem is now trivial since (4.2) produces the (generalized) limit s of the sequence (4.3) (Ref. 146, Theorem 12-8),

$$T_k^{(n)}(s_n,\omega_n) \;=\; s+\frac{c\Delta^k P_{k-1}(n)}{\Delta^k\{P_{k-1}(n)/\omega_n\}} \;=\; s,\quad k\in\mathbb{N},\quad n\in\mathbb{N}_0\,. \tag{4.4}$$

Unfortunately, the perfect remainder estimates satisfying (4.3) can only be found for practically more or less irrelevant model problems. In the case of realistic problems, we have to be more modest and can only hope to find remainder estimates that reproduce the leading order asymptotics of the actual remainders [Ref. 146, Eq. (7.3-1)],

$$r_n \;=\; s_n-s \;=\; \omega_n[c+\mathrm{O}(1/n)],\quad c\neq 0,\quad n\to\infty\,. \tag{4.5}$$

This asymptotic condition does not fix remainder estimates uniquely. All Levin-type transformations considered in this article are invariant under the transformation $\omega_n\to\gamma\omega_n$ with $\gamma\neq 0$. Accordingly, all Levin-type transformations considered here are homogeneous functions of degree one in the sequence elements and of degree zero in the remainder estimates [compare Ref. 146, Eq. (12.3-1)]. Moreover, given a sequence $\{r_n\}_{n=0}^{\infty}$ of remainders it is usually possible to find a variety of genuinely different sequences $\{\omega_n\}_{n=0}^{\infty}$, $\{\omega_n'\}_{n=0}^{\infty}$, $\{\omega_n''\}_{n=0}^{\infty}$,... of remainder estimates which all satisfy the asymptotic condition (4.5).

In some exceptional cases, explicit analytical expressions for remainder estimates can be found. Let us for instance assume that the elements of the sequence to be transformed are the partial sums $s_n=\Sigma_{k=0}^{n}a_k$ of an infinite series and that the terms a_k have a sufficiently simple analytical structure. Then it may be possible to derive an explicit expression for the truncation error, from which explicit remainder estimates satisfying (4.5) can be derived.

In principle, such an analytical approach would be highly desirable, in particular since it should then be possible to construct for a given sequence $\{s_n\}_{n=0}^{\infty}$ more effective remainder estimates $\{\tilde{\omega}_n^{(l)}\}_{n=0}^{\infty}$ that do not only reproduce the leading order asymptotics of the remainders according to (4.5), but several of the leading orders according to

$$r_n \;=\; s_n-s \;=\; \tilde{\omega}_n^{(l)}[c+\mathrm{O}(n^{-l})],\quad c\neq 0,\quad n\to\infty\,, \tag{4.6}$$

where $l>1$ is a fixed positive integer. Improved remainder estimates of that kind should lead to more efficient Levin-type transformations. Unfortunately, only relatively little work has been done on the asymptotics of truncation errors $\Sigma_{k=n+1}^{\infty}a_k$ of infinite series as $n\to\infty$ beyond the leading order. Moreover, in many applications of Levin-type transformations in particular in physics, only the numerical values of a finite string of sequence elements or series coefficients are available, but no explicit analytical expressions. In such a case, remainder estimates have to be constructed from the numerical values of the input data via simple rules.

Levin-type sequence transformations are not limited to strongly divergent perturbation expansions. They are able to accelerate the convergence of many series and sequences if suitable remainder estimates are used. In this context, it is helpful to introduce first some terminology which is common in the literature on convergence acceleration methods. Many practically relevant sequences $\{s_n\}_{n=0}^{\infty}$, which converge to some limit s, satisfy

$$\lim_{n\to\infty}\frac{s_{n+1}-s}{s_n-s} \;=\; \lim_{n\to\infty}\frac{r_{n+1}}{r_n} \;=\; \rho\,. \tag{4.7}$$

If $0<|\rho|<1$ holds, we say that the sequence $\{s_n\}_{n=0}^{\infty}$ converges *linearly*, if $\rho=1$ holds, we say that this sequence converges *logarithmically*, and if $\rho=0$ holds, we say that it converges *hyperlinearly*. Of course, $|\rho|>1$ implies that the sequence $\{s_n\}_{n=0}^{\infty}$ diverges.

In this article, only linearly and logarithmically convergent as well as divergent sequences are considered. Hyperlinearly convergent sequences as for example the partial sums of the power series for the exponential $\exp(z)$ normally converge so well that it is not worth while using sequence transformations.

On the basis of purely heuristic arguments Levin[99] and later Smith and Ford[140] suggested some simple remainder estimates which according to experience nevertheless work remarkably well in a large variety of cases. These simple remainder estimates can be motivated by considering simple model problems. For that purpose, let us assume that the elements of a sequence $\{s_n\}_{n=0}^{\infty}$ of partial sums $\Sigma_{\nu=0}^{n}a_\nu$ behave as follows:

$$s_n \;\sim\; s+z^{n+1}\,n^{\theta}\left[\alpha_0+\frac{\alpha_1}{n}+\frac{\alpha_2}{n^2}+\cdots\right],\quad n\to\infty\,. \tag{4.8}$$

This is a fairly general model sequence, which is able to describe the asymptotics of many practically relevant sequences as $n\to\infty$ and which Levin[99] probably had in mind when he introduced his simple remainder estimates. For $|z|<1$, the sequence (4.8) converges linearly to its limit s, for $z=1$ and $\mathrm{Re}(\theta)<0$, it converges logarithmically, and for $|z|>1$ it diverges.

From (4.8) we obtain via $a_n=\Delta s_{n-1}$ the leading orders of the asymptotic expansion of the terms of the infinite series $\Sigma_{\nu=0}^{\infty}a_\nu$. For $z=1$ and $\mathrm{Re}(\theta)<0$ (logarithmic convergence), we find with the help of the computer algebra system MAPLE

$$a_n=n^{\theta}\left\{\frac{\theta\alpha_0}{n}+\frac{(\theta-1)[2\alpha_1-\theta\alpha_0]}{2n^2}+\frac{(\theta-2)[6\alpha_2+(\theta-1)\{\theta\alpha_0-3\alpha_1\}]}{6n^3}+\mathrm{O}(n^{-3})\right\},$$
$$n\to\infty\,, \tag{4.9}$$

and for $|z|<1$ (linear convergence), we find

$$a_n=z^n\,n^{\theta}\left\{(z-1)\alpha_0+\frac{\theta\alpha_0+(z-1)\alpha_1}{n}+\frac{(\theta-1)[2\alpha_1-\theta\alpha_0]+2(z-1)\alpha_2}{2n^2}+\mathrm{O}(n^{-3})\right\},$$
$$n\to\infty\,. \tag{4.10}$$

If we compare (4.8) and (4.9), we see that in the case of logarithmic convergence the term $a_n=\Delta s_{n-1}=\mathrm{O}(n^{\theta-1})$ cannot reproduce the leading order of the remainder $r_n=s_n-s=\mathrm{O}(n^{\theta})$. However, the product $na_n=\mathrm{O}(n^{\theta})$ reproduces the leading order of the remainder of the model sequence (4.8). Thus, it is an obvious idea to use the remainder estimate[99]

$$\omega_n \;=\; (\beta+n)\Delta s_{n-1} \;=\; (\beta+n)a_n \tag{4.11}$$

in Levin's general transformation (2.18), yielding Levin's u transformation in the notation of [Ref. 146, Eq. (7.3-5)]:

$$u_k^{(n)}(\beta,s_n) \;=\; \mathcal{L}_k^{(n)}(\beta,s_n,(\beta+n)\Delta s_{n-1})\,,\quad k,n\in\mathbb{N}_0\,. \tag{4.12}$$

Since Levin's remainder estimate (4.11) reproduces the leading order of the remainder of the model sequence (4.8) for $z=1$ and $\mathrm{Re}(\theta)<0$ (logarithmic convergence), it is not surprising that the u transformation is an effective accelerator for many monotone, logarithmically convergent sequences and series.

In the case of linear convergence ($|z|<1$ in (4.8)), the asymptotic expansion (4.10) indicates that the term a_n itself and not the product na_n would be a natural estimate for the truncation error in (4.8). However, the Levin-type transformations considered in this article nevertheless accelerate convergence if instead of the "right" sequence $\{\omega_n\}_{n=0}^{\infty}$ of remainder estimates satisfying (4.5) "wrong" remainder estimates $\omega_n'=(n+\beta)^l\omega_n$ with $l\in\mathbb{N}_0$ are used (see Theorems 12-14–12-16 and the discussion on pp. 310–311 of Ref. 146). The use of "wrong" remainder estimates only leads—depending on the magnitude of l—to a decrease of the efficiency of the transformation process (compare for instance Ref. 146, Theorem 13-12). With the help of a generalization of Germain-Bonne's formal theory of convergence acceleration[68] it can be proved rigorously that the u transformation accelerates linear convergence (Ref. 146, Theorems 12-10, 12-11, and 12-16).

Moreover, the u transformation is also capable of summing effectively many alternating divergent series. According to Smith and Ford[140,141] the u transformation is among the most versatile and powerful sequence transformations that are currently known. This explains why Levin's u transformation is used internally in the computer algebra system Maple in the case of convergence problems (see for example Ref. 51, pp. 51 and 125 or Ref. 76, p. 258).

The remainder estimate (4.11) can also be inserted into the explicit expressions (2.21), (2.25), and (2.29) for $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$, yielding the u-type variants [Ref. 146, Eqs. (8.4-2) and (9.4-2)]

$$y_k^{(n)}(\beta,s_n) = \mathcal{S}_k^{(n)}(\beta,s_n,(\beta+n)\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0, \tag{4.13}$$

$$Y_k^{(n)}(\xi,s_n) = \mathcal{M}_k^{(n)}(\xi,s_n,(-\xi-n)\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0, \tag{4.14}$$

$${}_u\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \mathcal{C}_k^{(n)}(\alpha,\beta,s_n,(\beta+n)\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0. \tag{4.15}$$

In the case of the sequence transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)] we choose the u-type remainder estimates according to

$$\omega_n = (n+q_0)\Delta s_{n-1} = (n+q_0)a_n, \tag{4.16}$$

where $q_0\geqslant 0$ is a suitable constant. Inserting this into (1.1) yields

$$\begin{aligned}{}_u\mathcal{G}_k^{(n)}(q_m,s_n) &= \mathcal{G}_k^{(n)}(q_m,s_n,(n+q_0)\Delta s_{n-1})\\ &= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{s_{n+j}}{(n+j+q_0)\Delta s_{n+j-1}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{1}{(n+j+q_0)\Delta s_{n+j-1}}}, \quad k,n\in\mathbb{N}_0.\end{aligned} \tag{4.17}$$

As discussed in more detail in Sec. VI (see the discussion following (6.14)), this u-type transformation loses some important exactness properties if $q_0>0$ is essentially arbitrary and does not satisfy $q_0\in\{q_1,\ldots,q_m\}$ because then $[\Pi_{m=1}^{k-1}(n+q_m)]/(n+q_0)$ is rational in n and does not simplify to a polynomial of degree $k-2$ in n. Thus, an obvious idea would be to choose $q_0=q_1$. The other u-type transformations (4.12), (4.13), (4.14), and (4.15) all satisfy $q_0=q_1$.

The asymptotic expansion (4.10) indicates that in the case linear convergence the term a_n is a natural estimate for the truncation error of the sequence (4.8) with $|z|<1$. Thus, Levin[99] proposed for linearly convergent sequences and series the remainder estimate

$$\omega_n = \Delta s_{n-1} = a_n, \tag{4.18}$$

which yields Levin's t transformation in the notation of [Ref. 146, Eq. (7.3-7)]:

$$t_k^{(n)}(\beta,s_n) = \mathcal{L}_k^{(n)}(\beta,s_n,\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0. \tag{4.19}$$

The t transformation is an effective accelerator for linear convergence and in particular for alternating series.[140,141] With the help of a generalization of Germain–Bonne's formal theory of convergence acceleration[68] it can be proved rigorously that Levin's t transformation accelerates linear convergence (Ref. 146, Theorems 12-10, 12-11, and 12-16). It is also able to sum many alternating divergent series. However, a comparison of (4.8) and (4.9) indicates that the t transformation should fail to accelerate logarithmic convergence (for more details, see Ref. 146, Theorem 14-1).

The use of the remainder estimate (4.18) in the explicit expressions (2.21), (2.25), and (2.29) for $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ yields the t-type variants [Ref. 142, Eqs. (8.4-3) and (9.4-3)]

$$\tau_k^{(n)}(\beta,s_n) = \mathcal{S}_k^{(n)}(\beta,s_n,\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0, \tag{4.20}$$

$$T_k^{(n)}(\xi,s_n) = \mathcal{M}_k^{(n)}(\xi,s_n,\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0, \tag{4.21}$$

$${}_t\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\Delta s_{n-1}), \quad k,n\in\mathbb{N}_0. \tag{4.22}$$

In the case of the sequence transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ we obtain in this way,

$${}_t\mathcal{G}_k^{(n)}(q_m,s_n) = \mathcal{G}_k^{(n)}(q_m,s_n,\Delta s_{n-1}) = \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{s_{n+j}}{\Delta s_{n+j-1}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{1}{\Delta s_{n+j-1}}},$$

$$k,n\in\mathbb{N}_0. \tag{4.23}$$

Inspired by Aitken's Δ^2 formula,[1] Levin[99] introduced as a third simple remainder estimate

$$\omega_n = \frac{\Delta s_{n-1}\Delta s_n}{\Delta s_{n-1}-\Delta s_n} = \frac{a_n a_{n+1}}{a_n-a_{n+1}}. \tag{4.24}$$

The usefulness of this remainder estimate can be demonstrated by applying it to the model sequence (4.8). For $\zeta=1$ and $\mathrm{Re}(\theta)<0$ (logarithmic convergence) we obtain

$$\frac{a_n a_{n+1}}{a_n-a_{n+1}} = n^{\theta}\left\{-\frac{\theta\alpha_0}{\theta-1}-\frac{\theta\alpha_1}{(\theta-1)n}+\left[(\theta+1)\left\{\frac{\theta\alpha_0}{12}-\frac{(\theta-2)\alpha_2}{\theta-1}\right\}-\frac{{\alpha_1}^2}{\theta\alpha_0}\right]\frac{1}{(\theta-1)n^2}+\mathrm{O}(n^{-3})\right\}, \quad n\to\infty, \tag{4.25}$$

and for $|z|<1$ (linear convergence) we obtain

$$\frac{a_n a_{n+1}}{a_n-a_{n+1}} = z^{n+1}n^{\theta}\left\{-\alpha_0-\frac{\alpha_1}{n}-\left[\frac{z\theta\alpha_0}{(z-1)^2}+\alpha_2\right]\frac{1}{n^2}+\mathrm{O}(n^{-3})\right\}, \quad n\to\infty. \tag{4.26}$$

It is a remarkable feature of the remainder estimate (4.24) that it does not only reproduce the leading order of the model sequence (4.8), but both in the case of linear and logarithmic convergence also the next one. Thus, in the case of the model sequence (4.8) the reminder estimate (4.24) satisfies (4.6) with $l=2$, whereas Levin's other two remainder estimates (4.11) and (4.18) only satisfy (4.5). Of course, it would be desirable to find other remainder estimate which are also able to reproduce more than the leading order asymptotics of the truncation error. Further research into this direction should be of considerable interest.

The use of the remainder estimate (4.24) in (2.18) yields Levin's v transformation in the notation of [Ref. 146, Eq. (7.3-11)]:

$$v_k^{(n)}(\beta,s_n) = \mathcal{L}_k^{(n)}(\beta,s_n,\Delta s_{n-1}\Delta s_n/[\Delta s_{n-1}-\Delta s_n]), \quad k,n\in\mathbb{N}_0. \tag{4.27}$$

Levin's v transformation is an effective accelerator for many linearly and logarithmically convergent sequences and series. With the help of a generalization of Germain–Bonne's formal theory of convergence acceleration[68] it can be proved rigorously that the v transformation accelerates linear convergence (Ref. 146, Theorems 12-10 and 12-11). The v transformation is also able to sum many alternating divergent series. According to Smith and Ford,[140,141] the v transformation has similar properties as the u transformation, which means that it is among the most versatile and powerful sequence transformations that are currently known.

The use of the remainder estimate (4.24) in the explicit expressions (2.21), (2.25), and (2.29) for $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ yields the v-type variants [Ref. 146, Eqs. (8.4-5) and (9.4-5)]

$$\varphi_k^{(n)}(\beta,s_n) = \mathcal{S}_k^{(n)}(\beta,s_n,\Delta s_{n-1}\Delta s_n/[\Delta s_{n-1}-\Delta s_n]), \quad k,n\in\mathbb{N}_0, \tag{4.28}$$

$$\Phi_k^{(n)}(\xi,s_n) = \mathcal{M}_k^{(n)}(\xi,s_n,\Delta s_{n-1}\Delta s_n/[\Delta s_{n-1}-\Delta s_n]), \quad k,n\in\mathbb{N}_0, \tag{4.29}$$

$${}_v\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\Delta s_{n-1}\Delta s_n/[\Delta s_{n-1}-\Delta s_n]), \quad k,n\in\mathbb{N}_0. \tag{4.30}$$

In the case of the sequence transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ we obtain

$$\begin{aligned} {}_v\mathcal{G}_k^{(n)}(q_m,s_n) &= \mathcal{G}_k^{(n)}(q_m,s_n,\Delta s_{n-1}\Delta s_n/[\Delta s_{n-1}-\Delta s_n]) \\ &= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{(\Delta s_{n+j-1}-\Delta s_{n+j})s_{n+j}}{\Delta s_{n+j-1}\Delta s_{n+j}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{\Delta s_{n+j-1}-\Delta s_{n+j}}{\Delta s_{n+j-1}\Delta s_{n+j}}}, \quad k,n\in\mathbb{N}_0. \end{aligned} \tag{4.31}$$

The best simple estimate for the truncation error of a strictly alternating convergent series is the first term not included in the partial sum (Ref. 96, p. 259). Moreover, the first term neglected is also an estimate of the truncation error of a divergent hypergeometric series ${}_2F_0(a,b,-z)$ with $a,b,z>0$ (Ref. 40, Theorem 5.12-5). Accordingly, Smith and Ford[140] proposed the remainder estimate

$$\omega_n = \Delta s_n = a_{n+1}. \tag{4.32}$$

This remainder estimate can also be motivated via the model sequence (4.8). For $z=1$ and $\mathrm{Re}(\theta)<0$ (logarithmic convergence), we find

$$a_{n+1}=n^\theta\left\{\frac{\theta\alpha_0}{n}+\frac{(\theta-1)[2\alpha_1+\theta\alpha_0]}{2n^2}+\frac{(\theta-2)[6\alpha_2+(\theta-1)\{\theta\alpha_0+3\alpha_1\}]}{6n^3}+\mathrm{O}(n^{-3})\right\}, \quad n\to\infty, \tag{4.33}$$

and for $|z|<1$ (linear convergence), we find

$$a_{n+1}=z^{n+1}n^\theta\left\{(z-1)\alpha_0+\frac{z\theta\alpha_0+(z-1)\alpha_1}{n}+\frac{z(\theta-1)[2\alpha_1+\theta\alpha_0]+2(z-1)\alpha_2}{2n^2}+\mathrm{O}(n^{-3})\right\}, \quad n\to\infty. \tag{4.34}$$

The use of the remainder estimate (4.32) yields Levin's d transformation in the notation of [Ref. 146, Eq. (7.3-9)],

$$d_k^{(n)}(\beta,s_n) = \mathcal{L}_k^{(n)}(\beta,s_n,\Delta s_n), \quad k,n\in\mathbb{N}_0. \tag{4.35}$$

If we compare (4.33) with (4.9) and (4.34) with (4.10), we see that Levin's d transformation should have similar properties as Levin's t transformation. This is confirmed by experience: The d transformation is a powerful accelerator for linear convergence and in particular for alternating series, and is also able to sum many alternating divergent series, but fails to accelerate logarithmic convergence. With the help of a generalization of Germain–Bonne's formal theory of convergence acceleration[68] it can be proved rigorously that the d transformation accelerates linear convergence (Ref. 146, Theorems 12-10, 12-11, and 12-16).

The use of the remainder estimate (4.32) in the explicit expressions (2.21), (2.25), and (2.29) for $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ yields the d-type variants [Ref. 146, Eqs. (8.4-4) and (9.4-4)]

$$\delta_k^{(n)}(\beta,s_n) = \mathcal{S}_k^{(n)}(\beta,s_n,\Delta s_n), \quad k,n\in\mathbb{N}_0, \tag{4.36}$$

$$\Delta_k^{(n)}(\xi,s_n) = \mathcal{M}_k^{(n)}(\xi,s_n,\Delta s_n), \quad k,n\in\mathbb{N}_0, \tag{4.37}$$

$${}_d\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\Delta s_n), \quad k,n\in\mathbb{N}_0. \tag{4.38}$$

As already mentioned in Sec. I, the delta transformation (4.36) was found to be particularly powerful in the case of factorially and hyperfactorially divergent alternating power series as they for instance occur in the perturbation expansions of quantum physics[18,48–50,85,91,146–153,155,156,158,162,163] or in asymptotic expansions for special functions.[147,150,154,161]

In the case of the sequence transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ we obtain

$${}_d\mathcal{G}_k^{(n)}(q_m,s_n) = \mathcal{G}_k^{(n)}(q_m,s_n,\Delta s_n) = \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{s_{n+j}}{\Delta s_{n+j}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{1}{\Delta s_{n+j}}}, \quad k,n\in\mathbb{N}_0. \tag{4.39}$$

In practical applications it happens relatively often that asymptotic expressions $a_n^{(\infty)}$ for the terms a_n of a series are known that reproduce the leading order of a_n as $n\to\infty$. For example, the coefficients c_n of many divergent perturbation expansions, which are power series in some coupling constant g, satisfy (see for example, Ref. 65, Table I)

$$c_n = (-1)^n\,\Gamma(an+b)\,R^n\,[C+\mathrm{O}(1/n)], \quad n\to\infty, \tag{4.40}$$

where a, b, C, and R are known constants.

The remainder estimate (4.24), which leads to Levin's v transformation, is in some sense exceptional since reproduces not only the leading order of the truncation errors of the model sequence (4.8) as $n\to\infty$, but also the next one. Normally, we can only expect that the simple remainder estimates (4.11), (4.18), (4.24), and (4.32) reproduce the leading order of the remainder s_n-s. However, the leading order of the truncation error is also reproduced if we use in (4.11), (4.18), (4.24), and (4.32) not a_n and a_{n+1} but their limiting expressions $a_n^{(\infty)}$ and $a_{n+1}^{(\infty)}$. Whether this improves the transformation results or not, depends on the problem under consideration and cannot be decided by simple considerations. Nevertheless, it may well be worth a try. Ideas of that kind were discussed in more detail in Refs. 83, 149 and also by Čížek, Zamastil, and Skála.[50]

The t-type transformations (4.19), (4.20), (4.21), (4.22), and (4.23) use the last term a_n of the partial sum $s_n=\Sigma_{k=0}^{n}a_k$ as an estimate for the truncation error $r_n=-\Sigma_{k=n+1}^{\infty}a_k$, whereas the analogous d-type transformations (4.35), (4.36), (4.37), (4.38), and (4.39) use the first term a_{n+1} not included in the partial sum as the remainder estimate. Thus, it looks that t-type transformation utilize the available information in some sense more effectively than d-type transformation since they use a_{n+1} also for the construction of the next partial sum s_{n+1}. This is, however, a superficial judgment and it can be shown easily that t-type transformations are actually d-type transformations is disguise.

It follows from (2.13) that the t-type variant (4.23) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ can be expressed as follows:

$$ {}_t\mathcal{G}_k^{(n)}(s_n,\Delta s_{n-1}) = \frac{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\dfrac{s_n}{\Delta s_{n-1}}}{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\dfrac{1}{\Delta s_{n-1}}}, \quad k,n\in\mathbb{N}_0 . \tag{4.41}$$

Next, we use $s_n=s_{n-1}+\Delta s_{n-1}$ in the numerator on the right-hand side and take into account that Δ^k annihilates polynomials of degree $k-1$ in n. Thus,

$$ \Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\frac{s_n}{\Delta s_{n-1}} = \Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\left[\frac{s_{n-1}}{\Delta s_{n-1}}+\frac{\Delta s_{n-1}}{\Delta s_{n-1}}\right] \tag{4.42}$$

$$ = \Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\frac{s_{n-1}}{\Delta s_{n-1}}. \tag{4.43}$$

Inserting this into (4.41) shows that the t-type variant (4.23) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ actually corresponds to the d-type variant (4.39) with a shifted index $n'=n-1$ and modified parameters $q'_m=q_m+1$:

$$ {}_t\mathcal{G}_k^{(n)}(q_m,s_n)=\mathcal{G}_k^{(n-1)}(q_m+1,s_{n-1},\Delta s_{n-1})={}_d\mathcal{G}_k^{(n-1)}(q_m+1,s_{n-1}) \tag{4.44}$$

$$ =\frac{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\dfrac{(n+j+q_m)}{(n+k+q_m)}\right\}\dfrac{s_{n+j-1}}{\Delta s_{n+j-1}}}{\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\dfrac{(n+j+q_m)}{(n+k+q_m)}\right\}\dfrac{1}{\Delta s_{n+j-1}}}, $$

$$ k,n\in\mathbb{N}. \tag{4.45}$$

The other t-type transformations (4.19), (4.20), (4.21), and (4.22) can also be expressed by the corresponding d-type transformations (4.35), (4.36), (4.37), and (4.38) according to

$$ t_k^{(n)}(\beta,s_n) = \mathcal{L}_k^{(n-1)}(\beta+1,s_{n-1},\Delta s_{n-1}) = d_k^{(n-1)}(\beta+1,s_{n-1}), \tag{4.46}$$

$$ \tau_k^{(n)}(\beta,s_n) = \mathcal{S}_k^{(n-1)}(\beta+1,s_{n-1},\Delta s_{n-1}) = \delta_k^{(n-1)}(\beta+1,s_{n-1}), \tag{4.47}$$

$$ T_k^{(n)}(\xi,s_n) = \mathcal{M}_k^{(n-1)}(\xi+1,s_{n-1},\Delta s_{n-1}) = \Delta_k^{(n-1)}(\xi+1,s_{n-1}), \tag{4.48}$$

$$ {}_t\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \mathcal{C}_k^{(n-1)}(\alpha,\beta+1,s_{n-1},\Delta s_{n-1}) = {}_d\mathcal{C}_k^{(n-1)}(\alpha,\beta+1,s_{n-1}). \tag{4.49}$$

In these expressions, the case $n=0$ deserves special consideration. Since we tacitly assume $s_{-m}=0$ with $m\in\mathbb{N}$, the term with $j=0$ in the numerator sum of (4.45) vanishes for $n=0$. This can also be proved directly from the numerator sum in (4.23). If we write there $\Delta s_{n+j-1}=a_{n+j}$ and $s_{n+j}=\Sigma_{\nu=0}^{n+j}a_\nu$, we obtain for $n=0$:

$$\sum_{j=0}^{k} (-1)^j \binom{k}{j} \left\{ \prod_{m=1}^{k-1} (j+q_m) \right\} \sum_{\nu=0}^{j} \frac{a_\nu}{a_j}$$

$$= \sum_{j=0}^{k} (-1)^j \binom{k}{j} \left\{ \prod_{m=1}^{k-1} (j+q_m) \right\} \left[\sum_{\nu=0}^{j-1} \frac{a_\nu}{a_j} + \frac{a_j}{a_j} \right] \tag{4.50}$$

$$= \sum_{j=1}^{k} (-1)^j \binom{k}{j} \left\{ \prod_{m=1}^{k-1} (j+q_m) \right\} \sum_{\nu=0}^{j-1} \frac{a_\nu}{a_j}. \tag{4.51}$$

Here, we made use of the fact that $\Sigma_{\nu=0}^{j-1} a_\nu$ is for $j=0$ an empty sum which is zero. Thus, we obtain for the t-type variant of $\mathcal{G}_k^{(0)}(q_m, s_0, \omega_0)$ the following expression:

$${}_t\mathcal{G}_k^{(0)}(q_m, s_0) = \mathcal{G}_k^{(-1)}(q_m+1, s_{-1}, \Delta s_{-1}) = {}_d\mathcal{G}_k^{(-1)}(q_m+1, s_{-1}) \tag{4.52}$$

$$= \frac{\sum_{j=1}^{k} (-1)^j \binom{k}{j} \left\{ \prod_{m=1}^{k-1} \frac{(j+q_m)}{(k+q_m)} \right\} \frac{s_{j-1}}{\Delta s_{j-1}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \left\{ \prod_{m=1}^{k-1} \frac{(j+q_m)}{(k+q_m)} \right\} \frac{1}{\Delta s_{j-1}}}, \quad k \in \mathbb{N}. \tag{4.53}$$

The fact that t-type transformations are actually d-type transformations in disguise can also be deduced from the recursive scheme (3.10) which contains all the other recursive schemes of Sec. III as special cases. If we choose the initial conditions in (3.10a) according to $u_n = s_n/\Delta s_{n-1}$, then (3.10b) implies $G_1^{(n)} = \Delta[s_n/\Delta s_{n-1}] = \Delta[s_{n-1}/\Delta s_{n-1}]$. Thus, (3.10c) with $k \geqslant 1$ yields the same results as if we had started the recursion with the d-type initial conditions $u_n = s_{n-1}/\Delta s_{n-1}$.

Numerical cancellation increases the risk of losing accuracy. Therefore, it is probably wiser not to use the t-type initial conditions $u_n = s_n/\Delta s_{n-1}$ in the recursive scheme (3.10) or in any of its special cases, but instead the d-type initial conditions $u_n = s_{n-1}/\Delta s_{n-1}$.

V. RICHARDSON-TYPE TRANSFORMATIONS

Some of the most effective accelerators for logarithmically convergent sequences and series ($\rho = 1$ in (4.7)), which abound in scientific applications and which constitute formidable computational problems, can be derived with the help of interpolation theory. Thus, the existence of a function S of a continuous variable is postulated which coincides on a set of discrete arguments $\{x_n\}_{n=0}^{\infty}$ with the elements of the sequence $\{s_n\}_{n=0}^{\infty}$ to be transformed:

$$S(x_n) = s_n, \quad n \in \mathbb{N}_0. \tag{5.1}$$

This ansatz reduces the convergence acceleration problem to an extrapolation problem. If a finite string s_n, s_{n+1}, …, s_{n+k} of $k+1$ sequence elements is known, one can construct an approximation $S_k(x)$ to $S(x)$ which satisfies the $k+1$ interpolation conditions $S_k(x_{n+j}) = s_{n+j}$ with $0 \leqslant j \leqslant k$. Next, the value of $S_k(x)$ has to be determined for $x \to x_\infty$. If this can be done, $S_k(x_\infty)$ should provide a better approximation to the limit $s = s_\infty$ of the sequence $\{s_n\}_{n=0}^{\infty}$ than the last sequence element s_{n+k} used for its construction.

The most important interpolating functions are either polynomials or rational functions which lead to different convergence algorithm (see, for example, Ref. 146, Sec. 6). Here, only polynomial interpolation will be considered. Thus, it is assumed that the kth order approximant $S_k(x)$ is a polynomial of degree k in x,

$$S_k(x) = \gamma_0 + \gamma_1 x + \cdots + \gamma_k x^k, \quad k \in \mathbb{N}, \tag{5.2}$$

or equivalently that the model sequence for the Richardson extrapolation scheme,[115] whose construction will be sketched below, is a polynomial of degree k in the interpolation points x_n,

$$s_n = s + \sum_{j=0}^{k-1} c_j x_n^{j+1}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{5.3}$$

For polynomials, the most natural extrapolation point is $x_\infty = 0$. Accordingly, we assume that the interpolation points x_n satisfy the conditions

$$x_0 > x_1 > \cdots > x_m > x_{m+1} > \cdots > 0, \tag{5.4a}$$

$$\lim_{n\to\infty} x_n = 0. \tag{5.4b}$$

The choice $x_\infty = 0$ implies that the approximation to the limit $s = s_\infty$ in (5.3) is to be identified with the constant term γ_0 of the polynomial (5.2).

Several different methods for the construction of interpolating polynomials $S_k(x)$ are known (see, for example, Ref. 52, Chap. III). Since we are only interested in the constant term γ_0 of an interpolating polynomial $S_k(x)$ and since in most applications it is desirable to compute simultaneously a whole string of approximants $S_0(0), S_1(0), S_2(0), \ldots$ with increasing polynomial degree, the most economical choice is Neville's scheme[104] for the recursive computation of interpolating polynomials. If we set $x = 0$ in Neville's scheme, we obtain the following recursive scheme [see, for example, Ref. 33, p. 73 or Ref. 146, Eq. (6.1-5)]

$$\mathcal{N}_0^{(n)}(s_n, x_n) = s_n, \quad n \in \mathbb{N}_0, \tag{5.5a}$$

$$\mathcal{N}_{k+1}^{(n)}(s_n, x_n) = \frac{x_n \mathcal{N}_k^{(n+1)}(s_{n+1}, x_{n+1}) - x_{n+k+1} \mathcal{N}_k^{(n)}(s_n, x_n)}{x_n - x_{n+k+1}}, \quad k, n \in \mathbb{N}_0. \tag{5.5b}$$

In the literature on convergence acceleration, this variant of Neville's scheme is called Richardson extrapolation.[115] In Ref. 146, Sec. 7.4 it was shown that this recursive scheme can also be derived with the help of the of the annihilation operator approach described in Sec. II by using divided differences as annihilation operators.

In most applications, Richardson extrapolation is used in combination with the interpolation points $x_n = 1/(n+\beta)$ with $\beta > 0$. Then, the model sequence (5.3) assumes the following form:

$$s_n = s + \frac{1}{\beta+n} \sum_{j=0}^{k-1} \frac{c_j}{(\beta+n)^j}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{5.6}$$

This model sequence can be obtained from the model sequence (2.16) for Levin's sequence transformation by setting $\omega_n = 1/(\beta+n)$. Consequently, $\mathcal{N}_k^{(n)}$ with $x_n = 1/(\beta+n)$ is a special Levin transformation and can be expressed as the ratio of two finite sums according to (2.18). Since, however, the denominator of the ratio (2.18) can for $\omega_n = 1/(\beta+n)$ be expressed in closed form, $\mathcal{N}_k^{(n)}$ possesses an even simpler closed form expression as a finite sum [see, for example, Ref. 101, Lemma 2.1 on p. 313, or Ref. 146, Eq. (7.3-20)]

$$\begin{aligned} \Lambda_k^{(n)}(\beta, s_n) &= \mathcal{N}_k^{(n)}(s_n, 1/(\beta+n)) = \mathcal{L}_k^n(\beta, s_n, 1/(\beta+n)) \\ &= (-1)^k \sum_{j=0}^{k} (-1)^j \frac{(\beta+n+j)^k}{j!\,(k-j)!} s_{n+j}, \quad k, n \in \mathbb{N}_0. \end{aligned} \tag{5.7}$$

Moreover, the recursive scheme (5.5) assumes the following form [Ref. 146, Eq. (7.3-21)]:

$$\Lambda_0^{(n)}(\beta, s_n) = s_n, \quad n \in \mathbb{N}_0, \tag{5.8a}$$

$$\Lambda_{k+1}^{(n)}(\beta,s_n) = \Lambda_k^{(n+1)}(\beta,s_{n+1}) + \frac{\beta+n}{k+1}\Delta\Lambda_k^{(n)}(\beta,s_n), \quad k,n\in\mathbb{N}_0. \tag{5.8b}$$

In the case of doubly indexed quantities like $\Lambda_k^{(n)}$ it is always assumed that Δ only acts on the superscript n but not on the subscript k, i.e., $\Delta\Lambda_k^{(n)}=\Lambda_k^{(n+1)}-\Lambda_k^{(n)}$.

A Richardson-type variant of the sequence transformation (1.1) introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)] can be constructed easily. We only have set in (2.12) $\omega_n=1/(n+q_0)$, where q_0 is a suitable constant. This yields the model sequence

$$s_n = s + \sum_{j=0}^{k-1} \frac{c_j}{\prod_{m=1}^{j}(n+q_m)}, \quad k,n\in\mathbb{N}_0. \tag{5.9}$$

Thus, $\Delta^k\Pi_{m=0}^{k-1}(n+q_m)$ is the annihilation operator for the remainder of this model sequence, yielding the following Richardson-type variant of the sequence transformation introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)]:

$${}_R\mathcal{G}_k^{(n)}(q_m,s_n) = \mathcal{G}_k^{(n)}(q_m,s_n,n+q_0) = \frac{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}s_n}{\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}}, \quad k,n\in\mathbb{N}_0. \tag{5.10}$$

Of course, this transformation can be expressed as the ratio of two finite sums according to (1.1). However, the denominator of (5.10) can be expressed in closed form. First, we observe that the products in the difference operator representation (5.10) are polynomials of degree k in n, satisfying

$$\prod_{m=0}^{k-1}(n+q_m) = n^k + (q_0+q_1+\cdots+q_{k-1})n^{k-1} + \cdots. \tag{5.11}$$

Next, we use the well known relationship $\Delta^k n^k=k!$, which can for instance be derived by iterating the commutator relationship (3.4), and take into account that all polynomials of degree $0,1,\ldots,k-1$ in n are annihilated by Δ^k. Thus,

$$\Delta^k\prod_{m=0}^{k-1}(n+q_m) = k!. \tag{5.12}$$

With the help of (2.14) we then obtain from (5.10),

$${}_R\mathcal{G}_k^{(n)}(q_m,s_n) = \mathcal{G}_k^{(n)}(q_m,s_n,1/(n+q_0)) = (-1)^k\sum_{j=0}^{k-1}(-1)^j\frac{\prod_{m=1}^{k-1}(n+j+q_m)}{j!(k-j)!}s_{n+j}, \quad k,n\in\mathbb{N}_0. \tag{5.13}$$

If we set here $q_m=\beta$, we obtain the sequence transformation (5.7) according to

$${}_R\mathcal{G}_k^{(n)}(\beta,s_n) = \mathcal{G}_k^{(n)}(\beta,s_n,1/(\beta+n)) = \Lambda_k^{(n)}(\beta,s_n), \quad k,n\in\mathbb{N}_0. \tag{5.14}$$

We can derive a recursive scheme for ${}_R\mathcal{G}_k^{(n)}(q_m,s_n)$ by means of the techniques described in Sec. III. For that purpose, we express the numerator of the ratio on the right-hand side of (5.10) as follows:

$$Q_k^{(n)} = Q_k^{(n)}(q_m,s_n) = \Delta^k Y_k^{(n)}, \quad k,n\in\mathbb{N}_0, \tag{5.15}$$

$$Y_k^{(n)} = Y_k^{(n)}(q_m,s_n) = \prod_{m=0}^{k-1}(n+q_m)\,s_n, \quad k,n\in\mathbb{N}_0. \tag{5.16}$$

The quantities $Y_k^{(n)}$ satisfy for $k \geqslant 1$ the two-term recursion

$$Y_k^{(n)} = (n+q_{k-1})\, Y_{k-1}^{(n)}. \tag{5.17}$$

Next, we combine (5.15)–(5.17) with the commutator relationship (3.5), yielding

$$Q_k^{(n)} = \Delta^k (n+q_{k-1})\, Y_{k-1}^{(n)} \tag{5.18}$$

$$= [(n+k+q_{k-1})\, E - (n+q_{k-1})]\, \Delta^{k-1}\, Y_{k-1}^{(n)} \tag{5.19}$$

$$= (n+k+q_{k-1})\, Q_{k-1}^{(n+1)} - (n+q_{k-1})\, Q_{k-1}^{(n)}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{5.20}$$

Now, we only have to divide the recurrence formula (5.20) for the numerator of (5.10) by the denominator according to (5.12) to obtain the recursive scheme

$${}_R\mathcal{G}_k^{(0)}(q_m, s_n) = s_n, \quad n \in \mathbb{N}_0, \tag{5.21a}$$

$${}_R\mathcal{G}_{k+1}^{(n)}(q_m, s_n) = {}_R\mathcal{G}_k^{(n+1)}(q_m, s_{n+1}) + \frac{n+q_k}{k+1} \Delta\, {}_R\mathcal{G}_k^{(n)}(q_m, s_n), \quad k,n \in \mathbb{N}_0. \tag{5.21b}$$

If we choose in (5.21) $q_m = \beta$, we obtain the recursive scheme (5.8) for $\Lambda_k^{(n)}(\beta, s_n)$.

By specializing the parameters q_m in (5.13) and (5.21), other Richardson-type transformations and their recursive schemes can be obtained. If we choose $q_m = \chi + m$ with $\chi > 0$, we obtain the Richardson-type variant of the sequence transformation (2.21) [Ref. 146, Eq. (8.4-11)],

$$\mathcal{F}_k^{(n)}(\chi, s_n) = {}_R\mathcal{G}_k^{(n)}(\chi+m, s_n) = \mathcal{S}_k^{(n)}(\chi+1, s_n, 1/(\chi+n))$$

$$= (-1)^k \sum_{j=0}^{k} (-1)^j \frac{(\chi+n+j)_k}{j!\,(k-j)!}\, s_{n+j}, \quad k,n \in \mathbb{N}_0, \tag{5.22}$$

and its recursive scheme [Ref. 146, Eq. (8.4-12)]

$$\mathcal{F}_0^{(n)}(\chi, s_n) = s_n, \quad n \in \mathbb{N}_0, \tag{5.23a}$$

$$\mathcal{F}_{k+1}^{(n)}(\chi, s_n) = \mathcal{F}_k^{(n+1)}(\chi, s_{n+1}) + \frac{\chi+n+k}{k+1} \Delta\, \mathcal{F}_k^{(n)}(\chi, s_n), \quad k,n \in \mathbb{N}_0. \tag{5.23b}$$

If we choose in (5.13) and (5.21) $q_m = \zeta - m$ with $\zeta > 0$, we obtain the Richardson-type variant of the sequence transformation (2.25) [Ref. 146, Eq. (9.4-11)],

$$\mathcal{P}_k^{(n)}(\zeta, s_n) = {}_R\mathcal{G}_k^{(n)}(\zeta-m, s_n) = \mathcal{M}_k^{(n)}(\zeta-1, s_n, -1/(\zeta+n))$$

$$= \sum_{j=0}^{k} (-1)^j \frac{(-\zeta-n-j)_k}{j!\,(k-j)!}\, s_{n+j}, \quad k,n \in \mathbb{N}_0, \tag{5.24}$$

and its recursive scheme [Ref. 146, Eq. (9.4-12)]

$$\mathcal{P}_0^{(n)}(\zeta, s_n) = s_n, \quad n \in \mathbb{N}_0, \tag{5.25a}$$

$$\mathcal{P}_{k+1}^{(n)}(\zeta, s_n) = \mathcal{P}_k^{(n+1)}(\zeta, s_{n+1}) + \frac{\zeta+n-k}{k+1} \Delta\, \mathcal{P}_k^{(n)}(\zeta, s_n), \quad k,n \in \mathbb{N}_0. \tag{5.25b}$$

If we choose in (5.13) and (5.21) $q_m = \chi + m/\alpha$ with $\chi, \alpha > 0$, we obtain the Richardson-type variant of the sequence transformation (2.29),

$$
\begin{aligned}
{}_R\mathcal{C}_k^{(n)}(\alpha,\chi,s_n) &= {}_R\mathcal{G}_k^{(n)}(\chi+m/\alpha,s_n) = \mathcal{C}_k^{(n)}(\alpha,\chi+1,s_n,1/(\chi+n)) \\
&= \frac{(-1)^k}{\alpha^k}\sum_{j=0}^{k}(-1)^j\frac{(\alpha[\chi+n+j])_k}{j!(k-j)!}s_{n+j}, \quad k,n\in\mathbb{N}_0,
\end{aligned}
\tag{5.26}
$$

and its recursive scheme

$$
{}_R\mathcal{C}_0^{(n)}(\alpha,\chi,s_n) = s_n, \quad n\in\mathbb{N}_0, \tag{5.27a}
$$

$$
{}_R\mathcal{C}_{k+1}^{(n)}(\alpha,\chi,s_n) = {}_R\mathcal{C}_k^{(n+1)}(\alpha,\chi,s_{n+1}) + \frac{\chi+n+k/\alpha}{k+1}\Delta\,{}_R\mathcal{C}_k^{(n)}(\alpha,\chi,s_n), \quad k,n\in\mathbb{N}_0. \tag{5.27b}
$$

Depending upon the value of $\alpha>0$, ${}_R\mathcal{C}_k^{(n)}(\alpha,\chi,s_n)$ interpolates between the Richardson-type transformations $\Lambda_k^{(n)}(\beta,s_n)$ and $\mathcal{F}_k^{(n)}(\chi,s_n)$. If we choose in (5.26) $\alpha=1$ and compare the resulting expression with (5.22), we find

$$
{}_R\mathcal{C}_k^{(n)}(1,\chi,s_n) = \mathcal{F}_k^{(n)}(\chi,s_n), \tag{5.28}
$$

and if we use in (5.26),

$$
\lim_{\alpha\to\infty}\frac{(\alpha[\chi+n+j])_k}{\alpha^k} = \lim_{\alpha\to\infty}\prod_{m=0}^{k-1}(\chi+n+j+m/\alpha) = (\chi+n+j)^k \tag{5.29}
$$

together with $\chi=\beta$ and compare the resulting expression with (5.7), we find

$$
\lim_{\alpha\to\infty}{}_R\mathcal{C}_k^{(n)}(\alpha,\beta,s_n) = \Lambda_k^{(n)}(\beta,s_n). \tag{5.30}
$$

VI. RATIONAL APPROXIMANTS

In theoretical physics and in applied mathematics, Padé approximants[106] have become the standard tool to overcome problems with slowly convergent or divergent power series. Padé approximants can also be viewed as a special class of sequence transformations since they transform the partial sums

$$
f_n(z) = \sum_{\nu=0}^{n}\gamma_\nu z^\nu, \quad n\in\mathbb{N}_0, \tag{6.1}
$$

of a (formal) power series for some function f into a doubly indexed sequence of rational functions (see, for example, Ref. 3, Chap. 1):

$$
[l/m]_f(z) = \frac{P^{[l/m]}(z)}{Q^{[l/m]}(z)} = \frac{p_0+p_1z+\cdots+p_lz^l}{1+q_1z+\cdots+q_mz^m}, \quad l,m\in\mathbb{N}_0. \tag{6.2}
$$

We also obtain rational approximants if the u, t, d, and v variants considered in Sec. IV are applied to the partial sums (6.1). Nevertheless, there are some substantial differences between most sequence transformations and Padé approximants. Levin-type transformations can be computed via their explicit expressions, although it is normally preferable to compute them recursively. The coefficients $p_0,\ldots,p_l$ and $q_1,\ldots,q_m$ of the two Padé polynomials $P^{[l/m]}$ and $Q^{[l/m]}$ in (6.2) are, however, chosen in such a way that the Taylor expansion of the ratio $P^{[l/m]}(z)/Q^{[l/m]}(z)$ at $z=0$ agrees with the power series for f as far as possible:

$$Q^{[l/m]}(z)\,f(z) - P^{[l/m]}(z) \;=\; \mathrm{O}(z^{l+m+1})\,, \quad z\to 0\,. \tag{6.3}$$

This asymptotic condition leads to a system of $l+m+1$ linear equations. If this system of equations has a solution, it yields the coefficients of the polynomials $P^{[l/m]}(z)$ and $Q^{[l/m]}(z)$ (see, for example, Ref. 3, Chap. 1).

In most practical applications, Padé approximants are not computed via the defining system of equations, but with the help of recursive algorithms as for example, Wynn's epsilon algorithm.[167] Nevertheless, the accuracy-through-order relationship (6.3) guarantees that the Taylor expansion of $[l/m]_f(z)$ reproduces the partial sum $f_{l+m}(z)$ from which it was constructed. If a sequence transformation is applied to the partial sums of a (formal) power series, it is by no means obvious whether the resulting expression satisfies an accuracy-through-order relationship of the type of (6.3) (see, for example, the discussion in Ref. 157).

The accuracy-through-order relationship (6.3) is essential if Padé approximants are to be used for the prediction of unknown series coefficients, which was first described and utilized by Gilewicz.[69] This so-called Padé prediction is based on the fact that a Padé approximant is by construction analytic at the origin. Accordingly, the power series

$$[l/m]_f(z) \;=\; \sum_{\nu=0}^{\infty} \gamma_\nu^{[l/m]}\, z^\nu \tag{6.4}$$

converges in a neighborhood of $z=0$. The accuracy-through-order relationship (6.3) implies $\gamma_\nu^{[l/m]}=\gamma_\nu$ for $0\leqslant\nu\leqslant l+m$. The remaining coefficients $\gamma_{l+m+\mu+1}^{[l/m]}$ with $\mu\geqslant 0$ are in general different from the corresponding coefficients $\gamma_{l+m+\mu+1}$ of the power series for $f(z)$. If, however, the Padé approximants $[l/m]_f(z)$ converge more rapidly to $f(z)$ than the partial sums $f_{l+m}(z)$ from which they are constructed, then the coefficients $\gamma_{l+m+\mu+1}^{[l/m]}$ provide in particularly for smaller values of μ approximants to the corresponding series coefficients. It is important to note that Padé prediction is not restricted to convergent power series. Thus, Padé prediction can produce useful results even if the power series is a factorially divergent perturbation expansion.

In certain subfields of theoretical physics, the computation of more than a few coefficients of a perturbation expansion can be extremely difficult. Moreover, these coefficients are often affected by comparatively large relative errors. Under such adverse conditions, Padé approximants can be used to make predictions about the leading unknown coefficients of perturbation expansions as well as to make consistency checks for previously calculated coefficients. Further details as well as many examples can be found in Refs. 9, 38, 41–47, 53, 58–62, 85, 91, 93, 120–126, 143, 157, and references therein. Padé prediction can also be quite helpful in different contexts. For example, Padé prediction techniques developed in Ref. 157 were used in Ref. 9 to provide numerical evidence that the factorially divergent perturbation expansion for an anharmonic oscillator, whose Hamiltonian is non-Hermitian but $\mathcal{PT}$-symmetric,[7] is a Stieltjes series.

The prediction of unknown power series coefficients is not restricted to Padé approximants. In principle, any other rational approximant, that also satisfies an accuracy-through-order relationship of the type of (6.3), can be used. It seems that this idea was first formulated by Sidi and Levin[136] and by Brezinski.[25] Recently, it was found that Levin-type transformation like (4.35) and (4.36), which satisfy for $k\in\mathbb{N}$ and $n\in\mathbb{N}_0$ the following asymptotic order estimates as $z\to 0$ [Ref. 163, Eqs. (4.28) and (4.29)],

$$f(z) - d_k^{(n)}(\beta, f_n(z)) \;=\; \mathrm{O}(z^{k+n+2})\,, \tag{6.5}$$

$$f(z) - \delta_k^{(n)}(\beta, f_n(z)) \;=\; \mathrm{O}(z^{k+n+2})\,, \tag{6.6}$$

produce at least in some cases significantly more accurate predictions for unknown power series coefficients than Padé approximants.[85,91,156] Accordingly, it should be of interest to analyze not only the rational approximants, which result if Levin-type transformations are applied to power series, but also their accuracy-through-order relationships. In the case of Levin's t transformation,

this was already done by Sidi and Levin,[136] and the accuracy-through-order relationships for the u, t, v, and d variants of $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, and $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$ were studied in Ref. 150, Sec. 5.7, albeit by a less elegant method.

In this section, the u, t, v, and d variants of the sequence transformation $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ introduced by Čížek, Zamastil, and Skála [Ref. 50, Eq. (10)] are applied to (formal) power series and the accuracy-through-order properties of the resulting rational approximants are studied. Since the sequence transformations $\mathcal{L}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{S}_k^{(n)}(\beta,s_n,\omega_n)$, $\mathcal{M}_k^{(n)}(\xi,s_n,\omega_n)$, and $\mathcal{C}_k^{(n)}(\alpha,\beta,s_n,\omega_n)$ can be obtained from $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ by specializing the parameters q_m, all results for ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$, ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$, ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$, and ${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$ derived here can immediately be translated to the analogous results for the u, t, d, and v variants of the transformations mentioned above.

If we use the partial sums (6.1) of a (formal) power series $f(z)=\sum_{\nu=0}^{\infty}\gamma_\nu z^\nu$ as input data, the simple remainder estimates (4.16), (4.18), (4.24), and (4.32) for the u, t, v, and d variants of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ translate to $\omega_n=(n+q_0)\gamma_n z^n$, $\omega_n=\gamma_n z^n$, $\omega_n=\gamma_n\gamma_{n+1}z^{n+1}/[\gamma_n-z\gamma_{n+1}]$, and $\omega_n=\gamma_{n+1}z^{n+1}$. Of course, these remainder estimates can only be used if the coefficients of the power series for f satisfy $\gamma_n\neq 0$ for all $n\in\mathbb{N}_0$. In the following text, this will be tacitly assumed.

If we apply the u variant (4.17) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ to the partial sums (6.1) of the (formal) power series for f, we obtain

$$
\begin{aligned}
{}_u\mathcal{G}_k^{(n)}(q_m,f_n(z)) &= \mathcal{G}_k^{(n)}(q_m,f_n(z),(n+q_0)\gamma_n z^n)\\
&= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}f_{n+j}(z)}{(n+j+q_0)\gamma_{n+j}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}}{(n+j+q_0)\gamma_{n+j}}},\quad k,n\in\mathbb{N}.
\end{aligned}
\tag{6.7}
$$

${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is the ratio of two polynomials of degrees $k+n$ and k in z, and for its computation the partial sums $f_n(z)$, $f_{n+1}(z),\ldots,f_{n+k}(z)$ are needed. It resembles the Padé approximant $[k+n/k]$, whose computation with the help of Wynn's epsilon algorithm[167] requires, however, the partial sums $f_n(z),f_{n+1}(z),\ldots,f_{n+2k}(z)$.

In the case of the (modified) t variant (4.45) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$, we obtain for $n\geqslant 1$

$$
\begin{aligned}
{}_t\mathcal{G}_k^{(n)}(q_m,f_n(z)) &= \mathcal{G}_k^{(n-1)}(q_m+1,f_{n-1}(z),\gamma_n z^n)\\
&= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}f_{n+j-1}(z)}{\gamma_{n+j}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}}{\gamma_{n+j}}},\quad k\in\mathbb{N}_0,\quad n\in\mathbb{N},
\end{aligned}
\tag{6.8}
$$

and for $n=0$, we obtain from (4.53),

$$
\begin{aligned}
{}_t\mathcal{G}_k^{(0)}(q_m,f_0(z)) &= \mathcal{G}_k^{(-1)}(q_m+1,f_{-1}(z),\gamma_0 z^0)\\
&= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(j+q_m)}{(k+q_m)}\right\}\frac{z^{k-j}f_{j-1}(z)}{\gamma_j}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(j+q_m)}{(k+q_m)}\right\}\frac{z^{k-j}}{\gamma_j}},\quad k\in\mathbb{N}.
\end{aligned}
\tag{6.9}
$$

For $n\geqslant 1$, ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is the ratio of two polynomials of degrees $k+n-1$ and k in z, and for its computation the partial sums $f_{n-1}(z)$, $f_n(z),\ldots,f_{n+k}(z)$ are needed. For $n=0$, the degrees of

the numerator and denominator polynomials are $k-1$ and k, respectively. In that respect, ${}_t\mathcal{G}_k^{(0)}(q_m,f_0(z))$ resembles the Padé approximant $[k-1/k]$, which is of importance in the convergence theory of Stieltjes series (see, for example, Ref. 3, Theorem 5.2.3).

In the case of the d variant (4.39) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$, we obtain

$$\begin{aligned} {}_d\mathcal{G}_k^{(n)}(q_m,f_n(z)) &= \mathcal{G}_k^{(n)}(q_m,f_n(z),\gamma_{n+1}z^{n+1}) \\ &= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}f_{n+j}(z)}{\gamma_{n+j+1}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}}{\gamma_{n+j+1}}}, \quad k,n\in\mathbb{N}_0\,. \end{aligned} \tag{6.10}$$

${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is the ratio of two polynomials of degrees $k+n$ and k in z, and for its computation the partial sums $f_n(z)$, $f_{n+1}(z),\ldots,f_{n+k+1}(z)$ are needed.

In the case of the v variant (4.31) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$, we obtain

$$\begin{aligned} {}_v\mathcal{G}_k^{(n)}(q_m,f_n(z)) &= \mathcal{G}_k^{(n)}(q_m,f_n(z),\gamma_n\gamma_{n+1}z^{n+1}/[\gamma_n-z\gamma_{n+1}]) \\ &= \frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}(\gamma_{n+j}-z\gamma_{n+j+1})f_{n+j}(z)}{\gamma_{n+j}\gamma_{n+j+1}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}\frac{(n+j+q_m)}{(n+k+q_m)}\right\}\frac{z^{k-j}(\gamma_{n+j}-z\gamma_{n+j+1})}{\gamma_{n+j}\gamma_{n+j+1}}}, \\ & k,n\in\mathbb{N}_0\,. \end{aligned} \tag{6.11}$$

${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is the ratio of two polynomials of degrees $k+n+1$ and $k+1$ in z, and for its computation the partial sums $f_n(z)$, $f_{n+1}(z),\ldots,f_{n+k+1}(z)$ are needed.

Next, asymptotic order estimates of the type of (6.3) will be constructed for the rational approximants (6.7)–(6.11). Here, it must be taken into account that an accuracy-through-order relationship does not make any sense if the rational function reproduces exactly the function f represented by the power series. This is for instance the case if u, t, d, and v variants of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ are applied to the partial sums $\Sigma_{\nu=0}^{n}z^\nu=(1-z^{n+1})/(1-z)$ of the geometric series. For an analysis of these complications, let us consider the u variant (6.7). If we introduce the remainders of the partial sums (6.1) according to

$$r_n(z) = f_n(z)-f(z) = -\sum_{\nu=0}^{\infty}\gamma_{n+\nu+1}\,z^{n+\nu+1}, \tag{6.12}$$

then the difference between f and the u variant (6.7) can according to (4.2) be expressed as follows:

$$f(z)-{}_u\mathcal{G}_k^{(n)}(q_m,f_n(z)) = -z^{k+n}\,\frac{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}(n+j+q_m)\right\}\frac{r_{n+j}(z)}{(n+j+q_0)\gamma_{n+j}z^{n+j}}}{\displaystyle\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}(n+j+q_m)\right\}\frac{z^{k-j}}{(n+j+q_0)\gamma_{n+j}}}. \tag{6.13}$$

The denominator of this expression is by assumption of order O(1) as $z\to 0$. For the derivation of an order estimate of the numerator, we can use (2.14) to obtain

$$\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\prod_{m=1}^{k-1}(n+j+q_m)\right\}\frac{r_{n+j}(z)}{(n+j+q_0)\gamma_{n+j}z^{n+j}}$$

$$=(-1)^k\left[\Delta^k\left\{\prod_{m=1}^{k-1}(n+q_m)\right\}\frac{r_n(z)}{(n+q_0)\gamma_n z^n}\right]. \tag{6.14}$$

We now have to distinguish some special cases.

Let us first assume that the u type remainder estimate $\omega_n=(n+q_0)\gamma_n z^n$ is a perfect remainder estimate according to (4.3). Then, Δ^k acts on a polynomial of degree $k-1$ in n, which means that the right-hand side of (6.13) is annihilated. Accordingly, ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is exact for $k\geqslant 1$ and an accuracy-through-order relationship of the type of (6.3) makes no sense.

Let us now assume that the t type remainder estimate $\omega_n=\gamma_n z^n$ is a perfect remainder estimate according to (4.3), which is the case if the input data $\{f_n(z)\}_{n=0}^{\infty}$ are the partial sums $\Sigma_{\nu=0}^{n}z^\nu=(1-z^{n+1})/(1-z)$ of the geometric series. Then, we again have to distinguish two cases. If $q_0\in\{q_1,\ldots,q_{k-1}\}$, the ratio $\Pi_{m=1}^{k-1}(n+q_m)/(n+q_0)$ simplifies to yield a polynomial of degree $k-2$ in n which is annihilated by Δ^k. Accordingly, ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is for $k\geqslant 2$ exact for the partial sums of the geometric series and an accuracy-through-order relationship makes no sense. If $q_0\notin\{q_1,\ldots,q_{k-1}\}$, the ratio $\Pi_{m=1}^{k-1}(n+q_m)/(n+q_0)$ does not simplify to yield a polynomial and is not annihilated by Δ^k. Accordingly, ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ is in this case not exact for the geometric series.

The exactness for the geometric series is probably the most fundamental requirement for a sequence transformation in the case of linear convergence ($0<|\rho|<1$ in (4.7)). This follows from Germain–Bonne's formal theory of convergence acceleration[68] and its extension to Levin-type transformations (Ref. 146, Sec. 12). Consequently, it is probably a good idea that to choose q_0 in in $\omega_n=(n+q_0)\Delta s_{n-1}$ according to $q_0\in\{q_1,\ldots,q_m\}$. An obvious idea would be to choose $q_0=q_1$. The remainder estimates of the other u-type transformations (4.12), (4.13), (4.14), and (4.15) all satisfy $q_0=q_1$. Accordingly, these u variants are for $k\geqslant 1$ exact for the geometric series. This is also true for the t, d, and v variants (6.8)–(6.11) of $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$.

By analyzing expressions of the type of (6.13), accuracy-through-order relationships for ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$, ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$, ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$, and ${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$ can be derived (see, for example, Ref. 150, Sec. 5.7). However, this can be done more elegantly this via the theory of Padé-type approximants which were introduced by Brezinski in Ref. 22 and fully developed in the monograph.[23]

As is well known, the coefficients of the numerator and the denominator polynomials of a Padé approximants are chosen in such a way that the asymptotic order estimate (6.3) is satisfied, but it is not so well known that generalizations and modifications of Padé approximants can be obtained by suitably modifying the asymptotic condition (6.3). For example, let us consider the rational approximants

$$(l/m)_f(z)=\frac{\mathcal{U}^{(l/m)}(z)}{\mathcal{V}^{(l/m)}(z)}=\frac{u_0+u_1z+\cdots+u_lz^l}{v_0+v_1z+\cdots+v_mz^m},\quad l,m\in\mathbb{N}_0. \tag{6.15}$$

We assume that the two polynomials $\mathcal{U}^{(l/m)}(z)$ and $\mathcal{V}^{(l/m)}(z)$ are exactly of degrees l and m in z, or equivalently that $u_l\neq 0$ and $v_m\neq 0$. Let us now assume that the $m+1$ coefficients v_0, $v_1,\ldots,$ v_m of the denominator polynomial $\mathcal{V}^{(l/m)}(z)$ are chosen according to some rule. Then, only the $l+1$ coefficients u_0, $u_1,\ldots,$ u_l of the numerator polynomial $\mathcal{U}^{(l/m)}(z)$ have to be determined via the modified asymptotic condition

$$\mathcal{V}^{(l/m)}(z)\,f(z)-\mathcal{U}^{(l/m)}(z)=\mathrm{O}(z^{l+1}),\quad z\to 0, \tag{6.16}$$

yielding

$$\mathcal{U}^{(l/m)}(z) = \sum_{\lambda=0}^{l} v_\lambda z^\lambda f_{l-\lambda}(z) . \tag{6.17}$$

The rational function $(l/m)_f(z)$ is a so-called Padé-type approximant.[22,23]

Let us now set $l=k+n$ and $m=k$ with $k,n, \in \mathbb{N}_0$ in (6.15). Then, (6.17) implies

$$(k+n/k)_f(z) = \frac{\mathcal{U}^{(k+n/k)}(z)}{\mathcal{V}^{(k+n/k)}(z)} = \frac{\sum_{j=0}^{k} v_j z^j f_{k+n-j}(z)}{\sum_{j=0}^{k} v_j z^j} = \frac{\sum_{j=0}^{k} v_{k-j} z^{k-j} f_{n+j}(z)}{\sum_{j=0}^{k} v_{k-j} z^{k-j}} . \tag{6.18}$$

It follows from (6.7) and (6.10) that ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ and ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ possess the following general structure:

$$\mathbf{T}_k^{(n)}(z) = \frac{\sum_{j=0}^{k} \lambda_j^{(k,n)} z^{k-j} f_{n+j}(z)}{\sum_{j=0}^{k} \lambda_j^{(k,n)} z^{k-j}} = \frac{\sum_{j=0}^{k} \lambda_{k-j}^{(k,n)} z^{j} f_{n+k-j}(z)}{\sum_{j=0}^{k} \lambda_{k-j}^{(k,n)} z^{j}}, \quad k,n \in \mathbb{N}_0 . \tag{6.19}$$

Thus, ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ and ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ are Padé-type approximants of the type of $(k+n/k)_f(z)$ with $v_j=\lambda_{k-j}^{(k,n)}$.

It is a direct consequence of the defining asymptotic condition (6.16) that the Padé-type approximant $\mathbf{T}_k^{(n)}(z)$ satisfies the accuracy-through-order relationship

$$f(z) - \mathbf{T}_k^{(n)}(z) = O(z^{k+n+1}), \quad k,n \in \mathbb{N}_0, \quad z \to 0 . \tag{6.20}$$

This implies that ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$ as well as all the other u-type transformations satisfies the asymptotic order estimate

$$f(z) - {}_u\mathcal{G}_k^{(n)}(q_m,f_n(z)) = O(z^{k+n+1}), \quad k,n \in \mathbb{N}_0, \quad z \to 0 . \tag{6.21}$$

Thus, all coefficients $\gamma_0, \gamma_1, \ldots, \gamma_{k+n}$ of the power series $f(z)=\sum_{\nu=0}^{\infty}\gamma_\nu z^\nu$, that are used for the construction of ${}_u\mathcal{G}_k^{(n)}(q_m,f_n(z))$, are reproduced by a Taylor expansion around $z=0$.

For ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ we obtain the same asymptotic order estimate:

$$f(z) - {}_d\mathcal{G}_k^{(n)}(q_m,f_n(z)) = O(z^{k+n+1}), \quad k,n \in \mathbb{N}_0, \quad z \to 0 . \tag{6.22}$$

In the context of the prediction of unknown power series coefficients, this is a highly unwelcome result: For the computation of ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ we need the series coefficients $\gamma_0, \gamma_1, \ldots, \gamma_{n+k+1}$. Thus, the order term $O(z^{k+n+1})$ implies that a Taylor expansion of ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$ does not reproduce all coefficients used for its construction. Moreover, the order estimates (6.5) and (6.6), which were derived in Ref. 163 by directly analyzing the corresponding expressions without using the theory of Padé-type approximants, indicate that we should instead get the order estimate

$$f(z) - {}_d\mathcal{G}_k^{(n)}(q_m,f_n(z)) = O(z^{k+n+2}), \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0, \quad z \to 0 . \tag{6.23}$$

It is indeed possible to derive this seemingly irregular accuracy-through-order relationship by analyzing the Padé-type approximant $\mathbf{T}_k^{(n)}(z)$ more carefully. For that purpose, we rewrite (6.19) as follows:

$$\mathbf{T}_k^{(n)}(z) = f(z) - z^{k+n+1}\frac{\sum_{j=0}^{k}\lambda_j^{(k,n)}\sum_{\nu=0}^{\infty}\gamma_{n+j+\nu+1}z^{\nu}}{\sum_{j=0}^{k}\lambda_j^{(k,n)}z^{k-j}}. \tag{6.24}$$

The denominator on the right-hand side is by assumption of order O(1) as $z\to 0$. Accordingly, the asymptotic estimate (6.20) is normally optimal, and the improved asymptotic estimate (6.23) can only hold if the z-independent part of the numerator vanishes, or equivalently if $\Sigma_{j=0}^{k}\lambda_j^{(k,n)}\gamma_{n+j+1}=0$. For essentially arbitrary coefficients $\lambda_j^{(k,n)}$ this is certainly not true. However, in the case of all d-type transformations of this article we have $\lambda_j^{(k,n)}=(-1)^j\binom{k}{j}P_{k-1}(n+j)/\gamma_{n+j+1}$, where $P_{k-1}(n)$ is a suitable polynomial of degree $k-1$ in n. Then, we have for $k\geqslant 1$

$$\sum_{j=0}^{k}\lambda_j^{(k,n)}\gamma_{n+j+1} = \sum_{j=0}^{k}(-1)^j\binom{k}{j}P_{k-1}(n+j) = (-1)^k\Delta^k P_{k-1}(n) = 0. \tag{6.25}$$

This proofs the refined accuracy-through-order relationship (6.23).

As discussed in more detail in Sec. IV, t-type transformations are actually d-type transformations in disguise, and (4.44) implies

$${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z)) = {}_d\mathcal{G}_k^{(n-1)}(q_m+1,f_{n-1}(z)). \tag{6.26}$$

Accordingly, for $n\geqslant 1$ the asymptotic order estimate of ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$ follows from the asymptotic order estimate (6.23) of ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$:

$$f(z) - {}_t\mathcal{G}_k^{(n)}(q_m,f_n(z)) = f(z) - {}_d\mathcal{G}_k^{(n-1)}(q_m+1,f_{n-1}(z)) = \mathrm{O}(z^{k+n+1}),$$
$$k,n\in\mathbb{N},\quad z\to 0. \tag{6.27}$$

Thus, all coefficients $\gamma_0, \gamma_1,\ldots,\gamma_{k+n}$ of the power series $f(z)=\Sigma_{\nu=0}^{\infty}\gamma_\nu z^\nu$, that are used for the construction of ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$ with $n\geqslant 1$, are reproduced by a Taylor expansion around $z=0$.

Next, we analyze the case $n=0$ which is not covered by (6.27). A comparison of (6.9) and (6.19) shows that ${}_t\mathcal{G}_k^{(0)}(q_m,f_0(z))$ is not a Padé-type approximant—the term proportional to z^k is missing in the numerator sum—but a closely related rational function of the following kind:

$$\mathbf{T}_k^{(-1)}(z) = \frac{\sum_{j=0}^{k}\lambda_j^{(k,-1)}z^{k-j}f_{j-1}(z)}{\sum_{j=0}^{k}\lambda_j^{(k,-1)}z^{k-j}},\quad k\in\mathbb{N}. \tag{6.28}$$

Accordingly, the defining accuracy-through-order relationship (6.16) of Padé-type approximants cannot help us. However, $\mathbf{T}_k^{(-1)}(z)$ can be reformulated as follows:

$$\mathbf{T}_k^{(-1)}(z) = f(z) - z^k\frac{\sum_{j=0}^{k}\lambda_j^{(k,-1)}\sum_{\nu=0}^{\infty}\gamma_{j+\nu}z^{\nu}}{\sum_{j=0}^{k}\lambda_j^{(k,-1)}z^{k-j}},\quad k\in\mathbb{N}. \tag{6.29}$$

The ratio on the right-hand side is of order $\mathrm{O}(z^k)$ as $z\to 0$. This implies the asymptotic oder estimate $f(z)-{}_t\mathcal{G}_k^{(0)}(q_m,f_0(z))=\mathrm{O}(z^k)$ as $z\to 0$, which does not agree with (6.27) and which would be unsatisfactory since it indicates that not all coefficients $\gamma_0, \gamma_1,\ldots,\gamma_k$ are reproduced by a Taylor expansion of ${}_t\mathcal{G}_k^{(0)}(q_m,f_0(z))$. Instead, we need an order term $\mathrm{O}(z^{k+1})$. Accordingly, we have to show that the z-independent part $\Sigma_{j=0}^{k}\lambda_j^{(k,-1)}\gamma_j$ of the numerator on the right-hand side of (6.29) vanishes.

For that purpose, we take into account that a t-type transformations with $n=0$ is according to (4.44) or (6.26) actually a d-type transformations with $n=-1$. As remarked above, all d-type transformations satisfy $\lambda_j^{(k,n)}=(-1)^j\binom{k}{j}P_{k-1}(n+j)/\gamma_{n+j+1}$, where $P_{k-1}(n)$ is a suitable polynomial of degree $k-1$ in n. Thus, we obtain for $k\geqslant 1$ and $n=-1$:

$$\sum_{j=0}^{k}\lambda_j^{(k,-1)}\gamma_j = \sum_{j=0}^{k}(-1)^j\binom{k}{j}P_{k-1}(j-1) = (-1)^k\Delta^k P_{k-1}(n)\big|_{n=-1} = 0. \tag{6.30}$$

Inserting this into (6.29) yields

$$\mathbf{T}_k^{(-1)}(z) = f(z)-z^{k+1}\frac{\sum_{j=0}^{k}\lambda_j^{(k,-1)}\sum_{\nu=0}^{\infty}\gamma_{j+\nu+1}z^\nu}{\sum_{j=0}^{k}\lambda_j^{(k,-1)}z^{k-j}}, \quad k\in\mathbb{N}, \tag{6.31}$$

which proves the asymptotic order estimate

$$f(z)-{}_t\mathcal{G}_k^{(0)}(q_m,f_0(z)) = O(z^{k+1}), \quad k\in\mathbb{N}, \quad z\to 0. \tag{6.32}$$

Consequently, the asymptotic order estimate (6.27) holds also for $n=0$, and all series coefficients $\gamma_0,\ \gamma_1,\ldots,\ \gamma_{k+n}$ are reproduced by a Taylor expansion of ${}_t\mathcal{G}_k^{(n)}(q_m,f_n(z))$ which were used for its construction.

It follows from (6.11) that the rational approximant ${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$ possesses like all other v-type transformations of this article the following general structure:

$$\mathbf{V}_k^{(n)}(z) = \frac{\sum_{j=0}^{k}\lambda_j^{(k,n)}z^{k-j}f_{n+j}(z)+z\sum_{j=0}^{k}\mu_j^{(k,n)}z^{k-j}f_{n+j}(z)}{\sum_{j=0}^{k}\lambda_j^{(k,n)}z^{k-j}+z\sum_{j=0}^{k}\mu_j^{(k,n)}z^{k-j}}, \quad k,n\in\mathbb{N}_0. \tag{6.33}$$

Comparison with (6.19) shows that $\mathbf{V}_k^{(n)}(z)$ is no Padé-type approximant. Accordingly, the defining asymptotic condition (6.16) of Padé-type approximants cannot be applied. Fortunately, an analogous asymptotic order estimate for $\mathbf{V}_k^{(n)}(z)$ can be derived easily. For that purpose, we rewrite (6.33) as follows:

$$\mathbf{V}_k^{(n)}(z) = f(z)-z^{k+n+1}\frac{\sum_{j=0}^{k}\lambda_j^{(k,n)}\sum_{\nu=0}^{\infty}\gamma_{n+j+\nu+1}z^\nu+z\sum_{j=0}^{k}\mu_j^{(k,n)}\sum_{\nu=0}^{\infty}\gamma_{n+j+\nu+1}z^\nu}{\sum_{j=0}^{k}\lambda_j^{(k,n)}z^{k-j}+z\sum_{j=0}^{k}\mu_j^{(k,n)}z^{k-j}}. \tag{6.34}$$

The denominator on the right-hand side is by assumption of order O(1) as $z\to 0$. Accordingly, we obtain the asymptotic order estimate

$$f(z)-\mathbf{V}_k^{(n)}(z) = O(z^{k+n+1}), \quad k,n\in\mathbb{N}_0, \quad z\to 0, \tag{6.35}$$

which implies

$$f(z)-{}_v\mathcal{G}_k^{(n)}(q_m,f_n(z)) = O(z^{k+n+1}), \quad k,n\in\mathbb{N}_0, \quad z\to 0. \tag{6.36}$$

Now, we have the same problem as in the case of the suboptimal order estimate (6.22) for ${}_d\mathcal{G}_k^{(n)}(q_m,f_n(z))$: The order term $O(z^{k+n+1})$ in (6.36) implies that a Taylor expansion of ${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$ reproduces only $\gamma_0, \gamma_1,\ldots, \gamma_{n+k}$, whereas $\gamma_0, \gamma_1,\ldots, \gamma_{n+k+1}$ are needed for the computation of ${}_v\mathcal{G}_k^{(n)}(q_m,f_n(z))$. Thus, we need instead the order estimate

$$f(z) - {}_v\mathcal{G}_k^{(n)}(q_m,f_n(z)) = O(z^{k+n+2}), \quad k\in\mathbb{N}, \quad n\in\mathbb{N}_0, \quad z\to 0. \tag{6.37}$$

This refined asymptotic estimate can only be true if the z-independent part of the first numerator sum in (6.34) vanishes, or equivalently if $\Sigma_{j=0}^{k}\lambda_j^{(k,n)}\gamma_{n+j+1}=0$. For essentially arbitrary coefficients $\lambda_j^{(k,n)}$ this is certainly not true. However, in the case of the v-type transformations of this article we have just like in the case of the d-type transformations $\lambda_j^{(k,n)}=(-1)^j\binom{k}{j}P_{k-1}(n+j)/\gamma_{n+j+1}$ but $\mu_j^{(k,n)}=(-1)^{j+1}\binom{k}{j}P_{k-1}(n+j)/\gamma_{n+j}$, where $P_{k-1}(n)$ is a suitable polynomial of degree $k-1$ in n. Thus, (6.25) holds which proves the accuracy-through-order relationship (6.37).

In Sec. IV, it was mentioned that in some cases asymptotic expressions $a_n^{(\infty)}$ for the terms a_n of an infinite series $s=\Sigma_{\nu=0}^{\infty}a_\nu$ are known which reproduce the leading order asymptotics of a_n as $n\to\infty$, and that these asymptotic expressions can also be used in the simple remainder estimates (4.11), (4.18), (4.24), and (4.32) since they also reproduce the leading order asymptotics of the remainders $r_n=s_n-s$ as $n\to\infty$.

Thus, we now assume that asymptotic expressions $\gamma_n^{(\infty)}$ are known that reproduce the leading order asymptotics of the coefficients of the power series $f(z)=\Sigma_{\nu=0}^{\infty}\gamma_\nu z^\nu$ according to

$$\gamma_n = \gamma_n^{(\infty)}[c+O(1/n)], \quad c\neq 0, \quad n\to\infty. \tag{6.38}$$

If we use in $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ the u-, t-, v-, and d-type remainder estimates $\omega_n=(n+q_0)\gamma_n^{(\infty)}z^n$, $\omega_n=\gamma_n^{(\infty)}z^n$, $\omega_n=\gamma_n^{(\infty)}\gamma_{n+1}^{(\infty)}z^{n+1}/[\gamma_n^{(\infty)}-z\gamma_{n+1}^{(\infty)}]$, and $\omega_n=\gamma_{n+1}^{(\infty)}z^{n+1}$, we obtain rational approximants which closely resemble the u, t, v, and d variants (6.7), (6.8), (6.10), and (6.11), and which are also special cases of the rational functions $\mathbf{T}_k^{(n)}(z)$ and $\mathbf{V}_k^{(n)}(z)$ defined in (6.19) and (6.33), respectively. Consequently, these rational approximants satisfy for all $k,n\in\mathbb{N}_0$ the following asymptotic estimates as $z\to 0$:

$$f(z) - \mathcal{G}_k^{(n)}(q_m,f_n(z),(n+q_0)\gamma_n^{(\infty)}z^n) = O(z^{k+n+1}), \tag{6.39}$$

$$f(z) - \mathcal{G}_k^{(n)}(q_m,f_n(z),\gamma_n^{(\infty)}z^n) = O(z^{k+n+1}), \tag{6.40}$$

$$f(z) - \mathcal{G}_k^{(n)}(q_m,f_n(z),\gamma_{n+1}^{(\infty)}z^n) = O(z^{k+n+1}), \tag{6.41}$$

$$f(z) - \mathcal{G}_k^{(n)}(q_m,f_n(z),\gamma_n^{(\infty)}\gamma_{n+1}^{(\infty)}z^{n+1}/[\gamma_n^{(\infty)}-z\gamma_{n+1}^{(\infty)}]) = O(z^{k+n+1}). \tag{6.42}$$

Accordingly, all coefficients $\gamma_0, \gamma_1,\ldots, \gamma_{k+n}$ of the power series for $f(z)$, which were used for the construction of these rational approximants are reproduced by Taylor expansion.

Improved asymptotic estimates of the type of (6.23) or (6.37) for the d- and v-type variants do not hold here. The reason is that the coefficients $\lambda_j^{(k,n)}$ in (6.19) and (6.33) now satisfy $\lambda_j^{(k,n)}=(-1)^j\binom{k}{j}P_{k-1}(n+j)/\gamma_{n+j+1}^{(\infty)}$. In general, we have $\gamma_{n+j+1}^{(\infty)}\neq\gamma_{n+j+1}$, which implies that $\Sigma_{j=0}^{k}\lambda_j^{(k,n)}\gamma_{n+j+1}=0$ does not hold.

If we use in $\mathcal{G}_k^{(n)}(q_m,s_n,\omega_n)$ the remainder estimates $\omega_n=(n+q_0)\gamma_n^{(\infty)}z^n$, $\omega_n=\gamma_n^{(\infty)}z^n$, $\omega_n=\gamma_n^{(\infty)}\gamma_{n+1}^{(\infty)}z^{n+1}/[\gamma_n^{(\infty)}-z\gamma_{n+1}^{(\infty)}]$, and $\omega_n=\gamma_{n+1}^{(\infty)}z^{n+1}$, the poles of the resulting rational approximants are determined by the parameters q_m in the products $\Pi_{m=1}^{k-1}(n+q_m)$ and by the remainder estimates, but they do not depend on the coefficients γ_n of the power series for f. This highlights once more the crucial importance of the remainder estimates for the success or the failure of Levin-type transformations. In contrast, both the numerator and the denominator coefficients of a Padé approximant $[l/m]_f(z)$ depend via (6.3) on the coefficients of the partial sum $f_{l+m}(z)$ which was used for its construction.

VII. SUMMARY AND OUTLOOK

Levin[99] deserves credit for realizing that the efficiency of convergence acceleration and summation processes can be enhanced considerably by using as input data not only the elements of the sequence $\{s_n\}_{n=0}^{\infty}$ to be transformed, but also explicit estimates $\{\omega_n\}_{n=0}^{\infty}$ for the truncation errors of this sequence.

If the input data are the partial sums of an infinite series, and if sufficiently simple analytical expressions for the terms of this series are known, then it is possible to derive analytical estimates for the truncation errors of these series. In principle, the use of specially designed analytical remainder estimates would be highly desirable, although the resulting expressions are no longer generally applicable sequence transformations, but rather (optimized) approximation schemes for specific problems (see, for instance, the discussion in Ref. 159).

However, convergence acceleration and summation methods are needed most if only relatively few elements of a slowly convergent or divergent sequence are available, and if apart from the numerical values of the input data virtually nothing is known. This is a scenario which happens only too often if we try to sum divergent perturbation expansions of quantum physics. In such a situation there is obviously no chance of constructing analytical expressions for remainder estimates. Instead, we must construct the remainder estimates from the numerical values of the input data via simple rules. Fortunately, the simple remainder estimates proposed by Levin[99] and later Smith and Ford,[140] which are discussed in Sec. IV, normally do the job. In spite of their simplicity, they often work remarkably well.

If we approximate the remainder r_n of a sequence element s_n by the product $\omega_n z_n$ according to (2.8), where z_n is a so-called correction term, then we should take into account that our approximation scheme actually has two degrees of freedom. Levin[99] originally assumed that z_n is a truncated inverse power series according to (2.16). This is certainly a very natural idea, and it leads to a very powerful sequence transformation.

Nevertheless, in some cases Levin's transformation fails horribly for reasons which we do not completely understand. For example, it was found in Refs. 162 and 163 that Levin's transformation diverges if it is used for the summation of the perturbation expansions for the ground state energies of the anharmonic oscillators (compare also Ref. 148, Table II or the discussion in Ref. 150, Sec. 10.7). A similar divergence of Levin's transformation was observed by Čížek, Zamastil, and Skála (Ref. 50, p. 965) in the case of the hydrogen atom in an external magnetic field. Fortunately, Levin's choice for z_n is not the only possibility, and at least for some problems, alternative correction terms produce significantly better results. For example, the so-called delta transformation defined in (4.36) is based on the assumption that z_n is a truncated factorial series according to (2.19). As mentioned before, this delta transformation is a very effective transformation for slowly convergent and divergent alternating series. In particular, it produces very good summation results both in the case of the anharmonic oscillators[147,148,150,149,153,155,162,163] as well as in the case of the hydrogen atom in an external magnetic field (Ref. 50, Tables I and II).

The sequence transformation $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$ introduced by Čížek, Zamastil, and Skála[50] permits a unified treatment of the mathematical properties of all sequence transformations, whose correction terms are annihilated by difference operators of the type of

$$\hat{T} = \Delta^k P_{k-1}(n). \tag{7.1}$$

Here, $P_{k-1}(n)$ is a suitable polynomial of degree $k-1$ in n that can be obtained by specializing the parameters q_m in $\Pi_{m=1}^{k-1}(n+q_m)$. All Levin-type transformations considered in this article belong to this class of sequence transformations. Consequently, all their mathematical properties such as explicit expressions (Secs. II and V), recurrence formulas (Sec. III), and accuracy-through-order properties (Sec. VI) can be deduced from the corresponding properties of $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$ by specializing the parameters q_m.

In addition, new sequence transformations can be constructed by specializing the parameters q_m in $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$. For example, Čížek, Zamastil, and Skála (Ref. 50, Tables I and II) found that in the case of the hydrogen atom in an external magnetic field at least for some coupling

constants better summation results can be obtained by choosing $q_m = m^2$ instead of choosing $q_m = m$ which yields the delta transformation with $\beta = 1$. Such a quadratic dependence of the parameters q_m on m leads to a completely new sequence transformation. Thus, the sequence transformation $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$ introduced by Čížek, Zamastil, and Skála[50] does not only permit a unification of already known transformations, but it also opens up the path for promising new research.

As discussed in more details in the following article,[160] our current level of theoretical understanding does not permit to predict which one of the numerous variants of $\mathcal{G}_k^{(n)}(q_m, s_n, \omega_n)$ will give best results for a given convergence acceleration or summation problem. So, if we for example use one of the numerous Levin-type transformation for the summation of a divergent perturbation expansion, we are essentially conducting a numerical experiment. As every good experimentalist knows, a single experiment is only rarely able to provide a definite answer. Normally, a whole set of related experiments is needed to obtain convincing evidence. Of course, this applies also to our numerical experiments. Therefore, we should not insist with a quasireligious zeal on using only a single (Levin-type) transformation which we for some reason may prefer. Instead, it is usually a much better idea to compare the performance of several different transformations.

Levin-type transformations are not only very powerful but also very flexible. Experience shows that they can handle successfully a large variety of different convergence acceleration or summation problems. This is a direct consequence of the fact that the ansatz $\omega_n z_n$ for r_n according to (2.8) has two degrees of freedom which allows a considerable amount of fine-tuning. Nevertheless, Levin-type transformations are not a cure for all evils. Consequently, a good experimentalist should also take into account the possibility that Levin-type transformations may not work at all or that other transformations could produce better results.

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On solvable potentials related to SO(2,2). II. Natanzon potentials

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General Natanzon potentials related to the SO(2,2) group are studied. The S-matrices for systems under consideration are related to intertwining operators between Weyl equivalent most degenerate principal series representations of SO(2,2). © *2004 American Institute of Physics.* [DOI: 10.1063/1.1669057]

I. INTRODUCTION

The existence of Hamiltonians with nontrivial potentials which are exactly solvable is one of the most interesting problems in nonrelativistic quantum mechanics. By exactly solvable, one means those Hamiltonians for which the spectrum, eigenfunctions and the scattering matrices can be found explicitly. Apart from their beautiful mathematical structure, these models provide excellent tools for studying various physical phenomena.

In particular, the Hamiltonians with Natanzon potentials[1] are known to be exactly solvable, and much literature has been devoted to the study of these models.[2–11] An important point to stress is that they possess hidden algebraic structures responsible for solvability. Moreover, it has been shown by Wu *et al.*[5] that both bound and scattering problems for Natanzon potentials can be reduced to a representation theory problem of $\mathfrak{so}(2,2)$. It appears that knowledge of the interrelation between $\mathfrak{so}(2,2)$ algebra and an Euclidean algebra $\mathfrak{e}(2)\oplus\mathfrak{e}(2)$, which describes the asymptotic properties of the system, allows pure algebraic calculation of S-matrices. (This technique[12] is referred to as the Euclidean connection.) However, Natanzon potentials constructed in Ref. 5 is not the most general one related to $\mathfrak{so}(2,2)$. As we shall see, this lack of generality is due to the fact that only $\mathfrak{so}(2,2)\supset\mathfrak{so}(2)\oplus\mathfrak{so}(2)$ subgroup reduction were considered in that paper. It is also worth to point out that the Euclidean connection technique works out only in cases in which the reduction with respect to compact algebra is appropriate.

In a recent paper by one of the present authors[13] was proposed a way which allows pure algebraic calculation of S-matrices for the systems whose Hamiltonians are related to the Casimir operator C of some noncompact group G. In that paper the S-matrices for the systems under consideration are associated with intertwining operators A between Weyl equivalent principal series representations of G. At this stage we note that the operator A is said to intertwine the representations U^{χ} and $U^{\tilde{\chi}}$ of the group G (Ref. 14) if relation

$$AU^{\chi}(g)=U^{\tilde{\chi}}(g)A \quad \text{for all } g\in G \tag{1.1}$$

or

$$AdU^{\chi}(b)=dU^{\tilde{\chi}}(b)A \quad \text{for all } b\in\mathfrak{g} \tag{1.2}$$

holds, where dU^{χ} and $dU^{\tilde{\chi}}$ are the corresponding representations of the algebra $\mathfrak{g}$ of G.

It turns out that if Hamiltonian H of the system belongs to the center of the enveloping algebra of G, i.e.,

$$H=f(C), \tag{1.3}$$

then the S matrix coincide with intertwining operator between Weyl equivalent principal series representations of G. Moreover, it follows from Eq. (1.1) or (1.2) that if the matrix of the representation operator is diagonal in some subgroup basis then the matrix of the intertwining operator is also diagonal. This fact leads to the suggestion that there might exist a class of scattering systems for which

$$H=f(C)|_{\mathcal{H}}, \tag{1.4}$$

where $\mathcal{H}$ are the subspaces occurring in the subgroup reductions. This is exactly what happens in the algebraic approaches proposed in Refs. 15, 16, 17, 12. (As usual, H is linear on the second-order Casimir operator of G.) In this case the group G describes fixed energy states of a family of dynamical systems with different potential strength. This is why the present group G is called ''the potential group.'' [17,12]

It is clear that the scattering operators S for such systems are also related to the intertwining operators, but now

$$S=A|_{\mathcal{H}}. \tag{1.5}$$

Moreover, there also exist other solvable models for which scattering operators are given by (1.5) while the Hamiltonian of the systems are related to the Casimir operator C as[15]

$$Q(H-E)=(C-q)|_{\mathcal{H}}, \tag{1.6}$$

where q is an eigenvalue of C and Q is some nontrivial operator. Observe that if we choose $Q=\text{const}$ Eq. (1.6) reduces to (1.4) provided that H is linear on C.

Equations (1.1) and (1.2) have much restriction power, determining the intertwining operator up to a constant. Therefore, one can evaluate the S-matrix without writing a Schrödinger equation, or wave functions. Moreover, one can use the well-developed theory of intertwining operators for semisimple Lie groups[18–21] to obtain stringent restriction upon the structure of the scattering matrices for many-body systems associated with semisimple Lie groups, or even to determine it completely.[22]

In a previous paper[23] we gave the simple example of how the scattering problem for systems with the SO(2,2) ''potential group'' structure can be solved within the framework of group theory. We discussed the one-dimensional potential scattering of systems for which the Hamiltonians H can be written as

$$H\propto(C+1)|_{\mathcal{H}}, \tag{1.7}$$

where C is the Casimir operator of SO(2,2) and $\mathcal{H}$ is a subspace occurring in the $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(2)$, $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes E(1)$, $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$, $\mathrm{SO}(2,2)\supset\mathrm{SO}(1,1)\otimes E(1)$ or $\mathrm{SO}(2,2)\supset E(1)\otimes E(1)$ reduction. Here we show that the solution of the scattering problem in the case of models with algebraic structure proposed in (1.6) is also possible within this framework.

The content of the paper is arranged as follows: After the introduction, in Sec. II, we set out the basis of our approach. In Secs. III, IV, and V we discuss a class of quantum scattering problems related to most degenerate principal series representations of the group SO(2,2) in the reductions with respect to $\mathrm{SO}(2)\otimes\mathrm{SO}(2)$, $\mathrm{SO}(2)\otimes E(1)$, and $\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$. Finally, we have included in the Appendix some technical details of the calculation that for clarity were omitted from the main text.

II. MAIN IDEA

Let $R^{2,2}$ be a four-dimensional pseudo-Euclidean space with the bilinear form

$$[\xi,\eta]=\xi_1\eta_1+\xi_2\eta_2-\xi_3\eta_3-\xi_4\eta_4. \tag{2.1}$$

By SO(2,2) we denote the connected component of the group of linear transformation of $R^{2,2}$ preserving the form (2.1). We consider SO(2,2) as acting on $R^{2,2}$ on the right. In accordance with this we shall write the vector in the row form $\xi=(\xi_1,\xi_2,\xi_3,\xi_4)$.

Let us denote $\{g_{ij}(\theta)\}$ $i<j$, $i,j=1,2,3,4$ the one-parameter subgroups of SO(2,2) consisting of rotations or pseudorotations in the $\xi_i-\xi_j$-planes, that is, of transformations of the form

$$\xi_k'=\xi_k,\quad k\neq i,j,\quad \xi_i'=\xi_i\cos\theta+\xi_j\sin\theta,\quad \xi_j'=-\xi_i\sin\theta+\xi_j\cos\theta \tag{2.2}$$

or

$$\xi_k'=\xi_k,\ k\neq i,j,\quad \xi_i'=\xi_i\cosh\theta+\xi_j\sinh\theta,\quad \xi_j'=\xi_i\sinh\theta+\xi_j\cosh\theta, \tag{2.3}$$

respectively. The matrices

$$a_{ij}=\frac{d}{d\theta}g_{ij}(\theta)\bigg|_{\theta=0},\quad i<j \tag{2.4}$$

form a basis of the Lie algebra $\mathfrak{so}(2,2)$ of the group SO(2,2). Defining

$$\begin{aligned} a_1&=(a_{13}+a_{24})/2,\quad b_1=(a_{13}-a_{24})/2,\\ a_2&=(a_{23}-a_{14})/2,\quad b_2=(a_{23}+a_{14})/2,\\ a_3&=(a_{34}-a_{12})/2,\quad b_3=-(a_{12}+a_{34})/2, \end{aligned} \tag{2.5}$$

one has

$$\begin{aligned} [a_1,a_2]&=a_3,\quad [b_1,b_2]=b_3,\\ [a_2,a_3]&=-a_1,\quad [b_2,b_3]=-b_1,\\ [a_3,a_1]&=-a_2,\quad [b_3,b_1]=-b_2. \end{aligned} \tag{2.6}$$

The generators a_i and b_i separately form a Lie algebra of SO(2,1). In other words SO(2,2) is the product group of two SO(2,1) groups, i.e., $\mathrm{SO}(2,2)=\mathrm{SO}(2,1)\otimes\mathrm{SO}(2,1)$. Let us note at this point that the group SO(2,1) has three subgroups SO(2), SO(1,1), and $E(1)$ generated, for example, by a_3, a_1, and a_2+a_3, respectively, where $E(1)$ is an Euclidean group in one dimension. It is also worth noting that each UIR of SO(1.1) is doubly degenerate in principal series of UIR of SO(2.1).

The most degenerate UIR of SO(2,2) are known to form three series:[24,25] principal, supplementary, and discrete. It is also known that only the principal series of SO(2,2) describe scattering states. Consequently, the relevant unitary representations will be the principal series and we restrict the discussion to it.

The principal degenerate representation of SO(2,2) are characterized by the pair $\chi=(\rho,\varepsilon)$ where ε is equal to 0 or 1, while $0\leqslant\rho<\infty$. The representations specified by labels $\chi=(\rho,\varepsilon)$ and $\tilde{\chi}=(-\rho,\varepsilon)$ are equivalent. (The representations labeled by χ and $\tilde{\chi}$ have the same Casimir eigenvalues. Such representations are called Weyl equivalent.) For the sake of simplicity, we consider the representations with $\varepsilon=0$, although the case $\varepsilon=1$ can be also easily treated. We now return to our main theme.

We want to construct the Hamiltonians for which the relation

$$Q(H-E)=[C-j(j+2)]|_{\mathcal{H}} \tag{2.7}$$

holds, where j specifies the most degenerate principal series of SO(2,2) and $\mathcal{H}$ is a subspace occurring in subgroup reductions. The key to the construction of it lies in the observation that the Schrödinger energy eigenvalue equation for such systems is nothing but the condition imposed on

the carrier space of SO(2,2) to be irreducible. Thus in order to find the Hamiltonians for the systems under considerations we should look for a reducible representation of SO(2,2) containing the principal series.

Let us consider a quasiregular representation $T(g)$ of SO(2,2) realized in the Hilbert space of square-integrable functions $f(\xi)$ on hyperboloid Ξ,

$$\xi_1^2+\xi_2^2-\xi_3^2-\xi_4^2=1. \tag{2.8}$$

Generally, one can use for the construction of the quasiregular representation the carrier space $L^2(\Xi,d\mu)$ with any quasi-invariant measure $d\mu(\xi)$ on Ξ. The representations with different measure are unitarily equivalent. They are given by[26]

$$T(g)f(\xi)=(d\mu(\xi g)/d\mu(\xi))^{1/2}f(\xi g), \tag{2.9}$$

with the inner product

$$(f,f')=\int \overline{f(\xi)}f'(\xi)d\mu(\xi), \tag{2.10}$$

where $d\mu(\xi g)/d\mu(\xi)$ is the Radon–Nikodym derivative.

We can, without loss of generality, put

$$d\mu(\xi)=h(\xi)d\xi, \tag{2.11}$$

where $d\xi=d\xi_1 d\xi_2 d\xi_3/|\xi_4|$ is an invariant measure on Ξ. The requirement that the measure is quasi-invariant implies only the condition

$$h(\xi)\geqslant 0. \tag{2.12}$$

Then the (Hermitian) infinitesimal operators $A_{ij}=-i\,(d/d\theta)\,T(g_{ij}(\theta))|_{\theta=0}$ of the representation $T(g)$ corresponding to the one-parameter subgroups $g_{ij}(\theta)$ are given by

$$iA_{12}=\xi_2\frac{\partial}{\partial\xi_1}-\xi_1\frac{\partial}{\partial\xi_2}+\frac{1}{2h}\left(\xi_2\frac{\partial h}{\partial\xi_1}-\xi_1\frac{\partial h}{\partial\xi_2}\right),\quad iA_{14}=\xi_4\frac{\partial}{\partial\xi_1}+\frac{\xi_4}{2h}\frac{\partial h}{\partial\xi_1},$$

$$iA_{13}=\xi_3\frac{\partial}{\partial\xi_1}+\xi_1\frac{\partial}{\partial\xi_3}+\frac{1}{2h}\left(\xi_3\frac{\partial h}{\partial\xi_1}+\xi_1\frac{\partial h}{\partial\xi_3}\right),\quad iA_{24}=\xi_4\frac{\partial}{\partial\xi_2}+\frac{\xi_4}{2h}\frac{\partial h}{\partial\xi_2},$$

$$iA_{23}=\xi_3\frac{\partial}{\partial\xi_2}+\xi_2\frac{\partial}{\partial\xi_3}+\frac{1}{2h}\left(\xi_3\frac{\partial h}{\partial\xi_2}+\xi_2\frac{\partial h}{\partial\xi_3}\right),\quad iA_{34}=\xi_4\frac{\partial}{\partial\xi_3}+\frac{\xi_4}{2h}\frac{\partial h}{\partial\xi_3}.$$

We are taking ξ_1, ξ_2, and ξ_3 as the independent variables on Ξ.

We now require the representation space to be irreducible. (We note that the representation (2.9) is decomposed onto principal and discrete series of most degenerate UIR of SO(2,2).[24,25]) Such a restriction is obtained if all functions are eigenfunctions of the Casimir operator C

$$Cf=j(j+2)f, \tag{2.13}$$

where $C=A_{12}^2+A_{34}^2-A_{13}^2-A_{14}^2-A_{23}^2-A_{24}^2$. Since we are interested only in the continuous spectrum, we will put $j=-1-i\rho$. Next, imposing the reduction condition, one can extract corresponding one-dimensional potentials from the Casimir operator.

III. CLASS OF POTENTIALS RELATED TO $SO(2,2)\supset SO(2)\otimes SO(2)$ REDUCTION

As we mentioned above the quasiregular representations with different measure are unitarily equivalent. Although the representations with different measure are mathematically equivalent, they may be related to different physical problems. For this reason, we shall consider the quasiregular representation with different measure.

We want to diagonalize the $SO(2)\otimes SO(2)$ subgroup. Then, the reduction conditions are

$$A_3 f^{(1)}_{mk}=m f^{(1)}_{mk}, \quad B_3 f^{(1)}_{mk}=k f^{(1)}_{mk}, \tag{3.1}$$

where A_3 and B_3 are defined as

$$A_3=(A_{34}-A_{12})/2, \quad B_3=-(A_{12}+A_{34})/2. \tag{3.2}$$

(Here and in the following infinitesimal operators corresponding to generators a_i, b_i are denoted by A_i, B_i, respectively.) According to this we want $d\mu$ to be invariant under $SO(2)\otimes SO(2)$. We can, without loss of generality, put $d\mu(\xi)=h(r)d\xi$, where $r=\xi_1^2+\xi_2^2$. Then the generators A_{12} and A_{34} are given by

$$A_{12}=-i\left(\xi_2\frac{\partial}{\partial\xi_1}-\xi_1\frac{\partial}{\partial\xi_2}\right), \quad A_{34}=-i\xi_4\frac{\partial}{\partial\xi_3} \tag{3.3}$$

while

$$C=-\frac{\partial^2}{\partial\xi_1^2}-\frac{\partial^2}{\partial\xi_2^2}+\frac{\partial^2}{\partial\xi_3^2}+\left(\frac{\xi_1^2+\xi_2^2}{\xi_1 h}\frac{\partial h}{\partial\xi_1}+I\right)(I+2)-\frac{1}{\xi_1 h}\frac{\partial h}{\partial\xi_1}\left(\xi_1\frac{\partial}{\partial\xi_1}+\xi_2\frac{\partial}{\partial\xi_2}+1\right)$$
$$+\frac{(\xi_1^2+\xi_2^2)(\xi_1^2+\xi_2^2-1)}{2\xi_1\xi_2 h}\frac{\partial^2 h}{\partial\xi_1\partial\xi_2}-\frac{(\xi_1^2+\xi_2^2)(\xi_1^2+\xi_2^2-1)}{4\xi_1^2 h^2}\left(\frac{\partial h}{\partial\xi_1}\right)^2 \tag{3.4}$$

with

$$I=\xi_1\frac{\partial}{\partial\xi_1}+\xi_2\frac{\partial}{\partial\xi_2}+\xi_3\frac{\partial}{\partial\xi_3}, \tag{3.5}$$

where we have used

$$\frac{\partial h}{\partial\xi_2}=\frac{\xi_2}{\xi_1}\frac{\partial h}{\partial\xi_1}. \tag{3.6}$$

Since A_3 and B_3 are sought to be diagonal, we introduce in place of ξ_1, ξ_2, ξ_3 the variables x, α, β via

$$\xi_1=\frac{1}{\sqrt{1-z(x)}}\cos\frac{\alpha+\beta}{2}, \quad \xi_2=\frac{1}{\sqrt{1-z(x)}}\sin\frac{\alpha+\beta}{2},$$
$$\xi_3=\sqrt{\frac{z(x)}{1-z(x)}}\cos\frac{\beta-\alpha}{2}, \quad 0\leqslant\alpha, \quad \beta<2\pi, \quad 0\leqslant x<\infty, \tag{3.7}$$

where z is a differentiable function on R^+ with values in [0,1]. Then

$$A_3=-i\frac{\partial}{\partial\alpha}, \quad B_3=-i\frac{\partial}{\partial\beta} \tag{3.8}$$

as we expected. If we compute the Casimir operator C for this parametrization, it becomes

$$C=4\frac{z(1-z)^2}{\dot{z}^2}\left\{\frac{\partial^2}{\partial x^2}+\left(\frac{\dot{h}}{h}-\frac{\ddot{z}}{\dot{z}}+\frac{\dot{z}}{z}\right)\frac{\partial}{\partial x}\right.$$
$$\left.+\frac{\dot{z}^2}{4z^2}\left[\frac{\partial^2}{\partial\alpha^2}-2\frac{1+z}{1-z}\frac{\partial^2}{\partial\alpha\partial\beta}+\frac{\partial^2}{\partial\beta^2}\right]+\frac{1}{2h}\left[\ddot{h}-\frac{\dot{h}^2}{2h}-\left(\frac{\ddot{z}}{\dot{z}}-\frac{\dot{z}}{z}\right)\dot{h}\right]\right\}, \tag{3.9}$$

where dots represent derivatives with respect to x, i.e., $\dot{z}=dz/dx$, $\ddot{z}=d^2z/dx^2$, etc. In order to eliminate the term containing the first derivative we require

$$\frac{\dot{h}}{h}-\frac{\ddot{z}}{\dot{z}}+\frac{\dot{z}}{z}=0. \tag{3.10}$$

The solution to this equation is given by

$$h=\dot{z}z^{-1}. \tag{3.11}$$

(Since h must be positive we require that $\dot{z}>0$.) Substituting Eq. (3.11) into Eq. (3.9), one gets

$$C=\frac{4z(1-z)^2}{\dot{z}^2}\left[\frac{\partial^2}{\partial x^2}+\frac{\dot{z}^2}{4z^2}\left(\frac{\partial^2}{\partial\alpha^2}-2\frac{1+z}{1-z}\frac{\partial^2}{\partial\alpha\partial\beta}+\frac{\partial^2}{\partial\beta^2}+1\right)+\frac{1}{2}\frac{\dddot{z}}{\dot{z}}-\frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right]. \tag{3.12}$$

Thus, the principal series of SO(2,2) in SO(2)×SO(2) basis can be realized in the Hilbert space spanned by eigenfunctions of C, A_3, and B_3.

Let $\mathcal{H}^{(1)}_{mk}$ be a one-dimensional subspace spanned by $f^{(1)}_{mk}$ with fixed m and k. Then the Casimir operator restricted to $\mathcal{H}^{(1)}_{mk}$ becomes a differential operator in x alone; it is found that

$$C_{mk}=\frac{4z(1-z)^2}{\dot{z}^2}\left[\frac{\partial^2}{\partial x^2}+\dot{z}^2\frac{(1-z)+2mk(1+z)+(1-m^2-k^2)(1-z)}{4z^2(1-z)}+\frac{1}{2}\frac{\dddot{z}}{\dot{z}}-\frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right], \tag{3.13}$$

where C_{mk} denote the restriction of C to $\mathcal{H}^{(1)}_{mk}$. Then it is not difficult to see that a class of Natanzon hypergeometric potentials[1]

$$V(x)=-\frac{d^2}{dx^2}+\frac{fz(z-1)+h_o(1-z)+h_1z+1}{R}$$
$$+\left(a+\frac{a+(c_1-c_o)(2z-1)}{z(z-1)}-\frac{5\Delta}{4R}\right)\frac{z^2(1-z)^2}{R^2}, \tag{3.14}$$

which are defined in terms of six parameters f, h_o, h_1, a, c_o, c_1 and a function $z(x)$ satisfying

$$\dot{z}^2=\frac{4z^2(1-z)^2}{R(z)}, \tag{3.15}$$

where $\Delta=c_1^2-4c_oc_1$, $R(z)=a(z-1)z+c_o(1-z)+c_1z$, are related to C_{mk} as

$$(C_{mk}+\rho^2+1)=-\frac{4z(1-z)^2}{\dot{z}^2}(H-E),\quad H=-\frac{d^2}{dx^2}+V(x) \tag{3.16}$$

provided

$$1-(m+k)^2=aE-f,$$

$$1-(m-k)^2=c_0E-h_0, \tag{3.17}$$

$$1+\rho^2=c_1E-h_1.$$

(For details see Refs. 5 and 27.)

As a consequence, one find exactly solvable Hamiltonians (3.14) which have a ''broken symmetry'' in the sense that $H\neq f(C)|_{\mathcal{H}^{(1)}_{mk}}$. However, the Hamiltonians (3.14) have another kind of algebraic structure. It follows from (3.16) that

$$(C+\rho^2+1)|_{\mathcal{H}^{1}_{mk}}=Q(x)(H-E) \tag{3.18}$$

with m, k, and ρ given by (3.17) and

$$Q(x)=-\frac{4z(1-z)^2}{\dot{z}^2}. \tag{3.19}$$

Thus, the wave function of the Natanzon hypergeometric potential is related to the basis function $f^{(1)}_{mk}(\xi)$, while the S-matrix is (up to a ρ-dependent phase factor)

$$S=\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+k\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+k\right)} \tag{3.20}$$

(see Eq. (A17) of Ref. 23) where m, k, and ρ are given by (3.17). Moreover, from (A3), (A10), (3.11), and (3.7) follows that

$$f^{(1)}_{mk}(\xi)=\exp(im\alpha+ik\beta)\sqrt{\frac{z}{\dot{z}}}\int_0^{2\pi}\int_0^{2\pi}\left|\frac{\cos\frac{\theta+\varphi}{2}}{\sqrt{1-z}}-\frac{\sqrt{z}\cos\frac{\theta-\varphi}{2}}{\sqrt{1-z}}\right|^{-2-j} e^{im\varphi+ik\theta}d\varphi d\theta, \tag{3.21}$$

where $j=-1-i\rho$. Hence for the wave functions of the Natanzon potentials given in (3.14) we have

$$\Psi(x)\propto(\dot{z})^{-(1/2)}z^{(1+m-k)/2}(1-z)^{(2+j)/2}\,{}_2F_1\left(1+\frac{j}{2}-k,1+\frac{j}{2}+m;1+m-k;z\right), \tag{3.22}$$

where ${}_2F_1$ is the hypergeometric function.[28]

IV. CLASS OF POTENTIALS RELATED TO SO(2,2)⊃SO(2)⊗E(1) REDUCTION

Now, the reduction conditions are

$$A_3f^{(2)}_{m\lambda}=mf^{(2)}_{m\lambda}, \quad (B_2+B_3)f^{(2)}_{m\lambda}=\lambda f^{(2)}_{m\lambda}.$$

Hence we require the quasi-invariant measure $d\mu$ to be invariant under the transformations

$$\exp(a_3\varphi)=\begin{pmatrix} \cos\frac{\varphi}{2} & \sin\frac{\varphi}{2} & 0 & 0 \\ -\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} & 0 & 0 \\ 0 & 0 & \cos\frac{\varphi}{2} & -\sin\frac{\varphi}{2} \\ 0 & 0 & \sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} \end{pmatrix} \in \mathrm{SO}(2) \tag{4.1}$$

and

$$\exp[(b_2+b_3)t]=\begin{pmatrix} 1 & \frac{t}{2} & 0 & \frac{t}{2} \\ -\frac{t}{2} & 1 & \frac{t}{2} & 0 \\ 0 & \frac{t}{2} & 1 & \frac{t}{2} \\ \frac{t}{2} & 0 & -\frac{t}{2} & 1 \end{pmatrix} \in E(1). \tag{4.2}$$

According to this, we put $d\mu=h(r)d\xi$, where now $r=(\xi_1+\xi_3)^2+(\xi_2-\xi_4)^2$. As a check, one can immediately verify that such defined r is indeed invariant under the transformations given by (4.1) and (4.2). Then

$$2A_3=-i\left(\xi_4\frac{\partial}{\partial\xi_3}-\xi_2\frac{\partial}{\partial\xi_1}+\xi_1\frac{\partial}{\partial\xi_2}\right) \tag{4.3}$$

and

$$2(B_2+B_3)=-i\left[(\xi_4-\xi_2)\frac{\partial}{\partial\xi_1}+(\xi_3+\xi_1)\frac{\partial}{\partial\xi_2}+(\xi_2-\xi_4)\frac{\partial}{\partial\xi_3}\right]. \tag{4.4}$$

Since A_3 and B_2+B_3 are sought to be diagonal we introduce in place of ξ_1, ξ_2, ξ_3 the new variables x,φ,t by

$$\begin{aligned} \xi_1&=\frac{1+z}{2\sqrt{z}}\cos\frac{\varphi}{2}-\frac{t}{2\sqrt{z}}\sin\frac{\varphi}{2}, \\ \xi_2&=\frac{1+z}{2\sqrt{z}}\sin\frac{\varphi}{2}+\frac{t}{2\sqrt{z}}\cos\frac{\varphi}{2}, \\ \xi_3&=\frac{1-z}{2\sqrt{z}}\cos\frac{\varphi}{2}+\frac{t}{2\sqrt{z}}\sin\frac{\varphi}{2}, \end{aligned} \tag{4.5}$$

with $0\leqslant x<\infty$, $0<\varphi<2\pi$, $-\infty<t<\infty$, where $z(x)$ is a differentiable function on R^+ with values in $[0,1]$. Then $A_3=-i(\partial/\partial\varphi)$, $B_2+B_3=-i(\partial/\partial t)$, while

$$C=\frac{4z^2}{\dot{z}^2}\left\{\frac{\partial^2}{\partial x^2}+\left(\frac{\dot{h}}{h}-\frac{\ddot{z}}{\dot{z}}\right)\frac{\partial}{\partial x}+\dot{z}^2\left(\frac{\partial^2}{\partial t^2}-\frac{2}{z}\frac{\partial^2}{\partial\varphi\partial t}\right)+\frac{\dot{h}}{2h}\left[\frac{\ddot{h}}{\dot{h}}-\frac{\dot{h}}{2h}-\frac{\ddot{z}}{\dot{z}}\right]\right\}. \tag{4.6}$$

We now require

$$\frac{\dot{h}}{h}-\frac{\ddot{z}}{\dot{z}}=0,$$

which yields

$$h=-\dot{z}. \tag{4.7}$$

(Since h must be positive we require that $\dot{z}<0$.) Putting Eq. (4.7) into Eq. (4.6), one gets

$$C=\frac{4z^2}{\dot{z}^2}\left[\frac{\partial^2}{\partial x^2}+\dot{z}^2\left(\frac{\partial^2}{\partial t^2}-\frac{2}{z}\frac{\partial^2}{\partial\varphi\partial t}\right)+\frac{1}{2}\frac{\dddot{z}}{\dot{z}}-\frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right]. \tag{4.8}$$

Denote by $C_{m\lambda}$ a restriction of C on the one-dimensional subspace $\mathcal{H}^{(2)}_{m\lambda}$ spanned by $f^{(2)}_{m\lambda}$ with fixed m and λ,

$$C_{m\lambda}=\frac{4z^2}{\dot{z}^2}\left[\frac{\partial^2}{\partial x^2}-\dot{z}^2\left(\lambda^2-\frac{2m\lambda}{z}\right)+\frac{1}{2}\frac{\dddot{z}}{\dot{z}}-\frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right]. \tag{4.9}$$

Before proceeding further, note from (4.9) that $C_{m\lambda}$ is the Schrödinger-type if

$$\frac{z^2}{\dot{z}^2}=1.$$

The solution to this equation is given by

$$z=\exp(-x),\quad 0\leqslant x<\infty.$$

If we compute $C_{m\lambda}$ for this z, it becomes

$$C_{m\lambda}=4\frac{d^2}{dx^2}-4\lambda^2\exp(-2x)+8m\lambda\exp(-x)-1.$$

Hence the Hamiltonian

$$H=-\frac{d^2}{dx^2}+\lambda^2\exp(-2x)-2m\lambda\exp(-x)$$

is related to the Casimir operator as

$$H=-\tfrac{1}{4}(C+1)\big|_{\mathcal{H}^{(2)}_{m\lambda}}.$$

(We are using units with $2M=\hbar=1$.) Thus, the Mors Hamiltonian[29] has the SO(2,2) potential group structure; the scattering states that have the same energy but belong to different potential strengths are related to the UIR of the principal series of SO(2,2). However for a class of Hamiltonians the relation (2.7) can be satisfied by a proper choice of m, λ, and ρ as a function of the energy. It is not difficult to see that for Hamiltonians

$$H=-\frac{d^2}{dx^2}+\frac{g_2z^2+g_1z+h_o+1}{R}+\left(\frac{\sigma_1}{z}-\sigma_2-\frac{5\Delta}{R}\right)\frac{z^2}{R^2}, \tag{4.10}$$

where $R(z)=\sigma_2 z^2+\sigma_1 z+c_o$, $\Delta=\sigma_1^2-4\sigma_2 c_o$ and $z(x)$ satisfies

$$\dot{z}^2=\frac{4z^2}{R(z)} \tag{4.11}$$

the following relation holds:

$$C_{m\lambda}+\rho^2+1=-\frac{4z^2}{\dot{z}^2}(H-E), \tag{4.12}$$

provided

$$-8m\lambda=g_1-\sigma_1 E, \quad 4\lambda^2=g_2-\sigma_2 E, \quad 1+\rho^2=c_o E-h_o. \tag{4.13}$$

The interaction potentials given in (4.10) are Natanzon confluent potentials[1] which depends on six parameters h_o, c_o, g_1, σ_1, g_2, and σ_2. [In (4.10) we closely following the notation of Ref. 1.]

Thus, Natanzon confluent potentials in (4.11) are associated with the reduction into $\mathfrak{so}(2)\oplus\mathfrak{e}(1)$ in the sense that

$$(C+\rho^2+1)|_{\mathcal{H}^{(2)}_{m\lambda}}=Q(x)(H-E), \tag{4.14}$$

where

$$Q(x)=-\frac{4z^2}{\dot{z}^2}. \tag{4.15}$$

Hence S-matrices for these potentials are (up to a ρ-dependent phase factor)

$$S=|\lambda|^{-i\rho}\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)} \tag{4.16}$$

(see Eq. (A22) of Ref. 23). Moreover, it follows from (A3), (A16), (4.7), and (4.5) that

$$\Psi(x)\propto\sqrt{\dot{z}}\int_0^{2\pi}\int_{-\infty}^{\infty}\left|\sqrt{z}\cos\frac{\varphi}{2}-\frac{t}{\sqrt{z}}\sin\frac{\varphi}{2}\right|^{-2-j}e^{im\varphi+i\lambda t}d\varphi dt. \tag{4.17}$$

Hence, for the scattering solutions we have

$$\Psi(x)\propto\begin{cases}\dfrac{1}{\sqrt{\dot{z}}}W_{m,-(1+j)/2}(2z\lambda), & \text{if} \quad \lambda>0\\[2ex] \dfrac{1}{\sqrt{\dot{z}}}W_{-m,-(1+j)/2}(-2z\lambda), & \text{if} \quad \lambda<0,\end{cases} \tag{4.18}$$

where $W_{mn}(z)$ is the Whittaker function.[28]

It is also worth mentioning that the solution to the condition $Q=\text{const}$ is $\sigma_1=\sigma_2=0$. This gives rise to the Morse potential, which was already known to possess SO(2,2) as the potential group.

V. CLASS OF POTENTIALS RELATED TO SO(2,2)⊃SO(1,1)⊗SO(2) REDUCTION

The basis functions corresponding to the considered reduction are the eigenfunctions of C, A_1, and B_3, with

$$A_1 f^{(3)}_{m\nu\tau} = \nu f^{(3)}_{m\nu\tau}, \quad B_3 f^{(3)}_{m\nu\tau} = m f^{(3)}_{m\nu\tau}, \tag{5.1}$$

where $\tau = \pm 1$ is the multiplicity label. We now choose the quasi-invariant measure in (2.9) as $d\mu = h(r)d\xi$, with $r = \xi_1\xi_4 - \xi_2\xi_3$. Such a defined measure is invariant under the transformations given by

$$\exp(a_1 t) = \begin{pmatrix} \cosh\frac{t}{2} & 0 & \sinh\frac{t}{2} & 0 \\ 0 & \cosh\frac{t}{2} & 0 & \sinh\frac{t}{2} \\ \sinh\frac{t}{2} & 0 & \cosh\frac{t}{2} & 0 \\ 0 & \sinh\frac{t}{2} & 0 & \cosh\frac{t}{2} \end{pmatrix} \in \mathrm{SO}(1,1) \tag{5.2}$$

and

$$\exp(b_3 \varphi) = \begin{pmatrix} \cos\frac{\varphi}{2} & \sin\frac{\varphi}{2} & 0 & 0 \\ -\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} & 0 & 0 \\ 0 & 0 & \cos\frac{\varphi}{2} & \sin\frac{\varphi}{2} \\ 0 & 0 & -\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} \end{pmatrix} \in \mathrm{SO}(2). \tag{5.3}$$

Then

$$2A_1 = -i\left(\xi_3 \frac{\partial}{\partial \xi_1} + \xi_4 \frac{\partial}{\partial \xi_2} + \xi_1 \frac{\partial}{\partial \xi_3} \right), \tag{5.4}$$

and

$$2B_3 = -i\left(\xi_2 \frac{\partial}{\partial \xi_1} - \xi_1 \frac{\partial}{\partial \xi_2} + \xi_4 \frac{\partial}{\partial \xi_3} \right). \tag{5.5}$$

The parametrization that we see for hyperboloid (2.8) must be such as to make A_1, B_3, particularly simple

$$x_1=\frac{1}{\sqrt{1-z^2}}\cosh\frac{t}{2}\cos\frac{\varphi}{2}-\frac{z}{\sqrt{1-z^2}}\sinh\frac{t}{2}\sin\frac{\varphi}{2},$$

$$x_2=\frac{1}{\sqrt{1-z^2}}\sinh\frac{t}{2}\cos\frac{\varphi}{2}+\frac{z}{\sqrt{1-z^2}}\cosh\frac{t}{2}\sin\frac{\varphi}{2}, \tag{5.6}$$

$$x_3=\frac{1}{\sqrt{1-z^2}}\sinh\frac{t}{2}\cos\frac{\varphi}{2}-\frac{z}{\sqrt{1-z^2}}\cosh\frac{t}{2}\sin\frac{\varphi}{2}.$$

Then

$$A_1=-i\frac{\partial}{\partial t},\quad B_3=-i\frac{\partial}{\partial\varphi}, \tag{5.7}$$

while

$$C=\frac{(1-z^2)^2}{\dot z^2}\left\{\frac{\partial^2}{\partial x^2}+\left(\frac{\dot h}{h}-\frac{\ddot z}{\dot z}+\frac{2\dot z z}{1+z^2}\right)\frac{\partial}{\partial x}+\frac{4\dot z^2}{(1+z^2)^2}\left(\frac{\partial^2}{\partial t^2}-\frac{4z}{1-z^2}\frac{\partial^2}{\partial\varphi\partial t}-\frac{\partial^2}{\partial\varphi^2}\right)\right.$$
$$\left.+\frac{\dot h}{2h}\left[\frac{\ddot h}{\dot h}-\frac{\dot h}{2h}-\left(\frac{\ddot z}{\dot z}-\frac{2\dot z z}{1+z^2}\right)\right]\right\}. \tag{5.8}$$

Since we want the first derivative to vanish, we require

$$\frac{\dot h}{h}-\frac{\ddot z}{\dot z}+\frac{2\dot z z}{1+z^2}=0. \tag{5.9}$$

Hence the function h must be chosen to be

$$h=\frac{\dot z}{1+z^2}. \tag{5.10}$$

Substituting (5.10) into (5.8), one gets

$$C=\frac{(1-z^2)^2}{\dot z^2}\left\{\frac{\partial^2}{\partial x^2}+\frac{4\dot z^2}{(1+z^2)^2}\left(\frac{\partial^2}{\partial t^2}-\frac{4z}{1-z^2}\frac{\partial^2}{\partial\varphi\partial t}-\frac{\partial^2}{\partial\varphi^2}\right)-\frac{\dot z^2}{(1+z^2)^2}+\frac{1}{2}\frac{\dddot z}{\dot z}-\frac{3}{4}\left(\frac{\ddot z}{\dot z}\right)^2\right\}. \tag{5.11}$$

The restriction of C to a subspace $\mathcal{H}^{(3)}_{m\nu}$ spanned by $f^{(3)}_{m\nu\tau}, \tau=\pm1$, for given m and ν yields the differential operator $C_{m\nu}$,

$$C_{m\nu}=\frac{(1-z^2)^2}{\dot z^2}\left\{\frac{\partial^2}{\partial x^2}-\frac{\dot z^2}{(1+z^2)^2}\left(1+4\nu^2-4m^2-\frac{16zm\nu}{1-z^2}\right)+\frac{1}{2}\frac{\dddot z}{\dot z}-\frac{3}{4}\left(\frac{\ddot z}{\dot z}\right)^2\right\}. \tag{5.12}$$

Because of (2.7) we put

$$1+\nu^2-m^2=a_1E+b_1,$$

$$1+\rho^2/4=a_2E+b_2, \tag{5.13}$$

$$2m\nu=a_3E+b_3.$$

Then it is not difficult to see that the systems governed by Hamiltonians

$$H=-\frac{d^2}{dx^2}+\frac{(b_1-1)(1-v^2)-b_3v\sqrt{1-v^2}-b_2+5/4}{R}$$
$$+\frac{1}{2}\left(a_1-2a_2-\frac{a_2}{2(1-v^2)}-\frac{5\Delta}{8R}\right)\frac{(1-v^2)}{R^2}, \tag{5.14}$$

where $\Delta=a_3^2+4a_2(a_1-a_2)$, are related to SO(2,2) in the sense that

$$\left(C_{m\nu}+\rho^2+\frac{1}{4}\right)=-\frac{4(1-v^2)^2}{\dot{v}^2}[H-E] \tag{5.15}$$

provided

$$\dot{v}^2=\frac{(1-v^2)^2}{R}, \tag{5.16}$$

where $R=a_3v\sqrt{1-v^2}+a_1v^2+(a_2-a_1)$. To simplify notation we have put

$$v=\frac{2z}{(1+z^2)}. \tag{5.17}$$

Moreover, for the scattering solutions we have

$$\Psi_{\pm}(x)\propto\frac{(1-v^2)^{1/4}}{\sqrt{\dot{v}}}\mathfrak{Q}^{j/2+1}_{\pm i\nu,m}\left(\frac{\pm iv}{\sqrt{1-v^2}}\right), \tag{5.18}$$

where $\mathfrak{Q}^{j}_{m,n}(z)$ is the generalized Legendre function of the second kind as defined by Azimov.[30] The solution Ψ_+ describes waves incident from the left while Ψ_- describes waves that are incident from the right.

It should be noted that the potential functions of this class admit a double degeneracy of the wave function for every positive value of energy. The main reason for this is the fact that each UIR of SO(1,1) is twofold degenerate in principal series of UIR of SO(2,1). The scattering matrices can now be obtained as restriction of the intertwining operator onto $\mathcal{H}^{(3)}_{m\nu}$,

$$S=\begin{pmatrix}R & T\\ T & R\end{pmatrix}, \tag{5.19}$$

where

$$R=\frac{1}{\pi}\cosh\pi\nu\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\nu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\nu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)},$$

$$T=\frac{-i}{\pi}\sinh\frac{\pi\rho}{2}\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\nu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\nu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)}$$

(see Eq. (A27) of Ref. 23). According to this, the reflection and transmission coefficients are

$$|R|^2=\frac{\cosh^2\pi\nu}{\cosh^2\pi\nu+\sinh^2\pi\rho},\quad |T|^2=\frac{\sinh^2\pi\rho}{\cosh^2\pi\nu+\sinh^2\pi\rho}.$$

This class of solvable potentials includes as special cases important families of Ginocchio potentials.[2] Indeed, putting

$$a_1=\frac{1}{\gamma^4}-\frac{1}{\gamma^2},\ a_2=\frac{1}{\gamma^4},\ a_3=0,\ b_1=\delta(\delta+1)+\frac{3}{4},\ b_2=1,\ b_3=0$$

with $0<\gamma\leqslant 1$ and introducing Ginocchio's variable y

$$y=\frac{v}{\sqrt{v^2+\gamma^2(1-v^2)}} \tag{5.20}$$

we have

$$H=-\frac{d^2}{dx^2}+\gamma^2\delta(\delta+1)(1-y^2)+\frac{(1-y^2)(1-\gamma^2)}{4}[2-y^2(7-\gamma^2)+5(1-\gamma^2)y^4]. \tag{5.21}$$

Moreover, it follows from (5.16) and (5.20) that

$$\frac{dy}{dx}=(1-y^2)[1-(1-\gamma^2)y^2]. \tag{5.22}$$

We also mention that in the special case of $\gamma=1$ the Hamiltonian (5.21) reduces to the Pöschl–Teller Hamiltonian,[31]

$$H=-\frac{d^2}{dx^2}+\frac{\delta(\delta+1)}{\cosh^2 x}.$$

Observe that in this case $Q(x)=-4$. Moreover the solution to the condition $Q=\text{const}$ gives rise to the Scarf potential ($a_1=a_3=0$).[32]

VI. CONCLUSION

In this paper we have shown how the group theory can be used to obtain a class of one-dimensional Hamiltonians related to SO(2,2) in the sense of (2.7) and to solve the scattering problems. Using the quasiregular representation with any quasi-invariant measure, it was possible to treat a more general class of Natanzon potentials. We have seen how all the Natanzon potentials can quite easily be extracted from the Casimir operator. The relationship between the Hamiltonian and Casimir operators on the one hand and the scattering and intertwining operators on the other enabled us to write down an explicit expression for wave functions and scattering matrices for the systems under consideration. We have only considered $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(2)$, $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes E(1)$, and $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$ reductions but in a manner amenable to be immediately extended to other subgroup reductions.

Finally we note that the scattering problems related to the reductions $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$, $\mathrm{SO}(2,2)\supset E(1)\otimes\mathrm{SO}(1,1)$ and $\mathrm{SO}(2,2)\supset\mathrm{SO}(2,1)$ are somewhat more complicated than the one related to $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(2)$, $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes E(1)$ and $\mathrm{SO}(2,2)\supset E(1)\otimes E(1)$ reductions since the S-matrix in the former case is a unitary 2×2 matrix while in the latter it is a complex number of unit modulus. The reason for this is the fact that the subgroups SO(1,1) and SO(2,1) are degenerate in the principal series of SO(2,2).

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APPENDIX: THE BASIS FUNCTIONS OF THE PRINCIPAL SERIES REPRESENTATIONS ASSOCIATED WITH THE HYPERBOLOID

In this appendix we will give the integral representation for the basis functions of the most degenerate principal series representations induced by (2.9) which are related to the wave functions of the systems under consideration. The procedure will go as follows. We shall start with the most degenerate principal series representations of SO(2,2) associated with the cone.[24] For such realization of the principal series the basis functions have particularly simple form. Then the interrelation between two alternative realizations of the principal series allows us to obtain the integral representation mentioned above.

Since the representations (2.8) with different measure are unitarily equivalent we can, without loss of generality, put $d\mu(\xi)=d\xi$, where $d\xi=d\xi_1 d\xi_2 d\xi_3/|\xi_4|$ is an invariant measure on Ξ. In this case the Radon–Nikodym derivative equals to one and the representation, call it $\check{T}$, has the simple form

$$\check{T}(g)\check{f}(\xi)=\check{f}(\xi g) \tag{A1}$$

with inner product

$$(\check{f},\check{f}')=\int \overline{\check{f}(\xi)}\check{f}'(\xi)d\xi. \tag{A2}$$

Such defined quasiregular representation of course is unitarily equivalent to (2.9). The unitary mapping W which realizes the equivalence is given by

$$W: f\to\check{f}=h^{1/2}f. \tag{A3}$$

The principal series of most degenerate representation of SO(2,2) characterized by the pair $\chi=(\rho,\varepsilon)$, where ε is equal to 0 or 1, while $0\leqslant\rho<\infty$ can be realized in the space of infinitely differentiable functions $F(\zeta)$ on the cone $B=\{\zeta:\zeta\in R^{2,2},\ \zeta_1^2+\zeta_2^2-\zeta_3^2-\zeta_4^2=0\}$, homogeneous of degree $j=-1-i\rho$ and with parity ε

$$F(a\zeta)=|a|^j \operatorname{sign}^{\varepsilon} a F(\zeta). \tag{A4}$$

A representation operator U^χ is defined by

$$U^\chi(g)F(\zeta)=F(\zeta g). \tag{A5}$$

It is worth mentioning that the homogeneous functions on the cone are uniquely determined by their values on any contour Γ intersecting each generator at one point. Hence, U^χ can be realized in spaces of functions on these contours.

The interrelation between $U^\chi,\chi=(\rho,0)$, and the principal series representation induced by (A1) are given by integral transform[24,25]

$$\check{f}(\xi)=\int_\Gamma |[\xi,n]|^{-2-j}F(n)dn\equiv(IF)(\xi), \tag{A6}$$

where $[\cdot,\cdot]$ is given by (2.1) and Γ is arbitrary contour on the cone B which intersects every generator once; and dn is a quasi-invariant measure on Γ. Moreover the following intertwining relation is held:

$$IU=\check{T}I. \tag{A7}$$

Thus, Eq. (A6) allows us to obtain the integral representation for the basis functions of the principal series representations induced by (A1).

(i) The $SO(2,2)\supset SO(2)\times SO(2)$ reduction. According to this we introduce the spherical coordinate systems on the cone

$$\zeta=\omega n,\quad n=\left(\cos\frac{\psi+\varphi}{2},\ \sin\frac{\psi+\varphi}{2},\ \cos\frac{\psi-\varphi}{2},\ \sin\frac{\psi-\varphi}{2}\right),\tag{A8}$$

with $0\leqslant\omega<\infty$, $0<\psi\leqslant 2\pi$, $0<\varphi\leqslant 2\pi$. It follows from (A4) that the functions $F(\zeta)$ is uniquely determined by its values on the direct product of two circles Γ_S,

$$\Gamma_S=\left\{n:n\in B,n=\left(\cos\frac{\psi+\varphi}{2},\ \sin\frac{\psi+\varphi}{2},\ \cos\frac{\psi-\varphi}{2},\ \sin\frac{\psi-\varphi}{2}\right)\right\}.$$

Then

$$U^{\chi}(g)F(n)=(\omega_g)^j F(n_g),\tag{A9}$$

where ω_g and n_g are determined from parametrization (A5) of ng, i.e., from $ng=\omega_g n_g$. The Casimir $\acute{C}$ operator of the representation (A9) is identically a multiple of the unit $\acute{C}\equiv-\rho^2-\frac{1}{4}$, while $\acute{A}_3=-i(\partial/\partial\varphi)$, $\acute{B}_3=-i(\partial/\partial\psi)$. Therefore, the basis functions of (A9) in $SO(2,2)\supset SO(2)\times SO(2)$ reduction are $F^{(1)}_{mk}(n)=\exp(im\varphi+ik\psi)$. Then, due to (A6), we come to the following integral representation for the basis functions of the principal series representations induced by (A1),

$$\check{f}^{(1)}_{mk}(\xi)=\int_0^{2\pi}\left|\xi_1\cos\frac{\psi+\varphi}{2}+\xi_2\sin\frac{\psi+\varphi}{2}-\xi_3\cos\frac{\psi-\varphi}{2}-\xi_4\sin\frac{\psi-\varphi}{2}\right|^{-1-j}$$
$$\times\exp(im\varphi+ik\psi)d\varphi d\psi,\tag{A10}$$

where the upper index 1 refers to the $SO(2,2)\supset SO(2)\times SO(2)$ reduction. It is not difficult to see that the basis functions $\check{f}^{(1)}_{mk}$ are indeed the eigenfunctions of the set of commuting operators $\check{C}$, $\check{A}_3$, and $\check{B}_3$,

$$\check{C}\check{f}^{(1)}_{mk}=j(j+2)\check{f}^{(1)}_{mk},\quad \check{A}_3\check{f}^{(1)}_{mk}=m\check{f}^{(1)}_{mk},\quad \check{B}_3\check{f}^{(1)}_{mk}=k\check{f}^{(1)}_{mk},\tag{A11}$$

where

$$\check{C}=-\frac{\partial^2}{\partial\xi_1^2}-\frac{\partial^2}{\partial\xi_2^2}+\frac{\partial^2}{\partial\xi_3^2}+I(I+2),\quad I=\xi_1\frac{\partial}{\partial\xi_1}+\xi_2\frac{\partial}{\partial\xi_2}+\xi_3\frac{\partial}{\partial\xi_3},\tag{A12}$$

and

$$2\check{A}_3=-i\left(\xi_3\frac{\partial}{\partial\xi_1}+\xi_4\frac{\partial}{\partial\xi_2}+\xi_1\frac{\partial}{\partial\xi_3}\right),\quad 2\check{B}_3=-i\left(\xi_2\frac{\partial}{\partial\xi_1}-\xi_1\frac{\partial}{\partial\xi_2}+\xi_4\frac{\partial}{\partial\xi_3}\right).\tag{A13}$$

(ii) The reduction $SO(2,2)\supset SO(2)\times E(1)$. According to this, we introduce new coordinates on cone as follows:

$$\zeta=\omega n,n=\left(\cos\frac{\varphi}{2}-t\sin\frac{\varphi}{2},\ \sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2},\ \cos\frac{\varphi}{2}+t\sin\frac{\varphi}{2},\ -\sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2}\right),\tag{A14}$$

where $0\leqslant\omega<\infty$, $0<\varphi\leqslant 2\pi$, $-\infty<t<\infty$. Then the infinitesimal operators $\acute{A}_3$ and $\acute{B}_2+\acute{B}_3$ have the forms

$$\acute{A}_3=-i\frac{\partial}{\partial\varphi},\quad \acute{B}_2+\acute{B}_3=-i\frac{\partial}{\partial t}. \tag{A15}$$

By arguments very similar to those used to obtain (A10) we can show that

$$\check{f}^{(2)}_{m\lambda}(\xi)=\int_{-\infty}^{\infty}\int_0^{2\pi}\left|\xi_1\left(\cos\frac{\varphi}{2}-t\sin\frac{\varphi}{2}\right)+\xi_2\left(\sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2}\right)-\left(\xi_3\cos\frac{\varphi}{2}+t\sin\frac{\varphi}{2}\right)\right.$$
$$\left.-\xi_4\left(-\sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2}\right)\right|^{-1-j}e^{im\varphi}e^{i\lambda t}d\varphi dt, \tag{A16}$$

where the upper index 2 refers to the $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\times E(1)$ reduction. We note that

$$\check{C}\check{f}^{(2)}_{m\lambda}=j(j+2)\check{f}^{(2)}_{m\lambda},\quad \check{A}_3\check{f}^{(2)}_{m\lambda}=m\check{f}^{(2)}_{m\lambda},\quad (\check{B}_2+\check{B}_3)\check{f}^{(2)}_{m\lambda}=\lambda\check{f}^{(2)}_{m\lambda}, \tag{A17}$$

where

$$2\check{A}_3=-i\left(\xi_4\frac{\partial}{\partial\xi_3}-\xi_2\frac{\partial}{\partial\xi_1}+\xi_1\frac{\partial}{\partial\xi_2}\right),$$

$$2(\check{B}_2+\check{B}_3)=-i\left[(\xi_4-\xi_2)\frac{\partial}{\partial\xi_1}+(\xi_3+\xi_1)\frac{\partial}{\partial\xi_2}+(\xi_2-\xi_4)\frac{\partial}{\partial\xi_3}\right]$$

and $\check{C}$ is given by (A12).

(iii) The $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\times\mathrm{SO}(1,1)$ reduction. This case is somewhat more complicated than the previous one. We find that the parametrization $\zeta=\omega n$, $\omega>0$ covers only with two choices of n,

$$n^{\tau}=\left(\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}-\tau\sinh\frac{\beta}{2}\sin\frac{\varphi}{2},\ \tau\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}+\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}\right.$$
$$\left.-\tau\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},\ \tau\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}+\sinh\frac{\beta}{2}\sin\frac{\varphi}{2}\right),$$

$$\tau=\pm1,\ -\infty<\beta<\infty,0<\varphi\leqslant2\pi, \tag{A18}$$

while the expressions for $\acute{A}_1$ and $\acute{B}_3$ are given in both regions by $\acute{A}_1=-i(\partial/\partial\beta)$ and $\acute{B}_3=-i(\partial/\partial\varphi)$. Hence, we have the following integral representation for the basis functions corresponding to $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\times\mathrm{SO}(1,1)$ reduction:

$$\check{f}^{(3)}_{m\nu\tau}=\int_{-\infty}^{\infty}\int_0^{2\pi}|[\xi,n^{\tau}]|^{-2-j}\exp(im\varphi)\exp(i\nu\beta)d\varphi d\beta, \tag{A19}$$

where $\tau=\pm1$ is the multiplicity label and n^{τ} is given by (A18). Indeed, the functions $\check{f}^{(3)}_{m\nu\tau}$ are eigenfunctions of the set of commuting operators $\check{C}$, $\check{A}_1$, and $\check{B}_3$,

$$\check{C}f^{(3)}_{m\nu\tau}=j(j+2)f^{(3)}_{m\nu\tau},\quad \check{A}_1f^{(3)}_{m\nu\tau}=\nu f^{(3)}_{m\nu\tau},\quad \check{B}_3f^{(3)}_{m\nu\tau}=mf^{(3)}_{m\nu\tau}, \tag{A20}$$

where

$$2\check{A}_1 = -i\left(\xi_3\frac{\partial}{\partial\xi_1}+\xi_4\frac{\partial}{\partial\xi_2}+\xi_1\frac{\partial}{\partial\xi_3}\right),$$

$$2\check{B}_3 = -i\left(\xi_2\frac{\partial}{\partial\xi_1}-\xi_1\frac{\partial}{\partial\xi_2}+\xi_4\frac{\partial}{\partial\xi_3}\right),$$

and $\check{C}$ is given by (A12).

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Spectral properties of a short-range impurity in a quantum dot

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The spectral properties of the quantum mechanical system consisting of a quantum dot with a short-range attractive impurity inside the dot are studied in the zero-range limit. The Green function of the system is obtained in an explicit form. In the case of a spherically symmetric quantum dot, the dependence of the spectrum on the impurity position and strength of the impurity potential is analyzed in detail. The recovering of the confinement potential of the dot from the spectroscopy data is proven; the consequences of the hidden symmetry breaking by the impurity are considered. The effect of the positional disorder is analyzed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1647693]

I. INTRODUCTION

Quantum dots (i.e., nanostructures with charge carriers confinement in all spatial directions) have an atom-like energy spectrum and, therefore, make possible to fabricate quantum devices with energy level spacing much greater than the temperature smearing kT at work temperature T (see, e.g., Ref. 1). Moreover, dimension and shape of a quantum dot affect considerably the most important characteristics of the corresponding devices: Relaxation and recombination time, Auger recombination coefficient etc, thus a possibility arises to control such characteristics in manufacturing the devices.[2–4] Another way to control the properties of a quantum dot is instilling an impurity into the dot. Therefore, the investigation of spectral properties of a quantum dot with impurities as well as the dependence of the spectrum on the geometric parameters of the dot and physical characteristics of the impurity is an important problem of nano- and mesoscopic physics (see, e.g., in Refs. 5–7, and references therein). The case of a hydrogen-like impurity is one of the most extensively studied up to now; however, the spectral problem in this case has no exact solution. On the other hand, short-range impurities can be investigated in the framework of the point potential theory (also called the zero-range potential theory). An important peculiarity of the point potential method is that the spectral problem for a point perturbed Hamiltonian is explicitly soluble as soon as the Green function for the unperturbed operator is known in an explicit form.[8,9]

For modeling the geometric confinement of a quantum dot, quadratic (in other words, parabolic) potentials are successfully used[10] (see also examples of applications in Refs. 5–7, 11–15). The reason is that the self-consistent solution to the corresponding system of the Poisson and Schrödinger equations leads to the confinement potential having the form of a truncated parabolic potential.[16] Moreover, the Green function of the corresponding Hamiltonian $\hat{H}^0$,

$$\hat{H}^0 = -\frac{\hbar^2}{2\mu}\Delta + \frac{\mu\Omega^2}{2}r^2, \tag{1}$$

can be explicitly calculated[17–19] (here Ω is the frequency of the oscillator, μ denotes over the

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paper the mass of the considered charged particle). This makes possible to perform an exhaustive spectral analysis of the perturbation of $\hat{H}^0$ by a point potential of arbitrary position $\mathbf{q}$ and strength α [we denote this perturbation by $\hat{H}_\alpha(\mathbf{q})$] and to analyze the behavior of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$ as functions of $\mathbf{q}$ and α. This analysis is the main goal of the paper. Note that a quite particular case of the point perturbation of $\hat{H}^0$ at $\mathbf{q}=0$ (without obtaining any explicit form for the Green function) has been considered in Ref. 20. Point potential for modeling an impurity in a spherically symmetric quantum dot has been studied in the series of papers using the Green function representation by means of the Laplace transform of the propagator kernel, but this approach allows to analyze (with numerical methods) the lowest impurity level only.[6,13–15]

It should be noted that point perturbations of the one-dimensional harmonic oscillators have been studied in detail earlier. This study was started in Ref. 21, where the spectral properties of the point perturbed harmonic oscillator have been considered in the context of the one-dimensional models for the toponium physics and the Bose–Einstein condensation.[22] A strict mathematical justification of results from Ref. 21 was done in Refs. 23 and 24; see also in Ref. 25. Undoubtedly, our approach using the three-dimensional harmonic oscillator is more adequate for the analyzing the spectral properties of three-dimensional systems, in particular, the toponium. It should be noted also that the one-dimensional harmonic oscillator perturbed by a point potential with varying position and strength has been investigated in Refs. 26 and 27. A series of phenomena of low-dimensional condensed matter physics can be analyzed by means of the Hamiltonian of the perturbed oscillator: Impurity in a one-dimensional quantum well, one-dimensional channel in a two-dimensional heterostructure subjected to a perpendicular uniform magnetic field etc., see the bibliography in the cited papers for details. However, the analysis given in Refs. 26, and 27 is based on the properties of one-dimensional second-order differential operators and is not extended to the three-dimensional case.

The paper is organized as follows. Preliminary results are collected in Sec. II. In Sec. III we consider point perturbations of the operator

$$\hat{H}^0 = -\frac{\hbar^2}{2\mu}\Delta + V, \tag{2}$$

with an infinitely growing potential V. It turns out that the operator $\hat{H}_\alpha(\mathbf{q})$ can be defined and investigated for the more generic case when $\hat{H}^0$ is defined by Eq. (2). In Sec. IV some important properties of $\hat{H}_\alpha(\mathbf{q})$ are established. In particular, a complete description of the spectrum and eigenfunctions of $\hat{H}_\alpha(\mathbf{q})$ is given in Theorem 1. As a consequence of this theorem we get the falling of the considered particle on the attractive center as the potential strength α tends to $-\infty$; for a very particular case of the one-dimensional harmonic oscillator perturbed at the potential minimum this phenomenon was observed in Ref. 21. In Sec. V we define at fixed α a family of continuous functions such that the values of these functions at the point $\mathbf{q}$ form the complete family of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$. Some elementary properties of these functions are established in Theorem 2. The main results of the paper are contained in Sec. VI, where the point perturbations of the Hamiltonian of the harmonic oscillator are studied; the case of the isotropic harmonic oscillator (1) is considered in detail. These results are based on an explicit form of the Green function for the operator (1). The detailed analysis of the dependence of the point levels on the position $\mathbf{q}$ and on the strength α is given in Theorem 3. In particular, if $\mathbf{q}\neq 0$, then the point levels never coincide with the eigenvalues of the unperturbed operator $\hat{H}^0$. Therefore, we have here no accidental degeneracy of the levels, which is a peculiarity of the one-dimensional model for the toponium.[21,26] Hence, this degeneracy is an artifact of the one-dimensional model. Another interesting result is the asymptotic expression for the bound state of $\hat{H}_\alpha(\mathbf{q})$ [Eqs. (33), and (34)]. These equations show that at least for the isotropic harmonic oscillator its potential (i.e., the frequency Ω) can be recovered from the dependence of the ground state of the point perturbation on the support of the perturbation. Moreover, we argue that the form of the parabolic potential V may be recovered from the behavior of the excited energy for the ground state. Our conjecture is that this

property is true for a more general form of the potential V. In this connection it is of interest to note that the study of the excited energy is one of the main problems of the quantum dot physics.[6] The methods of Sec. VI allow us to analyze rigorously the phenomenon of so-called ''positional disorder'' in quantum dots (including nonisotropic ones). The relation of the degeneracy properties of the eigenvalues of $\hat{H}_\alpha(\mathbf{q})$ at $\mathbf{q}=0$ to the symmetry properties of the unperturbed operator $\hat{H}^0$ in the phase space is briefly discussed in the conclusion of Sec. VI. In particular, the appearance of states with nonzero dipole momentum is noted.

II. PRELIMINARIES

Here we present for the convenience of readers some basic properties of point perturbations of Schrödinger operators in $L^2(\mathbb{R}^3)$ (see, e.g., Refs. 8, 28–31 for details). We will consider only Schrödinger operators $\hat{H}^0$ of the form (2), where the potential V is subordinated to the conditions

(P1) $V\in L^p_{\mathrm{loc}}(\mathbb{R}^3)$ *for some* $p>3$;
(P2) $V_-=\min(V,0)\in L^2(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$.

Conditions (P1), (P2) are weaker than commonly used in applications conditions $V\in L^\infty_{\mathrm{loc}}(\mathbb{R}^3)$ and $V\geqslant c$ with $c\in\mathbb{R}$ but making use of (P1), (P2) requires no change in proving of main results below. It is well known that under these conditions $\hat{H}^0$ is semibounded from below and essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ (see in Ref. 32 Theorem X.28). Further we put, as a rule, $\hbar=1$, $\mu=1/2$ and denote the obtained operator $-\Delta+V$ by H^0. For the domain $\mathcal{D}(H^0)$ of H^0 we have $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)\subset C(\mathbb{R}^3)$. This inclusion implies that the Green function $G^0(\mathbf{x},\mathbf{y};\zeta)$ for H^0 (the integral kernel of the resolvent $R(\zeta)=(H^0-\zeta)^{-1}$) is a Carleman operator, this means that

$$\int_{\mathbb{R}^3}|G^0(\mathbf{x},\mathbf{y};\zeta)|^2\,d\mathbf{y}<+\infty \quad \text{for a.e. } \mathbf{x}\in\mathbb{R}^3. \tag{3}$$

Moreover, according to Theorem B.7.2 from Ref. 31, for every fixed ζ, $\zeta\in\mathbb{C}\backslash\mathrm{spec}\,(H^0)$, the function G^0 obeys the following properties:

(G1) *For every* $\zeta\in\mathrm{spec}(\mathrm{H}^0)$ *the function* $G^0(\mathbf{x},\mathbf{y};\zeta)$ *is continuous in the domain* $\{(\mathbf{x},\mathbf{y})\in\mathbb{R}^3\times\mathbb{R}^3:\mathbf{x}\neq\mathbf{y}\}$;
(G2) $|G^0(\mathbf{x},\mathbf{y};\zeta)|\leqslant c_2(\zeta)|\mathbf{x}-\mathbf{y}|^{-1}$;
(G3) *if* $|\mathbf{x}-\mathbf{y}|\geqslant d>0$, *then* $|G^0(\mathbf{x},\mathbf{y};\zeta)|\leqslant c_3(d,\delta,\zeta)\exp(-\delta|\mathbf{x}-\mathbf{y}|)$ *for some* $\delta>0$. *Moreover, if* $\mathrm{Re}\,\zeta<\Sigma\equiv\mathrm{infspec}(H^0)$, *then arbitrary* δ *with* $\delta^2/2<\Sigma-\mathrm{Re}\,\zeta$ *is suitable for this estimate.*

From (G1) we get, in particular, that (3) is valid for *every* $\mathbf{x}\in\mathbb{R}^3$.

The crucial role in the point potential theory is played by the regularized Green function

$$G^0_{\mathrm{reg}}(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\mathbf{y};\zeta)-\frac{1}{4\pi}\frac{1}{|\mathbf{x}-\mathbf{y}|}. \tag{4}$$

In the particular cases, e.g., if $V\in C^\infty(\mathbb{R}^3)$, it is known that at fixed ζ this function has a continuous extension on the whole space $\mathbb{R}^3\times\mathbb{R}^3$ (see, e.g., Ref. 33 or Theorem III.5.1 in Ref. 34). We need this property in the general situation and prove it under conditions (P1), (P2).

It is sufficient to prove that $G^0_{\mathrm{reg}}(\mathbf{x},\mathbf{y};\zeta)$ is continuous with respect to $(\mathbf{x},\mathbf{y})$ for some $\zeta=E_0<0$. Indeed, then for every $\zeta\in\mathbb{C}\backslash\mathrm{spec}\,(H^0)$

$$G^0(\mathbf{x},\mathbf{y};\zeta)=\int_{E_0}^{\zeta}\frac{\partial}{\partial\lambda}G^0(\mathbf{x},\mathbf{y};\lambda)\,d\lambda+G^0(\mathbf{x},\mathbf{y};E_0),$$

where the path of integration lies in the resolvent set $\mathbb{C}\backslash\mathrm{spec}\,(H^0)$. The function $(\partial G^0/\partial\lambda)(\mathbf{x},\mathbf{y};\lambda)$ is jointly continuous with respect to $(\mathbf{x},\mathbf{y})$ since it coincides with the integral kernel of $(H^0-\lambda)^{-2}$ and this kernel is continuous according to Theorem B.7.1 from Ref. 31.

It is easy to see that V can be represented in the form $V=V_1+W$, where $V_1\in C^\infty(\mathbb{R}^3)$ and obeys the property (P2) and $W\in L^p(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$. Denote $H^1=-\Delta+V_1$, $\Sigma_1=\mathrm{infspec}\,(H^1)$ and

by G^1 the Green function of H^1. Fix E_0, $E_0<\min(\Sigma,\Sigma^1)$, and introduce the function $F(\mathbf{x},\mathbf{y},\mathbf{z})=G^0(\mathbf{x},\mathbf{z};E_0)W(\mathbf{z})G^1(\mathbf{z},\mathbf{y};E_0)$. Using properties (G2), (G3), and the estimate

$$\int_{|\mathbf{y}-\mathbf{a}|\leqslant r}\frac{d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|^{\nu}}\leqslant\tilde{c}_{\nu}r^{3-\nu}, \tag{5}$$

where $0<\nu<3$, $r>0$, $\mathbf{a},\mathbf{x}\in\mathbb{R}^3$, it is easy to prove that $F(\mathbf{x},\mathbf{y},\cdot)\in L^1(\mathbb{R}^3)$ for all $\mathbf{x},\mathbf{y}\in\mathbb{R}^3$. In virtue of the Lippmann–Schwinger relation

$$G^0(\mathbf{x},\mathbf{y};E_0)=G^1(\mathbf{x},\mathbf{y};E_0)+\int_{\mathbb{R}^3}G^0(\mathbf{x},\mathbf{z};E_0)W(\mathbf{z})G^1(\mathbf{z},\mathbf{y};E_0)\,d\mathbf{z},$$

and the continuity of the regularized Green function for H^1, it remains to prove that the function

$$I(\mathbf{x},\mathbf{y})=\int_{\mathbb{R}^3}F(\mathbf{x},\mathbf{y},\mathbf{z})\,d\mathbf{z}$$

is continuous on $\mathbb{R}^3\times\mathbb{R}^3$. Moreover, (G1) shows that it remains to prove the continuity of I at points of the form $(\mathbf{x}_0,\mathbf{x}_0)$. To do this fix $\varepsilon>0$ and find $\eta>0$ such that the relations $|\mathbf{x}-\mathbf{x}_0|<\eta$, $|\mathbf{y}-\mathbf{x}_0|<\eta$ imply $|I(\mathbf{x},\mathbf{y})-I(\mathbf{x}_0,\mathbf{x}_0)|\leqslant\varepsilon$. Introduce the sets $B_1(\eta)=\{\mathbf{z}:|\mathbf{z}-\mathbf{x}_0|<\eta\}$, $B_2(\eta)=\mathbb{R}^3\backslash B_1(\eta)$, and for a measurable set $B\subset\mathbb{R}^3$ denote $I_B(\mathbf{x},\mathbf{y})=\int_B F(\mathbf{x},\mathbf{y},\mathbf{z})\,d\mathbf{z}$. Then

$$|I(\mathbf{x},\mathbf{y})-I(\mathbf{x}_0,\mathbf{y}_0)|\leqslant|I_{B_1(\eta)}(\mathbf{x},\mathbf{y})|+|I_{B_1(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|+|I_{B_2(\eta)}(\mathbf{x},\mathbf{y})-I_{B_2(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|\,.$$

If $\mathbf{x},\mathbf{y},\mathbf{z}\in B_1(\eta)$, then by (G2)

$$|F(\mathbf{x},\mathbf{y},\mathbf{z})|\leqslant f(\mathbf{z})\,|\mathbf{x}-\mathbf{y}|^{-1}|\mathbf{z}-\mathbf{y}|^{-1},$$

where $f\in L^p$, therefore relation (5) and the Cauchy–Schwartz inequality lead to the estimate $|I_{B_1(\eta)}(\mathbf{x},\mathbf{y})|+|I_{B_1(\eta)}(\mathbf{x}_0,\mathbf{y}_0)|\leqslant\text{const}\,\eta$. On the other hand, if $\mathbf{x},\mathbf{y}\in B_1(\eta/2)$, $\mathbf{z}\in B_2(\eta)$, then we have from (G3): $|F(\mathbf{x},\mathbf{y},\mathbf{z})|\leqslant g(\mathbf{z})\exp(-\delta|\mathbf{z}|)$, where $\delta>0$ and $g\in L^p$. Thus by (G1) and the Lebesgue majorization theorem, $I_{B_2(\eta)}(\mathbf{x},\mathbf{y})$ is a continuous function on $B_1(\eta/2)\times B_1(\eta/2)$, and the proof of continuity of G^0_{reg} is completed.

Let $\mathbf{q}\in\mathbb{R}^3$, then the restriction of H^0 to the domain $\{f\in\mathcal{D}(H^0):f(\mathbf{q})=0\}$ is a closed symmetric operator S with the deficiency indices (1,1). By definition, the *point perturbation of* H^0, *supported on* $\mathbf{q}$ is a self-adjoint extension of S different from H^0. All the point perturbations of H^0 supported on a given $\mathbf{q}\in\mathbb{R}^3$ form a one-parameter family $H_\alpha(\mathbf{q})$, $\alpha\in\mathbb{R}$, of self-adjoin operators such that the Green function G_α of $H_\alpha(\mathbf{q})$ is given by the formula

$$G_\alpha(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\mathbf{y};\zeta)-[Q(\zeta;\mathbf{q})-\alpha]^{-1}G^0(\mathbf{x},\mathbf{q};\zeta)G^0(\mathbf{q},\mathbf{y};\zeta)\,, \tag{6}$$

which is a consequence of the Krein resolvent formula. Here $Q(\zeta;\mathbf{q})=G^0_{\mathrm{reg}}(\mathbf{q},\mathbf{q};\zeta)$ is the so-called Krein $\mathcal{Q}$-function. The operator H^0 corresponds formally to $\alpha=\infty$; moreover, H^0 is the Friedrichs extension of S.

The extension parameter α has an important physical meaning, namely, H_α can be treated as the Hamiltonian H^0 perturbed by a zero-range potential, in this case α is the strength of this potential.[8,35,36] In place of the strength α, it is more convenient to use for applications so-called "scattering length" ℓ_s, $\ell_s=1/(4\pi\alpha)$ (see in Refs. 8, 35, and 36 again). More precisely,

$$\ell_s=\frac{\mu}{2\pi\hbar^2\alpha},$$

and we see that ℓ_s has actually the dimension of the length.

Note that according to the general results of the Krein self-adjoint extension theory, the function $\zeta \mapsto Q(\zeta;\mathbf{q})$ is analytic in the domain $\mathbb{C}\backslash\mathrm{spec}(H^0)$ for each $\mathbf{q}\in\mathbb{R}^3$ and $\partial Q(E;\mathbf{q})/\partial E>0$ if $E\in\mathbb{R}\backslash\mathrm{spec}(H^0)$.[37] Remark that $Q(\zeta;\mathbf{q})$ can be continuously extended to some points of $\mathrm{spec}(H^0)$. Further we assume that $Q(\zeta;\mathbf{q})$ is continuously extended to all regular points.

It is easy to prove that for every $\mathbf{q}\in\mathbb{R}^3$ the mapping $\zeta\mapsto G^0(\cdot,\mathbf{q};\zeta)$ is an analytic function from the domain $\mathbb{C}\backslash\mathrm{spec}\,(H^0)$ to the Hilbert space $L^2(\mathbb{R}^3)$. Denote $G^0(\cdot,\mathbf{q};\zeta)$ by $g_{\mathbf{q}}(\zeta)$, then we can rewrite (6) in an operator form

$$R_\alpha(\zeta)=R^0(\zeta)-[Q(\zeta;\mathbf{q})-\alpha]^{-1}|g_{\mathbf{q}}(\zeta)\rangle\langle g_{\mathbf{q}}(\zeta)|\,, \tag{7}$$

where $R_\alpha(\zeta)=(H_\alpha-\zeta)^{-1}$ and $R^0(\zeta)=(H^0-\zeta)^{-1}$.

Note, that $g_{\mathbf{q}}(\zeta)$ is a nonzero function for every $\mathbf{q}\in\mathbb{R}^3$ and $\zeta\in\mathbb{C}\backslash\mathrm{spec}\,(H^0)$. Indeed, otherwise we have $\varphi(\mathbf{q})=0$ for every $\varphi\in\mathcal{D}(H^0)$ that contradicts the inclusion $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)$.

In conclusion we mention a possibility to approximate the zero-range perturbation by potentials with decreasing support. For $V=0$ the corresponding procedure is described in Ref. 8 (Theorem 1.2.5). We sketch here the proof for H^0 with potential V having properties (P1), (P2).

Let $W\in L^2_{\mathrm{comp}}(\mathbb{R}^3)$, in particular, W is a Rollnik function (see in Ref. 32, Sec. X.2). Denote $v=|W|^{1/2}$, $u=v\,\mathrm{sign}(V)$, and let $\lambda(\varepsilon)$ be a real-analytic function in a neighborhood of zero such that $\lambda(0)=1$. For $\varepsilon>0$ consider the operator $H^\varepsilon\equiv H^\varepsilon(\mathbf{q})=H^0+\varepsilon^{-2}\lambda(\varepsilon)W(\varepsilon^{-1}(\mathbf{x}-\mathbf{q}))$. Then the resolvent $R^\varepsilon(\zeta)=(H^\varepsilon-\zeta)^{-1}$ $(\varepsilon>0)$ has the form

$$R^\varepsilon(\zeta)=R^0(\zeta)-\varepsilon\lambda(\varepsilon)A^\varepsilon[1+B^\varepsilon]^{-1}C^\varepsilon\,,$$

where A^ε, B^ε, C^ε are integral operators with the kernels $A^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=G^0(\mathbf{x},\varepsilon\mathbf{y}+\mathbf{q};\zeta)v(\mathbf{y})$, $C^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=G^0(\varepsilon\mathbf{x}+\mathbf{q},\mathbf{y};\zeta)u(\mathbf{x})$, $B^\varepsilon(\mathbf{x},\mathbf{y};\zeta)=\varepsilon\lambda(\varepsilon)G^0(\varepsilon\mathbf{x}+\mathbf{q},\varepsilon\mathbf{y}+\mathbf{q};\zeta)u(\mathbf{x})v(\mathbf{y})$. Define A^0 and C^0 putting $\varepsilon=0$ in the formulas above, and define B^0 by the integral kernel $B^0(\mathbf{x},\mathbf{y})=(4\pi|\mathbf{y}-\mathbf{x}|)^{-1}u(\mathbf{x})v(\mathbf{y})$. All the operators A^ε, B^ε and C^ε $(\varepsilon\geqslant 0)$ belong to the Hilbert–Schmidt class and $A^\varepsilon\to A^0$, $B^\varepsilon\to B^0$, $C^\varepsilon\to C^0$ with respect to the Hilbert–Schmidt norm as $\varepsilon\to+0$. Moreover, using (4) we can prove that with respect to this norm

$$B^\varepsilon=B^0+\varepsilon(\lambda'(0)B^0+Q(\zeta;\mathbf{q})|u\rangle\langle v|)+o(\varepsilon)\,.$$

Hence, the arguments using for the proof of Theorem 1.2.5 from Ref. 8 give the following result.

Theorem A:

(1) Let $\langle v|\varphi\rangle=0$ for all L^2-solutions φ of the equation $B^0\varphi=-\varphi$ (in particular, let -1 be not an eigenvalue of B_0). Then $H^\varepsilon(\mathbf{q})\to H^0$ in the norm-resolvent sense as $\varepsilon\to+0$;

(2) let -1 be a simple eigenvalue of B^0 and φ be a corresponding eigenfunction normalized by the condition $\langle\tilde{\varphi}|\varphi\rangle=-1$, where $\tilde{\varphi}=\varphi\,\mathrm{sign}(\mathrm{V})$. If $\langle v|\varphi\rangle\neq 0$, then $\lim_{\varepsilon\to+0}H^\varepsilon(\mathbf{q})=H_\alpha(\mathbf{q})$ in the norm-resolvent sense, where $\alpha=-\lambda'(0)|\langle v|\varphi\rangle|^{-2}$;

(3) let -1 be a multiple eigenvalue of B^0 with eigenfunctions $\varphi_1,\ldots,\varphi_n$ normalized by the conditions $\langle\tilde{\varphi}_j|\varphi_k\rangle=-\delta_{jk}$ $(\tilde{\varphi}_j=\varphi_j\,\mathrm{sign}(\mathrm{V}))$. If $\langle v|\varphi_j\rangle\neq 0$ for some j and $\lambda'(0)\neq 0$, then $\lim_{\varepsilon\to+0}H^\varepsilon(\mathbf{q})=H_\alpha(\mathbf{q})$ in the norm-resolvent sense, where

$$\alpha=-\lambda'(0)\left[\sum_{j=1}^{n}|\langle v|\varphi_j\rangle|^2\right]^{-1}.$$

■

III. POINT PERTURBATION IN THE CASE OF UNBOUNDED POTENTIAL *V*

Starting with this section we suppose additionally that

(P3) $\lim_{|\mathbf{r}|\to\infty}V(\mathbf{r})=+\infty$.

In this case $R^0(\zeta)$ is a compact operator for all $\zeta\in\mathbb{C}\backslash\mathrm{spec}(H^0)$ (the Strichartz theorem; see, e.g.,

in Ref. 38, Theorem XIII.69). Therefore, $\mathrm{spec}(H^0)$ consists of an unbounded sequence $\lambda_0<\lambda_1<\cdots<\lambda_n<\cdots$ of eigenvalues with finite multiplicity k_n. Consequently, $Q(\zeta;\mathbf{q})$ is a meromorphic function of ζ. We are going to find the poles of this function.

Denote by L_n the eigenspace associated with λ_n, and choose in L_n an orthonormal basis $F_{n,k}(\mathbf{r})$, $k=1,\ldots,k_n$. For every $\mathbf{q}\in\mathbb{R}^3$ we denote

$$\sigma(\mathbf{q})=\{\lambda_n\in\mathrm{spec}(H^0):\exists f\in L_n \quad \text{s.t.} \quad f(\mathbf{q})\neq 0\}$$

Lemma 1: The set of all poles of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ *coincides with* $\sigma(\mathbf{q})$.

Proof: Since $(\partial G^0/\partial\zeta)(\mathbf{x},\mathbf{y};\zeta)$ is the integral kernel for the operator $(H^0-\zeta)^{-2}$, we have according to the Mercer theorem

$$\frac{\partial}{\partial\zeta}G^0(\mathbf{x},\mathbf{y};\zeta)=\sum_{n=0}^{\infty}\sum_{k=1}^{k_n}(\lambda_n-\zeta)^{-2}F_{n,k}(\mathbf{x})\overline{F_{n,k}(\mathbf{y})},$$

where the series converges locally uniformly on $\mathbb{R}^3\times\mathbb{R}^3\times(\mathbb{C}\backslash\mathrm{spec}(H^0))$. Therefore,

$$\frac{\partial}{\partial\zeta}Q(\zeta;\mathbf{q})=\sum_{n=0}^{\infty}\sum_{k=1}^{k_n}(\lambda_n-\zeta)^{-2}|F_{n,k}(\mathbf{q})|^2, \tag{8}$$

and the series converges locally uniformly on $(\mathbb{C}\backslash\mathrm{spec}(H^0))\times\mathbb{R}^3$. The lemma follows from (8) immediately. ■

Lemma 2: For each $\mathbf{q}\in\mathbb{R}^3$ *the set* $\sigma(\mathbf{q})$ *is infinite. If* V *is bounded from below, then* $\lambda_0\in\sigma(\mathbf{q})$.

Proof: Consider the space of continuous functions $C(\mathbb{R}^3)$ with the topology of compact convergence. Due to the closed graph theorem and the relation $\mathcal{D}(H^0)\subset C(\mathbb{R}^3)$, the operator $R^0(-1):L^2(\mathbb{R}^3)\to C(\mathbb{R}^3)$ is continuous. Therefore, for every $f\in\mathcal{D}(H^0)$ the Fourier expansion for f with respect to the basis $(F_{n,k})_{n,k}$ converges locally uniformly. Assume that the set $\sigma(\mathbf{q})$ is finite; let $N=\max\{n:\lambda_n\in\sigma(\mathbf{q})\}$ and P be the orthogonal projection of $L^2(\mathbb{R}^3)$ on the subspace $M=L_0+\ldots+L_N$. Then for every $\varphi\in\mathcal{D}(H^0)$ the conditions $\varphi(\mathbf{q})=0$ and $(P\varphi)(\mathbf{q})=0$ are equivalent. Since M is finite dimensional, there is $h\in M$ such that for every $\varphi\in M$ the conditions $\varphi(\mathbf{q})=0$ and $\langle h\,|\,\varphi\rangle=0$ are also equivalent. Using the inclusion $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H^0)$ we see that there is a function $h\in L^2(\mathbb{R}^3)$ such that for every $\varphi\in C_0^\infty(\mathbb{R}^3)$ the conditions $\varphi(\mathbf{q})=0$ and $\langle h\,|\,\varphi\rangle=0$ are equivalent. Obviously, this is impossible, hence $\sigma(\mathbf{q})$ is infinite. If V is bounded from below, then by Theorem XIII.48 from Ref. 38 the eigenfunctions of H^0 corresponding to the ground state λ_0 have no zeros therefore $\lambda_0\in\sigma(\mathbf{q})$. ■

Another property of the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ we need further follows.

Lemma 3: The function $Q(\zeta;\mathbf{q})$ *tends to* $-\infty$ *as* $\zeta\to-\infty$, $\zeta\in\mathbb{R}$.

Proof: Since H^0 is the Friedrichs extension of S, the statement follows from Proposition 4 of Ref. 39. ■

IV. SPECTRAL PROPERTIES OF H_α AT FIXED POSITION OF THE POINT PERTURBATION

Here we describe the spectrum of $H_\alpha(\mathbf{q})$ for a fixed $\mathbf{q}\in\mathbb{R}^3$. Further, if it does not lead to a misunderstanding, we omit $\mathbf{q}$ from the notations.

Since H_α is a rank one perturbation of H^0, the spectrum of H_α is discrete. Moreover, an eigenvalue λ_n of H^0 of the multiplicity k_n is an eigenvalue of H_α of the multiplicity k_n-1, k_n or k_n+1 [if $k_n=1$, the first case means, of course, that λ_n does not belong to $\mathrm{spec}(H_\alpha)$]. For $\lambda\notin\mathrm{spec}(H^0)$ we see from (7) that λ is an eigenvalue of H_α if and only if $\zeta=\lambda$ is a solution to the equation

$$Q(\zeta;\mathbf{q})-\alpha=0. \tag{9}$$

Denote by $(\varepsilon_n)_{n\in\mathbb{N}}=(\varepsilon_n(\mathbf{q}))_{n\in\mathbb{N}}$ the strictly increasing sequence of all the poles of $Q(\zeta;\mathbf{q})$. Since $(\partial Q/\partial E)(E;\mathbf{q})>0$ for $E\in\mathbb{R}\backslash\mathrm{spec}(H^0)$, Eq. (9) has exactly one solution on each interval $(-\infty,\varepsilon_0),(\varepsilon_0,\varepsilon_1),\ldots$. Denote such solutions, which do not belong to $\mathrm{spec}(H^0)$, by $\mathcal{E}_0,\mathcal{E}_1,\ldots$, where $\mathcal{E}_0<\mathcal{E}_1<\cdots$. The following theorem completely describes the eigenvalues and the eigenfunctions of $H_\alpha(\mathbf{q})$.

Theorem 1: *Let $\mathbf{q}\in\mathbb{R}^3$ be fixed. The spectrum of $H_\alpha=H_\alpha(\mathbf{q})$ is discrete and consists of four nonintersecting parts $\sigma_1,\sigma_2,\sigma_3,\sigma_4$ described as follows.*

(1) σ_1 is the set of all solutions $\mathcal{E}_n$ to the Eq. (9), which do not belong to $\mathrm{spec}(H^0)$. *The multiplicity of $\mathcal{E}_n$ in the spectrum of H^0 is equal to 1.*
(2) σ_2 is the set of all $\lambda_n\in\sigma(\mathbf{q})$ that are multiple eigenvalues of H^0. The multiplicity of the eigenvalue $\lambda_n\in\sigma_2$ in the spectrum of H_α is equal to k_n-1.
(3) σ_3 consists of all λ_n, $\lambda_n\in\mathrm{spec}\,(H^0)\backslash\sigma(\mathbf{q})$, that are not solutions of (9). *The multiplicity of the eigenvalue λ_n in* $\mathrm{spec}(H_\alpha)$ *is equal to k_n.*
(4) σ_4 consists of all λ_n, $\lambda_n\in\mathrm{spec}\,(H^0)\backslash\sigma(\mathbf{q})$, such that λ_n is a solution of (9). *The multiplicity of the eigenvalue λ_n in* $\mathrm{spec}(H_\alpha)$ *is equal to k_n+1.*

The corresponding eigensubspaces are described as follows.

(1) The subspace spanned by the normalized eigenfunction

$$\Phi_n=\left[\frac{\partial Q}{\partial\zeta}(\mathcal{E}_n;\mathbf{q})\right]^{-1/2}g_{\mathbf{q}}(\mathcal{E}_n)\,.$$

(2) The orthogonal complement in L_n of the function

$$\Psi_n(\mathbf{x})=\sum_{k=1}^{k_n}\overline{F_{n,k}(\mathbf{q})}F_{n,k}(\mathbf{x})\,,$$

or, equivalently, the subspace of L_n of the form $\{f\in L_n: f(\mathbf{q})=0\}$.
(3) The subspace L_n.
(4) The direct sum of L_n and the space spanned by the function $g_{\mathbf{q}}(\lambda_n)$, which is orthogonal to L_n.

Proof: The proof is based on direct calculations with the help of following statements:
(A) *The orthoprojector $P(E_0)$ on the eigenspace of a self-adjoint operator T corresponding to an isolated eigenvalue E_0 has the form*

$$P(E_0)=-\mathrm{Res}[(T-\zeta)^{-1};\zeta=E_0].$$

(B) *Suppose P_1,P_2 and P_1+cP_2, where $c\in\mathbb{C}$, are orthoprojectors in a Hilbert space and $P_2\neq 0$, then c equals* 0, 1 *or* -1.

The first statement is well known; we omit the easy proof of the second one. Denote by $A(\zeta)$,

$$A(\zeta)=[Q(\zeta;\mathbf{q})-\alpha]^{-1}|g_{\mathbf{q}}(\zeta)\rangle\langle g_{\mathbf{q}}(\zeta)|,$$

the second term in the representation (7) of the resolvent. Further, denote for $E_0\in\mathbb{R}$

$$P_\alpha(E_0)=-\mathrm{Res}[R_\alpha(\zeta);\zeta=E_0]\,,$$

$$P^0(E_0)=-\mathrm{Res}[R^0(\zeta);\zeta=E_0]\,,$$

$$T(E_0)=\mathrm{Res}[A(\zeta);\zeta=E_0]\,;$$

therefore, according to (7)

$$P_\alpha(E_0)=P^0(E_0)+T(E_0)\,.$$

Start with the proof of the first assertion of Theorem. It is obvious that $\sigma_1 \subset \operatorname{spec}(H_\alpha)$. Let $\mathcal{E}_n \in \sigma_1$, then in a vicinity of $\mathcal{E}_n$ we have the following expansion:

$$Q(\zeta;\mathbf{q}) - \alpha = \frac{\partial}{\partial \zeta} Q(\mathcal{E}_n;\mathbf{q})(\zeta - \mathcal{E}_n) + O(\zeta - \mathcal{E}_n)^2. \tag{10}$$

Therefore,

$$T(\mathcal{E}_n) = \left[\frac{\partial}{\partial \zeta} Q(\mathcal{E}_n;\mathbf{q}) \right]^{-1} |g_{\mathbf{q}}(\mathcal{E}_n)\rangle\langle g_{\mathbf{q}}(\mathcal{E}_n)| . \tag{11}$$

Since obviously $P^0(\mathcal{E}_n) = 0$, we have $P_\alpha(\mathcal{E}_n) = T(\mathcal{E}_n)$ and the normalized eigenfunction corresponding to $\mathcal{E}_n$ is

$$\Phi_n = \left[\frac{\partial Q}{\partial \zeta}(\mathcal{E}_n;\mathbf{q}) \right]^{-1/2} g_{\mathbf{q}}(\mathcal{E}_n) . \tag{12}$$

Now consider an eigenvalue λ_n of H^0. In this case $P_\alpha(\lambda_n) = P^0(\lambda_n) + T(\lambda_n)$. According to (8), in a neighborhood W of λ_n we have the following representation

$$g_{\mathbf{q}}(\zeta) = \Psi_n(\cdot;\mathbf{q})(\lambda_n - \zeta)^{-1} + f(\zeta) ,$$

where f is analytic function in W with values in $L^2(\mathbb{R}^3)$ and

$$\Psi_n(\mathbf{x};\mathbf{q}) = \sum_{k=1}^{k_n} \overline{F_{n,k}(\mathbf{q})} F_{n,k}(\mathbf{x}) .$$

Consider the following three cases: (a) $\lambda_n \in \sigma(\mathbf{q})$; (b) $\lambda_n \notin \sigma(\mathbf{q})$ and $Q(\lambda_n;\mathbf{q}) - \alpha \neq 0$; (c) $\lambda_n \notin \sigma(\mathbf{q})$ and $Q(\lambda_n;\mathbf{q}) - \alpha = 0$.

Let us start with the case (a). Since λ_n is a pole of $Q(\cdot;\mathbf{q})$, we have $\Psi_n(\cdot;\mathbf{q}) \neq 0$ and therefore $T = cP$, where P is the orthoprojector on the one-dimensional space spanned by $\Psi_n(\cdot;\mathbf{q})$. Since $\Psi_n(\cdot;\mathbf{q}) \in L_n$, in virtue of statement (B) $c = -1$, and the assertion (2) of Theorem is proven.

In the case (b) according to Lemma 1, $F_{n,k}(\mathbf{q}) = 0$ for all $k = 1,\ldots,k_n$; hence $\Psi_n(\cdot,\mathbf{q}) = 0$ and $T(\lambda_n) = 0$. This implies assertion (3) of Theorem.

Finally, in the case (c) we can use (10)–(12) with $\zeta = \lambda_n$ instead of $\zeta = \mathcal{E}_n$, and obtain

$$T(\lambda_n) = |\Phi_n\rangle\langle\Phi_n| ,$$

according to (B), this get the statement (4) of Theorem. ■

For $n \in \mathbb{N}$ denote by A_n the set of all $\alpha \in \mathbb{R}$ such that the solution $\mathcal{E}_n \equiv \mathcal{E}_n(\alpha)$ of Equation (9) does not belong to the spectrum of H^0. Lemma 2 shows that $\mathbb{R} \backslash A_n$ is finite, moreover, if V bounded from below, then $A_0 = \mathbb{R}$.

For all $\mathbf{q} \in \mathbb{R}^3$ we will denote $\varepsilon_{-1}(\mathbf{q}) = \lambda_{-1} = -\infty$. Using Lemmas 1 and 3 we get immediately the following proposition.

Proposition 1: For each $n \in \mathbb{N}$ the function $\alpha \mapsto \mathcal{E}_n(\alpha)$ strictly increases on A_n. Moreover,

$$\lim_{\alpha \to +\infty} \mathcal{E}_n(\alpha) = \varepsilon_n , \qquad \lim_{\alpha \to -\infty} \mathcal{E}_n(\alpha) = \varepsilon_{n-1} .$$

■

Remark: For $n = 0$ we have an interesting phenomenon of falling the considered particle on the point $\mathbf{q}$ (the falling on the attractive center; cf. Ref. 21 for the case of a one-dimensional oscillator). Indeed, using estimate (b′) from Theorem B.7.1 of Ref. 31, we obtain without any difficulty $|\Phi_0(\mathbf{x})|^2 \to \delta(\mathbf{x} - \mathbf{q})$ in an appropriate space of distributions as $\alpha \to -\infty$ (and therefore

$\mathcal{E}_0 \to -\infty$). According to the standard interpretation of quantum mechanics, this relation means that the probability to find the particle in a domain not containing the point $\mathbf{q}$ tends to zero as $\mathcal{E}_0$ tends to $-\infty$.

V. DEPENDENCE OF THE SPECTRUM OF $H_\alpha(\mathbf{q})$ ON $\mathbf{q}$

Here we are going to analyze the dependence of the eigenvalues of H_α on $\mathbf{q}$. It is clear that $\mathcal{E}_n(\mathbf{q})$ are continuous branches of the multi-valued function defined by Eq. (9). This branches can intersect at values λ_n where a monodromy arises. To get a univalent enumeration of these branches, we modify the parametrization of the eigenvalues of H_α given by Theorem 1 (the enumeration of the numbers $\mathcal{E}_n(\mathbf{q})$ depends on the enumeration of poles $\varepsilon_n \in \mathrm{spec}(H^0)$, which in its turn depends obviously on $\mathbf{q}$). For $n=-1,0,\ldots$ consider the sets X_n defined as follows: $X_{-1} = \mathbb{R}^3$, and

$$X_n = \{\mathbf{q} \in \mathbb{R}^3 : \exists f \in L_n \text{ s.t. } f(\mathbf{q}) \neq 0\} = \{\mathbf{q} \in \mathbb{R}^3 : \lambda_n \in \sigma(\mathbf{q})\},$$

for $n \geqslant 0$. For all $n \in \mathbb{N}$ the set $\mathbb{R}^3 \backslash X_n$ is nowhere dense in $\mathbb{R}^3$ (see in Ref. 38, Theorem XIII.63). According to Lemma 1, for $n \geqslant 0$, the set X_n coincides with the set of all $\mathbf{q} \in \mathbb{R}^3$ such that λ_n is a pole of the function $Q(\cdot;\mathbf{q})$. Since we do not suppose the potential V is smooth, the function $Q(\zeta;\mathbf{q})$ on the set $(\lambda_{n-1},\lambda_n) \times (X_{n-1} \cap X_n)$, $n \geqslant 0$, is not, generally speaking, smooth. Nevertheless, it is monotone and real analytic with respect to the first argument ζ and continuous with respect to the second argument $\mathbf{q}$. In this case the following simple variant of Implicit Function Theorem is applicable (see in Ref. 40 for the proof):

Let J be an open nonempty interval of the real line $\mathbb{R}$, X be a topological space, and $F: J \times X \to \mathbb{R}$ be a separately continuous function such that each partial function $t \mapsto F(t,x)$, $x \in X$, is strictly monotone. Suppose that $F(t_0,x_0)=0$ for some $(t_0,x_0) \in J \times X$. Then there are an open neighborhood U of the point x_0 in X and a continuous function $f: U \to J$ such that (1) $F(f(x),x)=0$ for all $x \in U$; (2) if U' is another neighborhood of x_0, and $g: U' \to J$ is a function with the property: $F(g(x),x)=0$ for all $x \in U'$, then $U' \subset U$, and $f_{|U'} = g$.

According to this version of Implicit Function Theorem, for any $\mathbf{q} \in X_{n-1} \cap X_n$ there exists a unique solution $E_n(\mathbf{q})$ to Eq. (9) that belongs to $(\lambda_{n-1},\lambda_n)$ and $\mathbf{q} \mapsto E_n(\mathbf{q})$ is a continuous function in $X_{n-1} \cap X_n$.

Proposition 2: Every function $E_n(\mathbf{q})$, $n=0,1,\ldots$, has a continuous extension to the whole space $\mathbb{R}^3$.

Proof: Fix $n=0,1,\ldots$, and let a point $\mathbf{q}$, $\mathbf{q} \in \mathbb{R}^3 \backslash (X_{n-1} \cap X_n)$, be given. Choose a sequence $(\mathbf{q}_k)_{k \in \mathbb{N}}$ from $X_{n-1} \cap X_n$ which tends to $\mathbf{q}$. First we note that the sequence $(E_n(\mathbf{q}_k))_{k \in \mathbb{N}}$ is bounded in $\mathbb{R}$. It is trivial for $n>0$. If $n=0$, the sequence is bounded from above. We prove that it is bounded from below as well. Otherwise $E_0(\mathbf{q}_{k_l}) \to -\infty$ for some subsequence $(\mathbf{q}_{k_l})$. Since $Q(E;\mathbf{q}) \to -\infty$ as $E \to -\infty$, there exists $A < \lambda_0$ such that $Q(A;\mathbf{q}) < \alpha$. Then there exists $N \in \mathbb{N}$ such that $Q(A;\mathbf{q}_{k_l}) < \alpha$ and $E_0(\mathbf{q}_{k_l}) < A$ if $l \geqslant N$. Therefore, for $k \geqslant N$ we have

$$Q(E_0(\mathbf{q}_{k_l});\mathbf{q}_{k_l}) - \alpha < Q(A;\mathbf{q}_{k_l}) - \alpha < 0,$$

and we get a contradiction with the definition of $E_0(\mathbf{q}_{k_l})$.

By Bolzano–Weierstrass we can extract a subsequence $(\mathbf{q}_{k_l})$ from the sequence $(\mathbf{q}_k)$ such that the subsequence $(E_n(\mathbf{q}_{k_l}))$ has a limit, which we denote by E'. To prove that the sequence $(E_n(\mathbf{q}_k))$ tends to E' and E' is independent of the choice of a sequence $(\mathbf{q}_k)$ tending to $\mathbf{q}$ we need the following lemma concerning properties of E'.

Lemma 5: The limit E' has the properties:

(1) E' is not a pole of the function $\zeta \mapsto Q(\zeta;\mathbf{q})$;
(2) if $\lambda_{n-1} < E' < \lambda_n$, then E' is a unique solution of Eq. (9) in the interval $(\lambda_{n-1},\lambda_n)$;
(3) if $E' = \lambda_{n-1}$, then $\lim_{E \to E'} [Q(E;\mathbf{q}) - \alpha] \geqslant 0$;
(4) if $E' = \lambda_n$, then $\lim_{E \to E'} [Q(E;\mathbf{q}) - \alpha] \leqslant 0$.

Proof of the lemma:

(1) First consider the case $n>0$. The function $\tilde{Q}_n(\zeta;\mathbf{q})=[Q(\zeta;\mathbf{q})-\alpha](\zeta-\lambda_{n-1})(\zeta-\lambda_n)$ is continuous on the interval $(\lambda_{n-2},\lambda_{n+1})\times\mathbb{R}^3$. Since $\tilde{Q}_n(E_n(\mathbf{q}_{k_l});\mathbf{q}_{k_l})=0$, passing to the limit $l\to\infty$ we get $\tilde{Q}_n(E';\mathbf{q})=0$. Suppose $\zeta=E'$ is a pole of $Q(\zeta;\mathbf{q})$, then $\tilde{Q}_n(E';\mathbf{q})=\mathrm{Res}[Q(\zeta;\mathbf{q});\zeta=E']\neq 0$, and we get a contradiction. For $n=0$, we consider $\tilde{Q}_0(\zeta;\mathbf{q})=[Q(\zeta;\mathbf{q})-\alpha](\zeta-\lambda_0)$, and get the same result.
(2) It is sufficient to pass to the limit $l\to\infty$ in the identity $Q(E_n(\mathbf{q}_{k_l});\mathbf{q}_{k_l})=0$.
(3) In virtue of statement (1) of the lemma, the function $\zeta\mapsto Q(\zeta;\mathbf{q})$ is continuous in a neighborhood of E', and therefore there exists a limit $\lim_{\zeta\to\lambda_{n-1}}[Q(\zeta;\mathbf{q})-\alpha]=L$. Assume that $L<0$, then $Q(E,\mathbf{q})-\alpha<0$ for some $E\in(\lambda_{n-1},\lambda_n)$. Choose some m such that $E_n(\mathbf{q}_{k_m})<E$. Since $Q(\zeta;\mathbf{q})$ increases on the interval $(\lambda_{n-1},\lambda_n)$ as the function of ζ, we obtain a contradiction:

$$0=Q(E_n(\mathbf{q}_{k_m});\mathbf{q}_{k_m})-\alpha<Q(E;\mathbf{q}_{k_m})-\alpha<0\,.$$

Statement (4) can be proven similarly to (3). ■

Let us return to the proof of the proposition. We prove that if a sequence $(\mathbf{p}_k)_{k\in\mathbb{N}}$ from $X_{k-1}\cap X_k$ converges to the point $\mathbf{q}$, then $E_n(\mathbf{p}_k)\to E'$.

Suppose $E_n(\mathbf{p}_k)$ does not converge to E', then there exists a subsequence $(\mathbf{p}_{k_l})$ such that $E_n(\mathbf{p}_{k_l})\to E^*$, $E^*\neq E'$. Assume $E^*<E'$. Taking into account item (2) of Lemma 5 we get $E^*=\lambda_{n-1}$ or $E'=\lambda_n$. In both the cases we have

$$\lim_{\zeta\to E^*}[Q(\zeta;\mathbf{q})-\alpha]\geqslant 0 \quad\text{and}\quad \lim_{\zeta\to E'}[Q(\zeta;\mathbf{q})-\alpha]\leqslant 0.$$

Take some real numbers E_1 and E_2 such that $E^*<E_1<E_2<E'$. Then by the strict monotonicity of $\zeta\mapsto Q(\zeta;\mathbf{q})$ we have

$$0\leqslant Q(E_1;\mathbf{q})-\alpha<Q(E_2,\mathbf{q})-\alpha\leqslant 0\,.$$

This is a contradiction. ■

The following theorem is the main result of this section.

Theorem 2: *For each fixed $\alpha\in\mathbb{R}$ there is a sequence $(E_n(\mathbf{q}))_{n\in\mathbb{N}}$ of continuous functions of $\mathbf{q}\in\mathbb{R}^3$ with the following properties:*

(1) $\lambda_{n-1}\leqslant E_n(\mathbf{q})\leqslant\lambda_n$ *for all* $n\in\mathbb{N}$.
(2) For each $\mathbf{q}\in\mathbb{R}^3$ *the set consisting of all* $E_n(\mathbf{q})$ *and all the numbers* λ_n *with multiplicities* $k_n>1$ *form the complete collection of the eigenvalues of the operator* $H_\alpha(\mathbf{q})$.
(3) If $\lambda_{n-1}<E_n(\mathbf{q})<\lambda_n$, *then* $E_n(\mathbf{q})$ *is a unique solution of the Eq. (9) on the interval* $(\lambda_{n-1},\lambda_n)$.
(4) If $\zeta=\lambda_n$ *is a pole of the function* $\zeta\mapsto Q(\zeta;\mathbf{q})$, *then* $E_{n-1}(\mathbf{q})<\lambda_n<E_n(\mathbf{q})$.
(5) If $\zeta=\lambda_n$ *is not a pole of the function* $\zeta\mapsto Q(\zeta;\mathbf{q})$, *then we have the following assertions:*
(a) if $Q(\lambda_n;\mathbf{q})-\alpha<0$, *then* $E_n(\mathbf{q})=\lambda_n<E_{n+1}(\mathbf{q})$;
(b) if $Q(\lambda_n;\mathbf{q})-\alpha>0$, *then* $E_n(\mathbf{q})<\lambda_n=E_{n+1}(\mathbf{q})$;
(c) if $Q(\lambda_n;\mathbf{q})-\alpha=0$, *then* $E_n(\mathbf{q})=\lambda_n=E_{n+1}(\mathbf{q})$.

Proof: Consider the functions $E_n(\mathbf{q})$ given by Proposition 2. Then (1) is obvious by definition of $E_n(\mathbf{q})$. Assertion (2) follows from Theorem 1. Assertions (3) and (4) were proven in Lemma 5. It remains to prove (5).

Let λ_n be not a pole of $\zeta\mapsto Q(\zeta;\mathbf{q})$. Suppose $Q(\lambda_n;\mathbf{q})-\alpha<0$. For any positive integer m we choose a number E'_m such that $\lambda_n-1/m<E'_m<\lambda_n$; then $Q(E'_m;\mathbf{q})-\alpha<0$. Further, we choose points $\mathbf{q}_m\in\mathbb{R}^3$ such that λ_{n-1} and λ_n are not poles of the function $\zeta\mapsto Q(\zeta;\mathbf{q}_m)$ (that is $\mathbf{q}_m\in X_{m-1}\cap X_m$), and such that $|\mathbf{q}-\mathbf{q}_m|<1/m$ and $Q(E'_m;\mathbf{q}_m)-\alpha<0$. Then $\zeta=E_n(\mathbf{q}_m)$ is a solution

of the equation $Q(\zeta;\mathbf{q}_m)-\alpha=0$ lying in the interval $(\lambda_{n-1},\lambda_n)$. Since $Q(\zeta;\mathbf{q}_m)$ is a strictly monotone function of ζ on this interval, the inequalities $E'_m<E_n(\mathbf{q}_m)<\lambda_n$ take place for all m. Thus $E_n(\mathbf{q}_m)\to\lambda_n$ and $\mathbf{q}_m\to\mathbf{q}$ as $m\to\infty$; therefore, $\lambda_n=E_n(\mathbf{q})$ by the definition of the function $E_n(\mathbf{q})$. According to Lemma 5, $Q(\lambda_n;\mathbf{q})-\alpha\geqslant 0$, if $\lambda_n=E_{n+1}(\mathbf{q})$; therefore $\lambda_n<E_{n+1}(\mathbf{q})$. Hence, item (5a) is proved. The proofs of items (5b) and (5c) are similar. ■

Theorem 2 gives a useful description of the spectrum of H_α. Namely, denote by M the set $\{m\in\mathbb{N}: k_m>1\}$ and together with the functions $E_n(\mathbf{q})$ introduce a sequence of constant functions $\Lambda_m^{(k)}(\mathbf{q})=\lambda_m$, where $m\in M$, $k=1,\ldots,k_m-1$. Then $E_n(\mathbf{q})\leqslant\Lambda_n^{(k)}(\mathbf{q})\leqslant E_{n+1}(\mathbf{q})$ for all $n\in M$, $k=1,\ldots,k_n-1$, and for any fixed $\mathbf{q}\in\mathbb{R}^3$ the union of the sequences $(E_n(\mathbf{q}))_{n\in\mathbb{N}}$ and $(\Lambda_m^{(k)}(\mathbf{q}))_{m\in M,k=1,\ldots,k_m-1}$ forms the complete set of the eigenvalues of $H_\alpha(\mathbf{q})$ multiplicity counting. If $\mathbf{q}\in\cap_{n=0}^{\infty}X_n$, then every $E_n(\mathbf{q})$ is distinct from the numbers $\Lambda_m^{(k)}(\mathbf{q})$. Since $\mathbb{R}\backslash\cap_{n=0}^{\infty}X_n$ is the set of the first Baire category, for a generic $\mathbf{q}$ the point perturbation levels $E_n(\mathbf{q})$ are distinct from the levels of the unperturbed operator H^0.

VI. POINT PERTURBATIONS OF THE HARMONIC OSCILLATOR

Here we apply the results of the previous sections to the Hamiltonian (2) with the potential

$$V(\mathbf{r})=\frac{\mu\Omega_x^2}{2}x^2+\frac{\mu\Omega_y^2}{2}y^2+\frac{\mu\Omega_z^2}{2}z^2\,, \tag{13}$$

where Ω_j $(j=x,y,z)$ are the frequencies of the oscillator. The function V can be considered as a confinement potential of a quantum well in $\mathbb{R}^3$ with the characteristic sizes

$$L_j=\sqrt{\frac{\hbar}{2\mu\Omega_j}},\qquad j=x,y,z$$

(numbers $\sqrt{2}L_j$ are called also *length parameters* of the oscillator[41]). Therefore the operator with potential (13) can be used as the Hamiltonian of a (generally speaking, asymmetric) quantum dot.[1] It is convenient to pass to dimensionless coordinates $\mathbf{x}=\mathbf{r}/L$, where $L=\sqrt[3]{L_xL_yL_z}$. In the coordinates $\mathbf{x}=(x_1,x_2,x_3)$ the operator $\hat{H}^0$ takes the form $\hat{H}^0=\hbar\Omega H^0$, where

$$H^0=-\Delta+\tfrac{1}{4}(\omega_1^2x_1^2+\omega_2^2x_2^2+\omega_3^2x_3^2)\,,$$

$$\Omega=\sqrt[3]{\Omega_x\Omega_y\Omega_z}\,,\quad \omega_1=\frac{\Omega_x}{\Omega},\quad \omega_2=\frac{\Omega_y}{\Omega},\quad \omega_3=\frac{\Omega_z}{\Omega}$$

(hence, $\omega_1\omega_2\omega_3=1$).

Further we discuss the properties of H^0. The spectrum of this operator consists of the eigenvalues

$$\lambda_{n_1n_2n_3}=\omega_1(n_1+1/2)+\omega_2(n_2+1/2)+\omega_3(n_3+1/2)\,,$$

where $n_1,n_2,n_3\in\mathbb{N}$. The corresponding normalized eigenfunctions are

$$\Phi_{n_1n_2n_3}(\mathbf{x})=\varphi_{n_1}(x_1)\varphi_{n_2}(x_2)\varphi_{n_3}(x_3)\,,$$

where

$$\varphi_{n_j}(x_j)=\left(\frac{\omega_j}{2\pi}\right)^{1/4}(2^{n_j}n_j!)^{-1/2}\exp\left(-\frac{1}{4}\omega_jx_j^2\right)H_n\left(\sqrt{\frac{\omega_j}{2}}x_j\right)$$

is the oscillator function [$H_n(x)$ is the Hermite polynomial of degree n].

If the frequencies $\omega_1, \omega_2, \omega_3$ are independent over the ring $\mathbb{Z}$ (this is the generic case), then the spectrum of H^0 is simple; therefore, the multiplicity of the eigenvalues of $H_\alpha(\mathbf{q})$ does not exceed 2 and the part σ_2 of the spectrum $\mathrm{spec}\,(H_\alpha(\mathbf{q}))$ is always empty. On the other hand, since $H_n(0)=0$ if and only if n is odd, $\lambda_{n_1,n_2,n_3} \in \mathrm{spec}(H_\alpha(0))$ if and only if one of the numbers n_j $(j=1,2,3)$ is odd; hence, $\mathrm{spec}(H^0)\backslash\sigma(0)$ is always infinite. In addition, for all $n>0$ the set $\mathbb{R}^3\backslash X_n$ is infinite.

In general case, there are no explicit expressions for the Green functions of the harmonic oscillator in terms of commonly used elementary or special functions. Nevertheless, in a number of cases, the representation of the Green function $G^0(\mathbf{x},\mathbf{y};E)$ as the Laplace transform of the heat kernel $K(\mathbf{x},\mathbf{y};t)$ for H^0 is very useful to investigate some properties of the Krein $\mathcal{Q}$-function. The heat kernel for H^0 has the form (see, e.g., in Ref. 42):

$$K^0(\mathbf{x},\mathbf{y};t)=\prod_{j=1}^{3}\left(\frac{1}{4\pi \mathrm{sh}\omega_j t}\right)^{1/2}\exp\left(-\frac{\omega_j}{4\mathrm{sh}\omega_j t}((x_j^2+y_j^2)\mathrm{ch}\omega_j t-2x_j y_j)\right).$$

Using the heat kernel K^f for the free Hamiltonian $H^f=-\Delta$,

$$K^f(\mathbf{x},\mathbf{y};t)=(4\pi t)^{-3/2}\exp\left(-\frac{(\mathbf{x}-\mathbf{y})^2}{4t}\right),$$

and the $\mathcal{Q}$-function for H_f,

$$Q^f(\zeta)=-\frac{\sqrt{-\zeta}}{4\pi},$$

we get immediately from the formula

$$G(\mathbf{x},\mathbf{y};E)=\int_0^\infty e^{tE}K(\mathbf{x},\mathbf{y};t)\,dt,$$

that for $\mathrm{Re}\,\zeta<(\omega_1+\omega_2+\omega_3)/2$ the following representation of the $\mathcal{Q}$-function for H^0 takes place:

$$Q(\zeta;\mathbf{q})=-\frac{\sqrt{-\zeta}}{4\pi}+\frac{1}{(4\pi)^{3/2}}\int_0^\infty\left(\prod_{j=1}^{3}\left(\frac{1}{\mathrm{sh}\omega_j t}\right)^{1/2}\exp\left(-\frac{1}{2}q_j^2\omega_j\mathrm{th}\frac{\omega_j t}{2}\right)-\frac{1}{t^{3/2}}\right)e^{\zeta t}\,dt. \quad (14)$$

It is clear from (14) that $(\partial Q/\partial q_j)(E;\mathbf{q})<0$ for $q_j>0$, if $E<\lambda_0=(\omega_1+\omega_2+\omega_3)/2$. Since $\partial Q/\partial E>0$ for $E\in\mathbb{R}\backslash\mathrm{spec}\,(H^0)$, (9) implies that $\partial E_0/\partial q_j>0$. In particular, the depth of the lowest impurity level $\lambda_0-E_0(\mathbf{q})$ decreases if $|\mathbf{q}|$ increases in such a way that the inner product $\mathbf{a}\cdot\mathbf{q}$ remains positive for each vector $\mathbf{a}$ with positive coordinates. In the spherically symmetric case $\omega_1=\omega_2=\omega_3$, we have $\partial Q/\partial q<0$, where $q=|\mathbf{q}|>0$, and the depth decreases with increasing of q. This phenomenon was discovered numerically for a spherically symmetric quantum dot in Ref. 14 and called *positional disorder*. We see that the positional disorder is common to each parabolic quantum dot, not only to the spherically symmetric one. The similar result is valid in the two-dimensional case, i.e., for the case of impurities in a quantum well (see numerical results in Ref. 14). Our arguments are valid in the two-dimensional case also, thus we have a strict proof for the positional disorder in a two-dimensional quantum well.

The more detailed analysis is possible in the case of the *isotropic oscillator:* $\Omega_x=\Omega_y=\Omega_z$ $(=\Omega)$, i.e., in the case of a spherically symmetric quantum dot. In this case $\omega_1=\omega_2=\omega_3=1$ and the spectrum of H^0 consists of the eigenvalues

$$\lambda_n=n+\tfrac{3}{2},\quad n\in\mathbb{N},$$

where λ_n has the multiplicity $k_n=(n+1)(n+2)/2$. In this case there are natural units of length (namely, L) and of energy ($\hbar\Omega$). Therefore, the following very important scaling properties takes place. Denote by $\hat{Q}(\zeta;\mathbf{q})$ the Krein $\mathcal{Q}$-function for the operator $\hat{H}^0$ keeping the notation $Q(\zeta;\mathbf{q})$ for the $\mathcal{Q}$-function of H^0. Then

$$\hat{Q}(\zeta;\mathbf{q})=\frac{1}{\hbar\Omega L^3}Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=4\pi\frac{\mu}{2\pi\hbar^2 L}Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right).$$

Denote $\mu/(2\pi\hbar^2 L)$ by α^0; obviously, α^0 is strength of the point potential corresponding to the scattering length L. Then Eq. (9) takes the form

$$4\pi Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=\frac{\alpha}{\alpha^0}, \tag{15}$$

or, equivalently,

$$4\pi Q\left(\frac{\zeta}{\hbar\Omega};\frac{\mathbf{q}}{L}\right)=\frac{L}{\ell_s}.$$

Equation (15) shows that a change of the frequency Ω does not change the numerical values of energy levels in the spectrum of $\hat{H}^0$ if L is used as the unit of length, $\hbar\Omega$ as the unit of energy and α^0 as the unit of point potential strength.

In the case of isotropic oscillator, the set $\sigma(\mathbf{q})$ has a simple description:

Proposition 3: Let $\Omega_x=\Omega_y=\Omega_z$. *Then* $\sigma(\mathbf{q})=\{\lambda_{2n}: n\in\mathbb{N}\}$, *if* $\mathbf{q}=0$, *and* $\sigma(\mathbf{q})=\mathrm{spec}(H^0)$ *otherwise*.

Proof: Each λ_n is equal to $\lambda_{n_1n_2n_3}$, where $n_1+n_2+n_3=n$. If n is odd, then at least one of n_j is odd, and $\Psi_{n_1n_2n_3}(0)=0$. Therefore, $\lambda_n\notin\sigma(0)$. On the other hand, if n is even, then $\Psi_{n00}(0)\neq 0$, and therefore, $\lambda_n\in\sigma(0)$.

Let now $\mathbf{q}\neq 0$. First we remark that for all $n\in\mathbb{N}$ the following assertion is valid:

Lemma 6: If $H_n(x_0)=0$, *then* $H_{n+1}(x_0)\neq 0$.

Proof of the lemma: For all $n\in\mathbb{N}$ the following relation takes place:[43]

$$H'_{n+1}(x)=2(n+1)H_n(x).$$

If $H_n(x_0)=H_{n+1}(x_0)=0$, then $H'_n(x_0)=0$. Since $y=H_n(x)$ is a solution to the differential equation $y''-2xy'+2ny=0$, we have $H_n(x)=0$ for all x; but this is impossible. ■

Let us return to the proof of the proposition. Suppose that $\mathbf{q}\neq 0$; without loss of generality we can assume $q_2\neq 0$. Since $H_1(x)=0$ only for $x=0$, and $H_0(x)\neq 0$ for all x, we have $\lambda_0,\lambda_1\in\sigma(\mathbf{q})$. Let $n>1$. Suppose that $\Phi_{n-1,1,0}(\mathbf{q})=0$, then according to Lemma 6, $\Phi_{n,0,0}(\mathbf{q})\neq 0$. ■

Using Proposition 3 we can give the complete description of the spectrum $H_\alpha(\mathbf{q})$ in the case of an isotropic H^0. Moreover, in this case the explicit form of the Green function $G^0(\mathbf{x},\mathbf{x}';\zeta)$ is known, and therefore, we can give the explicit form of the Krein $\mathcal{Q}$-function and eigenfunction of $H_\alpha(\mathbf{q})$. In particular, the equation for the point perturbation levels $E_n(\mathbf{q})$ can be obtained in an explicit form. The mentioned Green function has the form[18]

$$G^0(\mathbf{x},\mathbf{y};\zeta)=-\frac{1}{2(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\left[\frac{U(-\zeta;\xi)U'(-\zeta;-\eta)+U'(-\zeta;\xi)U(-\zeta;-\eta)}{|\mathbf{x}-\mathbf{y}|}\right.$$
$$\left.+\frac{U(-\zeta;\xi)U'(-\zeta;-\eta)-U'(-\zeta;\xi)U(-\zeta;-\eta)}{|\mathbf{x}+\mathbf{y}|}\right], \tag{16}$$

where $\xi=(|\mathbf{x}+\mathbf{y}|+|\mathbf{x}-\mathbf{y}|)/2$, $\eta=(|\mathbf{x}+\mathbf{y}|-|\mathbf{x}-\mathbf{y}|)/2$, $U(\nu;z)$ is the parabolic cylinder function[44] (in the Whittaker notation $U(\nu;z)=D_{-\nu-1/2}(z)$), and U' denotes the derivative of U with respect to the second argument

$$U'(\zeta;y)=\frac{\partial}{\partial y}U(\zeta;y)\,.$$

Using (16), we get the following expression for the Q-function:

$$Q(\zeta;\mathbf{q})=-\frac{1}{8(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\Big[(q^2-4\zeta)U(-\zeta,q)U(-\zeta,-q)+4U'(-\zeta,q)U'(-\zeta,-q)$$
$$-\frac{2}{q}(U'(-\zeta,q)U(-\zeta,-q)-U(-\zeta,q)U'(-\zeta,-q))\Big], \tag{17}$$

where $q=|\mathbf{q}|$. Due to the symmetry of the problem, the $\mathcal{Q}$-function depends on q only, so we shall write often $Q(\zeta;q)$ instead of $Q(\zeta;\mathbf{q})$. Introducing the notation $\mathcal{U}(\zeta;y)=U(\zeta;y)U(\zeta;-y)$, we can rewrite (17) in the sometimes more useful form

$$Q(\zeta;\mathbf{q})=-\frac{1}{4(2\pi)^{3/2}}\Gamma\left(\frac{1}{2}-\zeta\right)\left[(q^2-4\zeta)\mathcal{U}(-\zeta;q)-\frac{1}{q}\mathcal{U}'(-\zeta;q)-\mathcal{U}''(-\zeta;q)\right], \tag{18}$$

where the prime denotes the derivative with respect to the second argument as before. Passing to limit we get at $q=0$

$$Q(\zeta;0)=-\frac{1}{\sqrt{8}\pi}\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}. \tag{19}$$

It is interesting to compare (19) with the Krein $\mathcal{Q}$-function $Q^{(1)}(\zeta;0)$ for the one-dimensional harmonic oscillator:[26]

$$Q^{(1)}(\zeta;0)=2^{-3/2}\frac{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}.$$

Curiously, in the case of the free Hamiltonian $H^0=-\Delta$, the $\mathcal{Q}$-functions Q_d for $d=1$ and for $d=3$ are also related as follows:

$$Q_1^{-1}(\zeta)=-8\pi Q_3(\zeta)\,. \tag{20}$$

Namely, for the free Hamiltonian $Q_1(\zeta)=(2\sqrt{-\zeta})^{-1}$, $Q_3(\zeta)=-(4\pi)^{-1}\sqrt{-\zeta}$. For $q\neq 0$ relation (20) for $\mathcal{Q}$-functions of the harmonic oscillators is violated.

It is useful to consider the behavior of the function $\zeta\mapsto Q(\zeta;q)$ near the singular points, i.e., near the poles and in a neighborhood of $-\infty$. Using properties of the parabolic cylinder functions,[43] we have

$$Q(\zeta;0)=-\frac{(2n+1)!!}{(2\pi)^{3/2}(2n)!!}\left(\frac{1}{\zeta-\lambda_{2n}}-\ln 2+1-\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k(1+2k)}+O(\zeta-\lambda_{2n})\right),$$

as $\zeta\to\lambda_{2n}$. If $\mathbf{q}\neq 0$, the coefficients for corresponding asymptotics are cumbrous enough, and we give the leading term only:

$$Q(\zeta;q)=-\frac{\exp(-q^2/2)}{(2\pi)^{3/2}2^{n+2}n!}(2(n+1)H_n^2(q/\sqrt{2})+\sqrt{2}(q^{-1}-q)H_n(q/\sqrt{2})H_{n+1}(q/\sqrt{2})$$
$$+H_{n+1}^2(q/\sqrt{2}))(\zeta-\lambda_n)^{-1}+O(1)\,, \tag{21}$$

as $\zeta\to\lambda_n$.

For $\mathrm{Re}\,\zeta\to-\infty$, we have

$$Q(\zeta;q)=-\frac{\sqrt{-\zeta}}{4\pi}\left(1-\frac{q^2}{8}\zeta^{-1}+\frac{8-q^4}{128}\zeta^{-2}+O(\zeta^{-3})\right). \tag{22}$$

It is important to note that the leading term in (22) coincides with the Krein $\mathcal{Q}$-function for the free Hamiltonian $-\Delta$.

Now consider the properties of the function $q\mapsto Q(\zeta;q)$. Since $U(\nu;z)$ is an entire function of z, the function $q\mapsto Q(\zeta;q)$ at $\zeta\notin\mathrm{spec}(H^0)$ can be extended to a real analytic even function on $\mathbb{R}$ [see (18)]. In particular,

$$\frac{\partial}{\partial q}Q(\zeta;0)=0\,.$$

As to the second derivative, we can obtain after some algebra

$$\frac{\partial^2}{\partial q^2}Q(\zeta;0)=\frac{1}{8\sqrt{6}\pi}\left[(4\zeta^2+1)\frac{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}-8\zeta\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}\right]. \tag{23}$$

For the fixed $\zeta\in\mathbb{R}\backslash\mathrm{spec}(H^0)$, the asymptotics of Q at $q\to\infty$ is given by

$$Q(\zeta;q)=-\frac{1}{8\pi}\left[q-\frac{2\zeta}{q}-\frac{1+2\zeta^2}{q^3}+O\left(\frac{1}{q^5}\right)\right]. \tag{24}$$

This follows from the asymptotics for $\mathcal{U}(\zeta;q)$ at $q\to\infty$:[45]

$$\mathcal{U}(\zeta;q)=\frac{\sqrt{2\pi}}{\Gamma\left(\frac{1}{2}+\zeta\right)}\left[\frac{1}{X}+O\left(\frac{1}{X^5}\right)\right],$$

where $X=\sqrt{q^2+4\zeta}$.

Further the following formula will be also useful

$$\frac{\partial Q}{\partial\zeta}(\zeta;0)=\frac{1}{4\sqrt{2}\pi}\frac{\Gamma\left(\frac{3}{4}-\frac{\zeta}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\zeta}{2}\right)}G\left(\frac{1}{2}-\zeta\right). \tag{25}$$

Here and below we use the standard notations[43]

$$G(z)=\psi\left(\frac{z}{2}+\frac{1}{2}\right)-\psi\left(\frac{z}{2}\right);\qquad \psi(z)=\frac{\Gamma'(z)}{\Gamma(z)}.$$

The plot of the graphs for the function $Q(\zeta;q)$ is shown in Figs. 1 and 2.

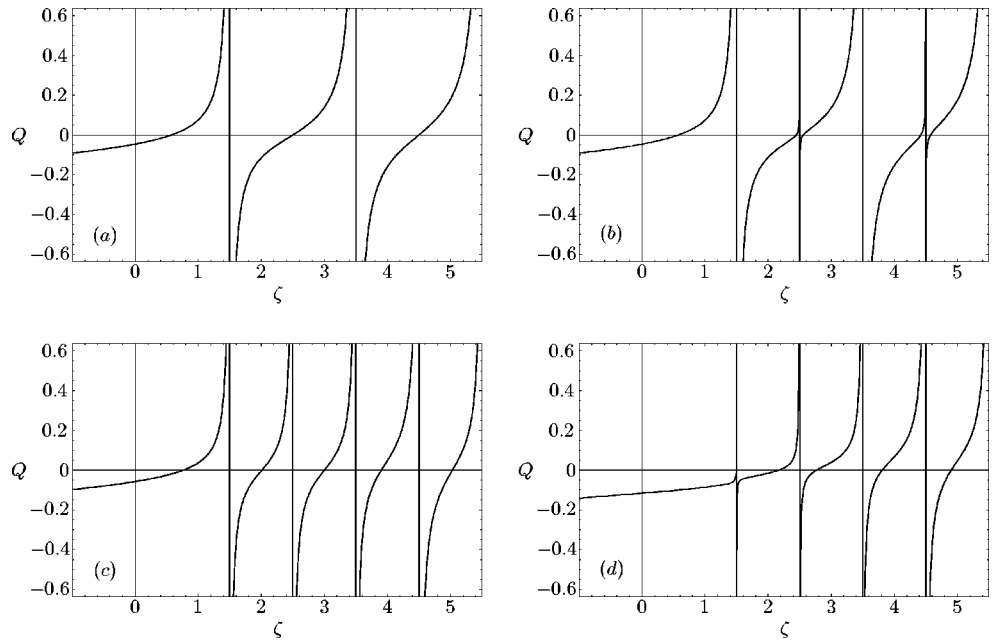

FIG. 1. Q as a function of ζ for (a) $q=0$, (b) $q=1/10$, (c) $q=1$, (d) $q=3$.

In the case of an isotropic oscillator, the functions $E_n(\mathbf{q})$ depend only on q and we will denote them by $E_n(q)$. Further properties of these functions [and, in particular, of the spectrum of $H_\alpha(\mathbf{q})$] for the isotropic case are given in Theorem 3 below, which is one of the main results of the article.

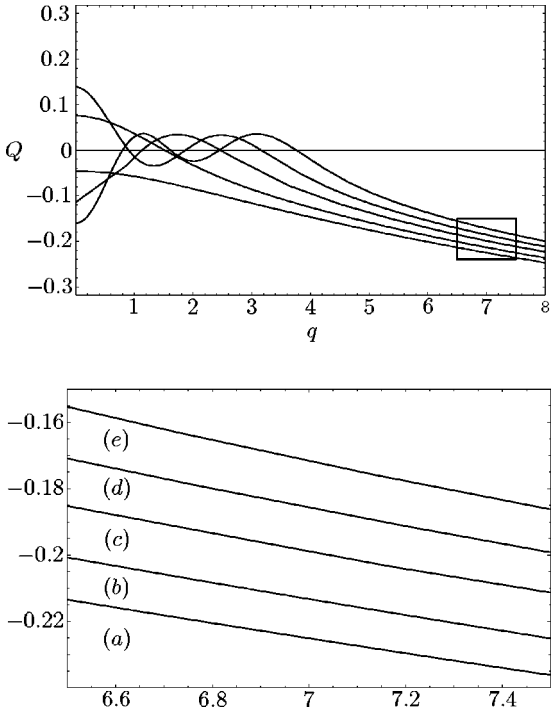

FIG. 2. Q as a function of q for (a) $\zeta=0$, (b) $\zeta=1$, (c) $\zeta=2$, (d) $\zeta=3$, (e) $\zeta=4$.

Theorem 3: *The following assertions take place.*

(1) The functions $E_n(q)$, $n\in\mathbb{N}$ *are real-analytic. If* $\alpha=0$ *and* $n>0$, *then in a vicinity of zero, these functions are continuous branches of a two-valued analytic function.*

(2a) $E_0(0)<\lambda_0$ *for each* α, $\alpha\in\mathbb{R}$.

(2b) If $\alpha>0$, *then* $E_{2n+1}(0)=\lambda_{2n+1}$ *and* $\lambda_{2n+1}<E_{2n+2}(0)<\lambda_{2n+2}\forall n\in\mathbb{N}$.

(2c) If $\alpha<0$, *then* $\lambda_{2n}<E_{2n+1}(0)<\lambda_{2n+2}$ *and* $E_{2n+2}(0)=\lambda_{2n+2}\forall n\in\mathbb{N}$.

(2d) If $\alpha=0$, *then* $E_{2n+1}(0)=E_{2n+2}(0)=\lambda_{2n+1}\forall n\in\mathbb{N}$.

(3a) If $\alpha\neq 0$, *then for any* $n>0$

$$\frac{\partial E_n}{\partial q}(0)=0\,. \tag{26}$$

If $n=0$, *then* (26) *is valid for any* α.

(3b) *If* $\alpha>0$ (*respectively,* $\alpha<0$), *then*

$$\frac{\partial^2 E_n}{\partial q^2}(0)=\frac{1}{8\sqrt{6}G\left(\frac{1}{2}-E_n(0)\right)}\left(\frac{4E_n^2(0)+1}{8\pi^2\alpha^2}-8E_n(0)\right), \tag{27}$$

for any even (respectively, odd) n. *If* $n=0$, *then* (27) *is valid for any* α.

(3c) *If* $\alpha=0$, *then* $(\partial E_{2n+1}/\partial q)(0)<0$, $(\partial E_{2n+2}/\partial q)(0)>0$, *and* $(|(\partial E_{2n+1}/\partial q)(0)|=|(\partial E_{2n+2}/\partial q)(0)|\forall n\in\mathbb{N}$.

(4) *If* $q\neq 0$, *then* $\lambda_{n-1}<E_n(q)<\lambda_n\forall n\in\mathbb{N}$.

(5) $\lim_{q\to\infty}E_n(q)=\lambda_n\forall n\in\mathbb{N}$.

Proof: Item (4) follows immediately from Proposition 3 and the definition of the functions E_n. Formula (19) shows that $Q(\zeta;0)=0$ if and only if $\zeta=\lambda_{2n+1}$ for some $n\in\mathbb{N}$; therefore, items (2a)–(2d) follow from Theorem 2. Using the standard version of the implicit function theorem and the Proposition 3 again, we see that $E_n(q)$ are real analytic at $q>0$. Moreover, item (3) of Theorem 2 implies that (i) $E_n(q)$ are real-analytic at $q=0$ for even n if $\alpha>0$, (ii) $E_n(q)$ are real-analytic at $q=0$ for odd n if $\alpha<0$, and (iii) $E_0(q)$ is real-analytic at $q=0$ for any α. In all these cases, the derivatives of E_n can be found from the equations

$$\frac{\partial Q}{\partial\zeta}\frac{\partial E_n}{\partial q}+\frac{\partial Q}{\partial q}=0\,,$$

$$\frac{\partial Q}{\partial\zeta}\frac{\partial^2 E_n}{\partial q^2}+\frac{\partial^2 Q}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+2\frac{\partial^2 Q}{\partial\zeta\partial q}\frac{\partial E_n}{\partial q}+\frac{\partial^2 Q}{\partial q^2}=0. \tag{28}$$

Since $(\partial Q/\partial q)(E;0)=0$ if $E\notin\mathrm{spec}(H^0)$, equation (26) follows from (28) in the considered cases. In virtue of (26), the second derivative of E_n is given by

$$\frac{\partial^2 E_n}{\partial q^2}(0)=-\frac{\partial^2 Q}{\partial q^2}\left(\frac{\partial Q}{\partial\zeta}\right)^{-1}(E_n(0);0). \tag{29}$$

Substituting (23) and (25) into (29) and using (9) we get (27).

Now consider the singular case when $E_n(0)$, $n\geqslant 1$, coincides with a point of the form λ_{2m+1}. In a neighborhood of the point $(E_n(0),0)$, introduce the function

$$\tilde{Q}_\alpha(\zeta;q)=\frac{Q(\zeta;q)-\alpha}{\Gamma\left(\frac{1}{2}-\zeta\right)},$$

which is smooth with respect to (ζ,q) and analytic with respect to the first argument ζ. In a vicinity of $(E_n(0),0)$ we have

$$\tilde{Q}_\alpha(E_n(q);q)=0\,. \tag{30}$$

Further,

$$\frac{\partial\tilde{Q}_\alpha}{\partial\zeta}=\frac{1}{\Gamma(1/2-\zeta)}\,\frac{\partial Q}{\partial\zeta}+(Q-\alpha)\frac{\Gamma'(1/2-\zeta)}{\Gamma^2(1/2-\zeta)}. \tag{31}$$

Since $(\partial Q/\partial\zeta)(\zeta;0)$ is a finite number at $\zeta=\lambda_{2m+1}$ and $\Gamma(1/2-\zeta)$ has a pole at λ_{2m+1}, the first term in (31) vanishes at the point $(\lambda_{2m+1},0)$. The value of the function $\Gamma'(1/2-\zeta)/\Gamma^2(1/2-\zeta)$ at $\zeta=\lambda_{2m+1}$ is a nonzero finite number. Finally, $Q(\lambda_{2m+1},0)=0$; thus $\partial\tilde{Q}_\alpha/\partial q$ vanishes at the point λ_{2m+1} if and only if $\alpha=0$. Therefore, if $\alpha\neq 0$, then each function $E_n(q)$ has an analytic continuation in a neighborhood of the point $q=0$. Since $q\mapsto\tilde{Q}_\alpha(\lambda_{2m+1};q)$ is an even function, we get easily (26).

Let now $\alpha=0$. Then

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}=\frac{1}{\Gamma(1/2-\zeta)}\,\frac{\partial^2 Q}{\partial\zeta^2}+2\,\frac{\Gamma'(1/2-\zeta)}{\Gamma^2(1/2-\zeta)}\,\frac{\partial Q}{\partial\zeta}-Q\,\frac{\Gamma''(1/2-\zeta)\Gamma(1/2-\zeta)-2\Gamma'^2(1/2-\zeta)}{\Gamma^3(1/2-\zeta)}. \tag{32}$$

It is easy to see that the first and last terms in (32) vanishes at the point $(\lambda_{2m+1},0)$, whereas the second one does not. Therefore, $\partial^2\tilde{Q}_0/\partial\zeta^2\neq 0$ at the point $(\lambda_{2m+1},0)$, and $E_n(q)$ being solutions of (30), are continuous branches a two-valued analytic function in a vicinity of $(\lambda_{2m+1},0)$. Obviously, at the point $(\lambda_{2m+1},0)$ the following relation is valid

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+2\,\frac{\partial^2\tilde{Q}_0}{\partial\zeta\partial q}\,\frac{\partial E_n}{\partial q}+\frac{\partial\tilde{Q}_0}{\partial\zeta}\,\frac{\partial^2 E_n}{\partial q^2}+\frac{\partial^2\tilde{Q}_0}{\partial q^2}=0\,.$$

Since $\partial\tilde{Q}_0/\partial\zeta=0$ at the considered point, we get the quadratic equation for $\partial E_n/\partial q$:

$$\frac{\partial^2\tilde{Q}_0}{\partial\zeta^2}\left(\frac{\partial E_n}{\partial q}\right)^2+\frac{\partial^2\tilde{Q}_0}{\partial q^2}=0\,.$$

As a result, we complete the proof of items (1) and (3c). It remains to prove (5). Fix $n\in\mathbb{N}$ and let ε, $0<\varepsilon<1$, is given. According to (24) we can choose $q_0>0$ such that $Q(\lambda_n-\varepsilon;q)-\alpha<0$ if $q\geqslant q_0$. Since $Q(E_n(q);q)-\alpha=0$ and the function $E\mapsto Q(E;q)$ increases in the interval $\lambda_{n-1}<E<\lambda_n$, we have $E_n(q)>\lambda_n-\varepsilon$ as $q\geqslant q_0$. Moreover, $E_n(q)<\lambda_n$, and the proof is completed. ■

The structure of $\mathrm{spec}(H_\alpha(q))$ given by Theorem 3 is presented in Table I. The peculiarities of this table at $q=0$ can be understood from the point of view the symmetry group of the problem. It is well known that for a generic spherically symmetric potential $V(\mathbf{r})$, the eigenvalues λ of the operator $H^0=-\Delta+V$ are parametrized by three quantum numbers: $\lambda=\lambda_{n_r,l,m}$, where n_r $(n_r=0,1,\ldots)$ is the so called principal (or total) quantum number; l $(l=0,1,\ldots)$ is the orbital quantum number, and m $(m=-l,-l+1,\ldots,l-1,l)$ is the magnetic quantum number. Each eigenvalue $\lambda_{n_r,l,m}$ is degenerate with multiplicity $2l+1$, namely, $\lambda_{n_r,l,m}=\lambda_{n_r,l,m'}$ if $m,m'\in\{-l,-l+1,\ldots,l-1,l\}$. This degeneracy is related to the invariance of H^0 with respect to the rotation group $\mathrm{SO}(3)$: eigensubspaces of H^0 carry an irreducible representation of this group. In general, $\lambda_{n_r,l,m}\neq\lambda_{n_r',l',m'}$ if $n_r\neq n_r'$ or $l\neq l'$. The eigenvalues of an isotropic harmonic oscillator have an additional (so-called accidental) degeneracy: Each eigensubspace L_n is decomposed on the sub-

TABLE I. The structure of $\mathrm{spec}(H_\alpha(q))$.

	$q=0$	$q\neq 0$
$\alpha>0$	$\sigma_1=\{E_{2n}(0): n\in\mathbb{N}\}$	$\sigma_1=\{E_n(q): n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}: n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}: n\in\mathbb{N}\}$
	$\sigma_3=\{\lambda_{2n+1}: n\in\mathbb{N}\}$	$\sigma_3=\varnothing$
	$\sigma_4=\varnothing$	$\sigma_4=\varnothing$
$\alpha=0$	$\sigma_1=\{1/2\}$	$\sigma_1=\{E_n(q): n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}: n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}: n\in\mathbb{N}\}$
	$\sigma_3=\varnothing$	$\sigma_3=\varnothing$
	$\sigma_4=\{\lambda_{2n+1}: n\in\mathbb{N}\}$	$\sigma_4=\varnothing$
$\alpha<0$	$\sigma_1=\{E_{2n+1}(0): n\in\mathbb{N}\}\cup\{E_0(0)\}$	$\sigma_1=\{E_n(q): n\in\mathbb{N}\}$
	$\sigma_2=\{\lambda_{2n+2}: n\in\mathbb{N}\}$	$\sigma_2=\{\lambda_{n+1}: n\in\mathbb{N}\}$
	$\sigma_3=\{\lambda_{2n+1}: n\in\mathbb{N}\}$	$\sigma_3=\varnothing$
	$\sigma_4=\varnothing$	$\sigma_4=\varnothing$

spaces $L_n^{(l)}$ with angular momentum $l=n,n-2,\ldots,0$ (if n is even) or $l=n,n-2,\ldots,1$ (if n is odd). This accidental degeneracy is related to the invariance of the Hamiltonian H^0 of an isotropic harmonic oscillator with respect to the group $\mathbb{U}(3)$. Indeed,

$$H^0=\sum_{j=1}^{3} a_j^+ a_j+\tfrac{3}{2},$$

where a_j^+ and a_j are standard creation and annihilation operators.[41] Therefore, H^0 is invariant with respect to the transformation

$$a_j\to a_j'=\sum_{j=1}^{3} u_{kj}a_j, \qquad a_j^+\to a'^+_j=\sum_{j=1}^{3} u_{kj}^* a_j^+,$$

where (u_{jk}) is a unitary matrix. If $q=0$, then $H_\alpha(0)$ is a spherically symmetric perturbation of H^0 that violates the $\mathbb{U}(3)$-symmetry. To prove this, we note that operators $a_j^+ a_k$ are generators of the Lie group $\mathfrak{u}(3)$. Therefore, if $H_\alpha(0)$ is invariant with respect to the considered representation of $\mathbb{U}(3)$, we must have $[H_\alpha(0),H^0]=0$. On the other hand it is easy to show that for $\zeta\in\mathbb{C}\backslash\mathbb{R}$ the operator $[R_\alpha(\zeta),R^0(\zeta)]$ has a nonzero integral kernel.

Since point perturbations cannot change states with nonzero angular momentum l (see, e.g., 8), the part σ_2 (at $q=0$) may contain only even eigenvalues λ_{2n} and we see this in Table I. Since all states from L_n have the same parity $(-1)^n$, the isotropic oscillator has no stationary states with a nonzero dipole momentum.[35] On the other hand every eigensubspace of $H_0(0)$ with eigenvalue from σ_4 have an eigenfunction with $l=0$ (this is the eigenfunction from item 4 of Theorem 1). Therefore, point perturbations of an isotropic harmonic oscillator can lead to an appearance of eigenstates with nonzero dipole momentum.

An alternative tool to understand the energy degeneracy of the three-dimensional isotropic oscillator gives the supersymmetry theory.[46–48] We will not dwell here on this approach, nevertheless note that the analysis performed in the cited papers requires a modification in the s-channel only.

The functions E_n depend not only on the position parameter q, but also on the strength α; we will denote these dependencies as $E_n=E_n(q,\alpha)$. If $E(q,\alpha_0)$ coincides with one of the numbers $\mathcal{E}_m$, then in a vicinity of α_0, the function $\alpha\mapsto E_n(q,\alpha)$ is a continuous branch of the inverse function to $E\mapsto Q(E;q)$. It is already known from Proposition 1 that the following limits take place:

$$\lim_{\alpha\to+\infty} E_n(q;\alpha)=\lambda_n, \qquad \lim_{\alpha\to-\infty} E_n(q;\alpha)=\lambda_{n-1},$$

where $\lambda_{-1}=-\infty$. Now we make more precise this behavior. From (22) we get the asymptotics of the function $E_0(q;\alpha)$ for the fixed $q\geqslant 0$ as $\alpha\to-\infty$,

$$E_0(q;\alpha)=-16\pi^2\alpha^2+\frac{q^2}{4}+\frac{1}{128\pi^2\alpha^2}+O\left(\frac{1}{\alpha^4}\right), \tag{33}$$

or in terms of the point perturbation of the initial operator (1)

$$E_0(q;\alpha)=-\frac{\hbar^2}{2\mu l_s^2}+\frac{\mu\Omega^2 q^2}{2}+\frac{\mu\Omega^2 l_s^2}{4}+O(l_s^4), \tag{34}$$

where the scattering length l_s tends to 0. Expression (34) means that up to the infinitely small term $O(l_s^2)$ the ground state of $\hat{H}_\alpha(\mathbf{q})$ equals to the ground state of the point perturbation of the free Hamiltonian $-\hbar^2\Delta/2\mu$ with the same scattering length l_s shifted by the potential $V(\mathbf{r})=\mu\Omega^2\mathbf{r}^2/2$ at the point $\mathbf{r}=\mathbf{q}$. Equation (34) shows that at least for the isotropic harmonic oscillator its potential can be recovered from the dependence of the ground state of the point perturbation on the position of the potential support. It is reasonable to suppose that this is true for more general forms of the potential V; we consider this conjecture elsewhere.

Now consider the behavior of $E_n(q;\alpha)$ in a vicinity of the poles of $Q(\zeta,q)$. We start with the general case $q\neq 0$. Using (21) we get as $\alpha\to\pm\infty$

$$\begin{aligned}E_n(q;\alpha)=\lambda_n^{\pm}-\frac{\exp(-q^2/2)}{(2\pi)^{3/2}2^{n+2}n!}&(2(n+1)H_n^2(q/\sqrt{2})+\sqrt{2}(q^{-1}-q)H_n(q/\sqrt{2})H_{n+1}(q/\sqrt{2})\\&+H_{n+1}^2(q/\sqrt{2}))\alpha^{-1}+O(\alpha^{-2}),\end{aligned} \tag{35}$$

where $\lambda_n^+=\lambda_n$ and $n\geqslant 0$ as $\alpha\to+\infty$, and $\lambda_n^-=\lambda_{n-1}$ and $n\geqslant 1$ as $\alpha\to-\infty$.

In the case $q=0$, we are in position to give a compact form for more precise asymptotics of $E_n(q;\alpha)$. Denote

$$\Lambda_n(\alpha)=\frac{(2n+1)!!}{(2\pi)^{3/2}(2n)!!}\alpha^{-1}-\left(\frac{(2n+1)!!}{(2\pi)^{3/4}(2n)!!}\right)^2\left(\ln 2-1+\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k(1+2k)}\right)\alpha^{-2}.$$

For eigenvalues with even indices we have

$$E_{2n}(0;\alpha)=\begin{cases}\lambda_{2n-1} \text{ for } \alpha\leqslant 0 \text{ and } n\geqslant 1\\ -16\pi^2\alpha^2+\dfrac{1}{128\pi^2}\alpha^{-2}+O(\alpha^{-4}) \text{ for } \alpha\to-\infty \text{ and } n=0\\ \lambda_{2n}-\Lambda_n(\alpha)+O(\alpha^{-3}) \text{ for } \alpha\to+\infty \text{ and } n\geqslant 0.\end{cases} \tag{36}$$

For the odd indices

$$E_{2n+1}(0;\alpha)=\begin{cases}\lambda_{2n+1} \text{ for } \alpha\geqslant 0\\ \lambda_{2n}-\Lambda_n(\alpha)+O(\alpha^{-3}) \text{ for } \alpha\to-\infty.\end{cases} \tag{37}$$

Formulas (35)–(37) explain peculiarities in the plots of functions E_n on Figs. 3 and 4. Note that in Eqs. (33)–(37) the remainder terms depend on n.

The isotropic harmonic oscillator has an equidistant spectrum. After the perturbation by a zero-range potential, the distances between energy levels are changed and become dependent on the energy index n. This is important in the connection with the problem of the controlled modulation of the binding energy of the impurity center in quantum dots, that can be used to design nonlinear opto-electronic active elements.[6] The asymptotic formulas (34)–(37) give very accurate expressions for the excited energies in the most interesting case of a deep zero-range well

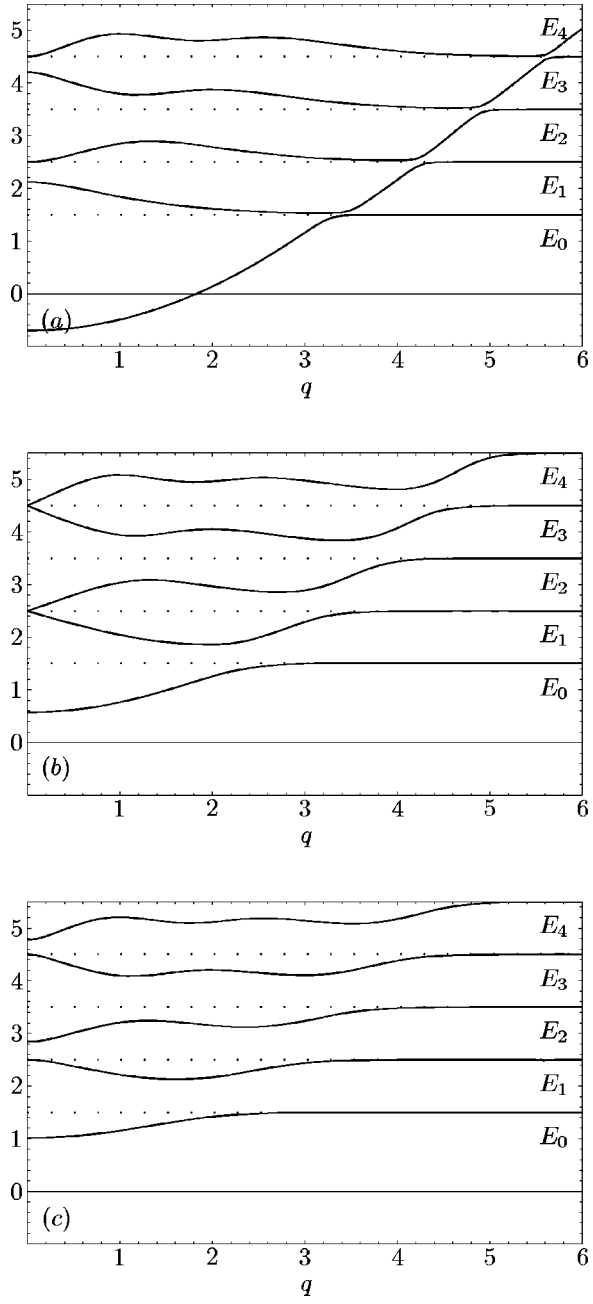

FIG. 3. E_n as a function of q for (a) $\alpha=-\alpha^0$, (b) $\alpha=0$, (c) $\alpha=\alpha^0$.

($\alpha\to-\infty$) as well as for the case of a shallow well ($\alpha\to+\infty$), which confirm numerical results from Ref. 6. Note also that Proposition 1 and Theorem 3 imply a remarkable distinction between the excited energy for the ground state and that for the other ones: The energy $E_1(q;\alpha)-E_0(q;\alpha)$ can take an arbitrary value depending on q and α; on the other hand, energies $\lambda_n-E_n(q;\alpha)$ and $E_{n+1}(q;\alpha)-\lambda_n(n\geqslant 1)$ are bounded by 1. Since at fixed α, $\alpha\ll-1$, the function $q\mapsto E_1(q;\alpha)-E_0(q;\alpha)$ is injective for moderate values of q, the position of an impurity in the quantum dot may be determined from the spectroscopy data.

We show the plot of the energies $E_1(q;\alpha)-E_0(q;\alpha)$ and $\lambda_1-E_1(q;\alpha)$ as functions of q and α on Figs. 5 and 6, respectively.

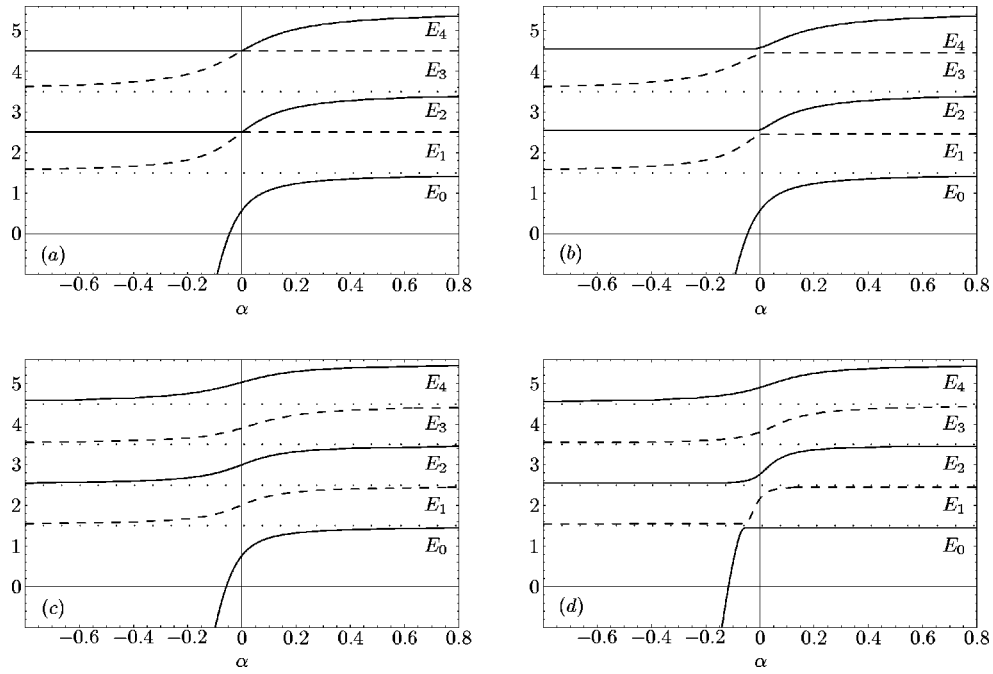

FIG. 4. E_n as a function of α for (a) $q=0$, (b) $q=1/10$, (c) $q=1$, (d) $q=3$.

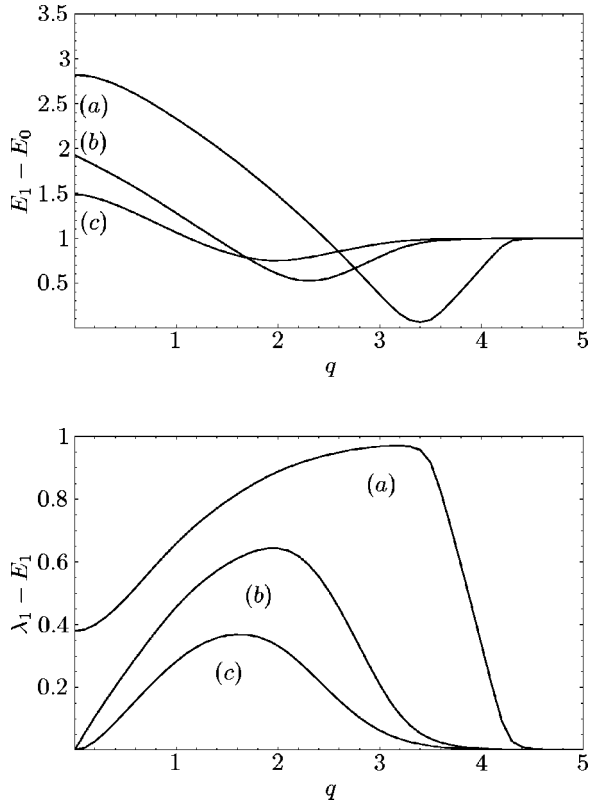

FIG. 5. The exciting energy as a function of q for (a) $\alpha=-\alpha^0$, (b) $\alpha=0$, (c) $\alpha=\alpha^0$.

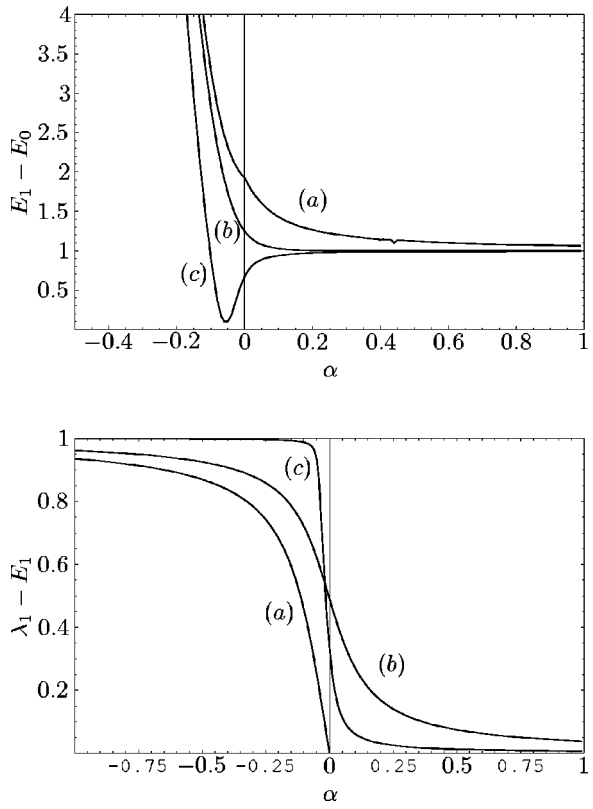

FIG. 6. The exciting energy as a function of α for (a) $q=0$, (b) $q=1$, (c) $q=3$.

In conclusion we give the following remark. Let $q:[0,\infty)\to\mathbb{R}$ be a smooth function obeying the conditions

(H1) $q\geqslant 0$ and the function $r\mapsto q(r)+r^2/4$ is nondecreasing;
(H2) $q'(r)\leqslant 0$, and let κ_0 and κ_1 be the first two eigenvalues of the operator $H^0+q=-\Delta+r^2/4+q(r)$. It is proven in Ref. 49 that $\kappa_0/\kappa_1<\lambda_0/\lambda_1$, if $q\neq 0$. Using Theorems 3 and A it is easy to construct smooth functions q with properties (H1) and
(H2a) $q'(r)\geqslant 0$, such that $\kappa_0/\kappa_1>\lambda_0/\lambda_1$.

ACKNOWLEDGMENTS

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Decoherence in a two-particle model

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We consider a simple one-dimensional quantum system consisting of a heavy and a light particle interacting via a point interaction. The initial state is chosen to be a product state, with the heavy particle described by a coherent superposition of two spatially separated wave packets with opposite momentum and the light particle localized in the region between the two wave packets. We characterize the asymptotic dynamics of the system in the limit of small mass ratio, with an explicit control of the error. We derive the corresponding reduced density matrix for the heavy particle and explicitly compute the (partial) decoherence effect for the heavy particle induced by the presence of the light one for a particular set up of the parameters. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1647692]

I. INTRODUCTION

Decoherence has become the terminology for the irreversible suppression of interference of the wave function of a quantum system due to the interaction with an ''environment.'' [7,3] The usual picture of decoherence, in the simple setting of a two particle system, goes as follows. Suppose one has a particle M with initial wave function $\varphi(x)=\varphi_l(x)+\varphi_r(x)$, representing the superposition of two wave packets φ_l, more or less supported ''on the left of the origin'' and heading to the right, and φ_r supported more or less on the ''right of the origin'' with an average velocity pointing to the left. Suppose that another particle m, described initially by the wave packet $\Phi(y)$, passes by and interacts with M. Assuming a small mass ratio between the second and the first particle, it is conceivable that the evolution of M will not be much affected by the interaction, while the scattering process undergone by the particle m will depend strongly on the position of the heavier particle. After interaction (which is assumed to be very fast) one then expects that the wave function describing the state of the system is of the type $\psi(x,y)=\varphi_l(x)\Phi_l(y)+\varphi_r(x)\Phi_r(y)$, where Φ_l and Φ_r will have spatial supports concentrated in distant regions for all later times. Therefore, in the configuration space of the entire system the entangled state will appear as the sum of two disjoint components and the possibility of interference of the heavy particle wave packets will be reduced.

Notice that the reduced density matrix of the particle M has in this ideal case negligible off-diagonal elements. In this sense, interference has been reduced and the motion of the particle M has become more ''classical.'' That is the way decoherence plays a role in the explanation of the emergence of classical behavior from quantum mechanics.

For the relevance of the mechanism of decoherence in the classical limit of Quantum Mechanics in the language of Bohmian Mechanics see Ref. 1.

In this respect it is an interesting problem to separate ''pure decoherence'' from the other

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effects which an environment usually produces, which are dissipation and fluctuation. That is, one would like to have the motion of the system not much affected by the interaction with the environment, while the environment produces decoherence. It is unclear whether these desiderata, namely a good decoherence rate and a more or less unperturbed motion can be consistently fulfilled in realistic physical models.[6]

Explicit models where one can rigorously establish decoherence in this sense have been worked out in the last years. One such model has been studied in Ref. 4 where the interaction of a particle with the radiation field has been considered. We shall now study another interaction which elaborates closer the idea of scattering of light particles (the environment) off a heavy particle (the system) (see Refs. 8, 5, and 11 for similar ideas).

We consider a very simple one-dimensional model of a system (a heavy particle of mass M) plus environment (one light particle of mass m) interacting via a short range force (δ-interaction). We consider this case as useful preparation for the treatment of a three-dimensional gas of light particles interacting with the heavy particle, which we shall address in subsequent work.

We wish to stress some features that make the two-particle model with δ-interaction (which has the advantage of being analytically easily accessible) particularly suitable as a model for decoherence:

(1) There exists a simple dimensionless parameter in the problem, namely the fraction of the masses $\epsilon = m/M$;
(2) letting ϵ become small while keeping M fixed allows to approximate the solution of the Schrödinger equation of the two body problem by a scattering solution in which the heavy particle acts as a scattering center for the light one. The error is $\mathcal{O}(\epsilon)$. The time scale on which this approximation holds is of course given by the time the light particle needs to pass the heavy particle. This approximation is the starting point of the analysis in Ref. 8;
(3) the decoherence effect (i.e., the amount by which the off diagonal elements of the reduced density matrix are reduced) can be explicitely computed [see (3.20) and the discussion following it] and is, in the relevant regime, of the order of $\alpha_0 m \hbar^{-2} \delta$, where δ is the initial spread of the light particle and α_0 is the strength of the potential [$(\alpha_0 m)^{-1}\hbar 2$ is the effective range of interaction] all of which can also be chosen ϵ-dependent.

We wish to warn the reader that the point interaction we look at here in form of the δ-potential is for finite α_0 not a hard core interaction. The case $\alpha_0 \to \infty$ corresponds to hard core.

The paper is organized as follows.

In Sec. II we introduce the model and characterize the asymptotic dynamics of the two-particle system for small mass ratio and state the main approximation result.

In Sec. III we show the attenuation of the off-diagonal terms in the reduced density matrix for the heavy particle and we compute explicitly the probability distribution for the position of the heavy particle, showing reduction of the interference effects with respect to the noninteracting case.

In Sec. IV we give the proof of the main result of the paper.

In the Appendix we recall the derivation of the explicit solution of the Schrödinger equation of the two-body system in interaction via a delta potential in dimension one.

II. EXPRESSION FOR SMALL MASS RATIO

In this section we shall study the Schrödinger equation for the two-particle system in one dimension described by the Hamiltonian

$$H = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2m}\Delta_r + \alpha_0 \delta(r-R), \quad \alpha_0 > 0. \tag{2.1}$$

In (2.1) we have denoted by R the position coordinate of the heavy particle with mass M and by r the position coordinate of the light particle with mass m. The interaction potential is chosen to be a repulsive point interaction of strenth α_0.

It is well known that (2.1) is a well defined positive and self-adjoint operator in $L^2(\mathbb{R}^2,drdR)$, which is also a solvable model.[2]

In fact, for an arbitrary initial state $\psi_0=\psi_0(r,R)$, the solution of the Schrödinger equation can be explicitely written as (see Ref. 10 and the Appendix)

$$\psi(t,r,R)=\int dr'dR'\,\psi_0(r',R')U_0^{\nu}\left(t,\frac{M}{\nu}(R-R')+\frac{\mu}{M}(r-r')\right)\cdot\left[U_0^{\mu}(t,(r-R)-(r'-R'))-\frac{\mu\alpha_0}{\hbar^2}\int_0^{\infty}du e^{-(\mu\alpha_0/\hbar^2)u}U_0^{\mu}(t,u+|r-R|+|r'-R'|)\right], \tag{2.2}$$

where we have introduced the reduced mass and the total mass of the system

$$\mu=\frac{mM}{m+M},\qquad \nu=m+M, \tag{2.3}$$

and the integral kernel of the free unitary group $U_0^{\mathcal{M}}(t)$ corresponding to the mass $\mathcal{M}>0$

$$U_0^{\mathcal{M}}(t,x-x')=e^{-i(t/\hbar)H_0^{\mathcal{M}}}(x-x')=\sqrt{\frac{\mathcal{M}}{2\pi i\hbar t}}e^{i(\mathcal{M}/2\hbar t)(x-x')^2},\qquad x,x'\in\mathbb{R}. \tag{2.4}$$

We are interested in the case of an initial state in a product form. Then we fix two real valued smooth functions (for ease of formulation we assume that they are in Schwartz space $\mathcal{S}$)

$$f,g\in\mathcal{S},\qquad \|f\|=\|g\|=1, \tag{2.5}$$

where $\|\cdot\|$ denotes the norm in $L^2(\mathbb{R})$. For later use, it will be convenient to choose g even. Using f and g we define now the states in such a way that we can easily read of the relevant physical scales, i.e., we code the states by the physical parameters $R_0,P_0,\sigma,r_0,q_0,\delta$ as follows:

$$f_{\sigma,R_0,P_0}(R)=\frac{1}{\sqrt{2}}[f^{+}_{\sigma,R_0,P_0}(R)+f^{-}_{\sigma,R_0,P_0}(R)], \tag{2.6}$$

$$f^{\pm}_{\sigma,R_0,P_0}(R)=\frac{1}{\sqrt{\sigma}}f\left(\frac{R\pm R_0}{\sigma}\right)e^{\pm i(P_0/\hbar)R}, \tag{2.7}$$

$$g_{\delta,r_0,q_0}(r)=\frac{1}{\sqrt{\delta}}g\left(\frac{r-r_0}{\delta}\right)e^{i(q_0/\hbar)r}, \tag{2.8}$$

$$\sigma,\delta,R_0,P_0,q_0>0,\quad r_0\in\mathbb{R},\qquad R_0>\sigma+\delta+|r_0|. \tag{2.9}$$

The choice (2.9) is not essential for the most part of the paper, but it sets already a geometrical picture which puts the results in the right perspective [see below (2.10)]. Later on we shall use this particular choice for computing effects. Note that the spread of the wave function of M is not given by σ but by R_0.

The initial state that we consider in the following is

$$\psi_0(r,R)=g_{\delta,r_0,q_0}(r)f_{\sigma,R_0,P_0}(R). \tag{2.10}$$

The initial state (2.10) is a (pure) product state for the whole system, i.e., no correlation is assumed between the two particles at time zero.

The heavy particle is assumed to be in a superposition of two spatially separated wave packets, one localized in $R=-R_0$ with mean value of the momentum P_0 and the other localized in $R=R_0$ with mean value of the momentum $-P_0$. The light particle is localized around r_0, in the region between the two wave packets, with positive mean momentum q_0.

To simplify the notation, in the rest of the paper we shall drop the dependence of the initial state on R_0, P_0, r_0, q_0. Moreover, for the convenience of the reader, we collect here some notation which will be used later on

$$\epsilon=\frac{m}{M}, \qquad \mu=\frac{\epsilon}{1+\epsilon}M, \qquad \nu=(1+\epsilon)M, \tag{2.11}$$

$$\alpha=\frac{\alpha_0 m}{\hbar^2}, \tag{2.12}$$

$$k_0=\frac{q_0}{\hbar}, \qquad K=\frac{P_0}{\hbar}+k_0, \tag{2.13}$$

$$T \;:\; L^2(\mathbb{R}^2, dr dR)\to L^2(\mathbb{R}^2, dx_1 dx_2),$$

$$(Th)(x_1,x_2)\equiv h\left(x_2+\frac{M}{m+M}x_1, x_2-\frac{m}{m+M}x_1\right), \tag{2.14}$$

$$\Delta^{\pm}=(\pm R_0-\sigma, \pm R_0+\sigma), \tag{2.15}$$

and finally c will denote a positive numerical constant.

We shall now characterize the asymptotic behavior of the wave function for small value of the mass ratio ϵ for the initial state (2.10). Letting m become small, keeping M fixed, the light particle moves with speed at least $v\sim\hbar/\delta m$ due to the uncertainty principle and the time by which the light particle passes M is of the order of R_0/v thus decreases with m, so that M does not change much its position during the passing of m.

The limit dynamics will hence describe a situation in which the light particle is scattered by the heavy one being in some fixed position, while the heavy particle moves freely. Nevertheless, we shall find that the free motion of the heavy particle is modified by the scattering event. In this heuristic argument we kept all the other physical parameters fixed except for the interaction strength. In fact, in order to keep the interaction effective on the light particle we need to scale α_0 in such a way that $\alpha_0 m\approx\mathcal{O}(1)$. There is of course no need to keep the other parameters fixed, in fact one may well imagine δ and R_0 increasing with m, so that the kinetic energy of m stays finite and the spread of the M increases. We shall not discuss such choices here, but the estimates are detailed enough, so that other scalings can be easily discussed. This might become relevant in a model where the heavy particle is immersed in a gas of light particles. In order to formulate the main result of this section, we define the integral operator

$$(W_+^{\gamma,x_0}h)(k)=\frac{1}{\sqrt{2\pi}}\int dx h(x)(e^{-ikx}+\mathcal{R}_\gamma(k)e^{-ix_0k}e^{i|k||x-x_0|}), \qquad \gamma>0,\ x_0\in\mathbb{R}, \tag{2.16}$$

$$\mathcal{R}_\gamma(k)=-\frac{\gamma}{\gamma-i|k|}, \tag{2.17}$$

where the integral kernel in (2.16) is the generalized eigenfunction of the Hamiltonian

$$H_{\gamma,x_0} = -\tfrac{1}{2}\Delta + \gamma\delta(\cdot - x_0), \tag{2.18}$$

and $\mathcal{R}_\gamma(k)$ is the corresponding reflection coefficient (see e.g., Ref. 2). Moreover we introduce the wave operator Ω_+^{γ,x_0} associated to H_{γ,x_0}, explicitly given by

$$(\Omega_+^{\gamma,x_0}h)(x) = [(W_+^{\gamma,x_0})^{-1}\tilde{h}](x), \tag{2.19}$$

where $\tilde{h}$ denotes the Fourier transform of h.

With the above notation the asymptotic wave function, which will be denoted by $\psi^a(t)$, is explicitely characterized in the following theorem.

Theorem 1: *Let $\sigma_1>0$, $\delta_1>0$, $\alpha_1>0$, $k_1<\infty$ and let the initial state be given by (2.10) with $\sigma\geqslant\sigma_1$, $\delta\geqslant\delta_1$, $\alpha\geqslant\alpha_1$, $k_0\leqslant k_1$.*

Then for any $t>0$ there exist time independent constants A, B such that

$$\|\psi(t)-\psi^a(t)\| < \left(\frac{A}{t}+B\right)\epsilon, \tag{2.20}$$

where

$$\begin{aligned}\psi^a(t,r,R) &= \sqrt{\frac{m}{i\hbar t}}\,e^{i(m/2\hbar t)\,r^2}\int dy\, f_\sigma(y)U_0^M(t,R-y)(W_+^{\alpha,y}g_\delta)\left(\frac{mr}{\hbar t}\right)\\ &= \sqrt{\frac{m}{i\hbar t}}\,e^{i(m/2\hbar t)\,r^2}\int dy\, f_\sigma(y)U_0^M(t,R-y)[(\Omega_+^{\alpha,y})^{-1}g_\delta]\left(\frac{mr}{\hbar t}\right).\end{aligned} \tag{2.21}$$

Remark 1: Note that $\psi^a(t,r,R)$ is close to what we described in the introduction. Think of f_σ as consisting of two well concentrated wave packets, then the light particle scattered wave function is correlated with the two average positions of the heavy particles, as one can see observing that the integration variable y in $[(\Omega_+^{\alpha,y})^{-1}g_\delta]$ appears as a scattering center.

The result of theorem 1 can be rephrased in terms of reduced density matrix for the heavy particle, which is defined by the integral operator $\hat{\rho}(t)$ in $L^2(\mathbb{R})$ given by the kernel

$$\hat{\rho}(t,R,R') = \int dr\,\psi(t,r,R)\overline{\psi}(t,r,R'). \tag{2.22}$$

We also introduce the integral operator $\hat{\rho}^a(t)$ defined by

$$\begin{aligned}\hat{\rho}^a(t,R,R') &= \int dr\,\psi^a(t,r,R)\overline{\psi^a}(t,r,R')\\ &= \int dy\, f_\sigma(y)U_0^M(t,R-y)\int dz\,\overline{f_\sigma}(z)\overline{U_0^M}(t,R'-z)\mathcal{I}(y,z),\end{aligned} \tag{2.23}$$

where

$$\mathcal{I}(y,z) \equiv \int dk\,(W_+^{\alpha,y}g_\delta)(k)\overline{(W_+^{\alpha,z}g_\delta)}(k) = ((\Omega_+^{\alpha,z})^{-1}g_\delta,(\Omega_+^{\alpha,y})^{-1}g_\delta). \tag{2.24}$$

Formula (2.24), obtained through heuristic considerations, has been the main ingredient in the description of scattering induced decoherence in Ref. 8.

Observe that, from (2.23) and (2.24) one has

$$\hat{\rho}^a(t) = U_0^M(t)\hat{\rho}_0^a U_0^M(-t), \tag{2.25}$$

where $\hat{\rho}_0^a$ is defined by the integral kernel

$$\hat{\rho}_0^a(y,z)=f_\sigma(y)\overline{f_\sigma}(z)\mathcal{I}(y,z). \tag{2.26}$$

It is easily seen that $\mathcal{I}(y,z)=\overline{\mathcal{I}}(z,y)$, $|\mathcal{I}(y,z)|\leqslant 1$ and the equality holds only if $y=z$. Then $\hat{\rho}_0^a$ is a self-adjoint and trace-class operator, with $Tr(\hat{\rho}_0^a)=1$; it is also positive since

$$\begin{aligned}(h,\hat{\rho}_0^a h)&=\int dy\overline{h}(y)\int dz h(z)f_\sigma(y)\overline{f_\sigma}(z)\int dk(W^{\alpha,y}g_\delta)(k)\overline{(W^{\alpha,z}g_\delta)}(k)\\&=\int dk\left|\int dy\overline{h}(y)f_\sigma(y)(W^{\alpha,y}g_\delta)(k)\right|^2.\end{aligned} \tag{2.27}$$

Moreover we have

$$Tr((\hat{\rho}_0^a)^2)=\int dydz|f_\sigma(y)|^2|f_\sigma(z)|^2|\mathcal{I}(y,z)|^2<1. \tag{2.28}$$

We conclude that $\hat{\rho}_0^a$ and its free evolution $\hat{\rho}^a(t)$ are density matrices describing mixture states and by Theorem 1, for any $t>0$, one has

$$Tr(|\hat{\rho}(t)-\hat{\rho}^a(t)|)<\left(\frac{A}{t}+B\right)\epsilon. \tag{2.29}$$

This means that in our asymptotic regime the motion of the heavy particle is a free evolution. On the other hand, the presence of the light particle has a relevant effect, since it produces a transition of the initial state of the heavy particle from $\hat{\rho}_0(y,z)=f_\sigma(y)\overline{f_\sigma}(z)$ to $\hat{\rho}_0^a(y,z)$. We shall see in the next section that this is the origin of the decoherence effect on the heavy particle.

Finally, it is worth to mention that the dynamics of the system can be equivalently described by the Wigner function. From (2.23) and (2.24) we see that the asymptotic form of the reduced Wigner function describing the motion of the heavy particle is the free evolution of

$$\hat{W}_0^a(R,P)=\frac{1}{2\pi}\int dxe^{iPx}f_\sigma\left(R-\frac{\hbar}{2}x\right)\overline{f_\sigma}\left(R+\frac{\hbar}{2}x\right)\mathcal{I}\left(R-\frac{\hbar}{2}x,R+\frac{\hbar}{2}x\right). \tag{2.30}$$

III. SIZE OF DECOHERENCE

Here we discuss an application of formulas (2.23) and (2.24) to a concrete example of quantum evolution and we give an explicit computation of the decoherence effect.

We shall consider the initial state (2.10) with the further assumptions (which are only done for ease of presentation)

$$f,g\in C_0^\infty(-1,+1) \tag{3.1}$$

and

$$\sigma \ll \frac{1}{\alpha} \ll R_0-|r_0|, \qquad \delta \ll R_0-|r_0|, \tag{3.2}$$

i.e., the spreading in position of the wave packets (which are superposed in a gross superposition) of the heavy particle is much smaller than the effective range of the interaction and this, in turn, is much smaller than the separation between the two particles. Moreover the light particle is well separated from each wave packet of the heavy one.

Notice that (3.2) obviously implies $\sigma/R_0\ll 1$.

Using assumptions (3.2) we can give an estimate of the basic object $\mathcal{I}(y,z)$ for $y,z\in\Delta^{\pm}$ and then we can find a more suitable expression for the reduced density matrix of the heavy particle. In order to formulate the result, we define the parameter

$$\Lambda=\int dk|\tilde{g}_{\delta}(k)|^2\mathcal{T}_{\alpha}(k)=1+\int dk|\tilde{g}_{\delta}(k)|^2\mathcal{R}_{\alpha}(k), \tag{3.3}$$

where

$$\mathcal{T}_{\gamma}(k)=-\frac{ik}{\gamma-ik}=1+\mathcal{R}_{\gamma}(k), \qquad \gamma>0, \tag{3.4}$$

is the transmission coefficient associated to a point interaction of strength γ (see e.g., Ref. 2). Then we have

Proposition 2: Assume (3.2). Then

$$\sup_{y,z\in\Delta^{\pm}}|\mathcal{I}(y,z)-1|<c\left(\alpha\sigma+\frac{1}{\alpha(R_0-|r_0|)}+\frac{\delta}{R_0-|r_0|}\right), \tag{3.5}$$

$$\sup_{y\in\Delta^{+},z\in\Delta^{-}}|\mathcal{I}(y,z)-\Lambda|=\sup_{y\in\Delta^{-},z\in\Delta^{+}}|\mathcal{I}(y,z)-\overline{\Lambda}|<c\left(\frac{1}{\alpha(R_0-|r_0|)}+\frac{\delta}{R_0-|r_0|}\right). \tag{3.6}$$

Proof: Using the shorthand notation $\beta=\alpha\delta$, we note that for $y\in\Delta^{-}$

$$\frac{1}{\sqrt{\delta}}(W_{+}^{\alpha,y}g_{\delta})\left(\frac{k}{\delta}\right)=e^{i(k_0\delta-k)r_0/\delta}\tilde{g}(k-k_0\delta)+\mathcal{R}_{\beta}(k)e^{i(k_0\delta+|k|)\,r_0/\delta-i(k+|k|)\,y/\delta}\tilde{g}(|k|+k_0\delta), \tag{3.7}$$

and for $y\in\Delta^{+}$

$$\frac{1}{\sqrt{\delta}}(W_{+}^{\alpha,y}g_{\delta})\left(\frac{k}{\delta}\right)=e^{i(k_0\delta-k)r_0/\delta}\tilde{g}(k-k_0\delta)+\mathcal{R}_{\beta}(k)e^{i(k_0\delta-|k|)\,r_0/\delta-i(k-|k|)\,y/\delta}\tilde{g}(|k|-k_0\delta), \tag{3.8}$$

where we have used the fact that

$$\tilde{g}_{\delta}(k)=\sqrt{\delta}\tilde{g}(k\delta-k_0\delta)e^{-i(k-k_0)r_0}. \tag{3.9}$$

Then for $y,z\in\Delta^{-}$ we have

$$\begin{aligned}\mathcal{I}(y,z)&=1+\int dk|\tilde{g}(|k|+k_0\delta)|^2|\mathcal{R}_{\beta}(k)|^2e^{-i(k+|k|)\,(y-z)/\delta}+\int dk\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(|k|+k_0\delta)\mathcal{R}_{\beta}\\&\quad\times(k)e^{i(k+|k|)\,(r_0-y)/\delta}+\int dk\bar{\tilde{g}}(|k|+k_0\delta)\tilde{g}(k-k_0\delta)\overline{\mathcal{R}_{\beta}}(k)e^{-i(k+|k|)\,(r_0-z)/\delta}\\&=1+\int_0^{\infty}dk|\tilde{g}(k+k_0\delta)|^2|\mathcal{R}_{\beta}(k)|^2(e^{-2ik\,(y-z)/\delta}-1)+\int_0^{\infty}dk\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(k+k_0\delta)\\&\quad\times\mathcal{R}_{\beta}(k)e^{2ik\,(r_0-y)/\delta}+\int_0^{\infty}dk\bar{\tilde{g}}(k+k_0\delta)\tilde{g}(k-k_0\delta)\overline{\mathcal{R}_{\beta}}(k)e^{-2ik\,(r_0-z)/\delta}\\&\equiv1+a_1+a_2+a_3,\end{aligned} \tag{3.10}$$

where we have used the identity $\mathcal{R}_\beta+\overline{\mathcal{R}_\beta}+2|\mathcal{R}_\beta|^2=0$ and the fact that $\tilde{g}$ is even.

Using (3.2) we easily estimate a_1

$$|a_1|\leqslant 2\,\frac{|y-z|}{\delta}\int_0^\infty dk|\tilde{g}(k+k_0\delta)|^2k|\mathcal{R}_\beta(k)|^2\leqslant 4\,\frac{\sigma}{\delta}\int_0^\infty dk|\tilde{g}(k+k_0\delta)|^2k|\mathcal{R}_\beta(k)|^2\leqslant 2\ \ \alpha\sigma. \tag{3.11}$$

For the estimate of a_2 it is convenient to integrate by parts

$$\begin{aligned}
|a_2|&=\left|\frac{1}{2i}\,\frac{\delta}{r_0-y}\int_0^\infty dk\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(k+k_0\delta)\mathcal{R}_\beta(k)\,\frac{d}{dk}e^{2ik(r_0-y)/\delta}\right|\\
&=\frac{\delta}{2|r_0-y|}\left|\int_0^\infty dk\,\frac{d}{dk}(\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(k+k_0\delta)\mathcal{R}_\beta(k))e^{2ik\,(r_0-y)/\delta}-|\tilde{g}(k_0\delta)|^2\right|\\
&\leqslant\frac{\delta}{R_0-|r_0|}\left[\frac{1}{2\pi}\left(\int dr|g(r)|\right)^2+\frac{1}{\beta}\int_0^\infty dk|\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(k+k_0\delta)|\right.\\
&\quad\left.+\int_0^\infty dk|\bar{\tilde{g}}'(k-k_0\delta)\tilde{g}(k+k_0\delta)|+\int_0^\infty dk|\bar{\tilde{g}}(k-k_0\delta)\tilde{g}'(k+k_0\delta)|\right]\\
&\leqslant\frac{\delta}{R_0-|r_0|}\left[\frac{1}{2\pi}\left(\int dr|g(r)|\right)^2+\frac{1}{\beta}\|g\|^2+2\|\tilde{g}'\|\right]\\
&\leqslant\frac{\delta}{R_0-|r_0|}\left(\frac{1}{\pi}+2\|\tilde{g}'\|\right)+\frac{1}{\alpha(R_0-|r_0|)}.
\end{aligned}\tag{3.12}$$

The term a_3 is analyzed exacly in the same way and then we get the estimate (3.5) for $y,z\in\Delta^-$. Since in the case $y,z\in\Delta^+$ the computation is similar we conclude that (3.5) holds.

In order to prove (3.6) we consider the case $y\in\Delta^+$ and $z\in\Delta^-$ (the case $y\in\Delta^-$ and $z\in\Delta^+$ can be treated exactly in the same way) and we obtain

$$\begin{aligned}
\mathcal{I}(y,z)&=1+\int dk\bar{\tilde{g}}(|k|+k_0\delta)\tilde{g}(|k|-k_0\delta)|\mathcal{R}_\beta(k)|^2e^{-2i|k|\,r_0/\delta+i(|k|-k)\,y/\delta+i(|k|+k)\,z/\delta}\\
&\quad+\int dk\bar{\tilde{g}}(k-k_0\delta)\tilde{g}(|k|-k_0\delta)\mathcal{R}_\beta(k)e^{-i(|k|-k)\,(r_0-y)/\delta}\\
&\quad+\int dk\bar{\tilde{g}}(|k|+k_0\delta)\tilde{g}(k-k_0\delta)\overline{\mathcal{R}_\beta}(k)e^{-i(|k|+k)\,(r_0-z)/\delta}\\
&=1+\int_0^\infty dk(|\tilde{g}(k-k_0\delta)|^2\mathcal{R}_\beta(k)+|\tilde{g}(k+k_0\delta)|^2\overline{\mathcal{R}_\beta}(k))\\
&\quad+\int_0^\infty dk\bar{\tilde{g}}(k+k_0\delta)\tilde{g}(k-k_0\delta)|\mathcal{R}_\beta(k)|^2e^{-2ik\,(r_0-z)/\delta}\\
&\quad+\int_0^\infty dk\bar{\tilde{g}}(k+k_0\delta)\tilde{g}(k-k_0\delta)\overline{\mathcal{R}_\beta}(k)e^{-2ik(r_0-z)/\delta}\\
&\quad+\int_0^\infty dk\bar{\tilde{g}}(k+k_0\delta)\tilde{g}(k-k_0\delta)|\mathcal{R}_\beta(k)|^2e^{-2ik\,(r_0-y)/\delta}\\
&\quad+\int_0^\infty dk\bar{\tilde{g}}(k+k_0\delta)\tilde{g}(k-k_0\delta)\mathcal{R}_\beta(k)e^{-2ik(r_0-y)/\delta}.
\end{aligned}\tag{3.13}$$

The estimate of the last four terms of (3.13) proceeds exactly as the estimate of a_2 in (3.12). On the other hand,

$$1+\int_0^\infty dk(|\tilde{g}(k-k_0\delta)|^2\mathcal{R}_\beta(k)+|\tilde{g}(k+k_0\delta)|^2\overline{\mathcal{R}_\beta}(k))=\int dk|\tilde{g}(k-k_0\delta)|^2\left(\frac{-ik}{\beta-ik}\right), \tag{3.14}$$

and this concludes the proof of the proposition. □

Proposition 2 allows us to find a further approximate form for the reduced density matrix.

Corollary 3: Under the assumptions (3.2) and for any $t\geqslant 0$ we have

$$[Tr((\hat{\rho}^a(t)-\hat{\rho}^f(t))^2)]^{1/2}<c\left(\alpha\sigma+\frac{1}{\alpha(R_0-|r_0|)}+\frac{\delta}{R_0-|r_0|}\right), \tag{3.15}$$

where

$$\hat{\rho}^f(t)=U_0^M(t)\hat{\rho}_0^f U_0^M(-t), \tag{3.16}$$

$$\hat{\rho}_0^f(y,z)=\frac{1}{2}f_\sigma^+(y)\overline{f_\sigma^+}(z)+\frac{1}{2}f_\sigma^-(y)\overline{f_\sigma^-}(z)+\frac{\Lambda}{2}f_\sigma^+(y)\overline{f_\sigma^-}(z)+\frac{\overline{\Lambda}}{2}f_\sigma^-(y)\overline{f_\sigma^+}(z). \tag{3.17}$$

Proof:

$$\begin{aligned}Tr((\hat{\rho}^a(t)-\hat{\rho}^f(t))^2)&=Tr((\hat{\rho}_0^a-\hat{\rho}_0^f)^2)\\&=\frac{1}{4}\int dydz|f_\sigma^+(y)\overline{f_\sigma^+}(z)(\mathcal{I}(y,z)-1)+f_\sigma^-(y)\overline{f_\sigma^-}(z)(\mathcal{I}(y,z)-1)\\&\quad+f_\sigma^+(y)\overline{f_\sigma^-}(z)(\mathcal{I}(y,z)-\Lambda)+f_\sigma^-(y)\overline{f_\sigma^+}(z)(\mathcal{I}(y,z)-\overline{\Lambda})|^2\\&\leqslant\sup_{y,z\in\Delta^+}|\mathcal{I}(y,z)-1|^2+\sup_{y,z\in\Delta^-}|\mathcal{I}(y,z)-1|^2+\sup_{y\in\Delta^+,z\in\Delta^-}|\mathcal{I}(y,z)-\Lambda|^2\\&\quad+\sup_{y\in\Delta^-,z\in\Delta^+}|\mathcal{I}(y,z)-\overline{\Lambda}|^2.\end{aligned} \tag{3.18}$$

Using proposition 2 we conclude the proof. □

From corollary 3 and theorem 1 we conclude that the reduced density matrix for the heavy particle in the position representation can be approximated by the density matrix

$$\begin{aligned}\hat{\rho}^f(t,R,R')&=\frac{1}{2}(U_0^M(t)f_\sigma^+)(R)(U_0^M(-t)\overline{f_\sigma^+})(R')+\frac{1}{2}(U_0^M(t)f_\sigma^-)(R)(U_0^M(-t)\overline{f_\sigma^-})(R')\\&\quad+\frac{\Lambda}{2}(U_0^M(t)f_\sigma^+)(R)(U_0^M(-t)\overline{f_\sigma^-})(R')+\frac{\overline{\Lambda}}{2}(U_0^M(t)f_\sigma^-)(R)(U_0^M(-t)\overline{f_\sigma^+})(R'),\end{aligned} \tag{3.19}$$

with an explicit control of the error.

If the interaction with the light particle is switched off, i.e., for $\alpha=0$, we have $\Lambda=1$ and then (3.19) reduces to the pure state corresponding to the coherent superposition of the free evolution of the two wave packets $f_\sigma^\pm$.

On the other hand, if $\alpha>0$ one easily sees that $0<|\Lambda|<1$ and then (3.19) is a mixed state for which the interference terms are reduced by the factor Λ and this is the typical manifestation of the (partial) decoherence effect induced by the light particle on the heavy one.

The relevant parameter Λ [see (3.3)] is defined in terms of the probability distribution of the momentum of the light particle $|\tilde{g}_\delta(k)|^2$ and of the transmission coefficient $\mathcal{T}_\alpha(k)$.

Then the decoherence effect is emphasized if the fraction of transmitted wave for the light particle is small.

In particular, rescaling the integration variable in (3.3), one can also write

$$\Lambda = 1 - \int dz |\tilde{g}(z)|^2 \frac{\alpha\delta}{\alpha\delta - i(z + k_0\delta)}. \tag{3.20}$$

Notice that decoherence is maximal when the wavelength of the light particle is smaller then or comparable to the scattering length of the interaction ($k_0 \sim \alpha$) and minimal for k_0 large with respect to α. Nevertheless it is worth stressing that (3.20) is an asymptotic formula whose effectivness is guaranteed only in the range of validity of the assumptions of theorem 1, from where it is derived.

For $k_0 \ll \alpha$ the effect of decoherence is given by

$$\Lambda \simeq \int dz |\tilde{g}(z)|^2 |\mathcal{T}_{\alpha\delta}(z)|^2 = 1 - \int dz |\tilde{g}(z)|^2 \frac{\alpha^2\delta^2}{\alpha^2\delta^2 + z^2}, \tag{3.21}$$

where we have used the fact that $\tilde{g}$ is even.

A further interesting question is the analysis of $\hat{\rho}^f(t)$ in the momentum representation. Since momentum is a constant of motion, the density matrix is simply given by

$$\begin{aligned}\frac{1}{\hbar}\tilde{\rho}_0^f\left(\frac{P}{\hbar}, \frac{P'}{\hbar}\right) &= \frac{1}{2\hbar}\tilde{f}_\sigma^+\left(\frac{P}{\hbar}\right)\overline{\tilde{f}_\sigma^+}\left(\frac{P'}{\hbar}\right) + \frac{1}{2\hbar}\tilde{f}_\sigma^-\left(\frac{P}{\hbar}\right)\overline{\tilde{f}_\sigma^-}\left(\frac{P'}{\hbar}\right) + \frac{\Lambda}{2\hbar}\tilde{f}_\sigma^+\left(\frac{P}{\hbar}\right)\overline{\tilde{f}_\sigma^-}\left(\frac{P'}{\hbar}\right) \\ &\quad + \frac{\overline{\Lambda}}{2\hbar}\tilde{f}_\sigma^-\left(\frac{P}{\hbar}\right)\overline{\tilde{f}_\sigma^+}\left(\frac{P'}{\hbar}\right).\end{aligned} \tag{3.22}$$

It is then clear that the decoherence effect is present also in the momentum representation and it is measured by the same parameter Λ.

Moreover, if $\tilde{f}_\sigma^+$ and $\tilde{f}_\sigma^-$ are well separated, one easily realizes that the probability distribution of the momentum remains essentially unchanged with respect to the unperturbed case $\Lambda = 1$, the error being of order ϵ.

We analyze now the evolution in the position representation of the heavy particle exploiting the approximate reduced density matrix $\hat{\rho}^f(t)$.

We shall explicitely show that the typical interference fringes produced by the superposition state when the interaction with the light particle is absent, i.e., for $\Lambda = 1$, are in fact reduced when the light particle is present, i.e., for $|\Lambda| < 1$.

In order to see the effect more clearly we assume

$$\frac{\sigma}{R_0} \ll \frac{\hbar}{\sigma P_0}. \tag{3.23}$$

The effect of the interference terms becomes more relevant when the supports of the two wave packets $U_0^M(t) f_\sigma^\pm$ have the maximal overlapping and this approximately happens at the time $t = \tau \equiv R_0 M / P_0$. Then, from (3.19), we consider

$$\begin{aligned}n(\tau, R) \equiv \hat{\rho}^f(\tau, R, R) = \tfrac{1}{2}[&|(U_0^M(\tau) f_\sigma^+)(R)|^2 + |(U_0^M(\tau) f_\sigma^-)(R)|^2 \\ &+ 2\Re(\Lambda (U_0^M(\tau) f_\sigma^+)(R) \overline{(U_0^M(\tau) f_\sigma^-)}(R))].\end{aligned} \tag{3.24}$$

Using (3.23) and a standard scattering estimate (see, e.g., Ref. 9) we obtain

$$\begin{aligned}(U_0^M(\tau) f_\sigma^+)(R) &= \sqrt{\frac{P_0\sigma}{2\pi\hbar R_0}} \int dx f\left(\frac{x + R_0}{\sigma}\right) e^{i(P_0/\hbar)x + i(P_0/2\hbar R_0)(R-x)^2} \\ &= \sqrt{\frac{P_0\sigma}{i\hbar R_0}} e^{i(P_0/\hbar)(R^2/2R_0 + R - R_0/2)} \tilde{f}\left(\frac{P_0\sigma}{\hbar R_0} R\right) + \mathcal{E}_0(R),\end{aligned} \tag{3.25}$$

$$\|\mathcal{E}_0\| < \frac{P_0\sigma^2}{2\hbar R_0}\|\Delta\tilde{f}\|. \tag{3.26}$$

Proceeding analogously for $(U_0^M(\tau)f_\sigma^-)(R)$ we find

$$n(\tau,R) = \frac{P_0\sigma}{\hbar R_0}\left|\tilde{f}\left(\frac{P_0\sigma}{\hbar R_0}R\right)\right|^2\left(1+|\Lambda|\cos\left(\frac{2P_0}{\hbar}R+\varphi\right)\right)+\mathcal{E}_1(R), \tag{3.27}$$

$$\|\mathcal{E}_1\|_{L^1} < c\ \frac{P_0\sigma^2}{\hbar R_0}, \tag{3.28}$$

where

$$\Lambda = |\Lambda|e^{i\varphi}. \tag{3.29}$$

For $|\Lambda|<1$, formula (3.27) shows that the presence of the light particle determines a reduction of the amplitude of the oscillations and a shift of the corresponding phases.

Notice that the shift is negligible if $k_0 \ll \alpha$.

IV. PROOF OF THEOREM 1

The proof of theorem 1 will be obtained through the proof of three lemmas.

Lemma 4: Given the initial state (2.10), for any $t \geqslant 0$ one has

$$\|\psi(t)-\psi_1(t)\| < C_1\,\epsilon, \tag{4.1}$$

where

$$\psi_1(t,r,R) = \int dy f_\sigma(y) U_0^\nu\left(t, \frac{M}{\nu}R+\frac{\mu}{M}r-y\right)\int dr' g_\delta(r'+y)U_{\alpha_0}^\mu(t,r-R,r') \tag{4.2}$$

and

$$C_1 = \left[\int dx x^2 \int dy \left|\frac{\partial}{\partial y}(f_\sigma(y)g_\delta(x+y))\right|^2\right]^{1/2}. \tag{4.3}$$

Proof: Using the relative and the center of mass coordinates [see (2.14)], from (A4) one has

$$(T\psi(t))(x_1,x_2) = (U_0^\nu(t)U_{\alpha_0}^\mu(t)T\psi_0)(x_1,x_2), \tag{4.4}$$

where $U_{\alpha_0}^\mu(t)$ is defined in (A10) of the Appendix and

$$(T\psi_0)(x_1,x_2) = f_\sigma\left(x_2-\frac{\mu}{M}x_1\right)g_\delta\left(x_2+\frac{M}{\nu}x_1\right). \tag{4.5}$$

Moreover

$$\begin{aligned}(T\psi_1(t))(x_1,x_2) &= \int dx_2' dx_1' f_\sigma(x_2')g_\delta(x_1'+x_2')U_0^\nu(t,x_2-x_2')U_{\alpha_0}^\mu(t,x_1,x_1') \\ &\equiv (U_0^\nu(t)U_{\alpha_0}^\mu(t)T\psi_{01})(x_1,x_2),\end{aligned} \tag{4.6}$$

where

$$\psi_{01}(r,R)=f_\sigma\left(\frac{M}{\nu}R+\frac{\mu}{M}r\right)g_\delta\left(r-R+\frac{M}{\nu}R+\frac{\mu}{M}r\right). \tag{4.7}$$

Then we have with $\mu/M=\epsilon/(1+\epsilon)$, $(M/\nu)-1=-\epsilon/(1+\epsilon)$

$$\begin{aligned}\|\psi(t)-\psi_1(t)\|^2&=\|T\psi(t)-T\psi_1(t)\|^2\\&=\|T\psi_0-T\psi_{01}\|^2\\&=\int dx_1dx_2\left|f_\sigma\left(x_2-\frac{\mu}{M}x_1\right)g_\delta\left(x_2+\frac{M}{\nu}x_1\right)-f_\sigma(x_2)g_\delta(x_1+x_2)\right|^2\\&=\int dx_1dx_2\left|f_\sigma\left(x_2-\frac{\epsilon}{1+\epsilon}x_1\right)g_\delta\left(x_2+x_1-\frac{\epsilon}{1+\epsilon}x_1\right)-f_\sigma(x_2)g_\delta(x_1+x_2)\right|^2\\&=\int dx_1dx_2\left|F\left(x_1,x_2-\frac{\epsilon}{1+\epsilon}x_1\right)-F(x_1,x_2)\right|^2,\end{aligned} \tag{4.8}$$

where $F(x_1,x_2)=f_\sigma(x_2)g_\delta(x_1+x_2)$. By a simple Plancherel argument, we have that

$$\begin{aligned}&\int dx_1dx_2\left|F\left(x_1,x_2-\frac{\epsilon}{1+\epsilon}x_1\right)-F(x_1,x_2)\right|^2\\&\quad=\int dx_1\int dk|\tilde F(x_1,k)\left(e^{-i(\epsilon/1+\epsilon)x_1k}-1\right)|^2\\&\quad\leqslant\int dx_1\int dk|\tilde F(x_1,k)|^2\left(\frac{\epsilon}{1+\epsilon}x_1k\right)^2=\left(\frac{\epsilon}{1+\epsilon}\right)^2\int dx_1x_1^2\int dx_2\left|\frac{\partial}{\partial x_2}F(x_1,x_2)\right|^2,\end{aligned} \tag{4.9}$$

from which the lemma follows. □

Since a small value of m in the interacting unitary group $U^\mu_{\alpha_0}(t)$ is equivalent to a large value of t, in the next lemma we use a typical scattering estimate to approximate $U^\mu_{\alpha_0}(t)$ in (4.2).

Lemma 5: Given the initial state (2.10), for any $t>0$ one has

$$\|\psi_1(t)-\psi_2(t)\|<\frac{C_2}{t}\epsilon, \tag{4.10}$$

where

$$\begin{aligned}\psi_2(t,r,R)=&\sqrt{\frac{m}{2\pi i\hbar t}}\sqrt{\frac{M}{2\pi i\hbar t}}e^{i(m/2\hbar t)r^2+i(M/2\hbar t)R^2}\int d\xi f_\sigma(\xi)e^{i(M/2\hbar t)\xi^2}e^{-i((M/\hbar t)R+(m/\hbar t)r)\xi}\\&\cdot\int dr'g_\delta(r'+\xi)\left(e^{-i(\mu/\hbar t)(r-R)r'}-\frac{e^{i(\mu/\hbar t)|r-R||r'|}}{1-i\dfrac{\hbar}{\alpha_0t}|r-R|}\right)\end{aligned} \tag{4.11}$$

and

$$\begin{aligned}C_2=c\frac{M}{\hbar}\Bigg\{&\int dxx^4|f_\sigma(x)|^2+\int dx|f_\sigma(x)|^2\Bigg[\int dyy^4|g_\delta(y+x)|^2+\frac{1}{\alpha^3}\left(\int dy|g_\delta(y+x)|\right)^2\\&+\frac{1}{\alpha}\left(\int dy|y||g_\delta(y+x)|\right)^2+\alpha\left(\int dyy^2|g_\delta(y+x)|\right)^2\Bigg]\Bigg\}^{1/2}.\end{aligned} \tag{4.12}$$

Proof: We shall first estimate the difference $\psi_1(t)-\hat\psi_2(t)$, where $\hat\psi_2(t)$ is explicitly given by

$$\hat{\psi}_2(t,r,R)=\sqrt{\frac{\mu}{2\pi i\hbar t}}e^{i(\mu/2\hbar t)(r-R)^2}\int dy f_\sigma(y)U_0^\nu\left(t,\frac{M}{\nu}R+\frac{\mu}{M}r-y\right)\int dr' g_\delta(r'+y)$$
$$\cdot\left(e^{-i(\mu/\hbar t)(r-R)r'}-\frac{e^{i(\mu/\hbar t)|r-R||r'|}}{1-i\dfrac{\hbar}{\alpha_0 t}|r-R|}\right). \tag{4.13}$$

From (4.2) we have

$$(T\psi_1)(t,x_1,x_2)=\int dy U_0^\nu(t,x_2-y)\varphi_1(t,x_1,y), \tag{4.14}$$

$$\varphi_1(t,x_1,x_2)=f_\sigma(x_2)\int dr' g_\delta(r'+x_2)U_{\alpha_0}^\mu(t,x_1,r'), \tag{4.15}$$

and analogously for $\hat{\psi}_2(t)$ we write

$$(T\hat{\psi}_2(t))(x_1,x_2)=\int dy U_0^\nu(t,x_2-y)\varphi_2(t,x_1,y), \tag{4.16}$$

$$\varphi_2(t,x_1,x_2)=\sqrt{\frac{\mu}{2\pi i\hbar t}}e^{i(\mu/2\hbar t)x_1^2}f_\sigma(x_2)\int dr' g_\delta(r'+x_2)\left(e^{-i(\mu/\hbar t)x_1 r'}-\frac{e^{i(\mu/\hbar t)|x_1||r'|}}{1-i\dfrac{\hbar|x_1|}{\alpha_0 t}}\right). \tag{4.17}$$

Using the isometric character of the operators T and $U_0^\nu(t)$ and the explicit expression of $U_{\alpha_0}^\mu(t)$ [see (A10)], we have

$$\begin{aligned}\|\psi_1(t)-\hat{\psi}_2(t)\|^2&=\|T\psi_1(t)-T\psi_2(t)\|^2\\&=\|\varphi_1(t)-\varphi_2(t)\|^2\\&\leqslant 2\int dx_1dx_2\left|f_\sigma(x_2)\int dr' g_\delta(r'+x_2)\right.\\&\quad\times\left.\left(U_0^\mu(t,x_1-r')-\sqrt{\frac{\mu}{2\pi i\hbar t}}e^{i(\mu/2\hbar t)x_1^2-i(\mu/\hbar t)x_1r'}\right)\right|^2\\&\quad+2\int dx_1dx_2\left|f_\sigma(x_2)\int dr' g_\delta(r'+x_2)\left(\frac{\mu\alpha_0}{\hbar^2}\int_0^\infty du e^{-(\mu\alpha_0/\hbar^2)u}\right.\right.\\&\quad\left.\left.\times U_0^\mu(t,u+|x_1|+|r'|)-\sqrt{\frac{\mu}{2\pi i\hbar t}}\frac{1}{1-i\dfrac{\hbar|x_1|}{\alpha_0 t}}e^{i(\mu/2\hbar t)x_1^2+i(\mu/\hbar t)|x_1||r'|}\right)\right|^2\\&\equiv(I)+(II).\end{aligned} \tag{4.18}$$

A standard estimate for the free unitary group (see, e.g., Ref. 9) gives

$$
\begin{aligned}
(I) &= \frac{\mu}{\pi\hbar t}\int dx_2 |f_\sigma(x_2)|^2 \int dx_1 \left| \int dr' g_\delta(r'+x_2)(e^{i(\mu/2\hbar t)\, r'^2}-1)e^{-i\,(\mu/\hbar t)\, x_1 r'}\right|^2 \\
&= \frac{1}{\pi}\int dx_2 |f_\sigma(x_2)|^2 \int d\overline{x_1} \left| \int dr' g_\delta(r'+x_2)(e^{i(\mu/2\hbar t)\, r'^2}-1)e^{-i\overline{x_1} r'}\right|^2 \\
&= 2\int dx_2 |f_\sigma(x_2)|^2 \int dr' |g_\delta(r'+x_2)|^2 |e^{i(\mu/2\hbar t)\, r'^2}-1|^2 \\
&\leqslant \frac{1}{2}\left(\frac{\mu}{\hbar t}\right)^2 \int dx_2 |f_\sigma(x_2)|^2 \int dr' r'^4 |g_\delta(r'+x_2)|^2 \\
&= \frac{\epsilon^2 M^2}{2(1+\epsilon)^2\hbar^2 t^2}\int dx_2 |f_\sigma(x_2)|^2 \int dr' r'^4 |g_\delta(r'+x_2)|^2,
\end{aligned}
\tag{4.19}
$$

where in the second line of (4.19) we used Plancherel theorem.

Concerning (II), we introduce the change of variables

$$
v = \frac{\mu\alpha_0}{\hbar^2}u, \qquad y_1 = \frac{\mu}{\hbar t}x_1, \tag{4.20}
$$

and use the identity

$$
\int_0^\infty dv\, e^{-v+i\,(\hbar|x_1|/\alpha_0 t)\, v} = \frac{1}{1-i\dfrac{\hbar|x_1|}{\alpha_0 t}}. \tag{4.21}
$$

Then

$$
\begin{aligned}
(II) &= \frac{1}{\pi}\int dx_2 |f_\sigma(x_2)|^2 \int dy_1 \left| \int dr' g_\delta(r'+x_2) e^{i|y_1||r'|}\right. \\
&\quad \cdot \left(e^{i(\mu/2\hbar t)\, r'^2}\int_0^\infty dv\, e^{-v+i\,[(1+\epsilon)/\alpha]\,|y_1|v + i[(1+\epsilon)m/2\hbar t\alpha^2]v^2 + i\,(m/\hbar t\alpha)\,|r'|v} \right. \\
&\quad \left.\left. - \int_0^\infty dv\, e^{-v+i1+\epsilon/\alpha\,|y_1|v}\right)\right|^2 \\
&\leqslant \frac{2}{\pi}\int dx_2 |f_\sigma(x_2)|^2 \int dy_1 \left| \int dr' g_\delta(r'+x_2) e^{i|y_1||r'|} e^{i(\mu/2\hbar t)\, r'^2}\int_0^\infty dv\, e^{-v+i[(1+\epsilon)/\alpha]\,|y_1|v}\right. \\
&\quad \left. \cdot (e^{i[(1+\epsilon)m/2\hbar t\alpha^2]v^2 + i(m/\hbar t\alpha)\,|r'|v} - 1)\right|^2 + \frac{2}{\pi}\int dx_2 |f_\sigma(x_2)|^2 \int dy_1 \left| \int dr' g_\delta(r'+x_2)\right. \\
&\quad \left. \times e^{i|y_1||r'|}(e^{i(\mu/2\hbar t)\, r'^2}-1)\frac{1}{1-i\dfrac{1+\epsilon}{\alpha}|y_1|}\right|^2 \equiv (III)+(IV).
\end{aligned}
\tag{4.22}
$$

The estimate of (IV) is trivial

$$
\begin{aligned}
(IV) &\leqslant \frac{1}{2\pi}\left(\frac{\mu}{\hbar t}\right)^2 \int dx_2 |f_\sigma(x_2)|^2 \int dy_1 \frac{1}{1+\left(\dfrac{1+\epsilon}{\alpha}\right)^2 y_1^2}\left(\int dr' r'^2 |g_\delta(r'+x_2)|\right)^2 \\
&\leqslant \frac{\epsilon^2 M^2 \alpha}{2(1+\epsilon)^3\hbar^2 t^2}\int dx_2 |f_\sigma(x_2)|^2 \left(\int dr' r'^2 |g_\delta(r'+x_2)|\right)^2.
\end{aligned}
\tag{4.23}
$$

For the estimate of (III) it is convenient to integrate by parts the integral in the variable v

$$(III)=\frac{2}{\pi}\int dx_2|f_\sigma(x_2)|^2\int dy_1\frac{1}{1+\left(\frac{1+\epsilon}{\alpha}\right)^2 y_1^2}\left|\int dr' g_\delta(r'+x_2)e^{i|y_1||r'|}e^{i(\mu/2\hbar t)\,r'^2}\right.$$
$$\left.\cdot\int_0^\infty dv e^{-v+i[(1+\epsilon)/\alpha]\,|y_1|v+i[(1+\epsilon)m/2\hbar t\alpha^2]v^2+i\,(m/\hbar t\alpha)\,|r'|v}\frac{(1+\epsilon)\mu}{\hbar t\alpha}\left(\frac{1+\epsilon}{\alpha}v+|r'|\right)\right|^2$$
$$\leqslant\frac{2(1+\epsilon)\mu^2}{\pi\hbar^2t^2\alpha}\int dx_2|f_\sigma(x_2)|^2\int dy_1\frac{1}{1+y_1^2}\left[\int dr'|g_\delta(r'+x_2)|\int_0^\infty dv e^{-v}\left(\frac{1+\epsilon}{\alpha}v+|r'|\right)\right]^2$$
$$\leqslant\frac{2\epsilon^2M^2}{(1+\epsilon)\hbar^2t^2\alpha}\int dx_2|f_\sigma(x_2)|^2\left[\int dr'|g_\delta(r'+x_2)|\left(\frac{1+\epsilon}{\alpha}+|r'|\right)\right]^2. \tag{4.24}$$

Finally, it remains to analyze the difference $\psi_2(t)-\hat{\psi}_2(t)$. Using the explicit expression of $U_0^\nu(t)$ we have

$$\psi_2(t,r,R)-\hat{\psi}_2(t,r,R)=\sqrt{\frac{m}{2\pi i\hbar t}}\sqrt{\frac{M}{2\pi i\hbar t}}e^{i(m/2\hbar t)\,r^2+i\,(M/2\hbar t)\,R^2}$$
$$\times\int d\xi f_\sigma(\xi)(e^{i(M/2\hbar t)\,\xi^2}-e^{i(\nu/2\hbar t)\,\xi^2})e^{-i[(M/\hbar t)\,R+\,(m/\hbar t)r]\xi}$$
$$\cdot\int dr' g_\delta(r'+\xi)\left(e^{-i\,(\mu/\hbar t)(r-R)r'}-\frac{e^{i(\mu/\hbar t)\,|r-R||r'|}}{1-i\frac{\hbar}{\alpha_0 t}|r-R|}\right). \tag{4.25}$$

Exploiting Plancherel theorem and the fact that the operator (2.16) is unitary one easily sees that

$$\|\psi_2(t)-\hat{\psi}_2(t)\|^2\leqslant\left(\frac{M}{2\hbar t}\right)^2\epsilon^2\int d\xi\xi^4|f_\sigma(\xi)|^2. \tag{4.26}$$

From (4.18), (4.19), (4.22), (4.23), (4.24), (4.26) we conclude the proof of the lemma. □

In the last step we approximate (4.13) using the fact that the coordinates of the heavy particle are slowly varying with respect to the coordinates of the light one.

Lemma 6: Given the initial state (2.10), for any $t>0$ we have

$$\|\psi_2(t)-\psi^a(t)\|<C_3(t)\,\epsilon, \tag{4.27}$$

where

$$C_3(t)=\left[\int dz z^2\int dx\left|\frac{\partial}{\partial x}(\tilde{f}_\sigma(z-x)\tilde{g}_\delta(x))\right|^2\right]^{1/2}+\frac{1}{\sqrt{2}\pi}\left\{\int dxdz\left[\frac{\alpha^2+z^2}{\alpha^2+x^2}\left(\int dr'|\zeta(z,r')|\right)^2\right.\right.$$
$$\left.\left.+\frac{\alpha^2z^2}{\alpha^2+x^2}\left(\int dr'|r'||\zeta(z,r')|\right)^2\right]\right\}^{1/2}, \tag{4.28}$$

with

$$C_3(t)<\frac{C_4}{t}+C_5 \tag{4.29}$$

and

$$\hat f_\sigma(\xi)=f_\sigma(\xi)e^{i(M/2\hbar t)\,\xi^2},\qquad \zeta(z,r')=\int d\xi \hat f_\sigma(\xi)g_\delta(r'+\xi)e^{-iz\xi}. \quad (4.30)$$

Proof: From (2.21) and (4.11) we have

$$\begin{aligned}\psi_2(t,r,R)-\psi^a(t,r,R)&=\sqrt{\frac{m}{2\pi i\hbar t}}\sqrt{\frac{M}{2\pi i\hbar t}}e^{i(m/2\hbar t)\,r^2+i\,(M/2\hbar t)\,R^2}\int d\xi f_\sigma(\xi)e^{i(M/2\hbar t)\,\xi^2}e^{-i[(M/\hbar t)R+\,(m/\hbar t)\,r]\xi}\\&\cdot\Bigg[\int dr' g_\delta(r'+\xi)(e^{-i(\mu/\hbar t)(r-R)r'}-e^{-i(m/\hbar t)rr'})+\int dr' g_\delta(r'+\xi)\\&\times\left(\frac{e^{i(\mu/\hbar t)\,|r-R||r'|}}{1-i\dfrac{\hbar}{\alpha_0 t}|r-R|}-\frac{e^{i(m/\hbar t)\,|r||r'|}}{1-i\dfrac{\hbar}{\alpha_0 t}|r|}\right)\Bigg]\equiv(\psi_2-\psi^a)_{fr}(t,r,R)+(\psi_2-\psi^a)_{in}(t,r,R).\end{aligned} \quad (4.31)$$

We will estimate separatly the two terms $(\psi_2-\psi^a)_{fr}(t)$ and $(\psi_2-\psi^a)_{in}(t)$.

Introducing the new integration variables

$$x=\frac{m}{\hbar t}r,\qquad z=\frac{MR+mr}{\hbar t}, \quad (4.32)$$

and the function $\hat f_\sigma(\xi)$ defined in (4.30), we have

$$\begin{aligned}\|(\psi_2-\psi^a)_{fr}(t)\|^2&=\frac{1}{(2\pi)^2}\int dxdz\left|\int d\xi\hat f_\sigma(\xi)e^{-iz\xi}\int dr' g_\delta(r'+\xi)\right.\\&\left.\times(e^{-i(x-[\epsilon/(1+\epsilon)]\,z)r'}-e^{-ixr'})\right|^2\\&=\frac{1}{2\pi}\int dxdz\left|\int d\xi\hat f_\sigma(\xi)e^{-iz\xi}\left(\tilde g_\delta\left(x-\frac{\epsilon}{1+\epsilon}z\right)e^{i(x-[\epsilon/(1+\epsilon)]\,z)\xi}-\tilde g_\delta(x)e^{ix\xi}\right)\right|^2\\&=\int dxdz\left|\tilde{\hat f}_\sigma\left(z-x+\frac{\epsilon}{1+\epsilon}z\right)\tilde g_\delta\left(x-\frac{\epsilon}{1+\epsilon}z\right)-\tilde{\hat f}_\sigma(z-x)\tilde g(x)\right|^2\\&=\int dxdz\left|G\left(x-\frac{\epsilon}{1+\epsilon}z,z\right)-G(x,z)\right|^2,\end{aligned} \quad (4.33)$$

where we introduced the function $G(x,z)=\tilde{\hat f}_\sigma(z-x)\tilde g(x)$.

Proceeding as in (4.9) we find

$$\|(\psi_2-\psi^a)_{fr}(t)\|^2\leqslant\left(\frac{\epsilon}{1+\epsilon}\right)^2\int dz z^2\int dx\left|\frac{\partial}{\partial x}(\tilde{\hat f}_\sigma(z-x)\tilde g(x))\right|^2. \quad (4.34)$$

For the estimate of $(\psi_2-\psi^a)_{in}(t)$ we use again the change of variables (4.32) and we introduce the function $\zeta(z,r')$ defined in (4.30).

Then we have

$$\|(\psi_2-\psi^a)_{in}\|^2\leqslant\frac{1}{(2\pi)^2}\int dxdz\left|\int dr'\zeta(z,r')\left(\frac{e^{i|x-[\epsilon/(1+\epsilon)]z||r'|}}{1-\frac{i}{\alpha}|(1+\epsilon)x-\epsilon z|}-\frac{e^{i|x||r'|}}{1-\frac{i}{\alpha}|x|}\right)\right|^2$$

$$\leqslant\frac{1}{2\pi^2}\int dxdz\left|\frac{1}{1-\frac{i}{\alpha}|(1+\epsilon)x-\epsilon z|}-\frac{1}{1-\frac{i}{\alpha}|x|}\right|^2\left(\int dr'|\zeta(z,r')|\right)^2$$

$$+\frac{1}{2\pi^2}\int dxdz\frac{\alpha^2}{\alpha^2+x^2}\left|\int dr'\zeta(z,r')(e^{i|x-[\epsilon/(1+\epsilon)]z||r'|}-e^{i|x||r'|})\right|^2$$

$$\leqslant\frac{\epsilon^2}{2\pi^2}\int dxdz\left[\frac{\alpha^2+z^2}{\alpha^2+x^2}\left(\int dr'|\zeta(z,r')|\right)^2+\frac{\alpha^2z^2}{\alpha^2+x^2}\left(\int dr'|r'||\zeta(z,r')|\right)^2\right], \tag{4.35}$$

where we have used the estimates

$$\left|\frac{1}{1-\frac{i}{\alpha}|(1+\epsilon)x-\epsilon z|}-\frac{1}{1-\frac{i}{\alpha}|x|}\right|^2=\frac{\alpha^2}{\alpha^2+x^2}\frac{(|x|-|(1+\epsilon)x-\epsilon z|)^2}{\alpha^2+((1+\epsilon)x-\epsilon z)^2}$$

$$\leqslant\epsilon^2\frac{\alpha^2}{\alpha^2+x^2}\frac{(x-z)^2}{\alpha^2+((1+\epsilon)x-\epsilon z)^2}\leqslant\left(\frac{\epsilon}{1+\epsilon}\right)^2\frac{\alpha^2+z^2}{\alpha^2+x^2} \tag{4.36}$$

and

$$|e^{i|x-[\epsilon/(1+\epsilon)]z||r'|}-e^{i|x||r'|}|\leqslant\frac{\epsilon}{1+\epsilon}|z||r'|. \tag{4.37}$$

The function $\zeta(z,r')$ is smooth and, using repeated integration by parts, one easily sees that it is rapidly decreasing when its first argument goes to infinity. The computation is long but straightforward and we omit the details. The conclusion is that the integral in the last line of (4.35) is finite. Along the same line one can verify that (4.29) holds, where the constants C_4, C_5 are independent of time and then the proof of the lemma follows.

Proof of theorem 1: This is now a simple consequence of lemmas 4, 5, 6. Furthermore the constants A,B can now be estimated, since they are given by $A=C_2+C_4$, $B=C_1+C_5$ [see (4.1), (4.10), (4.27), (4.29)] and then the dependence of A,B on the physical parameters characterising the initial state and the interaction can be seen from (4.3), (4.12), and (4.28).

We notice that, by simple rearrangments and rescaling, one can make such dependence more explicit. For instance, concerning C_1 one has

$$C_1^2=\int dz\int dy(z-y)^2|g'_\delta(z)f_\sigma(y)+g_\delta(z)f'_\sigma(y)|^2$$

$$\leqslant2(2R_0)^2\left(\int dz|g'_\delta\left(z|^2+\int dy|f'_\sigma(y)|^2\right)\right.$$

$$\leqslant16\left[\|g'\|^2\left(\frac{R_0}{\delta}\right)^2+\left(\frac{R_0q_0}{\hbar}\right)^2+2\|f'\|^2\left(\frac{R_0}{\sigma}\right)^2+2\left(\frac{R_0P_0}{\hbar}\right)^2\right], \tag{4.38}$$

where we have used the fact that $(z-y)^2\leqslant(2R_0)^2$ for $z\in supp\ \ g_\delta$, $y\in supp\ \ f_\sigma$ and we have rescaled the integration variables.

A longer but similar computation can also be done for the other constants C_2, C_4, C_5. □

APPENDIX: EXPLICIT SOLUTION OF THE TWO-BODY PROBLEM

We recall here the solution of the Schrödinger equation

$$i\hbar \frac{\partial \psi(t)}{\partial t} = H\psi(t), \qquad \psi(0)=\psi_0, \tag{A1}$$

where H is the self-adjoint Hamiltonian in $L^2(\mathbb{R}^2, drdR)$ given by (2.1). Using the unitary operator T [see (2.14)] one obviously has

$$THT^{-1} = H_0^{\nu} + H_{\alpha_0}^{\mu}, \qquad H_0^{\nu} = -\frac{\hbar^2}{2\nu}\Delta_{x_2}, \qquad H_{\alpha_0}^{\mu} = -\frac{\hbar^2}{2\mu}\Delta_{x_1} + \alpha_0\delta(x_1), \tag{A2}$$

where (x_1, x_2) are the relative and the center of mass coordinates

$$x_1 = r - R, \qquad x_2 = \frac{mr + MR}{m+M}. \tag{A3}$$

Then the solution of (A1) can be written as

$$\begin{aligned}\psi(t,r,R) &= (T^{-1}U_0^{\nu}(t)U_{\alpha_0}^{\mu}(t)T\psi_0)(r,R) \\ &= \int dr'dR'\,\psi_0(r',R')U_0^{\nu}\left(t, \frac{M}{\nu}(R-R') + \frac{\mu}{M}(r-r')\right)U_{\alpha_0}^{\mu}(t, r-R, r'-R'),\end{aligned} \tag{A4}$$

where the interacting unitary group $U_{\alpha_0}^{\mu}(t)$ is given by

$$U_{\alpha_0}^{\mu}(t,x,x') = e^{-i(t/\hbar)H_{\alpha_0}^{\mu}}(x,x'), \qquad x,x' \in \mathbb{R}. \tag{A5}$$

We remark that the evolution (A4) factorizes into a product of a free evolution in the center of mass coordinate and a one-body interacting evolution in the relative coordinate only if the initial state is of the form $\psi(r,R) = \psi_1[(M/\nu)R + (\mu/M)r]\psi_2(r-R)$.

In order to compute $(U_{\alpha_0}^{\mu}(t)\varphi_0)(x) \equiv \varphi(t,x)$ one has to solve the one-body Schrödinger equation

$$i\hbar \frac{\partial \varphi(t)}{\partial t} = -\frac{\hbar^2}{2\mu}\Delta_x\varphi(t) + \alpha_0\delta(x)\varphi(t), \qquad \varphi(0)=\varphi_0. \tag{A6}$$

Defining the rescaled wave function

$$\theta(s,z) = \varphi\left(\hbar s, \frac{\hbar}{\sqrt{\mu}}z\right), \tag{A7}$$

one finds that $\theta(s)$ satisfies the corresponding equation with $\mu = \hbar = 1$

$$i\frac{\partial \theta(s)}{\partial s} = -\frac{1}{2}\Delta_z\theta(s) + \alpha_0\frac{\sqrt{\mu}}{\hbar}\delta(z)\theta(s), \qquad \theta(0)=\theta_0, \quad \theta_0(z) = \varphi_0\left(\frac{\hbar}{\sqrt{\mu}}z\right). \tag{A8}$$

The solution of (5.8) can be found in Ref. 10.

$$\theta(s,z) = (\hat{U}_0^1(s)\theta_0)(z) - \alpha_0\frac{\sqrt{\mu}}{\hbar}\int_0^{\infty} dv\, e^{-\alpha_0(\sqrt{\mu}/\hbar)v}\int dz'\,\hat{U}_0^1(s, v+|z|+|z'|)\theta_0(z'), \tag{A9}$$

where $\hat{U}_0^1(s)$ is the free propagator with $\hbar=1$. Noticing that $(U^{\mu}_{\alpha_0}(t)\varphi_0)(x)=\varphi(t,x)=\theta(t/\hbar\,,(\sqrt{\mu}/\hbar)\,x)$ one has

$$(U^{\mu}_{\alpha_0}(t)\varphi_0)(x)=(U^{\mu}_0(t)\varphi_0)(x)-\frac{\mu\alpha_0}{\hbar^2}\int_0^{\infty}du e^{-(\mu\alpha_0/\hbar^2)u}\int dx' U^{\mu}_0(t,u+|x|+|x'|)\varphi_0(x'). \tag{A10}$$

Using (A4) and (A10), we finally obtain the complete solution (2.2) of the Schrödinger equation (A1).

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Continuum singularities of a mean-field theory of collisions

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Consider a complex energy z for an N-particle Hamiltonian H and let χ be any wave packet accounting for any channel flux. The time-independent mean-field (TIMF) approximation of the inhomogeneous, linear equation $(z-H)|\Psi\rangle=|\chi\rangle$ consists of replacing Ψ by a product or Slater determinant ϕ of single-particle states φ_i. This results, under the Schwinger variational principle, in self-consistent TIMF equations $(\eta_i-h_i)|\varphi_i\rangle=|\chi_i\rangle$ in single-particle space. The method is a generalization of the Hartree–Fock (HF) replacement of the N-body homogeneous linear equation $(E-H)|\Psi\rangle=0$ by single-particle HF diagonalizations $(e_i-h_i)|\varphi_i\rangle=0$. We show how, despite strong nonlinearities in this mean-field method, threshold singularities of the *inhomogeneous* TIMF equations are linked to solutions of the *homogeneous* HF equations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1666978]

I. INTRODUCTION

After the success of the mean-field approach for bound state systems in various fields of physics, it was only natural to try the mean-field concept for scattering states as well. The original attempt[1] was the time-dependent Hartree–Fock (TDHF) method, where one solves the single-particle equations of motion as *initial* value problem in time. From the resulting solutions at various impact parameters, one may then calculate the classical cross section. With no specification of the final state, the method is restricted to inclusive reactions. A serious, conceptual problem arises from spurious cross-channel correlations:[2,3] when projecting the TDHF Slater determinant for large times on an orthogonal set of channel wave functions, the expansion coefficients and the respective S-matrix vary in time *ad infinitum*. To overcome the shortcomings of TDHF, the time-dependent mean-field (TDMF) approach[2–4] expands the density in two sets of (biorthogonal) single-particle wave functions and solves the equations of motion as a *boundary* value problem in time, fixing initial and final densities. It has been proven that for TDMF an S-matrix can be defined which becomes asymptotically constant.[2] The problem with TDMF lies in combining self-consistency with given boundary conditions in time.[3,5] No practicable algorithm for this highly ''nonlocal'' problem exists up to date for use in actual numerical calculations. A third approach is the time-independent mean field (TIMF) method,[6] based on a Schwinger-type variational principle[7] for matrix elements of the resolvent or T-operator between given initial and final states. The method uses two sets of variational single-particle functions, analogous to TDMF, and leads to inhomogeneous equations of Hartree–Fock type which can be solved iteratively for given total energy of the system. TIMF is free of the conceptual and practical problems of TDHF and TDMF, respectively, and has been tested successfully on a number of simple systems. It can be extended to incorporate particle–hole correlations, as has also been done for TDHF, within a

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generalized random-phase-approximation.[8] The present paper goes beyond the above problems[9] by studying the continuum singularities of this TIMF approach for collisions.

Consider a finite number N of particles. Factorized wave packets (shifted Gaussians in momentum representation for example) make an overcomplete basis in their Hilbert space of wave functions. Hence, the calculation of a retarded Green's function amplitude $\mathcal{D}\equiv\langle\chi|(z-H)^{-1}|\chi\rangle$, where (i) χ is a product, $|\chi\rangle=\Pi_{i=1}^{N}|\chi_i\rangle$, and (ii) each single-particle wave function χ_i is real rather than complex, makes a fully generic problem. Such factorization simplifications are not physically restrictive and help in the analysis of a mean-field theory of collisions, the subject of this paper.

For the sake of simplicity, we deal so far with spinless, distinct particles only and short-range interactions v_{ij} for the Hamiltonian $H=\Sigma_{i=1}^{N}p_i^2/(2m_i)+\Sigma_{i>j=1}^{N}v_{ij}$. The case of identical particles can be treated later and, in the following, any reference to a Hartree method may be understood as a reference to a Hartree–Fock (HF) method if necessary. Again for simplicity, we consider the calculation of diagonal collision amplitudes only, $\langle\mathbf{k}|V(E^+-H)^{-1}V|\mathbf{k}\rangle$, Born term subtracted. Generalizations to distinct prior and post interactions, V,V', are kept for future work. The state $|\mathbf{k}\rangle$ is taken as a plane wave of relative motion in any two cluster channel ground state, and the product $|\chi\rangle\equiv V|\mathbf{k}\rangle$ is a square integrable state in the N-particle space. Finally, z is any complex number $E+i\Gamma$, and the usual limit E^+ at the end of any calculation reads $\Gamma\to+0$.

It is trivial to use the Schwinger variational principle[7] and show that $\mathcal{D}$ is the stationary value of the functional

$$\mathcal{F}\equiv\frac{\langle\Psi'|\chi\rangle\langle\chi|\Psi\rangle}{\langle\Psi'|(z-H)|\Psi\rangle} \tag{1}$$

under variations of Ψ,Ψ'. The corresponding Euler–Lagrange equations read, with retarded boundary conditions and arbitrary norms and phases of Ψ and Ψ'

$$(z-H)|\Psi\rangle=|\chi\rangle,\quad \langle\Psi'|(z-H)=\langle\chi|. \tag{2}$$

The variational equations which occur in the time-independent mean-field (TIMF)[6] theory of collisions read

$$(\eta_i-h_i)|\varphi_i\rangle=|\chi_i\rangle,\ \langle\varphi_i'|(\eta_i-h_i)=\langle\chi_i|,\ i=1,\ \ldots,N. \tag{3}$$

They are obtained from Eq. (1) when χ, and the approximation ϕ, respectively ϕ', chosen for Ψ, respectively Ψ', are products of single-particle orbitals, $\chi_i,\varphi_i,\varphi_i'$, respectively. Such TIMF equations are very simple.[6] Except for a single-particle density operator ρ defined nondiagonally as $\rho(\mathbf{r}',\mathbf{r})=\Sigma_i\varphi_i(\mathbf{r}')\varphi_i'^{*}(\mathbf{r})$, they are just Hartree(–Fock) equations completed by a right-hand side, representing the image of the channel in single-particle space. In the following, $\mathcal{F}$ is restricted to such factorized source functions χ and trial functions ϕ,ϕ' and will be labeled F. A saddle value under such a restriction of ϕ,ϕ' is not necessarily unique anymore. It will be denoted by D instead of $\mathcal{D}$ and may request an additional, identifying label. Now our claim is: *bound and unbound solutions of the usual Hartree(–Fock) equations*

$$(e_i-h_i)|\varphi_i\rangle=0, \tag{4}$$

induce singularities of the one-body variational conditions, Eqs. (3).

This reminds one, naturally, of the strict connection between the singularities of the linear, inhomogeneous problem $(z-H)|\Psi\rangle=|\chi\rangle$ in the N-body space and the solutions of the linear, homogeneous Schrödinger equation $(E-H)|\Psi\rangle=0$ in the same space. Because of the nonlinear nature of Eqs. (3)–(4) in single-particle space, our claim is not obvious, and will be qualified in this paper.

Actually, in a previous paper,[10] the claim was already substantiated in part: those energies E_H, for which a bound Hartree(–Fock) solution ϕ_H is found, generate poles of the approximate

amplitude D provided by saddle points of the restriction F. Furthermore $(z-E_H)D \to |\langle\chi|\phi_H\rangle|^2/\langle\phi_H|\phi_H\rangle$ when $z\to E_H$. Despite the nonlinearity of the approximation, such a residue at such a pole is almost expected. The analogy with the poles of $\mathcal{D}$ at exact eigenvalues for bound states is striking. We are now interested in a more difficult question, namely, is there a similar analogy at higher energies, when singularities of scattering and rearrangement collisions (thresholds, cuts) occur?

In Sec. II we briefly recall a very simple, soluble model,[11] used earlier among several other models to validate D as an approximation of $\mathcal{D}$. The model is reintroduced for pedagogical reasons first, to illustrate a derivation of Eqs. (3). Then, and mainly, it is used to provide a complete investigation of singularities, for it boils down to manipulations of polynomials. In Sec. III we introduce an enriched model, exactly soluble too. Section IV contains a generalization and discussion of the results obtained in Secs. II and III. Finally, Sec. V contains our conclusion.

II. FIRST MODEL, BARE PROPAGATION, SYMMETRIC MEAN FIELD, TWO-BODY THRESHOLD

In this soluble model, there are only two one-dimensional particles with just their kinetic energies, and different masses $m_i=1/(2a_i)$; hence, $H=a_1p_1^2+a_2p_2^2$. While the inversion of $z-H$ is numerically trivial and allows a good validation[11] of the TIMF approximation, the formal expression of $(z-H)^{-1}$ in terms of one-body propagators $(\eta_1-a_1p_1^2)^{-1}$ and $(\eta_2-a_2p_2^2)^{-1}$ is less trivial, as it demands a convolution. The TIMF method consists of replacing the convolution by just one product, namely,

$$(z-a_1p_1^2-a_2p_2^2)^{-1}|\chi_1\chi_2\rangle \propto (\eta_1-a_1p_1^2)^{-1}|\chi_1\rangle(\eta_2-a_2p_2^2)^{-1}|\chi_2\rangle\,. \tag{5}$$

This comes from variations $\delta/\delta\varphi_i$ of the functional F. An additional simplification results from a further remark: in those representations where χ and H are real, one finds from Eqs. (2) that $|\Psi'\rangle=|\Psi^*\rangle$, hence the possibility of just one trial function Ψ if one uses a Euclidean $(|)$ rather than a Hermitian $\langle|\rangle$ metric,

$$\mathcal{F}\equiv\frac{(\Psi|\chi)\,(\chi|\Psi)}{(\Psi|(z-H)|\Psi)}=\frac{(\chi|\Psi)^2}{(\Psi|(z-H)|\Psi)}\,. \tag{6}$$

For the present two-particle model, the factorization of χ into two single-particle wave packets with real wave functions χ_1,χ_2 allows us to use the following form of F:

$$F=\frac{(\chi_1\chi_2|\varphi_1\varphi_2)^2}{(\varphi_1\varphi_2|\,(z-a_1p_1^2-a_2p^2)\,|\varphi_1\varphi_2)}=\frac{(\chi_1|\varphi_1)^2(\chi_2|\varphi_2)^2}{z(\varphi_1|\varphi_1)(\varphi_2|\varphi_2)-(\varphi_1|a_1p_1^2|\varphi_1)(\varphi_2|\varphi_2)-(\varphi_1|\varphi_1)(\varphi_2|a_2p_2^2|\varphi_2)}\,. \tag{7}$$

We assume that χ_1,χ_2 are real in the momentum representation. The functional being insensitive to the norms and global phases of φ_1,φ_2, elementary manipulations of $\delta F/\delta\varphi_i$ yield, in the same momentum representation

$$\varphi_i(p)=\frac{\chi_i(p)}{\eta_i-a_ip^2}\,,\qquad i=1,2, \tag{8}$$

with

$$\eta_i=z-\frac{\int dp\;\varphi_j^2(p)\,a_jp^2}{\int dp\;\varphi_j^2(p)}=z-\eta_j-\frac{\int dp\;\chi_j^2(p)(a_jp^2-\eta_j)^{-1}}{\int dp\;\chi_j^2(p)(a_jp^2-\eta_j)^{-2}}\,,\qquad i=1,2,\ j=1,2,\ \text{and}\ j\neq i. \tag{9}$$

It is convenient at this stage to define the integrals

$$I_i = -(\chi_i|\varphi_i) = \int dp\, \frac{\chi_i^2(p)}{a_i p^2 - \eta_i}, \qquad i = 1,2, \tag{10}$$

and notice that Eqs. (9) then read

$$I_j \frac{d\eta_j}{dI_j} = z - \sum_{i=1}^{2} \eta_i, \qquad j = 1,2. \tag{11}$$

If furthermore one defines auxiliary variables ω_i by the conditions

$$\eta_i = a_i \omega_i^2, \quad \Im\omega_i > 0, \qquad i = 1,2, \tag{12}$$

then it is useful to define $J_j \equiv a_j I_j$. And, Eqs. (11) become

$$2\, a_j \omega_j J_j \frac{d\omega_j}{dJ_j} = z - \sum_{i=1}^{2} a_i\, \omega_i^2, \quad j = 1,2, \tag{13}$$

where a contour in the upper half plane of the complex variable p defines the integrals

$$J_j = \int dp\, \frac{\chi_j^2(p)}{p^2 - \omega_j^2}, \qquad j = 1,2. \tag{14}$$

The special cases $\Im\eta_j \to 0$, while $\Re\eta_j \geqslant 0$ define cuts in the complex η_j plane. These correspond to $\Im\omega_j \to 0$ in the ω_j plane.

When the two particles are identical, it may be interesting to symmetrize and antisymmetrize Eqs. (13) as

$$\sum_{i=1}^{2} a_i\, \omega_i\, J_i \frac{d\omega_i}{dJ_i} = z - \sum_{i=1}^{2} a_i\, \omega_i^2, \tag{15}$$

and

$$a_1\, \omega_1\, J_1 \frac{d\omega_1}{dJ_1} - a_2\, \omega_2\, J_2 \frac{d\omega_2}{dJ_2} = 0, \tag{16}$$

and identify cases where the mean field might break their symmetry. But, we shall keep the particles, and/or their channel wave packets distinct for a while.

A soluble model, involving only the manipulation of polynomials, is obtained if one chooses the forms of the wave packets as follows:

$$\chi_j(p) = \left[\frac{\gamma_j}{\pi[(p - K_j)^2 + \gamma_j^2]} \right]^{1/2}, \quad j = 1,2, \tag{17}$$

yielding the simple result

$$J_j = \frac{i\gamma_j}{\omega_j[(\omega_j - K_j)^2 + \gamma_j^2]} + \frac{1}{(K_j + i\gamma_j)^2 - \omega_j^2} = \frac{-\omega_j - i\gamma_j}{\omega_j(\omega_j - K_j + i\gamma_j)(\omega_j + K_j + i\gamma_j)}. \tag{18}$$

Resulting polynomial equations turn out to have a lower degree if $K_j = 0$, for then J_j becomes $J_j = -1/[\omega_j(\omega_j + i\gamma_j)]$. As will be found in this and the next sections, two kinds of singularities emerge: (i) "physical" ones, which essentially depend on z and are not very sensitive to "technical" parameters K_j, a_j, γ_j, and (ii) "technical" singularities, more sensitive to such parameters. The analytical continuation provided across η cuts[12] by this ω representation is clear.

Once Eqs. (13) have been solved, the saddle-point values of the functional read, using Eqs. (7)–(11)

$$D=\frac{(a_1\omega_1^2+a_2\omega_2^2-z)J_1J_2}{a_1a_2}. \tag{19}$$

The search for singularities of D as a function of the physical energy z thus consists of eliminating ω_1,ω_2 between Eqs. (13) and Eq. (19). The former reads, after elementary manipulations which take advantage of Eq. (18) when $K_1=K_2=0$

$$2a_1x^2y+a_1\gamma_2x^2-a_2\gamma_2y^2+2yz+\gamma_2z=0,\quad 2a_2y^2x+a_2\gamma_1y^2-a_1\gamma_1x^2+2xz+\gamma_1z=0, \tag{20}$$

where it was convenient to set $\omega_1=ix$, $\Re x>0$, and $\omega_2=iy$, $\Re y>0$. Equivalently, if we scale x and y into $x=\gamma_1x'$ and $y=\gamma_2y'$, respectively, the same equations read

$$(A_1x'^2+z)\,(1+2y')-A_2y'^2=0,\ (A_2y'^2+z)\,(1+2x')-A_1x'^2=0\,, \tag{21}$$

with $A_1\equiv a_1\gamma_1^2$ and $A_2\equiv a_2\gamma_2^2$. An elimination of y between Eqs. (20) gives

$$\begin{aligned}&2a_1^3\gamma_1x^7-a_1^2(4z-a_1\gamma_1^2+a_2\gamma_2^2)x^6-a_1z(8z-a_1\gamma_1^2+4a_2\gamma_2^2)x^4-2a_1\gamma_1z(3z+a_2\gamma_2^2)x^3\\&\quad-z^2(4z+a_1\gamma_1^2+4a_2\gamma_2^2)x^2-4z^2\gamma_1(z+a_2\gamma_2^2)x-\gamma_1^2z^2(z+a_2\gamma_2^2)=0,\end{aligned} \tag{22a}$$

$$y=-\frac{\gamma_2\,(a_1\,x^3+2\,x\,z+\gamma_1\,z)}{(2\,x+\gamma_1)\,(a_1\,x^2+z)}\ . \tag{22b}$$

The multiplicity of solutions is thus 7, which raises a problem for the identification of a solution, if possible unique, which accounts for a physical approximation.

In turn, if one inserts Eq. (18) into Eq. (19), one obtains D as a rational function of ω_1,ω_2, or x,y as well. Upon taking advantage of Eq. (22b), this rational fraction reduces into a rational fraction of x only, hence a polynomial relation between D and x, with degree 1 for D

$$\begin{aligned}&a_1^2a_2\gamma_2^2x^3(\gamma_1+x)^2(a_1x^3+\gamma_1z+2xz)D\\&\quad=4a_1^3x^7(x+\gamma_1)+a_1^2(a_1\gamma_1^2+a_2\gamma_2^2+12z)x^6+12a_1^2\gamma_1zx^5+a_1z(3a_1\gamma_1^2+4a_2\gamma_2^2\\&\qquad+12z)x^4+2a_1\gamma_1z(a_2\gamma_2^2+6z)x^3+z^2(3a_1\gamma_1^2+4a_2\gamma_2^2+4z)x^2\\&\qquad+4\gamma_1z^2(a_2\gamma_2^2+z)x+\gamma_1^2z^2(a_2\gamma_2^2+z).\end{aligned} \tag{23}$$

The same result is obtained if one uses Eq. (7) instead of Eq. (19).

An elimination of x between Eq. (23) and Eq. (22a) finally gives a direct, polynomial condition relating D and z

$$\begin{aligned}&z_1^2z_2^2(z_1+1)(z_2+1)(z_1+z_2+1)\overline{D}^7-4z_1z_2(z_1+1)(z_2+1)(z_1z_2-4z_1-4z_2-4)\overline{D}^6\\&\quad-4[3z_1^3z_2^2+3z_1^2z_2^3+(20z_1^3z_2+58z_1^2z_2^2+20z_1z_2^3)+(16z_1^3+88z_1^2z_2+88z_1z_2^2+16z_2^3)\\&\quad+(32z_1^2+84z_1z_2+32z_2^2)+16(z_1+z_2)]\overline{D}^5+16[3z_1^2z_2^2+39(z_1^2z_2+z_1z_2^2)\\&\quad+(32z_1^2+91z_1z_2+32z_2^2)+48(z_1+z_2)+16]\overline{D}^4+16[3z_1^2z_2+3z_1z_2^2-(8z_1^2+91z_1z_2+8z_2^2)\\&\quad-88(z_1+z_2)-64]\overline{D}^3+192[-z_1z_2+4(z_1+z_2)+8]\overline{D}^2-64(z_1+z_2+16)\overline{D}+256=0,\end{aligned} \tag{24}$$

where $z_i = a_i \gamma_i^2 / z$ and D is scaled as $D = \overline{D}/z$. The degree 7 for x in Eq. (22a) is correctly reflected here by the same degree for D (and $\overline{D}$). Conversely, given an amplitude D, the degree of the polynomial condition, Eq. (24), with respect to z, is 4. Hence, there are 7 approximate amplitudes offered by TIMF for each energy, while the inverse problem, ''given the TIMF amplitude, find the energy,'' has 4 solutions.

This model, although soluble, thus creates a complicated Riemann surface. Criteria are necessary to select one physical sheet, or physical pieces of sheets. Obvious candidates are the conditions $\Re x \geqslant 0, \Re y \geqslant 0$ when Eqs. (20) are solved. Concerning Eq. (24), the very definition of $\mathcal{D}$ demands that $\mathcal{D}$ be real and negative if z is real and negative. When $z > 0$ with a slight and positive imaginary part, then $\Im \mathcal{D}$ must be negative. Those roots D which show the same properties should thus help the identification of suitable sheets.

The argument is made much simpler if the ''technical'' parameters $a_1 \gamma_1^2$ and $a_2 \gamma_2^2$ are taken equal to some common value θ. This amounts, in some sense, to consider identical particles, although a_1 may still differ from a_2. Then, Eq. (24) factorizes as

$$[4 - 4(\theta + z)D + \theta(\theta + z)D^2]^2 [16 + 8(3\theta - 4z)D + 4(3\theta^2 + 10\theta z + 4z^2)D^2 + \theta^2(2\theta + z)D^3] = 0. \tag{25}$$

If θ is used as a unit for z and similarly $1/\theta$ is used as a unit for D, this reads as well

$$[4 - 4(1 + z)D + (1 + z)D^2] = 0, \tag{26a}$$

$$[16 + 8(3 - 4z)D + 4(3 + 10z + 4z^2)D^2 + (2 + z)D^3] = 0. \tag{26b}$$

The presence of a squared polynomial as the first factor in Eq. (25) reflects a ''symmetry breaking'' by the mean-field approximation. Indeed, when analyzing the corresponding solutions of Eqs. (20), one finds that each pair of roots $\{x,y\}$, with $x \neq y$, is accompanied by a pair $\{y,x\}$, generating the same value of D. Such a degeneracy thus makes, out of 4 of all the 7 solutions for $\{x,y\}$, two distinct values for D. All told, D then takes 5 distinct values. The remaining 3 solutions account for the degree 3 present in the second factor of Eq. (25). It is easy to verify that such 3 solutions are ''symmetric,'' namely, $x = y$. Notice that the symmetry breaking generates a rational inverse function

$$z_{bk} = \frac{(D_{bk} - 2)^2}{D_{bk}(4 - D_{bk})}, \tag{27}$$

while the symmetry conservation generates an equation of degree 2 for z. Since z_{bk} must be counted twice, one recovers the 4 solutions of the inverse problem.

It turns out that the symmetry breaking sector violates the double condition, $\Re x > 0$, $\Re y > 0$. Hence, the properties of this sector are listed in the Appendix only. Turning now to the symmetric amplitude D_{sy}, the choice of a physical branch is reasonably easy; see Figs. 1 and 2. In Fig. 1, the lower half plane contains a loop acceptable as a physical candidate. We verified that $\Re x > 0$ for this loop. Despite a suitable $\Re x > 0$ if $z > 0$, the other branch in Fig. 1 is clearly not acceptable, for it contains values D_{sy} with positive imaginary parts. Nor can one accept the third branch, seen in Fig. 2, despite its correct sign for $\Im D_{sy}$, for it violates both the limit $\mathcal{D} \to 0$ when $|z| \to \infty$ and the obvious condition ''$\Re \mathcal{D} < 0$ if z is real and negative.'' Furthermore, $\Re x$ is found unsatisfactory for this third branch.

Two values of z generate branching for D_{sy}. With a single root $D = -1/5$, reasonable, a double root $D = 16$, unphysical, occurs for $z = -27/16$, with expansion $D = 16 - 256/9\,(z + 27/16) \pm 8192/243\,[-(z + 27/16)^3]^{1/2}$. Hence, a familiar square-root cut can be used to disentangle the two corresponding sheets, both unphysical. The value $z = -27/16$ does not represent a natural threshold for the present model. More physical, obviously, is the triple-root singularity, $D = -2$, which occurs at $z = 0$, the true threshold. It is illustrated by Fig. 3, where a tiny imaginary

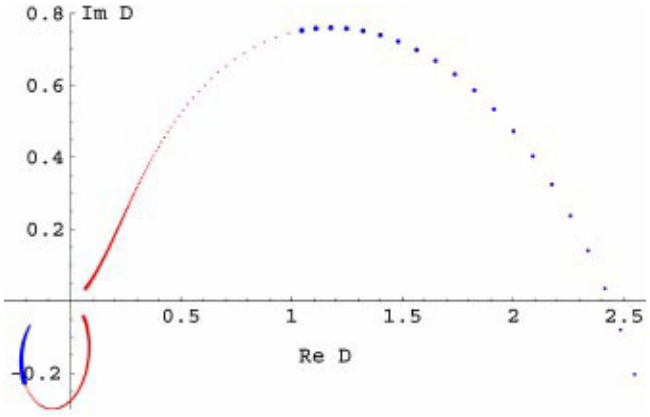

FIG. 1. Complex D plane. Two trajectories of symmetry conserving amplitudes as functions of $\Re z$ when $\Im z=1$. Growing blue dots: $\Re z$ grows from $-\infty$ to -0. Growing red dots: $\Re z$ increases from $+0$. The third trajectory lies far in the lower half. Color is available online at www-spht.cea.fr/articles/t02/148/

part $\Im z=0.0001$ was added in order to separate branches. It is noticed here that, although the physical branch gives real values of D_{sy} when $z<0$ and complex values of the same when $z>0$, there are always one real root and two complex conjugate roots on both sides in the vicinity of $z=0$. This happens indeed because the corresponding discriminant, $\Delta_3=256z^2(27+16z)^3/(2+z)^4$, actually changes sign, not for $z=0$, but rather for $z=-27/16$. This helps to understand the nature of the unphysical singularity occurring at $z=-27/16$. It gives an early ''warning'' of the (cubic) physical threshold singularity, $z=0$. An elementary, but slightly tedious calculation provides the expansions of the 3 branches in the vicinity of $z=0$, namely, $D=-2-j\,2^{2/3}\,3\,z^{1/3}+\mathcal{O}(z^{2/3})$, where j is either 1, or any one of its complex cubic roots $(-1\pm i\sqrt{3})/2$.

Consider Eqs. (21) and set $A_1=A_2$ to factorize the resultant, Eq. (22a). Then, scale x, y, and z as proportional to γ_1, γ_2, and A_1, respectively. For the sake of simple numbers, this strictly amounts to setting a common value $a_1=a_2=\gamma_1=\gamma_2=1$; hence, $A_1=A_2=1$, for those reduced equations which govern the scaled variables and parameters. For the symmetry sector, $x=y$, both equations, Eqs. (20), then boil down to $2x^3+2xz+z=0$. It is trivial to find that, at threshold $z\to 0$, all three roots have a leading term $x=(-z/2)^{1/3}+\mathcal{O}(z^{2/3})$, while, as already found,

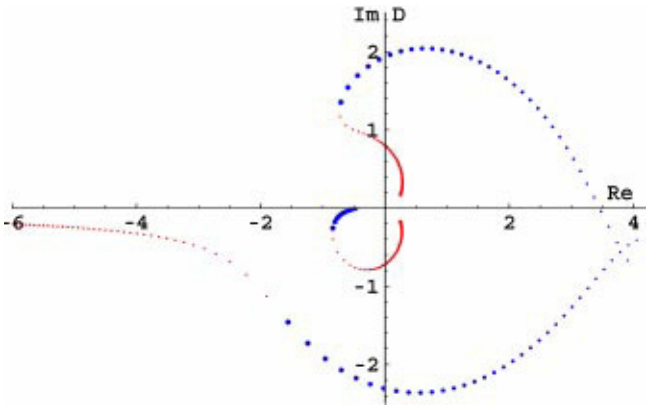

FIG. 2. Complex D plane. All trajectories D_{sy} when $\Im z=0.075$. Scales of trajectories made compatible by replacing radii from the origin by their square roots. Hence, for instance, announcing the double root $D=16$ when $z=-27/16$, blue branches cross each other near $\sqrt{D}=4$. Growing blue dots: $\Re z$ grows from $-\infty$ to -0. Growing red dots: $\Re z$ increases from $+0$.

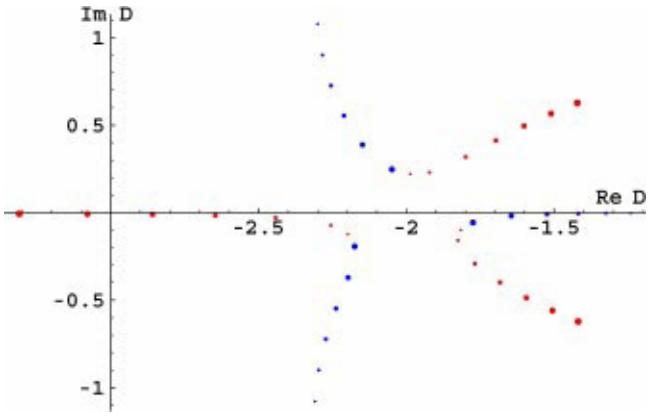

FIG. 3. Complex D plane. Triple merging $D_{sy}\rightarrow -2$, with $\Im z=0.0001$, $-0.09<\Re z<0.09$. Lower right branch physical.

$D_{sy}=-2+\mathcal{O}(z^{1/3})$. Obviously, below threshold, one must select the real root x, which gives a real amplitude. Conversely, above threshold, one must select that complex x which gives a retarded amplitude.

All told, for D_{sy}, cuts needed in the z plane are a cut from 0 to $+\infty$ for the cubic branching and, for instance, a "technical" cut from $-\infty$ to $-27/16$ to create an additional seam between the second and the third sheets.

Now we consider additional cuts, namely, those created by the condition $\Im\omega=0$, or, identically, by the condition $\Re x=0$. These occur because the solutions of realistic problems demand numerical, iterative calculations of η_i and φ_i before obtaining D. This means inversions of operators $(a_i\omega_i^2-h_i)$ in sequences of successive approximations of ω's (and self-consistent h's when potentials are involved). Obviously, every time $\Im\omega$ vanishes or becomes too small, numerical precautions are in order. Also, since the physical energy is on shell, $z=E+i0^+$, with a retardation boundary condition for many-body propagation, one would feel more comfortable with retardation also for the single-particle energies $\eta\propto\omega^2$. Advanced $\eta's$ are not to be ruled out *a priori*, because it is well known that mean-field approximations can be excellent while breaking many-body symmetries. But, clearly, branches of x's which cross such cuts $\Re x=0$ deserve some cautious scrutiny.

For the present case where $A_1=A_2$ for "symmetric" bare propagations, and still with simple numbers $a_i=\gamma_i=1$, our results are shown in Figs. 4 and 5. (For the academic, "symmetry breaking" case, see the Appendix and Figs. 13 and 14.) Figure 4 is a contour plot of the product $\Re x_1\Re x_2\Re x_3$ of the real parts of the 3 roots as functions of z in the z plane. Darker areas indicate an increasing positive product (two out of the three $\Re x$'s are <0), while the lighter areas mean a more and more negative one (one negative $\Re x$ only). The product vanishes along the contour line separating the light gray area from the moderate gray one. It will be noticed that this line contains the point $z=0$. Hence, the cut relevant to D and that relevant to x's both contain the two-body threshold. Notice, however, that, except at such a threshold, a real z induces complex η's. Namely, propagation energy cuts *do not follow the real axis* in the z plane.

The next figure, Fig. 5, shows the trajectories of the roots when we freeze $\Re z=0.1$, above threshold, and let $\Im z$ run from -1 to $+1$, hence allowing one $\Re x$, then a second one, to change their signs. The sizes of dots are coded as follows: minimal for $\Im z=-1$, growing until $\Im z=0$, minimal again for small positive values of $\Im z$, then growing again until $\Im z=1$. The lower branch is the best candidate for physical roots, because it provides a growing retardation, $0<\Im\eta\equiv\Im(-x^2)$, when $\Im z$ is positive and grows. As predicted from Fig. 4, there is an interval for $\Im z$ where 2 roots x have a positive $\Re x$.

To conclude this section, the main result derived from this elementary model with bare propagation of two particles lies in the systematic, *physical*, two-body threshold found at $z=0$ in the energy plane (z plane) for all the mean-field quantities, whether amplitudes D or propagation

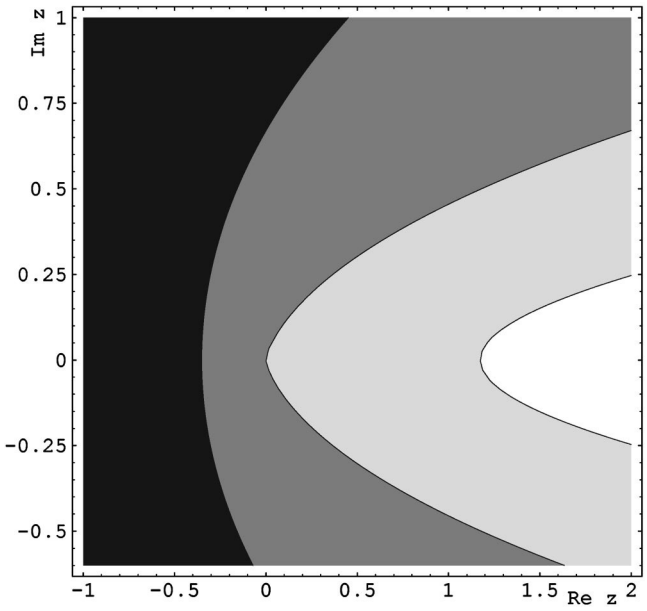

FIG. 4. Complex z plane. Cut caused by the condition $\Re x = 0$ for symmetry conserving roots. The cut is the contour line separating the lighter gray area from the darker gray one.

energies η. This threshold is, obviously, a common feature of both the exact problem and the corresponding Hartree problem. For amplitudes D, a cut in the z plane extends from the threshold 0 to $+\infty$, as seen in both the ''symmetric'' and ''breaking'' submodels. For propagation energies η, the cut starts from $z=0$, indeed, but deviates from the real semiaxis. For both Ds and η's, the cost of the nonlinearity of the TIMF approach is reflected in additional, unphysical, ''technical'' singularities. But, such unphysical singularities are not beyond interpretation either, as shown by the analytical properties listed in this section. Incidentally, as discussed earlier,[13] unphysical singularities may be washed out by a linear admixture of the various solutions of the nonlinear mean-field problem. The next sections will show even better how physical cuts remain a significant feature of the TIMF approximation.

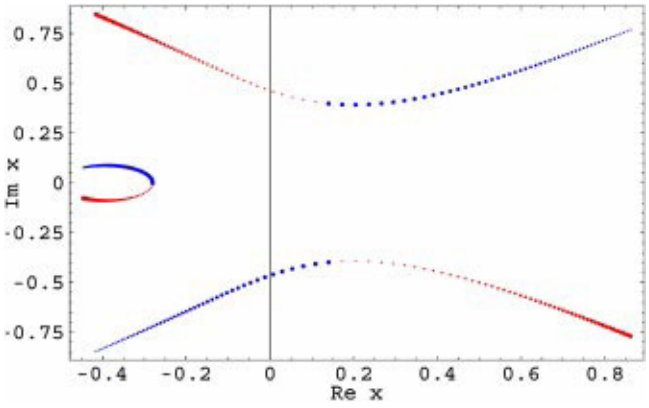

FIG. 5. Complex x plane. Trajectories of the symmetry conserving x's when $\Re z = 0.1$, while $\Im z$ crosses the cut shown by Fig. 4. Blue dots growing when $\Im z$ grows from -1 to 0. Red dots growing when $\Im z$ grows from 0 to 1.

III. SECOND SOLUBLE MODEL, ONE-BODY THRESHOLD

Here again we consider two one-dimensional particles, and particle 2 is still free with a pure kinetic energy $h_2=a_2p_2^2$ for its Hamiltonian. But, now the complete Hamiltonian $H=h_1+h_2$, while still separable, involves a bound state for particle 1, because we set $h_1=a_1p_1^2-\lambda|\chi_1\rangle\langle\chi_1|$, with an attractive enough potential. For technical reasons which will soon become clear, the form $\lambda|\chi_1\rangle\langle\chi_1|$ of this potential makes use of the same wave packet χ_1 taken as a channel wave packet. The numerical inversion of $z-H$ is still easy and allows another good validation of the TIMF approximation. The formal expression of $(z-H)^{-1}$ in terms of one-body propagators $(\eta_1-h_1)^{-1}$ and $(\eta_2-h_2)^{-1}$ demands again a convolution and the TIMF method consists in replacing the convolution by a product

$$(z-h_1-h_2)^{-1}|\chi_1\chi_2\rangle\propto(\eta_1-h_1)^{-1}|\chi_1\rangle\,(\eta_2-h_2)^{-1}|\chi_2\rangle. \tag{28}$$

This comes again from variations $\delta/\delta\varphi_i$ of the functional F. And, a further remark can be repeated: in those representations where χ and H are real, we obtain $|\Psi'\rangle=|\Psi^*\rangle$; see Eqs. (2). Hence, the possibility of just one trial function ϕ under a Euclidean rather than a Hermitian metric; see Eq. (6). The factorization of χ into two real wave packets χ_1,χ_2 essentially retains Eq. (7), which actually becomes

$$\begin{aligned}F&=\frac{(\chi_1\chi_2|\varphi_1\varphi_2)^2}{(\varphi_1\varphi_2|\,(z-h_1-h_2)\,|\varphi_1\varphi_2)}\\&=\frac{(\chi_1|\varphi_1)^2(\chi_2|\varphi_2)^2}{z(\varphi_1|\varphi_1)(\varphi_2|\varphi_2)-(\varphi_1|h_1|\varphi_1)(\varphi_2|\varphi_2)-(\varphi_1|\varphi_1)(\varphi_2|h_2|\varphi_2)}.\end{aligned} \tag{29}$$

We use the same χ_1,χ_2, real in the momentum representation. The functional being always insensitive to the norms and global phases of φ_1,φ_2, the same manipulations of $\delta F/\delta\varphi_i$ yield, in the same momentum representation

$$|\varphi_1)=(\eta_1-h_1)^{-1}|\chi_1),\quad(\eta_1-a_1p_1^2)|\varphi_1)=|\chi_1)-\lambda|\chi_1)(\chi_1|\varphi_1),$$

$$\varphi_1(p)=\frac{\chi_1(p)}{\eta_1-a_1p^2}[1-\lambda(\chi_1|\varphi_1)], \tag{30}$$

$$\varphi_2(p)=\frac{\chi_2(p)}{\eta_2-a_2p^2}, \tag{31}$$

where it is better, temporarily at least, to retain the factor $\nu=[1-\lambda(\chi_1|\varphi_1)]$ for φ_1. The same quantity ν, as will be seen shortly, cannot be discarded from the self-consistency conditions of the pair η_1,η_2

$$\eta_1=z-\frac{\int dp\;\varphi_2^2(p)\,a_2p^2}{\int dp\;\varphi_2^2(p)}=z-\eta_2-\frac{\int dp\;\chi_2^2(p)(a_2p^2-\eta_2)^{-1}}{\int dp\;\chi_2^2(p)(a_2p^2-\eta_2)^{-2}}, \tag{32}$$

$$\eta_2=z-\frac{(\varphi_1|h_1|\varphi_1)}{(\varphi_1|\varphi_1)}=z-\eta_1-\frac{(\varphi_1|(h_1-\eta_1)|\varphi_1)}{(\varphi_1|\varphi_1)}=z-\eta_1-\frac{(\chi_1|(h_1-\eta_1)^{-1}|\chi_1)}{(\chi_1|(h_1-\eta_1)^{-2}|\chi_1)}. \tag{33}$$

Indeed, it is necessary to consider the matrix element

$$\mathcal{I}_1=(\chi_1|(h_1-\eta_1)^{-1}|\chi_1), \tag{34}$$

and notice that Eqs. (32)–(33) become

$$I_2\frac{d\eta_2}{dI_2}=z-\eta_1-\eta_2=-\frac{(\chi_2|\varphi_2)}{(\varphi_2|\varphi_2)},\qquad \mathcal{I}_1\frac{d\eta_1}{d\mathcal{I}_1}=z-\eta_1-\eta_2=-\frac{(\chi_1|\varphi_1)}{(\varphi_1|\varphi_1)}. \tag{35}$$

The integrals I_1, I_2 were already defined by Eq. (10). Returning to $\mathcal{I}_1$, and to the factor ν which accounts for the separable potential present in h_1, an elementary manipulation of Eq. (30) gives

$$(\chi_1|\varphi_1)=-\mathcal{I}_1,\quad \mathcal{I}_1=\frac{I_1}{1-\lambda I_1}. \tag{36}$$

Again, we define auxiliary variables ω_i by Eq. (12) and integrals $J_j\equiv a_jI_j$ by contours in the upper half plane of the complex variable p. Then, Eqs. (35) become

$$2\,a_2\omega_2J_2\frac{d\omega_2}{dJ_2}=z-a_1\omega_1^2-a_2\omega_2^2,\quad 2\,a_1\omega_1\mathcal{I}_1\frac{d\omega_1}{d\mathcal{I}_1}=z-a_1\omega_1^2-a_2\omega_2^2. \tag{37}$$

It will be recalled here that a (unique) bound state occurs for h_1 for any positive value of λ, at an energy $\eta_0<0$, defined by the well-known condition

$$\frac{1}{\lambda}=\int dp\,\frac{\chi_1^2(p)}{a_1p^2-\eta_0}=\frac{J_1(\omega_0)}{a_1},\quad \eta_0=a_1\omega_0^2,\quad \Re\omega_0=0,\quad \Im\omega_0>0. \tag{38}$$

Indeed, the right-hand side is monotonically increasing when η_0 runs from $-\infty$ to 0 and the same right-hand side diverges at $\eta_0=0$, see Eq. (18), because of our choice of a Lorentzian form for χ_1^2. Accordingly, an explicit form of Eq. (38) is

$$\lambda+a_1\omega_0(\omega_0+i\gamma_1)=0,\quad \Re\omega_0=0,\quad \Im\omega_0>0, \tag{39}$$

or, in terms of η_0

$$(\eta_0+\lambda)^2+a_1\gamma_1^2\,\eta_0=0, \tag{40}$$

with obvious scaling properties. (Indeed, if the scale is set by λ for instance, it is convenient to define $A_1=a_1\gamma_1^2$, and the relevant scales are, obviously, A_1/λ and η_0/λ.) Threshold singularities are expected for Eqs. (32)–(33) when z reaches the one-body threshold η_0, besides the already-found two-body threshold $z=0$.

The saddle-point value D deduced from Eq. (29) reads, upon taking advantage of Eqs. (30)–(37)

$$D=(a_1\omega_1^2+a_2\omega_2^2-z)\,\mathcal{I}_1\,I_2\,. \tag{41}$$

This formula, Eq. (41), is an obvious generalization of Eq. (19). In the same way as we did in the previous section, we shall again eliminate ω_1 and ω_2, or rather the strictly equivalent variables $x=-i\omega_1$ and $y=-i\omega_2$, between Eqs. (37) and Eq. (41). It is then useful to define a parameter $A_2=a_2\gamma_2^2$, quite similar to A_1, and it is also easy to predict that the solution $D(z)$ scales in terms of A_1/λ, A_2/λ, z/λ, and λD. The Lorentzian choice for χ_1,χ_2, induces the following forms for Eqs. (37), when we replace a_1,a_2 by $A_1/\gamma_1^2, A_2/\gamma_2^2$, respectively:

$$A_1\gamma_2^2x^2+2A_1\gamma_2x^2y-A_2\gamma_1^2y^2+\gamma_1^2\gamma_2^2z+2\,\gamma_1^2\gamma_2yz=0, \tag{42a}$$

$$2\,\gamma_1\gamma_2^2\lambda x+A_2\gamma_1^2y^2+2A_2\gamma_1xy^2-A_1\gamma_2^2x^2+\gamma_1^2\gamma_2^2z+2\,\gamma_1\gamma_2^2xz=0, \tag{42b}$$

$$\frac{y}{\gamma_2}=-\frac{(\lambda\gamma_1^2+A_1x^2)\,x+(\gamma_1+2x)\gamma_1^2z}{(\gamma_1+2x)(A_1x^2+\gamma_1^2z)}. \tag{42c}$$

These scale obviously in terms of x/γ_1 and y/γ_2. It is then convenient to set $\gamma_1=\gamma_2=1$ in Eqs. (42).

Simultaneously, under the same replacement of a_1,a_2 by $A_1/\gamma_1^2, A_2/\gamma_2^2$, respectively, we can take advantage of Eqs. (36) and (18) (with $K_1=K_2=0$) to let Eq. (41) become

$$[\,A_1A_2(x^2y^2+\gamma_2x^2y+\gamma_1xy^2+\gamma_1\gamma_2xy)-A_2\gamma_1^2(y+\gamma_2)\lambda y\,]\,D+A_1\gamma_2^2x^2+A_2\gamma_1^2y^2+\gamma_1^2\gamma_2^2z=0. \tag{43}$$

Set $\gamma_1=\gamma_2=1$. The elimination of x and y between Eqs. (42)–(43) yields a degree 7 polynomial condition for D

$$\begin{aligned}\mathcal{P}(D,z,A_1,A_2,\lambda)\equiv{}&A_2^2(A_1+4\lambda)^2[\,(z+\lambda)^2+A_1z\,][\,(z+\lambda+A_2)^2+A_1(z+A_2)\,]D^7\\&-4A_2(A_1+4\lambda)[\,(z+\lambda)^2+A_1z\,][A_1A_2^2+5A_1A_2\lambda+8A_2^2\lambda+12A_2\lambda^2+4\lambda^3\\&+(-3A_1A_2-4A_2^2+4A_1\lambda+4A_2\lambda+4\lambda^2)z-4(A_1+2A_2+\lambda)z^2-4z^3]D^6\\&+\cdots-64z(A_1+A_2+20\lambda+16z)\,D+256z=0\,,\end{aligned} \tag{44}$$

which is too cumbersome to be listed here entirely. A factor $[(z+\lambda)^2+A_1z]$ forces its coefficients for both D^7 and D^6 to vanish when $z=\eta_0$; see Eq. (40). Hence, two roots D diverge at the expected one-body threshold. We also notice that for $z=0$ the two lowest degree coefficients of $\mathcal{P}$ vanish; hence, a double root $D=0$ occurs. But, for the sake of simplicity in this section, we shall not elaborate much on the exact nature of this two-body threshold singularity for this second model. Similarities with the behavior of the first model around $z=0$ are likely. In the following, we rather study in some detail the singularity at $z=\eta_0$.

The degree 7 for D is familiar from the model of the previous section. But, the degree for z is now 5 rather than 4. We verified that the limit $\lambda\to0$ factorizes $\mathcal{P}(D,z,A_1,A_2,\lambda)$ into a factor z and a polynomial with degree 4 for z.

It is convenient to set special values for a numerical investigation, for instance $a_1=\gamma_1=A_1=\gamma_2=1$ and $a_2=A_2=\lambda=2$. The full polynomial then reads

$$\begin{aligned}\mathcal{P}={}&3(1+z)(4+z)[27(3+z)(6+z)D+12(-108-9z+14z^2+2z^3)]D^6\\&-4(-2808+477z+5984z^2+3480z^3+690z^4+44z^5)\,D^5\\&+8(-584+1760z+3323z^2+1387z^3+200z^4+8z^5)D^4-8(-140+1195z+1471z^2+420z^3\\&+32z^4)\,D^3+32(-4+107z+82z^2+12z^3)D^2-16z(43+16z)D+64z.\end{aligned} \tag{45}$$

Here, the bound state lies at $\eta_0=-1$ with $\omega_0=i$. The second solution, $\omega_0=-2i, \eta_0=-4$, of Eqs. (39)–(40) violates the condition $\Re x>0$, and hence pertains to an unphysical sheet.

The 7 trajectories shown in Fig. 6 are those of the roots of $\mathcal{P}$, Eq. (45), when $\Re z$ runs from -7.5 to $+4$. This range suffices here to obtain a reasonable estimate of the root behavior when the energy runs from $-\infty$ to $+\infty$. For the sake of graphical convenience, a renormalization $D/(1+|D|)$ forces large Ds back to the trigonometric circle. Also, a small imaginary part $\Im z=0.2$ is set to enforce the rule $\Im\mathcal{D}<0$. Black dots (or lines when nearing dots fuse) correspond to $\Re z<-4.1$. Green and red ones correspond to $-3.9<\Re z<-1.1$ and $-0.9<\Re z$, respectively. Finally, blue and yellow ones investigate neighborhoods, $-4.1<\Re z<-3.9$ and $-1.1<\Re z<-0.9$, of expected singularities at $z=-4$ and $z=-1$, respectively. It turns out that Fig. 6 does not yield much information out of such ''blue'' and ''yellow'' segments, although it is clear that only two ''loops'' satisfy both rules $\Im D<0$, $\forall\Re z$ and $\lim_{|z|\to\infty}D=0$. Clearly, for a thorough investigation of all branchings and divergences, we should eliminate D between $\mathcal{P}$ and its derivative $\partial\mathcal{P}/\partial D$, then study the neigborhoods of all the roots of the obtained resultant

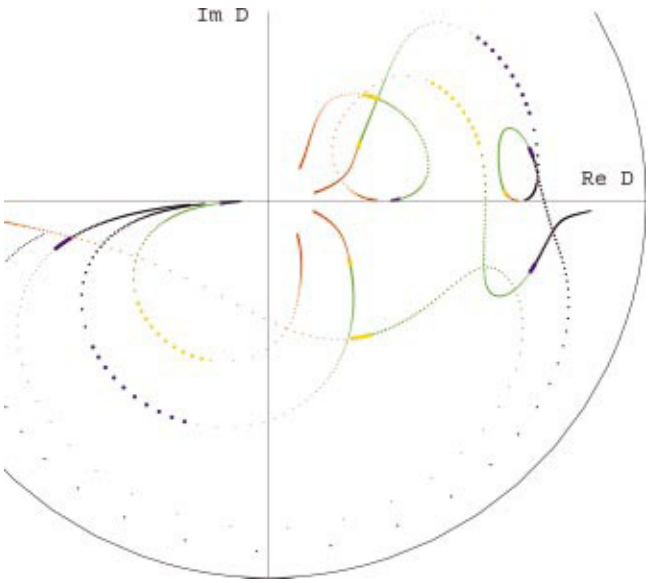

FIG. 6. (Color) Complex D plane. Trajectories of the 7 roots of Eq. (45) when $-7.5\leqslant \Re z\leqslant 4$ and $\Im z=0.2$. Black dots or lines correspond to $\Re z<-4.1$. Blue, green, yellow, and red ones correspond to $-4.1<\Re z<-3.9$, $-3.9<\Re z<-1.1$, $-1.1<\Re z<-0.9$, and $-0.9<\Re z$, respectively. Only two trajectories always keep $\Im D<0$ and cancel D when $|z|\to\infty$.

$$\mathcal{R}=z(1+z)^2(2+z)(3+z)(4+z)^2(6+z)(32+7z)^2\ \ (2\,426\,112+17\,293\,824z+54\,026\,784z^2 +121\,209\,152z^3+233\,641\,545z^4+328\,920\,768z^5+307\,812\,074z^6+191\,171\,112z^7 +79\,534\,245z^8+21\,923\,392z^9+3\,826\,944z^{10}+380\,928z^{11}+16\,384z^{12})^3\,. \tag{46}$$

This straightforward but lengthy task gives results too cumbersome to be published here, naturally. Still, it might be useful to compare Fig. 6 with a superposition of Figs. 2 and 11, keeping in mind that symmetry breaking double roots of the previous model will now be disentangled. Indeed, under the already-mentioned two criteria, namely, (i) $D\to 0$ if $|z|\to\infty$, and (ii) $\Im D<0$, only the ''tiny'' loops selected from Figs. 2 and 11 survive. Letting $\Im z\to 0$, we obtained graphical evidence that such two loops grow in such a way that their ''blue'' and ''yellow'' segments show the diverging roots predicted from the factor $(1+z)(4+z)$ in front of D^7 and D^6. With the same renormalization $D/(1+|D|)$, Fig. 7 confirms that two branches only are compatible with rules (i) and (ii), when we freeze $\Re z=-1$ and let $\Im z>0$ run. One of the ''good'' candidate roots diverges for $z=-1$; see the green segment in the lower left part of Fig. 7. The other good candidate, $D_1\simeq 0.31-0.21i$ (see the small green segment at the beginning of the smallest trajectory in the lower right angle of Fig. 7), is a simple root as a function of z in this area, and deserves little comment. The diverging root, however, because of its quadratic branching, deserves a study of its reciprocal, $d\equiv D^{-1}$. We set $z=-1+Z$ and expand $\mathcal{P}$, Eq. (45), at lowest orders with respect to d and Z

$$d^7\,\mathcal{P}(d^{-1},Z-1,A_1=1,A_2=2,\lambda=2)=270\,(2d^2+9Z)+\mathcal{O}(Z\,d)\,. \tag{47}$$

The neglected term is of order $Z^{3/2}$, because, obviously, the leading order of the double root is $d=\pm 3(-Z)^{1/2}/\sqrt{2}$, real below and imaginary above threshold, respectively. A similar, straightforward argument for the vicinity of the additional, but unphysical threshold at $z=-4$ yields the leading order $d=\pm 3(-4-z)^{1/2}/(2\sqrt{2})$.

Among all the singularities of this second model, we shall mainly discuss the physical threshold $z=-1$. Eliminate z between Eq. (42a) and Eq. (42b), or, equivalently, subtract the equations, Eqs. (37), from each other, hence

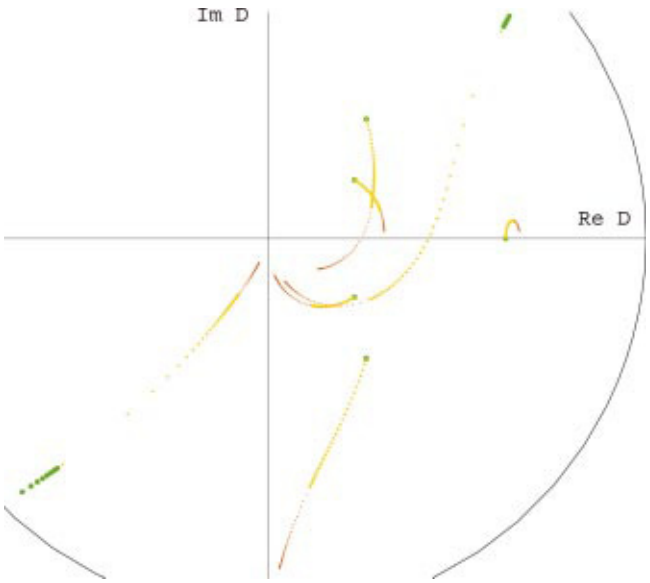

FIG. 7. (Color) Complex D plane. Trajectories of the 7 roots of Eq. (45) if $\Re z=-1$. Green, yellow, and red mean $0<\Im z<0.01$, $0.01<\Im z<2$, and $2<\Im z<8$, respectively. Again, only two trajectories maintain $\Im D<0$ and cancel D when $|z|\to\infty$.

$$a_2\omega_2 J_2\frac{d\omega_2}{dJ_2}=a_1\omega_1\mathcal{I}_1\frac{d\omega_1}{d\mathcal{I}_1}, \tag{48}$$

a relation similar to Eq. (16). To prove the statement that the static HF energy η_0 indeed defines a threshold solution of the TIMF equations, Eqs. (37), it is enough to set $\eta_1\to\eta_0$, $\eta_2\to 0$, and $z\to\eta_0$. This automatically induces $z-a_1\omega_1^2-a_2\omega_2^2\to 0$, naturally. Set $\gamma_1=\gamma_2=1$, for a trivial scaling. Then, Eq. (48) reads

$$\frac{A_2 y^2(1+y)}{1+2y}=\frac{x[A_1 x(1+x)-\lambda]}{1+2x}. \tag{49}$$

When $A_1=1$ and $A_2=\lambda=2$, we know that the limits of interest are $x\to 1$, $y\to 0$, and $z\to -1$. These satisfy the condition, $\Re x>0$; hence, only $\Re y$ must be investigated. Define $X=x-1$ and $Z=z+1$. Then, Eq. (49) boils down to $2y^2=X$, at leading orders in y and X. Accordingly, Eq. (42b), for instance, boils down to $2y^2+Z=0$. For $z<-1$ (below threshold) the solution $y\to\sqrt{(-z-1)/2}$ is acceptable, with, simultaneously, $x\to -z$. For $z>-1$ (above threshold), however, we find that a small, but positive $\Im z$ is necessary to allow the condition $\Re y>0$. This occurs because for $Z>0$ the leading order, $y^2\to -Z/2$, actually generates $\Im y$ only. An expansion up to higher orders is thus necessary for the knowledge of $\Re y$. A straightforward, but slightly lengthy calculation, yields

$$y=iZ'-\frac{i}{3}Z'^3-\frac{2}{3}Z'^4+\frac{13i}{18}Z'^5+\mathcal{O}(Z'^6), \tag{50}$$

where Z', a positive number, is defined as $Z'=\sqrt{Z/2}=\sqrt{(z+1)/2}$. The "formal conjugate" of this expansion

$$y=-iZ'+\frac{i}{3}Z'^3-\frac{2}{3}Z'^4-\frac{13i}{18}Z'^5+\mathcal{O}(Z'^6), \tag{51}$$

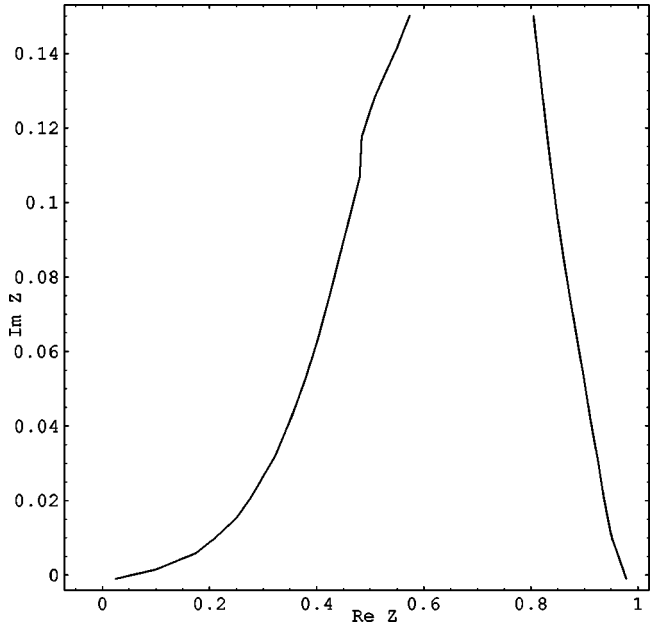

FIG. 8. Complex $Z \equiv z+1$ plane. Below the plotted line, both roots described by Eqs. (50)–(51) show $\Re y<0$. Above that line, one of them shows $\Re y>0$. The line contains both thresholds $Z=0$ and $Z=1$.

also holds, naturally. (Equivalently, it means the opposite choice of Z', namely, $Z'=-\sqrt{Z/2}$.) Both expansions induce a negative $\Re y$ as long as Z is real and positive. The sign of this $\Re y$ can be easily reversed, however, as soon as, above that threshold $z=-1$, an imaginary part $\Im z$ is implemented. Another slightly cumbersome calculation defines, upon taking advantage of either Eq. (50) or Eq. (51), the condition for the border at which one of such roots acquires a positive real part. This is illustrated by Fig. 8. Near to that threshold $z=-1$, the leading orders of the border condition give $(\Im z)^2=\frac{2}{9}(\Re z+1)^5$. Other numerical values for the parameters γ_i, A_i, etc. modify the numerical analysis, naturally, but leave intact the conclusion, namely, that $|\Im z|$ must have at least a nonvanishing value above the threshold if one needs one of these two roots to be compatible with the condition, $\Re y>0$.

We show in Fig. 9 the trajectories of y for $0<\Im z<\infty$ when $\Re z=-0.6$ is frozen at an intermediate value between the thresholds $z=-1$ and $z=0$. Only one branch is of interest, because all the other branches either stay in the $\Re y<0$ sector or the x partner root shows $\Re x<0$. The tiny blue segment at the beginning of this branch corresponds to $\Im z<0.03$, imaginary parts too small for letting y acquire a positive real part; see Fig. 8.

IV. A THEOREM

We return to the case where N is any finite particle number. The two-body interaction $V=\Sigma_{i>j}v_{ij}$ contained in the physical Hamiltonian H is assumed to be made of short-ranged potentials v_{ij}. Then, the TIMF mean fields U_i are also short ranged. For details of a further antisymmetrization with identical fermions, where the mean potential will be the same U for all particles, we refer to Ref. 8; the short range of U remains, whether one considers its direct or exchange part. At present, we still retain the case of distinct particles. Equation (3) reads again

$$(\eta_i-t_i-U_i)|\varphi_i\rangle=|\chi_i\rangle,\ \langle\varphi_i'|(\eta_i-t_i-U_i)=\langle\chi_i'|\,, \tag{52}$$

with

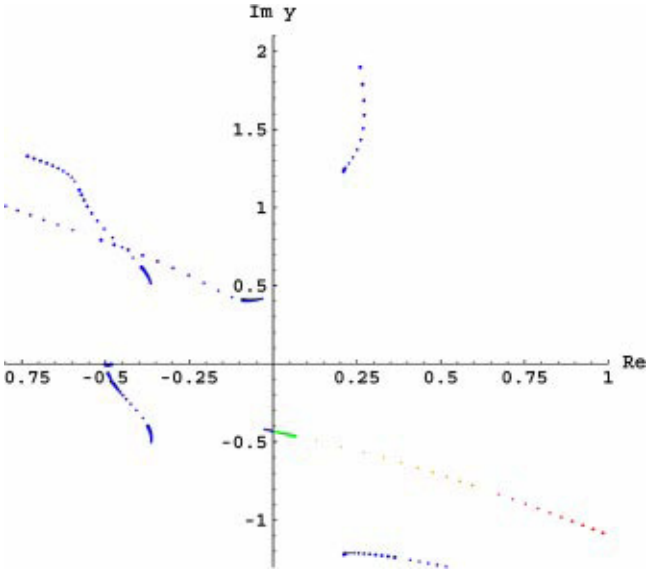

FIG. 9. Complex y plane. Trajectories of y when $\Re z=-0.6$ and $\Im z$ increases from 0. Blue lines are trajectories for which either $\Re x$ or $\Re y$ or both are negative. Only one branch, that long one in the lower right quadrant, survives the double condition, $\Re x>0$, $\Re y>0$. Tiny blue segment, $0<\Im z<0.03$. Green segment, $0.04<\Im z<0.2$. Orange one, $0.3<\Im z<1.8$. Red one, $2<\Im z<4$.

$$\eta_i = z - \frac{\langle \phi' | H | \phi \rangle}{\langle \phi' | \phi \rangle} + \frac{\langle \varphi_i' | (t_i + U_i) | \varphi_i \rangle}{\langle \varphi_i' | \varphi_i \rangle}. \tag{53}$$

Notice that we now process a generalized argument, since we can also study nondiagonal elements $\langle \chi' | (z-H)^{-1} | \chi \rangle$, where χ and χ' are products made of orbitals χ_i and χ_i', respectively. The Euclidean restriction is not implemented anymore. The trial functions ϕ and ϕ' are the products made of orbitals φ_i and φ_i', respectively. All such quantities and wave functions depend on z, but we stress here that, because of the short range of U_i, the spectrum of $h_i = t_i + U_i$ has a fixed continuum, extending from 0 to $+\infty$ on the real axis of the η_i complex plane. In general, U_i is complex and the poles of $(\eta_i - h_i)^{-1}$ need not be real; as a matter of fact, they move as functions of z (and of the choices of χ and χ'). But, the continuum cut for the spectrum of h_i always remains the same. It is therefore legitimate to ask the question, "What happens if one of the η_i's vanishes, hitting the threshold of the continuum of h_i?" Incidentally, it will be noticed that there are many trajectories (sheets) of such η_i's as functions of z. The multiplicity comes not only from the existence of N "momenta," $\omega_i \propto \pm\sqrt{\eta_i}$, with their $\pm$ ambiguity,[12] but it is also due to the nonlinearity of the mean-field theory. For instance, in our second model we found seven sheets; see the seven roots for each quantity $D(z)$, $x(z)$, $y(z)$ driven by z.

As a preliminary remark, we use Eqs. (53) to notice that the mismatch between any propagation energy η_i and the corresponding self-energy $\langle \varphi_i' | (t_i + U_i) | \varphi_i \rangle / \langle \varphi_i' | \varphi_i \rangle$ does not depend on i. Furthermore, we can take advantage of Eqs. (52) to relate the self- and propagation energies as

$$\frac{\langle \varphi_i' | (t_i + U_i) | \varphi_i \rangle}{\langle \varphi_i' | \varphi_i \rangle} = \eta_i + \frac{\mathcal{K}_i \, d\eta_i}{d\mathcal{K}_i}, \quad \mathcal{K}_i = \langle \chi_i' | (h_i - \eta_i)^{-1} | \chi_i \rangle = -\langle \varphi_i' | \chi_i \rangle = -\langle \chi_i' | \varphi_i \rangle. \tag{54}$$

In other terms, the mismatch is measured by the ratio $\langle \chi_i' | \varphi_i \rangle / \langle \varphi_i' | \varphi_i \rangle = \langle \varphi_i' | \chi_i \rangle / \langle \varphi_i' | \varphi_i \rangle$ as a function of η_i. When calculated at self-consistent $\eta_i(z)$'s, such ratios do not depend on i anymore.

Assume that the special vanishing η_s reads $\eta_s = i\varepsilon^2$, where ε is real, positive, and infinitesimal. This means that we select in the z complex plane a trajectory which in turn induces an η_s

trajectory leading to retarded, outgoing boundary conditions for that special φ_s and its partner φ'_s. For the sake of simplicity, set the inverse mass coefficient a_s to unity, or, equivalently, renormalize η_s and U_s accordingly. In physical three dimensions, the partial wave components $\varphi_{s\ell}$ are described by differential equations of the form

$$-\frac{d^2\varphi_{s\ell}}{dr^2}+\left[\frac{\ell(\ell+1)}{r^2}+U_{s\ell}(r)-i\varepsilon^2\right]\varphi_{s\ell}(r)$$
$$=\chi_{s\ell}(r)-\sum_{\ell'}\int_0^\infty dr'\,U_{s\ell\ell'}(r,r')\,\varphi_{s\ell'}(r'),\qquad \forall\ell\,, \tag{55}$$

where $U_{s\ell\ell'}$ is a short notation accounting for, if necessary, partial wave coupling and/or nonlocal parts of U_s. The source term χ_s is expanded in partial waves as well, naturally. It is then convenient to denote the right-hand sides of Eqs. (55) as source terms $\xi_{s\ell}(r)$. These are short ranged, obviously again. Similar equations hold for φ'_s.

For each ℓ, let $\sigma_{s\ell}(r)$ be the regular solution, usually normalized as $\sigma'_{s\ell}(0)=1$, of the homogeneous, left-hand side of Eqs. (55). The short range of U_s, and similar short ranges assumed for χ and χ', make it that, when $r\to\infty$, then $\varphi_{s\ell}(r)$ becomes $\simeq\exp[(i-1)\varepsilon r/\sqrt{2}]\int_0^\infty dr'\,\sigma_{s\ell}(r')\,\xi_{s\ell}(r')$, with a similar asymptotic formula for $\varphi'_{s\ell}$. Let C, a real and strictly positive number, be any convenient lower bound for the absolute values of these integrals $\int\sigma\xi$ and $\int\sigma\xi'$ in a neighborhood of $\varepsilon\to0$. This C exists, since such integrals are usually finite and nonvanishing when $\varepsilon=0$. It is clear that, as $\varepsilon\to0$, there are no longer any exponential decays or any asymptotic oscillations in the product $\varphi_s\varphi'_s$. Then, at this limit for ε, the integral $\langle\varphi'_s|\varphi_s\rangle$ diverges, while obviously an integral such as $\langle\chi'_s|\varphi_s\rangle$ remains finite. The "mismatch" cancels out.

This indicates that, for any $i\neq s$, the ratios $\mathcal{K}_i\,d\eta_i/d\mathcal{K}_i$ vanish simultaneously at their respective energies η_i. Besides threshold limits for each η_i, there is an easy interpretation for such a situation, namely, each among such $N-1$ propagation energies converges towards a bound state energy of its h_i. Indeed, let de_i be an infinitesimal difference between η_i and an isolated eigenvalue of h_i. Then, it is trivial, in an energy representation with biorthogonal eigenstates of h_i, to see that $\mathcal{K}_i$ diverges at order $(de_i)^{-1}$, while $d\mathcal{K}_i/d\eta_i$ diverges at order $(de_i)^{-2}$.

The situation is thus representative of a Hartree(–Fock) solution for the $N-1$ particle system. This is confirmed by the observation that, since $\langle\varphi'_s|\varphi_s\rangle$ diverges, the potential $U_{i/s}$ induced by particle s upon any particle $i\neq s$ vanishes. Indeed, the short range of v in the formula

$$U_{i/s}(r_i)=\frac{\int dr'\,v_{is}(r_i-r')\,\varphi'_s(r')\,\varphi_s(r')}{\langle\varphi'_s|\varphi_s\rangle}, \tag{56}$$

makes the numerator converge $\forall r_i$, while the denominator diverges. Any matrix element $\langle\varphi'_i\varphi'_s|v|\varphi_i\varphi_s\rangle$ will vanish too, for the same reason. Furthermore, the full matrix element $\langle\phi'|H|\phi\rangle/\langle\phi'|\phi\rangle$ can always be split as

$$\frac{\langle\phi'|H|\phi\rangle}{\langle\phi'|\phi\rangle}=\frac{\langle\phi'_{-s}|H_{-s}|\phi_{-s}\rangle}{\langle\phi'_{-s}|\phi_{-s}\rangle}+\frac{\langle\varphi'_s|(t_s+U_s)|\varphi_s\rangle}{\langle\varphi'_s|\varphi_s\rangle}, \tag{57}$$

where the subscript $-s$ refers to the subsystem where particle s is removed. At the limit under study, both η_s and $\mathcal{K}_s\,d\eta_s/d\mathcal{K}_s$ vanish. Hence, according to Eq. (54), the self-energy for particle s vanishes and the full matrix element $\langle\phi'|H|\phi\rangle/\langle\phi'|\phi\rangle$ reduces to the subsystem value, $\langle\phi'_{-s}|H_{-s}|\phi_{-s}\rangle/\langle\phi'_{-s}|\phi_{-s}\rangle$. Furthermore, setting $i=s$ in Eq. (53), we find that $z\to\langle\phi'_{-s}|H_{-s}|\phi_{-s}\rangle/\langle\phi'_{-s}|\phi_{-s}\rangle$. The threshold for the continuum of particle s in the z plane corresponds to the Hartree(–Fock) binding energy of the subsystem.

Conversely, if z converges towards a Hartree(–Fock) bound state energy of an $N-1$ particle system, it is easy to verify that at least one solution of the TIMF equations for the N particle system consists of a threshold wave for the additional particle, as a spectator of the static solution for the subsystem.

Notice that several special particles, not just one, can be forced into their continuum thresholds simultaneously. For instance, if particle s and s' are such that $\eta_s=\eta_{s'}=0$, then all potentials $U_{i/s}$ and $U_{i/s'}$, including $U_{s/s'}$ and $U_{s'/s}$, vanish, and $z=\langle \phi'_{-s-s'}|H_{-s-s'}|\phi_{-s-s'}\rangle/\langle \phi'_{-s-s'}|\phi_{-s-s'}\rangle$, a subsystem energy for $N-2$ particles.

It can also be noticed that such singularities do not depend upon the source terms χ and χ'. Indeed, the locations of such thresholds derive from homogeneous equations, where only H appears.

The present theorem can be phrased in a way which generalizes the theorem of Ref. 10: not only the mean-field binding energies of a system of N particles define singularities of the TIMF propagator, but the mean-field binding energies of its subsystems define thresholds of cuts where the additional particles become unbound.

V. DISCUSSION AND CONCLUSION

There are two parts in this work, namely, on the one hand, a couple of very special, analytical models, see Secs. II and III, and on the other hand, a theorem of a more general validity.

The systems described by our models are physically trivial, since they make noninteracting particles. But, their mathematical interest is different. As stated at the beginning of this work, it is important, for large particle numbers, to validate the replacement of convolutions by straight products, and our models allow a detailed study of all singularities and nonlinearities introduced by the mean-field approximation. We investigated three representations, namely what happens in (i) the z plane (propagation energy); see, for instance, Fig. 4; (ii) the D plane (TIMF amplitude); see, for instance, Fig. 1; (iii) pseudomomentum planes, such as, for instance the case of $x=-i\sqrt{\eta_1/a_1}$; see Fig. 5. Since our models automatically implement an analytic continuation from physical to unphysical sheets, there is no cut to consider in the pseudomomentum complex planes. It is obvious, however, that for both pseudomomenta x and y the imaginary axis represents both rims of the cut which would be necessary in their respective η plane. Accordingly (see for instance Fig. 8), values of z for which the real part of a pseudomomentum vanishes, or identically for which a propagation energy $\eta(z)$ becomes real and positive, make cuts in the z representation. The zoology of the TIMF solutions turns out to be surprisingly rich. The main two conclusions provided by the models can be listed as follows.

(i) Except when the many-body propagation energy z has too small an imaginary part, the TIMF equations always generate at least one branch of solutions where each single particle undergoes a retarded propagation and the TIMF amplitude D shows all suitable properties needed for a reasonable approximation of a Green's function matrix element; and

(ii) The threshold of a single-particle continuum induces the threshold of a cut singularity in the z representation; if one calls "projectile" that special particle becoming unbound, and "target" the system made by the other particle, the corresponding threshold value for the full propagation energy z is the binding energy of the "target."

The theorem derived in Sec. IV, valid for any particle number $N\geqslant 2$, extends this numerical and analytical evidence. Hence, the mean-field theory of collisions mimics the connection between singularities of the inhomogeneous problem $(z-H)|\Psi\rangle=|\chi\rangle$ and the solutions of the homogeneous Schrödinger equation $(E-H)|\Psi\rangle=0$. At this stage of our work, the similarity is restricted, however: we considered only partitions where a target is surrounded by one or several unbound particles, and we have not proven thresholds defined by mean-field energies of partitions $N_1+N_2=N$, $N_1\geqslant 2$, $N_2\geqslant 2$, into two clusters, each of them carrying its full internal energy. Nor have we considered even finer partitions $N_1+N_2+N_3=N$, with $N_1\geqslant 2$, $N_2\geqslant 2$, $N_3\geqslant 2$, and so on. Last

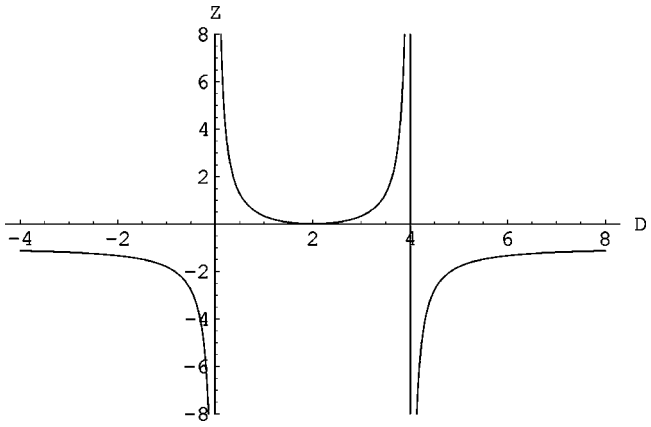

FIG. 10. Scaled energy z (unit θ) as a function of the "symmetry breaking" amplitude D (unit $1/\theta$).

but not least, the present work lacks a clear description of the shapes of the cuts beyond their thresholds. The preliminary result obtained at the stage of Fig. 8, with a "border equation" like $(\Im z)^2=\frac{2}{9}(\Re z+1)^5$, is an omen of subtle arguments yet to be phrased.

Despite such questions still open, the TIMF approximation now appears like a theory of collisions endowed with properties, such as poles and thresholds, with sound interpretations in terms of Hartree(–Fock) energies of subsystems. The special role played by single-particle energy propagators $(\eta-h)^{-1}$ in the definition of such properties is a logical consequence of the factorization of trial wave functions, an essential ingredient of practical approximations. With the present and foregoing studies, TIMF appears as a reliable and practicable alternative to resonating group (RGM) or generator coordinate (GCM) studies for application in nuclear astrophysics where there is still a demand for microscopic rather than phenomenological calculations of processes relevant to element synthesis.

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APPENDIX: THE SYMMETRY BREAKING BRANCH OF THE FIRST MODEL

For the symmetry breaking sector of the first model, we again set $a_i=\gamma_i=1$, scaling x,y,z and ensuring the factorization of the resultant, Eq. (22a). It is easy to analyze the singularities of the direct solution of Eq. (26a)

$$D_{bk}=2\pm 2\left(\frac{z_{bk}}{1+z_{bk}}\right)^{1/2}, \tag{A1}$$

in terms of one cut from -1 to 0 in the complex z plane, or, alternately, two cuts from $-\infty$ to -1 and from 0 to $+\infty$, and observe that the square-root singularity at $z=0$ seems to represent a very traditional threshold singularity. Less physical, the role of $z=-1$ is to reflect the discriminant $\Delta_2=4z/(1+z)$ of Eq. (26a).

In the forthcoming figures, we keep $\theta=1$, as a natural scale for energies and inverse amplitudes. Figure 10 shows the graph of z_{bk} when D_{bk} is real and takes on all values from $-\infty$ to $+\infty$. The symmetry axis at $D=2$ is obvious from Eq. (27). Since the physical amplitude is negative when z is negative, the right lower branch of the graph is clearly unphysical, while the left lower branch is a reasonable candidate for approximations. (Notice, however, that no real estimate of the

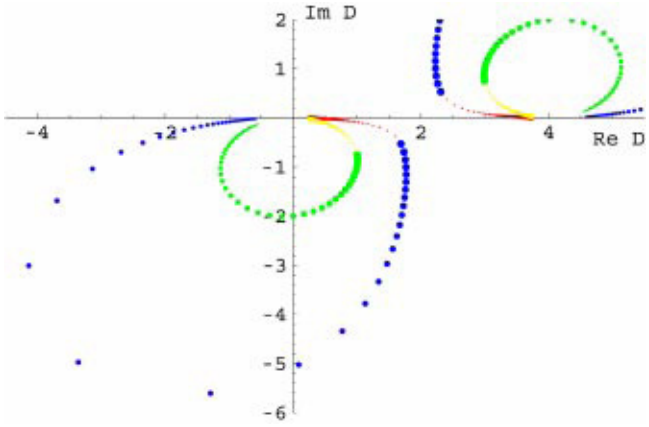

FIG. 11. Complex D plane. Trajectories of symmetry breaking D when $\Im z=0.075$ (outer loops) and $\Im z=0.4$ (inner ones). For $\Im z=0.075$, blue dots growing for $\Re z$ growing between $-\infty$ and 0^- and red ones growing for $\Re z$ growing from 0^+ to $+\infty$. For $\Im z=0.4$, blue and red replaced by green and yellow, respectively.

amplitude is offered for $-1\leqslant z\leqslant 0$.) In turn, the right upper branch is also ruled out, as $\mathcal{D}$ must vanish when $z\to+\infty$. This leaves the left upper branch as a tolerable candidate for physical approximates of the real (principal) part of $\mathcal{D}$ when z is positive.

Rather than considering inverse functions $z(D)$, we then show in Figs. 11–12 the trajectories, in a complex plane "D," of the solutions of Eq. (26a) when $\Re z$ takes on all values from $-\infty$ to $+\infty$ and $\Im z$ is frozen at some fixed value Γ. The physical situation corresponds to $\Gamma=0^+$, naturally, but Figs. 11–12 use larger values of Γ for graphical convenience. For Fig. 11, we use $\Gamma=0.075$ and $\Gamma=0.4$, which generate for D_{bk} two "outer loops" and two "inner loops," respectively. The role of $D=2$ as a symmetry center is obvious. The shrinking of the loops when Γ increases comes from the fact that, as $|z|\to\infty$, the dominant part of the symmetry breaking equation is $D(D-4)=0$. Conversely, the evolution of such loops into "angles" when $\Gamma\to 0$ is transparent in Fig. 12, obtained with $\Gamma=0.02$.

Only those solutions which lie in the lower half plane can be retained as physical candidates, according to the condition "if $\Im z>0$, then $\Im\mathcal{D}<0$." Hence, the general physical behavior of D_{bk} is as follows.

(i) When z is real and increases from $-\infty$ to -1, then D decreases from 0^- to $-\infty$;

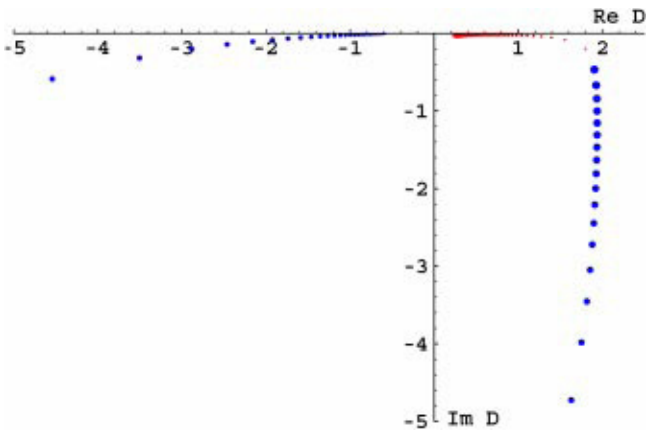

FIG. 12. Complex D plane. Lower loop trajectory of D_{bk} when $\Im z=0.02$ Blue dots growing for $\Re z$ growing between $-\infty$ and 0^-. Red ones growing for $\Re z$ growing from 0^+ to $+\infty$.

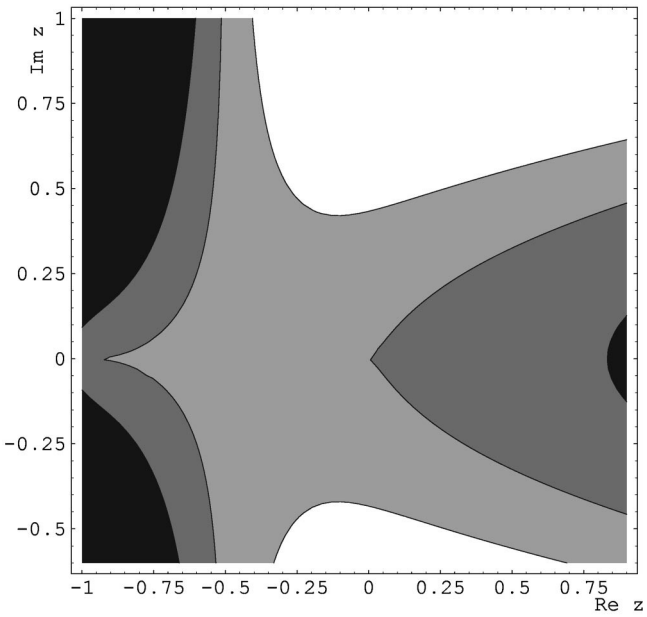

FIG. 13. Complex z plane. Cuts caused by the condition $\Re x=0$ for symmetry breaking roots. The cuts are the borders between light gray and darker gray areas.

(ii) When z is real and increases from -1 to 0, then D varies from $2-i\infty$ to 2; and
(iii) When $\Im z=0^+$ and $\Re z$ increases from 0 to $+\infty$, then D decreases from $2+i0^-$ to $i0^-$. This infinitesimal imaginary part hints that D_{bk} can at best approximate the principal part of $\mathcal{D}$. This was already deduced from Fig. 10.

The "breaking" factor of the factorizing resultant between Eqs. (20) reads

$$x^4-2\,x^3\,z-x^2\,z-2\,x\,z\,(1+z)-z\,(1+z)=0, \tag{A2}$$

keeping in mind that its roots must be paired as (x,y). Figure 13 displays a contour plot of the product of the corresponding four real parts of the roots as functions of z. The corresponding cut in the z plane is the border between the light gray and the darker gray areas. It is now made of two branches. The right-hand branch, while not located on the real axis of the z plane, again contains the two-body threshold $z=0$.

Then, Fig. 14 shows the trajectories of the four roots when we freeze $\Re z=0.1$ and let $\Im z$ run from -1 to $+1$, allowing z to cross twice the right-hand side cut shown by Fig. 13. The sizes of the dots are coded like those of Fig. 5: minimal for $\Im z=-1$, growing until $\Im z=0$, minimal again for small positive values of $\Im z$, growing again until $\Im z=1$. The "vertical" branch on the right-hand side of Fig. 14 has the unsatisfactory property that its "y partner," according to Eq. (22b), is the loop-like, tiny branch on the left-hand side of Fig. 14. Hence, $\Re x\,\Re y<0$. In turn, the two "horizontal" branches on Fig. 14 are "$x-y$" partners and are partly located inside the right-hand side of the complex x,y plane. But, actually the double condition, $\Re x>0$, $\Re y>0$, is never satisfied. It must be concluded that the symmetry breaking sector is unphysical.

A trivial manipulation of Eqs. (20) shows that the pairing of roots, for this sector and such special parameters, follows the rule

$$x\,y=z-x-y, \qquad \text{hence} \qquad y=\frac{z-x}{x+1}, \tag{A3}$$

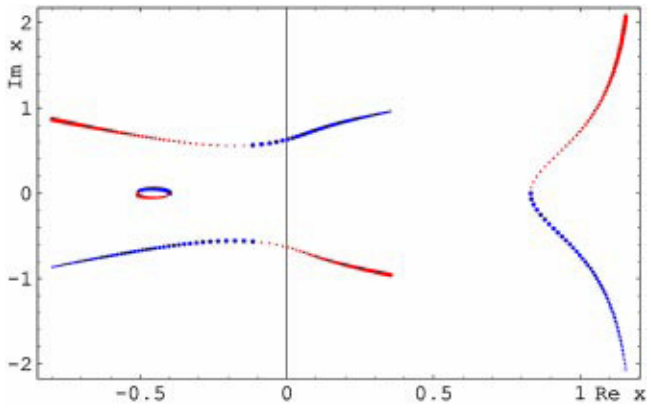

FIG. 14. Complex x plane. Trajectories of the symmetry breaking x's when $\Re z=0.1$, while $\Im z$ runs through one of the cuts shown by Fig. 13. Blue dots growing when $\Im z$ grows from -1 to 0. Red dots growing when $\Im z$ grows from 0 to 1.

which is its own inverse tranform, naturally. The rule is equivalent to Eq. (22b), but simpler. Then, if one defines $s\equiv x+y$, it is easy to reduce Eq. (A2) into

$$(z-s)^2=z(z+1), \qquad \text{or} \qquad z-s=\pm[z(z+1)]^{1/2}, \tag{A4}$$

while shortening Eq. (A3) into

$$x\,y=z-s=\pm[z(z+1)]^{1/2}. \tag{A5}$$

This means that Eq. (A2) factorizes into two distinct equations

$$x^2-x[z-(z+z^2)^{1/2}]+(z+z^2)^{1/2}=0\,, \tag{A6a}$$

$$x^2-x[z+(z+z^2)^{1/2}]-(z+z^2)^{1/2}=0\,. \tag{A6b}$$

It is easy to verify that each of these is invariant under the transform, Eq. (A3); hence, each yields a pair (x,y). A detailed analysis of all cases for such equations is trivial, but too lengthy to be published. Rather, it is enough and easy, actually, to set $\Im z=0$, and plot, for instance for Eq. (A6a), its two numerical roots as functions of z. It turns out that at least one of the roots always has a negative real part. The same phenomenon occurs for Eq. (A6b). All told, the symmetry breaking sector does not respect the constraints requested simultaneously for $\Re x$ and $\Re y$.

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Quantum indistinguishability from general representations of SU($2n$)

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A treatment of the spin-statistics relation in nonrelativistic quantum mechanics due to Berry and Robbins [Proc. R. Soc. London Ser. A **453**, 1771–1790 (1997)] is generalized within a group-theoretical framework. The construction of Berry and Robbins is reformulated in terms of certain locally flat vector bundles over n-particle configuration space. It is shown how families of such bundles can be constructed from irreducible representations of the group SU($2n$). The construction of Berry and Robbins, which leads to a definite connection between spin and statistics (the physically correct connection), is shown to correspond to the completely symmetric representations. The spin-statistics connection is typically broken for general SU($2n$) representations, which may admit, for a given value of spin, both Bose and Fermi statistics, as well as parastatistics. The determination of the allowed values of the spin and statistics reduces to the decomposition of certain zero-weight representations of a (generalized) Weyl group of SU($2n$). A formula for this decomposition is obtained using the Littlewood–Richardson theorem for the decomposition of representations of U($m+n$) into representations of U(m) $\times$U(n). © *2004 American Institute of Physics.* [DOI: 10.1063/1.1666979]

I. INTRODUCTION

In nonrelativistic quantum mechanics, the spin-statistics relation specifies the behavior of many-body wavefunctions for indistinguishable particles under the exchange of a pair of particle labels, and asserts that the wavefunctions either remain the same or change sign according to whether the spin of the particles, s, is integral or half-odd-integral. Nonrelativistic quantum mechanics can be formulated in a logically consistent way without the spin-statistics relation or else with the wrong (i.e., physically incorrect) spin-statistics relation. Therefore, if one is to derive the spin-statistics relation from within a nonrelativistic theory, the nonrelativistic theory must be reformulated, with postulates different from the standard ones. Whether such a reformulation serves to explain the spin-statistics relation is, to some extent, a matter of judgment, and depends on the naturalness and simplicity of the assumptions introduced.

Such a reformulation was presented by Berry and Robbins[3] (referred to in what follows as BR). In BR, the representation of spin was made to depend on position so that, in contrast to the standard formulation, the n-particle wavefunction was single-valued on configuration space. The statistics of the wavefunction was determined by a topological property of this position-dependent spin representation. A calculation showed that the statistics were in accord with the physically correct spin-statistics relation. The construction was based on Schwinger's representation of spin

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as number states of harmonic oscillators. Its implementation assumed without proof the solution of a certain topological problem; a solution was subsequently found by Atiyah.[2] The extension to relativistic wave equations was discussed by Anandan.[1]

To be compelling, a derivation of the spin-statistics relation should be based on general physical and mathematical principles, rather than a particular construction. In BR, it was suggested that certain properties of the construction introduced therein might be sufficient to ensure the correct spin-statistics relation. Later, it was shown that this is not the case,[4] as alternative constructions exist which possess these properties but yield the wrong statistics. Thus, a nonrelativistic derivation of the spin-statistics relation from general principles remains to be established along these lines. For a discussion of other nonstandard approaches to the spin-statistics relation, see Refs. 5 and 6. Our purpose here is to investigate a certain group-theoretical generalization of the construction in BR. We begin in Sec. II by framing the underlying requirement, namely, that wavefunctions be single-valued, in a geometrical context. The setting for the quantum description of n indistinguishable particles are certain vector bundles over configuration space, which we call n-spin bundles. n-spin bundles carry a representation of the spin-statistics group $\Sigma(n)$, which is (nearly) the group generated by permutations and independent rotations of n spinors (the precise definition is given in Sec. II A). The particular representation of $\Sigma(n)$ characterizes the spin and statistics of the particles. The statistics are then embodied in a topological property of the n-spin bundle, namely, the monodromy of its flat connection. This formulation is in the spirit of earlier treatments by Leinaas and Myrheim[13] and Sorkin.[17]

In Sec. III it is shown that n-spin bundles can be constructed from irreducible representations $\Gamma^{\mathbf{f}}$ of the group SU($2n$). The construction in BR is seen to be a particular case, corresponding to the completely symmetric representations of SU($2n$). For the completely symmetric representations, one obtains a definite connection between spin and statistics, indeed the physically correct connection. In contrast, an arbitrary representation of SU($2n$) does not necessarily engender a definite relation between spin and statistics; whether or not it does depends on the decomposition of certain representations of the spin-statistics group constructed from $\Gamma^{\mathbf{f}}$.

This decomposition is carried out in Sec. IV. The calculation involves the evaluation of integrals over characters of the spin-statistics group, and makes use of the Littlewood–Richardson formula for the decomposition of representations of U($k+l$) into representations of U(k) $\times$U(l). It turns out that for an arbitrary representation of SU($2n$) and a given value of spin, various choices of statistics may be realized, including parastatistics (which correspond to representations of the symmetric group of dimension greater than one).

Section V contains a summary and discussion of the results. A connection to a more general problem in representation theory is described in the Appendix.

Throughout this paper we will use the following notation: Given n elements $a_1,\ldots,a_n$ of a set $\mathcal{A}$, we let A denote the ordered n-tuple $(a_1,\ldots,a_n)$. The action of a permutation $\sigma\in S_n$ on A is denoted by $\sigma\cdot A$ and defined by

$$\sigma\cdot A=(a_{\sigma^{-1}(1)},\ldots,a_{\sigma^{-1}(n)}). \tag{1.1}$$

Many of the results presented here are discussed in greater detail by Harrison.[10]

II. BUNDLE DESCRIPTION OF *n*-PARTICLE QUANTUM MECHANICS

The configuration space C_n for n particles in three-dimensional space is the set of n-tuples $R=(\mathbf{r}_1,\ldots,\mathbf{r}_n)$. We will suppose the particles cannot coincide, so that $\mathbf{r}_j\neq\mathbf{r}_k$. If the particles are indistinguishable, then permuted configurations R and $\sigma\cdot R$ are to be regarded as being the same. We describe here a framework for quantum mechanics in which wavefunctions of identical particles are single-valued on configuration space; that is, the wavefunction at permuted configurations is the same.

We first introduce in Sec. II A the particular irreducible representations of the spin-statistics group $\Sigma(n)$, denoted by $Q^{s\lambda}$, which correspond to n identical spins. n-spin-s bundles with statistics λ are defined in Sec. II B. These are flat, Hermitian vector bundles over configuration

space whose fibers carry an irreducible representation of the spin-statistics group equivalent to $Q^{s\lambda}$. This representation is required to be compatible with indistinguishability and the flat connection. Wavefunctions are taken to be sections of the bundle, and operators representing quantum observables are defined on them. The relation to the standard formulation of quantum mechanics, as well as that of BR, is discussed.

A. Representations of the spin-statistics group for identical spinors

Let S_n denote the symmetric group. The irreducible representations, Λ^λ, of S_n are characterized by Young tableaux, λ, of n boxes (equivalently, partitions of n). Let d_λ denote the dimension of the representation Λ^λ. Let $|a\rangle$, $a=1,\ldots,d_\lambda$, denote an orthonormal basis for $\mathbb{C}^{d_\lambda}$ (with respect to the standard inner product). For $\sigma\in S_n$, we write

$$\Lambda^\lambda(\sigma)|a\rangle=\Lambda^\lambda_{a',a}(\sigma)|a'\rangle, \tag{2.1}$$

where here and elsewhere a sum over repeated indices is implied. We may take Λ^λ to be unitary, so that $\Lambda^\lambda_{a',a}(\sigma)$ is a unitary matrix.

Let

$$\mathrm{SU}(2)^n=\underbrace{\mathrm{SU}(2)\times\cdots\times\mathrm{SU}(2)}_{n\ \text{times}} \tag{2.2}$$

denote the direct product of n copies of SU(2). $\mathrm{SU}(2)^n$ describes the independent rotations of n spinors. Denote elements of $\mathrm{SU}(2)^n$ by $U=(u_1,\ldots,u_n)$, with $u_j\in\mathrm{SU}(2)$. States of n spinors, all of spin s, are unchanged if pairs of spinors are rotated through 2π, regardless of whether s is integral or half-odd-integral. Let $\mathrm{Nul}(n)\subset\mathrm{SU}(2)^n$ denote the subgroup generated by pairs of 2π-rotations. It consists of elements of the form

$$U_0=((-1)^{e_1}\mathrm{I}_2,\ldots,(-1)^{e_n}\mathrm{I}_2),\quad \text{where}\ \ (-1)^{e_1}\cdots(-1)^{e_n}=1 \tag{2.3}$$

(I_2 is the 2×2 identity matrix). The *n-spin group*, denoted by $\mathrm{Spn}(n)$, is defined by

$$\mathrm{Spn}(n)=\mathrm{SU}(2)^n/\mathrm{Nul}(n), \tag{2.4}$$

and represents in a one-to-one fashion the independent rotations of n spinors of the same spin. Given $U\in\mathrm{SU}(2)^n$, let

$$\overline{U}=U\ \ \mathrm{Nul}(n) \tag{2.5}$$

denote the corresponding element of $\mathrm{Spn}(n)$ [that is, $\overline{U}$ is the coset of $\mathrm{SU}(2)^n$ containing elements which differ from U by an even number of 2π rotations].

The *spin-statistics group*,

$$\Sigma(n)=\mathrm{Spn}(n)\rtimes S_n, \tag{2.6}$$

is the semidirect product of the n-spin group and the symmetric group. Elements are denoted by $(\overline{U},\sigma)$, where $U\in\mathrm{SU}(2)^n$ and $\sigma\in S_n$, and multiplication is given by

$$(\overline{U},\sigma)(\overline{U'},\sigma')=(\overline{U(\sigma\cdot U')},\sigma\sigma'). \tag{2.7}$$

[It is easy to check that the right-hand side of (2.7) is unchanged if U and U' are multiplied by an even number of 2π rotations.] For brevity, when $\mathrm{Spn}(n)$ and S_n are to be regarded as subgroups of $\Sigma(n)$, we will denote their elements simply by $\overline{U}$ and σ respectively, rather than by $(\overline{U},\mathrm{I}_{S_n})$ and $(\mathrm{I}_{\mathrm{Sp}(n)},\sigma)$.

The complete set of irreducible representations of the spin-statistics group can be obtained from the general representation theory of semidirect products (see, e.g., Ref. 16). Here we shall only be interested in representations whose restriction to $\mathrm{Spn}(n)$ describes n spinors all of spin s, where s is integral or half-odd-integral. It is easily established that each such irreducible representation of $\Sigma(n)$ is characterized by s and, additionally, by an irreducible representation λ of S_n. We denote this representation by $Q^{s\lambda}$, and describe it in the following.

$Q^{s\lambda}$ acts on the $(2s+1)^n d_\lambda$-dimensional vector space $\mathcal{V}^{s\lambda}$ given by

$$\mathcal{V}^{s\lambda}=\underbrace{\mathbb{C}^{2s+1}\otimes\cdots\otimes\mathbb{C}^{2s+1}}_{n\ \text{times}}\otimes\mathbb{C}^{d_\lambda}. \tag{2.8}$$

Let

$$|M,a\rangle=|m_1\rangle\otimes\cdots\otimes|m_n\rangle\otimes|a\rangle, \tag{2.9}$$

where $M=(m_1,\ldots,m_n)$ and m_j ranges between $-s$ and s in integer steps, denote a basis for $\mathcal{V}^{s\lambda}$ orthonormal with respect to the standard inner products on $\mathbb{C}^{2s+1}$ and $\mathbb{C}^{d_\lambda}$. For $\overline{U}\in\mathrm{Spn}(n)$, $Q^{s\lambda}(\overline{U})$ is given by

$$Q^{s\lambda}(\overline{U})|M,a\rangle=D^s_{m_1',m_1}(u_1)\cdots D^s_{m_n',m_n}(u_n)|M,a\rangle, \tag{2.10}$$

where $D^s_{m,m'}(u)$ denotes the standard spin-s representation of SU(2) on $\mathbb{C}^{2s+1}$, and $M'=(m_1',\ldots,m_n')$. [It is easy to check that the right-hand side of (2.10) is unchanged if $U=(u_1,\ldots,u_n)$ is multiplied by an element of $\mathrm{Nul}(n)$.] For $\sigma\in S_n$, $Q^{s\lambda}(\sigma)$ is given by

$$Q^{s\lambda}(\sigma)|M,a\rangle=\Lambda^\lambda_{a',a}|\sigma\cdot M,a'\rangle. \tag{2.11}$$

That is, the spin labels M are permuted while $|a\rangle$ transforms according to the representation Λ^λ of S_n. For a general element $(\overline{U},\sigma)\in\Sigma(n)$, the expression for $Q^{s\lambda}(\overline{U},\sigma)$ follows from (2.10) and (2.11) and the multiplication law (2.7).

B. *n*-spin-*s* bundles with statistics λ

For our purposes, a k-dimensional Hermitian vector bundle, $\mathcal{E}$, over the configuration space C_n will be regarded as a field of k-dimensional subspaces, $\mathcal{E}_R$, of a finite-dimensional Hilbert space, $\mathcal{V}$, depending smoothly on $R\in C_n$. $\mathcal{E}_R$ is called the fiber of $\mathcal{E}$ at R. A Hermitian inner product on $\mathcal{E}_R$ is induced by the Hermitian inner product on $\mathcal{V}$. A section of $\mathcal{E}$ is a function $|\Psi(R)\rangle$ on configuration space taking values in $\mathcal{E}_R$. The inner product of two sections is given by

$$\int_{C_n}\langle\Psi(R)|\Phi(R)\rangle\,dR. \tag{2.12}$$

The space of square-integrable sections forms a Hilbert space.

To represent spin s and statistics λ, each fiber $\mathcal{E}_R$ must carry a representation of the spin-statistics group unitarily equivalent to $Q^{s\lambda}$. Denote this representation by L_R. We require that L_R depend smoothly on R.

Operators representing spin, position and momentum may be defined on wavefunctions as follows. We consider the spin operators, denoted $\mathbf{S}^{op}=(\mathbf{s}_1^{op},\ldots,\mathbf{s}_n^{op})$, first. Consider the rotation of the rth spinor about an axis $\hat{\mathbf{e}}_a$ by an angle t holding the other spinors fixed. This is described by $U_{(r,a)}(t)=(u_1(t),\ldots,u_n(t))\in\mathrm{SU}(2)^n$, where

$$u_j(t)=\begin{cases}\exp(-\mathrm{i}t\sigma_a/2), & j=r,\\ \mathrm{I}_2, & \text{otherwise}\end{cases} \tag{2.13}$$

(here σ_1, σ_2, σ_3 are the Pauli matrices). Then $s^{op}_{r,a}$, the ath component of $\mathbf{s}^{op}_r$, is given by

$$\left|(s^{op}_{r,a}\Psi)(R)\right\rangle = \frac{1}{\mathrm{i}}\frac{d}{dt}\bigg|_{t=0} L_R(\overline{U}_{(r,a)}(t))\left|\Psi(R)\right\rangle. \tag{2.14}$$

As the representation L_R is unitary, $\mathbf{s}^{op}_j$, as defined by (2.14), is self-adjoint. The representation property of L_R implies that the standard commutation relations for spin are satisfied.

Position operators, $R^{op}=(\mathbf{r}^{op}_1,\ldots,\mathbf{r}^{op}_n)$, are defined componentwise by

$$\left|(r^{op}_{j,a}\Psi)(R)\right\rangle = r_{j,a}\left|\Psi(R)\right\rangle. \tag{2.15}$$

$\mathbf{r}^{op}_j$ is Hermitian with respect to the inner product (2.12), self-adjoint on a suitable domain, and the position operators commute amongst each other and with the spin operators.

The definition of momentum operators requires a Hermitian connection on $\mathcal{E}$. A Hermitian connection associates to piecewise smooth paths $R(t)\in C_n$ a family of unitary maps between the fibers $\mathcal{E}_{R(t)}$. These unitary maps describe the parallel transport of spinors along $R(t)$. Momentum operators may be defined in terms of the covariant derivative with respect to this connection.

A characteristic property of a connection is its curvature, which describes parallel transport around infinitesimal closed paths. Nonvanishing curvature corresponds physically to the presence of gauge (e.g., magnetic) fields. In order that our theory be capable of describing physics in the absence of fields, we shall require that $\mathcal{E}$ admit a flat connection. This condition is not automatically satisfied; the existence of a flat connection depends on the topology of the bundle (just as the fact that a two-torus admits a flat Riemannian metric, while a two-sphere does not, is a consequence of their different Euler characteristics).

For a flat connection, parallel transport around a closed path is trivial, provided the path is contractible. In C_n, every closed path is contractible (C_n is simply connected). Therefore, parallel-transport with respect to a flat connection on $\mathcal{E}$ is path-independent, and depends only on the endpoints of the path. Therefore, a flat Hermitian connection on $\mathcal{E}$ is characterized by unitary maps $T_{R'\leftarrow R}:\mathcal{E}_R\rightarrow\mathcal{E}_{R'}$ describing parallel transport from R to R'. Path independence then implies that

$$T_{R''\leftarrow R'}T_{R'\leftarrow R}=T_{R''\leftarrow R}. \tag{2.16}$$

Momentum operators $P^{op}=(\mathbf{p}^{op}_1,\ldots,\mathbf{p}^{op}_n)$ are defined as follows. Let

$$E_{(j,a)}=(0,\ldots,0,\hat{\mathbf{e}}_a,0,\ldots,0) \tag{2.17}$$

denote the tangent vector in configuration space on which the jth particle moves with unit velocity in the direction $\hat{\mathbf{e}}_a$ while the other particles stay fixed. Then the ath component of $\mathbf{p}^{op}_j$ is given by

$$\left|(p^{op}_{j,a}\Psi)(R)\right\rangle = \frac{d}{dt}\bigg|_0 (T_{R\leftarrow R+tE_{(j,a)}}\left|\Psi(R+tE_{(j,a)})\right\rangle). \tag{2.18}$$

$p^{op}_{j,a}$ is Hermitian with respect to the inner product (2.12) and is self-adjoint on a suitable domain. From (2.15) it is easily verified that the position and momentum operators satisfy the standard commutation relations. That the momentum operators commute amongst themselves follows from the fact that

$$T_{R\leftarrow R+tE}T_{R+tE\leftarrow R+tE+uF}=T_{R\leftarrow R+uF}T_{R+uF\leftarrow R+tE+uF}, \tag{2.19}$$

which in turn follows from the path independence (2.16) of the connection, provided the displacements tE and uF are small enough so as not to make the particles coincide.

The requirement that spin and momentum commute is equivalent to the requirement that parallel transport be compatible with the representation L_R. That is, we should have that $L_{R'}(\overline{U},\sigma)T_{R'\leftarrow R}=T_{R'\leftarrow R}L_R(\overline{U},\sigma)$.

As a basis for subsequent discussion, let us formulate the standard description of n-particle quantum mechanics within the framework described above. (In this case, the vector bundle description is unnecessary, of course, and appears artificial.) For this, take the fibers $\mathcal{E}_R$ to be everywhere equal to the fixed vector space $\mathcal{V}^{s\lambda}$. Take L_R, the representation of the spin-statistics group, to be everywhere equal to the standard representation $Q^{s\lambda}$. Parallel transport is everywhere taken to be trivial; i.e., $T_{R'\leftarrow R}$ is just the identity map on $\mathcal{V}^{s\lambda}$. Then $\mathcal{E}$ is just the Cartesian product $C_n\times\mathcal{V}^{s\lambda}$, and wavefunctions $|\Psi(R)\rangle$ are just $\mathcal{V}^{s\lambda}$-valued functions on C_n. Wavefunctions may be expanded in the standard basis $|M,a\rangle$ [cf. (2.9)],

$$|\Psi(R)\rangle=\sum_M\sum_{a=1}^{d_\lambda}\psi_{M,a}(R)|M,a\rangle. \tag{2.20}$$

The definitions (2.14), (2.15) and (2.18) of the position, spin and momentum operators yield the standard operations on the coefficients $\psi_{M,a}(R)$,

$$\mathbf{r}_j^{op}\psi^S_{M,a}(R)=\mathbf{r}_j\psi^S_{M,a}(R), \tag{2.21}$$

$$\mathbf{p}_j^{op}\psi^S_{M,a}(R)=-\mathrm{i}\nabla_{\mathbf{r}_j}\psi^S_{M,a}(R), \tag{2.22}$$

$$\mathbf{e}^{-\mathrm{i}\theta\mathbf{s}^{op}_{j,a}}\psi^S_{M,a}(R)=\sum_{m'=-s}^{s}D^s_{m_j,m'}(\mathrm{e}^{-\mathrm{i}\theta\cdot\sigma_a})\psi^S_{M',a}(R), \tag{2.23}$$

where, in (2.23), M' differs from M only in the jth component, in which m_j is replaced by m'.

We now introduce the requirement, basic to the formulation in BR, that for indistinguishable particles, the values of the wavefunction at permuted configurations should be the same. That is, we require that

$$|\Psi(\sigma\cdot R)\rangle=|\Psi(R)\rangle,\quad \sigma\in S_n. \tag{2.24}$$

(Note that for this condition to be sensible, the fibers at R and $\sigma\cdot R$ must be the same.) In this case, the wavefunction is single-valued as a function of configurations in which the particles are no longer labeled. Wavefunctions in the standard description are not single-valued in this sense. Indeed, in the standard description, the coefficients of the wavefunction at permuted configurations are related by

$$\psi_{M,a}(\sigma\cdot R)=\Lambda^\lambda_{a,a'}\psi_{\sigma^{-1}\cdot M,a'}(R), \tag{2.25}$$

so that the wavefunctions themselves satisfy

$$|\Psi(\sigma\cdot R)\rangle=L_{\sigma\cdot R}(\sigma)|\Psi(R)\rangle. \tag{2.26}$$

Descriptions based on single-valued wavefunctions, but physically equivalent to the standard description, are obtained by rewriting (2.26) as

$$|\Psi(\sigma\cdot R)\rangle=L_{\sigma\cdot R}(\sigma)T_{\sigma\cdot R\leftarrow R}|\Psi(R)\rangle. \tag{2.27}$$

In the standard description, (2.27) is the same as (2.26), since $T_{\sigma\cdot R\leftarrow R}$ is just the identity in this case. In contrast, for single-valued wavefunctions, (2.27) becomes

$$L^{-1}_{\sigma\cdot R}(\sigma)=T_{\sigma\cdot R\leftarrow R}. \tag{2.28}$$

Thus, for a description in terms of single-valued wavefunctions to be equivalent to the standard one, parallel transport is necessarily a nontrivial operation; between permuted configurations, parallel transport induces the corresponding permutation of spins.

Let us now formalize the preceding considerations. An n-spin-s bundle with statistics λ, denoted by $\mathcal{E}^{s\lambda}$, is defined to be a $(2s+1)d_\lambda$-dimensional Hermitian vector bundle over the configuration space C_n endowed with the following properties:

(A) There exists a smooth family, L_R, of unitary irreducible representations of the spin-statistics group $\Sigma(n)$ acting on the fibers $\mathcal{E}_R$, unitarily equivalent to $Q^{s\lambda}$.

(B) The fibers at permuted configurations are the same, i.e.,

$$\mathcal{E}_{\sigma\cdot R}=\mathcal{E}_R. \tag{2.29}$$

(C) There exists a flat Hermitian connection on $\mathcal{E}^{s\lambda}$, characterized by unitary maps $T_{R'\leftarrow R}$ describing parallel transport from R to R', satisfying the composition rule

$$T_{R''\leftarrow R'}T_{R'\leftarrow R}=T_{R''\leftarrow R}. \tag{2.30}$$

Parallel transport is compatible with the representation L_R in the sense that

$$L_{R'}(\overline{U},\sigma)T_{R'\leftarrow R}=T_{R'\leftarrow R}L_R(\overline{U},\sigma). \tag{2.31}$$

(D) Parallel transport between permuted fibers induces permutations, i.e.,

$$T_{\sigma\cdot R\leftarrow R}=L_{\sigma\cdot R}(\sigma^{-1}). \tag{2.32}$$

The Hilbert space $\mathcal{H}$ of wavefunctions describing n indistinguishable particles of spin s and statistics λ is the space of sections of $\mathcal{E}^{s\lambda}$ with inner product (2.12) satisfying the single-valuedness condition

$$|\Psi(\sigma\cdot R)\rangle=|\Psi(R)\rangle. \tag{2.33}$$

Observables are generated by combinations of the position, momentum and spin operators, $\mathbf{r}_j^{op}$, $\mathbf{p}_j^{op}$ and $\mathbf{s}_j^{op}$, given by (2.15), (2.22) and (2.14), respectively, which are invariant under permutations. These permutation-invariant operators preserve the single-valuedness condition (2.33).

To establish explicitly the equivalence between this formulation and the standard one, as well as the treatment in BR, it is useful to introduce a parallel-transported basis for the fibers $\mathcal{E}_R$. To this end, we fix a reference configuration $R_0\in C_n$. Since L_{R_0} is unitarily equivalent to $Q^{s\lambda}$, there exists an orthonormal basis $|M,a(R_0)\rangle$ of $\mathcal{E}_{R_0}$ for which

$$L_{R_0}(\overline{U},\sigma)|M,a(R_0)\rangle=Q^{s\lambda}_{M'a',Ma}(\overline{U},\sigma)|M',a'(R_0)\rangle. \tag{2.34}$$

A basis for $\mathcal{E}_R$ is defined via parallel transport as follows:

$$|M,a(R)\rangle=T_{R\leftarrow R_0}|M,a(R_0)\rangle. \tag{2.35}$$

Because the representation L_R is compatible with the flat connection, it follows that (2.34) holds for all R.

Wavefunctions $|\Psi(R)\rangle$ may be expanded in terms of this basis as

$$|\Psi(R)\rangle=\psi_{M,a}(R)|M,a(R)\rangle. \tag{2.36}$$

From the definitions (2.15), (2.18) and (2.14), it is readily verified that the position, momentum and spins operators act on the components $\psi_{M,a}(R)$ as the standard operators (2.21)–(2.23). The condition (2.32) implies that the components at permuted configurations are related as in (2.25), in accord with the standard formulation.

Apart from allowing parastatistics, the framework described here is equivalent to the one given in Sec. 2 of BR. There are, however, some differences in the formulation. In BR, properties (A)–(D) are expressed directly in terms of the parallel-transported basis. For example, instead of property (C), BR require that the parallel-transported basis satisfy

$$\langle M'(R)|\nabla_{\mathbf{r}_j} M(R)\rangle = 0. \tag{2.37}$$

In this way, the formalism and terminology of vector bundles is avoided.

An advantage of the present formulation is that properties required by physical considerations are distinguished from those which depend on convention. For example, (2.37) implies the existence of a flat connection, but it implies, additionally, that it is a particular connection which is flat—namely, the connection induced by the inner product on $\mathcal{V}$, according to which vectors are parallel-transported by translating them to an infinitesimally displaced fiber and there projecting them perpendicularly. This choice of connection, while convenient, is nevertheless a matter of convention, and is not required by physical considerations.

Finally, we note that we could, if we wished, impose the single-valuedness condition more directly by taking n-particle configuration space to be the identified configuration space $\overline{C}_n = C_n/S_n$ consisting of (unordered) sets $X=\{\mathbf{r},\mathbf{s},\ldots,\mathbf{t}\}$ of n distinct points in $\mathbb{R}^3$. (This is the point of view taken by Leinaas and Myrheim[13]) Then wavefunctions would become functions of X, or, more precisely, sections of an n-spin bundle over the identified configuration space $\overline{C}_n$. However, such a reformulation involves some additional mathematical complication, and, for this reason, we will confine our consideration of it to the following informal remarks.

The complication is due to the fact that there are no global Euclidean coordinates on $\overline{C}_n$; it is no longer sensible to refer to position, spin and momentum operators for a particular particle. In place of individual momenta, for example, one must introduce generalized momentum operators, which are related to covariant derivatives along smooth vector fields on $\overline{C}_n$. A formulation in terms of $\overline{C}_n$ does have some attractive aspects, though. Parallel transport between permuted fibers in C_n becomes transport from a single fiber to itself around a noncontractible closed path in $\overline{C}_n$. In this way, the statistics of the particles is reflected in the monodromy of the flat connection, a topological property of the bundle.

III. SPIN BUNDLES SU($2n$) REPRESENTATIONS

In this section we describe the construction of n-spin bundles from representations of SU($2n$). The construction is based on a connection between SU($2n$) and the spin-statistics group $\Sigma(n)$ (Sec. III A), which associates a representation $\Delta^{\mathbf{f}}$ of $\Sigma(n)$ to an irreducible representation $\Gamma^{\mathbf{f}}$ of SU($2n$) (Sec. III B). In general, the representation $\Delta^{\mathbf{f}}$ is reducible. n-spin bundles are constructed from the representations $\Gamma^{\mathbf{f}}$ and $\Delta^{\mathbf{f}}$ and an S_n-equivariant map from C_n to SU(n)/T(n) (Sec. III C).

Whether $\Gamma^{\mathbf{f}}$ determines a spin-statistics relation is discussed in Sec. III D. The question is related to the decomposition of $\Delta^{\mathbf{f}}$ into its irreducible components. A definite statistics for a given value of spin requires that $\Delta^{\mathbf{f}}$ should contain only one irreducible representation of $\Sigma(n)$ with that spin. This is the case for the completely symmetric representations, which correspond to the construction in BR. The general case is discussed in Sec. IV.

A. The spin-statistics group and SU($2n$)

Consider SU($2n$), the group of $2n$-dimensional unitary matrices of unit determinant. SU$(2)^n$ may be identified as a subgroup of SU($2n$), with $U=(u_1,\ldots,u_n)\in \mathrm{SU}(2)^n$ identified with the matrix

$$U=\begin{pmatrix} u_1 & & & \\ & u_2 & & 0 \\ & & \ddots & \\ & 0 & & u_n \end{pmatrix}. \tag{3.1}$$

[For simplicity, we will use the same symbol, in this instance U, for both an element of $\mathrm{SU}(2)^n$ and for the corresponding matrix in $\mathrm{SU}(2n)$, and will do the same for some other subgroups of $\mathrm{SU}(2n)$ to be introduced below. Taken in context this usage should not introduce any ambiguity.] Similarly, $\mathrm{SU}(n)$, the group of n-dimensional unitary matrices with unit determinant, may be identified with a subgroup of $\mathrm{SU}(2n)$, with $g\in\mathrm{SU}(n)$, with components denoted by g_{rt}, $1\leqslant r,t\leqslant t$, identified with the $\mathrm{SU}(2n)$-matrix

$$g=\begin{pmatrix} g_{11}\mathrm{I}_2 & \cdots & g_{1n}\mathrm{I}_2 \\ \vdots & \ddots & \vdots \\ g_{n1}\mathrm{I}_2 & \cdots & g_{nn}\mathrm{I}_2 \end{pmatrix}. \tag{3.2}$$

Finally, we let $T(n)$ denote the subgroup of diagonal matrices in $\mathrm{SU}(n)$. From (3.2), $T(n)$ may be identified as the subgroup of $\mathrm{SU}(2n)$ consisting of diagonal matrices of the form

$$t(\Theta)=\begin{pmatrix} \mathrm{e}^{\mathrm{i}\theta_1}\mathrm{I}_2 & & & \\ & \mathrm{e}^{\mathrm{i}\theta_2}\mathrm{I}_2 & & 0 \\ & & \ddots & \\ & 0 & & \mathrm{e}^{\mathrm{i}\theta_n}\mathrm{I}_2 \end{pmatrix}, \tag{3.3}$$

where $\Theta=(\theta_1,\ldots,\theta_n)$ is an n-tuple of phases satisfying

$$\mathrm{e}^{\mathrm{i}\theta_1}\cdots\mathrm{e}^{\mathrm{i}\theta_n}=1. \tag{3.4}$$

Note that $\mathrm{SU}(2)^n\cap T(n)$ is just the subgroup $\mathrm{Nul}(n)$ of null rotations, which consists of $\mathrm{SU}(2n)$-matrices of the form

$$U_0=\begin{pmatrix} (-1)^{e_1}\mathrm{I}_2 & & & \\ & (-1)^{e_2}\mathrm{I}_2 & & \\ & & \ddots & \\ & & & (-1)^{e_n}\mathrm{I}_2 \end{pmatrix}, \tag{3.5}$$

where $(-1)^{e_1}\cdots(-1)^{e_n}=1$.

Let $N(n)\subset\mathrm{SU}(n)$ denote the normalizer of $T(n)$ in $\mathrm{SU}(n)$, i.e., the subgroup of $\mathrm{SU}(n)$ which leaves $T(n)$ invariant under conjugation. It is straightforward to show that elements of $N(n)$ may be parametrized by a permutation $\sigma\in S_n$ and an n-tuple of phases $\Phi=(\phi_1,\ldots,\phi_n)$ satisfying

$$\mathrm{e}^{\mathrm{i}\phi_1}\cdots\mathrm{e}^{\mathrm{i}\phi_n}=\mathrm{sgn}(\sigma) \tag{3.6}$$

[here $\mathrm{sgn}(\sigma)$ denotes the parity of σ], and are of the form

$$y_{rt}(\sigma,\Phi)=\delta_{r,\sigma(t)}\mathrm{e}^{\mathrm{i}\phi_t}. \tag{3.7}$$

Multiplication in $N(n)$ is given by $y(\sigma,\Phi)y(\sigma',\Phi')=y(\sigma\sigma',\sigma'^{-1}\cdot\Phi+\Phi')$, so that, formally, $N(n)$ may be regarded as the semidirect product, $S_n\rtimes T(n)$. The quotient $N(n)/T(n)$, the Weyl group of $\mathrm{SU}(n)$, is isomorphic to S_n.

Let $M(n)$ denote the normalizer of $T(n)$ in $\mathrm{SU}(2n)$, i.e., the subgroup of $\mathrm{SU}(2n)$ which leaves $T(n)$ invariant under conjugation. Clearly $M(n)$ contains $N(n)$ as a subgroup. $M(n)$ also

contains the SU($2n$)-centralizer of $T(n)$, denoted by $Z(n)$, i.e., the subgroup of SU($2n$) whose elements commute with all elements of $T(n)$. It is straightforward to show that elements of $Z(n)$ are of the form $U\,t(\Theta)$, where $U\in \mathrm{SU}(2)^n$. and $t(\Theta)\in T(n)$. It is then straightforward to show that elements of $M(n)$ can be expressed as products of elements of $Z(n)$ and $N(n)$, and thus are of the form

$$x(U,\sigma,\Phi)=Uy(\sigma,\Phi), \tag{3.8}$$

where the phases Φ satisfy (3.6). Multiplication in $M(n)$ is given by

$$x(U,\sigma,\Phi)\,x(U',\sigma',\Phi')=x(U\sigma\cdot U',\sigma\sigma',\sigma'^{-1}\cdot\Phi+\Phi'). \tag{3.9}$$

The parametrization $x(U,\sigma,\Phi)$ of (3.8) is not unique. If U is replaced by UU_0, with $U_0\in \mathrm{Nul}(n)$ given by (3.5), and Φ is replaced by Φ', where $\phi_j'=\phi_j+e_j\pi$, then $x(U,\sigma,\Phi)$ is unchanged. In this way, we see that, formally, $M(n)$ is isomorphic to $\mathrm{SU}(2)^n\ltimes N(n)/\mathrm{Nul}(n)$.

From these considerations, it follows that the quotient $M(n)/T(n)$ is isomorphic to the spin-statistics group, i.e.,

$$\Sigma(n)=\mathrm{Spn}(n)\rtimes S_n\cong M(n)/T(n). \tag{3.10}$$

The isomorphism is given explicitly by

$$(\overline{U},\sigma)\mapsto x(U,\sigma,\Phi)T(n), \tag{3.11}$$

where $x(U,\sigma,\Phi)T(n)$ denotes a coset in $M(n)/T(n)$. This association between SU($2n$) and the spin-statistics group is the basis of the constructions to follow.

B. Representations of the spin-statistics group from representations of SU($2n$)

Let $\Gamma^{\mathbf{f}}$ denote a unitary irreducible representation of SU($2n$), labeled by a Young tableau $\mathbf{f}=(f_1,\ldots,f_{2n})$ of up to $2n$ rows (in fact, the last row of $\mathbf{f}$ may be taken to be empty). Let $\mathcal{V}$ denote the Hermitian inner product space on which $\Gamma^{\mathbf{f}}$ acts. (Of course, $\mathcal{V}$ depends on the choice of representation, but to simplify the notation we will not indicate this explicitly.)

Under the restriction of $\Gamma^{\mathbf{f}}$ to $T(n)$, $\mathcal{V}$ may be decomposed into a direct sum of orthogonal subspaces, $\mathcal{V}^K$, on which $\Gamma^{\mathbf{f}}(t(\Theta))$ is represented by the phase factor $\exp \mathrm{i}(K\cdot\Theta)$. Here $K=(k_1,\ldots,k_n)$ is an n-tuple of integers, and $K\cdot\Theta=\Sigma_j k_j\theta_j$. The subspace $\mathcal{V}^0$, corresponding to $K=(0,\ldots,0)$, consists of vectors which are invariant under $\Gamma^{\mathbf{f}}(T(n))$.

Let us determine the action of $M(n)$ on the subspaces $\mathcal{V}^K$. Given $x(U,\Phi,\sigma)\in M(n)$, it follows from (3.9) that

$$\begin{aligned}\Gamma^{\mathbf{f}}(t(\Theta))\Gamma^{\mathbf{f}}(x(U,\sigma,\Phi))\cdot\mathcal{V}^K&=\Gamma^{\mathbf{f}}(x(U,\sigma,\Phi))\Gamma^{\mathbf{f}}(t(\sigma^{-1}\cdot\Theta))\cdot\mathcal{V}^K\\&=\mathrm{e}^{\mathrm{i}(K\cdot(\sigma^{-1}\cdot\Theta))}\Gamma^{\mathbf{f}}(x(U,\sigma,\Phi))\cdot\mathcal{V}^K=\mathrm{e}^{\mathrm{i}(\sigma\cdot K)\cdot\Theta}\Gamma^{\mathbf{f}}(x(U,\sigma,\Phi))\cdot\mathcal{V}^K.\end{aligned} \tag{3.12}$$

Thus, under the action of $M(n)$, the subspaces $\mathcal{V}^K$ are mapped into one another according to

$$\Gamma^{\mathbf{f}}(x(U,\Phi,\sigma))\cdot\mathcal{V}^K=\mathcal{V}^{\sigma\cdot K}. \tag{3.13}$$

It follows from (3.13) that $\mathcal{V}^0$ is invariant under $M(n)$. Therefore $\Gamma^{\mathbf{f}}$ restricts to a representation of $M(n)$ on $\mathcal{V}^0$. Since $T(n)\subset M(n)$ belongs to the kernel of this representation [as $T(n)$ leaves vectors in $\mathcal{V}^0$ invariant], $\Gamma^{\mathbf{f}}(M(n))$ reduces to a representation of the quotient $M(n)/T(n)$, which we denote by $\Delta^{\mathbf{f}}$. Since $M(n)/T(n)\cong\Sigma(n)$ (cf. 3.10), $\Delta^{\mathbf{f}}$ is in fact a representation of the spin-statistics group. From (3.11), $\Delta^{\mathbf{f}}$ is given by

$$\Delta^{\mathbf{f}}(\overline{U},\sigma)=\Gamma^{\mathbf{f}}(x(U,\Phi,\sigma)). \tag{3.14}$$

In general, the representation $\Delta^{\mathbf{f}}$ of $\Sigma(n)$ is reducible. Let $\nu(\mathbf{f},s\lambda)$ denote the multiplicity with which the irreducible representation $Q^{s\lambda}$, given by (2.10), appears in the decomposition of $\Delta^{\mathbf{f}}$. This multiplicity will play a central role in what follows.

C. Construction of *n*-spin bundles

Let $\Xi: C_n \to \mathrm{SU}(n)/T(n)$ denote a smooth map from n-particle configuration space C_n to the coset space $\mathrm{SU}(n)/T(n)$. Such a map may be represented by $g(R)$, an $\mathrm{SU}(n)$-valued function on C_n which is smooth up to right multiplication by an element of $T(n)$. [That is, discontinuities in $g(R)$ can be removed locally by multiplying on the right by a discontinuous $T(n)$-valued function.] The symmetric group S_n acts on C_n as permutations (i.e., $R \mapsto \sigma \cdot R$) and on $\mathrm{SU}(n)/T(n)$ as the Weyl group [i.e., for $y(\sigma,\Phi) \in N(n)$, $g\,T(n) \mapsto g y^{-1}(\sigma,\Phi)\,T(n)$]. Ξ is said to be equivariant with respect to S_n if, for all $\sigma \in S_n$, $\Xi \circ \sigma = \sigma \circ \Xi$. In terms of $g(R)$, S_n-equivariance is equivalent to

$$g(\sigma \cdot R)\,T(n) = g(R) y^{-1}(\sigma,\Phi)\,T(n). \tag{3.15}$$

Atiyah[2] has shown that there exist continuous (and therefore smooth) S_n-equivariant maps from C_n to $\mathrm{SU}(n)/T(n)$. Let $g(R)$ represent any such equivariant map [the results which follow do not depend on the particular choice of $g(R)$].

As in Sec. III B, let $\Gamma^{\mathbf{f}}$ be an irreducible representation of $\mathrm{SU}(2n)$, and $\Delta^{\mathbf{f}}$ the associated representation of the spin-statistics group $\Sigma(n)$. Suppose $\nu(\mathbf{f},s\lambda) > 0$, i.e., $\mathcal{V}^0$ contains a subspace, which we denote by $\mathcal{V}^{s\lambda}$, which transforms under $\Delta^{\mathbf{f}}$ according to the irreducible representation $Q^{s\lambda}$ of $\Sigma(n)$. We may then construct an n-spin-s bundle $\mathcal{E}^{s\lambda}$ as follows. The fibers $\mathcal{E}^{s\lambda}_R \subset \mathcal{V}$ are given by

$$\mathcal{E}^{s\lambda}_R = \Gamma^{\mathbf{f}}(g(R)) \cdot \mathcal{V}^{s\lambda}. \tag{3.16}$$

Since $g(R)$ is smooth up to right multiplication by a $T(n)$-valued function and $\mathcal{V}^{s\lambda}$ is invariant under $\Gamma^{\mathbf{f}}(T(n))$, it follows that $\mathcal{E}^{s\lambda}_R$ depends smoothly on R.

Let us verify that $\mathcal{E}^{s\lambda}$ has the properties (A)–(D) listed in Sec. II B. For (A), we define the representation L_R on $\mathcal{E}^{s\lambda}_R$ by

$$L_R(\overline{U},\sigma) = \Gamma^{\mathbf{f}}(g(R)) \Delta^{\mathbf{f}}(\overline{U},\sigma) \Gamma^{\mathbf{f}^\dagger}(g(R)), \tag{3.17}$$

where $\Delta^{\mathbf{f}}(\overline{U},\sigma)$ is the representation of $\Sigma(n)$ given by (3.14). By assumption, $\Delta^{\mathbf{f}}$ is unitarily equivalent to $Q^{s\lambda}$ on $\mathcal{V}^{s\lambda}$, so it is evident from (3.17) that L_R is unitarily equivalent to $Q^{s\lambda}$ for all R. Since the right-hand side of (3.17) is unchanged if $g(R)$ is multiplied on the right by a (possibly discontinuous) $T(n)$-valued function, it is clear that L_R depends smoothly on R.

For (B), from the definition (3.16) and the equivariance property (3.15), we have that

$$\mathcal{E}^{s\lambda}_{\sigma \cdot R} = \Gamma^{\mathbf{f}}(g(\sigma \cdot R)) \cdot \mathcal{V}^{s\lambda} = \Gamma^{\mathbf{f}}(g(R)) \Gamma^{\mathbf{f}}(y^{-1}(\sigma,\Phi)) \cdot \mathcal{V}^{s\lambda} = \Gamma^{\mathbf{f}}(g(R)) \cdot \mathcal{V}^{s\lambda} = \mathcal{E}^{s\lambda}_R. \tag{3.18}$$

Thus the fibers at permuted configurations are the same.

For (C), we define the unitary maps $T_{R' \leftarrow R}$ describing flat parallel transport between the fibers at R and R' by

$$T_{R' \leftarrow R} = \Gamma^{\mathbf{f}}(g(R')) \Gamma^{\mathbf{f}^\dagger}(g(R)). \tag{3.19}$$

The right-hand side is unchanged if $g(R)$ is multiplied on the right by a $T(n)$-valued function, so $T_{R' \leftarrow R}$ is well defined and depends smoothly on R and R'. The composition law (2.30) is easily verified. Compatibility with the representations L_R [cf. (2.31)] follows from the definition of L_R in (3.17) and the representation property of $\Gamma^{\mathbf{f}}$.

For (D), from (3.19), parallel transport $T_{\sigma\cdot R\leftarrow R}$ between permuted fibers R and $\sigma\cdot R$ is given by $\Gamma^{\mathbf{f}}(g(\sigma\cdot R))\Gamma^{\mathbf{f}^\dagger}(g(R))$. The equivariance condition (3.15) implies this is equal to $\Gamma^{\mathbf{f}}(g(R))\Gamma^{\mathbf{f}}(y^{-1}(\sigma,\Phi))\Gamma^{\mathbf{f}^\dagger}(g(R))$. From (3.17), the condition (2.32) follows.

D. Spin-statistics relations from SU(2n) representations?

Given an irreducible representation $\Gamma^{\mathbf{f}}$ of SU($2n$), the preceding construction determines the statistics for spin s unambiguously, provided that there is just one representation $Q^{s\lambda}$ with spin s in the decomposition of $\Delta^{\mathbf{f}}$; equivalently, given $\mathbf{f}$ and s, the multiplicity $\nu(\mathbf{f},s,\lambda)$ should vanish for all but one λ.

This is the case for the completely symmetric representations of SU($2n$). The completely symmetric representations correspond to Young tableaux with a single row. Let Γ^d denote the representation for a single row of d boxes. Γ^d may be realized on the space $\mathcal{V}$ of homogeneous polynomials of degree d in $2n$ variables, $z=(z_1,\ldots,z_{2n})\in\mathbb{C}^{2n}$, and is given by $\Gamma^d(f)\cdot P(z)=P(f^{-1}\cdot z)$ for $f\in\mathrm{SU}(2n)$. Γ^d is unitary with respect to the inner product

$$\langle P,Q\rangle=\int_{\mathbb{C}^{2n}}\mathrm{e}^{-z^*\cdot z/2}P^*(z)Q(z)\,d^{4n}z \tag{3.20}$$

on $\mathcal{V}$.

An orthogonal basis for $\mathcal{V}$ is given by the monomials

$$\prod_{r=1}^{n} z_{1,r}^{a_r}z_{2,r}^{b_r}, \tag{3.21}$$

where the sum of the exponents a_j and b_j is given by d. The subspace $\mathcal{V}^0$, whose vectors are invariant under $T(n)$, consists of polynomials which are invariant under $z\mapsto t^{-1}(\Theta)\cdot z$, where

$$t^{-1}(\Theta)\cdot z=(\mathrm{e}^{-\mathrm{i}\theta_1}z_1,\mathrm{e}^{-\mathrm{i}\theta_1}z_2,\ldots,\mathrm{e}^{-\mathrm{i}\theta_n}z_{2n-1},\mathrm{e}^{-\mathrm{i}\theta_n}z_{2n}). \tag{3.22}$$

Such polynomials are linear combinations of the monomials (3.21) for which a_r+b_r is independent of r, so that $a_r+b_r=d/n$. Thus, for $\mathcal{V}^0$ to be nontrivial, d must be divisible by n.

Let us assume this is the case, so that d/n is integral. Then $s=d/2n$ is either integral or half-odd-integral. Let $m_r=a_r-s$. Then $a_r=s+m_r$ and $b_r=s-m_r$. It follows that $\mathcal{V}^0$ is spanned by the $(2s+1)^n$ monomials

$$\prod_{r=1}^{n} z_{1,r}^{s+m_r}z_{2,r}^{s-m_r}, \tag{3.23}$$

where $-s\leqslant m_r\leqslant s$ and $s\pm m_r$ is integral. Under Spn(n), $\mathcal{V}^0$ transforms as n spin-s spinors. As the dimension of $\mathcal{V}^0$ is $(2s+1)^n$, it follows that there is a single irreducible representation $Q^{s\lambda}$ with multiplicity one in the decomposition of $\Delta^{\mathbf{f}}$, and that $d_\lambda=1$, i.e., λ is either the completely symmetric or the completely antisymmetric representation of S_n.

λ may be determined by considering the action of permutations on an element of $\mathcal{V}^0$, for example,

$$P_s(z)\overset{\mathrm{def}}{=}z_2^{2s}z_4^{2s}\cdots z_{2n}^{2s}. \tag{3.24}$$

From (3.7), under $y^{-1}(\sigma,\Phi)$, the even components transform as $z_{2j}\mapsto\mathrm{e}^{-\mathrm{i}\phi_j}z_{2\sigma(j)}$. Thus, under $y(\sigma,\Phi)$, $P_s(z)$ is multiplied by the phase factor $\mathrm{e}^{2s\mathrm{i}\phi_1}\cdots\mathrm{e}^{2s\mathrm{i}\phi_n}$. From (3.6), this phase factor is just $\mathrm{sgn}^{2s}(\sigma)$. Thus, the completely symmetric representations of SU($2n$) of dimension $d=2ns$

lead to n-spin-bundles with spin s and Bose or Fermi statistics according to the parity of $2s$, in accord with the physically correct spin-statistics relation. This is precisely the result obtained in BR.

IV. CALCULATION OF THE MULTIPLICITIES

Given an arbitrary representation $\Gamma^{\mathbf{f}}$ of $\mathrm{SU}(2n)$, we wish to determine for which spins an n-spin-s bundle can be constructed, and, for those spins, whether the constructions have a definite type of statistics. To this end, we calculate the multiplicities $\nu(\mathbf{f},s\lambda)$ with which the irreducible representation $Q^{s\lambda}$ of $\Sigma(n)$ appears in the representation $\Delta^{\mathbf{f}}$. This is given by the following integral:

$$\nu(\mathbf{f},s\lambda)=\int_{\Sigma(n)} d\mu_{\Sigma(n)}\, X^{s\lambda *}(\overline{U},\sigma)X^{\mathbf{f}}(\overline{U},\sigma). \tag{4.1}$$

Here $X^{s\lambda}$ and $X^{\mathbf{f}}$ denote the characters of the $\Sigma(n)$-representations $Q^{s\lambda}$ and $\Delta^{\mathbf{f}}$, respectively, and $d\mu_{\Sigma(n)}$ denotes the normalized Haar measure on $\Sigma(n)$. Before evaluating the integral (4.1) in Sec. IV B, we first introduce some background material and notation.

A. Preliminaries

1. Character formula for U(k)

Irreducible representations of the k-dimensional unitary group $\mathrm{U}(k)$ are labeled by Young tableaux $\boldsymbol{\alpha}=(\alpha^1,\ldots,\alpha^k)$ of k rows (some of which may be empty), where $\alpha^1\geqslant\cdots\geqslant\alpha^k\geqslant 0$ specify the number of boxes in each row. Let

$$|\boldsymbol{\alpha}|=\alpha^1+\cdots+\alpha^k \tag{4.2}$$

denote the number of boxes in the tableau. Denote the eigenvalues of matrices in $\mathrm{U}(k)$ by $(\exp i\xi_1,\ldots,\exp i\xi_k)$, and their eigenphases by $\boldsymbol{\xi}=(\xi_1,\ldots,\xi_k)$. The characters $K_k^{\boldsymbol{\alpha}}$ of the irreducible representations are functions of $\boldsymbol{\xi}$ and are given by the Weyl character formula,

$$K_k^{\boldsymbol{\alpha}}(\boldsymbol{\xi})=\frac{\begin{vmatrix} e^{i(\alpha^1+k-1)\xi_1} & e^{i(\alpha^1+k-1)\xi_2} & \cdots & e^{i(\alpha^1+k-1)\xi_k} \\ e^{i(\alpha^2+k-2)\xi_1} & e^{i(\alpha^2+k-2)\xi_2} & \cdots & e^{i(\alpha^2+k-2)\xi_k} \\ \vdots & \vdots & & \vdots \\ e^{i\alpha^k\xi_1} & e^{i\alpha^k\xi_2} & \cdots & e^{i\alpha^k\xi_k} \end{vmatrix}}{\begin{vmatrix} e^{i(k-1)\xi_1} & e^{i(k-1)\xi_2} & \cdots & e^{i(k-1)\xi_k} \\ e^{i(k-2)\xi_1} & e^{i(k-2)\xi_2} & \cdots & e^{i(k-2)\xi_k} \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 \end{vmatrix}}. \tag{4.3}$$

Irreducible representations of $\mathrm{SU}(k)$ are obtained by restriction. On $\mathrm{SU}(k)$, the representation $\boldsymbol{\alpha}+r$, which is obtained by adding r columns of k boxes to $\boldsymbol{\alpha}$, is equivalent to the representation $\boldsymbol{\alpha}$. $\mathrm{SU}(k)$ representations can be uniquely labeled by Young tableaux of $k-1$ rows (some of which may be empty).

2. The Littlewood–Richardson theorem

Given an irreducible representation $\boldsymbol{\gamma}$ of $\mathrm{U}(k+l)$, its restriction to the subgroup $\mathrm{U}(k)\times\mathrm{U}(l)$ is, in general, reducible, and may be decomposed into a sum of tensor products of irreducible representations $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ of $\mathrm{U}(k)$ and $\mathrm{U}(l)$, respectively. In terms of characters, this decomposition takes the form

$$K^{\gamma}_{k+l}(\boldsymbol{\xi},\boldsymbol{\eta})=\sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} Y^{\gamma}_{\boldsymbol{\alpha}\boldsymbol{\beta}} K^{\boldsymbol{\alpha}}_{k}(\boldsymbol{\xi}) K^{\boldsymbol{\beta}}_{l}(\boldsymbol{\eta}), \tag{4.4}$$

where $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ denote the eigenphases of elements of U(k) and U(l), respectively. The coefficients $Y^{\gamma}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ in the decomposition are given by the Littlewood–Richardson theorem, according to which $Y^{\gamma}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ is the number of times that the tableau $\boldsymbol{\gamma}$ can be constructed from $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ by the following procedure: Boxes from the first row of $\boldsymbol{\beta}$ are added to $\boldsymbol{\alpha}$ so as to produce a new tableau, with the condition that no two boxes are placed in the same column of the new tableau. This is repeated with the second row of $\boldsymbol{\beta}$, with the additional condition that, on counting added boxes in the new tableau column-wise from right to left, and row-wise from top to bottom, the number of added boxes from the first row of $\boldsymbol{\beta}$ must always be greater than or equal to the number of added boxes from the second row. The procedure is continued for the other rows until all boxes from $\boldsymbol{\beta}$ have been added to $\boldsymbol{\alpha}$. It is evident that $\boldsymbol{\gamma}$ can be constructed in this way only if the number of boxes in $\boldsymbol{\gamma}$ equals the number of boxes in $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ together; that is, $Y^{\gamma}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ vanishes unless $|\boldsymbol{\gamma}| = |\boldsymbol{\alpha}| + |\boldsymbol{\beta}|$.

Equation (4.4) generalizes to the decomposition of irreducible representations $\boldsymbol{\gamma}$ of U($k_1 + \cdots + k_c$) restricted to the subgroup U(k_1)$\times\cdots\times$U(k_n), as follows:

$$K^{\gamma}_{k_1+\cdots+k_c}(\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_c)=\sum_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_c} Y^{\gamma}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_c} \prod_{b=1}^{c} K^{\boldsymbol{\alpha}_b}_{k_b}(\boldsymbol{\xi}_b). \tag{4.5}$$

Here the $\boldsymbol{\alpha}_b$'s are tableaux labeling irreducible representations of U(k_b), and the $\boldsymbol{\xi}_b$ denote the eigenphases of elements of U(k_b). The c-fold coefficients $Y^{\gamma}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_c}$ may be obtained from the twofold coefficients $Y^{\gamma}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ by performing the c-fold decomposition inductively.

With (4.5), the $(k_1+\cdots+k_c)$-fold determinants in the Weyl character formula (4.3) are reduced to sums of products of ratios of smaller, k_b-fold determinants. However, this simplification comes at a price; the Littlewood–Richardson coefficients are not easily calculated, and closed-form expressions for them are not known.

The original statement of the Littlewood–Richardson theorem appears in Ref. 14. A modern version with proof may be found in Ref. 15. The application of the Littlewood–Richardson theorem to the unitary groups is discussed by Hagen and MacFarlane[8] and Itzykson and Nauenberg.[11] A more detailed discussion of the rules for multiplying Young tableaux can be found in Ref. 9.

3. Characters for U(2) and SU(2)

We will need some results and notation particular to the groups SU(2) and U(2). Irreducible characters of SU(2) are denoted by $\chi^{s}_{\mathrm{SU}(2)}(\psi)$, where s is the spin and $e^{\pm i\psi}$ denotes the eigenvalues of elements of SU(2), and are given by

$$\chi^{s}_{\mathrm{SU}(2)}(\psi)=\frac{\sin((2s+1)\psi)}{\sin(\psi)}. \tag{4.6}$$

Irreducible representations of U(2) are labeled by tableaux $\boldsymbol{\alpha}=(\alpha^1,\alpha^2)$ of two rows. The U(2)-characters $K^{\boldsymbol{\alpha}}_{2}(\xi_1,\xi_2)$ are related to the SU(2)-characters $\chi^{s}_{\mathrm{SU}(2)}(\psi)$ by

$$K^{\boldsymbol{\alpha}}_{2}(+\psi+\theta,-\psi+\theta)=e^{i|\boldsymbol{\alpha}|\theta}\chi^{S(\boldsymbol{\alpha})}_{\mathrm{SU}(2)}(\psi), \tag{4.7}$$

where

$$S(\boldsymbol{\alpha})=(\alpha^1-\alpha^2)/2 \tag{4.8}$$

denotes the value of spin associated with the U(2)-representation $\boldsymbol{\alpha}$.

The Clebsch–Gordan coefficients $C(s_1,s_2,s_3)$ for SU(2) are defined by

$$C(s_1,s_2,s_3)=\frac{1}{\pi}\int_0^{2\pi} d\psi \sin^2(\psi)\chi^{s_1}_{\mathrm{SU}(2)}(\psi)\chi^{s_2}_{\mathrm{SU}(2)}(\psi)\chi^{s_3}_{\mathrm{SU}(2)}(\psi) \tag{4.9}$$

[note that $\sin^2(\psi)$ is the Haar measure with respect to classes of SU(2)], and give the multiplicity of the trivial representation in the decomposition of the tensor product of three SU(2)-representations with spins s_1, s_2 and s_3. It is an elementary result that $C(s_1,s_2,s_3)$ equals one if $|s_1-s_2|\leqslant s_3\leqslant s_1+s_2$, and is zero otherwise. We define the r-fold Clebsch–Gordan coefficients by

$$C(s_1,\ldots,s_r)=\frac{1}{\pi}\int_0^{2\pi} d\psi \sin^2(\psi)\chi^{s_1}_{\mathrm{SU}(2)}(\psi)\cdots\chi^{s_r}_{\mathrm{SU}(2)}(\psi). \tag{4.10}$$

These are given inductively by

$$C(s_1,\ldots,s_r,s_{r+1})=\sum_s C(s_1,\ldots,s_{r-1},s)C(s,s_r,s_{r+1}). \tag{4.11}$$

4. Cycle decomposition of permutations

The following notations will be used for permutations. Let $\sigma\in S_n$. Denote the factorization of σ into disjoint cycles by

$$\sigma=\hat{\sigma}_1\cdots\hat{\sigma}_{c(\sigma)}, \tag{4.12}$$

where $c(\sigma)$ denotes the number of cycles in the factorization. Denote the length of a cycle in the decomposition, say $\hat{\sigma}_b$, by $|\hat{\sigma}_b|$.

Let $\sigma\in S_n$ and $U=(u_1,\ldots,u_n)\in \mathrm{SU}(2)^n$. For each cycle $\hat{\sigma}_b$ in the factorization of σ, let $\hat{u}_b$ denote the product of the corresponding components of U, taken in the reverse order. That is, if $\hat{\sigma}_b=(jk\cdots l)$, then

$$\hat{u}_b=u_l\cdots u_k u_j. \tag{4.13}$$

Similarly, given an n-tuple of phases, $\Theta=(\theta_1,\ldots,\theta_n)$, let

$$\hat{\theta}_b=\theta_l+\cdots+\theta_k+\theta_j. \tag{4.14}$$

Clearly

$$\theta_1+\cdots+\theta_n=\hat{\theta}_1+\cdots+\hat{\theta}_{c(\sigma)}. \tag{4.15}$$

B. Evaluation of the integral

To evaluate the character integral (4.1), it will be convenient to regard $X^{s\lambda}$ and $X^{\mathbf{f}}$ as characters on $\mathrm{SU}(2)^n\rtimes\Sigma(n)$, i.e., as functions of U and σ rather than $\overline{U}$ and σ. Then

$$\nu(\mathbf{f},s\lambda)=\frac{1}{n!}\sum_{\sigma\in S_n}\int_{\mathrm{SU}(2)^n} du_1\cdots du_n X^{s\lambda}(U,\sigma)^* X^{\mathbf{f}}(U,\sigma), \tag{4.16}$$

where du_j denotes the normalized Haar measure on SU(2).

The character $X^{s\lambda}(U,\sigma)$ may be evaluated as follows. From (2.10) and (2.11),

$$\begin{aligned} X^{s\lambda}(U,\sigma)&=\sum_{a=1}^{d_\lambda}\sum_M \langle M,a|Q^{s\lambda}(U,\sigma)|M,a\rangle \\ &=\left(\sum_{a=1}^{d_\lambda}\Lambda_{a,a}(\sigma)\right)\left(\sum_M D^s_{m_{\sigma(1)},m_1}(u_1)\cdots D^s_{m_{\sigma(n)},m_n}(u_n)\right). \end{aligned} \tag{4.17}$$

The sum over a yields $\chi^{\lambda}_{S_n}(\sigma)$, the character of the S_n-representation Λ^{λ}. The sum over M factorizes into a product over the disjoint cycles $\hat{\sigma}_b$ of σ and yields

$$\mathrm{Tr}\, D^s(\hat{u}_1)\cdots \mathrm{Tr}\, D^s(\hat{u}_{c(\sigma)}), \tag{4.18}$$

where $\hat{u}_b \in \mathrm{SU}(2)$ is given by (4.13). Let $e^{\pm i\hat{\xi}_b}$ denote the eigenvalues of $\hat{u}_b$. Then

$$X^{s\lambda}(U,\sigma) = \chi^{\lambda}_{S_n}(\sigma) \prod_{b=1}^{c(\sigma)} \chi^{s}_{\mathrm{SU}(2)}(\hat{\xi}_b). \tag{4.19}$$

We note that $X^{s\lambda}(U,\sigma)$ is real, since the characters of S_n and SU(2) are real.

The character $X^{\mathbf{f}}(U,\sigma)$ in (4.16) may be expressed as

$$X^{\mathbf{f}}(U,\sigma) = \mathrm{Tr}\,(\Gamma^{\mathbf{f}}(x(U,\sigma,\Phi))P^0). \tag{4.20}$$

Here the trace is taken over the carrier space $\mathcal{V}$ of the representation $\Gamma^{\mathbf{f}}$, Φ denotes phases satisfying $e^{i\phi_1}\cdots e^{i\phi_n} = \mathrm{sgn}(\sigma)$, and P^0 denotes the Hermitian projection onto the subspace $\mathcal{V}^0$ given by

$$P^0 = \frac{1}{(2\pi)^{n-1}} \int d^{n-1}\Theta'\, \Gamma^{\mathbf{f}}(t(\Theta')), \tag{4.21}$$

where the Θ'-integral is taken over $0 \leqslant \theta'_j \leqslant 2\pi$ subject to the condition that $e^{i\theta'_1}\cdots e^{i\theta'_n} = 1$. Substituting (4.21) into (4.20) we get that

$$X^{\mathbf{f}}(U,\sigma) = \frac{1}{(2\pi)^{n-1}} \int d^{n-1}\Theta'\, \mathrm{Tr}\,\Gamma^{\mathbf{f}}(x(U,\sigma,\Theta'+\Phi)) = \frac{1}{(2\pi)^{n-1}} \int d^{n-1}\Theta\, \mathrm{Tr}\,\Gamma^{\mathbf{f}}(x(U,\sigma,\Theta)), \tag{4.22}$$

where the integral over $\Theta = (\theta_1,\ldots,\theta_n)$ in the last expression is restricted to $e^{i\theta_1}\cdots e^{i\theta_n} = \mathrm{sgn}(\sigma)$. It is convenient to incorporate this restriction using the identity

$$\frac{1}{(2\pi)^{n-1}} \int d^{n-1}\Theta = \sum_{q=-\infty}^{\infty} (\mathrm{sgn}\,\sigma)^q \frac{1}{(2\pi)^n} \int e^{iq(\theta_1+\cdots+\theta_n)}\,. \tag{4.23}$$

We note that as Θ on the right-hand side of (4.23) is unconstrained, $x(U,\sigma,\Theta)$ is, in general, an element of U($2n$) rather than SU($2n$). Let $\boldsymbol{\mu}$ denote the eigenphases of $x(U,\sigma,\Theta)$. Then $\mathrm{Tr}\,\Gamma^{\mathbf{f}}(x(U,\sigma,\Theta)) = K^{\mathbf{f}}_{2n}(\boldsymbol{\mu})$, and (4.22) becomes

$$X^{\mathbf{f}}(U,\sigma) = \sum_{q=-\infty}^{\infty} (\mathrm{sgn}\,\sigma)^q \frac{1}{(2\pi)^n} \int_0^{2\pi} d^n\Theta\, e^{-iq(\theta_1+\cdots\theta_n)} K^{\mathbf{f}}_{2n}(\boldsymbol{\mu}). \tag{4.24}$$

To determine the eigenphases $\boldsymbol{\mu}$ of $x(U,\sigma,\Theta)$, it is convenient to represent vectors in $\mathbb{C}^{2n}$ as linear combinations of terms $|v_j\rangle\otimes|j\rangle$, where $|v_j\rangle \in \mathbb{C}^2$ and $|j\rangle$ is an orthonormal basis for $\mathbb{C}^n$. From (3.7) and (3.8), the action of $x(U,\sigma,\Theta)$ is then given by

$$x(U,\sigma,\Theta)\sum_{j=1}^{n} |\xi_j\rangle\otimes|j\rangle = \sum_{j=1}^{n} e^{i\theta_j}(u_{\sigma(j)}|\xi_j\rangle)\otimes|\sigma(j)\rangle. \tag{4.25}$$

Let $\hat{\sigma}_b = (jk\cdots l)$ be a cycle in σ, and, as above, let $e^{\pm i\hat{\xi}_b}$ denote the eigenvalues of $\hat{u}_b$. Let $|\pm w_b\rangle \in \mathbb{C}^2$ denote the associated eigenvectors of $\hat{u}_b$. It is readily verified that $|\pm w_b\rangle\otimes|l\rangle$ are eigenvectors of $x^m(U,\sigma,\Theta)$, with eigenvalues $e^{im(\pm\hat{\xi}_b+\hat{\theta}_b)/|\hat{\sigma}_b|}$, if and only if m is a multiple of $|\hat{\sigma}_b|$.

In general, if $|v\rangle$ is an eigenvector of some positive integer power $|\hat{\sigma}_b|$ of a matrix M, with ρ the associated eigenvalue of $M^{|\hat{\sigma}_b|}$, and if $|v\rangle$ is not an eigenvector of any smaller positive power of M, then M has eigenvalues $e^{2\pi i p/|\hat{\sigma}_b|}\rho^{1/|\hat{\sigma}_b|}$, where $p=1,\ldots,|\hat{\sigma}_b|$. From these considerations we may deduce that to each cycle $\hat{\sigma}_b$ in σ are associated $2|\hat{\sigma}_b|$ eigenphases of $x(U,\sigma,\Theta)$, denoted by $\boldsymbol{\eta}_b=(\boldsymbol{\eta}_{b,1},\ldots,\boldsymbol{\eta}_{b,|\hat{\sigma}_b|})$ and given explicitly by

$$\boldsymbol{\eta}_{b,p}=\left(\frac{+\hat{\xi}_b+\hat{\theta}_b+2\pi p}{|\hat{\sigma}_b|},\frac{-\hat{\xi}_b+\hat{\theta}_b+2\pi p}{|\hat{\sigma}_b|}\right),\quad p=1,\ldots,|\hat{\sigma}_b|. \tag{4.26}$$

The full set of eigenvalues of $x(U,\sigma,\Theta)$ is

$$\boldsymbol{\mu}=(\boldsymbol{\eta}_1,\ldots,\boldsymbol{\eta}_{c(\sigma)}). \tag{4.27}$$

From (4.27) it is apparent that $x(U,\sigma,\Theta)\in \mathrm{U}(2n)$ is unitarily equivalent to the element of $\mathrm{U}(2|\sigma_1|)\times\cdots\times\mathrm{U}(2|\sigma_{c(\sigma)}|)$ with eigenphases $\boldsymbol{\eta}_1,\ldots,\boldsymbol{\eta}_{c(\sigma)}$ for the factors. From the Littlewood–Richardson formula (4.5), the character $K^{\mathbf{f}}_{2n}(\boldsymbol{\mu})$ in (4.24) is given by

$$K^{\mathbf{f}}_{2n}(\boldsymbol{\mu})=K^{\mathbf{f}}_{2n}(\boldsymbol{\eta}_1,\ldots,\boldsymbol{\eta}_{c(\sigma)})=\sum_{\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_{c(\sigma)}} Y^{\mathbf{f}}_{\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_{c(\sigma)}}\prod_{b=1}^{c(\sigma)} K^{\boldsymbol{\beta}_b}_{|\hat{\sigma}_b|}(\boldsymbol{\eta}_b), \tag{4.28}$$

where the $\boldsymbol{\beta}_b$'s are tableaux labeling representations of $\mathrm{U}(2|\hat{\sigma}_b|)$. As noted in Sec. IV A 2, the sum in (4.28) may restricted to those $\boldsymbol{\beta}_b$ satisfying

$$\sum_{b=1}^{c(\sigma)}|\boldsymbol{\beta}_b|=|\mathbf{f}|. \tag{4.29}$$

From (4.26), the characters $K^{\boldsymbol{\beta}_b}_{|\hat{\sigma}_b|}(\boldsymbol{\eta}_b)$ can themselves be expressed as a product of U(2)-characters by applying the Littlewood–Richardson theorem once more, as follows:

$$K^{\boldsymbol{\beta}_b}_{|\hat{\sigma}_b|}(\boldsymbol{\eta}_b)=K^{\boldsymbol{\beta}_b}_{|\hat{\sigma}_b|}(\boldsymbol{\eta}_{b,1},\ldots,\boldsymbol{\eta}_{b,|\hat{\sigma}_b|})=\sum_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}} Y^{\boldsymbol{\beta}_b}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}}\prod_{p=1}^{|\hat{\sigma}_b|} K^{\boldsymbol{\alpha}_p}_2(\boldsymbol{\eta}_{b,p}). \tag{4.30}$$

Here the $\boldsymbol{\alpha}_p$'s are tableaux labeling representations of U(2), and the sum in (4.30) may be restricted to those $\boldsymbol{\alpha}_p$ satisfying

$$\sum_{p=1}^{|\hat{\sigma}_b|}|\boldsymbol{\alpha}_p|=|\boldsymbol{\beta}_b|. \tag{4.31}$$

Finally, the U(2)-characters are given explicitly [cf. (4.7) and (4.26)] by

$$K^{\boldsymbol{\alpha}_p}_2(\boldsymbol{\eta}_{b,p})=e^{i|\boldsymbol{\alpha}_p|(2\pi p+\hat{\theta}_b)/|\hat{\sigma}_b|}\chi^{S(\boldsymbol{\alpha}_p)}_{\mathrm{SU}(2)}(\hat{\xi}_b/|\hat{\sigma}_b|). \tag{4.32}$$

To proceed, we substitute the expression (4.19) for $X^{s\lambda}(U,\sigma)$ and the expressions (4.24) and (4.28)–(4.32) for $X^{\mathbf{f}}(U,\sigma)$ into the integral (4.16). The integration over $\mathrm{SU}(2)^n$ can be arranged so that $\hat{u}_1,\ldots,\hat{u}_{c(\sigma)}\in\mathrm{SU}(2)$ are amongst the integration variables. Since the integrand depends only on the $\hat{u}_b$'s, any remaining SU(2)-integrals are trivially evaluated. Moreover, since the integrand depends only on the eigenphases $\hat{\xi}_b$, we can make the replacement

$$\int_{\mathrm{SU}(2)} d\hat{u}_b\to\frac{1}{\pi}\int_0^{2\pi} d\hat{\xi}_b\sin^2(\hat{\xi}_b). \tag{4.33}$$

Similarly, the Θ-integral in (4.16) can be arranged so that $\hat{\theta}_1,\ldots,\hat{\theta}_{c(\sigma)}$ are amongst the variables of integration; in view of (4.15), the integrand depends only on the $\hat{\theta}_b$'s, so the integrals over any remaining components of Θ are trivially evaluated. Finally, as the terms in the S_n-sum in (4.16) depend only the conjugacy class of σ and not on σ itself, we may make the replacement

$$\sum_{\sigma\in S_n}\rightarrow\sum_{[\sigma]\in S_n}\Omega_{[\sigma]}, \tag{4.34}$$

where $[\sigma]$ denotes the conjugacy class of σ and $\Omega_{[\sigma]}$ denotes the number of elements in $[\sigma]$ ($\Omega_{[\sigma]}$ may be explicitly expressed in terms of the cycle lengths $|\hat{\sigma}_1|,\ldots,|\hat{\sigma}_{c(\sigma)}|$). In this way, Eq. (4.16) for the multiplicities may be expressed as

$$\nu(\mathbf{f},s\lambda)=\frac{1}{n!}\sum_{[\sigma]\in S_n}\Omega_{[\sigma]}\chi^{\lambda}_{S_n}(\sigma)\sum_{q=-\infty}^{\infty}(\operatorname{sgn}\sigma)^q\sum_{\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_{c(\sigma)}}Y^{\mathbf{f}}_{\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_{c(\sigma)}}\prod_{b=1}^{c(\sigma)}I_b\,J_b\,. \tag{4.35}$$

The factor I_b, which contains the integral over θ_b, is given by

$$I_b=\frac{1}{2\pi}\int_0^{2\pi}d\hat{\theta}_b\,\mathrm{e}^{\mathrm{i}(|\boldsymbol{\beta}_b|/|\hat{\sigma}_b|-q)\hat{\theta}_b}, \tag{4.36}$$

where we have used (4.31). The factor J_b, which contains the integral over $\hat{\xi}_b$ and the sum over the U(2)-tableaux $\boldsymbol{\alpha}_p$, is given by

$$\begin{aligned}J_b=&\sum_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}}Y^{\boldsymbol{\beta}_b}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}}\,\mathrm{e}^{2\pi\mathrm{i}(\sum_{p=1}^{|\hat{\sigma}_b|}p|\boldsymbol{\alpha}_p|)/|\hat{\sigma}_b|}\times\frac{1}{\pi}\\&\times\int_0^{2\pi}d\hat{\xi}_b\sin^2(\hat{\xi}_b)\chi^{s}_{\mathrm{SU}(2)}(\hat{\xi}_b)\chi^{S(\boldsymbol{\alpha}_1)}_{\mathrm{SU}(2)}(\hat{\xi}_b/|\hat{\sigma}_b|)\cdots\chi^{S(\boldsymbol{\alpha}_{|\hat{\sigma}_b|})}_{\mathrm{SU}(2)}(\hat{\xi}_b/|\hat{\sigma}_b|).\end{aligned} \tag{4.37}$$

The $\hat{\theta}_b$-integral in (4.36) is trivial, and vanishes unless

$$q|\hat{\sigma}_b|=|\boldsymbol{\beta}_b|. \tag{4.38}$$

Summing over b in (4.38) and using (4.29), we get that

$$q=\frac{|\mathbf{f}|}{n}. \tag{4.39}$$

Since q is an integer, it follows that at least one of the I_b's must vanish [and, therefore, $\nu(\mathbf{f},s\lambda)$ must vanish] unless n divides $|\mathbf{f}|$. Assuming this to be so, the sum over q in (4.35) collapses to $q=|\mathbf{f}|/n$.

We consider next the expression for J_b. Since the integrand is 2π-periodic in $\hat{\xi}_b$, we can make the replacement

$$\int_0^{2\pi}d\hat{\xi}_b\rightarrow\int_0^{2\pi}d\hat{\psi}_b\,, \tag{4.40}$$

where $\hat{\psi}_b=\hat{\xi}_b/|\hat{\sigma}_b|$. Using the identity

$$\sin^2(r\hat{\psi}_b)\chi^{s}_{\mathrm{SU}(2)}(r\hat{\psi}_b)=\sin^2(\hat{\psi}_b)\chi^{rs+(r-1)/2}_{\mathrm{SU}(2)}(\hat{\psi}_b)\chi^{(r-1)/2}_{\mathrm{SU}(2)}(\hat{\psi}_b), \tag{4.41}$$

which follows from the definition (4.6), the resulting integral over $\hat{\psi}_b$ is of the form (4.10), and yields a $(|\hat{\sigma}_b|+2)$-fold Clebsch–Gordan coefficient. We obtain

$$J_b = \sum_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}} Y^{\boldsymbol{\beta}_b}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}} \mathrm{e}^{2\pi\mathrm{i}(\Sigma_{p=1}^{|\hat{\sigma}_b|} p|\boldsymbol{\alpha}_p|)/|\hat{\sigma}_b|} \times C(|\hat{\sigma}_b|s+\tfrac{1}{2}(|\hat{\sigma}_b|-1),\tfrac{1}{2}(|\hat{\sigma}_b|-1),S(\boldsymbol{\alpha}_1),\ldots,S(\boldsymbol{\alpha}_{|\hat{\sigma}_b|})). \tag{4.42}$$

From (4.35), (4.39) and (4.42), we get our main result for the multiplicities,

$$\nu(\mathbf{f},s\lambda) = \frac{1}{n!}\sum_{[\sigma]\in S_n} \Omega_{[\sigma]}\chi^{\lambda}_{S_n}(\sigma)(\operatorname{sgn}\sigma)^{|\mathbf{f}|/n}A_{[\sigma]}, \tag{4.43}$$

where

$$A_{[\sigma]} = \sum_{\substack{\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_{c(\sigma)} \\ |\boldsymbol{\beta}_b|=|\hat{\sigma}_b|\cdot|\mathbf{f}|/n}} Y^{\mathbf{f}}_{\boldsymbol{\beta}_1,\cdots,\boldsymbol{\beta}_{c(\sigma)}} \times \prod_{b=1}^{c(\sigma)} \left[\sum_{\boldsymbol{\alpha}_1,\cdots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}} Y^{\boldsymbol{\beta}_b}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_{|\hat{\sigma}_b|}} \mathrm{e}^{2\pi\mathrm{i}(\Sigma_{p=1}^{|\hat{\sigma}_b|} p|\boldsymbol{\alpha}_p|)/|\hat{\sigma}_b|} \times C(|\hat{\sigma}_b|s+\tfrac{1}{2}(|\hat{\sigma}_b|-1),\tfrac{1}{2}(|\hat{\sigma}_b|-1),S(\boldsymbol{\alpha}_1),\ldots,S(\boldsymbol{\alpha}_{|\hat{\sigma}_b|})) \right]. \tag{4.44}$$

For $\sigma=\mathrm{I}=(1)\cdots(n)$ (i.e., the identity element in S_n), the expression (4.44) simplifies considerably. In this case, $c(\sigma)=n$ and $|\sigma_b|=1$, so that each $\boldsymbol{\beta}_b$ is a U(2)-tableaux with $|\boldsymbol{\beta}_b| = |\mathbf{f}|/n$. The sum over $\boldsymbol{\alpha}_p$ collapses to $\boldsymbol{\alpha}=\boldsymbol{\beta}_b$, and the corresponding Clebsch–Gordan coefficient, $C(s,0,S(\boldsymbol{\beta}_b))$, vanishes unless $S(\boldsymbol{\beta}_b)=s$. It follows that the $\boldsymbol{\beta}_b$ must all coincide with the U(2)-tableaux $\boldsymbol{\beta}(\mathbf{f},n,s)$ given by

$$\boldsymbol{\beta}(\mathbf{f},s) = ((|\mathbf{f}|/2n+s),(|\mathbf{f}|/2n-s)). \tag{4.45}$$

We then obtain

$$A_{[I]} = Y^{\mathbf{f}}_{\underbrace{\boldsymbol{\beta}(\mathbf{f},s),\ldots,\boldsymbol{\beta}(\mathbf{f},s)}_{n\ \text{times}}}. \tag{4.46}$$

Some simplification in (4.44) also occurs for n-cycles in S_n, e.g., $\sigma=(12\cdots n)$, In this case $c(\sigma)=1$ and $|\hat{\sigma}|=n$, so that the sum over $\boldsymbol{\beta}$ collapses to $\boldsymbol{\beta}=\mathbf{f}$. We obtain

$$A_{[(12\cdots n)]} = \sum_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_n} Y^{\mathbf{f}}_{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_n} \mathrm{e}^{2\pi\mathrm{i}(\Sigma_{p=1}^{n} p|\boldsymbol{\alpha}_p|)/n} \times C(ns+\tfrac{1}{2}(n-1),\tfrac{1}{2}(n-1),S(\boldsymbol{\alpha}_1),\ldots,S(\boldsymbol{\alpha}_n)). \tag{4.47}$$

The sum $\Sigma_\lambda \nu(\mathbf{f},s\lambda)$ gives the number of n-spin-s representations, regardless of statistics. Using the character relation (see, e.g., Ref. 9),

$$\sum_{\lambda} \chi^{\lambda}(\sigma) = \begin{cases} n!, & \sigma=\mathrm{I}, \\ 0, & \text{otherwise}, \end{cases} \tag{4.48}$$

we obtain from (4.43) and (4.46) a simple expression for these summed multiplicities,

$$\sum_{\lambda} \nu(\mathbf{f},s\lambda) = Y^{\mathbf{f}}_{\underbrace{\boldsymbol{\beta}(\mathbf{f},s),\ldots,\boldsymbol{\beta}(\mathbf{f},s)}_{n \text{ times}}}. \tag{4.49}$$

C. Examples

In Sec. III D, we considered the case of completely symmetric representations, for which $\mathbf{f}=(d)$. There we showed that $\nu((d),s\lambda)$ vanishes unless $d=2ns$ and unless λ is the trivial (respectively, alternating) representation according to whether s is integral (respectively, half-odd-integral). This particular case is readily obtained from the general formulas (4.43) and (4.44). Instead of doing so, we sketch below the analogous calculation for the completely antisymmetric representations of SU(2n). The result turns out to be rather different from the symmetric case, in that only $s=\frac{1}{2}$ constructions are supported; the completely antisymmetric representations do not provide a systematic description for all spins. The $s=\frac{1}{2}$ statistics turn out to be bosonic in this case.

Completely antisymmetric representations of SU(2n) correspond to single-columned tableaux of between 1 and $2n-1$ rows (the $2n$-rowed tableau is equivalent to the trivial representation). Denote the d-rowed representation by $\mathbf{f}=(1)^d$. From (4.39), $\nu((1)^d,s\lambda)$ vanishes unless $d=n$ and, from (4.45) and (4.49), unless $s=\frac{1}{2}$. In this case, the expressions (4.43) and (4.44) simplify considerably. The sums over the $\boldsymbol{\alpha}_p$'s collapse to the single term where all the $|\boldsymbol{\alpha}_p|$'s are equal to one, and the sums over the $\boldsymbol{\beta}_b$'s collapse to the single term where $\boldsymbol{\beta}_b=(1)^{|\hat{\sigma}_b|}$. For these terms, the Littlewood–Richardson coefficients and Clebsch–Gordan coefficients appearing in (4.44) are all equal to one. We get that

$$A_{[\sigma]} = \prod_{b=1}^{c(\sigma)} \mathrm{e}^{2\pi \mathrm{i}(\Sigma_{p=1}^{|\hat{\sigma}_b|} p)/|\hat{\sigma}_b|} = \prod_{b=1}^{c(\sigma)} (-1)^{|\hat{\sigma}_b|+1} = \prod_{b=1}^{c(\sigma)} \operatorname{sgn}(\hat{\sigma}_b) = \operatorname{sgn}(\sigma). \tag{4.50}$$

Substituting the preceding into (4.43), we obtain

$$\nu\left((1)^n,\frac{1}{2}\lambda\right) = \frac{1}{n!} \sum_{[\sigma]\in S_n} \Omega_{[\sigma]} \chi^{\lambda}_{S_n}(\sigma), \tag{4.51}$$

which vanishes unless λ is the trivial representation of S_n.

This result can also be obtained by following the calculation of Sec. III D and regarding $z=(z_1,\ldots,z_{2n})$ as Grassmann variables. Equivalently, this may be regarded as the n-particle version of the ''anti-Schwinger'' construction of Ref. 4, wherein the raising/lower operators of Ref. 3 are made to satisfy anticommutation relations. The anticommutation relations are responsible for the restriction to $s=\frac{1}{2}$.

Next, we consider general representations for the case of two particles, $n=2$. For simplicity, we label the even and odd representations of S_2 by $\lambda=+$ and $\lambda=-$, respectively, with characters $\chi^{\pm}_{S_2}(\sigma)=\pm\operatorname{sgn}(\sigma)$. As in (4.45), let

$$\boldsymbol{\beta}(\mathbf{f},s) = ((|\mathbf{f}|/4+s),(|\mathbf{f}|/4-s)). \tag{4.52}$$

From (4.52) we can deduce that the multiplicities $\nu(\mathbf{f},s\pm)$ vanish unless $|\mathbf{f}|$ is even and $|\mathbf{f}|/4-s$ is a non-negative integer. From (4.43), (4.46) and (4.47), we get

$$\nu(\mathbf{f},s\pm) = \frac{1}{2} Y^{\mathbf{f}}_{\boldsymbol{\beta}(\mathbf{f},s),\boldsymbol{\beta}(\mathbf{f},s)} \pm \frac{(-1)^{2s}}{2} \sum_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2} Y^{\mathbf{f}}_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2} (-1)^{|\boldsymbol{\alpha}_1|} C(2s+\tfrac{1}{2},\tfrac{1}{2},S(\boldsymbol{\alpha}_1),S(\boldsymbol{\alpha}_2)). \tag{4.53}$$

The simplest cases are the tableaux $\mathbf{f}=(2,0)$ and $\mathbf{f}=(1,1)$ with $|\mathbf{f}|=2$. Then $s=\frac{1}{2}$ is the only permitted value of the spin, and $\boldsymbol{\beta}(\mathbf{f},s)$ contains a single box. The tableau (2,0) corresponds to a completely symmetric representation. As discussed in Sec. III D, this yields Fermi statistics for

spin-$\frac{1}{2}$, so that $\nu(\mathbf{f},\frac{1}{2}+)=0$ and $\nu(\mathbf{f},\frac{1}{2}-)=1$. Equation (4.53) is readily evaluated for the tableau (1,1), and one finds the opposite result, namely, Bose statistics for spin-$\frac{1}{2}$ (this case is equivalent to the ''anti-Schwinger construction'' discussed in Ref. 4).

For larger tableaux one typically finds that for each permitted value of spin, both multiplicities $\nu(\mathbf{f},s+)$ and $\nu(\mathbf{f},s-)$ are nonzero. Constructions based on such tableaux do not determine a spin-statistics relation. The smallest tableau where this occurs is $\mathbf{f}=(3,2,1)$ with $s=\frac{1}{2}$. Evaluation of (4.53) shows there is one Fermi and one Bose representation. In fact, for larger tableaux one typically finds that $\nu(\mathbf{f},s+)$ and $\nu(\mathbf{f},s-)$ are nearly equal, and there are arguments to suggest they are either exactly equal, or else differ by 1, according to whether their sum, given by $Y^{\mathbf{f}}_{\boldsymbol{\beta}(\mathbf{f},s),\boldsymbol{\beta}(\mathbf{f},s)}$, is even or odd. It turns out that most of the terms in the sum over tableaux in (4.53) cancel. First, since the summand is symmetric in $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$, apart from the sign factor $(-1)^{|\boldsymbol{\alpha}_1|}$, only terms for which $|\boldsymbol{\alpha}_1|$ and $|\boldsymbol{\alpha}_2|$ have the same parity contribute. Amongst these remaining terms, the sign factor is responsible for additional cancellations, due to the following fact: If $\boldsymbol{\alpha}_1+\boldsymbol{\epsilon}$ is the tableau obtained by adding one box to the first row of $\boldsymbol{\alpha}_1$, and $\boldsymbol{\alpha}_2-\boldsymbol{\epsilon}$ is the tableau obtained by removing one box from the first row of $\boldsymbol{\alpha}_2$, then the rules for multiplying tableaux imply that

$$Y^{\mathbf{f}}_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2}=Y^{\mathbf{f}}_{\boldsymbol{\alpha}_1+\boldsymbol{\epsilon},\boldsymbol{\alpha}_2-\boldsymbol{\epsilon}}. \tag{4.54}$$

Details may be found in Ref. 10.

To demonstrate the possibility of parastatistics, we consider the simplest case of three particles and the smallest SU(6) tableau, $\mathbf{f}=(2,1)$. From (4.45), it follows that $s=\frac{1}{2}$ is the only permitted value of spin, and that $\boldsymbol{\beta}(\mathbf{f},\frac{1}{2})=(1)$ consists of a single box. Let $\lambda=E$ denote the two-dimensional representation of S_3 [corresponding to the tableau (2,1)], with characters

$$\chi^E_{S_3}(\mathrm{I})=2,\quad \chi^E_{S_3}((12))=0,\quad \chi^E_{S_3}((123))=-1, \tag{4.55}$$

and classes

$$\Omega_{[\mathrm{I}]}=1,\quad \Omega_{[(12)]}=3,\quad \Omega_{[(123)]}=2 \tag{4.56}$$

(see, e.g., Ref. 9). From (4.43), (4.46) and (4.47), we get

$$\begin{aligned}\nu((2,1),\tfrac{1}{2}E)=&\ \tfrac{1}{6}Y^{(2,1)}_{(1),(1),(1)}\\ &-\tfrac{1}{6}\times 2\sum_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3} Y^{(2,1)}_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3}\mathrm{e}^{\mathrm{i}(2\pi/3)(|\boldsymbol{\alpha}_1|+2|\boldsymbol{\alpha}_2|)}C(\tfrac{5}{2},1,S(\boldsymbol{\alpha}_1),S(\boldsymbol{\alpha}_2),S(\boldsymbol{\alpha}_3)).\end{aligned} \tag{4.57}$$

There are four sets of U(2)-tableaux $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$ and $\boldsymbol{\alpha}_3$ which may be multiplied to obtain the SU(6) tableau (2,1) (including cases where one or more of the $\boldsymbol{\alpha}_j$ are empty, which we denote by $\boldsymbol{\alpha}_j=0$). For each combination we determine the Littlewood–Richardson coefficient $Y^{(2,1)}_{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3}$, the Clebsch-Gordan coefficient $C(\frac{5}{2},1,S(\boldsymbol{\alpha}_1),S(\boldsymbol{\alpha}_2),S(\boldsymbol{\alpha}_3))$, and the phase factor $\mathrm{e}^{\mathrm{i}(2\pi/3)(|\boldsymbol{\alpha}_1|+2|\boldsymbol{\alpha}_2|)}$. The results are summarized in the table below.

$\boldsymbol{\alpha}_1$	$\boldsymbol{\alpha}_2$	$\boldsymbol{\alpha}_3$	Y	C	$\mathrm{e}^{\mathrm{i}2\pi/3}$
(2,1)	0	0	1	0	1
(1,1)	(1)	0	1	0	$\mathrm{e}^{\mathrm{i}2\pi/3}$
(2)	(1)	0	1	1	$\mathrm{e}^{\mathrm{i}2\pi/3}$
(1)	(1)	(1)	2	1	1

(4.58)

Substituting (4.58) into (4.57), we obtain

$$\nu((2,1), \tfrac{1}{2}E) = 1. \tag{4.59}$$

That is, a 3-spin-$\frac{1}{2}$ bundle with parastatistics may be constructed from the representation $\Gamma^{(2,1)}$ of SU(6).

V. DISCUSSION

We have reformulated the quantum kinematics of BR for indistinguishable spinning particles in terms of vector bundles over n-particle configuration space. Within this geometrical framework, our main results concern a representation-theoretic generalization of the construction in BR. We have shown that n-spin bundles can be constructed from irreducible representations $\Gamma^{\mathbf{f}}$ of the group SU($2n$). The construction makes use of representations $\Delta^{\mathbf{f}}$ of the spin-statistics group $\Sigma(n)$ associated to $\Gamma^{\mathbf{f}}$, as well the existence of a continuous, S_n-equivariant map from $\mathrm{SU}(n)/T(n)$ to configuration space C_n.[2]

The construction in BR is based on particular representations of SU($2n$), namely, the completely symmetric representations. For a given number, n, of indistinguishable particles with spin s, there is a unique completely symmetric representation of SU($2n$), namely, the $2ns$-fold symmetric tensor product of SU($2n$) with itself, which leads to a description of the quantum kinematics (i.e., which supports an n-spin bundle with spin s). The statistics is necessarily in accord with the physically correct spin-statistics relation.

Representations of SU($2n$) other than the completely symmetric representations, corresponding to Young tableaux $\mathbf{f}$ of more than one row, typically support multiple values of spin s, and for a given spin may support distinct values of the statistics λ, including parastatistics. The values of spin and statistics supported by a given representation $\Gamma^{\mathbf{f}}$ are determined by the multiplicities $\nu(\mathbf{f}, s\lambda)$ of the irreducible representations of the spin-statistics group, $\Sigma(n)$, in the decomposition of $\Delta^{\mathbf{f}}$.

Our main calculation is an evaluation of the multiplicities $\nu(\mathbf{f}, s\lambda)$ using character methods. Equations (4.43) and (4.44) give the multiplicities as a finite sum over characters of the symmetric group S_n, the n-fold Clebsch–Gordan coefficients of SU(2), and the Littlewood–Richardson coefficients for the decomposition of representations of $\mathrm{U}(n+m)$ into representations of $\mathrm{U}(n) \times \mathrm{U}(m)$.

Our calculation is related to a more general problem in representation theory, namely, the decomposition of zero-weight representations of the Weyl group W of a compact, connected Lie group G associated with an irreducible representation of G. It would be interesting to see if alternative methods could be brought to bear on our calculation, as well as whether the methods used here might prove useful in other contexts. Our construction of n-spin-bundles is similarly related to the construction of flat zero-weight bundles over the coset space G/T (where T is a maximal torus of G), whose decomposition into a direct sum of subbundles irreducible under monodromy leads to the decomposition problem described above.

Concerning the spin-statistics relation, in the first instance our results are similar to those of Ref. 3. Within the group-theoretical framework considered here, the requisite properties introduced in Sec. II do not determine a connection between spin and statistics. When general representations of SU($2n$) are admitted alongside the completely symmetric representations, the spin-statistics relation is lost.

As argued in the Introduction, a derivation of the spin-statistics relation from a reformulation of quantum mechanics should be based on principles whose physical motivation is clear. The role played by the group SU($2n$) in our considerations is not well motivated in this respect. One could offer as motivation the fact that SU($2n$) incorporates both rotations of n spins [i.e., $\mathrm{SU}(2)^n$] and the permutations S_n, but of course it is not the only group which does so.

However, the role played by the completely symmetric representations deserves further consideration. They provide, at least as far as we have discerned, the only systematic means, within the given framework, of associating a representation to a particular value of spin. It is suggestive, too, that the scheme which works treats the spins in a completely symmetrical way; this would

seem appropriate for indistinguishable particles. Indeed, characteristic aspects of the completely symmetric representations may indicate a different approach to this nonrelativistic treatment of the spin-statistics relation, which we hope to report on in future.

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APPENDIX: GENERAL SETTING

The construction of n-spin bundles described in Sec. III is closely related to the following general problem (see, e.g., Ref. 12). Let Γ be an irreducible unitary representation on a vector space $\mathcal{V}$ of a compact Lie group G with maximal torus T. $\mathcal{V}$ may be decomposed into weight spaces, $\mathcal{V}^\mu$, labeled by weights μ of T. The zero-weight space $\mathcal{V}^0$ carries a representation Δ of the Weyl group, W, of G, which is, in general, reducible. One can then ask for the decomposition of this representation of the Weyl group into its irreducible components.

To each weight space $\mathcal{V}^\mu$ of the representation Γ is associated a Hermitian vector bundle $\mathcal{E}^\mu$ over G/T with Abelian G-invariant Hermitian connection. The curvature of this connection depends linearly on μ, and therefore vanishes on the zero-weight bundle $\mathcal{E}^0$. If G is simply connected, then $\mathcal{E}^0$ is trivial. However, the quotient bundle $\overline{\mathcal{E}^0}=\mathcal{E}^0/W$ over the quotient space $(G/T)/W$, while locally flat, may be nontrivial. For simply connected G, the fundamental group of the quotient space is just the Weyl group W, and the monodromy of the flat connection yields a representation of W, which is precisely the representation Δ described above.

This setting can be further generalized by regarding G as a subgroup of a Lie group F, and regarding Γ as the restriction to G of a representation of F. In this case, the natural structure group for the zero-weight bundle is the generalized Weyl group $V=M/T$, where M is the F-normalizer of T.

The construction of Sec. III is an example belonging to this more general setting, with $F=\mathrm{SU}(2n)$, $G=\mathrm{SU}(n)$, and $T=T(n)$. The Weyl group of $\mathrm{SU}(n)$ is just S_n, and the generalized Weyl group V is the spin-statistics group, $\Sigma(n)=\mathrm{SU}(2)^n\rtimes S_n/\mathrm{Nul}(n)$. The n-spin bundles are pullbacks, via the S_n-equivariant map $\Xi: C_n\to \mathrm{SU}(n)/T(n)$, of zero-weight bundles over $\mathrm{SU}(n)/T(n)$.

This point of view is elaborated below.

1. Generalized Weyl group

Let G be a compact, connected semisimple Lie group with maximal torus T. Let N denote the normalizer of T, and $W=N/T$ the Weyl group of G. Suppose G is a subgroup of a compact, connected Lie group F. Let M denote the F-normalizer of T, i.e., the subgroup of F which leaves T invariant under conjugation. We call

$$V=M/T \tag{A1}$$

the generalized Weyl group of G. Clearly the Weyl group W is a subgroup of V.

Let Z denote the F-centralizer of T, i.e., the subgroup of F whose elements commute with all elements of T. Z is a normal subgroup of M. Therefore, the group ZN, consisting of products zy of $z\in Z$ and $y\in N$, is a subgroup of M, and

$$ZN/T\cong Z/T\rtimes W, \tag{A2}$$

where in the semidirect product $Z/T\rtimes W$, an element $y\,T\in W$ acts on $z\,T\in Z/T$ according to $z\,T\to(yzy^{-1})\,T$. The isomorphism (A2) follows from consideration of the map

$$zy \in ZN \mapsto (z\,T, y\,T) \in Z/T \rtimes W. \tag{A3}$$

To show that this map is well defined, we need to check that $zy = z'y'$ implies that $z\,T = z'\,T$ and $y\,T = y'\,T$. But $zy = z'y'$ implies that $z' = z\tau$ and $y' = \tau^{-1}y$, where $\tau \in Z \cap N$. Since G is compact and connected, $Z \cap N = T$, so $\tau \in T$ as required. It is evident that the map preserves multiplication and that it is surjective. The kernel of the map consists of elements zy where $z, y \in T$, and therefore is just T itself, so that (A2) follows.

The spin-statistics group $\Sigma(n)$ is an example of a generalized Weyl group, with $F = \mathrm{SU}(2n)$, $G = \mathrm{SU}(n)$, and $T = T(n)$. The Weyl group W is isomorphic to S_n, Z/T is isomorphic to $\mathrm{Spn}(n)$, and V, the generalized Weyl group, is isomorphic to the semidirect product $\mathrm{Spn}(n) \rtimes S_n$, which is just $\tilde{\Sigma}(n)$.

2. Zero-weight representations of the generalized Weyl group

Let it be given $T \subset G \subset F$ and $N \subset M$ as above. Let $\mathfrak{f}$ denote the (real) Lie algebra of F, $\mathrm{Exp}: \mathfrak{f} \to F$ the exponential map, and ad the adjoint representation of F on $\mathfrak{f}$. Let $\mathfrak{g} \subset \mathfrak{f}$ denote the Lie algebra of G, and $\mathfrak{t} \subset \mathfrak{g}$ the Lie algebra of T (i.e., the Cartan subalgebra of G), with dual $\mathfrak{t}^*$. Denote the pairing between $\mu \in \mathfrak{t}^*$ and $\tau \in \mathfrak{t}$ by $\mu \cdot \tau$. The adjoint representation restricts to a representation of M on $\mathfrak{t}$, denoted $\mathrm{ad}(M)$. The co-adjoint representation of M on $\mathfrak{t}^*$, denoted $\mathrm{ad}^*(M)$, is defined by

$$(\mathrm{ad}^*(x) \cdot \mu) \cdot \tau = \mu \cdot (\mathrm{ad}(x) \cdot \tau). \tag{A4}$$

Let $\ker_{\mathfrak{t}}(\mathrm{Exp})$ denote the lattice in $\mathfrak{t}$ mapped to the identity in T. A weight μ of T is an element of τ^* which is integer-valued on $\ker_{\mathfrak{t}}(\mathrm{Exp})$. Irreducible representations of T are labeled by weights, and are given explicitly by $\mathrm{Exp}\,\tau \mapsto \exp(2\pi i \mu \cdot \tau)$.

Let Γ denote an irreducible unitary representation of F on a finite-dimensional Hilbert space $\mathcal{V}$. $\mathcal{V}$ may be decomposed into a direct sum of generalized weight spaces $\mathcal{V}^\mu$ on which $\Gamma(T)$ acts with weight μ. (In case $F = G$, this is the usual weight-space decomposition of $\mathcal{V}$.) Let $\mathcal{V}^0$ denote the zero-weight space, i.e., the subspace of vectors invariant under T, for which $\mu = 0$.

For $x \in M$ and $\mathrm{Exp}\,\tau \in T$, we have that

$$\begin{aligned}\Gamma(\mathrm{Exp}\,\tau) \cdot (\Gamma(x) \cdot \mathcal{V}^\mu) &= \Gamma(x) \cdot (\Gamma(\mathrm{Exp}\,(\mathrm{ad}\,(x^{-1}) \cdot \tau)) \cdot \mathcal{V}^\mu) \\ &= \exp(2\pi i \mu \cdot (\mathrm{ad}\,(x^{-1} \cdot \tau)))\Gamma(x) \cdot \mathcal{V}^\mu \\ &= \exp(2\pi i (\mathrm{ad}^*(x^{-1}) \cdot \mu) \cdot t)(\Gamma(x) \cdot \mathcal{V}^\mu),\end{aligned} \tag{A5}$$

so that

$$\Gamma(x) \cdot \mathcal{V}^\mu = \mathcal{V}^{\mathrm{ad}^*(x^{-1}) \cdot \mu}. \tag{A6}$$

It follows that the zero-weight space, $\mathcal{V}^0$, is invariant under M, so that Γ restricts to a representation of M on $\mathcal{V}^0$. Since T is contained in the kernel, $\Gamma(M)$ reduces to a representation of the generalized Weyl group $V = M/T$ on $\mathcal{V}^0$. Denote this representation by Δ^Γ. In general, Δ^Γ is reducible. Let Δ denote an irreducible representation of $\mathcal{V}$, and let $\nu(\Gamma, \Delta)$ denote the multiplicity of Δ in the decomposition of Δ^Γ into its irreducible components. The multiplicities $\nu(\Gamma, \Delta)$ are naturally associated with a pair of irreducible representations Γ and Δ of a compact connected Lie group F and the generalized Weyl group V. A natural question is how to compute them. In case $F = G = \mathrm{SU}(n)$, this question has been discussed by Kostant.[12]

3. Weight bundles over G/T

Associated to the weight space $\mathcal{V}^\mu$ is a vector bundle $\mathcal{E}^\mu$ over G/T. $\mathcal{E}^\mu$ is a subbundle of the trivial bundle $G/T \times \mathcal{V}$, with fibers $\mathcal{E}_{g\,T}$ given by $\Gamma(g) \cdot \mathcal{V}^\mu$. By virtue of its embedding in the

trivial bundle, there is an induced G-invariant connection on $\mathcal{E}^\mu$, according to which a vector $|\psi(t)\rangle \in \mathcal{E}_{g(t)\,T}$ is parallel transported along a curve $g(t)\,T \in G/T$ if and only if $|\dot{\psi}(t)\rangle$ is orthogonal (with respect to the inner product on $\mathcal{V}$) to the fiber $\mathcal{E}_{g(t)\,T}$.

It is straightforward to derive an explicit formula for parallel transport along a one-parameter subgroup,

$$g(t) = \mathrm{Exp}\,(t\xi), \tag{A7}$$

where $\xi \in \mathfrak{g}$. We note that Γ gives a representation on $\mathcal{V}$ of $\mathfrak{f}$, and, by restriction, of $\mathfrak{g}$, by anti-Hermitian linear transformations. We denote these Lie-algebra representations by Γ as well. Let $\mathfrak{t}^\perp \subset \mathfrak{g}$ denote the orthogonal complement of $\mathfrak{t}$ in $\mathfrak{g}$ with respect to the Killing form (as G is compact and semisimple, the Killing form is negative definite). It is a standard result (see, e.g., Ref. 7) that $\Gamma(\mathfrak{t}^\perp)$ maps $\mathcal{V}^\mu$ into a direct sum of orthogonal subspaces $\mathcal{V}^{\mu'}$ (the difference $\mu' - \mu$ is, in fact, a root of $\mathfrak{g}$). Given $\xi \in \mathfrak{g}$, let $\xi^{\mathfrak{t}} + \xi^{\mathfrak{t}^\perp}$ denote its (unique) decomposition into components in $\mathfrak{t}$ and $\mathfrak{t}^\perp$, respectively. Then, for $|\psi\rangle \in \mathcal{V}^\mu$, we have that

$$\Gamma(\xi)|\psi\rangle = 2\pi \mathrm{i}(\mu \cdot \xi^{\mathfrak{t}})|\psi\rangle + \{\text{ vectors orthogonal to } \mathcal{V}^\mu\}. \tag{A8}$$

It follows from (A8) that the parallel transport of $|\psi\rangle$ along $g(t)$ is given by

$$|\psi(t)\rangle = \exp(-2\pi \mathrm{i}\mu \cdot \xi^{\mathfrak{t}})\Gamma(g(t))|\psi\rangle. \tag{A9}$$

It follows that the induced connection (A9) is Abelian; under parallel transport around a closed curve in G/T, a vector in $\mathcal{E}^\mu$ returns to itself up to a phase factor.

Let

$$X_\xi(g\,T) = \frac{d}{dt}\mathrm{Exp}\,(t\xi)g\,T|_0,$$

$$X_\eta(g\,T) = \frac{d}{dt}\mathrm{Exp}\,(t\eta)g\,T|_0$$

denote tangent vector fields at $g\,T$ generated by the left action of G. From (A9) one can deduce that the scalar-valued curvature two-form Ω^μ on X_ξ, X_η is given by

$$\Omega^\mu(X_\xi, X_\eta)(g\,T) = \mathrm{i}\mu \cdot ([\xi, \eta]^{\mathfrak{t}} - [\xi^{\mathfrak{t}}, \eta^{\mathfrak{t}}]). \tag{A10}$$

Since the left-invariant vector fields span the tangent bundle of G/T, (A10) determines Ω^μ. The curvature form, like the connection, is invariant under the action of G.

4. Zero-weight bundle and representations of the generalized Weyl group

Suppose the representation Γ of F has a nontrivial zero-weight space $\mathcal{V}^0$. From (A10), the curvature of the associated zero-weight bundle $\mathcal{E}^0$ vanishes, so that induced connection on $\mathcal{E}^0$ is flat. In this case, parallel transport with respect to a flat connection depends only on the homotopy class of the path in G/T. If G/T is simply connected, parallel transport is path independent, and $\mathcal{E}^0$ is globally flat, and therefore trivial. This is the case if G itself is simply connected, as we will assume from now on. As G is compact and connected, $g(t) \in G$ can be expressed $\mathrm{Exp}\,(t\xi(t))$ for some $\xi(t) \in \mathfrak{g}$. It follows from (A9) that parallel transport in $\mathcal{E}$ along $g(t)\,T$ is given by

$$|\phi(t)\rangle = \Gamma(g(t))|\phi\rangle. \tag{A11}$$

The zero-weight bundle $\mathcal{E}^0$, in contrast to weight bundles with nonzero weights, descends from a bundle over G/T to a bundle over G/N. We denote this reduced bundle by $\overline{\mathcal{E}^0}$. $\overline{\mathcal{E}^0}$ is a

subbundle of the trivial bundle $G/N\times\mathcal{V}$, with fibers given by $\overline{\mathcal{E}}_{g\,N}=\Gamma(g)\mathcal{V}^0$. (Note that since N leaves $\mathcal{V}^0$ invariant, this expression does not depend on the choice of representative g for $g\,N$.) The flat connection on $\mathcal{E}$ passes to $\overline{\mathcal{E}}$.

In general, the G/N is not simply connected; its fundamental group is isomorphic to the Weyl group $W=N/T$, as follows from the fact that $G/N=(G/T)/(N/T)=(G/T)/W$, and G/T is simply connected by assumption. An isomorphism between W and $\pi_1(G/N,N)$, the fundamental group based at the identity coset $\mathrm{I}\,N$, is given explicitly as follows. Let $g(t)\,N$ denote a closed path in G/N beginning and ending at N. For definiteness, take $0\leqslant t\leqslant 1$ and $g(0)=\mathrm{I}$. Then $g(1)\,N=\mathrm{I}\,N$ implies that $g(1)\in N$. The map

$$g(t)\,N\mapsto g(1)\,T \tag{A12}$$

depends only on the homotopy class of $g(t)\,N$. It is easily verified that (A12) preserves group multiplication, and is $1-1$ (since T is connected and G is simply connected) and onto (since G is connected).

Because G/N is not simply connected, parallel transport with respect to the flat connection need not be trivial, and can depend on the homotopy class of the path. For closed paths, parallel transport generates a unitary representation of the fundamental group, the monodromy of the connection. In view of the preceding, the monodromy at the identity coset N is naturally regarded as a representation of the Weyl group W. We denote this representation by Δ^Γ, and compute it as follows. Given $y\in N$, let $g(t)\in G$ be a smooth path in G with $g(0)=\mathrm{I}$ and $g(1)=y$. From (A11), parallel transport in $\overline{\mathcal{E}}$ along $g(t)\,N$ is given by

$$|\psi(t)\rangle=\Gamma(g(t))|\psi\rangle. \tag{A13}$$

Δ^Γ is obtained from parallel transport at $t=1$, so that

$$\Delta^\Gamma(y)=\Gamma(y). \tag{A14}$$

This is just the restriction to N of the representation Δ^Γ of the generalized Weyl group V on $\overline{\mathcal{E}}_N$.

At an arbitrary fiber $\overline{\mathcal{E}}_{g\,N}$ of the quotient bundle we can define a unitary representation of the generalized Weyl group V, which we denote by $L_{g\,N}(y)$. For example, we can take $L_{g\,N}(y)=\Gamma(g)\Gamma(y)\Gamma^\dagger(g)$. A different choice of representative g for $g\,N$ would yield a different but equivalent representation. Therefore, there is a well-defined decomposition of $\overline{\mathcal{E}}$ into a direct sum of subbundles $\overline{\mathcal{E}}^\alpha$ whose fibers transform according to irreducible representations Δ of V. This decomposition is determined by the multiplicities $\nu(\Gamma,\Delta)$ discussed in Appendix Sec. 1.

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Bound states in coupled guides. I. Two dimensions

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Bound states that can occur in coupled quantum wires are investigated. We consider a two-dimensional configuration in which two parallel waveguides (of different widths) are coupled laterally through a finite length window and construct modes which exist local to the window connecting the two guides. We study both modes above and below the first cutoff for energy propagation down the coupled guide. The main tool used in the analysis is the so-called residue calculus technique, in which complex variable theory is used to solve a system of equations which is derived from a mode-matching approach. For bound states below the first cutoff a single existence condition is derived, but for modes above this cutoff (but below the second cutoff), two conditions must be satisfied simultaneously. A number of results have been presented which show how the bound-state energies vary with the other parameters in the problem.
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I. INTRODUCTION

Over the past decade or so there have been a number of theoretical investigations into the phenomena of bound states in quantum waveguides, and acoustic resonances (or trapped modes) in acoustic waveguides. Though the two physical phenomena occur on vastly different scales, they are intimately related. It is our intention in this and the following article to show how some of the techniques that have been developed for the calculation of resonant frequencies in the acoustic context can be used to provide accurate and efficient tools for the evaluation of bound-state energies in a particular class of quantum configurations.

Theoretical investigations into quantum wires and quantum waveguides became important when it became possible to manufacture crystalline structures of high purity within a semiconductor material which are of the order of tens of nanometers in size and on whose boundaries the wave functions are usually suppressed. As described in Duclos and Exner (1995), these properties make it reasonable to model the motion of an electron within such a microstructure as a free (spinless) particle in an infinite guide with a vanishing potential on the guide boundary. The underlying equation is of course the Schrödinger equation, but for stationary problems this reduces to the Helmholtz equation, and thus the situation has direct analogs in the theories of acoustic and electromagnetic waves. Of interest here is the possible existence of nontrivial solutions which have finite energy. In quantum waveguides such solutions are known as bound states and their existence was explicitly demonstrated for the first time in Exner and Šeba (1989) for the case of a curved, thin planar strip and a review of early theoretical work on bound states in curved quantum waveguides (in both two and three dimensions) can be found in Duclos and Exner (1995). Some early experimental work, in which computed bound-state energies were verified, is reported in Carini *et al.* (1992). The existence of bound states can have a significant influence on electron transport in mesoscopic systems.

In the acoustics literature, the same bounded solutions are typically referred to as acoustic resonances, and the study of this phenomenon dates back to the experimental and theoretical work of Parker (1966, 1967). In Parker's setup the guide was a rigid duct, so the appropriate boundary

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conditions on the guide walls were of Neumann rather than Dirichlet type. Also, rather than being curved, the duct was perturbed by the inclusion of one or more splitter plates of finite length. Parker showed that such a geometry could support a nontrivial solution which was localized near to the plate(s) and which could be excited by vortex shedding from the plate edges when a mean flow of a certain speed was created in the duct. These resonances are extremely important in a number of engineering applications such as flow-induced vibration in cooler tubes and the design of turbomachinery; see Parker and Stoneman (1989), and the references cited therein.

Parker's modes were rediscovered in the early 1990s in a completely different physical situation: linear water waves in a wall-sided channel containing an obstacle. Here, there are circumstances in which the depth dependence can be removed from the problem, leaving the Helmholtz equation to be solved in a two-dimensional parallel-plate waveguide in which is situated a bounded obstacle. If this is a strip, then the problem is identical to the one considered by Parker. After some initial work showing that shapes other than plates could support bounded solutions (in this context usually called trapped modes) Evans, Levitin, and Vassiliev (1994) proved that this was the case for a very wide class of geometries.

The early work on these trapped modes focused on geometries which were symmetric about the guide centerline. This allows for a decomposition of the problem into independent symmetric and antisymmetric parts, the latter exhibiting a cutoff frequency below which it is impossible for energy to escape down the guide. In more formal language, the operator in the antisymmetric problem has a continuous spectrum which is bounded away from zero, and the region below the continuous spectrum can be searched for discrete eigenvalues, corresponding to trapped modes. Perhaps the first function theoretical treatment of a problem of this type is that of Jones (1953), in which the author used comparison principles to prove the existence of discrete eigenvalues below the continuous spectrum for a class of semi-infinite guides.

The use of operator decomposition to create a gap below the continuous spectrum has proved extremely useful in the search for trapped modes/acoustic resonances and has been extended to cover a number of different situations; see, for example, Linton and McIver (1998); Groves (1998); Davies and Parnovski (1998). It is, however, merely a device which makes resonances relatively easy to find in certain situations, but it tells us nothing about the existence or otherwise of discrete eigenvalues embedded within the continuous spectra of the relevant operators. Little has been achieved for this more difficult problem, though some early progress is reported in Evans and Porter (1998); McIver *et al.* (2001), and McIver, Linton, and Zhang (2002), and this will be discussed in Sec. IV below.

The specific focus of our attention in this and the subsequent article is the study of coupled quantum waveguides and techniques that can be used to establish the existence of and compute the energies for bound states both in the discrete spectrum and embedded within the continuous spectrum. In two dimensions the guides we will consider consist of two straight parallel waveguides connected through a window in the common boundary. Experimental observations of a waveguide with a similar configuration can be found in Hirayama *et al.* (1992) and Hirayama *et al.* (1993). A numerical model, based on classical rebound effects in a straight wire for the experimental specification described in Hirayama *et al.* (1992), was provided in Takagaki and Ploog (1994).

One of the first theoretical treatments of resonances in coupled guides was that of Kunze (1993), who calculated the transmissivity of a wire coupled either to infinite space or to another wire via a small hole. Kunze showed that there are energies at which near resonances or quasi-bound states in the wire become possible, and that these states cause a sharp downward dip in the conductance of the wire. However, it is the treatment given by Exner *et al.* (1996) which forms the starting point for our work. Exner *et al.* studied the bound states and scattering problems in parallel quantum waveguides of unequal width coupled laterally through a boundary window. The same type of variational argument as that employed by Evans, Levitin, and Vassiliev (1994) was used to show that the system always has at least one bound state for any window width. Moreover, the boundary-value problem was solved using a mode-matching technique, which allows one to construct the corresponding wave functions and determine how the bound-state energies depend

on the parameters of the problem. Work by Bulla *et al.* (1997) showed that if the window was small enough so that only one simple eigenvalue below the continuous spectrum was present, this eigenvalue could be bounded from below, and this result was extended by Exner and Vugalter (1996), who showed that for a sufficiently small window a two-sided asymptotic estimate for the gap between the continuous spectrum and this eigenvalue could be obtained. The case of a coupled waveguide containing a finite number of windows in the common boundary was considered in Exner and Vugalter (1997), who showed that if the windows are small enough there is just one isolated eigenvalue. Upper and lower bounds of the gap between this eigenvalue and the continuous spectrum were found using a variational approach. Other extensions to this type of analysis, including the incorporation of a magnetic field, or three laterally coupled guides, have been treated in Popov (2002) and Popov and Frolov (2003).

We treat the same geometry as that considered in Exner *et al.* (1996) with a coupled guide of total width d formed by two parallel guides of width b and $d-b$ linked via a window of length $2a$ in their common boundary. After setting up the problem in Sec. II we investigate the existence of bound states below the first cutoff for the coupled guide in Sec. III. Our starting point is a mode-matching analysis, but rather than solve the resulting system of equations numerically as in Exner *et al.* (1996), we use the so-called residue calculus technique described in Mittra and Lee (1971) to derive an approximate solution which is extremely accurate unless a/d is very small. This approximation also provides a very useful insight into how to solve the full problem in a numerically efficient way, and we show how an exponentially convergent linear system can be derived. Numerical results are presented and comparisons between the approximate and full solutions made. We find that bound states occur for any values of the parameters a/d and b/d. We also use a variational argument to prove the existence of bound states for a sufficiently wide window and to provide estimates to the bound-state energies. It is shown that the upper bound of these estimates provides a very good approximation to the actual computed energies.

The residue calculus technique is readily adapted to the more difficult problem of searching for resonances above the first cutoff in the coupled guide, and bound states above the first cutoff and below the second cutoff are investigated in Sec. IV. The bound-state energies are shown to correspond to the intersection of two curves in parameter space, and we find that the number of parameters which can be fixed is reduced by 1. Thus, if we fix the b/d, then bound states occur only for specific window widths. The possible existence of resonances between the second and third cutoffs is also discussed. Here, we require the intersection of three lines and no solutions appear to exist.

When the two guides which are coupled have identical widths ($b/d=1/2$) the resulting problem has an extra symmetry, and this leads to some different results. Below the first cutoff there is essentially no difference and the results are just those obtained from the previous analysis in the limit as $b/d\to 1/2$, though the extra symmetry means that the equal-width problem could be solved rather more easily. However, above the cutoff we find that bound states are found in a different energy band, with those that were found for the unequal-width case disappearing as $b/d\to 1/2$. Some results for these new modes are presented.

II. FORMULATION

We consider a pair of two-dimensional waveguides of widths b and c, coupled laterally through a window of width $2a$ in their common boundary. The total width is $d=b+c$, and we assume without loss of generality that $b>d/2$. The case when $b=d/2$ can be treated more simply due to the extra symmetry in that case, and this in fact leads to a qualitative change in some of the results which will be explored in Sec. IV. Cartesian axes are chosen so that the x axis coincides with the lower boundary of the waveguide, and the y axis is chosen so that the waveguide is symmetric about the line $x=0$, as shown in Fig. 1. Our geometry is thus defined by two nondimensional parameters: the width of the window in the common boundary compared to the width of the whole guide, and the height of the window compared to the width of the full coupled guide ($2a/d$ and b/d, respectively).

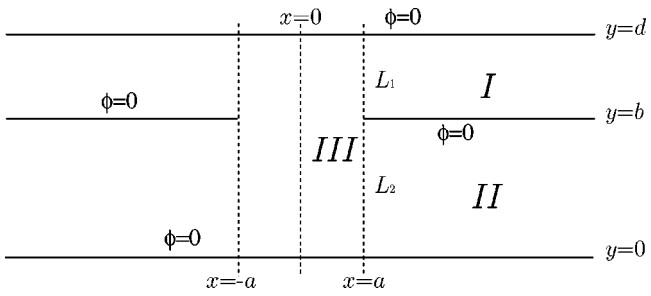

FIG. 1. Definition sketch.

Initially we shall seek a solution which is even (symmetric) about $x=0$, by considering the region $x>0$ and seeking a function $\phi(x,y)$ which satisfies

$$\frac{\partial \phi}{\partial x}=0 \quad \text{on} \quad x=0, \quad 0<y<d. \tag{2.1}$$

The function $\phi(x,y)$ must also satisfy the Helmholtz equation within the waveguide

$$(\nabla^2+k^2)\phi=0, \quad 0<y<d \quad \text{except on} \quad y=b, \quad x>a. \tag{2.2}$$

In the acoustic context $k=\omega/c$, where ω is the frequency of oscillation and c is the speed of sound, whereas in the related quantum-mechanical problem $k^2=2mE/\hbar^2$, in which m is the mass of the electron, and E is its total energy. In what follows, the parameter k will be referred to as the energy. The function ϕ satisfies Dirichlet boundary conditions on the waveguide walls

$$\phi=0 \quad \text{on} \quad y=0, \quad x>0, \tag{2.3}$$

$$\phi=0 \quad \text{on} \quad y=b, \quad x>a, \tag{2.4}$$

$$\phi=0 \quad \text{on} \quad y=d, \quad x>0, \tag{2.5}$$

and a radiation condition specifying that no waves propagate out to infinity

$$\phi\to 0 \quad \text{as} \quad x\to\infty, \tag{2.6}$$

which can be shown (using Green's theorem) to be equivalent in this problem to the statement that ϕ must possess finite energy

$$\int_\Omega |\nabla\phi|^2 \mathrm{d}\Omega<\infty, \tag{2.7}$$

where Ω is the interior of the coupled guide. We finally assume ϕ is nonsingular, and that

$$\nabla\phi=O(r^{-1/2}) \quad \text{as} \quad r\equiv\{(x-a)^2+(y-b)^2\}^{1/2}\to 0, \tag{2.8}$$

anticipating a singularity in the derivative of ϕ at the edge of the window.

It is useful to split the domain into three regions as shown in Fig. 1. Region *I* is $b<y<d$, $x>a$, region *II* is $0<y<b$, $x>a$, and region *III* is $0<y<d$, $0<x<a$. We can represent the function ϕ by a function ϕ_i $(i=1,2,3)$ in each region, with the following continuity conditions applied at the boundaries between the regions:

$$\phi_i=\phi_3, \quad \frac{\partial \phi_i}{\partial x}=\frac{\partial \phi_3}{\partial x}, \quad \text{on} \quad L_i, \quad i=1,2, \tag{2.9}$$

where L_1 is $x=a$, $b<y<d$, L_2 is $x=a$, $0<y<b$, and we will write L_3 for $L_1 \cup L_2$. We then introduce the complete orthogonal sets

$$\Psi_n^{(1)}(y)=2^{1/2}\sin \nu_n(d-y), \quad \nu_n=n\pi/c, \quad n\in\mathbb{N}, \tag{2.10}$$

$$\Psi_n^{(2)}(y)=2^{1/2}\sin \mu_n(b-y), \quad \mu_n=n\pi/b, \quad n\in\mathbb{N}, \tag{2.11}$$

$$\Psi_n^{(3)}(y)=2^{1/2}\sin \lambda_n(d-y), \quad \lambda_n=(n+1)\pi/d, \quad n\in\mathbb{N}_0, \tag{2.12}$$

which satisfy

$$\frac{1}{|L_i|}\int_{L_i}\Psi_n^{(i)}(y)\Psi_m^{(i)}(y)\mathrm{d}y=\delta_{mn}, \quad i=1,2,3, \tag{2.13}$$

where δ_{mn} is the Kronecker delta. Here and throughout, we use the symbol $\mathbb{N}$ for the set {1, 2, 3,...} and the symbol $\mathbb{N}_0$ for the set {0, 1, 2,...}.

Separation of variables shows that the eigenfunction expansions for the three regions can be written

$$\phi_1(x,y)=\sum_{n=1}^{\infty} U_n^{(1)}\frac{\mathrm{e}^{-\alpha_n(x-a)}}{-\alpha_n}\Psi_n^{(1)}(y), \quad \alpha_n=(\nu_n^2-k^2)^{1/2}, \tag{2.14}$$

$$\phi_2(x,y)=\sum_{n=1}^{\infty} U_n^{(2)}\frac{\mathrm{e}^{-\beta_n(x-a)}}{-\beta_n}\Psi_n^{(2)}(y), \quad \beta_n=(\mu_n^2-k^2)^{1/2}, \tag{2.15}$$

$$\phi_3(x,y)=\sum_{n=0}^{\infty} U_n^{(3)}\frac{\cosh \gamma_n x}{\gamma_n \sinh \gamma_n a}\Psi_n^{(3)}(y), \quad \gamma_n=(\lambda_n^2-k^2)^{1/2}, \tag{2.16}$$

where $U_n^{(i)}$, $i=1,2,3$, are unknown complex constants and various factors have been introduced for convenience. If we restrict the energy by

$$kb<\pi, \tag{2.17}$$

then, since $b>d/2$, the values of α_n and β_n, $n\in\mathbb{N}$ will all be real and positive. As these terms appear in the eigenfunction expansions as coefficients of negative exponentials, the restriction on energy produces exponential decay down the guide in both regions *I* and *II*. We define $kb=\pi$ as the first cutoff of the coupled waveguide and consider the case of bound states whose energies are below this cutoff.

III. BOUND STATES BELOW THE FIRST CUTOFF

If $kb<\pi$ then α_n, β_n, and γ_n, $n\in\mathbb{N}$, are all real and positive. However, provided $kd>\pi$, γ_0 will be purely imaginary and the corresponding mode will be oscillatory in region *III*. We thus anticipate that a necessary condition for the existence of bound states will be

$$\pi<kd<\frac{d\pi}{b}. \tag{3.1}$$

If we apply the continuity conditions (2.9), we obtain

$$\sum_{n=0}^{\infty} U_n^{(3)} \frac{\coth \gamma_n a}{\gamma_n} \Psi_n^{(3)}(y) = \begin{cases} \displaystyle\sum_{n=1}^{\infty} U_n^{(1)} \frac{\Psi_n^{(1)}(y)}{-\alpha_n}, & y \in L_1, \\ \displaystyle\sum_{n=1}^{\infty} U_n^{(2)} \frac{\Psi_n^{(2)}(y)}{-\beta_n}, & y \in L_2, \end{cases} \tag{3.2}$$

and

$$\sum_{n=0}^{\infty} U_n^{(3)} \Psi_n^{(3)}(y) = \begin{cases} \displaystyle\sum_{n=1}^{\infty} U_n^{(1)} \Psi_n^{(1)}(y), & y \in L_1, \\ \displaystyle\sum_{n=1}^{\infty} U_n^{(2)} \Psi_n^{(2)}(y), & y \in L_2. \end{cases} \tag{3.3}$$

We can convert (3.2) and (3.3) into an infinite system of linear algebraic equations by multiplying each by $\Psi_m^{(3)}$, $m \in \mathbb{N}_0$, and integrating over L_3. This leads to

$$U_m^{(3)} = \sum_{n=1}^{\infty} U_n^{(1)} d_{nm} + \sum_{n=1}^{\infty} U_n^{(2)} e_{nm}, \quad m \in \mathbb{N}_0, \tag{3.4}$$

$$U_m^{(3)} \frac{\coth \gamma_m a}{\gamma_m} = \sum_{n=1}^{\infty} \frac{U_n^{(1)}}{-\alpha_n} d_{nm} + \sum_{n=1}^{\infty} \frac{U_n^{(2)}}{-\beta_n} e_{nm}, \quad m \in \mathbb{N}_0, \tag{3.5}$$

where we have defined

$$d_{nm} = \frac{1}{d} \int_{L_1} \Psi_n^{(1)}(y) \Psi_m^{(3)}(y) \mathrm{d}y = \frac{2\nu_n (-1)^n \sin \lambda_m c}{d(\gamma_m^2 - \alpha_n^2)}, \quad m \in \mathbb{N}_0, \ n \in \mathbb{N}, \tag{3.6}$$

$$e_{nm} = \frac{1}{d} \int_{L_2} \Psi_n^{(2)}(y) \Psi_m^{(3)}(y) \mathrm{d}y = \frac{2\mu_n \sin \lambda_m c}{d(\gamma_m^2 - \beta_n^2)}, \quad m \in \mathbb{N}_0, \ n \in \mathbb{N}. \tag{3.7}$$

It is necessary that $\gamma_m \neq \alpha_n$ and $\gamma_m \neq \beta_n$ for any n and m and we can ensure this by assuming that b/d is irrational, although Evans, Linton, and Ursell (1993), Appendix D, show how continuity arguments can be used to remove this restriction so that the conditions for bound states that are obtained are valid for all values of b/d.

Eliminating $U_m^{(3)}$ from (3.4) and (3.5), and substituting for d_{nm} and e_{nm} from (3.6) and (3.7), we can derive

$$\sum_{n=1}^{\infty} U_n \left(\frac{1}{\alpha_n - \gamma_m} + \frac{\zeta_m}{\alpha_n + \gamma_m} \right) - \sum_{n=1}^{\infty} V_n \left(\frac{1}{\beta_n - \gamma_m} + \frac{\zeta_m}{\beta_n + \gamma_m} \right) = 0, \quad m \in \mathbb{N}_0, \tag{3.8}$$

where we have defined

$$U_n = \frac{U_n^{(1)} (-1)^n \nu_n}{\alpha_n}, \quad V_n = \frac{U_n^{(2)} \mu_n}{\beta_n}, \quad \zeta_m = \mathrm{e}^{-2\gamma_m a}. \tag{3.9}$$

So far we have only used the boundary conditions (2.1)–(2.6) and not the condition (2.8), which anticipates the singular behavior near the edge. Since $\Sigma_{n=1}^{\infty} n^{\tau} e^{-nx} = O(x^{-1-\tau})$ as $x \to 0+$ (see, e.g., Martin, 1995), consideration of the gradient of ϕ near the edge shows that

$$U_n, V_n = O(n^{-1/2}) \ \text{ as } \ n \to \infty. \tag{3.10}$$

A. Approximate solution

We now derive an approximate solution to (3.8) for large a, taking into account the asymptotic behavior required from (3.10). Note that since γ_m, $m\in\mathbb{N}$, is real, the terms ζ_m, $m\in\mathbb{N}$, appearing in (3.8) decay rapidly to zero as $a/d\to\infty$. A good approximation for large a is therefore to set $\zeta_m=0$ for $m\in\mathbb{N}$. The idea for this type of approximation (which is equivalent to assuming that the two edges at $x=\pm a$, $y=b$ can be treated independently) goes back to Hurd (1954), who was studying the propagation of electromagnetic surface waves along a comb grating. We would then have

$$\sum_{n=1}^{\infty}\left(\frac{U_n}{\alpha_n-\gamma_m}-\frac{V_n}{\beta_n-\gamma_m}\right)=-\delta_{m0}\zeta_0\sum_{n=1}^{\infty}\left(\frac{U_n}{\alpha_n+\gamma_0}-\frac{V_n}{\beta_n+\gamma_0}\right),\quad m\in\mathbb{N}_0, \tag{3.11}$$

a system of equations that can be solved explicitly using a method originally described in Whitehead (1951) and Berz (1951).

Consider the quantities

$$I_m=\lim_{N\to\infty}\frac{1}{2\pi\mathrm{i}}\int_{C_N}\frac{f(z)}{z-\gamma_m}\mathrm{d}z,\quad J_m=\lim_{N\to\infty}\frac{1}{2\pi\mathrm{i}}\int_{C_N}\frac{f(z)}{z+\gamma_m}\mathrm{d}z,\quad m\in\mathbb{N}_0, \tag{3.12}$$

where C_N is a sequence of contours (to be determined) on which $z\to\infty$ as $N\to\infty$ and $f(z)$ is a meromorphic function which is assumed to have the following properties:

(P1) $f(z)$ has simple poles at $z=\alpha_n$ and $z=\beta_n$, $n\in\mathbb{N}$;
(P2) $f(z)$ has simple zeros at $z=\gamma_n$, $n\in\mathbb{N}$, but not at $z=\gamma_0$; and
(P3) $f(z)=o(1)$ as $|z|\to\infty$ on C_N as $N\to\infty$.

Condition P3 ensures that $I_m=0$ and $J_m=0$. Applying Cauchy's residue theorem to the integrals in (3.12), we find

$$\sum_{n=1}^{\infty}\frac{R(f:\alpha_n)}{\alpha_n-\gamma_m}+\sum_{n=1}^{\infty}\frac{R(f:\beta_n)}{\beta_n-\gamma_m}+\delta_{m0}f(\gamma_0)=0, \tag{3.13}$$

$$\sum_{n=1}^{\infty}\frac{R(f:\alpha_n)}{\alpha_n+\gamma_m}+\sum_{n=1}^{\infty}\frac{R(f:\beta_n)}{\beta_n+\gamma_m}+f(-\gamma_m)=0, \tag{3.14}$$

where $R(f:z_0)$ represents the residue of $f(z)$ at $z=z_0$, and $m\in\mathbb{N}_0$, in each case. If we normalize $f(z)$ by setting

$$f(\gamma_0)=1, \tag{3.15}$$

then a comparison of (3.13) and (3.14) with (3.11) shows that the required solution of (3.11) is given by

$$U_n=R(f:\alpha_n),\quad V_n=-R(f:\beta_n),\quad n\in\mathbb{N}, \tag{3.16}$$

provided (3.10) is satisfied and

$$f(-\gamma_0)\zeta_0=-1. \tag{3.17}$$

If we can determine a suitable $f(z)$ and sequence of contours C_N, then (3.17) is the condition for the existence of bound states.

The method by which $f(z)$ can be constructed follows closely that given in Evans, Linton, and Ursell (1993), and we will simply note here that the a sequence of contours C_N can be constructed so that the function

$$f(z)=h_1 g(z), \tag{3.18}$$

where

$$h_1=\exp\left\{\frac{\gamma_0}{\pi}(b\ln(d/b)+c\ln(d/c))\right\}\prod_{n=1}^{\infty}\frac{(1-\gamma_0/\alpha_n)(1-\gamma_0/\beta_n)}{(1-\gamma_0/\gamma_n)}, \tag{3.19}$$

$$g(z)=\exp\left\{\frac{-z}{\pi}(b\ln(d/b)+c\ln(d/c))\right\}\prod_{n=1}^{\infty}\frac{(1-z/\gamma_n)}{(1-z/\alpha_n)(1-z/\beta_n)}, \tag{3.20}$$

has all the necessary properties. In fact, $f(z)=O(z^{-1/2})$ as $|z|\to\infty$ on C_N as $N\to\infty$. Note that the fact that $\gamma_n\sim(n+1)\pi/d$ rather than $n\pi/d$ (while $\alpha_n\sim n\pi/c$ and $\beta_n\sim n\pi/b$) is crucial.

The condition for the existence of bound states (3.17) is

$$f(\mathrm{i}\gamma')=-\mathrm{e}^{-2\mathrm{i}\gamma' a}, \tag{3.21}$$

where

$$\gamma'=\mathrm{i}\gamma_0=(k^2-(\pi/d)^2)^{1/2}, \tag{3.22}$$

and this reduces to

$$\gamma'(a-\Theta)=\chi+(n-\tfrac{1}{2})\pi, \quad n \text{ an integer}, \tag{3.23}$$

where

$$\Theta=\frac{1}{\pi}(b\ln(d/b)+c\ln(d/c)), \tag{3.24}$$

$$\chi=\sum_{n=1}^{\infty}\left(\tan^{-1}\left(\frac{\gamma'}{\gamma_n}\right)-\tan^{-1}\left(\frac{\gamma'}{\alpha_n}\right)-\tan^{-1}\left(\frac{\gamma'}{\beta_n}\right)\right). \tag{3.25}$$

For the case of antisymmetry about $x=0$, condition (2.1) is replaced by

$$\phi=0 \text{ on } x=0,\ 0<y<d, \tag{3.26}$$

and the system of equations (3.8) becomes

$$\sum_{n=1}^{\infty}U_n\left(\frac{1}{\alpha_n-\gamma_m}-\frac{\zeta_m}{\alpha_n+\gamma_m}\right)-\sum_{n=1}^{\infty}V_n\left(\frac{1}{\beta_n-\gamma_m}-\frac{\zeta_m}{\beta_n+\gamma_m}\right)=0,\ m\in\mathbb{N}_0. \tag{3.27}$$

The approximate existence condition (3.21) becomes

$$f(\mathrm{i}\gamma')=\mathrm{e}^{-2\mathrm{i}\gamma' a}, \tag{3.28}$$

with exactly the same function f as before, and this reduces to

$$\gamma'(a-\Theta)=\chi+n\pi, \quad n \text{ an integer}, \tag{3.29}$$

where Θ and χ are defined as before.

B. Full solution

The approximate solution derived above can be used as the basis for a very efficient numerical solution to the problem. The ideas behind the method are described in detail in Mittra and Lee (1971), and briefly in Jones (1994), Sec. 2.12. We form a solution to (3.8) by considering the quantities

$$I_m = \lim_{N\to\infty} \frac{1}{2\pi \mathrm{i}} \int_{C_N} f(z) \left(\frac{1}{z-\gamma_m} + \frac{\zeta_m}{z+\gamma_m} \right) \mathrm{d}z, \quad m \in \mathbb{N}_0, \tag{3.30}$$

where now $f(z)$ must satisfy

(P1) $f(z)$ has simple poles at $z=\alpha_n$ and $z=\beta_n$, $n\in\mathbb{N}$, and
(P2) $f(z)=o(1)$ as $|z|\to\infty$ on C_N as $N\to\infty$.

We now let

$$f(z) = g(z)h(z), \tag{3.31}$$

where $g(z)$ is given by (3.20) and

$$h(z) = 1 + \sum_{n=1}^{\infty} \frac{A_n}{z-\gamma_n}, \tag{3.32}$$

for some unknown constants A_n. The function $h(z)$ is chosen to cancel the zeros of $g(z)$ at γ_n, and we anticipate that as $a\to\infty$, $h(z)$ will tend rapidly to 1, since the exponential terms ζ_n will decay rapidly to zero. Thus, the constants A_m will also tend to zero rapidly as $a\to\infty$.

If we apply Cauchy's residue theorem to the integral in (3.30), we obtain

$$\sum_{n=1}^{\infty} R(f:\alpha_n) \left(\frac{1}{\alpha_n-\gamma_m} + \frac{\zeta_m}{\alpha_n+\gamma_m} \right) + \sum_{n=1}^{\infty} R(f:\beta_n) \left(\frac{1}{\beta_n-\gamma_m} + \frac{\zeta_m}{\beta_n+\gamma_m} \right) + f(\gamma_m) + \zeta_m f(-\gamma_m) = 0, \quad m \in \mathbb{N}_0. \tag{3.33}$$

Comparing (3.33) with (3.8), we see that $U_n = R(f:\alpha_n)$, $V_n = -R(f:\beta_n)$, $n\in\mathbb{N}$, provided (3.10) is satisfied and

$$f(\gamma_m) + \zeta_m f(-\gamma_m) = 0, \quad m \in \mathbb{N}_0. \tag{3.34}$$

For $m\in\mathbb{N}$ this is equivalent to an infinite system of equations for the unknowns A_m

$$A_m + B_m \sum_{n=1}^{\infty} \frac{A_n}{\gamma_m+\gamma_n} = B_m, \quad m \in \mathbb{N}, \tag{3.35}$$

where

$$B_m = 2\gamma_m \mathrm{e}^{2\gamma_m(\Theta-a)} \frac{(\alpha_m-\gamma_m)(\beta_m-\gamma_m)}{(\alpha_m+\gamma_m)(\beta_m+\gamma_m)} \prod_{\substack{n=1 \\ n\neq m}}^{\infty} \frac{(1+\gamma_m/\gamma_n)(1-\gamma_m/\alpha_n)(1-\gamma_m/\beta_n)}{(1+\gamma_m/\alpha_n)(1+\gamma_m/\beta_n)(1-\gamma_m/\gamma_n)}. \tag{3.36}$$

Unlike (3.8), this system of equations is real and the presence of the factor ζ_m in B_m shows that as $a\to\infty$, the coefficients A_m decay exponentially to zero. Moreover, the terms B_m decay exponentially as $m\to\infty$ and so the system can be solved very efficiently via a numerical truncation

technique. It can be proved, using the methods described in Evans (1992), Appendix B, and Evans, Linton, and Ursell (1993), Appendix C, that the infinite system (3.35) has a unique solution A_n with $\Sigma_{n=1}^{\infty} A_n^2 < \infty$ provided a/d is sufficiently large.

We now return to the one condition still to be satisfied, namely, (3.34) with $m=0$. This is

$$e^{2i\gamma' a} = -\frac{f(-i\gamma')}{f(i\gamma')}. \tag{3.37}$$

Now, since A_n and γ_n are real for $n \in \mathbb{N}$, we can write

$$\frac{h(-i\gamma')}{h(i\gamma')} = e^{2i\sigma}, \tag{3.38}$$

where

$$\sigma = \arg(h(-i\gamma')) = \arg\left(1 - \sum_{n=1}^{\infty} \frac{A_n}{\gamma_n + i\gamma'}\right). \tag{3.39}$$

Then, with χ and Θ as before, the condition for the existence of bound states (3.37) reduces to

$$\gamma'(a-\Theta) = \chi + \sigma + (n - \tfrac{1}{2})\pi, \quad n \text{ an integer.} \tag{3.40}$$

This condition differs from the approximate condition (3.23) by the inclusion of the term σ. This depends on a/d, but it is clear that as $a/d \to \infty$, $\sigma \to \arg(1) = 0$.

For the case of antisymmetry about $x=0$, (3.34) becomes

$$f(\gamma_m) - \zeta_m f(-\gamma_m) = 0, \quad m \in \mathbb{N}_0, \tag{3.41}$$

with the infinite system of equations equivalent to (3.35) being

$$A_m - B_m \sum_{n=1}^{\infty} \frac{A_n}{\gamma_m + \gamma_n} = -B_m, \quad m \in \mathbb{N}, \tag{3.42}$$

and B_m is given by (3.36) as before. The condition for antisymmetric modes, equivalent to (3.40), is thus

$$\gamma'(a-\Theta) = \chi + \sigma' + n\pi, \quad n \text{ an integer,} \tag{3.43}$$

where σ' is the argument of $h(-i\gamma')$ with the constants A_n given by the solution of (3.42).

C. Results

The systems of Eqs. (3.35) and (3.42) need to be solved by truncation but, due to the exponential convergence of the B_m terms, only a small truncation parameter is needed. In the following results a truncation parameter of 5 was used to assure high accuracy for all parameter values, but a 2×2 system is adequate unless a/d is very small. Figure 2 shows results for $b/d = 0.6$ and compares the nondimensional bound-state energies, kd/π, computed from the approximate solution (dashed lines) with those found from the full solution (solid lines). The two curves on the left of the figure correspond to the first symmetric (about $x=0$) mode, and the other two correspond to the first antisymmetric mode. For all but the smallest values of a/d, the results computed from the full and approximate methods are indistinguishable. Only when a/d is less than about 0.5 do the full solution and the approximate solution produce significantly different results.

In Fig. 3 a typical set of nondimensional bound-state energies, kd/π, computed from the full solutions (3.40) and (3.43), is plotted against a/d, for $b/d = 0.75$. The solid lines correspond to modes symmetric about $x=0$ and the dashed lines correspond to modes antisymmetric about x

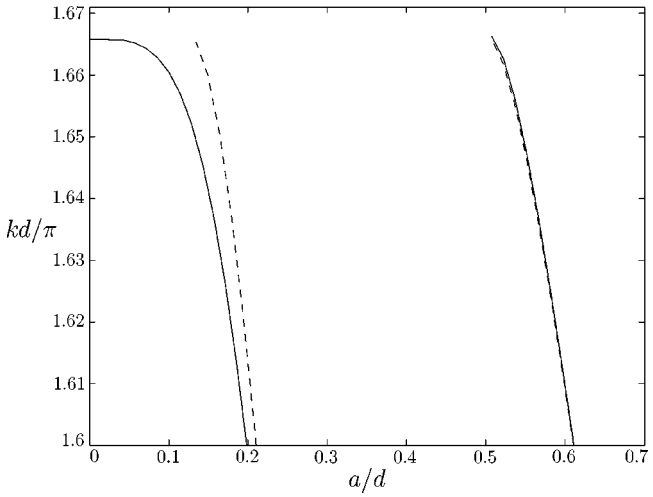

FIG. 2. A comparison of the nondimensional bound-state energies, kd/π, for modes symmetric and antisymmetric about $x=0$ for the approximate solution (dashed) and the full solution (solid) plotted against a/d when $b/d=0.6$.

$=0$. We see that as a/d increases the number of modes present also increases, and the modes appear alternatively symmetric and antisymmetric from the cutoff $kd=d\pi/b=4\pi/3$, and decrease towards $kd=\pi$.

The variation of nondimensional bound-state energies with b/d when $a/d=3$ is shown in Fig. 4. The solid lines represent symmetric modes, the dashed lines correspond to antisymmetric modes, and the dotted line represents the upper cutoff $kb=\pi$. It is clear that as b/d increases from 0.5, the number of modes present decreases and the energy of each of the modes decreases slightly. The figure shows that modes are present for any value of b/d in the interval $[0.5, 1)$.

D. Variational methods

Trapped modes occurring in two-dimensional acoustic waveguides containing long obstacles symmetric about the centerline were considered by Khallaf, Parnovski, and Vassiliev (2000). In their paper the authors use variational arguments to provide estimates for the trapped mode

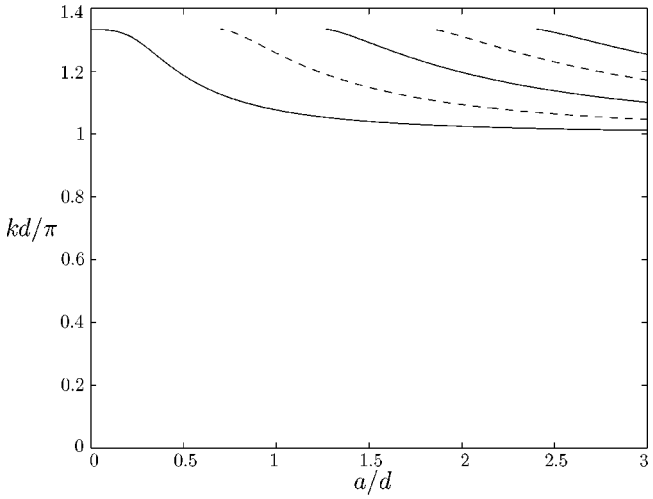

FIG. 3. Nondimensional bound-state energies, kd/π, for modes symmetric (—) and antisymmetric (– –) about $x=0$, plotted against a/d when $b/d=0.75$.

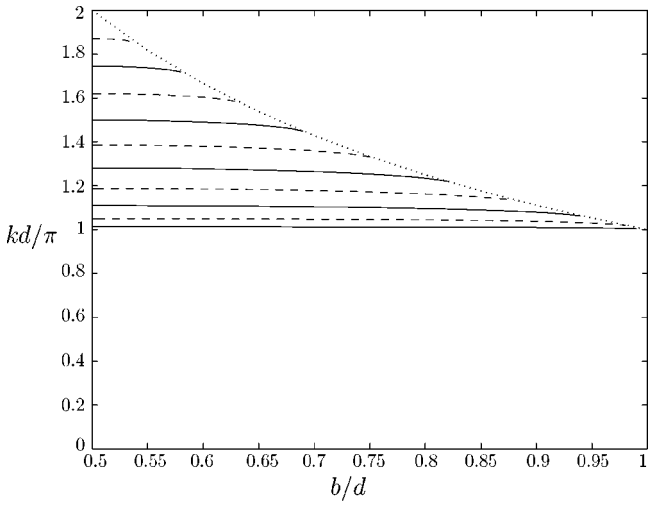

FIG. 4. Nondimensional bound-state energies, kd/π, for modes symmetric (—) and antisymmetric (––) about $x=0$, plotted against b/d when $a/d=3$. The dotted line is the curve $kb=\pi$.

frequencies and also to prove that the number of trapped modes occurring is asymptotically proportional to the obstacle's length. We will extend their method to provide estimates for the bound-state energies in our problem and to prove existence for a sufficiently large window. The main difference between the two problems is that the laterally coupled guide under consideration here is not symmetric about the centerline of the waveguide.

Our waveguide can be thought of as an unbounded domain Ω defined as

$$\Omega=\{(0,\infty)\times(0,d)\}\backslash\{[a,\infty)\times[b]\}, \tag{3.44}$$

where $a>0$ and $\frac{1}{2}<b/d<1$. We are trying to find estimates for values of λ for which there is a nontrivial solution $\phi(x,y)$ to the boundary-value problem

$$-\nabla^2\phi=\lambda\phi \quad \text{in} \quad \Omega, \tag{3.45}$$

subject to the boundary conditions (2.3)–(2.6), and (2.1) for symmetric modes or (3.26) for antisymmetric modes. In other words, we seek the eigenvalues of $-\nabla^2$ (defined on an appropriate domain) and since wave-like modes can propagate to infinity if $kb>\pi$, the continuous spectrum for either the symmetric or the antisymmetric problem is the semi-interval $[\pi^2/b^2,\infty)$.

We consider the Rayleigh quotient defined by

$$Q(\phi)=\frac{\displaystyle\int_\Omega|\nabla\phi|^2\mathrm{d}\Omega}{\displaystyle\int_\Omega|\phi|^2\mathrm{d}\Omega}, \tag{3.46}$$

and set

$$\lambda_1=\inf_{\phi\in\mathcal{H}_0^1\backslash\{0\}} Q(\phi). \tag{3.47}$$

(The symbol λ_n has a different meaning in this section than elsewhere in the paper.) Here, $\mathcal{H}_0^1$ is the Sobolev space consisting of all functions in $L^2(\Omega)$ which also have square-integrable first partial derivatives and which vanish on the boundary of Ω at the same places that the solution ϕ does. In particular, the symbol $\mathcal{H}_0^1$ represents different spaces in the symmetric and antisymmetric problems, since in the latter case functions in $\mathcal{H}_0^1$ must vanish on $x=0$, $0<y<d$. It is a standard result (see, e.g., Edmunds and Evans 1987, Chap. XI) that $\lambda_1>0$ is the lowest point of the

spectrum of our operator and, if $\lambda_1 < \pi^2/b^2$, then λ_1 must be an eigenvalue of the problem (the smallest) and the function φ_1 for which $Q(\varphi_1)=\lambda_1$ is the associated eigenfunction (bound state). We can define

$$\lambda_n = \inf_{\substack{\phi \in \mathcal{H}_0^1 \setminus \{0\} \\ \phi \perp \varphi_i,\, i=1,2,\ldots,n-1}} Q(\phi), \tag{3.48}$$

and if $\lambda_n < \pi^2/b^2$, λ_n is the nth eigenvalue for the problem (arranged in order of increasing size and accounting for multiplicity). If $\lambda_{n+1}=\pi^2/b^2$, there will be exactly n eigenvalues below the first cutoff. We label the eigenvalues below the continuous spectrum as $\lambda_{j,s}$ for the symmetric problem (and we assume that there are n_s of them) and $\lambda_{j,a}$ for the antisymmetric problem (of which there are n_a).

We now use the idea of Dirichlet–Neumann bracketing (see, e.g., Courant and Hilbert 1953) which is a consequence of the variational principle outlined above. The domain Ω is split into the regions *I*, *II*, and *III* defined previously and we consider the eigenvalues associated with each region separately when an artificial boundary condition is imposed on L_3. We denote the jth eigenvalue occurring in region i with a Dirichlet (respectively, Neumann) condition on L_3 as $\lambda_j^{i,D}$ (respectively, $\lambda_j^{i,N}$). We also define a counting function $N^{i,D}(\lambda)$ [respectively, $N^{i,N}(\lambda)$], as the number of eigenvalues less than λ in region i, with a Dirichlet (respectively, Neumann) condition on L_3. An extra subscript (s or a) will be used whenever it is necessary to distinguish between the symmetric and antisymmetric problems. If $\lambda < \pi^2/b^2$ we have

$$N^{I,D}(\lambda)+N^{II,D}(\lambda)+N_s^{III,D}(\lambda) \leqslant N_s(\lambda) \leqslant N^{I,N}(\lambda)+N^{II,N}(\lambda)+N_s^{III,N}(\lambda), \tag{3.49}$$

where $N_s(\lambda)$ is the total number of eigenvalues below λ for the symmetric problem. Note that $N_s(\pi^2/b^2)=n_s$.

A straightforward calculation shows that

$$\{\lambda_{j,s}^{III,D}\}_{j=1}^{\infty} = \{(n-1/2)^2\pi^2/a^2+(m\pi)^2/d^2\}_{n,m=1}^{\infty}, \tag{3.50}$$

$$\{\lambda_{j,s}^{III,N}\}_{j=1}^{\infty} = \{(n-1)^2\pi^2/a^2+(m\pi)^2/d^2\}_{n,m=1}^{\infty}, \tag{3.51}$$

and that there are no eigenvalues in regions *I* or *II*, and so (3.49) becomes

$$N_s^{III,D}(\lambda) \leqslant N_s(\lambda) \leqslant N_s^{III,N}(\lambda), \tag{3.52}$$

provided $\lambda < \pi^2/b^2$. It then follows (see, e.g., Behnke *et al.*, 2000) that

$$\lambda_{j,s}^{III,N} \leqslant \lambda_{j,s} \leqslant \lambda_{j,s}^{III,D}, \tag{3.53}$$

for all j for which $\lambda_{j,s} < \pi^2/b^2$. Hence

$$\frac{\pi^2}{a^2}(j-1)^2+\frac{\pi^2}{d^2} \leqslant \lambda_{j,s} \leqslant \frac{\pi^2}{a^2}(j-1/2)^2+\frac{\pi^2}{d^2}. \tag{3.54}$$

For the antisymmetric problem the eigenfunction expansions and eigenvalues can be recalculated and (3.54) becomes

$$\frac{\pi^2}{a^2}(j-1/2)^2+\frac{\pi^2}{d^2} \leqslant \lambda_{j,a} \leqslant \frac{\pi^2}{a^2}j^2+\frac{\pi^2}{d^2}. \tag{3.55}$$

The result of superimposing these intervals onto Fig. 3 is shown in Fig. 5. Each mode appears between two estimates as required, and it can be seen that as a/d increases along each curve, the estimate coming from the upper bound gives a better approximation to the energy.

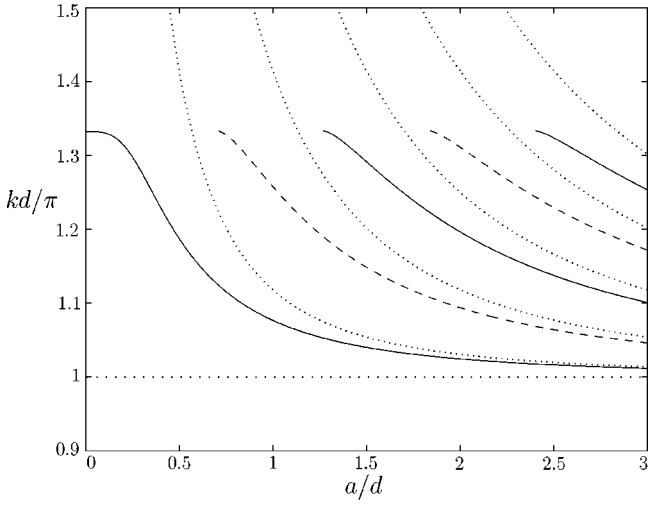

FIG. 5. Nondimensional bound-state energies, kd/π, for modes symmetric and antisymmetric about $x=0$ for the full solution (solid and dashed, respectively), and the estimated intervals (dotted), plotted against a/d when $b/d=0.75$.

Each interval of (3.54) and (3.55) whose right-end value is less than π^2/b^2 contains precisely one eigenvalue. Thus, there are at least n_s symmetric bound states provided

$$a/d > (n_s - \tfrac{1}{2})/\sqrt{d^2/b^2 - 1}. \tag{3.56}$$

Similarly, there are at least n_a antisymmetric bound states provided

$$a/d > n_a/\sqrt{d^2/b^2 - 1}. \tag{3.57}$$

As $b/d \to 1$, the required value of a/d tends to infinity in both cases. Similar results were found by Exner *et al.* (1996).

IV. BOUND STATES BELOW THE SECOND CUT-OFF

In this section we look for bound states whose energies are above the cutoff given by (2.17), i.e., $kb > \pi$. Any such mode corresponds to an eigenvalue embedded in the continuous spectrum of the relevant operator. Numerical evidence for the existence of an isolated trapped mode embedded in the continuous spectrum was given by Evans and Porter (1998) for the case of a rigid circular cylinder placed on the centerline of a guide with either Neumann or Dirichlet boundary conditions on its walls. In each case the trapped mode was shown to occur for a single cylinder radius and at a specific frequency.

More recently, McIver *et al.* (2001) showed that this trapped mode was not isolated, but part of a continuous branch of modes which exist for ellipses with varying aspect ratio. The ellipses are defined by two geometrical parameters a and b, say, where $(x/a)^2 + (y/b)^2 = 1$, and embedded trapped modes were found to exist for families of ellipses given by $a = a(b)$, with the corresponding frequency being of the form $k = k(b)$. Further examples of branches of embedded trapped modes in geometries defined by two geometrical parameters were computed in McIver, Linton, and Zhang (2002).

In general, it appears that for a given energy there will be a number of possible wave-like modes which can transmit the energy down the guide, and in order for a bound state to exist the amplitudes of these modes must be zero. If one considers a geometry defined by a sufficient number of parameters then it may be possible to determine relationships between these parameters which lead to bound states. The numbers of parameters needed will depend on the energy band considered and the boundary conditions for the problem (see, e.g., Linton *et al.*, 2002).

Here, we will use this idea to find bound states between the first and second cutoffs for a coupled waveguide (which is defined by two geometrical parameters). We set up the problem with eigenfunction expansions similar to those in Sec. II. The second cutoff is defined as the energy below which only one mode can propagate in the region $x>a$, i.e., one mode in either region *I* or region *II*. We also restrict the energy in such a way that two wave-like modes exist in the inner region, the reason for which will become clear later. Thus, we assume

$$2\pi<kd<\frac{d\pi}{c}, \quad \text{when} \quad 1/2<b/d\leqslant 2/3, \tag{4.1}$$

$$2\pi<kd<\frac{2d\pi}{b}, \quad \text{when} \quad 2/3\leqslant b/d<1. \tag{4.2}$$

For the symmetric problem the eigenfunction expansions for the three regions are

$$\phi_1(x,y)=\sum_{n=1}^{\infty} U_n^{(1)}\frac{e^{-\alpha_n(x-a)}}{-\alpha_n}\Psi_n^{(1)}(y), \quad \alpha_n=(\nu_n^2-k^2)^{1/2}, \tag{4.3}$$

$$\phi_2(x,y)=\sum_{n=2}^{\infty} U_n^{(2)}\frac{e^{-\beta_n(x-a)}}{-\beta_n}\Psi_n^{(2)}(y), \quad \beta_n=(\mu_n^2-k^2)^{1/2}, \tag{4.4}$$

$$\phi_3(x,y)=\sum_{n=0}^{\infty} U_n^{(3)}\frac{\cosh\gamma_n x}{\gamma_n\sinh\gamma_n a}\Psi_n^{(3)}(y), \quad \gamma_n=(\lambda_n^2-k^2)^{1/2}, \tag{4.5}$$

where $\Psi_n^{(1)}(y)$, $\Psi_n^{(2)}(y)$, and $\Psi_n^{(3)}(y)$ are given by (2.10)–(2.12). These expansions are the same as (2.14)–(2.16) except that the sum in region *II* starts from $n=2$, as we set the amplitude of the mode corresponding to β_1 equal to zero. With the restriction of frequency given by (4.1) and (4.2), γ_0 and γ_1 (and β_1) are purely imaginary whereas α_1, α_n, β_n and γ_n, $n\geqslant 2$ are all real and positive.

After matching on $x=a$, we obtain

$$\sum_{n=1}^{\infty} U_n\left(\frac{1}{\alpha_n-\gamma_m}+\frac{\zeta_m}{\alpha_n+\gamma_m}\right)-\sum_{n=2}^{\infty} V_n\left(\frac{1}{\beta_n-\gamma_m}+\frac{\zeta_m}{\beta_n+\gamma_m}\right)=0, \quad m\in\mathbb{N}_0, \tag{4.6}$$

where U_n, V_n, and ζ_m are defined in (3.9). The only difference between (4.6) and (3.8) is that the summation for V_n starts from $n=2$ instead of $n=1$. The condition (3.10) describing the behavior of U_n and V_n for large n remains the same.

We now consider the same quantities as in (3.30), except that now $f(z)$ must have simple poles at $z=\alpha_n$, $n\in\mathbb{N}$, and $z=\beta_n$, $n\geqslant 2$ as well as being $o(1)$ as $z\to\infty$. We choose

$$f(z)=\exp(-z\Theta)g(z)h(z), \tag{4.7}$$

where Θ is given by (3.24) and

$$g(z)=\frac{1}{1-z/\alpha_1}\prod_{n=2}^{\infty}\frac{1-z/\gamma_n}{(1-z/\alpha_n)(1-z/\beta_n)}, \quad h(z)=1+\sum_{n=2}^{\infty}\frac{A_n}{z-\gamma_n}. \tag{4.8}$$

The function $g(z)$ has the same behavior as $z\to\infty$, as that given in (3.20) since one linear factor has been removed from both the numerator and the denominator. Cauchy's residue theorem then gives

$$\sum_{n=1}^{\infty} R(f:\alpha_n)\left(\frac{1}{\alpha_n-\gamma_m}+\frac{\zeta_m}{\alpha_n+\gamma_m}\right)+\sum_{n=2}^{\infty} R(f:\beta_n)\left(\frac{1}{\beta_n-\gamma_m}+\frac{\zeta_m}{\beta_n+\gamma_m}\right)+f(\gamma_m)+\zeta_m f(-\gamma_m)$$
$$=0, \quad m\in\mathbb{N}_0, \tag{4.9}$$

and hence $U_n=R(f:\alpha_n)$ and $V_n=-R(f:\beta_n)$, provided (3.10) is satisfied and

$$f(\gamma_m)+\zeta_m f(-\gamma_m)=0, \quad m\in\mathbb{N}_0. \tag{4.10}$$

The coefficients A_n, $n=2,3,...$, can be found from a real, exponentially convergent system of equations

$$A_m+B_m\sum_{n=2}^{\infty}\frac{A_n}{\gamma_m+\gamma_n}=B_m, \quad m=2,3,..., \tag{4.11}$$

where

$$B_m=2\gamma_m e^{2\gamma_m(\Theta-a)}\frac{(\alpha_1-\gamma_m)(\alpha_m-\gamma_m)(\beta_m-\gamma_m)}{(\alpha_1+\gamma_m)(\alpha_m+\gamma_m)(\beta_m+\gamma_m)}\prod_{\substack{n=2\\ n\neq m}}^{\infty}\frac{(1-\gamma_m/\alpha_n)(1-\gamma_m/\beta_n)(1+\gamma_m/\gamma_n)}{(1+\gamma_m/\alpha_n)(1+\gamma_m/\beta_n)(1-\gamma_m/\gamma_n)}. \tag{4.12}$$

Whereas in the nonembedded case we had one extra condition to be satisfied, we now have two; namely (4.10) with $m=0$ and $m=1$. With $\gamma_j=-i\gamma_j'$, where $\gamma_j'=(k^2-\lambda_j^2)^{1/2}$, these conditions reduce to

$$e^{2i\gamma_j' a}=-\frac{f(-i\gamma_j')}{f(i\gamma_j')}, \quad j=0,1. \tag{4.13}$$

For bound states to exist, we must therefore have

$$\gamma_j'(a-\Theta)=\chi_j+\sigma_j+(n_j-\tfrac{1}{2})\pi, \quad j=0,1, \tag{4.14}$$

satisfied simultaneously, where

$$\chi_j=-\tan^{-1}\left(\frac{\gamma_j'}{\alpha_1}\right)+\sum_{n=2}^{\infty}\left(\tan^{-1}\left(\frac{\gamma_j'}{\gamma_n}\right)-\tan^{-1}\left(\frac{\gamma_j'}{\alpha_n}\right)-\tan^{-1}\left(\frac{\gamma_j'}{\beta_n}\right)\right), \tag{4.15}$$

$$\sigma_j=\arg(h(-i\gamma_j'))=\arg\left(1-\sum_{n=2}^{\infty}\frac{A_n}{\gamma_n+i\gamma_j'}\right), \tag{4.16}$$

and n_0 and n_1 are an arbitrary pair of integers.

For the case of antisymmetry about $x=0$, the conditions change to

$$\gamma_j'(a-\Theta)=\chi_j+\sigma_j'+n_j\pi, \quad j=0,1, \tag{4.17}$$

where σ_j' is the argument of $h(-i\gamma_j')$ with the A_n coefficients coming from

$$A_m-B_m\sum_{n=2}^{\infty}\frac{A_n}{\gamma_m+\gamma_n}=-B_m, \quad m=2,3,..., \tag{4.18}$$

and B_m given by (4.12).

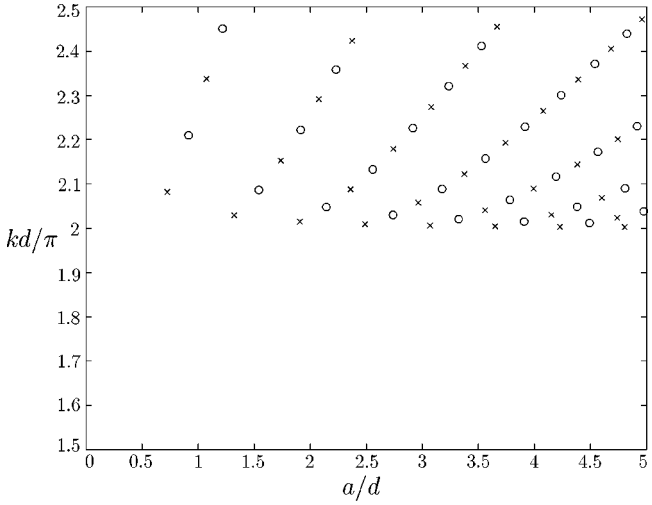

FIG. 6. Nondimensional bound-state energies for modes symmetric ($\times$) and antisymmetric ($\bigcirc$) about $x=0$ plotted against a/d, when $b/d=0.6$.

A. Results

For the numerical results in this section, the system of Eqs. (4.11) and (4.18) were truncated to 5×5 systems. However, in view of the fact that no modes are found for a/d smaller than about 0.7, the approximate solution in which we set $\sigma_j=0$, $j=0,1$, gives indistinguishable results.

In Fig. 6 a typical set of nondimensional bound-state energies, kd/π, are plotted against a/d when $b/d=0.6$, for which the relevant energy range is given by (4.1) as $2<kd/\pi<2.5$. The modes symmetric about $x=0$ are represented by a cross and the modes antisymmetric about $x=0$ are shown by a circle. A detailed view of just five of these bound states is given in Fig. 7, which also shows the solid lines corresponding to solutions of (4.14) and dashed lines corresponding to solutions of (4.17) for $j=0,1$, labeled with the corresponding n_0 and n_1 values. The bound states correspond to the intersections of two lines. Modes only exist for certain values of a/d, but as a/d increases the number of bound states present in a small a/d interval increases.

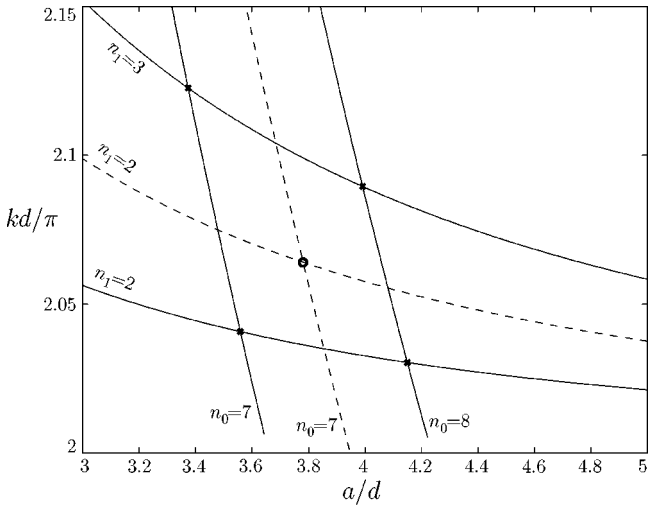

FIG. 7. A detailed view of part of Fig. 6 showing the curves corresponding to the solutions of (4.14) (solid curves) and (4.17) (dashed curves) for $j=0,1$, labeled with the corresponding n_0 and n_1 values. The embedded bound states are denoted by $\times$ (symmetric) and $\bigcirc$ (antisymmetric).

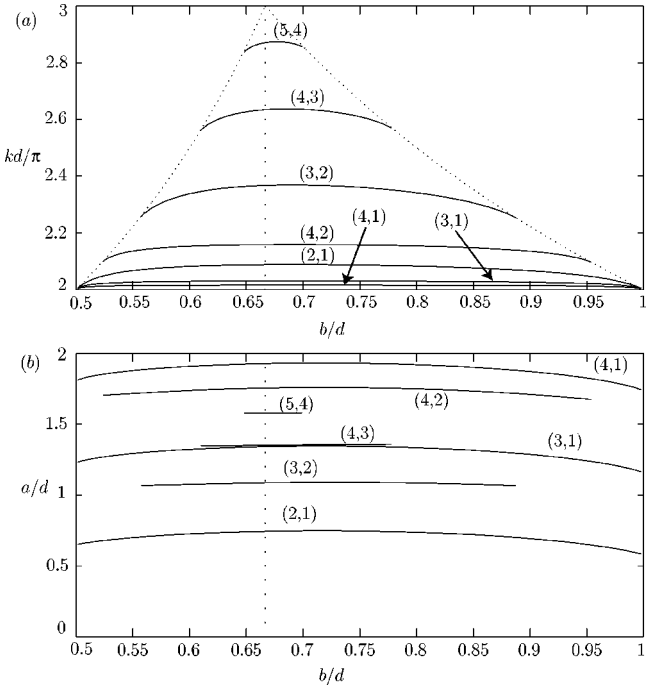

FIG. 8. Variation of (*a*) kd/π and (*b*) a/d with b/d for modes symmetric about $x=0$. The curves are labeled with the values of (n_0,n_1) used to generate them.

The bound states symmetric about $x=0$ obtained by keeping the integers n_0 and n_1 in (4.14) constant and varying either kd/π or a/d against b/d are shown in Figs. 8(a) and (b), respectively. The vertical dotted line corresponds to the value $b/d=2/3$, and the other two dotted lines correspond to the upper cutoffs given in (4.1) and (4.2). Only a selection of results for which $a/d<2$ are given. It can be seen from Fig. 8(a) that the highest energy states appear when (n_0,n_1) take the form $(N,N-1)$, with N large and the lower energies occur when $(n_0,n_1)=(N,1)$ with N large. Figure 8(b) shows that the lower values of a/d appear when (n_0,n_1) take the form $(N,N-1)$ with N small and as n_0 increases a/d increases. The figures also demonstrate that modes exist for any value of b/d in the range (0.5, 1) (but for only specific values of a/d).

In Linton *et al.* (2002) acoustic resonances were found between the second and third cutoffs for wave propagation down a rigid waveguide containing an off-center rigid plate aligned with the guide walls. The coupled waveguide problem under consideration here can be set up for energies between the second and third cutoffs, with three wave-like modes appearing in the region $x<a$ and two propagating modes in the region $x>a$. Using the same techniques as above, we find that bound states exist provided three conditions are satisfied simultaneously. However, these three conditions are found to be inconsistent.

B. The case $b/d=1/2$

If $2b=d$ the waveguide is symmetric about the midline parallel to the walls and this can be used to simplify the analysis. The problem can be decomposed into one symmetric about the midline and one antisymmetric about this line, and the latter problem is that of a parallel-plate waveguide with Dirichlet conditions on both walls, where there are no bound states. We thus restrict attention to the symmetric problem. Bound states below the first cutoff are precisely those which are obtained by letting $b/d\to 1/2$ in the preceding analysis.

However, in Sec. IV we found embedded bound states in the frequency range $2\pi<kd<d\pi/c$ when $1/2<b/d\leqslant 2/3$. These modes do not exist when $b/d=1/2$. The additional symmetry

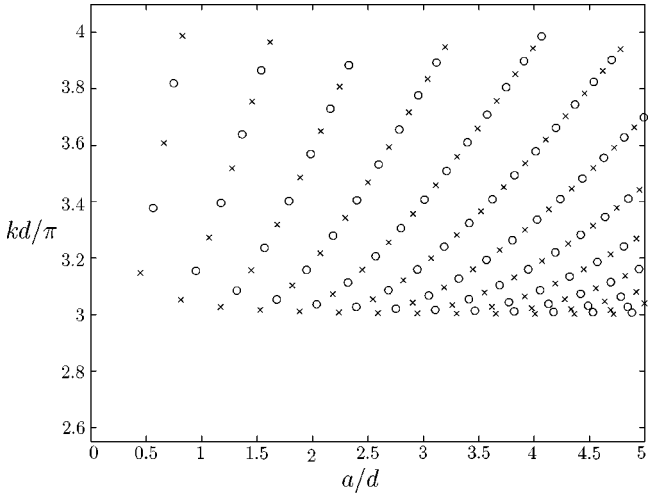

FIG. 9. Nondimensional bound-state energies, kd/π, for modes symmetric ($\times$) and antisymmetric ($\bigcirc$) about $x=0$ plotted against a/d when $b/d=1/2$.

in the problem when $b/d=0.5$ allows embedded modes to be found in a higher energy band in this case. In fact, we now require

$$3\pi<kd<4\pi, \tag{4.19}$$

to allow for two wave-like modes in the inner region and one in $x>a$. The problem is set up much as before; here, we will simply present some results.

In Fig. 9 the nondimensional bound-state energies are plotted against a/d. The modes symmetric about $x=0$ are shown by crosses and the modes antisymmetric about $x=0$ by circles. Just as in Fig. 7, the bound states correspond to the intersection of pairs of curves on which one of the two necessary conditions for bound states is satisfied. It can be seen that there are no bound states when a/d is below some critical value, and that bound states occur only for specific values of the plate length. As a/d increases, the number of bound states present in a small a/d interval increases as before.

V. CONCLUSION

In this article we have investigated the bound states that can occur in coupled quantum wires. Specifically, we have considered a two-dimensional configuration in which two parallel waveguides (of different widths) are coupled laterally through a finite length window and constructed modes which exist local to the window connecting the two guides. The geometry of the problem can be described in terms of the two parameters a/d and b/d, where the complete guide is made up of two guides of widths b and $d-b$, and the coupling window has length $2a$.

Initially we sought modes below the first cutoff for the guide. Modes for which the energy is below this cutoff cannot propagate down the guide and so if any are found they must be localized in space. The main tool used in the analysis is the residue calculus method, in which a function of a complex variable is constructed which has the property that when Cauchy's residue theorem is applied for some suitable contour, the system of equations derived from a mode-matching approach is obtained. The unknown coefficients then correspond to the residues of the complex function. If we assume that the window between the guides is long compared to the guide width, then this method allows us to solve the problem explicitly, and this approximate solution can then be used as the basis for a full numerical solution. This leads to an exponentially convergent system of equations and high accuracy can be achieved with only a very few equations. In fact, for all but the smallest values of a/d, the explicit approximate solution is quite sufficient.

A number of results have been presented which show that as the window length varies bound states occur alternately symmetric and antisymmetric about the line of symmetry of the guide, and that more modes appear as the window gets larger or as the widths of the two parts of the guide get closer together (i.e., as $b/d \to 1/2$). Using a variational principle we were able to provide upper and lower bounds for the bound-state energies and prove the existence of such states for a sufficiently large window. As a/d increases, the bound-state energies tend towards their upper bounds.

For modes whose energies are above the first cutoff we were able to use a similar residue calculus technique to compute bound-state energies. Here, we are seeking bound states whose energies are embedded in the continuous spectrum of the relevant operator, and this leads to the need to satisfy two conditions simultaneously, where there was only one below the cutoff. Below the cutoff we could fix either a/d or b/d and vary the other to get solutions. Above the cutoff, bound states occur for any values of $b/d \in (0.5,1)$ but only for specific values of the parameter a/d. When $b/d = 1/2$, the region in which these embedded modes occur is shifted to a higher energy band.

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Bound states in coupled guides. II. Three dimensions

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We compute bound-state energies in two three-dimensional coupled waveguides, each obtained from the two-dimensional configuration considered in paper I [J. Math. Phys. **45**, 1359–1379 (2004)] by rotating the geometry about a different axis. The first geometry consists of two concentric circular cylindrical waveguides coupled by a finite length gap along the axis of the inner cylinder, and the second is a pair of planar layers coupled laterally by a circular hole. We have also extended the theory for this latter case to include the possibility of multiple circular windows. Both problems are formulated using a mode-matching technique, and in the cylindrical guide case the same residue calculus theory as used in paper I is employed to find the bound-state energies. For the coupled planar layers we proceed differently, computing the zeros of a matrix derived from the matching analysis directly. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1675932]

I. INTRODUCTION

Here we extend the ideas from paper I [J. Math. Phys. **45**, 1359–1379 (2004)] to three dimensions and consider two distinct types of problem. First, we treat the case where the two-dimensional laterally coupled waveguide discussed in paper I is rotated about the x axis to produce a three-dimensional waveguide. The guide then consists of a pair of concentric circular cylindrical guides of widths b and d coupled by a finite gap in the inner cylinder. We seek bound states whose energies are below the first cutoff for wave propagation down the guide using the residue calculus technique. Second, we consider the case where the coupled waveguide considered in paper I is rotated about the y axis. The waveguide consists of two planar layers of widths b and $d-b$ coupled through a circular hole of radius a in the common boundary. In fact, we set up the problem for an arbitrary number of arbitrarily sized circular windows.

Early work on acoustic resonances in circular cylindrical waveguides was done by Ursell (1991), who considered a rigid cylinder with a rigid sphere placed on the axis. Using the method of multipole expansions, Ursell able to prove the existence of resonant states with certain angular variation, provided the sphere was sufficiently small. The method presented in this paper is similar to that used by Evans and Linton (1994), who developed an approximate solution for the existence of trapped modes in an infinitely long, rigid, circular cylindrical tube containing a concentric, rigid, open-ended circular cylinder of finite length. Linton and McIver (1998) proved that acoustic resonances can exist when any rigid, thin obstacle is placed in a rigid cylindrical waveguide of constant cross section in such a way that its normal is everywhere perpendicular to the generators of the cylinder. Similar results were also given in Groves (1998) and Davies and Parnovski (1998). The example of a cylindrical sleeve inside a circular cylindrical waveguide with Neumann conditions on all boundaries considered in Evans and Linton (1994) was recalculated using the residue calculus technique and extended to cover different angular variations.

In all the above examples, Neumann boundary conditions were imposed on the cylindrical waveguide. A cylindrical guide with Dirichlet conditions on the boundary was considered by Witsch (1990). Witsch used the same idea as Ursell in that he specified the angular variation to

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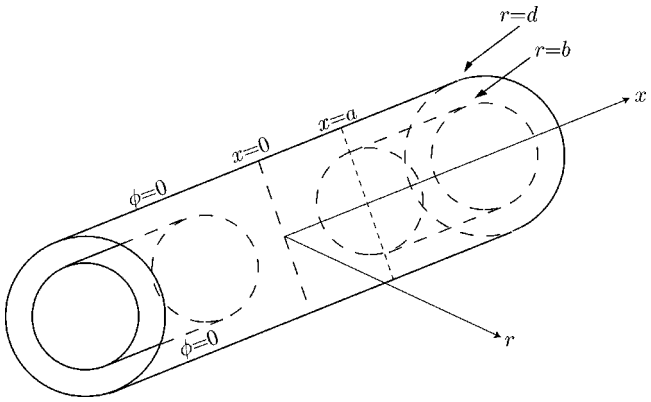

FIG. 1. Definition sketch.

produce a cutoff and then used a minimum–maximum principle to provide examples of eigenvalues that can occur in the waveguide.

Much less work has been done on the second problem. Exner and Vugalter (1997) considered the case when the hole was sufficiently small so that only one eigenvalue occurred below the continuous spectrum. The authors were then able to provide upper and lower asymptotic bounds on the gap between the eigenvalue and the continuous spectrum. Further asymptotic results were derived in Popov (2002).

II. COUPLED CYLINDRICAL GUIDES

In this section we consider a rotation of the waveguide used in paper I about the x axis. We introduce cylindrical polar coordinates (r,θ,x) so that the outer surface of the guide is at $r=d$. Inside the guide is placed an infinite, concentric cylinder of radius b $(<d)$, which has a gap of length $2a$ along its axis. The inner cylinder is placed so that its surface is at $r=b$ and the gap is at $-a<x<a$, as shown in Fig. 1. The resulting geometry is axisymmetric about the line $r=0$; hence, we are able to look for modes with angular variation $\cos m\theta$, where $m\in\mathbb{N}_0$. The quantity m is to be regarded as fixed in what follows.

The geometry is symmetric about $x=0$, allowing us only to consider the region $x>0$ and seek modes which are either symmetric or antisymmetric about $x=0$. We begin by seeking modes symmetric about $x=0$ by looking for nontrivial solutions $\phi(r,\theta,x)$, which satisfy

$$\frac{\partial\phi}{\partial x}=0 \quad \text{on } x=0,\ 0<r<d. \tag{2.1}$$

The function $\phi(r,\theta,x)$ must also satisfy the Helmholtz equation within the waveguide

$$(\nabla^2+k^2)\,\phi=0, \quad 0<r<d, x>0 \quad \text{except on } r=b,\ x>a, \tag{2.2}$$

and is subject to Dirichlet boundary conditions on the cylinders

$$\phi=0 \quad \text{on } r=b,\ x>a, \tag{2.3}$$

$$\phi=0 \quad \text{on } r=d,\ x>0, \tag{2.4}$$

and a radiation condition that stops waves propagating to infinity,

$$\phi\to 0 \quad \text{as } x\to\infty. \tag{2.5}$$

Finally, we assume that ϕ is nonsingular and

$$\frac{\partial \phi}{\partial \rho} = O(\rho^{-1/2}) \quad \text{as } \rho = [(x-a)^2 + (r-b)^2]^{1/2} \to 0, \tag{2.6}$$

anticipating singular behavior in the derivative of ϕ at the edge. The changes resulting from replacing (2.1) by an antisymmetric condition will be discussed later.

As in the two-dimensional case considered in paper I, we divide the interior of the guide into three parts. Region I is the annular region between the outer and inner cylinders, i.e., $\{r,\theta,x: b<r<d, x>a\}$, region II is the interior of the inner cylinder, i.e., $\{r,\theta,x: 0<r<b, x>a\}$, and region III is the gap of the inner cylinder, i.e., $\{r,\theta,x: 0<r<d, 0<x<a\}$. We can represent the function ϕ by a function $\phi_i(r,\theta,x) = \hat{\phi}_i(r,x)\cos m\theta$, $(i=1,2,3, m \in \mathbb{N}_0)$ in each region and apply the following continuity conditions at each region's boundary:

$$\hat{\phi}_i = \hat{\phi}_3, \quad \frac{\partial \hat{\phi}_i}{\partial x} = \frac{\partial \hat{\phi}_3}{\partial x}, \quad \text{on } L_i, \ \ i=1,2, \tag{2.7}$$

where L_1 is $x=a, b<r<d$, L_2 is $x=a, 0<r<b$, and we write $L_3 = L_1 \cup L_2$.

Complete orthogonal sets of functions of r in each of the three regions are defined in terms of Bessel functions as follows. Let ν_{mn} be the nth positive zero of the cross product $J_m(\eta d)\, Y_m(\eta b) - Y_m(\eta d)\, J_m(\eta b)$; then, functions appropriate for region I are

$$\Psi^{(1)}_{mn}(r) = p^{(1)}_{mn}[J_m(\nu_{mn} r)\, Y_m(\nu_{mn} b) - Y_m(\nu_{mn} r)\, J_m(\nu_{mn} b)], \quad n \in \mathbb{N}. \tag{2.8}$$

This function satisfies (2.3) and (2.4), and with

$$p^{(1)}_{mn} = \frac{\nu_{mn}\pi^{1/2}}{2^{1/2}} \left(\frac{J^2_m(\nu_{mn} b)}{J^2_m(\nu_{mn} d)} - 1 \right)^{-1/2}, \tag{2.9}$$

we have the orthogonality condition (see Jones, 1986, p. 228)

$$\int_{L_i} r\, \Psi^{(i)}_{mn}(r)\, \Psi^{(i)}_{ms}(r)\, \mathrm{d}r = \delta_{ns}, \quad n,s \in \mathbb{N}, \tag{2.10}$$

with $i=1$, where δ_{ns} is the Kronecker delta.

Similarly, for region II we let j_{mn} be the nth non-negative zero of $J_m(\eta)$ and define $\mu_{mn} b = j_{mn}$. We then define

$$\Psi^{(2)}_{mn}(r) = p^{(2)}_{mn}\ J_m(\mu_{mn} r), \quad n \in \mathbb{N}, \tag{2.11}$$

where

$$p^{(2)}_{mn} = \frac{2^{1/2}}{b\ J_{m+1}(\mu_{mn} b)}, \tag{2.12}$$

which satisfies (2.3) and the orthogonality condition (2.10) with $i=2$.

For region III we let $\lambda_{mn} d = j_{m,n+1}$, and define

$$\Psi^{(3)}_{mn}(r) = p^{(3)}_{mn}\ J_m(\lambda_{mn} r) \quad n \in \mathbb{N}_0, \tag{2.13}$$

where

$$p^{(3)}_{mn} = \frac{2^{1/2}}{d\ J_{m+1}(\lambda_{mn} d)}. \tag{2.14}$$

Then, $\Psi^{(3)}_{mn}$ satisfies (2.4) and the orthogonality condition (2.10) with $i=3$.

The appropriate eigenfunction expansions for $\hat{\phi}$ are now

$$\hat{\phi}_1(r,x)=\sum_{n=1}^{\infty} U_{mn}^{(1)}\frac{e^{-\alpha_{mn}(x-a)}}{-\alpha_{mn}}\Psi_{mn}^{(1)}(r), \quad \alpha_{mn}=(\nu_{mn}^2-k^2)^{1/2}, \tag{2.15}$$

$$\hat{\phi}_2(r,x)=\sum_{n=1}^{\infty} U_{mn}^{(2)}\frac{e^{-\beta_{mn}(x-a)}}{-\beta_{mn}}\Psi_{mn}^{(2)}(r), \quad \beta_{mn}=(\mu_{mn}^2-k^2)^{1/2}, \tag{2.16}$$

$$\hat{\phi}_3(r,x)=\sum_{n=0}^{\infty} U_{mn}^{(3)}\frac{\cosh\gamma_{mn}x}{\gamma_{mn}\sinh\gamma_{mn}a}\Psi_{mn}^{(3)}(r), \quad \gamma_{mn}=(\lambda_{mn}^2-k^2)^{1/2}. \tag{2.17}$$

For decay down the guide we require α_{mn} and β_{mn} to be real and positive for all n, and so we must have

$$kd<\nu_{m1}d \quad \text{and} \quad kd<\mu_{m1}d. \tag{2.18}$$

So as to allow one wave-like mode in the inner region, we also require γ_{m0} to be purely imaginary, but γ_{mn} to be real and positive for all other values of n, and hence

$$kd>\lambda_{m0}d=j_{m1}. \tag{2.19}$$

We therefore anticipate that a necessary condition for the existence of bound states is

$$j_{m1}<kd<\min(\mu_{m1}d,\nu_{m1}d). \tag{2.20}$$

A. Bound states below the first cutoff

We now use the continuity conditions (2.7) and proceed as in paper I. We obtain

$$U_{ms}^{(3)}=\sum_{n=1}^{\infty} U_{mn}^{(1)}\ d_{ns}+\sum_{n=1}^{\infty} U_{mn}^{(2)}\ e_{ns}, \quad s\in\mathbb{N}_0, \tag{2.21}$$

$$U_{ms}^{(3)}\frac{\coth\gamma_{ms}a}{\gamma_{ms}}=\sum_{n=1}^{\infty}\frac{U_{mn}^{(1)}}{-\alpha_{mn}}d_{ns}+\sum_{n=1}^{\infty}\frac{U_{mn}^{(2)}}{-\beta_{mn}}e_{ns}, \quad s\in\mathbb{N}_0, \tag{2.22}$$

where we have defined

$$d_{ns}=\frac{1}{d}\int_{L_1} r\Psi_{mn}^{(1)}(r)\Psi_{ms}^{(3)}(r)\,\mathrm{d}r, \tag{2.23}$$

$$e_{ns}=\frac{1}{d}\int_{L_2} r\Psi_{mn}^{(2)}(r)\Psi_{ms}^{(3)}(r)\,\mathrm{d}r. \tag{2.24}$$

Using various standard integrals, recurrence relations, and Wronskian relations for Bessel functions, we can show that, provided $\nu_{mn}\neq\lambda_{ms}$ and $\mu_{mn}\neq\lambda_{ms}$

$$d_{ns}=-\frac{2\,\nu_{mn}J_m(\lambda_{ms}b)}{(\nu_{mn}^2-\lambda_{ms}^2)\,\pi^{1/2}d\,J_{m+1}(\lambda_{ms}d)}\left(\frac{J_m^2(\nu_{mn}b)}{J_m^2(\nu_{mn}d)}-1\right)^{-1/2}, \quad s\in\mathbb{N}_0,\ n\in\mathbb{N}, \tag{2.25}$$

$$e_{ns}=\frac{2\,\mu_{mn}J_m(\lambda_{ms}b)}{d\,J_{m+1}(\lambda_{ms}d)\,(\mu_{mn}^2-\lambda_{ms}^2)}, \quad s\in\mathbb{N}_0,\ n\in\mathbb{N}. \tag{2.26}$$

Eliminating $U^{(3)}_{mn}$ from (2.21) and (2.22) and using (2.25) and (2.26), we obtain after some simplification

$$\sum_{n=1}^{\infty} U_{mn}\left(\frac{1}{\alpha_{mn}-\gamma_{ms}}+\frac{\zeta_{ms}}{\alpha_{mn}+\gamma_{ms}}\right)-\sum_{n=1}^{\infty} V_{mn}\left(\frac{1}{\beta_{mn}-\gamma_{ms}}+\frac{\zeta_{ms}}{\beta_{mn}+\gamma_{ms}}\right)=0, \tag{2.27}$$

where $s\in\mathbb{N}_0$ and we have defined

$$U_{mn}=\frac{U^{(1)}_{mn}\,\nu_{mn}}{\pi^{1/2}\,\alpha_{mn}}\left(\frac{J_m^2(\nu_{mn}b)}{J_m^2(\nu_{mn}d)}-1\right)^{-1/2},\quad V_{mn}=\frac{U^{(2)}_{mn}\,\mu_{mn}}{\beta_{mn}},\ \text{and}\ \zeta_{ms}=\mathrm{e}^{-2\gamma_{ms}a}. \tag{2.28}$$

The singular behavior required by condition (2.6) again influences the asymptotic behavior of U_{mn} and V_{mn} as $n\to\infty$. As in paper I, we can show that the edge condition is satisfied if both $U_{mn}=O(n^{-1/2})$ and $V_{mn}=O(n^{-1/2})$ as $n\to\infty$.

We now use the residue calculus technique of Mittra and Lee (1971), exactly as in paper I; the details are different but the procedure is essentially the same as before. We will make just one remark. The standard infinite product representation of the gamma function can be used to show that

$$\prod_{n=1}^{\infty}\frac{\left(1-\dfrac{zd}{(n+m/2+3/4)\pi}\right)}{\left(1-\dfrac{zc}{n\pi}\right)\left(1-\dfrac{zb}{(n+m/2-1/4)\pi}\right)}=\frac{\Gamma(m/2+7/4)\ \Gamma(1-zc/\pi)\ \Gamma(m/2+3/4-zb/\pi)}{\Gamma(m/2+7/4-zd/\pi)\ \Gamma(m/2+3/4)}, \tag{2.29}$$

and then the asymptotic forms [see Abramowitz and Stegun, 1965, Eqs. (9.5.12) and (9.5.27)]

$$\lambda_{mn}d=j_{m,n+1}\sim(n+m/2+3/4)\pi+O(1/n), \tag{2.30}$$

$$\mu_{mn}b=j_{mn}\sim(n+m/2-1/4)\pi+O(1/n), \tag{2.31}$$

$$\nu_{mn}(d-b)\sim n\pi+O(1/n) \tag{2.32}$$

as $n\to\infty$ can be used together with Stirling's formula to derive the necessary asymptotic form for the function $f(z)$ equivalent to (3.18) of paper I.

The condition for the existence of bound states turns out to be

$$\gamma'_m(a-\Theta)=\chi_m+\sigma_m+(n-\tfrac{1}{2})\pi,\quad n\ \text{an integer}, \tag{2.33}$$

where

$$\Theta=\frac{1}{\pi}(b\ln(d/b)+c\ln(d/c)), \tag{2.34}$$

$$\chi_m=\sum_{n=1}^{\infty}\left(\tan^{-1}\left(\frac{\gamma'_m}{\gamma_{mn}}\right)-\tan^{-1}\left(\frac{\gamma'_m}{\alpha_{mn}}\right)-\tan^{-1}\left(\frac{\gamma'_m}{\beta_{mn}}\right)\right), \tag{2.35}$$

and

$$\sigma_m=\arg\left(1-\sum_{n=1}^{\infty}\frac{A_{mn}}{\gamma_{mn}+\mathrm{i}\gamma'_m}\right), \tag{2.36}$$

where the coefficients A_{mn} are the solutions to the exponentially convergent system of equations

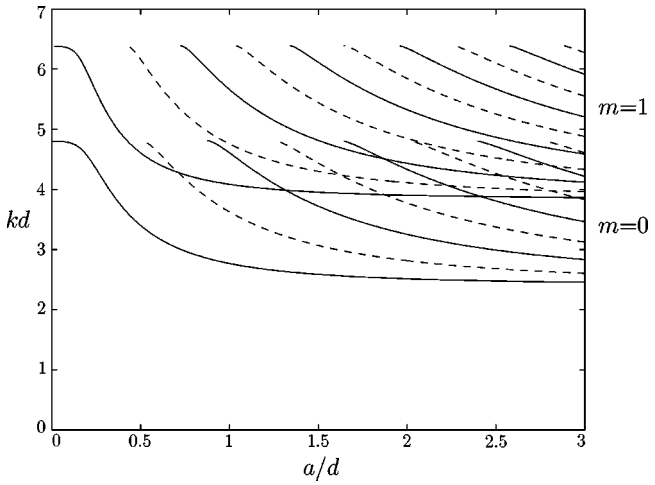

FIG. 2. Nondimensional bound-state energies for modes symmetric (—) and antisymmetric (– –) about $x=0$ plotted against a/d when $b/d=0.5$.

$$A_{ms}+D_{ms}\sum_{n=1}^{\infty}\frac{A_{mn}}{\gamma_{ms}+\gamma_{mn}}=D_{ms}, \quad s\in\mathbb{N}, \tag{2.37}$$

with

$$D_{ms}=2\gamma_{ms}\,\mathrm{e}^{2\gamma_{ms}(\Theta-a)}\frac{(\alpha_{ms}-\gamma_{ms})(\beta_{ms}-\gamma_{ms})}{(\alpha_{ms}+\gamma_{ms})(\beta_{ms}+\gamma_{ms})}$$
$$\times\prod_{\substack{n=1\\ n\neq s}}^{\infty}\frac{(1+\gamma_{ms}/\gamma_{mn})(1-\gamma_{ms}/\alpha_{mn})(1-\gamma_{ms}/\beta_{mn})}{(1+\gamma_{ms}/\alpha_{mn})(1+\gamma_{ms}/\beta_{mn})(1-\gamma_{ms}/\gamma_{mn})}. \tag{2.38}$$

For the case of antisymmetry about $x=0$, we replace the boundary condition (2.1) by

$$\phi=0 \quad \text{on } x=0, \quad 0<r<d, \tag{2.39}$$

and the equivalent condition to (2.33) is

$$\gamma_m'(a-\Theta)=\chi_m+\sigma_m'+n\pi, \quad n \text{ an integer}, \tag{2.40}$$

where χ_m and Θ are as before and σ_m' is as in (2.36) but with the coefficients A_{mn} coming from the system of equations

$$A_{ms}-D_{ms}\sum_{n=1}^{\infty}\frac{A_{mn}}{\gamma_{ms}+\gamma_{mn}}=-D_{ms}, \quad s\in\mathbb{N}. \tag{2.41}$$

B. Results

The results in this section are computed with the systems of equations (2.37) and (2.41) truncated to 5×5 systems. Typical results for the nondimensional bound-state energies when $m=0$ and 1 are shown in Figs. 2 and 3. In both figures the solid lines correspond to modes symmetric about $x=0$ and the dashed lines to modes antisymmetric about $x=0$.

In Fig. 2 nondimensional bound-state energies are plotted against a/d when $b/d=0.5$. As a/d increases, more and more modes appear alternately symmetric and antisymmetric about $x=0$ for each value of m. The upper and lower cutoffs for the existence of bound states are given by (2.20)

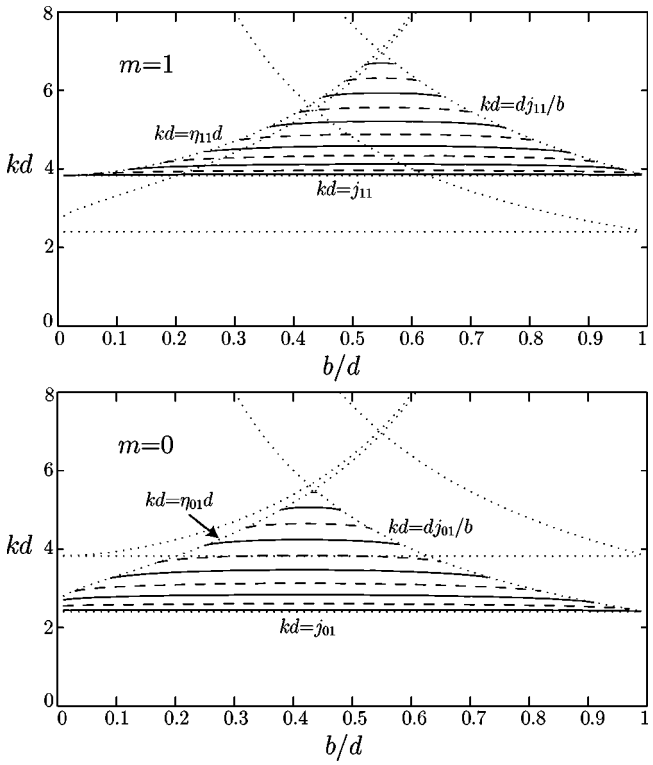

FIG. 3. Nondimensional bound-state energies for modes symmetric (—) and antisymmetric (– –) about $x=0$ plotted against b/d when $a/d=3$.

and depend on m. When $m=0$ the modes appear from the cutoff given by the minimum of $kd=j_{01}/0.5\approx 4.810$ and $kd=\nu_{01}d\approx 6.246$, i.e., $kd=2j_{01}$, and tend to $kd=j_{01}\approx 2.405$ as a/d increases. This minimum value changes, however, when $m=1$, as the upper cutoff becomes $kd=\nu_{11}d\approx 6.393$, which is less than $kd=2\,j_{11}\approx 7.663$. As a/d increases the modes corresponding to $m=1$ tend to $kd=j_{11}\approx 3.832$.

In Fig. 3 nondimensional bound-state energies are plotted against b/d when $a/d=3$. The upper plot corresponds to $m=1$ and the lower plot to $m=0$. The dotted lines appearing on both plots are the upper and lower cutoffs for the two different m values and show where the frequency ranges lie with respect to each other. When $b/d\to 0$ the only upper cutoff present for both plots is the one corresponding to $kd=\eta_{m1}$, whereas when $b/d\to 1$ the upper cutoff is shown by $kd=d\,j_{m1}/b$ for both values of m. When $m=0$ the upper cutoff changes from $kd=\eta_{01}d$ to $kd=j_{01}d/b$ when $b/d\approx 0.436$, and the largest number of modes appears at this value. Results for higher values of m show that as m increases, the value of b/d when the upper cutoff changes also increases.

III. LATERALLY COUPLED PLANAR WAVEGUIDES

We now turn our attention to the case where the two-dimensional laterally coupled waveguide considered in paper I is rotated about the y axis to produce a three-dimensional waveguide consisting of two planar layers of widths b and $c=d-b$ coupled laterally through a circular hole of radius a in the common boundary. We assume for convenience that $b>d/2$.

Circular cylindrical polar coordinates (r,θ,z) are introduced so that the waveguide is axisymmetric about $r=0$ and the planes lie at $z=0$, $z=b$ and $z=d$. We seek nontrivial solutions ϕ to

$$(\nabla^2+k^2)\,\phi=0,\quad 0<z<d,\quad r\geqslant 0\ \text{ except on } x=b,\quad r>a, \tag{3.1}$$

subject to the boundary conditions

$$\phi=0 \quad \text{on } z=0, \quad r\geqslant 0, \tag{3.2}$$

$$\phi=0 \quad \text{on } z=b, \quad r>a, \tag{3.3}$$

$$\phi=0 \quad \text{on } z=d, \quad r\geqslant 0, \tag{3.4}$$

and a radiation condition specifying that no waves propagate out to infinity

$$\phi\to 0 \quad \text{as } r\to\infty. \tag{3.5}$$

The guide is divided into three regions. Region I is $\{r,\theta,z: r>a, b<z<d\}$, region II is $\{r,\theta,z: r>a, 0<z<b\}$, and region III is $\{r,\theta,z: r<a, 0<z<d\}$. As the geometry is axisymmetric about $r=0$, we are able to look for a mode with angular variation $\cos m\theta$, $m\in\mathbb{N}_0$, and can write $\phi_i(r,\theta,z)=\hat{\phi}_i(r,z)\cos m\theta$ $(i=1,2,3)$, in each region and apply the continuity conditions

$$\hat{\phi}_i=\hat{\phi}_3, \quad \frac{\partial\hat{\phi}_i}{\partial r}=\frac{\partial\hat{\phi}_3}{\partial r}, \quad \text{on } L_i, \quad i=1,2, \tag{3.6}$$

where L_1 is $r=a, b<z<d$, L_2 is $r=a, 0<z<b$ and we write L_3 for $L_1\cup L_2$.

Suitable eigenfunction expansions in each region are

$$\hat{\phi}_1(r,z)=\sum_{n=1}^{\infty} U_{mn}^{(1)}\frac{K_m(\alpha_n r)}{\alpha_n K_m'(\alpha_n a)}\Psi_n^{(1)}(z), \quad \alpha_n=(\nu_n^2-k^2)^{1/2}, \tag{3.7}$$

$$\hat{\phi}_2(r,z)=\sum_{n=1}^{\infty} U_{mn}^{(2)}\frac{K_m(\beta_n r)}{\beta_n K_m'(\beta_n a)}\Psi_n^{(2)}(z), \quad \beta_n=(\mu_n^2-k^2)^{1/2}, \tag{3.8}$$

$$\hat{\phi}_3(r,z)=\sum_{n=0}^{\infty} U_{mn}^{(3)}\frac{I_m(\gamma_n r)}{\gamma_n I_m'(\gamma_n a)}\Psi_n^{(3)}(z), \quad \gamma_n=(\lambda_n^2-k^2)^{1/2}, \tag{3.9}$$

where I_m and K_m are modified Bessel functions and

$$\Psi_n^{(1)}(z)=2^{1/2}\sin\nu_n(d-z), \quad \nu_n=n\pi/c, \quad n\in\mathbb{N}, \tag{3.10}$$

$$\Psi_n^{(2)}(z)=2^{1/2}\sin\mu_n(b-z), \quad \mu_n=n\pi/b, \quad n\in\mathbb{N}, \tag{3.11}$$

$$\Psi_n^{(3)}(z)=2^{1/2}\sin\lambda_n(d-z), \quad \lambda_n=(n+1)\pi/d, \quad n\in\mathbb{N}_0, \tag{3.12}$$

which satisfy

$$\frac{1}{|L_i|}\int_{L_i}\Psi_n^{(i)}(y)\Psi_m^{(i)}(y)\,\mathrm{d}y=\delta_{mn}, \quad i=1,2,3. \tag{3.13}$$

As in paper I, we anticipate that a necessary condition for the existence of bound states will be

$$\pi<kd<\frac{d\pi}{b}, \tag{3.14}$$

since then γ_0 will be purely imaginary whereas α_n, β_n and γ_n, $n\in\mathbb{N}$, will all be real and positive. The mode corresponding to γ_0 will therefore be oscillatory in region III and all the other modes will decay away from the hole.

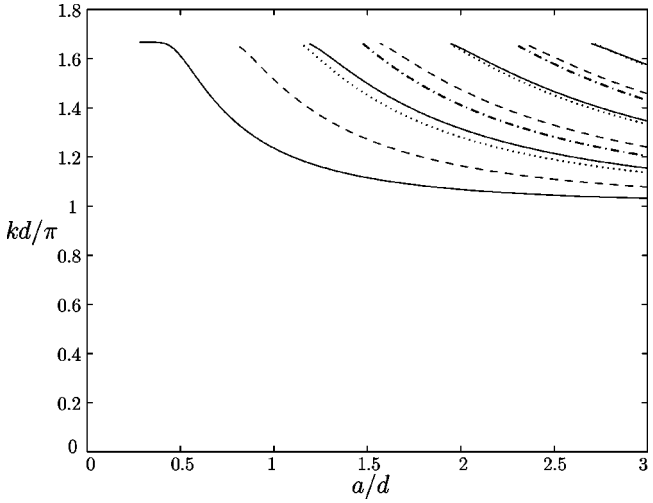

FIG. 4. Nondimensional bound-state energies, kd/π, plotted against a/d when $b/d=0.6$. The solid lines correspond to $m=0$, the dashed lines to $m=1$, the dotted lines to $m=2$, and the dot-dashed lines to $m=3$.

We now apply the continuity conditions (3.6), multiply each of the resulting equations by $\Psi_s^{(3)}, s\in\mathbb{N}_0$ and integrate over L_3, then eliminate $U_{ms}^{(3)}$ to obtain

$$\sum_{n=1}^{\infty} U_{mn}^{(1)} d_{ns}\left(\frac{I_m(\gamma_n a)}{\gamma_s I_m'(\gamma_s a)}-\frac{K_m(\alpha_n a)}{\alpha_n K_m'(\alpha_n a)}\right)+\sum_{n=1}^{\infty} U_{mn}^{(2)} e_{ns}\left(\frac{I_m(\gamma_n a)}{\gamma_s I_m'(\gamma_s a)}-\frac{K_m(\beta_n a)}{\beta_n K_m'(\beta_n a)}\right)=0,$$

$$s\in\mathbb{N}_0, \tag{3.15}$$

where d_{ns} and e_{ns} are given by

$$d_{ns}=\frac{1}{d}\int_{L_1}\Psi_n^{(1)}(y)\Psi_s^{(3)}(y)\,dy=\frac{2\nu_n(-1)^n\sin\lambda_s c}{d(\gamma_s^2-\alpha_n^2)},\quad s\in\mathbb{N}_0,\ \ n\in\mathbb{N}, \tag{3.16}$$

$$e_{ns}=\frac{1}{d}\int_{L_2}\Psi_n^{(2)}(y)\Psi_s^{(3)}(y)\,dy=\frac{2\mu_n\sin\lambda_s c}{d(\gamma_s^2-\beta_n^2)},\quad s\in\mathbb{N}_0,\ \ n\in\mathbb{N}. \tag{3.17}$$

Equation (3.15) is not amenable to the same residue calculus treatment as we have used in our other examples. Here, we solve it directly by truncating the value of n and $s+1$ with a truncation parameter N. We then have to find the values of kd for which the determinant of a (real) $2N\times 2N$ matrix is zero.

Figure 4 shows a typical set of nondimensional bound-state energies, kd/π, plotted against a/d when $b/d=0.6$. The results were computed using a truncation parameter $N=5$. The solid lines correspond to the modes when $m=0$, the dashed lines are when $m=1$, the dotted lines are when $m=2$, and the dot-dashed lines are for $m=3$. As the value of a/d is increased the bound states appear from the upper cutoff $kd=5\pi/3$ and tend to the lower cutoff $kd=\pi$. The results suggest that that bound states occur for all a/d except when the hole is small, and that as the value of m is increased the value of a/d below which modes do not exist increases.

However, Exner and Vugalter (1997) used variational techniques to show that for sufficiently small a/d there is just one bound state and that the ground-state eigenvalue, kd, then satisfies

$$\frac{d}{b}\left(1-\frac{1}{\pi^2}\exp(-c_1/a^3)\right)^{1/2}\leqslant kd\leqslant\frac{d}{b}\left(1-\frac{1}{\pi^2}\exp(-c_2/a^3)\right)^{1/2}, \tag{3.18}$$

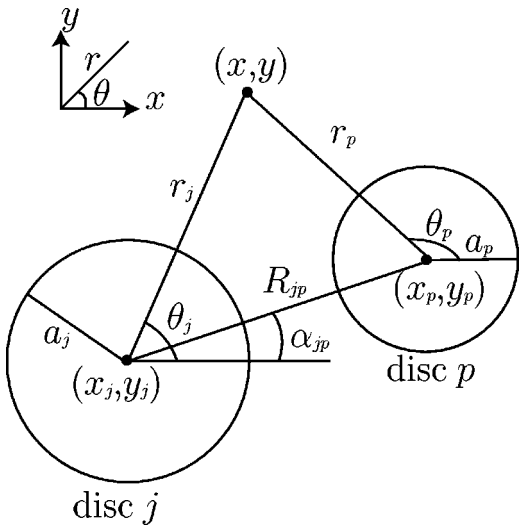

FIG. 5. Plan view of two disks.

for some positive c_1 and c_2. It is clear that for small windows, this will produce values of kd which differ from the upper cutoff by an extremely small amount and this explains why we were unable to compute bound-state energies when a/d is less than about 0.25.

It is fairly simple to extend the work above and consider the case of a pair of planar layers coupled laterally by a number of holes. For simplicity, we will consider the case where the two layers have the same width (i.e., $b/d=0.5$) and the additional symmetry allows us to consider the symmetric and antisymmetric parts of the solution independently. The antisymmetric part is trivial, and so the problem then reduces to that of a planar guide of width b with Dirichlet boundary conditions on both walls, except for a number of circular disks on one side on which Neumann conditions are applied. The method that we use to analyze multiple circular windows is a standard technique in studying the scattering of waves by arrays of circular cylinders; see, e.g., Linton and McIver (2001), Chap. 6.

We consider P ($\geqslant 1$) disks and introduce $P+1$ cylindrical polar coordinate systems, so that (r,θ,z) is centered at the origin and (r_j,θ_j,z), $j=1,\ldots,P$, are centered at the center of the jth disk, which is assumed to have radius a_j. The walls of the waveguide are at $z=0$ and $z=b$. The various parameters relating to the relative positions and sizes of the disks are shown in Fig. 5. The domain is divided up into $P+1$ parts and we represent the solution in the region above the jth disk by ϕ_j^I, $j=1,\ldots,P$ and the solution exterior to the disks by ϕ^{II}. We look for nontrivial solutions to the Helmholtz equation in the guide subject to the boundary conditions

$$\phi^{II}=0 \quad \text{on } z=0, \tag{3.19}$$

$$\phi_j^I=\phi^{II}=0 \quad \text{on } z=b, \quad j=1,\ldots,P, \tag{3.20}$$

$$\frac{\partial\phi_j^I}{\partial z}=0 \quad \text{on } z=0, \quad r_j<a_j, \quad j=1,\ldots,P, \tag{3.21}$$

$$\phi^{II}\to 0 \quad \text{as } r\to\infty. \tag{3.22}$$

We also need to apply continuity conditions at each region's boundary

$$\phi_j^I=\phi^{II}, \quad \frac{\partial\phi_j^I}{\partial r_j}=\frac{\partial\phi^{II}}{\partial r_j} \quad \text{on } r_j=a_j, \quad j=1,\ldots,P. \tag{3.23}$$

Separation of variables reveals that the appropriate eigenfunction expansions are

$$\phi_j^I = \sum_{m=-\infty}^{\infty} \sum_{n=0}^{\infty} A_{mn}^j \frac{I_m(\alpha_n r_j)}{\alpha_n I_m'(\alpha_n a_j)} \Psi_n^{(1)}(z)\, \mathrm{e}^{\mathrm{i}m\theta_j}, \quad j=1,\ldots,P, \tag{3.24}$$

$$\phi^{II} = \sum_{p=1}^{P} \sum_{m=-\infty}^{\infty} \sum_{n=0}^{\infty} B_{mn}^p \frac{K_m(\beta_n r_p)}{\beta_n K_m'(\beta_n a_p)} \Psi_n^{(2)}(z)\, \mathrm{e}^{\mathrm{i}m\theta_p}, \tag{3.25}$$

where $\alpha_n = (\mu_n^2 - k^2)^{1/2}$, $\beta_n = (\nu_n^2 - k^2)^{1/2}$, and

$$\Psi_n^{(1)}(z) = 2^{1/2} \sin \mu_n (b-z), \quad \mu_n = (n+\tfrac{1}{2})\pi/b, \quad n \in \mathbb{N}_0, \tag{3.26}$$

$$\Psi_n^{(2)}(z) = 2^{1/2} \sin \nu_n z, \quad \nu_n = n\pi/b, \quad n \in \mathbb{N}. \tag{3.27}$$

If we restrict the energy so that

$$\pi < kd < 2\pi, \tag{3.28}$$

then α_0 is purely imaginary, whereas α_n and β_n, $n \in \mathbb{N}$ will all be real and positive. This restriction allows for wave-like modes local to each disk, with decay as r becomes large.

In order to apply the continuity conditions (3.23), the eigenfunction expansion in region *II* must be written in terms of the coordinates r_j and θ_j. This can be achieved using Graf's addition theorem, which shows that provided $r_j < R_{jp}$ for all p, we can write

$$\begin{aligned}\phi^{II}(r_j,\theta_j,z) = &\sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} B_{mn}^j \frac{K_m(\beta_n r_j)}{\beta_n K_m'(\beta_n a_j)} \Psi_n^{(2)}(z)\, \mathrm{e}^{\mathrm{i}m\theta_j} \\ &+ \sum_{\substack{p=1 \\ p\neq j}}^{P} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{s=-\infty}^{\infty} B_{mn}^p \frac{I_s(\beta_n r_j)}{\beta_n K_m'(\beta_n a_j)} K_{m-s}(\beta_n R_{jp})\, \mathrm{e}^{\mathrm{i}s\theta_p} \Psi_n^{(2)}(z)\, \mathrm{e}^{\mathrm{i}(m-s)\alpha_{jp}},\end{aligned} \tag{3.29}$$

where R_{jp} is the distance between the centers of disks j and p, and α_{jp} is the angle of the center of disk p from disk j, measured as shown in Fig. 5.

We can then apply the matching conditions (3.23) and convert the resulting equations into an infinite system by multiplying each by $\Psi_t^{(1)}(z)\mathrm{e}^{-\mathrm{i}w\theta_j}$, $t \in \mathbb{N}_0$, $w \in \mathbb{Z}$, $j=1,\ldots,P$, and integrating over z in $(0,b)$ and θ_j in $(0, 2\pi)$. We obtain, after eliminating A_{mn}^j

$$\sum_{p=1}^{P} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} B_{mn}^p Z_{nmp,twj} = 0, \quad t \in \mathbb{N}_0, \quad w \in \mathbb{Z}, \quad j=1,\ldots,P, \tag{3.30}$$

where

$$Z_{nmp,twj} = \begin{cases} d_{tt} X_{twj} \delta_{mw} \delta_{nt} & p = j, \\ d_{nt} Y_{nmp,twj} & p \neq j, \end{cases} \tag{3.31}$$

$$X_{twj} = X_{t(-w)j} = \frac{I_w(\alpha_t a_j)}{\alpha_t I_w'(\alpha_t a_j)} - \frac{K_w(\beta_t a_j)}{\beta_t K_w'(\beta_t a_j)}, \tag{3.32}$$

$$Y_{nmp,twj} = K_{m-w}(\beta_n R_{jp})\, \mathrm{e}^{\mathrm{i}(m-w)\alpha_{jp}} \left(\frac{I_w(\alpha_t a_j) I_w'(\beta_n a_j)}{\alpha_t I_w'(\alpha_t a_j) K_m'(\beta_n a_j)} - \frac{I_w(\beta_n a_j)}{\beta_n K_m'(\beta_n a_j)} \right), \tag{3.33}$$

and

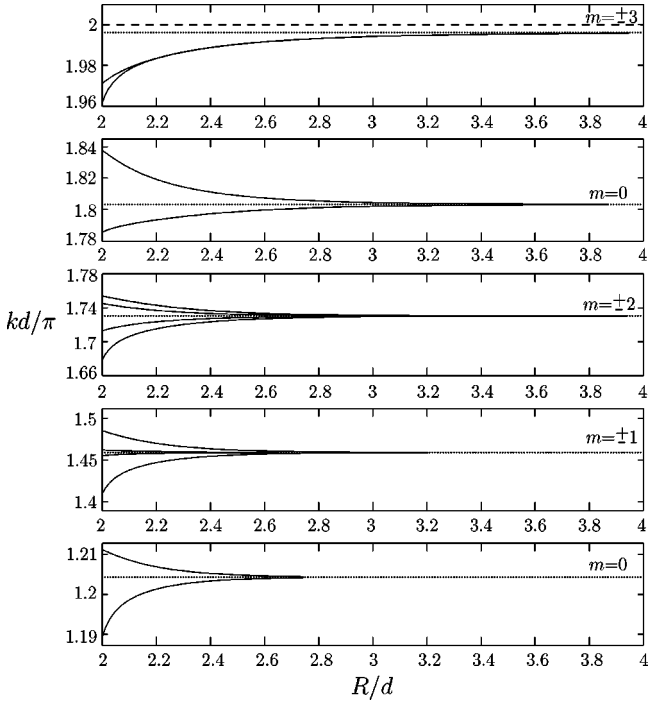

FIG. 6. Nondimensional bound-state energies, kd/π, plotted against R/d for the case of two identical windows with radius $a=d$. The dotted lines correspond to the bound states from the single-disk case with $a/d=1$ and are labeled with the appropriate values of m. The dashed line corresponds to the upper cutoff.

$$d_{nt}=\frac{2}{d}\int_0^{d/2}\Psi_n^{(2)}(z)\Psi_t^{(1)}(z)\,\mathrm{d}z=\frac{4\nu_n(-1)^t}{d(\mu_t^2-\nu_n^2)}. \tag{3.34}$$

A. Results

We solve (3.30) by introducing truncation parameters M and N so that m and w vary between $\pm M$, and n and $t+1$ vary between 1 and N. Then, we write

$$\lambda_1=n+N(m+M)+N(2M+1)(p-1), \tag{3.35}$$

$$\lambda_2=1+t+N(w+M)+N(2M+1)(j-1), \tag{3.36}$$

so that any positive integer λ_i between 1 and $N(2M+1)P$ corresponds to a unique triple (n,m,p) for $i=1$, or (t,w,j) for $i=2$. To find a solution of (3.30) we are required to find frequencies kd so that the determinant of the resulting $N(2M+1)P\times N(2M+1)P$ matrix is zero. For the results below, truncation parameters $N=5$ and $M=3$ were used.

We consider the case of two circular windows. In this situation the bound-state energies will be independent of the angle between the centers of the two disks (α_{12} and α_{21}, in Fig. 5). That this is the case can be demonstrated as follows. The matrix Z has a 2×2 block structure and, if we multiply the rows in the blocks corresponding to $j=1$ by $\exp(-\mathrm{i}m\alpha_{12})$, the rows in the blocks corresponding to $j=2$ by $\exp(-\mathrm{i}m\alpha_{21})$, the columns in the blocks corresponding to $p=1$ by $\exp(\mathrm{i}w\alpha_{21})$, and the columns in the blocks corresponding to $p=2$ by $\exp(\mathrm{i}w\alpha_{12})$, the resulting matrix is independent of the angles α_{12} and α_{21} and its determinant is a nonzero multiple of the determinant of Z and so will vanish for the same values of kd.

Figure 6 shows the nondimensional bound-state energies, kd/π plotted against nondimensional separation R/d for two identical windows with radius $a=d$. The dotted lines are the bound-state energies from the single-window case when $a/d=1$ and are labeled with the appro-

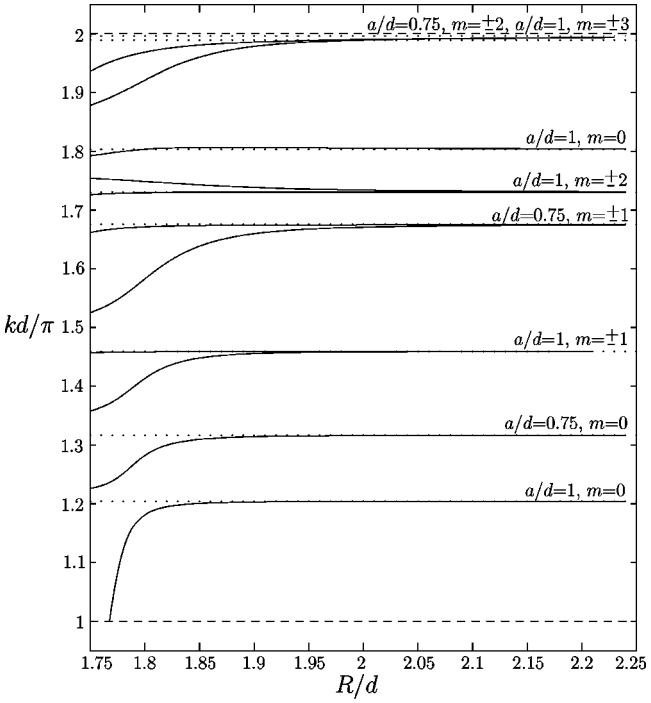

FIG. 7. Nondimensional bound-state energies, kd/π, plotted against R/d for the case of two windows of radii $a/d=1$ and $a/d=0.75$. The dotted lines correspond to the bound states from the single-window case with $a/d=1$ and $a/d=0.75$ and are labeled with the appropriate values of m. The dashed lines correspond to the upper and lower cutoffs.

priate values of m. They represent the limits for the energies as $R/d\to\infty$. The dashed line is the upper cutoff $kd=2\pi$. All possible modes appear in the figure. However, if we took a larger value of a/d we would have to use a larger truncation parameter M to find all the modes.

When the two disks are touching, i.e., when $R/d=2$, there are 14 bound states. There are two modes around each dotted line corresponding to $m=0$ and four modes around the other dotted lines (two for the positive value of m and two for the negative value of m). The exception occurs when $m=\pm 3$, as this mode is close to the upper cutoff and so only a single mode appears below the dotted line for each m. As the value of R/d is increased, which means that the disks are moved apart, each pair of modes converges towards the limiting case.

Figure 7 shows the nondimensional bound-state energies, kd/π plotted against R/d for two circular windows for which $a/d=1$ and $a/d=0.75$, respectively. The dotted lines are the bound-state energies from the single-window cases when $a/d=1$ and $a/d=0.75$, and are labeled with the appropriate values of m and again represent the limits for the energies as $R/d\to\infty$. The dashed lines are the upper and lower cutoffs. All possible modes appear in the figure. Between the two cutoffs we find that there are five modes from the single-window case with $a/d=1$ and three modes from the single-window case when $a/d=0.75$. When the two windows are touching, i.e., when $R/d=1.75$, the bound-state energies are very different from the single-window values, but as the separation is increased, the energies quickly approach the single-window values. Similar types of results were found by Evans and Porter (1997), who computed trapped modes in the vicinity of multiple cylinders in a channel.

IV. CONCLUSION

We have computed bound-state energies below the first cutoff in two three-dimensional coupled waveguides, each obtained from the two-dimensional configuration considered in paper I by rotating the geometry about a different axis.

First, we have studied bound states in a waveguide consisting of two concentric circular cylindrical waveguides coupled by a finite length gap along the axis of the inner cylinder. The same residue calculus method which was used in paper I was used to compute bound-state energies below the first cutoff for wave propagation down the guide. We were able to look for modes with a given angular variation $\cos m\theta$, $m \in \mathbb{N}_0$, and the bound states found are either symmetric or antisymmetric about the line of symmetry perpendicular to the axis of the cylinder. The available energy band for bound states is dependent on the values of m and the ratio of the two radii. The results show that bound states occur for any value of the gap length and ratio of radii, and the energies increase as m increases.

Second, we have considered the problem in which a pair of planar layers is coupled laterally by a circular hole. The sophisticated residue calculus theory is not available in this case, but we were able to compute bound states by searching for the zeros of the determinant of a matrix found from a mode-matching approach. For this problem we can again consider a given angular variation $\cos m\theta$, $m \in \mathbb{N}_0$, and find modes in each case.

We then extended the theory to cover the case of a number of circular windows connecting two planar guides of equal width and presented results for two circles, both when they have the same radius and when they do not. In both situations we find that when the windows are far apart the bound states are equivalent to those occurring in the single-window cases, but that the energies vary considerably as the windows are moved closer together.

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The magnetic Weyl calculus

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In the presence of a variable magnetic field, the Weyl pseudodifferential calculus must be modified. The usual modification, based on "the minimal coupling principle" at the level of the classical symbols, does not lead to gauge invariant formulas if the magnetic field is not constant. We present a gauge covariant quantization, relying on the magnetic canonical commutation relations. The underlying symbolic calculus is a deformation, defined in terms of the magnetic flux through triangles, of the classical Moyal product. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The correspondence principle of quantum mechanics asks that for a given physical system there should be a systematic way to convert classical observables into quantum observables. We use for this the rather vague term of *quantization*. For many given systems a true, manageable quantization is problematic, but there are important situations in which commonly accepted solutions exist. The purpose of the present article is to propose what we think to be the correct solution for the case of a nonrelativistic spinless particle, moving in $\mathbb{R}^N$, in the presence of a variable magnetic field. From the mathematical point of view, our results may be considered as a first step towards a quantization of symplectic manifolds.

General principles assert essentially that classical observables are functions in phase space, while quantum observables should be self-adjoint operators in some Hilbert space. Rather often, for some basic observables (positions, momenta,...) the prescription is either essentially unique (may be due to some commutation relations), or at least generally accepted. Thus, for many physical systems, quantization of all phase-space functions could be regarded as a sort of functional calculus. But since, as a rule, the basic observables do not commute, one cannot rely on the usual spectral theory to define this functional calculus. Roughly, quantization may be seen as the mathematical problem of defining functions of several noncommuting self-adjoint operators. Of course, the features of the physical system both impose constraints and offer empirical suggestions with respect to this procedure.

In the absence of any magnetic field, a nonrelativistic spinless particle moving in $\mathbb{R}^N$ is quantized through the Weyl pseudodifferential calculus. If f is a suitable function ("symbol") defined on the phase space $\mathbb{R}^{2N}$, the corresponding operator is defined to act in the Hilbert space $L^2(\mathbb{R}^N)$ by the formula

$$[\mathfrak{Op}(f)u](x) := \int_{\mathbb{R}^{2N}} dy \quad dp \quad e^{i(x-y)\cdot p} f\left(\frac{x+y}{2}, p\right) u(y). \tag{1}$$

In a certain sense (which can be made precise and which will be discussed below), we may write $\mathfrak{Op}(f) = f(Q,P)$ and interpret it as the action on the symbol f of the functional calculus associated to the family of operators $(Q_1,\ldots,Q_N,P_1,\ldots,P_N)$, where Q_j is the multiplication by the jth coordinate and $P_j := -i\partial_j$. The well-known rules of commutation between these position

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and momentum quantum observables play a decisive role in determining the explicit formula above. They are thus also basic in deducing the explicit product rule $(f,g)\mapsto f\circ g$ and involution $f\mapsto f^\circ$ leading to $\mathfrak{Op}(f)\mathfrak{Op}(g)=\mathfrak{Op}(f\circ g)$ and $\mathfrak{Op}(f)^*=\mathfrak{Op}(f^\circ)$.

When a magnetic field B is turned on, we are faced with the problem of modifying the formula for $\mathfrak{Op}(f)$ in a way taking into account the presence of the magnetic field in a correct, physical way. A mistaken procedure which appears from time to time in the literature is the following: One chooses a vector potential A corresponding to the magnetic field ($B=dA$) and, by an (unjustified) application of the minimal coupling principle, one sets $\mathfrak{Op}_A(f):=\mathfrak{Op}(f_A)$, with $f_A(x,p):=f(x,p-A(x))$. This is meant to be the action on f of the functional calculus associated with the family $Q_1,\ldots,Q_N,\Pi_1,\ldots,\Pi_N$, where $\Pi_j:=P_j-A_j(Q)$ is the jth component of the vector potential. But the resulting formula

$$[\mathfrak{Op}_A(f)u](x):=\int_{\mathbb{R}^{2N}}dy\quad dk\quad e^{i(x-y)\cdot k}f\left(\frac{x+y}{2},k-A\left(\frac{x+y}{2}\right)\right)u(y) \tag{2}$$

$$=\int_{\mathbb{R}^{2N}}dy\quad dp\quad e^{i(x-y)\cdot p}e^{i(x-y)\cdot A((x+y)/2)}f\left(\frac{x+y}{2},p\right)u(y) \tag{3}$$

cannot be the right one, since it lacks gauge covariance: If one chooses another vector potential A' associated to B, differing from the initial one by the gradient of a scalar function, $A'=A+\nabla\rho$, then *the expected formula* $e^{i\rho}\mathfrak{Op}_A(f)e^{-i\rho}=\mathfrak{Op}_{A'}(f)$ *does not hold*. In fact, this formula is restored if one replaces the phase factor $e^{i(x-y)\cdot A((x+y)/2)}$ by $e^{i(x-y)\cdot\int_0^1 dsA((1-s)x+sy)}$. It is reassuring to note that $-(x-y)\cdot\int_0^1 dsA((1-s)x+sy)$ is in fact the circulation $\Gamma^A([x,y])$ of the vector potential A through the segment leading from x to y. Thus the formula we propose instead of (2) is

$$[\mathfrak{Op}^A(f)u](x):=\int_{\mathbb{R}^{2N}}dy\quad dp\quad e^{i(x-y)\cdot p}e^{-i\Gamma^A([x,y])}f\left(\frac{x+y}{2},p\right)u(y). \tag{4}$$

The main purpose of our article is to give an explanation of these facts. As a prologue for doing this, in the next section we review some facts related to canonical commutation relations and Weyl calculus when no magnetic field is present. The main topic will be the justification of the formula for $\mathfrak{Op}(f)$ as a sort of integrated form of *the Weyl system*, which is a family of unitary operators $\{W(\xi)\}_\xi$ indexed by the points of the phase space and containing the relevant information on the commutation relations between the operators Q and P. We claim no originality (see, for example, Ref. 18); we include this here because it seems to be an argument largely ignored, which is basic to our approach. The symbolic calculus beyond the Weyl prescription is the famous Moyal product. Other references emphasizing the connection between quantum mechanics and pseudodifferential theory are Refs. 15 and 10.

When a magnetic field is present, the Weyl system has to be modified. Instead of the group of translations, appearing naturally in the formula giving $W(\xi)$ [see (8)], one has to work with the magnetic translations, forming a sort of generalized projective representation of $\mathbb{R}^N$. This is presented in the Sec. III.

In Sec. IV, the formula $\mathfrak{Op}^A$ for the functional calculus with magnetic field is deduced. For this we apply the same strategy as in Sec. II, but using now the magnetic Weyl system, introduced in Sec. III. The setting relies on the choice of a vector potential, but now gauge covariance is available; equivalent vector potentials lead to unitarily equivalent operators. The basic expression for $\mathfrak{Op}^A(f)$ requires rather strong conditions on the function f. But for large classes of magnetic fields one can extend it, as in the nonmagnetic case, to all tempered distributions, by a suitable interpretation of $\mathfrak{Op}^A(f)$ as a linear continuous operator from the Schwartz space $\mathcal{S}(\mathbb{R}^N)$ to its dual. This is based on a study of the distribution kernel of this operator. These and some other fundamental facts are also considered in Sec. IV.

Beyond these operators lies a symbolic calculus which is *manifestly gauge invariant*, being defined only in terms of the magnetic field. The composition is a magnetic correction of the Moyal product, while the involution is just the usual complex conjugation of functions. In Sec. V we study this symbolic calculus. Once again an important problem is to extend the formulas when obvious integrability conditions are not satisfied. This is a more complicated task for the product than it was for the quantization itself, especially if one aims at obtaining *-algebras. We postpone the application of the machinery of oscillatory integrals and classical symbol function spaces to a future article. For our present purposes the strategy of extension by duality methods (see Refs. 13 and 14 for the nonmagnetic case) is more fruitful. It will lead to a large, interesting *-algebra of distributions which will be called *the magnetic Moyal algebra*.

Of course, for certain problems, a well-justified norm on (restricted) *-algebras of symbols could be very useful. It happens that this is easier to achieve after performing a partial Fourier transform. Surprisingly, one naturally encounters certain C^*-algebras which were studied in pure mathematics, with little connection with physics. These are special types of twisted crossed products, associated to twisted actions of $\mathbb{R}^N$ on suitable Abelian C^*-algebras of position observables. They were already related to quantum magnetic fields in Ref. 23; see also Refs. 11, 5 and 6 for related works. In a future publication we shall extend their study and outline the connection with our pseudodifferential calculus.

Concerning the difference between the expressions (2) [or (3)] and (4) some comments are necessary. In Sec. IV D we shall outline some situations when they give the same result. By admitting the convenient assumption that the components of A are smooth functions with tempered growth, both (2) and (4) can be extended to any tempered distribution f. Then *we shall have* $\mathfrak{Op}_A(f)=\mathfrak{Op}^A(f)$ *for all* f *if and only if* A *is linear* (this is one of the most important cases appearing usually in the literature). Remark that this condition corresponds to a constant magnetic field, but *it is not gauge invariant*: for some other A' with $dA'=B=\text{const}$, $\mathfrak{Op}_{A'}$ and $\mathfrak{Op}^{A'}$ will be different! (The pseudodifferential calculus corresponding to a linear A was developed in Ref. 7 in connection with some problems in pure PDE theory; in fact the term ''magnetic field'' is never explicitly mentioned.) One will also have $\mathfrak{Op}_A(f)=\mathfrak{Op}^A(f)$ *for any* A if f is a polynomial of order $\leqslant 2$. The most studied magnetic operators are the Schrödinger magnetic Hamiltonians $(P-A(Q))^2+V(Q)$, cf. Ref. 1 and 24, for instance. They are obtained by quantizing the sum between a quadratic function depending only on p and a function depending only on x, so no care is needed in this case. However, even their study may involve applying the Weyl calculus to more complicated symbols. Anyhow, for polynomials of order three in p, (2) and (4) already give different results. We remark that using the Weyl calculus coupled with the minimal coupling principle [as in (2)] for a nonconstant magnetic field and a complicated symbol is still legitimate as long as this is a technical tool and not the quantization of the classical observable represented by the symbol. This is often the case in solid state physics, in arguments concerning the Peierls substitution, as in Refs. 12 and 29.

Our feeling is that the magnetic Weyl calculus elaborated in this article is both an interesting mathematical object and a significant formalism for theoretical physics. From the mathematical point of view, we consider it interesting to use our calculus for some specific classes of symbols and obtain more detailed results and also to connect it with strict deformation quantization. Moreover, obtaining precise estimations on the C^*-norm of the objects in the Moyal algebra and some variants of Calderon–Vaillancourt theorems is of much interest in spectral analysis, deformation quantization and semiclassical limit. These results may be then applied for quantum Hamiltonians (of Schrödinger or relativistic type) and obtain spectral and propagation information and to study their semiclassical limit and its dependence on the chosen quantization procedure. In this article we intended to be accessible to people that are only vaguely familiar with pseudodifferential theory; more technical developments or applications are deferred to future works. We were encouraged in this attitude by a discussion with Joseph Avron and Omri Gat. A paper devoted to some C^*-algebras aspects of our magnetic Weyl calculus is in preparation in collaboration with Serge Richard.

II. CANONICAL COMMUTATION RELATIONS AND PSEUDODIFFERENTIAL CALCULUS WITHOUT MAGNETIC FIELDS

One of the main virtues of the standard pseudodifferential calculus (in Weyl form) lies in the fact that it gives an answer to a fundamental problem in quantum mechanics. It can be figured out as the quantization of a physical system composed of a nonrelativistic particle without internal structure, moving in a Euclidean configuration space. We review this topic briefly, since it gives a solid motivation for our later treatment of the case in which a magnetic field is added. Further details may be found in Refs. 10 and 18, for example. At the root of this approach lie the canonical commutation relations satisfied by the basic observables of the system, the positions and the momenta, and this is the main point we want to emphasize.

A. Framework

We have in view an N-dimentional nonrelativistic particle without internal structure (called simply *a particle*) that is described classically in *the phase space* $\Xi := X \times X^\star$, where $X := \mathbb{R}^N$ is *the configuration space* and $X^\star$ is its dual. The space Ξ is naturally endowed with the symplectic form $\sigma: \Xi \times \Xi \to \mathbb{R}$ given by

$$\sigma((q',p'),(q'',p'')) := q'' \cdot p' - q' \cdot p'',$$

where $q \cdot p$ denotes the canonical pairing on $X \times X^\star$.

The classical observables are (smooth) real functions defined on Ξ. A particular role is played by the Poisson bracket

$$\{f,g\} := \sigma(\nabla f, \nabla g) = \sum_{j=1}^{N} (\partial_{p_j} f \ \partial_{q_j} g - \partial_{p_j} g \ \partial_{q_j} f).$$

Real functions of class C^∞ on the phase space form an infinite-dimentional Lie algebra under the pointwise vector operations and the Poisson bracket.

The associated quantum system is described on the Hilbert space $\mathcal{H} = L^2(X)$ in terms of the family of self-adjoint operators $(Q_j)_{j=1,\ldots,N}$ and $(P_j)_{j=1,\ldots,N}$ (here Q_j is the operator of multiplication with the jth component of the variable in $\mathcal{H}$ and $P_j := -i\partial_j$). The operators $(Q_j, P_j)_{j=1,\ldots,N}$ are the quantum version of the classical observables position and momenta, given by the the canonical variables in phase space $q_1, \ldots, q_N, p_1, \ldots, p_N$. These canonical variables satisfy the relations

$$\{q_i, q_j\} = 0, \ \{p_i, p_j\} = 0, \ \{p_i, q_j\} = \delta_{ij}, \quad i,j = 1, \ldots, N,$$

and the corresponding quantum observables should satisfy at their turn

$$i[Q_i, Q_j] = 0, \ i[P_i, P_j] = 0, \ i[P_i, Q_j] = \delta_{ij}, \ i,j = 1, \ldots, N,$$

as they actually do, at least formally.

B. The Weyl system

In principle, the choice of the Hilbert space $L^2(X)$ and of the explicit form of the operators Q_j and P_j should be justified. It is widely accepted the vague prescription that to the canonical variables q_j and p_j one should ascribe self-adjoint operators $\mathfrak{Op}(q_j)$ and $\mathfrak{Op}(p_j)$ acting in some Hilbert space $\mathcal{H}$, satisfying

$$i[\mathfrak{Op}(q_i), \mathfrak{Op}(q_j)] = 0, \ i[\mathfrak{Op}(p_i), \mathfrak{Op}(p_j)] = 0, \ i[\mathfrak{Op}(p_i), \mathfrak{Op}(q_j)] = \delta_{ij}, \ i,j = 1, \ldots, N. \quad (5)$$

But an axiomatic approach relying on this formula is hard to conceive. The typical difficulties related to the (inevitable) nonboundedness of the operators $\mathfrak{Op}(q_j)$ and $\mathfrak{Op}(p_j)$ cannot be solved by *a priori* arguments.

For this and for several other reasons, it is preferable to rephrase all in terms of bounded operators. For $q \in X$ and $p \in X^\star$, let us set $U(q) := e^{-iq\cdot P}$ and $V(p) := e^{-iQ\cdot p}$. These are unitary operators in $L^2(X)$ given explicitly by

$$[U(q)u](y) = u(y-q) \quad \text{and} \quad [V(p)u](y) = e^{-iy\cdot p}u(y), \quad u \in L^2(X),\ y \in X. \tag{6}$$

The maps $q \mapsto U(q)$ and $p \mapsto V(p)$ are strongly continuous unitary representations of X, respectively X^*, in $L^2(X)$ and *the Weyl form of the canonical commutation relations,*

$$U(q)V(p) = e^{iq\cdot p}\ V(p)U(q), \quad q \in X,\ p \in X^\star, \tag{7}$$

holds. Now there is no ambiguity in addressing the abstract problem of the classification of triples $(\mathcal{H},U,V)$, where $\mathcal{H}$ is a Hilbert space and $U: X \to \mathcal{U}(\mathcal{H})$, $V: X^\star \to \mathcal{U}(\mathcal{H})$ are strongly continuous unitary representations satisfying (7). And there is a simple answer, given by the Stone–von Neumann Theorem (for a more explicit statement and for the proof we look to Ref. 10): If one also assumes irreducibility of the family $\{U(q),V(p) \mid q \in X, p \in X^\star\}$, then any solution is unitarily equivalent to (6) (which is called *the Schrödinger representation*). And a non-irreducible triple is just a multiple of this Schrödinger representation.

A convenient way to condense the two objects U and V into a single one is to define *the Weyl system* $\{W(\xi) \mid \xi \in \Xi\} \subset \mathcal{U}(\mathcal{H})$ by

$$W(q,p) := e^{(i/2)\,q\cdot p}\ U(-q)V(p) = e^{-(i/2)\,q\cdot p}\ V(p)U(-q), \quad q \in X, \quad p \in X^\star. \tag{8}$$

A short calculation shows that W satisfies

$$W(\xi)W(\eta) = e^{(i/2)\,\sigma(\xi,\eta)}\ W(\xi+\eta), \qquad \xi,\eta \in \Xi, \tag{9}$$

i.e., W is a projective representation of the group Ξ with two-cocycle (phase factor) $e^{(i/2)\,\sigma}$.

Of course, W can be defined for any abstract triple $(\mathcal{H},U,V)$. But, as a consequence of the Stone–von Neumann Theorem, it is enough to work with the Schrödinger representation. The corresponding W will be called *the Schrödinger Weyl system* and is explicitly given on $L^2(X)$ by

$$[W(q,p)u](y) = e^{-i((1/2)\,q+y)\cdot p}\ u(y+q). \tag{10}$$

The representations U and V can be recovered easily from W by $U(q) = W(-q,0)$ and $V(p) = W(0,p)$. One easily justifies the formula $W(\xi) = e^{-i\sigma(\xi,R)}$, where $R = (Q,P)$; $\sigma(\xi,R)$ signifies here the (suitable defined) self-adjoint operator $Q\cdot p - q\cdot P$.

The Weyl system is a convenient way to codify the commutation relations between the basic operators Q and P. In the next paragraph, the quantization by pseudodifferential operators will be obtained as an integrated form of this Weyl system.

C. Pseudodifferential operators

If a family of self-adjoint operators $S_1,\ldots,S_m$ is given such that for any i,j, S_i and S_j commute, then one can define a functional calculus for this family by one of the two formulas

$$f(S) = \int_{\mathbb{R}^m} f(\lambda)\,dE_S(\lambda) = \int_{\mathbb{R}^m} dt\ \check{f}(t)e^{-it\cdot S}.$$

Here E_S is the spectral measure (on $\mathbb{R}^m$) of the family $S_1,\ldots,S_m$, under suitable assumptions $t\cdot S := t_1S_1 + \cdots + t_mS_m$ is a well-defined self-adjoint operator and $\check{f}$ is the inverse Fourier tranform of f, conveniently normalized.

If, once again, $S_1,\ldots,S_m$ are self-adjoint, but they no longer commute, there is usually no reasonable spectral measure E_S. One can try to use the operator version of the Fourier inversion formula to define a functional calculus. The key point would be the ability of defining a suitable

analog of $e^{-it\cdot S}$. This strategy is outlined in Ref. 2 (see also Ref. 3) for very general situations. But the properties of the resulting functional calculus are quite modest if the commutation relations of the operators S_j have no interesting peculiarities.

We shall show how this program can be implemented for the case $m=2N$, $S_j=Q_j$ if $j=1,\ldots,N$ and $S_j=P_j$ for $j=N+1,\ldots,2N$. In an analoguous but more complicated way, in Sec. IV we shall do the same for $S_j=Q_j$ if $j=1,\ldots,N$ and $S_j=\Pi_j^A$ for $j=N+1,\ldots,2N$, with $\Pi_j^A=P_j-A_j(Q)$ the jth component of the magnetic momentum defined by a vector potential A. But we stop for a moment to fix some conventions on Fourier transforms that will also be useful later on.

In fact, we are faced with two problems: normalization and the choice of a good definition on the symplectic space. The Lebegue measures on X, $X^\star$ and Ξ are not the most convenient Haar (=positive, translational invariant Borel) measures, since they lead to the appearance of spurious constants. Let us start with two arbitrary Haar measures dx on X and dp on X^*. One defines at the level of tempered distributions

$$\mathcal{F}_X,\overline{\mathcal{F}}_X:\mathcal{S}'(X)\to\mathcal{S}'(X^*),\ \mathcal{F}_{X^\star},\overline{\mathcal{F}}_{X^\star}:\mathcal{S}'(X^\star)\to\mathcal{S}'(X),$$

uniquely determined by the following actions on integrable functions:

$$(\mathcal{F}_X u)(p)=\int_X dx\ \ e^{-ix\cdot p}u(x),\ \ (\overline{\mathcal{F}}_X u)(p)=\int_X dx\ \ e^{ix\cdot p}u(x),$$

$$(\mathcal{F}_{X^\star} v)(x)=\int_{X^\star} dp\ \ e^{-ix\cdot p}v(p),\ \ (\overline{\mathcal{F}}_{X^\star} v)(p)=\int_{X^\star} dp\ \ e^{ix\cdot p}v(p).$$

It is easily shown that there exists $c>0$ such that

$$\overline{\mathcal{F}}_{X^*}\circ\mathcal{F}_X=c\ \ \mathrm{id}_{\mathcal{S}'(X)}\qquad\text{and}\qquad\mathcal{F}_X\circ\overline{\mathcal{F}}_{X^\star}=c\ \ \mathrm{id}_{\mathcal{S}'(X^\star)}.$$

Thus, by redefining dx and dp, one gets $\mathcal{F}_X^{-1}=\overline{\mathcal{F}}_{X^\star}$ and $\mathcal{F}_{X^\star}^{-1}=\overline{\mathcal{F}}_X$. We fix such a choice for dx and dp, but obviously $d\xi:=dx\otimes dp$ does not depend on this choice. We also set the symplectic Fourier transforms

$$\mathcal{F}_\Xi,\mathcal{F}_\Xi^{-1}:\mathcal{S}'(\Xi)\to\mathcal{S}'(\Xi),$$

$$(\mathcal{F}_\Xi f)(\xi)=(\mathcal{F}_\Xi^{-1}f)(\xi):=\int_\Xi d\eta\ \ e^{i\sigma(\xi,\eta)}f(\eta)$$

and note that $\mathcal{F}_\Xi=\mathcal{I}\circ(\overline{\mathcal{F}}_X\otimes\mathcal{F}_{X^\star})$, where $\mathcal{I}:\mathcal{S}'(X^\star\times X)\to\mathcal{S}'(X\times X^\star)$, $(\mathcal{I}g)(x,p):=g(p,x)$.

Now, for any Weyl system $(\mathcal{H},W)$ we define (at least) for functions $f:\Xi\to\mathbb{C}$ with integrable symplectic Fourier transform

$$\mathfrak{Op}(f):=\int_\Xi d\xi\ \ (\mathcal{F}_\Xi^{-1}f)(\xi)\ \ W(\xi).\tag{11}$$

We do not insist on the precise interpretation of this formula; this will be done later on in the more complicated magnetic case.

Once again, by the Stone–von Neumann theorem, we are satisfied with the case of the Schrödinger representation. By introducing the explicit form of the Schrödinger Weyl system, one gets immediatly for any $u\in L^2(X)$

$$[\mathfrak{Op}(f)u](x)=\int_X dy\int_{X^\star} dp\ \ e^{i(x-y)\cdot p}f\left(\frac{x+y}{2},p\right)u(y)\tag{12}$$

and this is exactly the Weyl prescription to quantize classical symbols.

We note that $\mathfrak{Op}(f)$ is an integral operator with kernel $K_f(x,y) := [(1\otimes \overline{\mathcal{F}}_{X^*})f]((x+y)/2, x-y)$.

Then, by an elementary application of Schwartz's kernel theorem, one gives a sense to $\mathfrak{Op}(f)$ for any $f\in\mathcal{S}'(\Xi)$ as a continuous linear operator from $\mathcal{S}(X)$ to $\mathcal{S}'(X)$. In fact, all these operators are of the form $\mathfrak{Op}(f)$ for some unique tempered distribution f.

D. The Moyal algebra

We turn now to the symbolic calculus. It is easy to see that by setting

$$(f\circ g)(\xi) := 4^N \int_\Xi d\eta \int_\Xi d\zeta \;\; e^{-2i\sigma(\xi-\eta,\xi-\zeta)} f(\eta) g(\zeta) \tag{13}$$

one will have $\mathfrak{Op}(f)\mathfrak{Op}(g) = \mathfrak{Op}(f\circ g)$, and that $\mathfrak{Op}(f)^* = \mathfrak{Op}(f^\circ)$, with $f^\circ(x) := \overline{f(x)}$.

The noncommutative composition law $\circ$ is often called *the Moyal product* (or *the Weyl product*). It makes sense for suitable symbols, say $f,g\in\mathcal{S}(\Xi)$. For many purposes it is useful to extend it to larger classes of functions and distributions. The standard approach (see Refs. 10, 18, 19, 28 and many others) is via oscillatory integrals. Better suited to our setting is the approach by duality of Refs. 4, 13 and 14 that we review now briefly.

Let us denote by $(\cdot,\cdot)$ the duality $\mathcal{S}'(X)\times\mathcal{S}(X)\to\mathbb{C}$. By a simple calculation we see that for any three functions f, g and h in $\mathcal{S}(\Xi)$ we have

$$(f, g\circ h) = (f\circ g, h) = (h, f\circ g) = (h\circ f, g) = (g, h\circ f).$$

Thus, we can extend $\circ$ to mappings $\mathcal{S}(\Xi)\times\mathcal{S}'(\Xi)\to\mathcal{S}'(\Xi)$ and $\mathcal{S}'(\Xi)\times\mathcal{S}(\Xi)\to\mathcal{S}'(\Xi)$ by $(f\circ G, h) := (G, h\circ f)$ and $(F\circ g, h) := (F, g\circ h)$, for $f,g,h\in\mathcal{S}(\Xi)$ and $F,G\in\mathcal{S}'(\Xi)$. This is already useful and allows composing n symbols if all except one are in the Schwartz space.

Now set $\mathcal{M}(\Xi) := \{F\in\mathcal{S}'(\Xi) \,|\, F\circ\mathcal{S}(\Xi)\subset\mathcal{S}(\Xi) \text{ and } \mathcal{S}(\Xi)\circ F\subset\mathcal{S}(\Xi)\}$. Just by some abstract nonsense one checks that $\mathcal{M}(\Xi)$ is a *-algebra under (the extension of) the Moyal product $\circ$ and the involution $^\circ$. In Ref. 13 $\mathcal{M}(\Xi)$ is called *the Moyal algebra* and some of its properties are studied. In particular it is shown that $\mathcal{M}(\Xi)$ is stable under all sorts of Fourier transforms, and it contains all the distributions with compact support and (thus) large classes of analytic functions. It also contains the family of C^∞ functions on Ξ with all the derivatives dominated by the same (arbitrary) polynomial.

We will reconsider this topic in greater detail in Sec. V, where the magnetic field will also be present.

III. THE MAGNETIC WEYL SYSTEM

We consider a quantum particle without internal structure moving in $X=\mathbb{R}^N$, in the presence of a variable magnetic field. The *magnetic field* is described by a closed continuous field of two-forms B defined on $\mathbb{R}^N$. In the standard coordinate system on $\mathbb{R}^N$, it is represented by a continuous function taking real antisymmetric matrix values and verifying the cocycle relation $\partial_j B_{kl} + \partial_k B_{lj} + \partial_l B_{jk} = 0$ in a distributional sense. The reader will verify for himself that many constructions and assertions will still be valid for locally integrable fields; we assumed continuity for simplicity and to have a uniform framework.

It is well-known that any such field B may be written as the (distributional) differential dA of a field of one-forms A, *the vector potential*, that is highly nonunique (the gauge ambiguity); by using coordinates, one has $B_{jk} = \partial_j A_k - \partial_k A_j$ for each $j,k = 1,\ldots,N$.

In this section we shall deduce a formula for the analog of the Weyl system of Sec. II B, but in which the magnetic field is also taken into account. One may proceed as in Sec. II B, with the single modification which consists in replacing the translations by the magnetic translations [exponentials of $q\cdot\Pi^A$, where $\Pi^A := P - A(Q)$ is the magnetic momentum]. Just for a change, we

proceed in a different, but equivalent, way. First we get directly the formula for our magnetic Weyl system by exponentiating the self-adjoint operators $\sigma[(q,p),(Q,\Pi^A)]=Q\cdot p-q\cdot(P-A(Q))$, $(q,p)\in\Xi$. Then the magnetic translations and the magnetic form of the Weyl commutation relations are deduced as consequences.

The magnetic translations have long since appeared in the physical literature (see Refs. 22 and 31, for example), especially in connection with problems in solid state physics. Most of the time they were used for the case of a constant field; some references are Refs. 5, 6, 16, 17 and 26.

We stress that the new objects appearing in the magnetic case are two phase factors: One is defined as the imaginary exponential of the circulation of the vector potential; it enters the definition of the magnetic translations, the magnetic Weyl system and (as a consequence, in Sec. IV) in the expression of the magnetic pseudodifferential operators. The other one, an imaginary exponential of the flux of the magnetic field, appears in connection with multiplicative properties of the magnetic translations and of the magnetic Weyl system and (as a consequence, in Sec. V) in the expression of the composition law defining the symbolic calculus. We hope that our treatment will constitute a source of unification of the various ''nonintegrable phase factors'' scattered in the literature on quantum magnetic fields.

A. The magnetic Weyl system

Given a k-form C on X and a compact k-surface $\gamma\subset X$, we define

$$\Gamma^C(\gamma):=\int_\gamma C$$

(this integral having a well-defined invariant meaning). We shall mainly encounter circulations of one-forms along linear segments ($\gamma=[x,y]$) and fluxes of two-forms through triangles ($\gamma=\langle x,y,z\rangle$).

We denote by $\mathcal{H}$ the Hilbert space $L^2(X)$. For each $t\in\mathbb{R}$ we define

$$W_t^A:\Xi\to\mathcal{U}(\mathcal{H}),\quad W_t^A(x,p):=e^{-it(Q+tx/2)\cdot p}\Lambda^A(Q;tx)e^{itx\cdot P},\tag{14}$$

where we introduced the exponential of the circulation of the vector potential

$$\Lambda^A(q;x):=e^{-i\Gamma^A([q,q+x])}=e^{-ix\cdot\int_0^1 ds\ A(q+sx)}.\tag{15}$$

We make the convention that the vector potential will always be taken continuous. This is, indeed, always possible, since B is supposed continuous, by *the transversal gauge*

$$A_i(x)=-\sum_{j=1}^N\int_0^1 ds\ B_{ij}(sx)sx_j.\tag{16}$$

Noncontinuous vector potentials are not really useful in our framework, but they could also be handled either directly or by exploiting gauge covariance.

The next lemma says that $\{W_t^A(x,p)\}_{t\in\mathbb{R}}$ is the evolution group of the self-adjoint operator $Q\cdot p-x\cdot\Pi^A$, suitably defined.

Lemma 1: We have $W_t^A(x,p)=e^{-it\sigma[(x,p),(Q,\Pi^A)]}$, *where the self-adjoint operator* $\sigma[(x,p),(Q,\Pi^A)]$ *is the closure of the restriction at* $\mathcal{S}(X)$ *of the sum* $S+T$, *with* $S=Q\cdot p+x\cdot A(Q)$ *and* $T=-x\cdot P$.

Proof: It is known that $S+T$ is indeed essentially self-adjoint on $C_c^\infty(X)$ (see Refs. 21 and 8). Thus, we can apply Trotter's formula (see Ref. 27, Th. VII.31). We set $S=a(Q)$ and calculate

$$
\begin{aligned}
&(e^{-(i/n)\,ta(Q)}e^{(i/n)\,tx\cdot P})^n\\
&\quad=e^{-(i/n)\,ta(Q)}e^{(i/n)\,tx\cdot P}e^{-(i/n)\,ta(Q)}e^{-(i/n)\,tx\cdot P}\\
&\qquad\cdot e^{2i/n\,tx\cdot P}e^{-(i/n)\,ta(Q)}e^{-(2i/n)\,tx\cdot P}\\
&\qquad\times e^{(3i/n)\,tx\cdot P}\cdots e^{[(n-1)i/n]\,tx\cdot P}e^{-(i/n)\,ta(Q)}e^{-[(n-1)i/n]\,tx\cdot P}e^{(ni/n)\,tx\cdot P}\\
&\quad=e^{-(it/n)[a(Q)+a(Q+\,tx/n)+\cdots+a(Q+\,(n-1)tx/n)]}e^{itx\cdot P}.
\end{aligned}
$$

One notes the appearance of a Riemman sum at the exponent, hence the last expression converges strongly to $e^{-i\int_0^t ds\;\; a(Q+sx)}e^{itx\cdot P}$. The proof is ended by remarking that

$$
\int_0^t ds\;\;\{(y+sx)\cdot p+x\cdot A(y+sx)\}=ty\cdot p+\frac{t^2}{2}x\cdot p+\Gamma^A[y,y+tx].
$$

■

Another, more annoying, proof would consist in showing that for all $\xi\in\Xi$, $t\mapsto W_t(\xi)$ is a strongly continuous unitary group in $\mathcal{H}$ and then doing the necessary derivations.

We note the obvious formula $W_t^A(\xi)=W_1^A(t\xi)$. The operator $W_1^A(\xi)$ will be denoted simply by $W^A(\xi)$.

Definition 2: The family $\{W^A(\xi)\}_{\xi\in\Xi}$ will be called *the magnetic Weyl system associated to the vector potential A*. We write down here, for further use, the action of $W^A(\xi)$ on vectors $u\in\mathcal{H}=L^2(X)$:

$$
[W^A(x,p)u](y)=e^{-i(y+x/2)\cdot p}e^{-i\Gamma^A([y,y+x])}u(y+x). \tag{17}
$$

The usual Weyl system was a projective representation of Ξ. Now the situation is of the same nature, but more involved. For $x,y,q\in X$, let us define

$$
\Omega^B(q;x,y):=e^{-i\Gamma^B(\langle q,q+x,q+x+y\rangle)}. \tag{18}
$$

We note that this is a continuous function of q for fixed x and y, thus it defines a multiplication operator in $\mathcal{H}$.

Proposition 3: For any $\xi=(x,k),\eta=(y,l)\in\Xi$ *one has*

$$
W^A(\xi)W^A(\eta)=e^{(i/2)\,\sigma(\xi,\eta)}\Omega^B(Q;x,y)W^A(\xi+\eta). \tag{19}
$$

Proof: By the Stokes theorem coupled with the relation $B=dA$, one gets for any $x,y,q\in X$ the equality $\Omega^B(q;x,y)=\Lambda^A(q;x)\Lambda^A(q+x;y)[\Lambda^A(q;x+y)]^{-1}$. Then (19) follows by a routine calculation. ■

Let us denote by $C(X;U(1))$ the group (with pointwise multiplication) of all continuous functions on X, taking values in $U(1)$, the multiplicative group of complex numbers of modulus 1. One can interpret Ω^B as a function $\Omega^B:X\times X\to C(X;U(1))$. This function satisfies the following two-cocycle conditions:

$$
\begin{gathered}
\Omega^B(q;x,0)=\Omega^B(q;0,y)=1,\\
\Omega^B(q;x+y,z)\Omega^B(q;x,y)=\Omega^B(q+x;y,z)\Omega^B(q;x,y+z).
\end{gathered} \tag{20}
$$

They follow easily by direct calculations (for the second one use the Stokes theorem for the closed two-form B and the tetrahedron of vertices $q,q+x,q+x+y$ and $q+x+y+z$), but are also easy consequences of Proposition 3. We also note that $\Omega^B(q;x,-x)=1$.

B. The magnetic canonical commutation relations

By restricting to X, respectively $X^\star$, we recover the usual *magnetic translations*, respectively, the unitary group, generated by the position operators:

$$\begin{aligned} U^A(x) &:= W^A(-x,0) = \Lambda^A(Q;-x)e^{-ix\cdot P} = \Lambda^A(Q;-x)U(x), \\ V(p) &:= W^A(0,p) = e^{-iQ\cdot p}. \end{aligned} \tag{21}$$

One has, analogously to (8),

$$W^A(x,p) := e^{(i/2)\,x\cdot p}\ \ U^A(-x)V(p) = e^{-(i/2)\,x\cdot p}\ \ V(p)U^A(-x), \quad x\in X,\ \ p\in X^\star. \tag{22}$$

We get easily from (19) (or by direct calculation) the commutation rules

$$V(p)V(k) = V(k)V(p), \quad U^A(x)V(p) = e^{ix\cdot p}V(p)U^A(x) \tag{23}$$

and

$$U^A(x)U^A(y) = \Omega^B(Q;-x,-y)U^A(x+y), \tag{24}$$

that are the magnetic extension of the Weyl form of the canonical commutation relations.

For any $x\in X$ and any $p\in X^\star$, the applications $\mathbb{R}\ni t\mapsto U^A(tx)\in\mathcal{U}(\mathcal{H})$ and $\mathbb{R}\ni t\mapsto V(tp)\in\mathcal{U}(\mathcal{H})$ are one-parameter unitary groups on $\mathcal{H}$. We define self-adjoint generators (choosing $x=e_j$, resp. $p=\epsilon_j$ the jth element of the canonical orthogonal basis in $\mathbb{R}^N$)

$$\begin{aligned} Q_j &:= i\frac{\partial}{\partial t}\bigg|_{t=0} V(t\epsilon_j), \\ \Pi_j^A &:= i\frac{\partial}{\partial t}\bigg|_{t=0} U^A(te_j) = P_j - A_j(Q). \end{aligned} \tag{25}$$

On the common domain formed of C^∞-functions with compact support we have the following commutation relations:

$$i[Q_j,Q_k]=0, \quad i[Q_j,\Pi_k]=\delta_{jk} \quad i[\Pi_j,\Pi_k]=B_{jk}(Q). \tag{26}$$

If the magnetic field is not constant (or at least polynomial), they are much more complex than in the nonmagnetic case; the successive commutators of the components of B with the magnetic momenta are nontrivial.

IV. MAGNETIC PSEUDODIFFERENTIAL OPERATORS

Our intention is to elaborate a functional calculus for the *noncommutative* family of self-adjoint operators $\{Q_j,\Pi_k\}_{j,k=1}^N$. We shall call it *the Weyl calculus with magnetic field*. As in the nonmagnetic case, we obtain it by an analog of the Fourier inversion formula, the magnetic Weyl system of the preceding section playing the part of the imaginary exponential. The resulting formula has the right gauge covariance. The operators involved are all integral operators and by the kernel theorem they can also be defined for symbols which are tempered distributions. The problem of identifying finite-rank, Hilbert–Schmidt and compact operators is also addressed. For this, an extension of the classical Fourier–Wigner transform (cf. Ref. 10) is of great help. It also shows *a posteriori* the irreducibility of our magnetic Weyl system. In the final part of the section we compare the magnetic Weyl calculus and the composition of the usual Weyl caculus with the minimal coupling prescription. They are different but, striking enough, they give the same result in many important cases. This explains perhaps the fact that the quantization of observables in a magnetic field has not been treated properly before in a suitable generality. We note, however, that

in Ref. 22 one finds (in a nonsystematic setting) the right attitude for the case of periodic symbols depending only on p. We thank George Nenciu for drawing our attention to this reference.

Let us finally remark that for a constant magnetic field, using a linear vector potential, one is lead to a change of the canonic symplectic form of the space $\Xi = X \times X^\star$, while for nonconstant magnetic fields one is quantizing a symplectic manifold (with a nonconstant symplectic form of the special type $\sigma_B := \sigma + B$) associated to the same linear space Ξ.

A. The functional calculus

We define the linear mapping

$$\mathfrak{Op}^A : \mathcal{F}_\Xi L^1(\Xi) \to \mathcal{B}(L^2(X)), \quad \mathfrak{Op}^A(f) := \int_\Xi d\xi \ \ (\mathcal{F}_\Xi^{-1} f)(\xi) \ \ W^A(\xi) \tag{27}$$

in a weak sense: if $u, v \in \mathcal{H} := L^2(X)$, then $\langle v, \mathfrak{Op}^A(f) u \rangle = \int_\Xi d\xi \ \ (\mathcal{F}_\Xi^{-1} f)(\xi) \langle v, W^A(\xi) u \rangle$. It clearly satisfies the estimate $\|\mathfrak{Op}^A(f)\| \leqslant \|\mathcal{F}_\Xi^{-1} f\|_{L^1}$.

Using the expression of the operators $W^A(\xi)$ given in (14) and (15) we obtain, at least formally, the explicit form of the operators $\mathfrak{Op}^A(f)$,

$$(\mathfrak{Op}^A(f) u)(x) = \int_X dy \int_{X^\star} dk \ \ e^{i(x-y)\cdot k} \tilde{\Lambda}^A(x,y) f\left(\frac{x+y}{2}, k\right) u(y), \tag{28}$$

where $\tilde{\Lambda}^A(x,y) := e^{-i\Gamma^A([x,y])} = \Lambda^A(x; y-x)$. For $A = 0$ this is the usual Weyl prescription to quantize a classical symbol, encountered in the theory of pseudodifferential operators. For general (continuous) A this is, in our opinion, the right formula that should stand for $f(Q, \Pi^A)$.

In fact, the precise sense of (27) and (28) and of their equivalence depends on our assumptions on f and u. In the next paragraphs, under certain hypothesis on the magnetic field, we shall cover the very general case in which f is a tempered distribution; then both formulas will make sense with a suitable reinterpretation and actually define the same object. If f is subject to suitable strong decay assumptions, then no special condition is needed (except our standing convention that A is continuous). All is smooth, for example, if f is in the Schwartz class $\mathcal{S}(\Xi)$. On the other hand, once again without any assumption on the magnetic field, (27) can be extended straightforwardly to f's that are Fourier transforms of bounded complex measures on Ξ. Now, of course, (28) needs a reinterpretation.

To advocate our choice of the mapping $\mathfrak{Op}^A$, an important point is to note *gauge covariance*:

Proposition 4: Let A and A' be two continuous vector potentials defining the same continuous magnetic field: $dA = B = dA'$. *Then there exists a real C^1-function ρ on X such that $A' = A + \nabla\rho$ and we have $e^{i\rho(Q)} W^A(\xi) e^{-i\rho(Q)} = W^{A+\nabla\rho}(\xi)$ for all $\xi \in \Xi$ and $e^{i\rho(Q)} \mathfrak{Op}^A(f) e^{-i\rho(Q)} = \mathfrak{Op}^{A+\nabla\rho}(f)$ for all $f \in \mathcal{F}_\Xi L^1(\Xi)$.*

Proof: It is well-known (cf. Ref. 20, for example) that if $dA = B = dA'$ and A, A' have L^1_{loc}-components, then there exists ρ (in some suitable local Sobolev space that does not matter here) such that $A' - A = \nabla\rho$ in a distributional sense. Now, since in our case A and A' are continuous, ρ will be of class C^1 by a simple argument. The two identities are verified by trivial calculations based on the relation

$$e^{i\rho(Q)} e^{ix\cdot P} e^{-i\rho(Q)} = e^{-i[\rho(Q+x)-\rho(Q)]} e^{ix\cdot P} = e^{-ix\cdot \int_0^1 ds \ \ \nabla\rho(Q+sx)} e^{ix\cdot P}.$$

■

Remark: One implements Planck's constant, at the level of the physical momentum, by setting $P = \hbar D := -i\hbar\nabla$. This gives for the magnetic Weyl system

$$W^A_\hbar(x,p) = e^{-i(Q + (\hbar/2)x)\cdot p} e^{-(i/\hbar)\Gamma^A([Q, Q+\hbar x])} e^{i\hbar x\cdot D}$$

and the $\hbar$-dependent magnetic two-cocycle will be $\Omega_\hbar^B(q;x,y)=e^{-(i/\hbar)\,\Gamma^B(\langle q,q+\hbar x,q+\hbar x+\hbar y\rangle)}$. We collect here, for the convenience of the reader, formulas for the magnetic Weyl calculus,

$$(\mathfrak{Op}_\hbar^A(f)u)(x)=\hbar^{-N}\int_X dy\int_{X^\star}dk\;\; e^{(i/\hbar)(x-y)\cdot k}e^{-(i/\hbar)\,\Gamma^A([x,y])}f\left(\frac{x+y}{2},k\right)u(y),$$

and for the magnetic Moyal product (subject of Sec. V),

$$(f\circ_\hbar^B g)(\xi)=\left(\frac{2}{\hbar}\right)^{2N}\int_\Xi d\eta\int_\Xi d\zeta\;\; e^{-2(i/\hbar)\,\sigma(\xi-\eta,\xi-\zeta)}e^{-(i/\hbar)\,\Gamma^B(\langle q-y+x,x-q+y,y-x+q\rangle)}f(\eta)g(\zeta).$$

In the sequel $\hbar$ will always be 1.

Remark: One often uses instead of (1) *the τ-quantizations* ($\tau\in[0,1]$), given by (cf. Ref. 28)

$$[\mathfrak{Op}_{(\tau)}(f)u](x):=\int_{\mathbb{R}^{2N}}dy\;\; dp\;\; e^{i(x-y)\cdot p}f((1-\tau)x+\tau y,p)u(y).$$

They are somehow connected with the ordering of Q and P in the expression of $f(Q,P)$. The cases $\tau=0$ and $\tau=1$ are called respectively *the right* and *the left quantization*. Rather often, in texbooks, only the case $\tau=0$ is treated. But the Weyl prescription $\mathfrak{Op}\equiv\mathfrak{Op}_{(1/2)}$ is preferred in quantum mechanics because of its nice property $\mathfrak{Op}(f)^*=\mathfrak{Op}(\overline{f})$.

We obtain the magnetic analog of $\mathfrak{Op}_{(\tau)}$ by replacing $W^A(\xi)$ with

$$W_{(\tau)}^A(x,p):=e^{i(1-\tau)x\cdot p}U^A(-x)V(p)=e^{-i\tau x\cdot p}V(p)U^A(-x),\quad x\in X,p\in X^\star.$$

A short formal calculation shows that the definition $\mathfrak{Op}_{(\tau)}^A(f):=\int_\Xi d\xi\;\;(\mathcal{F}_\Xi^{-1}f)(\xi)\;\;W_{(\tau)}^A(\xi)$ leads to

$$[\mathfrak{Op}_{(\tau)}^A(f)u](x):=\int_{\mathbb{R}^{2N}}dy\;\; dp\;\; e^{i(x-y)\cdot p}e^{-i\Gamma^A([x,y])}f((1-\tau)x+\tau y,p)u(y),$$

which allows a rigorous treatment analogous to that given for $\mathfrak{Op}^A\equiv\mathfrak{Op}_{(1/2)}^A$ in the sequel.

B. The distribution kernel

$\mathfrak{Op}^A(f)$ is an integral operator having a kernel that can be defined in terms of f and "the phase function" $\tilde{\Lambda}^A$. In fact, let us introduce the one-to-one linear change of variables $(x,y)\mapsto S(x,y):=(x+y/2,x-y/2)$ and denote by the same symbol S the induced transformation on functions $(S\Phi)(x,y):=\Phi(S(x,y))=\Phi(x+y/2,x-y/2)$. The explicit form of the inverse is $S^{-1}(x,y)=((x+y)/2,x-y)$. We can now define [on $\mathcal{S}(\Xi)$ for instance] the map

$$K^A:=\tilde{\Lambda}^A S^{-1}(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star}),\tag{29}$$

composed of a partial Fourier transform, a change of variables and a multiplication operator. It is easy to verify that $\mathfrak{Op}^A(f)$ is the integral operator with kernel K^Af. For functions Φ defined on $X\times X$ we shall denote by $\mathfrak{Int}(\Phi)$ the integral operator on $L^2(X)$ with kernel Φ, so that one can write $\mathfrak{Op}^A(f)=\mathfrak{Int}(K^Af)$.

For further use we shall introduce two more notations, trying to emphasize the special role played by the phase factor $\tilde{\Lambda}^A$. We define "the zero magnetic field analog" of K^A, the map $K:=S^{-1}(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star})$ and the magnetic integral operator associated to a kernel Φ as $\mathfrak{Int}^A(\Phi):=\mathfrak{Int}(\tilde{\Lambda}^A\Phi)$. With these notations one may write for any $f\in\mathcal{S}(\Xi)$

$$\mathfrak{Op}^A(f)=\mathfrak{Int}(K^Af)=\mathfrak{Int}^A(Kf).\tag{30}$$

We use now these facts to extend the operation $\mathfrak{Op}^A$ to distributions. Let us assume that the components of the magnetic field are C^∞_{pol} functions, i.e., they are indefinitely derivable and any derivative is polynomially bounded. These types of functions are also called *with tempered growth*; their main virtue is that by multiplication they leave the Schwartz space $\mathcal{S}$ invariant, hence they define by duality multiplication operators on $\mathcal{S}'$. The formula (16) for the transversal gauge shows that the vector potential A can also be chosen of class C^∞_{pol}. By easy calculations, $\widetilde{\Lambda}^A$ will also be C^∞_{pol} in both variables. Then it is clear that K^A defines isomorphisms $\mathcal{S}(\Xi)\tilde{\to}\mathcal{S}(X\times X)$ and $\mathcal{S}'(\Xi)\tilde{\to}\mathcal{S}'(X\times X)$.

On the other hand, let us recall that for any finite dimensional vector space $\mathcal{V}$, the spaces $\mathcal{S}(\mathcal{V})$ and $\mathcal{S}'(\mathcal{V})$ are nuclear and we have linear topological isomorphisms (see, for example, Ref. 30, Theorem 51.6 and its Corollary)

$$\mathcal{S}(X)\otimes\mathcal{S}(X)\cong\mathcal{S}(X\times X),\quad \mathcal{S}'(X)\otimes\mathcal{S}'(X)\cong\mathcal{S}'(X\times X). \tag{31}$$

Here the tensor product is the closure of the algebraic tensor product for the injective or the projective topologies that coincide in this case (we refer to Ref. 30, Theorem 50.1). We shall be interested in the following spaces of linear continuous operators: $\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$, $\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]$ and $\mathcal{L}[\mathcal{S}(X)]\cong\mathcal{L}[\mathcal{S}'(X)]$. On all these spaces we consider the topology of uniform convergence on bounded sets. It is easy to see that we have the continuous linear injections

$$\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]\subset\mathcal{B}[L^2(X)]\subset\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]. \tag{32}$$

The conclusions of Sec. 50 in Ref. 30 and the Corollary of Theorem 51.6 in Ref. 30 imply that, isomorphically,

$$\mathfrak{Int}:\mathcal{S}(X\times X)\tilde{\to}\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)],\quad \mathfrak{Int}:\mathcal{S}'(X\times X)\tilde{\to}\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]. \tag{33}$$

By putting together the information above about the operations K^A and $\mathfrak{Int}$, we get the following result concerning our functional calculus:

Proposition 5: If the potential vector A is of class C^∞_{pol}, the map $\mathfrak{Op}^A$ defines linear topological isomorphisms

$$\mathfrak{Op}^A:\mathcal{S}(\Xi)\tilde{\to}\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)],\quad \mathfrak{Op}^A:\mathcal{S}'(\Xi)\tilde{\to}\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)].$$

So "any" operator is (in a unique way) a magnetic pseudodifferential operator of the form $\mathfrak{Op}^A(f)$ for some tempered distribution f and the regularizing operators are exactly those with symbol in the Schwartz space.

Gauge covariance can be extended to this setting; we leave the details to the reader:

Proposition 6: Let A and A' be two vector potentials of class C^∞_{pol} defining the same magnetic field, $dA=B=dA'$. Then there exists a real function $\rho\in C^\infty_{pol}(X)$ such that $A'=A+\nabla\rho$ and $e^{i\rho(Q)}\mathfrak{Op}^A(f)e^{-i\rho(Q)}=\mathfrak{Op}^{A+\nabla\rho}(f)$ for any $f\in\mathcal{S}'(\Xi)$; this second identity is valid in $\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$.

C. The magnetic Fourier–Wigner transformation and special classes of operators

Definition 7: (a) For any pair of vectors u,v from $\mathcal{H}=L^2(X)$ we define the function

$$\mathcal{W}^A_{u,v}:\Xi\to\mathbb{C},\quad \mathcal{W}^A_{u,v}(\xi):=\langle v,W^A(\xi)u\rangle, \tag{34}$$

called *the magnetic Fourier–Wigner transform of the couple* (u,v).

(b) The map $(v,u)\mapsto\mathcal{W}^A_{u,v}$ will be called *the magnetic Fourier–Wigner transformation* (defined by the vector potential A).

In fact $\mathfrak{Op}^A(f)$ was defined by $\langle v,\mathfrak{Op}^A(f)u\rangle=\int_\Xi d\xi\ \ (\mathcal{F}^{-1}_\Xi f)(\xi)\mathcal{W}^A_{u,v}(\xi),\ \ u,v\in\mathcal{H}$.

Proposition 8: (*a*) *The magnetic Fourier–Wigner transformation extends to a unitary operator* $\mathcal{W}^A:L^2(X\times X)\to L^2(\Xi)$.

(*b*) *If A is of class* C^∞_{pol}, *then the magnetic Fourier–Wigner transformation defines isomorphisms* $\mathcal{W}^A:\mathcal{S}(X\times X)\to\mathcal{S}(\Xi)$ *and* $\mathcal{W}^A:\mathcal{S}'(X\times X)\to\mathcal{S}'(\Xi)$.

Proof: Using the explicit form of $W^A(\xi)$ we obtain

$$\mathcal{W}^A_{u,v}=[(\mathbf{1}\otimes\mathcal{F}_X)\mathfrak{I}S(\tilde{\Lambda}^A)^{-1}](u\otimes\overline{v}), \tag{35}$$

where $\mathfrak{I}$ is the composition with the change of variables $(x,y)\mapsto(y,x)$ on $X\times X$. Under the right asumption, each of the maps $\mathbf{1}\otimes\mathcal{F}_X$, $\mathfrak{I}$, S and $(\tilde{\Lambda}^A)^{-1}$ is an isomorphism between the corresponding spaces. One also uses the reinterpretation $\mathcal{W}^A_{u,v}\equiv\mathcal{W}^A_{u\otimes\overline{v}}$. ■

An important direct consequence of this result is the following.

Corollary 9: The Weyl system with magnetic field $W^A:\Xi\to\mathcal{U}[L^2(X)]$ *is irreducible, i.e., there are no nontrivial subspaces of* $L^2(X)$ *invariant under all the operators* $\{W^A(\xi)|\xi\in\Xi\}$.

Proof: Suppose that $\mathcal{K}$ is a closed nontrivial subspace of $L^2(X)$, invariant under all the operators $W^A(\xi)$, $\xi\in\Xi$. Let $v\in\mathcal{K}^\perp$ be different from 0. Then for any $u\in\mathcal{K}\backslash\{0\}$ we have $W^A(\xi)u\in\mathcal{K}$ for any $\xi\in\Xi$, so that

$$\mathcal{W}^A_{u,v}(\xi)=\langle v,W^A(\xi)u\rangle=0,\quad\forall\xi\in\Xi.$$

Thus we deduce that $\|\mathcal{W}^A_{u,v}\|_{L^2(\Xi)}=0$. But $\|\mathcal{W}^A_{u,v}\|_{L^2(\Xi)}=\|u\|\|v\|$ and we get a contradiction. ■

Remark: The Fourier–Wigner transformation also serves to express the operators $\mathfrak{Op}^A(F)$ in a convenient way. Let us stick, for example, to the case in which A has tempered growth. Then for all $u,v\in\mathcal{S}(X)$ and $F\in\mathcal{S}'(\Xi)$, one has $\langle v,\mathfrak{Op}^A(F)u\rangle=\langle\overline{\mathcal{W}^A_{u,v}},\mathcal{F}^{-1}_\Xi F\rangle$, the left-hand-side being interpreted as the anti-duality between $\mathcal{S}(X)$ and $\mathcal{S}'(X)$, while the right-hand-side as the anti-duality between $\mathcal{S}(\Xi)$ [cf. Proposition 8, (b)] and $\mathcal{S}'(\Xi)$.

We shall identify now finite-rank, Hilbert–Schmidt and compact operators.

Proposition 10: (*a*) *For any* $u,v\in\mathcal{H}$ *we have* $|u\rangle\langle v|=\mathfrak{Op}^A(\mathcal{F}_\Xi\mathcal{W}^A_{u,v})$.

(*b*) $\mathfrak{Op}^A$ *induces a unitary map from* $L^2(\Xi)$ *to* $\mathcal{B}_2(\mathcal{H})$, *the ideal of Hilbert–Schmidt operators.*

(*c*) *The family* $\mathfrak{Op}^A[\mathcal{F}_\Xi L^1(\Xi)]$ *is dense in the closed ideal* $\mathcal{K}(\mathcal{H})$ *of all compact operators in* $\mathcal{H}$.

Proof: (a) The operator $|u\rangle\langle v|$ is an integral operator having the kernel $u\otimes\overline{v}$. Thus

$$|u\rangle\langle v|=\mathfrak{Int}(u\otimes\overline{v})=\mathfrak{Op}^A[(K^A)^{-1}(u\otimes\overline{v})].$$

One has

$$(K^A)^{-1}(u\otimes\overline{v})=(\mathbf{1}\otimes\mathcal{F}_X)S(\tilde{\Lambda}^A)^{-1}(u\otimes\overline{v})=(\mathbf{1}\otimes\mathcal{F}_X)\mathfrak{I}(\mathbf{1}\otimes\overline{\mathcal{F}_{X\star}})(\mathbf{1}\otimes\mathcal{F}_X)\mathfrak{I}S(\tilde{\Lambda}^A)^{-1}(u\otimes\overline{v}).$$

But, by a simple calculation, one gets $(\mathbf{1}\otimes\mathcal{F}_X)\mathfrak{I}(\mathbf{1}\otimes\overline{\mathcal{F}_{X\star}})=\mathcal{F}_\Xi$. The point (a) follows by taking (35) into account.

(b) On the intersection $\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)$ we have $\mathfrak{Op}^A=\mathfrak{Int}\circ K^A$, where $K^A:L^2(\Xi)\to L^2(X\times X)$ is unitary and $\mathfrak{Int}:L^2(X\times X)\to\mathcal{B}_2(\mathcal{H})$ is also unitary (a classical result). But $\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)$ is dense in $L^2(\Xi)$.

(c) By (b), for all $f\in\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)$ the operator $\mathfrak{Op}^A(f)$ is Hilbert–Schmidt, hence compact. The space $\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)$ is dense in $L^2(\Xi)$, thus $\mathfrak{Op}^A[\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)]$ is dense in $\mathcal{B}_2(\mathcal{H})$ with respect to the Hilbert–Schmidt norm, hence also with respect to the operator norm. It follows that $\mathfrak{Op}^A[\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)]$ is dense in $\mathcal{K}(\mathcal{H})$. But $\mathfrak{Op}^A[\mathcal{F}_\Xi L^1(\Xi)]$ is also contained in $\mathcal{K}(\mathcal{H})$, since $\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)$ is dense in $\mathcal{F}_\Xi L^1(\Xi)$ and $\|\mathfrak{Op}^A(f)\|_{\mathcal{B}(\mathcal{H})}\leqslant\|f\|_{\mathcal{F}_\Xi L^1}:=\|\mathcal{F}^{-1}_\Xi f\|_{L^1}$, $\forall f$. ■

We see that $\mathfrak{Op}^A$ has a strong tendency towards irreducibility: $\mathcal{K}(\mathcal{H})$ is, of course, irreducible, thus, by density, $\mathfrak{Op}^A[\mathcal{F}_\Xi L^1(\Xi)\cap L^2(\Xi)]$ is also an irreducible family of operators in $\mathcal{H}$. Other results of this type may be obtained by density.

D. The correct form of the minimal coupling principle

The loose form of the minimal coupling principle says that "when a magnetic field $B=dA$ is turned on, one should replace the canonical variable p with $p-A(x)$." The question is, of course, at which stage should this replacement be performed when quantization of a classical observable f is intended. The wrong answer is to compose $f:\Xi\to\mathbb{C}$ with the change of variables $(x,p)\mapsto(x,p-A(x))$ and then apply the Weyl calculus. As seen in the Introduction, this would give a gauge non-covariant formula. The right approach is to apply to f itself a modified (magnetic) Weyl calculus. And this modification is governed actually by the sound, elementary form of the minimal coupling principle: the quantum observable P is replaced by $\Pi^A=P-A(Q)$ and this object determines the expression of the Weyl system W^A, used in the definition of $f(Q,\Pi^A)$. One could say that this is correct, since W^A summarizes the commutation relations of the family of operators $(Q_1,\ldots,Q_N;\Pi_1^A,\ldots,\Pi_N^A)$ for which a functional calculus is requested.

However, one could ask for a more sophisticated (and not so clear ideologically) form of the minimal coupling principle: find a transformation T^A acting on phase-space functions such that, for any f, $f(Q,\Pi^A)$ is obtained (also) by Weyl quantizing the symbol $T^Af\equiv f^A$. A brief examination of this topic follows.

Let us assume, for convenience, that B and A are of class C^∞_{pol}. Both $\mathfrak{Op}^A$ and $\mathfrak{Op}$ are one-to-one (even isomorphic) from $\mathcal{S}'(\Xi)$ to $\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$. Using notations from Sec. IV B, one has

$$\mathfrak{Op}^A(f)=\mathfrak{Op}(f^A)\Leftrightarrow\mathfrak{Int}(K^Af)=\mathfrak{Int}(Kf^A)\Leftrightarrow f^A=K^{-1}K^Af.$$

By using explicit formulas for K^A and K and the identity $S\tilde{\Lambda}^AS^{-1}=\tilde{\Lambda}^A\circ S$, one gets $f^A=T^Af$, with

$$T^A:\mathcal{S}'(\Xi)\to\mathcal{S}'(\Xi),\quad T^A:=(\mathbf{1}\otimes\mathcal{F}_X)(\tilde{\Lambda}^A\circ S)(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star}).$$

Formally (or for suitable f's)

$$(T^Af)(x,p)=\int_X\int_{X^\star}dydk\;\; e^{iy\cdot[k-p+\int_{-1/2}^{1/2}dt\;\; A(x+ty)]}f(x,k)$$

$$=\int_X dy\;\; e^{-iy\cdot[p-\int_{-1/2}^{1/2}dt\;\; A(x+ty)]}(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star})]f(x,y).$$

One should compare this rather complicated formula (a sort of minimal coupling principle for all observables) with

$$(M^Af)(x,p):=f(x,p-A(x))=\int_X\int_{X^\star}dydk\;\; e^{iy\cdot[k-p+A(x)]}f(x,k).$$

The rigorous expression behind this formal integral is

$$M^A:\mathcal{S}'(\Xi)\to\mathcal{S}'(\Xi),\quad M^A:=(\mathbf{1}\otimes\mathcal{F}_X)\Sigma^A(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star}),$$

with $\Sigma^A(x,y)=e^{iy\cdot A(x)}$, $x,y\in X$.

A comparison of the explicit formulas for T^A and M^A shows once again the difference between the correct and the mistaken quantizations in a magnetic field: *The correct one involves circulations of the magnetic potential A through segments* $[x_1,x_2]$, *while for the wrong one the same circulations are calculated by using the constant value* $A_{x_1,x_2}:=A((x_1+x_2/2))$, *taken at the middle of the respective segment.*

One has a complete characterization of the vector potentials for which the wrong quantization is good:

Lemma 11: One has $T^A=M^A$ [*which is equivalent to* $\mathfrak{Op}^A(f)=\mathfrak{Op}(M^Af)$, $\forall f\in\mathcal{S}'(\Xi)$] *if and only if* A *is linear*.

Proof: $\mathbf{1}\otimes\mathcal{F}_X$ and $\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star}$ being one-to-one, we have $T^A=M^A$ if and only if $\tilde{\Lambda}^A\circ S=\Sigma^A$, i.e., if and only if $y\cdot\int_{-1/2}^{1/2}dt\ [A(x+ty)-A(x)]=0$, $\forall x,y\in X$. A simple application of Taylor's formula shows that this is equivalent to the annulation of all the second derivatives of all the components of A. ■

One of the most important examples is the constant magnetic field. In this case, everybody would choose a linear potential vector A and no care is needed in the choice of the quantization procedure. Most articles involving a functional calculus in a magnetic field are written for constant B *and* linear A. Note, however, that the identity $T^A=M^A$ *is not gauge invariant.*

However, one can have $T^Af=M^Af$ for any A for certain special functions f. This is obviously true if f depends only on the variable $x\in X$. Actually, in this case $\mathfrak{Op}^A(f)=\mathfrak{Op}(M^Af)=f(Q)$. Let us give some more interesting examples.

Proposition 12: Let f *be a polynomial of order* m *in* p, *not depending on the variable in* X. *If* $m\leqslant 2$, *then* $T^Af=M^Af$, *hence* $\mathfrak{Op}^A(f)=\mathfrak{Op}(M^Af)$. *This is no longer true for* $m=3$.

Proof: Let us consider the monomial $f_\alpha(x,p):=p^\alpha$. Then we have $(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star})f_\alpha=(-i\partial)^\alpha\delta$, thus $(T^Af)(x,p)=[(i\partial_y)^\alpha e^{-i\tau^A(x,p;y)}]|_{y=0}$ and $(M^Af)(x,p)=[(i\partial_y)^\alpha e^{-i\mu^A(x,p;y)}]|_{y=0}$, where the two phases are defined by $\tau^A(x,p;y):=y\cdot[p-\int_{-1/2}^{1/2}dt\ A(x+ty)]$ and $\mu^A(x,p;y):=y\cdot[p-A(x)]$. We concentrate on the cases $m=1,2,3$. The following list of relations is needed:

$$i\partial_{y_j}e^{-i\varphi}=(\partial_{y_j}\varphi)e^{-i\varphi},\quad i^2\partial_{y_k}\partial_{y_j}e^{-i\varphi}=(i\partial_{y_k}\partial_{y_j}\varphi+\partial_{y_k}\varphi\ \ \partial_{y_j}\varphi)e^{-i\varphi},$$

$$i^3\partial_{y_l}\partial_{y_k}\partial_{y_j}e^{-i\varphi}=(-\partial_{y_l}\partial_{y_k}\partial_{y_j}\varphi+i\partial_{y_j}\varphi\ \ \partial_{y_l}\partial_{y_k}\varphi+i\partial_{y_k}\varphi\ \ \partial_{y_l}\partial_{y_j}\varphi+i\partial_{y_l}\varphi\ \ \partial_{y_k}\partial_{y_j}\varphi+\partial_{y_l}\varphi\ \ \partial_{y_k}\varphi\ \ \partial_{y_j}\varphi)e^{-i\varphi}.$$

Note that $\partial_{y_j}\mu^A(x,p;y)=p_j-A_j(x)$, while the higher-order derivatives vanish.

A simple calculation gives

$$\partial_{y_j}\tau^A(x,p;y)=p_j-\int_{-1/2}^{1/2}dt\ \ A_j(x+ty)-\sum_{n=1}^{N}y_n\int_{-1/2}^{1/2}tdt\ \ (\partial_jA_n)(x+ty),$$

and by taking the value in $y=0$ one gets $[\partial_{y_j}\tau^A(x,p;y)]|_{y=0}=[\partial_{y_j}\mu^A(x,p;y)]|_{y=0}=p_j-A_j(x)$. Thus $T^Af=M^Af$ for any first-order polynomial. This is not amaizing: $\mathfrak{Op}^A(p_j)=\Pi^A$ was accepted as a basic principle.

One also has

$$\partial_{y_k}\partial_{y_j}\tau^A(x,p;y)=-\int_{-1/2}^{1/2}tdt\ \ (\partial_jA_k+\partial_kA_j)(x+ty)-\sum_{n=1}^{N}y_n\int_{-1/2}^{1/2}t^2dt\ \ (\partial_k\partial_jA_n)(x+ty).$$

By "miracle" this term vanishes in $y=0$; then straightforwardly $T^Af=M^Af$ also for second-order polynomials. This is significant, since most of the time people considered the case $f(x,p)=|p|^2$, leading to the magnetic Laplacian $\Delta^A=(\Pi^A)^2$; no care is needed in this case.

The situation changes drastically for third order polynomials. One has

$$\partial_{y_l}\partial_{y_k}\partial_{y_j}\tau^A(x,p;y)=-\int_{-1/2}^{1/2}t^2dt\ \ (\partial_k\partial_jA_l+\partial_l\partial_jA_k+\partial_l\partial_kA_j)(x+ty)$$
$$-\sum_{n=1}^{N}y_n\int_{-1/2}^{1/2}t^3dt\ \ (\partial_l\partial_k\partial_jA_n)(x+ty),$$

which in $y=0$ takes the value $-\frac{1}{12}(\partial_k\partial_jA_l+\partial_l\partial_jA_k+\partial_l\partial_kA_j)(x)$. In this case $T^Af\neq M^Af$. ■

V. THE MAGNETIC MOYAL ALGEBRA

We come now to an important point in the development of our functional calculus. The product of the operators $\mathfrak{Op}^A(f)$ and $\mathfrak{Op}^A(g)$ is again an integral operator with a kernel $K^A(f \circ^B g)$, which can formally be associated to the function on Ξ obtained by the following noncommutative composition law, called *the magnetic Moyal product of the functions f and g*:

$$(f\circ^B g)(\xi)=4^N\int_\Xi d\eta\int_\Xi d\zeta\ \ e^{-2i\sigma(\xi-\eta,\xi-\zeta)}e^{-i\Gamma^B(\langle q-y+x,x-q+y,y-x+q\rangle)}f(\eta)g(\zeta)$$

$$=4^N\int_\Xi d\eta\int_\Xi d\zeta\ \ e^{-2i\sigma(\eta,\zeta)}e^{-i\Gamma^B(\langle q-x-y,q+x-y,q+y-x\rangle)}f(\xi-\eta)g(\xi-\zeta);\quad (36)$$

here $\xi=(q,p)$, $\eta=(x,k)$, $\zeta=(y,l)$. Thus we have $\mathfrak{Op}^A(f\circ^B g)=\mathfrak{Op}^A(\underline{f})\mathfrak{Op}^A(g)$. We can also define an involution (the same as in the nonmagnetic case) by $f^\circ(\xi):=\overline{f(\xi)}$ such that $\mathfrak{Op}^A(f^\circ)=\mathfrak{Op}^A(f)^*$.

The integral defining $f\circ^B g$ is absolutely convergent only for restricted classes of symbols. One seeks to extend the composition law $\circ^B$ to large classes of distributions in such a way as to obtain (together with the involution $^\circ$) *-algebras. For any choice of a magnetic potential, the functional calculus with magnetic field will be a representation of these *-algebras. But the algebras themselves are completely intrinsic, being defined only in terms of the magnetic field. We shall do this extension by duality, following the approach of Refs. 4 and 13 (see also Refs. 14 and 9) valid in the absence of the magnetic field. We obtain a magnetic analog of the Moyal algebra outlined in Sec. II D; the terminology is that of the references above and it is suggested by some early fundamental work of Moyal (cf. Ref. 25).

The standard technique of extending the composition law, based on oscillatory integrals and classes of symbols, is less appropriate for our present purposes. But we intend to deal with this topic in a subsequent publication.

A. The magnetic Moyal product

Before discussing rigorously the sense of formula (36) for various assumptions on f, g and B, we make some formal remarks. Note that if $B=0$, (36) reduces to the usual composition of symbols (13) in the Weyl quantization. The magnetic correction consists of a phase factor defined in terms of the flux of the magnetic field through suitable triangles. The associativity of the above composition law comes from the two-cocycle condition, the second identity in (20). For this just notice that $e^{-i\Gamma^B(\langle q-y+x,x-q+y,y-x+q\rangle)}=\Omega^B(q-y+x;2y-2q,2q-2x)$ and do the right calculation. Finally, it is easy to check that $\mathfrak{Op}^A(f\circ^B g)=\mathfrak{Op}^A(f)\mathfrak{Op}^A(g)$ whenever everything is well-defined.

In general, if no special assumption on B is imposed, it is not so easy to define and use sharply the magnetic Moyal product. For $f,g\in\mathcal{F}_\Xi L^1(\Xi)$ both $\mathfrak{Op}^A(f)$ and $\mathfrak{Op}^A(g)$ are defined as bounded linear operators in $\mathcal{H}=L^2(X)$, but it is not clear if their product is of the form $\mathfrak{Op}^A(h)$ for some h (eventually in $\mathcal{F}_\Xi L^1(\Xi)$). On the other hand, if $f,g\in L^1(\Xi)$, then the integral in (36) is absolutely convergent and defines a bounded continuous function on Ξ. However, we do not see why this function should be integrable and, anyway, applying $\mathfrak{Op}^A$ to all these is problematic. One can also take advantage of Proposition 10(b) to endow $L^2(\Xi)$ with the structure of a *-algebra, the composition law coinciding with (36) on suitable subsets.

In fact many other solutions exist but *they do not seem to be natural enough in the present framework*. In a future publication we will give another (equivalent) form of the magnetic Moyal product (a ''very twisted convolution'') for which it will be relatively easy to define nice normed *-algebras. Their pull-backs in the pseudo-differential representation involve a partial Fourier transformation that does not have an explicitly expressible range. So we postpone the study of magnetic composition laws for general (continuous) magnetic fields and turn to a special case which is, however, very comprehensive.

Proposition 13: Assume that the components of the magnetic field B are of class C^∞_{pol}.

(*a*) *For any* $f,g\in\mathcal{S}(\Xi)$ *one has* $f\circ^B g\in\mathcal{S}(\Xi)$. *The map* $\circ^B:\mathcal{S}(\Xi)\times\mathcal{S}(\Xi)\to\mathcal{S}(\Xi)$ *is bilinear and continuous.*

(*b*) *For any continuous vector potential* A *such that* $dA=B$, *one has* $\mathfrak{Op}^A(f\circ^B g)=\mathfrak{Op}^A(f)\mathfrak{Op}^A(g)$.

Proof: One can prove that $\mathcal{S}(\Xi)\circ^B\mathcal{S}(\Xi)\subset\mathcal{S}(\Xi)$ directly, estimating $\xi^\alpha\partial^\beta(f\circ^B g)$ by involved manipulations in (36). This also gives the required continuity. We prefer to outline a simpler proof, based on integral kernels.

Let us choose $A\in C^\infty_{\mathrm{pol}}(X,X^\star)$ such that $dA=B$; this is possible by (16). We know that the maps $K^A:=\widetilde{\Lambda}^A S^{-1}(\mathbf{1}\otimes\overline{\mathcal{F}}_{X^\star}):\mathcal{S}(\Xi)\to\mathcal{S}(X\times X^\star)$, $\mathfrak{Int}:\mathcal{S}(X\times X^\star)\to\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]$ and $\mathfrak{Op}^A:\mathcal{S}(\Xi)\to\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]$ are topological isomorphisms and that $\mathfrak{Op}^A=\mathfrak{Int}\circ K^A$. One checks easily that $K^A(f\circ^B g)=K^A(f)\ddagger K^A(g)$, where $(L\ddagger M)(x,y):=\int_X dz\ L(x,z)M(z,y)$ is the composition rule of integral kernels (leading to the product of the integral operators involved). These facts and the continuity of $\ddagger:\mathcal{S}(X\times X^\star)\times\mathcal{S}(X\times X^\star)\to\mathcal{S}(X\times X^\star)$ imply both the points (a) and (b) for $A\in C^\infty_{\mathrm{pol}}(X,X^\star)$.

The general case of a continuous A in (b) is solved by gauge covariance, cf. Proposition 4 (we consider here $\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]$ embedded in $\mathcal{B}[L^2(X)]$). ■

Since $\mathcal{S}(\Xi)$ is obviously stable under involution, $(\mathcal{S}(\Xi),\circ^B,^\circ)$ is a *-algebra (all the axioms are easily verified) and $\mathfrak{Op}^A:\mathcal{S}(\Xi)\to\mathcal{L}[\mathcal{S}'(X),\mathcal{S}(X)]$ is a *-isomorphism. Unfortunately, $\mathcal{S}(\Xi)$ is too small for many purposes. For instance, functions depending only on x or on p are not included.

B. Extension by duality

We start extending by duality the magnetic Moyal product with an asymmetric version: we shall compose a Schwartz test function with a tempered distribution. The result is *a priori* a tempered distribution, but we shall be able to get more precise information in certain cases. The components of the magnetic field will be always considered to be in C^∞_{pol}, thus the conclusions of Proposition 13 hold.

The duality approach is facilitated by the next lemma:

Lemma 14: For any functions f *and* g *in* $\mathcal{S}(\Xi)$ *we have*

$$\int_\Xi d\xi\ \ (f\circ^B g)(\xi)=\int_\Xi d\xi\ \ (g\circ^B f)(\xi)=\int_\Xi d\xi\ \ f(\xi)g(\xi)=\langle\overline{f},g\rangle\equiv(f,g).$$

Proof: Of course, one needs only to show that $\int_\Xi d\xi\ \ (f\circ^B g)(\xi)=\int_\Xi d\xi\ \ f(\xi)g(\xi)$; the other identities are trivial consequences.

The calculation will be straightforward by regularization. We choose sequences $(a_n)_{n\in\mathbb{N}}\in\mathcal{S}(X)$, $(b_n)_{n\in\mathbb{N}}\in\mathcal{S}(X^\star)$ such that $a_n\to 1$ in $\mathcal{S}'(X)$ and $b_n\to 1$ in $\mathcal{S}'(X^\star)$. Then it is shown easily that

$$\int_X\int_{X^\star}dq\ \ dp\ \ (f\circ^B g)(q,p)a_n(q)b_m(p)\to\int_X\int_{X^\star}dq\ \ dp\ \ f(q,p)g(q,p)$$

for $n,m\to\infty$. For this we use the explicit formula for $f\circ^B g$, Fubini's theorem, the fact that the Fourier transforms of a_n and b_m converge respectively to the distribution δ and the annulation of $\Gamma^B(\langle q-y+x,x-q+y,y-x+q\rangle)$ for $x=y$. We leave the details to the reader. ■

Corollary 15: For any three functions f, g *and* h *in* $\mathcal{S}(\Xi)$ *we have*

$$(f\circ^B g,h)=(f,g\circ^B h)=(g,h\circ^B f).$$

Proof: Easy consequence of the lemma, the associativity of $\circ^B$ and the symmetry of $(\cdot,\cdot)$. ■

Definition 16: For any distribution $F\in\mathcal{S}'(\Xi)$ and any function $f\in\mathcal{S}(\Xi)$ we define

$$(F\circ^B f,h):=(F,f^\circ\circ^B h),\quad (f\circ^B F,h):=(F,h\circ^B f^\circ),\quad \forall h\in\mathcal{S}(\Xi).$$

By using Proposition 13(a) and the definition it is straightforward to see the following.

Proposition 17: The above definition provides two bilinear continuous mappings $\mathcal{S}'(\Xi)\times\mathcal{S}(\Xi)\to\mathcal{S}'(\Xi)$, *resp.* $\mathcal{S}(\Xi)\times\mathcal{S}'(\Xi)\to\mathcal{S}'(\Xi)$.

One easily checks that $(F\circ^B g)^\circ = g^\circ\circ^B F^\circ$ and $(g\circ^B F)^\circ = F^\circ\circ^B g^\circ$, for all $F\in\mathcal{S}'(\Xi)$ and $g\in\mathcal{S}(\Xi)$. Associativity results as $(f_1\circ^B F)\circ^B f_2 = f_1\circ^B(F\circ^B f_2)$, for $f_1, f_2\in\mathcal{S}(\Xi)$, $F\in\mathcal{S}'(\Xi)$ obviously hold, so one can define unambiguously $f_1\circ^B\cdots\circ^B f_n$ if one f_j is a tempered distribution and all the others are Schwartz test functions. Lemma 14 implies immediately that $1\circ^B f = f = f\circ^B 1$, $\forall f\in\mathcal{S}(\Xi)$.

Proposition 18: For any vector potential A with tempered growth, $\mathfrak{Op}^A$ *is an involutive linear continuous map*: $\mathcal{S}'(\Xi)\mapsto\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$, *satisfying* $\mathfrak{Op}^A(F\circ^B g)=\mathfrak{Op}^A(F)\mathfrak{Op}^A(g)$ *and* $\mathfrak{Op}^A(g\circ^B F)=\mathfrak{Op}^A(g)\mathfrak{Op}^A(F)$ *for all* $F\in\mathcal{S}'(\Xi)$ *and* $g\in\mathcal{S}(\Xi)$.

Proof: We already know that $\mathfrak{Op}^A:\mathcal{S}'(\Xi)\mapsto\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$ is an isomorphism of topological vector spaces. The involution on $\mathcal{L}[\mathcal{S}(X),\mathcal{S}'(X)]$ is defined by antiduality ($\langle T^*v,u\rangle=\langle v,Tu\rangle$, $\forall u,v\in\mathcal{S}(X)$). Then the formula $\mathfrak{Op}^A(F)^*=\mathfrak{Op}^A(F^\circ)$ follows readily from the Remark in Sec. IV C. The relations $\mathfrak{Op}^A(F\circ^B g)=\mathfrak{Op}^A(F)\mathfrak{Op}^A(g)$ and $\mathfrak{Op}^A(g\circ^B F)=\mathfrak{Op}^A(g)\mathfrak{Op}^A(F)$ follow by approximating $F\in\mathcal{S}'(\Xi)$ with elements f_n of $\mathcal{S}(\Xi)$; all the continuity properties which are needed are already proved.

C. The magnetic Moyal *-algebras

Definition 19: (a) The spaces of distributions

$$\mathcal{M}_L(\Xi) := \{F\in\mathcal{S}'(\Xi) \;\mid\; F\circ^B f\in\mathcal{S}(\Xi),\quad \forall f\in\mathcal{S}(\Xi)\}$$

and

$$\mathcal{M}_R(\Xi) := \{F\in\mathcal{S}'(\Xi) \;\mid\; f\circ^B F\in\mathcal{S}(\Xi),\quad \forall f\in\mathcal{S}(\Xi)\}$$

will be called, respectively, *the left* and *the right magnetic Moyal algebras*.

(b) Their intersection

$$\mathcal{M}(\Xi) := \mathcal{M}_L(\Xi)\cap\mathcal{M}_R(\Xi)$$

will be called *the magnetic Moyal algebra*.

The three spaces above depend on the magnetic field so, in principle, they would deserve an index B.

For any two distributions F and G in $\mathcal{M}(\Xi)$ we can extend the magnetic Moyal product by

$$(F\circ^B G,h) := (F,G\circ^B h),\quad \forall h\in\mathcal{S}(\Xi).$$

Proposition 20: The set $\mathcal{M}(\Xi)$ *together with the composition law* $\circ^B$ *defined as above and the complex conjugation* $F\mapsto F^\circ$ *is an unital *-algebra, containing* $\mathcal{S}(\Xi)$ *as a self-adjoint two-sided ideal*.

All the verifications are trivial. Since the constant functions are obviously in $\mathcal{M}(\Xi)$, it is already clear that the *-algebra $\mathcal{S}(\Xi)$ is enlarged. We shall see in Sec. V D that this enlargement is substantial.

We study now the behavior of $\mathfrak{Op}^A$ on symbols belonging to the magnetic Moyal algebra.

Proposition 21: $\mathfrak{Op}^A$ *is an isomorphism of *-algebras betweeen* $\mathcal{M}(\Xi)$ *and* $\mathcal{L}[\mathcal{S}(X)]\cap\mathcal{L}[\mathcal{S}'(X)]$.

Proof: Let us denote simply $\mathcal{S}=\mathcal{S}(X)$ and $\mathcal{S}'=\mathcal{S}'(X)$. We identify $\mathcal{L}(\mathcal{S})\equiv\mathcal{L}(\mathcal{S},\mathcal{S})$ with the family of all the elements $T\in\mathcal{L}(\mathcal{S},\mathcal{S}')$ such that $T\mathcal{S}\subset\mathcal{S}$. By the closed graph theorem, such a T will automatically be continuous (and linear) as a mapping $\mathcal{S}\mapsto\mathcal{S}$. $\mathcal{L}(\mathcal{S})$ is obviously an algebra with the composition of operators.

Another algebra is $\mathcal{L}(\mathcal{S}')\equiv\mathcal{L}(\mathcal{S}',\mathcal{S}')$, which may be identified with the family of elements $T\in\mathcal{L}(\mathcal{S},\mathcal{S}')$ that admit a continuous extension to $\mathcal{S}'$. We recall that the involution on $\mathcal{L}(\mathcal{S},\mathcal{S}')$ is defined by antiduality $(\langle T^*u,w\rangle=\langle u,Tw\rangle,\ \forall u,w\in\mathcal{S})$. Then, plainly, $\mathcal{L}(\mathcal{S})^*=\mathcal{L}(\mathcal{S}')$ and $\mathcal{L}(\mathcal{S}')^*=\mathcal{L}(\mathcal{S})$. Thus $\mathcal{L}(\mathcal{S})\cap\mathcal{L}(\mathcal{S}')$ is a *-algebra.

We know that $\mathfrak{Op}^A$ is one-to-one; we calculate now $\mathfrak{Op}^A[\mathcal{M}(\Xi)]$. By the definition of $\mathcal{M}(\Xi)$ and Proposition 5, T is in $\mathfrak{Op}^A[\mathcal{M}(\Xi)]$ if and only if $T\mathcal{L}(\mathcal{S}',\mathcal{S})\subset\mathcal{L}(\mathcal{S}',\mathcal{S})$ and $\mathcal{L}(\mathcal{S}',\mathcal{S})T\subset\mathcal{L}(\mathcal{S}',\mathcal{S})$. The last inclusion is equivalent to $T^*\mathcal{L}(\mathcal{S}',\mathcal{S})\subset\mathcal{L}(\mathcal{S}',\mathcal{S})$. It is easy to see that $T\mathcal{L}(\mathcal{S}',\mathcal{S})\subset\mathcal{L}(\mathcal{S}',\mathcal{S})$ if and only if $T\in\mathcal{L}(\mathcal{S})$. One implication is trivial and the other one follows once again from the closed graph theorem and from the fact that for any $v\in\mathcal{S}$ there exist $u\in S'$ and $S\in\mathcal{L}(\mathcal{S}',\mathcal{S})$ such that $Su=v$. Then, by taking also T^* into account, we see that $\mathfrak{Op}^A[\mathcal{M}(\Xi)]=\mathcal{L}(\mathcal{S})\cap\mathcal{L}(\mathcal{S}')$.

Let $F,G\in\mathcal{M}(\Xi)$. We calculate for $u\in\mathcal{S}'$ and $h\in\mathcal{S}(\Xi)$

$$\mathfrak{Op}^A(F\circ^B G)[\mathfrak{Op}^A(h)u]=\mathfrak{Op}^A(F\circ^B G\circ^B h)u=\mathfrak{Op}^A(F)[\mathfrak{Op}^A(G\circ^B h)u]$$
$$=[\mathfrak{Op}^A(F)\mathfrak{Op}^A(G)]\mathfrak{Op}^A(h)u,$$

where we used Proposition 18. Since any $v\in\mathcal{S}$ can be written as $\mathfrak{Op}^A(h)u$ for some $u\in\mathcal{S}'$ and $h\in\mathcal{S}(\Xi)$, the multiplicative property of $\mathfrak{Op}^A$ on $\mathcal{M}(\Xi)$ is shown.

The involutivity of $\mathfrak{Op}^A$ is valid on $\mathcal{S}'(\Xi)$, as remarked before. ■

Remark: Propositions 20 and 21 are the most important results. We note here rapidly some extra results concerning the magnetic Moyal algebras, all of an elementary nature. One also defines by duality products of the form $F_1\circ^B G\circ^B F_2\in\mathcal{S}'(\Xi)$ for $F_1\in\mathcal{M}_R(\Xi)$, $F_2\in\mathcal{M}_L(\Xi)$ and $G\in\mathcal{S}'(\Xi)$; $\mathcal{S}'(\Xi)$ is a $(\mathcal{M}_R(\Xi),\mathcal{M}_L(\Xi))$-bimodule. In fact $\mathcal{M}_L\circ^B\mathcal{M}_L\subset\mathcal{M}_L$ and $\mathcal{M}_R\circ^B\mathcal{M}_R\subset\mathcal{M}_R$, hence $\mathcal{M}_L$ and $\mathcal{M}_R$ are algebras. But they are different and correspond to each other by complex conjugation, so $\mathcal{M}$ is optimally defined as a *-algebra by the present methods. The proof of Proposition 21 also leads to $\mathfrak{Op}^A\mathcal{M}_L(\Xi)=\mathcal{L}(\mathcal{S})$ and $\mathfrak{Op}^A\mathcal{M}_R(\Xi)=\mathcal{L}(\mathcal{S}')$.

The next striking result shows once more the importance of the magnetic Moyal algebras.

Proposition 22: One has $\mathcal{S}'(\Xi)\circ^B\mathcal{S}(\Xi)\subset\mathcal{M}_R(\Xi)$ *and* $\mathcal{S}(\Xi)\circ^B\mathcal{S}'(\Xi)\subset\mathcal{M}_L(\Xi)$.

Proof:

$$\mathfrak{Op}^A[\mathcal{S}'(\Xi)\circ^B\mathcal{S}(\Xi)]=\mathfrak{Op}^A[\mathcal{S}'(\Xi)]\mathfrak{Op}^A[\mathcal{S}(\Xi)]=\mathcal{L}(\mathcal{S},\mathcal{S}')\mathcal{L}(\mathcal{S}',\mathcal{S})=\mathcal{L}(\mathcal{S}')\subset\mathfrak{Op}^A\mathcal{M}_R(\Xi),$$

thus $\mathcal{S}'(\Xi)\circ^B\mathcal{S}(\Xi)\subset\mathcal{M}_R(\Xi)$. The other inclusion is proved analogously. ■

We note that both the inclusions are strict. For zero magnetic field $f\circ G$ is smooth if $f\in\mathcal{S}(\Xi)$ and $G\in\mathcal{S}'(\Xi)$, cf. Ref. 13.

D. Some important subclasses

We keep the setting of the preceding paragraphs, i.e., the components of B (and those of A when necessary) are of class C^∞_{pol}. Simple examples show readily that $\mathcal{M}(\Xi)$ is much larger than $\mathcal{S}(\Xi)$. One shows easily that if $f(x,p)=f_1(x)$ depends only on the variable in X, then $\mathfrak{Op}^A(f)=f_1(Q)$. If f_1 has tempered growth, then $f_1(Q)\in\mathcal{L}(\mathcal{S})\cap\mathcal{L}(\mathcal{S}')$, thus $f\in\mathcal{M}(\Xi)$ by Proposition 21. It is also quite obvious that $\mathcal{F}_\Xi L^1(\Xi)\subset\mathcal{M}(\Xi)$, since $W^A(\xi)$ is a continuous operator in $\mathcal{S}$ for all $\xi\in\Xi$. Actually, the same argument would also show that Fourier transforms of bounded, complex measures on Ξ are also in the magnetic Moyal algebra. In the sequel we shall outline a less evident example.

Let $C^\infty_{\mathrm{pol,u}}(\Xi)\subset\mathcal{S}'(\Xi)$ be the space of indefinitely derivable complex functions on Ξ having uniform polynomial growth at infinity; i.e., $f\in C^\infty_{\mathrm{pol,u}}(\Xi)$ when it is indefinitely derivable and there exists $m\in\mathbb{N}$ (depending on f) such that for any multi-index $a\in\mathbb{N}^{2N}$ one has $|(\partial^a f)(\xi)|\leqslant C_a\langle\xi\rangle^m$ for all $\xi\in\Xi$.

Proposition 23: $C^\infty_{\mathrm{pol,u}}(\Xi)\subset\mathcal{M}(\Xi)$.

Proof: First we reduce our proof to a precise estimate. Classes of functions $\mathcal{T}(\Xi)$ will be denoted briefly by $\mathcal{T}$.

For any $m\in\mathbb{R}$ we set $S_0^m:=\{f\in C^\infty|\langle\cdot\rangle^{-m}\partial^a f\in L^\infty,\ \forall a\in\mathbb{N}^{2N}\}$ and $R_0^m:=\{f\in C^\infty|\langle\cdot\rangle^{-m}\partial^a f\in L^1,\ \forall a\in\mathbb{N}^{2N}\}$. The reason for introducing these function spaces is the fact that $C^\infty_{\mathrm{pol,u}}(\Xi)=\cup_{m\in\mathbb{R}}S_0^m=\cup_{m\in\mathbb{R}}R_0^m$. This follows from $R_0^m\subset S_0^m\subset R_0^{m+2N+\varepsilon}$, valid for any $m\in\mathbb{R}$ and any $\varepsilon>0$, which is shown by trivial estimates. So the proposition will be proved if we show that $R_0^m\subset\mathcal{M},\ \forall m\in\mathbb{R}$.

In fact the spaces S_0^m were introduced only for comparison. They are the first constituents of $C^\infty_{\mathrm{pol,u}}$ you would think of, but technically the classes R_0^m are better suited, since L^1-inequalities in initial spaces are within reach (for example we have $\|f\circ^B g\|_\infty\leqslant\|f\|_1\|g\|_1$). R_0^m is a locally convex space with the family of norms $\{r_n^m\}_{n\in N}$, where $r_n^m(f):=\Sigma_{|a|\leqslant n}\|\partial^a[\langle\cdot\rangle^{-m}f]\|_1$ (other, equivalent, family is obtained by writing ∂^a and $\langle\cdot\rangle^{-m}$ in reversed order.)

Since $\mathcal{S}$ is dense in R_0^m, to show that $R_0^m\subset\mathcal{M}$ it will be sufficient to prove that for any $g\in\mathcal{S}$ the mappings $\mathcal{S}\ni f\mapsto f\circ^B g\in\mathcal{S}$ and $\mathcal{S}\ni f\mapsto g\circ^B f\in\mathcal{S}$ are continuous if on the initial space $\mathcal{S}$ we consider the topology induced from R_0^m. We shall treat the first mapping; in fact this is enough, since R_0^m is left invariant by complex conjugation.

In the sequel we shall always write $\xi=(q,p)$, $\eta=(x,k)$ and $\zeta=(y,l)$. We also set $\phi^B(q,x,y):=e^{-i\Gamma^B(\langle q-y+x,x-q+y,y-x+q\rangle)}$; it is a function in C^∞_{pol} with $|\phi^B(q,x,y)|=1$. By taking into account the discussion above and the form of the seminorms on $\mathcal{S}$, we see that it is enough to prove that for any $g\in\mathcal{S}$, $\alpha,\beta,\gamma,\delta\in\mathbb{N}^N$ and $m\in\mathbb{R}$ (we shall take m to be an even positive integer) there exist $n\in\mathbb{N}$ and $C<\infty$ (they both depend on everything) such that

$$\|q^\alpha p^\beta\partial_q^\gamma\partial_p^\delta(f\circ^B g)\|_\infty\leqslant Cr_n^m(f).$$

Now the proof will proceed in several steps:

Step 1: A simple calculation gives

$$[q^\alpha p^\beta\partial_q^\gamma\partial_p^\delta(f\circ^B g)](q,p)=\sum_{\gamma'\leqslant\gamma}C_{\gamma'}^{\alpha\beta\gamma\delta}\int_\Xi\int_\Xi d\eta\ \ d\zeta\ \ q^\alpha p^\beta(k-l)^{\gamma'}(y-x)^\delta \times e^{-2i\sigma(\xi-\eta,\xi-\zeta)}(\partial_q^{\gamma-\gamma'}\phi^B)(q,x,y)f(\eta)g(\zeta).$$

The Leibnitz rule was used, as well as the two identities

$$\partial_p^\delta e^{-2i\sigma(\xi-\eta,\xi-\zeta)}=(2i)^{|\delta|}(y-x)^\delta e^{-2i\sigma(\xi-\eta,\xi-\zeta)},$$

$$\partial_q^{\gamma'}e^{-2i\sigma(\xi-\eta,\xi-\zeta)}=(2i)^{|\gamma'|}(k-l)^{\gamma'}e^{-2i\sigma(\xi-\eta,\xi-\zeta)}.$$

Step 2: Having in view the form of r_n^m, we write $f(\eta)=\langle\eta\rangle^m[\langle\eta\rangle^{-m}f(\eta)]$ (m even). By developing, the factor $\langle\eta\rangle^m$ contributes with terms of the form $x^\mu k^\nu$. Thus, we need to estimate objects as

$$\int_\Xi\int_\Xi d\eta\ \ d\zeta\ \ q^{\alpha_1}x^{\alpha_2}(y-x)^{\alpha_3}p^{\alpha_4}k^{\alpha_5}(k-l)^{\alpha_6}e^{-2i\sigma(\xi-\eta,\xi-\zeta)}\varphi(q,x,y)[\langle\eta\rangle^{-m}f(\eta)]g(\eta).$$

Here φ is C^∞_{pol} in all the variables; the zeroth order derivative is no longer bounded and this will cause some complications.

Step 3: The heart of the proof lies in exploiting the nice properties of the factor $e^{-2i\sigma(\xi-\eta,\xi-\zeta)}$ by integrations by parts (an oscillatory integral technique). This works efficiently only with respect to certain of the variables. We produce these variables by making linear combinations of other, non-convenient ones. Let us write, for instance, $p=(p-l)+l$, $k-l=(k-p)+(p-l)$ and $k=(k-l)+l=(k-p)+(p-l)+l$. Then, plainly, we are reduced to estimating terms of the form

$$\int_\Xi \int_\Xi d\eta \;\; d\zeta \;\; q^{\beta_1} x^{\beta_2} (y-x)^{\beta_3} l^{\beta_4} (p-k)^{\beta_5} (p-l)^{\beta_6} e^{-2i\sigma(\xi-\eta,\xi-\zeta)} \varphi(q,x,y)$$
$$\times [\langle \eta \rangle^{-m} f(\eta)] g(\eta).$$

Step 4: We use

$$(p-k)^{\beta_5}(p-l)^{\beta_6} e^{-2i\sigma(\xi-\eta,\xi-\zeta)} = (2i)^{-|\beta_5|}(-2i)^{-|\beta_6|} \partial_y^{\beta_5} \partial_x^{\beta_6} [e^{-2i\sigma(\xi-\eta,\xi-\zeta)}].$$

After an integration by parts and an application of Leibnitz's rule we see that we are reduced to bound terms as

$$\int_\Xi \int_\Xi d\eta \;\; d\zeta \;\; \psi(q,x,y) e^{-2i\sigma(\xi-\eta,\xi-\zeta)} \partial_x^{\gamma_1} [\langle \eta \rangle^{-m} f(\eta)] l^{\gamma_2} (\partial_y^{\gamma_3} g)(\zeta)$$

for some unbounded C^∞_{pol}-function ψ. Actually, only the polynomial estimate on ψ itself will count now.

Step 5: Polynomial bounds are very democratic with respect to the choice of variables; use for example inequalities of the form $\langle x+y \rangle \leqslant 2^{1/2} \langle x \rangle \langle y \rangle$. Thus we can write

$$\psi(q,x,y) = \left[\frac{\psi(q,x,y)}{\langle y \rangle^j \langle q-x \rangle^j \langle q-y \rangle^j} \right] \;\; [\langle y \rangle^j \langle q-x \rangle^j \langle q-y \rangle^j]$$

and the first factor will be bounded for j large enough. By developing, we need to estimate

$$\int_\Xi \int_\Xi d\eta \;\; d\zeta \;\; \rho(q,x,y)(q-x)^{\delta_1}(q-y)^{\delta_2} e^{-2i\sigma(\xi-\eta,\xi-\zeta)} \partial_x^{\delta_3} [\langle \eta \rangle^{-m} f(\eta)] y^{\delta_4} l^{\delta_5} (\partial_y^{\delta_6} g)(\zeta),$$

where now ρ is bounded.

Step 6: But one has

$$(q-x)^{\delta_1}(q-y)^{\delta_2} e^{-2i\sigma(\xi-\eta,\xi-\zeta)} = (-2i)^{-|\delta_1|}(2i)^{-|\delta_2|} \partial_l^{\delta_1} \partial_k^{\delta_2} e^{-2i\sigma(\xi-\eta,\xi-\zeta)}.$$

We perform our last integration by parts, reducing ourselves to estimate

$$\int_\Xi \int_\Xi d\eta \;\; d\zeta \;\; \rho(q,x,y) e^{-2i\sigma(\xi-\eta,\xi-\zeta)} \partial_k^{\delta_2} \partial_x^{\delta_3} [\langle \eta \rangle^{-m} f(\eta)] y^{\delta_4} [\partial_l^{\delta_1} \partial_y^{\delta_6} (l^{\delta_5} g)](\zeta).$$

Step 7: Obviously, this integral is dominated for any ξ by $\| \partial_k^{\delta_2} \partial_x^{\delta_3} \times [\langle \cdot \rangle^{-m} f] \|_1 \;\; \| y^{\delta_4} [\partial_l^{\delta_1} \partial_y^{\delta_6} (l^{\delta_5} g)] \|_1$. The first factor is part of the norm $r_n^m(f)$ for some large n and the second is one of the seminorms of g in $\mathcal{S}$. The proposition is proved and, as a bonus, we found out that $(f,g) \mapsto f \circ^B g$ extends to a bilinear *jointly continuous* mapping: $R_0^m \times \mathcal{S} \to \mathcal{S}$. ■

The class $C^\infty_{\mathrm{pol,u}}(\Xi)$ is indeed convenient. It has a very explicit definition and it contains all the polynomials in x and p. It also contains the classical symbol spaces $S^m(\Xi) := \{ f \in C^\infty(\Xi) \,|\, |(\partial^a f)(\xi)| \leqslant C_a \langle \xi \rangle^{m-|a|}, \;\; \forall a \in \mathbb{N}^{2N} \}$ for all m.

The magnetic Moyal algebra is large indeed, but many distributions, even with a good behavior at infinity, are not inside. The one-rank projection $|u\rangle\langle u|$ is in $\mathcal{L}(\mathcal{S})$ if and only if $u \in \mathcal{S}$. Thus, by Proposition 21, there are plenty of elements in $L^2(\Xi)$ not belonging to $\mathcal{M}(\Xi)$.

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Note added. After inserting the preprint of this paper on the mp-arc electronic archieve, T. A. Osborn brought to our attention the paper ''Symplectic area, quantization, and dynamics in electromagnetic fields,'' J. Math. Phys. **43**, 756–788 (2002) by M. V. Karasev and T. A. Osborn and the more recent preprint ''Quantum Magnetic Algebras and Magnetic Curvature,'' arXiv:quant-ph/0311053 by the same authors, where a gauge invariant quantization in the presence of an inhomogeneous electromagnetic tensor is developed in a way similar to ours. The above papers are concerned mainly with the geometric aspects related to this calculus and some interesting connections with grupoids. Our approach motivated by C^*-algebraic methods in spectral analysis for quantum Hamiltonians [see our previous paper: M. Măntoiu and R. Purice, *The Algebra of Observables in a Magnetic Field*, Mathematical Results in Quantum Mechanics (Taxco, 2001), Contemporary Mathematics Vol. 307 (AMS, Providence, RI, 2002), pp. 239–245] aims mainly to the analytic aspects of this quantization procedure (the main results of our Sec V).

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On the absolutely continuous and negative discrete spectra of Schrödinger operators on the line with locally integrable globally square summable potentials

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For one-dimensional Schrödinger operators with potentials q subject to $\Sigma_{n=-\infty}^{\infty}(\int_n^{n+1}|q(x)|dx)^2<\infty$, we prove that the absolutely continuous spectrum is $[0,\infty)$, extending the 1999 result due to Dieft–Killip. As a by-product we show that under the same condition the sequence of the negative eigenvalues is 3/2-summable improving the relevant result by Lieb–Thirring. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1650048]

I. INTRODUCTION

The main object of our consideration is the Schrödinger operator,

$$H=-d^2/dx^2+q(x), \quad \text{on } \mathbb{R}:=(-\infty,\infty), \tag{1.1}$$

with a real slowly decaying potential q. For the background information, literature, and open problems we refer to the recent surveys[12,13] by Simon. In this paper we will be concerned with the essential support of the absolutely continuous (a.c.) spectrum $\sigma_{\text{a.c.}}(H)$ of H for L_2-type potentials without smoothness assumptions. It was proved in 1999 by Dieft–Killip[2] that

$$q\in L_2(\mathbb{R})+L_1(\mathbb{R})\Rightarrow\sigma_{\text{a.c.}}(H)=\mathbb{R}_+:=[0,\infty), \tag{1.2}$$

settling down one conjecture due to Kiselev–Last–Simon[8] which drew considerable attention. We are unable to review here the extensive literature devoted to it and refer the interested reader to, e.g., Christ–Kiselev,[1] Killip,[6] and the literature cited therein. Relevant to our note, the best Christ–Kiselev result is

$$q\in l_p(L_1(\mathbb{R})), \quad 1<p<2\Rightarrow\sigma_{\text{a.c.}}(H)=\mathbb{R}_+, \tag{1.3}$$

where $l_p(L_1)$ stands for the Birman–Solomyak class $(0<p\leqslant\infty)$,

$$f\in l_p(L_1(\mathbb{R}))\Leftrightarrow\left\{\int_n^{n+1}|f(x)|dx\right\}\in l_p(\mathbb{Z}), \quad \mathbb{Z}=\{0,\pm1,\pm2,\dots\}.$$

Since $L_2+L_1\subset l_2(L_1)$ there is a certain mismatch between (1.2) and (1.3). Killip[7] informed the author about his conjecture that (1.3) holds for $p=2$. In the present article we give an affirmative answer to this question. Actually we prove even more.

Theorem 1: *Let q be real valued and from $l_2(L_1(\mathbb{R}))$. Then*

$$\sigma_{\text{a.c.}}(H)=\mathbb{R}_+, \tag{1.4}$$

and the negative discrete spectrum $\{-\kappa_j^2\}$ satisfies

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$$\sum_j \kappa_j^3 < \infty. \tag{1.5}$$

Note that (1.5) extends the Lieb–Thirring bounds,[9]

$$\sum_j \kappa_j^3 \leqslant C \int_{\mathbb{R}} q^2(x)dx,$$

to include $l_2(L_1)$ potentials. The improved bounds will be given in Ref. 11.

We note that a complete treatment of rather general Dirac operators with square summable potentials was recently done by Denisov[3] who besides a proper analog of (1.2) also proved the existence of relevant wave operators.

II. A LEMMA ON A WKB-TYPE ASYMPTOTICS

The following technical lemma will play a crucial role in our consideration.

Lemma 1: Let $q \in l_2(L_1(\mathbb{R}_+))$, then the equation,

$$-u'' + q(x)u = \lambda^2 u, x \in \mathbb{R}_+, \tag{2.1}$$

has a solution $\Psi(x,\lambda)$ which can be represented in the domain Λ of all points (x,λ), $x \in \mathbb{R}_+$ and $\lambda \in \mathbb{C}_+ := \{\lambda \in \mathbb{C}: \operatorname{Im}\lambda > 0\}$ such that

$$(\operatorname{Im}\lambda)^{-1}(2 + (\operatorname{Im}\lambda)^{-1})^2 \|q\chi_x\|^2_{l_2(L_1)} < 1/4 \tag{2.2}$$

[where χ_x is the indicator of (x,∞)] in the form

$$\Psi(x,\lambda) = y(x,\lambda)\exp\left\{ i\lambda x + \int_0^x Q(s,\lambda)ds \right\}, \tag{2.3}$$

where

$$Q(x,\lambda) := -\int_x^\infty e^{2i\lambda(s-x)} q(s)ds, \tag{2.4}$$

and $y(x,\lambda)$ is some continuous function satisfying $((x,\lambda) \in \Lambda)$,

$$|y(x,\lambda) - 1| \leqslant 4(\operatorname{Im}\lambda)^{-1}(2 + (\operatorname{Im}\lambda)^{-1})^2 \|q\chi_x\|^2_{l_2(L_1)}. \tag{2.5}$$

Proof: Let us prove first that if $q \in l_2(L_1(\mathbb{R}_+))$ then $Q(\cdot,\lambda) \in L_2(\mathbb{R})$ for every $\operatorname{Im}\lambda > 0$. Indeed, by Jensen's inequality,

$$\begin{aligned}
|Q(x,\lambda)|^2 &= \left| \sum_{n \geqslant 0} \int_n^{n+1} e^{2i\lambda s} q(s+x)ds \right|^2 \\
&\leqslant \left\{ \sum_{n \geqslant 0} e^{-2n \operatorname{Im}\lambda} \left(\int_n^{n+1} |q(s+x)|ds \right) \right\}^2 \\
&\leqslant \sum_{n \geqslant 0} e^{-2n \operatorname{Im}\lambda} \cdot \sum_{n \geqslant 0} e^{-2 \operatorname{Im}\lambda n} \left(\int_n^{n+1} |q(s+x)|ds \right)^2 \\
&= \frac{1}{1 - e^{-2 \operatorname{Im}\lambda}} \sum_{n \geqslant 0} e^{-2 \operatorname{Im}\lambda n} \left(\int_n^{n+1} |q(s+x)|ds \right)^2.
\end{aligned} \tag{2.6}$$

Integrating (2.6) with respect to x one has

$$\|Q(\cdot,\lambda)\|_2^2 \leqslant \left(1+\frac{1}{2\operatorname{Im}\lambda}\right)\sum_{n\geqslant 0} e^{-2\operatorname{Im}\lambda n}\int_0^\infty\left(\int_n^{n+1}|q(s+x)|ds\right)^2 dx. \tag{2.7}$$

Observe now that

$$\begin{aligned}\int_0^\infty\left(\int_n^{n+1}|q(s+x)|ds\right)^2 dx &= \sum_{m\geqslant 0}\int_m^{m+1}\left(\int_x^{x+1}|q|\right)^2 dx\\ &\leqslant \sum_{m\geqslant 0}\left(\int_m^{m+2}|q|\right)^2\\ &\leqslant 2\sum_{m\geqslant 0}\left\{\left(\int_m^{m+1}|q|\right)^2+\left(\int_{m+1}^{m+2}|q|\right)^2\right\}\\ &= 4\sum_{m\geqslant 0}\left(\int_m^{m+1}|q|\right)^2\\ &= 4\|q\|_{l_2(L_1)}^2.\end{aligned} \tag{2.8}$$

Plugging (2.8) into (2.7), one has

$$\|Q(\cdot,\lambda)\|_2^2 \leqslant \left(1+\frac{1}{2\operatorname{Im}\lambda}\right)\sum_{n\geqslant 0} e^{-\operatorname{Im}\lambda n}\cdot 4\|q\|_{l_2(L_1)}^2 \leqslant \left(2+\frac{1}{\operatorname{Im}\lambda}\right)^2\|q\|_{l_2(L_1)}^2,$$

that is

$$\|Q^2(\cdot,\lambda)\|_1 \leqslant \|Q(\cdot,\lambda)\|_2^2 \leqslant \left(2+\frac{1}{\operatorname{Im}\lambda}\right)^2\|q\|_{l_2(L_1)}^2. \tag{2.9}$$

By inspection

$$\Theta(x,\lambda) := \exp\left\{i\lambda x+\int_0^x Q(s,\lambda)ds\right\}$$

is a solution to

$$-u''+(q(x)+Q^2(x,\lambda))u=\lambda^2 u. \tag{2.10}$$

If $u_1(x,\lambda)=\Theta(x,\lambda)$ is a solution to (2.10) then as the other solution we choose

$$u_2(x,\lambda)=\Theta(x,\lambda)\int_0^x \Theta^{-2}(s,\lambda)ds.$$

Rewriting the original equation (2.1) as

$$-u''+(q(x)+Q^2(x,\lambda))u-\lambda^2 u=Q^2(x,\lambda)u, \tag{2.11}$$

by variation of parameters one easily verifies (formally) that (2.11) implies ($y=\Theta^{-1}u$)

$$y(x,\lambda)=1+\int_x^\infty K(x,s,\lambda)y(s,\lambda)ds, \tag{2.12}$$

with the kernel

$$K(x,s,\lambda) := Q^2(s,\lambda)\cdot\Theta^2(s,\lambda)\int_x^s \Theta^{-2}(t,\lambda)dt. \tag{2.13}$$

To justify this formal computation it is enough to show that $K(x,\cdot,\lambda)\in L_1$ for every $x\in\mathbb{R}_+$, $\lambda\in\mathbb{C}_+$. By (2.9), $Q^2(\cdot,\lambda)\in L_1$ and it is only left to demonstrate that $\Theta^2(s,\lambda)\int_x^s\Theta^{-2}(t,\lambda)dt$ is bounded. Indeed,

$$\begin{aligned}\left|\Theta^2(s,\lambda)\int_x^s\Theta^{-2}(t,\lambda)dt\right| &= \left|\int_x^s \exp^2\left\{i\lambda(s-t)+\int_t^s Q(t,\lambda)dt\right\}dt\right| \\ &\leqslant \left|\int_0^{s-x}\exp^2\left\{-\operatorname{Im}\lambda\, t\left(1-\frac{1}{\operatorname{Im}\lambda}\|Q(\cdot,\lambda)\|_\infty\right)\right\}\right| \\ &\leqslant \int_0^\infty \exp(-\operatorname{Im}\lambda\, t)dt = \frac{1}{\operatorname{Im}\lambda}\end{aligned}$$

and, by (2.9), we have

$$\|K(x,\cdot,\lambda)\|_1 \leqslant \frac{1}{\operatorname{Im}\lambda}\|Q^2(\cdot,\lambda)\|_1 \leqslant \frac{1}{\operatorname{Im}\lambda}\left(2+\frac{1}{\operatorname{Im}\lambda}\right)^2\|q\|^2_{l_2(L_1)}.$$

The standard iteration procedure completes the proof. ■

Remark 1: One can easily see that, up to a factor, solution (2.3) has the WKB-type asymptotic behavior,

$$\Psi(x,\lambda)\sim\exp\left\{i\lambda x+\frac{1}{2i\lambda}\int_0^x q(s)ds\right\},\quad x\to\infty, \tag{2.14}$$

for every $\lambda\in\mathbb{C}_+$. We, by no means, claim that Lemma 1 proves (2.14) for almost all real λ for every potential q from $l_2(L_1(\mathbb{R}_+))$. Theorem 1 would be immediately proven then. It is a very difficult open question and the best known result here belongs to Christ–Kiselev.[1] Using some very elaborate techniques, they showed that (2.14) holds for a.e. real λ for $q\in l_p(L_1(\mathbb{R}_+))$,$1<p<2$. This was exactly their way to prove (1.3). Our approach requires (2.14) only for $\lambda\in\mathbb{C}_+$.

III. PROOF OF THEOREM 1

We employ the standard approach. We first get all necessary formulas for the truncated potentials $\tilde{q}$ defined as

$$\tilde{q}(x)=q(x)\chi_{[-a,a]}(x),\quad a>0;$$

$\chi_{[-a,a]}$ denotes the characteristic function of $[-a,a]$, and then pass to the limit when $\tilde{q}\to q$ (i.e., $a\to\infty$). In the sequel, we agree to put $\tilde{}$ on top of every object related to $\tilde{q}$.

Let us evaluate the transmission coefficient $\tilde{T}(\lambda)$ for $\lambda\in\mathbb{C}_+$ in two different ways. Following Faddeev–Zhakharov[4] (adopting the convention $\int := \int_{-\infty}^{\infty}$),

$$\tilde{T}(\lambda)=\prod_j\frac{\lambda+i\tilde{\kappa}_j}{\lambda-i\tilde{\kappa}_j}\exp\left\{i\int\frac{\tilde{f}(k)}{k-\lambda}dk\right\}, \tag{3.1}$$

where $-\tilde{\kappa}_j^2$ are negative eigenvalues of $\tilde{H}$ and

$$\tilde{f}(k) := \frac{1}{\pi}\log|\tilde{T}(k)|^{-1}. \tag{3.2}$$

Due to the general properties of the transmission coefficient, the function $\tilde{f}$ is integrable, nonnegative, and even and hence

$$\int \frac{\widetilde{f}(k)}{k-\lambda}dk=-\frac{1}{\lambda}\int \widetilde{f}(k)dk+\frac{1}{\lambda^2}\int \frac{k^2\widetilde{f}(k)}{k-\lambda}dk=-\frac{1}{\lambda}\int \widetilde{f}(k)dk+\frac{2}{\lambda}\int_0^\infty \frac{k^2\widetilde{f}(k)}{k^2-\lambda^2}dk. \quad (3.3)$$

We have used here the obvious identity

$$\frac{1}{k-\lambda}=-\frac{k}{\lambda^2}-\frac{1}{\lambda}+\frac{1}{\lambda^2}\frac{k^2}{k-\lambda}.$$

By the first Buslaev–Faddeev–Zhakharov trace formula,[4]

$$-2\sum_j \widetilde{\kappa}_j+\int \widetilde{f}(k)dk=\frac{1}{2}\int \widetilde{q}(x)dx, \quad (3.4)$$

and (3.3) can be continued,

$$\int \frac{\widetilde{f}(k)}{k-\lambda}dk=-\frac{1}{\lambda}\int \widetilde{f}(k)dk+\frac{2}{\lambda}\int_0^\infty \frac{k^2\widetilde{f}(k)}{k^2-\lambda^2}dk=-\frac{2}{\lambda}\sum_j \widetilde{\kappa}_j-\frac{1}{2\lambda}\int \widetilde{q}(x)dx+\frac{2}{\lambda}\int_0^\infty \frac{k^2\widetilde{f}(k)}{k^2-\lambda^2}dk. \quad (3.5)$$

Plugging (3.5) into (3.1) one has

$$\widetilde{T}(\lambda)=\prod_j \frac{\lambda+i\widetilde{\kappa}_j}{\lambda-i\widetilde{\kappa}_j}e^{2i/\lambda\widetilde{\kappa}_j}\cdot \exp\left\{\frac{2i}{\lambda}\int_0^\infty \frac{k^2\widetilde{f}(k)}{k^2-\lambda^2}dk\right\}\exp\left\{\frac{1}{2i\lambda}\int \widetilde{q}(x)dx\right\}. \quad (3.6)$$

On the other hand, following Hinton–Klaus–Shaw,[5]

$$\widetilde{T}(\lambda)=\frac{2i\lambda}{\widetilde{m}_+(\lambda^2)+\widetilde{m}_-(\lambda^2)}(\widetilde{F}_+(\lambda)\widetilde{F}_-(\lambda))^{-1}, \quad (3.7)$$

where $\widetilde{m}_\pm$ are the Weyl m-functions associated with $-d^2/dx^2+\widetilde{q}(x), u(\pm 0)=0$ on $L_2(\mathbb{R}_\pm)$ and $\widetilde{F}_\pm$ are the Jost functions of $\widetilde{H}=-d^2/dx^2+\widetilde{q}(x)$ on $L_2(\mathbb{R})$ corresponding to $\pm\infty$, respectively. We recall that for $q\in L_1(\mathbb{R})$ the equation

$$-u''+q(x)u=\lambda^2 u, x\in\mathbb{R}, \quad \operatorname{Im}\lambda^2\geqslant 0,$$

has two linearly independent solutions $u_\pm(x,\lambda)$, referred to as Jost, subject to

$$u_\pm(x,\lambda)=e^{\pm i\lambda x}(1+o(1)), x\to\pm\infty.$$

Functions $F_\pm$ and $m_\pm$ are related to $u_\pm$ by

$$F_\pm(\lambda):=u_\pm(0,\lambda), \quad m_\pm(\lambda^2):=\pm\frac{d}{dx}\log u_\pm(x,\lambda)\big|_{x=0}. \quad (3.8)$$

Evaluate now $\widetilde{F}_+(\lambda)\widetilde{F}_-(\lambda)$ in (3.7). Since $\widetilde{F}_+$ and $\widetilde{F}_-$ are similar we handle only $\widetilde{F}_+$. Directly by definition (2.4), one verifies that

$$\int_0^a \widetilde{Q}(s,\lambda)ds=\frac{1}{2i\lambda}\int_0^a \widetilde{q}(s)ds-\frac{\widetilde{Q}(a,\lambda)-\widetilde{Q}(0,\lambda)}{2i\lambda}=\frac{1}{2i\lambda}\int_0^a \widetilde{q}(s)ds+\frac{1}{2i\lambda}\widetilde{Q}(0,\lambda), \quad (3.9)$$

where we have observed that $\widetilde{Q}(a,\lambda)=0$. Comparing u_+ with the solution Ψ from Lemma 1, one has

$$\tilde{u}_+(x,\lambda)=\tilde{\Psi}(x,\lambda)\exp\left\{-\int_0^a \tilde{Q}(s,\lambda)ds\right\}$$
$$=\tilde{\Psi}(x,\lambda)\exp\left\{-\frac{1}{2i\lambda}\int_0^\infty \tilde{q}(s)ds\right\}\exp\left\{\frac{1}{2i\lambda}\int_0^\infty e^{2i\lambda s}\tilde{q}(s)ds\right\}. \tag{3.10}$$

It follows from (3.8), (3.9), and (2.2) that

$$\tilde{F}_+(\lambda)=\tilde{y}_+(\lambda)\exp\left\{-\frac{1}{2i\lambda}\int_0^\infty \tilde{q}(s)ds\right\}\exp\left\{\frac{1}{2i\lambda}\int_0^\infty e^{2i\lambda s}\tilde{q}(s)ds\right\}, \tag{3.11}$$

where $\tilde{y}_+(\lambda):=\tilde{y}(+0,\lambda)$. Analogously,

$$\tilde{F}_-(\lambda)=\tilde{y}_-(\lambda)\exp\left\{-\frac{1}{2i\lambda}\int_{-\infty}^0 \tilde{q}(s)ds\right\}\exp\left\{\frac{1}{2i\lambda}\int_{-\infty}^0 e^{-2i\lambda s}\tilde{q}(s)ds\right\}$$

with some function $\tilde{y}_-$ admitting a similar to the (2.3) estimate. Thus

$$(\tilde{F}_+(\lambda)\tilde{F}_-(\lambda))^{-1}=\tilde{y}^{-1}(\lambda)\exp\left\{\frac{1}{2i\lambda}\int \tilde{q}(x)dx\right\}\exp\left\{\frac{i}{2\lambda}\int e^{2i\lambda|x|}\tilde{q}(x)dx\right\}, \tag{3.12}$$

where $\tilde{y}:=\tilde{y}_+\tilde{y}_-$. Inserting (3.12) into (3.7), we finally arrive at

$$\tilde{T}(\lambda)=\tilde{y}^{-1}(\lambda)\frac{2i\lambda}{\tilde{m}_+(\lambda^2)+\tilde{m}_-(\lambda^2)}\exp\left\{\frac{1}{2i\lambda}\int \tilde{q}(x)dx\right\}\exp\left\{\frac{i}{2\lambda}\int e^{2i\lambda|x|}\tilde{q}(x)dx\right\}. \tag{3.13}$$

Equate now the right hand sides of (3.6) and (3.13). Taking $\lambda=i$ and observing that the divergent factor $\exp\{-\frac{1}{2}\int\tilde{q}(x)dx\}$ drops out from both sides, we obtain

$$\prod_j \frac{1+\tilde{\kappa}_j}{1-\tilde{\kappa}_j}e^{-2\tilde{\kappa}_j}\cdot\exp\left\{2\int_0^\infty\frac{k^2}{1+k^2}\tilde{f}(k)dk\right\}=\left\{\frac{-2\tilde{y}^{-1}(i)}{\tilde{m}_+(-1)+\tilde{m}_-(-1)}\right\}\exp\left\{\frac{1}{2}\int e^{-2|x|}\tilde{q}(x)dx\right\}. \tag{3.14}$$

Taking notice that due to basic facts of perturbation theory a change of the potential q on a finite interval does not effect the conclusions of the theorem, we alter, if needed, our potential to satisfy condition (2.2) for $\lambda=i$ for all $x\geqslant 0$ and $\sup|\tilde{\kappa}_j|<1$. This makes every factor in (3.14) positive and one can pass in (3.14) to the logarithms

$$\sum_j\left(\log\frac{1+\tilde{\kappa}_j}{1-\tilde{\kappa}_j}-2\tilde{\kappa}_j\right)+\int_0^\infty\frac{2k^2}{1+k^2}\tilde{f}(k)dk=\frac{1}{2}\int e^{-2|x|}\tilde{q}(x)dx+2\tilde{\omega}, \tag{3.15}$$

where

$$\tilde{\omega}:=-\tilde{y}^{-1}(i)\{\tilde{m}_+(-1)+\tilde{m}_-(-1)\}^{-1}. \tag{3.16}$$

The sum in (3.15) has the lower bound $\frac{2}{3}\Sigma_j\tilde{\kappa}_j^3$. Indeed, setting for the time being $\alpha=\tilde{\kappa}_j$ one has

$$\log\frac{1+\alpha}{1-\alpha}-2\alpha=\log(1+\alpha)-\log(1-\alpha)-2\alpha$$
$$=\sum_{n\geqslant 0}(-1)^n\frac{\alpha^n}{n+1}+\sum_{n\geqslant 0}\frac{\alpha^n}{n+1}-2\alpha$$
$$=2\sum_{n\geqslant 1}\frac{\alpha^{2n+1}}{2n+1}\geqslant\frac{2}{3}\alpha^3,$$

and thus

$$\sum_j\left(\log\frac{1+\tilde\kappa_j}{1-\tilde\kappa_j}-2\tilde\kappa_j\right)\geqslant\frac{2}{3}\sum_j\tilde\kappa_j^3.$$

It follows from (3.15) that

$$\frac{1}{3}\sum_j\tilde\kappa_j^3+\int_0^\infty\frac{k^2}{1+k^2}\tilde f(k)dk\leqslant\frac{1}{4}\int e^{-2|x|}\tilde q(x)dx+\tilde\omega. \tag{3.17}$$

Show now that the right hand side of (3.17) is uniformly bounded as $\tilde q\to q$. Indeed, by (2.2) and (2.5),

$$|\tilde y(i)|^{-1}=|\tilde y_+(i)|^{-1}|\tilde y_-(i)|^{-1}\leqslant 2\cdot 2=4.$$

The other factor in (3.16) goes to $(m_+(-1)+m_-(-1))^{-1}$ due to the general properties of the Weyl m-function[14] and hence $\tilde\omega$ is uniformly bounded as $\tilde q\to q$. Since

$$\int e^{-2|x|}\tilde q(x)dx\to\int e^{-2|x|}q(x)dx,\quad \tilde q\to q,$$

we see that the right hand side of (3.17) is uniformly bounded too. Since both terms on the left hand side of (3.17) are positive, recalling (3.2), we arrive at

$$\int_0^\infty\frac{k^2}{1+k^2}\log|\tilde T(k)|^{-1}dk\leqslant C, \tag{3.18}$$

$$\sum_j\tilde\kappa_j^3\leqslant C, \tag{3.19}$$

with some finite constant C dependent only on q. Estimate (3.18) allows one now to use a lemma by Deift–Killip[2] (see also Ref. 10). Thus (1.4), i.e., $\sigma_{\text{a.c.}}(H)=\mathbb{R}_+$, is proven.

It is left to establish (1.5). We can actually pass to the limit in (3.19). To this end consider the operator $H_-:=-d^2/dx^2+q_-(x)$ where q_- is the negative part of q. In obvious notation, estimate (3.19) for $\tilde H_-$ reads (with possibly different constant) as

$$\sum_j(\tilde\kappa_j^{(-)})^3\leqslant C. \tag{3.20}$$

But $0<a<b$ implies $q_-(x)\chi_{[-a,a]}(x)\geqslant q_-(x)\chi_{[-b,b]}(x)$, which, in turn, yields

$$-d^2/dx^2+q_-(x)\chi_{[-a,a]}(x)\supseteq -d^2/dx^2+q_-(x)\chi_{[-a,a]}(x),$$

and it follows from the standard fact of perturbation theory that $\tilde{\kappa}_j^{(-)}$ is a nondecreasing function of the cutoff point a for every fixed j. The latter combined with the uniform bound (3.20) immediately yields

$$\sum_j (\kappa_j^{(-)})^3 \leqslant C. \tag{3.21}$$

What is left to observe that, by the same perturbation principal, $\kappa_j \leqslant \kappa_j^{(-)}$ (since $H_- \subseteq H$) and (3.21) implies (1.5). The theorem is proven.

Remark 2: Identity (3.15) can actually be viewed as the first formula in a certain chain of sum rules. Our elementary arguments provide a short-cut to Theorem 1 but yet are not fine enough to derive those formulas in a compact form. The adequate approach is rather operator theoretical and will be discussed in Ref. 11 where we also plan to improve on the results of Ref. 10 in the spirit of Theorem 1. At this point we only notice that (3.15) resembles the second (sic) Buslaev–Faddeev–Zhakharov trace formula

$$\frac{1}{3}\sum_j \tilde{\kappa}_j^3 + \int_0^\infty k^2 \tilde{f}(k)\,dk = \frac{1}{16}\int \tilde{q}^2(x)\,dx,$$

which was the main new insight of Ref. 2 proving (1.2) and which higher order analogs were used in Ref. 10.

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Quantum-mechanical scattering in exterior domains with impenetrable periodic boundaries and short-range potentials

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We study the scattering of a nonrelativistic particle in an exterior domain (=open connected subset) $\Omega \subset \mathbf{R}^{\nu}(\nu \geqslant 2)$ containing a half-space and contained in another half-space, and having an impenetrable periodic boundary $\partial\Omega$. "Impenetrable" means that (generalized) homogeneous Dirichlet conditions are imposed on $\partial\Omega$. We prove the existence and completeness of the wave operators $W_{\pm} = \lim_{t \to \pm\infty} \exp(itH_1)\mathcal{P}\exp(-itH_0)$ corresponding to the scattering of a nonrelativistic particle in Ω by the combined effect of the boundary and a short-range potential present in Ω. Here $H_0 = -\Delta$ is the negative distributional Laplacian in the Hilbert space $\mathcal{H}_0 = L^2(\mathbf{R}^{\nu})$, $H_1 = -\Delta_{\mathrm{D}}(\Omega) + V$, $\Delta_{\mathrm{D}}(\Omega)$ being the Dirichlet Laplacian in the Hilbert space $\mathcal{H} = L^2(\Omega)$, V an operator of multiplication in $\mathcal{H}$ by a bounded measurable function $V(x)$ on Ω having the periodicity of the boundary, and $\mathcal{P}: \mathcal{H}_0 \to \mathcal{H}$ an identification operator. The operators $W_{\pm}$ model the quantum-mechanical scattering of low-energy atoms by crystal surfaces, with V modeling the interaction between the incident particles and the surface atoms. This interaction is idealized by assuming that $V(x)$ depends solely on x_{ν} when $x_{\nu} > a$, a being a sufficiently large positive constant, and x_{ν} the component of $x \in \mathbf{R}^{\nu}$ directed perpendicularly to the surfaces of the above two half-spaces. Under this and other hypotheses on Ω and V stated precisely in the paper, we prove that $W_{\pm}$ exist as partially isometric operators whose initial sets have a transparent physical meaning. Moreover, we prove the following: (a) $\mathrm{Ran}\, W_{\pm} = \mathcal{H}_{\mathrm{scatt}}$; and (b) $W_{\pm}$ are asymptotically complete, in the sense that $\mathcal{H} = \mathcal{H}_{\mathrm{scatt}} \oplus \mathcal{H}_{\mathrm{surf}}$. Here $\mathcal{H}_{\mathrm{scatt}}$ and $\mathcal{H}_{\mathrm{surf}}$ are suitably defined subspaces of scattering and surface states of $\mathcal{H}$. These results are proved by using direct-integral techniques, asymptotic methods from the theory of ODEs, and methods analogous to those of Lyford. The present paper generalizes an earlier one by the author for the case $V = 0$. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Theoretical studies of classical scattering, both acoustic and electromagnetic, by corrugated surfaces go at least as far back as Lord Rayleigh and have an enormous literature.[1] Quantum mechanical scattering of low-energy atomic beams by crystal surfaces, modeled as impenetrable corrugated surfaces, has also received much attention.[2] Much less work has been done on scattering by such surfaces at a rigorous mathematical level. This includes research by Wilcox[3,4] and the present author.[5,6]

In Ref. 5, we studied quantum-mechanical scattering of nonrelativistic particles by an impenetrable periodic boundary, i.e., such that the pertinent wave functions obeyed (generalized) homogeneous Dirichlet conditions thereon. In the present paper we generalize this work to the case in which a short-range potential is present, which models the interaction between the particle and the

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surface atoms of a crystal. In more detail, we consider the quantum-mechanical scattering of such a particle in an exterior domain (=open connected subset) $\Omega\subset\mathbf{R}^\nu(\nu\geqslant 2)$ with an impenetrable corrugated boundary $\partial\Omega$ by the combined effect of the boundary and a short-range potential present in Ω. ''Impenetrable'' means that the particle's wave function obeys (generalized) homogeneous Dirichlet conditions on $\partial\Omega$. Our point of view will be that of time-dependent two-Hilbert-space scattering theory, in which the scattering is described by the wave operators

$$W_\pm = W_\pm(H_1,H_0;\mathcal{P}) = s-\lim_{t\to\pm\infty}\exp(itH_1)\mathcal{P}\exp(-itH_0). \tag{1.1}$$

Here H_0 is the ''unperturbed'' Hamiltonian, defined as the negative distributional Laplacian $-\Delta$ in $\mathcal{H}_0=L^2(\mathbf{R}^\nu)$, while $H_1=H+V$ is the corresponding ''perturbed'' Hamiltonian, H being the negative Dirichlet Laplacian $-\Delta_{\mathrm{D}}(\Omega)$ in $\mathcal{H}=L^2(\Omega)$ and V a maximal operator of multiplication in $\mathcal{H}$ by a real-valued measurable function, also denoted by V, which models the above short-range interaction between the particle and the surface atoms. Moreover, $\mathcal{P}$: $\mathcal{H}_0\to\mathcal{H}$ is a suitable bounded operator (identification operator).

As to Ω, we assume that it contains a half-space and is contained in another half-space. We also suppose that it has the periodicity property $(\tilde{x},x_\nu)\in\Omega\Rightarrow(\tilde{x}+n,x_\nu)\in\Omega$ for all $n\in\mathbf{Z}^{\nu-1}$, where we write $x\in\mathbf{R}^\nu$ as $(\tilde{x},x_\nu)\in\mathbf{R}^{\nu-1}\times\mathbf{R}$, x_ν being in a direction perpendicular to the boundaries of these half-spaces. No smoothness or regularity conditions are imposed on $\partial\Omega$ by virtue of a theorem of Lyford,[7] as we shall explain in more detail in Sec. II. As to the potential function V, we assume it to be periodic in the sense that $V(x)=V(\tilde{x},x_\nu)=V(\tilde{x}+n,x_\nu)$ for all $x\in\Omega$ and all $n\in\mathbf{Z}^{\nu-1}$. We also suppose that $V(x)$ has certain boundedness and integrability properties, and depends only on x_ν for $x_\nu>a$, where a is a sufficiently large positive constant. The last condition allows us to use powerful results on the asymptotic behavior of solutions of ODEs in the relevant proofs. On the other hand, it is a physically reasonable requirement, since for a large class of short-range potentials with the mentioned periodicity property, $V(\tilde{x},x_\nu)$ tends pointwise to a function independent of $\tilde{x}$ for $x_\nu\to\infty$.[8]

Our principal results are Theorems 3.1 and 3.2. The former asserts the completeness of the wave operators (1.1), and more precisely that $\mathrm{Ran}\,W_+=\mathrm{Ran}\,W_-=\mathcal{H}_{\mathrm{scatt}}$. Here $\mathcal{H}_{\mathrm{scatt}}$ is the subspace of scattering states, consisting of those functions $f\in\mathcal{H}$ that are evanescent from each region bounded by $\partial\Omega$ and a plane $x_\nu=\mathrm{const}$. Theorem 3.2 states that $W_\pm$ are asymptotically complete, i.e., that $\mathcal{H}_{\mathrm{scatt}}$ is the orthogonal complement with respect to $\mathcal{H}$ of the subspace $\mathcal{H}_{\mathrm{surf}}$ of surface states. The latter subspace, first introduced in Ref. 9, consists of all $f\in\mathcal{H}$ that remain ''close'' to $\partial\Omega$ for all time. [Rigorous definitions of $\mathcal{H}_{\mathrm{scatt}}$ and $\mathcal{H}_{\mathrm{surf}}$ are given by Eqs. (3.4) and (3.5), respectively.]

The organization of this paper is as follows. In Sec. II we define the self-adjoint operators H,H^0,H_1,V needed to construct $W_\pm$ in (1.1). Section III has two subsections. In Sec. III A we state Theorems 3.1 and 3.2, and Sec. III B is devoted to an overview of the methods of proof of these theorems, which rely heavily on direct-integral methods. A proof of Theorem 3.1 is given in Sec. IV by using a theorem of Lyford[10] based on work of Birman and Belopol'skii[11] and employing a version of a theorem of Stinespring.[12] In preparation for proving Theorem 3.2, we devote Sec. V to studying the spectrum of a family of self-adjoint operators $h_\theta[\theta\in(0,1)^{\nu-1}]$ defined in Sec. II, whose direct integral is unitarily equivalent to H, and prove that each h_θ has an empty singular continous spectrum. In Sec. V the asymptotic properties of solutions of a second-order ODE satisfied by the expansion coefficients of certain locally square-integrable functions play an important role. In particular, the above spectral and asymptotic properties are essential ingredients of the proof of Theorem 3.2 presented in Sec. VI. There are three appendixes. Appendix A explains our function-space notation, while Appendixes B and C state, respectively, a key local compactness property and a lemma on asymptotic solutions of ODEs of the above type, both of these results being used in Sec. V.

II. SELF-ADJOINTNESS OF A HAMILTONIAN OF A NONRELATIVISTIC PARTICLE IN AN EXTERIOR DOMAIN Ω WITH AN IMPENETRABLE PERIODIC BOUNDARY AND SUBJECTED TO A SHORT-RANGE POTENTIAL

For future reference, it is convenient to restate here the assumed properties of the exterior domain $\Omega\subset\mathbf{R}^{\nu}(\nu\geqslant 2)$ that were mentioned in Sec. I:

(I) $\mathbf{R}^{\nu-1}\times[\beta,\infty)\subset\Omega\subset\mathbf{R}^{\nu-1}\times[\alpha,\infty)$, for some $0<\alpha<\beta<1/2$.

(II) (Periodicity) Write the points $x\in\mathbf{R}^{\nu}(\nu\geqslant 2)$ as $(\tilde{x},x_{\nu})$, where $\tilde{x}\in\mathbf{R}^{\nu-1}$,

$$x_{\nu}\in\mathbf{R}.\ \text{For all}\ \ n\in\mathbf{Z}^{\nu-1},\ \ (\tilde{x},x_{\nu})\in\Omega\Rightarrow(\tilde{x}+n,x_{\nu})\in\Omega.$$

We consider a nonrelativistic particle in Ω whose evolution is governed by a self-adjoint Hamiltonian operator H_1 acting in the Hilbert space $\mathcal{H}=L^2(\Omega)$, and defined as the operator sum

$$H_1=H+V, \tag{2.1}$$

where (in suitable units) H denotes the kinetic energy operator of the particle, confined in Ω by the surface $\partial\Omega$ on which we impose a generalized homogeneous Dirichlet condition, and V models its interaction with the surface atoms.

More precisely,

$$H=-\Delta_{\mathrm{D}}(\Omega), \tag{2.2}$$

where $\Delta_{\mathrm{D}}(\Omega)$ is the Dirichlet Laplacian in $\mathcal{H}$, acting by Δ (distributional Laplacian) on the functions in its domain,

$$D(\Delta_{\mathrm{D}}(\Omega))=L^2(\Delta;\Omega)\cap H_0^1(\Omega). \tag{2.3}$$

Here $L^2(\Delta;\Omega)$ denotes the Hilbert space defined in Appendix A and $H_0^1(\Omega)$ the usual Sobolev space. These and other function spaces used in this paper are defined in that appendix. By (2.2), (2.3), and a remarkable theorem of Lyford,[7] the operator H is self-adjoint for an *arbitrary domain* $\Omega\subset\mathbf{R}^{\nu}$, and not merely for the domain Ω considered here.

We define V as a maximal operator of multiplication in $L^2(\Omega)$ by a real-valued measurable function on Ω, which will also be denoted by V and assumed to satisfy the following requirement.

Condition 1: V has the periodicity property

$$V(x)=V(\tilde{x},x_{\nu})=V(\tilde{x}+n,x_{\nu}),\ \ x\in\Omega,n\in\mathbf{Z}^{\nu-1}, \tag{2.4a}$$

is bounded on Ω, and has the integrability property

$$V\big|\omega\in L^2(\omega). \tag{2.4b}$$

Here ω denotes the irregular semi-infinite cylinder $\omega=\{x=(\tilde{x},x_{\nu})\in\Omega:\tilde{x}\in(0,1)^{\nu-1}\}$, whose axis is parallel to the x_{ν} axis.

Remarks: (1) The properties of the function V which are stated in this condition and the fact that it is real-valued entail that the corresponding operator V is bounded and self-adjoint, and hence that its domain is $\mathcal{H}$. Thus H_1, as the operator sum of the (unbounded) self-adjoint operator H and V is itself self-adjoint. Indeed, V is infinitesimally small wrt H, or $V\ll H$ in symbols.[13]

(2) If the function V had not been required to be essentially bounded, H_1 could have been defined by (2.1), understood in the sense of quadratic forms. However, this would greatly complicate the treatment of the problems discussed in the paper. The boundedness of this function is very natural from a physical viewpoint, since for the models of atomic crystal surfaces of interest here, the atomic cores lie in the complement $\mathbf{R}^{\nu}\backslash\Omega$ of Ω, and hence Ω contains no infinite singularities of V.[2] Finally, the integrability condition (2.4b), which is reasonable for short-range potentials, plays an important role in the proof of the key Lemma 4.2.

III. SCATTERING BY IMPENETRABLE PERIODIC BOUNDARIES WITH SHORT-RANGE POTENTIALS: MAIN RESULTS AND STRATEGY OF PROOF

A. Statement of main results

As mentioned in Sec. I, Theorems 3.1 and 3.2 are our principal results. Before stating them, we make some definitions and a further assumption on V.

Let K_1, K_2 be self-adjoint operators in the respective Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, K_1 having a purely absolutely continous spectrum, and let $B:\mathcal{H}_1\to\mathcal{H}_2$ be a bounded operator. We define the wave operators

$$W_{\pm}(K_2,K_1;B)=s-\lim_{t\to\pm\infty}\exp(itK_2)\,B\exp(-itK_1), \tag{3.1}$$

if they exist. The wave operators studied in this paper have the form (3.1).

Theorems 3.1 and 3.2 deal with properties of the wave operators,

$$W_{\pm}:=W_{\pm}(H_1,H_0;\mathcal{P}), \tag{3.2}$$

which, as mentioned in the Introduction, describe scattering by the impenetrable periodic boundary $\partial\Omega$ when the short-range potential V acts in the exterior domain Ω. As in Sec. II, $H_0=-\Delta$, the negative distributional Laplacian acting in the Hilbert space $\mathcal{H}_0=L^2(\mathbf{R}^\nu)$, and $\mathcal{P}:\mathcal{H}_0\to\mathcal{H}=L^2(\Omega)$ is defined by

$$(\mathcal{P}f)(x)=\begin{cases} f(x), & x\in\Omega,\\ 0, & x\in\mathbf{R}^\nu\backslash\Omega,\end{cases}$$
$$f\in\mathcal{H}_0,\quad x\in\Omega. \tag{3.3a}$$

For any measurable subset $A\subset\mathbf{R}^\nu$, we identify $L^2(A)$ with the subspace of $L^2(\mathbf{R}^\nu)$ composed of all f such that $f(x)=0$ a.e. on $\mathbf{R}^\nu\backslash A$. Thus, the requirements $\mathcal{P}:\mathcal{H}_0\to\mathcal{H}$ and (3.3a) are consistent.

By Theorem 3.1, the wave operators (3.2) can be written as $W_{\pm}(H_1,H_0;J)$, a form that has certain technical advantages. Here $J:\mathcal{H}_0\to\mathcal{H}$ is given by

$$(Jf)=\begin{cases} j(x_\nu)f(x), & x=(\tilde{x},x_\nu)\in\Omega,\\ 0, & x\in\mathbf{R}^\nu\backslash\Omega,\end{cases} \tag{3.3b}$$

where $j\in C^\infty(\mathbf{R})$ is such that

$$j(y)=\begin{cases} 0, & y\leqslant 1/2,\\ 1, & y\geqslant 1.\end{cases} \tag{3.3c}$$

The requirements $J:\mathcal{H}_0\to\mathcal{H}$ and (3.3b) are therefore consistent.

An important role in what follows is played by the subspaces $\mathcal{H}_{\text{scatt}}$, $\mathcal{H}_{\text{surf}}$ of scattering and surface states, respectively, defined by

$$\mathcal{H}_{\text{scatt}}=\{f\in L^2(\Omega):\ \lim_{t\to\pm\infty}\|\exp(-itH_1)f\|_{\Omega_r}=0,1<r<\infty\}, \tag{3.4}$$

$$\mathcal{H}_{\text{surf}}=\{f\in L^2(\Omega):\ \lim_{t\to\pm\infty}\|\exp(-itH_1)f\|_{\Omega\backslash\Omega_r}=0,1<r<\infty\}, \tag{3.5}$$

whose physical significance was mentioned in Sec. I. Here $\|\cdot\|_M$ denotes the $L^2(M)$ norm for a measurable subset $M\subset\mathbf{R}^\nu$ and $M_r=\{(\tilde{x},x_\nu)\in\mathbf{R}^\nu:x_\nu<r\}$. We will also use the notation $M_{r,\infty}=\{x\in M:x_\nu>r\}$.

Besides assuming that V satisfies condition **1**, we will suppose that it has the following property, unless we make an explicit statement to the contrary.

Condition 2: $V(\tilde{x},x_\nu)=w(x_\nu)\forall x=(\tilde{x},x_\nu)\in\omega_{a,\infty}$, where $w\in C^\infty((a,\infty))\cap L^1((a,\infty))$ and $a>1$ is a constant.

Remarks: We have already commented on the mathematical convenience and physical reasonableness of this condition in Sec. I. The infinite differentiability of w in condition 2 is imposed for ease of exposition, while the integrability requirement therein plays an essential role in proving various key lemmas.

Theorem 3.1: Let conditions 1 and 2 be satisfied. Then we have the following:

(a) The operators $W_\pm=W_\pm(H_1,H_0;\mathcal{P})$ exist and equal $W_\pm(H_1,H_0;J)$;

(b) $W_\pm$ are complete in the usual sense:

$$(W_\pm)^*W_\pm=E_\pm, \tag{3.6a}$$

$$W_\pm(W_\pm)^*=P_{\text{scatt}}, \tag{3.6b}$$

where $E_\pm$ and P_{scatt} are projection operators having domains $\mathcal{H}_0$ and $\mathcal{H}$, respectively, with $E_\pm\mathcal{H}_0=\mathcal{H}_\pm$ and $P_{\text{scatt}}\mathcal{H}=\mathcal{H}_{\text{scatt}}$. The initial sets of the partially isometric operators $W_\pm$ are explicitly given by

$$\mathcal{H}_\pm=\{f\in\mathcal{H}_0:\hat{f}(k)=0,\ \text{for a.e. } k=(k_1,\ldots,k_\nu)\in\mathbf{R}^\nu,\quad \text{with } k_\nu\lessgtr 0\}, \tag{3.7}$$

$\hat{f}$ denoting the $L^2(\mathbf{R}^\nu)$ Fourier transform of f:

$$\hat{f}(k)=(2\pi)^{-\nu/2}L^2(\mathbf{R}^\nu)-\lim_{r\to\infty}\int_{[-r\cdot r]^\nu}\exp(-ik\cdot x)f(x)dx. \tag{3.8}$$

Remark: Equation (3.7) has a transparent physical meaning. Intuitively, in order for a wave packet f_t in Ω evolving as $\exp(-itH_0)f$ for large negative times, to arrive "near" $\partial\Omega$ at time $t=0$, its Fourier transform $\hat{f}_t$ must have for $t\to\infty$ support intersecting the region of momentum space with $k_\nu<0$ in a set of positive measure. Again intuitively, if a wave packet g_t in Ω, which was "near" $\partial\Omega$ at $t=0$ is scattered, then the support of $\hat{g}_t$ must, for large positive times, intersect the momentum–space region with $k_\nu>0$ in a set of positive measure. This interpretation reinforces our contention that the wave operators $W_\pm(H_1,H_0;\mathcal{P})$ are appropriate for describing quantum-mechanical scattering of nonrelativistic particles by the impenetrable periodic surface $\partial\Omega$ in the framework of the present model.

Theorem 3.2: Let conditions 1, 2 be satisfied. Then $W_\pm$ are asymptotically complete, in the sense that

$$\mathcal{H}=\mathcal{H}_{\text{scatt}}\oplus\mathcal{H}_{\text{surf}}. \tag{3.9}$$

B. Methods of proof

A central idea in the proofs of Theorems 3.1 and 3.2 is to replace the study of the wave operators $W_\pm(H^0,H_0;\mathcal{P})$, in the technically more convenient form $W_\pm(H_1,H_0;J)$, by that of $W_\pm(H_1,H_0;J^0)$ and the related infinite family $\{W_\pm(h^1_\theta,h^0_\theta;\eta),\theta\in G\}$ of wave operators constructed by direct-integral methods. Here $H^0=-\Delta_{\text{D}}(\Omega^0)$, the negative Dirichlet Laplacian in the Hilbert space $\mathcal{H}^0=L^2(\Omega^0)$, acting by the negative distributional Laplacian on the functions in its domain, defined by (2.3), with Ω replaced by Ω^0, the half-space $\{(\tilde{x},x_\nu)\in R^\nu:x_\nu>0\}$. Furthermore, $J^0:\mathcal{H}^0\to\mathcal{H}=L^2(\Omega)$ is defined as J was in (3.3b), but with $\mathcal{H}_0$ replaced by $\mathcal{H}^0$. The above family of wave operators indexed by θ will be defined later in this section, after we introduce the necessary direct-integral machinery on which our proofs are heavily dependent.[14]

We define the single-fiber direct integrals,

$$\mathcal{K}^0=\int_G^{\oplus} L^2(\omega^0)d\theta, \tag{3.10a}$$

$$\mathcal{K}=\int_G^{\oplus} L^2(\omega)d\theta, \tag{3.10b}$$

of Hilbert spaces, where $d\theta$ is a Lebesgue measure in $\mathbf{R}^{\nu-1}$ and where we note the relation

$$\omega^0 := G\times\mathbf{R}_+ \supset \omega = \Omega\cap\omega^0, \tag{3.11}$$

between the cylinders ω^0 and ω, G denoting the open $(\nu-1)$-dimensional cube $(0,1)^{\nu-1}$. Note that $\omega^0\backslash\omega$ is bounded, as follows from (3.11) and properties (I) and (II) of Ω. This boundedness is important for our purposes.

We define the unitary operators U^0, U with domains $\mathcal{H}^0=L^2(\Omega^0)$, $\mathcal{H}=L^2(\Omega)$ and ranges $\mathcal{K}^0$, $\mathcal{K}$, respectively, as follows. For $f\in L^2(\Omega)$ of bounded support, we set

$$(Uf)_\theta(x)=\sum_{n\in\mathbf{Z}^{\nu-1}} \exp(-2\pi i n\cdot\theta) f(\tilde{x}+n,x_\nu),$$
$$\theta\in G,\quad x=(\tilde{x},x_\nu)\in\omega, \tag{3.12}$$

where only a finite number of terms in the sum in (3.12) are nonvanishing on ω. The set of all such f's is dense in $L^2(\Omega)$, and it is easy to prove that U can be extended to the whole of $L^2(\Omega)$ as a unitary operator onto $\mathcal{K}$. The operator U^0 is defined in the same way as U, except with Ω, ω replaced by Ω^0, ω^0, respectively. U^0, U have the crucial properties

$$U^0H^0(U^0)^{-1}=\int_G^{\oplus} h_\theta^0 d\theta, \tag{3.13a}$$

$$UHU^{-1}=\int_G^{\oplus} h_\theta d\theta, \tag{3.13b}$$

where h_θ^0 and h_θ are self-adjoint operators in $L^2(\omega^0)$, $L^2(\omega)$, respectively. The operator h_θ ($\theta\in G$) has domain

$$D(h_\theta)=\{f\in L^2(\Delta;\omega)\cap H^1(\omega): f \text{ has an extension,}$$
$$\tilde{f}\in L^2_{\mathrm{loc}}(\Delta;\overline{\Omega})\cap H^1_{0,\mathrm{loc}}(\overline{\Omega}), \text{ with property } P_\theta\}, \tag{3.14}$$

and acts as the negative distributional Laplacian on every $f\in D(h_\theta)$.

A function $g:\Omega\to\mathbf{C}$ is said to have property P_θ ($\theta\in G$) if it has the form $f(x)=f(\tilde{x},x_\nu)$ $=\exp(2\pi i\theta\cdot\tilde{x})\times u(\tilde{x},x_\nu)$, where $u(\tilde{x}+n,x_\nu)=u(\tilde{x},x_\nu)$ $\forall n\in\mathbf{Z}^{\nu-1}$.

Each h_θ^0 ($\theta\in G$) is defined in the same way as h_θ, except with ω replaced by ω^0 (Ref. 15).

An obvious formal consequence of Eqs. (3.13b) and (2.1), that is easily derived rigorously, is that

$$UH_1U^{-1}=\int_G^{\oplus} h_\theta^1 d\theta, \tag{3.15}$$

where each h_θ^1 is a self-adjoint operator defined as the operator sum,

$$h_\theta^1=h_\theta+v_\theta,\quad \theta\in G, \tag{3.16}$$

v_θ denoting the maximal operator of multiplication in $L^2(\omega)$ by the bounded, real, measurable function $v_\theta = V|\omega$. Since $UVU^{-1} = \int_G^\oplus v_\theta \, d\theta$, as one shows by using the periodicity property (2.4a) and arguments similar, but simpler, than those used to prove (3.13b), and since $V \ll H$, we infer that $v_\theta \ll h_\theta$,[16] and hence that each h_θ^1 is self-adjoint by the Kato–Rellich theorem.

The relation

$$U \exp(itH_1)U^{-1} = \int_G^\oplus \exp(ith_\theta^1) d\theta, \quad t \in \mathbf{R}, \tag{3.17a}$$

formally expected in view of (3.15), follows immediately from two facts. First, it holds if its rhs is replaced by $\exp(itUH_1U^{-1})$.[17] Second, $\exp(itUH_1U^{-1}) = U\exp(itH_1)U^{-1}$.[18] Analogously,

$$U^0 \exp(itH^0)(U^0)^{-1} = \int_G^\oplus \exp(ith_\theta^0) d\theta, \quad t \in \mathbf{R}. \tag{3.17b}$$

Relations (3.17) will be used to prove Theorem 3.1.

The connection between the wave operators $W_\pm(H_1, H_0; \mathcal{P}) = W_\pm(H_1, H_0; J)$ and $W_\pm(H, H; J^0)$ that is of interest for our purposes is expressed by the relation

$$W_\pm(H_1, H_0; J) = W_\pm(H_1, H^0; J^0) W_\pm(H^0, H_0; \mathcal{P}_0), \tag{3.18}$$

following from the existence of the wave operators on the rhs of (3.18) and the fact that $J = J^0\mathcal{P}_0$. The existence of $W_\pm(H, H; J^0)$ will be proved in Sec. IV, while that of $W_\pm(H^0, H_0; \mathcal{P}^0)$, describing scattering from a flat surface, was proved previously.[19] A decisive step in proving Theorem 3.1 is to show that the wave operators $W_\pm(h_\theta^1, h_\theta^0; \eta)$ $(\theta \in G)$ are partial isometries that are complete in the usual sense, where $\eta: L^2(\omega^0) \to L^2(\omega)$ is defined by

$$(\eta f)(x) = \begin{cases} j(x_\nu) f(x), & x = (\tilde{x}, x_\nu) \in \omega, \\ 0, & x \in \omega^0 \setminus \omega, \end{cases} \qquad f \in L^2(\omega^0). \tag{3.19}$$

The fact that in the present Dirichlet context ω posseses the local compactness property for every bounded subset of $H^1(\omega)$ (Lemma B.1) is crucial in the proof of Theorem 3.1, which is based on a variant of results of Birman and Belopol'skii.[11] Once the completeness of the operators $W_\pm(h_\theta^1, h_\theta^0; \eta)$ is proved, Theorem 3.1 readily follows. As mentioned in Sec. I, a key step in demonstrating Theorem 3.2 is to show that each h_θ^1 $(\theta \in G)$ has an empty singular continous spectrum, a fact asserted by Lemma 5.4.

IV. PROOF OF THEOREM 3.1

It is based on Lemmas 4.1 and 4.2 and Eq. (6.3a). These lemmas concern properties of the wave operators,

$$W_\pm^\theta := W_\pm(h_\theta^1, h_\theta^0; \eta), \quad \theta \in G, \tag{4.1}$$

$$\mathcal{W}_\pm = W_\pm(H_1, H^0; J^0), \tag{4.2}$$

where $J^0 = J|\Omega^0$ and $\eta = J|\omega^0$, in accord with (3.19). Equation (6.3a), in whose derivation the absence of the singular continous spectrum of the h_θ^1 plays an essential role, asserts the equality of the projection operators P_{ac} and P_{scatt}. Here

$$UP_{\mathrm{ac}}U^{-1} = \int_G^\oplus P_{\mathrm{ac}}(h_\theta^1) d\theta, \tag{4.3}$$

$P_{\mathrm{ac}}(h_\theta^1)$ denoting the orthogonal projection from $L^2(\omega)$ onto the subspace of the absolute continuity of $L^2(\omega)$ wrt h_θ^1. Definition (4.3) makes sense because each function $\theta \mapsto P_{\mathrm{ac}}(h_\theta^1)$ from G into the space of bounded linear operators in $L^2(\omega)$ is measurable and each $P_{\mathrm{ac}}(h_\theta^1)$ is bounded.[20]

Lemma 4.1: Suppose that condition 1 holds and that $\forall\, \theta \in G$ the wave operators $W_\pm^\theta$ in (4.1) exist and are partial isometries that are complete in the usual sense:

$$(W_\pm^\theta)^* W_\pm^\theta = I_{L^2(\omega^0)}, \tag{4.4a}$$

$$W_\pm^\theta (W_\pm^\theta)^* = P_{\mathrm{ac}}(h_\theta^1), \tag{4.4b}$$

where $I_{L^2(\omega^0)}$ is the unit operator in $L^2(\omega^0)$. Then the wave operators $\mathcal{W}_\pm$ in (4.2) exist and are complete in the sense that

$$(\mathcal{W}_\pm)^* \mathcal{W}_\pm = I_{L^2(\Omega^0)}, \tag{4.5a}$$

$$\mathcal{W}_\pm (\mathcal{W}_\pm)^* = P_{\mathrm{ac}}, \tag{4.5b}$$

where $I_{L^2(\Omega^0)}$ is the unit operator in $L^2(\Omega^0)$.

Proof: Define

$$\mathcal{W}_t = \exp(itH_1) J^0 \exp(-itH^0), \quad t \in \mathbf{R}, \tag{4.6}$$

and note that

$$U J^0 (U^0)^{-1} = \mathcal{J} := \int_G^\oplus \eta_\theta \, d\theta, \tag{4.7}$$

where $\eta_\theta = \eta(\theta \in G)$. To prove (4.7), it suffices to show that $UJ^0 f = \mathcal{J} U^0 f$ when $f \in L^2(\Omega^0)$ is equivalent to a function of bounded support, as can be done by using, in particular, (3.12) and the fact that for each such f only a finite number of summands in (3.12) do not vanish a.e.

By (4.6), (3.17), and (4.7),

$$\mathcal{W}_t = U^{-1} \left(\int_G^\oplus \mathcal{W}_t^\theta \, d\theta \right) U^0, \quad t \in \mathbf{R}, \tag{4.8}$$

where

$$\mathcal{W}_t^\theta = \exp(ith_\theta^1)\, \eta_\theta \exp(-ith_\theta^0), \quad \theta \in G, \quad t \in \mathbf{R}. \tag{4.9}$$

Supposing that $\mathcal{W}_\pm^\theta = s - \lim_{t \to \pm\infty} \mathcal{W}_t^\theta$ exists for each $\theta \in G$, and using (4.8) and unitarity, we see that

$$\begin{gathered} \| \mathcal{W}_{t_1} f - \mathcal{W}_{t_2} f \|_\Omega^2 = \int_G \| \mathcal{W}_{t_1} g_\theta - \mathcal{W}_{t_2} g_\theta \|_\omega^2 \, d\theta, \\ f \in L^2(\Omega^0), \quad t_1, t_2 \in \mathbf{R}, \end{gathered} \tag{4.10}$$

where $g = U^0 f \in \mathcal{K}^0 g$ [see (3.10a)]. Now,

$$\|\mathcal{W}_{t_1} g_\theta - \mathcal{W}_{t_2} g_\theta\|_\omega \leqslant 2\|g_\theta\|_\omega, \tag{4.11}$$

at each such t_1, t_2, θ, since $\|\mathcal{W}_t g_\theta\|_\omega \leqslant 1$ for $t \in \mathbf{R}$, $\theta \in G$. By (4.10), (4.11), and dominated convergence,

$$\lim_{t_1, t_2 \to \pm\infty} \|\mathcal{W}_{t_1} f - \mathcal{W}_{t_2} f\|_\Omega^2 = \int_G \lim_{t_1, t_2 \to \pm\infty} \|\mathcal{W}_{t_1}^\theta g_\theta - \mathcal{W}_{t_2}^\theta g_\theta\|_\omega^2 \, d\theta = 0. \tag{4.12}$$

Hence, $\mathcal{W}_\pm$ exists if $\mathcal{W}_\pm^\theta$ exist for each $\theta \in G$.

Next, we show that if Eqs. (4.4) hold for every such θ, then so do (4.5). Indeed, from (4.8) we find taking strong limits and again using dominated convergence:

$$\mathcal{W}_\pm = U^{-1}\left(\int_G^\oplus \mathcal{W}_\pm^\theta \, d\theta \right) U^0, \tag{4.13a}$$

which implies

$$(\mathcal{W}_\pm)^* = (U^0)^{-1}\left(\int_G^\oplus (\mathcal{W}_\pm^\theta)^* d\theta \right) U. \tag{4.13b}$$

But (4.13), (4.4), and (4.3) entail (4.5). □

Lemma 4.2: Equations (4.4) hold $\forall\, \theta \in G$ if condition 1 is satisfied.

Before proving this lemma, we will use it to prove Theorem 3.1.

Proof of Theorem 3.1: (a) Since $W_\pm(H_1, H^0; J^0)$ exist by Lemmas 4.1 and 4.2, and $W_\pm(H^0, H_0; \mathcal{P}_0)$ exists, $W_\pm(H_1, H_0; J)$ exists by (3.18). That $W_\pm(H_1, H_0; \mathcal{P}) = W_\pm(H_1, H_0; J)$ follows by arguments virtually identical to those invoked in an analogous connection in the proof of part (a) of Theorem 2.1 of Ref. 5.

(b) By $W_\pm(H_1, H_0; \mathcal{P}) = W_\pm(H_1, H_0; J)$, (3.18), (4.5), and the corollary to Lemma B.1 in Appendix B of Ref. 5 there follows a modified version of Eqs. (3.6) with P_{scatt} replaced by P_{ac}. This result and (6.3a) entail that Eqs. (3.6) hold in their originally stated form. [We remind the reader that (6.3a) is derived in Sec. VI under the assumption that conditions 1 and 2 hold.] Equation (3.7) follows by arguments similar to ones adduced in the proof of part (b) of Theorem 2.1 of Ref. 5. □

Proof of Lemma 4.2: Assume that **1** is satisfied. Then Lemma 4.2 holds if statements (i)–(iii) below are true for all $\theta \in G$ and all bounded intervals $\delta \subset \mathbf{R}$:[10]

(i) $\eta D(h_\theta^0) \subset D(h_\theta^1)$, $\eta^* D(h_\theta^1) \subset D(h_\theta^0)$.

(ii) $(\eta^* \eta - I_{L^2(\omega^0)}) E(\delta; h_\theta^0)$ and $(\eta \eta^* - I_{L^2(\omega)}) E(\delta; h_\theta^1)$ are compact, where $E(\delta; h_\theta^0), E(\delta; h_\theta^1)$ are the spectral measures of h_θ^0, h_θ^1, respectively.

(iii) $(h_\theta^1 \eta - \eta h_\theta^0) E(\delta; h_\theta^0)$ is trace class.

We proceed to prove (i)–(iii), fixing $\theta \in G$ and a bounded interval $\delta \subset \mathbf{R}$ until further notice.

Proof of (i): Since $D(h_\theta^1) = D(h_\theta)$, the relations (i) hold in the present case since they do in the case $V = 0$ (Ref. 5, pp. 2878–2879).

Proof of (ii): The first property (ii) was proved when $V = 0$ (Ref. 5, p. 2879). Hence we only need to establish the compactness of $(\eta \eta^* - I_{L^2(\omega)}) E(\delta; h_\theta^1)$. Since $\eta \eta^* - I_{L^2(\omega)}$ is multiplication by a $C^\infty(\omega)$ function of bounded support, it suffices to show that for an arbitrary sequence $\{g_m\}_{m \in \mathbf{N}}$ bounded in $L^2(\omega)$ ($\mathbf{N}$ = the positive integers), the sequence $\{u_m = E(\delta; h_\theta^1) g_m\}_{m \in \mathbf{N}}$ is precompact in $L^2(\omega(r))$ for large enough $r > 0$. Here is the proof. We first show that $\{u_m\}_{m \in \mathbf{N}}$ is bounded in $H^1(\omega)$. Obviously, it is bounded in $L^2(\omega)$. Also, by $u_m \in D(h_\theta^1) = D(h_\theta) \subset D_\theta$, $\forall m \in \mathbf{N}$, (3.16), the boundedness of the operators v_θ and $h_\theta^1 E(\delta; h_\theta^1)$ and that of the sequence $\{u_m\}_{m \in \mathbf{N}}$ in $L^2(\omega)$, it follows that

$$\begin{aligned}\|\nabla u_m\|_\omega^2 &= \langle \nabla u_m, \nabla u_m\rangle_\omega \\ &= \langle u_m, h_\theta u_m\rangle_\omega \\ &\leqslant \langle u_m, h_\theta^1 u_m\rangle_\omega + |\langle u_m, v_\theta u_m\rangle_\omega| \\ &\leqslant \langle u_m, h_\theta^1 u_m\rangle_\omega + \text{const}\|u_m\|_\omega^2 \leqslant \text{const}\|u_m\|_\omega^2 \leqslant \text{const},\end{aligned} \tag{4.14}$$

where "const" is independent of m, and where $\|\cdot\|_M$, $\langle\cdot\rangle_M$ denote the norm and inner product in $L^2(M)$, respectively, for a measurable subset $M\subset\mathbf{R}^\nu$.[21] Hence $\{u_m\}$ is bounded in $H^1(\omega)$. By Lemma B.1, we thus conclude that $\{u_m\}$ is precompact in $L^2(\omega(r))$ for each $r>0$ for which $\omega(r)\neq\varnothing$.

Proof of (iii): We continue to assume that $\theta\in G$ is fixed and that $\delta\subset\mathbf{R}$ is a fixed bounded interval. We will need the fact (Ref. 5, p. 2876) that the spectral measure $E(\cdot;h_\theta^0)$ of h_θ^0 is given by

$$\begin{gathered}(E(\delta;h_\theta^0)f)(x) = \sum_{n\in\mathbf{Z}^{\nu-1}} \int_{\mathbf{R}_+} \chi_\delta(\kappa_n(\xi)) w_n(x,\xi)\tilde{f}_n(\xi)\,d\xi, \\ f\in L^2(\omega^0), \quad \text{a.e. } x\in\omega^0,\end{gathered} \tag{4.15}$$

where

$$\begin{gathered}\tilde{f}_n(\xi) = L^2(\mathbf{R}_+) - \lim_{r\to\infty} \int_{\omega^0(r)} w_n(x,\xi) f(x)\,dx, \\ w_n(x,\xi) = (2/\pi)^{1/2} \exp[2\pi i(n+\theta).\tilde{x}]\sin\xi x_\nu, \\ f\in L^2(\omega_0), \quad n\in\mathbf{Z}^{\nu-1}, \quad \text{a.e. } \xi\in\mathbf{R}_+ .\end{gathered} \tag{4.16}$$

Here χ_δ is the characteristic function of the interval δ, $\kappa_{n\theta}(\xi)=\xi^2+4\pi^2|n+\theta|^2$, and $\mathbf{R}_+ = [0,\infty)$. The θ-dependence of various functions is suppressed for notational convenience. Since δ is bounded, only a finite number of terms in the sum (4.15) are nonzero for a.e. $x\in\omega^0$.

Note that the mapping $\mathcal{U}$ from $L^2(\omega^0)$ onto $\mathcal{C}=\Sigma_{n\in\mathbf{Z}^{\nu-1}}\oplus L^2(\mathbf{R}_+)$ defined by $\mathcal{U}f = \{\tilde{f}_n\}_{n\in\mathbf{Z}^{\nu-1}}$ is unitary. Hence condition (iii) is equivalent to the condition that

$$(h_\theta^1\eta - \eta h_\theta^0)E(\delta;h_\theta^0)\mathcal{U}^*$$

be trace class from $\mathcal{C}$ to $L^2(\omega^0)$. In turn, the latter condition is equivalent to requiring that the mapping

$$\tilde{f}_n \to (h_\theta^1\eta - \eta h_\theta^0)\int_{\mathbf{R}_+} \tilde{f}_n(\xi) w_n(\cdot,\xi)\chi_\delta(\kappa_n(\xi))\,d\xi$$

be trace class from $L^2(\mathbf{R}_+)$ to $L^2(\omega)$ for each $n\in\mathbf{Z}^{\nu-1}$. This equivalence follows from the facts that only a finite number of summands in (4.15) are nonvanishing a.e. on ω^0 and that the sum of a finite number of trace class operators with the same domains and ranges is trace class. Hence we fix $n\in\mathbf{Z}^{\nu-1}$ and proceed as follows. We first remark that

$$\begin{gathered}(h_\theta^1\eta - \eta h_\theta^0)\int_{\mathbf{R}_+} \tilde{f}_n(\xi) w_n(\cdot,\xi)\chi_\delta(\kappa_n(\xi))\,d\xi = \int_{\mathbf{R}_+} M_n(\cdot,\xi)\tilde{f}_n(\xi)\,d\xi := B_n\tilde{f}_n, \\ f\in L^2(\omega^0), \quad n\in\mathbf{Z}^{\nu-1},\end{gathered} \tag{4.17a}$$

where

$$M_n = M_n'(x,\xi) + M_n''(x,\xi), \tag{4.17b}$$

and where

$$M_n'(x,\xi) = -\{[d^2 j(x_\nu)/dx_\nu{}^2] w_n(x,\xi) + 2[d^2 j(x_\nu)/dx_\nu{}^2] \partial w_n(x,\xi)/\partial\xi]\} \chi_\delta(\kappa_n(\xi)), \tag{4.17c}$$

$$M_n''(x,\xi) = V(x) j(x_\nu) w_n(x,\xi) \chi_\delta(\kappa_n(\xi)), \tag{4.17d}$$

$\forall n \in \mathbf{Z}^{\nu-1}, x \in \omega^0, \xi \in \mathbf{R}_+$, where, by definition, $V(x) = 0$ on $\omega^0 \backslash \omega$. Equations (4.17) can be readily justified. Indeed, note that $\int_{\mathbf{R}_+} \tilde{f}_n(\xi) w_n(x,\xi) \chi_\delta(\kappa_n(\xi)) d\xi$ is an infinitely differentiable function of x on ω by dominated convergence. Consequently, the operator $h_\theta^1 \eta - \eta h_\theta^0$ acts on this function (which is in its domain) by $(-\Delta + V|\omega) j + j\Delta$, where Δ may be interpreted as the usual, rather than the weak Laplacian, and may be taken inside the integral sign by dominated convergence. Given these facts, (4.17) follows by a brief calculation.

Write $B_n = B_n' + B_n''$, where B_n', B_n'' are defined by (4.17a), but with M_n replaced by M_n', M_n'', respectively. Thus, in order to prove (iii) it suffices to show that B_n', B_n'' are trace class. This will now be done for B_n'', the proof for B_n' being analogous.

Note that

$$\int_{\mathbf{R}_+} \left(\int_\omega |M_n''(x,\xi)|^2 \, dx \right) d\xi < \infty, \tag{4.18}$$

in view of (4.17d), $V|\omega \in L^2(\omega)$, the boundedness of j, w_n, and the fact that $\chi_\delta(\kappa_n(\cdot))$ is of bounded support. Note also that as a mapping from $\mathbf{R}_+$ to $L^2(\omega)$, $M_n''(\cdot\,,\xi)$ is continuous and has a continuous first derivative $\partial M_n''(\cdot\,,\xi)/\partial\xi$ on this support. The proof of these two facts is elementary. By a version of a theorem of Stinespring[12] due to Lyford,[22] these properties of $M_n''(\cdot\,,\xi)$ imply that B_n'' is trace class.

V. SPECTRUM OF $h_\theta^1 (\theta \in G)$

A. Preliminary remarks

In this section, we will once more fix $\theta \in G$, which again allows us to simplify the notation by omitting θ from various symbols. In particular, we write

$$k_n = 4\pi^2 |n + \theta|^2, \quad n \in \mathbf{Z}^{\nu-1}. \tag{5.1}$$

If $f \in L^2_{\mathrm{loc}}(\overline{\omega})$ has an extension to $L^2_{\mathrm{loc}}(\overline{\Omega})$ having property P_θ, then it has the $L^2_{\mathrm{loc}}(\overline{\omega}_{1,\infty})$-convergent series representation

$$f(x) = \sum_{n \in \mathbf{Z}^{\nu-1}} f_n(x_\nu) \eta_n(\tilde{x}), \quad \text{a.e. } x \in \omega_{1,\infty}, \tag{5.2a}$$

in the open cylindrical subset $\omega_{1,\infty}$ of ω, where we recall that $\omega_{r,\infty} = \{x \in \omega : x_\nu > r\}$ and where

$$f_n(x_\nu) = \int_G \eta_n(\tilde{x}) f(\tilde{x}, x_\nu) d\tilde{x}, \quad n \in \mathbf{Z}^{\nu-1}, \quad \text{a.e. } x_\nu > 1, \tag{5.2b}$$

the set of functions

$$\eta_n(\tilde{x}) = \exp[2\pi i (n + \theta).\tilde{x}], \quad \tilde{x} \in G, \ n \in \mathbf{Z}^{\nu-1}, \tag{5.2c}$$

being a complete orthonormal set in $L^2(G)$.

By condition 2, $V(x)=w(x_\nu), \forall x \in \omega_{a,\infty}$ for a fixed $a>1$, where $w \in C^\infty((a,\infty))$. Suppose that this condition holds and that f is as stated in the previous paragraph, and in addition is a weak (and therefore strict) solution of the elliptic equation,

$$-\Delta f + w(x_\nu) f = \zeta f, \quad x \in \omega_{a,\infty}, \tag{5.3}$$

for some $\zeta \in \mathbf{C}$. Then the restriction of f to $\omega_{a,\infty}$ is equivalent to a $C^\infty(\omega_{a,\infty})$ function,[23] with which we will identify it w.l.g. This fact, the P_θ property of f, and (5.1), (5.2b), and (5.2c) entail (via differentiation under the integral sign and partial integration) that $\int_G \Delta f(\tilde{x},x_\nu).\eta_n(\tilde{x})d\tilde{x} = -d^2 f_n(x_\nu)/dx_\nu^2 + k_n f_n(x_\nu)$ for $x_\nu > a$. In turn, this leads to

$$\frac{d^2 f_n(x_\nu)}{dx_\nu^2} - [k_n - \zeta + w(x_\nu)] f_n(x_\nu) = 0, \quad x_\nu > a, \ \ n \in \mathbf{Z}^{\nu-1}, \tag{5.4}$$

with the aid of (5.2b) and (5.3). Our discussions of the spectrum of h_θ^1 in this section depend in an essential way on the asymptotic behavior of the solutions of this ODE for $x_\nu \to \infty$.

B. Point spectrum of h_θ^1

By Lemma 4.2, the absolutely continuous spectrum of h_θ^1 coincides with the spectrum of h_θ^0, since the latter spectrum is purely absolutely continuous. In this and the next section, we will discuss the singular spectrum of h_θ^1. The main result of the present section, stated in Lemma 5.1, is that the eigenvalues of h_θ^1 in suitable intervals are isolated and have finite multiplicity. This result will be used in Sec. V C to show that the singular continuous spectrum of h_θ^1 is empty.

Lemma 5.1: Let conditions 1, 2 be satisfied. Let $I \subset \mathbf{R}$ be a compact interval $[A,B]$ or a semi-infinite interval of the form $(-\infty,B]$, no k_n's being contained in either of these intervals [recall (5.1)]. Then h_θ^1 has a finite number of eigenvalues in I, each having finite multiplicity.

Proof: It will be by contradiction. Let $\{\phi_m\}_{m \in \mathbf{N}}$ be an infinite orthonormal set of eigenfunctions of h_θ^1 with eigenvalues λ_m lying in a compact interval $[A,B]$ or $(-\infty,B]$ not containing any k_n's. We claim that $\{\phi_m\}_{m \in \mathbf{N}}$ is bounded in $H^1(\omega)$. This follows from two facts. First, since the ϕ_m are orthonormal, this sequence is trivially bounded in $L^2(\omega)$. Second, for each $m \in \mathbf{N}$,

$$\|\nabla \phi_m\|_\omega^2 = \langle \phi_m, -\Delta \phi_m \rangle_\omega = \langle \phi_m, h_\theta^1 \phi_m - v_\theta \phi_m \rangle_\omega = \lambda_m + |\langle \phi_m, v_\theta \phi_m \rangle_\omega| \leqslant B + \text{const}, \tag{5.5}$$

where "const" is independent of m. The first equality in (5.5) follows from $\phi_m \in D(h_\theta^1)$ and the formula mentioned in Ref. 21, and to derive the rest of (5.5) we have used (3.16), $v_\theta \ll h_\theta$, the boundedness of v_θ, $\lambda_m \leqslant B$, and the fact that $\|\phi_m\|_\omega = 1$.

Next, we use the boundedness of $\{\phi_m\}_{m \in \mathbf{N}}$ in $H^1(\omega)$ and other arguments to show that this sequence has a subsequence that is Cauchy in $L^2(\omega)$. This is absurd and will thus complete the proof of the lemma.

Since each $\phi_m \in L^2(\omega)$ and its Fourier coefficients $(\phi_m)_n(x_\nu)$ in the expansion (5.2a) satisfy a differential equation of the type (5.4) (with ζ replaced by λ_m), and in view of Lemma C.1 [see especially Eqs. (C.3a) and (C.4a)] and the definition of $\sqrt{z}(z \in \mathbf{C})$ in Appendix C, it follows that

$$\phi_m(\tilde{x},x_\nu) = \phi_m(\tilde{x},b+y) = \sum_{n \in Z^{\nu-1}, k_n > \lambda_m} C_{mn} \exp(-\sqrt{k_n - \lambda_m}\, y)[1 + \rho(y, k_n - \lambda_m)]\, \eta_n(\tilde{x}),$$
$$x \in \omega_{b,\infty}, \tag{5.6}$$

in the $L^2(\omega_{b,\infty})$ sense. Here $b > a$ is a constant, $y = x_\nu - b > a - b$ [i.e., J in Lemma C.1 is $(a-b,\infty) \supset [0,\infty)$ in the present case], the C_{mn} are constants, and

$$|\rho(y,\kappa)| = \exp\left(\int_y^\infty |q(\xi)|\, d\xi/\kappa \right) - 1, \quad \kappa > 0, \ \ y \geqslant 0, \tag{5.7}$$

where $q(y)=w(x_\nu)$. Since $\int_0^\infty |q(\xi)|d\xi<\infty$ by 2, (5.7) makes sense. Using (5.6) and the orthonormality of the $\eta_n(\tilde{x})$, and choosing $r>0$ so large that

$$0<\rho(r,p)<1/2, \tag{5.8a}$$

where $p=\min\{\sqrt{k_n-B}:k_n>B\}$, we obtain

$$\begin{aligned}\|\phi_m\|^2_{\omega_{b+r,\infty}} &= \sum_{n\in\mathbf{Z}^{\nu-1},k_n>\lambda_m} |C_{mn}|^2 \int_r^\infty \exp(-2\sqrt{k_n-\lambda_m}y).[1+\rho(y,k_n-\lambda_m)] \\ &\leqslant \sum_{n\in\mathbf{Z}^{\nu-1},k_n>\lambda_m} |C_{mn}|^2 \exp(-2\sqrt{k_n-\lambda_m}r).[1+\rho(r,p)]^2/2\sqrt{k_n-\lambda_m} \\ &< (9/8) \sum_{n\in\mathbf{Z}^{\nu-1},k_n>\lambda_m} |C_{mn}|^2 \exp(-2\sqrt{k_n-\lambda_m}r)/\sqrt{k_n-\lambda_m}. \end{aligned} \tag{5.9a}$$

Actually, we will choose $r>0$ even larger, and in fact so large that

$$0<\rho(r/2,p)<1/2, \tag{5.8b}$$

which implies (5.8a). Doing this and proceeding similarly to the way in which we derived (5.8a), we see that both

$$\|\phi_m\|_{\omega_{b+r/2,\infty}} > (1/8) \sum_{n\in\mathbf{Z}^{\nu-1}} |C_{mn}|^2 \exp(\sqrt{k_n-\lambda_m}r)/\sqrt{k_n-\lambda_m}, \tag{5.9b}$$

and (5.9a) hold. By (5.9a) and (5.9b),

$$\|\phi_m\|^2_{\omega_{b+r,\infty}} < 9\exp(-pr)\|\phi_m\|^2_{\omega_{b+r/2,\infty}} \leqslant 9\exp(-pr)\|\phi_m\|^2_{\omega} \leqslant 9\exp(-pr). \tag{5.10}$$

Now, the sequence $\{\phi_m\}_{m\in\mathbf{N}}$ is bounded in $H^1(\omega)$ and each $\phi_m\in D(h_\theta)$. Hence, by the local compactness (LC) property of ω (Lemma B.1), $\{\phi_m\}_{m\in\mathbf{N}}$ has a subsequence $\{\phi_m\}_{m\in\mathcal{T}}$ that is Cauchy in $L^2_{\mathrm{loc}}(\overline{\omega})$. That is,

$$\|\phi_m-\phi_n\|_{\omega_{b+s}}\to 0, \quad \text{for } m,n\in\mathcal{J} \quad \text{and } m,n\to\infty, \tag{5.11}$$

$\forall s>0$, where $\mathcal{J}\subset\mathbf{N}$ is independent of s by the LC property. Henceforth, the indices m,n will be assumed to be in $\mathcal{J}$.

It is now easy to show that $\{\phi_m\}_{m\in\mathcal{T}}$ is Cauchy in $L^2(\omega)$. Indeed, note that for an arbitrary $\varepsilon>0$ there exists $n_0\in\mathcal{J}$, such that

$$\begin{aligned}\|\phi_m-\phi_n\|^2_{\omega_{b+r,\infty}} &= \|\phi_m\|^2_{\omega_{b+r,\infty}} + \|\phi_n\|^2_{\omega_{b+r,\infty}} + 2\|\phi_m\|_{\omega_{b+r,\infty}}\cdot\|\phi_n\|_{\omega_{b+r,\infty}} \\ &\leqslant 36\exp(-pr)\leqslant \varepsilon^2/2, \quad \forall m,n\geqslant n_0, \end{aligned} \tag{5.12}$$

if r is large enough. W.l.g., we will assume that r is so large that (5.12), as well as (5.8b), and therefore also (5.8a), obtain. Moreover, by (5.11) there exists $n_1\in\mathcal{J}$ such that

$$\|\phi_m-\phi_n\|^2_{\omega_{b+r}} \leqslant \varepsilon^2/2, \quad \forall m,n\geqslant n_1. \tag{5.13}$$

An immediate consequence of (5.11) and (5.13) is that the subsequence $\{\phi_m\}_{m\in\mathcal{J}}$ is Cauchy in $L^2(\omega)$. Since this is impossible, h^1_θ has a finite number of eigenvalues in I, each having finite multiplicity. □

C. Absence of the singular continous spectrum of h_θ^1

This fact is asserted by Lemma 5.4. A key preliminary step in its proof is Lemma 5.3, which states an important boundedness property of the resolvent of h_θ^1 at points of the complex plane approaching certain points of the real axis. In this section we assume that conditions 1 and 2 are satisfied.

Before proving Lemmas 5.3 and 5.4, we introduce some terminology. We first define the set

$$\mathcal{D}_\theta=\{f\in L^2_{\mathrm{loc}}(\Delta;\overline{\omega})\cap H^1_{\mathrm{loc}}(\overline{\omega}):\ f\ \text{has an extension,}$$

$$\text{to } L^2_{\mathrm{loc}}(\Delta;\overline{\Omega})\cap H^1_{0,\mathrm{loc}}(\overline{\Omega})\ \text{with property } P_\theta\}. \tag{5.14}$$

Second, $f\in L^2_{\mathrm{loc}}(\overline{\omega})$ will be said to satisfy the outgoing (resp., incoming) radiation condition in ω if

$$f_n(x_\nu)\sim\begin{cases}\text{const}\exp(-\sqrt{k_n-\lambda}\,x_\nu), & \text{if } k_n>\lambda,\\ \text{const}\exp(\pm i\sqrt{|k_n-\lambda|}\,x_\nu), & \text{if } k_n<\lambda,\end{cases} \tag{5.15}$$

holds for $x_\nu\to\infty$ with the $+$ (resp., $-$) sign for some $\lambda\in\mathbf{R}$ and all $n\in\mathbf{Z}^{\nu-1}$. Third, we set

$$\Lambda=\{\lambda\in\mathbf{R}:\ \lambda\notin\sigma_p(h_\theta^1),\lambda\neq k_n,\forall n\in\mathbf{Z}^{\nu-1}\}, \tag{5.16}$$

where $\sigma_p(h_\theta^1)$ denotes the point spectrum of h_θ^1.

The next lemma will be used to prove Lemma 5.3.

Lemma 5.2: Suppose that $f\in\mathcal{D}_\theta$ satisfies the incoming or outgoing radiation condition in ω and that the equation

$$-\Delta f+\tilde{V}f=\lambda f \tag{5.17}$$

holds for some $\lambda\in\Lambda$ in the distributional sense, where $\tilde{V}$ is the maximal operator of multiplication by the function $V|\omega$, V denoting the function with properties 1, 2 that was introduced in Sec. III A. Then $f=0$.

Proof: We will prove the lemma by contradiction in the case when $f\in\mathcal{D}_\theta$ satisfies the outgoing radiation condition. It can be proved similarly when the incoming radiation condition obtains. Obviously, the Fourier coefficients $f_n(x_\nu)$ of $f(x)$ satisfy the ODE (5.4) with ζ replaced by $\lambda\forall y=x_\nu-b\geqslant 0$. Moreover, using Lemma C.1 [particularly (C.3a) and (C.3b)], we see that in the present case f has the $L^2_{\mathrm{loc}}(\overline{\omega}_{b,\infty})$-convergent series representation,

$$f(x)=\sum_{n\in\mathbf{Z}^{\nu-1}}\gamma_n\exp(\sigma_n\sqrt{|k_n-\lambda|}y)[1+\rho_n(y)]\,\eta_n(\tilde{x}),\quad \text{a.e. } x\in\omega_{b,\infty}, \tag{5.18a}$$

where the γ_n's are constants and $\sigma_n=-1$, i in the respective cases $k_n>\lambda$, $k_n<\lambda$ (the only ones possible since $\lambda\in\Lambda$), and where $\rho_n(y)=o(1)$ as $y\to\infty$. Again using Lemma C.1 and arguments analogous to those adduced to derive (5.18a), one can show that $\partial f/\partial x_\nu$ is represented by the $L^2_{\mathrm{loc}}(\overline{\omega}_{b,\infty})$-convergent series:

$$\frac{\partial f(x)}{\partial x_\nu}=\sum_{n\in Z^{\nu-1}}\gamma_n\sigma_n\sqrt{|k_n-\lambda|}\exp(\sigma_n\sqrt{|k_n-\lambda|}y)[1+\tilde{\rho}_n(y)]\,\eta_n(\tilde{x}),$$

$$\text{a.e. } x\in\omega_{b,\infty}, \tag{5.18b}$$

where each $\tilde{\rho}_n(y)=o(1)$ as $y\to\infty$. Note that the only summands in (5.18a) and (5.18b) not vanishing a.e. are those for which either $k_n>\lambda$ or $k_n<\lambda$, since $\lambda\in\Lambda$.

By Lemma C.5 of Ref. 5, (5.18), and the orthonormality of the η_n, it follows that

$$\int_G \left[\overline{f} \frac{\partial f(x)}{\partial x_\nu} - f \frac{\partial \overline{f}(x)}{\partial x_\nu} \right] (\tilde{x}, x_\nu) d\tilde{x} = \sum_{n \in \mathbf{Z}^{\nu-1}} \left[\overline{f}_n \frac{df_n}{dx_\nu} - f_n \frac{d\overline{f}_n}{dx_\nu} \right] (x_\nu) = 0, \quad x_\nu > b. \tag{5.19}$$

Using the reality of the summands in (5.18b) when $k_n > \lambda$, one sees that the contribution of such summands to the sum in (5.19) vanishes. On the other hand, the contribution of the terms with $k_n < \lambda$, for which $\sigma_n = i$, has the form shown on the lhs of the equation,

$$\sum_{n \in Z^{\nu-1}, k_n < \lambda} |\gamma_n|^2 [1 + \psi_n(y)] = 0, \ x_\nu > b \tag{5.20}$$

(except for an unimportant factor $2i$). Here $\psi_n(y) = o(1)$ as $y \to \infty$. Since the sum (5.20) contains only a finite number of nonvanishing terms, we conclude that $\gamma_n = 0$ if $k_n < \lambda$. By this result and (5.18a),

$$f(x) = \sum_{n \in \mathbf{Z}^{\nu-1}, k_n > \lambda} \gamma_n \exp(-\sqrt{k_n - \lambda} y)[1 + \rho_n(y)] \eta_n(\tilde{x}), \quad \text{a.e. } x \in \omega_{b,\infty}. \tag{5.18c}$$

Consequently, $f \in L^2(\omega_{b,\infty})$. Since $f \in L^2_{\mathrm{loc}}(\overline{\omega})$ holds as well, we conclude that $f \in L^2(\omega)$. Moreover, since $\Delta f = v(x) f + \lambda f$ a.e. on ω and $v \in L^2(\omega)$, we see that $\Delta f \in L^2(\omega)$, and hence that $f \in L^2(\Delta; \omega)$. Now, $f \in \mathcal{D}_\theta$ by hypothesis and $\mathcal{D}_\theta \cap L^2(\Delta; \omega) = D(h_\theta)$ by Lemma 7.2 of Ref. 5 (where "$\subset$," "$\cap$" should read "$\cap$," "$\subset$," respectively). Therefore, $f \in D(h_\theta) = D(h^1_\theta)$ and $h^1_\theta f = \lambda f$. But since $\lambda \notin \sigma_p(h^1_\theta)$, it follows that $f = 0$. □

The next lemma states in a precise fashion the boundedness property of the resolvent $R_\zeta = (h^1_\theta - \zeta 1_{L^2(\omega)})^{-1}$ alluded to above.

Lemma 5.3: Let $[\gamma, \delta] \subset \Lambda$ be a compact interval and $b \in (a, \infty)$. Suppose $f \in L^2(\omega)$, $\operatorname{supp} f \subset \omega_b$, and $\|f\|_{\omega_b} = 1$. Then

$$\|R_{\lambda \pm i\sigma} f\|_{1,\omega_c} \leqslant K_{bc}, \tag{5.21}$$

$\forall c \in (b, \infty)$, provided that $\lambda \in [\gamma, \delta]$ and $\sigma \in (0,1)$, where K_{bc} is a constant independent of λ, σ, f. (See Appendix A for the definition of $\|\cdot\|_{1,A}$.)

Proof: We will prove it by contradiction for the case of the + sign in (5.21), the proof for the − sign being similar. Suppose the lemma is false for some finite $c > b \geqslant a > 1$, where a is the constant in condition 2. Then there exist sequences $\{\zeta_k = \lambda_k + i\sigma_k\}_{k \in \mathbf{N}}$ and $\{f_k\}_{k \in \mathbf{N}}$, with $\lambda_k \in [\gamma, \delta]$, $\sigma_k \in (0,1)$ and $\|f_k\|_{\omega_c} = 1$, $\operatorname{supp} f_k \subset \omega_b$ $\forall k \in \mathbf{N}$, such that

$$\|R_{\zeta_k} f_k\|_{1,\omega_b} \geqslant k, \tag{5.22}$$

for each such k. Since $[\gamma, \delta] \times (0,1) \in \mathbf{R}^2$ is bounded, $\{\zeta_k\}_{k \in \mathbf{N}}$ will be assumed to converge w.l.g. Hence $\lambda_k \to \lambda \in [\gamma, \delta]$ and $\sigma_k \downarrow 0 (k \to \infty)$. For $\sigma_k \to \sigma \neq 0$ would contradict (5.22).

Define

$$u_k = \|R_{\zeta_k} f_k\|^{-1}_{1,\omega_c} R_{\zeta_k} f_k, \quad g_k = \|R_{\zeta_k} f_k\|^{-1}_{1,\omega_c} f_k, \quad k \in \mathbf{N}. \tag{5.23}$$

Hence $\|u_k\|_{1,\omega_c} = 1$ for all such k and $g_k \to 0$ in $L^2(\omega)$ as $k \to \infty$. Now $u_k \in D(h_\theta) \subset D_\theta$. Since the sequence $\{u_k\}_{k \in \mathbf{N}}$ is obviously bounded in $H^1(\omega)$, Lemma B.1 implies that it has a subsequence $\{u_k\}_{k \in \mathcal{K}}$, independent of c and Cauchy in $L^2(\omega_c)$. Directly from the definitions,

$$-\Delta u_k + w(y) u_k = \zeta_k u_k + g_k = \zeta_k u_k, \quad k \in N, \quad \text{a.e. } x \in \omega_{b,\infty}, \tag{5.24}$$

since supp $f_k \subset \omega_b$. Taking into account (5.24), condition 2, and Lemma C.1, together with the facts that $u_k \in L^2(\omega)$ and that $\mathrm{Re}\sqrt{k_n-\zeta_k}>0$, $\forall n \in \mathbf{Z}^{\nu-1} \forall k \in \mathbf{N}$, since $\mathrm{Im}\,\zeta_k \neq 0$ at each such k (recall the second sentence of the second paragraph of Appendix C), it follows that every such u_k is represented by the $L^2(\omega_{b,\infty})$-convergent series,

$$u_k(x)=\sum_{n\in\mathbf{Z}^{\nu-1}} (u_k)_n(x_\nu)\,\eta_n(\tilde{x}), \quad \text{a.e. } x\in\omega_{b,\infty}, \tag{5.25a}$$

where

$$(u_k)_n(x_\nu)=C_{kn}\exp(-\sqrt{k_n-\zeta_k}\,y)[1+\rho_{kn}(y)],$$
$$n\in\mathbf{Z}^{\nu-1}, \quad y\geqslant 0. \tag{5.25b}$$

Here

$$\rho_{kn}(y)\leqslant Q(y)=\exp\left(\int_y^\infty |w(\xi)|\,d\xi/P\right)-1, \quad y\geqslant 0, \tag{5.25c}$$

with $P=\min\{\sqrt{|k_m-\zeta_j|}, m\in\mathbf{Z}^{\nu-1}, j\in\mathbf{N}, \mathrm{Re}\,\zeta_j\in[\gamma,\delta], \mathrm{Im}\,\zeta_j\in(0,1)\}$.

We claim that

$$\|u_k\|_{b+jr,b+(j+1)r}\leqslant\|u_k\|_{b+r,b+2r}, \quad j=0,1,2,3,\ldots, \tag{5.26}$$

if r is so large that

$$0<Q(r)<1, \quad \exp(-2rP)\frac{[1+Q(r)]^2}{[1-Q(r)]^2}\leqslant 1. \tag{5.27}$$

This claim can be proved similarly to (5.9a).

Since $\{u_k\}_{k\in\mathcal{K}}$ is Cauchy in $L^2(\omega_c)$ and (5.26) holds, this subsequence is also Cauchy in $L^2_{\mathrm{loc}}(\overline{\omega})$. By $\Delta u_k=-[\zeta_k+V(x)]u_k$ (a.e. $x\in\omega$), $\{u_k\}_{k\in\mathcal{K}}$ is Cauchy in $L^2_{\mathrm{loc}}(\Delta;\overline{\omega})$ as well. Therefore, $u_k\to u\in\mathcal{D}_\theta$ in $L^2_{\mathrm{loc}}(\Delta;\overline{\omega})$ by Lemma 7.1 of Ref. 5, with

$$-\Delta u(x)+V(x)u=\lambda u(x), \quad \text{a.e. } x\in\omega, \tag{5.28}$$

$\lambda\in[\gamma,\delta]$ denoting the limit of the sequence $\{\zeta_k\}_{k\in\mathbf{N}}$ as above.

We now show that u satisfies the outgoing radiation condition, and hence that $u=0$ by Lemma 5.2. But since $\|u_k\|_{1,\omega_b}=1$ $(k\in\mathcal{K})$, this is absurd and will complete the proof.

We will write $y=x_\nu$ for convenience. Since $u_k\to u$ in $L^2_{\mathrm{loc}}(\overline{\omega})$, it follows that $(u_k)_n\to u_n \in L^2_{\mathrm{loc}}(\overline{\mathbf{R}}_+)$ by Schwarz's inequality, where $\mathbf{R}_+=[0,\infty)$. By a standard smoothness argument, this entails pointwise convergence: $(u_k)_n(y)\to u_n(y)$ for $y\geqslant 0$ as $k\to\infty$. We thus have for each such y by (5.24), (5.28), and other arguments, analogous to those used to prove (5.4):

$$\frac{d^2(u_k)}{dy^2}-[k_n-\zeta_k+w(y)](u_k)_n=0, \tag{5.29a}$$

$$\frac{d^2u_n}{dy^2}-[k_n-\lambda+w(y)]u_n=0. \tag{5.29b}$$

Fixing $n\in\mathbf{Z}^{\nu-1}$, and since $\lambda\in\Lambda$, either $k_n>\lambda$ [case (a)] or $k_n<\lambda$ [case (b)]. We note that

$$\exp(-\sqrt{k_n-\zeta_k}\,y)\sim\begin{cases}\exp(i\sqrt{|k_n-\lambda|}\,y) & \text{in case (a)},\\ \exp(-\sqrt{|k_n-\lambda|}\,y) & \text{in case (b)},\end{cases} \tag{5.30}$$

as $k\to\infty$. By the pointwise convergence property of $(u_k)_n(y)$, together with (5.25b), (5.30), and Lemma C.1, it follows that $u_n(y)$ can be written as the linear combination,

$$u_n(y)=C_n'\exp(i\sqrt{|k_n-\lambda|}y)[1+\rho_n^+(y)]+D_n'\exp(-i\sqrt{|k_n-\lambda|}y)[1+\rho_n^+(y)]$$
$$\equiv C_n'u_n^+(y)+D_n'u_n^-(y), \tag{5.31}$$

where $\rho_n^\pm(y)=o(y)$ as $y\to\infty$ and $u_n^\pm(y)$ are linearly independent solutions of (5.29b) for $y\geqslant 0$. Note also that by (C5) and the definition of $u_n^+(y)$,

$$u_n(y)=\lim_{k\to\infty}\{C_{nk}\exp(-\sqrt{k_n-\zeta_k}y)[1+\rho_{kn}(y)]\}=C_nu_n^+(y), \tag{5.32}$$

at each such y, where the limit $C_{kn}\to C_n\in\mathbf{C}$ as $k\to\infty$ exists.[24] By (5.31) and (5.32),

$$C_nu_n^+(y)=C_n'u_n^+(y)+D_n'u_n^-(y),\quad y\geqslant 0. \tag{5.33}$$

But (5.33) and the linear independence of $u_n^\pm(y)$ implies that $D_n'=0$. Hence $u(y)$ satisfies the outgoing radiation condition. □

The main result of this section is as follows.

Lemma 5.4: h_θ^1 has an empty singular continuous spectrum.

Proof: Follows from Lemma 5.3 by the same arguments used to prove Lemma 7.6 in Ref. 5.□

VI. PROOF OF THEOREM 3.2

It will be given after some preliminary remarks, definitions, and lemmas. We will assume that conditions 1 and 2 hold throughout this section.

Denoting by $\mathcal{H}_{\rm ac}(h_\theta^1)$ and $\mathcal{H}_p(h_\theta^1)$ the subspace of absolute continuity of $L^2(\omega)$ wrt h_θ^1 and the closed span of the eigenfunctions of h_θ^1, respectively, it follows that

$$L^2(\omega)=\mathcal{H}_{\rm ac}(h_\theta^1)\oplus\mathcal{H}_p(h_\theta^1),\quad \theta\in G, \tag{6.1}$$

since the subspace of singular continuity of $L^2(\omega)$ wrt h_θ^1 is the zero subspace by Lemma 5.4.[25] The projection operators $P_{\rm ac}$, P_s with domain $\mathcal{H}=L^2(\Omega)$ play an important role in this section. The former operator was defined in (4.3), and we define

$$UP_sU^{-1}=\int_G^\oplus P_p(h_\theta^1)d\theta, \tag{6.2}$$

where U is the unitary operator from $\mathcal{H}$ onto the single-fiber direct integral $\int_G^\oplus L^2(\omega)d\theta$ of Hilbert spaces introduced in Sec. III B and $P_p(h_\theta^1)$ the projection from $L^2(\omega)$ into $\mathcal{H}_p(h_\theta^1)$. Needless to say, P_s exists for reasons analogous to those guaranteeing the existence of $P_{\rm ac}$ that were mentioned in Sec. IV. As a byproduct of results in the present section, we will see that the equations

$$\mathrm{Ran}\,P_{\rm ac}=\mathcal{H}_{\rm scatt}, \tag{6.3a}$$

$$\mathrm{Ran}\,P_s=\mathcal{H}_{\rm surf} \tag{6.3b}$$

hold, the first of which was used to prove Theorem 3.1.

The next three lemmas are needed to prove Theorem 3.2.

Lemma 6.1: (a) $\mathcal{H}_{\rm scatt}$ and $\mathcal{H}_{\rm surf}$ are mutually orthogonal subspaces of $\mathcal{H}$.

Proof: The same as that of Lemma 8.1, Ref. 5.

Lemma 6.2: $\mathrm{Ran}\,P_{\rm ac}\subset\mathcal{H}_{\rm scatt}$.

Proof: Let $f\in\mathrm{Ran}\,P_{\rm ac}$. Then $g:=Uf=\int_G^\oplus g_\theta\,d\theta$ is such that $g_\theta\in\mathcal{H}_{\rm ac}(h_\theta^1)$ for a.e. $\theta\in G$. Fix $\theta\in G$ for which this holds and fix $a\geqslant 1$. Let X_a be the operator of multiplication in $L^2(\omega)$ by the characteristic function of $\omega_a=\{x\in\omega: x_\nu<a\}$. Let $[c,d]\subset\mathbf{R}$ be compact, with $c=\inf$ of the spec-

trum of h_θ^1, and denote by $E(\cdot;h_\theta^1)$ the spectral measure of h_θ^1. Then by the LC property of ω (defined as stated in the Remark to Lemma B.1), $X_a E([c,d];h_\theta^1)$ is a compact operator in $L^2(\omega)$. By $g_\theta \in \mathcal{H}_{\mathrm{ac}}(h_\theta^1)$ and the Riemann–Lebesgue lemma, $s-\lim_{t\to\pm\infty} X_a E([c,d];h_\theta^1)\exp(-ith_\theta^1)g_\theta = 0$. Since $X_a E([c,d];h_\theta^1)$ is compact, $s-\lim_{t\to\pm\infty} X_a E([c,d];h_\theta^1)\exp(-ith_\theta^1)g_\theta=0$. Since $s-\lim_{d\to\infty} E([c,d];h_\theta^1)=I_{L^2_{(\omega)}}$, it follows that[26]

$$\lim_{t\to\pm\infty} \|\exp(-ith_\theta^1)g_\theta\|_{\omega_a}=0. \tag{6.4}$$

By (3.17a) and (3.12),

$$\|\exp(-itH_1)f\|_{\Omega_a}^2=\int_G \|\exp(-ith_\theta^1)g_\theta\|_{\omega_a}^2\, d\theta, \tag{6.5}$$

if f is of bounded support, but a simple density argument allows us to drop this requirement. By (6.5), together with

$$\|\exp(-ith_\theta^1)g_\theta\|_{\omega_a}\leqslant\|g_\theta\|_{\omega_a}, \tag{6.6}$$

and the dominated convergence theorem, we infer that

$$\lim_{t\to\pm\infty} \|\exp(-itH_1)f\|_{\Omega_a}^2=\int_G \lim_{t\to\pm\infty} \|\exp(-ith_\theta^1)g_\theta\|_{\omega_a}^2\, d\theta=0, \tag{6.7}$$

and hence that $f\in\mathcal{H}_{\mathrm{scatt}}$. □

Lemma 6.3: $\mathrm{Ran}\, P_s\subset\mathcal{H}_{\mathrm{surf}}$.

Proof: Similar to that of a result of Davies and Simon.[27]

Proof of Theorem 3.2: By (6.1) and Lemmas 6.1–6.3,

$$\mathcal{H}=\mathrm{Ran}\, P_{\mathrm{ac}}\oplus\mathrm{Ran}\, P_s\subset\mathcal{H}_{\mathrm{scatt}}\oplus\mathcal{H}_{\mathrm{surf}}, \tag{6.8}$$

which immediately implies

$$\mathcal{H}=\mathcal{H}_{\mathrm{scatt}}\oplus\mathcal{H}_{\mathrm{surf}}, \tag{6.9}$$

thus proving Theorem 3.2. □

Equations (6.3) are direct consequences of Lemma 6.1, (6.4), and (6.5).

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APPENDIX A: FUNCTION SPACE NOTATION

For a measurable subset $A\subset\mathbf{R}^\nu(\nu\geqslant 2)$, the norm and inner product in the complex vector space $L^2(A)$ will be written as

$$\|\cdot\|_A,\ \langle\ \rangle_A,$$

respectively. $L^2(\Delta;A)$ denotes the complex Hilbert space of all $f\in L^2(A)$ such that $\Delta f\in L^2(A)$, equipped with the norm

$$\|f\|_{\Delta;A}=(\|f\|_A^2+\|\Delta f\|_A^2)^{1/2},$$

where Δ and all other partial differential operators in this appendix should be understood in the distributional sense.

The only Sobolev spaces used in this paper are $H^1(A)$ and $H_0^1(A)\subset H^1(A)$. The norm of $H^1(A)$ is denoted by

$$\|f\|_{1,A}=\left(\|f\|_A^2+\sum_{i=1}^{\nu}\|\partial f/\partial x_i\|_A^2\right)^{1/2}.$$

$L^2_{\mathrm{loc}}(\Delta;\overline{A})$ denotes the Fréchet space of (equivalence classes of) complex-valued functions f on A with $f|A(r)$, $\partial f/\partial x_i|A(r)\in L^2(A(r))$ $[r>0,A(r)\neq\varnothing]$, whose topology is generated by the seminorms

$$\|\cdot\|_{1,A(r)},\quad r>0,\quad A(r)\neq\varnothing.$$

We also need $H^1_{\mathrm{loc}}(\overline{A})$, the Fréchet space composed of all such functions f on A with $f|A(r)$, $\partial f/\partial x_i|A(r)\in L^2(A(r))$ for all such r, whose topology is generated by the seminorms

$$\|\cdot\|_{1,A(r)},\quad r>0,\quad A(r)\neq\varnothing.$$

Finally, $H^1_{0,\mathrm{loc}}(\overline{A})$ is a (closed) subspace of $H^1_{\mathrm{loc}}(\overline{A})$ that is the completion of $C_0^\infty(A)$ in the $H^1_{\mathrm{loc}}(\overline{A})$ topology.

For Fréchet spaces, $\overline{A}$ has been used to indicate integrability up to the boundary.

APPENDIX B: LOCAL COMPACTNESS OF ω

The main purpose of this appendix is to state Lemma B.1, which we use to prove Lemmas 5.1 and 5.3.

An open subset $A\subset\mathbf{R}^\nu(\nu\geqslant 2)$ is said to have the local compactness (LC) property for a bounded subset $B\subset H^1(A)$ if B is precompact in $L^2(A(r))$ for each $r>0$, with $A(r)\neq\varnothing$, i.e., if for each such r every sequence $\{f_n\}_{n\in\mathbf{N}}\subset B$ has a subsequence $\{f_{n_k}\}$ such that $\{f_{n_k}|A(r)\}$ is Cauchy in $L^2(A(r))$.

Lemma B.1: ω has the LC property for every bounded subset $H^1(\omega)\subset D(h_\theta)$, $\forall\,\theta\in G$.

Remarks: In the case $A=\omega$ considered in the lemma, the above definition of LC is equivalent to that obtained by replacing $\omega(r)$ by ω_r.

Proof: This is a special case of Lemma 4.6 of Ref. 5.

APPENDIX C: LEMMA ON ASYMPTOTIC SOLUTIONS OF A SECOND-ORDER ODE

The lemma stated in this appendix is used in the proofs of Lemmas 5.1–5.3. In it and throughout the paper, we define the square root of a complex number z by $\sqrt{z}=\exp(i\phi/2)\sqrt{|z|}$ for $\phi:=\arg z\in(-\pi,\pi)$ and set $\sqrt{z}=i\sqrt{|z|}$ for $z<0$. It is important to note that this definition implies that $\mathrm{Re}\,\sqrt{z}>0$ if $\mathrm{Im}\,\sqrt{z}\neq 0$.

Lemma C.1: Let $z\in\mathbf{C}\backslash\{0\}$ and suppose that $q\in C^1(J)$ is absolutely integrable over J, where $J\supset[0,\infty)$ is an open interval. Then for $0\leqslant y<\infty$ the differential equation,

$$\frac{d^2u}{dy^2}-[z+q(y)]u=0, \tag{C1}$$

has two solutions $u_\pm(y;z)$, linearly independent over this interval, satisfying the initial conditions

$$u_\pm(y;0)=1,\quad \frac{du_\pm(y;0)}{dy}=\pm\sqrt{z}, \tag{C2}$$

and such that

$$u_{\pm}(y;z)=\exp(\pm\sqrt{z}y)[1+\rho_{\pm}(y;z), \tag{C3a}$$

$$\frac{du_{\pm}(y;z)}{dy}=\pm\sqrt{z}\exp(\sqrt{z}y)[1+\sigma_{\pm}(y;z)], \tag{C3b}$$

where $\rho_{\pm}(y)$, $\sigma_{\pm}(y)$ are $o(1)$ as $y\to\infty$ and are real for $0\leqslant y<\infty$ if $z>0$. Moreover,

$$|\rho_{-}(y;z)|\leqslant\exp\left(\int_y^{\infty}|q(\xi)|d\xi/\sqrt{|z|}\right)-1, \tag{C4a}$$

$$|\sigma_{-}(y;z)|\leqslant\exp\left(\int_0^{\infty}|q(\xi)|d\xi/\sqrt{|z|}\right)\left[\exp\left(\int_y^{\infty}|q(\xi)|d\xi/\sqrt{|z|}\right)-1\right] \tag{C4b}$$

for y in the latter interval. Finally, if $(z_j)_{j\in\mathbf{N}}\subset\mathbf{C}\backslash\{0\}$ denotes a sequence converging to $\hat{z}\in\mathbf{C}\backslash\{0\}$, then

$$\lim_{j\to\infty}u_{-}(y;z_j)=u_{-}(y;\hat{z}), \tag{C5}$$

for $0\leqslant y\leqslant\infty$.

Remark: Properties of $\rho_{+}(y;z)$, $\sigma_{+}(y;z)$, and $u_{+}(y;z)$ analogous to those stated in (C4a), (C4b), and (C5), respectively, are readily derivable, but will not be needed.

Proof: Proofs of Eqs. (C3) are given in Ref. 28 for the case when $\mathrm{Re}\,\sqrt{z}\neq 0$. These equations follow more easily by integral-equation arguments. In the remaining case, namely $z=-1$, they are readily proved by the integral-equation approach used to derive (C4), which we now sketch.[29] To prove (C4a), one sets $u_{-}(y;z)=\exp(-\sqrt{z}y)U(y;z)$, constructs a singular Volterra integral equation for $U(y;z)$, and obtains an estimate for this function by solving it by successive approximations. Inequality (C4b) follows by differentiating the above expression for $u_{-}(y;z)$ and using this estimate and one for $\partial U(y;z)/\partial y$ that is derivable analogously. Finally, (C5) follows by a standard uniform-convergence argument using the solution of the said Volterra equation. □

[1] For a selected list of references, see., e.g., J. A. DeSanto, *Methods and Applications of Scattering Theory*, edited by J. A. DeSanto *et al.* (Springer-Verlag, Berlin, 1980), p. 60.

[2] See, e.g., G. Boato *et al.*, J. Phys. C **6**, L394 (1973); R. I. Masel *et al.*, Surf. Sci. **46**, 681 (1974); J. Chem. Phys. **64**, 45 (1976).

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[8] See, e.g., R. I. Masel *et al.*, J. Chem. Phys. **64**, 45 (1976), particularly Eq. (32), p. 51.

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[12] W. F. Stinespring, J. Reine Angew. Math. **200**, 200 (1958), Theorem 2.

[13] Here we are using the well-known terminology of M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness* (Academic, New York, 1975), p. 162. Henceforth we will use it without comment.

[14] For the general theory of direct integrals, see J. Dixmier, *Les algèbres d'operateurs dans l'espace Hilbertien*, 2nd ed. (Gauthier-Villars, Paris, 1969), Chap. II. For most (but not all) of our needs, the treatment in M. Reed and B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators* (Academic, New York, 1978), Sec. XIII.16, suffices.

[15] The self-adjointness of the h_θ's, the measurability of the functions $\theta\mapsto h_\theta$, and (3.13a) are asserted by Lemmas 4.2, C.1 (where "$\theta\mapsto H_\theta$" should read "$\theta\mapsto h_\theta$"), and 4.5 of Ref. 5. The corresponding properties of the h_θ^0's are provable similarly.

[16] Reed and Simon, Ref. 14, Theorem XIII.85 (g), p. 284.

[17] Reed and Simon, Ref. 14, Theorem XIII.85 (c), p. 284.

[18] This relation follows from the definition $\exp(itA)=s-\lim_{n\to\infty}[1-(itA/n)]^{-n}$ $(t\in\mathbf{R})$ for a self-adjoint operator A in a separable Hilbert space. See, e.g., T. Kato, *Perturbation Theory of Linear Operators* (Springer-Verlag, New York, 1966), Chap. IX, Sec. 1, paragraphs 2,3.

[19] See Ref. 5, Appendix B.1.

[20] The measurability of these functions follows from (4.4b) (which holds by Lemma 4.2) and the fact that each function $\theta\mapsto W_\theta^\pm$ is measurable, i.e., that for all $f\in L^2(\omega^0)$, $g\in L^2(\omega)$, the functions $\theta\mapsto\langle g,W_\theta^\pm f\rangle_\omega$ are measurable in the usual sense. The latter property follows from the measurability of $\theta\mapsto h_\theta^0$, $\theta\mapsto h_\theta$, and the existence of the $W_\theta^\pm$'s as strong limits.

[21] The second equality (4.14) is a special case of the formula $\langle\nabla f,\nabla g\rangle_\omega=\langle f,-\Delta g\rangle_\omega$, holding $\forall f,g\in D(h_\theta)$ by the alternative definition (4.8) of $D(h_\theta)$ in Ref. 5.

[22] W. C. Lyford, Math. Ann. **236**, 255 (1978), Theorem 3.3.

[23] M. Reed and B. Simon, Ref. 14, Theorem IX. 26, p. 54.

[24] The fact that $C_{kn}\to C_n$ as $k\to\infty$ for each n follows from two facts. First, the limit as $k\to\infty$ of the y-dependent factor of C_{kn} inside the brackets $\{\cdot\}$ in (5.31) exists and is not identically zero by (C5). Second, let $\{c_k\},\{d_k\},\{e_k\}$ be sequences in $\mathbf{C}$ such that $d_k\to d\neq 0$, $e_k\to e$. Then $\lim_k c_k=e/d$.

[25] M. Reed and B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis* (Academic, New York, 1972), Theorem VII.4, p. 230.

[26] The derivation of (6.4) is analogous to that of Lemma 1.6 in W. C. Lyford, Math. Ann. **216**, 229 (1975).

[27] E. B. Davies and B. Simon, Ref. 9, Proposition 6.1.

[28] P. Hartman, *Ordinary Differential Equations* (Birkhäuser, Boston, 1982), Corollary 9.2, p. 381.

[29] Compare with E. Hille, *Lectures on Ordinary Differential Equations* (Addison-Wesley, Reading, MA, 1969), especially pp. 172, 173, 444, 445.

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Supersymmetric field-theoretic models on a supermanifold

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We propose the extension of some structural aspects that have successfully been applied in the development of the theory of quantum fields propagating on a general space–time manifold so as to include superfield models on a supermanifold. We only deal with the limited class of supermanifolds which admit the existence of a smooth body manifold structure. Our considerations are based on the Catenacci–Reina–Teofillatto–Bryant approach to supermanifolds. In particular, we show that the class of supermanifolds constructed by Bonora–Pasti–Tonin satisfies the criteria which guarantee that a supermanifold admits a Hausdorff body manifold. This construction is the closest to the physicist's intuitive view of superspace as a manifold with some anticommuting coordinates, where the odd sector is topologically trivial. The paper also contains a new construction of superdistributions and useful results on the wavefront set of such objects. Moreover, a generalization of the spectral condition is formulated using the notion of the wavefront set of superdistributions, which is equivalent to the requirement that all of the component fields satisfy, on the body manifold, a microlocal spectral condition proposed by Brunetti–Fredenhagen–Köhler. © *2004 American Institute of Physics.*
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I. INTRODUCTION

There are topics in the physical literature which do not exhaust themselves, but always deserve new analyses. Among these, the program to a quantum gravity theory has a significant part, remaining an open problem of physics and an active area of current research. In spite of the fact that many attempts have been made to include gravity in the quantization program, a satisfactory and definitive theory still does not exist. Many lines of research in quantum gravity developed over the last decades, under different names, such as the Supergravity, Kaluza–Klein, String, Twistors, D-brane, Loop Quantum Gravity, Noncommutative Geometry and Topos theories, have elucidated the role of quantum gravity, without, however, providing conclusive results (see, for instance, Ref. 1 for a recent review of the status of quantum gravity). Whereas these good ideas stay only as good promises in the direction of a final theory of the quantum gravity, and since the relevant scale of the Standard Model, or any of its supersymmetric extensions, is much below the typical gravity scale, it seems appropriate to treat, in an intermediate step, some aspects of gravity in quantum field theory by considering the approach which describes the matter quantum fields under the influence of a gravitational background. This framework has a wide range of physical applicability, the most prominent being the gravitational effect of particle creation in the vicinity of blackholes, raised up for the first time by Hawking.[2]

The study of quantum field theories on a general manifold has become an area of intensive

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research activity, and a substantial progress has been made on a variety of interesting problems. In particular, great strides have been made towards the understanding of the question of how the spectral condition can be defined. While most of the Wightman axioms can be implemented on a curved space–time, the spectral condition (which expresses the positivity of the energy) represents a serious conceptual problem. On a flat space–time the Poincaré covariance, in particular the translations, guarantees the positivity of the spectrum, and fixes a unique vacuum state; but on a general curved space–time, due the absence of a global Poincaré group, there does not exist a useful notion of a vacuum state. As a result, the concept of particles becomes ambiguous, and the problem of the physical interpretation becomes much more difficult. One possible resolution to this difficulty is to choose some quantities other than particles content to label quantum states. Such an advice was given by Wald[3] with the purpose of finding the expectation value of the energy-momentum tensor. For free fields, this approach leads to the concept of Hadamard states. The latter are thought to be good candidates for describing physical states, at least for free quantum field theories in curved spacetime, according to the work of DeWitt and Brehme[4] (see Refs. 5, 6, 7 for a general review and references). In a seminal work, Radzikowski[8] showed that the global Hadamard condition can be locally characterized in terms of the wavefront set, and proved a conjecture by Kay[9] that a locally Hadamard quasifree Klein–Gordon state on any globally hyperbolic curved space–time must be globally Hadamard. His proof relies on a general *wavefront set spectrum condition* for the two-point distribution, which has made the connection with the spectral condition much more transparent (see also Refs. 10, 11).

The wavefront set was introduced by the mathematicians Hörmander and Duistermaat around 1971 (Refs. 12, 13) in their studies on the propagation of singularities of pseudodifferential operators, which rely on what is now known as a microlocal point of view. This subject is growing of importance, with a range of applications going beyond the original problems of linear partial equations. In particular, the link with quantum field theories on a curved space–time is now firmly established, especially after Radzikowski's work. A considerable amount of recent papers devoted to this subject[10,11,14–20] emphasizes the importance of the microlocal technique to solving some previously unsolved problems.

At the same time, it seems that not so much attention has been drawn to supersymmetric theories in this direction. Much of the progress made in understanding the physics of elementary particles has been achieved through a study of supersymmetry. The latter is a subject of considerable interest amongst physicists and mathematicians. It is not only fascinanting in its own right; in the 30 years that have passed since its proposal, supersymmetry has been studied intensively in the belief that such theories may play a part in a unified theory of the fundamental forces, and many issues are understood much better now. Although no clear signal has been observed up to now, supersymmetry is believed to be detectable, at least if certain minimal models of particle physics turn out to be realized in nature, and calculations and phenomenological analysis of supersymmetry models are well-justified in view of the forthcoming generation of machines, as the new super collider LHC being buit at CERN, which is expected to operate in a few years time and will have probably enough high energy to reveal some of the predicted supersymmetry particles, such as neutralinos, sleptons and may be indirectly squarks. It also has proven to be a tool to link the quantum field theory and noncommutative geometry.[21,22] Furthermore, in recent years the supersymmetry have been instrumental in uncovering nonperturbative aspects of quantum theories.[23,24] All of this gives strong motivations for trying to get a deeper understanding of the structure and of the properties of supersymmetric field theories.

This work is inspired in the structurally significant, recent results on quantum fields propagating in a globally hyperbolic, curved space–time, and represents a natural attempting to construct a generalization of some of the conventional mathematical structures used in quantum field theory, such as manifolds, so as to include superfield models in supermanifolds (curved superspaces). These structural questions are not without physical interest and relevance! It is the purpose of the present paper to study how such a construction can be achieved.

The outline of the paper is as follows: We shall begin in Sec. II by describing some global properties of supermanifolds according to Rogers,[25] and the problem of constructing their bodies

in the sense of Catenacci *et al.*[26] and Bryant.[27] Then, by working with a class of G^∞ supermanifolds constructed by Bonora–Pastin–Tonin[28] (BPT-supermanifolds), we demonstrate that this class of supermanifolds satisfies the criteria which guarantee that a supermanifold admits a Hausdorff body manifold. In Sec. III, superdistributions on superspace are defined. We derive some results not contained in Ref. 29. In particular, we generalize straightforwardly the notion of distributions defined on a manifold to distributions defined on a supermanifold. In Sec. IV, we discuss the algebraic formalism so as to include supersymmetry on a supermanifold. The results from this section may be seen as a natural extension of the ''Haag–Kastler–Dimock'' axioms[30,31] for local ''observables'' to supermanifolds. In Sec. V, we summarize some basics on the description of Hadamard (super)states. The focus of the Sec. VI will be on the extension of the Hörmander's description of the singularity structure (wavefront set) of a distribution to include the supersymmetric case. This fills a gap in the literature between the usual textbook presentation of the singularity structure of superfunctions and the rigorous mathematical treatment based on microlocal analysis. In Sec. VII, we present the characterization of a type of microlocal spectral condition for a superstate ω^{susy} with m-point superdistribution ω_m^{susy} on a supermanifold, in terms of the wavefront set of superdistributions, which is equivalent to the requirement that all of the component fields satisfy the microlocal spectral conditions[11] on the body manifold. This is in accordance with the DeWitt's remark[32] which asserts that in physical applications of supersymmetric quantum field theories, the spectral condition of the GNS-Hilbert superspace is restricted to the ordinary GNS-Hilbert space that sits inside the GNS-Hilbert superspace. Finally, Sec. VIII contains our final considerations.

II. NOTIONS OF SUPERMANIFOLDS

This section introduces some few basic fundamentals on the theory of supermanifolds. We follow here the work of Rogers[25] which is both general and mathematically rigorous. Rogers' theory has an advantage, a supermanifold is an ordinary Banach manifold endowed with a Grassmann algebra structure, so that the topological constructions have their standard meanings. In this context see also Refs. 32–39.

We start by introducing first some definitions and concepts of a Grassmann–Banach algebra, i.e., a Grassmann algebra endowed with a Banach algebra structure. This leads to the key concept of supercommutative superalgebra.

Definition 2.1: An algebra is said to be a supercommutative superalgebra Λ*—or a* $\mathbb{Z}_2$*-graded commutative algebra—if* Λ *is the direct sum* $\Lambda=\Lambda_0\oplus\Lambda_1$ *of two complementary subspaces such that* $\mathbb{1}\in\Lambda_0$ *and* $\Lambda_0\Lambda_0\subset\Lambda_0$, $\Lambda_0\Lambda_1\subset\Lambda_1$, $\Lambda_1\Lambda_1\subset\Lambda_0$. *Moreover, for all homegeneous element* x, y *in* Λ, $xy=(-1)^{|x||y|}yx$, *where* $|x|=0$ *if* $x\in\Lambda_0$ *and* $|x|=1$ *if* $x\in\Lambda_1$. *In particular, it follows that the square of odd elements is zero*.

Elements from Λ_0 and Λ_1 are said to be homegeneous if they have a definite parity, i.e., an element $x\in\Lambda_0$ is said to have *even* parity, while an element $x\in\Lambda_1$ is said to have *odd* parity. Products of homogeneous elements of the same parity are even and of elements of different parities are odd.

We shall assume that the superalgebra Λ is a Banach space with norm $\|\cdot\|$ satisfying the condition

$$\|xy\|\leqslant\|x\|\|y\|\ ,\forall x,y\in\Lambda;\quad \|\mathbb{1}\|=1\ .$$

Let L be a finite positive integer and $\mathcal{G}$ denote a Grassmann algebra, such that $\mathcal{G}$ can naturally be decomposed as the direct sum $\mathcal{G}=\mathcal{G}_0\oplus\mathcal{G}_1$, where $\mathcal{G}_0$ consists of the even (commuting) elements and $\mathcal{G}_1$ consists of the odd (anti-commuting) elements in $\mathcal{G}$, respectively. Let M_L denote the set of sequences $\{(\mu_1,\ldots,\mu_k)|1\leqslant k\leqslant L;\mu_i\in\mathbb{N};1\leqslant\mu_1<\cdots<\mu_k\leqslant L\}$. Let Ω represent the empty sequence in M_L, and (j) denote the sequence with just one element j. A basis of $\mathcal{G}$ is given by monomials of the form $\{\xi_\Omega,\xi^{\mu_1}\xi^{\mu_2},\ldots,\xi^{\mu_1}\xi^{\mu_2}\cdots\xi^{\mu_k}\}$ for all $\mu\in M_L$, such that $\xi_\Omega=\mathbb{1}$ and $\xi^{(i)}\xi^{(j)}+\xi^{(j)}\xi^{(i)}=0$ for $1\leqslant i,j\leqslant L$. Futhermore, there is no other independent relations among the generators. By $\mathcal{G}_L$ we denote the Grassmann algebra with L generators, where the even and the

odd elements, respectively, take their values. L being assumed a finite integer (the number of generators L could be possibly infinite), it means that the sequence terminates at $\xi^1\cdots\xi^L$ and there are only 2^L distinct basis elements. An arbitrary element $q\in\mathcal{G}_L$ has the form

$$q=q_{\mathbf{b}}+\sum_{(\mu_1,\ldots,\mu_k)\in M_L} q_{\mu_1,\ldots,\mu_k}\xi^{\mu_1}\cdots\xi^{\mu_k}\ , \tag{2.1}$$

where $q_{\mathbf{b}}, q_{\mu_1\cdots\mu_k}$ are real numbers. An even or odd element is specified by 2^{L-1} real parameters. The number $q_{\mathbf{b}}$ is called the body of q, while the remainder $q-q_{\mathbf{b}}$ is the soul of q, denoted $s(q)$. The element q is invertible if, and only if, its body is nonzero.

With reference to supersymmetric field theories, the commuting variable x has the form

$$x=x_{\mathbf{b}}+x_{ij}\xi^i\xi^j+x_{ijkl}\xi^i\xi^j\xi^k\xi^l+\cdots\ , \tag{2.2}$$

where $x_{\mathbf{b}}, x_{ij}, x_{ijkl},\ldots$ are real variables. Similarly, the anticommuting variables (in the Weyl representation) θ and $\overline{\theta}=(\theta)^*$ have the form

$$\theta=\theta_i\xi^i+\theta_{ijk}\xi^i\xi^j\xi^k+\cdots\ ,\quad \overline{\theta}=\overline{\theta}_i\xi^i+\overline{\theta}_{ijk}\xi^i\xi^j\xi^k+\cdots\ , \tag{2.3}$$

where $\theta_i, \theta_{ijk},\ldots$ are complex variables. The summation over repeated indices is to be understood unless otherwise stated.

Remark 2.1: As pointed out by Vladimirov–Volovich,[40] from the physical point of view, superfields are not functions of $\theta_i, \theta_{ijk},\ldots$ and $x_{\mathbf{b}}, x_{ij}, x_{ijkl},\ldots$, but only depend on these variables through θ and x, as it occurs with ordinary complex analysis where analytic functions of the complex variables $z=x+iy$ are not arbitrary functions of the variables x and y, but functions that depend on x and y through z. ■

The Grassmann algebra may be topologized. Consider the complete norm on $\mathcal{G}_L$ defined by[41]

$$\|q\|_p=\left(|q_{\mathbf{b}}|^p+\sum_{(\mu)=1}^{L}|q_{\mu_1\cdots\mu_k}|^p\right)^{1/p}\ . \tag{2.4}$$

A useful topology on $\mathcal{G}$ is the topology induced by this norm. The norm $\|\cdot\|_1$ is called the Rogers norm and $\mathcal{G}_L(1)$ the Rogers algebra.[25] The Grassmann algebra $\mathcal{G}$ equipped with the norm (2.4) becomes a Banach space. In fact $\mathcal{G}$ becomes a Banach algebra, i.e., $\|\mathbb{1}\|=1$ and $\|qq'\|\leqslant\|q\|\|q'\|$ for all $q,q'\in\mathcal{G}$.

Definition 2.2: A Grassmann–Banach algebra is a Grassmann algebra endowed with a Banach algebra structure.

A superspace must be constructed using as a building block a Grassmann–Banach algebra $\mathcal{G}_L$ and not only a Grassmann algebra.

Definition 2.3: Let $\mathcal{G}_L=\mathcal{G}_{L,0}\oplus\mathcal{G}_{L,1}$ be a Grassmann–Banach algebra. Then the (m,n)-dimensional superspace is the topological space $\mathcal{G}_L^{m,n}=\mathcal{G}_{L,0}^m\times\mathcal{G}_{L,1}^n$, which generalizes the space $\mathbb{R}^m$, consisting of the Cartesian product of m copies of the even part of $\mathcal{G}_L$ and n copies of the odd part.

For an (m,n)-dimensional superspace, a typical element of this set used in physics is denoted by $(z)=(z_1,\ldots,z_{m+n})=(x_1,\ldots,x_m,\theta_1,\ldots,\theta_{n/2},\overline{\theta}_1,\ldots,\overline{\theta}_{n/2})$. For instance, for the (4,4)-dimensional Minkowski superspace, which is the space of, e.g., $N=1$ Wess–Zumino model formulated in superfield language and modeled as $\mathcal{G}_L^{4,4}=\mathcal{G}_{L,0}^4\times\mathcal{G}_{L,1}^4$, $(z)=(x_1,\ldots,x_4,\theta_1,\theta_2,\overline{\theta}_1,\overline{\theta}_2)$. The norm on $\mathcal{G}_L^{4,4}$ is defined by $\|z\|=\Sigma_{i=1}^4\|x_i\|+\Sigma_{j=1}^2\|\theta_j\|+\Sigma_{k=1}^2\|\overline{\theta}_k\|$. The topology on $\mathcal{G}_L^{4,4}$ is the topology induced by this norm—which is also the product topology.

In supersymmetric quantum field theory, superfields are functions in superspace usually given by their (terminating) standard expansions in powers of the odd coordinates

$$F(x,\theta,\overline{\theta})=\sum_{(\gamma)=0}^{\Gamma} f_{(\gamma)}(x)(\theta)^{(\gamma)}\ , \tag{2.5}$$

where $(\theta)^{(\gamma)}$ comprises all monomials in the anticommuting variables θ and $\overline{\theta}$ (belonging to odd part of a Grassmann–Banach algebra) of degree $|\gamma|$; $f_{(\gamma)}(x)$ is called a component field, whose Lorentz properties are determined by those of $F(x,\theta,\overline{\theta})$ and by the power (γ) of (θ). The following notation, extended to more than one θ variable, is used (2.5): $(\theta)=(\theta_1,\overline{\theta_1},\ldots,\theta_n,\overline{\theta_n})$, and (γ) is a multi-index $(\gamma_1,\overline{\gamma_1},\ldots,\gamma_n,\overline{\gamma_n})$ with $|\gamma|=\Sigma_{r=1}^{n}(\gamma_r+\overline{\gamma_r})$ and $(\theta)^{(\gamma)}=\Pi_{r=1}^{n}\theta_r^{\gamma_r}\overline{\theta}_r^{\overline{\gamma}_r}$. In Eq. (2.5), for a (4,4)-dimensional superspace, $\Gamma=(2,2)$.

Rogers[25] considered superfields in $\mathcal{G}_L^{m,n}$ as G^∞ superfunctions, i.e., functions whose coefficients $f_{(\gamma)}(x)$ of their expansions are smooth functions of $\mathbb{R}^m$ into $\mathcal{G}_L$, extended from $\mathbb{R}^m$ to all of $\mathcal{G}_L^{m,0}$ by z-continuation,[25] which maps functions of real variables into functions of variables in $\mathcal{G}_L^{m,0}$.

Definition 2.4: Let U be an open set in $\mathcal{G}_L^{m,0}$ and let $\epsilon:\mathcal{G}_L^{m,0}\to\mathbb{R}^m$ be the body projection which associates to each m-tuple $(x_1,\ldots,x_m)\in\mathcal{G}_L^{m,0}$ an m-tuple $(\epsilon(x_1),\ldots,\epsilon(x_m))\in\mathbb{R}^m$. Let V be an open set in $\mathbb{R}^m$ with $V=\epsilon(U)$. We get through z-continuation—or "Grassmann analytic continuation"—of a function $f\in C^\infty(V,\mathcal{G}_L)$ a function $z(f)\in G^\infty(U,\mathcal{G}_L)$, which admits an expansion in powers of the soul of x

$$z(f)(x_1,\ldots,x_m)=\sum_{i_1=\cdots=i_m=0}^{L}\frac{1}{i_1!\cdots i_m!}[\partial_1^{i_1}\cdots\partial_m^{i_m}]f(\epsilon(x))s(x_1)^{i_1}\cdots s(x_m)^{i_m}\ ,$$

where $s(x_i)=(x_i-\epsilon(x_i))$ and $\epsilon(x_i)=(x_i)_{\mathbf{b}}$.

One should keep always in mind that the continuation involves only the even variables $z:C^\infty(\epsilon(U))\to G^\infty(U)$, and that $z(f)(x_1,\ldots,x_m)$ is a supersmooth function if their components are smooth for soulless values of x. This justifies the formal manipulations in the physics literature, where superfields are manipulated as if their even arguments were ordinary numbers:[37] a supersmooth function is completely determined when its components are known on the body of superspace.

According to Definition 2.4, the superfield $F(x,\theta,\overline{\theta})\in G^\infty(U,\mathcal{G}_L)$ admits an expansion

$$F(x,\theta,\overline{\theta})=\sum_{(\gamma)=0}^{\Gamma} z(f_{(\gamma)})(x)(\theta)^{(\gamma)}\ ,$$

but here with suitable $f_{(\gamma)}\in C^\infty(\epsilon(U),\mathcal{G}_L)$.

Now, we are going to consider some helpful aspects about supermanifolds, based on the work of Rogers,[25] replacing the simple superspace $\mathcal{G}_L^{m,n}$ by a more general supermanifold. Rogers used the concept of G^∞ superfunctions to define the concept of G^∞ supermanifolds (which can be considered as Banach real manifolds C^∞ modeled on $\mathcal{G}_L^{m,n}$ of dim $N=2^{L-1}(m+n)$), with a structure allowing for the definitions of neighboring points and continuous superfunctions. An (m,n)-dimensional G^∞ supermanifold generalizes the concept of an m-dimensional C^∞ manifold: just as a manifold is a Hausdorff topological space such that every point has a neighborhood homeomorphic to $\mathbb{R}^m$ and has local coordinates $(x_1(p),\ldots,x_m(p))$ in $\mathbb{R}^m$, a supermanifold is a topological space which locally looks like $\mathcal{G}_L^{m,n}$ (but not necessarily in its global extent) and has local coordinates $(x_1(p),\ldots,x_m(p),\theta_1(p),\ldots,\theta_n(p))$ in $\mathcal{G}_L^{m,n}$, and whose transition functions fulfill a suitable supersmoothness condition.

Definition 2.5: A supermanifold is in general a paracompact Hausdorff topological space $\mathcal{M}$, together with an atlas of charts $\{(X_\alpha,k_\alpha)|\alpha\in I\}$, over a Grassmann–Banach algebra $\mathcal{G}_L$, where the X_α cover $\mathcal{M}$ and each coordinate function k_α is a homeomorphic local map from X_α onto an open subset $\tilde{X}_\alpha\subset\mathcal{G}_L^{m,n}$, also Hausdorff.

The existence of infinitely differentiable coordinates systems makes the supermanifold differentiable. The differentiable structure in this topological space is due to G^r ($r=p$ or $p=\infty$) structure of transition functions, $k_\beta \circ k_\alpha^{-1}$, between overlapping coordinate patches, $k_\alpha(X_\alpha \cap X_\beta)$ and $k_\beta(X_\alpha \cap X_\beta)$, required to be supersmooth morphisms for any $\alpha,\beta \in I$. The local coordinates are:

$$u_i = p_i \circ k_\alpha \mapsto (i=1,\ldots,m),$$

$$v_j = p_{j+m} \circ k_\alpha \mapsto (j=1,\ldots,n).$$

In this sense $\mathcal{G}_L^{m,n}$ is an example of G^∞ supermanifold, unlike of the coarse topology in the DeWitt sense[32] whose structure cannot be even a metric one.

Definition 2.6: Let $\tilde{X}_\alpha$ be an open in $\mathcal{G}_L^{m,n}$ and $f:\tilde{X}_\alpha \to \mathcal{G}_L$, then:

(a) f is called G^0 in $\tilde{X}_\alpha$ if f is continuous in $\tilde{X}_\alpha$.

(b) f is called G^1 in $\tilde{X}_\alpha$ if exist $m+n$ functions $G_k f:\tilde{X}_\alpha \to \mathcal{G}_L$, $k=1,\ldots,m+n$ and functions $\eta:\mathcal{G}_L^{m,n} \to \mathcal{G}_L$ such that

$$f(a+h,b+k) = f(a,b) + \sum_{i=1}^{m} h_i\{G_i f(a,b)\} + \sum_{j=1}^{n} k_j\{G_{j+m} f(a,b)\} + \|h,k\|\eta(h,k),$$

and $\eta(h,k) \to 0$ when $\|h,k\| \to 0$. In this sense, $G_i f \to f_i'$.

We can generalize to G^p, with finite p in the following: f is G^p in $\tilde{X}_\alpha$ if is possible choose $G_k f$ which are G^{p-1} with $f \in G^1$ em $\tilde{X}_\alpha$. If it is true to all p, f is called G^∞. In fact, any function which is absolutely convergent (power series) is G^∞ on $\tilde{X}_\alpha$, in other words,

$$f(z) = \sum_{k_1 \cdots k_{m+n}=0}^{\infty} a_{k_1 \cdots k_{m+n}} z_1^{k_1} \cdots z_{m+n}^{k_{m+n}},$$

$$f:\tilde{X}_\alpha \to \mathcal{G}_L, \quad \tilde{X}_\alpha \subset \mathcal{G}_L^{m,n} \quad \text{and} \quad a_{k_1 \cdots k_{m+n}} \in \mathcal{G}_L.$$

Another important fact is the C^∞ structure:

$$[D^p f(z)][\ell^1,\ell^2,\ldots,\ell^p] = \sum_{k_1 \ldots k_p=1}^{m+n} l_{k_1}^1 \cdots l_{k_p}^p (G_{k_p} G_{k_{p-1}} \cdots G_{k_1} f)(z),$$

for all $z \in \tilde{X}_\alpha$ open in $\mathcal{G}_L^{m,n}$ and $l_{k_1}^1 \cdots l_{k_p}^p \in (\mathcal{G}_L^{m,n})^p$. The latter denotes a product space of p copies of $\mathcal{G}_L^{m,n}$. In this way the p derivative of $f \in \mathcal{L}[(\mathcal{G}_L^{m,n})^p, \mathcal{G}_L]$ are elements of continuous p-linear maps of $(\mathcal{G}_L^{m,n})^p$ into $\mathcal{G}_L$. This formalism is interesting and agrees to the Hörmander's one[42] (p. 11), where $f^{(p)} \in L^p(X_\alpha, X_\beta)$, are elements of continuous p-linear forms from X_α to X_β.

Remark 2.2: The discussion of differentiability by Jadczyk–Pilch[33] is simpler than the one given by Rogers.[25] In particular, knowing already that a function f is a C^∞ map between Banach spaces, it is needed only to look at its first derivative to know whether f is supersmooth or not, while according to Rogers an investigation of all derivatives is necessary. However, the concept of supersmoothness by Jadczyk–Pilch, and the concept of G^∞ differentiability by Rogers are equivalent. ■

The body of a supermanifold: Now that the general idea of structure on a supermanifold has been introduced, it is time to restrict our attention to the case of fundamental interest: the problem of constructing the body of a G^∞ supermanifold which serves as the physical space–time. Roughly speaking, the body of a supermanifold $\mathcal{M}$ is an ordinary C^∞ space–time manifold $\mathcal{M}_0$ obtained from $\mathcal{M}$ getting rid of all the soul coordinates. Because of its extreme generality, Rogers' theory includes many topologically exotic supermanifolds which are not physically useful, admitting the

possibility of nontrivial topology in the anticommuting directions and classes of supermanifolds without a body manifold. But, intuition suggests that only a bodied G^∞ supermanifold can be physically relevant!

The question of the existence of the body of a supermanifold was clarified in the papers by Catenacci *et al.*[26] and Bryant.[27] Their approach is independent of the atlas used, and it is based on the fact that any G^∞ supermanifold $\mathcal{M}$ admits a foliation $\mathfrak{F}$. This type of structure is defined and related to the natural notions of quotient and substructure on a supermanifold. As with many important concepts in mathematics, there are several equivalent ways of defining the notion of a foliation. The simplest and most geometric is the following:

Definition 2.7: Let $\mathcal{M}$ be an (m,n)-dimensional supermanifold of class G^r, $0\leqslant r\leqslant p$. A foliation of class G^r, and of codimension m, is a decomposition of $\mathcal{M}$ into disjoint connected subsets $\{\mathfrak{L}_\alpha\}_{\alpha\in A}$, called the leaves of the foliation, such that each point of $\mathcal{M}$ has a neighborhood U and a system of G^r coordinates $(x,\theta): U\to\mathcal{G}^m_{L,0}\times\mathcal{G}^n_{L,1}$ such that for each leaf $\mathfrak{L}_\alpha$, the components of $U\cap\mathfrak{L}_\alpha$ are described by surfaces on which all the body coordinates $\epsilon(x_1),\ldots,\epsilon(x_m)$ are constant. We denote the foliation by $\mathfrak{F}=\{\mathfrak{L}_\alpha\}_{\alpha\in A}$.

The coordinates referred to in Definition 2.7 are said to be distinguished by the foliation $\mathfrak{F}$. Under certain regularity conditions on $\mathfrak{F}$, the quotient space $\mathcal{M}/\mathfrak{F}$ can be given the structure of an ordinary m-dimensional differentiable manifold $\mathcal{M}_0$, which is called the body manifold of $\mathcal{M}$ (for details see Ref. 26). A G^∞ supermanifold whose $\mathfrak{F}$ foliation is regular is called regular itself. On regular supermanifolds the following theorem holds:

Theorem 2.8 (Catenacci–Reina–Teofilatto Theorem): *Let $\mathcal{M}$ be a regular G^∞ supermanifold. Then its body $\mathcal{M}_0$ is a C^∞ manifold.* □

As stated by Bryant,[27] the necessity of regularity of the soul foliation in the sense of Catenacci–Reina–Teofilatto is not sufficient to guarantee that a supermanifold admits a body manifold. He derived necessary and sufficient conditions, namely, that leaves should be closed and do not accumulate, for the existence of a Hausdorff body manifold.

Theorem 2.9 (Bryant Theorem 2.5): *Suppose that $\mathcal{M}$ is a supermanifold. In order that $\mathcal{M}$ admits a body manifold, it is necessary and sufficient that the leaves of the soul foliations are closed in $\mathcal{M}$ and do not accumulate.* □

For our purposes, it will be sufficient to consider the class of G^∞ supermanifolds constructed by Bonora–Pasti–Tonin[28] (we shall call BPT-supermanifolds for brevity), which has important applications in theoretical physics—and fulfills Theorems 2.8 and 2.9, as we shall verify presently. These supermanifolds consist of the Grassmann extensions of *any* ordinary C^∞ space–time manifold. From a given m-dimensional physical space–time, one constructs first an $(m,0)$-dimensional supermanifold, and the (m,n)-dimensional supermanifold by taking the direct product with $\mathcal{G}^{0,n}_L$. This construction is the closest to the physicist's intuitive view of superspace as a manifold with some anticommuting coordinates, with the odd Grassmann variables being topologically trivial.

Remark 2.3: As a matter of fact, in any model involving fermions in a general space–time, the supermanifold will need to be that constructed from the spinor bundle of the manifold in the way which we recall now: Let $\mathcal{M}$ be an m-dimensional body manifold and E be an n-dimensional vector bundle over $\mathcal{M}$. Suppose that $\{U_\alpha\}$ is a covering of $\mathcal{M}$ by coordinate neighborhoods which are also trivialization neighborhoods of E. Then, the corresponding (m,n)-dimensional supermanifold has coordinate transition functions

$$x^i_\alpha=\phi^i_{\alpha\beta}(x_\beta),$$

where $\phi_{\alpha\beta}$ is the z continuation of the transition function for M and

$$\theta^i_\alpha=g_{\alpha\beta}{}^i{}_j(x_\beta)\,\theta^j_\alpha,$$

with $g_{\alpha\beta}: U_\alpha\cap U_\beta\to Gl(n)$ being the transition function for E. It is worthwhile to note that the BPT-supermanifolds are examples of this construction when the bundle E is trivial. ■

For the convenience of the reader, we recall here the construction of Bonora–Pasti–Tonin.[28] Let $\{(U_\alpha,\psi_\alpha)|\alpha\in I\}$ be an atlas for $\mathcal{M}_0$. For each $\alpha\in I$ consider the subset X_α of the Cartesian product $U_\alpha\times\mathcal{G}_L^{m,0}$ defined by

$$X_\alpha=\{(x,\overline{x})|x\in U_\alpha,\overline{x}\in\mathcal{G}_L^{m,0},\quad\text{and}\quad\epsilon(\overline{x})=\psi_\alpha(x)\},\tag{2.6}$$

and define $k_\alpha:X_\alpha\to\mathcal{G}_L^{m,0}$ by $k_\alpha(x,\overline{x})=\overline{x}$ for $(x,\overline{x})\in X_\alpha$. k_α is a homeomorphism and its image is an open subset of $\mathcal{G}_L^{m,0}$.

An important property of the z-continuation is the composition of functions. Let U be an open set in $\mathbb{R}^m$, and let the map $f:\mathbb{R}^m\to\mathcal{G}_L^{k,0}$ be represented by the set of C^∞ functions $\{f_i(x_1,\ldots,x_m),i=1,\ldots,m\}$. Define $z(f)$ as the set of functions $\{z(f_i)\}$. Let V be an open set in $\mathbb{R}^n$, and consider the maps $f:U\to V$ and $g:V'\to\mathcal{G}_L^{k,0}$, respectively, where $V'\subseteq V$, and both f,g are C^∞ functions. Then

$$z(g\circ f)=z(g)\circ z(f).\tag{2.7}$$

Now consider the disjoint union $M=\cup_{\alpha\in I}X_\alpha$. Two points of M are equivalent if and only if $(x,\overline{x})\sim(x',\overline{x'})$, such that $(x,\overline{x})\in X_\alpha$ and $(x',\overline{x'})\in X_\beta$ and $x=x'$, $\overline{x'}=z(\psi_\beta\circ\psi_\alpha^{-1})(\overline{x})$. Of course M is a Hausdorff space. Then consider the space $\mathcal{M}_G$ equal to the space M modulo the equivalence relation above. The k_α's provide $\mathcal{M}_G$ with a G^∞ differentiability structure, so that $\mathcal{M}_G$ is a G^∞ $(m,0)$ supermanifold. Let $\pi_G:\mathcal{M}_G\to\mathcal{M}_0$ be a continuous and open projection. Locally $\pi_G|_{X_\alpha}(x,\overline{x})=x$ for $(x,\overline{x})\in X_\alpha$. Since $\mathcal{M}_G$ is a *regular* supermanifold, we find straightforwardly that $\pi_G\circ k_\alpha^{-1}=\psi_\alpha^{-1}\circ\epsilon$ for $\overline{x}\in k_\alpha(X_\alpha)$. This can be expressed by the commutative diagram:

$$\begin{array}{ccc} X_\alpha & \xleftarrow{k_\alpha^{-1}} & \mathcal{G}_L^{m,0} \\ \pi_G\downarrow & & \downarrow\epsilon \\ U_\alpha & \xleftarrow{\psi_\alpha^{-1}} & \mathbb{R}^m \end{array}$$

Finally, we construct the (m,n)-dimensional supermanifold $\mathcal{M}$ by taking the direct product of $\mathcal{M}_G$ with $\mathcal{G}_L^{0,n}$. The projection $\pi_S:\mathcal{M}\to\mathcal{M}_0$ is the composite map $\pi_G\circ\gamma$, where $\gamma:\mathcal{M}\to\mathcal{M}_G$ is the projection onto the first factor. The map γ is G^∞, unlike π_G which is a C^∞ function but not a G^∞.

Corollary 2.10: Let $\mathcal{M}$ be a BPT-supermanifold. Then the leaves of the soul foliation are regular, closed in $\mathcal{M}$ and do not accumulate.

Proof: First of all, it is worthwhile noticing that, according to the construction of Bonora–Pasti–Tonin, two points of a BPT-supermanifold are in the same leaf if, and only if, they are equivalents in the sense defined above. Then the soul foliation can be defined by $\mathcal{M}/\sim\overset{\text{def}}{=}\mathcal{M}/\mathfrak{F}$. Once verified the corollary, we see that a BPT-supermanifold possesses an ordinary body manifold defined by soul foliation $\mathcal{M}_0\overset{\text{def}}{=}\mathcal{M}/\mathfrak{F}$, where $\mathcal{M}_0$ denotes the body manifold.

In order to show that the leaves of a BPT-supermanifold are closed, the following considerations are needed: we say that the soul foliation of a BPT-supermanifold is a Hausdorff space, and that the structure of their supermanifold is regular. This can be verified through the following theorem by Bryant[27] (Theorem 3.2): Suppose that $\mathcal{M}$ is a supermanifold of dimension (m,n) and $\Gamma=\{U_i,\phi_i\}$ is a good atlas; then the following conditions are equivalent: (i) $\Gamma=\{U_i,\phi_i\}$ is a regular superstructure on $\mathcal{M}$, (ii) when s and t lie in U_i, $s\approx t$ implies $s\sim t$, and (iii) the body map $\epsilon:\mathcal{M}\to\mathcal{M}/\mathfrak{F}$ is locally modeled on $\epsilon_0:B^{m,n}\to\mathbb{R}^m$ in the sense that exist homeomorphisms $\overline{\phi_i}:\epsilon U_i\to\epsilon_0\phi_i U_i$ such that $\overline{\phi_i}\circ\epsilon_{|U_I}=\epsilon_0\circ\phi$. When these conditions are satisfied, $\mathcal{M}/\mathfrak{F}$ is Hausdorff and is a smooth manifold of dimension m with charts $\{\epsilon U_i,\overline{\phi_i}\}$. For the case of the equivalence relation $(s\sim t)$ of a BPT-supermanifold, we see that it must be $\approx$ in the Bryant sense because embodies $\sim$ and is transitive. Then $\approx$ implies $\sim$ on the same charts. This means that the conditions of the Theorem 3.2 by Bryant must be properties of the BPT foliation, and hence is

Hausdorff and regular. Now, the fact that the leaves of a BPT-supermanifold are closed is clear: each point $(\epsilon(s))$ of $\mathcal{M}/\sim$ is closed, given that the BPT-supermanifolds is a Hausdorff space, and the inverse application theorem guarantees that a leaf is necessarily closed, since being F the leaf in $\mathcal{M}$, $F=\epsilon^{-1}\epsilon(s)$ where ϵ^{-1} is a continuous map.

Finally, we shall verify that the leaves of a BPT-supermanifold do not accumulate. First, we shall suppose that the leaves of soul foliation accumulate[43] in a given pair of points, e.g., $s_+, s_- \in \mathcal{M}$. Note that as $\mathcal{M}/\mathfrak{F}$ is Hausdorff, given two points $x \in \mathcal{M}/\mathfrak{F}$ and $y \in \mathcal{M}/\mathfrak{F}$ with $x \neq y$, we can separate them by disjoint open sets. Choice, for example, $\epsilon s_+ = x$ and $\epsilon s_- = y$, where $\epsilon: \mathcal{M} \to \mathcal{M}/\mathfrak{F}$. Then, we also can choose $s_+ \in F' \cup \Sigma_+$ (a transverse submanifold) and $s_- \in F' \cup \Sigma_-$ (another transverse submanifold). If this is true, s_+, s_- must be in the same leaf, by indicating that $\epsilon s_+ = \epsilon s_-$ contradicting the statement which a soul foliation is Hausdorff. Hence, the leaves do not accumulate. In order to complete the prove, we examine the condition $\epsilon s_+ = \epsilon s_-$. Due the possibility of choosing arbitrary transverse submanifolds, we select $\Sigma(s)$ and $\Sigma(t)$ through the some disjoint neighborhoods of s and t, resp., such that does not exist a U_i which intersects $\Sigma(s)$ and $\Sigma(t)$. But $\epsilon s_+ = \epsilon s_-$ implies that s and t are in the same chart U_i, so the leaves do not accumulate since $\Sigma(s) \cup \Sigma(t) = \varnothing$. □

The existence of a body manifold places us in a position to consider physically interpretable field theories on supermanifolds. In order to establish applicability in a physical system, we need to impose some restrictions regarding to the body manifold $\mathcal{M}_0$, associated with the supermanifold $\mathcal{M}$. Apart from another aspects, the causality principle plays a crucial role in our construction. Therefore, we restrict our body manifold, $(\mathcal{M}_0, g_0)$, to be globally hyperbolic Lorentz manifold, by consisting of a four-dimensional smooth manifold $\mathcal{M}_0$ (any dimension would be possible) that can be smoothly foliated by a family of acausal Cauchy surfaces[6] and a smooth metric g_0 with signature $(+, -, -, -)$. This means that the body manifold must be topologically equivalent to the Cartesian product of $\mathbb{R}$ and a smooth spacelike hypersurface Σ (a Cauchy surface). Σ intersects any endless timelike curve at most once. A four-dimensional globally hyperbolic Lorentz manifold is orientable and time orientable, i.e., at each $x \in \mathcal{M}_0$ we may designate a future and past light cone continuously. Moreover, $\mathcal{M}_0$ is assumed to have a spin structure, so that one can consider spinors defined on it. It can be shown that a four-dimensional globally hyperbolic Lorentz manifold admits a spin structure.[44] In fact, Geroch[44] pointed out that a *noncompact, parallelizable* four-dimensional manifold admits a spin structure. Geroch's parallelizability criterion applies to a four-dimensional globally hyperbolic Lorentz manifold.

Remark 2.4: As it has been emphasized in Ref. 10, a natural background geometry that admits a supersymmetric extension of its isometry group can only be of the anti–de Sitter (AdS) type. In other words, the global supersymmetry should not be compatible with most spacetimes, an exception being the AdS space. This requirement seems to be an extremely restrictive condition, since the AdS space has problems with closed timelike curves, apparently violating causality and leading to problems during quantization. Namely, boundary conditions at infinity are needed. Nevertheless, one should remind that this result refers to extended supergravity theories with gauged SO(N) internal symmetry;[45] this is not, however, our case in this paper. Furthermore, this result can mainly be justified by the heuristic form of introducing the superspace (which may be bypassed taking into account the Rogers' theory of a global supermanifold). As stressed by Bruzzo,[39] "...the usual ways of dealing with superspace field theories are highly unsatisfactory from a mathematical point of view. The superspace is defined formally, and, for instance, general coordinate transformations are mathematically not well defined. As a consequence, there is now room for studying global topological properties of superspace." As it shall be tackled further on, Sec. IV, the mathematical structure of the supermanifolds chosen here leads to a natural formulation of superdiffeormorphisms, G^{∞}, from $(\mathcal{M}, g)$ to $(\mathcal{M}', g')$, from the z-continuation of ordinary diffeomorphisms, so that these structures become, projectively, well-defined isometries whenever $\mathcal{M}' = \mathcal{M}$ and restricted to the ordinary body manifold. ■

III. SUPERDISTRIBUTIONS

In this section, as a natural next step, we extend the definition of the objects most widely used in physics: distributions. We define superdistributions on supermanifolds over the Grassmann–Banach algebra $\mathcal{G}_L$, as continuous linear mappings to $\mathcal{G}_L$ from the test function space of G^∞ superfunctions with compact support. We derive some results not contained in Ref. 29.

A. Distributions on a manifold

To prepare for the extension of the theory of distributions to supermanifolds, we first consider their definition on manifolds. Following Ref. 42, the space–time manifold $\mathcal{M}_0$ (here $\mathcal{M}_0$ denotes an ordinary manifold obtained from a supermanifold $\mathcal{M}$ by throwing away all the soul coordinates) is a Hausdorff space covered by charts (X_α, k_α), where the open sets X_α are homeomorphic neighborhoods to open sets in $\mathbb{R}^n$. A C^∞ structure on $\mathcal{M}_0$ is a family $\mathcal{F}=\{(X_\alpha,k_\alpha)|\alpha\in I\}$, called an atlas, of homeomorphisms k_α, called coordinate functions, of open sets $X_\alpha\subset\mathcal{M}_0$ on open sets $\tilde{X}_\alpha\subset\mathbb{R}^n$, such that (i) if $k_\alpha, k_\beta\in\mathcal{F}$, then the map $k_\beta\circ k_\alpha^{-1}: k_\alpha(X_\alpha\cap X_\beta)\to k_\beta(X_\alpha\cap X_\beta)$ is infinitely differentiable, (ii) $\mathcal{M}_0=\cup_{\alpha\in I}X_\alpha$. Let $f\in C_0^\infty(\mathbb{R}^n)$ denotes the set of C^∞ functions of compact support on $\tilde{X}_\alpha\subset\mathbb{R}^n$. Then, we can represent each f by functions $\overline{f}$ of compact support on $\mathcal{M}_0$ by $f=\overline{f}\circ k_\alpha^{-1}$, for each k_α, where $\overline{f}\in C_0^\infty(\mathcal{M}_0)$. Elements of $\mathcal{D}'(\mathcal{M}_0)$, the topological dual of $C_0^\infty(\mathcal{M}_0)$, are distributions u on $\mathcal{M}_0$, by which we mean collections $\{u_{k_\alpha}\}_{k_\alpha\in\mathcal{F}}$ of distributions $u_{k_\alpha}\in\mathcal{D}'(\tilde{X}_\alpha)$ such that u is uniquely determined by the u_{k_α} and relations $u=u_{k_\alpha}\circ k_\alpha$. Moreover, since for any other coordinate system one has $u=u_{k_\beta}\circ k_\beta$ in $(X_\alpha\cap X_\beta)$, it follows that $u_{k_\beta}=(k_\alpha\circ k_\beta^{-1})^* u_{k_\alpha}=u_{k_\alpha}\circ(k_\alpha\circ k_\beta^{-1})$ in $(X_\alpha\cap X_\beta)$.

B. Distributions on the flat superspace

With the purpose of defining superdistributions on supermanifolds, we must first consider superdistributions on an open set $U\subset\mathcal{G}_L^{m,n}$, where $\mathcal{G}_L^{m,n}$ denotes the flat superspace. We begin by introducing the concept of superdistributions as the dual space of supersmooth functions in $\mathcal{G}_L^{m,0}$, with compact support, equipped with an appropriate topology, called *test superfunctions*. This can be done relatively straightforward in analogy to the notion of distributions as the dual space to the space $C_0^\infty(U)$ of functions on an open set $U\subset\mathbb{R}^m$ which have compact support, since the spaces $\mathcal{G}_L^{m,0}$ and $\mathcal{G}_L^{m,n}$ are regarded as ordinary vector spaces of $2^{L-1}(m)$ and $2^{L-1}(m+n)$ dimensions, respectively, over the real numbers.

Let $\Omega\subset\mathbb{R}^m$ be an open set. $\Omega=\epsilon(U)$ regarded as a subset of $\mathcal{G}_L^{m,0}$, it is identified with the body of some domain in superspace. Let $C_0^\infty(\Omega,\mathcal{G}_L)$ be the space of $\mathcal{G}_L$-valued smooth functions with compact support in $\mathcal{G}_L$. Every function $f\in C_0^\infty(\Omega,\mathcal{G}_L)$ can be expanded in terms of the basis elements of $\mathcal{G}_L$ as

$$f(x)=\sum_{(\mu_1,\ldots,\mu_k)\in M_L^0} f_{\mu_1,\ldots,\mu_k}(x)\xi^{\mu_1}\cdots\xi^{\mu_k}, \tag{3.1}$$

where $M_L^0\overset{\text{def}}{=}\{(\mu_1,\ldots,\mu_k)|0\leqslant k\leqslant L;\mu_i\in\mathbb{N};1\leqslant\mu_1<\cdots<\mu_k\leqslant L\}$ and $f_{\mu_1,\ldots,\mu_k}(x)$ is in the space $C_0^\infty(\Omega)$ of real-valued smooth functions on Ω with compact support. Thus, it follows that the space $C_0^\infty(\Omega,\mathcal{G}_L)$ is isomorphic to the space $C_0^\infty(\Omega)\otimes\mathcal{G}_L$.[29] In accordance with definition 2.4, the smooth functions of $C_0^\infty(\Omega,\mathcal{G}_L)$ can be extended from $\Omega\subset\mathbb{R}^m$ to $U\subset\mathcal{G}_L^{m,0}$ by Taylor expansion.

In order to define superdistributions, we need to give a suitable topological structure to the space $G_0^\infty(U,\mathcal{G}_L)$ of $\mathcal{G}_L$-valued superfunctions on an open set $U\subset\mathcal{G}_L^{m,0}$ which have compact support. According to a proposition by Rogers, every G^∞ superfunction on a compact set $U\subset\mathcal{G}_L^{m,0}$ can be considered as a real-valued C^∞ function on $U\subset\mathbb{R}^N$, where $N=2^{L-1}(m)$, regarding $\mathcal{G}_L^{m,0}$ and $\mathcal{G}_L$ as Banach spaces. In fact, the identification of $\mathcal{G}_L^{m,0}$ with $\mathbb{R}^{2^{L-1}(m)}$ is possible.[26] We have here an example of functoriality. Indeed, let X and Y denote a G^∞ supermanifold and a Banach

manifold C^∞, respectively. Then with each supermanifold X we associate a Banach manifold Y, via a *covariant* functorial relation $\lambda: X \to Y$, and with each G^∞ map ϕ defined on X, a C^∞ map $\lambda(\phi)$ defined on Y.[26]

Following, we shall first consider only the subset C_K^∞ of $C_0^\infty(U \subset \mathbb{R}^N)$ which consists of functions with support in a fixed compact set K. Since by construction C_K^∞ is a Banach space, the functions C_K^∞ have a natural topology given by the finite family of norms

$$\|\phi\|_{K,m} = \sup_{\substack{|p| \leq m \\ x \in K}} |D^p \phi(x)| \ , \quad D^p = \frac{\partial^{|p|}}{\partial x_1^{p_1} \cdots \partial x_m^{p_m}}, \tag{3.2}$$

where $p = (p_1, p_2, \ldots, p_m)$ is a m-tuple of non-negative integers, and $|p| = p_1 + p_2 + \cdots + p_m$ defines the order of the derivative. Next, let U be considered as a union of compact sets K_i which form an increasing family $\{K_i\}_{i=1}^\infty$, such that K_i is contained in the interior of K_{i+1}. That such family exist follows from the Lemma 10.1 of Ref. 46. Therefore, we think of $C_0^\infty(U \subset \mathbb{R}^N)$ as $\cup_i C_{K_i}^\infty(U \subset \mathbb{R}^N)$. We take the topology of $C_0^\infty(U \subset \mathbb{R}^N)$ to be given by the strict inductive limit topology of the sequence $\{C_{K_i}^\infty(U \subset \mathbb{R}^N)\}$. Of another way, we may define convergence in $C_0^\infty(U \subset \mathbb{R}^N)$ of a sequence of functions $\{\phi_k\}$ to mean that for each k, one has supp $\phi_k \subset K \subset U \subset \mathbb{R}^N$ such that for a function $\phi \in C_0^\infty(U \subset \mathbb{R}^N)$ we have $\|\phi - \phi_k\|_{K,m} \to 0$ as $k \to \infty$. This notion of convergence generates a topology which makes $C_0^\infty(U \subset \mathbb{R}^N)$, certainly, a topological vector space.

Now, let F and E be spaces of smooth functions with compact support defined on $U \subset \mathcal{G}_L^{m,0}$ and $U \subset \mathbb{R}^N$, respectively. If $\lambda: \mathsf{E} \to \mathsf{F}$ is a *contravariant* functor which associates with each smooth function of compact support in E, a smooth function of compact support in F, then we have a map

$$\|\phi\|_{K,m} \to \|\lambda(\phi)\|_{K,m}, \tag{3.3}$$

providing $G_0^\infty(U, \mathcal{G}_L)$ with a limit topology induced by a finite family of norms.

We now take a result by Jadczyk–Pilch,[33] later refined by Hoyos *et al.*,[34] which establishes as a natural domain of definition for supersmooth functions a set of the form $\epsilon^{-1}(\Omega)$, where Ω is open in $\mathbb{R}^m$. Let $\epsilon^{-1}(\Omega)$ be the domain of definition for a superfunction $f \in G_0^\infty(\epsilon^{-1}(\Omega), \mathcal{G}_L)$, where $\epsilon^{-1}(\Omega)$ is an open subset in $\mathcal{G}_L^{m,0}$ and Ω is an open subset in $\mathbb{R}^m$, and let $\tilde{\phi} \in C_0^\infty(\Omega, \mathcal{G}_L)$ denotes the restriction of ϕ to $\Omega \subset \mathbb{R}^m \subset \mathcal{G}_L^{m,0}$. Then, it follows that $(\partial_1^{p_1} \cdots \partial_m^{p_m} \phi)^{\sim} = \partial_1^{p_1} \cdots \partial_m^{p_m} \tilde{\phi}$, where the derivatives on the right-hand side are with respect to m real variables. Now, suppose $\Omega = \cup_i \tilde{K}_i$ where each $\tilde{K}_i$ is open and has compact closure in $\tilde{K}_{i+1}$. It follows that $C_0^\infty(\Omega, \mathcal{G}_L) = \cup_i C_{\tilde{K}_i}^\infty(\Omega, \mathcal{G}_L)$. Then, one can give $C_0^\infty(\Omega, \mathcal{G}_L)$ a limit topology induced by finite family of norms[29]

$$\|\tilde{\phi}\|_{\tilde{K},m} = \sup_{\substack{|p| \leq m \\ x \in \tilde{K}}} |D^p \tilde{\phi}(x)| = \sup_{\substack{|p| \leq m \\ x \in \tilde{K}}} \left\{ \sum_{(\mu_1, \ldots, \mu_k) \in M_L^0} |D^p \tilde{\phi}_{\mu_1, \ldots, \mu_k}(x)| \right\}. \tag{3.4}$$

Finally, a suitable topological structure to the space $G_0^\infty(U, \mathcal{G}_L)$ of $\mathcal{G}_L$-valued superfunctions on an open set $U \subset \mathcal{G}_L^{m,n}$ which have compact support, it is obtained immediately by the natural identification of $\mathcal{G}_L^{m,n}$ with $\mathbb{R}^{2^{L-1}(m+n)}$ and by the obvious extension of the construction above, which allows us define a limit topology induced to the space $G_0^\infty(U, \mathcal{G}_L)$ by finite family of norms,

$$\|\lambda(\phi)\|_{K,m+n} = \sup_{\substack{|p| \leq m+n \\ z \in K}} |D^p(\lambda(\phi))(z)| \ , \quad D^p = \frac{\partial^{|q|+|r|}}{\partial x_1^{q_1} \cdots \partial x_m^{q_m} \partial \theta_1^{r_1} \cdots \partial \theta_n^{r_n}} \ . \tag{3.5}$$

The derivatives $\partial^{|q|}/\partial x_1^{q_1} \cdots \partial x_m^{q_m}$ commute while the derivatives $\partial^{|r|}/\partial \theta_1^{r_1} \cdots \partial \theta_n^{r_n}$ anticommute, and $|p| = |q| + |r| = \Sigma_{i=1}^m q_i + \Sigma_{j=1}^n r_j$ defines the total order of the derivative, with $r_j = 0,1$.

We are now ready to define a superdistribution in an open subset U of $\mathcal{G}_L^{m,n}$. The set of all superdistributions in U will be denoted by $\mathfrak{D}'(U)$. A superdistribution is a continuous linear functional $u:G_0^\infty(U)\to\mathcal{G}_L$, where $G_0^\infty(U)$ denotes the test superfunction space of $G^\infty(U)$ superfunctions with compact support in $K\subset U$. The continuity of u on $G_0^\infty(U)$ is equivalent to its boundedness on a neighborhood of zero, i.e., the set of numbers $u(\phi)$ is bounded for all $\phi\in G_0^\infty(U)$. The last statement translates directly into:

Proposition 3.1: A superdistribution u in $U\in\mathcal{G}_L^{m,n}$ is a continuous linear functional on $G_0^\infty(U)$ if and only if to every compact set $K\subset U$, there exists a constant C and $(m+n)$ such that

$$|u(\phi)|\leqslant C\sup_{\substack{|p|\leqslant m+n\\ z\in K}}|D^p(\phi)(z)|,\quad \phi\in G_0^\infty(K).$$

Proof: First, it is worth keeping in mind that $\mathcal{G}_L$ can be identified with $\mathbb{R}^{2^{L-1}}$.[26] In fact, a number system assuming values in some Grassmann algebra with L generators is specified by 2^{L-1} real parameters. Let F and E be spaces of smooth functions with compact support defined on $K\subset U\subset\mathcal{G}_L^{m,n}$ and $K\subset U\subset\mathbb{R}^{2^{L-1}(m+n)}$, respectively. If we have a functorial relation $\lambda:\mathsf{F}\to\mathsf{E}$ and a linear functional $\tilde{u}:\mathsf{E}\to\mathbb{R}^{2^{L-1}}$, we can compose λ with $\tilde{u}$ to obtain the pullback of $\tilde{u}$ by λ, i.e., $u=\lambda^*\tilde{u}=\tilde{u}\circ\lambda$, and hence a linear functional $\lambda^*\tilde{u}:\mathsf{F}\to\mathbb{R}^{2^{L-1}}$. Then, the statement follows if $\tilde{u}$ is continuous on E. But this clear from proposition 21.1 of Ref. 46, which can be applied *verbatim* for a functional $\tilde{u}$ on E. □

C. Distributions on a supermanifold

Next we will obtain an extension of basic results about superdistributions on the flat superspace in the case of general supermanifolds.

Definition 3.2: Let $\mathcal{M}$ a G^∞ supermanifold. For every coordinate system $p_i\circ k_\alpha$ in $\mathcal{M}$ one has a distribution $u_{k_\alpha}\in\mathfrak{D}'(\tilde{X}_\alpha)$ where $\tilde{X}_\alpha$ is an open from $\mathcal{G}_L^{m,n}$ such that

$$u_{k_\beta}=\{(p_i\circ k_\alpha)\circ(k_\beta^{-1}\circ p_i^{-1})\}^*u_{k_\alpha},\quad (i=1,\ldots,m+n),\tag{3.6}$$

in $k_\beta(X_\alpha\cap X_\beta)$, where p_i is a projection into each copies (i) from $\mathcal{G}^{m,n}$, such that $x_i=p_i\circ k_\alpha$ and $y_j=p_{j+m}\circ k_\alpha$, with $(i=1,\ldots,m;j=1,\ldots,n)$. We call the system u_{k_α} a distribution u in $\mathcal{M}$. The set of every distribution in $\mathcal{M}$ is denoted by $\mathfrak{D}'(\mathcal{M})$.

Theorem 3.3: *Let $\tilde{X}_\alpha,\alpha\in I$, be an arbitrary family of open sets in $\mathcal{G}_L^{m,n}$, and set $\tilde{X}=\cup_{\alpha\in I}\tilde{X}_\alpha$. If $u_\alpha\in\mathfrak{D}'(\tilde{X}_\alpha)$ and $u_\alpha=u_\beta$ in $(\tilde{X}_\alpha\cap\tilde{X}_\beta)$ for all $\alpha,\beta\in I$, then there exists one and only one $u\in\mathfrak{D}'(\tilde{X})$ such that u_α is the restriction of u to $\tilde{X}_\alpha$ for every α.*

To prove this theorem, it is interesting to state the following results:

Lemma 3.4: Let $\tilde{X}_1,\ldots,\tilde{X}_k$ be open sets in $\mathcal{G}_L^{m,n}$ and let $\phi\in G_0^\infty(\cup_1^k\tilde{X}_\alpha)$. Then one can find $\phi_\alpha\in G_0^\infty(\tilde{X}_\alpha),\alpha=1,\ldots,k$, such that $\phi=\Sigma_1^k\phi_\alpha$ and if $\phi\geqslant 0$ can take all $\phi_\alpha\geqslant 0$.

Proof: We can choose compact sets $K_1,\ldots,K_k$ with $K_\alpha\subset\tilde{X}_\alpha$, so that the supp $\phi\subset\cup_1^k K_\alpha$. Every point in supp ϕ has a compact neighborhood contained in some $\tilde{X}_\alpha$, a finite number of such neighborhoods can be chosen which cover all of supp ϕ. The union of those which belong to X_α is a compact set $K_\alpha\subset\tilde{X}_\alpha$. Now, if $\tilde{X}$ is an open set in $\mathcal{G}_L^{m,n}$ and K is a compact subset, then one can find $\phi\in G_0^\infty(\tilde{X})$ with $0\leqslant\phi\leqslant 1$ so that $\phi=1$ in a neighborhood of K. So, we can choose $\psi_\alpha\in G_0^\infty(\tilde{X}_\alpha)$ with $0\leqslant\psi_\alpha\leqslant 1$ and $\psi_\alpha=1$ in K_α, then the functions

$$\phi_1=\phi\psi_1,\phi_2=\phi\psi_2(1-\psi_1),\ldots,\phi_k=\phi\psi_k(1-\psi_1)\cdots(1-\psi_{k-1})$$

have the required properties since

$$\sum_1^k \phi_\alpha - \phi = -\phi \prod_1^k (1-\psi_\alpha) = 0,$$

because either ϕ or some $1-\psi_\alpha$ is zero at any point. □

Corollary 3.5: Let $\tilde{X}_1,\ldots,\tilde{X}_k$ be open sets in $\mathcal{G}_L^{m,n}$ and K a compact subset $\subset \tilde{X}_\alpha$. Then one can find $\phi_\alpha \in G_0^\infty(\tilde{X}_\alpha)$ so that $\phi_\alpha \geqslant 0$ and $\Sigma_1^k \phi_\alpha \leqslant 1$ with equality in a neighborhood of K. □

Proof of the Theorem 3.3: If u is a distribution, then

$$u(\phi) = \sum u_\alpha(\phi_\alpha), \quad \text{if} \quad \phi = \sum \phi_\alpha \quad (\text{where } \phi_\alpha \in G_0^\infty(\tilde{X}_\alpha)),$$

and the sum is finite. By the Lemma 3.4, every $\phi \in G_0^\infty(\tilde{X})$ can be written as such a sum. If $\Sigma \phi_\alpha = 0 \Rightarrow \Sigma u_\alpha(\phi_\alpha) = 0$, then we conclude that $\Sigma u_\alpha(\phi_\alpha)$ is independent of how we choose the sum. Let $K = \cup \operatorname{supp} \phi$ compact set $K \subset \tilde{X}$ and using the corollary 3.5, we can choose $\psi_\beta \in G_0^\infty(\tilde{X}_\beta)$ such that $\Sigma \psi_\beta = 1$ in K and the sum is finite. Then $\psi_\beta \phi_\alpha \in G_0^\infty(\tilde{X}_\alpha \cap \tilde{X}_\beta)$ so $u_\alpha(\psi_\beta \phi_\alpha) = u_\beta(\psi_\beta \phi_\alpha)$. Hence

$$\sum u_\alpha(\phi_\alpha) = \sum \sum u_\alpha(\phi_\alpha \psi_\beta) = \sum \sum u_\beta(\phi_\alpha \psi_\beta) = \sum u_\beta\left(\psi_\beta \sum \phi_\alpha\right) = 0.$$

We have shown that if $\Sigma \phi_\alpha = 0 \Rightarrow \Sigma u_\alpha(\phi_\alpha)$ is zero, then u is unique. In order to show that u is distribution, choose a compact set $K \subset \tilde{X}$ and a function $\psi_\beta \in G_0^\infty(\tilde{X}_\beta)$ with $\Sigma \psi_\beta = 1$ in K and finite sum. If $\phi \in G_0^\infty(K)$ we have $\phi = \Sigma \phi \psi_\beta$ with $\phi \psi_\beta \in G_0^\infty(\tilde{X}_\beta)$ so that the first equation this proof gives

$$u(\phi) = \sum u_\beta(\phi \psi_\beta),$$

but, if u_β is a distribution, then

$$|u_\beta(\phi \psi_\beta)| \leqslant C \sup_{\substack{|p| \leqslant m+n \\ z \in K}} |D^p(\phi \psi_\beta)(z)|, \quad \phi \psi_\beta \in G_0^\infty(\tilde{X}_\beta),$$

where $\sup D^p \phi$ can be estimated in terms of ϕ, and so we conclude that

$$|u(\phi)| \leqslant C \sup_{\substack{|p| \leqslant m+n \\ z \in K}} |D^p \phi(z)|, \quad \phi \in G_0^\infty(K).$$

This completes our proof. □

Theorem 3.6: *Let $\mathcal{F}$ be an atlas for $\mathcal{M}$. If for every $p_i \circ k \in \mathcal{F}$ one has a distribution $u_k \in \mathfrak{D}'(\tilde{X}_k)$ and the above definition is true when $p_i \circ k$ and $p_i' \circ k'$ belongs to $\mathcal{F}$, then there is one, and only one, distribution $u \in \mathfrak{D}'(\mathcal{M})$ such that $u \circ (k^{-1} \circ p_i^{-1}) = u_k$ for every $p_i \circ k \in \mathcal{F}$.*

Proof: Let $\psi \in G^\infty$ be a coordinate system in $\mathcal{M}$. Theorem 3.3 states that there exists one, and only one, distribution $U_\psi \in \mathfrak{D}'(\tilde{X}_\psi)$ in such a way for every $p_i \circ k$, $U_\psi = ((p_i \circ k) \circ \psi^{-1})^* u_k$ in $\psi(X_\psi \cap X_k) \subset \tilde{X}_\psi$. If $\psi \in \mathcal{F} \rightarrow U_\psi = u_\psi$, we can choose $p_i \circ k = \psi$. Now, one defines u as a distribution, since U_ψ satisfies (3.6) for both coordinate systems $p_i \circ k$ and $p_i' \circ k'$. □

IV. ALGEBRAIC FRAMEWORK ON A SUPERMANIFOLD

In the usual treatment of quantum field theory in flat spacetime, the existence of a unitary representation of the restricted Poincaré group, $\mathcal{P}_+^\uparrow$, with generators P_μ fulfilling the spectral condition $\mathrm{sp} P_\mu \subset \overline{V}_+$, is very essential. This unitary operator plays a key role in picking out a preferred vacuum state, i.e., a state which is invariant under all translations. We choose a complete

system of physical states, with positive energies, just when it is possible to define this vacuum state and consequently the Fock space, $\mathcal{F}$. One then defines observables as operators on $\mathcal{F}$ which act upon the states. However, the characterization of the vacuum involves global aspects, and in the case of a curved space–time it is not evident how to select a distinguished state. As already mentioned in the Introduction, due the absence of a *global* Poincaré group there is no analogous selection criterium on a curved spacetime: no vacuum state can be used as reference. To understand the significance of this point under another point of view, we take into account that, initially, a theory defined on a globally hyperbolic Lorentz manifold could be reduced to the tangent space at a given point, one neglecting the gravitational effects. One finds that the tangent space theory reduces to a free quantum field theory in a Minkowski space which has local translation invariance and a distinguished invariant state could be established by a *local* unitary mapping. Nevertheless, this unitary operator depends on the region and there exists no unitary operator which does the mapping for all open regions simultaneously. Therefore, the problem of how to characterize the physical states arises. For the discussion of this problem on a general manifold, the setting of the so-called algebraic approach to quantum field theory (see Refs. 6, 7, 47) is particularly appropriate, because it treats all states on equal footing, especially the states arising of unitarily inequivalent representations.

The algebraic approach envolves the theory of $*$-algebras and their states and Hilbert space representations. In this framework the basic objects are the algebras generated by observables localized in a given spacetime region. Fields are not mentioned in this setting and are regarded as a type of coordinates of the algebras. The basic assumption is that *all physical* information must already be encoded in the structure of the local observables. Haag and Kastler introduced a mathematical structure for the set of observables of a physical system by proposing the now so-called Haag–Kastler axioms[30] for nets of C^* algebras, later generalized by Dimock[31] for local observables to globally hyperbolic manifolds. Recently, a new approach to the model independent description of quantum field theories has been introduced by Brunetti–Fredenhagen–Verch,[48] which incorporates in a local sense the principle of general covariance of general relativity, thus giving rise to the concept of a locally covariant quantum field theory. The usual Haag–Kastler–Dimock framework can be regained from this new approach as a special case.

In this section, we intend to discuss the algebraic formalism so as to include supersymmetry on a supermanifold. A straight formulation on a supermanifold can be performed over the algebraic approach easily, since the construction of the algebra *does not depend "a priori" of the manifold*. Let us describe a physical theory in a general supermanifold from an extended formulation of the ordinary theory in curved space–time. An observable algebra can be generated from $\Phi_{sd}(f_{sf})$, where Φ_{sd} are superdistributions (superfields) and f_{sf} test superfunctions. A complete superalgebra, like above, is represented by $\mathfrak{A}_{sa}=\overline{\cup_{\mathcal{O}}\mathfrak{A}_{sa}(\mathcal{O})}$, where $\mathfrak{A}_{sa}$ denotes the superalgebra, with $\mathcal{O}\subset\mathcal{M}$ denoting a bounded open region on a supermanifold $\mathcal{M}$. We shall assume we have assigned to every bounded open region $\mathcal{O}$ in $\mathcal{M}$ the following properties:

(P.1) All $\mathfrak{A}_{sa}(\mathcal{O})$ are $*$-superalgebras containing a common unit element, where it is assumed that the following condition of isotony holds:

$$\mathcal{O}_1\subset\mathcal{O}_2\Rightarrow\mathfrak{A}_{sa}(\mathcal{O}_1)\hookrightarrow\mathfrak{A}_{sa}(\mathcal{O}_2).$$

This condition expresses the fact that the set, which we call in an improper way, of supersymmetric ''observables'' increases with the size of the localization region. (Certainly the set of physically interesting observables are obtained taking the body.)

(P.2) We define the essential notion of locality so that the restriction of a compact region $\mathcal{O}\in\mathcal{M}$ to a compact region of the body of the supermanifold, $\mathcal{O}_{\mathbf{b}}\in\mathcal{M}_0$, is causally separated from another compact region $\mathcal{O}'_{\mathbf{b}}\in\mathcal{M}_0$. This implies in the spacelike commutativity, $[\mathfrak{A}_{sa}(\mathcal{O}),\mathfrak{A}_{sa}(\mathcal{O}')]=0$. We see that this requirement is important, because only with this restriction we can work with causality: the notion of a suitable proper time curve which intersects the Cauchy surface in a global hyperbolic spacetime makes sense only on the body manifold. So, there we can establish an evolution of Cauchy surfaces to give us a criterion to

define a Hadamard form to the vacuum state. A superdistribution on a supermanifold as a two-point function shows us that the causality is well-defined in this context. Therefore, we now state: if $\mathcal{O}_{\mathbf{b}}$ is causally dependent on $\mathcal{O}'_{\mathbf{b}}$, then $\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})\subset\mathfrak{A}_{\mathrm{sa}}(\mathcal{O}')$.

(P.3) Following Dimock,[31] we require that there be an $\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})$ for each supermanifold $\mathcal{M}$ equipped with some supermetric g, which generalizes the Lorentz metric, in a diffeomorphic class. Let $k:\mathcal{M}_0\to\mathcal{M}'_0$ be a C^∞ diffeomorphism on the body manifold, such that $k^*(g'_0)=g_0$, where g_0 is a metric of signature $(+,-,-,-)$ of the body manifold. Then $z(k):\mathcal{M}\to\mathcal{M}'$ is a G^∞ superdiffeomorphism $z(k)$ from $(\mathcal{M},g)$ to $(\mathcal{M}',g')$ such that $z(k)^*(g')=g$, and there is an isomorphism $\alpha_{z(k)}:\mathfrak{A}_{\mathrm{sa}}\to\hat{\mathfrak{A}}_{\mathrm{sa}}$ such that $\alpha_{z(k)}[\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})]=\hat{\mathfrak{A}}_{\mathrm{sa}}(z(k)(\mathcal{O}))$. One can also show that $z(\mathrm{id}_{\mathcal{M}_0})=\mathrm{id}_{\mathcal{M}}$, where $\mathrm{id}_{\mathcal{M}_0}(\mathrm{id}_{\mathcal{M}})$ are the identity functions on $\mathcal{M}_0(\mathcal{M})$, respectively. Hence, $\alpha_{z(\mathrm{id}_{\mathcal{M}_0})}=\alpha_{(\mathrm{id}_{\mathcal{M}})}$ and, by Eq. (2.7), we have $\alpha_{z(k_1)}\circ\alpha_{z(k_2)}=\alpha_{z(k_1\circ k_2)}$.

It is interesting, in a particular way, to choose a suitable $*$-algebra for a formulation of quantum fields in connection to the Gårding–Wightman approach.[49] In quantum field theory, it is natural to work with tensor product over test functions, since is usual the presence of more than one field. Therefore, we introduce a tensor algebra of smooth superfunctions of compact support over $\mathcal{O}\in\mathcal{M}$, where $\mathcal{O}$ is an open region in a supermanifold. Let f_m be a test superfunction in $\mathfrak{D}_m(\mathcal{O})$, so that $F=\oplus_{m\in\mathbb{N}}f_m(z_1,\ldots,z_m)\in\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})$, where here $z_i=(x_i,\theta_i,\overline{\theta_i})$ denotes the supercoordinates. In a same way we take $\omega_m(z_1,\ldots,z_m)\in\mathfrak{D}'_m(\mathcal{O})$, here $\mathfrak{D}'_m$ is the dual space of $\mathfrak{D}_m$ consisting of m-point superdistributions $\omega=\{\omega_m\}_{m\in\mathbb{N}}$, such that ω_m belongs to the dual algebra denoted by $\mathfrak{A}'_{\mathrm{sa}}(\mathcal{O})$. As we are working on involutive superalgebras, let us define the operation of involution $(*)$ by $f_m^*(z_1,\ldots,z_m)=\overline{f_m(z_m,\ldots,z_1)}$, where $f_m^*=\overline{f_m}$ denotes the complex conjugation.

A superstate ω in this class of algebra is a normalized positive linear functional $\omega:\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})\to\mathcal{G}_L$, with $\omega(F^*F)\geqslant 0$ for all $F\in\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})$. The normalization means that $\omega^0=1$. This net of algebra is the Borchers–Uhlmann one.[50] Such an algebra does not contain any specific dynamical information, which can be obtained by specifying a vacuum state on it. Once the vacuum state has been specified, through the GNS construction which fixes a Hilbert superspace and a vacuum vector, one can extract from the corresponding time-ordered, advanced or retarded superfunctions the desired information.

A superstate is said to satisfy the essential property of *local commutativity* if and only if for all $m\geqslant 2$ and all $1\leqslant i\leqslant m-1$ we have

$$\omega_m(f_1\otimes\cdots\otimes f_i\otimes f_{i+1}\otimes\cdots\otimes f_m)=\omega_m(f_1\otimes\cdots\otimes f_{i+1}\otimes f_i\otimes\cdots\otimes f_m),$$

for all $f_i\in G_0^\infty(\mathcal{O})$, such that the restriction of each f_i on compact regions of the body of supermanifold implies that the supp $f_i|_{\mathcal{O}_{\mathbf{b}}}$ and supp $f_{i+1}|_{\mathcal{O}_{\mathbf{b}}}$ are spacelike separated. Furthermore, a superstate ω is ''quasifree'' if the one-point superdistribution and all the truncated m-point superdistributions for $m\neq 2$ vanish, i.e., all m-point superdistributions are obtained from the two-point superdistribution via relation:

$$\omega_{2m+1}(f_1\otimes\cdots\otimes f_m)=0\quad\text{for } m\geqslant 0,$$

$$\omega_{2m}(f_1\otimes\cdots\otimes f_m)=\sum_{\substack{i_1<\cdots<i_{2m}\\ i_k<j_k\\ i_1,\ldots,j_{2m}\ \text{distinct}}}\omega_2(f_{i_1}\otimes f_{j_1})\omega_2(f_{i_2}\otimes f_{j_2})\cdots\omega_2(f_{i_{2m}}\otimes f_{j_{2m}}),$$

for $m\geqslant 1$.

It is a well-known result that the physical model can be described by the GNS construction, showing us how the Hilbert space is constructed and defining what are the operators (just the algebra representation) acting in this space. According to conventional prescription, for getting the

Hilbert space we choose the quotient between the observable algebra and the ideal $\mathcal{N}_\omega$ (to guarantee the scalar product existence). In this stage the problem of several inequivalent representation persists. In flat superspaces, the super-Poincaré invariance of the vacuum state picks out the correct representation.[51] In general supermanifolds the case is more delicated; we will look for (super)Hadamard structures. This is motivated by the ordinary general manifold case. At last, we choose an acceptable Hilbert superspace from the algebraic properties via GNS construction by the following identification:

$$\omega_m(f_1\otimes\cdots\otimes f_m)=\langle\Omega_\omega,\pi_\omega(f_1)\cdots\pi_\omega(f_m)\Omega_\omega\rangle,$$

where here Ω_ω is a distinguished vector in Hilbert superspace, and π_ω is the representation of the elements $F\in\mathfrak{A}_{\mathrm{sa}}(\mathcal{O})$ which play the role of self-adjoint linear operator acting in the Hilbert superspace over test superfunctions. In addition, we use the physical requirements on the body manifold in order to define whole set of superstates which are supposed to be distinguished by a certain generalized form of the spectral condition.[11]

Remark 4.1: The main features of Hilbert superspaces relevant for our purposes are summarized as follows: (i) when the Grassmann algebra $\mathcal{G}_L$ is endowed with the Rogers norm, every Hilbert superspace is of the form $\mathscr{H}=\mathcal{H}\otimes\mathcal{G}_L$, where $\mathcal{H}$ is an ordinary Hilbert space (the existence of such a subspace $\mathcal{H}$ of $\mathscr{H}$ called a base Hilbert space is important in physical applications[52]), (ii) the $\mathcal{G}_L$-valued inner product $\langle\cdot,\cdot\rangle:\mathscr{H}\times\mathscr{H}\to\mathcal{G}_L$ respects the body operation $\langle x_{\mathbf{b}},y_{\mathbf{b}}\rangle=\langle x,y\rangle_{\mathbf{b}}$ and $\langle x,x\rangle_{\mathbf{b}}\geqslant 0$ for all $\in\mathscr{H}$, so that $x\in\mathscr{H}$ has nonvanishing body if and only if $\langle x,x\rangle_{\mathbf{b}}>0$. For generalizations of some basic results of the theory of Hilbert space to Hilbert superspaces we refer to the recent paper,[41] and references therein. ■

V. HADAMARD (SUPER)STATES

As already emphasized, the Hadamard state condition provides a framework in which we may improve our understanding to the problem concerning the determination of physically acceptable states. The motivation for which we adopt the Hadamard structure of the vacuum state in curved space–time quantum field theory is quite simple. In general, as we lost the possibility of picking out a good representation for the model due the fact that now we have no more an invariant structure over the action of an isometry group (in the flat case, the global Poincaré group), we must get another condition to choose. Since we are able to describe some aspects of a manifold observing the evolution of the Cauchy surface (CS) coming from an asymptotic flat space, a new kind of invariance becomes natural, and this invariance arises from the preservation of some particular structure while the CS geometry is changing in determinated manifolds.

In particular, for states whose expectation values of the energy-momentum tensor operator can be defined by using the point separation prescription for renormalization, Fulling *et al.*[53] showed that if such states have a singularity structure of the Hadamard form in an open neighborhood of a Cauchy surface, then they have their forms preservated independently of the Cauchy evolution. In this case, the states are said to have the Hadamard form if they can be expressed as

$$\Delta_{\mathrm{Had}}(x_1,x_2)=\frac{U(x_1,x_2)}{\sigma(x_1,x_2)}+V(x_1,x_2)\ \ln|\sigma(x_1,x_2)|+W(x_1,x_2),$$

where $\sigma(x_1,x_2)$ is one-half of the square of the geodesic distance between x_1 to x_2. In flat space–time or in the $x_1\to x_2$ limit in curved space–time, $\sigma=\frac{1}{2}(x_1-x_2)^2$. It is clear that this sing supp $\Delta_{\mathrm{Had}}=\{(x_1,x_2)|\sigma=\frac{1}{2}(x_1-x_2)^2=0\}$ (we recall that the singular support of a distribution $u\in\mathcal{D}'(X)$ is the smallest closed subset Y of X such that $u|_{X\setminus Y}$ is of class C^∞). U, V, and W are regular functions for all choices of x_1 and x_2. The functions U and V are geometrical quantities independent of the quantum state, and only W carries information about the state. Therefore, for free quantum field models in ordinary globally hyperbolic manifolds, the Hadamard form plays an important role: it is a strong candidate to describe an acceptable physical representation.

The search for the Hadamard form in the superspace case is simple, since the latter is, in general, obtainable by applying the function $\delta^2(\overline{\theta}-\overline{\theta'})$ (or $\delta^2(\theta-\theta')$) and an exponential structure $e^{E(\partial_x,\theta,\overline{\theta})}$ to the ordinary Hadamard form Δ_{Had} (see proposition 7.3 below and Refs. 54, 55 for details), such that the *singularity structure region is not affected*, i.e., it has a short distance behavior analogous to the short distance behavior discussed in the case of a general spacetime manifold.[56] This issue is recaptured in Sec. VI. Since we can deal with a supermanifold which has a body manifold being a globally hyperbolic one (to guarantee this we just report to the construction of Bonora–Pasti–Tonin[28]), it is important to establish that only *projectively* super-Hadamard structures make sense. The obvious explanation for this statement is that the structure must cover the global time notion, and consequently the argument of causality, but over a supermanifold the notion of causal curves are not well defined unless projectively. The tool to extend the Hadamard structure to the supersymmetric environment arises from the fact that the existence and uniqueness of the Grassmannian continuation (z-continuation) for C^∞ functions is checked. By a body projection, we always get the ordinary Hadamard structure such that the latter must be invariant by CS evolution on the body manifold. This is a consistent result, since we will show in the next section, through an alternative and equivalent characterization of the Hadamard condition due Radzikowski[8] which involves the notion of the wavefront set of a superdistribution, that the structure of singularity is not changed and is condensed in the ordinary region of any Green superfunction, corroborating to the fact that only on the body of a supermanifold the causality makes sense.

VI. MICROLOCAL ANALYSIS IN SUPERSPACE

Important progress in understanding the significance of the Hadamard form relates it to Hörmander's concept of wavefront sets and microlocal analysis,[8] in a particular way by the wavefront set of their two-point functions. It satisfies the Hadamard condition if its wavefront set contains only positive frequencies propagating forward in time and negative frequencies backward in time.

The focus in this section will be on the extension of the Hörmander's description of the singularity structure (wavefront set) of a distribution to include the supersymmetric case. The well-known result that the singularities of a superdistribution may be expressed in a very simple way through the ordinary distribution is proved by functional analytical methods, in particular the methods of microlocal analysis formulated in superspace language.

A. Standard facts on microlocal analysis

The study of singularities of solutions of differential equations is simplified and the results are improved by taking what is now known as microlocal analysis. This leads to the definition of the wavefront set, denoted (WF), of a distribution, a refined description of the singularity spectrum. A similar notion was developed in other versions by Sato,[57] Iagolnitzer,[58] and Sjöstrand.[59] The definition, as known nowadays, is due to Hörmander. He used this terminology due to an existing analogy between his studies on the ''propagation'' of singularities and the classical construction of propagating waves by Huyghens.

The key point of the microlocal analysis is the transference of the study of singularities of distributions from the configuration space only to the rather phase space, by exploring in frequency space the decay properties of a distribution at infinity and the smoothness properties of its Fourier transform. For a distribution u we introduce its wavefront set $\mathrm{WF}(u)$ as a subset in phase space $\mathbb{R}^n\times\mathbb{R}^n$. The functorially correct definition of phase space is $\mathbb{R}^n\times(\mathbb{R}^n)^*$. We shall here ignore any attempt to distinguish between $\mathbb{R}^n$ and $(\mathbb{R}^n)^*$. We shall be thinking of points (x,k) in phase space as specifying those singular directions k of a ''bad'' behavior of the Fourier transform $\hat{u}$ at infinity that are responsible for the nonsmoothness of u at the point x in position space. So we shall usually want $k\neq 0$. A relevant point is that $\mathrm{WF}(u)$ is independent of the coordinate system chosen, and it can be described locally.

As it is well-known,[42,60] a distribution of compact support, $u \in \mathcal{E}'(\mathbb{R}^n)$, is a smooth function if, and only if, its Fourier transform, $\hat{u}$, rapidly decreases at infinity (i.e., as long as supp u does not touch the singularity points). By a fast decay at infinity, one must understand that for all positive integer N exists a constant C_N, which depends on N, such that

$$|\hat{u}(k)| \leqslant (1+|k|)^{-N} C_N, \quad \forall\, N \in \mathbb{N};\ k \in \mathbb{R}^n. \tag{6.1}$$

If, however, $u \in \mathcal{E}'(\mathbb{R}^n)$ is not smooth, then the directions along which $\hat{u}$ does not fall off sufficiently fast may be adopted to characterize the singularities of u.

For distributions does not necessarily of compact support, still we can verify if its Fourier transform rapidly decreases in a given region V through the technique of localization. More precisely, if $V \subset X \subset \mathbb{R}^n$ and $u \in \mathcal{D}'(X)$, we can restrict u to a distribution $u|_V$ in V by setting $u|_V(\phi) = u(\phi)$, where ϕ is a smooth function with support contained in a region V, with $\phi(x) \neq 0$, for all $x \in V$. The distribution ϕu can then be seen as a distribution of compact support on $\mathbb{R}^n$. Its Fourier transform will be defined as a distribution on $\mathbb{R}^n$, and must satisfy, in absence of singularities in $V \in \mathbb{R}^n$, the property (6.1). From this point of view, all development is local in the sense that only the behavior of the distribution on the arbitrarily small neighborhood of the singular point, in the configuration space, is relevant.

Let $u \in \mathcal{D}'(\mathbb{R}^n)$ be a distribution and $\phi \in C_0^\infty(V)$ a smooth function with support $V \subset \mathbb{R}^n$. Then, ϕu has compact support. The Fourier transform of ϕu produces a smooth function in frequency space.

Lemma 6.1: Consider $u \in \mathcal{D}'(\mathbb{R}^n)$ and $\phi \in C_0^\infty(V)$. Then $\widehat{\phi u}(k) = u(\phi e^{-ikx})$. Moreover, the restriction of u to $V \subset \mathbb{R}^n$ is smooth on V if, and only if, for every $\phi \in C_0^\infty(V)$ and each positive integer N there exists a constant $C(\phi, N)$, which depends on N and ϕ, such that $|\widehat{\phi u}(k)| \leqslant (1+|k|)^{-N} C(\phi, N)$, for all $N \in \mathbb{N}$ and $k \in \mathbb{R}^n$. □

If $u \in \mathcal{D}'(\mathbb{R}^n)$ is singular in x, and $\phi \in C_0^\infty(V)$ is $\phi(x) \neq 0$; then ϕu is also singular in x and has compact support. However, in some directions in k-space $\widehat{\phi u}$ until will be asymptotically limited. This is called the set of *regular directions* of u.

Definition 6.2: Let $u(x)$ be an arbitrary distribution, not necessarily of compact support, on an open set $X \subset \mathbb{R}^n$. Then, the set of pairs composed by singular points x in configuration space and by its associated nonzero singular directions k in Fourier space

$$\mathrm{WF}(u) = \{(x,k) \in X \times (\mathbb{R}^n \backslash 0) \,|\, k \in \Sigma_x(u)\}, \tag{6.2}$$

is called **wavefront set** *of u. $\Sigma_x(u)$ is defined to be the complement in $\mathbb{R}^n \backslash 0$ of the set of all $k \in \mathbb{R}^n \backslash 0$ for which there is an open conic neighborhood M of k such that $\widehat{\phi u}$ rapidly decreases in M, for $|k| \to \infty$.*

Remarks 6.1: We will now collect some basic properties of the wavefront set:

(1) The $\mathrm{WF}(u)$ is conic in the sense that it remains invariant under the action of dilatations, i.e., when we multiply the second variable by a positive scalar. This means that if $(x,k) \in \mathrm{WF}(u)$ then $(x, \lambda k) \in \mathrm{WF}(u)$ for all $\lambda > 0$.
(2) From the definition of $\mathrm{WF}(u)$, it follows that the projection onto the first variable, $\pi_1(\mathrm{WF}(u)) \to x$, consists of those points that have no neighborhood wherein u is a smooth function, and the projection onto the second variable, $\pi_2(\mathrm{WF}(u)) \to \Sigma_x(u)$, is the cone around k attached to a such point denoting the set of high-frequency directions responsible for the appearance of a singularity at this point.
(3) The wavefront set of a smooth function is the empty set.
(4) For all smooth function ϕ with compact support $\mathrm{WF}(\phi u) \subset \mathrm{WF}(u)$.
(5) For any partial linear differential operator P, with C^∞ coefficients, we have
$$\mathrm{WF}(Pu) \subseteq \mathrm{WF}(u)\ .$$
(6) If u and v are two distributions belonging to $\mathcal{D}'(\mathbb{R}^n)$, with wavefront sets $\mathrm{WF}(u)$ and $\mathrm{WF}(v)$, respectively; then the wavefront set of $(u+v) \in \mathcal{D}'(\mathbb{R}^n)$ is contained in $\mathrm{WF}(u) \cup \mathrm{WF}(v)$.

(7) If U,V are open set of $\mathbb{R}^n$, $u\in\mathcal{D}'(V)$, and $\chi:U\to V$ a diffeomorphism such that $\chi^*u\in\mathcal{D}'(U)$ is the distribution pulled back by χ, then $\mathrm{WF}(\chi^*u)=\chi^*\mathrm{WF}(u)$. ■

Another result, which we merely state, is needed to complete this briefing on microlocal analysis.

Theorem 6.3 (Wavefront set of pushforwards of a distribution): *Let $f:X\to Y$ be a submersion, and let $u\in\mathcal{E}'(X)$. Then*

$$\mathrm{WF}(f_*u)\subset\{(f(x),\eta)|x\in X,(x,{}^tf'_x\eta)\in\mathrm{WF}(u)\ \text{or}\ {}^tf'_x\eta=0\},$$

where ${}^tf'_x$ denotes the transpose matrix of the Jacobian matrix f'_x of f. □

B. Wavefront set of a superdistribution

It is already well-known that the singularity structure of Feynman (or more precisely Wightman) superfunctions is completely associated with the ''bosonic'' sector of the superspace. Although claims exist that the result is completely obvious, we do not think that a clear proof is available in the literature, to the best of our knowledge. In fact, there is a certain gap in the scientific literature between the usual textbook presentation of the singularity structure of superfunctions and the very mathematical treatement based on microlocal analysis. The purpose of the present subsection is to fill this gap. As expected, our result confirms that the decay properties of an ordinary distribution hold also to the case of a superdistribution, i.e., no new singularity appear by taking into account the structure of the superspace.

Lemma 6.4: Let $X\subset\mathcal{G}_L^{m,0}$ be an open set, and u be a superdistribution on X taking values in $\mathcal{G}_L$, i.e., a linear functional $u:G_0^\infty(X)\to\mathcal{G}_L$. Let ϕ be a supersmooth function with compact support $K\subset X$. Then ϕu is also supersmooth on K, if its components $(\phi u)(\epsilon(x))$ are smooth on a compact set $K'\subset\Omega$, where Ω is the body of superspace. Therefore, the following estimate holds:

$$|\widehat{\phi u}(k)|\leqslant(1+|k_{\mathbf{b}}|)^{-N}C(N,\phi)\ .$$

Indication of Proof: A schematic proof may be constructed along the lines suggested by DeWitt:[32] from definition 2.4 follows that functions of x are in one-to-one correspondence with functions of $x_{\mathbf{b}}$; this implies that in working with integrals over $\mathcal{G}_L^{m,0}$ one may for many purposes proceed as if one were working over the body of superspace, $\Omega=\{(x,0,0)\in X|\epsilon(x)\in\mathbb{R}^m\}$. Because $\phi u(x)$ vanishes at infinity, independently of their souls, the contour in $\mathcal{G}_{L,0}^m$ may be displaced to coincide with Ω, without affecting the value of the integral. So, the theory of the Fourier transforms remains unchanged in form. For the sake of simplicity, we take the case for which $s(x)=(x-\epsilon(x))$ is a smooth singled-valued function of $\epsilon(x)=x_{\mathbf{b}}$ and $L=2$ is the number of generators of $\mathcal{G}_2^{1,0}$. This implies

$$\begin{aligned}\widehat{\phi u}(k)&=\int dx\ e^{ikx}\phi u(x)\\&=\int dx_{\mathbf{b}}\ e^{ik_{\mathbf{b}}x_{\mathbf{b}}}(\phi u(x_{\mathbf{b}})+i\,x_{\mathbf{b}}\phi u(x_{\mathbf{b}})k_{ij}\xi^i\xi^j)\\&=\widehat{\phi u}(k_{\mathbf{b}})+(\widehat{\phi u})'(k_{\mathbf{b}})k_{ij}\xi^i\xi^j\ .\end{aligned}$$

The proof follows one making use of repeated integrations-by-parts generalizing the fact $-i\,k_{\mathbf{b}}^{-1}(d/dx_{\mathbf{b}}\,e^{ik_{\mathbf{b}}x_{\mathbf{b}}})=e^{ik_{\mathbf{b}}x_{\mathbf{b}}}$,

$$\widehat{\phi u}(k)=\frac{(i)^{|\beta|}}{k_{\mathbf{b}}^\beta}\left\{\int dx_{\mathbf{b}}\ e^{-ik_{\mathbf{b}}x_{\mathbf{b}}}(D^\beta_{x_{\mathbf{b}}}(\phi u(x_{\mathbf{b}}))+D^\beta_{x_{\mathbf{b}}}(x_{\mathbf{b}}\phi u(x_{\mathbf{b}}))k_{ij}\xi^i\xi^j)\right\}.$$

Taking the absolute value of both sides and using the Banach algebra property of $\mathcal{G}_L$, we get the estimate

$$|\widehat{\phi u}(k)| \leqslant |\widehat{\phi u}(k_{\mathbf{b}})| + |(\widehat{\phi u})'(k_{\mathbf{b}})||k_{ij}|$$
$$\leqslant (1+|k_{\mathbf{b}}|)^{-|\beta|}\left(\sup_{\substack{|\beta|\leqslant m \\ x_{\mathbf{b}}\in K'}} |D^{\beta}_{x_{\mathbf{b}}}(\phi u(x_{\mathbf{b}}))| + \sup_{\substack{|\beta|\leqslant m \\ x_{\mathbf{b}}\in K'}} |D^{\beta}_{x_{\mathbf{b}}}(x_{\mathbf{b}}\phi u(x_{\mathbf{b}}))||k_{ij}| \right). \quad (6.3)$$

This inequality clearly implies our assertion. Hence, in order that (6.3) be smooth, we only need that $\widehat{\phi u}(k)$ be rapidly decreasing as $|k_{\mathbf{b}}|\to\infty$. The proof may be generalized to include the case in which $s(x)$ is a multivalued function of the body and L is finite arbitrarily. We finish the proof by observing that as expected the soul part of k has a polynomial behavior. □

Lemma 6.5: By replacing $\mathcal{G}_L^{m,0}$ by $\mathcal{G}_L^{m,n}$ in the Lemma 6.4, then in this case the following estimate holds:

$$|\widehat{\phi u}(k,\theta,\overline{\theta})| \leqslant (1+|k_{\mathbf{b}}|)^{-N} C(N,\phi_{(\gamma)})\|\theta_1\|\|\overline{\theta}_1\|\cdots\|\theta_n\|\|\overline{\theta}_n\| \ .$$

Proof: First, we note that both u and ϕ are G^{∞} superfunctions which can be expanded as a polinomial in the odd coordinates whose coefficients are functions defined over the even coordinates,

$$u(x,\theta,\overline{\theta}) = \sum_{(\gamma)=0}^{\Gamma} z(u_{(\gamma)})(x)(\theta)^{(\gamma)} \quad \text{and} \quad \phi(x,\theta,\overline{\theta}) = \sum_{(\gamma)=0}^{\Gamma} z(\phi_{(\gamma)})(x)(\theta)^{(\gamma)} \ .$$

Then, the proof follows essentially by similar arguments to the proof of the previous lemma, taking into account the polinomial behavior of odd variables, θ and $\overline{\theta}$. In fact, $\phi u(x,\theta,\overline{\theta})$ is *linear* function in each odd coordinates separately, because each odd coordinate is nilpotent, and no higher power of a odd coordinate can appear, i.e., $\phi u(x,\theta,\overline{\theta})$ is an absolutely convergent serie in the odd coordinates w.r.t. the Rogers norm $\|\cdot\|_1$. Indeed, $\phi u(x,\theta,\overline{\theta})$ is analytic in the odd coordinates. This suggests that to take the Fourier transform of $\phi u(x,\theta,\overline{\theta})$ on the even variables must be sufficient to infer on the smoothness properties of $\phi u(x,\theta,\overline{\theta})$:

$$\widehat{\phi u}(k,\theta,\overline{\theta}) = \sum_{(\gamma)=0}^{\Gamma}\sum_{(\mu)=0}^{L} (\widehat{\phi u})_{(\gamma),(\mu)}(k_{\mathbf{b}})(\xi)^{(\mu)}(\theta)^{(\gamma)}$$
$$= \sum_{(\gamma)=0}^{\Gamma}\left[\int dx_{\mathbf{b}}\ e^{ik_{\mathbf{b}}x_{\mathbf{b}}}((\phi u)_{(\gamma)}(x_{\mathbf{b}}) + i\,x_{\mathbf{b}}(\phi u)_{(\gamma)}(x_{\mathbf{b}})k_{ij}\xi^i\xi^j + \cdots)\right](\theta)^{(\gamma)}. \quad (6.4)$$

Then, taking the absolute value of both sides of (6.4), we obtain from the Banach algebra property of $\mathcal{G}_L$ and for each integer N the estimate

$$|\widehat{\phi u}(k,\theta,\overline{\theta})| = \left|\sum_{(\gamma)=0}^{\Gamma}\sum_{(\mu)=0}^{L} (\widehat{\phi u})_{(\gamma),(\mu)}(k_{\mathbf{b}})(\xi)^{(\mu)}(\theta)^{(\gamma)}\right|$$
$$\leqslant \sum_{(\gamma)=0}^{\Gamma}\sum_{(\mu)=0}^{L} |(\widehat{\phi u})_{(\gamma),(\mu)}(k_{\mathbf{b}})|\|(\theta)^{(\gamma)}\|$$
$$\leqslant (1+|k_{\mathbf{b}}|)^{-N} C(N,\phi_{(\gamma)})\|\theta_1\|\|\overline{\theta}_1\|\cdots\|\theta_n\|\|\overline{\theta}_n\|. \quad (6.5)$$

This proves the lemma. □

So, the odd sector of superspace does not produce any effect on the singular structure of u. Combining the results above, we have proven.

Theorem 6.6: *The singularities of a superdistribution u are located at specific values of the body of x, the coordinates of the* **physical space–time**, *independently of the odd coordinates.* □

Comment 6.1: That the body of the superspace is responsible for carrying all its singular structure is not too surprising. Apparently, there exists no reason to have superspaces whose topological properties are substantially different from its body, which is responsible for carrying all observables, reflecting some measurable properties of the model. ■

We sum up the preceding discussion as follows:

Definition 6.7 (Wavefront set of a superdistribution): The wavefront set $\mathrm{WF}(u)$ *of a superdistribution* u *in a superspace* $\mathcal{M}$ *is the complement of the set of all regular directed points in the cotangent bundle* $T^*\mathcal{M}_0$, *where* $\mathcal{M}_0=\epsilon(\mathcal{M})$ *is the body of superspace, excluding the trivial point* $k_{\mathbf{b}}=0$.

There is a more precise version of definition 6.7. As we have seen in Sec. III all of the foregoing definitions and statements about supermanifolds may be converted into corresponding definitions and statements about ordinary manifolds, since associated with a supermanifold $\mathcal{M}$ of dimension (m,n) is a family of ordinary manifolds, of dimensions $N=2^{L-1}(m+n)$, $(L=1,2,\ldots)$. The resulting manifold is called the Lth skeleton of $\mathcal{M}$ and denoted by $\mathcal{S}_L(\mathcal{M})$.[32] With the aid of the family of skeletons we can define the pushforward (or direct image) of a superdistribution. Let $X\subset\mathcal{S}_L(\mathcal{M})$ and $Y\subset\mathcal{M}_0$ be open sets and let ϵ be the natural projection from $\mathcal{S}_L(\mathcal{M})$ (or $\mathcal{M}$) to $\mathcal{M}_0$, the body map. If we introduce local coordinates $x=(x_1,\ldots,x_N)$ in X, then Y is defined by $x_{\mathbf{b}}=(x_1,\ldots,x_m)$. There is a local relationship between the body and the skeletons given by

$$\mathcal{S}_L(X)\overset{\text{diff.}}{=}Y\times\mathbb{R}^{2^{L-1}(m+n)-m}\ .$$

Now, let u be a superdistribution on X, then the pushforward ϵ_*u defined by $\epsilon_*u(\varphi)=u(\epsilon^*\varphi)$, $\varphi\in C_0^\infty(Y)$, it is a superdistribution on Y. Using these concepts, we can establish the following:

Corollary 6.8: Let $\epsilon: X\subset\mathcal{S}_L(\mathcal{M})\to Y\subset\mathcal{M}_0$ *be the body projection, and let* $u\in\mathfrak{D}'(X)$. *Then*

$$\mathrm{WF}(\epsilon_*u)\subset\{(x_{\mathbf{b}},k_{\mathbf{b}})\in T^*\mathcal{M}_0\backslash 0\,|\,\exists\, x'=(x_{m+1},\ldots,x_{N'}),(x_{\mathbf{b}},x',k_{\mathbf{b}},0)\in\mathrm{WF}(u)\},$$

where $N'=2^{L-1}(m+n)-m$.

Proof: If $x=(x_{\mathbf{b}},x')$, where $x_{\mathbf{b}}\in Y$, $x'\in\mathbb{R}^{N'}$ and $\epsilon: X\to Y$ is the body map, then the Jacobian matrix is of the form $\epsilon'_x=(1,0)$ and the statement follows by theorem 6.3. Thus, with any superspace $\mathcal{M}$ and body of superspace $\mathcal{M}_0$ the singularities of a superdistribution ϵ_*u are located in a natural way in the set of projections of those points of the wavefront set of the superdistribution u where singular directions are parallel to the $x_{\mathbf{b}}$-axis. □

Example 6.1: For the model of Wess–Zumino, which consist of a chiral superfield Φ in self-interaction, the Feynman superpropagators, in flat superspace, are[54]

$$\begin{aligned}
\Delta^{\mathrm{F}}_{\Phi\Phi}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})&=-i\,m\,\delta^2(\theta-\theta')e^{i(\theta\sigma^\mu\overline{\theta}-\theta'\sigma^\mu\overline{\theta'})\partial_\mu}\Delta_{\mathrm{F}}(x-x'),\\
\Delta^{\mathrm{F}}_{\overline{\Phi}\Phi}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})&=e^{i(\theta\sigma^\mu\overline{\theta}+\theta'\sigma^\mu\overline{\theta'}-2\theta\sigma^\mu\overline{\theta'})\partial_\mu}\Delta_{\mathrm{F}}(x-x'),\\
\Delta^{\mathrm{F}}_{\overline{\Phi}\overline{\Phi}}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})&=i\,m\,\delta^2(\overline{\theta}-\overline{\theta'})e^{-i(\theta\sigma^\mu\overline{\theta}-\theta'\sigma^\mu\overline{\theta'})\partial_\mu}\Delta_{\mathrm{F}}(x-x'),
\end{aligned}\tag{6.6}$$

where $\delta^2(\theta-\theta')=(\theta-\theta')^2$, with $x,\theta,\overline{\theta}$ having the form (2.2) and (2.3), respectively. According to our analysis, the wavefront set of Feynman superprogators have the form

$$\mathrm{WF}(\Delta^{\mathrm{F}}_{\mathrm{susy}})=\{(x_{\mathbf{b}},k_{\mathbf{b}};x'_{\mathbf{b}},-k'_{\mathbf{b}};x,0;x',0)\,|\,(x_{\mathbf{b}},k_{\mathbf{b}};x'_{\mathbf{b}},-k'_{\mathbf{b}})\in\mathrm{WF}(\Delta^{\mathrm{F}}_{\mathrm{susy}}|_{\mathcal{M}_0})\},$$

where $\mathrm{susy}=(\Phi\Phi;\overline{\Phi}\Phi;\overline{\Phi}\overline{\Phi})$, $x=(x_{m+1},\ldots,x_{N'})$, $x'=(x'_{m+1},\ldots,x'_{N'})$, $\Delta^{\mathrm{F}}_{\mathrm{susy}}|_{\mathcal{M}_0}\equiv\epsilon_*\Delta^{\mathrm{F}}_{\mathrm{susy}}$ is the direct image of Feynman superpropagators on the body of superspace, and $\mathrm{WF}(\Delta^{\mathrm{F}}_{\mathrm{susy}}|_{\mathcal{M}_0})\subset O\cup D$,[8] with the off-diagonal piece given by

$$O=\{(x_{\mathbf{b}},k_{\mathbf{b}};x'_{\mathbf{b}},-k'_{\mathbf{b}})\in T^*\mathcal{M}_0^2|(x_{\mathbf{b}},k_{\mathbf{b}})\sim(x'_{\mathbf{b}},k'_{\mathbf{b}}),x_{\mathbf{b}}\neq x'_{\mathbf{b}},$$

$$k_{\mathbf{b}}\in\overline{V}_{\pm}\quad\text{if}\quad x_{\mathbf{b}}\in J_{\pm}(x'_{\mathbf{b}})\},$$

where the equivalence relation $(x_{\mathbf{b}},k_{\mathbf{b}})\sim(x'_{\mathbf{b}},k'_{\mathbf{b}})$ means that there is a lightlike geodesic γ connecting $x_{\mathbf{b}}$ and $x'_{\mathbf{b}}$, such that at the point $x_{\mathbf{b}}$ the covector $k_{\mathbf{b}}$ is tangent to γ and $k'_{\mathbf{b}}$ is the vector parallel transported along the curve γ at $x'_{\mathbf{b}}$ which is again tangent to γ.

The diagonal piece is given by

$$D=\{(x_{\mathbf{b}},k_{\mathbf{b}};x_{\mathbf{b}},-k_{\mathbf{b}})\in T^*\mathcal{M}_0^2\backslash 0|x_{\mathbf{b}}\in\mathcal{M}_0,k_{\mathbf{b}}\in T^*\mathcal{M}_0^2\backslash 0\}.$$

For this reason, the Feynman superpropagators are singular only for pairs of points on the body of superspace that can be connected by a lightlike geodesic. ■

We end this section quoting the main lesson on the microlocal analysis that we can use, i.e., the one about how the wavefront set may be lifted from superdistributions on open sets of $\mathcal{G}_L^{m,n}$ to superdistributions on a smooth supermanifold $\mathcal{M}$. Such an extension can be achieved in analogy with the ordinary case. Let $\mathcal{O}$ be an open neighborhood of $z\in\mathcal{M}$, which is assumed without loss generality to be covered by a single coordinate patch, and $u\in\mathfrak{D}'(\mathcal{O})$ be a superdistribution. Then, there exists a diffeomorphism $\chi:\mathcal{O}\to U\subset\mathcal{G}_L^{m,n}$, so that $\chi^*u\in\mathfrak{D}'(U)$ is the superdistribution pulled back by χ. Therefore $\mathrm{WF}(\chi^*u)=\chi^*\mathrm{WF}(u)$. Now, let ϕ be a supersmooth function with compact support contained within $\mathcal{O}$ with $\phi(z)\neq 0$—one should keep always in mind that each component $\phi_{(\gamma)}(\epsilon(x))$ of $\phi(z)$ is a smooth function and with support contained within $\mathcal{O}_{\mathbf{b}}$, where $\mathcal{O}_{\mathbf{b}}$ denotes an open neighborhood of $x_{\mathbf{b}}\in\mathcal{M}_0$. Hence, the superdistribution $u\phi$ can be seen as a superdistribution on $\mathcal{G}_L^{m,n}$ which is of compact support, and given that there are no points belonging to the $\mathrm{WF}(u)$, the Fourier transform, $\widehat{u\phi}$, of $u\phi$ is well defined as a superdistribution on $\mathcal{G}_L^{m,n}$ and satisfies the Lemma 6.5.

VII. A TYPE OF MICROLOCAL SPECTRAL CONDITION

We come back to the question of the Hadamard superstates. As repeatedly stated in this paper, Hadamard states have acquired a prominent status in connection with the spectral condition, and are recognized as defining the class of physical states for quantum field theories on a globally hyperbolic space–time. Important progress in understanding the significance of Hadamard states was achieved by Radzikowski (with some gaps filled by Köhler[10]) who succeeded in characterizing the class of these states in terms of the wavefront set of their two-point function ω_2 satisfying a certain condition. He called this condition the wavefront set spectral condition (WFSSC). He proposed that a quasifree state ω of the Klein–Gordon field over a globally hyperbolic manifold is a Hadamard state if and only if its two-point distribution ω_2 has wavefront set

$$\mathrm{WF}(\omega_2)=\{(x_1,k_1);(x_2,k_2)\in T^*\mathcal{M}_0^2\backslash\{0\}|(x_1,k_1)\sim(x_2,-k_2)\quad\text{and}\quad k_1^0\geqslant 0\},\qquad(7.1)$$

so that x_1 and x_2 lie on a single null geodesic γ, $(k_1)^\mu=g^{\mu\nu}(k_1)_\nu$ is tangent to γ and future pointing, and when k_1 is parallel transported along γ from x_1 to x_2 yields $-k_2$. If $x_1=x_2$, we have $k_1^2=0$ and $k_1=k_2$. Radzikowski in fact showed that this condition is similar to the spectral condition of axiomatic quantum field theory.[49]

Note that Eq. (7.1) restricts the singular support of $\omega_2(x_1,x_2)$ to points x_1 and x_2 which are null related. Hence, ω_2 must be smooth for all other points. This is known be true for theory of quantized fields on Minkowski space for spacelike related points. The key is the Bargman–Hall–Wightman theorem which shows that this is obtainable by applying complex Lorentz transformations to the primitive domain of analyticity determined by the spectral condition. However, a similar prediction on the smoothness does not exist for timelike related points. Radzikowski suggested to extend the right-hand side of Eq. (7.1) to all causally related points, in order to include possible singularities at timelike related points.

The microlocal characterization of Hadamard states may be applied equally well to a n-point function, with $n>2$. This generalization was achieved by Brunetti *et al.*[11] They suggested a prescription which we recall now. Let $\mathcal{G}_m$ denotes the set of all finite graphs,[61] into some Lorentz manifold $\mathcal{M}_0$, whose vertices represent points in the set $V=\{x_1,\ldots,x_m\}\in\mathcal{M}_0$, and whose edges e represent connections between pairs x_i,x_j by smooth curves (geodesics) $\gamma(e)$ from x_i to x_j. To each edge e one assigns a covariantly constant causal covector field k_e which is future directed if $i<j$, but not related to the tangent vector of the curve. If e^{-1} denotes the edge with opposite direction as e, then the corresponding curve $\gamma(e^{-1})$ is the inverse of $\gamma(e)$, which carries the momentum $k_{e^{-1}}=-k_e$.

Definition 7.1 [μSC (Ref. 11)]: A state ω with m-point distribution ω_m is said to satisfy the Microlocal Spectral Condition if, and only if, for any m

$$\mathrm{WF}(\omega_m)\subseteq\Gamma_m,$$

where Γ_m is the set $\{(x_1,k_1),\ldots,(x_m,k_m)\}$ for which there exists a graph $G\in\mathcal{G}_m$ as described above with $k_i=\Sigma k_e(x_i)$ where the sum runs over all edges which have the point x_i as their sources. The trivial momentum configuration $k_1=\cdots=k_m=0$ is excluded.

Passing from a smooth manifold to a smooth supermanifold, it seems reasonable to require that a superstate satisfies a certain type of microlocal spectrum condition. A completely analogous statement to definition 7.1 can be achieved, once more with the aid of the family of skeletons, $\mathcal{S}_L(\mathcal{M})$, and the graph theory. Let $\mathcal{G}_r$ be a set of finite "*supergraphs*," into some $\mathcal{S}_L(\mathcal{M})$, whose vertices represent points in the set $V=\{x_1,\ldots,x_r\}\in\mathcal{S}_L(\mathcal{M})$. Locally the traditional notion of a supergraph drawing is that its vertices are represented by points in the hyperplane $\mathbb{R}^{2^{L-1}(m+n)}$, its edges are represented by curves—that are piecewise linear—between these points, and different curves meet only in common endpoints. If $\epsilon_0:\mathbb{R}^{2^{L-1}(m+n)}\to\mathbb{R}^m$ is the canonical projection, then $\tilde{G}=\epsilon_0 G$ is a graphy composed by the projection of those points of a supergraph whose edges e represent connections between pairs $x_{\mathbf{b}_i},x_{\mathbf{b}_j}\in\mathbb{R}^m$ by curves from $x_{\mathbf{b}_i}$ to $x_{\mathbf{b}_j}$. Then, according to Brunetti *et al.*,[11] an immersion of a graph $\tilde{G}$ into the body manifold $\mathcal{M}_0$ is an assignment of vertices of $\tilde{G}$ to points in $\mathcal{M}_0$, and of the edges of $\tilde{G}$ to piecewise smooth curves in $\mathcal{M}_0$, $e\to\gamma(e)$ with source $s(\gamma(e))=x_{\mathbf{b}}(s(e))$ and target $t(\gamma(e))=x_{\mathbf{b}}(t(e))$, respectively, together with a covariantly constant causal covector field $k_{\mathbf{b}_e}$ on γ such that: (i) if e^{-1} denotes the edge with opposite direction as e, then the corresponding curve $\gamma(e^{-1})$ is the inverse of $\gamma(e)$; (ii) for every edge e the covector $k_{\mathbf{b}_e}$ is directed toward future if $x_{\mathbf{b}}(s(e))<x_{\mathbf{b}}(t(e))$; (iii) $k_{\mathbf{b}_{e^{-1}}}=-k_{\mathbf{b}_e}$. Using this construction, we establish:

Definition 7.2 (susyμSC): A superstate ω^{susy} with r-point superdistribution ω_r^{susy} is said to satisfy a supersymmetric microlocal spectral condition if, and only if, for any r,

$$\mathrm{WF}(\omega_r^{\mathrm{susy}})=\{(x_{\mathbf{b}_1},x_1',k_{\mathbf{b}_1},0);\ldots;(x_{\mathbf{b}_r},x_r',k_{\mathbf{b}_r},0)\,|\,\mathrm{WF}(\epsilon_*\omega_r^{\mathrm{susy}})\subseteq\tilde{\Gamma}_r\},$$

where $\tilde{\Gamma}_r$ is the set $\{(x_{\mathbf{b}_1},k_{\mathbf{b}_1});\ldots;(x_{\mathbf{b}_r},k_{\mathbf{b}_r})\}$ for which there exists a graph $\tilde{G}$ as described above with $k_{\mathbf{b}_i}=\Sigma k_{\mathbf{b}_e}(x_{\mathbf{b}_i})$ where the sum runs over all edges which have the point $x_{\mathbf{b}_i}$ as their sources. The trivial momentum configuration $k_{\mathbf{b}_1}=\cdots=k_{\mathbf{b}_r}=0$ is excluded.

Remarks 7.1: We would like to call attention to two important points:

(1) Definition 7.2 indicates that for a superstate ω^{susy} the (susyμSC) is equivalent to the requirement that all of the component fields satisfy the microlocal spectral conditions[11] on the body manifold. This observation is significant because it is in agreement with the DeWitt's remark which asserts that, in physical applications of supersymmetric quantum field theories, the spectral condition of the GNS-Hilbert superspace is restricted to the ordinary GNS-Hilbert space that sits inside the GNS-Hilbert superspace.

(2) Definition 7.2 provides us with a "global" microlocal spectral condition. In our setting the word "global" means that the singular support of all component fields is embodied in

WF($\epsilon_* \omega_m^{\text{susy}}$). This is typical feature of supersymmetric theories in superspace language. For instance, for the chiral superfield of Wess–Zumino,[54] in analogy to the scalar component field, the Hadamard condition for a spinorial component field is formulated in terms of its two-point distribution ω_2. The latter are obtainable by applying the adjoint of the spinorial operator to a suitable auxiliary Hadamard state of the squared spinorial equation. For fixed spinor indices the wavefront set of the latter is contained in the r.h.s. of Eq. (7.1) and derivatives do not enlarge the wavefront set. ■

Next we give a example of an application of our definiton. We restrict ourselves to the simplest case of massive chiral/antichiral fields of the Wess–Zumino model in flat superspace, leaving other cases as the Wess–Zumino model, or supersymmetric gauge theories in curved superspace for future works.

The free Wess–Zumino model in flat superspace: The simplest $N=1$ supersymmetric model in four dimension is the free model of Wess–Zumino,[54] which consists of a chiral superfield $\Phi(x,\theta,\overline{\theta})$, resp., antichiral superfield $\overline{\Phi}(x,\theta,\overline{\theta})$, obeying the differential constraint $\overline{D}_{\dot{\alpha}}\Phi=0$, resp., $D_\alpha\Phi=0$. As usual,

$$D_\alpha=\frac{\partial}{\partial\theta^\alpha}-i\sigma^\mu_{\alpha\dot{\alpha}}\overline{\theta}^{\alpha}\partial_\mu, \quad \overline{D}_{\dot{\alpha}}=-\frac{\partial}{\partial\overline{\theta}^{\alpha}}+i\theta^\alpha\sigma^\mu_{\alpha\dot{\alpha}}\partial_\mu, \tag{7.2}$$

is a supersymmetric covariant derivatives. Our notations and conventions are those of Ref. 56. The elements of the $N=1$ superspace are parametrized by even and odd coordinates $z^M=(x^\mu,\theta^\alpha,\overline{\theta^\alpha})$, with $\mu=(0,\ldots,3)$, $\alpha=(1,2)$, $\dot{\alpha}=(\dot{1},\dot{2})$, where θ and its complex conjugate $\overline{\theta}$, are odd coordinates and by construction they anticommute with each other. In this case the body manifold is $\mathbb{R}^m$ and the body map is the augmentation map $\epsilon:\mathcal{G}_L^{m,n}\to\mathbb{R}^m$.

The superfield $\Phi(z)$ is a function mapping superspace into the even part of a Grassmann algebra.[25] With the help of the commutation rule $\overline{D}_\alpha\,(e^{-i\theta\sigma^\mu\overline{\theta}\partial_\mu}\phi)=e^{-i\theta\sigma^\mu\overline{\theta}\partial_\mu}(-\partial/\partial\overline{\theta^\alpha})\phi$, the chiral superfield can be expanded in powers of the odd coordinates as

$$\Phi(z)=e^{-i\theta\sigma^\mu\overline{\theta}\partial_\mu}(\varphi(x)+\theta\psi(x)+\theta^2F(x)), \tag{7.3}$$

with $\varphi\overset{\text{def}}{=}2^{-1/2}(A+iB)$ and $F\overset{\text{def}}{=}2^{-1/2}(D-iE)$. A, B, and ψ are, respectively, the scalar, pseudoscalar, and spin-1/2 physical component fields of Φ, whereas D and E are their scalar and pseudoscalar auxiliary components. The latter are necessary for a classical off-shell closure of the supersymmetry algebra (they do not correspond to propagating degrees of freedom in that appear through nonderivative terms).

As above, the antichiral superfield $\overline{\Phi}(z)$, with the help of the commutation rule $D_\alpha\,(e^{i\theta\sigma^\mu\overline{\theta}\partial_\mu}\phi)=e^{i\theta\sigma^\mu\overline{\theta}\partial_\mu}(\partial/\partial\theta^\alpha)\phi$, can be expanded in component fields:

$$\overline{\Phi}(z)=e^{i\theta\sigma^\mu\overline{\theta}\partial_\mu}(\varphi^*(x)+\overline{\theta\psi}(x)+\overline{\theta}^2F^*(x)). \tag{7.4}$$

The quantum version of the Wess–Zumino model is based on the classical field equations

$$\frac{1}{16}\overline{D}^2\overline{\Phi}+\frac{m}{4}\Phi=0, \quad \frac{1}{16}D^2\Phi+\frac{m}{4}\overline{\Phi}=0. \tag{7.5}$$

Applying the operator D^2 to the first equation (resp., $\overline{D}^2$ to the second equation), multiplying the second equation by $4m$ (resp., the first equation), and using the commutation relation $[D^2,\overline{D}^2]=8iD\sigma^\mu\overline{D}\partial_\mu+16\Box$; one may combine them in order to find

$$(\Box_x+m^2)\Phi=0, \quad (\Box_x+m^2)\overline{\Phi}=0. \tag{7.6}$$

To our classical superfields Φ and $\overline{\Phi}$, we associate quantum superfields, an operator-valued ''superdistributions,'' smeared with ''supertest'' functions,

$$F(z)=e^{-i\theta\sigma^{\mu}\overline{\theta}\partial_{\mu}}(f(x)+\theta\chi(x)+\theta^{2}h(x)),$$

$$\overline{F}(z)=e^{i\theta\sigma^{\mu}\overline{\theta}\partial_{\mu}}(f^{*}(x)+\overline{\theta\chi}(x)+\overline{\theta}^{2}h^{*}(x)), \tag{7.7}$$

with $F(z),\overline{F}(z)\in G_{0}^{\infty}(U,\mathcal{G}_{L})$, the $\mathcal{G}_{L}$-valued superfunctions on an open set $U\subset\mathcal{G}_{L}^{m,n}$ which have compact support.

For all $F(z),G(z)\in G_{0}^{\infty}(U,\mathcal{G}_{L})$, we define the commutation relations

$$[\Phi(\overline{F}),\Phi(\overline{G})]=\int d\mu(z)d\mu(z')\ \Delta_{\Phi\Phi}^{\mathrm{PJ}}(z,z')\overline{F}(z)\overline{G}(z'),$$

$$[\overline{\Phi}(F),\Phi(\overline{G})]=\int d\mu(z)d\mu(z')\ \Delta_{\overline{\Phi}\Phi}^{\mathrm{PJ}}(z,z')F(z)\overline{G}(z'), \tag{7.8}$$

$$[\overline{\Phi}(F),\overline{\Phi}(G)]=\int d\mu(z)d\mu(z')\ \Delta_{\overline{\Phi}\overline{\Phi}}^{\mathrm{PJ}}(z,z')F(z)G(z'),$$

where $d\mu(z)\overset{\mathrm{def}}{=}d^{8}z=d^{4}xd^{2}\theta d^{2}\overline{\theta}$. We call $\Delta_{\Phi\Phi}^{\mathrm{PJ}}$, $\Delta_{\overline{\Phi}\Phi}^{\mathrm{PJ}}$, and $\Delta_{\overline{\Phi}\overline{\Phi}}^{\mathrm{PJ}}$ the Pauli–Jordan superdistributions, fundamental solutions of the homogeneous equations (7.6). In fact they are two-point distributions, elements of $\mathfrak{D}'(U)$.

The vacuum expectation value of the product $\Phi(F)\Phi(G)$ satisfies the relation

$$(\Omega,\Phi(F)\Phi(G)\Omega)=(w_{2}^{\mathrm{susy}}(z,z'),F(z)G(z')). \tag{7.9}$$

The distribution $w_{2}^{\mathrm{susy}}(z,z')$ extends the Wightman formalism. For this reason, we call $w_{2}^{\mathrm{susy}}(z,z')$ Wightman superdistribution of two-points.

The Wightman superdistribution of n-points will be symbolically written under the form[51]

$$w_{n}^{\mathrm{susy}}(z_{1},,\ldots,z_{n})=(\Omega,\Phi(x_{1};\theta_{1},\overline{\theta}_{1})\cdots\Phi(x_{n};\theta_{n},\overline{\theta}_{n})\Omega), \tag{7.10}$$

and

$$w_{n}^{\mathrm{susy}}(F_{n})=\int\prod_{i=1}^{n}d\mu_{i}\ w_{n}^{\mathrm{susy}}(z_{1},\ldots,z_{n})F_{n}(z_{1},\ldots,z_{n}). \tag{7.11}$$

In this definition, we have fixed the order in which we take the superdistribution and the supertest function.

Proposition 7.3: The two-point Hadamard, Pauli–Jordan, and Wightman superdistributions have the following dependence in $x,\theta,\overline{\theta}$:

$$\Delta_{\Phi\Phi}^{X}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})=-i\,m\,\delta^{2}(\theta-\theta')e^{i(\theta\sigma^{\mu}\overline{\theta}-\theta'\sigma^{\mu}\overline{\theta'})\partial_{\mu}}\Delta_{X}(x-x'),$$

$$\Delta_{\overline{\Phi}\Phi}^{X}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})=e^{i(\theta\sigma^{\mu}\overline{\theta}+\theta'\sigma^{\mu}\overline{\theta'}-2\theta\sigma^{\mu}\overline{\theta'})\partial_{\mu}}\Delta_{X}(x-x'), \tag{7.12}$$

$$\Delta_{\overline{\Phi}\overline{\Phi}}^{X}(x,\theta,\overline{\theta};x',\theta',\overline{\theta'})=i\,m\,\delta^{2}(\overline{\theta}-\overline{\theta'})e^{-i(\theta\sigma^{\mu}\overline{\theta}-\theta'\sigma^{\mu}\overline{\theta'})\partial_{\mu}}\Delta_{X}(x-x'),$$

where $X=(\mathrm{Had,PJ,W})$.

Idea of proof: We start from (6.6) and use the fact that in terms of even and odd solutions of the homogeneous wave equation, the function $\Delta_{\mathrm{F}}(x-x')$ can be written as

$$\Delta_F(x-x') = \tfrac{1}{2}[\, i\,\Delta_{\mathrm{Had}}(x-x') + \varepsilon(x^0-x^{0'})\Delta_{\mathrm{PJ}}(x-x')]. \tag{7.13}$$

Then, by replacing (7.13) in (6.6), we immediately get the Hadamard and Pauli–Jordan superdistribution as stated. The Wightman superdistribution is obtained directly from the fact the $\Delta_{\mathrm{PJ}}(x-x') = \Delta_W(x-x') - \Delta_W(x-x')$ and $\Delta_{\mathrm{Had}}(x-x') = -i(\Delta_W(x-x') + \Delta_W(x-x'))$. □

Proposition 7.4: Let ω^{susy} be a state for the quantum Wess–Zumino model on the flat superspace, whose r-point superdistributions ω_r^{susy} satisfy the Wightman axioms.[62] *Then ω^{susy} satisfies definition 7.2.*

Proof: This is an immediate consequence of corollary 6.8 above and theorem 4.6 of Ref. 11.□

VIII. FINAL CONSIDERATIONS

Having proposed an extension of some structural aspects that have successfully been applied in the development of the theory of quantum fields propagating on a general space–time manifold so as to include superfield models on a supermanifold, it would be interesting to consider the perturbative treatment of interacting quantum superfield models, in particular the formulation of renormalization theory on supermanifolds. The main problem which still remains in this rather restrictive framework is the mathematically consistent definition of all powers of Wick ''superpolynomials'' and their time-ordered products for the noninteracting theory, which serve as building blocks for a perturbative definition of interacting superfields. Another work devoted to its solution is in progress,[64] such that covariance with respect to supersymmetry is manifestly preserved. The renormalization scheme underlying our construction is the one of Epstein–Glaser. It is formulated, unlike the other renormalization schemes, in configuration space. Therefore, it becomes appropriate to define carefully perturbative renormalization on a generic spacetime manifold. Recently, Brunetti and Fredenhagen[16] (with some gaps filled by Hollands and Wald[65]) have shown that the Wick polynomials and their time-ordered products can be defined in globally hyperbolic spacetimes. By the methods of this paper we can define powers of Wick ''superpolynomials'' and their time-ordered products for the noninteracting theory.

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[61] A graph is a pair $G=(V,E)$, where the elements of V are the *vertices* (or *nodes*, or *points*) of the graph G, and the elements of E are its *edges* (or *lines*). The numbers of vertices of a graph is its order, and graphs are finite or infinite according to their order.
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Variational derivation of relativistic fermion–antifermion wave equations in QED

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We present a variational method for deriving relativistic two-fermion wave equations in a Hamiltonian formulation of QED. A reformulation of QED is performed, in which covariant Green functions are used to solve for the electromagnetic field in terms of the fermion fields. The resulting modified Hamiltonian contains the photon propagator directly. The reformulation permits one to use a simple Fock-space variational trial state to derive relativistic fermion–antifermion wave equations from the corresponding quantum field theory. We verify that the energy eigenvalues obtained from the wave equation agree with known results for positronium. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1649794]

I. INTRODUCTION

The description of relativistic bound and quasibound (i.e., unstable) few body systems continues to be an active area of research. The traditional method of treating relativistic bound states in quantum field theory (QFT) is by means of the Bethe–Salpeter (BS) equation. However, this approach has a number of difficulties, including the appearance of relative-time coordinates and negative-energy solutions. In practice, the interaction kernels (potentials) in the BS equation are obtained from covariant perturbation theory, which may be of questionable validity for strongly coupled systems. In addition, the BS formalism is difficult to implement for systems of more than two particles.

An alternative approach might be the variational method, which is nonperturbative in principle. The variational method has not been widely used in quantum field theory, in contrast to nonrelativistic systems describable by the Schrödinger theory, in part because of the difficulty of constructing realistic yet tractable trial states.

It has been pointed out in previous publications[1,2] that various models in QFT, including QED, can be reformulated, using mediating-field Green functions, into a form particularly convenient for variational calculations. This approach was applied recently to the study of relativistic two-body states in the scalar Yukawa (Wick–Cutkosky) theory.[3–5] In the present paper we shall implement this approach to the realistic QED theory, where comparison with experimentally verified results are possible. In particular, we shall use the reformulated QED Hamiltonian to derive a relativistic fermion–antifermion wave equation and discuss its solution.

The reformulation of QED is presented in Sec. II, while the Hamiltonian and equal time quantization are given in Sec. III. In Sec. IV we use the variational principle with simple Fock-space trial states to derive the relativistic fermion–antifermion equations, and present their ''partial wave'' decomposition for all possible J^{PC} states. The relativistic radial equations are presented in Sec. V, while their nonrelativistic and semirelativistic limits are given in Sec. VI. In Sec. VII the energy eigenvalues are shown to yield the correct fine and hyperfine structure for all states. Concluding remarks are given in Sec. VIII.

II. REFORMULATION OF FIELD EQUATIONS AND LAGRANGIAN

The Lagrangian of QED is ($\hbar = c = 1$)

$$\mathcal{L} = \overline{\psi}(x)(i\gamma^\mu \partial_\mu - m - e\gamma^\mu A_\mu(x))\psi(x) - \tfrac{1}{4}(\partial_\alpha A_\beta(x) - \partial_\beta A_\alpha(x))(\partial^\alpha A^\beta(x) - \partial^\beta A^\alpha(x)). \quad (1)$$

The corresponding Euler–Lagrange equations of motion are the coupled Dirac–Maxwell equations,

$$(i\gamma^{\mu}\partial_{\mu}-m)\psi(x)=e\gamma^{\mu}A_{\mu}(x)\psi(x), \tag{2}$$

and

$$\partial_{\mu}\partial^{\mu}A^{\nu}(x)-\partial^{\nu}\partial_{\mu}A^{\mu}(x)=j^{\nu}(x), \tag{3}$$

where

$$j^{\nu}(x)=e\overline{\psi}(x)\gamma^{\nu}\psi(x). \tag{4}$$

Equations (2) and (3) can be decoupled in part by using the well-known formal solution[6,7] of the Maxwell equation (3), namely,

$$A_{\mu}(x)=A^{0}_{\mu}(x)+\int d^{4}x' D_{\mu\nu}(x-x')j^{\nu}(x'), \tag{5}$$

where $D_{\mu\nu}(x-x')$ is a Green function (or photon propagator in QFT terminology), defined by

$$\partial_{\alpha}\partial^{\alpha}D_{\mu\nu}(x-x')-\partial_{\mu}\partial^{\alpha}D_{\alpha\nu}(x-x')=g_{\mu\nu}\delta^{4}(x-x'), \tag{6}$$

and $A^{0}_{\mu}(x)$ is a solution of the homogeneous (or "free field") equation (3) with $j^{\mu}(x)=0$.

We recall, in passing, that Eq. (6) does not define the covariant Green function $D_{\mu\nu}(x-x')$ uniquely. For one thing, one can always add a solution of the homogeneous equation [Eq. (6) with $g_{\mu\nu}\rightarrow 0$]. This allows for a certain freedom in the choice of $D_{\mu\nu}$, as is discussed in standard texts (e.g., Refs. 6 and 7). In practice, the solution of Eq. (6), like that of Eq. (3), requires a choice of gauge. However, we do not need to specify one at this stage.

Substitution of the formal solution (5) into Eq. (2) yields the "partly reduced" equations,

$$(i\gamma^{\mu}\partial_{\mu}-m)\psi(x)=e\gamma^{\mu}\left(A^{0}_{\mu}(x)+\int d^{4}x' D_{\mu\nu}(x-x')j^{\nu}(x')\right)\psi(x), \tag{7}$$

which is a nonlinear Dirac equation. To our knowledge no exact (analytic or numeric) solution of Eq. (7) for classical fields have been reported in the literature. However, approximate solutions have been discussed by various authors, particularly Barut and co-workers (see Refs. 8, 9, and citations therein). In any case, our interest here is in the quantized field theory.

The partially reduced equation (7) is derivable from the stationary action principle

$$\delta S[\psi]=\delta\int d^{4}x\mathcal{L}_{R}=0 \tag{8}$$

with the Lagrangian density

$$\mathcal{L}_{R}=\overline{\psi}(x)(i\gamma^{\mu}\partial_{\mu}-m-e\gamma_{\mu}A^{\mu}_{0}(x))\psi(x)-\frac{1}{2}\int d^{4}x' j^{\mu}(x')D_{\mu\nu}(x-x')j^{\nu}(x) \tag{9}$$

provided that the Green function is symmetric in the sense that

$$D_{\mu\nu}(x-x')=D_{\mu\nu}(x'-x) \qquad \text{and} \qquad D_{\mu\nu}(x-x')=D_{\nu\mu}(x-x'). \tag{10}$$

One can proceed to do conventional covariant perturbation theory using the reformulated QED Lagrangian (9). The interaction part of (9) has a somewhat modified structure from that of the usual formulation of QED. Thus, there are two interaction terms. The last term of (9) is a "current–current" interaction which contains the photon propagator sandwiched between the fer-

mionic currents. As such, it corresponds to Feynman diagrams without external photon lines. The term containing A_0^μ corresponds to diagrams that cannot be generated by the term containing $D_{\mu\nu}$, including diagrams involving external photon lines (care would have to be taken not to double count physical effects). However, we shall not pursue covariant perturbation theory in this work. Rather, we shall consider a variational approach that allows one to derive relativistic few-fermion equations, and to study their bound and scattering solutions.

III. HAMILTONIAN OF THE QUANTIZED THEORY IN THE EQUAL-TIME FORMALISM

We consider this theory in the quantized, equal-time formalism. To this end we write down the Hamiltonian density corresponding to the Lagrangian (9), with the term for the free $A_0^\mu(x)$ field suppressed since it will not contribute to the results presented in this paper. The relevant expression is

$$\mathcal{H}_R = \mathcal{H}_0 + \mathcal{H}_I, \tag{11}$$

where

$$\mathcal{H}_0 = \psi^\dagger(x)(-i\boldsymbol{\alpha}\cdot\nabla + m\beta)\psi(x), \tag{12}$$

$$\mathcal{H}_I = \frac{1}{2}\int d^4x' j^\mu(x') D_{\mu\nu}(x-x') j^\nu(x). \tag{13}$$

We construct a quantized theory by the imposition of anticommutation rules for the fermion fields, namely,

$$\{\psi_\alpha(\mathbf{x},t), \psi_\beta^\dagger(\mathbf{y},t)\} = \delta_{\alpha\beta}\delta^3(\mathbf{x}-\mathbf{y}), \tag{14}$$

while all other vanish. In addition, if $A_0^\mu \neq 0$, there would be the usual commutation rules for the A_0^μ field, and commutation of the A_0^μ field operators with the ψ field operators.

To specify our notation, we quote the usual Fourier decomposition of the field operators, namely,

$$\psi(x) = \sum_s \int \frac{d^3p}{(2\pi)^{3/2}}\left(\frac{m}{\omega_p}\right)^{1/2}[b_{\mathbf{p}s}u(\mathbf{p},s)e^{-ip\cdot x} + d_{\mathbf{p}s}^\dagger v(\mathbf{p},s)e^{ip\cdot x}], \tag{15}$$

with $p = p^\mu = (\omega_p, \mathbf{p})$, and $\omega_p = \sqrt{m^2+\mathbf{p}^2}$. Dirac spinors u and v for free particles of mass m, where $(\gamma^\mu p_\mu - m)u(\mathbf{p},s) = 0$, $(\gamma^\mu p_\mu + m)v(\mathbf{p},s) = 0$, are normalized such that

$$u^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma) = v^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma) = \frac{\omega_p}{m}\delta_{s\sigma}, \tag{16}$$

$$u^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma) = v^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma) = 0. \tag{17}$$

The creation and annihilation operators $b^\dagger$, b of the (free) fermions of mass m, and $d^\dagger$, d for the corresponding antifermions, satisfy the usual anticommutation relations. The nonvanishing ones are

$$\{b_{\mathbf{p}s}, b_{\mathbf{q}\sigma}^\dagger\} = \{d_{\mathbf{p}s}, d_{\mathbf{q}\sigma}^\dagger\} = \delta_{s\sigma}\delta^3(\mathbf{p}-\mathbf{q}). \tag{18}$$

IV. VARIATIONAL PRINCIPLE AND FERMION–ANTIFERMION TRIAL STATES

Unfortunately we do not know how to obtain exact eigenstates of the Hamiltonian (11). Therefore we shall resort to a variational approximation, based on the variational principle

$$\delta\langle\psi|\hat{H} - E|\psi\rangle_{t=0} = 0. \tag{19}$$

For a fermion–antifermion system, the simplest Fock-space trial state that can be written down in the rest frame is

$$|\psi_T\rangle = \sum_{s_1 s_2} \int d^3\mathbf{p} F_{s_1 s_2}(\mathbf{p}) b^\dagger_{\mathbf{p}s_1} d^\dagger_{-\mathbf{p}s_2}|0\rangle, \tag{20}$$

where $F_{s_1 s_2}$ are four adjustable functions. We use this trial state to evaluate the matrix elements needed to implement the variational principle (19), namely,

$$\langle\psi_T|:\hat{H}_0 - E:|\psi_T\rangle = \sum_{s_1 s_2} \int d^3\mathbf{p} F^*_{s_1 s_2}(\mathbf{p}) F_{s_1 s_2}(\mathbf{p})(2\omega_p - E) \tag{21}$$

and

$$\langle\psi_T|:\hat{H}_I:|\psi_T\rangle = \frac{e^2 m^2}{(2\pi)^3} \sum_{s_1' s_2' s_1 s_2} \int \frac{d^3\mathbf{p} d^3\mathbf{p}'}{\omega_p \omega_{p'}} F^*_{s_1 s_2}(\mathbf{p}) F_{s_1' s_2'}(\mathbf{p}') \times \begin{pmatrix} -\overline{u}(\mathbf{p}, s_1)\gamma^\mu u(\mathbf{p}', s_1') D_{\mu\nu}(p - p')\overline{v}(-\mathbf{p}', s_2')\gamma^\nu v(-\mathbf{p}, s_2) \\ +\overline{u}(\mathbf{p}, s_1)\gamma^\mu v(-\mathbf{p}, s_2) D_{\mu\nu}(p + p')\overline{v}(-\mathbf{p}', s_2')\gamma^\nu u(\mathbf{p}', s_1') \end{pmatrix}, \tag{22}$$

where $p = (\omega_p, \mathbf{p})$, $p' = (\omega_{p'}, \mathbf{p}')$, with $\mathbf{p} + \mathbf{p}' = 0$ (i.e., $p + p' = (2\omega_p, 0)$) in the rest frame, and

$$D_{\mu\nu}(x - x') = \int \frac{d^4 k}{(2\pi)^4} D_{\mu\nu}(k) e^{-ik\cdot(x - x')}. \tag{23}$$

We have normal-order the entire Hamiltonian, since this circumvents the need for mass renormalization which would otherwise arise. Not that there is difficulty with handling mass renormalization in the present formalism (as shown in various earlier papers; see, for example, Ref. 10, and citations therein). It is simply that we are not interested in mass renormalization here, since it has no effect on the two-body bound state energies that we obtain in this paper. Furthermore, the approximate trial state (20), which we use in this work, is incapable of sampling loop effects. Thus, the normal-ordering of the entire Hamiltonian does not ''sweep under the carpet'' loop effects, since none arise at the present level of approximation, that is with the trial state $|\psi_T\rangle$ specified in Eq. (20).

The variational principle (19) leads to the following equation:

$$\sum_{s_1 s_2} \int d^3\mathbf{p}(2\omega_p - E) F_{s_1 s_2}(\mathbf{p})\, \delta F^*_{s_1 s_2}(\mathbf{p}) - \frac{m^2}{(2\pi)^3} \sum_{\sigma_1 \sigma_2 s_1 s_2} \int \frac{d^3\mathbf{p} d^3\mathbf{q}}{\omega_p \omega_q} F_{\sigma_1 \sigma_2}(\mathbf{q})(-i)\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q})\, \delta F^*_{s_1 s_2}(\mathbf{p}) = 0, \tag{24}$$

where $\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q})$ is an invariant ''matrix element,'' which contains two terms:

$$\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q}) = \mathcal{M}^{\text{ope}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q}) + \mathcal{M}^{\text{ann}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q}), \tag{25}$$

where

$$\mathcal{M}^{\text{ope}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q}) = -\overline{u}(\mathbf{p}, s_1)(-ie\gamma^\mu) u(\mathbf{q}, \sigma_1) i D_{\mu\nu}(p - q)\overline{v}(-\mathbf{q}, \sigma_2)(-ie\gamma^\nu) v(-\mathbf{p}, s_2), \tag{26}$$

$$\mathcal{M}^{\text{ann}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p}, \mathbf{q}) = \overline{u}(\mathbf{p}, s_1)(-ie\gamma^\mu) v(-\mathbf{p}, s_2) i D_{\mu\nu}(p + q)\overline{v}(-\mathbf{q}, \sigma_2)(-ie\gamma^\nu) u(\mathbf{q}, \sigma_1), \tag{27}$$

correspond to the usual one-photon exchange and virtual annihilation Feynman diagrams.

At this point it is worthwhile to make a few comments about our Eq. (24) and to compare its general features with other two-fermion equations, particularly field-theory based approaches. Firstly we note that the present variational derivation leads to momentum-space Salpeter-type equations, with at most four independent components $F_{s_1 s_2}(\mathbf{p})$. The equations have only positive-energy solutions, as is evident from Eq. (24) with the interaction turned off, in which case only $E=2\omega_p>0$ is obtained. This is in contrast to the BS equation, which is a 16-component equation and contains both positive, negative and mixed energy solutions.

The interaction kernels, represented by the covariant $\mathcal{M}$-matrices, result from the variational derivation, that is, they are not put in by hands. This is in contrast to two fermion equations, which are not derived from a underlying quantum field theory, such as various two-body generalizations of the one-body Dirac equation. There are many such equations on the market, for example the eight component two-fermion equation of Pilkuhn.[11] In these treatments QFT effects, such as the virtual annihilation interaction [Eq. (27)] do not arise naturally but need to be added in.

The fact that only the lowest order (''tree level'') diagrams appear in our Eq. (24) is a reflection of the fact that we have used the simplest possible variational ansatz (20). Even so, it is important to note that, because of the reformulation discussed in Secs. II and III, their derivation does not require additional Fock-space terms in the variational state (20) as is the case in traditional (nonreformulated) treatments (e.g., Refs. 12–14).

In the nonrelativistic limit, the functions $F_{s_1 s_2}$ can be written as

$$F_{s_1 s_2}(\mathbf{p})=F(\mathbf{p})\Lambda_{s_1 s_2}, \tag{28}$$

where the nonzero elements of Λ_{ij} for total spin singlet ($S=0$) states are $\Lambda_{12}=-\Lambda_{21}=1/\sqrt{2}$, while for the spin triplet ($S=1$) states the nonzero elements are $\Lambda_{11}=1$ for $m_s=+1$, $\Lambda_{12}=\Lambda_{21}=1/\sqrt{2}$ for $m_s=0$, and $\Lambda_{22}=1$ for $m_s=-1$. We use the notation that the subscripts 1 and 2 of Λ correspond to $m_s=1/2$ and $m_s=-1/2$ (or $\uparrow$ and $\downarrow$) respectively. Substituting (28) into (24), the variational procedure, after multiplying the result by $\Lambda_{s_1 s_2}$ and summing over s_1 and s_2, gives the equation

$$(2\omega_p-E)F(\mathbf{p})=\frac{1}{(2\pi)^3}\int d^3\mathbf{q}\,\mathcal{K}(\mathbf{p},\mathbf{q})F(\mathbf{q}), \tag{29}$$

where

$$\mathcal{K}(\mathbf{p},\mathbf{q})=-i\frac{m^2}{\omega_p\omega_q}\sum_{s_1 s_2\sigma_1\sigma_2}\Lambda_{s_1 s_2}\mathcal{M}_{s_1 s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})\Lambda_{\sigma_1\sigma_2}. \tag{30}$$

To lowest-order in $|\mathbf{p}|/m$ (i.e., in the nonrelativistic limit), the kernel (30) reduces to $\mathcal{K}=e^2/|\mathbf{p}-\mathbf{q}|^2$, and so (29) reduces to the (momentum-space) Schrödinger equation

$$\left(\frac{\mathbf{p}^2}{2\mu}-\varepsilon\right)F(\mathbf{p})=\frac{1}{(2\pi)^3}\int d^3\,\mathbf{q}\,\frac{e^2}{|\mathbf{p}-\mathbf{q}|^2}F(\mathbf{q}), \tag{31}$$

where $\varepsilon=E-2m$ and $\mu=m/2$. This verifies that the relativistic two-fermion equation (24) has the expected nonrelativistic limit.

In the relativistic case we do not complete the variational procedure in (24) at this stage to get equations for the four adjustable functions $F_{s_1 s_2}$, because they are not independent in general. Indeed we require that the trial state be an eigenstate of the total angular momentum operator (in relativistic form), its projection, parity and charge conjugation, namely, that

$$\begin{bmatrix} \hat{\mathbf{J}}^2 \\ \hat{J}_3 \\ \hat{\mathcal{P}} \\ \hat{\mathcal{C}} \end{bmatrix} |\psi_T\rangle = \begin{bmatrix} J(J+1) \\ m_J \\ P \\ C \end{bmatrix} |\psi_T\rangle, \tag{32}$$

where $m_J = J, J-1, \ldots, -J$ as usual. We present explicit forms for the operators $\hat{\mathbf{J}}^2$, $\hat{J}_3$ in Appendix A. The form for $\hat{\mathbf{J}}^2$, Eq. (109), in particular, is not readily found in standard texts and reference books.

The functions $F_{s_1s_2}(\mathbf{p})$ can be written in the general form

$$F_{s_1s_2}(\mathbf{p}) = \sum_{\ell_{s_1s_2}} \sum_{m_{s_1s_2}} f_{s_1s_2}^{\ell_{s_1s_2} m_{s_1s_2}}(p) Y_{\ell_{s_1s_2}}^{m_{s_1s_2}}(\hat{\mathbf{p}}), \tag{33}$$

where $Y_{\ell_{s_1s_2}}^{m_{s_1s_2}}(\hat{\mathbf{p}})$ are the usual spherical harmonics. Here and henceforth we will use the notation $p = |\mathbf{p}|$, etc. (four-vectors will be written as p^μ). The orbital indexes $\ell_{s_1s_2}$ and $m_{s_1s_2}$ depend on the spin indexes s_1 and s_2 and are specified by equations (32). The radial coefficients $f_{s_1s_2}^{\ell_{s_1s_2} m_{s_1s_2}}(p)$ in the expansion (33) also depend on the spin variables.

Substitution of (33) into (20) and then into (32) leads to two categories of relations among the adjustable functions, as shown in Appendixes A and B. It follows that, for trial states of the form (20), the total spin of the system is a good quantum number, and the states of the system separate into singlet states with the total spin $S=0$ (parastates) and into triplet states with $S=1$ (orthostates). We should point out that this phenomenon is characteristic of the fermion antifermion systems, which are charge conjugation eigenstates, and does not arise for systems like $\mu^+ e^-$.

A. The singlet states

In this case $\ell_{s_1s_2} \equiv \ell = J$, $m_{11} = m_{22} = 0$ and $m_{12} = m_{21} = m_J$. The nonzero components of $F_{s_1s_2}(\mathbf{p})$ are $F_{\uparrow\downarrow}(\mathbf{p}) \equiv F_{12}(\mathbf{p})$, $F_{\downarrow\uparrow}(\mathbf{p}) \equiv F_{21}(\mathbf{p})$ and have the form

$$F_{s_1s_2}(\mathbf{p}) = f_{s_1s_2}^{(\mathrm{sgl})J}(p) Y_J^{m_{s_1s_2}}(\hat{\mathbf{p}}), \tag{34}$$

where the relations between $f_{12}^{(\mathrm{sgl})J}(p)$ and $f_{21}^{(\mathrm{sgl})J}(p)$ involve the Clebsch–Gordan (C–G) coefficients $C_{Jm_J}^{(\mathrm{sgl})Jm_{s_1s_2}}$, that is

$$f_{s_1s_2}^{(\mathrm{sgl})J}(p) = C_{Jm_J}^{(\mathrm{sgl})Jm_{s_1s_2}} f^J(p), \tag{35}$$

as is shown in Appendix A. We see that the spin and radial variables separate for the singlet states in the sense that the factors $f_{s_1s_2}^{(\mathrm{sgl})J}(p)$ have a common radial function $f^J(p)$. Thus, for the singlet states we obtain

$$F_{s_1s_2}(\mathbf{p}) = C_{Jm_J}^{(\mathrm{sgl})Jm_{s_1s_2}} f^J(p) Y_J^{m_J}(\hat{\mathbf{p}}). \tag{36}$$

The C–G coefficients $C_{Jm_J}^{(\mathrm{sgl})Jm_{s_1s_2}}$ have a simple form: $C_{Jm_J}^{(\mathrm{sgl})Jm11} = C_{Jm_J}^{(\mathrm{sgl})Jm22} = 0$, $C_{Jm_J}^{(\mathrm{sgl})Jm12} = -C_{Jm_J}^{(\mathrm{sgl})Jm21} = 1$ (see Appendix A). Therefore for the singlet states we can write expression (20) in the explicit form

$$|\psi_T\rangle = \int d^3\mathbf{p} f^J(p) Y_J^{m_J}(\hat{\mathbf{p}}) (b_{\mathbf{p}\uparrow}^\dagger d_{-\mathbf{p}\downarrow}^\dagger - b_{\mathbf{p}\downarrow}^\dagger d_{-\mathbf{p}\uparrow}^\dagger)|0\rangle. \tag{37}$$

These states are characterized by the quantum numbers J, m_J parity $P=(-1)^{J+1}$ and charge conjugation $C=(-1)^J$. As we can see, the quantum numbers ℓ (orbital angular momentum), and total spin S are good quantum numbers for the singlet states as well. The spectroscopical notation is ${}^1J_J$.

B. The triplet states

The solution of the system (32) for $S=1$ leads to two cases (Appendix A), namely, $\ell_{s_1s_2} \equiv \ell = J$, for which

$$F_{s_1s_2}(\mathbf{p}) = f^{(\mathrm{tr})J}_{s_1s_2}(p) Y^{m_{s_1s_2}}_J(\hat{\mathbf{p}}), \tag{38}$$

and $\ell_{s_1s_2} \equiv \ell = J \mp 1$, for which

$$F_{s_1s_2}(\mathbf{p}) = f^{J-1}_{s_1s_2}(p) Y^{m_{s_1s_2}}_{J-1}(\hat{\mathbf{p}}) + f^{J+1}_{s_1s_2}(p) Y^{m_{s_1s_2}}_{J+1}(\hat{\mathbf{p}}), \tag{39}$$

where

$$m_{11} = m_J - 1, \; m_{12} = m_{21} = m_J, \;\; m_{22} = m_J + 1. \tag{40}$$

The expressions for $f^{\ell}_{s_1s_2}(p)$ in both cases involve the C–G coefficients $C^{(\mathrm{tr})\ell m_s}_{Jm_J}$ for $S=1$ listed in Appendix A, that is

$$f^{(\mathrm{tr})\ell}_{s_1s_2}(p) = C^{(\mathrm{tr})\ell m_s}_{Jm_J} f^{\ell}(p), \tag{41}$$

where the index m_s is defined as

$$\begin{aligned} m_s &= +1, \text{ when } \; m_{s_1s_2} = m_{11}, \\ m_s &= 0, \text{ when } \; m_{s_1s_2} = m_{12} = m_{21}, \\ m_s &= -1, \text{ when } \; m_{s_1s_2} = m_{22}. \end{aligned} \tag{42}$$

Thus, for the triplet states with $\ell = J$,

$$F_{s_1s_2}(\mathbf{p}) = C^{(\mathrm{tr})Jm_s}_{Jm_J} f^J(p) Y^{m_{s_1s_2}}_J(\hat{\mathbf{p}}). \tag{43}$$

These functions correspond to states, which can be characterized by the quantum numbers J, m_J, parity $P=(-1)^{J+1}$ and charge conjugation $C=(-1)^{J+1}$. The orbital angular momentum ℓ, as well as the total spin $S=1$, are good quantum numbers in this case. The spectroscopic notation for these states is ${}^3J_J$.

For the triplet states with $\ell = J \mp 1$ we obtain the result

$$F_{s_1s_2}(\mathbf{p}) = C^{(\mathrm{tr})(J-1)m_s}_{Jm_J} f^{J-1}(p) Y^{m_{s_1s_2}}_{J-1}(\hat{\mathbf{p}}) + C^{(\mathrm{tr})(J+1)m_s}_{Jm_J} f^{J+1}(p) Y^{m_{s_1s_2}}_{J+1}(\hat{\mathbf{p}}), \tag{44}$$

which involves two radial functions $f^{J-1}(p)$ and $f^{J+1}(p)$ corresponding to $\ell = J-1$ and $\ell = J+1$. This means that ℓ is not a good quantum number. Such states are characterized by quantum numbers J, m_J, $P=(-1)^J$, charge conjugation $C=(-1)^J$ and spin $S=1$. In spectroscopic notation, these states are a mixture of ${}^3(J-1)_J$ and ${}^3(J+1)_J$ states.

The requirement that the states be charge conjugation eigenstates [the last equation of (32)] is intimately tied to the conservation of total spin. Indeed, a linear combination of singlet and triplet states like

$$F_{s_1s_2}(\mathbf{p}) = C_1 f^{(\mathrm{sgl})J}_{s_1s_2}(p) Y_J^{m_{s_1s_2}}(\hat{\mathbf{p}}) + C_2 f^{(\mathrm{tr})J}_{s_1s_2}(p) Y_J^{m_{s_1s_2}}(\hat{\mathbf{p}}), \tag{45}$$

satisfies the first three equations of (32). However, it is unacceptable for describing a fermion–antifermion system because the first and the second terms in (45) have different charge conjugation. For a system of two particles of different mass (such as $\mu^+ e^-$) charge conjugation is not applicable, so that the total spin would not be conserved.

V. THE RELATIVISTIC RADIAL EQUATIONS AND APPLICATION TO POSITRONIUMLIKE SYSTEMS

We return to Eq. (24) and replace the functions $F_{s_1s_2}(p)$ by the expression (36) for singlet states and by (43) and (44) for triplet states. The variational procedure then leads to the following results:

For the singlet states $\ell = J$, $P = (-1)^{J+1}$, $C = (-1)^J$, the radial equations are

$$(2\omega_p - E) f^J(p) = \frac{m^2}{(2\pi)^3} \int \frac{q^2 dq}{\omega_p \omega_q} \mathcal{K}^{(\mathrm{sgl})}(p,q) f^J(q), \tag{46}$$

where the kernel

$$\mathcal{K}^{(\mathrm{sgl})}(p,q) = -i \sum_{s_1s_2\sigma_1\sigma_2 m_J} \int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, C^{(\mathrm{sgl})s_1s_2\sigma_1\sigma_2}_{Jm_J} \mathcal{M}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q}) Y_J^{m_J *}(\hat{\mathbf{p}}) Y_J^{m_J}(\hat{\mathbf{q}}) \tag{47}$$

is defined by the invariant M-matrix and the coefficients

$$C^{(\mathrm{sgl})s_1s_2\sigma_1\sigma_2}_{Jm_J} \equiv C^{(\mathrm{sgl})Jm_\sigma}_{Jm_J} C^{(\mathrm{sgl})Jm_s}_{Jm_J} \Big/ \sum_{\nu_1\nu_2 m_J} (C^{(\mathrm{sgl})Jm_\nu}_{Jm_J})^2. \tag{48}$$

Here we have summed over m_J, because of the $(2J+1)$-fold energy degeneracy.

For the triplet states, we obtain different equations for the $\ell = J$, and $\ell = J \mp 1$ cases. Thus for the states with $\ell = J$, $P = (-1)^{J+1}$, $C = (-1)^{J+1}$ the result is

$$(2\omega_p - E) f^J(p) = \frac{m^2}{(2\pi)^3} \int \frac{q^2 dq}{\omega_p \omega_q} \mathcal{K}^{(\mathrm{tr})}(p,q) f^J(q), \tag{49}$$

where the kernel $K^{(\mathrm{tr})}$ is formally like that of (47), namely,

$$\mathcal{K}^{(\mathrm{tr})}(p,q) = -i \sum_{s_1s_2\sigma_1\sigma_2 m_J} C^{(\mathrm{tr})s_1s_2\sigma_1\sigma_2}_{Jm_J} \int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, \mathcal{M}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q}) Y_J^{m_{s_1s_2}*}(\hat{\mathbf{p}}) Y_J^{m_{\sigma_1\sigma_2}}(\hat{\mathbf{q}}). \tag{50}$$

However it involves different C–G coefficients, namely,

$$C^{(\mathrm{tr})s_1s_2\sigma_1\sigma_2}_{Jm_J} = C^{(\mathrm{tr})Jm_\sigma}_{Jm_J} C^{(\mathrm{tr})Jm_s}_{Jm_J} \Big/ \sum_{\nu_1\nu_2 m_J} (C^{(\mathrm{tr})Jm_\nu}_{Jm_J})^2. \tag{51}$$

For the triplet states with $\ell = J \mp 1$, we have two independent radial functions $f^{J-1}(p)$ and $f^{J+1}(p)$. Thus the variational equation (24) leads to a system of coupled equations for $f^{J-1}(p)$ and $f^{J+1}(p)$. It is convenient to write them in matrix form,

$$(2\omega_p - E)\mathbb{F}(p) = \frac{m^2}{(2\pi)^3} \int \frac{q^2 dq}{\omega_p \omega_q} \mathbb{K}(p,q)\mathbb{F}(q), \tag{52}$$

where

$$\mathbb{F}(p)=\begin{bmatrix} f^{J-1}(p) \\ f^{J+1}(p) \end{bmatrix}, \tag{53}$$

and

$$\mathbb{K}(p,q)=\begin{bmatrix} \mathcal{K}_{11}(p,q) & \mathcal{K}_{12}(p,q) \\ \mathcal{K}_{21}(p,q) & \mathcal{K}_{22}(p,q) \end{bmatrix}. \tag{54}$$

The kernels K_{ij} are similar in form to (47) and (50), that is

$$\mathcal{K}_{ij}(p,q)=-i\sum_{\sigma_1\sigma_2 s_1 s_2 m_J} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j}\int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, \mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q}) Y^{m_{\sigma_1\sigma_2}}_{\ell_j}(\hat{\mathbf{q}}) Y^{m_{s_1 s_2}*}_{\ell_i}(\hat{\mathbf{p}}). \tag{55}$$

However the coefficients $C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j}$ are defined by expression

$$C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j}=C^{(\mathrm{tr})\ell_j m_\sigma}_{J m_J} C^{(\mathrm{tr})\ell_i m_s}_{J m_J} \Big/ \sum_{s_1 s_2 m_J} (C^{(\mathrm{tr})\ell_i m_s}_{J m_J})^2, \tag{56}$$

where $\ell_1=J-1$, $\ell_2=J+1$ and m_S is as defined in Eq. (42). The system (52) reduces to a single equation for $J=0$ since $f^{J-1}(p)=0$ in that case.

Our Eq. (24), or its radial components (46), (49), (52), contain the relativistic two-body kinematics (kinetic energy, recoil effects) exactly, but the dynamics are included approximately due to the limited nature of our trial state (20). This limitation is reflected in the fact that the interaction kernels of our equations contain only ''tree-level'' Feynman diagrams. Nevertheless our Eqs. (46), (49), (52) have no negative-energy solutions, in contrast to the BS equation. They are variationally derived, hence the energy eigenvalues obtained from them will give meaningful values for any strength of the coupling.

To our knowledge, it is not possible to obtain analytic solutions of the relativistic radial momentum-space equations (46), (49), and (52). Thus one must resort to numerical or other approximation methods. Numerical solutions of such equations are discussed, for example, in Ref. 10, while a variational approximation has been employed in Ref. 5. However, in this paper we will concentrate on perturbative $O(\alpha^4)$ solutions, since it is important to verify that our equations yield the correct fine structure for systems like positronium.

Our equations will yield energies which are incomplete beyond $O(\alpha^4)$, because our variational trial state (20), as mentioned, reflects only ''tree-level'' Feynman diagrams, that is no radiative corrections are incorporated. One could, of course, augment them by the addition of invariant matrix elements corresponding to higher-order Feynman diagrams (including radiative corrections) to the existing $\mathcal{M}$-matrices in the kernels of our equations, as is done in the BS formalism. Indeed, such an approach has been used in a similar, though not variational, treatment of positronium by Zhang and Koniuk.[15] These authors show that the inclusion of invariant matrix elements corresponding to single-loop diagrams yields positronium energy eigenstates which are accurate to $O(\alpha^5, \alpha^5 \ln \alpha)$. However such augmentation of the kernels ''by hand'' would be contrary to the spirit of the present variational treatment, and we shall not pursue it in this work.

VI. SEMIRELATIVISTIC EXPANSIONS AND THE NONRELATIVISTIC LIMIT

For perturbative solutions of our radial equations, it is necessary to work out expansions of the relevant expressions to first order beyond the nonrelativistic limit. This shall be summarized in the present section. We perform the calculation in the Coulomb gauge, in which the photon propagator has the form[16]

$$D_{00}(\mathbf{k})=\frac{1}{\mathbf{k}^2}, \quad D_{0j}(\mathbf{k})=0, \quad D_{ij}(k^\mu)=\frac{1}{k^\mu k_\mu}\left(\delta_{ij}-\frac{k_i k_j}{\mathbf{k}^2}\right), \tag{57}$$

where $k^\mu=(\omega_p-\omega_q,\mathbf{p}-\mathbf{q})$.

To expand the amplitudes $\mathcal{M}$ of (26) and (27) to one order of $(p/m)^2$ beyond the nonrelativistic limit, we take the free-particle spinors to be

$$u(\mathbf{p},i)=\begin{bmatrix}\left(1+\dfrac{\mathbf{p}^2}{8m^2}\right)\\ \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m}\end{bmatrix}\varphi_i,\quad v(\mathbf{p},i)=\begin{bmatrix}\dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m}\\ \left(1+\dfrac{\mathbf{p}^2}{8m^2}\right)\end{bmatrix}\chi_i, \tag{58}$$

as discussed in Appendix C. In this approximation the photon propagator takes on the form

$$D_{00}(\mathbf{p}-\mathbf{q})=\frac{1}{(\mathbf{p}-\mathbf{q})^2},\qquad D_{ij}(\mathbf{p}-\mathbf{q})\simeq-\frac{1}{(\mathbf{p}-\mathbf{q})^2}\left(\delta_{ij}-\frac{(p-q)_i(p-q)_j}{(\mathbf{p}-\mathbf{q})^2}\right). \tag{59}$$

Corresponding calculations give for the orbital part of the $\mathcal{M}$-matrix

$$\mathcal{M}^{\mathrm{ope(orb)}}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})=ie^2\left\{\frac{1}{(\mathbf{p}-\mathbf{q})^2}+\frac{1}{m^2}\left(\frac{1}{4}+\frac{\mathbf{q}\cdot\mathbf{p}}{(\mathbf{p}-\mathbf{q})^2}+\frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}\right)\right\}\delta_{s_1\sigma_1}\delta_{s_2\sigma_2}. \tag{60}$$

The terms of the expansion linear in spin correspond to the spin–orbit interaction:

$$\mathcal{M}^{\mathrm{ope(s-o)}}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})=\frac{3e^2}{4m^2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\frac{(\boldsymbol{\sigma}^{(+)}-\boldsymbol{\sigma}^{(-)})\cdot(\mathbf{p}\times\mathbf{q})}{(\mathbf{p}-\mathbf{q})^2}\varphi_{\sigma_1}\chi_{s_2}. \tag{61}$$

Here $\boldsymbol{\sigma}^{(+)}$ and $\boldsymbol{\sigma}^{(-)}$ are positron and electron spin matrices, respectively, defined as follows: $\boldsymbol{\sigma}^{(+)}\varphi_{\sigma_1}\chi_{s_2}=(\boldsymbol{\sigma}^{(+)}\varphi_{\sigma_1})\chi_{s_2}$, $\boldsymbol{\sigma}^{(-)}\varphi_{\sigma_1}\chi_{s_2}=\varphi_{\sigma_1}(\boldsymbol{\sigma}^{(-)}\chi_{s_2})$. The quadratic spin terms or spin–spin interaction terms are

$$\mathcal{M}^{\mathrm{ope(s-s)}}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})=\frac{ie^2}{4m^2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\left\{-\frac{(\boldsymbol{\sigma}^{(+)}\cdot(\mathbf{p}-\mathbf{q}))(\boldsymbol{\sigma}^{(-)}\cdot(\mathbf{p}-\mathbf{q}))}{(\mathbf{p}-\mathbf{q})^2}+\boldsymbol{\sigma}^{(+)}\cdot\boldsymbol{\sigma}^{(-)}\right\}\varphi_{\sigma_1}\chi_{s_2}. \tag{62}$$

Lastly, the virtual annihilation contribution is given by

$$\mathcal{M}^{\mathrm{ann}}_{s_1s_2\sigma_1\sigma_2}(p,q)=-\frac{ie^2}{4m^2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\{\boldsymbol{\sigma}^{(+)}\cdot\boldsymbol{\sigma}^{(-)}\}\varphi_{\sigma_1}\chi_{s_2}, \tag{63}$$

where we have excluded a divergent term, which appears in the Coulomb gauge calculation. This divergence is an artifact of the Coulomb gauge. It does not arise, for example, in the Lorentz gauge, where only expression (63) is obtained. However the Lorentz gauge is not convenient for obtaining all other $O(\alpha^4)$ corrections because it contains spurious degrees of freedom (longitudinal polarization) of the photon.

We have used expressions (60)–(63) to obtain the corresponding radial kernels. Details of the calculations can be found in Appendix D. We use the notation $z=(p^2+q^2)/2pq$, and $Q_\lambda(z)$ is the Legendre function of the second kind.[17] The contributions of the various terms to the kernel are as follows:

Singlet states with $\ell=J$ $(J\geqslant 0)$, $P=(-1)^{J+1}$, $C=(-1)^J$.

Orbital term

$$\mathcal{K}^{(\mathrm{sgl})(\mathrm{o})}(p,q)=\frac{2\pi e^2}{pq}Q_J(z)+\frac{\pi e^2}{m^2}\left(-\frac{J-3}{2}\left(\frac{p}{q}+\frac{q}{p}\right)Q_J(z)+(J+1)Q_{J+1}(z)-2\delta_{J,0}\right). \tag{64}$$

Spin–orbit interaction

$$\mathcal{K}^{(\mathrm{sgl})(\mathrm{s-o})}(p,q)=0. \tag{65}$$

Spin–spin interaction

$$\mathcal{K}^{(\mathrm{sgl})(\mathrm{s-s})}(p,q)=\frac{2\pi e^2}{m^2}\delta_{J,0}. \tag{66}$$

Triplet states with $\ell=J$ $(J\geqslant 1)$, $P=(-1)^{J+1}$, $C=(-1)^{J+1}$.

Orbital term

$$K^{(\mathrm{tr})(\mathrm{o})}(p,q)=\frac{2\pi e^2}{pq}Q_J(z)+\frac{\pi e^2}{m^2}\left(-\frac{J-3}{2}\left(\frac{p}{q}+\frac{q}{p}\right)Q_J(z)+(J+1)Q_{J+1}(z)\right). \tag{67}$$

Spin–orbit interaction

$$K^{(\mathrm{tr})(\mathrm{s-o})}(p,q)=-\frac{3\pi e^2}{m^2}\frac{1}{2J+1}\{Q_{J+1}(z)-Q_{J-1}(z)\}. \tag{68}$$

Spin–spin interaction

$$\mathcal{K}^{(\mathrm{tr})(\mathrm{s-s})}(p,q)=\frac{\pi e^2}{2m^2}\left(\frac{p}{q}+\frac{q}{p}\right)Q_J(z)-\frac{\pi e^2}{m^2}\frac{1}{2J+1}\{JQ_{J+1}(z)+(J+1)Q_{J-1}(z)\}. \tag{69}$$

Triplet states with $\ell=J-1$ $(J\geqslant 1)$, $\ell=J+1$ $(J\geqslant 0)$, $P=(-1)^J$, $C=(-1)^J$.

The off-diagonal elements of the kernel matrix [Eqs. (52)–(54)], K_{12} and K_{21} which are responsible for mixing of states with $\ell=J-1$ and $\ell=J+1$, get a nonzero contribution from the spin-spin interactions only:

$$\mathcal{K}_{12}(p,q)=\mathcal{K}_{21}(p,q)=\frac{\pi e^2}{5m^2}\frac{\sqrt{J(J+1)}}{(2J+1)}\left(\frac{p}{q}Q_{J+1}(z)+\frac{q}{p}Q_{J-1}(z)-2Q_J(z)\right). \tag{70}$$

The contributions to the diagonal elements of the kernel matrix are the following:

Orbital terms

$$\mathcal{K}_{11}^{(\mathrm{o})}(p,q)=\frac{2\pi e^2}{pq}Q_{J-1}(z)+\frac{\pi e^2}{m^2}\left(-\frac{J-4}{2}\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J-1}(z)+JQ_J(z)-2\delta_{J-1,0}\right), \tag{71}$$

$$\mathcal{K}_{22}^{(\mathrm{o})}(p,q)=\frac{2\pi e^2}{pq}Q_{J+1}(z)+\frac{\pi e^2}{m^2}\left(-\frac{J-2}{2}\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J+1}+(J+2)Q_{J+2}\right). \tag{72}$$

Spin–orbit interaction

$$\mathcal{K}_{11}^{(\mathrm{s-o})}(p,q)=\frac{3\pi e^2}{m^2}\frac{J-1}{2J-1}(Q_J(z)-Q_{J-2}(z)), \tag{73}$$

$$\mathcal{K}_{22}^{(\mathrm{s-o})}(p,q)=-\frac{3\pi e^2}{m^2c^2}\frac{J+2}{2J+3}(Q_{J+2}(z)-Q_J(z)). \tag{74}$$

Spin–spin interaction

$$\mathcal{K}_{11}^{(\mathrm{s-s})}(p,q)=\frac{\pi e^2}{2m^2}\frac{1}{2J+1}\left(\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J-1}(z)-2Q_J(z)\right), \tag{75}$$

$$\mathcal{K}_{22}^{(\mathrm{s-s})}(p,q)=\frac{\pi e^2}{2m^2}\frac{1}{2J+3}\left(\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J+1}(z)-2Q_{J+2}(z)\right). \tag{76}$$

Annihilation term

$$\mathcal{K}^{\mathrm{ann}}(p,q)=-\frac{2\pi e^2}{m^2}\delta_{J-1,0}. \tag{77}$$

We note that in the nonrelativistic limit only the first terms of the orbital part of the kernels survive. They have the common form $2\pi i e^2 Q_\ell(z)/pq$, hence all radial equations reduce to the form

$$(2\omega_p-E)f^\ell(p)=\frac{m^2e^2}{\pi\omega_p p}\int_0^\infty dq\,\frac{q}{\omega_q}Q_\ell(z)f^\ell(q). \tag{78}$$

Recalling, also, that

$$\omega_p=\sqrt{m^2+\mathbf{p}^2}\simeq m\left(1+\frac{1}{2}\left(\frac{\mathbf{p}}{m}\right)^2\right), \tag{79}$$

we obtain, in the nonrelativistic limit, the momentum-space Schrödinger radial equations

$$\left(\frac{\mathbf{p}^2}{2\mu}-\varepsilon\right)f^\ell(p)=\frac{\alpha}{\pi}\frac{1}{p}\int_0^\infty dq\,q\,Q_J(z)f^\ell(q), \tag{80}$$

where $\alpha=e^2/4\pi$, $\mu=m/2$, $\varepsilon=E-2m$.

VII. ENERGY LEVELS: FINE AND HYPERFINE STRUCTURE

The relativistic energy eigenvalues $E_{n,J}$ can be calculated from the expression

$$\begin{aligned}E\int_0^\infty dp\,p^2 f^J(p)f^J(p)=&\int_0^\infty dp\,p^2\,2\omega_p f^J(p)f^J(p)\\&-\frac{m^2}{(2\pi)^3}\int_0^\infty\frac{dpp^2}{\omega_p}\int_0^\infty dq\,\frac{q^2}{\omega_q}\mathcal{K}^{(\mathrm{sgl,tr})}(p,q)f^J(p)f^J(q)\end{aligned} \tag{81}$$

for the singlet and $\ell=J$ triplet states.

For the $\ell=J\mp1$ triplet states the corresponding result is [see Eq. (52)]

$$\begin{aligned}E\int_0^\infty dp\,p^2\mathbb{F}^\dagger(p)\mathbb{F}(p)=&\int_0^\infty dp\,p^2\,2\omega_p\mathbb{F}^\dagger(p)\mathbb{F}(p)\\&-\frac{m^2}{(2\pi)^3}\int_0^\infty\frac{dpp^2}{\omega_p}\int_0^\infty dq\,\frac{q^2}{\omega_q}\mathbb{K}(p,q)\mathbb{F}^\dagger(p)\mathbb{F}(q).\end{aligned} \tag{82}$$

To obtain results for E to $O(\alpha^4)$ we use the forms of the kernels expanded to $O(p^2/m^2)$ [Eqs. (64)–(77)] and replace $f^\ell(p)$ by their nonrelativistic (Schrödinger) form (see (D10), Appendix D). The most important integrals that we used for calculating (81) and (82), are given in Appendix D. In Appendix E we show that the contribution of kernels K_{12} and K_{21} in (82), is zero at $O(\alpha^4)$. Thus, the energy corrections for the triplet states with $\ell=J-1$ and $\ell=J+1$ can be calculated independently.

The results will be presented in the form $\Delta\varepsilon=E-2m+\alpha^2m/4n^2$.

A. Singlet states ($\ell = J$ ($J \geqslant 0$), $P = (-1)^{J+1}$, $C = (-1)^J$)

The kinetic energy corrections

$$\Delta\varepsilon_K^{(\mathrm{sgl})} = -\frac{\alpha^4 m}{8}\left(\frac{1}{2J+1}\frac{1}{n^3} - \frac{3}{8}\frac{1}{n^4}\right). \tag{83}$$

The potential energy corrections

$$\Delta\varepsilon_P^{(\mathrm{sgl})(\mathrm{o})} = -\frac{\alpha^4 m}{8}\left(\left(\frac{3}{2J+1} - 2\delta_{J,0}\right)\frac{1}{n^3} - \frac{1}{n^4}\right), \tag{84}$$

$$\Delta\varepsilon_P^{(\mathrm{sgl})(\mathrm{s-o})} = 0, \tag{85}$$

$$\Delta\varepsilon_P^{(\mathrm{sgl})(\mathrm{s-s})} = -\frac{\alpha^4 m}{4}\frac{\delta_{J,0}}{n^3}. \tag{86}$$

The total energy corrections

$$\Delta\varepsilon^{(\mathrm{sgl})} = -\frac{\alpha^4 m}{8}\left(\frac{4}{2J+1}\frac{1}{n^3} - \frac{11}{8n^4}\right). \tag{87}$$

B. Triplet states ($\ell = J$ ($J \geqslant 1$), $P = (-1)^{J+1}$, $C = (-1)^{J+1}$)

The kinetic energy corrections

$$\Delta\varepsilon_K^{(\mathrm{tr})} = -\frac{\alpha^4 m}{8}\left(\frac{1}{2J+1}\frac{1}{n^3} - \frac{3}{8}\frac{1}{n^4}\right). \tag{88}$$

The potential energy corrections

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{o})} = -\frac{\alpha^4 m}{8}\left(\left(\frac{3}{2J+1} - 2\delta_{J,0}\right)\frac{1}{n^3} - \frac{1}{n^4}\right), \tag{89}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-o})} = -\frac{\alpha^4 m}{8}\frac{3}{J(J+1)(2J+1)}\frac{1}{n^3}, \tag{90}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-s})} = \frac{\alpha^4 m}{8}\frac{1}{J(J+1)(2J+1)}\frac{1}{n^3}. \tag{91}$$

The total energy corrections

$$\Delta\varepsilon^{(\mathrm{tr})} = -\frac{\alpha^4 m}{8}\left(\left(\frac{4}{2J+1} + \frac{2}{J(J+1)(2J+1)}\right)\frac{1}{n^3} - \frac{11}{8}\frac{1}{n^4}\right). \tag{92}$$

C. Triplet states ($\ell = J-1$ ($J \geqslant 1$), $P = (-1)^J$, $C = (-1)^J$)

The kinetic energy corrections

$$\Delta\varepsilon_K^{(\mathrm{tr})(J-1)} = -\frac{\alpha^4 m}{8}\left(\frac{1}{2J-1}\frac{1}{n^3} - \frac{3}{8}\frac{1}{n^4}\right). \tag{93}$$

The potential energy corrections

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{o})(J-1)}=-\frac{\alpha^4 m}{8}\left[\left(\frac{3}{2J-1}-2\,\delta_{J,1}\right)\frac{1}{n^3}-\frac{1}{n^4}\right], \tag{94}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-o})(J-1)}=\frac{\alpha^4 m}{8}\,\frac{3(1-\delta_{J,1})}{J(2J-1)}\,\frac{1}{n^3}, \tag{95}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-s})(J-1)}=-\frac{\alpha^4 m}{8}\left(\frac{1-\delta_{J,1}}{J(2J+1)(2J-1)}-\frac{2}{3}\,\delta_{J,1}\right)\frac{1}{n^3}, \tag{96}$$

$$\Delta\varepsilon^{(\mathrm{ann})}=\frac{\alpha^4 m}{4}\,\frac{1}{n^3}\,\delta_{J,1}. \tag{97}$$

The total energy corrections

$$\Delta\varepsilon^{(\mathrm{tr})(J-1)}=-\frac{\alpha^4 m}{8}\left(\left(\frac{4}{2J-1}-\frac{2(3J+1)}{J(2J+1)(2J-1)}-2\,\delta_{J,1}\right)\frac{1}{n^3}-\frac{11}{8}\,\frac{1}{n^4}\right). \tag{98}$$

D. Triplet states ($\ell=J+1$ ($J\geqslant 0$), $P=(-1)^J$, $C=(-1)^J$)

The kinetic energy corrections

$$\Delta\varepsilon_K^{(\mathrm{tr})(J+1)}=-\frac{\alpha^4 m}{8}\left(\frac{1}{2J+3}\,\frac{1}{n^3}-\frac{3}{8}\,\frac{1}{n^4}\right). \tag{99}$$

The potential energy corrections

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{o})(J+1)}=-\frac{\alpha^4 m}{8}\left[\frac{3}{2J+3}\,\frac{1}{n^3}-\frac{1}{n^4}\right], \tag{100}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-o})(J+1)}=-\frac{\alpha^4 m}{8}\,\frac{3}{(J+1)(2J+3)}\,\frac{1}{n^3}, \tag{101}$$

$$\Delta\varepsilon_P^{(\mathrm{tr})(\mathrm{s-s})(J+1)}=-\frac{\alpha^4 m}{8}\,\frac{1}{(J+1)(2J+3)(2J+1)}\,\frac{1}{n^3}. \tag{102}$$

The total energy corrections

$$\Delta\varepsilon^{(\mathrm{tr})(J+1)}=-\frac{\alpha^4 m}{8}\left(\frac{2}{2J+3}\left(2+\frac{3J+2}{(J+1)(2J+1)}\right)\frac{1}{n^3}-\frac{11}{8}\,\frac{1}{n^4}\right). \tag{103}$$

These results are in agreement with the well-known positronium fine structure results.[18,19]

VIII. CONCLUDING REMARKS

We have considered a reformulation of electrodynamics, in which covariant Green functions are used to solve the field equations for the mediating electromagnetic field in terms of the fermion field. This leads to a reformulated Hamiltonian with an interaction term in which the photon propagator appears sandwiched between fermionic currents.

The variational method within a Hamiltonian formalism of quantum field theory is used to determine approximate eigensolutions for bound relativistic fermion–antifermion states. The reformulation enables us to use the simplest possible trial state to derive a relativistic momentum-space Salpeter-type equation for a positroniumlike system. The invariant $\mathcal{M}$ matrices corresponding to one-photon exchange and virtual annihilation Feynman diagrams arise directly in the interaction kernel of this equation.

The trial states are chosen to be eigenstates of the total angular momentum operator $\hat{\mathbf{J}}^2$ and $\hat{J}_3$, along with parity and charge conjugation. A general relativistic reduction of the wave equations to radial form is given. For given J there is a single radial equation for total spin zero singlet states, but for spin triplet states there are, in general two coupled equations. We show how the classification of states follows naturally from the system of eigenvalue equations obtained with our trial state.

It is not possible, as far as we know, to obtain analytic solutions of our relativistic radial equations nor the resulting eigenvalues of the particle–antiparticle system described. However, it is possible to obtain $O(\alpha^4)$ corrections analytically for all states using perturbation theory. The results agree with well known results for positronium, obtained on the basis of the Bethe–Salpeter equation,[19] which lends credence to the validity of our variationally derived equations.

The method presented here can be generalized to include effects higher order in alpha by using dressed propagators in place of the bare propagators. This shall be the subject of a forthcoming work.

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APPENDIX A: TOTAL ANGULAR MOMENTUM OPERATOR IN RELATIVISTIC FORM

The total angular momentum operator is defined by expression

$$\hat{\mathbf{J}}=\int d^3\mathbf{x}:\psi^\dagger(x)(\hat{\mathbf{L}}+\hat{\mathbf{S}})\psi(x):, \tag{A1}$$

where $\hat{\mathbf{L}}=\hat{\mathbf{x}}\times\hat{\mathbf{p}}$ and $\hat{\mathbf{S}}=\frac{1}{2}\hat{\boldsymbol{\sigma}}$ are the orbital angular momentum and spin operators. We use the standard representation for the Pauli matrices

$$\hat{\boldsymbol{\sigma}}=\begin{bmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{bmatrix}, \tag{A2}$$

$$\sigma_1=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad \sigma_2=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\qquad \sigma_3=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}. \tag{A3}$$

Using the field operator $\psi(x)$ in the form (15), after tedious calculations we obtain

$$\begin{aligned}
\hat{J}_1&=\int d^3\mathbf{q}\begin{pmatrix}\hat{L}_{q1}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\\ +\frac{1}{2}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\downarrow})\end{pmatrix},\\
\hat{J}_2&=\int d^3\mathbf{q}\begin{pmatrix}\hat{L}_{q2}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\\ +\dfrac{i}{2}(-b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}-d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\uparrow})\end{pmatrix},\\
\hat{J}_3&=\int d^3\mathbf{q}\begin{pmatrix}\hat{L}_{q3}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\\ +\frac{1}{2}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}-b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}-d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\end{pmatrix}.
\end{aligned} \tag{A4}$$

Here $\hat{\mathbf{L}}_q$ is the orbital angular momentum operator in momentum representation:

$$(\hat{\mathbf{L}}_q)_i\equiv\hat{L}_{qi}=-i(\mathbf{q}\times\nabla_q)_i\,. \tag{A5}$$

Note that these expressions are valid for any t, since the time-dependent phase factors of the form $e^{i\omega_q t}$ cancel out.

For the operator $\hat{\mathbf{J}}^2=\hat{J}_1^2+\hat{J}_2^2+\hat{J}_3^2$ we have

$$\hat{\mathbf{J}}^2=\int d^3\mathbf{q}\begin{pmatrix}(\hat{\mathbf{L}}_q^2+\frac{3}{4})(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\\ +\hat{L}_{q-}b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}+\hat{L}_{q+}b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}+\hat{L}_{q-}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\downarrow}+\hat{L}_{q+}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\uparrow}\\ +\hat{L}_{q3}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow}-b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}+d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}-d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\end{pmatrix}$$
$$+\frac{1}{2}\int d^3\mathbf{q}'d^3\mathbf{q}\begin{pmatrix}2\hat{\mathbf{L}}_{q'}\cdot\hat{\mathbf{L}}_q\begin{pmatrix}b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow}\\ +b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow}\end{pmatrix}\\ +\frac{1}{2}(b^\dagger_{q'\uparrow}b_{q'\uparrow}d^\dagger_{q\uparrow}d_{q\uparrow}-b^\dagger_{q'\uparrow}b_{q'\uparrow}d^\dagger_{q\downarrow}d_{q\downarrow})\\ -\frac{1}{2}(b^\dagger_{q'\downarrow}b_{q'\downarrow}d^\dagger_{q\uparrow}d_{q\uparrow}-b^\dagger_{q'\downarrow}b_{q'\downarrow}d^\dagger_{q\downarrow}d_{q\downarrow})\\ +b^\dagger_{q'\uparrow}b_{q'\downarrow}d^\dagger_{q\downarrow}d_{q\uparrow}+b^\dagger_{q'\downarrow}b_{q'\uparrow}d^\dagger_{q\uparrow}d_{q\downarrow}\\ +\hat{L}_{q'+}\begin{pmatrix}b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\uparrow}+b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\uparrow}\\ +b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}d^\dagger_{\mathbf{q}'\uparrow}d_{\mathbf{q}'\uparrow}+b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}d^\dagger_{\mathbf{q}'\downarrow}d_{\mathbf{q}'\downarrow}\end{pmatrix}\\ +\hat{L}_{q'-}\begin{pmatrix}b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\downarrow}+b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\downarrow}\\ +b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}d^\dagger_{\mathbf{q}'\uparrow}d_{\mathbf{q}'\uparrow}+b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}d^\dagger_{\mathbf{q}'\downarrow}d_{\mathbf{q}'\downarrow}\end{pmatrix}\\ +(\hat{L}_{q'3}+\hat{L}_{q3})(b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow}-b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow})\\ -(\hat{L}_{q'3}-\hat{L}_{q3})(b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}d^\dagger_{\mathbf{q}\downarrow}d_{\mathbf{q}\downarrow}-b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}d^\dagger_{\mathbf{q}\uparrow}d_{\mathbf{q}\uparrow})\end{pmatrix}, \tag{A6}$$

where

$$\hat{L}_{q+}=\hat{L}_{q1}+i\hat{L}_{q2}, \qquad \hat{L}_{q-}=\hat{L}_{q1}-i\hat{L}_{q2}. \tag{A7}$$

The requirement that the trial state (20) be an eigenstate of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ leads to the system of equations

$$\begin{gathered}(\hat{L}_3+1)F_{11}=m_JF_{11},\\ \hat{L}_3F_{12}=m_JF_{12},\\ \hat{L}_3F_{21}=m_JF_{21},\\ (\hat{L}_3-1)F_{22}=m_JF_{22},\\ (J(J+1)-\hat{\mathbf{L}}^2-2-2\hat{L}_3)F_{11}=\hat{L}_-(F_{12}+F_{21}),\\ (J(J+1)-\hat{\mathbf{L}}^2-1)F_{12}=F_{21}+\hat{L}_+F_{11}+\hat{L}_-F_{22},\\ (J(J+1)-\hat{\mathbf{L}}^2-1)F_{21}=F_{12}+\hat{L}_+F_{11}+\hat{L}_-F_{22},\\ (J(J+1)-\hat{\mathbf{L}}^2-2+2\hat{L}_3)F_{22}=\hat{L}_+(F_{12}+F_{21}).\end{gathered} \tag{A8, A9}$$

Substitution of the expressions (33) for $F_{s_1s_2}$ and use of Eq. (A8) gives

$$m_{12}=m_{21}=m_J,\ \ m_{11}=m_J-1,\ \ m_{22}=m_J+1, \tag{A10}$$

$$\ell_{11}=\ell_{22}=\ell_{12}=\ell_{21}=\ell, \tag{A11}$$

and

$$(J(J+1)-\ell(\ell+1)-2m_J)f^{\ell}_{11}(p)=\sqrt{(\ell-m_J+1)(\ell+m_J)}f^{\ell}_{12}(p)+\sqrt{(\ell-m_J+1)(\ell+m_J)}f^{\ell}_{21}(p),$$

$$\begin{aligned}(J(J+1)-\ell(\ell+1)-1)f^{\ell}_{12}(p)&=f^{\ell}_{21}(p)+\sqrt{(\ell+m_J)(\ell-m_J+1)}f^{\ell}_{11}(p)\\&\quad+\sqrt{(\ell-m_J)(\ell+m_J+1)}f^{\ell}_{22}(p),\\(J(J+1)-\ell(\ell+1)-1)f^{\ell}_{21}(p)&=f^{\ell}_{12}(p)+\sqrt{(\ell+m_J)(\ell-m_J+1)}f^{\ell}_{11}(p)\\&\quad+\sqrt{(\ell-m_J)(\ell+m_J+1)}f^{\ell}_{22}(p),\end{aligned} \tag{A12}$$

$$(J(J+1)-\ell(\ell+1)+2m_J)f^{\ell}_{22}(p)=\sqrt{(\ell+m_J+1)(\ell-m_J)}f^{\ell}_{12}(p)+\sqrt{(\ell+m_J+1)(\ell-m_J)}f^{\ell}_{21}(p).$$

The singlet states correspond to the solution $f^{\ell}_{11}(p)=f^{\ell}_{22}(p)=0$, $f^{\ell}_{12}(p)=-f^{\ell}_{21}(p)$ of this system with $\ell=J$ $(J\geqslant 0)$.

For the triplet states the solutions are $f^{\ell}_{12}(p)=f^{\ell}_{21}(p)\equiv f^{\ell}(p)$, and, for $\ell=J-1$ $(J\geqslant 1)$:

$$(J-m_J)f^{J-1}_{11}(p)=\sqrt{(J-m_J)(J+m_J-1)}f^{J-1}(p), \tag{A13}$$

$$(J+m_J)f^{J-1}_{22}(p)=\sqrt{(J+m_J)(J-m_J-1)}f^{J-1}(p), \tag{A14}$$

for $\ell=J$ $(J\geqslant 1)$:

$$m_J f^{J}_{11}(p)=-\sqrt{(J+m_J)(J-m_J+1)}f^{J}(p), \tag{A15}$$

$$m_J f^{J}_{22}(p)=\sqrt{(J-m_J)(J+m_J+1)}f^{J}(p), \tag{A16}$$

for $\ell=J+1$ $(J\geqslant 0)$:

$$(J+1+m_J)f^{J+1}_{11}(p)=-\sqrt{(J-m_J+2)(J+m_J+1)}f^{J+1}(p), \tag{A17}$$

$$(J+1-m_J)f^{J+1}_{22}(p)=-\sqrt{(J-m_J+1)(J+m_J+2)}f^{J+1}(p). \tag{A18}$$

It is convenient to introduce the table of coefficients $C^{(\mathrm{tr})\ell m_s}_{Jm_J}$:

	$m_s=+1$	$m_s=0$	$m_s=-1$
$\ell=J-1$	$\sqrt{\frac{(J+m_J-1)(J+m_J)}{J(2J-1)}}$	$\sqrt{\frac{(J-m_J)(J+m_J)}{J(2J-1)}}$	$\sqrt{\frac{(J-m_J-1)(J-m_J)}{J(2J-1)}}$
$\ell=J$	$-\sqrt{\frac{(J+m_J)(J-m_J+1)}{J(J+1)}}$	$\frac{m_J}{\sqrt{J(J+1)}}$	$\sqrt{\frac{(J-m_J)(J+m_J+1)}{J(J+1)}}$
$\ell=J+1$	$\sqrt{\frac{(J-m_J+1)(J-m_J+2)}{(J+1)(2J+3)}}$	$-\sqrt{\frac{(J-m_J+1)(J+m_J+1)}{(J+1)(2J+3)}}$	$\sqrt{\frac{(J+m_J+2)(J+m_J+1)}{(J+1)(2J+3)}}$

These coefficients coincide with the usual Clebsch–Gordan coefficients for $S=1$ except for a factor 2 in the denominator, which we absorb into the normalization constant.

APPENDIX B: PARITY AND CHARGE CONJUGATION

We consider the application of the parity operator to the trial state (20):

$$\hat{\mathcal{P}}|\psi_T\rangle=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b^\dagger_{ps_1}\hat{\mathcal{P}}^{-1}\hat{\mathcal{P}}d^\dagger_{-ps_2}\hat{\mathcal{P}}^{-1}\hat{\mathcal{P}}|0\rangle. \tag{B1}$$

Making use of the properties

$$\hat{\mathcal{P}}b^\dagger_{ps_1}\hat{\mathcal{P}}^{-1}=\eta^P b^\dagger_{-ps_1},\qquad \hat{\mathcal{P}}d^\dagger_{-ps_2}\hat{\mathcal{P}}^{-1}=-\eta^P d^\dagger_{ps_2},\qquad \hat{\mathcal{P}}|0\rangle=|0\rangle, \tag{B2}$$

where η^P is the intrinsic parity ($(\eta^P)^2=1$), it follows that

$$\begin{aligned}\hat{\mathcal{P}}|\psi_T\rangle&=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle\\&=-\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(-\mathbf{p})b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle\\&=P\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle,\end{aligned} \tag{B3}$$

where the parity eigenvalue P depends on the symmetry of $F_{s_1s_2}(p)$ in different states:

For the singlet states ($\ell=J$) we get from (36) $F_{s_1s_2}(-p)=(-1)^JF_{s_1s_2}(p)$, so that $P=(-1)^{J+1}$.

For the triplet states with $\ell=J$ we get from (38) $F_{s_1s_2}(-p)=(-1)^JF_{s_1s_2}(p)$, hence $P=(-1)^{J+1}$.

For the triplet states with $\ell=J\pm1$ we get from (39) $F_{s_1s_2}(-p)=(-1)^{J+1}F_{s_1s_2}(p)$, therefore $P=(-1)^J$.

Charge conjugation is associated with the interchange of the particle and antiparticle. Applying the charge conjugation operator to the trial state (20) we get

$$\hat{\mathcal{C}}|\psi_T\rangle=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{C}}b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle \tag{B4}$$

$$=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{C}}b^\dagger_{ps_1}\hat{\mathcal{C}}^{-1}\hat{\mathcal{C}}d^\dagger_{-ps_2}\hat{\mathcal{C}}^{-1}\hat{\mathcal{C}}|0\rangle. \tag{B5}$$

Using the relations

$$\hat{\mathcal{C}}b^\dagger_{ps_1}\hat{\mathcal{C}}^{-1}=\eta^C d^\dagger_{ps_1},\qquad \hat{\mathcal{C}}d^\dagger_{-ps_2}\hat{\mathcal{C}}^{-1}=\eta^C b^\dagger_{-ps_2},\qquad \hat{\mathcal{C}}|0\rangle=|0\rangle, \tag{B6}$$

where $(\eta^C)^2=1$, we obtain

$$\begin{aligned}\hat{\mathcal{C}}|\psi_T\rangle&=\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})\hat{\mathcal{C}}b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle\\&=-\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_2s_1}(\mathbf{p})b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle\\&=C\sum_{s_1s_2}\int d^3\mathbf{p}F_{s_1s_2}(\mathbf{p})b^\dagger_{ps_1}d^\dagger_{-ps_2}|0\rangle,\end{aligned} \tag{B7}$$

where the charge conjugation quantum number C depends on the symmetry of $F_{s_1s_2}(p)$ in different states:

For the singlet states ($\ell=J$) we get from (36) $F_{s_1s_2}(-p)=(-1)^{J+1}F_{s_1s_2}(p)$, hence $C=(-1)^J$.

For the triplet states with $\ell = J$ we get from (38) $F_{s_1 s_2}(-p) = (-1)^J F_{s_1 s_2}(p)$, therefore $C = (-1)^{J+1}$.

For the triplet states with $\ell = J \pm 1$ we get from (39) $F_{s_1 s_2}(-p) = (-1)^{J+1} F_{s_1 s_2}(p)$, so that $C = (-1)^J$.

APPENDIX C: EXPANSION OF THE SPINORS

We recall the form of the particle spinors:

$$u(\mathbf{p},i) = N_{\mathbf{p}} \begin{bmatrix} 1 \\ \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{\omega_p + m} \end{bmatrix} \varphi_i , \tag{C1}$$

where

$$\varphi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \varphi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad N_{\mathbf{p}} = \sqrt{\frac{\omega_p + m}{2m}}. \tag{C2}$$

The antiparticle or ''positron'' representation for the $v_i(p)$ spinors has the form

$$v(\mathbf{p},i) = N_{\mathbf{p}} \begin{bmatrix} \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{\omega_p + m} \\ 1 \end{bmatrix} \chi_i , \tag{C3}$$

where

$$\chi_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad \chi_2 = -\begin{bmatrix} 1 \\ 0 \end{bmatrix}. \tag{C4}$$

The normalization is

$$\overline{u}(\mathbf{p},i) u(\mathbf{p},j) = \delta_{ij} , \qquad \overline{v}(\mathbf{p},i) v(\mathbf{p},j) = -\delta_{ij} . \tag{C5}$$

Expanding in powers of p/m and keeping the lowest non-trivial order terms,

$$\frac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{\omega_p + m} \simeq \frac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m}, \tag{C6}$$

$$N_{\mathbf{p}} = \sqrt{\frac{\omega_p + m}{2m}} \simeq 1 + \frac{\mathbf{p}^2}{8m^2}, \tag{C7}$$

we obtain the result

$$u(\mathbf{p},i) \simeq \left(1 + \frac{\mathbf{p}^2}{8m^2}\right) \begin{bmatrix} 1 \\ \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m} \end{bmatrix} \varphi_i = \begin{bmatrix} \left(1 + \dfrac{\mathbf{p}^2}{8m^2}\right) \\ \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m} \end{bmatrix} \varphi_i , \tag{C8}$$

$$v(\mathbf{p},i) \simeq \left(1 + \frac{\mathbf{p}^2}{8m^2}\right) \begin{bmatrix} \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m} \\ 1 \end{bmatrix} \chi_i = \begin{bmatrix} \dfrac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2m} \\ \left(1 + \dfrac{\mathbf{p}^2}{8m^2}\right) \end{bmatrix} \chi_i . \tag{C9}$$

APPENDIX D: SOME USEFUL IDENTITIES AND INTEGRALS

The following identity is useful for evaluating the $\mathcal{M}$ matrices:

$$\frac{((\mathbf{p}-\mathbf{q})\cdot\mathbf{p})^2}{(\mathbf{p}-\mathbf{q})^4}=\frac{\mathbf{p}^2}{(\mathbf{p}-\mathbf{q})^2}-\frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}. \tag{D1}$$

The angular integration in (47), (50), (55) involves the following integrals:

$$\int d\hat{\mathbf{p}}\,d\hat{\mathbf{q}}\,\mathsf{F}(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})Y_{J'}^{m_J'}(\hat{\mathbf{q}})Y_J^{m_J*}(\hat{\mathbf{p}})=2\pi\delta_{J'J}\delta_{m_J'm_J}\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\mathsf{F}(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}), \tag{D2}$$

$$\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}}{(\mathbf{p}-\mathbf{q})^2}P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})=\frac{1}{|\mathbf{p}||\mathbf{q}|}\left(\frac{J+1}{2J+1}Q_{J+1}(z)+\frac{J}{2J+1}Q_{J-1}(z)\right), \tag{D3}$$

$$\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})=\frac{(J+1)(J+2)}{2(2J+1)}Q_{J+1}(z)-\frac{J(J-1)}{2(2J+1)}Q_{J-1}(z), \tag{D4}$$

where $\mathsf{F}(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})$ is an arbitrary function of $\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}$, $P_J(x)$ is the Legendre polynomial, and $Q_J(z)$ is the Legendre function of the second kind of order J.

The following integrals are needed for the calculation of the relativistic energy corrections:

$$\int_0^\infty\int_0^\infty dp\,dq\,p^2q^2f^J(p)f^J(q)=2\pi\left(\frac{\alpha\mu}{n}\right)^3\delta_{J,0}, \tag{D5}$$

$$\int_0^\infty\int_0^\infty dp\,dq\,pqf^J(p)f^J(q)Q_J(z_1)=\frac{\pi\alpha\mu}{n^2}, \tag{D6}$$

$$\int_0^\infty\int_0^\infty dp\,dq\,p^2q^2f^J(p)f^J(q)Q_J(z_1)=\int_0^\infty\int_0^\infty dp\,dq\,p^3qf^J(p)f^J(q)Q_J(z_1)$$
$$=\pi\left(\frac{\alpha\mu}{n}\right)^3\left(\frac{4}{2J+1}-\frac{1}{n}\right), \tag{D7}$$

$$\int_0^\infty\int_0^\infty dp\,dq\,p^2q^2f^J(p)f^J(q)Q_{J-1}(z_1)=\pi\left(\frac{\alpha\mu}{n}\right)^3\left(\frac{2}{J}-\frac{1}{n}\right), \tag{D8}$$

$$\int_0^\infty\int_0^\infty dp\,dq\,p^2q^2f^J(p)f^J(q)Q_{J+1}(z_1)=\pi\left(\frac{\alpha\mu}{n}\right)^3\left(\frac{2}{J+1}-\frac{1}{n}\right). \tag{D9}$$

Here f^J is the nonrelativistic hydrogenlike radial wave function in momentum space[19]

$$f^J(p)\equiv f_n^J(p)=\left(\frac{2}{\pi}\frac{(n-J-1)!}{(n+J)!}\right)^{1/2}\frac{n^{J+2}p^J2^{2(J+1)}J!}{(n^2p^2+1)^{J+2}}\mathcal{G}_{n-J-1}^{J+1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right), \tag{D10}$$

where $G_{n-J-1}^{J+1}(x)$ are Gegenbauer functions.

APPENDIX E: $\mathcal{K}_{12}$, $\mathcal{K}_{21}$ KERNELS FOR $\ell=J\mp1$ STATES

The contribution of the kernel $\mathcal{K}_{12}$ to the energy correction is

$$\int dp\,dq\,p^2q^2\mathcal{K}_{12}(p,q)f^{J-1}(p)f^{J+1}(q), \tag{E1}$$

where

$$\mathcal{K}_{12}(p,q)=\sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12}\int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, \mathcal{M}^{\text{ope(s-s)}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q}) Y^{m_{\sigma_1\sigma_2}}_{J+1}(\hat{\mathbf{q}}) Y^{m_{s_1 s_2}*}_{J-1}(\hat{\mathbf{p}}). \tag{E2}$$

This requires the following integral:

$$\sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12}\int d^3\mathbf{p}\, d^3\mathbf{q}\, f^{J-1}(p) Y^{m_{s_1 s_2}*}_{J-1}(\hat{\mathbf{p}}) \mathcal{M}^{\text{ope(s-s)}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q}) f^{J+1}(q) Y^{m_{\sigma_1\sigma_2}}_{J+1}(\hat{\mathbf{q}}). \tag{E3}$$

We calculate this form in coordinate space. The Fourier transform of $\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q})$ is

$$\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q})=\int d^3\mathbf{r}\, d^3\mathbf{r}'\, \mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{r},\mathbf{r}') e^{-i(\mathbf{p}-\mathbf{q})\cdot(\mathbf{r}-\mathbf{r}')}, \tag{E4}$$

where the $M_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{r},\mathbf{r}')$ matrix is a local operator in general,[16] that is

$$\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{r},\mathbf{r}')=\mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}'). \tag{E5}$$

We apply this transformation to the $\mathcal{M}^{\text{ope(s-s)}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q})$ matrix [see Eq. (62)]. Because of the angular integration in (E2), only the first term in (62) survives. The Fourier transformation of that term is

$$\frac{(\boldsymbol{\sigma}^{(+)}\cdot(\mathbf{p}-\mathbf{q}))(\boldsymbol{\sigma}^{(-)}\cdot(\mathbf{p}-\mathbf{q}))}{4m^2(\mathbf{p}-\mathbf{q})^2} \quad \rightarrow \quad 3\frac{(\boldsymbol{\sigma}^{(+)}\cdot\mathbf{r})(\boldsymbol{\sigma}^{(-)}\cdot\mathbf{r})}{16\pi m^2 r^5}. \tag{E6}$$

Furthermore,

$$\int d^3\mathbf{p} f^{J-1}(p) Y^{m_{s_1 s_2}*}_{J-1}(\hat{\mathbf{p}}) e^{-i\mathbf{p}\cdot\mathbf{r}}=R^{J-1}_n(r) Y^{m_{s_1 s_2}*}_{J-1}(\hat{\mathbf{r}}), \tag{E7}$$

$$\int d^3\mathbf{q} f^{J+1}(q) Y^{m_{s_1 s_2}*}_{J+1}(\hat{\mathbf{q}}) e^{-i\mathbf{q}\cdot\mathbf{r}}=R^{J+1}_n(r) Y^{m_{s_1 s_2}}_{J+1}(\hat{\mathbf{r}}), \tag{E8}$$

where

$$R^{\ell}_n(r)=-\frac{2}{n^2}\sqrt{\frac{(n-\ell-1)!}{((n+\ell)!)^3}} e^{-r/n}\left(\frac{2r}{n}\right)^{\ell} L^{2\ell+1}_{n+\ell}\left(\frac{2r}{n}\right). \tag{E9}$$

The associated Laguerre function $L^{\mu}_{\lambda}(\rho)$ is related to the confluent hypergeometric function by

$$L^{\mu}_{\lambda}(\rho)=(-1)^{\mu}\frac{(\lambda!)^2}{\mu!(\lambda-\mu)!}F(-\lambda+\mu,\mu+1;\rho). \tag{E10}$$

The generating function for the Laguerre function is

$$U_{\mu}(\rho,u)\equiv(-1)^{\mu}\frac{u^{\mu}}{(1-u)^{\mu+1}}\exp\left(-\frac{u\rho}{1-u}\right)=\sum_{\lambda=\mu}^{\infty}\frac{L^{\mu}_{\lambda}(\rho)}{\lambda!}u^{\lambda}, \tag{E11}$$

hence

$$\sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12} \int d^3\mathbf{p}\, d^3\mathbf{q}\, f^{J-1}(p) Y^{m_{s_1 s_2}}_{J-1}{}^{*}(\hat{\mathbf{p}}) \mathcal{M}^{\mathrm{ope(s-s)}}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q}) f^{J+1}(q) Y^{m_{\sigma_1\sigma_2}}_{J+1}(\hat{\mathbf{q}})$$

$$= \sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12} \int d^3\mathbf{r}\, R_n^{J-1}(r) Y^{m_{s_1 s_2}}_{J-1}{}^{*}(\hat{\mathbf{r}}) \times \left(3\alpha \frac{(\boldsymbol{\sigma}^{(+)}\cdot\mathbf{r})(\boldsymbol{\sigma}^{(-)}\cdot\mathbf{r})}{16\pi m^2 r^5} \right) R_n^{J+1}(r) Y^{m_{s_1 s_2}}_{J+1}(\hat{\mathbf{r}})$$

$$= \frac{3\alpha}{16\pi m^2} \int dr\, r^2 \frac{1}{r^3} R_n^{J-1}(r) R_n^{J+1}(r)$$

$$\times \sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12} \int d\hat{\mathbf{r}}\, Y^{m_{s_1 s_2}}_{J-1}{}^{*}(\hat{\mathbf{r}}) (\boldsymbol{\sigma}^{(+)}\cdot\hat{\mathbf{r}}) (\boldsymbol{\sigma}^{(-)}\cdot\hat{\mathbf{r}}) Y^{m_{s_1 s_2}}_{J+1}(\hat{\mathbf{r}}). \tag{E12}$$

It follows that

$$\sum_{\sigma_1\sigma_2 s_1 s_2} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J 12} \int d\hat{\mathbf{r}} Y^{m_{s_1 s_2}}_{J-1}{}^{*}(\hat{\mathbf{r}}) (\boldsymbol{\sigma}^{(+)}\cdot\hat{\mathbf{r}}) (\boldsymbol{\sigma}^{(-)}\cdot\hat{\mathbf{r}}) Y^{m_{s_1 s_2}}_{J+1}(\hat{\mathbf{r}}) = \frac{1}{15} \frac{\sqrt{J(J+1)}}{2J+1}, \tag{E13}$$

but

$$\int_0^\infty dr\, r^2 \frac{1}{r^3} R_n^{J-1}(r) R_n^{J+1}(r) = 0. \tag{E14}$$

The last expression can be proved in the following way. Let us consider the more general case

$$\int_0^\infty dr\, r^{\beta+2} R_n^{\ell}(r) R_n^{\ell'}(r). \tag{E15}$$

The generating function for $R_n^{\ell}(r)$ is

$$G_{n\ell}(r,u) = -\frac{2}{n^2} \sqrt{\frac{(n-\ell-1)!}{((n+\ell)!)^3}} e^{-r/n} \left(\frac{2r}{n}\right)^{\ell} (-1)^{2\ell+1} \frac{u^{2\ell+1}}{(1-u)^{2\ell+2}} \exp\left\{ -\frac{u}{1-u} \frac{2r}{n} \right\}. \tag{E16}$$

Then we consider the expression

$$\int_0^\infty dr r^{\beta+2} G_{n\ell}(r,u) G_{n\ell'}(r,v) = \int_0^\infty dr r^{\beta+2} \frac{4}{n^4} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^3((n+\ell')!)^3}} e^{-2r/n} \left(\frac{2r}{n}\right)^{\ell+\ell'}$$

$$\times \frac{u^{2\ell+1} v^{2\ell'+1}}{(1-u)^{2\ell+2}(1-v)^{2\ell'+2}} \exp\left\{ -\left(\frac{u}{1-u} + \frac{v}{1-v} \right) \frac{2r}{n} \right\}$$

$$= \frac{4}{n^4} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^3((n+\ell')!)^3}} \frac{u^{2\ell+1} v^{2\ell'+1}}{(1-u)^{2\ell+2}(1-v)^{2\ell'+2}}$$

$$\times \int_0^\infty dr \left(\frac{2r}{n}\right)^{\beta+2+\ell+\ell'} \exp\left\{ -\left(1 + \frac{u}{1-u} + \frac{v}{1-v} \right) \frac{2r}{n} \right\}. \tag{E17}$$

It is well known that

$$\int_0^\infty d\rho \rho^\beta e^{-\rho} = \Gamma(\beta+1), \tag{E18}$$

therefore

$$\int_0^\infty dr \left(\frac{2r}{n}\right)^{\beta+2+\ell+\ell'} \exp\left\{-\left(1+\frac{u}{1-u}+\frac{v}{1-v}\right)\frac{2r}{n}\right\}$$
$$= \left(\frac{n}{2}\right)^{\beta+3} \left(\frac{(1-u)(1-v)}{1-uv}\right)^{\beta+3+\ell+\ell'} \Gamma(\beta+3+\ell+\ell') \tag{E19}$$

and

$$\int_0^\infty dr r^{\beta+2} G_{n\ell}(r,u) G_{n\ell'}(r,v) = \frac{2^{-\beta-1}}{n^{-\beta+1}} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^3((n+\ell')!)^3}}$$
$$\times \frac{u^{2\ell+1} v^{2\ell'+1} (1-u)^{\beta+1-\ell+\ell'} (1-v)^{\beta+1+\ell-\ell'}}{(1-uv)^{\beta+3+\ell+\ell'}}$$
$$\times \Gamma(\beta+3+\ell+\ell'). \tag{E20}$$

We expand this expression in a series,

$$\int_0^\infty dr r^{\beta+2} G_{n\ell}(r,u) G_{n\ell'}(r,v) = \sum_{\eta\eta'} C_{\eta\eta'}(n,\beta,\ell,\ell') u^\eta u^{\eta'}. \tag{E21}$$

It is not difficult to show[20] that the coefficient $C_{n+\ell,n+\ell'}$ represents the integral

$$C_{n+\ell,n+\ell'}(n,\beta,\ell,\ell') = \int_0^\infty dr r^{\beta+2} R_n^\ell(r) R_n^{\ell'}(r). \tag{E22}$$

Simple but tedious calculations show that this coefficient is zero for $\beta=-3$, $\ell=J-1$, $\ell'=J+1$. Thus the kernel $\mathcal{K}_{12}$ does not contribute to the energy corrections to $O(\alpha^4)$. The same result is obtained for the kernel $\mathcal{K}_{21}$.

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Ideally embedded space–times

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Due to the growing interest in embeddings of space–time in higher-dimensional spaces we consider a specific type of embedding. After proving an inequality between intrinsically defined curvature invariants and the squared mean curvature, we extend the notion of ideal embeddings from Riemannian geometry to the indefinite case. Ideal embeddings are such that the embedded manifold receives the least amount of tension from the surrounding space. Then it is shown that the de Sitter spaces, a Robertson–Walker space–time and some anisotropic perfect fluid metrics can be ideally embedded in a five-dimensional pseudo-Euclidean space. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1668333]

I. INTRODUCTION

In recent years the ideas of Kaluza and Klein have received new attention. Shortly after the publication of the general theory of relativity Kaluza proposed to unify gravity and electromagnetism by adding an extra dimension. Klein suggested that this fifth dimension would be compactified and unobservable on experimentally accessible energy scales. This idea of compactifying the extra dimension has dominated the search for a unified theory and lead to the 11-dimensional supergravity theory and more recent ten-dimensional superstring theory (see Ref. 1 for an overview).

Instead of compactifying the extra dimensions other approaches have been developed. In the space-time-matter (STM) theory[2] the $(3+1)$-dimensional cosmologies may be recovered from the geometry of $(4+1)$-dimensional, vacuum general relativity. Matter in four dimensions is induced by the shape of the embedded hypersurface and the five-dimensional Ricci flat geometry. More recently the Randall–Sundrum scenario has gained a lot of support. In Refs. 3 and 4 they try to solve the hierarchy problem between the observed Planck and weak scales by embedding the three-brane in a nonfactorizable five-dimensional metric.

From a mathematical point of view the theory of embeddings starts with the definition of a manifold by Riemann. Shortly after the publication of his famous Habilitationsschrift (see, e.g., Ref. 5 for a translation) Schläfli[6] conjectured that any n-dimensional Riemannian manifold could be locally and isometrically embedded in a d-dimensional Euclidean space with $d=n(n+1)/2$. This was proven by Janet and Cartan and extended to manifolds with indefinite metric by Friedman.[7] The Janet–Cartan theorem as it became known implies that we at maximum need ten dimensions to locally and isometrically embed any four-dimensional space–time.

A lesser known theorem by Campbell and Magaard[8] states that any analytical Riemannian space $V_n(s,t)$ can be locally and isometrically embedded in a Ricci flat Riemannian space $V_{n+1}(\tilde{s},\tilde{t})$, with $\tilde{s}=s+1,\tilde{t}=t$ or $\tilde{s}=s,\tilde{t}=t+1$. This theorem has obvious applications in STM theory.[9] For further generalizations of the Campbell–Magaard theorem to embedding spaces

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which are Einstein, scalar field sourced or have nondegenerate Ricci tensor see Refs. 10–12.

In applications of the embedding theorems one often starts from a given metric and looks for the embedding space with the minimal dimension or one puts restrictions on the source type.[13–15] In the following we will take a different approach by putting a restriction on the type of embedding. Using some recently defined intrinsic curvature invariants on a manifold we prove an inequality between intrinsic and extrinsic curvatures of an embedded Lorentzian manifold in a pseudo-Euclidean space. For a proof in the Riemannian case see Ref. 16. An embedding for which the equality holds is called ideal and in this case the shape operators take on specified forms. The space–times which satisfy such an ideal embedding in a five-dimensional space are determined. In the remainder all embeddings are local and isometric.

II. Λ-CURVATURES OF CHEN

Starting from a Lorentzian manifold (M,g) with signature $(m-1(+),1(-))$ isometrically embedded in a pseudo-Euclidean space (E_n,η) of signature $(n-1,1)$ or $(m-1,n-m+1)$ we will introduce the intrinsically defined Λ-curvature invariants of Chen.[17]

We denote the Levi-Civita connection on M with ∇ and on E_n with $\tilde{\nabla}$. The covariant derivative in E_n between two tangent vectors X and Y on M can be decomposed in a tangential and normal part,

$$\tilde{\nabla}_X Y = \nabla_X Y + \Omega(X,Y),$$

with $\Omega: TM \times TM \to N(M)$ the second fundamental form. If we choose an orthonormal basis $\{\xi_A\}$ in the normal space $N(M)$ of M and denote the signature of the basis vectors with $\varepsilon_A = \eta(\xi_A,\xi_A) = \pm 1$, we can define Ω as

$$\Omega(X,Y) = \sum_{A=m+1}^{n} \varepsilon_A \eta(\tilde{\nabla}_X Y, \xi_A)\xi_A. \tag{1}$$

In the following greek indices run from 1 to m, latin indices from 1 to n and capital indices from $m+1$ to n, unless otherwise stated.

The integrability conditions for the existence of an embedding are given by the Gauss–Codazzi–Ricci equations,[18,19]

$$R_{\alpha\beta\gamma\mu} = \sum_A \varepsilon_A \{\Omega^A_{\alpha\gamma}\Omega^A_{\beta\mu} - \Omega^A_{\alpha\mu}\Omega^A_{\beta\gamma}\}, \tag{2}$$

$$\nabla_\gamma \Omega^A_{\alpha\beta} - \nabla_\beta \Omega^A_{\alpha\gamma} = \sum_B \varepsilon_B \{S^{BA}{}_\gamma \Omega^B_{\alpha\beta} - S^{BA}{}_\beta \Omega^B_{\alpha\gamma}\}, \tag{3}$$

$$\nabla_\beta S^{BA}{}_\alpha - \nabla_\alpha S^{BA}{}_\beta = \sum_C \varepsilon_C \{S^{CB}{}_\beta S^{CA}{}_\alpha - S^{CB}{}_\alpha S^{CA}{}_\beta\} + g^{\gamma\mu}\{\Omega^B_{\gamma\beta}\Omega^A_{\mu\alpha} - \Omega^B_{\gamma\alpha}\Omega^A_{\mu\beta}\}, \tag{4}$$

with S^{AB}_{α} the torsion vector. For an interpretation of this vector as a gauge field in a Kaluza–Klein view of embeddings see Ref. 20 and as a real connection on space–time see Ref. 21.

The mean curvature vector is defined as

$$\vec{H} = \sum_A \varepsilon_A g^{\alpha\beta}\Omega^A_{\alpha\beta}\,\xi_A.$$

Let $\{e_\alpha\}$ be an orthonormal basis of M. The sectional curvature of a two-plane spanned by the orthonormal vectors $\{e_\alpha, e_\beta\}$ is defined by

$$K(e_\alpha \wedge e_\beta) = \varepsilon_{\alpha\beta} g(R(e_\alpha, e_\beta)e_\beta, e_\alpha),$$

with $\varepsilon_{\alpha\beta} = \varepsilon_\alpha \varepsilon_\beta$. The scalar curvature of an r-plane section L spanned by the orthonormal vectors $\{e_1, \ldots, e_r\}$ is defined as

$$\tau(L) = \sum_{\alpha<\beta} K(e_\alpha \wedge e_\beta), \quad 1 \leqslant \alpha < \beta \leqslant r.$$

The scalar curvature of the whole Lorentzian manifold is denoted by R. Denote the constant $c(n_1, \ldots, n_k)$ by

$$c(n_1, \ldots, n_k) = \frac{2\left(m + k - \sum_{j=1}^{k} n_j\right)}{m + k - 1 - \sum_{j=1}^{k} n_j}.$$

We are now in a situation to define the Λ-curvature invariants of Chen in the pseudo-Riemannian case as

$$\Lambda(n_1, \ldots, n_k) = c(n_1, \ldots, n_k)[R - \inf\{\tau(L_1) + \cdots + \tau(L_k) | L_j \text{ a non-null } n_j\text{-plane section, } L_i \perp L_j\}],$$

and

$$\hat{\Lambda}(n_1, \ldots, n_k) = c(n_1, \ldots, n_k)[R - \sup\{\tau(L_1) + \cdots + \tau(L_k) | L_j \text{ a non-null } n_j\text{-plane section, } L_i \perp L_j\}].$$

Note that in our definition the plane sections can be timelike or spacelike. Let $\{e_1, \ldots, e_m, \xi_{m+1}, \ldots, \xi_n\}$ be an orthonormal basis of E_n. Because we have space–time applications in mind we take M to be time-orientable, i.e., there exists a global nowhere-zero timelike vector field which we denote with e_m. From (1) we have

$$\Omega^A_{m\alpha} = -\eta(e_m, \tilde{\nabla}_{e_\alpha} \xi_A) = -\eta(e_\alpha, \tilde{\nabla}_{e_m} \xi_A),$$

with $A = m+1, \ldots, n$ and $\alpha = 1, \ldots, m-1$.

Definition II.1: An embedding $x: (M, g) \to (E_{n-1,1}, \eta)$ is called causal-type preserving if $\tilde{\nabla}_{e_\alpha} \xi_A$ is spacelike, $\forall\, A = m+1, \ldots, n$ and $\forall\, \alpha = 1, \ldots, m-1$.

Definition II.2: An embedding $x: (M, g) \to (E_{m-1,n-m+1}, \eta)$ is called causal-type preserving if $\tilde{\nabla}_{e_m} \xi_A$ is timelike, $\forall\, A = m+1, \ldots, n$.

From the above we see that causal-type preserving embeddings have $\Omega^A_{m\alpha} = 0$, $\forall\, \alpha = 1, \ldots, m-1$.

III. IDEAL EMBEDDINGS

We can now formulate and prove an inequality relating the above intrinsically defined curvature invariants and the square of the extrinsic mean curvature of the embedded manifold.

Theorem III.1: *Let $x: (M, g) \to (E_n, \eta)$ be a causal-type preserving embedding of a Lorentzian m-dimensional manifold in a n-dimensional pseudo-Euclidean manifold. For any k-tuple $(n_1, \ldots, n_k)$ we have that*

$$\|H\|^2 \geqslant \Lambda(n_1, \ldots, n_k), \tag{5}$$

if (E_n, η) has signature $(n-1, 1)$ and

$$\|H\|^2 \leqslant \hat{\Lambda}(n_1, \ldots, n_k), \tag{6}$$

if (E_n, η) has signature $(m-1, n-m+1)$.

Proof: Starting from the Gauss equation (2) w.r.t. an orthonormal basis $\{e_1,\ldots,e_m,\xi_{m+1},\ldots,\xi_n\}$ we can express the scalar curvature of M as

$$\begin{aligned}2R&=\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}R_{\alpha\beta\alpha\beta}\\&=\sum_{A=m+1}^{n}\varepsilon_A\left(\sum_{\alpha=1}^{m}\varepsilon_\alpha\Omega^A_{\alpha\alpha}\right)^2-\sum_{A=m+1}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^A_{\alpha\beta})^2\\&=\|H\|^2-\Omega^2.\end{aligned}\tag{7}$$

If we put, with $k\geqslant 1$,

$$\phi=2R-\frac{m+k-1-\sum_{j=1}^{k}n_j}{m+k-\sum_{j=1}^{k}n_j}\|H\|^2,$$

$$\gamma=m+k-\sum_{j=1}^{k}n_j,$$

it is a small calculation to show that

$$\|H\|^2=\gamma(\phi+\Omega^2).\tag{8}$$

We choose ξ_{m+1} along $\vec{H}$ and put $a_\alpha=\varepsilon_\alpha\Omega^{m+1}_{\alpha\alpha}$. Equation (8) becomes

$$\begin{aligned}\varepsilon_{m+1}\left(\sum_{\alpha=1}^{m}a_\alpha\right)^2=\gamma\Bigg\{&\phi+\varepsilon_{m+1}\sum_{\alpha=1}^{m}(a_\alpha)^2+\varepsilon_{m+1}\sum_{\alpha\neq\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{m+1}_{\alpha\beta})^2\\&+\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^A_{\alpha\beta})^2\Bigg\}.\end{aligned}\tag{9}$$

If we use the notation

$$\overline{a}_1=a_1,$$

$$\overline{a}_2=a_2+\cdots+a_{n_1},$$

$$\overline{a}_3=a_{n_1+1}+\cdots+a_{n_1+n_2},$$

$$\vdots$$

$$\overline{a}_{k+1}=a_{n_1+\cdots+n_{k-1}+1}+\cdots+a_{n_1+\cdots+n_k},$$

$$\overline{a}_{k+2}=a_{n_1+\cdots+n_k+1},$$

$$\vdots$$

$$\overline{a}_\gamma=a_{m-1},$$

$$\overline{a}_{\gamma+1}=a_m,$$

we have

$$\left(\sum_{\alpha=1}^{\gamma+1}\overline{a}_\alpha\right)^2=\left(\sum_{\alpha=1}^{m}a_\alpha\right)^2,$$

and

$$\sum_{\alpha=1}^{\gamma+1}(\overline{a}_\alpha)^2=\sum_{\alpha=1}^{m}(a_\alpha)^2+\sum_{2\leqslant\alpha_1\neq\beta_1\leqslant n_1}a_{\alpha_1}a_{\beta_1}+\sum_{\alpha_2\neq\beta_2\in Q_2}a_{\alpha_2}a_{\beta_2}+\cdots+\sum_{\alpha_k\neq\beta_k\in Q_k}a_{\alpha_k}a_{\beta_k},$$

with $Q_1=\{1,\ldots,n_1\}$, $Q_2=\{n_1+1,\ldots,n_1+n_2\}$, $\ldots$, $Q_k=\{n_1+\cdots+n_{k-1}+1,\ldots,n_1+\cdots+n_k\}$. Equation (9) becomes

$$\begin{aligned}\varepsilon_{m+1}\left(\sum_{\alpha=1}^{\gamma+1}\overline{a}_\alpha\right)^2=\gamma\Bigg\{&\phi+\varepsilon_{m+1}\sum_{\alpha=1}^{\gamma+1}(\overline{a}_\alpha)^2+\varepsilon_{m+1}\sum_{\alpha\neq\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{m+1}_{\alpha\beta})^2\\&+\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{A}_{\alpha\beta})^2-\varepsilon_{m+1}\sum_{2\leqslant\alpha_1\neq\beta_1\leqslant n_1}a_{\alpha_1}a_{\beta_1}-\cdots\\&-\varepsilon_{m+1}\sum_{\alpha_k\neq\beta_k\in Q_k}a_{\alpha_k}a_{\beta_k}\Bigg\}.\end{aligned}\tag{10}$$

We need the following algebraic lemma:

Lemma III.1:[16] *If* $\overline{a}_1,\ldots,\overline{a}_n,c$ *are* $n+1$ $(n\geqslant 2)$ *real numbers such that*

$$\left(\sum_{i=1}^{n}\overline{a}_i\right)^2=(n-1)\left(\sum_{i=1}^{n}(\overline{a}_i)^2+c\right),$$

we have that $2\overline{a}_1\overline{a}_2\geqslant c$ *and equality holds iff* $\overline{a}_1+\overline{a}_2=\overline{a}_3=\cdots=\overline{a}_n$.

Two separate cases appear. We first look at the case when $\vec{H}$ is spacelike, i.e., $\varepsilon_{m+1}=1$. Using the above lemma Eq. (10) becomes

$$\begin{aligned}\overline{a}_1\overline{a}_2\geqslant\frac{1}{2}\phi+\frac{1}{2}\sum_{\alpha\neq\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{m+1}_{\alpha\beta})^2+\frac{1}{2}\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{A}_{\alpha\beta})^2\\-\frac{1}{2}\sum_{2\leqslant\alpha_1\neq\beta_1\leqslant n_1}a_{\alpha_1}a_{\beta_1}-\cdots-\frac{1}{2}\sum_{\alpha_k\neq\beta_k\in Q_k}a_{\alpha_k}a_{\beta_k}.\end{aligned}$$

Because

$$\sum_{\alpha_j\neq\beta_j}a_{\alpha_j}a_{\beta_j}=2\sum_{\alpha_j<\beta_j}a_{\alpha_j}a_{\beta_j},$$

we have

$$\sum_{j=1}^{k}\sum_{\alpha_j<\beta_j\in Q_j}a_{\alpha_j}a_{\beta_j}\geqslant\frac{1}{2}\phi+\sum_{\alpha<\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{m+1}_{\alpha\beta})^2+\frac{1}{2}\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega^{A}_{\alpha\beta})^2.\tag{11}$$

Let L_j be an n_j-dimensional subspace of T_pM such that

$$L_j=\text{span}\{e_{n_1+\cdots+n_{j-1}+1},\ldots,e_{n_1+\cdots+n_j}\}.$$

The scalar curvature of the plane section is given by

$$\tau(L_j)=\sum_{\alpha_j<\beta_j\in Q_j}\varepsilon_{\alpha_j\beta_j}\sum_{A=m+1}^{n}\varepsilon_A[\Omega^A_{\alpha_j\alpha_j}\Omega^A_{\beta_j\beta_j}-(\Omega^A_{\alpha_j\beta_j})^2].$$

Then, using the above notation we find

$$\begin{aligned}\tau(L_1)+\cdots+\tau(L_k)=&\sum_{j=1}^{k}\sum_{\alpha_j<\beta_j\in Q_j}a_{\alpha_j}a_{\beta_j}-\sum_{j=1}^{k}\sum_{\alpha_j<\beta_j\in Q_j}\varepsilon_{\alpha_j\beta_j}(\Omega^{m+1}_{\alpha_j\beta_j})^2\\&+\sum_{j=1}^{k}\sum_{\alpha_j<\beta_j\in Q_j}\varepsilon_{\alpha_j\beta_j}\sum_{A=m+2}^{n}\varepsilon_A[\Omega^A_{\alpha_j\alpha_j}\Omega^A_{\beta_j\beta_j}-(\Omega^A_{\alpha_j\beta_j})^2].\end{aligned}$$

If we use the inequality (11) and the notation

$$Q_{k+1}=\{n_1+\cdots+n_k+1,\ldots,m\},$$

$$Q=Q_1\cup\cdots\cup Q_k\cup Q_{k+1},$$

$$Q^2=(Q_1\times Q_1)\cup\cdots\cup(Q_k\times Q_k)\cup(Q_{k+1}\times Q_{k+1}),$$

$$\nabla^2=(Q\times Q)/Q^2,$$

we have

$$\tau(L_1)+\cdots+\tau(L_k)\geqslant\frac{1}{2}\phi+\frac{1}{2}\sum_{A=m+1}^{n}\varepsilon_A\sum_{(\alpha,\beta)\in\nabla^2}\varepsilon_{\alpha\beta}(\Omega^A_{\alpha\beta})^2+\frac{1}{2}\sum_{A=m+2}^{n}\varepsilon_A\sum_{j=1}^{k}\left(\sum_{\alpha\in Q_j}\varepsilon_\alpha\Omega^A_{\alpha\alpha}\right)^2.\tag{12}$$

The signature of the embedding space E_n is chosen to be $(n-1,1)$ such that all $\varepsilon_A=1$ and the condition of causal-type preserving ensures that the terms with possible minus signs appearing on the right-hand side vanish. We have

$$\tau(L_1)+\cdots+\tau(L_k)\geqslant\tfrac{1}{2}\phi.$$

This holds for all mutually orthogonal subspaces L_j, in particular for the infimum,

$$\|H\|^2\geqslant\Lambda(n_1,\ldots,n_k).\tag{13}$$

The case when $\vec{H}$ is timelike is analogous and we find, instead of (12),

$$\begin{aligned}\tau(L_1)+\cdots+\tau(L_k)\leqslant&\frac{1}{2}\phi+\frac{1}{2}\sum_{A=m+1}^{n}\varepsilon_A\sum_{(\alpha,\beta)\in\nabla^2}\varepsilon_{\alpha\beta}(\Omega^A_{\alpha\beta})^2\\&+\frac{1}{2}\sum_{A=m+2}^{n}\varepsilon_A\sum_{j=1}^{k}\left(\sum_{\alpha_j\in Q_j}\varepsilon_{\alpha_j}\Omega^A_{\alpha_j\alpha_j}\right)^2.\end{aligned}$$

We choose the signature of the embedding space to be $(m-1,n-m+1)$, i.e., all normal directions are timelike. We find

$$\tau(L_1)+\cdots+\tau(L_k)\leqslant\tfrac{1}{2}\phi.$$

This holds again for all mutually orthogonal subspaces, in particular for the supremum,

$$\|H\|^2\leqslant\hat{\Lambda}(n_1,\ldots,n_k).\tag{14}$$

It remains to show the inequality when $k=0$. Starting from (7) and again choosing ξ_{m+1} along $\vec{H}$, we find

$$2R=\|H\|^2-\varepsilon_{m+1}\sum_{\alpha=1}^{m}(a_\alpha)^2-\varepsilon_{m+1}\sum_{\alpha\neq\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega_{\alpha\beta}^{m+1})^2-\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega_{\alpha\beta}^{A})^2, \tag{15}$$

with $a_\alpha=\varepsilon_\alpha\Omega_{\alpha\alpha}^{m+1}$. We have

$$\sum_{\alpha=1}^{m}(a_\alpha)^2=\left(\sum_{\alpha=1}^{m}a_\alpha\right)^2-2\sum_{\alpha<\beta=1}^{m}a_\alpha a_\beta=\varepsilon_{m+1}\|H\|^2+\sum_{\alpha<\beta=1}^{m}(a_\alpha-a_\beta)^2-(m-1)\sum_{\alpha=1}^{m}(a_\alpha)^2,$$

$$m\sum_{\alpha=1}^{m}(a_\alpha)^2=\varepsilon_{m+1}\|H\|^2+\sum_{\alpha<\beta=1}^{m}(a_\alpha-a_\beta)^2\geqslant\varepsilon_{m+1}\|H\|^2.$$

If $\vec{H}$ is spacelike, (15) with the above inequality becomes

$$2R\leqslant\frac{m-1}{m}\|H\|^2-\sum_{\alpha\neq\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega_{\alpha\beta}^{m+1})^2-\sum_{A=m+2}^{n}\varepsilon_A\sum_{\alpha,\beta=1}^{m}\varepsilon_{\alpha\beta}(\Omega_{\alpha\beta}^{A})^2.$$

The signature of the embedded space is chosen to be $(n-1,1)$ and because of the condition of causal-type preserving, we find

$$\|H\|^2\geqslant\frac{2m}{m-1}R=\Lambda(0). \tag{16}$$

The proof for the timelike case is similar. ◇

Notice that due to our choice of signature for the embedded space E_n, $\vec{H}$ is always non-null. So we exclude the case of quasi-minimal embeddings.

If there is equality we can determine the form of the second fundamental forms.

Corollary III.1: There is equality in (5) or (6) at a point $p\in M$ iff there exists an orthonormal basis at p such that the second fundamental forms take the form

$$\Omega_{m+1}=\begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{pmatrix},$$

with $a_1+\cdots+a_{n_1}=a_{n_1+1}+\cdots+a_{n_1+n_2}=\cdots=a_{n_1+\cdots+n_{k-1}+1}+\cdots+a_{n_1+\cdots+n_k}=a_{n_1+\cdots+n_k+1}=\cdots=a_m$ *and*

$$\Omega_r=\begin{pmatrix} A_{r1} & & & & & & \\ & A_{r2} & & & & & \\ & & \ddots & & & & \\ & & & A_{rk} & & & \\ & & & & 0 & & \\ & & & & & \ddots & \\ & & & & & & 0 \end{pmatrix},$$

with $Trace(A_{rj})=0$, $r=m+2,\ldots,n$, $j=1,\ldots,k$.

As in Ref. 17 we have the following.

Definition III.1: An isometric embedding $x:(M,g)\to(E_n,\eta)$ *is called an ideal embedding if and only if there exists a* k*-tuple* $(n_1,\ldots,n_k)$ *such that in a neighborhood* U *of a point* $p\in M$ *there is equality in (5) or (6), respectively.*

If the pseudo-Euclidean embedding space has signature $(n-1,1)$, an ideally embedded manifold M means that the squared mean curvature of M is minimal. Because $\vec{H}$ measures the tension on M from the surrounding space an ideal embedding in $E_{n-1,1}$ can be considered as *a best way of living in a best world* for the neighborhood U.[17] In the case of an embedding space with signature $(n-m+1,m-1)$ the situation is reversed. An ideally embedded manifold receives the maximum possible amount of tension from the surrounding space at each point of M. Although this situation is not *ideal* we reserve the notation for both occasions.

IV. IDEALLY EMBEDDED SPACE–TIMES

Using the above notion of ideal embedding gives us a natural set of second fundamental forms to consider. Notice that this is the reverse situation usually adopted in the literature. There one often starts from a given metric and looks for the minimal embedding, i.e., with the least extra dimensions, or one puts some constraints on the curvature tensor through the choice of matter and/or Petrov type (although see Ref. 22 for a different approach).

We will restrict our manifold M to be a four-dimensional space–time embedded in a five-dimensional pseudo-Euclidean space. The torsion vector is zero in this case, so (4) is trivially satisfied and (3) simplifies significantly. We further only study those cases when there is equality for a k-tuple with only spacelike plane sections. The case with a timelike plane section in the k-tuple will be considered separately.

We denote the orthonormal basis of an ideally embedded space–time M for which the second fundamental forms take their special forms as $\{e_\alpha\}=\{\vec{w},\vec{v},\vec{q},\vec{u}\}$ with $u_\alpha u^\alpha=-1$. From the above corollary we have three possible cases:
(i) equality with $k=0$,

$$\Omega_{\alpha\beta}=\mu g_{\alpha\beta};$$

(ii) equality with $k=1$, $n=2$,

$$\Omega_{\alpha\beta}=(\mu-\lambda)w_\alpha w_\beta+\lambda v_\alpha v_\beta+\mu q_\alpha q_\beta-\mu u_\alpha u_\beta;$$

(iii) equality with $k=1$, $n=3$,

$$\Omega_{\alpha\beta}=(\mu-\lambda-\nu)w_\alpha w_\beta+\lambda v_\alpha v_\beta+\nu q_\alpha q_\beta-\mu u_\alpha u_\beta.$$

Before we determine the metrics which can be ideally embedded with one of the above second fundamental forms we mention two results which limit the possible outcomes.

Theorem VI.1:[23] *No nonflat vacuum metric can be embedded in a five-dimensional pseudo-Euclidean space.*

Theorem IV.2:[13] *There are no embedding class one solutions of the Einstein–Maxwell equations with a non-null electromagnetic field.*

A. Case i

If we take as shape operator

$$\Omega_{\alpha\beta}=\mu g_{\alpha\beta},$$

i.e., the embedding is umbilical, the Codazzi equations (3) become

$$g_{\alpha\beta}\nabla_\gamma\mu=g_{\alpha\gamma}\nabla_\beta\mu,$$

or contracting over α and β gives $\nabla_\gamma\mu=0$. The Gauss equations (2) give

$$R_{\alpha\beta\gamma\delta}=2\varepsilon\mu^2 g_{\alpha[\gamma}g_{\delta]\beta},$$

with μ a constant. The space–time is a space of constant curvature, a de Sitter space if $\varepsilon=1$ or an anti-de Sitter space if $\varepsilon=-1$ (Ref. 15, p. 103). Due to our assumption of time-orientability the space obtained from the de Sitter space in which points are identified by reflection through the origin of the embedding space is excluded (Ref. 24, p. 130).

B. Case ii

With respect to the orthonomal basis $\{w^\alpha,v^\alpha,q^\alpha,u^\alpha\}$, u^α timelike, the second fundamental form becomes

$$\Omega_{\alpha\beta}=-\mu u_\alpha u_\beta+\mu q_\alpha q_\beta+\lambda v_\alpha v_\beta+(\mu-\lambda)w_\alpha w_\beta.$$

If we decompose the covariant derivatives,

$$\nabla_\beta u_\alpha=w_\alpha A_\beta+v_\alpha B_\beta+q_\alpha C_\beta,$$

$$\nabla_\beta w_\alpha=u_\alpha A_\beta+v_\alpha D_\beta+q_\alpha E_\beta,$$

$$\nabla_\beta v_\alpha=u_\alpha B_\beta-w_\alpha D_\beta+q_\alpha F_\beta,$$

$$\nabla_\beta q_\alpha=u_\alpha C_\beta-w_\alpha E_\beta-v_\alpha F_\beta,$$

the Codazzi equations give

$$\lambda A_\alpha=\nabla_w\mu\, u_\alpha+\lambda A_v\, v_\alpha-\nabla_u\lambda\, w_\alpha,$$

$$(\lambda-\mu)B_\alpha=-\nabla_v\mu\, u_\alpha-\nabla_u\lambda\, v_\alpha-\lambda A_v\, w_\alpha,$$

$$(2\lambda-\mu)D_\alpha=\lambda A_v\, u_\alpha+(2\lambda-\mu)D_q\, q_\alpha-\nabla_w\lambda\, v_\alpha-\nabla_v(\mu-\lambda)\, w_\alpha, \tag{17}$$

$$\lambda E_\alpha=-\nabla_w\mu\, q_\alpha+(2\lambda-\mu)D_q\, v_\alpha+\nabla_q\lambda\, w_\alpha,$$

$$(\lambda-\mu)F_\alpha=\nabla_v\mu\, q_\alpha+\nabla_q\lambda\, v_\alpha-(2\lambda-\mu)D_q\, w_\alpha,$$

and

$$\nabla_u\mu=\nabla_q\mu=0,$$

with A_v, D_q scalars and $u^\alpha\nabla_\alpha=\nabla_u$, etc. There is no equation for C_α.

The Ricci identities $2\nabla_{[\gamma}\nabla_{\beta]}z_\alpha=z^\sigma R_{\sigma\alpha\beta\gamma}$, with z^α one of the basis vectors, give

$$\nabla_{[\alpha}A_{\beta]}-D_{[\alpha}B_{\beta]}-E_{[\alpha}C_{\beta]}=\varepsilon\mu(\mu-\lambda)\, u_{[\beta}w_{\alpha]}, \tag{18}$$

$$\nabla_{[\alpha}B_{\beta]}+D_{[\alpha}A_{\beta]}-F_{[\alpha}C_{\beta]}=\varepsilon\mu\lambda\, u_{[\beta}v_{\alpha]}, \tag{19}$$

$$\nabla_{[\alpha}C_{\beta]}+E_{[\alpha}A_{\beta]}+F_{[\alpha}B_{\beta]}=\varepsilon\mu^2\, u_{[\beta}q_{\alpha]}, \tag{20}$$

$$\nabla_{[\alpha}D_{\beta]}+B_{[\alpha}A_{\beta]}-F_{[\alpha}E_{\beta]}=\varepsilon\lambda(\mu-\lambda)\, w_{[\beta}v_{\alpha]}, \tag{21}$$

$$\nabla_{[\alpha}E_{\beta]}+C_{[\alpha}A_{\beta]}+F_{[\alpha}D_{\beta]}=\varepsilon\mu(\mu-\lambda)\, w_{[\beta}q_{\alpha]}, \tag{22}$$

$$\nabla_{[\alpha}F_{\beta]}+C_{[\alpha}B_{\beta]}-E_{[\alpha}D_{\beta]}=\varepsilon\mu\lambda\, v_{[\beta}q_{\alpha]}. \tag{23}$$

1. If $\lambda=\mu\neq 0$

From the Codazzi equations we find $\nabla_v\mu = A_v = D_q = 0$ and

$$\nabla_\beta w_\alpha = \nabla_w \ln\lambda\,(u_\alpha u_\beta - v_\alpha v_\beta - q_\alpha q_\beta).$$

Let us denote the projection operator on the timelike hypersurface orthogonal to w^α by $h_\alpha^\beta = \delta_\alpha^\beta - w_\alpha w^\beta$. From the Gauss equations we find that

$$w^\alpha R_{\alpha\beta\gamma\delta}=0\,,$$

and so w^α is a constant vector field (see Ref. 15, p. 553), i.e., $\nabla_\beta w_\alpha = 0$ or $\lambda=\mu=\text{const}$. If we denote with ${}^3R_{\alpha\beta\gamma\delta}$ the Riemann tensor of the timelike hypersurface, the Gauss equations give

$${}^3R_{\alpha\beta\gamma\delta} = R_{\alpha\beta\gamma\delta} = 2\varepsilon\lambda^2 h_{\alpha[\gamma}h_{\delta]\beta}\,.$$

The timelike three-space is a space of constant curvature. We can then choose coordinates such that the metric reads

$$\mathrm{d}s^2 = \mathrm{d}z^2 + \frac{\mathrm{d}y^2+\mathrm{d}x^2-\mathrm{d}t^2}{[1+\frac{1}{4}\varepsilon\lambda^2(y^2+x^2-t^2)]^2}, \tag{24}$$

with $\lambda=\text{const}$. Because the embedding is quasi-umbilical (i.e., there exist functions ϕ and ψ such that $\Omega_{\alpha\beta}=\phi g_{\alpha\beta}+\psi w_\alpha w_\beta$) the metric is conformally flat.[25] The Ricci tensor is

$$R_{\alpha\beta} = 2\varepsilon\lambda^2 h_{\alpha\beta}\,,$$

with Segré type A1, [1(11,1)], and the energy-momentum tensor does not satisfy any of the known energy conditions.[24] Due to the observation that the Universe is accelerating, cosmological models with such a strange equation of state are recently under investigation.

2. If $\lambda=0$, $\mu\neq 0$

From the Codazzi equations we find $\nabla_w\mu = D_q = 0$ and

$$\nabla_\beta v_\alpha = \nabla_v \ln\mu\,(u_\alpha u_\beta - w_\alpha w_\beta - q_\alpha q_\beta).$$

This is the previous case with the roles of v^α and w^α interchanged.

3. If $\mu=2\lambda\neq 0$

The Codazzi equations give $A_v=\nabla_v\lambda=\nabla_w\lambda=0$. Then $A_\alpha=B_\alpha=D_\alpha=E_\alpha=F_\alpha=0$. The Ricci identity (18) gives $\lambda=0$, so we must take $\mu\neq 2\lambda$.

4. If $\lambda\neq 0$, $\mu-\lambda\neq 0$ and $\mu-2\lambda\neq 0$

Let $p_\alpha^\beta = \delta_\alpha^\beta - v_\alpha v^\beta - w_\alpha w^\beta$ be the projection operator on the two-space V_2 orthogonal to v^α and w^α. The second fundamental forms of the embedding of V_2 in the space–time (M,g) are

$$\Omega^v_{\alpha\beta} = p^\gamma_{(\alpha}p^\sigma_{\beta)}\nabla_\gamma v_\sigma = \frac{\nabla_v\mu}{\lambda-\mu}p_{\alpha\beta}\,,$$

and

$$\Omega^w_{\alpha\beta} = -\frac{\nabla_w\mu}{\lambda}p_{\alpha\beta}\,.$$

Using the Gauss equations we find for the Riemann tensor of the timelike two-space V_2,

$$ {}^2R_{\alpha\beta\gamma\delta}=2\left\{\varepsilon\mu^2+\left(\frac{\nabla_v\mu}{\lambda-\mu}\right)^2+\left(\frac{\nabla_w\mu}{\lambda}\right)^2\right\}p_{\alpha[\gamma}p_{\delta]\beta}. \tag{25}$$

It is a small calculation to show that the coefficient has zero-derivative in the u and q directions. The two-space V_2 is a space of constant curvature. We can choose coordinates such that

$$ w_\alpha=(e^{\phi(y,z)},0,0,0),\ v_\alpha=(0,e^{\xi(y,z)},0,0), $$

and the metric reads

$$ \mathrm{d}s^2=e^{2\phi(y,z)}\mathrm{d}z^2+e^{2\xi(y,z)}\mathrm{d}y^2+Y^2(y,z)\{\mathrm{d}x^2-\Sigma^2(x,k)\mathrm{d}t^2\}, \tag{26}$$

with $\Sigma(x,k)=\sin(x)$, x or $\sinh(x)$ if $k=1$, 0 or -1 and

$$ kY^{-2}=\varepsilon\mu^2+\left(\frac{\nabla_v\mu}{\lambda-\mu}\right)^2+\left(\frac{\nabla_w\mu}{\lambda}\right)^2. $$

These metrics have a group G_3 working on the two-surface of constant curvature and therefore have Petrov type D or O. Because the two-surface is timelike the energy-momentum content cannot be a perfect fluid, a null electromagnetic field or pure radiation (see Ref. 15, Chap. 15) and due to Theorems IV.1 and IV.2 also vacuum and an electromagnetic non-null field are not possible. We can, however, interpret this space–time as filled with an anisotropic perfect fluid satisfying the strong energy condition if and only if the extra dimension is timelike ($\varepsilon=-1$) and μ and λ satisfy any of the following conditions:

(1) $\lambda>0,\ \mu>\lambda$,
(2) $\lambda>0,\ -\lambda\leqslant\mu\leqslant\frac{1}{2}\lambda$,
(3) $\lambda<0,\ \frac{1}{2}\lambda\leqslant\mu\leqslant-\lambda$,
(4) $\lambda<0,\ \mu<\lambda$.

C. Case iii

With respect to an orthonormal tetrad $\{w^\alpha,v^\alpha,q^\alpha,u^\alpha\}$ the shape operator takes the form

$$ \Omega_{\alpha\beta}=-\mu u_\alpha u_\beta+\nu q_\alpha q_\beta+\lambda v_\alpha v_\beta+(\mu-\lambda-\nu)w_\alpha w_\beta. \tag{27}$$

If we use the same decompositions of the covariant derivatives as in the previous case, the Codazzi equations give

$$ (\lambda+\nu)A_\alpha=\nabla_w\mu\,u_\alpha+\nabla_u(\mu-\lambda-\nu)\,w_\alpha+(\lambda+\nu)A_v\,v_\alpha+(\lambda+\nu)A_q\,q_\alpha, $$

$$ (\mu-\lambda)B_\alpha=-\nabla_v\mu\,u_\alpha+(\lambda+\nu)A_v\,w_\alpha+\nabla_u\lambda\,v_\alpha+(\mu-\lambda)B_q\,q_\alpha, $$

$$ (\mu-\nu)C_\alpha=-\nabla_q\mu\,u_\alpha+(\lambda+\nu)A_q\,w_\alpha+(\mu-\lambda)B_q\,v_\alpha+\nabla_u\nu\,q_\alpha, $$

$$ (\mu-2\lambda-\nu)D_\alpha=-(\lambda+\nu)A_v\,u_\alpha+\nabla_v(\mu-\lambda-\nu)\,w_\alpha+\nabla_w\lambda\,v_\alpha+(\mu-2\lambda-\nu)D_q\,q_\alpha, $$

$$ (\mu-\lambda-2\nu)E_\alpha=-(\lambda+\nu)A_q\,u_\alpha+\nabla_q(\mu-\lambda-\nu)\,w_\alpha+(\mu-2\lambda-\nu)D_q\,v_\alpha+\nabla_w\nu\,q_\alpha, $$

$$ (\lambda-\nu)F_\alpha=-(\mu-\lambda)B_q\,u_\alpha+(\mu-2\lambda-\nu)D_q\,w_\alpha+\nabla_q\lambda\,v_\alpha+\nabla_v\nu\,q_\alpha, $$

with A_v, A_q, B_q, D_q scalars. The Ricci identities are

$$ \nabla_{[\alpha}A_{\beta]}-D_{[\alpha}B_{\beta]}-E_{[\alpha}C_{\beta]}=\varepsilon\mu(\mu-\lambda-\nu)\,u_{[\beta}w_{\alpha]}, \tag{28}$$

$$ \nabla_{[\alpha}B_{\beta]}+D_{[\alpha}A_{\beta]}-F_{[\alpha}C_{\beta]}=\varepsilon\mu\lambda\,u_{[\beta}v_{\alpha]}, \tag{29}$$

$$\nabla_{[\alpha}C_{\beta]}+E_{[\alpha}A_{\beta]}+F_{[\alpha}B_{\beta]}=\varepsilon\mu\nu\, u_{[\beta}q_{\alpha]}, \tag{30}$$

$$\nabla_{[\alpha}D_{\beta]}+B_{[\alpha}A_{\beta]}-F_{[\alpha}E_{\beta]}=\varepsilon\lambda(\mu-\lambda-\nu)\, w_{[\beta}v_{\alpha]}, \tag{31}$$

$$\nabla_{[\alpha}E_{\beta]}+C_{[\alpha}A_{\beta]}+F_{[\alpha}D_{\beta]}=\varepsilon\nu(\mu-\lambda-\nu)\, w_{[\beta}q_{\alpha]}, \tag{32}$$

$$\nabla_{[\alpha}F_{\beta]}+C_{[\alpha}B_{\beta]}-E_{[\alpha}D_{\beta]}=\varepsilon\nu\lambda\, v_{[\beta}q_{\alpha]}. \tag{33}$$

Using the Gauss equations we find the Ricci tensor,

$$R_{\alpha\beta}=\varepsilon\{-\mu^2u_\alpha u_\beta+\nu(2\mu-\nu)q_\alpha q_\beta+\lambda(2\mu-\lambda)v_\alpha v_\beta+(\mu-\lambda-\nu)(\mu+\lambda+\nu)w_\alpha w_\beta\}. \tag{34}$$

In the generic case the Segré type is A1, [111,1]. We will restrict the calculations in the following to perfect fluid space–times. This means μ, λ and ν must satisfy one of the following conditions:

$$\text{(A)}\quad \mu=3\lambda,\ \ \nu=\lambda,$$

$$\text{(B)}\quad \mu=-\lambda,\ \ \nu=\lambda,$$

$$\text{(C)}\quad \mu=-\nu,\ \ \lambda=-3\nu,$$

$$\text{(D)}\quad \mu=-\lambda,\ \ \nu=-3\lambda.$$

The cases B, C, and D are the same with the roles of the spacelike vectors interchanged. Before we study the above cases in detail we give first the decomposition of the covariant derivative of the timelike direction u^α into its irreducible parts if $\lambda+\nu\neq0$, $\mu-\lambda\neq0$ and $\mu-\nu\neq0$.

The acceleration reads

$$\dot{u}_\alpha=\frac{\nabla_q\mu}{\mu-\nu}q_\alpha+\frac{\nabla_v\mu}{\mu-\lambda}v_\alpha-\frac{\nabla_w\mu}{\lambda+\nu}w_\alpha, \tag{35}$$

the expansion

$$\theta=\frac{\nabla_u(\mu-\lambda-\nu)}{\lambda+\nu}+\frac{\nabla_u\lambda}{\mu-\lambda}+\frac{\nabla_u\nu}{\mu-\nu}, \tag{36}$$

the shear

$$\begin{aligned}\sigma_{\alpha\beta}=&\left\{\frac{2\nabla_u(\mu-\lambda-\nu)}{3(\lambda+\nu)}-\frac{\nabla_u\lambda}{3(\mu-\lambda)}-\frac{\nabla_u\nu}{3(\mu-\nu)}\right\}w_\alpha w_\beta+\frac{(\mu+\nu)A_v}{\mu-\lambda}w_{(\alpha}v_{\beta)}+\frac{(\mu+\lambda)A_q}{\mu-\nu}w_{(\alpha}q_{\beta)}\\&+\left\{-\frac{\nabla_u(\mu-\lambda-\nu)}{3(\lambda+\nu)}+\frac{2\nabla_u\lambda}{3(\mu-\lambda)}-\frac{\nabla_u\nu}{3(\mu-\nu)}\right\}v_\alpha v_\beta+\frac{(2\mu-\lambda-\nu)B_q}{\mu-\nu}v_{(\alpha}q_{\beta)}\\&+\left\{-\frac{\nabla_u(\mu-\lambda-\nu)}{3(\lambda+\nu)}-\frac{\nabla_u\lambda}{3(\mu-\lambda)}+\frac{2\nabla_u\nu}{3(\mu-\nu)}\right\}q_\alpha q_\beta,\end{aligned}$$

and the vorticity

$$\omega_{\alpha\beta}=\frac{(\mu-2\lambda-\nu)A_v}{\mu-\lambda}w_{[\alpha}v_{\beta]}+\frac{(\mu-\lambda-2\nu)A_q}{\mu-\nu}w_{[\alpha}q_{\beta]}+\frac{(\lambda-\nu)B_q}{\mu-\nu}v_{[\alpha}q_{\beta]}. \tag{37}$$

1. If $\mu=-\lambda$ and $\nu=\lambda\neq 0$

From the Codazzi equations we find $B_q=D_q=0$ and $\nabla_v\lambda=\nabla_q\lambda=0$. Projecting the Ricci identity (29) on $u^\alpha v^\beta$ and (30) on $u^\alpha q^\beta$ gives $A_v^2=A_q^2$. If we further project (29) on $u^\alpha q^\beta$ we find $A_vA_q=0$, so

$$A_v=A_q=0\ .$$

Combining (28), (29) and (31) gives

$$(\nabla_w \ln\lambda)^2=4(\nabla_u \ln\lambda)^2, \tag{38}$$

$$\nabla_u\nabla_w \ln\lambda=\tfrac{3}{2}\nabla_u \ln\lambda\ \nabla_w \ln\lambda, \tag{39}$$

and (29) then becomes

$$2\nabla_u\nabla_u \ln\lambda-3(\nabla_u \ln\lambda)^2-4\varepsilon\lambda^2=0. \tag{40}$$

If we differentiate (38) in the direction of u^α and use (39) and (40) we find $\lambda=0$. This case does not lead to ideally embedded perfect fluid space–times.

2. If $\mu=3\lambda$ and $\nu=\lambda$

From the Codazzi equations we find $A_v=A_q=B_q=0$ and $\nabla_w\lambda=\nabla_v\lambda=\nabla_q\lambda=0$. We find that u^α is geodesic, hypersurface orthogonal and shearfree. The expansion of the timelike congruence with tangent u^α is given by $\theta=\frac{3}{2}\nabla_u \ln\lambda$. From the Ricci identities we have the equation

$$2\nabla_u\nabla_u \ln\lambda+(\nabla_u \ln\lambda)^2-12\varepsilon\lambda^2=0\ . \tag{41}$$

It follows that if $\theta=0$, $\lambda=0$ and space–time is flat. Therefore we take $\theta\neq 0$. We then choose coordinates adapted to the timelike vector, $u_\alpha=(0,0,0,u_4)$. The metric becomes

$$\mathrm{d}s^2=h_{ij}\mathrm{d}x^i\mathrm{d}x^j-(u_4)^2\mathrm{d}t^2\ ,$$

with $i,j=1,2,3$. Then $\theta=\theta(t)$, $\lambda=\lambda(t)$ and $u_4=u_4(t)$. The second fundamental form of the embedding of the spacelike hypersurface orthogonal to u^α in (M,g) is

$$\Omega^u_{ij}=\tfrac{1}{3}\theta h_{ij}\ .$$

The Riemann tensor of the three-space reads

$${}^3R_{ijkl}=2\{\varepsilon\lambda^2-\tfrac{1}{9}\theta^2\}h_{i[k}h_{l]j}\ ;$$

the spacelike hypersurface is a space of constant curvature. The metric can be written, after a coordinate transformation $u_4(t)\mathrm{d}t\to\mathrm{d}t$, as

$$\mathrm{d}s^2=a^2(t)\{\mathrm{d}r^2+\Sigma^2(r,k)(\mathrm{d}\phi^2+\sin^2(\phi)\mathrm{d}\psi^2)\}-\mathrm{d}t^2\ , \tag{42}$$

with

$$ka^{-2}=\varepsilon\lambda^2-\tfrac{1}{9}\theta^2, \tag{43}$$

and $\Sigma(r,k)=\sin(r),r$ or $\sinh(r)$ if $k=1,0$ or -1. This metric is a Robertson–Walker metric (see Ref. 26 for the first results on the embedding of R-W models in flat five-dimensional spaces). Combining (41) and (43) $a(t)$ must be a solution of

$$(\partial_t a)^2=\varepsilon c^2a^6-k, \tag{44}$$

with $c=\text{const}$ and $\lambda=ca^2$. From the expression of the Ricci tensor (34) and the Einstein equations we can write the energy ρ and pressure p of the perfect fluid as

$$\kappa\rho=3c^2a^4 \quad \text{and} \quad \kappa p=-7c^2a^4,$$

with $\varepsilon=+1$.

V. CONCLUSION

In the study of embeddings of a space–time in some higher-dimensional space attention has focused primarily on intrinsic properties of the submanifold (e.g., the source type or Petrov type). But the fact that we embed our space–time metric in a greater space gives us the opportunity to consider also extrinsic properties of our model. From this viewpoint an ideal embedding seems to be the most natural and simple type of embedding to study. Ideally embedded space–times receive the least amount of tension from the surrounding space. We found that ideally embedded hypersurfaces in a pseudo-Euclidean space contain the de Sitter spaces and a Robertson–Walker model. Embeddings of the de Sitter and Robertson–Walker models were already considered by Ponce de Leon.[27] It was later realized that his five-dimensional embedding space was flat[2,28] and this was used in, e.g., Ref. 29 to study the structure of the Big Bang.

Furthermore, a class of anisotropic perfect fluid models containing a timelike two-surface of constant curvature has also been shown to be ideally embedded. Because the nonflat vacuum models were excluded from our study due to Theorem IV.1 we will study them in a future paper.

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Homotopy structure of 5d vacua

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It is shown that flat zero-energy solutions (vacua) of the 5d Kaluza–Klein theory admit a nontrivial homotopy structure generated by certain Kaluza–Klein excitations. These vacua consist of an infinite set of homotopically different space–times denoted by $\mathcal{M}_5^{(n)}$, among which $\mathcal{M}_5^{(0)}$ and $\mathcal{M}_5^{(1)}$ are especially identified as $M_4 \times S^1$ and M_5, the vacuum states of the 5d Kaluza–Klein theory and the 5d general relativity, respectively (where M_k represents the k-dimensional Minkowski space).
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The 5d Kaluza–Klein theory is distinguished from the ordinary 5d general relativity by the fact that the background vacuum is assumed to be the product $M_4 \times S^1$ instead of M_5, where M_k represents the k-dimensional Minkowski space. Having zero energy, the manifolds $M_4 \times S^1$ and M_5 are both qualified for the vacuum state of the 5d theory of gravity. Classically, there is no way to determine which is more appropriate than the other. The only basis for choosing $M_4 \times S^1$ as the vacuum state of the 5d Kaluza–Klein theory is that it includes the compactified dimension which is crucial in order to admit an internal gauge group U(1) in the reduced theory. In fact, the compactification is an essential ingredient of any higher dimensional theory (including string theory) based on the Kaluza–Klein theory. The particle spectrum is then obtained by expanding around the vacuum $M_4 \times S^1$; one finds a finite number of massless modes and an infinite tower of massive (excitation) modes. In traditional theories the low-energy physics would be mostly governed by the dynamics of the massless modes alone, because the energy scale of the massive modes is about the order of the Planck scale. However, this is not to be the case anymore once we adopt the scenario that extra dimensions be very large. Recently, it has been suggested that the old hierarchy problem can be solved in the framework of higher-dimensional theories by taking extra dimensions to be very large.[1] In this scenario the energy scale of the massive modes (which is of the order of the inverse of the radius of S^1) could sufficiently lower down to the level of low energy physics, and one can imagine that the massive modes perhaps play an important role even in the low energy limit. In this paper, we examine the effect of the massive excitations on the geometry or topology of the background space–time $M_4 \times S^1$. Then we end up with a remarkable result that 5d vacua admit a nontrivial homotopy structure; 5d vacua consist of an infinite set of homotopically different space–times denoted by $\mathcal{M}_5^{(n)}$, where $\mathcal{M}_5^{(0)}$ and $\mathcal{M}_5^{(1)}$ are especially identified as $M_4 \times S^1$ and M_5, respectively. It is also conjectured that $M_4 \times S^1$ may not be the true physical vacuum of the 5d Kaluza–Klein theory.

We start the discussion with a metric

$$\begin{aligned} ds^2 &= -dt^2 + dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2) + \Phi^2(x^\alpha, x^5)[dx^5 + A_\mu(x^\alpha, x^5)dx^\mu]^2 \\ &= \overset{4}{g}_{\mu\nu} dx^\mu dx^\nu + \Phi^2[dx^5 + A_\mu dx^\mu]^2 \\ &= \overset{4}{\eta}_{ab} \omega^a \omega^b + (\omega^5)^2 \quad (\mu, \nu, \alpha = 0,1,2,3; a, b = 0,1,2,3), \end{aligned} \tag{1}$$

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where $\overset{4}{\eta}_{ab}$ is the 4d flat Minkowski metric, and

$$\omega^a = e^a_\mu dx^\mu, \quad \omega^5 = \Phi(dx^5 + A_\mu dx^\mu) \tag{2}$$

are basis one-forms of the orthonormal frame. From Eq. (1) we see that the fields Φ and A_μ have x^5-dependence, meaning that they include massive modes. In the reduced 4d sector, Φ and A_μ are identified as the Brans–Dicke scalar and the U(1) gauge potential, respectively. The vierbein $e^a{}_\mu$, on the other hand, are functions of x^α alone,[2] so they commute with ∂_5. The nonvanishing components of Riemann tensor are then calculated in the orthonormal frame to give[3]

$$\overset{5}{R}_{abcd} = -\tfrac{1}{2}(\hat{f}_{ab}\hat{f}_{cd} + \hat{f}_{a[c}\hat{f}_{bd]}), \tag{3}$$

$$\overset{5}{R}_{abc5} = \mathcal{D}_{[a}\hat{f}_{b]c} - F_c\hat{f}_{ab}, \tag{4}$$

$$\overset{5}{R}_{a5b5} = -\mathcal{D}_{(a}F_{b)} - \tfrac{1}{4}\hat{f}_{ac}\hat{f}^c{}_b - F_aF_b, \tag{5}$$

where $\hat{f}_{ab}$ is defined by $\hat{f}_{ab} \equiv \Phi f_{ab}$ and

$$f_{ab} = e_a{}^\mu e_b{}^\nu (D_\mu A_\nu - D_\nu A_\mu) \equiv e_a{}^\mu e_b{}^\nu f_{\mu\nu} \quad (D_\mu \equiv \partial_\mu - A_\mu\partial_5), \tag{6}$$

$$F_a = e_a{}^\mu(\partial_\mu\Phi - \partial_5\hat{A}_\mu)/\Phi \equiv e_a{}^\mu F_\mu \quad (\hat{A}_\mu \equiv \Phi A_\mu), \tag{7}$$

$$\mathcal{D}_a = e_a{}^\mu(\nabla_\mu - A_\mu\partial_5) \equiv e_a{}^\mu\mathcal{D}_\mu, \tag{8}$$

and, in Eq. (8), ∇_μ represents the ordinary covariant derivative associated with the metric $\overset{4}{g}_{\mu\nu}$. Also, $f_{\mu\nu}$ in Eq. (6) is a generalization of the Maxwell field strength; it takes the same form as the conventional Maxwell field strength except that the ordinary derivative ∂_μ is replaced by the covariant derivative[4] D_μ. Without x^5-dependency the derivative D_μ reduces to ∂_μ, and consequently $f_{\mu\nu}$ becomes the conventional Maxwell field strength.

Now we look for flat (vacuum) solutions which satisfy the equations $\overset{5}{R}_{abcd} = \overset{5}{R}_{abc5} = \overset{5}{R}_{a5b5} = 0$. A set of the simplest solutions to these equations may be obtained by setting

$$f_{\mu\nu} = D_\mu A_\nu - D_\nu A_\mu = 0, \tag{9}$$

$$F_\mu = \frac{1}{\Phi}(\partial_\mu\Phi - \partial_5\hat{A}_\mu) = 0, \tag{10}$$

and in particular Eq. (9) is immediately solved by an ansatz

$$A_t = A_\theta = A_\phi = 0, \quad A_r = A_r(r, x^5), \quad \Phi = \Phi(r, x^5). \tag{11}$$

Equation (11) is actually the most general ansatz preserving spherical symmetry, and A_μ in Eq. (11) may be regarded as a pure gauge in the sense that it gives $f_{\mu\nu} = 0$. With this ansatz, the metric in Eq. (1) can be recast into the form

$$ds^2 = -dt^2 + d\hat{r}^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2) + \frac{\Phi^2}{1 + \hat{A}_r^2}(dx^5)^2 \quad (\hat{A}_r \equiv \Phi A_r), \tag{12}$$

where $d\hat{r}$ is defined by

$$d\hat{r}=(1+\hat{A}_r{}^2)^{1/2}dr+\frac{\Phi\hat{A}_r}{(1+\hat{A}_r{}^2)^{1/2}}dx^5. \tag{13}$$

Equation (13) indicates that the variable $\hat{r}$ is a function of r and x^5, i.e., $\hat{r}=f(r,x^5)$ with

$$\frac{\partial f}{\partial r}=(1+\hat{A}_r{}^2)^{1/2}, \quad \frac{\partial f}{\partial x^5}=\frac{\Phi\hat{A}_r}{(1+\hat{A}_r{}^2)^{1/2}}. \tag{14}$$

With the aid of Eq. (10) one then finds from the equations in (14) that the condition $\partial^2 f/\partial r\partial x^5 = \partial^2 f/\partial x^5\partial r$ implies that $\partial_r\hat{A}_r=0$; i.e., $\hat{A}_r$ must be a function of x^5 alone:

$$\hat{A}_r\equiv Y(x^5). \tag{15}$$

Thus the equations in (14) are now integrated to give

$$f=\hat{r}=r(1+Y^2)^{1/2}+g(x^5), \tag{16}$$

$$\Phi=rY'+\frac{(1+Y^2)^{1/2}}{Y}g', \tag{17}$$

where $g(x^5)$, which has been introduced as an integral constant, is an arbitrary function of x^5 alone, and the ''prime'' in Eq. (17) denotes the x^5-derivative. Note that $\hat{A}_r$ and Φ in Eqs. (15) and (17) indeed describe the flat solution satisfying $\overset{5}{R}_{ABCD}=0$; one can readily check that they satisfy Eq. (10). Now we impose the condition

$$\lim_{Y,Y'\to 0}\ \Phi=\text{const}\equiv\Phi_0, \tag{18}$$

which suggests that the solution we are to find is the one that reduces to the Kaluza–Klein vacuum $M_4\times S^1$ as $A_\mu\to 0$; note that $M_4\times S^1$ with $A_\mu=0$ and $\Phi=$const is also a solution to Eq. (10). The condition in Eq. (18) immediately implies that

$$g'=\Phi_0 Y, \tag{19}$$

and therefore Φ in Eq. (17) becomes

$$\Phi=rY'+\Phi_0(1+Y^2)^{1/2}. \tag{20}$$

Using all this, one can show that the metric in Eq. (12) can be converted into the form

$$ds^2=-dt^2+\left(1-\frac{\Phi_0^2Y^2}{R^2}\right)d\rho^2+\frac{\rho^2}{1+Y^2}(d\theta^2+\sin^2\theta d\phi^2)+R^2\left(dx^5+\frac{\Phi_0 Y}{R^2}d\rho\right)^2, \tag{21}$$

where ρ and R are defined by

$$\rho=\hat{r}-g=r(1+Y^2)^{1/2}, \tag{22}$$

$$R=\left[\Phi_0^2Y^2+\left(\rho\frac{Y'}{1+Y^2}+\Phi_0\right)^2\right]^{1/2}. \tag{23}$$

So far, the function $Y(x^5)$ and the constant Φ_0 have been entirely arbitrary except that they should satisfy the condition (18). Now let us take

$$Y_n(x^5)=\tan\frac{nx^5}{2R_c},\quad \Phi_0=\delta_{n0}\quad (n=0,1,2,...), \tag{24}$$

where R_c represents the compactification radius of the fifth-dimension [note that Eq. (24) respects the condition (18) as $n\to 0$]. By Eqs. (15), (20), and (24), the gauge field A_r becomes

$$A_r(r,x^5)=a_n(r)\sin\frac{nx^5}{R_c} \tag{25}$$

with

$$a_n(r)=\frac{R_c}{nr+2R_c\delta_{n0}}, \tag{26}$$

which shows that taking $Y_n(x^5)$ as in Eq. (24) implies that we are considering a situation where the nth excitation of the gauge field (together with the scalar field induced by this gauge field) is present in the background space–time $M_4\times S^1$ [see Eq. (1)]. In this case the field $\Phi(r,x^5)$ takes the form

$$\Phi(r,x^5)=\frac{nr}{2R_c}\sec^2\frac{nx^5}{2R_c}+\delta_{n0}, \tag{27}$$

and we see that $A_r\to 0$, $\Phi\to 1$ for $n=0$. Namely, the $n=0$ state simply describes the compactified vacuum $M_4\times S^1$ without any gauge or scalar field. For $n\neq 0$, on the other hand, both fields are present in the form of $A_r\sim 1/r$ and $\Phi\sim r$, respectively [the presence of the gauge excitation necessarily demands the presence of the scalar field with a behavior of $\Phi\sim r$, as can be checked from Eq. (10)]. Then, what happens to the space–time by the presence of these excitations Φ and A_r? By Eq. (24), the metric (21) simplifies to

$$ds^2=-dt^2+d\rho^2+\rho^2\sin^2\chi_n(d\theta^2+\sin^2\theta d\phi^2)+(\rho d\chi_n+\delta_{n0}dx^5)^2 \tag{28}$$

with χ_n defined by

$$\chi_n(x^5)=\frac{nx^5}{2R_c}+\frac{\pi}{2}, \tag{29}$$

which, after all, implies that the metric (28) is equivalent under (24) to the metric in Eq. (1) with Φ and A_μ given by Eqs. (25) and (27). Indeed, for $n=0$, it reduces to the flat $M_4\times S^1$:

$$ds^2_{(0)}=-dt^2+d\rho^2+\rho^2(d\theta^2+\sin^2\theta d\phi^2)+(dx^5)^2, \tag{30}$$

which is just the metric in Eq. (1) with $A_\mu=0$, $\Phi=1$. For $n\neq 0$, on the other hand, the metric (28) becomes

$$ds^2_{(n)}=-dt^2+d\rho^2+\rho^2[d\chi_n^2+\sin^2\chi_n(d\theta^2+\sin^2\theta d\phi^2)], \tag{31}$$

the 5d flat Minkowski metric! The topology of space–time has been changed by the nonzero excitation modes. The toroidal compactification $M_4\times S^1$ in Eq. (1) has been converted into the noncompact space–time described by the metric in Eq. (31). Furthermore, let us change the variable $x^5\to y_n$ by the equation

$$y_n=x^5+\frac{\pi R_c}{n}. \tag{32}$$

Under Eq. (32), the metric (1) [with A_r and Φ given by Eqs. (25) and (27)] takes the same form as before, i.e.,

$$ds^2 = -dt^2 + dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2) + \Phi^2(r, y_n)[dy_n + A_r(r, y_n)dr]^2 \tag{33}$$

with[5]

$$A_r(r, y_n) = -a_n(r)\sin\frac{ny_n}{R_c}, \quad \Phi(r, y_n) = \frac{nr}{2R_c}\csc^2\frac{ny_n}{2R_c} + \delta_{n0}, \tag{34}$$

but χ_n in (31) is now written [from (29)] as

$$\chi_n(y) = \frac{ny_n}{2R_c} \quad (0 \leqslant y_n \leqslant 2\pi R_c). \tag{35}$$

This is remarkable. Equation (35) suggests that the 5d vacua admit a nontrivial homotopy structure. Note that the angle χ_n varies from 0 to $n\pi$ as y_n makes a single turn from 0 to $2\pi R_c$ around S^1, which in turn means that the set of variables (χ_n, θ, ϕ) in (31) covers the hypersurface S^3 n times when (y_n, θ, ϕ) in (33) covers $S^2 \times S^1$ just once. The 3d manifold described by (χ_n, θ, ϕ) can be regarded as a three-loop $\alpha_n(t_1, t_2, t_3)$, where t_i, the coordinates of 3d cube I_3, are defined by the map: $t_1 = y_n/2\pi R_c$, $t_2 = \theta/\pi$ and $t_3 = \phi/2\pi$, which is an homeomorphism $f: S^2 \times S^1 \to I_3$. A collection of these three-loops which cover S^3 n times constitutes the nth equivalence class of the third homotopy group $\pi_3(S^3)$. The spatial subsector of the space–time described by Eq. (31) is essentially a pile of such three-loops. This suggests that the space–time described by Eq. (31) (let us call it $\mathcal{M}_5^{(n)}$) belongs to the $n \neq 0$ homotopy class of $\pi_3(S^3)$, though $M_4 \times S^1$ with no excitations especially belongs to the $n = 0$ class since it is obtained by simply taking[6] $n = 0$. Further, for $n = 1$, it is obvious from Eq. (35) that $\mathcal{M}_5^{(n)}$ is precisely identified as the ordinary 5d Minkowski space M_5. But note that, in general, $\mathcal{M}_5^{(n)}$ is not M_5 itself; $\mathcal{M}_5^{(n)}$ is an n-fold cover of M_5. Namely, it is a fiber bundle over M_5 with fiber F a discrete set of n points. In short, 5d vacua consist of an infinite set of homotopically different space–times $\mathcal{M}_5^{(n)}$, among which the cases of $n = 0$ and $n = 1$ are especially identified as the background vacua of the 5d Kaluza–Klein theory and the 5d general relativity, respectively; i.e., $M_4 \times S^1 = \mathcal{M}_5^{(0)}$, and $M_5 = \mathcal{M}_5^{(1)}$. Such a homotopy structure manifests itself once there is a defect, or a point particle at $\rho = 0$. With a defect or point particle at $\rho = 0$, the spatial subsector of M_5 is not simply connected, and the three-loops which contain $\rho = 0$ are not shrinkable. So each $\mathcal{M}_5^{(n)}$, a pile of such three-loops which enclose the point $\rho = 0$ n times, belongs to a different homotopy class.

Though the above discussion has its own right in 5d Kaluza–Klein theories, it may be applied to any other higher dimensional theories with toroidal compactification. For instance, in the 11-dimensional theory compactified on $X \times S^1/Z_2$ (or equivalently, in the strong coupling limit of the $E_8 \times E_8$ heterotic string) it is believed that the radius of the orbifold S^1 is larger than the volume of the Calabi–Yau manifold X, and there is a regime where our space–time appears five-dimensional.[7,8] To the lowest order of the 11d Newton constant κ, the (5d sector of the) ground state metric takes the form of the 5d Kaluza–Klein vacuum $M_4 \times S^1$. So in this case the vacua of the theory could admit the homotopy structure under discussion. If this is the case, it then follows that the T-duality could break down due to the presence of the excitations. Note that for $n \neq 0$ the compactified dimension S^1 disappears due to the excitation modes; the map $f: S^2 \times S^1 \to S^3$ takes S^1 to the great circle of S^3. Thus the winding number (of the closed string) is not a topological number here and consequently the term corresponding to winding modes does not exist in the mass formula, and it leads to the conjecture that the T-duality might break down in the presence of excitations.

So far, we have considered only the (excitations of the) Kaluza–Klein components (i.e., 5d metric components) as the source of the topology change of the space–time. But in the 5d bulk space–time there also exist other fields besides the Kaluza–Klein components.[8] For instance, we may consider the case where a 5d U(1) gauge field[9] $\mathcal{A}_\mu$ exists in the bulk space–time, with field

strength $\mathcal{F}_{\mu\nu}$ (see, for instance, Ref. 10), and it takes the place of the Kaluza–Klein vector A_μ. Indeed, disregarding the components $\mathcal{F}_{\mu 5}$, one finds that the 4d effective action for $\mathcal{A}_\mu$ takes the same form as the action for A_μ, which suggests that the homotopy structure of the 5d vacua can be generated even by (the excitations of) bulk fields, rather than Kaluza–Klein components.

The result of this paper is quite analogous to the case of the θ-vacua of the Yang–Mills theory. In both cases the vacua admit the same homotopy structure with an infinite set of homotopy classes each of which is characterized by an integer n. In the Yang–Mills theory the integer n is identified with the Pontryagin index $q \sim Tr\int d^4x F^{\mu\nu}\tilde{F}_{\mu\nu}$, and the vacua belonging to different homotopy classes are connected by a Euclidean (instanton) solution. In the present paper the integer n is simply an excitation number of the pure gauge A_μ, and the instanton solution interconnecting two different vacua does not exist here. But notice that in our case there exist gauge transformations which mix the massive and massless modes[11] of A_μ, and consequently the space–times belonging to different classes can be mixed by such gauge transformations. The gauge transformation which mixes the massive and massless modes can be generated by allowing gauge parameter ξ to depend on x^5. For instance, the transformation which mixes the nth and $(n-k)$th modes (in the Fourier exponential series) of A_μ takes the form (see Ref. 11)

$$\delta_k A_{\mu n} = \delta_{nk}\partial_\mu \xi_k + i(n-2k)\xi_k A_{\mu(n-k)}/R_c, \tag{36}$$

where $A_{\mu n}$ and ξ_n are the nth components of the Fourier exponential series

$$A_\mu(x^\alpha, x^5) = \sum_n A_{\mu n}(x^\alpha) e^{inx^5/R_c}, \tag{37}$$

$$\xi(x^\alpha, x^5) = \sum_n \xi_n(x^\alpha) e^{inx^5/R_c}, \tag{38}$$

respectively, and δ_k represents the transformation induced by ξ_k. Since $\mathcal{M}_5^{(n)}$ is equivalent to $\mathcal{M}_5^{(0)}$ plus the nth excitation (in the Fourier sine-series) of A_μ, the transformation (36) apparently mixes $\mathcal{M}_5^{(n)}$ with other space–times belonging to different classes. This is quite remarkable. Note that a gauge transformation essentially does not change the physics of a system. But the above argument suggests that $\mathcal{M}_5^{(n)}$ is not invariant under a ''large'' gauge transformation of the form (36), which immediately leads us to suspect that space–times $\mathcal{M}_5^{(n)}$ (most importantly $\mathcal{M}_5^{(0)} = M_4 \times S^1$ and $\mathcal{M}_5^{(1)} = M_5$) may not be the physical states of the theory. Namely, the suggested conjecture is that $M_4 \times S^1$ may not be the true physical vacuum of the 5d Kaluza–Klein theory; it serves as a vacuum only when we do not consider the ''large'' gauge transformation. The physical vacuum of the 5d Kaluza–Klein theory may perhaps be a superposition of an infinite number of $\mathcal{M}_5^{(n)}$, analogously to the case of the θ-vacua of the Yang–Mills theory.

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[6] Equation (35) [i.e., the variable change $x^5 \to y_n$ in Eq. (32)] is in fact applicable to the $n = 0$ case either. Note that since $\lim_{n\to 0} n y_n = \pi R_c$ from (32), we see that the metric (33) reduces to the flat $M_4 \times S^1$ as $n \to 0$. This is the same result that we obtain from the metric (1) with A_r and Φ given by Eqs. (25) and (27).

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Classification of static plane symmetric space–times according to their matter collineations

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In this paper we classify static plane symmetric space–times according to their matter collineations. These have been studied for both cases when the energy–momentum tensor is nondegenerate and also when it is degenerate. It turns out that the nondegenerate case yields either *four*, *five*, *six*, *seven*, or *ten* independent matter collineations in which *four* are isometries and the rest are proper. There exists three interesting cases where the energy–momentum tensor is degenerate but the group of matter collineations is finite-dimensional. The matter collineations in these cases are either *four*, *six*, or *ten*. © *2004 American Institute of Physics.*
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I. INTRODUCTION

There exists a large body of literature on classification of space–times according to their isometries or Killing vectors (KVs) and the groups admitted by them.[1–4] These investigations of symmetries played an important role in the classification of space–times, giving rise to many interesting results with useful applications. As curvature and Ricci tensors play a significant role in understanding the geometric structure of metrics, the energy–momentum tensor enables us to understand the physical structure of space–times. Symmetries of the energy–momentum tensor (also called matter collineations) provide conservation laws on matter fields. These enable us to know how the physical fields, occupying certain region of space–times, reflect the symmetries of the metric.[5]

Some recent literature[6–12] shows keen interest in the study of matter collineations (MCs). In one of the recent papers,[12] the study of MCs has been taken for spherically symmetric space–times and some interesting results have been obtained. In this paper, we address the same problem for static plane symmetric space–times. It turns out that static plane symmetric space–times admit a MC Lie algebra of 10, 7, 6, 5, and 4 dimensions apart from the infinite-dimensional algebras.

Let (M,g) be a space–time, where M is a smooth, connected, Hausdorff four-dimensional manifold and g is a smooth Lorentzian metric of signature $(+\ -\ -\ -)$ defined on M. The manifold M and the metric g are assumed smooth (C^{∞}). We shall use the usual component notation in local charts, and a covariant derivative with respect to the symmetric connection Γ associated with the metric g will be denoted by a semicolon and a partial derivative by a comma. A smooth vector field ξ is said to preserve a matter symmetry[13] on M if, for each smooth local diffeomorphism ϕ_t associated with ξ, the tensors T and $\phi_t^* T$ are equal on the domain U of ϕ_t, i.e., $T=\phi_t^* T$. Equivalently, a vector field ξ^a is said to generate a matter collineation if it satisfies the following equation:

$$\pounds_{\xi} T_{ab}=0, \tag{1}$$

where $\pounds$ is the Lie derivative operator, ξ^a is the symmetry or collineation vector. Every KV is an

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MC but the converse is not true, in general. Collineations can be proper (nontrivial) or improper (trivial). We define a proper MC to be a MC which is not a KV, or a homothetic vector (HV). The MC Eq. (1) can be written in component form as

$$T_{ab,c}\xi^c + T_{ac}\xi^c_{,b} + T_{cb}\xi^c_{,a} = 0 \quad (a,b,c = 0,1,2,3). \tag{2}$$

A plane symmetric space–time is a Lorentzian manifold possessing a physical stress–energy tensor. This admits $SO(2)\otimes\Re^2$ as the minimal isometry group in such a way that the group orbits are spacelike surfaces of constant curvature. The metric for static plane symmetric space–times is given in the form[3]

$$ds^2 = e^{\nu(x)}\,dt^2 - dx^2 - e^{\mu(x)}(dy^2 + dz^2), \tag{3}$$

where ν and μ are arbitrary functions of x. The surviving components of the energy–momentum tensor, given in Appendix A, are T_0, T_1, T_2, T_3, where $T_3 = T_2$ and we have used the notation $T_{aa} = T_a$ for the sake of simplicity.

The MC equations can be written as follows:

$$T_{0,1}\xi^1 + 2T_0\xi^0_{,0} = 0, \tag{4}$$

$$T_0\xi^0_{,1} + T_1\xi^1_{,0} = 0, \tag{5}$$

$$T_0\xi^0_{,2} + T_2\xi^2_{,0} = 0, \tag{6}$$

$$T_0\xi^0_{,3} + T_2\xi^3_{,0} = 0, \tag{7}$$

$$T_{1,1}\xi^1 + 2T_1\xi^1_{,1} = 0, \tag{8}$$

$$T_1\xi^1_{,2} + T_2\xi^2_{,1} = 0, \tag{9}$$

$$T_1\xi^1_{,3} + T_2\xi^3_{,1} = 0, \tag{10}$$

$$T_{2,1}\xi^1 + 2T_2\xi^2_{,2} = 0, \tag{11}$$

$$T_2(\xi^2_{,3} + \xi^3_{,2}) = 0, \tag{12}$$

$$T_{2,1}\xi^1 + 2T_2\xi^3_{,3} = 0. \tag{13}$$

These are the first order nonlinear partial differential equations in four variables $\xi^a(x^b)$. We solve these equations for the nondegenerate case, when

$$\det(T_{ab}) = T_0T_1T_2^2 \neq 0, \tag{14}$$

and for the degenerate case, where $\det(T_{ab}) = 0$. The rest of the paper is organized as follows. The next section contains a solution of MC equations when the energy–momentum tensor is nondegenerate. In Sec. III, MC equations are solved for the degenerate energy–momentum tensor and Sec. IV provides some examples admitting proper MCs for the nondegenerate case. Finally, Sec. V contains a summary and discussion of the results obtained.

II. MATTER COLLINEATIONS IN THE NONDEGENERATE CASE

In this section, we shall evaluate MCs only for those cases which have a nondegenerate energy–momentum tensor, i.e., $\det(T_{ab}) \neq 0$. To this end, we set up the general conditions for the solution of MC equations for the nondegenerate case.

When we solve Eqs. (4)–(13) simultaneously, after some algebraic computations, we arrive at the following solution:

$$\xi^0=-\frac{T_2}{T_0}\left[\frac{1}{2}(y^2+z^2)\dot{A}_1+z\dot{A}_2+y\dot{A}_3\right]+A_4, \tag{15}$$

$$\xi^1=-\frac{T_2}{T_1}\left[\frac{1}{2}(y^2+z^2)A_1'+zA_2'+yA_3'\right]+A_5, \tag{16}$$

$$\xi^2=\tfrac{1}{2}z^2(c_1y+c_3)+z(c_2y+c_4)-\tfrac{1}{6}c_1y^3-\tfrac{1}{2}c_3y^2+yA_1+A_3, \tag{17}$$

$$\xi^3=-\tfrac{1}{2}y^2(c_1z+c_2)-y(c_3z+c_4)+\tfrac{1}{6}c_1z^3+\tfrac{1}{2}c_2z^2+zA_1+A_3, \tag{18}$$

where c_1,c_2,c_3,c_4 are arbitrary constants and $A_\mu=A_\mu(t,x)$, $\mu=1,2,3,4,5$ are integration functions. Here an overdot and a prime indicate the differentiation with respect to time and the x coordinate, respectively. When we replace these values of ξ^a in MC, Eqs. (4)–(13), we obtain the following constraints on A_μ:

$$\frac{T_0'}{T_1}A_i'+2\ddot{A}_i=0 \quad (i=1,2,3), \tag{19}$$

$$\dot{A}_i=\sqrt{\frac{T_0}{T_2}}f_i(t),\ \ A_i'=\frac{\sqrt{T_1}}{T_2}g_i(t), \tag{20}$$

$$\dot{A}_4=-\frac{T_0'}{2T_0\sqrt{T_1}}g_5(t),\ \ A_4'=-\frac{\sqrt{T_1}}{T_0}\dot{g}_5(t), \tag{21}$$

$$c_1=0,\ \ T_2'A_1'=0, \tag{22}$$

$$\frac{T_2'}{T_2}A_5+2A_1=0, \tag{23}$$

$$\frac{T_2'}{T_2\sqrt{T_1}}g_2(t)-2c_2=0, \tag{24}$$

$$\frac{T_2'}{T_2\sqrt{T_1}}g_3(t)+2c_3=0, \tag{25}$$

$$\frac{T_2'}{T_2\sqrt{T_1}}g_5(t)+2A_1=0, \tag{26}$$

$$\frac{T_0'}{T_2\sqrt{T_1}}g_i(t)+2\ddot{A}_i=0, \tag{27}$$

where $f_i(t),g_i(t)$, $g_5(t)$ are integration functions. Thus the problem of working out MCs for all possibilities of A_i,A_4,A_5 is reduced to solving the set of Eqs. (15)–(18) subject to the above constraints. We would solve these to classify MCs of the plane symmetry manifolds.

From Eqs. (24)–(26), there arise two main cases:

$$(1)\quad \left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' \neq 0;\ (2)\quad \left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0.$$

Case (1): In this case, we have $T_2' \neq 0$ and hence Eq. (22) gives $A_1 = A_1(t)$. Using these in Eq. (26), it follows that

$$\frac{T_2'}{T_0\sqrt{T_1}} g_5(t) + 2A_1(t) = 0, \tag{28}$$

which implies that $g_5 = 0$ and $A_1 = 0$. Thus we have from Eqs. (21) and (23) $A_5 = 0$, $A_4 = c_0$. Also, Eqs. (24) and (25) yield

$$g_2 = 0 = g_3,\ c_2 = 0 = c_3. \tag{29}$$

Now from Eqs. (19) and (20), we have

$$A_j' = 0,\ \ddot{A}_j = 0,\ \dot{f}_j = 0\ \ (j = 2,3), \tag{30}$$

which gives

$$A_j(t,x) = \sqrt{\frac{T_0}{T_2}} c_j t + c_{j+2}. \tag{31}$$

Since $A_j'(t,x) = 0$ which implies that either

$$(a)\quad \left(\frac{T_0}{T_2}\right)' = 0,\quad \text{or}\ (b)\quad \left(\frac{T_0}{T_2}\right)' \neq 0.$$

In the first case 1(a), we have the following MCs:

$$\begin{gathered}\xi_{(1)} = \partial_t,\ \ \xi_{(2)} = \partial_y,\ \ \xi_{(3)} = \partial_z,\ \ \xi_{(4)} = z\partial_y - y\partial_z, \\ \xi_{(5)} = t\partial_z - \frac{T_2}{T_0} z\partial_t,\quad \xi_{(6)} = t\partial_y - \frac{T_2}{T_0} y\partial_t.\end{gathered} \tag{32}$$

Thus we obtain six independent MCs in which four are the usual isometries of the plane symmetry and the rest are the proper MCs. The MCs for the case 1(b) turns out to be the same as the minimal isometries for the plane symmetry.

Case (2): This case implies that $T_2'/T_2\sqrt{T_1} = \alpha$, where α is an arbitrary constant and can have the following two subcases according as α is nonzero or zero.

$$(a)\quad \alpha \neq 0,\quad (b)\quad \alpha = 0.$$

For the case 2(a), we use Eqs. (20), (22), (24), and (25) so that

$$g_2 = 2c_2/\alpha,\ g_3 = -2c_3/\alpha,\ A_1' = 0, \tag{33}$$

and

$$\left(\frac{T_2}{T_0}\right)' \dot{A}_i = 0. \tag{34}$$

The last equation further gives us the following two possibilities:

$$\text{(i)} \quad \left(\frac{T_2}{T_0}\right)' \neq 0, \quad \text{(ii)} \quad \left(\frac{T_2}{T_0}\right)' = 0.$$

In the first case 2a(i), Eqs. (20), (21), (23), (25), (36), and (37) imply that

$$A_5 = c_5,\ T_0' A_i' = 0,\ A_5 = -\frac{2c_5}{\alpha\sqrt{T_1}},\ A_4' = 0, \tag{35}$$

and

$$\dot{A}_4 = \frac{T_0'}{\alpha T_0 \sqrt{T_1}} c_5. \tag{36}$$

This last equation implies that for $(T_0'/T_0\sqrt{T_1})' \neq 0$, we have the same MCs as KVs. When $T_0'/T_0\sqrt{T_1} = \beta$, where β is an arbitrary constant, this further gives the following two subcases:

$$(*) \quad \beta \neq 0; \quad (**) \quad \beta = 0.$$

The case 2ai(*), in addition to the usual isometries of plan symmetry, gives the following one proper MC:

$$\xi_{(5)} = \frac{\beta}{\alpha} t\partial_t - \frac{2}{\alpha\sqrt{T_1}}\partial_x + y\partial_y + z\partial_z. \tag{37}$$

For the case 2ai(**), we have $T_0 = \text{const}$ and we obtain the following MCs:

$$\xi_{(5)} = yz + \left(\frac{z^2}{2} - \frac{y^2}{2} - \frac{2}{\alpha^2 T_2}\right)\partial_z,$$

$$\xi_{(6)} = yz - \left(\frac{z^2}{2} - \frac{y^2}{2} + \frac{2}{\alpha^2 T_2}\right)\partial_y, \tag{38}$$

$$\xi_{(7)} = y\partial_y + z\partial_z.$$

This implies that we have seven independent MCs in which three are the proper MCs.

In the case 2a(ii), we obtain $T_2 = \gamma T_0$, where γ is an arbitrary constant and this yields the following MCs:

$$\xi_{(5)} = \frac{1}{2}\left(t^2 - \frac{4}{\alpha^2 T_0} - \gamma y^2 - \gamma z^2\right)\partial_t + \frac{2}{\alpha\sqrt{T_1}}\partial_x + ty\partial_y + tz\partial_z,$$

$$\xi_{(6)} = \frac{1}{\gamma} tz\partial_t + \frac{2}{\alpha^2\sqrt{T_1}} z\partial_x + yz\partial_y - \frac{1}{2}\left(\frac{t^2}{\gamma} + \frac{4}{\alpha^2 T_2} + y^2 - z^2\right)\partial_z,$$

$$\xi_{(7)} = z\partial_t - t\partial_z,$$

$$\xi_{(8)} = \frac{1}{\gamma} ty\partial_t + \frac{2}{\alpha^2\sqrt{T_1}} y\partial_x - \frac{1}{2}\left(\frac{t^2}{\gamma} + \frac{4}{\alpha^2 T_2} - y^2 + z^2\right)\partial_y - yz\partial_z,$$

$$\xi_{(9)} = y\partial_t - t\partial_y,$$

$$\xi_{(10)}=t\partial_t+\frac{2}{\alpha\sqrt{T_1}}\partial_x+y\partial_y+z\partial_z. \tag{39}$$

This shows that we have ten independent MCs including six proper MCs.

The case 2(b) implies that $T_2=\text{const}$ which yields that either

$$\text{(i)}\quad \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'=0 \quad \text{or} \quad \text{(ii)}\quad \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'\neq 0$$

For the first possibility 2b(i), we have $(\sqrt{T_0})'/\sqrt{T_1}=\delta$, where δ is an arbitrary constant and gives two possibilities according to whether it is nonzero or zero:

$$(*)\quad \delta\neq 0, \quad (**)\quad \delta=0.$$

For the case 2bi(*), we obtain the following MCs:

$$\begin{aligned}
\xi_{(5)}&=\frac{T_2}{\sqrt{T_0}}z\sin\delta t\partial_t-\frac{T_2}{\sqrt{T_1}}z\cos\delta t\partial_x+\frac{T_0}{\delta}\cos\delta t\partial_z,\\
\xi_{(6)}&=\frac{T_2}{\sqrt{T_0}}z\cos\delta t\partial_t+\frac{T_2}{\sqrt{T_1}}z\sin\delta t\partial_x-\frac{T_0}{\delta}\sin\delta t\partial_z,\\
\xi_{(7)}&=\frac{T_2}{\sqrt{T_0}}y\sin\delta t\partial_t-\frac{T_2}{\sqrt{T_1}}y\cos\delta t\partial_x+\frac{T_0}{\delta}\cos\delta t\partial_y,\\
\xi_{(8)}&=\frac{T_2}{\sqrt{T_0}}y\cos\delta t\partial_t+\frac{T_2}{\sqrt{T_1}}y\sin\delta t\partial_x-\frac{T_0}{\delta}\sin\delta t\partial_y,\\
\xi_{(9)}&=\frac{1}{\sqrt{T_0}}\sin\delta t\partial_t-\frac{1}{\sqrt{T_1}}\cos\delta t\partial_x,\\
\xi_{(10)}&=\frac{1}{\sqrt{T_0}}\cos\delta t\partial_t+\frac{1}{\sqrt{T_1}}\sin\delta t\partial_x,
\end{aligned} \tag{40}$$

which yields ten independent MCs having six proper MCs.

In the case of 2bi(**), we have the following MCs:

$$\begin{aligned}
\xi_{(5)}&=\frac{T_2}{\sqrt{T_1}}z\partial_x-\int\sqrt{T_1}dx\partial_z,\\
\xi_{(6)}&=\frac{T_2}{\sqrt{T_1}}y\partial_x-t\partial_z,\\
\xi_{(7)}&=\frac{T_2}{\sqrt{T_1}}z\partial_t-\int\sqrt{T_1}dx\partial_y,\\
\xi_{(8)}&=\frac{T_2}{\sqrt{T_1}}y\partial_t-t\partial_y,
\end{aligned} \tag{41}$$

$$\xi_{(9)}=\frac{1}{T_0}\int \sqrt{T_1}dx\partial_t-\frac{1}{\sqrt{T_1}}t\partial_x,$$

$$\xi_{(10)}=\frac{1}{\sqrt{T_1}}\partial_x,$$

giving ten independent MCs with six proper MCs.

The case 2b(ii) further implies the following two possibilities:

$$(*)\quad \left(\frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\right)'=0;\quad (**)\quad \left(\frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\right)'\neq 0.$$

For 2bii(*), we have $(T_0/2)\sqrt{T_1}(T_0'/T_0\sqrt{T_1})'=\epsilon$, where ϵ is an integration constant and gives further two cases when

$$(+)\quad \epsilon=0 \qquad \text{and} \quad (++)\quad \epsilon\neq 0.$$

In the case 2bii*(+), we have $T_0'/T_0\sqrt{T_1}=\chi\neq 0$, and this gives the following MCs:

$$\xi_{(5)}=\left(\frac{1}{\chi T_0}-\frac{\chi}{4}t^2\right)\partial_t+\frac{1}{\sqrt{T_1}}t\partial_x,$$

$$\xi_{(6)}=\frac{\chi}{2}t\partial_t+\frac{1}{\sqrt{T_1}}\partial_x, \tag{42}$$

yielding six independent MCs.

For the case 2bii*(++), we obtain

$$\xi_{(5)}=\left(\frac{1}{T_0}\partial_t-\frac{1}{\sqrt{T_1}}\partial_x\right)e^{\sqrt{\eta}t},$$

$$\xi_{(6)}=\left(\frac{1}{T_0}\partial_t+\frac{1}{\sqrt{T_1}}\partial_x\right)e^{-\sqrt{\eta}t}, \tag{43}$$

giving six independent MCs.

In the case 2bii(**), we get MCs equal to the KVs.

III. MATTER COLLINEATIONS IN THE DEGENERATE CASE

In this section only those cases will be considered for which the energy–momentum tensor is degenerate, i.e., $\det(T_{ab})=0$. Thus we would discuss the space–times when at least one of the T_a or their combination is zero. When $T_a=0$, we have trivially every direction is an MC. The remaining cases can be classified as follows: (1) When only one T_a is nonzero; (2) when two T_a's are nonzero; and (3) when three T_a's are nonzero.

Case (1): This can further be grouped as follows: (a) $T_0\neq 0$, $T_i=0$; (b) $T_1\neq 0$, $T_j=0$, $(i=1,2,3)$, $(j=0,2,3)$.

The case 1(a) yields two possibilities according as $T_0'=0$ or $T_0'\neq 0$. For the first possibility, we get

$$\xi^0=c_0,\quad \xi^i=\xi^i(x^a). \tag{44}$$

The second possibility implies that

$$\xi^0=\xi^0(t),\quad \xi^1=-\frac{2T_0}{T_0'}\dot{\xi}^0(t),\quad \xi^k=\xi^k(x^a)\quad (k=2,3). \tag{45}$$

Thus we have infinite-dimensional MCs.

The case 1(b) can be solved trivially and gives

$$\xi^1=\frac{c_1}{\sqrt{T_1}},\quad \xi^j=\xi^j(x^a), \tag{46}$$

which implies infinite-dimensional MCs.

Case (2): This case can be divided into the following cases: (a) $T_l=0,\ T_k\neq 0$ ($l=0,1$ and $k=2,3$); (b) $T_l\neq 0,\ T_k=0$.

In the first case, if we take $T_2=$const, then we have the following MCs:

$$\xi^l=\xi^l(x^a),\quad \xi^2=c_0z+c_1,\quad \xi^3=-c_0y+c_2, \tag{47}$$

which gives infinite-dimensional MCs. For $T_2'\neq 0$, we again have infinite-dimensional MCs given by

$$\xi^0=\xi^0(x^a), \tag{48}$$

$$\xi^1=-\frac{T_2}{T_2'}(f'(u)+g'(u)), \tag{49}$$

$$\xi^2=f(u)+g(v), \tag{50}$$

$$\xi^3=\iota(-f(u)+g(v))+c_0, \tag{51}$$

where $u=y+\iota z$ and $v=y-\iota z$.

For the second case 2(b), it follows from Eqs. (4)–(7) and (9)–(10) that $\xi^l=\xi^l(t,x)$, $\xi^k=\xi^k(x^a)$. Also, Eq. (8) yields $\xi^1=f(t)/T_1$. If we use this value in Eqs. (4)–(5) and eliminate ξ^0, we have

$$\ddot{f}(t)=\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'f(t). \tag{52}$$

From this equation, we see that for $f=0$, we have infinite-dimensional MCs given by

$$\xi^0=c_0,\quad \xi^l=0,\quad \xi^k=\xi^k(x^a). \tag{53}$$

For $f(t)\neq 0$, we have

$$\frac{\ddot{f}(t)}{f(t)}=\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'=\alpha, \tag{54}$$

where α is an arbitrary constant. This gives two possibilities: either $\alpha=0$ or $\alpha\neq 0$. For the first possibility, we obtain $T_0'/2T_0\sqrt{T_1}=\beta$, an arbitrary constant. This again yields the infinite-dimensional MCs given by

$$\xi^0=c_1\left(-\frac{\beta}{2}t^2-\int\frac{\sqrt{T_1}}{T_0}dx\right)-c_2\beta t+c_0, \tag{55}$$

$$\xi^l=\frac{1}{T_1}(c_1t+c_2), \tag{56}$$

$$\xi^k=\xi^k(x^a). \tag{57}$$

When $\alpha\neq 0$, we have infinite-dimensional MCs as follows:

$$\xi^0=-\frac{T_0'}{2T_0\sqrt{\alpha T_1}}(c_1e^{\sqrt{\alpha}t}-c_2e^{-\sqrt{\alpha}t}+c_3), \tag{58}$$

$$\xi^l=\frac{1}{T_1}(c_1e^{\sqrt{\alpha}t}+c_2e^{-\sqrt{\alpha}t}), \tag{59}$$

$$\xi^k=\xi^k(x^a). \tag{60}$$

Case (3): This case can be divided as follows: (a) $T_0=0,\ T_i\neq 0$; (b) $T_1=0,\ T_j\neq 0$.

In the case 3(a), it is easy to see that Eqs. (4)–(7) imply that ξ^0 is an arbitrary function of four variables while $\xi^i=\xi^i(x,y,z)$. Further, it follows from Eqs. (8)–(11) and (13) that

$$A_1(y,z)_{,kk}-\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\frac{T_2}{\sqrt{T_1}}A_1(y,z)=0. \tag{61}$$

From here we have two possibilities—either $A_1=0$ or $A_1\neq 0$. For the first possibility, we have the following MCs:

$$\xi^0=\xi^0(x^a),\quad \xi^1=0,\quad \xi^2=c_1z+c_2,\quad \xi^3=-c_1y+c_3. \tag{62}$$

When $A_1\neq 0$, we obtain

$$\frac{A_1(y,z)_{,kk}}{A_1(y,z)}=\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\frac{T_2}{\sqrt{T_1}}=\alpha, \tag{63}$$

where α is an arbitrary constant which may be zero or nonzero. The possibility $\alpha=0$ implies that $T_2'/T_2\sqrt{T_1}=\beta$, an arbitrary constant and we have the following MCs:

$$\xi^0=\xi^0(x^a), \tag{64}$$

$$\xi^1=\frac{1}{\sqrt{T_1}}((c_1y+c_2)z+c_3y+c_4), \tag{65}$$

$$\xi^2=-\left[\left(\frac{\beta}{4}y^2+\int\sqrt{T_1}T_2dx\right)c_1z+\frac{\beta c_2}{2}yz+\left(\frac{\beta}{4}(y^2-z^2)+\int\sqrt{T_1}T_2dx\right]c_3+\frac{\beta c_4}{2}y-c_5z+c_7, \tag{66}$$

$$\xi^3=-\left[\left(\frac{\beta}{4}z^2+\int\sqrt{T_1}T_2dx\right)c_1y+\frac{\beta c_3}{2}yz+\left(\frac{\beta}{4}(z^2-y^2)+\int\sqrt{T_1}T_2dx\right)c_2+\frac{\beta c_4}{2}z\right]+c_5y+c_6. \tag{67}$$

For $\alpha\neq 0$, the MCs are given by

$$\xi^0=\xi^0(x^a),\quad \xi^1=0,\quad \xi^2=c_0z+c_1,\quad \xi^3=-c_0y+c_2. \tag{68}$$

In the case 3(b), when $T_0=\gamma$ and $T_2=\delta$, where γ and δ are arbitrary constants, we have the following MCs:

$$\xi^0=c_4y+c_5z+c_0, \tag{69}$$

$$\xi^1=\xi^1(x^a), \tag{70}$$

$$\xi^2=c_1z-\frac{\delta c_4}{\gamma}t+c_3, \tag{71}$$

$$\xi^3=-c_1y-\frac{\delta c_5}{\gamma}t+c_3. \tag{72}$$

If $T_0'\neq 0$ and $T_2'=0$, the MCs are given by

$$\xi^0=f(t),\quad \xi^1=-\frac{2T_0}{T_0'}\dot{f}(t),\quad \xi^2=c_1z+c_2,\quad \xi^3=-c_1y+c_3. \tag{73}$$

When $T_2'\neq 0$ and $T_0'T_2/T_0T_2'=\epsilon=0$, we obtain the following MCs:

$$\xi^0=c_0, \tag{74}$$

$$\xi^1=-\frac{2T_2}{T_2'}(f'(u)+g'(v)), \tag{75}$$

$$\xi^2=f(u)+g(v), \tag{76}$$

$$\xi^3=-\iota(f(u)-g(v))+c_1, \tag{77}$$

where $u=y+\iota z$ and $v=y-\iota z$. For $T_2'\neq 0$, $\epsilon\neq 0$ and $(T_0/T_2)'\neq 0$, the proper MCs are given by

$$\begin{aligned}\xi_{(5)}&=t\partial_t-\frac{2T_0}{T_0'}\partial_x,\\ \xi_{(6)}&=\iota(z\partial_y-y\partial_z).\end{aligned} \tag{78}$$

This gives two proper MCs. If $T_2'\neq 0$, $T_0=\lambda T_2$ and $T_0'\neq 0$, we get

$$\begin{aligned}\xi_{(5)}&=\frac{1}{\lambda}\left[ty\partial_t-\frac{2T_2}{T_2'}y\partial_x+\frac{1}{2}(y^2-z^2-\lambda t^2)\partial y+yz\,\partial z\right],\\ \xi_{(6)}&=tz\partial_t-\frac{2T_2}{T_2'}z\partial_x+yz\,\partial y-\frac{1}{2}(y^2-z^2-\lambda t^2)\partial z,\\ \xi_{(7)}&=t\partial t-\frac{2T_2}{T_2'}\partial_x+y\partial y+z\partial z,\\ \xi_{(8)}&=\frac{1}{2\lambda}(y^2+z^2-\lambda t^2)\partial_t+\frac{2T_2}{T_2'}t\partial_x-ty\,\partial y-tz\,\partial z,\\ \xi_{(9)}&=\frac{1}{\lambda}y\partial t-t\,\partial y,\end{aligned} \tag{79}$$

$$\xi_{(10)}=\frac{1}{\lambda}z\partial t-t\,\partial t,$$

which yields six proper MCs. Finally, when $T_2'\neq 0$ and $(T_0'T_2/T_0T_2')'\neq 0$, we have four independent MCs which are exactly the isometries of the plane symmetry. It is interesting to note that the last three subcases of this case give finite-dimensional MCs even for the degenerate case.

IV. EXAMPLES ADMITTING PROPER MCs

In this section we construct examples which admit proper MCs for the nondegenerate energy–momentum tensor. It can be seen from Eq. (A3) that the energy–momentum tensor will be nonzero when neither of the metric functions ν and μ are constants. If we choose these ν and μ such that $\nu=a\ln x+b$, $\mu=c\ln x+d$, where a,b,c,d are constants with $a\neq c$ then

$$\frac{T_2'}{T_2\sqrt{T_1}}=\frac{2(c-2)}{\sqrt{c(c+2a)}}=\text{const}=\alpha\neq 0, \tag{80}$$

$$\frac{T_0'}{T_0\sqrt{T_1}}=\frac{2(a-2)}{\sqrt{c(c+2a)}}=\text{const}=\beta\neq 0. \tag{81}$$

This shows that $\alpha\neq\beta$ as $a\neq c$ and hence the metric

$$ds^2=x^a\,dt^2-dx^2-x^c(dy^2+dz^2), \tag{82}$$

admits five MCs. It is pointed out that this metric possesses four KVs and therefore we have one proper MC given by Eq. (37). It can easily be shown that this space–time satisfies the conditions of the case 2ai(*).

If we choose $c=2$ and $a\geqslant 0$ but $a\neq 2$ in Eq. (82), it admits six MCs whereas this metric has four isometries and hence in this case we have two proper MCs as given by Eq. (42). The resulting space–time will satisfy the constraints of the case 2bii*(+).

When we choose $a=2$ and $c\geqslant 0$ but $c\neq 2$ in the metric given by Eq. (82), it yields seven MCs in which four are the usual isometries while the remaining three are the proper MCs. This satisfies the conditions of the case 2ai(**). Finally, if we choose $\nu=ax=\mu$, then we obtain ten independent MCs and the constraint equations for the case 2a(ii) are satisfied. The corresponding space–time will take the following form:

$$ds^2=e^{ax}(dt^2-dy^2-dz^2)-dx^2. \tag{83}$$

This is the well known anti-de Sitter metric which has ten KVs and consequently in this case we have no proper MC.

V. DISCUSSION AND CONCLUSION

It is known[14] that when we classify plane symmetric space–times according to their KVs, we get metrics which admit ten isometries (the spaces of constant curvature), a space–time which admits seven KVs (the Einstein metric) and a metric which has five KVs. There do not exist metrics admitting G_9 and G_8 as the maximal isometry groups.[15,16] The metric admitting five isometries is given by

$$ds^2=e^{\nu(x)}dt^2-dx^2-e^{2(x/a)}(dy^2+dz^2)\quad(a\neq 0), \tag{84}$$

where a is an arbitrary constant.

If we take μ to be constant and $\nu(x)$ either $\ln\cosh^2 ax$, or $2ax$ or $\ln\cos^2 ax$, we obtain three different metrics corresponding to each value of ν with six KVs each. This corresponds to the

TABLE I. MCs for the nondegenerate case.

Cases	MCs	Constraints
1a	6	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' \neq 0,\ \left(\frac{T_0}{T_2}\right)' = 0$
1b	4	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' \neq 0,\ \left(\frac{T_0}{T_2}\right)' \neq 0$
2ai*	5	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} \neq 0,\ \left(\frac{T_2}{T_0}\right)' \neq 0,\ \frac{T_0'}{T_0\sqrt{T_1}} \neq 0$
2ai**	7	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} \neq 0,\ \left(\frac{T_2}{T_0}\right)' \neq 0,\ \frac{T_0'}{T_0\sqrt{T_1}} = 0$
2aii	10	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} \neq 0,\ \left(\frac{T_2}{T_0}\right)' = 0$
2bi*	10	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} = 0,\ \left(\frac{(\sqrt{T_0})'}{T_1}\right)' = 0,\ \frac{(\sqrt{T_0})'}{T_1} \neq 0$
2bi**	10	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} = 0,\ \left(\frac{(\sqrt{T_0})'}{T_1}\right)' = 0,\ \frac{(\sqrt{T_0})'}{T_1} = 0$
2bii*+	6	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} = 0,\ \left(\frac{(\sqrt{T_0})'}{T_1}\right)' \neq 0,$ $\left(\frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\right)' = 0,\ \frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)' = 0$
2bii*++	6	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} = 0,\ \left(\frac{(\sqrt{T_0})'}{T_1}\right)' \neq 0,$ $\left(\frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\right)' = 0,\ \frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)' \neq 0$
2bii**	4	$\left(\frac{T_2'}{T_2\sqrt{T_1}}\right)' = 0,\ \frac{T_2'}{T_2\sqrt{T_1}} = 0,\ \left(\frac{(\sqrt{T_0})'}{T_1}\right)' \neq 0,$ $\left(\frac{T_0}{2}\sqrt{T_1}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\right)' \neq 0$

degenerate case. The six isometries of each metric are given by Eqs. (B2), (B3), and (B3) in Appendix B. These isometries satisfy the algebra $SO(2)\circledS R^2]\otimes SO(1,2)$ isomorphic to $SO(2)\circledS R^2]\otimes SO(3)$ over complex fields. If we choose μ and ν both to be constant, then the space–time turns out to the Minkowski space–time. All metrics other than those given above admit only the minimal isometry group G_4 satisfying the algebra $[SO(2)\circledS R^2]\otimes R$.

In a recent paper,[12] some interesting results have been obtained when we classify spherically symmetric space–times according to their energy–momentum tensor. In this paper, we have extended the same procedure to classify static plane symmetric space–times according to their MCs.

In the nondegenerate case, we obtain either four, five, six, seven, or ten independent MCs. These contain the usual four isometries of the plane symmetry and the rest are the proper MCs. For the degenerate energy–momentum tensor, most of the cases give infinite-dimensional MCs. The cases worth mentioning are those where we have a finite number of MCs even when the energy–momentum tensor is zero. We obtain three such different cases having either four, six, or ten independent MCs. The results are summarized in the form of Tables I and II given below.

From these tables, it follows that each case has different constraints on the energy–momentum tensor. Finally, we have constructed some particular examples satisfying constraints of the four different cases given by 2ai(*), 2ai(**), 2a(ii), and 2bii*(+). We have seen that the constraints

TABLE II. MCs for the degenerate case (only finite cases).

Cases	MCs	Constraints
3bi	6	$T_1=0,\ T_j\neq 0 (j=0,2,3),\ T_2'\neq 0,\ \frac{T_0'T_2}{T_0T_2'}\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0$
3bii	10	$T_1=0,\ T_j\neq 0,\ T_2'\neq 0,\ T_0=\lambda T_2,\ T_0'\neq 0$
3biii	4	$T_1=0,\ T_j\neq 0,\ T_2'\neq 0,\ \frac{T_0'T_2}{T_0T_2'}\neq 0$

of the case 2ai(*) give one proper MC, the case 2ai(**) yields three proper MCs and the constraints of the case 2bii*(+) give two proper MCs. However, the constraints of the case 2a(ii) yield an anti–de Sitter metric which has ten isometries and hence there is no proper MC in this case. In all other cases, we would have four isometries and find the proper MCs immediately.

When the rank of T_a is 3, i.e. $T_1=0$, we obtain the following metric:

$$ds^2=e^{\nu}dt^2-dx^2-e^{-2\nu}(dy^2+dz^2), \tag{85}$$

where ν is an arbitrary function of x only. It can be easily verified that this class of metrics represent perfect fluid dust solutions. The energy–density for the above metrics is given as

$$\rho=(2\nu''-3\nu'^2)e^{\nu/2}. \tag{86}$$

It is remarked here that the general solution of the constraint equations does not necessarily give the interesting metrics. It may not even be necessary to get solved constraints generically. However, it would be interesting to solve the constraints involved or more examples should be constructed.

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APPENDIX A

The surviving components of the Ricci tensor are

$$\begin{aligned} R_0&\equiv R_{00}=\tfrac{1}{4}e^{\nu}(2\nu''+\nu'^2+2\nu'\mu'),\\ R_1&\equiv R_{11}=-\tfrac{1}{4}(2\nu''+\nu'^2+4\mu''+2\mu'^2),\\ R_2&\equiv R_{22}=-\tfrac{1}{4}e^{\mu}(2\mu''+2\mu'^2+\nu'\mu'),\\ R_{33}&=R_{22}. \end{aligned} \tag{A1}$$

The Ricci scalar is given by

$$R=\tfrac{1}{2}(2\nu''+\nu'^2+2\nu'\mu'+3\mu'^2+4\mu''). \tag{A2}$$

Using Einstein field equations, the nonvanishing components of energy–momentum tensor T_{ab} are

$$T_0\equiv T_{00}=-\tfrac{1}{4}e^{\nu}(4\mu''+3\mu'^2),$$

$$T_1 \equiv T_{11} = \tfrac{1}{4}(\mu'^2 + 2\nu'\mu'),$$
$$T_2 \equiv T_{22} = \tfrac{1}{4}e^{\mu}(2\nu'' + \nu'^2 + \nu'\mu' + \mu'^2 + 2\mu''), \tag{A3}$$
$$T_{33} = T_{22}.$$

APPENDIX B

The four independent KVs associated with the plane symmetric space–times are given by[3]

$$\xi_{(1)} = \partial_t, \quad \xi_{(2)} = \partial_y, \quad \xi_{(3)} = \partial_z, \quad \xi_{(4)} = z\partial_y - y\partial_z. \tag{B1}$$

The six independent KVs associated with the plane symmetric space–times with ν either $\ln\cosh^2 ax$, or $2ax$ or $\ln\cos^2 ax$ and μ to be constant are given by

$$\xi_{(1)} = \partial_t, \quad \xi_{(2)} = \partial_y, \quad \xi_{(3)} = \partial_z, \quad \xi_{(4)} = z\partial_y - y\partial_z,$$
$$\xi_{(5)} = \cos at\,\partial_x - \sin at \tanh ax\,\partial_t, \tag{B2}$$
$$\xi_{(6)} = \sin at\,\partial_x - \cos ax \tanh ax\,\partial_t;$$

$$\xi_{(1)} = \partial_t, \quad \xi_{(2)} = \partial_y, \quad \xi_{(3)} = \partial_z,$$
$$\xi_{(4)} = z\partial_y - y\partial_z, \quad \xi_{(5)} = 2t\partial_x - at^2\partial_t, \tag{B3}$$
$$\xi_{(6)} = \partial_x - at\partial_t;$$

$$\xi_{(1)} = \partial_t, \quad \xi_{(2)} = \partial_y, \quad \xi_{(3)} = \partial_z, \quad \xi_{(4)} = z\partial_y - y\partial_z,$$
$$\xi_{(5)} = \cosh at\,\partial_x + \sin at \tan ax\,\partial_t, \tag{B4}$$
$$\xi_{(6)} = \sinh at\,\partial_x + \cos ax \tan ax\,\partial_t.$$

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Symmetries of the energy-momentum tensor of cylindrically symmetric static space–times

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We investigate matter symmetries of cylindrically symmetric static space–times. These are classified for both cases when the energy-momentum tensor is nondegenerate and also when it is degenerate. It is found that the nondegenerate energy-momentum tensor gives either *three*, *four*, *five*, *six*, *seven* or *ten* independent matter collineations in which *three* are isometries and the rest are proper. The worth mentioning cases are those where we obtain the group of matter collineations finite dimensional, even the energy-momentum tensor is degenerate. These are either *three*, *four*, *five* or *ten*. Some examples are constructed satisfying the constraints on the energy-momentum tensor. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Let M be a space–time manifold with Lorentz metric g of signature $(+,-,-,-)$. It is assumed that the manifold M, and the metric g, are smooth. There has been recent significant interest in the study of the various symmetries (in particular, Ricci and matter collineations) that arise in the exact solutions of Einstein's field equations (EFEs)

$$R_{ab}-\tfrac{1}{2}Rg_{ab}\equiv G_{ab}=\kappa T_{ab} \quad (a,b=0,1,2,3), \tag{1}$$

where κ is the gravitational constant, G_{ab} is the Einstein tensor, R_{ab} is the Ricci, and T_{ab} is the matter (energy-momentum) tensor. Also, $R=g^{ab}R_{ab}$ is the Ricci scalar. We have assumed here that the cosmological constant $\Lambda=0$. The theoretical basis for the study of the affine, conformal, projective, curvature (CCs) and Ricci collineations (RCs) has been analyzed and many examples have been discovered.[1–5] The symmetries of the energy-momentum tensor have recently been studied.

We define a differentiable vector field ξ on M to be a *matter collineation* if

$$\pounds_{\xi}T_{ab}=0, \tag{2}$$

where $\pounds$ is the Lie derivative operator, ξ^a is the symmetry or collineation vector. The study of matter collineations (MCs) derives from the mathematical interest in the invariance attributes of a geometrical object, i.e., Einstein tensor. Since the Einstein tensor is related to the matter content of the space–time by the EFEs, the investigation of MCs seems to be more relevant from the viewpoint of physics.

The study of symmetries played an important role in the classification of space–times, giving rise to many interesting results with useful applications. It is well known that two different collineations are not in general equivalent. For example, a Killing vector (KV) is a MC but the converse does not hold. Collineations have been classified by means of their relative properness by Katzin *et al.*[6,7] This classification indicates that the basic collineation is the KVs. The role of isometries is to restric the general form of the metric. Consequently, the number of independent

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field equations would reduce and it would be easy to find the exact solutions. It is noted that there are well-known metrics which do not have isometries.[8] This does not imply that they do not admit higher symmetries. The symmetry properties given by KVs lead to conservation laws.[9–11] A large number of solutions of the EFEs with different symmetry structures have been found[10] and classified according to their properties.[12] Symmetries of the energy-momentum tensor (also called matter collineations) provide conservation laws on matter fields. These enable us to know how the physical fields, occupying in certain region of space–times, reflect the symmetries of the metric.[13]

There is a large body of recent literature which shows interest in the study of MCs.[14–23] In a recent paper,[22] the study of MCs has been taken for spherically symmetric space–times and some interesting results have been obtained. We have also classified plane symmetric static space–times according to their MCs.[23] In this paper, we extend the procedure to calculate MCs of cylindrically symmetric static space–times both for nondegenerate and also for degenerate cases. Here we would not give details of the calculations as the procedure has been given in different papers.[22,23]

The MC Eq. (2) can be written in component form as

$$T_{ab,c}\xi^c + T_{ac}\xi^c_{,b} + T_{cb}\xi^c_{,a} = 0. \tag{3}$$

The most general form of cylindrically symmetric static space–time is given by

$$ds^2 = e^{\nu(r)}\,dt^2 - dr^2 - e^{\lambda(r)}\,d\theta^2 - e^{\mu(r)}\,dz^2. \tag{4}$$

The only nonzero components of the energy-momentum tensor, given in Appendix A, are T_{00}, T_{11}, T_{22}, T_{33}. We can write the MC equations as follows:

$$T_0'\xi^1 + 2T_0\xi^0_{,0} = 0, \tag{5}$$

$$T_1'\xi^1 + 2T_1\xi^1_{,1} = 0, \tag{6}$$

$$T_2'\xi^1 + 2T_2\xi^2_{,2} = 0, \tag{7}$$

$$T_3'\xi^1 + 2T_3\xi^3_{,3} = 0, \tag{8}$$

$$T_0\xi^0_{0,1} + T_1\xi^1_{,0} = 0, \tag{9}$$

$$T_0\xi^0_{,2} + T_2\xi^2_{,0} = 0, \tag{10}$$

$$T_0\xi^0_{,3} + T_3\xi^3_{,0} = 0, \tag{11}$$

$$T_1\xi^1_{,2} + T_2\xi^2_{,1} = 0, \tag{12}$$

$$T_1\xi^1_{,3} + T_3\xi^3_{,1} = 0, \tag{13}$$

$$T_2\xi^2_{,3} + T_3\xi^3_{,2} = 0, \tag{14}$$

where prime $'$ indicates differentiation with respect to r. These yield the first order nonlinear coupled partial differential equations in four variables $\xi^a(x^b)$. The components of the energy-momentum tensor depend only on r. Here we have used the notation $T_{aa} = T_a$ for the sake of brevity. We solve this set of equations for the nondegenerate case, when

$$\det(T_{ab}) = T_0T_1T_2T_3 \neq 0 \tag{15}$$

and for the degenerate case, where $\det(T_a) = 0$.

The rest of the paper is organized as follows. The next section contains brief comments and results about MCs. In Sec. III, we shall solve the MC equations when the energy-momentum

tensor is nondegenerate and in the next section MC equations are solved for the degenerate energy-momentum tensor. In Sec. V, we shall solve some of the constraints on energy-momentum tensor to obtain exact solution of EFEs. Section VI contains a summary and discussion of the results obtained.

II. SOME GENERAL COMMENTS

Let ξ be a matter collineation. All KVs, homothetic vectors and special conformal Killing vectors are MCs. However, the converse is not always true. In this case, the MC is called proper or nontrivial. The study of MCs has many associated problems. Here we list these in comparison with the other symmetries.

(1) When we define affine and conformal vector fields on M we usually assume that the vector field is at least C^2 and C^3, respectively. Then it follows from Hall *et al.*[4] that ξ^a must be a smooth vector field on M. However, for $k \in Z^+$ there exist MCs on smooth space–times which are C^k but not C^{k+1}.
(2) We know that an affine and conformal vector fields ξ^a on M are uniquely determined by specifying ξ^a and $\xi^a{}_{;b}$ and, respectively, by specifying ξ^a and the components of its first two covariant derivatives $\xi^a{}_{;b}$ and $\xi^a{}_{;bc}$ at some point $p \in M$. However, the value of ξ^a and all its derivatives at some point $q \in M$ may not be enough to determine uniquely a MC ξ^a on M. The fact is that two MCs which agree on a nonempty open subset of M may not agree on M.
(3) The set of all MCs on M is a vector space but in a similar way to the sets of CCs and RCs, and unlike the sets of affine and conformal vector fields, it could be infinite dimensional and could fail to be a Lie algebra. The problem here arises from the fact that such collineations must be C^1 in order that the defining equations make sense. It is unfortunate that a matter, Ricci or curvature collineation might turn out to be precisely C^1 and so the differentiability may be destroyed under the Lie bracket operation. On the other hand, if we assume that MCs are C^∞ then we recover the Lie algebra structure but we are then forced to expel the collineations which are not smooth. The infinite dimensionality may also lead to problems related to the orbits of the resulting local diffeomorphism.[4,24]
(4) If the energy-momentum tensor is of rank 4 everywhere then we can think of this tensor as a metric on the space–time M. It then follows from the theory of Killing vectors that the family of MCs is, in fact, a Lie algebra of smooth vector fields on M, of finite dimension, $\leqslant 10$, and, in addition, $\neq 9$ by Fubini's theorem.[12]

III. MATTER COLLINEATIONS IN THE NONDEGENERATE CASE

In this section, we shall evaluate MCs only for those cases which have nondegenerate energy-momentum tensor, i.e., $T_a \neq 0$.

When we solve Eqs. (5)–(14) simultaneously, we get the following constraint equation:

$$T_0' \xi^1_{,23} = 0. \tag{16}$$

This equation implies that either
(1) $T_0' = 0$,
or
(2) $T_0' \neq 0$.

Case 1: In the first case we have $T_0 = -k_1$, where k_1 is a nonzero constant which implies that the MC equations yield the following four possibilities:

$$(a_1) \quad T_2' = 0, \quad T_3' = 0,$$

$$(a_2) \quad T_2' = 0, \quad T_3' \neq 0,$$

$$(a_3)\quad T_2'\neq 0,\quad T_3'=0,$$

$$(a_4)\quad T_2'\neq 0,\quad T_3'\neq 0.$$

Subcase 1(a_1): This implies that $T_2=k_2$ and $T_3=k_3$, where k_2 and k_3 are nonzero constants. In this case, in addition to the nonproper MCs $\xi_{(1)}$, $\xi_{(2)}$, $\xi_{(3)}$ given in Appendix B, we obtain the following proper MCs:

$$\xi_{(4)}=\theta\partial_t+\frac{k_1}{k_2}t\partial_\theta,$$

$$\xi_{(5)}=-\frac{1}{k_1}\int\sqrt{T_1}\mathrm{d}r\,\partial_t+\frac{1}{\sqrt{T_1}}t\partial_r,$$

$$\xi_{(6)}=z\partial_t+\frac{k_1}{k_3}t\partial_z,$$

$$\xi_{(7)}=\frac{1}{\sqrt{T_1}}\partial_r, \tag{17}$$

$$\xi_{(8)}=\frac{\theta}{\sqrt{T_1}}\partial_r-\frac{1}{k_2}\int\sqrt{T_1}\mathrm{d}r\,\partial_\theta,$$

$$\xi_{(9)}=\frac{z}{\sqrt{T_1}}\partial_r-\frac{1}{k_3}\int\sqrt{T_1}\mathrm{d}r\,\partial_z,$$

$$\xi_{(10)}=z\partial_\theta-\frac{k_2}{k_3}\theta\partial_z.$$

Thus we have 10 independent MCs in which seven are proper.

Subcase 1(a_2): It follows that $T_2=k_2$, $T_3'\neq 0$ which further yields the following two cases:

$$(b_1)\quad\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$$

$$(b_2)\quad\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0.$$

The case $1a_2(b_1)$ gives

$$\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=\alpha_1,$$

where α_1 is an arbitrary constant which may be

$$(c_1)\quad\alpha_1>0,\quad(c_2)\quad\alpha_1=0,\quad\text{or}\quad(c_3)\quad\alpha_1<0.$$

The first option $1a_2b_1(c_1)$, when $\alpha_1>0$, gives the following proper MCs:

$$\xi_{(4)}=\theta\partial_t+\frac{k_1}{k_2}t\partial_\theta,$$

$$\xi_{(5)}=\frac{e^{\sqrt{\alpha_1}z}}{\sqrt{T_1}}\partial_r-\frac{T_3'e^{\sqrt{\alpha_1}z}}{2\sqrt{\alpha_1}T_3\sqrt{T_1}}\partial_z, \tag{18}$$

$$\xi_{(6)}=\frac{e^{-\sqrt{\alpha_1}z}}{\sqrt{T_1}}\partial_r+\frac{T_3'e^{-\sqrt{\alpha_1}z}}{2\sqrt{\alpha_1}T_3\sqrt{T_1}}\partial_z.$$

The second option $1a_2b_1(c_2)$, when $\alpha_1=0$, yields the following three proper MCs:

$$\xi_{(4)}=\theta\partial_t+\frac{k_1}{k_2}t\partial_\theta,$$

$$\xi_{(5)}=\frac{1}{T_1}\partial_r-\alpha_2z\partial_z, \tag{19}$$

$$\xi_{(6)}=\frac{z}{\sqrt{T_1}}\partial_r-\left(\int\frac{\sqrt{T_1}}{T_3}\mathrm{d}r+\alpha_2\frac{z^2}{2}\right)\partial_z,$$

where $\alpha_2=T_3'/2T_3\sqrt{T_1}$ is a nonzero constant.

The third option $1a_2b_1(c_3)$ gives the same MCs as the first case $1a_2b_1(c_1)$.

When we solve MC equations for the case $1a_2(b_2)$, we have only one proper MC given by

$$\xi_{(4)}=\theta\partial_t+\frac{k_1}{k_2}t\partial_\theta. \tag{20}$$

Subcase 1(a_3): The subcase $1(a_3)$ is similar to the subcase $1(a_2)$ and MCs follow by interchanging θ and z coordinates.

Subcase 1(a_4): Here we have $T_2'\neq0$, $T_3'\neq0$ which gives rise to the following two possibilities:

$$(b_1)\quad\left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$$

$$(b_2)\quad\left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'\neq0.$$

The first possibility $1a_4(b_1)$ implies that $(T_2/\sqrt{T_1})(T_2'/2T_2\sqrt{T_1})'=\alpha_3$, where α_3 is an arbitrary constant such that

$$(c_1)\ \ \alpha_3>0,\quad (c_2)\ \ \alpha_3=0,\quad \text{or}\ \ (c_3)\ \ \alpha_3<0.$$

When α_3 is positive, $1a_4b_1(c_1)$, it further gives the following two options:

$$(d_1)\quad\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$$

$$(d_2)\quad\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq0.$$

For the option $1a_4b_1c_1(d_1)$, we obtain similar result to the case $1a_2(b_1)$. The option $1a_4b_1c_1(d_2)$ gives the following two cases:

$$(e_1)\ \frac{T_2}{T_3}=\text{constant}\neq 0,\quad (e_2)\ \frac{T_2}{T_3}\neq\text{constant}.$$

The case $1a_4b_1c_1d_2(e_1)$ yields one proper MC,

$$\xi_{(4)}=z\partial_\theta-\frac{T_2}{T_3}\theta\partial_z, \tag{21}$$

and the case $1a_4b_1c_1d_2(e_2)$ gives three independent MCs.

The case $1a_4b_1(c_2)$, when $\alpha_3=0$, yields $T_2'/2T_2\sqrt{T_1}=\alpha_4$, where α_4 is a nonzero constant which gives either

$$(d_1)\ \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$$

or

$$(d_2)\ \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0.$$

The first possibility $1a_4b_1c_2(d_1)$ further divides into three cases according to $(T_3/\sqrt{T_1})\,(T_3'/2T_3\sqrt{T_1})'=\alpha_1$,

$$(e_1)\ \alpha_1>0,\quad (e_2)\ \alpha_1=0,\quad \text{or}\ (e_3)\ \alpha_1<0.$$

The case $1a_4b_1c_2d_1(e_1)$, when $\alpha_1>0$, MCs turn out to be similar to the case $1a_2b_1(c_1)$. When $\alpha_1=0$, i.e., in the case $1a_4b_1c_2d_1(e_2)$, we have further two options, either

$$(f_1)\ \frac{T_3}{T_2}=k=\text{constant}\neq 0,\quad \text{or}\ (f_2)\ \frac{T_3}{T_2}\neq\text{constant}.$$

In the option $1a_4b_1c_2d_1e_2(f_1)$, we obtain the following four proper MCs:

$$\begin{aligned}
\xi_{(4)}&=-z\partial_\theta+\frac{\theta}{k}\partial_z,\\
\xi_{(5)}&=\frac{1}{\sqrt{T_1}}\partial_r-\alpha_2\theta\partial_\theta-\alpha_2 z\partial_z,\\
\xi_{(6)}&=\frac{\theta}{\sqrt{T_1}}\partial_r-\alpha_2\theta z\partial_z-\left(\int\frac{\sqrt{T_1}}{T_2}\mathrm{d}r+\alpha_2\frac{\theta^2}{2}-k\alpha_2\frac{z^2}{2}\right)\partial_\theta,\\
\xi_{(7)}&=\frac{z}{\sqrt{T_1}}\partial_r-\alpha_2\theta z\partial_\theta-\left(\int\frac{\sqrt{T_1}}{T_2}\mathrm{d}r-\alpha_2\frac{\theta^2}{2k}+\alpha_2\frac{z^2}{2}\right)\partial_z.
\end{aligned} \tag{22}$$

For the option $1a_4b_1c_2d_1e_2(f_2)$, there is only one proper MC

$$\xi_{(4)}=\frac{1}{\sqrt{T_1}}\partial_r+\theta\partial_\theta-\alpha_2 z\partial_z. \tag{23}$$

The case $1a_4b_1c_2d_1(e_3)$, when $\alpha_1<0$, yields similar solution as the case $1a_2b_1(c_3)$. The option $1a_4b_1c_2(d_2)$ gives similar result as the case $1a_4b_1c_1(d_2)$. The possibility $1a_4b_1(c_3)$, when $\alpha_3<0$, also gives similar solution as the case $1a_2b_1(c_1)$.

In the case $1a_4(b_2)$, we have either

$$(c_1)\ \frac{T_2}{T_3}=\text{constant}, \quad \text{or}\ \ (c_2)\ \frac{T_2}{T_3}\neq\text{constant}.$$

For the case $1a_4b_2(c_1)$, it coincides with $1a_4b_1c_1(d_2)$ and in the case $1a_4b_2(c_2)$, we get minimal MCs, i.e., three.

Case 2: Now we evaluate MCs for the case when $T_0'\neq 0$. This case implies that $\xi^1_{,23}=0$. Using this value in Eqs. (12)–(14), we obtain

$$\left(\frac{T_2}{T_3}\right)'\xi^2_{,3}=0. \tag{24}$$

This implies that either

$$(a_1)\ \left(\frac{T_2}{T_3}\right)'=0, \quad \text{or}\ \ (a_2)\ \left(\frac{T_2}{T_3}\right)'\neq 0.$$

Subcase 2(a_1): This yields $T_2/T_3=k_1$, where k_1 is a nonzero constant. Solving MC equations using this value, we obtain the following two cases:

$$(b_1)\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0, \quad (b_2)\quad \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0.$$

The case $2a_1(b_1)$ implies that $T_2'/2T_2\sqrt{T_1}=\beta_1$, a constant which yields that either

$$(c_1)\ \ \beta_1=0, \quad \text{or}\ \ (c_2)\ \ \beta_2\neq 0.$$

For the case $2a_1b_1(c_1)$, when $\beta_1=0$, it yields the following two groups:

$$(d_1)\quad \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'=0, \quad (d_2)\ \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'\neq 0.$$

The first group $2a_1b_1c_1(d_1)$ gives 10 independent MCs in which seven are proper given by

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$

$$\xi_{(5)}=\frac{1}{\sqrt{T_0}}\theta\sin k_2t\partial_t-\frac{1}{\sqrt{T_1}}\theta\cos k_2t\partial_r+\frac{\sqrt{T_0}}{k_2T_2}\cos k_2t\partial_\theta,$$

$$\xi_{(6)}=-\frac{1}{\sqrt{T_0}}\theta\cos k_2t\partial_t-\frac{1}{\sqrt{T_1}}\theta\sin k_2t\partial_r+\frac{\sqrt{T_0}}{k_2T_2}\sin k_2t\partial_\theta,$$

$$\xi_{(7)}=\frac{1}{k_1\sqrt{T_0}}z\sin k_2t\partial_t-\frac{1}{k_1\sqrt{T_1}}z\cos k_2t\partial_r+\frac{\sqrt{T_0}}{k_2T_2}\cos k_2t\partial_\theta, \tag{25}$$

$$\xi_{(8)}=-\frac{1}{k_1\sqrt{T_0}}z\cos k_2t\partial_t-\frac{1}{k_1\sqrt{T_1}}z\sin k_2t\partial_r+\frac{\sqrt{T_0}}{k_2T_2}\sin k_2t\partial_\theta,$$

$$\xi_{(9)}=\frac{1}{\sqrt{T_0}}\sin k_2 t\partial_t+\frac{1}{\sqrt{T_1}}\cos k_2 t\partial_r,$$

$$\xi_{(10)}=\frac{1}{\sqrt{T_0}}\cos k_2 t\partial_t+\frac{1}{\sqrt{T_1}}\sin k_2 t\partial_r,$$

where $k_2=(\sqrt{T_0})'/\sqrt{T_1}$ is a nonzero constant. The second group $2a_1b_1c_1(d_2)$ gives further two possibilities:

$$(e_1)\quad \frac{T_0}{2\sqrt{T_1}}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'=\text{constant}=\beta_2,$$

$$(e_2)\quad \frac{T_0}{2\sqrt{T_1}}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\neq\text{constant}.$$

In the first possibility $2a_1b_1c_1d_2(e_1)$, we further have two options according to

$$(f_1)\ \ \beta_2=0,\quad (f_2)\ \ \beta_2\neq 0.$$

The option $2a_1b_1c_1d_2e_1(f_1)$ gives six independent MCs in which three proper MCs are given by

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$

$$\xi_{(5)}=\left(\frac{1}{\beta_3 T_0}-\frac{\beta_3}{4}t^2\right)\partial_t+\frac{1}{\sqrt{T_1}}t\partial_r, \tag{26}$$

$$\xi_{(6)}=-\frac{\beta_3}{2}t\partial_t+\frac{1}{\sqrt{T_1}}\partial_r,$$

where $\beta_3=T_0'/T_0\sqrt{T_1}$ is a nonzero constant. The possibility $2a_1b_1c_1d_2e_1(f_2)$ also gives six independent MCs. The three proper MCs are

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$

$$\xi_{(5)}=-\frac{T_0'}{2\sqrt{\beta_2}T_0\sqrt{T_1}}e^{\sqrt{\beta_2}t}\partial_t+\frac{1}{\sqrt{T_1}}e^{\sqrt{\beta_2}t}\partial_r, \tag{27}$$

$$\xi_{(6)}=\frac{T_0'}{2\sqrt{\beta_2}T_0\sqrt{T_1}}e^{-\sqrt{\beta_2}t}\partial_t+\frac{1}{\sqrt{T_1}}e^{-\sqrt{\beta_2}t}\partial_r.$$

The case $2a_1b_1c_1d_2(e_2)$ yields the same result as the case $1a_4b_1c_1(d_2)$, i.e., one proper MC.

The possibility $2a_1b_1(c_2)$, i.e., nonzero value of the constant β_1, gives us two more options:

$$(d_1)\ \ \left(\frac{T_2}{T_0}\right)'=0,\quad (d_2)\ \ \left(\frac{T_2}{T_0}\right)'\neq 0.$$

The first option $2a_1b_1c_2(d_1)$ gives 10 independent MCs. The seven proper MCs are

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$

$$\xi_{(5)}=k_3\theta\partial_t+t\partial_\theta,$$

$$\xi_{(6)}=\frac{k_3}{k_1}z\partial_t+t\partial_z,$$

$$\xi_{(7)}=\frac{1}{2}\left(t^2-\frac{4}{\beta_1^2T_0}+k_3\theta^2+\frac{k_3}{k_1}z^2\right)\partial_t-\frac{2}{\beta_1\sqrt{T_1}}t\partial_r+t\theta\partial_\theta+tz\partial_z, \tag{28}$$

$$\xi_{(8)}=-k_1t\theta\partial_t+\frac{2k_1}{\beta_1\sqrt{T_1}}\theta\partial_r+\frac{1}{2}\left(-\frac{k_1}{k_3}t^2+\frac{4k_1}{\beta_1^2T_2}-k_1\theta^2+z^2\right)\partial_\theta-k_1\theta z\partial_z,$$

$$\xi_{(9)}=tz\partial_t-\frac{2}{\beta_1\sqrt{T_1}}z\partial_r+\theta z\partial_\theta+\frac{1}{2}\left(\frac{k_1}{k_3}t^2-\frac{4k_1}{\beta_1^2T_2}-k_1\theta^2+z^2\right)\partial_z,$$

$$\xi_{(10)}=t\partial_t-\frac{2}{\beta_1\sqrt{T_1}}\partial_r+\theta\partial_\theta+z\partial_z,$$

where $k_3=-T_2/T_0$ is a constant.

The second option $2a_1b_1c_2(d_2)$ further yields two possibilities,

$$(e_1)\ \left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'=0,\quad (e_2)\ \left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\neq 0.$$

If it is zero, i.e., the case $2a_1b_1c_2d_2(e_1)$, we have the following two proper MCs:

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$
$$\xi_{(5)}=\frac{\beta_4}{\beta_1}t\partial_t-\frac{2}{\beta_1\sqrt{T_1}}\partial_r+\theta\partial_\theta+z\partial_z, \tag{29}$$

where $\beta_4=T_0'/T_0\sqrt{T_1}$ is a constant such that $\beta_1\neq\beta_4$. If it is nonzero, i.e., $2a_1b_1c_2d_2(e_2)$, we have the same result as for the case $1a_4b_1c_1(d_2)$.

The case $2a_1(b_2)$, when $(T_2'/2T_2\sqrt{T_1})'\neq 0$, implies that $T_2'\neq 0$ which results the following two possibilities:

$$(c_1)\ \left(\sqrt{\frac{T_0}{T_2}}\right)'=0,\quad (c_2)\ \left(\sqrt{\frac{T_0}{T_2}}\right)'\neq 0.$$

The first possibility $2a_1b_2(c_1)$ gives six independent MCs in which three are the usual isometries and the remaining three are proper MCs given by

$$\xi_{(4)}=z\partial_\theta-k_1\theta\partial_z,$$
$$\xi_{(5)}=\theta\partial_t+k_4^2t\partial_\theta, \tag{30}$$
$$\xi_{(6)}=z\partial_t+k_1k_4^2t\partial_z,$$

where $k_4=\sqrt{T_0/T_2}$ is a constant. The second possibility $2a_1b_2(c_2)$ gives one proper MC as in the case $1a_1b_1c_1(d_2)$.

Subcase 2(a_2): Here we have $(T_2/T_3)'\neq 0$. If we use this constraint in MC Eqs. (7), (8), and (14), we have

$$T_2'\xi^1_{,3}=0=T_3'\xi^1_{,2}. \tag{31}$$

This gives rise to the following three possibilities:

$$(b_1)\quad T_2'=0,\quad T_3'\neq 0,$$

$$(b_2)\quad T_2'\neq 0,\quad T_3'=0,$$

$$(b_3)\quad T_2'\neq 0,\quad T_3'\neq 0.$$

In the first case, we can write

$$\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'=\gamma_1,\quad \frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=\gamma_2, \tag{32}$$

where γ_1 and γ_2 are arbitrary constants. From here we have the following four different cases:

$$(c_1)\quad \gamma_1=0,\quad \gamma_2=0,$$

$$(c_2)\quad \gamma_1\neq 0,\quad \gamma_2=0,$$

$$(c_3)\quad \gamma_1=0,\quad \gamma_2\neq 0,$$

$$(c_4)\quad \gamma_1\neq 0,\quad \gamma_2\neq 0.$$

The first case $2a_2b_1(c_1)$ can be divided into the following two options according to

$$(d_1)\quad \left(\frac{T_0}{T_3}\right)'=0,\quad \text{or}\quad (d_2)\quad \left(\frac{T_0}{T_3}\right)'\neq 0.$$

The first option $2a_2b_1c_1(d_1)$ gives seven independent MCs in which four are proper,

$$\begin{aligned}
\xi_{(4)}&=\left(\frac{\gamma_3}{2}t^2-\int\frac{\sqrt{T_1}}{T_0}dr+\frac{\gamma_3}{2k_1}z^2\right)\partial_t+\frac{1}{\sqrt{T_1}}t\partial_r+\gamma_3tz\partial_z,\\
\xi_{(5)}&=\gamma_3tz\partial_t+\frac{1}{\sqrt{T_1}}z\partial_r+\left(\frac{k_1\gamma_3}{2}t^2-\int\frac{\sqrt{T_1}}{T_3}\mathrm{d}r+\frac{\gamma_3}{2}z^2\right)\partial_z,\\
\xi_{(6)}&=\gamma_3t\partial_t+\frac{1}{\sqrt{T_1}}\partial_r+\gamma_3z\partial_z,\\
\xi_{(7)}&=z\partial_t+k_1t\partial_z,
\end{aligned} \tag{33}$$

where $k_1=-T_0/T_3$ and $\gamma_3=-T_0'/2T_0\sqrt{T_1}$ are constants. The second option $2a_2b_1c_1(d_2)$ yields only one proper MC given by

$$\xi_{(4)}=\gamma_3t\partial_t+\frac{1}{\sqrt{T_1}}t\partial_r+\gamma_4tz\partial_z, \tag{34}$$

where $\gamma_4=-T_3'/2T_3\sqrt{T_1}$.

In the case $2a_2b_1(c_2)$, when $\gamma_1\neq 0$, $\gamma_2=0$, we have either

$$(d_1)\quad \gamma_1>0,\quad \text{or}\quad (d_2)\quad \gamma_1<0.$$

For $2a_2b_1c_2(d_1)$, when $\gamma_1>0$, we obtain three independent MCs which are the usual isometries.

The case $2a_2b_1c_2(d_2)$, when $\gamma_1<0$, we have two options

$$(e_1)\ \left(\frac{T_0}{T_3}\right)'=0,\quad \text{or}\ (e_2)\ \left(\frac{T_0}{T_3}\right)'\neq 0.$$

For the case $2a_2b_1c_2d_2(e_1)$, we have only one proper MC given by

$$\xi_{(4)}=\frac{1}{k_1}z\partial_t+t\partial_z. \tag{35}$$

In the case $2a_2b_1c_2d_2(e_2)$, we obtain the minimal symmetry.

The case $2a_2b_1(c_3)$, when $\gamma_1=0$, $\gamma_2\neq 0$, is similar to the previous case $2a_2b_1(c_2)$ by interchanging t and z.

The case $2a_2b_1(c_4)$, when $\gamma_1\neq 0$, $\gamma_2\neq 0$, yields the following four different possibilities:

$$(d_1)\ \ \gamma_1>0,\quad \gamma_2>0,$$

$$(d_2)\ \ \gamma_1>0,\quad \gamma_2<0,$$

$$(d_3)\ \ \gamma_1<0,\quad \gamma_2>0,$$

$$(d_4)\ \ \gamma_1<0,\quad \gamma_2<0.$$

The first possibility further gives two options according to

$$(e_1)\ \ \gamma_2T_0\int\frac{\sqrt{T_1}}{T_0}\mathrm{d}r+\frac{T_3'}{2\sqrt{T_1}}=0,$$

$$\text{or}\ (e_2)\ \ \gamma_2T_0\int\frac{\sqrt{T_1}}{T_0}\mathrm{d}r+\frac{T_3'}{2\sqrt{T_1}}\neq 0.$$

The first option $2a_2b_1c_4d_1(e_1)$ gives the minimal symmetry. The second option $2a_2b_1c_4d_1(e_2)$ further gives two possibilities,

$$(f_1)\ \left(\frac{T_0}{T_3}\right)'=0,\quad (f_2)\ \left(\frac{T_0}{T_3}\right)'\neq 0.$$

The case $2a_2b_1c_4d_1e_2(f_1)$ yields four independent MCs in which the proper MC is given by

$$\xi_{(4)}=z\partial_t+k_1t\partial_z. \tag{36}$$

For the case $2a_2b_1c_4d_1e_2(f_2)$, we have three independent MCs.

All other cases $2a_2b_1c_4(d_2-d_4)$ are similar to the previous case $2a_2b_1c_4(d_1)$.

The case $2a_2(b_2)$, when $T_2'\neq 0$, $T_3'=0$, is similar to the first case $2a_2(b_1)$.

In the third case $2a_2(b_3)$, when $T_2'\neq 0$, $T_3'\neq 0$, we further have the following two possibilities:

$$(c_1)\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\quad \left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=0,$$

$$(c_2)\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,\quad \left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\neq 0.$$

For the first possibility $2a_2b_3(c_1)$, we obtain the following three options:

$$(d_1)\ \left(\frac{T_2}{T_0}\right)'=0,\quad \left(\frac{T_3}{T_0}\right)'\neq 0,$$

$$(d_2)\ \left(\frac{T_2}{T_0}\right)'\neq 0,\quad \left(\frac{T_3}{T_0}\right)'=0,$$

$$(d_3)\ \left(\frac{T_2}{T_0}\right)'\neq 0,\quad \left(\frac{T_3}{T_0}\right)'\neq 0.$$

The first option $2a_2b_3c_1(d_1)$ yields five independent MCs in which three are the usual KVs and the remaining are the proper MCs given by

$$\xi_{(4)}=\gamma_3 t\partial_t+\frac{1}{\sqrt{T_1}}\partial_r+\gamma_3\theta\partial_\theta+\gamma_4 z\partial_z,$$
$$\xi_{(5)}=k_2\theta\partial_t+t\partial_\theta, \tag{37}$$

where $k_2=-T_2/T_0$ is a nonzero constant. The second option $2a_2b_3c_1(d_2)$ is similar to the first one. The third case $2a_2b_3c_1(d_3)$ implies that either

$$(e_1)\ \left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'=0,\quad \text{or}\ (e_2)\ \left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\neq 0.$$

For the first option $2a_2b_3c_1d_3(e_1)$, we get one proper MC given by

$$\xi_{(4)}=\gamma_3 t\partial_t+\frac{1}{\sqrt{T_1}}\partial_r+\gamma_3\theta\partial_\theta+\gamma_4 z\partial_z. \tag{38}$$

In the second option $2a_2b_3c_1d_3(e_2)$, we obtain the minimal symmetry.

The case $2a_2b_3(c_2)$ also yields the same three possibilities,

$$(d_1)\ \left(\frac{T_2}{T_0}\right)'=0,\quad \left(\frac{T_3}{T_0}\right)'\neq 0,$$

$$(d_2)\ \left(\frac{T_2}{T_0}\right)'\neq 0,\quad \left(\frac{T_3}{T_0}\right)'=0,$$

$$(d_3)\ \left(\frac{T_2}{T_0}\right)'\neq 0,\quad \left(\frac{T_3}{T_0}\right)'\neq 0.$$

It is to be noted that we have excluded the possibility when both are constants as this leads T_2/T_3 to be constant which gives a contradiction. The first case $2a_2b_3c_2(d_1)$ gives only one proper MC, i.e.,

$$\xi_{(4)}=k_2\theta\partial_t+t\partial_\theta. \tag{39}$$

The second case $2a_2b_3c_2(d_2)$ is similar to the previous one and the third case $2a_2b_3c_2(d_3)$ gives the minimal MCs.

IV. MATTER COLLINEATIONS IN THE DEGENERATE CASE

In this section only those cases will be considered for which $\det(T_{ab})=0$ which implies that at least one of the components of the energy-momentum tensor is zero, i.e., $T_a=0$. The trivial case is that when all T_a are zero. In this case, every direction is in a MC. The remaining cases can be divided into three main groups:

(1) when at least one of T_a is nonzero;
(2) when at least two of T_a are nonzero;
(3) when three of T_a are nonzero.

Case 1: This case can further be divided into the following four subcases:

$$(a_1)\quad T_0=0,\quad T_1=0,\quad T_2=0,\quad T_3\neq 0,$$

$$(a_2)\quad T_0=0,\quad T_1=0,\quad T_2\neq 0,\quad T_3=0,$$

$$(a_3)\quad T_0=0,\quad T_1\neq 0,\quad T_2=0,\quad T_3=0,$$

$$(a_4)\quad T_0\neq 0,\quad T_1=0,\quad T_2=0,\quad T_3=0.$$

When we use the values of $1(a_1)$ in MC equations, we obtain $\xi^3=\xi^3(z)$ and Eq. (9) gives

$$\xi^1=-\frac{2T_3}{T_3'}\xi^3_{,3}(z), \tag{40}$$

where $T_3'\neq 0$ and ξ^0, ξ^1 are arbitrary functions of t,r,θ,z. This gives infinite dimensional MCs. The second case $1(a_2)$ is similar to the first one if we interchange the indices 2 and 3.

The third case $1(a_3)$ gives $\xi^1=\xi^1(r)$ and Eq. (7) yields

$$\xi^1=\frac{c_1}{\sqrt{T_1}}, \tag{41}$$

where ξ^0, ξ^2, ξ^3 are arbitrary functions of t,r,θ,z which gives infinite dimensional MCs. The fourth case $1(a_4)$ yields the similar result as the case $1(a_1)$ by interchanging the indices 0 and 3. Thus we obtain infinite dimensional MCs in all the possibilities of the case 1.

Case 2: This case has the following six possibilities:

$$(a_1)\quad T_0=0,\quad T_1=0,\quad T_2\neq 0,\quad T_3\neq 0,$$

$$(a_2)\quad T_0=0,\quad T_1\neq 0,\quad T_2=0,\quad T_3\neq 0,$$

$$(a_3)\quad T_0=0,\quad T_1\neq 0,\quad T_2\neq 0,\quad T_3=0,$$

$$(a_4)\quad T_0\neq 0,\quad T_1=0,\quad T_2=0,\quad T_3\neq 0,$$

$$(a_5)\quad T_0\neq 0,\quad T_1=0,\quad T_2\neq 0,\quad T_3=0,$$

$$(a_6)\quad T_0\neq 0,\quad T_1\neq 0,\quad T_2=0,\quad T_3=0.$$

When we replace the information of the subcase $2(a_1)$ in MC equations, we obtain $\xi^0=\xi^0(t,r,\theta,z)$, $\xi^2=\xi^2(\theta,z)$, $\xi^3=\xi^3(\theta,z)$, and

$$\left(\frac{T_3}{T_2}\right)'\xi^3_{,2}=0. \tag{42}$$

From here we have two options:

$$(b_1)\ \left(\frac{T_3}{T_2}\right)'=0, \quad (b_2)\ \left(\frac{T_3}{T_2}\right)'\neq 0.$$

For the first option $2a_1(b_1)$, MC equations yield

$$\xi^2_{,22}+\frac{1}{c}\xi^2_{,33}=0, \tag{43}$$

$$\xi^3_{,22}+\frac{1}{c}\xi^3_{,33}=0, \tag{44}$$

where $c=T_3/T_2$ is a nonzero constant. If $c>0$, Eqs. (43) and (44) yield the following solution:

$$\xi^2=f_+\left(\theta+\frac{\iota z}{\sqrt{c}}\right)+f_-\left(\theta-\frac{\iota z}{\sqrt{c}}\right), \tag{45}$$

$$\xi^3=g_+\left(\theta+\frac{\iota z}{\sqrt{c}}\right)+g_-\left(\theta-\frac{\iota z}{\sqrt{c}}\right). \tag{46}$$

Replacing the value of ξ^2 in Eq. (8), we obtain

$$\xi^1=-\frac{2T_2}{T_2'}\left[f_{+,2}\left(\theta+\frac{\iota z}{\sqrt{c}}\right)+f_{-,2}\left(\theta-\frac{\iota z}{\sqrt{c}}\right)\right], \tag{47}$$

where $T_2'\neq 0$ and $\xi^0=\xi^0(t,r,\theta,z)$. If we take $T_2=$constant, MC equations give the following solution:

$$\begin{gathered}\xi^0=\xi^0(t,r,\theta,z), \quad \xi^1=\xi^1(t,r,\theta,z),\\ \xi^2=c_1z+c_2, \quad \xi^3=c_1\theta+c_3.\end{gathered} \tag{48}$$

The option $2a_1(b_2)$ further divides into three cases,

$$(c_1)\ \ T_2'=0, \quad T_3'\neq 0,$$

$$(c_2)\ \ T_2'\neq 0, \quad T_3'=0,$$

$$(c_3)\ \ T_2'\neq 0, \quad T_3'\neq 0.$$

In the case $2a_1b_2(c_1)$, we get the following solution:

$$\begin{gathered}\xi^0=\xi^0(t,r,\theta,z), \quad \xi^1=\frac{T_3}{T_3'}f(z),\\ \xi^2=c_1, \quad \xi^3=-\frac{1}{2}\int f(z)dz+c_2.\end{gathered} \tag{49}$$

The case $2a_1b_2(c_2)$ gives the similar results as the case $2a_1b_2(c_1)$ by interchanging θ and z.

If we solve MC equations for the possibility $2a_1b_2(c_3)$, we have the following solution:

$$\xi^0=\xi^0(t,r,\theta,z), \quad \xi^1=\frac{T_2}{T_2'}c_1,$$
$$\xi^2=c_1\theta+c_2, \quad \xi^3=c_3z+c_4. \tag{50}$$

For the subcase $2(a_2)$, we further have the following two options from MC equations:

$$(b_1)\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$$
$$(b_2)\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0.$$

Also $\xi^0=\xi^0(t,r,\theta,z)$, $\xi^1=\xi^1(r,z)$, $\xi^2=\xi^2(r)$, $\xi^3=\xi^3(r,z)$. The first possibility $2a_2(b_1)$ gives $(T_3/\sqrt{T_1})\,(T_3'/2T_3\sqrt{T_1})'=c$, where c is an arbitrary constant which implies that either

$$(c_1)\ \ c>0, \quad (c_2)\quad c=0, \quad \text{or} \quad (c_3)\quad c<0.$$

The case $2a_2b_1(c_1)$ yields the following solution:

$$\xi^0=\xi^0(t,r,\theta,z),$$
$$\xi^1=\frac{1}{\sqrt{T_1}}(c_1e^{\sqrt{c}z}+c_2e^{-\sqrt{c}z}), \quad \xi^2=\xi^2(r,z), \tag{51}$$
$$\xi^3=-\frac{T_3'}{2\sqrt{c}T_3\sqrt{T_1}}(c_1e^{\sqrt{c}z}-c_2e^{-\sqrt{c}z})+c_3.$$

For the case $2a_2b_1(c_2)$, when $c=0$, we obtain

$$\xi^0=\xi^0(t,r,\theta,z),$$
$$\xi^1=\frac{1}{\sqrt{T_1}}(c_1z+c_2), \quad \xi^2=\xi^2(r,z), \tag{52}$$
$$\xi^3=-c_1\int\frac{\sqrt{T_1}}{T_3}\mathrm{d}r-\frac{T_3'}{2T_3\sqrt{T_1}}\left(c_1\frac{z^2}{2}+c_2z\right)+c_3.$$

In the case $2a_2b_1(c_3)$, when $c<0$, the solution is similar to the previous case $2a_2b_1(c_2)$.

The second possibility $2a_2(b_2)$ gives

$$\xi^0=\xi^0(t,r,\theta,z), \quad \xi^1=0,$$
$$\xi^2=\xi^2(r,z), \quad \xi^3=c_1. \tag{53}$$

The subcase $2(a_3)$ gives similar results as the case $2(a_2)$ by interchanging the indices 2 and 3.

The subcases $2(a_4)$ and $2(a_5)$ yield results similar to the case $2(a_1)$ if we interchange indices 0, 2 and 0, 3, respectively.

The subcase $2(a_6)$ would give similar result as the case $2(a_2)$ by interchanging the indices 0, 3. It is to be noted that we again have infinite dimensional MCs in the case 2.

Case 3: The case, when only one component of the energy-momentum tensor is zero, we have four different subcases:

$$(a_1)\quad T_0=0,\quad T_1\neq 0,\quad T_2\neq 0,\quad T_3\neq 0,$$

$$(a_2)\quad T_0\neq 0,\quad T_1=0,\quad T_2\neq 0,\quad T_3\neq 0,$$

$$(a_3)\quad T_0\neq 0,\quad T_1\neq 0,\quad T_2=0,\quad T_3\neq 0,$$

$$(a_4)\quad T_0\neq 0,\quad T_1\neq 0,\quad T_2\neq 0,\quad T_3=0.$$

The first subcase gives $\xi^0=\xi^0(t,r,\theta,z)$ with the following two possibilities:

$$(b_1)\quad \left[\frac{T_2}{\sqrt{T_1}}\left(-\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$$

$$(b_2)\quad \left[\frac{T_2}{\sqrt{T_1}}\left(-\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'\neq 0.$$

In the first possibility $3a_1(b_1)$, we have $(T_2/\sqrt{T_1})[-(T_2'/2T_2\sqrt{T_1})]'=\alpha_1$, where α_1 is an arbitrary constant which can be such that

$$(c_1)\quad \alpha_1>0,\quad (c_2)\quad \alpha_1=0,\quad (c_3)\quad \alpha_1<0.$$

The case $3a_1b_1(c_1)$, when $\alpha_1>0$ gives further three options according to $\alpha_2=(T_3/\sqrt{T_1})\times[-(T_3'/2T_3\sqrt{T_1})]'$,

$$(d_1)\quad \alpha_2>0,\quad (d_2)\quad \alpha_2=0,\quad (d_3)\quad \alpha_2<0.$$

The first option $3a_1b_1c_1(d_1)$, when $\alpha_2>0$, gives either

$$(e_1)\quad \sqrt{\frac{\alpha_1}{\alpha_2}}+\sqrt{\frac{\alpha_2}{\alpha_1}}=0,\quad \text{or}\quad (e_2)\quad \sqrt{\frac{\alpha_1}{\alpha_2}}+\sqrt{\frac{\alpha_2}{\alpha_1}}\neq 0.$$

For the first case $3a_1b_1c_1d_1(e_1)$, we obtain

$$\begin{aligned}&\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=0,\\ &\xi^2=c_1z+c_2,\quad \xi^3=c_1\theta+c_3.\end{aligned}\tag{54}$$

In the second case $3a_1b_1c_1d_1(e_2)$, we have the solution

$$\begin{aligned}&\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=0,\\ &\xi^2=c_1z+c_2,\quad \xi^3=-c_1k_1\theta+c_3,\end{aligned}\tag{55}$$

where $k_1=T_2/T_3$ is a constant.

The second option $3a_1b_1c_1(d_2)$, when $\alpha_2=0$, yields the following solution:

$$\begin{aligned}&\xi^0=\xi^0(t,r,\theta,z),\\ &\xi^1=\frac{1}{\sqrt{T_1}}[e^{\iota\sqrt{\alpha_1}\theta}(c_1z+c_2)+e^{-\iota\sqrt{\alpha_1}\theta}(c_3z+c_4)],\\ &\xi^2=-\frac{\iota T_2'\sqrt{T_1}}{2T_2\sqrt{T_1}}[e^{\iota\sqrt{\alpha_1}\theta}(c_1z+c_2)-e^{-\iota\sqrt{\alpha_1}\theta}(c_3z+c_4)]+c_5,\end{aligned}\tag{56}$$

$$\xi^3=-\alpha_3\left[e^{\iota\sqrt{\alpha_1}\theta}\left(c_1\frac{z^2}{2}+c_2z\right)+e^{-\iota\sqrt{\alpha_1}\theta}\left(c_3\frac{z^2}{2}+c_4z\right)\right]-[c_1e^{\iota\sqrt{\alpha_1}\theta}+c_3e^{-\iota\sqrt{\alpha_1}\theta}]\int\frac{\sqrt{T_1}}{T_3}dr+c_6,$$

where $\alpha_3=T_3'/2T_3\sqrt{T_1}$ is a constant.

The third option $3a_1b_1c_1(d_3)$, for $\alpha_2<0$, is similar to the first option $3a_1b_1c_1(d_1)$.

Now we come to the case $3a_1b_1(c_2)$ when $\alpha_1=0$ which gives $\alpha_4=-(T_2'/2T_2\sqrt{T_1})$, a constant such that

$$(d_1)\ \ \alpha_4=0,\quad (d_2)\ \ \alpha_4\neq 0.$$

In the case $3a_1b_1c_2(d_1)$, we have $\alpha_2=(T_3/\sqrt{T_1})[-(T_3'/2T_3\sqrt{T_1})]'$ which yields the following options:

$$(e_1)\ \ \alpha_2>0,\quad (e_2)\ \ \alpha_2=0,\quad (e_3)\ \ \alpha_2<0.$$

For the case $3a_1b_1c_2d_1(e_1)$, when $\alpha_2>0$, we have the following MCs:

$$\xi^0=\xi^0(t,r,\theta,z),$$

$$\xi^1=\frac{1}{\sqrt{T_1}}[e^{\iota\sqrt{\alpha_2}\theta}(c_1z+c_2)+e^{-\iota\sqrt{\alpha_2}\theta}(c_3z+c_4)],$$

$$\xi^2=0, \tag{57}$$

$$\xi^3=-\frac{T_3'}{\iota 2\sqrt{\alpha_2}T_3\sqrt{T_1}}(c_1e^{\iota\sqrt{\alpha_2}z}-c_2e^{-\iota\sqrt{\alpha_2}z}).$$

The case $3a_1b_1c_2d_1(e_2)$, when $\alpha_2=0$, we have further two possibilities according to $\alpha_5=-T_3'/2T_3\sqrt{T_1}$, a constant such that

$$(f_1)\ \ \alpha_5=0,\quad (f_2)\ \ \alpha_5\neq 0.$$

For the case $3a_1b_1c_2d_1e_2(f_1)$, we get the following result:

$$\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=\frac{1}{\sqrt{T_1}}(c_1\theta+c_2z+c_3),$$

$$\xi^2=-\frac{c_1}{T_2}\int\sqrt{T_1}dr,\quad \xi^3=-\frac{c_2}{T_3}\int\sqrt{T_1}dr. \tag{58}$$

For α_5 to be nonzero, i.e., the case $3a_1b_1c_2d_1e_2(f_2)$, we obtain

$$\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=\frac{1}{\sqrt{T_1}}(c_1z+c_2),$$

$$\xi^2=0,\quad \xi^3=\alpha_5\left(c_1\frac{z^2}{2}+c_2z\right)-c_1\int\frac{\sqrt{T_1}}{T_3}dr. \tag{59}$$

The case $3a_1b_1c_2d_1(e_3)$ when $\alpha_2<0$ is similar to the case $3a_1b_1c_2d_1(e_1)$.

In the case $3a_1b_1c_2(d_2)$ when $\alpha_2\neq 0$, we have $\alpha_2=(T_3/\sqrt{T_1})[-(T_3'/2T_3\sqrt{T_1})]'$, a constant which gives the following three options:

$$(e_1)\ \ \alpha_2>0,\quad (e_2)\ \ \alpha_2=0,\quad (e_3)\ \ \alpha_2<0.$$

The case $3a_1b_1c_2d_2(e_1)$ yields the following solution:

$$\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=0,$$
$$\xi^2=(c_1z+c_2),\quad \xi^3=-\frac{T_2}{T_3}c_1\theta+c_3. \tag{60}$$

The case $3a_1b_1c_2d_2(e_2)$, when $\alpha_2=0$, gives the following MCs:

$$\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=\frac{c_1}{T_1},$$
$$\xi^2=(\alpha_3c_1\theta+c_2),\quad \xi^3=\alpha_3c_1z+c_3. \tag{61}$$

The last possibility $3a_1b_1c_2d_2(e_3)$ when α_2 is negative yields similar solution to the positive case $3a_1b_1c_2d_2(e_1)$.

The case $3a_1b_1(c_3)$, when $\alpha_1<0$, is similar to the case $3a_1b_1(c_1)$.

The case $3a_1(b_2)$ yields the following solution:

$$\xi^0=\xi^0(t,r,\theta,z),\quad \xi^1=0,$$
$$\xi^2=c_1z+c_2,\quad \xi^3=c_3\theta+c_4. \tag{62}$$

The case $3(a_2)$ when $T_0\neq0$, $T_1=0$, $T_2\neq0$, $T_3\neq0$ gives the following two options:

$$(b_1)\ \ T_0'=0,\quad (b_2)\ \ T_0'\neq0.$$

The first option $3a_2(b_1)$ gives either

$$(c_1)\ \left(\frac{T_2'T_3}{T_2T_3'}\right)'=0,\quad \text{or}\ \ (c_2)\ \left(\frac{T_2'T_3}{T_2T_3'}\right)'\neq0.$$

The case $3a_2b_1(c_1)$ gives one proper MC,

$$\xi_{(4)}=-\frac{2T_2}{T_2'}\beta_1\partial_r+\beta_1\theta\partial_\theta+z\partial_z, \tag{63}$$

where $\beta_1=T_2'T_3/T_2T_3'$. For the case $3a_2b_1(c_2)$, we have either

$$(d_1)\ \ T_2'=0=T_3',\quad \text{or}\ \ (d_2)\ \ T_2'\neq0,\quad T_3'\neq0.$$

The case $3a_2b_1c_2(d_1)$ yields infinite dimensional MCs. For the case $3a_2b_1c_2(d_2)$, we get three MCs which are the usual KVs.

The case $3a_2(b_2)$ divides into four groups:

$$(c_1)\ \left(\frac{T_0}{T_2}\right)'=0,\quad \left(\frac{T_0}{T_3}\right)'=0,$$
$$(c_2)\ \left(\frac{T_0}{T_2}\right)'=0,\quad \left(\frac{T_0}{T_3}\right)'\neq0,$$
$$(c_3)\ \left(\frac{T_0}{T_2}\right)'\neq0,\quad \left(\frac{T_0}{T_3}\right)'=0,$$

$$(c_4)\ \left(\frac{T_0}{T_2}\right)'\neq 0,\quad \left(\frac{T_0}{T_3}\right)'\neq 0.$$

The first group $3a_2b_2(c_1)$ gives 10 independent MCs in which seven are proper MCs given by

$$\xi_{(4)}=-\frac{k_1}{k_2}z\partial_\theta+\theta\partial_z,$$

$$\xi_{(5)}=\theta\partial_t+k_1t\partial_\theta,$$

$$\xi_{(6)}=z\partial_t+k_2t\partial_z,$$

$$\xi_{(7)}=\left(\frac{\theta^2}{2}+\frac{k_1z^2}{2k_2}+k_1\frac{t^2}{2}\right)\partial_t-\frac{2k_1T_0}{T_0'}t\partial_r+k_1t\theta\partial_\theta+k_1tz\partial_z, \tag{64}$$

$$\xi_{(8)}=t\theta\partial_t-\frac{2T_0}{T_0'}\theta\partial_r+\left(k_1\frac{t^2}{2}+\frac{\theta^2}{2}-\frac{k_1}{k_2}\frac{z^2}{2}\right)\partial_\theta+\theta z\partial_z,$$

$$\xi_{(9)}=tz\partial_t-\frac{2T_0}{T_0'}z\partial_r+\theta z\partial_\theta+\left(k_2\frac{t^2}{2}-\frac{k_2}{k_1}\frac{\theta^2}{2}+\frac{z^2}{2}\right)\partial_z,$$

$$\xi_{(10)}=t\partial_t-\frac{2T_0}{T_0'}\partial_r+\theta\partial_\theta+z\partial_z,$$

where $k_1=-T_0/T_2$ and $k_2=-T_0/T_3$ are nonzero constants.

The second group $3a_2b_2(c_2)$ when $(T_0/T_2)'=0$, $(T_0/T_3)'\neq 0$ can give two more possibilities whether

$$(d_1)\ \left(\frac{T_3'T_0}{T_3T_0'}\right)'=\text{constant},\quad (d_2)\ \left(\frac{T_3'T_0}{T_3T_0'}\right)'\neq\text{constant}.$$

The case $3a_2b_2c_2(d_1)$, we have two proper MC given by

$$\xi_{(4)}=\theta\partial_t+k_1t\partial_\theta,$$
$$\xi_{(5)}=t\partial_t-\frac{2T_0}{T_0'}\partial_r+\theta\partial_\theta+cz\partial_z, \tag{65}$$

where $T_0/T_3=c$ is an arbitrary constant. If it is not constant, i.e., the case $3a_2b_2c_2(d_2)$, we obtain only one proper MC given by

$$\xi_{(4)}=\theta\partial_t+k_1t\partial_\theta. \tag{66}$$

The third group $3a_2b_2(c_3)$ when $(T_0/T_2)'\neq 0$, $(T_0/T_3)'=0$ would give the similar solution as the previous one $3a_2b_2(c_2)$.

The last group $3a_2b_2(c_4)$ when $(T_0/T_2)'\neq 0$, $(T_0/T_3)'\neq 0$ would give the following four possibilities:

$$(d_1)\ \left(\frac{T_0'T_2}{T_0T_2'}\right)'\neq 0,\quad \left(\frac{T_0'T_3}{T_0T_3'}\right)'\neq 0,$$

$$(d_2)\ \left(\frac{T_0'T_2}{T_0T_2'}\right)'\neq 0,\quad \left(\frac{T_0'T_3}{T_0T_3'}\right)'=0,$$

$$(d_3)\ \left(\frac{T_0'T_2}{T_0T_2'}\right)'=0,\quad \left(\frac{T_0'T_3}{T_0T_3'}\right)'\neq 0,$$

$$(d_4)\ \left(\frac{T_0'T_2}{T_0T_2'}\right)'=0,\quad \left(\frac{T_0'T_3}{T_0T_3'}\right)'=0.$$

In the first possibility $3a_2b_2c_4(d_1)$, we have either

$$(e_1)\ \frac{T_2}{T_3}=\text{constant},\quad \text{or}\ (e_2)\ \frac{T_2}{T_3}\neq\text{constant}.$$

The case $3a_2b_2c_4d_1(e_1)$ gives one proper MC. The proper MC is

$$\xi_{(4)}=z\partial_\theta-\frac{T_2}{T_3}\theta\partial_z. \tag{67}$$

For the case $3a_2b_2c_4d_1(e_2)$, we get three MCs which are KVs. The possibilities $3a_2b_2c_4(d_2)$ and $3a_2b_2c_4(d_3)$ are similar to the case $3a_2b_2c_4(d_1)$.

In the last possibility $3a_2b_2c_4(d_4)$, we obtain five MCs in which two are proper, i.e.,

$$\begin{aligned}\xi_{(4)}&=z\partial_\theta-\frac{T_2}{T_3}\theta\partial_z,\\ \xi_{(5)}&=t\partial_t-\frac{2T_0}{T_0'}\partial_r+\frac{1}{\beta_2}\theta\partial_\theta+\frac{1}{\beta_2}\partial_z,\end{aligned} \tag{68}$$

where $T_0'T_2/T_0T_2'=\beta_2$, a constant. We also take T_2/T_3 to be constant.

The subcases $3(a_3)$ and $3(a_4)$ can be proceeded as the subcase $3(a_1)$ and would give similar results.

V. EXAMPLES OF FINITE DIMENSIONAL MATTER COLLINEATIONS

We see from Secs. III and IV that when we find MCs for the cylindrically symmetric static space–times, we obtain different constraints on the energy-momentum tensor. If we solve these constraints, we can have exact solutions of EFEs or a class of solutions that can be obtained. In this section, we would attempt to solve some of these constraints to get explicit forms of the metrics. We are not providing the details. Instead we provide a list of solutions and their properties satisfying the constraints.

(1) When we solve the constraints of the case $2a_1b_2(c_2)$, we obtain the following metric:
$$\mathrm{d}s^2=\cosh^2 cr\,\mathrm{d}t^2-\mathrm{d}r^2-(\cosh cr)^{-1}\,\mathrm{d}\theta^2-(\cosh cr)^{-1}\,\mathrm{d}z^2, \tag{69}$$
where c is an arbitrary constant. This metric admits four MCs and also four isometries. This implies that there is no proper MC in this example but it has seven RCs. This metric has an anisotropic fluid with energy-density positive for $0\leqslant r<(1/c)\tanh^{-1}(2/\sqrt{7})$ and negative for $r\geqslant(1/c)\tanh^{-1}(2/\sqrt{7})$.

(2) If we solve the constraints of the case $2a_2b_3c_1d_3(e_1)$, the space–time would be
$$\mathrm{d}s^2=(r/r_0)^{2a}\,\mathrm{d}t^2-\mathrm{d}r^2-(r/r_0)^{2b}\,\mathrm{d}\theta^2-(r/r_0)^{2c}\,\mathrm{d}z^2, \tag{70}$$
where a, b, c, and r_0 are arbitrary constants such that $a,b,c\neq 0,1$. The components of the energy-momentum tensor for this metric are given in Appendix B. This metric has four MCs with three KVs giving one proper MC.

(3) If we choose the values of a, b, c such that $a=1$, $b=c\neq 1$ in Eq. (70), we get a metric which admits seven MCs and four KVs satisfying the constraints $1a_4b_1c_2d_1e_2(f_1)$. This gives three proper MCs. It is obvious from the energy-momentum tensor given in Eq. (B2) that the energy density will be positive for $0<b<2/3$.

(4) When we take $a=b=c\neq 0,1$ in Eq. (70), we obtain a metric which satisfies the constraints given in $2a_1b_1c_2(d_1)$. This space–time admits 10 MCs with six KVs and hence we have four proper MCs in this example. It can be seen from the energy-momentum tensor that it becomes singular at $r=0$.

(5) If we take $b=c\neq 0,1$ in Eq. (70), we get a metric satisfying the constraints of the case $2a_1b_1c_2d_2(e_1)$ admitting five MCs but three KVs. This is another example admitting proper MCs. We must take $0<b<2/3$ to make the energy-density positive. It is to be noted that the resulting metric would represent a perfect fluid for $b=a(a-1)/(a+1)$ and non-null electromagnetic field when $b=a+1$.

(6) Taking $\nu=\lambda=\mu$ in Eq. (4), it satisfies the constraints of the case $2a_1b_2(c_1)$. This metric admits six MCs and also six KVs.

(7) When we choose $a=b\neq c$ such that $a,c\neq 0,1$ in Eq. (70), we obtain a metric satisfying the constraints of the case $2a_2b_3c_1(d_1)$. This metric admits five MCs with four isometries hence giving one proper MC.

(8) If we take either $\nu=\lambda$ or $\nu=\mu$ in Eq. (4), we have the solution of the constraints given by $2a_2b_3c_2(d_1)$. This metric admits four MCs and four isometries.

(9) Now solving the constraints of the case $2a_2b_3c_2(d_2)$, we obtain the following solution:

$$ds^2=(\cosh cr)^{-1}dt^2-dr^2-\cosh^2 cr\,d\theta^2-(\cosh cr)^{-1}dz^2. \tag{71}$$

It has four MCs and also four KVs but seven RCs. This space–time represents anisotropic tachyonic fluid.

(10) If we take $a=-\frac{1}{4}$, $b=c=\frac{1}{2}$ in Eq. (70), we get $T_1=0$ which gives the degenerate case and hence satisfies the constraints of the case $3a_2b_2c_4(d_4)$. This metric admits five MCs and four KVs. Thus we have one proper MC in this degenerate case.

VI. CONCLUSION

We know from the classification of cylindrically symmetric static space–times according to their isometries that we either get three, four, five, six, seven or ten isometries. The ten and seven KVs are admitted by the well known anti–de Sitter and anti-Einstein universes, respectively. The six isometries are admitted by the Bertotti–Robinson metric with the isometry group $SO(1,1)\times)\Re^3\otimes SO(3)$. There is one class of metrics depending on one arbitrary function with six isometries given by

$$ds^2=e^{\nu}(dt^2-dr^2-d\theta^2-dz^2). \tag{72}$$

There are three cases of five dimensional isometry groups. There are also three classes of metrics depending upon two arbitrary functions having four dimensional isometry groups given by

$$ds^2=e^{\nu}dt^2-dr^2-e^{\mu}(d\theta^2-dz^2), \tag{73}$$

$$ds^2=e^{\nu}(dt^2-dz^2)-dr^2-e^{\lambda}d\theta^2, \tag{74}$$

$$ds^2=e^{\nu}(dt^2-d\theta^2)-dr^2-e^{\mu}dz^2. \tag{75}$$

All other metrics admit minimal isometry group G_3.

This paper presents a complete classification of cylindrically symmetric static space–times according to their MCs. We have solved MC equations for both nondegenerate and degenerate cases. The explicit forms of MCs are given in each case. We have also written the corresponding constraints on the energy-momentum tensor in each case. Finally, we have attempted to solve some of these constraints to find the exact solution of EFEs.

TABLE I. MCs of case (1) for the nondegenerate energy-momentum tensor.

Cases	MCs	Constraints
$1(a_1)$	10	$T_0'=0,\ T_2'=0=T_3'$
$1a_2b_1(c_1)$	6	$T_0'=0,\ T_2'=0,\ T_3'\neq 0,$ $\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,\quad \frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=\alpha_1>0$
$1a_2b_1(c_2)$	6	$T_0'=0,\ T_2'=0,\ T_3'\neq 0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_1=0$
$1a_2b_1(c_3)$	6	$T_0'=0,\ T_2'=0,\ T_3'\neq 0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,\quad \alpha_1<0$
$1a_2(b_2)$	4	$T_0'=0,\ T_2'=0,\ T_3'\neq 0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0$
$1(a_3)$	$1(a_2)$	$T_0'=0,\ T_2'\neq 0,\ T_3'=0$
$1a_4b_1c_1(d_1)$	6	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\quad \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=\alpha_3>0,$ $\left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0$
$1a_4b_1c_1d_2(e_1)$	4	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\quad \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3>0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0,\quad \frac{T_2}{T_3}=\text{constant}\neq 0$
$1a_4b_1c_1d_2(e_2)$	3	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\quad \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3>0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0,\quad \frac{T_2}{T_3}\neq\text{constant}$
$1a_4b_1c_2d_1(e_1)$	6	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\quad \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3=0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_1>0$
$1a_4b_1c_2d_1e_2(f_1)$	7	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3=0,\ \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,\ \alpha_1=0,\ \frac{T_3}{T_2}=\text{constant}$
$1a_4b_1c_2d_1e_2(f_2)$	4	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3=0,\ \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,\quad \alpha_1=0,\quad \frac{T_3}{T_2}\neq\text{constant}$
$1a_4b_1c_2d_1(e_3)$	6	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\quad \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3=0,\ \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'=0,\ \alpha_1<0$

TABLE I. (*Continued*).

Cases	MCs	Constraints
$1a_4b_1c_2(d_2)$	4	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,$ $\alpha_3=0,\quad \left[\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right]'\neq 0$
$1a_4b_1(c_3)$	6	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'=0,\ \alpha_3<0$
$1a_4b_2(c_1)$	4	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'\neq 0,\ \frac{T_2}{T_3}=\text{constant}$
$1a_4b_2(c_2)$	3	$T_0'=0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left[\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right]'\neq 0,$ $\frac{T_2}{T_3}\neq \text{constant}$

When the energy-momentum tensor is nondegenerate (Sec. III), we obtain either three, four, five, six, seven or ten independent MCs. Out of these MCs, we obtain three isometries and the rest are the nontrivial (proper) MCs. In the degenerate case (Sec. IV), most of the possibilities lead to infinite dimensional MCs. However, there are some worth mentioning cases where we obtain finite dimensional MCs even with degenerate energy-momentum tensor. In these cases, we get either three, four, five or ten independent MCs in which three are the usual KVs and the rest are the proper MCs.

The summary of the results can be given in the form of Tables I–V.

It is seen from Tables I–V that each case has different constraints on the energy-momentum tensor. If we solve these constraints, we may have exact solution of EFEs. We have attempted (Sec. V) 10 different constraints to obtain the energy-momentum tensor and the corresponding space–time. These cases are given by $1a_4b_1c_2d_1e_2(f_1)$, $2a_1b_1c_2(d_1)$, $2a_1b_1c_2d_2(e_1)$, $2a_1b_2(c_1)$, $2a_1b_2(c_2)$, $2a_2b_3c_1(d_1)$, $2a_2b_3c_2(d_1)$, $2a_2b_3c_2(d_2)$, $2a_2b_3c_1d_3(e_1)$, $3a_2b_2c_4(d_4)$. It turns out that the cases $2a_1b_2(c_1)$, $2a_1b_2(c_2)$, $2a_2b_3c_2(d_1)$, $2a_2b_3c_2(d_2)$, $2a_2b_3c_1d_3(e_1)$ provide no proper MC. However, the cases $2a_2b_3c_1(d_1)$ and $3a_2b_2c_4(d_4)$ yield one proper MC, the case $2a_1b_1c_2d_2(e_1)$ gives two proper MCs, the case $1a_4b_1c_2d_1e_2(f_1)$ yields three proper MCs and the case $2a_1b_1c_2(d_1)$ gives four proper MCs. It is interesting to note that $3a_2b_2c_4(d_4)$ is the case where $T_1=0$, i.e., the degenerate case but this provides finite dimensional MCs and we obtain one proper MC in this case.

We have attempted some of the constraints to obtain exact solutions of EFEs which give finite dimensional MCs. We have discussed some of the physical properties of the resulting space–times. It would be interesting to look for more solutions of the constraints or examples should be constructed to satisfy the constraints.

APPENDIX A

The surviving components of the Ricci tensor are

$$
\begin{aligned}
R_{00}&=\tfrac{1}{4}e^{\nu}(2\nu''+\nu'^2+\nu'\lambda'+\nu'\mu'),\\
R_{11}&=-\tfrac{1}{4}(2\nu''+2\lambda''+2\mu''+\nu'^2+\lambda'^2+\mu'^2),\\
R_{22}&=-\tfrac{1}{4}e^{\lambda}(2\lambda''+\nu'\lambda'+\lambda'^2+\lambda'\mu'),\\
R_{33}&=-\tfrac{1}{4}e^{\mu}(2\mu''+\nu'\mu'+\lambda'\mu'+\mu'^2).
\end{aligned}
\tag{A1}
$$

TABLE II. MCs of case (2) for the nondegenerate energy-momentum tensor.

Cases	MCs	Constraints
$2a_1b_1c_1(d_1)$	10	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \frac{T_2'}{2T_2\sqrt{T_1}}=\beta_1=0,\ \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'=0$
$2a_1b_1c_1d_2e_1(f_1)$	6	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1=0,\ \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'\neq 0,$ $\frac{T_0}{2\sqrt{T_1}}\left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'=\beta_2=\text{constant},\ \beta_2=0$
$2a_1b_1c_1d_2e_1(f_2)$	6	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1=0,\ \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'\neq 0,$ $\beta_2=\text{constant},\ \beta_2\neq 0$
$2a_1b_1c_1d_2(e_2)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1=0,\ \left(\frac{(\sqrt{T_0})'}{\sqrt{T_1}}\right)'\neq 0,$ $\beta_2\neq\text{constant}$
$2a_1b_1c_2(d_1)$	10	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1\neq 0,\ \left(\frac{T_2}{T_0}\right)'=0$
$2a_1b_1c_2d_2(e_1)$	5	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1\neq 0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'=0$
$2a_1b_1c_2d_2(e_2)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,\ \beta_1\neq 0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_0'}{T_0\sqrt{T_1}}\right)'\neq 0$
$2a_1b_2(c_1)$	6	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,\ \left(\sqrt{\frac{T_0}{T_2}}\right)'=0$
$2a_1b_2(c_2)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'=0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,\ \left(\sqrt{\frac{T_0}{T_2}}\right)'\neq 0$
$2a_2b_1c_1(d_1)$	7	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'=\gamma_1=0,$ $\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=\gamma_2=0,\ \left(\frac{T_0}{T_3}\right)'=0$
$2a_2b_1c_1(d_2)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1=0,\ \gamma_2=0,\ \left(\frac{T_0}{T_3}\right)'\neq 0$
$2a_2b_1c_2(d_1)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2=0,\ \gamma_1>0$
$2a_2b_1c_2d_2(e_1)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2=0,\ \gamma_1<0,\ \left(\frac{T_0}{T_3}\right)'=0$
$2a_2b_1c_2d_2(e_2)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2=0,\ \gamma_1<0,\ \left(\frac{T_0}{T_3}\right)'\neq 0$
$2a_2b_1(c_3)$	$2a_2b_1(c_2)$	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1=0,\ \gamma_2\neq 0$
$2a_2b_1c_4d_1(e_1)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1>0,$ $\gamma_2>0,\ \gamma_2T_0\int\frac{\sqrt{T_1}}{T_0}dr+\frac{T_3'}{2\sqrt{T_1}}=0$
$2a_2b_1c_4d_1e_2(f_1)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1>0,$ $\gamma_2>0,\ \gamma_2T_0\int\frac{\sqrt{T_1}}{T_0}dr+\frac{T_3'}{2\sqrt{T_1}}\neq 0,\ \left(\frac{T_0}{T_3}\right)'=0$

TABLE II. (*Continued.*)

Cases	MCs	Constraints
$2a_2b_1c_4d_1e_2(f_2)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1>0,\ \gamma_2>0,$ $\gamma_2 T_0\int \frac{\sqrt{T_1}}{T_0}dr+\frac{T_3'}{2\sqrt{T_1}}\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0$
$2a_2b_1c_4(d_2)$	$2a_2b_1c_4(d_1)$	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1>0,\ \gamma_2<0$
$2a_2b_1c_4(d_3)$	$2a_2b_1c_4(d_1)$	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1<0,\ \gamma_2>0$
$2a_2b_1c_4(d_4)$	$2a_2b_1c_4(d_1)$	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'=0,\ T_3'\neq 0,\ \gamma_1\neq 0,\ \gamma_2\neq 0,\ \gamma_1<0,\ \gamma_2<0$
$2a_2(b_2)$	$2a_2(b_1)$	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'=0$
$2a_2b_3c_1(d_1)$	5	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=0,\ \left(\frac{T_2}{T_0}\right)'=0,\ \left(\frac{T_3}{T_0}\right)'\neq 0$
$2a_2b_3c_1(d_2)$	5	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_3}{T_0}\right)'=0$
$2a_2b_3c_1d_3(e_1)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_3}{T_0}\right)'\neq 0,\ \left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'=0$
$2a_2b_3c_1d_3(e_2)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_3}{T_0}\right)'\neq 0,\ \left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\neq 0$
$2a_2b_3c_2(d_1)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\neq 0,\ \left(\frac{T_2}{T_0}\right)'=0,\ \left(\frac{T_3}{T_0}\right)'\neq 0$
$2a_2b_3c_2(d_2)$	4	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\neq 0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_3}{T_0}\right)'=0$
$2a_2b_3c_2(d_3)$	3	$T_0'\neq 0,\ \left(\frac{T_2}{T_3}\right)'\neq 0,\ T_2'\neq 0,\ T_3'\neq 0,\ \left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\neq 0,$ $\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\neq 0,\ \left(\frac{T_2}{T_0}\right)'\neq 0,\ \left(\frac{T_3}{T_0}\right)'\neq 0$

TABLE III. MCs of case (1) for the degenerate energy-momentum tensor.

Cases	MCs	Constraints
$1(a_1)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2=0,\ T_3\neq 0$
$1(a_2)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2\neq 0,\ T_3=0$
$1(a_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2=0,\ T_3=0$
$1(a_4)$	Infinite No. of MCs	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3=0$

The Ricci scalar is given by

$$R=\tfrac{1}{2}(2\nu''+2\lambda''+2\mu''+\nu'^2+\lambda'^2+\mu'^2+\nu'\lambda'+\nu'\mu'+\lambda'\mu'). \tag{A2}$$

Using Einstein field equations (1), the nonvanishing components of energy-momentum tensor T_{ab} are

TABLE IV. MCs of case (2) for the degenerate energy-momentum tensor.

Cases	MCs	Constraints
$2a_1(b_1)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_3}{T_2}\right)'=0$
$2a_1b_2(c_1)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_3}{T_2}\right)'\neq 0,$ $T_2'=0,\ T_3'\neq 0$
$2a_1b_2(c_2)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_3}{T_2}\right)'\neq 0,$ $T_2'\neq 0,\ T_3'=0$
$2a_1b_2(c_3)$	Infinite No. of MCs	$T_0=0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_3}{T_2}\right)'\neq 0,$ $T_2'\neq 0,\ T_3'\neq 0$
$2a_2b_1(c_1)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2=0,\ T_3\neq 0,$ $\left(\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right)'=0,\ \frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=c>0$
$2a_2b_1(c_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2=0,\ T_3\neq 0,$ $\left(\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right)'=0,\ c=0$
$2a_2b_1(c_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2=0,\ T_3\neq 0,$ $\left(\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right)'=0,\ c<0$
$2a_2(b_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2=0,\ T_3\neq 0,$ $\left(\frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'\right)'\neq 0$
$2(a_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3=0$
$2(a_4)$	Infinite No. of MCs	$T_0\neq 0,\ T_1=0,\ T_2=0,\ T_3\neq 0$
$2(a_5)$	Infinite No. of MCs	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3=0$
$2(a_6)$	Infinite No. of MCs	$T_0\neq 0,\ T_1\neq 0,\ T_2=0,\ T_3=0$

TABLE V. MCs of case (3) for the degenerate energy-momentum tensor.

Cases	MCs	Constraints
$3a_1b_1c_1d_1(e_1)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'=\alpha_1>0,\ \frac{T_3}{\sqrt{T_1}}\left(\frac{T_3'}{2T_3\sqrt{T_1}}\right)'=\alpha_2>0,$ $\sqrt{\frac{\alpha_1}{\alpha_2}}+\sqrt{\frac{\alpha_2}{\alpha_1}}=0$
$3a_1b_1c_1d_1(e_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1>0,\ \alpha_2>0,\sqrt{\frac{\alpha_1}{\alpha_2}}+\sqrt{\frac{\alpha_2}{\alpha_1}}\neq 0$
$3a_1b_1c_1(d_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,\ \alpha_1>0,\ \alpha_2=0$
$3a_1b_1c_1(d_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,\ \alpha_1>0,\ \alpha_2<0$
$3a_1b_1c_2d_1(e_1)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,\ \alpha_1=0,$ $-\frac{T_2'}{2T_2\sqrt{T_1}}=\alpha_4=0,\quad \alpha_2>0$
$3a_1b_1c_2d_1e_2(f_1)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4=0,\ \alpha_2=0,\quad -\frac{T_3'}{2T_3\sqrt{T_1}}=\alpha_5=0$
$3a_1b_1c_2d_1e_2(f_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4=0,\ \alpha_2=0,\ \alpha_5\neq 0$
$3a_1b_1c_2d_1(e_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4=0,\ \alpha_2<0$
$3a_1b_1c_2d_2(e_1)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4\neq 0,\ \alpha_2>0$
$3a_1b_1c_2d_2(e_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4\neq 0,\ \alpha_2=0$
$3a_1b_1c_2d_2(e_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,$ $\alpha_1=0,\quad \alpha_4\neq 0,\ \alpha_2<0$
$3a_1b_1(c_3)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'=0,\ \alpha_1<0,$
$3a_1(b_2)$	Infinite No. of MCs	$T_0=0,\ T_1\neq 0,\ T_2\neq 0,\ T_3\neq 0,\ \left(\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'\right)'\neq 0$
$3a_2b_1(c_1)$	4	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'=0,\ \left(\frac{T_2'T_3}{T_2T_3'}\right)'=0$

TABLE V. (*Continued*.)

Cases	MCs	Constraints
$3a_2b_1c_2(d_1)$	Infinite No. of MCs	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ T_0'=0,\ \left(\frac{T_2'T_3}{T_2T_3'}\right)'\neq 0,\quad T_2'=0=T_3'$
$3a_2b_1c_2(d_2)$	3	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'=0,\ \left(\frac{T_2'T_3}{T_2T_3'}\right)'\neq 0,\quad T_2'\neq 0,\quad T_3'\neq 0$
$3a_2b_2(c_1)$	10	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'=0,\ \left(\frac{T_0}{T_3}\right)'=0$
$3a_2b_2c_2(d_1)$	5	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'=0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,\ \left(\frac{T_0}{T_2}\right)'=0$
$3a_2b_2c_2(d_2)$	4	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\ T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'=0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0$
$3a_2b_2(c_3)$	$3a_2b_2(c_2)$	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'=0$
$3a_2b_2c_4d_1(e_1)$	4	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,$ $\left(\frac{T_0'T_2}{T_0T_2'}\right)'\neq 0,\ \left(\frac{T_0'T_3}{T_0T_3'}\right)'\neq 0,\ \frac{T_2}{T_3}=\text{constant}$
$3a_2b_2c_4d_1(e_2)$	3	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,$ $\left(\frac{T_0'T_2}{T_0T_2'}\right)'\neq 0,\ \left(\frac{T_0'T_3}{T_0T_3'}\right)'\neq 0,\ \frac{T_2}{T_3}\neq\text{constant}$
$3a_2b_2c_4(d_2)$	4	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,$ $\left(\frac{T_0'T_2}{T_0T_2'}\right)'\neq 0,\ \left(\frac{T_0'T_3}{T_0T_3'}\right)'=0$
$3a_2b_2c_4(d_3)$	4	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,$ $\left(\frac{T_0'T_2}{T_0T_2'}\right)'=0,\ \left(\frac{T_0'T_3}{T_0T_3'}\right)'\neq 0$
$3a_2b_2c_4(d_4)$	5	$T_0\neq 0,\ T_1=0,\ T_2\neq 0,\ T_3\neq 0,\quad T_0'\neq 0,\ \left(\frac{T_0}{T_2}\right)'\neq 0,\ \left(\frac{T_0}{T_3}\right)'\neq 0,$ $\left(\frac{T_0'T_2}{T_0T_2'}\right)'=0,\ \left(\frac{T_0'T_3}{T_0T_3'}\right)'=0$
$3(a_3)$	$3(a_1)$	$T_0\neq 0,\ T_1\neq 0,\ T_2=0,\ T_3\neq 0$
$3(a_4)$	$3(a_1)$	$T_0\neq 0,\ T_1\neq 0,\ T_2\neq 0,\ T_3=0$

$$
\begin{aligned}
T_{00} &= -\tfrac{1}{4}e^{\nu}(2\lambda''+2\mu''+\lambda'^2+\mu'^2+\lambda'\mu'),\\
T_{11} &= \tfrac{1}{4}(\nu'\lambda'+\nu'\mu'+\lambda'\mu'),\\
T_{22} &= \tfrac{1}{4}e^{\lambda}(2\nu''+2\mu''+\nu'^2+\mu'^2+\nu'\mu'),\\
T_{33} &= \tfrac{1}{4}e^{\mu}(2\nu''+2\lambda''+\nu'^2+\lambda'^2+\nu'\lambda').
\end{aligned}
\tag{A3}
$$

APPENDIX B

Linearly independent KVs associated with the static cylindrical symmetric space–times are given by[12]

$$\xi_{(1)}=\partial_t,$$
$$\xi_{(2)}=\partial_\theta, \tag{B1}$$
$$\xi_{(3)}=\partial_z.$$

The components of the energy-momentum tensor for the metric in Eq. (70) are

$$T_0=(r/r_0)^{2a}(b+c-b^2-c^2-bc)/r^2,$$
$$T_1=(ab+bc+ca)/r^2,$$
$$T_2=-(r/r_0)^{2b}(a+c-a^2-c^2-ac)/r^2, \tag{B2}$$
$$T_3=-(r/r_0)^{2c}(a+b-a^2-b^2-ab)/r^2.$$

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Geodesic flow on (super-) Bott–Virasoro group and Harry Dym family

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We show various Harry Dym type equations and Super Harry Dym equations, introduced by Brunelli, Das, and Popowicz [2003 Supersymmetric extensions of the Harry Dym hierarchy, J. Math. Phys. **44**, 4756–4767 (2003)], follow from the geodesic flows on the Bott–Virasoro group and its supersymmetric generalization, superconformal group. In fact, their bi-Hamiltonian structures can be derived from the Lie Poisson structures on the (super-) Bott–Virasoro orbit. We also show that that m^2KdV or Calogero–Degasperis equation is also connected to the Bott–Virasoro group. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The connection between the geodesic equation of the Bott–Virasoro group and the periodic Korteweg–de Vries (KdV) equation follows from the work of Ovsienko and Khesin,[21] Segal,[26,27] Witten,[28] and others.[10,12,13]

The following three systems, the KdV equation, the Camassa–Holm equation, and the Harry Dym equation, are related to various hydrodynamical approximations of the famous Euler equation of an incompressible ideal fluid, and all these equations follow from the geodesic flows on the Bott–Virasoro group.[11,14,20,21]

It is known that the geodesic motion on the group of all volume preserving Hilbert diffeomorphisms of some Sobolev class H^s yields the hydrodynamics of an incompressible ideal fluid. This was formally derived by Arnold.[2] Later, Ebin–Marsden[8] established a proper geometric setting for this problem.

Ovsienko and Khesin[21] showed that the KdV equation is the Euler–Poincaré equation (cf. Refs. 17, 18) for a central extension of the group Diff(S^1) group of diffeomorphisms of the circle parametrized by $x:0\leqslant x\leqslant 2\pi$. For all practical purposes we restrict ourselves to the space of orientation preserving C^∞, the diffeomorphism of S^1, denoted by Diff$_+(S^1)$.

It is natural to consider the Lie algebra $\Omega\mathcal{G}$ of vector fields on S^1 as its algebra. The dual of this algebra is identifed with space of quadratic differential forms $u(x)dx^{\otimes 2}$ by the following pairing:

$$\left\langle u(x)dx^2, \quad f(x)\frac{d}{dx}\right\rangle = \int_0^{2\pi} u(x)f(x)dx.$$

The Lie algebra of vector fields on S^1, $\Omega\mathcal{G}$, has a unique nontrivial central extension by means of $\mathbf{R}$,

$$0\to\mathbf{R}\to\widehat{\Omega\mathcal{G}}\to\Omega\mathcal{G}\to 0,$$

described by the Gelfand–Fuks cocycle (cf. Refs. 11, 12),

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$$\omega_1\left(f\frac{d}{dx},g\frac{d}{dx}\right)=\int_{S^1}f'g''\,dx.$$

The extended Lie algebra of vector fields is called the Virasoro algebra.

The elements of $\hat{\Omega}\mathcal{G}$ can be identifed with the pairs (2π periodic function, real number). The commutator in $\hat{\Omega}\mathcal{G}$ takes the form

$$\left[\left(f(x)\frac{d}{dx},a\right),\left(g(x)\frac{d}{dx},b\right)\right]=\left(fg'-gf',\int_{S^1}f'g''\right). \tag{1}$$

The dual space $\hat{\Omega}\mathcal{G}^*$ can be identified to the set

$$\{(\lambda,u)|\lambda\in\mathbf{R}\ \text{ and } u\ \text{ is a quadratic diffferential}\}.$$

A pairing between a point $(\lambda,f(x)(d/dx))\in\hat{\Omega}\mathcal{G}$ and a point $(\mu,u\,dx^{\otimes 2})$ is given by

$$\lambda\mu+\int_{S^1}f(x)u(x)dx.$$

Theorem 1.1: *There exists a group* $\hat{\mathrm{Diff}}_+(S^1)$ *which is a central extension of* $\mathrm{Diff}_+(S^1)$ *given by Bott's cocycle,*

$$c:\mathrm{Diff}_+(S^1)\times\mathrm{Diff}_+(S^1)\to\mathbf{R},$$

such that

$$c(\sigma_1,\sigma_2)=\int_{S^1}\log(\sigma_1\circ\sigma_2)'d\log\sigma_1', \tag{2}$$

for $\sigma_i\in\mathrm{Diff}_+(S^1)$. *This cocycle satisfes* $c(\sigma_1,\sigma_1^{-1})=0$.

The next theorem follows from the work of Lazutkin and Pankratova.[15]

Theorem 1.2: *The space* $\hat{\Omega}\mathcal{G}^*$ *can be identifed with the* $\hat{\Omega}\mathcal{G}$*-module of Hill's operators,*

$$\{\mu\partial_x^2+q\},$$

acting on distributions of weight $-\frac{1}{2}$ *as* $\hat{\mathrm{Diff}}_+(S^1)$ *modules.*

The theories of infinite-dimensional super integrable system have drawn lots of interst in the last two decades. As a consequence a number of well known integrable equations have been generalized into supersymmetric integrable systems. Ovsienko and Khesin[21] showed that supersymmetric KdV equation, introduced by Kupershmidt, can be obtained as a geodesic flow of an invariant L^2 metric on the group of superconformal transformations of two-dimensional domains.

In an interesting paper Brunelli–Das–Popowicz[3] proposed a supersymmetric version for the well known Harry Dym system. In this paper, we show that these equations also arise as a geodesic flow on the group of a superconformal group.

II. GEODESIC FLOWS AND HARRY DYM EQUATIONS

Let G be a Lie group and $\mathfrak{g}$ be its corresponding Lie algebra and its dual is denoted by $\mathfrak{g}^*$.

The dual space $\mathfrak{g}^*$ to any Lie algebra $\mathfrak{g}$ carries a natural Lie–Poisson structure:

$$\{f,g\}_{\mathrm{LP}}(\mu):=\langle[df,dg],\mu\rangle,$$

for any $\mu\in\mathfrak{g}^*$ and $f,g\in C^\infty(S^1)$.

Lemma 2.1: The Hamiltonian vector field on $\mathfrak{g}^*$ *corresponding to a Hamiltonian function* f*, computed with respect to the Lie–Poisson structure is given by*

$$\frac{d\mu}{dt} = ad^*_{df}\mu. \tag{3}$$

Proof: It follows from the following identities:

$$i_{X_f} dg|_\mu = L_{X_f} g|_\mu = \{f,g\}_{\mathrm{LP}}(\mu) = \langle [dg,df],\mu\rangle = \langle dg, ad^*_{df}\mu\rangle.$$

This implies that $X_f = ad^*_{df}\mu$. Thus the Hamiltonian equation $d\mu/dt = X_f$ yields our result. □

Let I be an inertia operator,

$$I:\mathfrak{g}\to\mathfrak{g}^*,$$

and then $\mu\in\mathcal{G}^*$ evolve by

$$\frac{d\mu}{dt} = (I^{-1}\mu)\cdot\mu, \tag{4}$$

where the right hand side denotes the coadjoint action of $\mathfrak{g}$ on $\mathfrak{g}^*$. This equation is called the Euler–Poincaré equation.

Definition 2.2: The Euler–Poincaré equation on $\mathfrak{g}^*$ *corresponding to the Hamiltonian* $H(\mu) = \frac{1}{2}\langle I^{-1}\mu,\mu\rangle$ *is given by*

$$\frac{d\mu}{dt} = -ad^*_{I^{-1}\mu}\mu.$$

It characterizes an evolution of a point $\mu\in\mathfrak{g}^*$.

Proposition 2.3: Let ΩG *be infnite-dimensional Lie group equipped with a right invariant metric. A curve* $t\to c(t)$ *in* ΩG *is a geodesic of this metric iff* $u(t) = d_{c_t}R_{c_t^{-1}}\dot{c}(t)$ *satisfes*

$$\frac{d}{dt}u(t) = -ad^*_{u(t)}u(t). \tag{5}$$

The Euler–Poincaré equation is the Hamiltonian flow on the coadjoint orbits on the dual of Bott–Virasoro algebra generated by the Hamiltonian

$$H(u\partial_x, a) = \frac{1}{2}\int_{S^1} u^2\,dx + a^2,$$

where a is just a constant.

Lemma 2.4:

$$ad^*_{(\lambda, f(x)\,(d/dx))}(\mu,u) = (0, \tfrac{1}{2}\mu f''' + 2\,f'u + 2\,fu') \equiv (0,\tilde{u}). \tag{6}$$

Proof: It follows from the definition

$$\left\langle ad^*_{(\lambda,f(x)\,(d/dx))}(\mu,u(x)dx^2),\left(\nu,g(x)\frac{d}{dx}\right)\right\rangle=\left\langle(\mu,u\,dx^2),ad_{(\lambda,f(x)\,(d/dx))}\left(\nu,g(x)\frac{d}{dx}\right)\right\rangle$$
$$=\left\langle(\mu,u),\left(\frac{1}{2}\int_{S^1}f'g''dx,\left[f(x)\frac{d}{dx},g(x)\frac{d}{dx}\right]\right)\right\rangle$$
$$=\mu\frac{1}{2}\int_{S^1}f'g''\,dx+\int_{S^1}\left[f(x)\frac{d}{dx},g(x)\frac{d}{dx}\right]u(x)dx.$$

□

The coadjoint action leaves the parameter μ invariant, so we fix $\mu=1$ and by the abusing the notation we continue to denote it by $\hat{\Omega}\mathcal{G}^*$.

On the coadjoint orbit in $\hat{\Omega}\mathcal{G}^*$ we define the Lie–Poisson structure:

$$\{f,g\}(u(x),1)=\int\left[\left(\frac{\delta f}{\delta u}\right)\left(\frac{\delta g}{\delta u}\right)'-\left(\frac{\delta g}{\delta u}\right)\left(\frac{\delta f}{\delta u}\right)'+\left(\frac{\delta f}{\delta u}\right)'\left(\frac{\delta g}{\delta u}\right)''\right]dx,$$

where $\delta f/\delta u(x)$ is called the Fréchet derivative and it is defined by

$$\frac{d}{d\epsilon}f(u+\epsilon v,\lambda)\big|_{\epsilon=0}=\int\frac{\delta f}{\delta u}(x)v(x)dx.$$

Using Eq. (4), we know

$$\tilde{u}=\tfrac{1}{2}f'''+2\,f'u+\xi u'=(\tfrac{1}{2}\partial_x^3+2u\partial_x+u_x)f.$$

The operator $(\frac{1}{2}\partial_x^3+2u\partial_x+u_x)$ is called a symplectic operator. The Euler–Poincaré equation is the Hamiltonian flow on the coadjoint orbits in $\hat{\Omega}\mathcal{G}^*$ generated by the Hamiltonian

$$H(u)=\tfrac{1}{2}\langle(1,u(dx)^{\otimes 2}),(1,u(dx)^{\otimes 2})\rangle.$$

Theorem 2.5: *The Euler–Poincaré equation gives the KdV equation, it is a Hamiltonian flow on the coadjoint orbits in $\hat{\Omega}\mathcal{G}^*$ for the Hamiltonian function $H(u)=\frac{1}{2}u^2$.*

The Harry Dym equation is given by

$$w_t=(w^{-1/2})_{xxx}. \tag{7}$$

This can be written as

$$w_t=\partial^3\left(\frac{\delta H_1}{\delta w}\right)=(\partial w+w\partial)\frac{\partial H_2}{\delta w},$$

where

$$H_1=\int_{S^1}dx(2w^{1/2}),$$

$$H_2=\int_{S^1}dx\left(\frac{1}{8}w^{-5/2}w_x^2\right).$$

Theorem 2.6: *The Euler–Poincaré equation gives the Harry Dym equation, it is a Hamiltonian flow on the coadjoint orbits in* $\Omega\mathcal{G}^*$ *(centerless) for the Hamiltonian function* $H(w)=\int_{S^1}dx(\frac{1}{8}w^{-5/2}w_x^2)$.

Clarkson, Fokas, and Ablowitz[7] proposed a generalization of the Harry Dym equation,

$$w_t=2(w^{-1/2})_{xxx}+\gamma w^{1/2}w_x+\alpha w^{-3/2}w_x+\delta w_x, \tag{8}$$

where γ, α, and δ are coefffents. This equation reduces to the Harry Dym equation when $\gamma=\alpha=\delta=0$.

Theorem 2.7: *The Euler–Poincaré equation yields the generalized Harry Dym equation or Clarkson–Fokas–Ablowitz equation*[7] $(\delta=0)$, *for the Hamiltonian function,*

$$H(w)=\int_{S^1}dx\left(\frac{1}{8}w^{-5/2}w_x^2\right)-\alpha\int_{S^1}dx\,w^{-1/2}+\frac{2}{3}\gamma\int_{S^1}dx\,w^{3/2}.$$

Remark: One can incorporate δw_x term through lightcone coordinate, that is, defining

$$\frac{\partial}{\partial t'}=\frac{\partial}{\partial t}-\gamma\frac{\partial}{\partial x}.$$

Another interesting equation, the Hunter–Zheng equation (cf. Ref. 2) also follows from the same Hamiltonian structure with a Hamiltonian,

$$H=\frac{1}{2}\int_{S^1}(\partial^{-2}w)(\partial^{-1}w)^2\,dx.$$

Let us study the bihamiltonian structure of Harry Dym equation.[22]

Definition 2.8: Let M_P *be a Poisson manifold endowed with two Poisson bracket* $\{\cdot,\cdot\}_0$ *and* $\{\cdot,\cdot\}_1$. *We say that* M_P *is a bi-Hamiltonian manifold if the linear combination,*

$$\{f,g\}_\lambda:=\{f,g\}_0+\lambda\{f,g\}_1,$$

of these brackets satisfes Jacobi identity for any value λ *then* $\{\cdot,\cdot\}_\lambda$ *is called a Poisson pencil.*

In other words, a dynamical system,

$$\frac{d\mu}{dt}=\mathcal{X}_{\mathrm{H}}(\mu),$$

on M is called bi-Hamiltonian if the vector field $\mathcal{X}_{\mathrm{H}}$ is Hamiltonian with respect to both the Poisson brackets $\{\cdot,\cdot\}_0$ and $\{\cdot,\cdot\}_1$.

Let us consider Poisson pencil $\{\cdot,\cdot\}_\lambda$ is the deformation of $\{\cdot,\cdot\}_0$ and the Casimir function of $\{\cdot,\cdot\}_0$.

Let $H(\lambda)$ be the one parameter families of function such that

$$\{H(\lambda),f\}_\lambda=0.$$

Let $H(\lambda)=\Sigma_k H_k\lambda^{-k}$ and suppose $G(\lambda)$ be the another Casimir element on the Poisson pencil then from the recurence relation it can be proved[6] that

$$\{H_k,G_j\}_1=\{H_{k+1},G_j\}_0=0.$$

Hence, we say that the coefficients of the Laurent expansion of the Casimir function of the pencil are in involution with respect to both the basis brackets.

Let us assume $\{\cdot,\cdot\}_0$ to be a constant Poisson bracket.

Definition 2.9: The constant Poisson bracket associated to a point $\mu_0 \in \mathfrak{g}^*$ *is the bracket* $\{\cdot,\cdot\}_0$ *on the dual space* $\mathfrak{g}^*$ *defined by*

$$\{f,g\}_0(\mu) := \langle [df,dg], \mu_0 \rangle,$$

for any two smooth functions f *and* g *on the dual space for any* $\mu \in \mathfrak{g}^*$.

Remark: The constant bracket depends on the choice of the ''freezing'' point μ_0, while the Lie–Poisson bracket is defned by the Lie algebra structure only.

The following proposition was shown by Khesin and Misiolek.[14]

Proposition 2.10: The brackets $\{\cdot,\cdot\}_{LP}$ *and* $\{\cdot,\cdot\}_0$ *are compatible for every "freezing" point* μ_0.

Freezing at the point $(u\,dx^2,a)=(0,1)$ yields a truncated Hamiltonian operator,

$$\mathcal{O}_0 = \partial^3.$$

Theorem 2.11: *The Euler–Poincaré equation corresponds to "freezing" at the point* $(u\,dx^2,a)=(0,1)$ *yields a Harry Dym flow with respect to* $H=\int_{S^1} 2w^{1/2}$.

III. SUPER HARRY DYM EQUATION

Let us consider a Lie superalgebra, the Neveu–Schwarz superalgebra,[16] which contains the Virasoro algebra as its even part.

The first and foremost characteristic property of super algebra is that all the additive groups of its basic and derived structures are $\mathbb{Z}_2$ graded. A vector superspace is a $\mathbb{Z}_2$ graded vector space $V=V_0+V_1$. An element v of V_0 (resp., V_1) is said to be even (resp., odd). The super commutator of a pair of elements $v,w \in V$ is defined to be the element

$$[v,w] = vw - (-1)^{\overline{vw}} wv.$$

The Neveu–Schwartz superalgebra has two parts: bosonic (even) and fermionic (odd). These are given by

$$S\hat{\mathcal{G}}_B = \mathrm{Vect}(S^1) \oplus \mathbf{R}, \tag{9}$$

$$S\hat{\mathcal{G}}_F = C^\infty(S^1). \tag{10}$$

The Neveu–Schwarz superalgebra is an algebra on the space $\mathrm{Vect}(S^1)\oplus C^\infty(S^1)\oplus \mathbf{R}$ with the bilinear operation

$$\left[\begin{pmatrix} f(x)\dfrac{d}{dx} \\ \phi(x) \\ \lambda \end{pmatrix}, \begin{pmatrix} g(x)\dfrac{d}{dx} \\ \psi(x) \\ \mu \end{pmatrix} \right] = \begin{pmatrix} (fg'-f'g+\psi\phi)\dfrac{d}{dx} \\ \left(\left(f\psi'-\dfrac{1}{2}f'\psi\right)-\left(g\phi'-\dfrac{1}{2}g'\phi\right)\right) \\ \left(a_1\displaystyle\int_{S^1} f'g''+a_2\int_{S^1} fg'\,dx \right. \\ \left. \quad +2b_1\displaystyle\int_{S^1}\phi'\psi'\,dx+b_2\int_{S^1}\phi\psi\,dx\right) \end{pmatrix}. \tag{11}$$

Note that this algebra is the extension of $s\,\mathrm{Vect}(S^1)$ by the super Gelfand–Fuchs cocycle,

$$c_{\text{Super}}\left(\left(f(x)\frac{d}{dx},\phi(x)\right),\left(g(x)\frac{d}{dx},\psi(x)\right)\right)$$
$$=a_1\int_{S^1}f'g''\,dx+a_2\int_{S^1}fg'\,dx+2b_1\int_{S^1}\phi'\psi'\,dx+b_2\int_{S^1}\phi\psi\,dx,$$

where the even part of this cocycle is cohomologous to the Gelfands–Fuchs cocycle and, therefore, the corresponding central extension is isomorphic to the Virasoro algebra. Indeed, the first order term is a coboundary.

On this algebra, the ad-invariant, bilinear L^2 norm is given by

$$\left\langle\left(f(x)\frac{d}{dx},\phi(x),a\right),\left(g(x)\frac{d}{dx},\psi(x),b\right)\right\rangle_{L^2}=\int_{S^1}fg\,dx+\int_{S^1}\phi\partial_x^{-1}\psi\,dx+ab.$$

Lemma 3.1:

$$ad_{\hat{f}}^{*}\hat{u}=\begin{pmatrix}2uf'(x)+u'f+af'''+\frac{1}{2}\psi'\phi+\frac{3}{2}\psi\phi'\\ f\psi'+\frac{3}{2}f'\psi+u\phi+b\phi''\end{pmatrix},\tag{12}$$

where a and b are constants.

Hence the super Hamiltonian operator associated to superconformal group is given by

$$\mathcal{O}_{\text{super}}=\begin{pmatrix}\partial u+u\partial+a\partial^3 & \frac{1}{2}\partial\psi+\psi\partial\\ \frac{1}{2}\partial\psi+\psi\partial & u+b\partial^2\end{pmatrix}.\tag{13}$$

Let us consider a ''super freezing'' point,

$$(u\,dx^2,\phi(x),a,b)=(0,0,1,1).$$

Corresponding to this point we defne the constant Poisson bracket $\{\cdot,\cdot\}_0$. This bracket yields the super Harry Dym equation,

$$\begin{pmatrix}w\\ \psi\end{pmatrix}_t=\begin{pmatrix}\partial^3\dfrac{\delta H_1}{\delta w}\\ \partial^2\dfrac{\delta H_1}{\delta\psi}\end{pmatrix}=\begin{pmatrix}\partial^3(w^{-1/2})\\ \partial^2(\psi_x w^{-3/2})\end{pmatrix}.$$

The second Hamiltonian structure is

$$\mathcal{O}_{\text{sHD}}=\begin{pmatrix}\partial u+u\partial & \frac{1}{2}\partial\psi+\psi\partial\\ \frac{1}{2}\partial\psi+\psi\partial & u\end{pmatrix},\tag{14}$$

and the corresponding super Hamiltonian

$$\mathcal{H}=\frac{1}{8}\int_{S^1}(u_x^2u^{-5/2}-16\psi_x\psi_{xx}w^{-5/2}-15\psi\psi_xw_{xx}w^{-7/2}+15\psi\psi_{xx}w_xw^{-7/2})dx$$

yields super Harry Dym equation.[3]

IV. RECIPROCAL TRANSFORMATION AND INTEGRABLE FLOWS CONNECTED TO BOTT–VIRASORO GROUP

In this section we show how several other integrable systems are connected to the geodesic flows on the Bott–Virasoro group via reciprocal transformation. Reciprocal transformations are a useful tool in the study of integrable partial differential equations. These transformations have been extensively employed in contimuum mechanics not only to solve nonlinear boundary value problems. These applications are described in detail in the works of Rogers *et al.*[23,24] In our present context, reciprocal transformation is shown to be a key component[25] to connect the Harry Dym system and modified modified KdV (or m^2KdV) or Calogero–Degasperis system.[4]

Consider the following ''modified'' Gelfands–Fuchs cocycle (cf. Refs. 12, 13) on Vect(S^1):

$$\omega_{m\mathrm{GF}}\left(f(x)\frac{d}{dx},g(x)\frac{d}{dx}\right)=\int_{S^1}(af'g''+bf'g)dx. \tag{15}$$

It is easy to check that the modified action of Vect(S^1) on $\mathrm{vir}^*_{\mathrm{reg}}$ is given by the following lemma.

Lemma 4.1:

$$ad^*_{f(x)\,d/dx\,,\lambda}(u\,dx^2,\mu)=(\mu(af_{xxx}+bf_x)+4f'u+2\,fu',0). \tag{16}$$

Let us choose a specific hyperplane in $\mathrm{vir}^*_{\mathrm{reg}}$ such that $a=1,b=-1$.

Freezing at the point $(u\,dx^2,\mu)=(0,1)$ yields a truncated Hamiltonian operator,

$$\mathcal{O}=(\partial^3-\partial).$$

Theorem 4.2: *The Euler–Poincaré equation corresponds to "freezing" at the point* $(u\,dx^2,a)=(0,1)$ *yields a Camassa–Holm flow,*

$$w_t=(\partial^3-\partial)w^{-1/2}, \tag{17}$$

with respect to $H=\int_{S^1}2w^{1/2}$.

The integrable shallow-water equation investigated in Camassa and Holm,[5] namely,

$$m_t=-(m\partial+\partial m)u,\ \text{where}\ m=u-u_{xx}+\tfrac{1}{2}k \tag{18}$$

has an associated hierarchy determined from the recursion operator $R=\mathcal{O}_2\mathcal{O}_1^{-1}$, where

$$\mathcal{O}_1=\partial-\partial^3,\ \text{where}\ \mathcal{O}_2=m\partial+\partial m$$

are the first and second Hamiltonian operators. Applying the recursion operator R three times (cf. Ref. 1), starting from the shallow-water wave equation (18), gives the equation (17). In the standard Dym equation, the term ∂ is absent. The equation (18) is also called the Fuchsteinner–Fokas–Camassa–Holm equation.[5,9]

Let us substitute $w=A^2\rho^2$ in the Camassa–Holm equation (17). We obtain

$$\rho_t=\alpha\rho^{-1}[(\rho^{-1})_{xxx}-(\rho^{-1})_x], \tag{19}$$

where $2A^3\alpha=1$.

Under the reciprocal transformation

$$dX=\rho dx+\alpha[\rho^{-1}(\rho^{-1})_{xx}-\tfrac{1}{2}[(\rho^{-1})_x]^2-\tfrac{1}{2}(\rho^{-1})^2]dt,\quad dT=dt,$$

and $\Lambda=1/\rho$, we obtain

$$\Lambda_T+\alpha[\Lambda\{(\Lambda)_{XX}-1/2\,(A\Lambda)_X^2-\Lambda^2/2\}]_X=0. \tag{20}$$

Let us set

$$\theta=-A\Lambda,$$

so that

$$\theta_T+\alpha[\,\theta_{XXX}-(1/2)\,\theta_X^3-(3/2)\,e^{-2\theta}\theta_X]=0. \tag{21}$$

The choice $\alpha=-1$ delivers the m^2KdV equation.

Thus, we have seen that the m^2KdV or Calogero–Degasperis equation[4] is also connected to the geodesic flow on the Bott–Virasoro group.

V. CONCLUSION AND OUTLOOK

In this paper we have shown how several Harry Dym type equations are connected to the geodesic flows on the Bott–Virasoro group. We have also studied their superanalogs. These are connected to the geodesic flows on the superconformal group.

This result should be generalized to include deformed integrable systems. Recently Manna and Neveu[19] derived a new integrable classical $1+1$-dimensional equation, given by

$$u_{xxt}=u_x-uu_{xxx}-2u_xu_{xx}+\lambda\partial^2(u_x^3),$$

from the columnar approximation of the Euler equations of an incompressible fluid with surface tension. It would be challenging to connect the Manna–Neveu equation with the Bott–Virasoro group.

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Superfluidity of a Fermi liquid from the viewpoint of a hierarchy of equations for reduced density matrices

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The hierarchy of equations for reduced density matrices relevant to thermodynamic equilibrium with account taken of the spin obtained earlier is modified in order to describe the state of a Fermi system with a condensate. Although the procedure is to some extent analogous with the one carried out by the author earlier for a Bose liquid peculiarities relevant to Fermi statistics complicate considerably the treatment. As in the case of the Bose liquid the condensate phase can be superfluid as well as nonsuperfluid, the physical causes of superfluidity being identical. A new mechanism of fermion pairing that acts even in the case of a purely repulsive Hamiltonian is pointed out. Special attention is given to the thermodynamics of a superfluid Fermi system. The example of a hard-sphere system is used to find out the form of phase diagrams, the character of the phase transition to a condensate phase and the properties of the last. Noticeable dissimilarities from a Bose system with the same Hamiltonian are revealed. Application of the present approach to superconductivity is discussed as well.
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I. INTRODUCTION

In a recent paper[1] to be referred to as I a hierarchy of equations for *s*-particle reduced density matrices describing a system of nonzero-spin particles at thermodynamic equilibrium was derived, the hierarchy being a quantum analogue of the equilibrium Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy. The hierarchy derived is an extension of the hierarchy obtained earlier[2] for spinless particles. The approach proposed in Ref. 2 permitted one not only to deduce the hierarchy but also to construct relevant thermodynamics. In a subsequent publication[3] the approach was used for treatment of Bose condensation and thereupon of superfluidity in Bose systems, a new explanation of the phenomenon being proposed on this basis. At the same time it was shown that the condensate cannot form in the case of spinless fermions and thereby superfluidity cannot exist in this case. Therefore, in order to consider superfluidity in fermionic systems on a base of the approach it was necessary first to incorporate the spin into its framework. This being done in I our aim in the present paper is to study superfluidity of a Fermi liquid leaning upon ideas of Ref. 3, which can provide a new method for studying the phenomenon.

The superfluidity of Fermi systems itself is worthy of special attention since in nature there is a fermionic system, liquid helium-3, which can be superfluid. However, still more important is the fact that consideration of systems comprising noncharged fermions (just noncharged particles are implied in the present paper) represents an essential step towards a treatment of such a phenomenon as superconductivity.

Theoretical studies of superconductivity are based mainly upon ideas of the Bardeen–Cooper–Schrieffer (BCS) theory[4] and of Bogolyubov's method,[5] of which the latest developments are reflected in different reviews.[6–8] In the present paper we shall proceed from the general principles formulated in Refs. 2 and 3 and we shall have no need of resorting to any extra ideas or argumentation of the type presented in the references cited just above. Doubtlessly, different

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approaches in the theory of superconductivity are of obvious physical interest as long as they enable one to obtain further insight into the essence of the phenomenon, which may have considerable utility especially in the light of problems of high-temperature superconductivity.

The organization of the paper is as follows. In Sec. II we modify the hierarchy obtained in I in order to take account of the situation in which there is an exceptional state, a condensate, proceeding along the lines of Ref. 3 and without resorting to Cooper's idea that fermions combine into pairs that behave like bosons. Nevertheless the condensate can form although the reason for this is more complicated than in the case of bosons owing to the Pauli exclusion principle. The existence of the condensate leads to the possibility of superfluidity just as in Ref. 3. In Sec. III we consider the thermodynamics of a state with condensate. Section IV illustrates application of the general theory established in the preceding sections using, as an example, a system of hard spheres wherein triplet correlations are neglected. In particular we shall construct a phase diagram where a region relevant to the condensate phase will be seen. Since the same example was considered in Ref. 3 this will enable us to compare the fermionic and bosonic condensate phases and to reveal that they exhibit different features. The results obtained and some other relevant questions are discussed in the concluding section.

This paper should be considered to be the second part of a work, the first part being paper I. For this reason we neither repeat the ideas of the present approach nor discuss previous results obtained with its help because all of this can be found in the introduction to paper I. When it is not stipulated explicitly the definitions and notation of I are implied. For the sake of convenience, when referring to an equation of paper I we shall place I in front; so we shall write, e.g., (I.2.16) implying Eq. (2.16) of I.

II. GENERAL EQUATIONS AND THEIR ANALYSIS

A. Hierarchy of equations in the presence of a condensate

When the spin of particles is taken into account the reduced density matrices $R_s(\mathbf{X}_s,\mathbf{X}_s')$ in a condition of thermodynamic equilibrium have the form of (I.2.16), namely,

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\nu,\Gamma_s} n_s(\varepsilon_\nu^{(s)})\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\nu\Gamma_s}(\mathbf{X}_s'). \tag{2.1}$$

In this equation the quantities $\varepsilon_\nu^{(s)}$ are eigenvalues of Eq. (I.2.11) and, therefore, ν is in reality a set of numbers that characterize eigenfunctions of Eq. (I.2.11). For this reason the quantities $\varepsilon_\nu^{(s)}$ and thereby $n_s(\varepsilon_\nu^{(s)})$ are defined initially on a discrete point set in the relevant ν-space whose dimensionality depends on the number s. In paper I (see also Ref. 2) it is assumed that in a state of thermodynamic equilibrium the functions $n_s(\varepsilon_\nu^{(s)})$ are universal functions, which implies that n_s's are continuous functions of a continuous variable z, i.e. $n_s=n_s(z)$ while $z=\varepsilon_\nu^{(s)}$ in (2.1).

According to the ideas of Ref. 3 the initial character of $\varepsilon_\nu^{(s)}$ may manifest itself in that the quantity $n_s(\varepsilon_\nu^{(s)})$ has an outlier at a certain $\nu=\nu_0$ depending on the number s, which amounts to saying that $n_s(\varepsilon_{\nu_0}^{(s)})=\Delta n_s+n_s(z_0)$ where $n_s(z_0)$ is the limit of $n_s(z)$ as $z\to z_0=\varepsilon_{\nu_0}^{(s)}$. The part of the system described by Δn_s will be called the condensate according to the commonly accepted terminology. In this case Eq. (2.1) can be recast as

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=R_s^{(c)}(\mathbf{X}_s,\mathbf{X}_s')+R_s^{(n)}(\mathbf{X}_s,\mathbf{X}_s'), \tag{2.2}$$

with

$$R_s^{(c)}(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\Gamma_s}\Phi_s^{(\Gamma_s)}(\mathbf{X}_s)\Phi_s^{(\Gamma_s)*}(\mathbf{X}_s'), \tag{2.3}$$

$$R_s^{(n)}(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\nu,\Gamma_s} n_s(\varepsilon_\nu^{(s)})\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\nu\Gamma_s}(\mathbf{X}_s'), \tag{2.4}$$

where the superscript (c) means the condensate fraction and (n) the normal one, the functions $n_s(z)$ in (2.4) being continuous now. When writing down (2.3) we imply that there is no external field that would act on the spins; thereby all solutions with $\nu=\nu_0$ and different spin projections are singled out, none of them being distinguished anyhow. Upon assuming that $\Delta n_s>0$ the unknown quantities Δn_s are incorporated into the functions $\Phi_s^{(\Gamma_s)}(\mathbf{X}_s)$ of (2.3) which because of this differ from $\Psi_{\nu_0\Gamma_s}(\mathbf{X}_s)$ in the normalization. Therefore, according to (I.A10) they have the form

$$\Phi_s^{(\Gamma_s)}(\mathbf{X}_s)=\frac{1}{s!}\sum_{P_{r\sigma}}^{(s)}(\pm)^p\mathsf{P}_{r\sigma}\chi_{\Gamma_s}(\Sigma_s)\varphi_s(\mathbf{x}_s), \tag{2.5}$$

while the functions $\varphi_s(\mathbf{x}_s)$ satisfy the equation following from (I.2.11)

$$\frac{\hbar^2}{2m}\sum_{j=1}^{(s)}\nabla_j^2\varphi_s(\mathbf{x}_s)+[\varepsilon_{(s)}-U_s(\mathbf{x}_s)]\varphi_s(\mathbf{x}_s)=0, \tag{2.6}$$

in which $\varepsilon_{(s)}$ is written for $\varepsilon_{\nu_0}^{(s)}$.

If, by analogy with ν_0, several sets of numbers ν are exceptional the relevant functions will be labeled with an index λ. In this case instead of (2.2) and (2.3) one will have

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\lambda,\Gamma_s}\Phi_{s,\lambda}^{(\Gamma_s)}(\mathbf{X}_s)\Phi_{s,\lambda}^{(\Gamma_s)*}(\mathbf{X}_s')+R_s^{(n)}(\mathbf{X}_s,\mathbf{X}_s'). \tag{2.7}$$

Analogously with (2.2) we introduce also diagonal elements of the density matrices summed up over the spin coordinates defined in (I.2.5):

$$\rho_s(\mathbf{x}_s)=\rho_s^{(c)}(\mathbf{x}_s)+\rho_s^{(n)}(\mathbf{x}_s), \tag{2.8}$$

where upon implying (2.3)

$$\rho_s^{(c)}(\mathbf{x}_s)=\sum_{\Sigma_s,\Gamma_s}|\Phi_s^{(\Gamma_s)}(\mathbf{X}_s)|^2. \tag{2.9}$$

As long as Eq. (2.4) is identical to (2.1) with the same presumptions as to the continuity of $n_s(z)$, for $R_s^{(n)}(\mathbf{X}_s,\mathbf{X}_s')$ we have the same formulas as the ones of I for $R_s(\mathbf{X}_s,\mathbf{X}_s')$. Therefore, the expression for $\rho_s^{(n)}(\mathbf{x}_s)$ coincides with (I.2.27), namely,

$$\rho_s^{(n)}(\mathbf{x}_s)=\frac{1}{2\pi i(2\pi\hbar)^{3s}s!}\int d\mathbf{m}_s\int_C dz n_s(z)\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$$
$$\times\sum_P^{(s)}(\pm)^p\kappa(P)\exp\left[\frac{i}{\hbar}\sum_{k=1}^{s}\mathbf{r}_k(\mathbf{p}_k-\mathsf{P}\mathbf{p}_k)\right], \tag{2.10}$$

with $\kappa(P)=\Sigma_{\Sigma_s}\delta(\mathsf{P}\Sigma_s,\Sigma_s)$ and the function $\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$ satisfying Eq. (I.2.26):

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2\upsilon_s+\frac{i\hbar}{m}\sum_{j=1}^{s}\mathbf{p}_j\nabla_j\upsilon_s+\left[z-\frac{1}{2m}\sum_{k=1}^{s}\mathbf{p}_j^2-U_s(\mathbf{x}_s)\right]\upsilon_s=1. \tag{2.11}$$

When deriving Eq. (I.2.24) from a hierarchy of equations for $R_s(\mathbf{X}_s,\mathbf{X}_s')$ of (2.1) no continuity condition was implied for $n_s(\varepsilon_\nu^{(s)})$ and consequently this equation can be used as it stands:

$$\rho_s(\mathbf{x}_s)\nabla_1U_s(\mathbf{x}_s)=\rho_s(\mathbf{x}_s)\nabla_1\sum_{j=2}^{s}K(|\mathbf{r}_1-\mathbf{r}_j|)+\int\rho_{s+1}(\mathbf{x}_{s+1})\nabla_1K(|\mathbf{r}-\mathbf{r}_{s+1}|)d\mathbf{r}_{s+1}, \tag{2.12}$$

upon supposing that there is no external field $V^{(e)}(\mathbf{r})$. It will be recalled that $K(|\mathbf{r}_i-\mathbf{r}_j|)$ is the two-body potential that describes interaction between particles.

Thus, just as in I we have again obtained a hierarchy of equations for diagonal elements of reduced density matrices at thermodynamic equilibrium, which contains $\rho_s(\mathbf{x}_s)$, $U_s(\mathbf{x}_s)$, $v_s(\mathbf{x}_s,\mathbf{m}_s,z)$ and now $\varphi_s(\mathbf{x}_s)$ in addition. The equations are (2.5), (2.6), (2.8)–(2.12). Equations (2.9), (2.5), and (2.6) determine $\rho_s^{(c)}(\mathbf{x}_s)$ as a functional of the effective potential $U_s(\mathbf{x}_s)$ via an auxiliary function $\varphi_s(\mathbf{x}_s)$ while Eqs. (2.10) and (2.11) determine $\rho_s^{(n)}(\mathbf{x}_s)$ as a functional of the same potential $U_s(\mathbf{x}_s)$ via an auxiliary function $v_s(\mathbf{x}_s,\mathbf{m}_s,z)$. Eq. (2.12) yields a functional dependence of $U_s(\mathbf{x}_s)$ on the full functions $\rho_s(\mathbf{x}_s)$ and $\rho_{s+1}(\mathbf{x}_{s+1})$ of (2.8) thus closing the set of equations and at the same time connecting the sth and $(s+1)$th members of the hierarchy. Note that Eq. (2.12) has a form similar to that of an equation of the classical BBGKY hierarchy.[2] It remains to determine the functions $n_s(z)$, the quantities $\varepsilon_{(s)}$, the normalization of $\varphi_s(\mathbf{x}_s)$, and conditions on solutions of Eq. (2.6), the conditions on solutions of Eq. (2.11) being discussed in Ref. 2 seeing that Eq. (2.11) coincides with Eq. (2.22) of this last reference.

B. Supplementary equations and conditions

In order to find the quantities and conditions listed at the end of the preceding subsection we turn to the interrelation between the reduced density matrices that follows from (I.2.4) at $n=s+1$:

$$(N-s+1)R_{s-1}(\mathbf{X}_{s-1},\mathbf{X}'_{s-1})=\sum_{\sigma_s=1}^{\kappa}\int_V R_s(\mathbf{X}_{s-1},\mathbf{r}_s,\sigma_s,\mathbf{X}'_{s-1},\mathbf{r}_s,\sigma_s)d\mathbf{r}_s, \tag{2.13}$$

where we have made the replacement $s\to s-1$ for convenience sake.[9] In virtue of the linearity of Eq. (2.13) one can require it to be satisfied by $R_s^{(c)}$ and $R_s^{(n)}$ separately.

As long as $R_s^{(n)}$ obeys the same equations as R_s in I Eq. (2.13) permits one to arrive at an equation for $n_s(z)$ identical with (I.2.29). In order to solve this equation uniquely an extra condition on $n_s(z)$ is required. To obtain the condition in question one may reason exactly as in Sec. IV of Ref. 2. Let the system be made up of two mutually noninteracting subsystems A and B, so that the wave function of the system is of the form $\Psi=\Psi_A\Psi_B$. In this case the density matrices should break up into two factors according to the definition of (I.2.2):

$$R_s(\mathbf{X}_s,\mathbf{X}'_s)=C_s^{s_a,s_b}R_{s_a}(\mathbf{X}_{s_a}^{(a)},\mathbf{X}_{s_a}^{(a)\prime})R_{s_b}(\mathbf{X}_{s_b}^{(b)},\mathbf{X}_{s_b}^{(b)\prime}), \tag{2.14}$$

where $s=s_a+s_b$, the constant $C_s^{s_a,s_b}$ depends on the manner in which one normalizes R_{s_a} and R_{s_b} (see Appendix A), the index a refers to the subsystem A and b to B. For simplicity we assume that the subsystem A alone has a condensate. Then as in (2.2)–(2.4) we shall have

$$R_{s_a}(\mathbf{X}_{s_a}^{(a)},\mathbf{X}_{s_a}^{(a)\prime})=\sum_{\Gamma_{s_a}}\Phi_{s_a}^{(\Gamma_{s_a})}(\mathbf{X}_{s_a}^{(a)})\Phi_{s_a}^{(\Gamma_{s_a})*}(\mathbf{X}_{s_a}^{(a)\prime})+\sum_{\nu_a,\Gamma_{s_a}}n_{s_a}(\varepsilon_{\nu_a}^{(s_a)})\Psi_{\nu_a\Gamma_{s_a}}(\mathbf{X}_{s_a}^{(a)})\Psi^*_{\nu_a\Gamma_{s_a}}(\mathbf{X}_{s_a}^{(a)\prime}), \tag{2.15}$$

$$R_{s_b}(\mathbf{X}_{s_b}^{(b)},\mathbf{X}_{s_b}^{(b)\prime})=\sum_{\nu_b,\Gamma_{s_b}}n_{s_b}(\varepsilon_{\nu_b}^{(s_b)})\Psi_{\nu_b\Gamma_{s_b}}(\mathbf{X}_{s_b}^{(b)})\Psi^*_{\nu_b\Gamma_{s_b}}(\mathbf{X}_{s_b}^{(b)\prime}). \tag{2.16}$$

Upon substituting this into (2.14) and taking into account that $\varepsilon_\nu^{(s)}=\varepsilon_{\nu_a}^{(s_a)}+\varepsilon_{\nu_b}^{(s_b)}$ in the present case[2] we shall obtain an expression of the type (2.7) only if

$$n_s(\varepsilon_{\nu_a}^{(s_a)}+\varepsilon_{\nu_b}^{(s_b)})\propto n_{s_a}(\varepsilon_{\nu_a}^{(s_a)})n_{s_b}(\varepsilon_{\nu_b}^{(s_b)}). \tag{2.17}$$

This relation together with (I.2.29) entail Eqs. (I.2.30) and (I.2.31) (details are given in Appendix A), namely,

$$n_s(z)=A_s e^{-z/\tau},\quad A_s=s!\left(\frac{\rho}{\kappa}\right)^{s-1}\left(\frac{2\pi\hbar^2}{m\tau}\right)^{3(s-1)/2}A;\quad n_1(z)\equiv n(z)=Ae^{-z/\tau},\tag{2.18}$$

where $\rho=N/V$ is the average number density, A and τ are constants.

Having found $n_s(z)$ we now turn to the relationship of (2.13) as applied to the condensate part $R_s^{(c)}(\mathbf{X}_s,\mathbf{X}_s')$. Upon placing Eq. (2.3) there and assuming that $s\ll N$ we have, for $s>1$,

$$\sum_{\Gamma_{s-1}}\Phi_{s-1}^{(\Gamma_{s-1})}(\mathbf{X}_{s-1})\Phi_{s-1}^{(\Gamma_{s-1})*}(\mathbf{X}_{s-1}')=\frac{1}{N}\sum_{\sigma_s=1}^{\kappa}\sum_{\Gamma_s}\int_V\Phi_s^{(\Gamma_s)}(\mathbf{X}_{s-1},\mathbf{r}_s,\sigma_s)\Phi_s^{(\Gamma_s)*}(\mathbf{X}_{s-1}',\mathbf{r}_s,\sigma_s)d\mathbf{r}_s.\tag{2.19}$$

Let us find first $\Phi_1^{(\gamma)}(\mathbf{r},\sigma)$ that, according to (2.5), is of the form

$$\Phi_1^{(\gamma)}(\mathbf{r},\sigma)=\delta_{\gamma\sigma}\varphi_1(\mathbf{r}).\tag{2.20}$$

It will be recalled that the spin variable σ and the spin index γ run from 1 to $\kappa=2S+1$ where S is the particle spin. As in I we limit ourselves to consideration of a spatially uniform boundless system upon putting[2] $U_1=0$. Then Eq. (2.6) at $s=1$ becomes

$$\frac{\hbar^2}{2m}\nabla^2\varphi_1(\mathbf{r})+\varepsilon_{(1)}\varphi_1(\mathbf{r})=0.\tag{2.21}$$

We take a solution of this equation which gives $\rho_1^{(c)}=\rho_c=$constant. Analogously to Eq. (2.8) of Ref. 3 this solution is of the form $\varphi_1(\mathbf{r})=C\exp(i\mathbf{p}_0\mathbf{r}/\hbar)$ with $\mathbf{p}_0^2=2m\varepsilon_{(1)}$. The constant C that can be considered to be real because a factor like $e^{i\alpha}$ plays no part for (2.3) may be expressed in terms of ρ_c by (2.9). We introduce the result into (2.20):

$$\Phi_1^{(\gamma)}(\mathbf{r},\sigma)=\delta_{\gamma\sigma}\sqrt{\frac{\rho_c}{\kappa}}\exp\left(\frac{i}{\hbar}\mathbf{p}_0\mathbf{r}\right),\quad \varepsilon_{(1)}=\frac{\mathbf{p}_0^2}{2m}.\tag{2.22}$$

Here we have also written down the quantity $\varepsilon_{(1)}$ as a function of $\mathbf{p}_0$. Below we shall see that all quantities relevant to the condensate are expressed in terms of the condensate density ρ_c and of the vector $\mathbf{p}_0$.

Next, referring again to (2.5) one has

$$\Phi_2^{(\gamma_1,\gamma_2)}(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2)=\tfrac{1}{2}[\delta_{\gamma_1\sigma_1}\delta_{\gamma_2\sigma_2}\varphi_2(\mathbf{r}_1,\mathbf{r}_2)\pm\delta_{\gamma_1\sigma_2}\delta_{\gamma_2\sigma_1}\varphi_2(\mathbf{r}_2,\mathbf{r}_1)].\tag{2.23}$$

We turn now to the relationship (2.19) putting $s=2$. At given $\mathbf{r}_{s-1}=\mathbf{r}_1$ and $\mathbf{r}_{s-1}'=\mathbf{r}_1'$ the main contribution to the integral in (2.19) as $V\to\infty$ results from regions where $|\mathbf{r}_1-\mathbf{r}_2|$ and $|\mathbf{r}_1'-\mathbf{r}_2|$ are large (cf. Sec. IV of Ref. 2). In these regions $U_2\to 0$, and Eq. (2.5) at $s=2$ becomes

$$\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)\varphi_2^{(\infty)}(\mathbf{r}_1,\mathbf{r}_2)+\varepsilon_{(2)}\varphi_2^{(\infty)}(\mathbf{r}_1,\mathbf{r}_2)=0,\tag{2.24}$$

the superscript (∞) denoting the limiting value of φ_s. By analogy with the solution of Eq. (2.21) the solution of (2.24) can be taken to be

$$\varphi_2^{(\infty)}(\mathbf{r}_1,\mathbf{r}_2)=B_2\exp\left[\frac{i}{\hbar}(\mathbf{q}_1\mathbf{r}_1+\mathbf{q}_2\mathbf{r}_2)\right],\quad \varepsilon_{(2)}=\frac{\mathbf{q}_1^2+\mathbf{q}_2^2}{2m}.\tag{2.25}$$

It should be observed that the solution of (2.24) need not have any symmetry since the symmetry required will emerge after substitution into (2.23). If (2.22) and (2.23) together with (2.25) are inserted into (2.19) at $s=2$, one will obtain that $\mathbf{q}_1=\mathbf{q}_2=\mathbf{p}_0$ and, besides,

$$B_2=\sqrt{\frac{2\rho_c\rho}{\kappa(\kappa\pm1)}},\quad \varepsilon_{(2)}=\frac{\mathbf{p}_0^2}{m}. \tag{2.26}$$

Some comment at this point is in order. In Ref. 3 it was pointed out that in the case of spinless fermions the condensate could not form. This follows directly from (2.26): if one puts $\kappa=1$ (i.e., $S=0$) implying the lower sign in (2.26), then the expression for B_2 makes no sense unless $\rho_c=0$.[10] Existence of the spin of fermions (the spin factor $\kappa\geqslant2$) leads to the result that $B_2\neq0$ if $\rho_c\neq0$. In other words, the spin permits one to surmount the difficulty that arises at $s=2$ in the case of spinless fermions.

If, however, one goes on reasoning in parallel with Ref. 3 farther, in the case of spin-half fermions ($\kappa=2$) one will again encounter an analogous difficulty now at the next stage [$s=3$ in (2.19)]. The difficulty consists in the following. In Ref. 3 when considering an equation identical with (2.6) in the limit of large $|\mathbf{r}_j-\mathbf{r}_k|$'s, one implied simplest asymptotic solutions having the form $\varphi_s^{(\infty)}(\mathbf{x}_s)\propto\exp(i\Sigma\mathbf{q}_k\mathbf{r}_k/\hbar)$ [cf. (2.25)] which always turned out symmetric in $\mathbf{r}_k$ because $\mathbf{q}_k=\mathbf{p}_0$ [see Eq. (2.9) of Ref. 3]. On the other hand if the function $\varphi_s(\mathbf{x}_s)$ in (2.5) is symmetric, in order that $\Phi_s^{(\Gamma_s)}(\mathbf{X}_s)$ be antisymmetric it is necessary that the function relevant to the spin variables shall be antisymmetric. The latter function can be expressed in terms of spinors. When $S=1/2$, however, there is no antisymmetric spinor of rank 3 (see Ref. 11). If $S>1/2$ (i.e., $\kappa>2$) analogous difficulties occur for $s>3$. It would seem that there is no solution to Eq. (2.19) appropriate for fermions.

However, just if $s\geqslant3$ there emerges a favourable circumstance. All solutions of Eq. (2.6) at $s=2$ can be taken to be symmetric or antisymmetric as in the case of the Schrödinger equation[11] that Eq. (2.6) is identical with. It easy to see that antisymmetric solutions are not appropriate for our purposes.[12] In the event that $s\geqslant3$, in addition to symmetric and antisymmetric solutions an equation of the (2.6) type always admits solutions that have no such symmetries.[11] Just these last solutions are helpful for us.

For $s\geqslant3$ we shall take solutions of (2.6) subject to the conditions

$$\varphi_s(\mathbf{x}_s)\to D_s\varphi_{s-1}(\mathbf{x}_{s-1})\exp\left(\frac{i}{\hbar}\mathbf{p}_0\mathbf{r}\right),\quad \text{as}\ \ |\mathbf{r}_s|\to\infty, \tag{2.27}$$

$$\varphi_s(\mathbf{x}_s)\to0,\quad \text{as}\ \ |\mathbf{r}_j|\to\infty\ \ \text{with}\ \ j\neq s, \tag{2.28}$$

where D_s is a constant to be chosen later. The physical bearings of the conditions of (2.27) and (2.28) will be discussed below. Note that the conditions are not symmetric in all $\mathbf{r}_1,\ldots,\mathbf{r}_s$. We place Eq. (2.27) into (2.6), letting $|\mathbf{r}_s|\to\infty$ and making use of the obvious fact[2] that $U_s(\mathbf{x}_s)\to U_{s-1}(\mathbf{x}_{s-1})$ in this limit since $U_1=0$. As a result we have

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s-1}\nabla_j^2\varphi_{s-1}(\mathbf{x}_{s-1})+\left[\varepsilon_{(s)}-\frac{\mathbf{p}_0^2}{2m}-U_{s-1}(\mathbf{x}_{s-1})\right]\varphi_{s-1}(\mathbf{x}_{s-1})=0. \tag{2.29}$$

Upon comparing this with Eq. (2.6) written for $\varphi_{s-1}(\mathbf{x}_{s-1})$ we see that the condition of (2.27) is possible if

$$\varepsilon_{(s)}=\varepsilon_{(s-1)}+\frac{\mathbf{p}_0^2}{2m}. \tag{2.30}$$

Because we know $\varepsilon_{(1)}$ and $\varepsilon_{(2)}$ by (2.22) and (2.26), this relation determines all $\varepsilon_{(s)}$.

We revert now to the right-hand side of (2.19). Again, as in the $s=2$ case, the main contribution to the integral as $V\to\infty$ is due to regions where $|\mathbf{r}_s|$ is large, and thereby the limiting expressions of (2.27) and (2.28) have to be used with account taken of the fact that the vector $\mathbf{r}_s$ is permuted according to (2.5). By virtue of (2.28) all permutations that involve $\mathbf{r}_s$ will give integrals that increase more slowly than V in the limit as $V\to\infty$. For this reason we ought to retain only those permutations that do not affect $\mathbf{r}_s$, which implies making use of (2.27). Then the integral in (2.19) is calculated at once while the summation over σ_s and γ_s is readily carried out thanks to (I.2.12). If one compares the result with the left-hand side of (2.19) wherein (2.5) is put one will see that (2.19) is fulfilled if

$$D_s = s\sqrt{\frac{\rho}{\kappa}}. \tag{2.31}$$

Thus, we have satisfied the last condition to which the density matrices are to be subjected, the condition being (2.19). Together with this, we have uniquely formulated the problem concerning solution of Eq. (2.6) for $s\geqslant 3$: the quantities $\varepsilon_{(s)}$ are defined by (2.30) while the limiting form of $\varphi_s(\mathbf{x}_s)$ must be that of (2.27) and (2.28) wherein D_s is given by (2.31). We see that calculation of $\varphi_{s-1}(\mathbf{x}_{s-1})$ determines the boundary conditions for $\varphi_s(\mathbf{x}_s)$ from which the normalization of $\varphi_s(\mathbf{x}_s)$ follows as well. For $s=2$ the boundary condition is (2.25) with (2.26), while for $s=1$ the solution is known by virtue of (2.22). Just as in Ref. 3 there remain four arbitrary constants τ, A, ρ_c, and $\mathbf{p}_0$ which are to be found from thermodynamic considerations and the normalization condition of (I.2.6).

C. Analysis and discussion of the results obtained

Turning now to the discussion of the physical bearings of the conditions of (2.27) and (2.28) let us first consider the case $s=3$ when $\mathbf{r}_s=\mathbf{r}_3$. The condition of (2.27) is usual and means that, when particle 3 moves away, particles 1 and 2 are described by the wave function $\varphi_2(\mathbf{r}_1,\mathbf{r}_2)$. The condition (2.28) is rather unusual in our case. The fact that a wave function vanishes at infinity implies that there is a bound state. Therefore, the condition of (2.28) amounts to saying that particles 1 and 2 form a bound state in the presence of particle 3 even if there is no bound state when particle 3 is absent [the above function $\varphi_2(\mathbf{r}_1,\mathbf{r}_2)$ corresponds to the scattering of particles according to the discussion of Eq. (3.6) obtained below]. The possibility of such a situation is quite understandable physically. Let us suppose that the interaction between each pair of particles is attractive but rather weak, so that they cannot form a bound state. Approach of a third particle diminishes the potential energy, and thereby the first two particles may form a bound state when the third is near. The aforesaid does not signify that all particles break up into pairs. The condition of (2.28) for $s=4$ is equivalent to saying that three particles form a bound state in the presence of a fourth particle. If one puts $s=5$ in (2.28) one will conclude that four particles form a bound state when a fifth particle is near, and so on. It should be emphasized that the above argument is a simplification, and is presented here for illustrative purposes only. In the matter of an interacting N-body system one cannot speak of states of two, three, etc. particles. The conditions of (2.27) and (2.28) merely imply special correlations that arise in the case under study. From the dynamical point of view there occurs permanent formation and disintegration of groups of bound particles.

Nevertheless from the foregoing it follows that the condition of (2.28) can be fulfilled only if there exists an attractive interaction between the particles. However, this does not at all amount to saying that the interparticle potential $K(\mathbf{r})$ must have an attractive part. The point is that (2.6) contains an effective potential $U_s(\mathbf{x}_s)$, and not $K(\mathbf{r})$. Even in the case of hard spheres the potential $U_s(\mathbf{x}_s)$ has an attractive part which is due to the shielding effect (for an explanation of this effect see, e.g., Ref. 13, Sec. 8.6). Of course, other causes for the existence of an effective attraction in the event of a purely repulsive Hamiltonian are possible. In the BCS theory such an attraction is ascribed to an electron–phonon interaction. As is known it is difficult to explain high-temperature

superconductivity in the framework of the BCS theory. Perhaps, in the last case an important role is played just by the shielding effect that is manifested at any density and temperatures regardless of the Hamiltonian.

Let us make a few remarks in addition. As was shown in Ref. 2, in the case of a Bose system the normal phase cannot exist at temperatures $\theta \approx 0$. For this reason, as the temperature is lowered there must necessarily emerge a condensate phase. With this corresponds the fact that in the boson case the condensate phase exists whatever the interaction potential $K(\mathbf{r})$ is[3] [it occurs even in an ideal gas when $K(\mathbf{r}) \equiv 0$]. In the case of a Fermi system the situation is different. According to I the fermionic normal phase can exist even at $\theta = 0$. Consequently the fermionic condensate phase need not exist necessarily for any $K(\mathbf{r})$. The fermionic condensate phase occurs only when the conditions of (2.27) and (2.28) can be fulfilled. In particular, these conditions cannot be satisfied in an ideal gas. Therefore, the condensate phase cannot form in an ideal Fermi gas as is obvious in advance.

Equation (2.6) can have a solution corresponding to (2.27) and (2.28) in the case of bosons as well. In Ref. 3 it was stated that condensate phases of different types are possible. The solution corresponding to (2.27) and (2.28) provides an extra possible type of the condensate phase for bosons.

If the spin S of fermions is such that $\kappa > 2$ (i.e., $S > 1/2$), symmetric solutions with the simplest limiting form $\varphi_s^{(\infty)}(\mathbf{x}_s) \propto \exp(i\Sigma \mathbf{q}_k \mathbf{r}_k / \hbar)$ as in Ref. 3 are possible up to $s = \kappa$. Only when $s \geqslant \kappa$, solutions must have the limiting form of (2.27) and (2.28). Therefore, a variety of condensate phases may be obtained, depending on the integer s at which (2.27) and (2.28) begin to hold. Realized is the phase that provides an absolute minimum of the appropriate thermodynamic potential.

In the event of a Fermi liquid one can repeat the considerations expounded in Sec. IV of Ref. 3. Consequently, condensate phases of different types, either superfluid ($\mathbf{p}_0 \neq 0$) or nonsuperfluid ($\mathbf{p}_0 = 0$), may happen even in the case $\kappa = 2$.

It might seem at first sight that the first summand in (2.2) corresponds to condensation of fermions in one level, which contradicts the Pauli exclusion principle. In fact there is no contradiction. In paper I (see also Ref. 2) it was emphasized that the quantities $n_s(\varepsilon_\nu^{(s)})$ are no occupation numbers of levels for there are no single-particle levels in an interacting system, so that one cannot speak of condensation of particles in a level. Let us explain the absence of any contradiction with the Pauli principle in more detail. The principle stems from the antisymmetry of fermion wave functions (if states of two fermions coincide the wave function vanishes identically owing to the antisymmetry). In our case all fermion density matrices (and thereby the wave function itself) are antisymmetric with respect to the variables denoted briefly as $\mathbf{X}_s$ and $\mathbf{X}_s'$, which is immediately seen from (I.A10) and (2.5). Just the requirement that $R_s^{(c)}(\mathbf{X}_s, \mathbf{X}_s')$ should not vanish identically compelled us to resort to limiting conditions of types (2.27) and (2.28). In the case of bosons that are not subjected to the Pauli principle, simpler solutions used in Ref. 3 (see also above) are possible.

Concluding the section let us calculate the momentum of the system. To this end, by making use of (2.22) and (2.2)–(2.4), first we find the density matrix R_1:

$$R_1(\mathbf{r}, \sigma, \mathbf{r}', \sigma') = \frac{\delta_{\sigma\sigma'}}{\kappa} \left\{ \rho_c \exp\left[\frac{i}{\hbar} \mathbf{p}_0 (\mathbf{r} - \mathbf{r}') \right] + \rho_n \exp\left[-\frac{m\tau(\mathbf{r} - \mathbf{r}')^2}{2\hbar^2} \right] \right\}. \tag{2.32}$$

The second term is written here with the help of formulas of the next section. The momentum $\mathbf{P}$ of the system can be computed by Eq. (2.13) of Ref. 3 with additional summation over the spin projections, so that $\mathbf{P} = \rho_c V \mathbf{p}_0$. Just as in the boson case of Ref. 3 the situation is analogous with that in which there are $N_c = \rho_c V$ particles that move at a speed of $\mathbf{p}_0 / m$ without any dissipation of energy.

It is worthy of remark that according to (2.32) the density matrices exhibit off-diagonal long range order (ODLRO) since they do not vanish in the limit as $|\mathbf{r} - \mathbf{r}'| \to \infty$. ODLRO is due only to

the condensate fraction because the first summand alone in (2.32) displays this feature. As is known the existence of ODLRO is characteristic of superfluidity.[14]

III. THERMODYNAMICS

A. Transformation of equations

Before proceeding to thermodynamics it is worthwhile to transform some of the equations obtained above. To this end instead of $\varphi_s(\mathbf{x}_s)$ with $s\geqslant 3$ we set up functions $u_s(\mathbf{x}_s)$ according to

$$\varphi_s(\mathbf{x}_s)=u_s(\mathbf{x}_s)\exp\left(\frac{i}{\hbar}\mathbf{p}_0\sum_{k=1}^{s}\mathbf{r}_k\right). \tag{3.1}$$

When substituted into (2.6) with account taken of (2.30), this yields the equation

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2 u_s(\mathbf{x}_s)+\frac{i\hbar\mathbf{p}_0}{m}\sum_{j=1}^{s}\nabla_j u_s(\mathbf{x}_s)-U_s(\mathbf{x}_s)u_s(\mathbf{x}_s)=0. \tag{3.2}$$

Note that this last equation coincides with Eq. (2.10) obtained in Ref. 3 for the boson case. The relevant boundary conditions follow from (2.27) and (2.28):

$$u_s(\mathbf{x}_s)\to D_s u_{s-1}(\mathbf{x}_{s-1}) \quad \text{as} \quad |\mathbf{r}_s|\to\infty, \tag{3.3}$$

$$u_s(\mathbf{x}_s)\to 0, \quad \text{as} \quad |\mathbf{r}_j|\to\infty \quad \text{with} \quad j\neq s. \tag{3.4}$$

At $s=2$ it is more convenient to use another normalization of u_2 upon writing, instead of (3.1),

$$\varphi_2(\mathbf{r}_1,\mathbf{r}_2)=\sqrt{\frac{2\rho_c\rho}{\kappa(\kappa\pm 1)}}\,u_2(\mathbf{r}_1,\mathbf{r}_2)\exp\left[\frac{i}{\hbar}\mathbf{p}_0(\mathbf{r}_1+\mathbf{r}_2)\right]. \tag{3.5}$$

It should be observed that $u_2(\mathbf{r}_1,\mathbf{r}_2)$ is to be symmetric by virtue of (2.25). In the case of homogeneous media we deal with, $u_2(\mathbf{r}_1,\mathbf{r}_2)$ depends only upon the difference $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$, while Eq. (3.2) becomes

$$\frac{\hbar^2}{m}\nabla^2 u_2(\mathbf{r})-U_2(\mathbf{r})u_2(\mathbf{r})=0, \tag{3.6}$$

with the condition that $u_2(\mathbf{r})\to 1$ as $|\mathbf{r}|\to\infty$, which follows from (2.25) and (2.26). Such an equation with this condition is characteristic of the problem of scattering of a particle with the propagation vector $\mathbf{k}=0$ by a fixed force field as was noted in Ref. 3. In particular instead of (3.6) one may use Eq. (2.12) of this reference.

In uniform media one can put[2] $U_1=0$, so that Eq. (2.11) with $s=1$ is readily solved to yield

$$\nu_1(\mathbf{p},z)=\frac{1}{z-\mathbf{p}^2/2m}. \tag{3.7}$$

Now we calculate $\rho_1^{(n)}$ by (2.10) with the help of the residue theorem upon inserting (2.18) for $n_1(z)\equiv n(z)$. Next, recalling that $\rho_1^{(c)}=\rho_c$ we find ρ_1 by (2.8) and put it in the normalization condition of (I.2.6) with the result that $\rho=\rho_c+\rho_n$ where $\rho=N/V$ and

$$\rho_n=\frac{\sqrt{\pi}}{2}A\kappa\omega\tau^{3/2} \quad \text{with} \quad \omega=\frac{m^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}. \tag{3.8}$$

In like fashion one gets (2.32) if use is made of (I.3.3) for $R_1^{(n)}$.

Calculation of thermodynamic quantities requires a knowledge of the pair density matrix $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$. We substitute (2.5) and (3.5) into (2.8) with (2.9) and use the symmetry of $u_2(\mathbf{r}_1,\mathbf{r}_2)=u_2(\mathbf{r}_2-\mathbf{r}_1)$ [see the remark following (3.5)]. We take (I.3.12) to calculate $\rho_2^{(n)}$. As a result we obtain the following expression for the pair correlation function $g(\mathbf{r})=\rho_2(\mathbf{r})/\rho^2$:

$$g(\mathbf{r})=\frac{\rho_c}{\rho}u_2^2(\mathbf{r})+\frac{1}{2\pi i(2\sqrt{2}\pi\hbar)^3\rho}\int d\mathbf{q}\int_C dz n(z)\upsilon(\mathbf{r},\mathbf{q},z)\left[\kappa\pm\exp\left(\frac{i}{\hbar}\mathbf{q}\mathbf{r}\right)\right], \tag{3.9}$$

while $\upsilon(\mathbf{r},\mathbf{q},z)$ obeys Eq. (I.3.13) in which $U_2(\mathbf{r})$ replaces $U_2(|\mathbf{r}|)$ since the functions are not spherically symmetric if $\mathbf{p}_0\neq 0$.

The second term in (3.9) may be reduced to a form analogous with the right-hand side of Eq. (I.3.14). For use later we need (3.9) in the case of a spherical symmetry of $U_2(\mathbf{r})$ on condition that the spectrum is continuous. In this case one can use (I.3.16) for the second term in (3.9) with the result that

$$g(\mathbf{r})=f_c u_2^2(\mathbf{r})+\frac{1}{\pi\sqrt{2}\rho}\sum_{l=0}^{\infty}[\kappa\pm(-1)^l](2l+1)\int_0^{\infty}n\left(\frac{\hbar^2k^2}{m}\right)R_{kl}^2(r)dk, \tag{3.10}$$

where $f_c=\rho_c/\rho$ while R_{kl} satisfies Eq. (I.3.17) with the boundary condition of (I.3.18).

B. The thermodynamics of a superfluid Fermi system

General ideas as to constructing thermodynamics in the framework of the present approach were expounded in paper I. Modifications needed in order to take into account the presence of a condensate can be made by analogy with the thermodynamics of a superfluid Bose system presented in Ref. 3. The sole difference with Ref. 3 comes about because of the spin of particles. All thermodynamic formulas of Ref. 3 remain, however, as they stand because the factor κ in (2.32) cancels out owing to summation over the spin projections. Let us summarize the main features of thermodynamics in the present case referring to Ref. 3 for details.

In the preceding section it was established that the density matrices are characterized by four parameters τ, A, ρ_c, and p_0 where p_0 is the magnitude of the vector $\mathbf{p}_0$ (the direction of $\mathbf{p}_0$ plays no role in uniform media). The external parameters are implied to be the average number density $\rho=N/V$ and the temperature θ in units of energy ($\theta=k_BT$). The parameter A is expressed in terms of ρ_c by (3.8) with $\rho_n=\rho-\rho_c$. Instead of ρ_c we shall use $f_c=\rho_c/\rho$ while instead of τ it is more convenient to employ $\tilde{\tau}=\rho_n\tau/\rho=(1-f_c)\tau$.

If there is a superflow characterized by the vector $\mathbf{p}_0$ the system cannot be isotropic. We assume an axial symmetry with the z axis oriented along $\mathbf{p}_0$, so that $g(\mathbf{r})=g(r_\perp,z)$ where $r_\perp=\sqrt{x^2+y^2}$ (by r is meant $|\mathbf{r}|$). It turns out that all thermodynamic quantities can, instead of $g(r_\perp,z)$, be expressed in terms of two spherically symmetric functions (we presume that the interaction potential $K(|\mathbf{r}|)$ is spherically symmetric), namely,

$$\overline{g}(r)=\frac{1}{r}\int_0^r g(\sqrt{r^2-z^2},z)dz,\quad \tilde{g}(r)=\frac{3}{r^3}\int_0^r g(\sqrt{r^2-z^2},z)z^2dz. \tag{3.11}$$

It will be noted that in the case of a spherical symmetry

$$\overline{g}(r)=\tilde{g}(r)=g(r). \tag{3.12}$$

The parameters p_0, $\tilde{\tau}$, and f_c can be found from the following equations:

$$f_c p_0^2=\pi m\rho\int_0^{\infty}r^3\frac{dK}{dr}[\tilde{g}(r)-\overline{g}(r)]dr, \tag{3.13}$$

$$2\theta\frac{\partial\tilde{\tau}}{\partial\theta}+3\rho\frac{\partial\tilde{\tau}}{\partial\rho}-2\tilde{\tau}=\frac{\pi\rho}{3}\int_0^\infty dr r^2\left\{K(r)\left[3(\tilde{g}-\overline{g})-12\rho\frac{\partial\overline{g}}{\partial\rho}+r\left(3\frac{\partial\overline{g}}{\partial r}+\frac{\partial\tilde{g}}{\partial r}\right)\right]\right.$$
$$\left.+r\frac{dK}{dr}\left[2\theta\left(3\frac{\partial\overline{g}}{\partial\theta}-\frac{\partial\tilde{g}}{\partial\theta}\right)+3\rho\left(\frac{\partial\overline{g}}{\partial\rho}-\frac{\partial\tilde{g}}{\partial\rho}\right)\right]\right\}, \tag{3.14}$$

$$\frac{\partial}{\partial f_c}\int_0^\infty r^2\left(2K+r\frac{dK}{dr}\right)\overline{g}(r,\tilde{\tau},f_c,p_0,\rho)dr=0. \tag{3.15}$$

When writing down (3.15) we assumed that $g(\mathbf{r})$ as given by (3.9) does not depend explicitly upon θ while depending on other parameters.

Equation (3.15) plays another important role as well, namely, it yields a line in the ρ-θ plane where a solution relevant to the condensate phase bifurcates off the high-temperature solution. This line represents a phase transition line if the transition is second order. To obtain the equation of the line, in Eq. (3.15) one should put $f_c=0$, $\overline{g}(r)=g(r)$ and $\tilde{\tau}=\tau(\theta,\rho)$ with $\tau(\theta,\rho)$ relevant to the high-temperature phase and given by equations of I. The equality $\tilde{\tau}=\tau(\theta,\rho)$ on the line serves also as boundary condition for Eq. (3.14).

Having solved Eqs. (3.13)–(3.15) one may compute the internal energy E by

$$E=\frac{3}{2}\tilde{\tau}N+2\pi N\rho\int_0^\infty r^2K(r)\overline{g}(r)dr+\frac{\pi}{2}N\rho\int_0^\infty r^3\frac{dK}{dr}[\tilde{g}(r)-\overline{g}(r)]dr. \tag{3.16}$$

The pressure p that is isotropic although there is a flow in the superfluid is given by

$$p=\rho\tilde{\tau}-\frac{\pi\rho^2}{3}\int_0^\infty r^3\frac{dK}{dr}[3\overline{g}(r)-\tilde{g}(r)]dr. \tag{3.17}$$

With $E(\theta,\rho)$ and $p(\theta,\rho)$ at our disposal we can calculate the Helmholtz free energy F with the help of a formula of Appendix B of I and thereupon all thermodynamic quantities.

It should be observed that in the condensate phase the quantity τ plays a secondary part insofar as the function $n(z)$ of (2.18) characterizes now only a part of the particles. The role of τ goes over to $\tilde{\tau}$, which can be seen by comparing (3.16) and (3.17) with (I.3.7) especially when (3.12) holds.

In summary, we see that the equations for density matrices of Sec. II and the equations of the present section permit one to attain a full structural and thermodynamic description of a superfluid Fermi systems, and one has no need of resorting to any extra ideas or argumentation besides those formulated initially in Refs. 2 and 3.

IV. HARD SPHERES UNDER THE NEGLECT OF TRIPLET CORRELATIONS

A. General consideration

In the present section we are coming to an example that illustrates how the general equations derived in the preceding sections can be handled in order to produce concrete physical results. We shall consider a system of hard spheres in which triplet correlations are neglected, the same example being used in paper I as well as in Refs. 2 and 3

In the case of hard spheres

$$K(r)=\begin{cases}\infty & \text{if } r<a\\ 0 & \text{if } r>a.\end{cases} \tag{4.1}$$

If the triplet correlations are disregarded then $U_2(r)=K(r)$ according to I, which drastically simplifies the matter of finding $g(r)$ by (3.10) and of solving Eqs. (3.13)–(3.15).

Before proceeding further a word should be said in this connection. When discussing the conditions of (2.27) and (2.28) we emphasized the specific nature of correlations necessary for the conditions to be feasible, in particular if $s=3$. For this reason, if triplet correlations are negligible the condensate phase could not exist. At the same time when studying the thermodynamics of a hard-sphere system the neglect of triplet correlations may prove to be not a bad approximation even for a condensate phase. The reason lies in the fact that from Eqs. (3.13)–(3.17) it follows that all thermodynamic quantities are determined by integrals of the type

$$I=\int_0^\infty r^n\tilde{K}(r)G(r)dr, \tag{4.2}$$

where $\tilde{K}(r)=K(r)$ or dK/dr, and $G(r)$ depends on $g(r)$ and its derivatives [below we consider the case in which (3.12) holds]. For the hard-sphere potential of (4.1) one has $\tilde{K}(r)\equiv 0$ if $r>a$ and $G(r)\equiv 0$ if $r<a$. Consequently in this instance, only values of the functions at $r=a$ contribute to the integral of (4.2). When two hard spheres come in contact, locations of other hard spheres are of little importance to the two spheres. For this reason the contact value $g(a)$ of the pair correlation function should not depend appreciably upon triplet correlations. This is corroborated by the fact that different quantities calculated in paper I and Ref. 2 upon neglecting the triplet correlations coincide rather well with the ones computed by other authors without disregarding these correlations.

Below we shall find $g(r)$ upon discarding the triplet correlations, with the intention of using solely the contact value $g(a)$. Of course, without special investigation one cannot wholly rely upon all results so obtained: some of them might be rather qualitative than quantitative. In particular, one cannot pass to the limit $a\to 0$ in the formulas deduced below inasmuch as the value $a=0$ corresponds to an ideal gas while the condensate phase cannot exist in an ideal Fermi gas (see Sec. II C).

If $U_2(r)=K(r)$ with $K(r)$ given by (4.1), Eq. (3.6) has a unique solution

$$u_2(r)=1-\frac{a}{r}, \tag{4.3}$$

subject to two conditions, namely, $u_2(a)=0$ and $u_2(r)\to 1$ as $r\to\infty$.

In the approximation used $U_2(\mathbf{r})$ does not depend on $u_2(\mathbf{r})$, hence the second term in (3.10) will differ from (I.5.1) only because of the value of A given now by (3.8). Upon denoting the right-hand side of (I.5.1) with A from (I.3.6) by $g_{\mathrm{I}}(r)$ we are led to

$$g(r)=1-\frac{2af_c}{r}\left(1-\frac{a}{2r}\right)+(1-f_c)[g_{\mathrm{I}}(r)-1]. \tag{4.4}$$

This function corresponds to a spherical symmetry, which entails $p_0=0$ on account of (3.12) and (3.13). Consequently, in the case considered in the present section we shall have a condensate phase without superfluidity just as in the analogous case of bosons treated in Ref. 3. It should be emphasized, however, that this result does nowise amount to saying that the hard-sphere condensate phase is necessarily nonsuperfluid. The result merely signifies that the exact value of p_0 cannot be found if the triplet correlations are disregarded. We note in passing that Eq. (4.4) shows that if $f_c\neq 0$ the decay of spatial correlations is slow as $r\to\infty$, they decay proportionally to $1/r$. Therefore, the condensate phase is characterized by long-range correlations.

We calculate now the integrals entering into Eqs. (3.13)–(3.17) implying (3.12). Upon denoting the first term of (3.10) as $g_c(r)$, in Appendix B it is shown that in the case of the potential of (4.1) and of any continuous function $f(r)$ one has

$$\int_0^\infty f(r)K(r)\frac{\partial g_c}{\partial r}dr=\frac{\rho_c\hbar^2 f(a)}{\rho m a^2}. \tag{4.5}$$

A similar integral in which g_c is replaced by the second term of (3.10) may be calculated like (I.5.2). As a result, integrating by parts we obtain for spin-half fermions

$$\int_0^\infty r^3 g(r)\frac{dK}{dr}dr=-\frac{a\hbar^2}{m}[f_c+(1-f_c)H_2(\overline{\tau})], \tag{4.6}$$

with $\overline{\tau}=a^2m\tau/\hbar^2$ and $H_2(\xi)$ defined in (I.5.6). When integrating by parts we used the fact that in the present case, as can be shown analogously with (I.5.2) and (4.5), one has

$$\int_0^\infty r^2 g(r)K(r)dr=0. \tag{4.7}$$

All of these and (3.12) allow Eq. (3.14) to be reduced to the form

$$2\theta\frac{\partial\tilde{\tau}}{\partial\theta}+3\rho\frac{\partial\tilde{\tau}}{\partial\rho}-2\tilde{\tau}=\frac{4\pi a\hbar^2\rho}{3m}\left\{f_c+(1-f_c)H_2(\overline{\tau})-\frac{a^2m\theta}{\hbar^2}H_2'(\overline{\tau})\frac{\partial\tilde{\tau}}{\partial\theta}\right.$$
$$\left.-[1-H_2(\overline{\tau})+\overline{\tau}H_2'(\overline{\tau})]\theta\frac{\partial f_c}{\partial\theta}\right\}, \tag{4.8}$$

where the prime over $H_2'(\overline{\tau})$ denotes differentiation with respect to the argument. The noteworthy is the fact that (4.8) is akin to Eq. (5.3) of Ref. 3. The internal energy E and the pressure p may be calculated by (3.16) and (3.17) with the help of (4.5) and (4.6), so that

$$E=\frac{3}{2}\tilde{\tau}N,\quad p=\rho\tilde{\tau}+\frac{2\pi a\hbar^2}{3m}\rho^2[f_c+(1-f_c)H_2(\overline{\tau})]. \tag{4.9}$$

The quantity $\overline{\tau}$ that figures in (4.8) and (4.9) can be expressed in terms of the parameters $\tilde{\tau}$ and f_c defined in Sec. III:

$$\overline{\tau}=\frac{a^2m\tilde{\tau}}{\hbar^2(1-f_c)}. \tag{4.10}$$

B. Phase transition

Having established general formulas for a hard-sphere system with condensate let us elucidate now the question as to whether a solution with $f_c>0$ can branch off the high-temperature (normal) solution considered in Sec. V of I, i.e., whether a phase transition to the condensate phase is possible. To this end one has to examine Eq. (3.15) following a remark in Sec. III. Substituting Eqs. (4.6), (4.7), and (4.10) reduces Eq. (3.15) to the form

$$H_2(\overline{\tau})-1-\overline{\tau}H_2'(\overline{\tau})=0. \tag{4.11}$$

According to (I.5.5) the function $f(\xi)=H_2(\xi)-1-\xi H_2'(\xi)$ is positive if $\xi\to\infty$, while $f(\xi)<0$ at $\xi=0$ with regard to (I.5.7). Therefore, the equation $f(\xi)=0$ has at least one solution. A numerical calculation shows that the equation has a unique solution which is $\xi=\xi_0\equiv 0.395\,628\,3$. Now Eq. (4.11) amounts to $\overline{\tau}=\xi_0$. Recall that in the case of spinless bosons Eq. (5.4) of Ref. 3 identical with (4.11) had no solution, and thereupon the condensate phase emerged at another point. According to Appendix C in the condensate phase under study $(\partial p/\partial V)_\theta<0$. Therefore, the condensate phase is stable and the bifurcation line is a second-order phase transitions line [a first-order transition implies the existence of a region where $(\partial p/\partial V)_\theta>0$: see, e.g., the solid curve in Fig. 1 of Ref. 3; a van der Waals isotherm serves as another example].

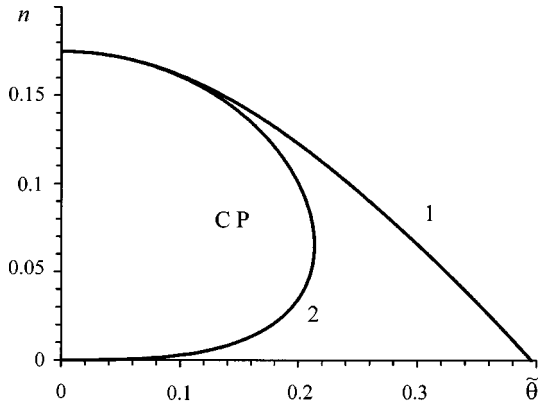

FIG. 1. Line of phase transitions to the condensate phase (CP) in the phase diagram: $\tilde{\theta}=a^2m\theta/\hbar^2$, $n=\pi a^3\rho$. Curve 1 corresponds to Eqs. (4.12) and (4.13), curve 2 corresponds to the approximate equation of (4.15).

In order to find the equation of that line it is necessary to insert the value of $\overline{\tau}$ relevant to the normal phase into Eq. (4.11), that is, into the equation $\overline{\tau}=\xi_0$. We shall consider the normal phase in the approximation corresponding to (I.5.21), which is equivalent to using the well-known method of pseudopotentials. Then

$$\tau=\tau_{\mathrm{id}}+\frac{2\pi a\hbar^2\rho}{3m}, \tag{4.12}$$

where τ_{id} is given by (I.3.10) with $\kappa=2$, that is to say, by

$$\tau_{\mathrm{id}}=\frac{2}{3}\left(\frac{\rho}{2\omega}\right)^{2/3}\frac{G_1(\alpha)}{G_0^{5/3}(\alpha)}, \quad \rho=2\omega\theta^{3/2}G_0(\alpha), \tag{4.13}$$

with α playing the role of a parameter.

After placing (4.12) and (4.13) in the equation $\overline{\tau}=\xi_0$ that amounts to $\tau=\xi_0\hbar^2/a^2m$ we obtain the phase transition line represented by curve 1 in Fig. 1 upon having recourse to numerical calculation. Note that $\tau_{\mathrm{id}}=\theta$ when $\rho=0$ according to (4.13), and thereby at $n=0$ the line terminates at $\tilde{\theta}=\xi_0$. It should be pointed out that if $a\to 0$, that is, if $n\to 0$ we arrive at an ideal gas. At the outset of this section we mentioned that the condensate phase could not occur in an ideal gas. Consequently, one should view the small values of n in Fig. 1 with caution. On the other hand Fig. 1 indicates that the condensate phase in a hard-sphere fermionic system will be observed only if values of n are not too large.

Insofar as the temperatures are supposed to be low, one may use the expansion (I.5.19) instead of the rather complex (4.12) and (4.13). The approximation of (4.12) corresponds to retaining corrections of order $n^{1/3}$, so that in the same approximation by (I.5.19) one has

$$\tau=\frac{2}{5}\left(\frac{3\rho}{4\omega}\right)^{2/3}+\frac{\pi^2\theta^2}{6}\left(\frac{4\omega}{3\rho}\right)^{2/3}+\frac{2\pi a\hbar^2\rho}{3m}. \tag{4.14}$$

In this case one can obtain the equation of the phase transition line in explicit form by equating (4.14) and $\xi_0\hbar^2/a^2m$. In the notation of Fig. 1 this gives

$$\tilde{\theta}=\sqrt{3}\left(\frac{3n}{\pi^2}\right)^{1/3}\sqrt{\xi_0-\frac{1}{5}(3\pi n)^{2/3}-\frac{2}{3}n}. \tag{4.15}$$

The line corresponding to this equation is presented in Fig. 1 by curve 2. At large n curves 1 and 2 are close to each other, however at small n they diverge drastically. This is due to the fact

that the expansion of (I.5.19) fails for small ρ because it is an expansion in powers of θ/ε_0 whereas $\varepsilon_0 \propto \rho^{2/3}$. At the same time curve 2 may reflect the real physical picture better since the curve shows that the condensate phase does not exist if n is too small. However, it is not clear without special analysis whether the use of (4.14) yields all quantities correctly for any ρ and θ.

C. Properties of the condensate phase

Let us turn now to investigation of the condensate phase. In the condensate phase Eq. (4.11) provides a relationship between $\tilde{\tau}$ and f_c according to Sec. III. As (4.11) signifies that $\overline{\tau}=\xi_0$, thanks to (4.10) we have

$$f_c = 1 - \frac{a^2 m \tilde{\tau}}{\xi_0 \hbar^2}. \tag{4.16}$$

Transforming Eq. (4.8) for $\tilde{\tau}$ we note that in the case under study the functions $H_2(\overline{\tau})$ and $H_2'(\overline{\tau})$ are merely constants, which will be denoted as

$$h_2^{(0)} = H_2(\xi_0) = 2.089\,748, \quad h_2 = H_2'(\xi_0) = 2.754\,475. \tag{4.17}$$

Substituting (4.16) and (4.17) into (4.8) yields

$$2\theta\left(1+\frac{2}{3}\pi h_2 a^3 \rho\right)\frac{\partial \tilde{\tau}}{\partial \theta} + 3\rho \frac{\partial \tilde{\tau}}{\partial \rho} - 2\left(1+\frac{2}{3}\pi h_2 a^3 \rho\right)\tilde{\tau} = \frac{4\pi a \hbar^2 \rho}{3m}, \tag{4.18}$$

where we have used the relation $h_2^{(0)} = 1 + \xi_0 h_2$ following from (4.11). We met with equations of the type (4.18) more than once in paper I and Ref. 2 and solved them with the help of the method of characteristics. So, the general solution of (4.18) is

$$\tilde{\tau} = \rho^{2/3} \exp\left(\frac{4}{9}\pi h_2 a^3 \rho\right)\left\{\Phi\left[\frac{\theta}{\rho^{2/3}} \exp\left(-\frac{4}{9}\pi h_2 a^3 \rho\right)\right] + \frac{4\pi\hbar^2}{3m h_2^{1/3}} \nu[a(h_2\rho)^{1/3}]\right\}, \tag{4.19}$$

where $\Phi(x)$ is an arbitrary function and

$$\nu(x) = \int_0^x \exp\left(-\frac{4}{9}\pi \xi^3\right) d\xi. \tag{4.20}$$

The last integral can be calculated analytically in the limits as $x \to 0$ and $x \to \infty$.

In order to find $\Phi(x)$ we must, according to a note in Sec. III about the boundary condition to Eq. (3.14), equate (4.19) and (4.12) on the phase transition line, that is, on curve 1 of Fig. 1. As a result we get the following equations for $\tilde{\tau}(\theta, \rho)$:

$$\tilde{\tau} = \frac{\hbar^2}{m} \rho^{2/3} \exp\left(\frac{4}{9}\pi h_2 a^3 \rho\right)\left\{\frac{\xi_0}{y^2} \exp\left(-\frac{4}{9}\pi h_2 y^3\right) + \frac{4\pi}{3 h_2^{1/3}}[\nu(a h_2^{1/3} \rho^{1/3}) - \nu(h_2^{1/3} y)]\right\}, \tag{4.21}$$

$$2\pi y^3 + \frac{(2\pi^2)^{2/3} G_1(a)}{G_0^{5/3}(\alpha)} y^2 - 3\xi_0 = 0, \tag{4.22}$$

$$\theta = \frac{\hbar^2}{m}\left[\frac{\pi^2 \rho}{\sqrt{2} G_0(\alpha)}\right]^{2/3} \exp\left[\frac{4}{9}\pi h_2 (a^3\rho - y^3)\right]. \tag{4.23}$$

These equations determine the dependence of $\tilde{\tau}$ on θ and ρ via two parameters α and y. For given θ and ρ we solve (4.22) and (4.23) for y upon eliminating α, whereupon we find $\tilde{\tau}$ by (4.21). The parameter α varies from $-\infty$ to $+\infty$ while the parameter y changes from 0 (this is the line n

$=0$) to $y_0=0.381\,814\,7$ (this is the line $\tilde{\theta}=0$). On the phase transition line $y=a\rho^{1/3}$, so that (4.21) yields $\tilde{\tau}=\xi_0\hbar^2/a^2m$, as it should. It is convenient to organize real calculation as follows. For a given α one finds y by solving the cubic equation of (4.22) (one is to choose the positive root that exists always and is unique). Taking a value of ρ one computes θ by (4.23) and moreover the relevant value of $\tilde{\tau}$ by (4.21).

If one proceeds on (4.14) the $\tilde{\tau}(\theta,\rho)$ dependence is given by the two equations

$$\tilde{\tau}=\frac{\hbar^2}{m}\left\{\rho^{2/3}\left[\frac{1}{5}(3\pi^2)^{2/3}+\frac{\pi^{2/3}m^2\theta^2}{3\hbar^4(3\rho^2)^{2/3}}-\frac{2}{3}\pi y\right]+\frac{4\pi a\rho}{3}\right\}, \tag{4.24}$$

$$2\pi y^3+\left[\frac{3}{5}(3\pi^2)^{2/3}+\frac{\pi^{2/3}m^2\theta^2}{\hbar^4(3\rho^2)^{2/3}}\right]y^2-3\xi_0=0. \tag{4.25}$$

Here one has only one parameter y that varies within the same limits as above. In principle, upon solving the cubic equation of (4.25) for y and substituting the result into (4.24) one could obtain the function $\tilde{\tau}(\theta,\rho)$ in explicit form; however, the formula will be fairly complex. Since Eqs. (4.24) and (4.25) do not much simplify the matter, in the following we carry out our investigation on the basis of Eqs. (4.21)–(4.23) that are more exact.

The properties of the function $\tilde{\tau}(\theta,\rho)$ as given by (4.21)–(4.23) are considered in Appendix C. As mentioned above, $\tilde{\tau}=\xi_0\hbar^2/a^2m$ on the phase transition line. Then Eq. (4.16) gives $f_c=0$ as it should. In Appendix C it is shown that $\partial\tilde{\tau}/\partial\theta>0$, and thereupon f_c increases with decreasing temperature. At $\theta=0$ one has $\tilde{\tau}>0$, and therefore, f_c never reaches the value $f_c=1$ (except the case $\rho=0$). The value of $\tilde{\tau}$ at $\theta=0$ can be found by (4.21) and (4.22) upon putting $\alpha=+\infty$. Then (4.22) entails $y=y_0$ [see the discussion following (4.23)] while (4.21) gives the desired value of $\tilde{\tau}$. Now Eq. (4.16) yields the value of f_c at $\theta=0$. This last value changes from 0 at the point where curve 1 of Fig. 1 intersects the n axis, to 1 at the point $n=\tilde{\theta}=0$.

Let us consider the heat capacity $C_V=(\partial E/\partial\theta)_\rho$. The internal energy E is given in (4.9), so that $C_V=\frac{3}{2}N\partial\tilde{\tau}/\partial\theta$. As mentioned above $\partial\tilde{\tau}/\partial\theta>0$, therefore, $C_V>0$ as it should. We may calculate the heat-capacity jump in the phase transition

$$\Delta C_V=C_V^{(c)}-C_V^{(n)}, \tag{4.26}$$

where $C_V^{(c)}$ and $C_V^{(n)}$ are the heat capacities of the condensate and normal phases, respectively, at the phase transition point. Calculation with the use of (4.21)–(4.23) and (4.12) (in the normal phase $E=\frac{3}{2}\tau N$), and of (C2) as well, yields rather a complicated formula, namely,

$$\Delta C_V=\frac{a\rho^{1/3}GN[(1+4\pi h_2a^3\rho/3)G_0^{5/3}+h_2a^2(2\pi^2\rho)^{2/3}(3G_0^2/G_{-1}-G_1)]}{2G_0G_{-1}[(4\pi)^{1/3}G_1+3a\rho^{1/3}G_0^{5/3}+(2\pi^2)^{2/3}h_2a^3\rho G/3G_{-1}]}, \tag{4.27}$$

with $G=G(\alpha)$ defined in Appendix C. Here the parameter α is determined by Eq. (4.23) with $y=a^3\rho$, which then coincides with the second equation of (4.13). Since $G>0$ and $3G_0^2-G_1G_{-1}>0$ (for the Fermi case), from (4.27) one has $\Delta C_V>0$, which corresponds with the Landau theory of phase transitions. The results of numerical calculations of C_V for two values of $n=\pi a^3\rho$ are shown in Fig. 2. We see that the transition from the normal to the condensate phase possesses all properties of an ordinary second-order phase transition.

We cannot compare the results obtained with experimental data on liquid ^{3}He because for liquid ^{3}He $n=0.83$ (see Ref. 2) whereas the hard-sphere condensate phase wherein triplet correlations are negligible can exist only if $n\leqslant 0.1749$ according to Fig. 1. When n is great the role of the triplet correlations becomes essential and the results of this section cannot be applied. Nevertheless it is of interest to estimate the real temperatures that correspond to the phase diagram of Fig. 1. If we take $a=2.56$ Å characteristic of helium[2] the temperature expressed in kelvins will be

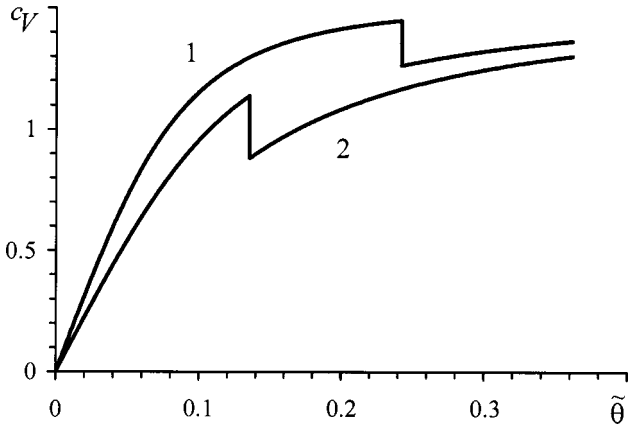

FIG. 2. Temperature dependence of the heat capacity $c_V = C_V/N$ for different values of n. Curve 1: $n = 0.1$, curve 2: $n = 0.15$. The jump of c_V corresponds to the phase transition. The notation is the same as in Fig. 1.

$$T = \frac{\hbar^2}{k_B m a^2}\tilde{\theta} = 2.454\tilde{\theta},$$

where k_B is the Boltzmann constant and the ^{3}He atom mass is taken for m. Consequently the maximum temperature for curve 1 of Fig. 1 ($\tilde{\theta} = 0.3956$) is $T = 0.971$ K, and for curve 2 ($\tilde{\theta} = 0.2136$) it is $T = 0.524$ K. These temperatures far exceed those at which superfluid phases in liquid ^{3}He are observed. Low densities, i.e., small n, when the triplet correlations can be neglected are characteristic of a vapor state. Perhaps the vapor state of ^{3}He would pass into a condensate phase at temperatures close to the ones obtained above.

Concluding the section let us compare the boson and fermion condensate phases [implying the potential $U_2(r)$ considered in the section]. In the boson case[3] the transformation into the condensate phase is a first-order phase transition, the condensate fraction f_c reaches unity even when $\theta \neq 0$, properties of the condensate phase are strongly affected by details of the correlations (in order to find completely E and p for the phase even in a first approximation it is necessary to know the exact value of τ in the normal phase). In the fermion case the transformation into the condensate phase is a second-order phase transition, the condensate fraction f_c never reaches unity even at $\theta = 0$, properties of the condensate phase are not very sensitive to details of the correlations [we were able to find completely the expression for $\tilde{\tau}$ by confining ourselves to the terms written down in (4.12), which amounts to saying that the influence of higher powers of a is alike in the normal and condensate phases]. We see that the properties of the boson and fermion condensate phases differ appreciably even though the interparticle potential is the same.

V. CONCLUDING REMARKS

The present paper shows that the approach proposed in Ref. 2 and extended in paper I in order to take the spin of particles into account enables one to investigate the condensate phase in Fermi systems and superfluidity of these systems, the treatment of the fermionic superfluid being in principle the same as that of a bosonic superfluid. The present theory does not resort to Cooper's idea of fermion pairing although there are some elements of pair formation in the theory but the phenomenon as a whole is rather intricate (see Sec. II C). If one reasons in terms of pairing the present theory indicates at once that, besides the well known mechanism of pairing connected with an electron–phonon interaction and other known mechanisms,[6] a completely different mechanism is possible which acts even in the case of a purely repulsive Hamiltonian. This last mechanism is due to a specific collective effect, namely the shielding effect, and can be efficacious at any temperature whatsoever the Hamiltonian is.

The physical causes of fermion superfluidity and possible peculiarities of the phenomenon are wholly analogous with the ones of boson superfluidity discussed in Ref. 3. At the same time, even if a boson system and a fermion one are described by one and the same Hamiltonian the character of the phase transition to the condensate phase and the properties of this last phase may differ appreciably for the two systems.

The study of fermion superfluidity is an essential step towards a theory of such an important phenomenon as superconductivity, based upon the ideas of the present approach. In the theory, account must be taken of the fact that metals have a crystalline structure whereas only spatially uniform systems were considered in the present paper. Note that some results concerning the study of a crystal on the basis of the approach proposed in Ref. 2 are already published.[15]

Of even greater importance is the fact that a superflow of charged particles is an electrical current, and thereby it always creates a magnetic field. Consequently in order to study superconductivity it is necessary to incorporate electromagnetic interactions in the framework of the present approach. Inasmuch as the quantum hierarchy for reduced density matrices the present approach is based upon is, to a considerable extent, analogous with the classical BBGKY hierarchy[2] one may treat the electromagnetic interactions leaning upon this analogy and resorting, for example, to methods of the theory of plasmas where the classical BBGKY hierarchy is widely employed for charged particle systems.

However, some considerations may be expressed even now as to the influence of the magnetic field upon the phenomena in question. In Ref. 3 it was mentioned that formation of cells with closed superflows in a confined volume would most likely be energetically unprofitable. If, however, the superflow is created by charged particles there appears a magnetic field. For this reason the formation of a pattern of closed streamlines with opposite currents in different cells will be energetically favourable because, owing to this, the magnetic field and thereupon the magnetic energy of the system might decrease just as in the case of a ferromagnet when magnetic domains form.

Reasoning along these lines one can offer a simple explanation for the Meissner effect (a magnetic field does not penetrate into the bulk of a superconductor). An external magnetic field, by acting on the supercurrents in the cells, reconstructs the pattern until the resultant magnetic field within the body (the external field plus that due to the supercurrents) vanishes. This is analogous to the case of a conductor in equilibrium into the interior of which an electrostatic field cannot penetrate. One may also draw a parallel between the action of the magnetic field on the supercurrents and on the ''molecular currents'' in a diamagnetic molecule; inasmuch as the direction of the supercurrent can be arbitrary the superconductior is a perfect diamagnetic while in the molecule the molecular currents are fixed by the structure of the molecule. Of course a full explanation of the Meissner effect and of its peculiarities requires an analysis of the above hierarchy with account taken of electromagnetic interactions.

It is also worth noting that, by analogy with the existence of a critical velocity in Bose systems, there should be a critical supercurrent in charged Fermi systems. When the supercurrent exceeds the critical value, fermion superfluidity (i.e., superconductivity in this instance) breaks down. The value of the critical supercurrent is determined by a formula analogous with (3.13) (cf. Ref. 3).

APPENDIX A: THE CONDITION OF (2.17) ON THE FUNCTIONS $n_s(z)$

In Ref. 2 and paper I the relation of (2.17) was discussed rather briefly. For this reason we consider the relation first for the nondegenerate case, i.e., for the case in which there is no condensate, in more detail.

First of all we find the constant $C_s^{s_a,s_b}$ that figures in Eq. (2.14). If one normalizes R_{s_a} and R_{s_b} in the same manner as R_s, that is, according to (I.2.2) then

$$C_s^{s_a,s_b}=\frac{N!(N_a-s_a)!(N_b-s_b)!}{(N-s)!N_a!N_b!}, \tag{A1}$$

where N_a and N_b are the number of particles in the subsystems A and B, respectively ($N=N_a+N_b$). Equation (A1) can be readily got by integrating (2.14) and applying (I.2.3) to both the sides.

Upon introducing a coefficient of proportionality we rewrite (2.17) as

$$n_s(\varepsilon_{\nu_a}^{(s_a)}+\varepsilon_{\nu_b}^{(s_b)})=B_s^{s_a,s_b}n_{s_b}(\varepsilon_{\nu_a}^{(s_a)})n_{s_b}(\varepsilon_{\nu_b}^{(s_b)}). \tag{A2}$$

In order to find the coefficient $B_s^{s_a,s_b}$ we remark first that to one eigenvalue $\varepsilon_\nu^{(s)}$ of Eq. (I.2.11) correspond $s!$ eigenfunctions $\psi_\nu(\mathbf{x}_s)$ obtained by permutation of s arguments. This degeneracy must be taken into account when one substitutes expressions of the type (2.1) together with (A1) and (A2) into (2.14). To make the number of terms on the left of Eq. (2.14) equal to the one on the right the left side of (2.14) is to be divided by $s!$ and the right side by $s_a!\ s_b!$, so that

$$B_s^{s_a,s_b}=\frac{s!}{s_a!s_b!}C_s^{s_a,s_b}=\frac{\mu_s}{\mu_{s_a}\mu_{s_b}} \quad \text{with} \quad \mu_s=\frac{s!N!}{(N-s)!}\approx s!N^s. \tag{A3}$$

When writing the last expression for μ_s account is taken of the fact that $s\ll N$.

To solve the functional equation of (A2) we denote $\varepsilon_{\nu_a}^{(s_a)}$ by x and $\varepsilon_{\nu_b}^{(s_b)}$ by y, take the logarithm of both the sides and differentiate with respect to x:

$$\frac{1}{n_s(x+y)}\frac{dn_s(x+y)}{d(x+y)}=\frac{1}{n_{s_a}(x)}\frac{dn_{s_a}(x)}{dx}.$$

The right-hand side does not depend on y, hence the left-hand side cannot depend on y either, that is to say, upon $x+y=z$. Therefore,

$$\frac{1}{n_s(z)}\frac{dn_s(z)}{dz}=\text{const.} \tag{A4}$$

Denoting this last constant by $-1/\tau$ and integrating Eq. (A4) yields

$$n_s(z)=A_s e^{-z/\tau}. \tag{A5}$$

To determine the constant A_s we place (A5) into (A2), which gives on account of (A3)

$$\frac{A_s}{\mu_s}=\frac{A_{s_a}}{\mu_{s_a}}\frac{A_{s_b}}{\mu_{s_b}}. \tag{A6}$$

If one writes the indices as arguments and recalls that $s=s_a+s_b$ one will see that Eq. (A6) is identical with Eq. (A2) on condition that one sets $B_s^{s_a,s_b}=1$. Therefore, for A_s/μ_s one will have an expression of the type (A5) with $A_s=1$ and a new constant D instead of $e^{-1/\tau}$, which amounts to saying that $A_s=\mu_s D^s$. Upon substituting this into (A5), using the approximate expression for μ_s of (A3) and introducing a new constant $\zeta=ND$ one has finally

$$n_s(z)=s!\zeta^s e^{-z/\tau}. \tag{A7}$$

The constant ζ can be found by placing (A7) into (I.2.29) with the result that

$$\zeta=\frac{\rho}{\kappa}\left(\frac{2\pi\hbar^2}{m\tau}\right)^{3/2}. \tag{A8}$$

If in paper I one inserts A of (I.3.6) into (I.2.30) one will obtain an expression for $n_s(z)$ that wholly coincides with the one given by (A7) and (A8). This shows that in the nondegenerate case in order to determine the functions $n_s(z)$ uniquely one need not resort to the normalization condition of (I.2.6) that has led to (I.3.6).

We turn now to the degenerate case, that is, to the case in which there is a condensate. First of all it will be noted that the functions $n_s(z)$ satisfy a normalization condition which follows from (2.1) if use is made of (I.2.3):

$$\sum_{\nu} n_s(\varepsilon_{\nu}^{(s)}) = \frac{N!}{(N-s)!}, \tag{A9}$$

where we imply that $\Psi_{\nu\Gamma_s}(\mathbf{X}_s)$'s are normalized to unity. If we assume that $n_s(\varepsilon_{\nu_0}^{(s)}) = \Delta n_s + n_s(z_0)$ as at the outset of Sec. II, the normalization of the continuous part of $n_s(z)$ changes according to (A9). As long as the quantities Δn_s are not known in advance we have no prior knowledge of the new normalization of $n_s(z)$ in (2.4). However, the remark following (2.22) suggests that there is only one parameter, namely ρ_c, that determines the normalization of functions relevant to the condensate fraction because the vector $\mathbf{p}_0$ does not affect the normalization. Therefore the functions $n_s(z)$ contain only one unknown factor as well and Eq. (A2) should be recast as

$$n_s(\varepsilon_{\nu_a}^{(s_a)} + \varepsilon_{\nu_b}^{(s_b)}) = B \;\; B_s^{s_a,s_b} n_{s_a}(\varepsilon_{\nu_a}^{(s_a)}) n_{s_b}(\varepsilon_{\nu_b}^{(s_b)}), \tag{A10}$$

with an unknown coefficient B.

Now we shall arrive again at (A5) but A_s will contain an extra factor, owing to B, that cannot be determined from (I.2.29) because any constant factor in $n_s(z)$ cancels out when $n_s(z)$ is substituted into (I.2.29). Instead of (A7) and (A8), in the degenerate case Eq. (I.2.29) yields (2.18) with a constant A that should be found otherwise. In Sec. III A is calculated from the normalization condition of (I.2.6).

APPENDIX B: DERIVATION OF EQ. (4.5)

Instead of (4.1) we assume the potential

$$K(r) = \begin{cases} K_m & \text{if } r < a \\ 0 & \text{if } r > a. \end{cases} \tag{B1}$$

We consider spherically symmetric solutions. Upon putting $U_2(r) = K(r)$ in (3.6) and writing $u_2(r) = \chi(r)/r$ we get

$$\frac{d^2\chi}{dr^2} - \frac{m}{\hbar^2} K(r)\chi(r) = 0. \tag{B2}$$

Since $u_2 \to 1$ as $r \to \infty$, this equation yields for $r > a$

$$u_2(r) = 1 - \frac{C_1}{r}. \tag{B3}$$

If $r < a$, (B2) leads to the following expression for $u_2(r)$ finite at $r = 0$:

$$u_2(r) = \frac{C_2}{r} \sinh br, \quad b^2 = \frac{m}{\hbar^2} K_m. \tag{B4}$$

As usual the constants C_1 and C_2 are specified by the condition that $u_2(r)$ and its derivative shall be continuous at $r = a$. As a result, when $r < a$

$$u_2(r)=\frac{\sinh br}{br\cosh ba}. \tag{B5}$$

We consider now an integral of the form

$$\int_0^\infty f(r)K(r)\frac{\partial g_c}{\partial r}dr=K_m\frac{\rho_c}{\rho}\int_0^a f(r)\frac{du_2^2}{dr}dr \tag{B6}$$

with an arbitrary function $f(r)$ assumed to be continuous. On the right we have made use of (B1) and replaced $g_c(r)$ by the first term of (3.9). From (B5) it follows that if $r<a$ the function $u_2(r)$ is exponentially small when $b\to\infty$. For this reason only the value of $f(r)$ at $r=a$ is of importance for the integral in (B6). Upon putting $f(r)=f(a)$ the integral is easily evaluated and leads to (4.5) in the limit as $K_m\to\infty$.

APPENDIX C: THE FUNCTION $\tilde{\tau}(\theta,\rho)$ OF (4.21)–(4.23)

If one regards y as a function of θ and ρ, from (4.22) and (4.23) one gets, on account of formulas presented in Appendix F of Ref. 2,

$$\left[6G_1+9\left(\frac{2}{\pi}G_0^5\right)^{1/3}y+2\pi h_2y^3\frac{G}{G_{-1}}\right]\frac{\partial y}{\partial\theta}=-\frac{3Gy}{2\theta G_{-1}}, \tag{C1}$$

where $G=5G_1(\alpha)G_{-1}(\alpha)-9G_0^2(\alpha)$. A numerical calculation shows that $G>0$. Consequently $\partial y/\partial\theta<0$ (in this inequality and below we assume that $\rho\neq 0$). Therefore, y is maximum at $\theta=0$, when $y=y_0$ [see the discussion following (4.23)].

Upon keeping ρ constant and inspecting (4.21) one sees readily that $\tilde{\tau}$ decreases with increasing y, which entails that $\partial\tilde{\tau}/\partial\theta>0$. Therefore, $\tilde{\tau}$ is minimum at $\theta=0$. Substituting $y=y_0$ into (4.21) one obtains numerically that $\tilde{\tau}>0$ at $\theta=0$. Hence, always $\tilde{\tau}>0$.

By analogy with (C1), from (4.21) to (4.23) it follows that

$$\frac{\partial\tilde{\tau}}{\partial\theta}=\frac{2^{1/3}GG_0^{2/3}(3\xi_0+2\pi\xi_0h_2y^3+2\pi y^3)}{\pi^{4/3}y^2G_{-1}[6G_1+9(2G_0^5/\pi)^{1/3}y+2\pi h_2y^3G/G_{-1}]}. \tag{C2}$$

This confirms again that $\partial\tilde{\tau}/\partial\theta>0$. Likewise one can calculate the derivative $\partial\tilde{\tau}/\partial\rho$. One obtains, however, an expression for it which is much more complicated than (C2) and difficult for analytical investigation. A numerical calculation shows that $\partial\tilde{\tau}/\partial\rho>0$.

The pressure p is given by (4.9). With reference to (4.16) and (4.17), one has

$$p=\rho\left(1+\frac{2}{3}\pi h_2a^3\rho\right)\tilde{\tau}+\frac{2\pi a\hbar^2\rho^2}{3m}. \tag{C3}$$

Since $\tilde{\tau}>0$ and $\partial\tilde{\tau}/\partial\rho>0$ it follows immediately from this that $\partial p/\partial\rho>0$, i.e., $(\partial p/\partial V)_\theta<0$.

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Existence of Gibbs state for continuous gas with many-body interaction

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A continuous infinite system of point particles interacting via finite-range many-body potentials of superstable type is considered in the framework of classical statistical mechanics. We prove that for any temperature and chemical activity there exists at least one Gibbs state. © *2004 American Institute of Physics.*
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I. INTRODUCTION

One of the basic problems of equilibrium statistical mechanics is the construction of Gibbs states for continuous particle systems with many-body interactions. In the pioneering works by Greenberg[7] and Moral[13] the problem was analyzed via Kirkwood–Salsburg equations (KSE). For sufficiently small activity parameter z they proved existence of unique solution of KSE, but with rather unnatural assumptions on the potentials which, in fact, take place only for finite range and positive interactions. In Ref. 17 the convergence of the Brydges–Federbush-type cluster expansion is proved for dilute continuous systems with n-body ($n \leqslant M$) interaction. The proof requires a stable potential satisfying an integrability condition and exponential decay of the many-body potentials at large distances. In the following paper[15] the authors consider the system of hard-core spheres interacting via infinite group of many body potentials (for all n) which are bounded and integrable. They prove the convergence of the Mayer series for the pressure in thermodynamic limit and establish the region of analyticity in the activity z. In the recent work by Belitsky and Pechersky[3] the problem of existence and uniqueness of Gibbs state in $\mathbb{R}^d$ with finite group of n-body interactions was investigated using the technique of Dobrushin's type.[4,5]

In this work we give a simple proof of the existence of Gibbs state with infinite group of many body potentials. We establish some kind of modified Ruelle's bound for finite volume correlation functions. It gives a possibility to prove existence of at least one Gibbs measure in thermodynamic limit. We consider these results as some further development in solving the problem.

In the next section we define the system and formulate main results. Section III is devoted to the proof of these results. The basic technical lemma is outlined in the Appendix.

II. CORRELATION FUNCTIONS

A. Configuration space

Let $\mathbb{R}^d$ be a d-dimensional Euclidean space. By $\mathcal{O}(\mathbb{R}^d)$ and $\mathcal{B}(\mathbb{R}^d)$ we denote the family of all open and Borel sets, respectively. $\mathcal{O}_c(\mathbb{R}^d)$, $\mathcal{B}_c(\mathbb{R}^d)$ denote the systems of all sets in $\mathcal{O}(\mathbb{R}^d)$, $\mathcal{B}(\mathbb{R}^d)$, respectively, which are bounded.

The set of positions $\{x_i\}_{i \in \mathbb{N}}$ of identical particles is considered to be a locally finite subset in $\mathbb{R}^d$ and the set of all such subsets creates the configuration space:

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$$\Gamma=\Gamma_{\mathbb{R}^d}:=\{\gamma\subset\mathbb{R}^d\,|\,|\gamma\cap\Lambda|<\infty,\ \text{for all}\ \ \Lambda\in\mathcal{B}_c(\mathbb{R}^d)\},$$

where $|A|$ denotes the cardinality of the set A. The symbol $|\cdot|$ may also represent the Lebesgue measure of the set, but the meaning will always be clear from the context. For any $\Lambda\in\mathcal{B}(\mathbb{R}^d)$ we denote by γ_Λ the projection of γ on Λ and the corresponding configuration space by Γ_Λ. We also need to define the space of finite configurations Γ_0:

$$\Gamma_0=\bigsqcup_{n\in\mathbb{N}_0}\Gamma^{(n)},\quad \Gamma^{(n)}:=\{\eta\subset\mathbb{R}^d\ \mid\ |\eta|=n\},\quad \mathbb{N}_0=\mathbb{N}\cup\{0\}.$$

For every $\Lambda\in\mathcal{B}_c(\mathbb{R}^d)$ one can define a mapping $N_\Lambda:\Gamma\to\mathbb{N}_0$ of the form

$$N_\Lambda(\eta):=|\eta\cap\Lambda|.$$

The Borel σ-algebra $\mathfrak{B}(\Gamma)$ is equal to $\sigma(N_\Lambda|\Lambda\in\mathfrak{B}_c(\mathbb{R}^d))$ and additionally one may introduce the following filtration

$$\mathfrak{B}_\Lambda(\Gamma):=\sigma(N_{\Lambda'}|\Lambda'\in\mathcal{B}_c(\mathbb{R}^d),\ \Lambda'\subset\Lambda),$$

see Refs. 10 and 11 for details.

By $\mathfrak{B}(\cdot)$ we denote the corresponding σ-algebras on Γ_Λ and Γ_0. For a given intensity measure $\sigma=z\,dx$ $(z>0)$ on $\mathcal{B}(\mathbb{R}^d)$ and any $n\in\mathbb{N}$ the product measure $\sigma^{\otimes n}$ can be considered by restriction as a measure on

$$\widetilde{(\mathbb{R}^d)^n}=\{(x_1,\ldots,x_n)\in(\mathbb{R}^d)^n|\ x_k\neq x_l\ \text{if}\ k\neq l\}$$

and hence as a measure $\sigma^{(n)}$ on $\Gamma^{(n)}$ through the map

$$\mathrm{sym}_n:\widetilde{(\mathbb{R}^d)^n}\ni(x_1,\ldots,x_n)\mapsto\{x_1,\ldots,x_n\}\in\Gamma^{(n)},$$

cf. Ref. 8. For simplicity we will write $(x)_n$ instead of $\{x_1,\ldots,x_n\}\in\Gamma^{(n)}$.

Define the Lebesgue–Poisson measure λ_σ on $\mathfrak{B}(\Gamma_0)$ by the formula:

$$\lambda_\sigma:=\sum_{n\geqslant 0}\frac{1}{n!}\sigma^{(n)}.$$

The restriction of λ_σ to $\mathfrak{B}(\Gamma_\Lambda)$ we also denote by λ_σ. For a more detailed structure of the configuration spaces $\Gamma,\Gamma_0,\Gamma_\Lambda$, see Ref. 1.

B. Interactions and Hamiltonians

We consider a general type of many-body interaction specified by a family of k-body potentials $V_k:\mathbb{R}^{dk}\to\mathbb{R}$, $k\geqslant 2$. About the potentials $\{V_k\}_{k\geqslant 2}$ we will assume:

A1. Finite range: There exists a constant $R>0$, such that for any $k\geqslant 2$

$$V_k(x_1,\ldots,x_k)\equiv 0,\ \text{if}\ \ \mathrm{diam}\{x_1,\ldots,x_k\}>R.$$

A2. Continuity:

$$V_k\in C(\widetilde{(\mathbb{R}^d)^k}),\quad k\geqslant 2.$$

A3. Symmetry: For any $k\geqslant 2$, any $(x_1,\ldots,x_k)\in(\mathbb{R}^d)^k$, and any permutation π of numbers $\{1,\ldots,k\}$

$$V_k(x_1,\ldots,x_k)=V_k(x_{\pi(1)},\ldots,x_{\pi(k)}).$$

A4. Translation invariance: For any $k\geqslant 2$, any $(x_1,\ldots,x_k)\in(\mathbb{R}^d)^k$, and any $a\in\mathbb{R}^d$

$$V_k(x_1,\ldots,x_k)=V_k(x_1+a,\ldots,x_k+a).$$

We are able now to introduce the Hamiltonian $U^V:\Gamma_0\to\mathbb{R}\cup\{\infty\}$, which corresponds to the family of potentials $V:=\{V_k\}_{k\geqslant 2}$ and which is defined by

$$U^V(\eta)=\sum_{k\geqslant 2}\sum_{\{x_1,\ldots,x_k\}\subset\eta}V_k(x_1,\ldots,x_k),\quad \eta\in\Gamma_0,\quad |\eta|\geqslant 2.$$

For the fixed family of potentials V we will write for short $U=U^V$ and for $\Lambda\in\mathcal{B}_c(\mathbb{R}^d)$, $\eta\in\Gamma_\Lambda$ we will sometimes write $U_\Lambda(\eta)$ instead of $U(\eta)$.

A5. Strong superstability: For any $k\geqslant 2$ the potential V_k can be represented as

$$V_k=V_k^+ + V_k^{(\mathrm{st})},$$

where V_k^+ is a non-negative function such that for any $(x_1,\ldots,x_k)\in(\mathbb{R}^d)^k\setminus\widetilde{(\mathbb{R}^d)^k}$

$$V_k^+(x_1,\ldots,x_k)=+\infty,$$

and $V_k^{(\mathrm{st})}$ is stable, i.e., there exists a constant $B\geqslant 0$ such that for any configuration $\eta\in\Gamma_0$ holds

$$U^{V^{(\mathrm{st})}}(\eta)\geqslant -B|\eta|.$$

Let $\lambda\in\mathbb{R}_+$ be arbitrary. For each $r\in\mathbb{Z}^d$ we define an elementary cube

$$\Delta(r)=\{x\in\mathbb{R}^d\,|\,\lambda(r^i-1/2)\leqslant x^i<\lambda(r^i+1/2)\}.$$

These cubes form a partition of $\mathbb{R}^d$, which we denote by $\overline{\Delta_\lambda}$. We will sometimes write Δ instead of $\Delta(r)$, if a cube Δ is considered to be arbitrary and there is no reason to emphasize that it is centered at the concrete point $r\in\mathbb{Z}^d$. By $\mathcal{J}_\lambda(\mathbb{R}^d)$ we denote all finite unions of cubes of the form $\Delta(r)$ (such sets are used in the construction of the Jordan measure).

Let $N\in\mathbb{N}$ and $k\geqslant N+1$ be arbitrary. For any $X_N=\cup_{j=1}^N\Delta_j\in\mathcal{J}_\lambda(\mathbb{R}^d)$ we define

$$I_k^{k_1,\ldots,k_N|\overline{k}}(\Delta_1,\ldots,\Delta_N) := \sup_{(x)_{k_i}^i\subset\Delta_i,\ 1\leqslant i\leqslant N}\ {\sum_{\substack{\Delta_j'\subset X_N^c,\\ 1\leqslant j\leqslant\overline{k}}}}^{*}\ \sup_{y_1\in\Delta_1',\ldots,y_{\overline{k}}\in\Delta_{\overline{k}}'}|V_k^{(\mathrm{st}),-}(x_1^1,\ldots,x_{k_N}^N,y_1,\ldots,y_{\overline{k}})|, \tag{1}$$

where $\overline{k}\geqslant 1$, $k_i\geqslant 1, i=1,\ldots,N$ such that $k_1+\cdots+k_N+\overline{k}=k$, and

$$v_k^{k_1,\ldots,k_N}(\Delta_1,\ldots,\Delta_N):=\inf_{(x)_{k_i}^i\subset\Delta_i,1\leqslant i\leqslant N,}V_k^+(x_1^1,\ldots,x_{k_N}^N), \tag{2}$$

where $k_i\in\mathbb{N}_0$, $(x)_{k_i}^i=\{x_1^i,\ldots,x_{k_i}^i\}$, $1\leqslant i\leqslant N$ such that $k_1+\cdots+k_N=k$. $V_k^{(\mathrm{st}),-}$ denotes the negative part of $V_k^{(\mathrm{st})}$, and the symbol Σ^* means that the sum extends only over different cubes, i.e., $\Delta_i'\neq\Delta_j'$, $i\neq j$, $1\leqslant i,j\leqslant\overline{k}$.

A6. Attraction–repulsion relation: There exists $\lambda=\lambda_0>0$, such that for any $N\in\mathbb{N}$ and any $X_N=\cup_{j=1}^N\Delta_j\in\mathcal{J}_{\lambda_0}(\mathbb{R}^d)$ (we omit dependence on the cubes in the notations of (1) and (2)) the following holds:

(i) for an arbitrary $\Delta\in\overline{\Delta_{\lambda_0}}$ and any $k\geqslant 2$

$$V_k(x_1,\ldots,x_k)\geqslant 0,\qquad \{x_1,\ldots,x_k\}\subset\Delta;$$

(ii) for an arbitrary $k \geqslant N+1$

$$v_k^{k_1,\dots,k_N} \geqslant 4\overline{I}^{(N)}_{k;\,k_1,\dots,k_N}, \qquad v_{N+1}^{k_1,\dots,k_N} \geqslant 4(\overline{I}^{(N)}_{N+1}+B), \tag{3}$$

and

$$\overline{I}^{(N)}_{k;\,k_1,\dots,k_N} = \sum_{l\geqslant 1} l I_{k+l}^{k_1,\dots,k_N|\,l} < \infty, \qquad \overline{I}^{(N)}_{N+1} = \sum_{l\geqslant 1} l I_{N+l}^{1,\dots,1|\,l} < \infty, \tag{4}$$

$$k_1+\cdots+k_N = k.$$

In the sequel we write $\overline{\Delta}$ instead of $\overline{\Delta}_{\lambda_0}$.

Remark 2.1: By the definition, $V_k^{\mathrm{st},-}$ describes attractive part of the k-body interaction. Therefore, $\overline{I_k^{k_1,\dots,k_N|k}}(\Delta_1,\dots,\Delta_N)$ describes only the attractive part of the k-body interaction of fixed particles in cubes $\Delta_1,\dots,\Delta_N$ with "dilute configuration," i.e., no more than one particle is located in any cube Δ from $X_N^c = \mathbb{R}^d \backslash X_N$, $X_N = \cup_{j=1}^N \Delta_j$. Then, condition (4) means that the energy of the k-body interaction decreases sufficiently fast with k. From the assumption **A6** *and the definition of $\overline{I}^{(N)}_{k;\,k_1,\dots,k_N}$ therein, it is clear that at least one cube from $\Delta_1,\dots,\Delta_N$ contains more than one particle, and so $v_k^{k_1,\dots,k_N}$ should be greater than contributions of all $k+l$-body attractive energies of interaction $(l \in N)$ for sufficiently small λ.*

Remark 2.2: From the definition of $\overline{I_k^{k_1,\dots,k_N|k}}(\Delta_1,\dots,\Delta_N)$ (see (1)) it is clear that

$$\overline{I_k^{k_1,\dots,k_N|k}}(\Delta_1,\dots,\Delta_N) \leqslant C_k \lambda^{-d\overline{k}}, \qquad \lambda \to 0,$$

where $C_k = C_k(\lambda) \geqslant 0$ are some constants. Moreover, if $V_k^{(\mathrm{st}),-}$ is bounded from below on $(\mathbb{R}^d)^k \backslash \widetilde{(\mathbb{R}^d)^k}$, then $C_k(\lambda)$ has the following limit at $\lambda \to 0$:

$$C_k(0) = \int_{(\mathbb{R}^d)^{\overline{k}}} |V_k^{(\mathrm{st}),-}(x_1^1,\dots,x_{k_N}^N, y_1,\dots,y_{\overline{k}})| dy_1 \cdots dy_{\overline{k}},$$

where $x_1^1,\dots,x_{k_N}^N$ some fixed points in $\mathbb{R}^d$. For example, if we would have only pair potential, to satisfy (3) the positive part of the potential $V_2^+(x_1,x_2)$ should behave like $|x_1-x_2|^{-d-\varepsilon}$, $|x_1-x_2| \to 0$, for some $\varepsilon > 0$.

In the case of all orders of interactions, the k-body potentials, for $k \geqslant 3$, can be chosen in such a way that constants C_k, $k \geqslant 3$ have behavior like $C^k/k!$, for some constant $C > 0$. Under such condition, $\overline{I_k^{k_1,\dots,k_N|k}}(\Delta_1,\dots,\Delta_N)$ will behave like $\lambda^{-d} C^{k+1} e^{C\lambda^{-d}}/k!$. Therefore, to satisfy (3), the positive part of the potentials $V_k^+(x_1,\dots,x_k)$ should behave like

$$|x_i - x_j|^{-d-\varepsilon} \frac{C^{k+1}}{k!} e^{C|x_i-x_j|^{-d-\varepsilon}}, \qquad |x_i - x_j| \to 0, \quad 1 \leqslant i,j \leqslant k$$

for some $\varepsilon > 0$.

For a given $\overline{\gamma} \in \Gamma$ define the interaction energy between $\eta \in \Gamma_\Lambda$, $\Lambda \in \mathcal{B}_c(\mathbb{R}^d)$ and $\overline{\gamma}_{\Lambda^c} = \overline{\gamma} \cap \Lambda^c$, $\Lambda^c = \mathbb{R}^d \backslash \Lambda$ as

$$W_\Lambda(\eta|\overline{\gamma}) = \sum_{k\geqslant 2} \sum_{\substack{m+n=k \\ m,n\geqslant 1}} \sum_{\substack{\{x_1,\dots,x_m\}\subset \eta \\ \{y_1,\dots,y_n\}\subset \overline{\gamma}_{\Lambda^c}}} V_k(x_1,\dots,x_m,y_1,\dots,y_n).$$

Define

$$U_\Lambda(\eta|\overline{\gamma}) = U_\Lambda(\eta) + W_\Lambda(\eta|\overline{\gamma}).$$

A7. The order of interaction: For any $\Lambda \in \mathcal{B}_c(\mathbb{R}^d)$, $\eta \in \Gamma_\Lambda$ and $\overline{\gamma} \in \Gamma$ the interaction energy $W_\Lambda(\eta|\overline{\gamma})$ does not become $-\infty$ and the partition function

$$Z_\Lambda(\overline{\gamma}) = \int_{\Gamma_\Lambda} \exp\{-U_\Lambda(\eta| \ \overline{\gamma})\}\lambda_\sigma(d\eta) < \infty.$$

Remark 2.3: Assumption **A7** *is important only for the next chapter, where the precise definition of the Gibbs state on the configuration space* Γ *will be given. In fact, for the results of the present paper we do not need fulfillment of* **A7** *for all* $\overline{\gamma} \in \Gamma$, *but only for empty boundary configurations. In turn, this fact is automatically ensured by assumption* **A5**.

C. Gibbs specification and correlation functions

Let $\Lambda \in \mathcal{B}_c(\mathbb{R}^d)$ and let $\overline{\gamma} \in \Gamma$. The finite volume Gibbs state with boundary configuration $\overline{\gamma}$ for U, $z>0$ and $\beta>0$ is

$$\mu_\Lambda(d\eta| \ \overline{\gamma}) = \frac{\exp\{-\beta U_\Lambda(\eta| \ \overline{\gamma})\}}{Z_\Lambda(\overline{\gamma})}\lambda_{z\sigma}(d\eta).$$

Under assumption **A7**, the finite volume Gibbs state is well defined. When $\overline{\gamma}=\varnothing$, let $\mu_\Lambda(d\eta|\varnothing) \equiv \mu_\Lambda(d\eta)$.

The corresponding finite-volume correlation functions for boundary configuration $\overline{\gamma} \in \Gamma$ have the following form:

$$\rho^\Lambda(\eta|\overline{\gamma}) = \frac{1}{Z_\Lambda(\overline{\gamma})}\int_{\Gamma_\Lambda} e^{-\beta U(\eta \cup \gamma|\overline{\gamma})}\lambda_\sigma(d\gamma), \qquad \eta \in \Gamma_\Lambda. \tag{5}$$

Let $\{\pi_\Lambda\}$ denote the specification associated with z, β and the Hamiltonian U (see Ref. 14), which is defined on Γ by

$$\pi_\Lambda(A| \ \overline{\gamma}) = \int_{A'} \mu_\Lambda(d\eta| \ \overline{\gamma}),$$

where $A' = \{\eta \in \Gamma_\Lambda : \ \eta \cup (\overline{\gamma}_{\Lambda^c}) \in A\}$, $A \in \mathfrak{B}(\Gamma)$.

A probability measure μ on Γ is called a Gibbs state for U, β and z if

$$\mu(\pi_\Lambda(A| \ \overline{\gamma})) = \mu(A)$$

for every $A \in \mathfrak{B}(\Gamma)$ and every $\Lambda \in \mathcal{B}_c(\mathbb{R}^d)$.

This relation is the well known (DLR)-equation (Dobrushin–Lanford–Ruelle equation), see Ref. 6 for more details. The class of all Gibbs states which correspond to the specifications $\{\pi_\Lambda\}_{\Lambda \in \mathcal{B}_c(\mathbb{R}^d)}$ we denote by $\mathcal{G}(V,z,\beta)$.

D. Main results

Theorem 2.1: *Suppose that the interaction family V satisfies the assumptions* **A1–A6**. *Then, for any* $\Lambda \in \mathcal{J}_{\lambda_0}(\mathbb{R}^d)$ *and any* $\beta,z>0$ *there exists a constant* $\xi = \xi(\beta,z)$ *(independent of* Λ*) such that the finite volume correlation function* $\rho^\Lambda(\eta) = \rho^\Lambda(\eta|\varnothing)$ *satisfies the following inequality:*

$$\rho^\Lambda(\eta) \leqslant \xi^{|\eta|} e^{-(1/2)U^+(\eta)}, \quad \eta \in \Gamma_\Lambda. \tag{6}$$

Remark 2.4: The estimate (6) without exponent factor at the right-hand side is the well-known Ruelle bound.[18] *We call (6) a generalized Ruelle bound. For the two-body interaction it was obtained in Refs. 1 and 16.*

As a consequence of Theorem 2.1 the following theorem is fulfilled.

Theorem 2.2: *Let the interaction family V satisfy* **A1–A6**. *Then for any* $z>0$ *and* $\beta>0$

$$\mathcal{G}(V,z,\beta)\neq\varnothing.$$

Proof: Existence of the corresponding Gibbs state follows from the arguments which are based on the following observation. Let $\psi\in L^1(\mathbb{R}^d)\cap C(\mathbb{R}^d)$ be any positive function such that $\psi(x)\leqslant 1, x\in\mathbb{R}^d$, and let $\alpha(t)$, $t\in\mathbb{R}_+$ be any continuous decreasing function with the following conditions:

(1) $\alpha_0:=\lim_{t\to 0+}\alpha(t)=+\infty$;
(2) $\alpha_+:=\lim_{t\to+\infty}\alpha(t)\geqslant 1$.

Define,

$$\Gamma^{\alpha,\psi}=\left\{\gamma\in\Gamma\;\middle|\;\sum_{\{x,y\}\subset\gamma}\psi(x)\alpha(|x-y|)\psi(y)<\infty\right\}$$

and

$$E^{\alpha,\psi}(\gamma)=\sum_{\{x,y\}\subset\gamma}\psi(x)\alpha(|x-y|)\psi(y),\quad\gamma\in\Gamma^{\alpha,\psi}.$$

As shown in Ref. 9, for any $0<D<\infty$ the set

$$\{\gamma\in\Gamma\,|\,|E^{\alpha,\psi}(\gamma)|\leqslant D\}$$

is precompact in Γ, which is Polish space.

In this paper we consider α as any continuous decreasing function such that

$$\alpha(|x-y|)\leqslant e^{(1/2)\,V_2^+(x,y)}.$$

Obviously, chosen in such a way, this function satisfies the conditions above. Using the properties of the so-called *K*-transform (see Ref. 8) and the Theorem 2.1, for any $\Lambda\in\mathcal{J}_{\lambda_0}(\mathbb{R}^d)$ we have

$$\int_\Gamma E^{\alpha,\psi}(\gamma)\,d\mu_\Lambda(\gamma)=\int_{\mathbb{R}^{2d}}\psi(x)\alpha(|x-y|)\psi(y)\rho_\Lambda^{(2)}(\{x,y\})\,dx\,dy<C,$$

where $C\in\mathbb{R}_+$ is some constant.

Therefore, by Prokhorov theorem the family of measures

$$\{\mu_\Lambda\,|\,\Lambda\in\mathcal{J}_{\lambda_0}(\mathbb{R}^d)\}$$

is precompact, which implies the existence of at least one limit measure μ when $\Lambda\nearrow\mathbb{R}^d$. We will prove that corresponding limit measure is Gibbsian. Let μ_{Λ_n}, $n\geqslant 1$, where $\Lambda_n\nearrow\mathbb{R}^d$, $n\to\infty$ be the sequence which converges (in the sense of the Prokhorov theorem) to the measure μ, and let ρ^{Λ_n}, ρ be the corresponding correlation functions. It is well-known (see Ref. 6) that probability measure μ on Γ is Gibbs, iff μ fulfills the *Georgii–Nguyen–Zessin* equation (GNZ), i.e., for all positive, $\mathcal{B}(\mathbb{R}^d)\times\mathfrak{B}(\Gamma)$ measurable functions H the following holds

$$\int_\Gamma\sum_{x\in\gamma}H(x,\gamma)\mu(d\gamma)=\int_\Gamma\int_{\mathbb{R}^d}H(x,\gamma\cup\{x\})e^{-\beta W(\{x\}|\gamma)}\sigma(dx)\mu(d\gamma).\tag{7}$$

Moreover, using the Mecke formula (see Ref. 6), one can show that (7) holds for any measure μ_{Λ_n}, $n\geqslant 1$.

Let $\Lambda \in \mathcal{B}_c(\mathbb{R}^d)$. The σ-algebra $\mathfrak{B}(\Gamma)$ is generated by sets of the form $A \cap \tilde{A}$ with $A \in \mathfrak{B}_\Lambda(\Gamma)$, $\tilde{A} \in \mathfrak{B}_{\mathbb{R}^d \setminus \Lambda}(\Gamma)$ and every measure on Γ is uniquely determined by its values on these sets.

Let us prove (7) for the function $H(x,\gamma) = \mathbb{1}_\Lambda(x)\mathbb{1}_A(\gamma)\mathbb{1}_{\tilde{A}}(\gamma)$. Let $n \in \mathbb{N}$ be arbitrary. Using the properties of the K-transform (see Ref. 8) we have

$$\int_{\Gamma_{\Lambda_n}} \sum_{x \in \gamma} \mathbb{1}_\Lambda(x)\mathbb{1}_A(\gamma)\mathbb{1}_{\tilde{A}}(\gamma)\mu_{\Lambda_n}(d\gamma) \leqslant \int_{\Gamma_{\Lambda_n}} \sum_{x \in \gamma} \mathbb{1}_\Lambda(x)\mu_{\Lambda_n}(d\gamma) = \int_\Lambda \rho^{\Lambda_n}(x)\sigma(dx) \leqslant z\xi|\Lambda|. \tag{8}$$

The right-hand side of (7) for the measure μ_{Λ_n} is bounded by

$$\int_{\mathbb{R}^d} \mathbb{1}_\Lambda(x) \int_{\Gamma_{\Lambda_n}} e^{-\beta W(\{x\}|\gamma)} \mu_{\Lambda_n}(d\gamma)\sigma(dx) = \int_{\mathbb{R}^d} \mathbb{1}_\Lambda(x)\rho^{\Lambda_n}(x)\sigma(dx) \leqslant z\xi|\Lambda|, \tag{9}$$

where we have used the definition of the correlation function and Fubini theorem. Hence, there exists some subsequence $\{\mu_{\Lambda_{n_k}}\}_{k \geqslant 1}$ which ensures the fulfillment of (7) for the limit measure μ. The proof for the general positive function H follows from the fact that any positive measurable function can be approximated by the simple functions.

III. THE PROOF OF THEOREM 2.1

The proof is based on the expansion of the Lebesgue–Poisson integral for the correlation functions (5) into the series over some kind of dense configurations (see Ref. 16 and definition (3.4) therein).

A. Cluster expansion in densities of configurations

The main idea of the construction consists in the use of the fact that if two or more particles are in one elementary cube $\Delta \in \overline{\Delta}$ then Gibbs factor $\exp[-\beta V_2(x_i,x_j)] \sim \exp[-\beta b]$, where

$$b = \inf_{\Delta \in \overline{\Delta}} \inf_{x_1,x_2 \in \Delta} V_2^+(x_1,x_2) \tag{10}$$

and $b \to \infty$, when $\lambda \to 0$. The configurations with this property will be called *dense* configurations, as opposed to *dilute* configurations, in which no more than one particle is situated in any cube. The main technical idea consists in separation of the dilute parts of configurations from the dense parts. In order to do this we define an indicator function for the configuration γ_Λ, $\Lambda \in \mathcal{J}_{\lambda_0}(\mathbb{R}^d)$ in the cube Δ:

$$\chi_n^\Delta(\gamma_\Lambda) = \chi_n^\Delta(\gamma_\Delta) = \begin{cases} 1, & \text{for } |\gamma_\Delta| = n, \\ 0, & \text{otherwise.} \end{cases}$$

Then the indicator for *dilute* configurations is defined as

$$\chi_-^\Delta(\gamma_\Delta) = \chi_0^\Delta(\gamma_\Delta) + \chi_1^\Delta(\gamma_\Delta)$$

and for *dense* configurations as

$$\chi_+^\Delta(\gamma_\Delta) = \sum_{n \geqslant 2} \chi_n^\Delta(\gamma_\Delta).$$

To obtain decomposition we use the following partition of the unity:

$$1 = \prod_{\Delta\subset\Lambda}[\chi^{\Delta}_{-}(\gamma_\Delta)+\chi^{\Delta}_{+}(\gamma_\Delta)] = \sum_{\omega}\prod_{\Delta\subset\Lambda}\chi^{\Delta}_{\omega(\Delta)}(\gamma_\Delta), \tag{11}$$

where ω is the map from $\overline{\Delta}\cap\Lambda := \{\Delta\in\overline{\Delta}:\Delta\subset\Lambda\}$ into the set $\{+,-\}$, such that $\omega(\Delta)=+$ or $-$ for any $\Delta\in\overline{\Delta}\cap\Lambda$. Inserting (11) into (5) for $\overline{\gamma}=\varnothing$, we get

$$\rho^{\Lambda}(\eta) = \frac{1}{Z_\Lambda}\sum_{\omega}\int_{\Gamma_\Lambda}\prod_{\Delta\subset\Lambda}\chi^{\Delta}_{\omega(\Delta)}(\gamma_\Delta)e^{-\beta U(\eta\cup\gamma)}\lambda_\sigma(d\gamma), \tag{12}$$

where $Z_\Lambda = Z_\Lambda(\varnothing)$. Now we define the set

$$X = \bigcup_{\Delta\subset\Lambda\,:\,\omega(\Delta)=+}\Delta.$$

Then the sum over ω can be rewritten as the sum over all possible sets X in Λ. Namely,

$$\rho^{\Lambda}(\eta) = \frac{1}{Z_\Lambda}\sum_{\varnothing\subseteq X\subseteq\Lambda}\int_{\Gamma_\Lambda}\tilde{\chi}^{X}_{+}(\gamma)\tilde{\chi}^{X^c}_{-}(\gamma)e^{-\beta U(\eta\cup\gamma)}\lambda_\sigma(d\gamma),$$

where

$$\tilde{\chi}^{X}_{\pm}(\gamma) = \prod_{\Delta\subset X}\chi^{\Delta}_{\pm}(\gamma_\Delta).$$

For any $X\in\mathcal{J}_{\lambda_0}(\mathbb{R}^d)$, $X\subseteq\Lambda$ define graph $G_R(X)$ with vertices in the centers of all elementary cubes $\Delta\subset X$ and lines $l(\Delta,\Delta')$ iff $\mathrm{dist}(\Delta,\Delta')\leqslant R$. The number of lines depends on graph $G_R(X)$.

Definition 3.1: The set X is called R-connected if the corresponding graph $G_R(X)$ is connected in ordinary way.

R-connected set X is denoted by X^R. Then, every set X can be represented as some fixed partition

$$\{X\}^R_n := \{X^R_1,\ldots,X^R_n|\,\mathrm{dist}(X^R_i,X^R_j)>R,\quad \text{for}\quad i\neq j\},$$

and so the sum over all possible X in Λ can be rewritten as the sum over all possible sets $\{X\}^R_n$ (for $n=0, X=\varnothing$). Furthermore, we replace the sum over all such sets by the sum over $X^R_1,\ldots,X^R_n$ independently, and remove the conditions $\mathrm{dist}(X^R_i,X^R_j)>R$ by introducing the *hard-core* potential

$$\chi^{\mathrm{cor}}_R(X)_n = \begin{cases} 0, & \text{there exists } X^R_i, X^R_j,\ i\neq j,\ \mathrm{dist}(X^R_i,X^R_j)\leqslant R,\\ 1, & \text{otherwise.}\end{cases}$$

Then we get

$$\rho^{\Lambda}(\eta) = \frac{1}{Z_\Lambda}\sum_{n\geqslant 0}\frac{1}{n!}\sum_{X^R_1\subseteq\Lambda}\cdots\sum_{X^R_n\subseteq\Lambda}\chi^{\mathrm{cor}}_R(X)_n\int_{\Gamma_\Lambda}\tilde{\chi}^{X}_{+}(\gamma)\tilde{\chi}^{X^c}_{-}(\gamma)e^{-\beta U(\eta\cup\gamma)}\lambda_\sigma(d\gamma). \tag{13}$$

In the sequel, having in mind only R-connected components of X, we drop index R in the notation X^R_i, and summation $\Sigma_{X_1\subseteq\Lambda}\cdots\Sigma_{X_n\subseteq\Lambda}$, for simplicity, will be denoted by $\Sigma_{(X)_n}$. Now, the last step in arranging our decomposition is as follows. Define the set

$$X_0 = \bigcup_{\Delta\subset\Lambda\,:\,\mathrm{dist}(\Delta,\,\eta)\leqslant R}\Delta.$$

This set is fixed for fixed variable of the correlation function $\rho^{\Lambda}(\eta)$. Now, for every $n\geqslant 0$ we split the sum over $(X)_n$ into two sums. The first one is over those X_j, which do not intersect the

region X_0 and the second one over those which intersect X_0. To distinguish the sets X_j which do not intersect and do intersect X_0, the latter sets are denoted by Y_j. There are $n!/k!(n-k)!$ possibilities when any k sets X_j do not intersect X_0 and $(n-k)$ sets Y_j intersect X_0. So the final expansion is the following:

$$\rho^{\Lambda}(\eta) = \frac{1}{Z_\Lambda}\sum_{n\geqslant 0}\sum_{k=0}^{n}\frac{1}{k!(n-k)!}\sum_{(X)_k}\sum_{(Y)_{n-k}}\chi_R^{\mathrm{cor}}((X)_k,(Y)_{n-k}) \times\int_{\Gamma_\Lambda}\lambda_\sigma(d\gamma)\tilde{\chi}_+^X(\gamma)\tilde{\chi}_-^{X^c}(\gamma)e^{-\beta U(\eta\cup\gamma)}, \tag{14}$$

where

$$X=\tilde{X}_k\cup\tilde{Y}_{n-k}:=\left[\bigcup_{i=1}^{k}X_i\right]\bigcup\left[\bigcup_{j=1}^{n-k}Y_j\right].$$

B. The main estimates

As the first step, let us split the exponent in (14) into four parts: the part which corresponds to the positive part of the energy of the configuration η, the interactions of the particles inside the region $X_0\cup\tilde{Y}_{n-k}$, inside $\Lambda\backslash(X_0\cup\tilde{Y}_{n-k})$ and interactions between them. Note that interaction between $X_0\cup\tilde{Y}_{n-k}$ and $\tilde{X}_k$ is zero due to the finite range of potential. Therefore, considering $\gamma\in\Gamma_\Lambda : \gamma\cap\eta=\varnothing$ we get

$$e^{-\beta U(\eta\cup\gamma)}=e^{-\beta U^+(\eta)}E_1E_2E_0,$$

where

$$E_1(X_0\cup\tilde{Y}_{n-k})=e^{-\beta U^{\mathrm{st}}(\eta)}\prod_{l=1}^{n-k}e^{\beta W(\eta\,|\,\gamma_{Y_l})-1/2\,\beta U^+(\gamma_{Y_l})-\beta U^{\mathrm{st}}(\gamma_{Y_l})},$$

$$E_2(X_0\cup\tilde{Y}_{n-k}|(X_0\cup X)^c)=e^{-\beta W(\eta\,|\,\gamma_{X_0\backslash\tilde{Y}_{n-k}})}\prod_{l=1}^{n-k}e^{-\beta[1/2\,U^+(\gamma_{Y_l})+W(\gamma_{Y_l}\,|\,\gamma_{X^c})]},$$

and

$$E_0(\tilde{Y}_{n-k}^c)=e^{-\beta U(\gamma_{\Lambda\backslash\tilde{Y}_{n-k}})}.$$

Lemma 3.1:

$$E_1\leqslant e^{\beta B|\eta|}\prod_{l=1}^{n-k}\prod_{\Delta\subset Y_l}e^{\beta B|\gamma_\Delta|-(1/2)\,\beta U^+(\gamma_\Delta)}. \tag{15}$$

Proof: Using **A5** we have

$$U^{(\mathrm{st})}(\eta\cup\gamma_{\tilde{Y}_{n-k}})\geqslant -B\left(|\eta|+\sum_{l=1}^{n-k}\sum_{\Delta\subset Y_l}|\gamma_\Delta|\right)$$

and

$$W^+(\eta|\gamma_{\tilde{Y}_{n-k}})\geqslant 0,\quad U^+(\gamma_{Y_l})\geqslant\sum_{\Delta\subset Y_l}U^+(\gamma_\Delta).$$

■

Lemma 3.2: For any $\gamma\in\Gamma$ *and* $\overline{\gamma}\in\overline{\Gamma}_{X^c}$, $X\in\mathcal{J}_{\lambda_0}(\mathbb{R}^d)$, $X\subseteq\Lambda$

$$\tfrac{1}{4}U^+(\gamma_X)+W(\gamma_X|\overline{\gamma})\geqslant-\overline{I|\gamma_X|}, \tag{16}$$

where $\overline{I}:=\overline{I}_2^{(1)}$ (*see (4)), and*

$$\overline{\Gamma}_{X^c}=\{\gamma\in\Gamma_{X^c}\,|\;\;|\gamma\cap\Delta|\leqslant 1,\quad\text{for all}\;\;\Delta\subset X^c\}.$$

■

Proof: See Appendix.

Let us define

$$\partial\eta=\bigcup_{\Delta\,:\,\eta\cap\Delta\neq\varnothing}\Delta.$$

Now using the property of infinite divisibility of measure λ_σ and estimate (16) we can calculate the part of integral in (14)

$$\begin{aligned}
&e^{-(1/2)\,\beta U^+(\eta)}\int_{\Gamma_{\tilde{Y}_{n-k}}}\tilde{\chi}_+^{\tilde{Y}_{n-k}}(\gamma)E_1E_2\lambda_\sigma(d\gamma)\\
&\leqslant e^{-(1/4)\,\beta U^+(\eta)+\beta|\eta|\overline{I}}\int_{\Gamma_{\tilde{Y}_{n-k}}}\tilde{\chi}_+^{\tilde{Y}_{n-k}}(\gamma)e^{-\beta W(\eta\,|\,\gamma_{(X_0\cap\partial\eta)\setminus\tilde{Y}_{n-k}})}E_1\\
&\quad\times\prod_{l=1}^{n-k}e^{-\beta[(1/2)\,U^+(\gamma_{Y_l})+W(\gamma_{Y_l}\,|\,\gamma_{X^c})]}\lambda_\sigma(d\gamma).
\end{aligned}\tag{17}$$

Assumption **A6**, estimate (15), and trivial inequality

$$U^+(\eta)\geqslant\sum_{\Delta\subset\partial\eta}U^+(\eta_\Delta)$$

gives us the bound for the integral (17),

$$e^{\beta|\eta|(\overline{I}+B)+\beta\Sigma_{\Delta\subset\partial\eta}\overline{I}|\eta_\Delta|}\prod_{l=1}^{n-k}\prod_{\Delta\subset Y_l}I_\Delta,$$

where

$$I_\Delta=\int_{\Gamma_\Delta}\chi_+^\Delta(\gamma_\Delta)e^{-\beta\,(1/2)\,U^+(\gamma_\Delta)+\beta(B+\overline{I})|\gamma_\Delta|}\lambda_\sigma(d\gamma). \tag{18}$$

Focusing only on the two-body positive part of interaction and taking into account the definition (10) we can estimate the last integral by

$$I_\Delta\leqslant\varepsilon_1=\tfrac{1}{2}z^2\lambda_0^{2d}e^{-\beta(1/2)\,b-2\overline{I}-2B)}\exp\{z\lambda_0^d e^{-\beta(3/2)}\,b-\overline{I}-B)\}, \tag{19}$$

which is finite due to **A6**.

Now taking the maximum of E_0 in variable $\tilde{Y}_{n-k}$ (we denote this maximum by $\overline{Y}_{n-k}$) and using elementary estimate

$$\chi_R^{\mathrm{cor}}((X)_k,(Y)_{n-k})\leqslant\chi_R^{\mathrm{cor}}(X)_k \tag{20}$$

we can estimate the sum over $(Y)_{n-k}$ by the following lemma:

Lemma 3.3 (e.g., Ref. 12):

$$\sum_{Y\cap X_0\neq\varnothing} \varepsilon_1^{|Y|/\lambda^d} \leqslant |\eta| c(d)\left(\frac{R}{\lambda}\right)^d \frac{\varepsilon}{1-\varepsilon} = |\eta| K, \tag{21}$$

where $c(d)$ *is a constant which depends only on* d *and* $\varepsilon = 4c(d)(R/\lambda)^d \varepsilon_1$.

For the *proof* in our case, see Ref. 16.

The last step is as follows. The expansion like (13) can be constructed for partition function Z_{Λ_1} with $\Lambda_1 \subset \Lambda$. Denote it by

$$Z_{\Lambda_1} = \sum_{k\geqslant 0} \frac{1}{k!} Z^{(k)}_{\Lambda_1}. \tag{22}$$

Taking into account all previous estimates we get

$$\begin{aligned}
\rho^{\Lambda}(\eta) &\leqslant \frac{1}{Z_\Lambda} e^{-(1/2)\beta U^+(\eta_\Lambda)+\beta(2\bar{I}+B)|\eta|} \sum_{n\geqslant 0} \sum_{k=0}^{n} \frac{(|\eta|K)^{n-k}}{k!(n-k)!} Z^{k}_{\Lambda\setminus\bar{Y}_{n-k}} \\
&= \frac{1}{Z_\Lambda} e^{-(1/2)\beta U^+(\eta_\Lambda)+\beta(2\bar{I}+B)|\eta|} \sum_{k\geqslant 0} \frac{1}{k!} \sum_{l\geqslant 0} \frac{(|\eta|K)^{l}}{l!} Z^{k}_{\Lambda\setminus\bar{Y}_{l}} \\
&= e^{-(1/2)\beta U^+(\eta_\Lambda)+\beta(2\bar{I}+B)|\eta|} \sum_{l\geqslant 0} \frac{(|\eta|K)^{l}}{l!} \frac{Z_{\Lambda\setminus\bar{Y}_l}}{Z_\Lambda}.
\end{aligned} \tag{23}$$

The fact that $Z_{\Lambda_1} \leqslant Z_{\Lambda_2}$ for $\Lambda_1 \subset \Lambda_2$ gives the inequality

$$\rho^{\Lambda}(\eta) \leqslant e^{-(1/2)\beta U^+(\eta)} e^{|\eta|(\beta(2\bar{I}+B)+K)}.$$

■

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APPENDIX: PROOF OF THE LEMMA 3.2

Let $X = \cup_{j=1}^{N} \Delta_j$. Consider the configuration γ with $|\gamma_X| = m, |\gamma_{\Delta_1}| = m_1, \ldots, |\gamma_{\Delta_N}| = m_N$, $m_j \geqslant 1$ for $j = 1, \ldots, N$ and $m_1 + \cdots + m_N = m$. Let in the k-body interaction be involved $\bar{k} \geqslant 1$ particles from the dilute configuration $\bar{\gamma}_{X^c} \in \bar{\gamma}_{X^c}$ and, correspondingly, q_1 particles of γ_X from Δ_1, which are situated in the points $x_1^{(1)}, \ldots, x_{q_1}^{(1)} \in \Delta_1$, $\ldots$, q_N particles $x_1^{(N)}, \ldots, x_{q_N}^{(N)}$ from Δ_N. It is clear that $q_1 + \cdots + q_N + \bar{k} = k$ and $0 \leqslant q_i \leqslant m_i$, $\bar{k} \geqslant 1$. Then the interaction energy between m particles of the configuration γ_X and $\bar{k}$ particles of dilute configuration $\bar{\gamma}_{X^c}$ can be written in the following form:

$$\begin{aligned}
W_k(\gamma_X|\bar{\gamma}_{X^c}) = &\sum_{\substack{0\leqslant q_i\leqslant m_i,\,\bar{k}\geqslant 1 \\ q_1+\cdots+q_N+\bar{k}=k}} \sum_{\{x_1^{(1)},\ldots,x_{q_1}^{(1)}\}\in\gamma_{\Delta_1}} \cdots \sum_{\{x_1^{(N)},\ldots,x_{q_N}^{(N)}\}\in\gamma_{\Delta_N}} \\
&\times \sum_{\{y_1,\ldots,y_{\bar{k}}\}\in\bar{\gamma}_{X^c}} V_k(x_1^{(1)},\ldots,x_{q_1}^{(1)},\ldots,x_1^{(N)},\ldots,x_{q_N}^{(N)},y_1,\ldots,y_{\bar{k}}).
\end{aligned}$$

Then taking into account (1) we obtain

$$-W_k(\gamma_X|\overline{\gamma}_{X^c}) \leqslant \sum_{\substack{0\leqslant q_i\leqslant m_i,\ \overline{k}\geqslant 1 \\ q_1+\cdots+q_N+\overline{k}=k}} \prod_{i=1}^{N} C_{m_i}^{q_i} I_k^{q_1,\ldots,q_N|\overline{k}}(\Delta_1,\ldots,\Delta_N), \tag{A1}$$

where $C_m^k = m!/k!(m-k)!$. Let in the sequence $q_1,\ldots,q_N$ be nonzero correspondingly $q_{l_i}=k_{l_i}$ particles from Δ_{l_i}, $i=1,\ldots,M$ involved in k-body interaction. Changing in (A1) to the summation over $k_{l_1},\ldots,k_{l_M}$:

$$-W_k(\gamma_X|\overline{\gamma}_{X^c}) \leqslant \sum_{M=1}^{\min\{N,\,k-1\}} \sum_{1\leqslant l_1<l_2<\cdots<l_M\leqslant N} \sum_{\substack{1\leqslant k_{l_i}\leqslant m_{l_i},\ \overline{k}\geqslant 1 \\ k_{l_1}+\cdots+k_{l_M}+\overline{k}=k}} \prod_{i=1}^{M} C_{m_{l_i}}^{k_{l_i}} I_k^{k_{l_1},\ldots,k_{l_M}|\overline{k}}(\Delta_{l_1},\ldots,\Delta_{l_M}). \tag{A2}$$

Let among the cubes $\Delta_1,\ldots,\Delta_N$ be N_1 cubes with only one point of γ inside. Without loss of generality, we suppose that $m_j=1$, $j=N-N_1+1,\ldots,N$. We suppose also that $1\leqslant N_1<N$. Split the summation over $1\leqslant l_1<l_2<\cdots<l_M\leqslant N$ into the summation over $1\leqslant l_1<l_2<\cdots<l_S\leqslant N-N_1$ over cubes $\Delta_1,\ldots,\Delta_{N-N_1}$ and the summation over $1\leqslant l_1'<l_2'<\cdots<l_{S'}'\leqslant N_1$ over cubes $\Delta_1',\ldots,\Delta_{N_1}'$. It is clear that $S+S'=M$ and S can take integer values from 0 to M. Therefore, we get additionally $M+1$ sums over S. Every value of $1\leqslant l_1'<\cdots<l_{S'}'\leqslant N_1$ corresponds to the dilute configuration. Hence, using the definition (1) we can apply the following formula:

$$\sum_{1\leqslant l_1'<l_2'<\cdots<l_{S'}'\leqslant N_1} I_k^{k_{l_1},\ldots,k_{l_S},1,\ldots,1|\overline{k}}(\Delta_{l_1},\ldots,\Delta_{l_S},\Delta_{l_1'},\ldots,\Delta_{l_{S'}'}) \leqslant I_k^{k_{l_1},\ldots,k_{l_S}|\overline{k}+S'}(\Delta_{l_1},\ldots,\Delta_{l_S}),$$

yielding

$$-W_k(\gamma_X|\overline{\gamma}_{X^c}) \leqslant \sum_{M=1}^{\min\{N-N_1,\,k-1\}} \sum_{1\leqslant l_1<l_2<\cdots<l_M\leqslant N-N_1} \sum_{l=0}^{\min\{N_1,\,k-M-1\}} \sum_{\substack{1\leqslant k_{l_i}\leqslant m_{l_i},\ \overline{k}\geqslant 1 \\ k_{l_1}+\cdots+k_{l_M}+\overline{k}+l=k}} \prod_{i=1}^{M} C_{m_{l_i}}^{k_{l_i}}$$

$$\times I_k^{k_{l_1},\ldots,k_{l_M}|\overline{k}+l}(\Delta_{l_1},\ldots,\Delta_{l_M}) + N_* \sum_{l_1'=1}^{\min\{N_1,\,k-1\}} I_k^{1|k-1}(\Delta_{l_1}'),$$

where $N_*=\min\{N,k-1\}$. Collecting the terms with $M=1$, $k_{l_1}=1$ in the first sum and the last sum, and selecting also the terms with $k_{l_1}=k_{l_2}=\cdots=k_{l_M}=1$, summing up all inequalities in $k\geqslant 2$ and taking into account that $N_*\leqslant k-1$, we get

$$-W(\gamma_X|\overline{\gamma}_{X^c}) \leqslant \overline{I}|\gamma_X| + W_1 + W_2,$$

where

$$W_1 = \sum_{M=2}^{N-N_1} \sum_{1\leqslant l_1<l_2<\cdots<l_M\leqslant N-N_1} \prod_{i=1}^{M} C_{m_{l_i}}^{1} \sum_{k\geqslant M+1} (k-M) I_k^{1,\ldots,1|k-M}(\Delta_{l_1},\ldots,\Delta_{l_M}),$$

$$W_2 = \sum_{M=1}^{N-N_1} \sum_{1\leqslant l_1<l_2<\cdots<l_M\leqslant N-N_1} \sum_{k\geqslant M+1} \sum_{\substack{1\leqslant k_{l_i}\leqslant m_{l_i} \\ k_{l_1}+\cdots+k_{l_M}=k}} \prod_{i=1}^{M} C_{m_{l_i}}^{k_{l_i}} \times \sum_{l\geqslant 1} l I_{k+l}^{k_{l_1},\ldots,k_{l_M}|l}(\Delta_{l_1},\ldots,\Delta_{l_M}).$$

Using the same arguments, one can get almost the same inequality for the positive part of energy:

$$U^+(\gamma_X)\geqslant U_0,$$

where

$$U_0=\sum_{M=1}^{N-N_1}\sum_{1\leqslant l_1<l_2<\cdots<l_M\leqslant N-N_1}\sum_{k\geqslant M+1}\sum_{\substack{1\leqslant k_{l_i}\leqslant m_{l_i}\\ k_{l_1}+\cdots+k_{l_M}=k}}\prod_{i=1}^{M}C_{m_{l_i}}^{k_{l_i}}\times v_k^{k_{l_1},\ldots,k_{l_M}}(\Delta_{l_1},\ldots,\Delta_{l_M}).$$

Now it is clear from the assumptions **A6** that

$$\tfrac{1}{4}U_0\geqslant W_1,\quad \text{and}\quad \tfrac{1}{4}U_0\geqslant W_2,$$

which gives (16). It is not difficult to see (using direct computation) that condition $1\leqslant N_1<N$ is not essential in the proof of Lemma 3.2. ■

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Equilibrium states for the Bose gas

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The generating functional of the cyclic representation of the canonical commutation relations (CCR) representation for the thermodynamic limit of the grand canonical ensemble of the free Bose gas with attractive boundary conditions is rigorously computed. We use it to study the condensate localization as a function of the homothety point for the thermodynamic limit using a sequence of growing convex containers. The Kac function is explicitly obtained proving nonequivalence of ensembles in the condensate region in spite of the condensate density being zero locally. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1649793]

I. INTRODUCTION

The interest in the phenomenon of standard Bose Einstein Condensation (BEC) revived in recent years is due to the spectacular experimental work on Bosons in traps. We refer, e.g., to Refs. 9 and 12 for experimental and theoretical state of affairs. A renewed interest in old problems connected with the phase transition accompanying BEC is at order. The generic model for BEC is the free Bose gas as already was pointed out by Bose and Einstein in 1925. On the level of mathematical physics, the understanding of the phase transition started with the well known paper of Araki and Woods,[1] where the generating functionals of the cyclic representations of the canonical commutation relations corresponding to the equilibrium states of the free Bose gas are computed for periodic boundary conditions. Lewis and Pulé[7,8,11] computed the grand canonical equilibrium states for a set of boundary conditions including the Dirichlet and Neumann boundary conditions but not the attractive boundary conditions. They are using the Kac method. An important consequence of their result is the explicit computation of a nontrivial Kac density showing nonequivalence of the canonical and grand-canonical ensembles in the condensate region. The next result is found in Ref. 3, where the same conclusion was obtained for generalized condensations in some models of imperfect gases with diagonal interactions.

In the present paper we complete this computation of the equilibrium states for the free Bose gas with *attractive* boundary conditions. About the relevance of this type of boundary conditions, see, e.g., Refs. 4 and 10. This model has a particular type of condensation, namely, condensation in quantum states corresponding to isolated points in the spectrum. It is well known[5,10] that in this case the condensate is situated at the ''boundary'' and *not* uniformly spread out everywhere in space. We give a precise formulation of the generating functional in the frame of the theory of generating functionals on the CCR in order to catch up the condensate. Finally we derive also that there is *nonequivalence* of ensembles, something which was unclear until now because of the fact that the quantum fluctuations show a pattern[6] completely different from the free Bose gas with Dirichlet or Neumann boundary conditions. The intuition behind this fact is related to a wondering peculiarity of the free Bose gas with *attractive* boundary conditions.[5,10] If one takes the thermo-

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dynamic limit using a sequence of growing convex domains with the point of homothety at the origin of the coordinates, then *locally* the condensation density is always equal to zero. As a by-product, our computations imply that the condensate is spatially situated in a region logarithmically close to the boundary of these increasing domains. In the present paper we take different positions of the homothety point for cubic containers to show that the density of this logarithmic stratum of condensate inherits also a spacial anisotropy due to the choice of cubic containers. Finally remark that for the rotating bucket case,[11] one has also the effect of the condensate being increased at the boundary. But this is an effect of large angular momentum and not of the boundary conditions as in our case.

II. CCR-REPRESENTATIONS AND THE GENERATING FUNCTIONAL

For details about the CCR algebra, we refer to Ref. 2.

Let h be a complex pre-Hilbert space with inner product $(\cdot,\cdot)$. A representation of the CCR over h on a Hilbert space $\mathcal{H}$ is a map $f\mapsto W(f)$ of h into the group $\mathcal{U}(\mathcal{H})$ of unitary operators on a Hilbert space $\mathcal{H}$ satisfying the Weyl relations:

$$W(f_1)W(f_2)=\exp\left\{-\frac{\mathrm{i}}{2}\mathrm{Im}(f_1,f_2)\right\}W(f_1+f_2) \tag{2.1}$$

such that for each $f\in h$ the map $\lambda\mapsto W(\lambda f)$ of $\mathbb{R}$ into $\mathcal{U}(\mathcal{H})$ is strongly continuous. By Stone's theorem, this continuity condition implies the existence of self-adjoint operators $\Phi(f)$ such that

$$W(f)=\exp\{\mathrm{i}\Phi(f)\}. \tag{2.2}$$

These $\Phi(f)$ are called field operators. The map $f\mapsto\Phi(f)$ is linear over $\mathbb{R}$, but not linear over $\mathbb{C}$. Using the $\Phi(f)$ we can now define the creation and annihilation operators $a^*(f)$ and $a(f)$ for $f\in h$ by

$$a^*(f)=2^{-1/2}\{\Phi(f)-\mathrm{i}\Phi(\mathrm{i}f)\}, \tag{2.3}$$

$$a(f)=2^{-1/2}\{\Phi(f)+\mathrm{i}\Phi(\mathrm{i}f)\}. \tag{2.4}$$

A state on the CCR-algebra is a linear functional $\omega: h\to\mathbb{C}$ with the properties

$$\omega(A^*A)\geqslant 0,\quad \omega(\mathbf{1})=1,\quad \text{for } A \text{ linear combinations of the } W(f),\ f\in h.$$

A representation $(W,\mathcal{H},\Omega)$ is called a cyclic representation if Ω is a cyclic vector. A vector Ω is cyclic if the set $\{W(f)\Omega\}_{f\in h}$ is dense in $\mathcal{H}$. To each cyclic representation $(W,\mathcal{H},\Omega)$ of the CCR corresponds a generating functional $\mathbb{E}: h\to\mathbb{C}$ given by

$$\mathbb{E}(f)=\omega(W(f))=(\Omega,W(f)\Omega). \tag{2.5}$$

Proposition 2.1: A functional $\mathbb{E}: h\to\mathbb{C}$ is the generating functional of a cyclic representation of the CCR if and only if it satisfies the following conditions:

(i) $\mathbb{E}(0)=1$,

(ii) $\forall f\in h: \lambda\mapsto\mathbb{E}(\lambda f)$ *is continuous,*

(iii) $\forall$ *finite sets of complex numbers* $c_1,\ldots,c_n$ *and elements* $f_1,\ldots,f_n\in h$: $\Sigma_i\Sigma_j\mathbb{E}(f_i-f_j)\mathrm{e}^{(\mathrm{i}/2)\,\mathrm{Im}(f_i,f_j)}\overline{c_i}c_j\geqslant 0$.

III. KAC-DENSITY AND EQUIVALENCE OF ENSEMBLES

A. Concrete setup

Let $\Lambda_L^\nu=[-L/2,L/2]^\nu$ be a bounded region in $\mathbb{R}^\nu$ with volume $V=L^\nu$. We put $h_L=\mathcal{L}^2(\Lambda_L^\nu)$ for the Hilbert space of the wave functions in Λ_L^ν with the scalar product $(f,g)_{h_L}:=\int_{\Lambda_L^\nu}dx^\nu\overline{f(x)}g(x)$. Then $\Lambda_L^\nu\subseteq\Lambda_{L'}^\nu$ and $h_L\subseteq h_{L'}$ whenever $L\leqslant L'$ via natural imbedding.

Let t_L^σ be the self-adjoint extension of the operator $-\Delta_L$ (with domain $\mathrm{dom}(-\Delta_L)=C_0^\infty(\Lambda_L^\nu)$) determined by the boundary conditions $\partial_n\phi+\sigma\phi=0$ on $\partial\Lambda_L^\nu$. Here ∂_n is the directional derivative in the direction of the outward normal n to $\partial\Lambda_L^\nu$. If the parameter $\sigma<0$, we say that the boundary $\partial\Lambda_L^\nu$ is *attractive*.

First we have to solve the one-dimensional one-body eigenvalue problem on $\Lambda_L=[-L/2,L/2]$:

$$(t_L^\sigma\phi)(x)=\lambda\phi(x)$$

with boundary conditions ($\sigma<0$):

$$\begin{cases}\left(\dfrac{d\phi}{dx}-\sigma\phi\right)_{x=-L/2}=0,\\ \left(\dfrac{d\phi}{dx}+\sigma\phi\right)_{x=L/2}=0.\end{cases}$$

Due to these attractive boundary conditions, there are two negative eigenvalues tending to the same limit $-\sigma^2$ (when $L\to\infty$) and an infinite number of positive eigenvalues (for $L|\sigma|>2$):

$$\epsilon_L(0)<\epsilon_L(1)<0<\epsilon_L(2)<\epsilon_L(3)<\cdots,$$

$$\epsilon_L(0)=-\sigma^2-O(e^{-L|\sigma|}),$$

$$\epsilon_L(1)=-\sigma^2+O(e^{-L|\sigma|}),$$

$$k\geqslant 2:\quad \left(\frac{(k-1)\pi}{L}\right)^2<\epsilon_L(k)<\left(\frac{k\pi}{L}\right)^2. \tag{3.1}$$

The corresponding eigenfunctions $\{\phi_k^L\}_{k\in\mathbb{Z}_+}$ form a basis in h_L and are given by

$$\phi_0^L(x)=\sqrt{\frac{2}{L}}\left(1+\frac{\sinh(L|\sigma|)}{L|\sigma|}\right)^{-1/2}\cosh(-|\sigma|x),$$

$$\phi_1^L(x)=\sqrt{\frac{2}{L}}\left(-1+\frac{\sinh(L|\sigma|)}{L|\sigma|}\right)^{-1/2}\sinh(-|\sigma|x),$$

$$\phi_k^L(x)=\begin{cases}\sqrt{\dfrac{2}{L}}\left(1+\dfrac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1/2}\cos(\sqrt{\epsilon_L(k)}x), & \text{for } k \text{ even},\\ \sqrt{\dfrac{2}{L}}\left(1-\dfrac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1/2}\sin(\sqrt{\epsilon_L(k)}x), & \text{for } k \text{ odd}.\end{cases}$$

The eigenvalues and the wave functions of the corresponding multidimensional case have the form

$$E_L(\mathbf{k}) = \sum_{i=1}^{\nu} \epsilon_L(k_i),$$

$$\psi_{\mathbf{k}}^L(\mathbf{x}) = \prod_{i=1}^{\nu} \phi_{k_i}^L(x_i),$$

where $\mathbf{k} = \{k_i\}_{i=1}^{\nu} \in \mathbb{Z}_+^{\nu}$ and $\mathbf{x} = \{x_i\}_{i=1}^{\nu} \in \Lambda_L^{\nu}$.

B. Kac density

The Kac density relates expectation values of observables in the *canonical ensemble* and those in the *grand canonical ensemble*. The canonical equilibrium state for a free Bose gas in a cube Λ_L^{ν} of volume $V = L^{\nu}$ with total particle density ρ and inverse temperature β is given by

$$\omega_{L,\beta,\rho}^{\mathrm{can}}(A) = \frac{\mathrm{Tr}_{\mathcal{H}_{L,B}^{(n)}} A^{(n)} \mathrm{e}^{-\beta T_L^{\sigma,(n)}}}{\mathrm{Tr}_{\mathcal{H}_{L,B}^{(n)}} \mathrm{e}^{-\beta T_L^{\sigma,(n)}}}, \quad \text{where } n = [V\rho], \mathrm{dom}(A^{(n)}) \subset \mathcal{H}_L^{(n)}, \tag{3.2}$$

and $T_L^{\sigma,(n)}$ is the n-particle free Bose gas Hamiltonian in the cube Λ_L^{ν} with boundary conditions defined by σ. Now we consider the grand canonical equilibrium state at chemical potential μ and inverse temperature β,

$$\omega_{L,\beta,\mu}^{\mathrm{g.c.}}(A) = \frac{\mathrm{Tr}_{\mathcal{F}_{L,B}} A \exp\{-\beta(T_L^{\sigma} - \mu N_L)\}}{\mathrm{Tr}_{\mathcal{F}_{L,B}} \exp\{-\beta(T_L^{\sigma} - \mu N_L)\}}, \quad \mathrm{dom}(A) \subset \mathcal{F}_{L,B}. \tag{3.3}$$

Here $T_L^{\sigma} = \Sigma_{\mathbf{k} \in \mathbb{Z}_+^{\nu}} E_L(\mathbf{k}) a^*(\psi_{\mathbf{k}}^L) a(\psi_{\mathbf{k}}^L)$ is the free Bose gas Hamiltonian and $N_L = \Sigma_{\mathbf{k} \in \mathbb{Z}_+^{\nu}} N_{L,\mathbf{k}} = \Sigma_{\mathbf{k} \in \mathbb{Z}_+^{\nu}} a^*(\psi_{\mathbf{k}}^L) a(\psi_{\mathbf{k}}^L)$, is the particle number operator in $\mathcal{F}_{L,B}$, the boson Fock space over $\mathcal{L}^2(\Lambda_L^{\nu})$:

$$\mathcal{F}_{L,B} = \mathcal{F}_B(\mathcal{L}^2(\Lambda_L^{\nu})) = \bigoplus_{n=0}^{\infty} \mathcal{H}_{L,B}^{(n)} \tag{3.4}$$

with $\mathcal{H}_{L,B}^{(n)}$ the symmetrized n-particle Hilbert space appropriate for bosons and $\mathcal{H}_{L,B}^{(0)} = \mathbb{C}$.

Notice that in the thermodynamic limit $L \to \infty$ the canonical ensemble state $\omega_{\beta,\rho}^{\mathrm{can}}(\cdot)$ may not coincide with the equilibrium state of the grand canonical ensemble state $\omega_{\beta,\overline{\mu}(\beta,\rho)}^{\mathrm{g.c.}}(\cdot)$ for the corresponding particle density ρ. Here $\overline{\mu}(\beta,\rho) = \lim_{L\to\infty} \overline{\mu}_L(\beta,\rho)$ and $\overline{\mu}_L(\beta,\rho)$ is a solution of the grand canonical particle density equation (see also (3.22))

$$\rho = \omega_{L,\beta,\overline{\mu}_L(\beta,\rho)}^{\mathrm{g.c.}}(N_L/V). \tag{3.5}$$

By virtue of (3.4) the states (3.2) and (3.3) are related by

$$\omega_{L,\beta,\mu}^{\mathrm{g.c.}}(A) = \int_{\mathbb{R}_+} K_{L,\beta,\mu}^{\mathrm{g.c.}}(d\xi)\ \omega_{L,\beta,\xi}^{\mathrm{can}}(A^{([V\xi])}), \tag{3.6}$$

where $A^{(n)} = A \lceil \mathcal{H}_{L,B}^{(n)}$ is a restriction of the operator A on the subspace $\mathcal{H}_{L,B}^{(n)}$ and

$$K_{L,\beta,\mu}^{\mathrm{g.c.}}(\xi) = \frac{\sum_{n=0}^{[V\xi]} \exp(n\beta\mu) \mathrm{Tr}_{\mathcal{H}_{L,B}^{(n)}} \exp(-\beta T_L^{(n)})}{\mathrm{Tr}_{\mathcal{F}_{L,B}} \exp\{-\beta(T_L - \mu N_L)\}}. \tag{3.7}$$

For a given grand canonical density (3.5), the measure (3.7) takes the form

$$K_{L,\beta,\rho}(d\xi) := K^{\text{g.c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}(d\xi) = d\xi\, K_{L,\beta}(\xi;\rho), \tag{3.8}$$

and the limit $K_\beta(x;\rho) = \lim_{L\to\infty} K_{L,\beta}(x;\rho)$ is known as the *Kac density*, see, e.g., Ref. 7. If the Kac density happens to be a δ-function with support at ρ, then clearly one has (*strong*) equivalence of ensembles:

$$\omega^{\text{g.c.}}_{\beta,\bar{\mu}(\beta,\rho)}(A) = \omega^{\text{can}}_{\beta,\rho}(A). \tag{3.9}$$

Otherwise there is only *weak* equivalence of ensembles, see Ref. 3.

The limit $\rho_c(\beta) := \lim_{\mu\to-\nu\sigma^2} \lim_{L\to\infty} \omega^{\text{g.c.}}_{L,\beta,\mu}(N_L/V)$ is the critical density for the free Bose gas in a box with attractive boundary conditions. We shall show that in the model the canonical and the grand canonical ensembles are *not* equivalent in the *presence* of the Bose condensate, i.e., for $\rho > \rho_c(\beta)$, or for $\beta > \beta_c(\rho)$, where $\rho_c(\beta_c(\rho)) = \rho$. The nonequivalence of ensembles in the case of the free Bose gas with *attractive boundaries* is not the same phenomenon as in the case of the one with, for example Dirichlet, $\sigma = \infty$, or Neumann, $\sigma = 0$, boundary conditions. In the case of the attractive boundary conditions ($\sigma < 0$), the condensation phenomenon is a *surface effect* (not a bulk effect as in the free Bose gas with $\sigma = \infty$ or $\sigma = 0$): the condensate is located near the walls, see Sec. IV B.

To determine the Kac density, we have to calculate (see (3.6))

$$\begin{aligned}\omega^{\text{g.c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}(W(f)) &= \int_{\mathbb{R}_+} K_{L,\beta,\rho}(d\xi)\ \omega^{\text{can}}_{L,\beta,\xi}(W(f)) \\ &= \int_{\mathbb{R}_+} d\xi\ K_{L,\beta}(\xi;\rho)\,\omega^{\text{can}}_{L,\beta,\xi}(W(f))\end{aligned} \tag{3.10}$$

for any test function $f \in C_0^\infty(\mathbb{R}^\nu)$, the C^∞-functions on $\mathbb{R}^\nu$ with compact support. Therefore we first must calculate the limit of the expectation value of the exponential function:

$$\omega^{\text{g.c.}}_{\beta,\rho}(W(f)) := \lim_{L\to\infty} \omega^{\text{g.c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}(W(f)) \tag{3.11}$$

with $\{\bar{\mu}_L(\beta,\rho)\}_L$ solutions of the density equation (3.5).

This is possible because the states $\omega^{\text{g.c.}}_{L,\beta,\mu}$, where $\mu < -\nu\sigma^2$, are *quasifree states*, and these are easily obtained by using the *truncated functionals* $\omega_{L,\beta,\rho}(\cdots)_T$, see, e.g., Ref. 2. The functionals are defined by the recursion relations:

$$\omega^{\text{g.c.}}_{L,\beta,\mu}(A_1\cdots A_n) = \sum_{\tau\in P_n} \prod_{J\in\tau} \omega^{\text{g.c.}}_{L,\beta,\mu}(A_{j(1)},\ldots,A_{j(|J|)})_T \tag{3.12}$$

for all A_i ($i = 1,2$) creation or annihilation operators and $n \in \mathbb{N}$. The sum $\tau \in P_n$ is over all partitions τ of a set of n elements into ordered subsets $J = \{j(1),\ldots,j(|J|)\} \in \tau$. One can verify that the truncated functionals associated to the equilibrium states $\omega^{\text{g.c.}}_{L,\beta,\mu}$ satisfy

$$\begin{aligned}&\omega^{\text{g.c.}}_{L,\beta,\mu}(a^\sharp(f))_T = \omega^{\text{g.c.}}_{L,\beta,\mu}(a^\sharp(f)) = 0, \\ &\omega^{\text{g.c.}}_{L,\beta,\mu}(a^*(f_1),a^*(f_2))_T = \omega^{\text{g.c.}}_{L,\beta,\mu}(a(f_1),a(f_2))_T = 0, \\ &\omega^{\text{g.c.}}_{L,\beta,\mu}(a^*(f_1),a(f_2))_T = \left\langle f_2, \frac{1}{e^{\beta(t^\sigma_L-\mu)}-1} f_1 \right\rangle_{h_L},\end{aligned} \tag{3.13}$$

with $f, f_1, f_2, \ldots \in h_L$, the space of testfunctions with support in Λ_L^ν, $a^\sharp = \{a \text{ or } a^*\}$ and t_L^σ is the self-adjoint extension of the Laplacian $-\Delta_L$ corresponding to attractive boundary conditions $\sigma < 0$ on $\partial\Lambda_L^\nu$. Then the nontrivial two-point functions (3.13) are explicitly given by

$$\omega_{L,\beta,\mu}^{\text{g.c.}}(a^*(f_1), a(f_2))_T = \omega_{L,\beta,\mu}^{\text{g.c.}}(a^*(f_1)a(f_2)) = \sum_{\mathbf{k}\in\mathbb{Z}_+^\nu} \overline{\hat{f}_2(\mathbf{k})}\hat{f}_1(\mathbf{k}) \frac{1}{e^{\beta(E_L(\mathbf{k})-\mu)}-1}, \tag{3.14}$$

where the transformation $f(\mathbf{x}) \mapsto \hat{f}(\mathbf{k})$ of $f \in C_0^\infty(\mathbb{R}^\nu)$, is now defined by

$$\hat{f}(\mathbf{k}) := (\psi_{\mathbf{k}}^L, f)_{h_L} = \int_{\Lambda_L^\nu} d\mathbf{x}\, \overline{\psi_{\mathbf{k}}^L(\mathbf{x})} f(\mathbf{x}), \tag{3.15}$$

the Fourier transforms for the basis of t_L^σ (see Sec. III A). Now,

$$\omega_{L,\beta,\mu}^{\text{g.c.}}(W(f)) = \omega_{L,\beta,\mu}^{\text{g.c.}}(e^{i\Phi(f)}) = \exp \sum_{n=1}^{\infty} \frac{i^n}{n!} \omega_{L,\beta,\rho}(\underbrace{\Phi(f), \Phi(f), \ldots, \Phi(f)}_{\text{n times}})_T, \tag{3.16}$$

where the $\omega_{L,\beta,\mu}^{\text{g.c.}}(\Phi(f), \Phi(f), \ldots, \Phi(f))_T$ are the n-point truncated field correlation functions. Because of the fact that $\omega_{L,\beta,\mu}^{\text{g.c.}}$ is a quasifree state, only the two-point truncated correlation function is nonvanishing, yielding

$$\omega_{L,\beta,\mu}^{\text{g.c.}}(W(f)) = \exp(-\tfrac{1}{2}\omega_{L,\beta,\mu}^{\text{g.c.}}(\Phi(f), \Phi(f))_T). \tag{3.17}$$

By virtue of (2.3) and (2.4) it can be rewritten in terms of the creation and annihilation operators $a^*(f)$ and $a(f)$,

$$\omega_{L,\beta,\mu}^{\text{g.c.}}(\Phi(f), \Phi(f))_T = \tfrac{1}{2}(f,f)_{h_L} + \omega_{L,\beta,\mu}^{\text{g.c.}}(a^*(f)a(f)) \tag{3.18}$$

so that the explicit form of the generating functional (3.17) becomes

$$\omega_{\beta,\mu}^{\text{g.c.}}(W(f)) = \lim_{L\to\infty} \omega_{L,\beta,\mu}^{\text{g.c.}}(W(f)) = \exp(-\tfrac{1}{4}(f,f)_{h_L} - \tfrac{1}{2}\lim_{L\to\infty} \omega_{L,\beta,\mu}^{\text{g.c.}}(a^*(f)a(f))). \tag{3.19}$$

A last remark about the thermodynamic limit. Notice that the grand-canonical ensemble for the free Bose gas exists only for $\mu < \inf \operatorname{spec}(t_L^\sigma)$. Therefore, the solution of Eq. (3.5) verifies the inequality $\overline{\mu}_L(\beta,\rho) < -\nu\sigma^2$. Since the *critical density*,

$$\lim_{\mu\to -\nu\sigma^2} \lim_{L\to\infty} \omega_{L,\beta,\mu}^{\text{g.c.}}\left(\frac{N_L}{L^\nu}\right) = \rho_c(\beta) \tag{3.20}$$

for the free Bose gas with attractive boundary conditions $\sigma < 0$ is *finite* for all dimensions greater then, or equal to one,[5,10] Bose–Einstein condensation occurs for $\rho > \rho_c(\beta)$,

$$\rho_0(\beta) := \rho - \rho_c(\beta) = \lim_{L\to\infty} 2^\nu \omega_{L,\beta,\overline{\mu}_L(\beta,\rho)}^{\text{g.c.}}\left(\frac{N_{L,\mathbf{0}}}{L^\nu}\right) > 0, \tag{3.21}$$

where $N_{L,\mathbf{0}}$ is the number-operator on $\mathcal{F}_{L,B}$ of the zero mode $\mathbf{k} = \mathbf{0}$. The factor 2^ν is due to the asymptotic degeneracy of the $\inf \operatorname{spec}(t_L^\sigma) = -\nu\sigma^2 + O(e^{-L|\sigma|})$ for $L \to \infty$, see Sec. III A. Notice that (3.21) implies that the solution of (3.5) for $\rho > \rho_c(\beta)$ has the asymptotics,

$$\overline{\mu}_L(\beta,\rho) = -\nu\sigma^2 - \frac{2^\nu}{\beta(\rho-\rho_c(\beta))L^\nu} + o(L^{-\nu}). \tag{3.22}$$

We use this result in the computations of the thermodynamic limit of the generating functional below.

We conclude this section by the following statement about the explicit form of the Kac density for the thermodynamic limit of the free Bose gas in the *cubic* box with *attractive* boundary conditions.

Theorem 3.1: *For the free Bose gas T_L^σ with attractive boundary conditions $\sigma<0$ the limiting Kac density has the form*

$$K_\beta(\xi;\rho)=\begin{cases}\delta(\xi-\rho), & \text{for } \rho<\rho_c(\beta),\\ \dfrac{2^\nu\theta(\xi-\rho_c(\beta))}{(2^\nu-1)!(\rho-\rho_c(\beta))}\left[\dfrac{2^\nu(\xi-\rho_c(\beta))}{\rho-\rho_c(\beta)}\right]^{2^\nu-1}\exp\left\{-\dfrac{2^\nu(\xi-\rho_c(\beta))}{\rho-\rho_c(\beta)}\right\}, & \text{for } \rho\geqslant\rho_c(\beta).\end{cases} \tag{3.23}$$

Here $\theta(z\leqslant 0)=0$ and $\theta(z>0)=1$.

Proof: By the identity (3.10), the Kac density $K_\beta(\xi;\rho)$ is related to the thermodynamic limit of the characteristic function of the particle density N_L/V for $t\in\mathbb{R}^1$,

$$\begin{aligned}\lim_{L\to\infty}\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(\exp(itN_L/V))&=\int_{\mathbb{R}_+}K_{\beta,\rho}(d\xi)\ \omega^{\text{can}}_{\beta,\xi}(\exp(it\xi))\\ &=\int_{\mathbb{R}_+}d\xi\ K_\beta(\xi;\rho)\exp(it\xi).\end{aligned} \tag{3.24}$$

To calculate the limit in the left-hand side of (3.24), we use that the state $\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(\cdot)$ is quasifree. Then

$$\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(\exp(itN_L/V))=\prod_{\mathbf{k}\in\mathbb{Z}^\nu_+}\left\{\frac{1-\exp[-\beta(E_L(\mathbf{k})-\overline{\mu}_L(\beta,\rho))]}{1-\exp[-\beta(E_L(\mathbf{k})-\overline{\mu}_L(\beta,\rho)-it/\beta L^\nu)]}\right\}. \tag{3.25}$$

Since the 2^ν lowest energy-levels, i.e., the levels for which $\mathbf{k}\in\mathbb{K}_{\leqslant 2^\nu}=\{\mathbf{k}\in\mathbb{Z}^\nu_+ : k_i=0,1;\ i=1,\ldots,\nu\}$ are exponentially degenerated when $L\to\infty$: $E_L(\mathbf{k}\in\mathbb{K}_{\leqslant 2^\nu})=-\nu\sigma^2+O(e^{-L|\sigma|})$, by virtue of (3.22) and (3.25) we get that

$$\lim_{L\to\infty}\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(\exp(itN_L/V))=\begin{cases}\exp(it\rho), & \text{for } \rho<\rho_c(\beta),\\ [1-it2^{-\nu}(\rho-\rho_c(\beta))]^{-2^\nu}\exp(it\rho_c(\beta)), & \text{for } \rho\geqslant\rho_c(\beta).\end{cases} \tag{3.26}$$

Therefore, by (3.24), the Kac density (3.23) is the Fourier transformation of the right-hand side of (3.26).

IV. THE GENERATING FUNCTIONAL

A. Condensate and generating functional

We are interested in the thermodynamic limit of the generating functional $\omega^{\text{g.c.}}_{\beta,\rho}(W(f))=\lim_{L\to\infty}\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(W(f))$ for any $f\in C_0^\infty(\mathbb{R}^\nu)$. To this end we choose the box Λ_L^ν with L large enough such that the $\Lambda_f:=\text{supp}(f)$ is contained in Λ_L^ν. We consider here the generating functional $\omega^{\text{g.c.}}_{\beta,\rho}(W(f))$ for f an element in $C_0^\infty(\mathbb{R}^\nu)$.

Theorem 4.1: *The generating functional $\omega^{\text{g.c.}}_{\beta,\rho}(W(f))$ on $C_0^\infty(\mathbb{R}^\nu)$ is given by*

$$\omega^{\text{g.c.}}_{\beta,\rho}(W(f))=\exp(-\tfrac{1}{4}(f,f))\exp(-\tfrac{1}{2}(f,g_\sigma(\beta,\rho)f)), \tag{4.1}$$

with operator $g_\sigma(\beta,\rho)$ on $\mathcal{L}^2(\mathbb{R}^\nu)$ defined by

$$(g_\sigma(\beta,\rho)f)(\mathbf{x})=\int_{\mathbb{R}^\nu} d\mathbf{y} G_\sigma(\beta,\rho)(\|\mathbf{x}-\mathbf{y}\|)f(\mathbf{y}),$$

$$G_\sigma(\beta,\rho)(r)=(4\pi\beta)^{-\nu/2}\sum_{n=1}^{\infty} \mathrm{e}^{-r^2/4n\beta}\frac{\mathrm{e}^{-n\beta\overline{\mu}(\beta,\rho)}}{n^{\nu/2}}, \tag{4.2}$$

where $\overline{\mu}(\beta,\rho)<-\nu\sigma^2$ *for* $\rho<\rho_c(\beta)$ *and* $\overline{\mu}(\beta,\rho)=-\nu\sigma^2$ *for* $\rho\geqslant\rho_c(\beta)$ *are limiting solutions of the grand canonical density equation (3.5).*

Proof: In order to determine the generating functional $\omega^{\mathrm{g.c.}}_{\beta,\rho}(W(f))$, we have to compute $\lim_{L\to\infty}\omega^{\mathrm{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(f)a(f))$, see (3.19). Since the attractive boundary conditions $\sigma<0$ create a gap in the spectrum $\mathrm{spect}(t_L^\sigma)$, and, respectively, in $\mathrm{spect}(T_L^\sigma)$, the calculations need a separation of the negative eigenvalues from the positive part of the spectrum.

We consider first the one-dimensional case, when there are only two negative eigenvalues tending to $-\sigma^2$ for $L\to\infty$, see Sec. III A. By virtue of (3.14) one gets for a given $f\in C_0^\infty(\mathbb{R}^1)$ that

$$\begin{aligned}\lim_{L\to\infty}\omega^{\mathrm{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(f)a(f))&=\lim_{L\to\infty}\sum_{k\in\mathbb{Z}^1_+}|\hat{f}(k)|^2\frac{1}{\mathrm{e}^{\beta(\epsilon_L(k)-\overline{\mu}_L(\beta,\rho))}-1}\\&=\lim_{L\to\infty}\Bigg(|\hat{f}(0)|^2\frac{1}{\mathrm{e}^{\beta(\epsilon_L(0)-\overline{\mu}_L(\beta,\rho))}-1}+|\hat{f}(1)|^2\frac{1}{\mathrm{e}^{\beta(\epsilon_L(1)-\overline{\mu}_L(\beta,\rho))}-1}\\&\quad+\sum_{n=1}^{\infty}\mathrm{e}^{n\beta\overline{\mu}_L(\beta,\rho)}\sum_{k=2}^{\infty}\mathrm{e}^{-n\beta\epsilon_L(k)}|\hat{f}(k)|^2\Bigg).\end{aligned} \tag{4.3}$$

As mentioned before, we choose Λ_L large enough such that $\mathrm{supp}(f)=\Lambda_f$ is contained in Λ_L. Then one estimates that $|\hat{f}(0)|^2$ has an asymptotics of the order of $O(e^{-L|\sigma|})$ for large L since

$$\begin{aligned}|\hat{f}(0)|^2&=\left|\int_{\Lambda_f}dx f(x)\overline{\phi_0^L(x)}\right|^2\\&=\frac{2}{L}\left(1+\frac{\sinh(L|\sigma|)}{L|\sigma|}\right)^{-1}\left|\int_{\Lambda_f}dx f(x)\cosh(-|\sigma|x)\right|^2\\&=4|\sigma|e^{-L|\sigma|}\left|\int_{\Lambda_f}dx f(x)\cosh(-|\sigma|x)\right|^2+o(e^{-L|\sigma|}).\end{aligned} \tag{4.4}$$

The integral in the last expression is independent of L, because $\mathrm{supp}(f)$ is finite and inside the box Λ_L. Similarly one gets for $L\to\infty$ that

$$|\hat{f}(1)|^2=4|\sigma|e^{-L|\sigma|}\left|\int_{\Lambda_f}dx f(x)\sinh(-|\sigma|x)\right|^2+o(e^{-L|\sigma|}). \tag{4.5}$$

Consider now the coefficients of $|\hat{f}_L(0)|^2$ and of $|\hat{f}_L(1)|^2$ in (4.3). If $\rho<\rho_c(\beta)$, then $\overline{\mu}(\beta,\rho)<-\sigma^2$, i.e., $\epsilon_L(0)-\overline{\mu}_L(\beta,\rho)>0$ for large L. Therefore, by virtue of (4.3), (4.4), and (4.5), both of those terms are of the order $O(e^{-L|\sigma|})$ for large L. If $\rho\geqslant\rho_c(\beta)$, then $\overline{\mu}_L(\beta,\rho)=-\sigma^2+O(L^{-1})$, and one gets for large L,

$$\left\{|\hat{f}(0)|^2\frac{1}{\mathrm{e}^{\beta(\epsilon_L(0)-\overline{\mu}_L(\beta,\rho))}-1}+|\hat{f}(1)|^2\frac{1}{\mathrm{e}^{\beta(\epsilon_L(1)-\mu_L(\beta,\rho))}-1}\right\}\simeq\tfrac{1}{2}\rho_0(\beta)L\{|\hat{f}(0)|^2+|\hat{f}(1)|^2\}, \tag{4.6}$$

where $\rho_0(\beta)=\rho-\rho_c(\beta)$ is the condensate density. Therefore, again by virtue of (4.4) and (4.5), these terms vanish in the limit $L\to\infty$.

Consider now the last term in the limit (4.3). By virtue of (3.15) for $\nu=1$ (see Sec. III A) we can represent the sum over $k\geqslant 2$ in the following explicit form:

$$\frac{2}{L}\sum_{\{k\geqslant 2:\ \text{even}\}}\left(1+\frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1}\overline{\hat{F}_{L\ \text{even}}(k)}\hat{F}_{L\ \text{even}}(k)\mathrm{e}^{-s\epsilon_L(k)}$$
$$+\frac{2}{L}\sum_{\{k\geqslant 2:\ \text{odd}\}}\left(1-\frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1}\overline{\hat{F}_{L\ \text{odd}}(k)}\hat{F}_{L\ \text{odd}}(k)\mathrm{e}^{-s\epsilon_L(k)}, \tag{4.7}$$

where $s=n\beta$ and

$$\hat{F}_{L\ \text{even}}(k):=\int_{\Lambda_f}dx\cos(\sqrt{\epsilon_L(k)}x)f(x),\ \hat{F}_{L\ \text{odd}}(k):=\int_{\Lambda_f}dx\sin(\sqrt{\epsilon_L(k)}x)f(x). \tag{4.8}$$

Since the spectrum $\{\epsilon_L(k)\}_{k\geqslant 2}$ verifies the conditions (3.1) and $f\in C_0^\infty(\mathbb{R}^1)$, the first and the second series of terms in (4.7) are Darboux–Riemann sums for the corresponding integrals:

$$\lim_{L\to\infty}\left\{\frac{2}{L}\sum_{\{k\geqslant 2:\ \text{even}\}}\left(1+\frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1}\overline{\hat{F}_{L\ \text{even}}(k)}\,\hat{F}_{L\ \text{even}}(k)\mathrm{e}^{-s\epsilon_L(k)}\right.$$
$$\left.+\frac{2}{L}\sum_{\{k\geqslant 2:\ \text{odd}\}}\left(1-\frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L}\right)^{-1}\overline{\hat{F}_{L\ \text{odd}}(k)}\,\hat{F}_{L\ \text{odd}}(k)\mathrm{e}^{-s\epsilon_L(k)}\right\}$$
$$=\frac{1}{\pi}\int_0^\infty dk\,\overline{\mathrm{Re}(\mathrm{e}^{ik\cdot},f)_{h_L}}\,\mathrm{Re}(\mathrm{e}^{ik\cdot},f)_{h_L}\mathrm{e}^{-sk^2}+\frac{1}{\pi}\int_0^\infty dk\,\overline{\mathrm{Im}(\mathrm{e}^{ik\cdot},f)_{h_L}}\,\mathrm{Im}(\mathrm{e}^{ik\cdot},f)_{h_L}\mathrm{e}^{-sk^2}. \tag{4.9}$$

The last expression of (4.9) yields

$$\frac{1}{2\pi}\int_{-\infty}^\infty dk\,\overline{(\mathrm{e}^{ik\cdot},f)_{h_L}}\,(\mathrm{e}^{ik\cdot},f)_{h_L}\mathrm{e}^{-sk^2}=(4\pi s)^{-1/2}\int_{\mathbb{R}^1}dx\int_{\mathbb{R}^1}dy\,\overline{f(x)}f(y)\exp\left\{-\frac{|x-y|^2}{4s}\right\}. \tag{4.10}$$

Finally, taking into account (4.4)–(4.6), (4.10), and the fact that $\overline{\mu}(\beta,\rho)\leqslant-\sigma^2<0$, we get for the limit (4.3) in the one-dimensional case:

$$\omega^{\mathrm{g.c.}}_{\beta,\rho}(a^*(f)a(f))=(f,g_{\sigma,\nu=1}(\beta,\rho)f)_{h_L}, \tag{4.11}$$

where $g_{\sigma,\nu=1}(\beta,\rho)$ is the integral operator on $\mathcal{L}^2(\mathbb{R}^1)$ defined by

$$(g_{\sigma,\nu=1}(\beta,\rho)f)(x)=\int_{\mathbb{R}^1}dy\ \ G_{\sigma,\nu=1}(\beta,\rho)(|x-y|)f(y)\ ,$$

$$G_{\sigma,\nu=1}(\beta,\rho)(r)=(4\pi\beta)^{-1/2}\sum_{n=1}^\infty\mathrm{e}^{-r^2/4n\beta}\frac{\mathrm{e}^{-n\beta\overline{\mu}(\beta,\rho)}}{n^{1/2}}\ .$$

Using the results for the one-dimensional case, one computes the two-point correlation function $\omega^{\mathrm{g.c.}}_{\beta,\rho}(a^*(f)a(f))$ in the ν-dimensional case. Since the first 2^ν wave functions $\{\psi^L_{\mathbf{k}}(\mathbf{x})\}_{\mathbf{k}\in\mathbb{Z}^\nu_+}$ have the same exponential behavior as in the one-dimensional case and since $\inf_L\mathrm{spect}(t^\sigma_L)=-\nu\sigma^2$, see Sec. III A, we get

$$\lim_{L\to\infty}\omega^{\mathrm{g.c.}}_{L,\beta,\bar{\mu}(\beta,\rho)}(a^*(f)a(f))=\lim_{L\to\infty}\sum_{\mathbf{k}\in\mathbb{Z}^\nu_+}|\hat{f}(\mathbf{k})|^2\frac{1}{\mathrm{e}^{\beta(E_L(\mathbf{k})-\mu_L(\beta,\rho))}-1}$$

$$=\sum_{n=1}^{\infty}\mathrm{e}^{-n\beta\nu\bar{\mu}(\beta,\rho)}(4\pi n\beta)^{-\nu/2}\int_{\mathbb{R}^\nu}d\mathbf{x}\int_{\mathbb{R}^\nu}d\mathbf{y}\overline{f(\mathbf{x})}f(\mathbf{y})$$

$$\times\exp\left\{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4n\beta}\right\},$$

which implies (4.2). By virtue of (3.19) this finishes the proof of (4.1) and of the theorem for any particle density ρ.

Theorem 4.1 tells us that the condensate is not traceable by considering only strictly local observables. The characteristic functional on the CCR-C*-algebra of quasilocal observables coincides with the one without condensate. The reason for this is that the condensate is not homogeneous but located in the vicinity of the container boundary.

In order to catch up the presence of the condensate or to get a complete picture of the system, one has to extend the algebra of observables to the weak closure of the CCR-C*-algebra with respect to the limit Gibbs states. In the next paragraph we compute the limit functional on the relevant nonlocalized observables, and obtain a complete picture yielding the existence of sufficiently many fields in the representation of any w^*-limit point of Gibbs states as L tends to infinity. In fact our strategy will be to make a relevant choice of the *homothety point* for the thermodynamic limit of convex containers, in order to catch up the condensate.

Above and below we considered only the easy shape container limit, namely cubic boxes. Because of the particular inhomogeneous spreading of the condensate in the neighborhood of the box boundary, it is clear that this thermodynamic limit treatment can be very much shape dependent. In this paper we do not enter into the details of this specific problem.

B. Condensate localization

Remark 4.2: It sounds curious that in spite of the nonzero condensate density for $\rho>\rho_c(\beta)$, *(3.21), there is no trace of it in the generating functional (4.1). This is in contrast to the Kac density (3.23), which explicitly depends on the condensate density* $\rho-\rho_c(\beta)$. *To understand this difference one has to take into account that (4.1) is localized on the support of the function* $f\in C_0^\infty(\mathbb{R}^\nu)$, *whereas the Kac density is a global function, depending on the condensate even if it is localized at "infinity," sticked to the attractive boundaries.*

In order to make this statement rigorous we start first with the one-dimensional case. Let the function $f\in C_0^\infty(\mathbb{R}^1)$ be such that $\mathrm{supp}(f)=(-\delta,\delta)\subset(-L/2,L/2)$ and $\delta<(\ln L)/2|\sigma|$. Consider its shift over a distance $\gamma_L(\sigma):=L/2-(2|\sigma|)^{-1}\ln L$:

$$f_{\tau_{\gamma_L(\sigma)}}(x)\equiv(\tau_{\gamma_L(\sigma)}f)(x):=f(x-[L/2-(2|\sigma|)^{-1}\ln L]). \tag{4.12}$$

Then $f_{\tau_{\gamma_L(\sigma)}}\in C_0^\infty(-L/2,L/2)$.

To get the generating functional we compute now the limit of the corresponding two-point function (3.19):

$$\lim_{L\to\infty}\omega^{\mathrm{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(\tau_{\gamma_L(\sigma)}f)a(\tau_{\gamma_L(\sigma)}f))$$

$$=\lim_{L\to\infty}\sum_{k=0}^{\infty}|\hat{f}_{\tau_{\gamma_L(\sigma)}}(k)|^2\frac{1}{e^{\beta(\epsilon_L(k)-\mu_L(\beta,\rho))}-1}$$

$$=\lim_{L\to\infty}\left(|\hat{f}_{\tau_{\gamma_L(\sigma)}}(0)|^2\frac{1}{e^{\beta(\epsilon_L(0)-\overline{\mu}_L(\beta,\rho))}-1}+|\hat{f}_{\tau_{\gamma_L(\sigma)}}(1)|^2\frac{1}{e^{\beta(\epsilon_L(1)-\overline{\mu}_L(\beta,\rho))}-1}\right.$$

$$\left.+\sum_{k=2}^{\infty}|\hat{f}_{\tau_{[\gamma_L(\sigma)]}}(k)|^2\frac{1}{e^{\beta(\epsilon_L(k)-\mu_L(\beta,\rho))}-1}\right). \tag{4.13}$$

Remark 4.3: Notice that in contrast to (4.3), the shift (4.12) corresponds simply to the choice of a new point of homothety for the thermodynamic limit (4.13). In (4.3), the point of homothety coincides with the origin of coordinates $x=0$, whereas in (4.13) this point is $L/2-(2|\sigma|)^{-1}\ln L$.

Now, and in contrast to (4.4), $|\hat{f}_{\tau_{\gamma_L(\sigma)}}(0)|^2$ goes like L^{-1} for large L. Indeed,

$$|\hat{f}_{\tau_{\gamma_L(\sigma)}}(0)|^2=\left|\int_{\gamma_L(\sigma)-\delta}^{\gamma_L(\sigma)+\delta}dx(\tau_{\gamma_L(\sigma)}f)(x)\phi_0^L(x)\right|^2=|\sigma|L^{-1}\left|\int_{-\delta}^{\delta}dxf(x)e^{|\sigma|x}\right|^2+o(L^{-1}).$$

Remark that for $\rho>\rho_c(\beta)$ the first term in (4.13) remains now *finite* in the limit $L\to\infty$. Taking into account (3.21) and (3.22) one gets

$$\lim_{L\to\infty}|\hat{f}_{\tau_{\gamma_L(\sigma)}}(0)|^2\frac{1}{e^{\beta(\epsilon_L(0)-\overline{\mu}_L(\beta,\rho))}-1}=\frac{\rho_0(\beta,\rho)}{2}|\sigma|\left|\int_{-\delta}^{\delta}dxf(x)e^{|\sigma|x}\right|^2. \tag{4.14}$$

The same reasoning for the second term in formula (4.13) gives a similar result:

$$\lim_{L\to\infty}|\hat{f}_{\tau_{\gamma_L(\sigma)}}(1)|^2\frac{1}{e^{\beta(\epsilon_L(1)-\overline{\mu}_L(\beta,\rho))}-1}=\frac{\rho_0(\beta,\rho)}{2}|\sigma|\left|\int_{-\delta}^{\delta}dxf(x)e^{|\sigma|x}\right|^2. \tag{4.15}$$

By the same computations as used in the proof of Theorem 4.1, the third term in (4.13) yields for $\rho>\rho_c(\beta)$:

$$\lim_{L\to\infty}\sum_{k=2}^{\infty}|\hat{f}_{\tau_{\gamma_L(\sigma)}}(k)|^2\frac{1}{e^{\beta(\epsilon_L(k)-\overline{\mu}_L(\beta,\rho))}-1}$$

$$=\sum_{n=1}^{\infty}e^{-n\beta\sigma^2}(4\pi n\beta)^{-1/2}\int_{\mathbb{R}^1}dx\int_{\mathbb{R}^1}dyf(x)\overline{f(y)}\exp\left\{-\frac{|x-y|^2}{4n\beta}\right\}. \tag{4.16}$$

Hence the two-point function for the one-dimensional problem becomes

$$\lim_{L\to\infty}\omega^{\mathrm{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(\tau_{\gamma_L(\sigma)}f)a(\tau_{\gamma_L(\sigma)}f))$$

$$=\rho_0(\beta,\rho)|\sigma|\left|\int_{\mathbb{R}^1}dxf(x)e^{|\sigma|x}\right|^2+(f,g_{\sigma,\nu=1}(\beta,\rho)f), \tag{4.17}$$

see (4.11) for the definition of the operator $g_{\sigma,\nu=1}(\beta,\rho)$.

It is evident that one gets the same result for the shift of $\mathrm{supp}(f)=(-\delta,\delta)$ over a distance $-\gamma_L(\sigma)=-L/2+(2|\sigma|)^{-1}\ln L$, i.e.,

$$\lim_{L\to\infty} \omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(\tau_{\pm\gamma_L(\sigma)}f)a(\tau_{\pm\gamma_L(\sigma)}f))$$

$$=\rho_0(\beta,\rho)|\sigma|\left|\int_{\mathbb{R}^1} dx f(x)\mathrm{e}^{\pm|\sigma|x}\right|^2+(f,g_{\sigma,\nu=1}(\beta,\rho)f), \tag{4.18}$$

where

$$(\tau_{\pm\gamma_L(\sigma)}f)(x):=f(x\mp[L/2-(2|\sigma|)^{-1}\ln L]). \tag{4.19}$$

Therefore, taking the thermodynamic limit $L\to\infty$ at one of the homothety points $\pm\gamma_L(\sigma)$, we get that the generating functional depends on the Bose-condensate density for $\rho\geqslant\rho_c(\beta)$:

$$\lim_{L\to\infty} \omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(W(\tau_{\pm\gamma_L(\sigma)}f))=\exp(-\tfrac{1}{4}(f,f))\exp(-\tfrac{1}{2}C^{\pm}_{\sigma,\nu=1}(f)-\tfrac{1}{2}(f,g_{\sigma,\nu=1}f)), \tag{4.20}$$

where, by virtue of (4.18), one has

$$C^{\pm}_{\sigma,\nu=1}(f)=\rho_0(\beta,\rho)|\sigma|\left|\int_{\mathbb{R}^1} dx f(x)\mathrm{e}^{\pm|\sigma|x}\right|^2. \tag{4.21}$$

Remark 4.4: Notice that this result is due to a fine (logarithmic) tuning of the position of the homothety points $\pm\gamma_L(\sigma)$. *Indeed, take* $\pm\gamma_L(a\sigma)$, *for* $0<a<1$, *i.e., the homothety points are more distant from the boundary* $\pm L/2$. *Taking into account the explicit form of the eigenfunctions for* $k=0,1$ *one finds that now* $|\hat{f}_{\tau_{\pm\gamma_L(a\sigma)}}(k=0,1)|^2$ *goes for large* L *like* $L^{-1/a}$. *This implies that both limits (4.14) and (4.15), and hence (4.21), vanish. So, the generating functional (4.20) has the same form as for thermodynamic limit with the homothety point at the origin. In contrast to that, the choice* $1<a$ *means that the homothety points are closer to the boundaries* $\pm L/2$. *Then* $|\hat{f}_{\tau_{\pm\gamma_L(a\sigma)}}(k=0,1)|^2$ *goes slower then* L^{-1}. *This implies that both limits (4.14) and (4.15), and hence (4.21), becomes infinite. So, for* $\rho\geqslant\rho_c(\beta)$ *the generating functional (4.20) is zero, whereas for* $\rho<\rho_c(\beta)$ *it is nontrivial with* $C^{\pm}_{\sigma,\nu=1}(f)=0$.

To interpret these results, consider the *local* particle density:

$$\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(x)a(x))=\sum_{k\in\mathbb{Z}^{\nu=1}_+}\frac{|\phi^L_k(x)|^2}{\mathrm{e}^{\beta(\epsilon_L(k)-\overline{\mu}_L(\beta,\rho))}-1}. \tag{4.22}$$

Here $a(x)$ is the Bose-field operator such that $a(f)=\int_{\mathbb{R}^{\nu=1}}dx\overline{f(x)}a(x)$ for $f\in C^\infty_0(\Lambda^{\nu=1}_L)$ and $N(x)=a^*(x)a(x)$ is the local number operator, cf. (3.14). Then by (3.5) and (3.14), the global density is

$$\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}\left(\frac{N_L}{L}\right)=\frac{1}{L}\int_{\Lambda^{\nu=1}_L} dx\,\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(x)a(x)). \tag{4.23}$$

Consider the thermodynamic limit of the *local* particle density at the *origin* of the coordinates $x=0$. Taking into account the explicit form of the eigenfunctions, one gets that

$$\rho(\beta,\rho;x=0):=\lim_{L\to\infty}\omega^{\text{g.c.}}_{L,\beta,\overline{\mu}_L(\beta,\rho)}(a^*(x=0)a(x=0))=\frac{1}{\pi}\int_{\mathbb{R}^1_+} dk\frac{1}{\mathrm{e}^{\beta(k^2-\overline{\mu}(\beta,\rho))}-1} \tag{4.24}$$

for $\rho<\rho_c(\beta)$, and

$$\rho(\beta,\rho;x=0)=\lim_{L\to\infty}\omega^{\text{g.c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}(a^*(x=0)a(x=0))$$

$$=\frac{1}{\pi}\int_{\mathbb{R}^1_+}dk\,\frac{1}{e^{\beta(k^2+\sigma^2)}-1}=\rho_c(\beta) \tag{4.25}$$

for $\rho\geqslant\rho_c(\beta)$ by (3.22). By inspection of (4.24) and (4.25) based on the explicit formulas for the eigenfunctions one readily gets that

$$\rho(\beta,\rho;x)=\rho(\beta,\rho;x=0) \tag{4.26}$$

for any x in a *bounded* domain D, containing the origin of the coordinates $x=0$. In particular we get that the limiting *local* density for $x\in D$ corresponding to the first two modes ($k=0,1$) is

$$\rho_0(\beta,\rho;x):=\lim_{L\to\infty}\sum_{k=0,1}\frac{|\phi^L_k(x=0)|^2}{e^{\beta(\epsilon_L(k)-\bar{\mu}_L(\beta,\rho))}-1}=0. \tag{4.27}$$

On the other hand, the *global* Bose–Einstein condensation density (3.21) is also related exactly to these two modes:

$$\rho_0(\beta,\rho)=\lim_{L\to\infty}\frac{1}{L}\sum_{k=0,1}\frac{1}{e^{\beta(\epsilon_L(k)-\bar{\mu}_L(\beta,\rho))}-1}=\rho-\rho_c(\beta)>0, \tag{4.28}$$

which is not present in (4.25).

Consider now the local density of the Bose–Einstein condensation (4.27) at the homothety points $\pm\gamma_L(\sigma)$. Then taking into account the explicit form of the eigenfunctions $\phi^L_{k=0,1}(x)$ and (3.22), we get that, in contrast to (4.27), the *local condensate* density is

$$\lim_{L\to\infty}\sum_{k=0,1}\frac{|\phi^L_k(x=\pm\gamma_L(\sigma))|^2}{e^{\beta(\epsilon_L(k)-\mu_L(\beta,\rho))}-1}=\rho_0(\beta,\rho)|\sigma|. \tag{4.29}$$

The same arguments as above show that this condensate local density varies from *zero* to *infinity* when the parameter a in the homothety point positions $\pm\gamma_L(a\sigma)$ varies in the same interval.

Remark 4.5: These observations can be interpreted as follows: the Bose–Einstein condensate for attractive boundary conditions $\sigma<0$ is localized in a logarithmically narrow domain in the vicinity of the boundary. In other words this kind of condensation is a surface phenomenon. At the same time globally it is very "visible," since the Kac density indicates a nonequivalence of ensembles in the presence of the condensate, see Theorem 3.1.

For the generalization to the ν-dimensional case, we start with the corresponding *local condensate* density:

$$\rho_0(\beta,\rho;\mathbf{x}):=\lim_{L\to\infty}\sum_{\mathbf{k}\in\{\mathbb{Z}^\nu_+\,:\,k_\alpha=0,1\,;\,\alpha=1,\ldots,\nu\}}\frac{|\psi^L_{\mathbf{k}}(\mathbf{x})|^2}{e^{\beta(E_L(\mathbf{k})-\bar{\mu}_L(\beta,\rho))}-1}. \tag{4.30}$$

Let $\mathbf{x}$ belong to a bounded domain D^ν, containing the origin of the coordinates $\mathbf{x}=\mathbf{0}$. Then using the explicit expressions for the eigenfunctions $\psi^L_{\mathbf{k}}(\mathbf{x})$, see Sec. III.A, and by the same arguments as above for $\nu=1$, we obtain that the limit (4.30) is *zero* for all densities $\rho>0$.

The *product* structure: $\psi^L_{\mathbf{k}}(\mathbf{x})=\Pi^\nu_{i=1}\phi^L_{k_i}(x_i)$, implies that this conclusion does not change if we consider instead of $\mathbf{x}\in D^\nu$, the condensate density in the vicinity of the points corresponding to the shifts where at *least one* among the ν arguments remains *unshifted*.

On the other hand, this structure and the asymptotics of $\phi^L_{k=0,1}(x)$ for $|x|\to\infty$ yields also that for any $\mathbf{k}\in\{\mathbb{Z}^\nu_+:k_\alpha=0,1\,;\,\alpha=1,\ldots,\nu\}$ one gets

$$\left(\prod_{\alpha=1}^{\nu}\tau_{\pm\gamma_L(a_\alpha\sigma)}\psi_{\mathbf{k}}^L\right)(\mathbf{x}=0)=|\sigma|^{\nu/2}L^{-(1/2)(a_1^{-1}+a_2^{-1}+\cdots+a_\nu^{-1})}+o(L^{-(1/2)(a_1^{-1}+a_2^{-1}+\cdots+a_\nu^{-1})}) \tag{4.31}$$

as $L\to\infty$. Then, by virtue of (3.22), the limit for the local condensate density becomes *nontrivial:*

$$\lim_{L\to\infty}\sum_{\mathbf{k}\in\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\ \alpha=1,\ldots,\nu\}}\frac{\left|\left(\prod_{\alpha=1}^{\nu}\tau_{\pm\gamma_L(a_\alpha\sigma)}\psi_{\mathbf{k}}^L\right)(\mathbf{x}=0)\right|^2}{e^{\beta(E_L(\mathbf{k})-\mu_L(\beta,\rho))}-1}=|\sigma|^\nu(\rho-\rho_c(\beta))>0, \tag{4.32}$$

if and only if

$$a_1^{-1}+a_2^{-1}+\cdots+a_\nu^{-1}=\nu. \tag{4.33}$$

This means that the condensate (up to logarithmic deviations) is localized essentially in the *corners* of the hypercube Λ_L^ν, where $L\to\infty$. We proved the following statement:

Theorem 4.6: *Let* $\mathbf{x}$ *be in a bounded domain* D^ν*, containing the origin of the coordinates* $\mathbf{x}=\mathbf{0}$*, then the thermodynamic limit of the local particle density is*

$$\rho(\beta,\rho;\mathbf{x}):=\lim_{L\to\infty}\sum_{\mathbf{k}\in\mathbb{Z}_+^\nu}\frac{|\psi_{\mathbf{k}}^L(\mathbf{x})|^2}{e^{\beta(E_L(\mathbf{k})-\mu_L(\beta,\rho))}-1}=\frac{1}{\pi^\nu}\int_{\mathbb{R}_+^\nu}d\mathbf{k}\frac{1}{e^{\beta(\mathbf{k}^2-\overline{\mu}(\beta,\rho))}-1}, \tag{4.34}$$

where $\overline{\mu}(\beta,\rho)<-\nu\sigma^2$ *for* $\rho<\rho_c(\beta)$ *and* $\overline{\mu}(\beta,\rho)=-\nu\sigma^2$ *for* $\rho\geqslant\rho_c(\beta)$*. Thus* $\rho(\beta,\rho;\mathbf{x})=\rho_c(\beta)$ *for* $\rho\geqslant\rho_c(\beta)$*, i.e., the local condensate density* $\rho_0(\beta,\rho;\mathbf{x})=0$ *for any* $\rho>0$*. Whereas at the homothety points corresponding to the shifts* $\Pi_{\alpha=1}^\nu\tau_{\pm\gamma_L(a_\alpha\sigma)}$ *with parameters satisfying (4.33), the local condensate density (4.32) is nontrivial. Moreover, besides being inhomogeneous it is also anisotropic and essentially localized in the directions of the corners of the hypercube* $\Lambda_{L\to\infty}^\nu$*. Varying the parameters* $\{a_\alpha\}_{\alpha=1}^\nu$ *in the range* $(0,+\infty)$ *one finds this local condensate density varying from zero to infinity.*

Now we extend Theorem 4.1 on the basis of our discussion above of the condensate localization and Theorem 4.6. Similar to the one-dimensional case, see Remark 4.4, our relevant localized observable in the ν-dimensional case will be a function $f\in\mathcal{C}_0^\infty(\mathbb{R}^\nu)$ such that $\mathrm{supp}(f)=(-\delta_1,\delta_1)\times(-\delta_2,\delta_2)\times\cdots\times(-\delta_\nu,\delta_\nu)\subset\Lambda_L^\nu$ and with $\delta=\max_{i=1,\ldots,\nu}\delta_i$ such that $\delta<(\ln L)/2|\sigma|$. Consider in each coordinate the shift over a distance $\gamma_L(\sigma)=L/2-(2|\sigma|)^{-1}\ln L$:

$$\left(\prod_{\alpha=1}^{\nu}\tau_{\gamma_L(\sigma)}f\right)(\mathbf{x})=f(x_1-(L/2-(2|\sigma|)^{-1}\ln L),\ldots,x_\nu-(L/2-(2|\sigma|)^{-1}\ln L)),$$

then $\Pi_{\alpha=1}^\nu\tau_{\gamma_L(\sigma)}f\in\mathcal{C}_0^\infty(\Lambda_L^\nu)$.

To get the generating functional in the ν-dimensional case, we compute the limit of the corresponding two-point correlation function:

$$\lim_{L\to\infty}\omega^{\text{g. c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}\left(a^*\left(\prod_{\alpha=1}^{\nu}\tau_{\gamma_L(\sigma)}f\right)a\left(\prod_{\alpha=1}^{\nu}\tau_{\gamma_L(\sigma)}f\right)\right)$$

$$=\lim_{L\to\infty}\sum_{\mathbf{k}\in\mathbb{Z}_+^\nu}\left|\prod_{\alpha=1}^{\nu}(\hat{f}_{\tau_{\gamma_L(\sigma)}})(\mathbf{k})\right|^2\frac{1}{e^{\beta(E_L(\mathbf{k})-\bar{\mu}_L(\beta,\rho))}-1}$$

$$=\lim_{L\to\infty}\left(\sum_{\mathbf{k}\in\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\alpha=1,\ldots,\nu\}}\left|\prod_{\alpha=1}^{\nu}(\hat{f}_{\tau_{\gamma_L(\sigma)}})(\mathbf{k})\right|^2\frac{1}{e^{\beta(E_L(\mathbf{k})-\bar{\mu}_L(\beta,\rho))}-1}\right.$$

$$\left.+\sum_{n=1}^{\infty}e^{n\beta\bar{\mu}_L(\beta,\rho)}\sum_{\mathbf{k}\in\mathbb{Z}_+^\nu\setminus\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\ \alpha=1,\ldots,\nu\}}e^{-n\beta E_L(\mathbf{k})}\left|\prod_{\alpha=1}^{\nu}(\hat{f}_{\tau_{\gamma_L(\sigma)}})(\mathbf{k})\right|^2\right). \tag{4.35}$$

This thermodynamic limit depends on the homothety point corresponding to the shifts $\Pi_{\alpha=1}^{\nu}\tau_{\pm\gamma_L(a_\alpha\sigma)}$ with parameters $a_\alpha=1$. Notice that the factor $|\Pi_{\alpha=1}^{\nu}\hat{f}_{\tau_{\gamma_L(\sigma)}}(\mathbf{k})|^2$ is of the order $O(L^{-\nu})$ for large L:

$$\left|\prod_{\alpha=1}^{\nu}\hat{f}_{\tau_{\gamma_L(\sigma)}}(\mathbf{k})\right|^2=\left|\int_{\gamma_L(\sigma)-\delta_1}^{\gamma_L(\sigma)+\delta_1}dx_1\cdots\int_{\gamma_L(\sigma)-\delta_\nu}^{\gamma_L(\sigma)+\delta_\nu}dx_\nu\prod_{\alpha=1}^{\nu}(\tau_{\gamma_L(\sigma)}f)(\mathbf{x})\overline{\psi^L_{\mathbf{k}}(\mathbf{x})}\right|^2$$

$$=|\sigma|^\nu L^{-\nu}\left|\int_{\text{supp}(f)}d\mathbf{x}\,f(\mathbf{x})\prod_{\alpha=1}^{\nu}e^{|\sigma|x_\alpha}\right|^2+o(L^{-\nu}), \tag{4.36}$$

and for any $\mathbf{k}\in\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\alpha=1,\ldots,\nu\}$. Hence, by the same reasoning, which implies (4.32), the first 2^ν terms in (4.35) give

$$\lim_{L\to\infty}\sum_{\mathbf{k}\in\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\alpha=1,\ldots,\nu\}}\left|\prod_{\alpha=1}^{\nu}(\hat{f}_{\tau_{\gamma_L(\sigma)}})(\mathbf{k})\right|^2\frac{1}{e^{\beta(E_L(\mathbf{k})-\bar{\mu}_L(\beta,\rho))}-1}$$

$$=\rho_0(\beta,\rho)|\sigma|^\nu\left|\int_{\mathbb{R}^\nu}d\mathbf{x}\,f(\mathbf{x})\prod_{i=1}^{\nu}e^{|\sigma|x_i}\right|^2. \tag{4.37}$$

For the last term in (4.35), we perform the computations as in Theorem 4.1, yielding

$$\lim_{L\to\infty}\sum_{\mathbf{k}\in\mathbb{Z}_+^\nu\setminus\{\mathbb{Z}_+^\nu:k_\alpha=0,1;\ \alpha=1,\ldots,\nu\}}\left|\prod_{\alpha=1}^{\nu}\hat{f}_{\tau_{\gamma_L(\sigma)}}(\mathbf{k})\right|^2\frac{1}{e^{\beta(E_L(\mathbf{k})-\bar{\mu}_L(\beta,\rho))}-1}$$

$$=\sum_{n=1}^{\infty}e^{-n\nu\beta\sigma^2}(4\pi n\beta)^{-\nu/2}\int_{\mathbb{R}^\nu}d\mathbf{x}\int_{\mathbb{R}^\nu}d\mathbf{y}f(\mathbf{x})\overline{f(\mathbf{y})}\exp\left\{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4n\beta}\right\}. \tag{4.38}$$

So, taking the thermodynamic limit $L\to\infty$ at one of the homothety points $\{\pm\gamma_L(\sigma)\}_{\alpha=1}^{\nu}$, we get now the generating functional for $\rho\geqslant\rho_c(\beta)$:

$$\lim_{L\to\infty}\omega^{\text{g. c.}}_{L,\beta,\bar{\mu}_L(\beta,\rho)}\left(\prod_{\alpha=1}^{\nu}W(\tau_{\pm\gamma(\sigma)}f)\right)$$

$$=\exp(-\tfrac{1}{4}(f,f))\exp(-\tfrac{1}{2}C_\sigma^{\pm}(\beta,\rho)(f)-\tfrac{1}{2}(f,g_\sigma(\beta,\rho)f)) \tag{4.39}$$

with

$$C_{\sigma}^{\pm}(\beta,\rho)(f)=\rho_0(\beta,\rho)|\sigma|^{\nu}\left|\int_{\mathbb{R}^{\nu}}d\mathbf{x}\,f(\mathbf{x})\prod_{\alpha=1}^{\nu}\mathrm{e}^{\pm|\sigma|x_{\alpha}}\right|^2. \tag{4.40}$$

Remark 4.7: Again this result is due to a fine (logarithmic) tuning of the position of the homothety points $\{\pm\gamma_L(\sigma)\}_{\alpha=1}^{\nu}$ *in the corner directions of the hypercube* Λ_L^{ν}. *Indeed, take as in Theorem 4.6 the shifts* $\Pi_{\alpha=1}^{\nu}\tau_{\pm\gamma_L(a_{\alpha}\sigma)}$, *with* $\Sigma_{\alpha=1}^{\nu}(a_{\alpha})^{-1}>\nu$, *i.e., the homothety points are more distant from the corners of the hypercube. Taking into account the explicit form of the eigenfunctions for* $\mathbf{k}\in\{\mathbb{Z}_+^{\nu}:k_{\alpha}=0,1;\alpha=1,\ldots,\nu\}$, *one finds now that* $|\Pi_{\alpha=1}^{\nu}\hat{f}_{\tau_{\gamma_L(a_{\alpha}\sigma)}}(\mathbf{k})|^2$ *with* $\mathbf{k}\in\{\mathbb{Z}_+^{\nu}:k_{\alpha}=0,1;\alpha=1,\ldots,\nu\}$ *goes like* $L^{-(a_1^{-1}+a_2^{-1}+\cdots+a_{\nu}^{-1})}$ *for large* L. *This implies that the limits of the first* 2^{ν} *terms (4.37), and hence (4.40), vanish. So, the generating functional (4.39) has the same form as for the thermodynamic limit with the homothety point at the origin* $\mathbf{x}=\mathbf{0}$. *In contrast to that, the choice* $0<\Sigma_{\alpha=1}^{\nu}(a_{\alpha})^{-1}<\nu$ *means that the homothety points are too close to the corners of the hypercube* Λ_L^{ν}. *Then* $|\Pi_{\alpha=}^{\nu}\hat{f}_{\tau_{\pm\gamma_L(a_{\alpha}\sigma)}}(\mathbf{k})|^2$ *with* $\mathbf{k}\in\{\mathbb{Z}_+^{\nu}:k_{\alpha}=0,1;\alpha=1,\ldots,\nu\}$ *goes to zero slower then* $L^{-\nu}$. *This implies that the limit (4.40) becomes infinite. So, for* $\rho\geqslant\rho_c(\beta)$ *the generating functional (4.39) is zero, whereas for* $\rho<\rho_c(\beta)$ *it is nontrivial with* $C_{\sigma}^{\pm}(f)=0$.

Therefore, we proved the following theorem:

Theorem 4.8: *The generating functional* $\lim_{L\to\infty}\omega_{L,\beta,\bar{\mu}_L(\beta,\rho)}^{\mathrm{g.\,c.}}(\Pi_{\alpha=1}^{\nu}W(\tau_{\pm\gamma(a_{\alpha}\sigma)}f))$ *on* $C_0^{\infty}(\mathbb{R}^{\nu})$ *is given by*

$$\lim_{L\to\infty}\omega_{L,\beta,\bar{\mu}_L(\beta,\rho)}^{\mathrm{g.\,c.}}\left(\prod_{\alpha=1}^{\nu}W(\tau_{\pm\gamma(a_{\alpha}\sigma)}f)\right)$$

$$=\exp(-\tfrac{1}{4}(f,f))\exp(-\tfrac{1}{2}C_{\mathbf{a}\sigma}^{\pm}(\beta,\rho)(f)-\tfrac{1}{2}(f,g_{\sigma}(\beta,\rho)f)), \tag{4.41}$$

with

$$C_{\mathbf{a}\sigma}^{\pm}(\beta,\rho)(f)=\rho_0(\beta,\rho)|\sigma|^{\nu}\left|\int_{\mathbb{R}^{\nu}}d\mathbf{x}\,f(\mathbf{x})\prod_{i=1}^{\nu}\mathrm{e}^{\pm|\sigma|x_i}\right|^2\chi_{\nu}(\mathbf{a}),$$

$$(g_{\sigma}(\beta,\rho)f)(\mathbf{x})=\int_{\mathbb{R}^{\nu}}d\mathbf{y}G_{\sigma}(\beta,\rho)(\|\mathbf{x}-\mathbf{y}\|)f(\mathbf{y}),$$

$$G_{\sigma}(\beta,\rho)(r)=(4\pi\beta)^{-\nu/2}\sum_{n=1}^{\infty}\mathrm{e}^{-r^2/4n\beta}\frac{\mathrm{e}^{-n\beta\nu\sigma^2}}{n^{\nu/2}}.$$

Here $\bar{\mu}(\beta,\rho)<-\nu\sigma^2$ *for* $\rho<\rho_c(\beta)$ *and* $\bar{\mu}(\beta,\rho)=-\nu\sigma^2$ *for* $\rho\geqslant\rho_c(\beta)$ *are the limiting solutions of the grand canonical density equation (3.5),* $\rho_0(\beta,\rho)=0$ *for* $\rho<\rho_c(\beta)$ *whereas* $\rho_0(\beta,\rho)=\rho-\rho_c(\beta)$ *for* $\rho\geqslant\rho_c(\beta)$ *and the function* $\chi_{\nu}(\mathbf{a})=0,1,+\infty$, *respectively, for* $\nu<\Sigma_{\alpha=1}^{\nu}(a_{\alpha})^{-1}$, $\nu=\Sigma_{\alpha=1}^{\nu}(a_{\alpha})^{-1}$, *and* $\nu>\Sigma_{\alpha=1}^{\nu}(a_{\alpha})^{-1}$.

V. CONCLUDING REMARKS

The main results of our analysis for the free Bose gas with attractive boundary conditions are contained in the Theorems 3.1, 4.1, and 4.8.

In Theorem 3.1, we obtain a Kac density function showing nonequivalence of the canonical and the grand canonical ensemble in the presence of the condensate even if the condensate density is locally zero.

We learn from Theorem 4.1 that the condensation is not visible in the expectation values of strictly localized observables because the Bose condensate is situated near the boundary of an ''infinite container.'' Nevertheless one should observe the effects of condensation in the equilibrium states, i.e., in the generating functional.

Theorem 4.8 yields the answer. We make precise for which type of observables the equilibrium states show their dependence on the condensate. This completes the rigorous analysis of the problem of (non)equivalence of ensembles for the free Bose gas with attractive boundary conditions and the inhomogeneous condensate localization.

Finally we repeat that we analyzed only the problem taking the thermodynamic limits in the sense of homothetically increasing cubes, with the consequence that the condensate is situated anisotropically in the direction of the corners of these cubes and is ''localized at infinity.'' To prove this we tune the homothety point position at the logarithmic (in the units of the cube size) distance from the cube boundary. If instead one looks for the limit of spherical containers, this anisotropy in the positioning of the condensate should disappear. Does one expect spontaneous spherical symmetry breaking of the equilibrium states in this case?

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Noncommutative geometry of super-Jordanian $OSp_h(2/1)$ covariant quantum space

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Extending a recently proposed procedure of construction of various elements of differential geometry on noncommutative algebras, we obtain these structures on noncommutative superalgebras. As an example, a quantum superspace covariant under the action of super-Jordanian $OSp_h(2/1)$ is studied. It is shown that there exist a two-parameter family of torsionless connections, and the curvature computed from this family of connections is bilinear. It is also shown that the connections are not compatible with the metric. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Noncommutative geometry is one of the active fields in recent theoretical physics and mathematics. The physical interests seem to be focused on noncommutative differential geometry, since it plays crucial roles in the context of string theory and quantum gravity.[1,2] There exists various approaches to noncommutative differential calculus. For instance, Connes' approach involves the Dirac operator,[1] Dubois–Violette's method is based on derivations,[3] and studies based on quantum groups also exist.[4–6] Analogs of Riemannian connection, curvature and metric on noncommutative algebra $\mathcal{A}$ were introduced in Ref. 7, where the authors used only the left $\mathcal{A}$-module structure of the differential forms. On the other hand, the $\mathcal{A}$-bimodule structure of an algebra of differential forms was used to define a linear connection for a particular differential calculus based on derivations.[8] Mourad also made essential use[9] of the $\mathcal{A}$-bimodule structure to define linear connection, torsion, and curvature on a noncommutative algebra $\mathcal{A}$. In the procedure used in Ref. 9, a noncommutative generalization of the permutation operator on two copies of one-forms was introduced. The generalized permutation operator plays a role in defining the noncommutative differential geometry. A general notion of connection based on a generalized transposition operator was introduced in Ref. 10. The above methodology was found to be useful in other approaches to the noncommutative differential calculi. Furthermore, it was extended to other studies concerning differential calculi on noncommutative algebras such as $SL_q(2)$ covariant quantum plane,[11] two-parameter quantum plane,[12] Jordanian h-deformed quantum plane,[13,14] matrix geometries,[15] and so on. The curvatures corresponding to the connections were also studied[8,9,16] in this context.

In the present work, we follow the line of investigation developed in Refs. 8, 9, 16 to study the noncommutative differential geometry associated with the quantized supergroups. It will be seen that the ideas used there are also appropriate for studying noncommutative differential geometry on quantum superspaces. Following Refs. 8, 9, 16 we can naturally define linear connections, torsions, curvatures, and metrics on noncommutative quantum superspaces. As an example, we will study the quantum superspace covariant under the action of super-Jordanian deformation of OSp(2/1). The super-Jordanian $OSp_h(2/1)$ is introduced as a Hopf algebra dually related to the recently obtained triangular deformation of Lie superalgebra osp(2/1);[17] and it coincides with the deformed OSp(2/1) supergroup studied by Juszczak and Sobczyck.[18] We obtain the most general

form of linear connections on the quantum superspace covariant under the action of $\mathrm{OSp}_h(2/1)$. The curvatures and the metric will also be studied in the sequel.

We first briefly review the construction of a linear connection in a commutative geometry.[9] Let $\mathcal{M}$ be a manifold, and $C(\mathcal{M})$ be an algebra of functions on $\mathcal{M}$. The set of k-forms is denoted by Ω^k. The covariant derivative D is a linear map from Ω^1 to $\Omega^1 \otimes_{C(\mathcal{M})} \Omega^1$ obeying the Leibnitz rule

$$D(f\xi) = df \otimes \xi + fD\xi, \quad f \in C(\mathcal{M}), \quad \xi \in \Omega^1. \tag{1.1}$$

Since functions commute with forms, the Leibnitz rule may also be recast as

$$D(\xi f) = \sigma(\xi \otimes df) + (D\xi) f, \tag{1.2}$$

where σ is a permutation acting on $\Omega^1 \otimes_{C(\mathcal{M})} \Omega^1$:

$$\sigma(\xi \otimes \eta) = \eta \otimes \xi, \quad \xi, \eta \in \Omega^1; \tag{1.3}$$

and the exterior derivative d is nilpotent: $d^2 = 0$. In the context of commutative geometry the two Leibnitz rules (1.1) and (1.2) are equivalent. However, in the noncommutative setting this is not the case, as functions and forms do not commute. The noncommutative covariant derivative is constructed in such a way that it is required[9] to satisfy the two Leibnitz rules. Reflecting the noncommutative nature of functions and forms, the operator σ can no longer be represented by a simple permutation element. It needs to be modified for noncommutative quantum spaces.

Suppose the manifold $\mathcal{M}$ is parallelizable and let ω^i be an arbitrary basis element of Ω^1. The covariant derivative of a one-form is then uniquely determined by $D\omega^i$. The linear connection is defined by $\Gamma^i = -D\omega^i$. Namely, the covariant derivative defines the linear connection. Throughout this article, we use the terms ''linear connection'' and ''covariant derivative'' synonymously. Let π be a projection of $\Omega^1 \otimes_{C(\mathcal{M})} \Omega^1$ onto Ω^2 such that $\pi(\xi \otimes \eta) = \xi \wedge \eta$. Then the map $\Theta: \Omega^1 \to \Omega^2$ defined by $\Theta = d - \pi \circ D$ is a bimodule homomorphism, that is, it maintains $\Theta(f\xi) = f\Theta(\xi)$ and $\Theta(\xi f) = \Theta(\xi) f$, where $f \in C(\mathcal{M})$. The torsion is defined by $\Theta(\omega^i)$. This construction of linear connections will be extended to noncommutative superspaces associated with quantum supergroups.

This paper is organized as follows: In the next section, we extend the differential geometry on noncommutative algebras to noncommutative superalgebras. The super-Jordanian deformation of OSp(2/1) is introduced in Sec. III. The quantum superspace which is covariant under the action of super-Jordanian $\mathrm{OSp}_h(2/1)$ is introduced, and the differential calculus on it in the sense of Wess–Zumino is constructed in Sec. IV. The linear connection on the quantum superspace is studied in Sec. V, and it is observed that the most general torsionless connection is a member of a two-parameter family. In Sec. VI, the curvature obtained from the linear connection is calculated and it is shown that the curvature is bilinear. The metric of the quantum superspace is also studied. We show that the covariant derivative is not compatible with the metric. Section VII contain the concluding remarks.

II. NONCOMMUTATIVE EXTENSION OF SUPERSPACE GEOMETRY

Let $\mathcal{A}$ be a noncommutative algebra with $\mathbb{Z}_2$ grading. The grading is specified by parity of elements of $\mathcal{A}$. An even (odd) element $f \in \mathcal{A}$ has a parity $\hat{f} = 0\ (1)$. It is assumed that a differential calculus over $\mathcal{A}$, describing, in particular, the one-forms and their commutation relations with the elements of $\mathcal{A}$, has been constructed. Let $\Omega^k(\mathcal{A})$ and d denote the space of k-forms over $\mathcal{A}$ and the exterior derivative, respectively. The covariant derivative D is defined as a map $D: \Omega^1 \to \Omega^1 \otimes_{\mathcal{A}} \Omega^1$ subject to the following Leibnitz rules:

$$D(f\xi) = df \otimes \xi + (-1)^{\hat{f}} fD\xi, \tag{2.1}$$

$$D(\xi f) = (-1)^{\hat{\xi}} \sigma(\xi \otimes df) + (D\xi) f, \quad f \in \Omega^0, \quad \xi \in \Omega^1, \tag{2.2}$$

where $\sigma:\Omega^1\otimes_{\mathcal{A}}\Omega^1\to\Omega^1\otimes_{\mathcal{A}}\Omega^1$ refers to a noncommutative generalization of the permutation map. The covariant derivative changes the parity of a k-form ξ by unity: $\widehat{D\xi}=\hat{\xi}+1$, (mod 2). In the commutative case where $\sigma(\xi\otimes\eta)=(-1)^{\hat{\xi}\hat{\eta}}\eta\otimes\xi$, the two Leibnitz rules (2.1) and (2.2) are equivalent up to an overall sign

$$D(\xi f)=(-1)^{\hat{\xi}\hat{f}}D(f\xi). \tag{2.3}$$

Using the definition of the covariant derivative, one can show that the map σ is $\mathcal{A}$-bilinear

$$\sigma(f\xi\otimes\eta)=f\sigma(\xi\otimes\eta),\quad \sigma(\xi\otimes\eta f)=\sigma(\xi\otimes\eta)f,\quad f\in\Omega^0,\quad \xi,\eta\in\Omega^1. \tag{2.4}$$

We now demonstrate the first relation in (2.4). The second relation in (2.4) follows similarly. For arbitrary elements $f,g\in\Omega^0$ and $\xi\in\Omega^1$, we compute $D(f\xi g)$ in two different ways. Regarding it as $D(f\cdot\xi g)$, we apply (2.1) and obtain

$$D(f\xi g)=df\otimes\xi g+(-1)^{\hat{f}}fD(\xi g)=df\otimes\xi g+(-1)^{\hat{f}+\hat{\xi}}f\sigma(\xi\otimes dg)+(-1)^{\hat{f}}f(D\xi)g.$$

Alternately, for the choice $D(f\xi g)=D(f\xi\cdot g)$ the Leibnitz rule (2.2) yields

$$D(f\xi g)=(-1)^{\hat{f}+\hat{\xi}}\sigma(f\xi\otimes dg)+df\otimes\xi g+(-1)^{\hat{f}}f(D\xi)g.$$

As the above two computations must give identical results, it follows $\sigma(f\xi\otimes dg)=f\sigma(\xi\otimes dg)$.

The covariant derivative may be extended as a linear map from the n-fold tensored space $\otimes^n\Omega^1$ to the $(n+1)$-fold tensored space $\otimes^{(n+1)}\Omega^1$. This is done recurrently while maintaining the following extension of the Leibnitz rule

$$D(\omega\otimes\omega')=D\omega\otimes\omega'+(-1)^{\hat{\omega}}\sigma_{12}(\omega\otimes D\omega'), \tag{2.5}$$

where $\omega\in\Omega^1$, $\omega'\in\otimes^{n-1}\Omega^1$ and σ_{12} has a nontrivial structure in the first two sectors:

$$\sigma_{12}=\sigma\otimes\underbrace{1\otimes 1\otimes\cdots\otimes 1}_{n-1\text{ times}}. \tag{2.6}$$

Let π be a projection of $\Omega^1\otimes_{\mathcal{A}}\Omega^1$ onto Ω^2 defined by the wedge product on the forms

$$\pi(\xi\otimes\eta)=\xi\wedge\eta. \tag{2.7}$$

The noncommutativity of $\mathcal{A}$, in general, demands $\xi\wedge\eta\neq-\eta\wedge\xi$. Employing the projection operator π, we define the torsion Θ of the covariant derivative D as a map $\Theta:\Omega^1\to\Omega^2$

$$\Theta:\Omega^1\to\Omega^2,\quad \Theta=d-\pi\circ D. \tag{2.8}$$

The torsion is always left $\mathcal{A}$-linear, whereas the condition

$$\pi\circ(\sigma-1)=0 \tag{2.9}$$

is necessary for it to be right $\mathcal{A}$-linear. More explicitly, the torsion satisfies the relations

$$\Theta(f\xi)=(-1)^{\hat{f}}f\Theta(\xi),\quad \Theta(\xi f)=\Theta(\xi)f,\quad f\in\Omega^0,\ \xi\in\Omega^1. \tag{2.10}$$

The condition (2.9) is necessary for the validity of the second relation in (2.10). Note that the relation (2.9) has a sign difference from the nongraded case.[11,15] Since the proof is straightforward, we show only the second relation. The exterior derivative acts on the one-form ξf as follows:

$$d(\xi f)=(d\xi)f+(-1)^{\hat{\xi}}\xi\wedge df=(d\xi)f+(-1)^{\hat{\xi}}\pi(\xi\otimes df),$$

while the action of $\pi\circ D$ on ξf reads

$$\pi\circ D(\xi f)=\pi((-1)^{\hat{\xi}}\sigma(\xi\otimes df)+(D\xi)f).$$

Consequently, it follows

$$\Theta(\xi f)=\Theta(\xi)f-(-1)^{\hat{\xi}}\pi\circ(\sigma-1)(\xi\otimes df).$$

It is thus evident that condition (2.9) needs to be satisfied for the torsion Θ to be right $\mathcal{A}$-linear.

The curvature is defined by the following map:[16]

$$\pi_{12}D^2 \;:\; \Omega^1\to\Omega^2\otimes_{\mathcal{A}}\Omega^1, \tag{2.11}$$

where $\pi_{12}=\pi\otimes 1$. The torsionless condition $\Theta=0$ and the validity of the constraint (2.9) require the curvature to be left $\mathcal{A}$-linear:

$$\pi_{12}D^2(f\xi)=f\pi_{12}D^2(\xi),\quad f\in\Omega^0,\;\; \xi\in\Omega^1. \tag{2.12}$$

We demonstrate this below. Employing the Leibnitz rule (2.5), we compute

$$D^2(f\xi)=Ddf\otimes\xi+(-1)^{\widehat{df}}\sigma_{12}(df\otimes D\xi)+(-1)^{\hat{f}}df\otimes D\xi+fD^2\xi.$$

The left-hand side in (2.12) now reads

$$\pi_{12}D^2(f\xi)=\pi\circ Ddf\otimes\xi-(-1)^{\hat{f}}\pi_{12}\circ(\sigma_{12}-1)(df\otimes D\xi)+f\pi_{12}D^2(\xi).$$

The first and second terms in the above expression vanish because of the torsionless condition and the constraint (2.9), respectively. Thus the curvature is left $\mathcal{A}$-linear. In general, the curvature is not right $\mathcal{A}$-linear. It is, however, known that there exist some cases for nongraded $\mathcal{A}$ where the curvature is right $\mathcal{A}$-linear.[11] We will find such an example for graded $\mathcal{A}$ in the following sections.

Now let us define a metric. A metric g is a nondegenerate $\mathcal{A}$-bilinear map

$$g \;:\; \Omega^1\otimes_{\mathcal{A}}\Omega^1\to\mathcal{A}. \tag{2.13}$$

The metric is said to be nondegenerate if the following conditions hold: $g(\xi\otimes\eta)=0$ for all $\eta\in\Omega^1$ implies $\xi=0$, and, simultaneously, $g(\xi\otimes\eta)=0$ for all $\xi\in\Omega^1$ implies $\eta=0$. Symmetry of the metric is defined by using the extended permutation σ. A metric satisfying $g\circ\sigma=g$ ($g\circ\sigma=-g$) is known to be symmetric (skew-symmetric) in nature. If the following diagram is commutative, the covariant derivative D is said to be compatible with the metric g, or, in short, D is said to be metric:

$$\begin{array}{ccc}
\Omega^1\otimes_{\mathcal{A}}\Omega^1 & \overset{D}{\longrightarrow} & \Omega^1\otimes_{\mathcal{A}}\Omega^1\otimes_{\mathcal{A}}\Omega^1 \\
g\downarrow & & 1\otimes g\downarrow \\
\mathcal{A} & \overset{d}{\longrightarrow} & \Omega^1.
\end{array}$$

More explicitly, the above compatibility condition reads

$$d\circ g=(1\otimes g)\circ D. \tag{2.14}$$

In the following sections an example of the differential geometry described here will be presented. In this example, the algebra $\mathcal{A}$ is taken to be a quantum superspace covariant under the action of a quantum supergroup $OSp_h(2/1)$. The example will be constructed so as to keep the covariance of all relations.

III. SUPER-JORDANIAN DEFORMATION OF OSp(2/1)

In this section we introduce a quantum deformation of the supergroup OSp(2/1). The conventions adopted here regarding the graded Yang–Baxter equation are same as in Refs. 19 and 20. The quantum supergroup discussed here is the dual Hopf algebra to the super-Jordanian deformed $U_h(\mathrm{osp}(2/1))$ algebra introduced recently. The study of super-Jordanian osp(2/1) algebra was initiated by Kulish.[21] It was further developed by the works of the present authors[17] and Borowiec *et al.*[22] In Ref. 17, the universal $\mathcal{R}$ matrix of the $U_h(\mathrm{osp}(2/1))$ algebra was obtained up to $O(h^3)$ where h is the deformation parameter. Its limiting classical value is described by $h\to 0$. The fundamental representation of the generators of the $U_h(\mathrm{osp}(2/1))$ algebra is obtained by mapping the deformed algebra on its classical counterpart. Although the two deformation maps given in Ref. 17 provide two distinct sets of matrices for the fundamental representation, the pertinent R matrices computed for these two cases are identical. All the terms in the universal $\mathcal{R}$ matrix $O(h^3)$ and above vanish in the fundamental representation, and, therefore, the R matrix in the said representation is determined by the terms up to $O(h^2)$. The R matrix, thus obtained, is given by

$$R=\left(\begin{array}{ccc|ccc|ccc}
1 & \cdot & -h & \cdot & h & \cdot & h & \cdot & h^2/2 \\
\cdot & 1 & \cdot & \cdot & \cdot & -h & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & -h \\
\hline
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & h & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & -h \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & h \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{array}\right), \tag{3.1}$$

where the dot $(\cdot)$ is used instead of 0 for better readability. The R matrix (3.1) solves the graded Yang–Baxter equation. The inverse of this R matrix is given by $R^{-1}=R(-h)$; and identifying $h=-p$ in (3.1) the R-matrix given in Ref. 18 is reproduced. In Ref. 21, a contraction technique is applied to the R matrix in the fundamental representation of the $U_q(\mathrm{osp}(2/1))$ algebra to obtain a triangular $\tilde{R}$ matrix, which maintains the relation $\tilde{R}^{k\ell}_{ij}=R^{\ell k}_{ji}$ with the R matrix given in (3.1).

Now we explicitly write down the nonstandard deformed supergroup $OSp_h(2/1)$. Since the R matrix (3.1) is the inverse of the one used in Ref. 18, the quantum supergroup $OSp_h(2/1)$ is identical to the one given in Ref. 18, where the deformed supergroup $OSp_h(2/1)$ is constructed by the FRT (Ref. 23) method. Let the inverse scattering matrix T in the fundamental representation of the super-Jordanian deformed $OSp_h(2/1)$ is given by

$$T=(t^i_j)=\left(\begin{array}{ccc} a & \alpha & b \\ \gamma & e & \beta \\ c & \delta & d \end{array}\right), \tag{3.2}$$

where $\hat{i}=0(1)$ for $i=\{1,3\}(\{2\})$, and $\hat{t}^i_j=\hat{i}+\hat{j}$. Thus the entries a,b,c,d,e are even elements, whereas α, β, γ, δ are odd ones. The RTT relation and deformed orthosymplectic conditions

$$T^{\mathrm{st}}JT=J,\quad TJ^{-1}T^{\mathrm{st}}=J^{-1},\quad J=\begin{pmatrix}0&0&1\\0&1&0\\-1&0&-h/2\end{pmatrix} \tag{3.3}$$

determine the relations among the entries of T. The supertransposition of T is defined by $(T^{\mathrm{st}})^i_j=(-1)^{\hat{i}(\hat{i}+\hat{j})}t^j_i$. The matrix J corresponds to the matrix C^{-1} in Ref. 18. An error contained in C of Ref. 18 is corrected. It follows from this definition that $(AB)^{\mathrm{st}}=B^{\mathrm{st}}A^{\mathrm{st}}$, $((A^{\mathrm{st}})^{\mathrm{st}})^i_j=(-1)^{\hat{i}+\hat{j}}A^i_j$. Note that the matrix J has the property

$$(-1)^{\hat{a}+\hat{b}}J_{ab}=J_{ab}. \tag{3.4}$$

This simplifies many relations in the later computations. Following Ref. 18 we express the elements e,β, and γ in terms of the remaining elements a,b,c,d,α. The commutation relations satisfied by the elements a,b,c,d,α and δ are summarized as

$$\begin{gathered}[a,b]=h(1-a^2),\quad [a,c]=hc^2,\quad [a,d]=h(cd-ca),\\ [a,\alpha]=0,\quad [a,\delta]=hc\delta,\quad [b,c]=h(ca+dc),\\ [b,d]=h(d^2-1),\quad [b,\alpha]=h\alpha a,\quad [b,\delta]=h(d\delta+c\alpha),\\ [c,d]=-hc^2,\quad [c,\alpha]=-hc\delta,\quad [c,\delta]=0,\\ [d,\alpha]=h(\delta a-\delta d),\quad [d,\delta]=h\delta c,\quad \{\alpha,\delta\}=h(ac-\delta^2),\\ \alpha^2=\frac{h}{2}(a^2-1),\quad \delta^2=\frac{h}{2}c^2.\end{gathered} \tag{3.5}$$

The other entries of T may be algebraically solved as follows:

$$e=1+\alpha\delta-\frac{h}{2}ac,\quad \beta=\alpha d-\delta b-h\delta d-\frac{h}{2}\gamma,\quad \gamma=\alpha c-\delta a-h\delta c. \tag{3.6}$$

Relations analogous to the classical supergroup OSp(2/1) exist for the nonstandard deformation:

$$ad-bc+\alpha\delta+\frac{h}{2}ac=1,\quad e^{-1}=\left(1-\alpha\delta+\frac{h}{2}ac\right)\left(1-\frac{h^2}{4}c^2\right)^{-1},\quad \alpha\delta+\beta\gamma=\frac{h}{2}(ac-dc). \tag{3.7}$$

For completeness, we also give the commutation relations involving the elements e,β, and γ:

$$\begin{gathered}[a,e]=h\gamma\delta,\quad [b,e]=h(\beta\delta+\gamma\alpha),\quad [c,e]=0,\\ [d,e]=h\gamma\delta,\quad [e,\alpha]=h(e\delta+\gamma a),\quad [e,\beta]=h(d\delta+\gamma e),\\ [e,\gamma]=hc\delta,\quad [e,\delta]=hc\gamma,\quad [a,\beta]=h(\gamma d-\gamma a),\\ [b,\beta]=h\beta d,\quad [c,\beta]=-hc\gamma,\quad [d,\beta]=0,\\ \{\alpha,\beta\}=h(ea-ed),\quad \{\beta,\gamma\}=-h(dc+\gamma^2),\quad \{\beta,\delta\}=hce,\\ [a,\gamma]=h\gamma c,\quad [b,\gamma]=h(\beta c+\gamma a),\quad [c,\gamma]=0,\\ [d,\gamma]=hc\gamma,\quad \{\alpha,\gamma\}=-hce,\quad \{\gamma,\delta\}=0,\\ \beta^2=\frac{h}{2}(1-d^2),\gamma^2=-\frac{h}{2}c^2.\end{gathered} \tag{3.8}$$

As a consequence of the grading, the RTT relation

$$\sum_{x,y} (-1)^{\hat{y}(\hat{x}+\hat{i})} R_{xy}^{k\ell}\, t_i^x\, t_j^y = \sum_{x,y} (-1)^{\hat{y}(\hat{k}+\hat{x})} t_y^\ell\, t_x^k\, R_{ij}^{xy} \tag{3.9}$$

involves extra sign factors in the tensor products of T and the identity matrix.

The coalgebra mappings of the quantum supergroup $OSp_h(2/1)$ are, as usual, given by

$$\Delta(T) = T \dot{\otimes} T, \quad \epsilon(T) = \mathrm{diag}(1,1,1). \tag{3.10}$$

The antipode is obtained from the coproduct:

$$S(T) = \begin{pmatrix} d+\frac{h}{2}c & -\beta-\frac{h}{2}\gamma & -b-\frac{h}{2}(a-d)+\frac{h^2}{4}c \\ \delta & e & -\alpha+\frac{h}{2}\delta \\ -c & \gamma & a-\frac{h}{2}c \end{pmatrix} = J^{-1}T^{\mathrm{st}}J. \tag{3.11}$$

It is easy to see that $TS(T) = S(T)T = \mathrm{diag}(1,1,1)$.

IV. DIFFERENTIAL CALCULUS ON QUANTUM SUPERSPACE

In this section, a quantum superspace covariant under the action of $OSp_h(2/1)$ is introduced and a differential calculus in the sense of Wess and Zumino[6] is constructed. The quantum superspace is a graded algebra, denoted by $\mathcal{A}$, generated by two odd (θ_1, θ_2) and one even (x) elements. The defining relations of the algebra $\mathcal{A}$ read

$$[\theta_1, x] = -hx\theta_2, \quad \{\theta_1, \theta_2\} = 0, \quad [\theta_2, x] = 0,$$

$$\theta_1^2 = -\frac{h}{2}(x^2 - 2\theta_1\theta_2), \quad \theta_2^2 = 0. \tag{4.1}$$

It is straightforward to verify that the relations (4.1) are preserved under the action of $OSp_h(2/1)$ from the left

$$\begin{pmatrix} \theta_1' \\ x' \\ \theta_2' \end{pmatrix} = \begin{pmatrix} a & \alpha & b \\ \gamma & e & \beta \\ c & \delta & d \end{pmatrix} \begin{pmatrix} \theta_1 \\ x \\ \theta_2 \end{pmatrix}. \tag{4.2}$$

The quantum superspace (4.1) has an important difference from that associated to the Jordanian quantum supergroup $GL_h(1/1)$ discussed in Refs. 24 and 25. In the quantum superspace covariant under the action of $GL_h(1/1)$, the deformation parameter h is a Grassmann variable, whereas the quantity h in (4.1) commute with all elements of the quantum superspace.

A scalar element φ exists in the quantum superspace $\mathcal{A}$:

$$\varphi \equiv X^{\mathrm{st}} J X = x^2 - 2\theta_1\theta_2, \tag{4.3}$$

where

$$X = \begin{pmatrix} \theta_1 \\ x \\ \theta_2 \end{pmatrix}, \quad X^{\mathrm{st}} = (-\theta_1, x, -\theta_2). \tag{4.4}$$

Then it is easy to show that φ is preserved by the left action of $\mathrm{OSp}_h(2/1)$. Note that the parity of components of X is $\hat{X}^i = 1 + \hat{i} \pmod 2$. The fourth relation in (4.1) implies that θ_1^2 is also a scalar in the algebra $\mathcal{A}$. Employing a solution of the nongraded Yang-Baxter equation the defining relations (4.1) of the algebra $\mathcal{A}$ may be written in a compact form:

$$X^i X^j = \sum_{k,\ell} B^{ij}_{k\ell} X^\ell X^k, \quad B_{12}B_{13}B_{23} = B_{23}B_{13}B_{12}, \tag{4.5}$$

where the matrix B reads

$$B(h) = \left(\begin{array}{ccc|ccc|ccc} -1 & \cdot & -h & \cdot & -h & \cdot & h & \cdot & -h^2/2 \\ \cdot & 1 & \cdot & \cdot & \cdot & -h & \cdot & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & -h \\ \hline \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & h & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & -h \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & h \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 \end{array}\right). \tag{4.6}$$

The matrix B is related to the R matrix of the deformed supergroup $\mathrm{OSp}_h(2/1)$ as

$$R(h)^{k\ell}_{xy} = (-1)^{1+\hat{k}+(1+\hat{x})\hat{y}} (B(h)^{-1})^{k\ell}_{xy} = (-1)^{1+\hat{k}+\hat{y}+\hat{k}\hat{l}} B(-h)^{k\ell}_{xy}, \tag{4.7}$$

where the last equality follows from the relation $(B(h)^{-1})^{k\ell}_{xy} = (-1)^{\hat{k}\hat{\ell}+\hat{x}\hat{y}} B(-h)^{k\ell}_{xy}$.

The differential calculus on quantum space is an algebra generated by coordinates X^i, differentials $\Xi^i \equiv dX^i$ and derivatives $\partial_i = \partial/\partial X^i$. The parity of differentials and derivatives are, in general, $\hat{\Xi}^i = 1 + \hat{X}^i$, $\hat{\partial}_i = \hat{X}^i$. The differential calculus on quantum superspace using solutions of the nongraded Yang–Baxter equation is developed in Ref. 26. These authors require the exterior derivative d, which maps a k-form to a $(k+1)$-form, to maintain three properties: (i) nilpotency, (ii) graded Leibnitz rule

$$d(f \wedge g) = (df) \wedge g + (-1)^{\hat{f}} f \wedge dg, \quad f \in \Omega^p, \ g \in \Omega^q, \tag{4.8}$$

and (iii) its action on a function $f(X^i)$ is given by $df = \Sigma_i \Xi^i \partial_i f$. Employing these properties, the following commutation relations among X^i, Ξ^i and ∂_i may be determined:

$$\Xi^i \wedge \Xi^j = \sum_{k,\ell} (-1)^{\hat{X}^i + \hat{\Xi}^\ell} B^{ij}_{k\ell} \Xi^\ell \wedge \Xi^k, \quad X^i \Xi^j = \sum_{k,\ell} (-1)^{\hat{X}^i} B^{ij}_{k\ell} \Xi^\ell X^k,$$

$$\partial_j X^i = \delta_{ij} + \sum_{k,\ell} B^{i\ell}_{kj} X^k \partial_\ell, \quad \partial_j \Xi^i = \sum_{k,\ell} (-1)^{\hat{X}^j} (B^{-1})^{ki}_{j\ell} \Xi^\ell \partial_k,$$

$$\partial_i \partial_j = \sum_{k,\ell} B^{k\ell}_{ij} \partial_\ell \partial_k. \tag{4.9}$$

Our convention of the matrix B differs from that in Ref. 26. We use the Yang–Baxter equation of the form (4.5), whereas the Yang–Baxter equation in the braid group form $F_{12}F_{23}F_{12} = F_{23}F_{12}F_{23}$ is used in Ref. 26. They are related as $F^{k\ell}_{ij} = B^{k\ell}_{ji}$. The relations (4.9) are covariant under the action of the super-Jordanian $\mathrm{OSp}_h(2/1)$:

$$X'^i=\sum_j t^i_j X^j, \quad \Xi'^i=\sum_j (-1)^{\hat{i}+\hat{j}} t^i_j \Xi^j, \quad \partial'_i=\sum_j (-1)^{\hat{i}+\hat{j}}((T^{st})^{-1})^i_j \partial_j. \tag{4.10}$$

To show the covariance, we need RTT-type relations for T and T^{st} with the matrix B. They are obtained via (3.9) and (4.5):

$$\sum_{i,j} (-1)^{\hat{b}+\hat{j}+\hat{i}\hat{j}+\hat{b}\hat{i}} t^a_i t^b_j B^{ij}_{cd}=\sum_{i,j} (-1)^{\hat{c}+\hat{i}+\hat{c}\hat{d}+\hat{d}\hat{i}} B^{ab}_{ij} t^j_d t^i_c, \tag{4.11}$$

$$\sum_{i,j} (-1)^{\hat{i}+\hat{a}+\hat{i}\hat{j}+\hat{i}\hat{b}} \tau^a_i \tau^b_j B^{cd}_{ij}=\sum_{i,j} (-1)^{\hat{d}+\hat{j}+\hat{d}\hat{i}+\hat{c}\hat{d}} B^{ij}_{ab} \tau^j_d \tau^i_c, \tag{4.12}$$

$$\sum_{i,j} (-1)^{\hat{i}+\hat{b}\hat{i}+\hat{c}\hat{i}+\hat{d}\hat{j}} \tau^a_i t^b_j B^{jd}_{ci}=\sum_{i,j} (-1)^{\hat{c}+\hat{i}+\hat{j}+\hat{i}\hat{c}} B^{bi}_{ja} t^j_c \tau^i_d, \tag{4.13}$$

$$\sum_{i,j} (-1)^{\hat{c}+\hat{i}+\hat{j}+\hat{c}\hat{i}} (B^{-1})^{ib}_{aj} t^j_c \tau^i_d=\sum_{i,j} (-1)^{\hat{i}+\hat{b}\hat{i}+\hat{c}\hat{i}+\hat{j}\hat{d}} \tau^a_i t^b_j (B^{-1})^{dj}_{ic}, \tag{4.14}$$

where $\tau=(T^{\mathrm{st}})^{-1}$. Introducing the notations $\xi_1=d\theta_1$, $\eta=dx$, $\xi_2=d\theta_2$, the explicit form of the $OSp_h(2/1)$ covariant differential calculus on the quantum superspace $\mathcal{A}$ is summarized as follows:

(1) Coordinates

$$[\theta_1,x]=-hx\theta_2, \quad \{\theta_1,\theta_2\}=0, \quad [\theta_2,x]=0,$$
$$\theta_1^2=-\frac{h}{2}(x^2-2\theta_1\theta_2), \quad \theta_2^2=0. \tag{4.15}$$

(2) Differentials

$$\xi_1\wedge\eta-\eta\wedge\xi_1=h\eta\wedge\xi_2, \quad \xi_1\wedge\xi_2-\xi_2\wedge\xi_1=h\xi_2\wedge\xi_2,$$
$$\eta\wedge\xi_2-\xi_2\wedge\eta=0, \quad \eta\wedge\eta=-\frac{h}{2}\xi_2\wedge\xi_2. \tag{4.16}$$

(3) Coordinates and differentials

$$[\theta_1,\xi_1]=h\left(\theta_1\xi_2+x\eta-\theta_2\xi_1-\frac{h}{2}\theta_2\xi_2\right), \quad \{\theta_1,\eta\}=hx\xi_2,$$
$$[\theta_1,\xi_2]=h\theta_2\xi_2, \quad [x,\xi_1]=-h\theta_2\eta, \quad [x,\eta]=-h\theta_2\xi_2,$$
$$[x,\xi_2]=0, \quad [\theta_2,\xi_1]=-h\theta_2\xi_2,$$
$$\{\theta_2,\eta\}=0, \quad [\theta_2,\xi_2]=0. \tag{4.17}$$

(4) Derivatives and coordinates

$$\partial_1\theta_1=1-\theta_1\partial_1+h\theta_2\partial_1, \quad \partial_1 x=x\partial_1, \quad \partial_1\theta_2=-\theta_2\partial_1,$$
$$\partial_x\theta_1=\theta_1\partial_x-hx\partial_1, \quad \partial_x x=1+x\partial_x+h\theta_2\partial_1, \quad \partial_x\theta_2=\theta_2\partial_x,$$
$$\partial_2\theta_1=-\theta_1\partial_2-h\left(\theta_1\partial_1+x\partial_x+\theta_2\partial_2+\frac{h}{2}\theta_2\partial_1\right),$$
$$\partial_2 x=x\partial_2-h\theta_2\partial_x, \quad \partial_2\theta_2=1-\theta_2\partial_2+h\theta_2\partial_1,$$
$$\text{where } \partial_1=\frac{\partial}{\partial\theta_1}, \ \partial_x=\frac{\partial}{\partial x}, \ \partial_2=\frac{\partial}{\partial\theta_2}. \tag{4.18}$$

(5) Derivatives and differentials

$$\partial_1\xi_1=\xi_1\partial_1-h\xi_2\partial_1,\quad \partial_1\eta=-\eta\partial_1,\quad \partial_1\xi_2=\xi_2\partial_1,$$
$$\partial_x\xi_1=\xi_1\partial_x-h\eta\partial_1,\quad \partial_x\eta=\eta\partial_x+h\xi_2\partial_1,\quad \partial_x\xi_2=\xi_2\partial_x,$$
$$\partial_2\xi_1=\xi_1\partial_2+h\left(\xi_1\partial_1+\eta\partial_x+\xi_2\partial_2+\frac{h}{2}\xi_2\partial_1\right),$$
$$\partial_2\eta=-\eta\partial_2+h\xi_2\partial_x,\quad \partial_2\xi_2=\xi_2\partial_2-h\xi_2\partial_1. \tag{4.19}$$

(6) Derivatives

$$\partial_1^2=0,\quad \partial_1\partial_x=\partial_x\partial_1,\quad \partial_1\partial_2=-\partial_2\partial_1,$$
$$\partial_x\partial_2=\partial_2\partial_x-h\partial_1\partial_x,\qquad \partial_2^2=h(\partial_1\partial_2-\tfrac{1}{2}\partial_x^2). \tag{4.20}$$

V. $OSp_h(2/1)$ SYMMETRIC TORSIONLESS CONNECTIONS

We have seen that a scalar $\varphi(\sim\theta_1^2)$ exists in the quantum superspace $\mathcal{A}$. This scalar is an $OSp_h(2/1)$ invariant zero-form. Invariant one and two-forms under the action of the deformed supergroup $OSp_h(2/1)$ also exist in the differential calculus $\mathcal{A}$:

$$\varrho=\sum_{a,b} J_{ab}X^a\Xi^b=\theta_1\xi_2+x\eta-\theta_2\xi_1-\frac{h}{2}\theta_2\xi_2, \tag{5.1}$$

$$\chi=\sum_{a,b} J_{ab}\Xi^a\wedge\Xi^b=0. \tag{5.2}$$

It is evident that the invariant two-form χ is trivial. It is straightforward to verify the invariance of ϱ and χ under the transformation (4.10). Note that the ϱ appears on the right-hand side of the first relation in (4.17). It is easy to find the commutation relations between the invariant forms and the basis elements (X^a,Ξ^a). For the zero-form φ these relations read

$$X^a\varphi=\varphi X^a,\quad \Xi^a\varphi=\varphi\Xi^a. \tag{5.3}$$

The commutation properties of the invariant one-form ϱ are succinctly given by

$$X^a\varrho=(-1)^{\hat{X}^a}\varrho X^a,\quad \Xi^a\wedge\varrho=(-1)^{\hat{\Xi}^a}\varrho\wedge\Xi^a. \tag{5.4}$$

In a more expanded version the above relations read

$$[x,\varrho]=\{\theta_i,\varrho\}=0,\quad i=(1,2), \tag{5.5}$$

$$\eta\wedge\varrho+\varrho\wedge\eta=0,\quad \xi_i\wedge\varrho-\varrho\wedge\xi_i=0. \tag{5.6}$$

It is also straightforward to verify the relation

$$\varrho\wedge\varrho=0. \tag{5.7}$$

In order to determine the covariant derivative, it is necessary to find the action of the extended permutation σ on $\Omega^1\otimes\Omega^1$. This can be done by applying the covariant derivative D on the second relation in (4.9). Using the Leibnitz rules, we obtain

$$\Xi^i\otimes\Xi^j+(-1)^{\hat{X}^i}X^iD\Xi^j=\sum_{k,\ell}(-1)^{\hat{X}^i}B^{ij}_{k\ell}\ \{(-1)^{\hat{\Xi}^\ell}\sigma(\Xi^\ell\otimes\Xi^k)+(D\Xi^\ell)X^k\}.$$

This relation implies that the action of σ on $\Xi^\ell\otimes\Xi^k$, and the commutation relations between X^i and $D\Xi^j$ may be consistently described as

$$\Xi^i\otimes\Xi^j=\sum_{k,\ell}\ (-1)^{\hat{X}^i+\hat{\Xi}^\ell}B^{ij}_{k\ell}\ \ \sigma(\Xi^\ell\otimes\Xi^k), \tag{5.8}$$

$$X^iD\Xi^j=\sum_{k,\ell}\ B^{ij}_{k\ell}\ \ (D\Xi^\ell)X^k. \tag{5.9}$$

Using the property (4.7) the exchange relation (5.8) may be solved yielding the action of σ on the tensored space of one-forms as follows:

$$\sigma(\Xi^k\otimes\Xi^\ell)=\sum_{i,j}\ (-1)^{\hat{i}\hat{j}}R^{\ell k}_{ij}\ \ \Xi^i\otimes\Xi^j\equiv\sum_{i,j}\ \check{R}^{k\ell}_{ij}\ \ \Xi^i\otimes\Xi^j. \tag{5.10}$$

The matrix $\check{R}$ has two important properties, namely, $\check{R}$ is idempotent and satisfies a nongraded Yang–Baxter equation

$$\check{R}^2=1,\quad \check{R}_{12}\check{R}_{23}\check{R}_{12}=\check{R}_{23}\check{R}_{12}\check{R}_{23}. \tag{5.11}$$

As a consequence of the exchange of the superscripts in the definition (5.10) of $\check{R}$, it satisfies a different form of Yang–Baxter equation from the one obeyed by R. The operator σ, therefore, exhibits identical properties:

$$\sigma^2=1,\quad \sigma_{12}\sigma_{23}\sigma_{12}=\sigma_{23}\sigma_{12}\sigma_{23}. \tag{5.12}$$

The map σ may now be explicitly written as follows:

$$\begin{aligned}
\sigma(\xi_1\otimes\xi_1)&=\xi_1\otimes\xi_1-h\left(\xi_1\otimes\xi_2+\eta\otimes\eta-\xi_2\otimes\xi_1-\frac{h}{2}\xi_2\otimes\xi_2\right),\\
\sigma(\xi_1\otimes\eta)&=\eta\otimes\xi_1+h\xi_2\otimes\eta,\\
\sigma(\xi_1\otimes\xi_2)&=\xi_2\otimes\xi_1+h\xi_2\otimes\xi_2,\\
\sigma(\eta\otimes\xi_1)&=\xi_1\otimes\eta-h\,\eta\otimes\xi_2,\\
\sigma(\eta\otimes\eta)&=-\eta\otimes\eta-h\xi_2\otimes\xi_2,\\
\sigma(\eta\otimes\xi_2)&=\xi_2\otimes\eta,\\
\sigma(\xi_2\otimes\xi_1)&=\xi_1\otimes\xi_2-h\xi_2\otimes\xi_2,\\
\sigma(\xi_2\otimes\eta)&=\eta\otimes\xi_2,\\
\sigma(\xi_2\otimes\xi_2)&=\xi_2\otimes\xi_2.
\end{aligned} \tag{5.13}$$

The map σ being $\mathcal{A}$-bilinear, the following relations hold:

$$\begin{aligned}
&\sigma(\xi_1\otimes\varrho)=\varrho\otimes\xi_1,\quad \sigma(\eta\otimes\varrho)=-\varrho\otimes\eta,\quad \sigma(\xi_2\otimes\varrho)=\varrho\otimes\xi_2,\\
&\sigma(\varrho\otimes\xi_1)=\xi_1\otimes\varrho,\quad \sigma(\varrho\otimes\eta)=-\eta\otimes\varrho,\quad \sigma(\varrho\otimes\xi_2)=\xi_2\otimes\varrho,\\
&\sigma(\varrho\otimes\varrho)=-\varrho\otimes\varrho.
\end{aligned} \tag{5.14}$$

The explicit form of the map σ being known, the relations (5.12) and (2.9) may be verified by direct computation.

To derive the action of the covariant derivative D on Ξ^a, we compare the relation (5.9) with (4.5) and the second relation in (4.9). The comparison suggests that $D\Xi^a$ contains X^a and Ξ^a as factors. Another important observation is that $D\Xi^a$ has the same transformation property as X^a under the action of $\mathrm{OSp}_h(2/1)$ namely,

$$D\Xi'^a = \sum_i t_i^a D\Xi^i. \tag{5.15}$$

Thus the most general form of $D\Xi^a$ may be given by

$$D\Xi^a = c_0 X^a \varpi + c_1(-1)^{\hat{a}}\Xi^a \otimes \varrho + c_2 \varrho \otimes \Xi^a, \tag{5.16}$$

where c_i $(i=0,1,2)$ are real parameters and $\varpi \in \Omega^1 \otimes \Omega^1$ satisfies

$$\varpi' = \varpi, \quad X^a \varpi = \varpi X^a. \tag{5.17}$$

It is not difficult to see that each term on the right-hand side of (5.16) has the same transformation property as X^a under the action of the deformed supergroup $\mathrm{OSp}_h(2/1)$. Furthermore, each term of (5.16) satisfies the same commutation relation as (5.9). As we have seen in the beginning of this section, the $\mathrm{OSp}_h(2/1)$ invariant two-form χ is trivial so that the only possible choice for ϖ is given by

$$\varpi = \varrho \otimes \varrho. \tag{5.18}$$

In this way, we have seen that (5.16) and (5.18) describe the most general linear connection.

Let us recall that our main interest is in torsionless connections, as the torsion-free condition is necessary for making the curvature left $\mathcal{A}$-linear. We restrict the linear connection obtained above to be torsion-free: $\Theta\Xi^a = 0$. As the nilpotency of d constrains $d\Xi^a = 0$, we obtain

$$\Theta\Xi^a = -\pi \circ D\Xi^a = -c_0 \varrho \wedge \varrho - c_1(-1)^{\hat{\Xi}^a}\Xi^a \wedge \varrho - c_2 \varrho \wedge \Xi^a = -(c_1+c_2)\varrho \wedge \Xi^a = 0, \tag{5.19}$$

where we have used the relations (5.4) and (5.7). The torsion-free condition thus requires $c_2 = -c_1$. Therefore, the general form of the $\mathrm{OSp}_h(2/1)$ symmetric torsionless connections is given by the following two-parameter family:

$$D\Xi^a = c_0 X^a \varrho \otimes \varrho + c_1((-1)^{\hat{a}}\Xi^a \otimes \varrho - \varrho \otimes \Xi^a). \tag{5.20}$$

More explicitly these connections read

$$\begin{aligned} D\xi_1 &= c_0\theta_1 \varrho \otimes \varrho + c_1(\xi_1 \otimes \varrho - \varrho \otimes \xi_1), \\ D\eta &= c_0 x \varrho \otimes \varrho - c_1(\eta \otimes \varrho + \varrho \otimes \eta), \\ D\xi_2 &= c_0\theta_2 \varrho \otimes \varrho + c_1(\xi_2 \otimes \varrho - \varrho \otimes \xi_2). \end{aligned} \tag{5.21}$$

For the torsionless connections (5.20), it is easy to see

$$D\varrho = \sum_{a,b} J_{ab}\,\Xi^a \otimes \Xi^b + (c_0\varphi - 2c_1)\varrho \otimes \varrho. \tag{5.22}$$

Applying (2.7), (5.2), (5.7) it immediately follows that

$$\pi(D\varrho) = 0. \tag{5.23}$$

VI. CURVATURE AND METRIC

A two-parameter family of $OSp_h(2/1)$ symmetric torsion-free connections was obtained in the previous section. Since the generalized permutation operator σ satisfies the relation (2.9), the curvature computed from the connections are left $\mathcal{A}$-linear. Recall that curvatures are, in general, not right $\mathcal{A}$-linear. In the present case, however, the curvature is also right $\mathcal{A}$-linear. We exhibit this by explicit computation. We also discuss the metric on the quantum superspace $\mathcal{A}$. It, however, turns out that the connections are not compatible with the metric.

To obtain the curvature, we apply $\pi_{12}D$ on (5.20). Each term is computed separately and listed below:

$$\pi_{12}D(X^a\varrho\otimes\varrho)=\Xi^a\wedge\varrho\otimes\varrho-\sum_{b,c}\ (-1)^{\hat{X}^a}J_{bc}\,X^a\varrho\wedge\Xi^b\otimes\Xi^c,$$

$$\pi_{12}D((-1)^{\hat{a}}\Xi^a\otimes\varrho)=\sum_{b,c}\ J_{bc}\,\Xi^a\wedge\Xi^b\otimes\Xi^c+(c_0\varphi-2c_1)\Xi^a\wedge\varrho\otimes\varrho,$$

$$\pi_{12}D(\varrho\otimes\Xi^a)=-c_1\Xi^a\wedge\varrho\otimes\varrho.$$

Combining the above results, the curvature is obtained as follows:

$$\pi_{12}D^2\Xi^a=(c_0-c_1^2+c_0c_1\varphi)\Xi^a\wedge\varrho\otimes\varrho+(c_0(-1)^{\hat{a}}X^a\varrho+c_1\Xi^a)\wedge\Lambda, \tag{6.1}$$

where

$$\Lambda=\sum_{a,b}\ J_{ab}\,\Xi^a\otimes\Xi^b=\xi_1\otimes\xi_2+\eta\otimes\eta-\xi_2\otimes\xi_1-\frac{h}{2}\xi_2\otimes\xi_2. \tag{6.2}$$

Note that $\pi(\Lambda)=\chi=0$. Expanding the first term in the right-hand side of (6.1) as

$$\Xi^a\wedge\varrho\otimes\varrho=\sum_{b,c}\ (-1)^{\hat{X}^b}J_{bc}\,\Xi^aX^b\wedge\varrho\otimes\Xi^c,$$

we express the curvature in terms of a two-form ω

$$\pi_{12}D^2\Xi^a=\sum_b\ \omega_b^a\otimes\Xi^b, \tag{6.3}$$

where

$$\omega_b^a=\sum_k\ J_{kb}\{(-1)^{\hat{k}}\{c_0(-1)^{\hat{a}}X^a\Xi^k-(c_0-c_1^2+c_0c_1\varphi)\Xi^aX^k\}\wedge\varrho+c_1\Xi^a\wedge\Xi^k\}. \tag{6.4}$$

We now prove that the curvature obtained above is right $\mathcal{A}$-linear. To this end, we note that the following relation may be established by direct computation:

$$[X^a,\Lambda]=0. \tag{6.5}$$

Employing the second relation in (4.9), in conjunction with the left $\mathcal{A}$-linearity of the curvature, we obtain

$$\pi_{12}D^2(\Xi^bX^a)=\sum_{i,j}\ (-1)^{\hat{X}^i}(B^{-1})_{ij}^{ab}X^i\pi_{12}D^2\Xi^j. \tag{6.6}$$

Substituting (6.1) into (6.6), and then transferring X^i to the right via Eqs. (4.9), (5.3), (5.4), (6.5), we demonstrate the intended result

$$\pi_{12}D^2(\Xi^b X^a)=(\pi_{12}D^2\Xi^b)X^a, \tag{6.7}$$

establishing the right $\mathcal{A}$-linearity of the curvature. In the above computation we have used the fact that the matrices B_{ij}^{ab} and $(B^{-1})_{ij}^{ab}$ maintain the following relationship regarding the parity of their indices: $\hat{a}+\hat{b}=\hat{i}+\hat{j}$.

Let us now turn to the metric, which is considered as a bilinear map $g:\Omega^1\otimes_{\mathcal{A}}\Omega^1\to\mathcal{A}$. To completely determine the metric we need to know the action of the map g on the basis elements of $\Omega^1\otimes\Omega^1$. Setting $g^{ab}=g(\Xi^a\otimes\Xi^b)$, we require that g^{ab} to be invariant under the action of $\mathrm{OSp}_\hbar(2/1)$:

$$g'^{ab}\equiv g(\Xi'^a\otimes\Xi'^b)=\sum_{k,\ell} g((-1)^{\hat{a}+\hat{k}}t_k^a\,\Xi^k\otimes(-1)^{\hat{b}+\hat{\ell}}t_\ell^b\,\Xi^\ell)=\sum_{k,\ell}(-1)^{\hat{a}+\hat{b}+\hat{k}+\hat{\ell}}t_k^a\,g^{k\ell}(t^{st})_\ell^b.$$

The above result, in conjunction with the identity (3.3), immediately yields $g'^{ab}=g^{ab}$, provided we choose $g^{k\ell}=(-1)^{\hat{k}+\hat{\ell}}(J^{-1})_{k\ell}=(J^{-1})_{k\ell}$. The $\mathrm{OSp}_\hbar(2/1)$ invariant metric, therefore, is given by

$$g^{ab}=g(\Xi^a\otimes\Xi^b)=(J^{-1})_{ab}=\begin{pmatrix}-\frac{h}{2} & 0 & -1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{pmatrix}. \tag{6.8}$$

Denoting the components of g^{-1} by g_{ab}, we note that the invariant one-form ϱ may be written in terms of the metric

$$\varrho=\sum_{a,b} g_{ab}X^a\Xi^b.$$

The structure of the metric (6.8) implies

$$d\circ g(\Xi^a\otimes\Xi^b)=0. \tag{6.9}$$

The compatibility condition (2.14) now reads

$$(1\otimes g)\circ D(\Xi^a\otimes\Xi^b)=0. \tag{6.10}$$

To compute the left-hand side in (6.10), we start by ordering the one-forms in the expression of ϱ to the left:

$$\varrho=\xi_2\theta_1+\eta x-\xi_1\theta_2+\frac{h}{2}\xi_2\theta_2=\sum_{a,b}(-1)^{\hat{X}^b}J_{ab}\,\Xi^aX^b. \tag{6.11}$$

We now readily obtain

$$g(\varrho\otimes\Xi^a)=X^a,\quad g(\Xi^a\otimes\varrho)=(-1)^{\hat{X}^a}X^a. \tag{6.12}$$

Following (2.5) the action of the covariant derivative on $\Omega^1\otimes\Omega^1$ is given as

$$D(\Xi^a\otimes\Xi^b)=D\Xi^a\otimes\Xi^b+(-1)^{\hat{\Xi}^a}\sigma_{12}(\Xi^a\otimes D\Xi^b). \tag{6.13}$$

Substituting (5.20) into (6.13), we observe that, as a consequence of the bilinearity of g, we may treat the first (proportional to c_0) and the second (proportional to c_1) terms in the right hand side of (5.20) separately. For the choice $c_1=0$, we then obtain

$$D(\Xi^a\otimes\Xi^b)=c_0(X^a\varrho\otimes\varrho\otimes\Xi^b+\varrho\otimes\Xi^a\otimes\varrho X^b),$$

which, in turn, yields

$$(1\otimes g)\circ D(\Xi^a\otimes\Xi^b)=(-1)^{\hat{X}^a}2c_0\varrho X^aX^b. \tag{6.14}$$

For the alternate choice $c_0=0$, it follows that

$$D(\Xi^a\otimes\Xi^b)=c_1\{(-1)^{\hat{a}}\Xi^a\otimes\varrho\otimes\Xi^b-2\varrho\otimes\Xi^a\otimes\Xi^b+(-1)^{\hat{a}+\hat{b}}\sigma_{12}(\Xi^a\otimes\Xi^b\otimes\varrho)\}.$$

The right-hand side in (6.10) now reads

$$(1\otimes g)\circ D(\Xi^a\otimes\Xi^b)=c_1\{(-1)^{\hat{a}}\Xi^aX^b-2g^{ab}\varrho+(-1)^{\hat{a}+\hat{b}}(1\otimes g)\circ\sigma_{12}(\Xi^a\otimes\Xi^b\otimes\varrho)\}. \tag{6.15}$$

The last term is computed by using (5.13) and (6.12). The result is listed below:

$$(1\otimes g)\circ D(\xi_1\otimes\xi_1)=0,$$

$$(1\otimes g)\circ D(\xi_1\otimes\eta)=c_1(\xi_1x+\eta\theta_1-h\xi_2x),$$

$$(1\otimes g)\circ D(\xi_1\otimes\xi_2)=c_1\left(\eta x-\frac{h}{2}\xi_2\theta_2+\varrho\right),$$

$$(1\otimes g)\circ D(\eta\otimes\xi_1)=-c_1(\xi_1x+\eta\theta_1+h\eta\theta_2),$$

$$(1\otimes g)\circ D(\eta\otimes\eta)=-c_1(2\eta x-h\xi_2\theta_2+2\varrho),$$

$$(1\otimes g)\circ D(\eta\otimes\xi_2)=-c_1(\eta\theta_2+\xi_2x),$$

$$(1\otimes g)\circ D(\xi_2\otimes\xi_1)=-c_1\left(\eta x-\frac{h}{2}\xi_2\theta_2+\varrho\right),$$

$$(1\otimes g)\circ D(\xi_2\otimes\eta)=c_1(\eta\theta_2+\xi_2x),$$

$$(1\otimes g)\circ D(\xi_2\otimes\xi_2)=0. \tag{6.16}$$

Together with (6.14), it has been shown that $(1\otimes g)\circ D\neq 0$, except for the trivial choice $c_0=c_1=0$. Thus the covariant derivative D is not compatible with the metric.

VII. CONCLUDING REMARKS

In the present work we have studied noncommutative spaces, linear connections, curvatures, and metrics associated with the quantized supergroups. Our approach is a naive extension of the differential geometry developed in Refs. 8, 9, 16. We have demonstrated that the ideas of these authors may be appropriately adapted to study the geometric objects related to the quantum supergroups. Specifically, we applied the extended differential geometry to the quantum superspace covariant under the quantum supergroup $OSp_h(2/1)$. We have seen that our particular example has a two-parameter family of $OSp_h(2/1)$ symmetric torsion-free connections. It turned

out that the curvature of the connection was bilinear. The connection was, however, not compatible with the metric. These properties are specific to our example. There could be other quantum superspace endowed with linear connections compatible with metric.

It may be of interest to recall the results related to the quantum spaces covariant under quantized SL(2) groups, and compare them with the present results. It is well-known that SL(2) admits two inequivalent deformations: the standard q-deformation and the Jordanian h-deformation. The quantum space for q-deformed SL(2) has a one-parameter family of torsionless linear connections and it has been shown that there can be no compatible metric,[11] whereas the quantum space of h-deformed SL(2) is more classical. It has a two-parameter family of torsion-free linear connections. A one-parameter subfamily of these connections is known to be compatible with a metric.[14] On the other hand, the Lie superalgebra osp(2/1) admits three inequivalent deformations.[27] We are thus able to consider three deformations of the supergroup OSp(2/1): q-deformation,[20] h-deformation,[28] and super-Jordanian deformation. The q and h-deformations have the SL(2) counterparts, while super-Jordanian does not. The super-Jordanian deformation can be regarded as an algebra intermediate between q and h-deformations. We have seen that the quantum space for super-Jordanian $\mathrm{OSp}_h(2/1)$ is less classical since the connections are not metric. This leads us to the anticipate that the quantum space for h-deformed OSp(2/1) has connections which are metric, while the connections on the quantum spaces related to the standard q-deformed supergroup $\mathrm{OSp}_q(2/1)$ are not metric. This will be presented in a future work.

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Existence and uniqueness of global solution of the Hasegawa–Mima equation

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The Hasegawa–Mima equation is the simplest nonlinear model to investigate drift waves and drift-wave turbulence. In this article, we establish the existence and uniqueness of a global weak solution for the Cauchy problem of the two-dimensional Hasegawa–Mima equation. Moreover, if the background particle density is homogeneous in the x-direction, there is a unique global regular solution. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1667607]

I. INTRODUCTION

We consider the existence and uniqueness of a global solution for the following two-dimensional (2D) Hasegawa–Mima equation,

$$\partial_t(u-\Delta u)+k\partial_y u+\{u,\Delta u\}=0, \qquad (x,y)\in R^2, \quad t>0, \tag{1}$$

with initial datum

$$u(x,y,t=0)=u_0(x,y), \tag{2}$$

where k is a constant, Δ is the 2D Laplacian, and $\{\cdot,\cdot\}$ denotes the Poisson bracket

$$\{f,g\}=(\partial_x f)(\partial_y g)-(\partial_x f)(\partial_y g).$$

Equation (1) is the simplest and powerful 2D turbulent system. In plasma,[6] Eq. (1) describes the time evolution of drift wave, and u describes the electrostatic fluctuations, where $k=\partial_x \ln n_0$ and n_0 is the background particle density.[13] In geophysical fluids,[12] Eq. (1) describes the temporal evolution of geostrophic motion and is called the quasi-geostrophic potential vorticity equation for the Rossby wave, and u is the geostrophic stream function. If we eliminate the term u_t of Eq. (1), then Eq. (1) is changed into the Euler equation for inviscid incompressible homogeneous fluids. The Euler equation has been actively studied by many authors (see Refs. 2–4, 10, 14, and 15 and references therein). The Hasegawa–Mima equation has been actively studied by way of numerical simulation and analysis of Fourier ansatz, and some important characteristics of the 2D turbulence have been found (see, e.g., Refs. 1, 5–8, and 11–13 and references therein), but rigorous results are lacking. In the present work, we establish that Cauchy problem (1) and (2) is global well-posed. Our main results are stated as follows.

Theorem 1: *Let $k=0$, initial data $u_0\in H^m(R^2)\cap W^2_\infty(R^2)$. Then for all time $T>0$ and integer $m\geqslant 3$ there is a unique regular solution u of problem (1) and (2) such that $u\in L^\infty([0,T];H^m(R^2))$, $u_t\in L^\infty([0,T];H^{m-1}(R^2))$.*

Theorem 2: *Let initial data $u_0\in H^2(R^2)$. Then for all time $T>0$ there is a weak solution u of problem (1) and (2) such that $u\in L^\infty([0,T];H^2(R^2))$ and $u_t\in L^\infty([0,T];H^1(R^2))$. If u_0*

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$\in H^2(R^2)\cap W^2_\infty(R^2)$, *then the weak solution* u *of problem (1) and (2) is unique and for all* $2\leqslant p<\infty$ *we have* $u\in L^\infty([0,T];W^2_p(R^2))$. *Moreover, if* $u_0\in H^2(R^2)\cap W^2_\infty(R^2)$ *and* $k=0$, *then* $u\in L^\infty([0,T];H^2(R^2)\cap W^2_\infty(R^2))$.

Definition 1: Let $T>0$, $u_0\in H^m(R^2)$, $m\geqslant 2$, *and function* $u\in L^\infty([0,T];H^m(R^2))$ *such that*

$$\int_0^T\int_{R^2}((u-\Delta u)\phi_t+ku\phi_y+\{u,\phi\}\Delta u)dx\ \ dy\ \ dt+\int_{R^2}u_0\phi(x,y,0)dx\ \ dy=0,$$
$$\forall\phi\in C^1([0,T];C_0^\infty(R^2)),\qquad \phi(x,y,t)|_{t=T}=0. \tag{3}$$

If $m=2$, *the function* u *is said to be a weak solution of (1) and (2) in the interval* $[0,T]$. *If* $m\geqslant 3$, *the function* u *is said to be a regular solution of (1) and (2) in the interval* $[0,T]$.

We first establish the existence and uniqueness of the global solution for the perturbed Hasegawa–Mima equation

$$\partial_t(u-\Delta u)+k\partial_y u+\{u,\Delta u\}-\lambda\Delta(u-\Delta u)=0 \tag{4}$$

with initial datum

$$u(x,y,t=0)=u_0(x,y), \tag{5}$$

where constant $0<\lambda<1$, and obtain the uniform *a priori* estimates for the solution of problem (4) and (5) relative to the coefficient λ. Let $\lambda\to 0$, and then Theorems 1 and 2 are proved.

In this paper, we use a variety of function spaces: Lebesgue space $L^p=L^p(R^2)$, Sobolev spaces $H^k(R^2)$ and $W^k_p(R^2)$, and the spaces $L^q([0,T];X)$ and $C([0,T];X)$, where X is one of the spaces just mentioned. In order to simplify the exposition, different positive constants might be denoted by the same letter C; if necessary, by $C(\cdots)$ denote the constant depending only on the quantities appearing in parentheses. The rest of this work is organized as follows. In Sec. II, we establish *a priori* estimates. In Sec. III, we establish the existence and uniqueness of solution for the problem (4) and (5). In Sec. IV, we give the proof of Theorems 1 and 2.

II. *A PRIORI* ESTIMATES

In this section, we establish *a priori* estimates of solutions for the problem (4) and (5).

Lemma 1: Let initial data $u_0\in H^m(R^2)$ $(m\geqslant 2)$ *and* u *be the smooth solution of problem (4) and (5). Then we have that*

$$\|u(\cdot,t)\|_{H^2}+\lambda\int_0^t\|u(\cdot,\tau)\|_{H^3}d\tau\leqslant C(\|u_0\|_{H^2}),\qquad \forall t\geqslant 0. \tag{6}$$

If $u_0\in H^2(R^2)\cap W^2_\infty(R^2)$, *then for all* $2<p<\infty$ *we have that*

$$\|u(\cdot,t)\|_{W^2_p}\leqslant C(\|u_0\|_{H^2},\|u_0\|_{W^2_\infty})(1+pt^2),\qquad \forall t\geqslant 0. \tag{7}$$

Moreover, if $u_0\in H^2(R^2)\cap W^2_\infty(R^2)$ *and* $k=0$, *then we have that*

$$\|u(\cdot,t)\|_{W^2_\infty}\leqslant C(\|u_0\|_{H^2},\|u_0\|_{W^2_\infty}),\qquad \forall t\geqslant 0. \tag{8}$$

Here constants $C(\cdots)$ *are independent of* p *and* λ.

Proof: Taking the scalar product of the function $2u$ and the equation (4), and then integrating the result over R^2 for the space variable (x,y) and over $[0,t]$ for the temporal variable t, we have

$$\|u(\cdot,t)\|_{L^2}^2+\|\nabla u(\cdot,t)\|_{L^2}^2+2\lambda\int_0^t(\|\nabla u(\cdot,\tau)\|_{L^2}^2+\|\Delta u(\cdot,\tau)\|_{L^2}^2)d\tau=\|u_0\|_{L^2}^2+\|\nabla u_0\|_{L^2}^2,\quad \forall t\geqslant 0, \tag{9}$$

where we have used the fact

$$\int_{R^2}\{u,\Delta u\}u(x,y,t)\ \ dxdy=0,\qquad \forall t\geqslant 0.$$

Similarly, taking the scalar product of $-2\Delta u$ and the equation (4), and then integrating the result over R^2 for the space variable (x,y) and over $[0,t]$ for the temporal variable t, we have

$$\begin{aligned}&\|\nabla u(\cdot,t)\|_{L^2}^2+\|\Delta u(\cdot,t)\|_{L^2}^2+2\lambda\int_0^t(\|\Delta u(\cdot,\tau)\|_{L^2}^2+\|\nabla\Delta u(\cdot,\tau)\|_{L^2}^2)d\tau\\&\quad=\|\Delta u_0\|_{L^2}^2+\|\nabla u_0\|_{L^2}^2,\qquad \forall t\geqslant 0,\end{aligned} \tag{10}$$

where we have used the following fact:

$$\int_{R^2}\{u,\Delta u\}\Delta u(x,y,t)\ \ dxdy=0,\qquad \forall t\geqslant 0.$$

Putting together (9) and (10), we obtain (6).

Now taking the scalar product of $p|u-\Delta u|^{p-2}(u-\Delta u)$ (for all $2<p<\infty$) and the equation (4), and then integrating the result over R^2 for the space variable (x,y), we get

$$\begin{aligned}&\frac{d}{dt}\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}^p-p\lambda\int_{R^2}\Delta(u-\Delta u)\cdot|u-\Delta u|^{p-2}(u-\Delta u)\ \ dx\ \ dy\\&\quad\leqslant pk\|\nabla u(\cdot,t)\|_{L^p}\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}^{p-1},\quad \forall t\geqslant 0,\end{aligned} \tag{11}$$

where we have used the following fact:

$$\int_{R^2}\{u,\Delta u\}|u-\Delta u|^{p-2}(u-\Delta u)(x,y,t)\ \ dxdy=0,\qquad \forall t\geqslant 0.$$

Note that

$$\begin{aligned}\|\nabla u(\cdot,t)\|_{L^p}^p&=-(p-1)\int_{R^2}(|\partial_x u|^{p-2}u\cdot\partial_x^2 u+|\partial_y u|^{p-2}u\cdot\partial_y^2 u)\ dx\ \ dy\\&\leqslant p\|\nabla u(\cdot,t)\|_{L^p}^{p-2}\|u(\cdot,t)\|_{L^p}(\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}+\|u(\cdot,t)\|_{L^p}),\end{aligned} \tag{12}$$

$$\|u(\cdot,t)\|_{L^p}\leqslant\|u(\cdot,t)\|_{L^2}^{2/p}\|u(\cdot,t)\|_{L^\infty}^{(p-2)/p}\leqslant\|u(\cdot,t)\|_{L^2}+\|u(\cdot,t)\|_{L^\infty}. \tag{13}$$

Integrating by parts, we get

$$\begin{aligned}&-p\lambda\int_0^t\int_{R^2}\Delta(u-\Delta u)\cdot|u-\Delta u|^{p-2}(u-\Delta u)\ \ dx\ \ dy\ \ d\tau\\&\quad=p(p-1)\lambda\int_0^t\int_{R^2}(\nabla(u-\Delta u))^2|u-\Delta u|^{p-2}\ \ dx\ \ dy\ \ d\tau\geqslant 0.\end{aligned} \tag{14}$$

Inserting (6) and (12)–(14) into (11), for all $2<p<\infty$ we get

$$\frac{d}{dt}\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}\leqslant Ck\sqrt{p}(1+\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}^{1/2}),\quad \forall t\geqslant 0, \tag{15}$$

where constant C is independent of λ and p.

In the case $k=0$, using (6), (13), and (15) and the following fact,

$$\begin{aligned}\|u_0-\Delta u_0\|_{L^p}\leqslant\|u_0\|_{L^p}+\|\Delta u_0\|_{L^p}&\leqslant C\|u_0\|_{H^1}+\|\Delta u_0\|_{L^2}^{2/p}\|\Delta u_0\|_{L^\infty}^{(p-2)/p}\\&\leqslant C\|u_0\|_{H^1}+\|\Delta u_0\|_{L^2}+\|\Delta u_0\|_{L^\infty},\end{aligned} \tag{16}$$

we get

$$\|\Delta u(\cdot,t)\|_{L^p(R^2)}\leqslant C,\qquad \forall t\geqslant 0,\quad 2\leqslant p<\infty, \tag{17}$$

where constant C is independent of λ and p. Fixing $N>0$, one has

$$\|\Delta u(\cdot,t)\|_{L^p(B_N)}\leqslant\|\Delta u(\cdot,t)\|_{L^p(R^2)}\leqslant C,\qquad \forall t\geqslant 0,\quad 2\leqslant p<\infty,$$

where constant C is independent of N, λ and p; $B_N=\{(x,y)\in R^2|\ \ x^2+y^2\leqslant N^2\}$. Let $p\to\infty$. We get

$$\|\Delta u(\cdot,t)\|_{L^\infty(B_N)}=\lim_{p\to\infty}\|\Delta u(\cdot,t)\|_{L^p(B_N)}\leqslant C,\qquad \forall t\geqslant 0,$$

where constant C is independent of N and λ. Let $N\to\infty$. We have

$$\|\Delta u(\cdot,t)\|_{L^\infty(R^2)}=\lim_{N\to\infty}\|\Delta u(\cdot,t)\|_{L^\infty(B_N)}\leqslant C,\qquad \forall t\geqslant 0. \tag{18}$$

Estimate (8) is proved.

In the case $k\neq 0$, using (15) and (16), for all $2<p<\infty$ one has

$$\|u(\cdot,t)-\Delta u(\cdot,t)\|_{L^p}\leqslant C(1+pt^2),\qquad \forall t\geqslant 0, \tag{19}$$

where constant C is independent of λ and p. Putting together (6), (13), and (19), we get estimate (7).

This completes the proof of Lemma 1.

Lemma 2: Let initial data $u_0\in H^m(R^2)\cap W_\infty^2(R^2)$ $(m\geqslant 3)$ and u be the smooth solution of problem (4) and (5). Then for all time $0<T<\infty$ one has the following estimates:

$$\|\nabla\Delta u(\cdot,t)\|_{L^2}^2+\lambda\int_0^t\|\Delta^2 u(\cdot,s)\|_{L^2}^2 ds\leqslant C(T,\|u_0\|_{H^3},\|u_0\|_{W_\infty^2}),\qquad \forall t\in[0,T], \tag{20}$$

where constant $C(\cdots)$ is independent of λ in the case $k=0$.

Proof: Differentiating Eq. (4) with respect to (x,y), we get

$$\partial_t\nabla(u-\Delta u)+k\partial_y\nabla u+\{u,\nabla\Delta u\}+\{\nabla u,\Delta u\}-\lambda\nabla\Delta(u-\Delta u)=0. \tag{21}$$

Taking the scalar product of $-2\nabla\Delta u$ and the equation (21), and then integrating the result over R^2 for the space variable (x,y), we have

$$\begin{aligned}&\frac{d}{dt}(\|\Delta u(\cdot,t)\|_{L^2}^2+\|\nabla\Delta u(\cdot,t)\|_{L^2}^2)+2\lambda(\|\nabla\Delta u(\cdot,t)\|_{L^2}^2+\|\Delta^2 u(\cdot,t)\|_{L^2}^2)\\&\quad\leqslant 2\|\partial^2 u(\cdot,t)\|_{L^\infty}\|\nabla\Delta u(\cdot,t)\|_{L^2}^2,\end{aligned} \tag{22}$$

where ∂^2 denotes the differential operator of the second order: $\partial^\alpha=\partial_x^{\alpha_1}\partial_y^{\alpha_2}$, $\alpha_1+\alpha_2=2$, and we have used the following facts:

$$\int_{R^2}\partial_y\nabla u\cdot\nabla\Delta u \quad dx \quad dy=0, \qquad \int_{R^2}\{u,\nabla\Delta u\}\cdot\nabla\Delta u \quad dx \quad dy=0, \quad \forall t\geqslant 0.$$

In the case $k=0$, inserting estimate (8) into (22) and employing Gronwall's inequality, we get (20), where the constant C is independent of λ.

In the case $k\neq 0$, applying estimate (6), Gagliardo–Nirenberg's inequality and Hölder's inequality, one has that

$$\begin{aligned}
&\|\partial^2 u(\cdot,t)\|_{L^\infty}\leqslant C\|\Delta u(\cdot,t)\|_{L^2}^{1/2}\|\Delta^2 u(\cdot,t)\|_{L^2}^{1/2},\\
&\|\nabla\Delta u(\cdot,t)\|_{L^2}\leqslant C\|\Delta u(\cdot,t)\|_{L^2}^{1/2}\|\Delta^2 u(\cdot,t)\|_{L^2}^{1/2},\\
&\|\partial^2 u(\cdot,t)\|_{L^\infty}\|\nabla\Delta u(\cdot,t)\|_{L^2}^2\leqslant C\|\Delta u(\cdot,t)\|_{L^2}^{3/2}\|\Delta^2 u(\cdot,t)\|_{L^2}^{3/2}\\
&\qquad\leqslant\lambda\|\Delta^2 u(\cdot,t)\|_{L^2}^2+C(\lambda).
\end{aligned}\tag{23}$$

Putting together (22) and (23), we obtain (20).

The proof of this lemma is completed.

Lemma 3: Let initial data $u_0\in H^m(R^2)\cap W_\infty^2(R^2)$ $(m\geqslant 2)$ and u be the smooth solution of problem (4) and (5). One then has the following estimates:

$$\|u(\cdot,t)\|_{H^m}^2+\lambda\int_0^t\|u(\cdot,\tau)\|_{H^{m+1}}^2 d\tau\leqslant C(T,\|u_0\|_{H^m}), \qquad \forall T>0, \quad t\in[0,T], \tag{24}$$

where constant $C(\cdots)$ is independent of λ in the case $k=0$.

Proof: This lemma is proved by mathematical induction as follows. For the case of $2\leqslant m\leqslant 3$, estimates (24) have been proved in Lemmas 1 and 2. Assume that (24) is valid for the case $m=M\geqslant 3$.

Differentiating Eq. (4) with respect to (x,y), we get

$$\partial_t\partial^\alpha(u-\Delta u)+k\partial_y\partial^\alpha u+\sum_{\beta_1+\beta_2=\alpha}\{\partial^{\beta_1}u,\partial^{\beta_2}\Delta u\}-\lambda\partial^\alpha\Delta(u-\Delta u)=0, \tag{25}$$

where α, β_1 and β_2 are multi-index and ∂^α is a differential operator of the $(M-1)$th order. Taking the scalar product of $-2\partial^\alpha\Delta u$ and the equation (25), and then integrating the result over R^2 for the space variable (x,y), we have

$$\begin{aligned}
&\frac{d}{dt}(\|\partial^\alpha\nabla u(\cdot,t)\|_{L^2}^2+\|\partial^\alpha\Delta u(\cdot,t)\|_{L^2}^2)+2\lambda(\|\partial^\alpha\Delta u(\cdot,t)\|_{L^2}^2+\|\partial^\alpha\nabla\Delta u(\cdot,t)\|_{L^2}^2)\\
&\leqslant 2\sum_{\beta_1+\beta_2=\alpha,\ 1\leqslant|\beta_1|\leqslant M-2}\|\nabla\partial^{\beta_1}u(\cdot,t)\|_{L^\infty}\|\nabla\partial^{\beta_2}\Delta u(\cdot,t)\|_{L^2}\|\partial^\alpha\Delta u(\cdot,t)\|_{L^2}\\
&\quad+2\|\nabla\partial^\alpha u(\cdot,t)\|_{L^4}\|\nabla\Delta u(\cdot,t)\|_{L^4}\|\partial^\alpha\Delta u(\cdot,t)\|_{L^2}\\
&\leqslant C(1+\|u(\cdot,t)\|_{H^{M+1}}^2),
\end{aligned}\tag{26}$$

where we have used the induction assumption and the following facts:

$$\int_{R^2}\partial_y\partial^\alpha u\cdot\partial^\alpha\Delta u \quad dx \quad dy=0, \qquad \int_{R^2}\{u,\partial^\alpha\Delta u\}\cdot\partial^\alpha\Delta u \quad dx \quad dy=0, \quad \forall t\geqslant 0,$$

$$\|\nabla\partial^{\beta_1}u(\cdot,t)\|_{L^\infty}\leqslant C\|\nabla\partial^{\beta_1}u(\cdot,t)\|_{H^2},$$

$$\|\nabla\partial^{\alpha}u(\cdot,t)\|_{L^4}\leqslant C\|\nabla\partial^{\alpha}u(\cdot,t)\|_{L^2}^{1/2}\|\nabla\partial^{\alpha}u(\cdot,t)\|_{H^1}^{1/2},$$

$$\|\nabla\Delta u(\cdot,t)\|_{L^4}\leqslant C\|\nabla\Delta u(\cdot,t)\|_{L^2}^{1-1/2(M-2)}\|\nabla\Delta u(\cdot,t)\|_{H^{M-2}}^{1/2(M-2)}.$$

Summing over $|\alpha|=M-1$ in (26) and applying Gronwall's inequality, we have

$$\|u(\cdot,t)\|_{H^{M+1}}^2+\lambda\int_0^t\|u(\cdot,\tau)\|_{H^{M+2}}^2d\tau\leqslant C(T,\|u_0\|_{H^{M+1}}),\qquad \forall T>0,\quad t\in[0,T],\tag{27}$$

where constant $C(\cdots)$ is independent of λ in the case $k=0$.

By induction, this lemma is proved.

III. SOLUTION OF THE PERTURBED HASEGAWA–MIMA EQUATION

It is easy to check that $e^{t\lambda\Delta}$ is the analytic semigroup generated by $\lambda\Delta$ in $L^p(R^2)$ $(2\leqslant p<\infty)$. In what follows, we apply the abstract semigroup theory and its methods to establish the existence and uniqueness of the local solution (in time t) for the problem (4) and (5). Thanks to the estimate (24), we can extend the local solution to the global solution.

Lemma 4: Let $u_0\in H^m(R^2)$, $m\geqslant 4$. Then for all time $0<T<\infty$ there exists a unique solution u of problem (4) and (5) such that $u\in C([0,T];H^m(R^2))$. Moreover, if $k=0$, then we have

$$\sup_{0\leqslant t\leqslant T}\|u(\cdot,t)\|_{H^m}\leqslant C,\tag{28}$$

where constant C is independent of λ.

Proof: Let $w=u-\Delta u$. Then $u=(1-\Delta)^{-1}w$ and Eqs. (4) and (5) are rewritten

$$\partial_t w+k\partial_y(1-\Delta)^{-1}w+\{(1-\Delta)^{-1}w,w\}-\lambda\Delta w=0,\tag{29}$$

$$w(x,y,t)|_{t=0}=w_0(x,y)=u_0-\Delta u_0.\tag{30}$$

As is well known, $\lambda\Delta$ generates a analytic semigroup $S(t)=e^{t\lambda\Delta}$ in $L^2(R^2)$. Let

$$Y=\{w|w\in C([0,T];H^m(R^2)),\quad t^\alpha w(t)\in C^\alpha((0,T];H^m(R^2)),\quad w(0)=w_0,$$

$$\|w\|_{C([0,T];H^m)}+[t^\alpha w]_{C^\alpha((0,T];H^m)}\leqslant\rho,\quad 0<\alpha<1,\quad m\geqslant 2\}.$$

Define a nonlinear operator Γ on Y, by $\Gamma(w)=v$, where v is the solution of the following problem:

$$\partial_t v+k\partial_y(1-\Delta)^{-1}w+\{(1-\Delta)^{-1}w,w\}-\lambda\Delta v=0,\qquad w(0)=w_0.$$

Note that $\xi/(1+|\xi|^2)$ is a multiplier for $L^p(R^2)$ $(1<p<\infty)$. We have

$$\|\nabla(1-\Delta)^{-1}w(\cdot,t)\|_{L^p}\leqslant C\|w(\cdot,t)\|_{L^p},\qquad \forall p>1.$$

By Theorem 4.3.5 of Ref. 9 (pp. 137–139), for every $w\in Y$, $\Gamma(w)\in C([0,T];H^m(R^2))$ and $t^\alpha\Gamma(w)\in C^\alpha((0,T];H^m(R^2))$. Then, repeating the same procedure as that produced in the proof of Theorem 8.1.1 of Ref. 9 (pp. 290–294), there exists $T>0$ and $\rho>0$ such that $\Gamma: Y\to Y$ is a contraction, i.e., there exists $T>0$ and a unique local solution u of problem (4) and (5) such that $u\in C([0,T];H^m(R^2))$ $(m\geqslant 4)$. Employing the estimates of Lemma 3, we can extend this local solution into a unique global solution such that this global solution satisfies the estimate (28).

This completes the proof of the lemma.

Lemma 5: Let $u_0 \in H^2(R^2)$. *Then for all time* $0<T<\infty$ *there exists a solution* u *of problem (4) and (5) such that* $u \in C([0,T];H^2(R^2))$ *and*

$$\sup_{0\leqslant t\leqslant T} \|u(\cdot,t)\|_{H^2} \leqslant C. \tag{31}$$

Moreover, if $u_0 \in H^2(R^2)\cap W^2_\infty(R^2)$, *then the solution* u *of (4) and (5) is unique and for all* $2<p<\infty$ *we have*

$$\sup_{0\leqslant t\leqslant T} \|u(\cdot,t)\|_{W^2_p} \leqslant C(1+pT^2), \tag{32}$$

$$\sup_{0\leqslant t\leqslant T} \|u(\cdot,t)\|_{W^2_\infty} \leqslant C \qquad \textit{only for the case of } k=0. \tag{33}$$

Here the above constants C *are independent of* T, p *and* λ.

Proof: Let $u_{0\epsilon}=\eta_\epsilon * u_0$, $\epsilon>0$, $\eta_\epsilon(x,y)=(1/\epsilon^2)\,\eta_\epsilon(x/\epsilon, y/\epsilon)$, where η is the standard mollifier. Then $u_{0\epsilon}\in H^4(R^2)$, $\|u_{0\epsilon}\|_{L^\infty}\leqslant\|u_0\|_{L^\infty}$ and $\|u_{0\epsilon}-u_0\|_{H^2}\to 0$ as $\epsilon\to 0$.

Consider Eq. (4) with initial datum

$$u(x,y,0)=u_{0\epsilon}(x,y). \tag{34}$$

Applying the results of Lemma 4, for all time $0<T<\infty$ there exists a unique solution u_ϵ of the problem (4) and (34) such that $u_\epsilon\in C([0,T];H^4(R^2))$. Thanks to the estimates (6)–(8), let $\epsilon\to 0$. We obtain that there exists a global solution u for the problem (4) and (5) such that $u\in C([0,T];H^2(R^2))$ and $\sup_{0\leqslant t\leqslant T}\|u(\cdot,t)\|_{H^2}\leqslant C$; moreover, if $u_0\in H^2(R^2)\cap W^2_\infty(R^2)$, then for all $2<p<\infty$ we have

$$\sup_{0\leqslant t\leqslant T} \|u(\cdot,t)\|_{W^2_p} \leqslant C(1+pT^2),$$

$$\sup_{0\leqslant t\leqslant T} \|u(\cdot,t)\|_{W^2_\infty} \leqslant C \qquad \text{only for the case of } k=0,$$

where constants C are independent of λ.

Assume that there are two solutions u and v of problem (4) and (5) such that

$$u,v\in C([0,T];W^2_p(R^2)), \qquad \forall p\in[2,\infty), \quad 0<T<\infty,$$

$$\sup_{0\leqslant t\leqslant T} \max\{\|u(\cdot,t)\|_{H^2},\|v(\cdot,t)\|_{H^2}\}\leqslant C, \tag{35}$$

$$\sup_{0\leqslant t\leqslant T} \max\{\|u(\cdot,t)\|_{W^2_p},\|v(\cdot,t)\|_{W^2_p}\}\leqslant C(1+pT^2), \qquad \forall p>2, \tag{36}$$

where constants C are independent of λ. Let $w=u-v$. Then w is the solution of the following problem:

$$\partial_t(w-\Delta w)+k\partial_y w+\{u,\Delta w\}+\{w,\Delta v\}-\lambda\Delta(w-\Delta w)=0, \tag{37}$$

$$w(x,y,0)=0. \tag{38}$$

Taking the scalar product of $2w$ and the equation (37), and then integrating the result over R^2 for the space variable (x,y), we have

$$\frac{d}{dt}\|w(\cdot,t)\|_{H^1}^2+\lambda\int_{R^2}|(|\nabla w|^2+|\Delta w|^2)(x,y,t)\quad dx\quad dy$$
$$\leqslant C(1+pt^2)^{1+2/p}\|\nabla w(\cdot,t)\|_{L^2}^{2-2/p},\qquad \forall p>2,\quad t\geqslant 0, \tag{39}$$

where we have used estimate (35) and (36) and the following facts:

$$\int_{R^2}\{w,\Delta v\}w\quad dx\quad dy=0,$$

$$\int_{R^2}\{u,\Delta w\}w\quad dx\quad dy=\int_{R^2}((u_{xx}-u_{yy})w_xw_y+u_{xy}(w_yw_y-w_xw_x))\quad dx\quad dy$$
$$\leqslant\|\Delta u(\cdot,t)\|_{L^p}\|\nabla w(\cdot,t)\|_{L^{2p/(p-2)}}\|\nabla w(\cdot,t)\|_{L^2}$$
$$\leqslant C(1+pt^2)^{1+2/p}\|\nabla w(\cdot,t)\|_{L^2}^{2-2/p},\qquad \forall p>2.$$

From (39), we get

$$\|w(\cdot,t)\|_{H^1}^2\leqslant(Cp^2(1+t^2)^2t)^p,\qquad \forall p>2,\quad t\geqslant 0, \tag{40}$$

where constant C is independent of time t, p and λ. Therefore, there exists a $T>0$ such that $C(1+T^2)^2T\leqslant\frac{1}{2}$. Let $p\to\infty$. One then has

$$\|w(\cdot,t)\|_{H^1}^2=0,\qquad \forall t\in[0,T]. \tag{41}$$

This completes the proof of uniqueness of solution for problem (4) and (5).

Repeating the same procedure as that produced in the proof of Lemma 5, we can prove the following lemma.

Lemma 6: Let $u_0\in H^3(R^2)\cap W_\infty^2(R^2)$. Then for all time $0<T<\infty$ there is a unique solution u of problem (4) and (5) such that $u\in C([0,T];H^3(R^2))$. Moreover, if $k=0$, then

$$\sup_{0\leqslant t\leqslant T}\|u(\cdot,t)\|_{H^3}+\sup_{0\leqslant t\leqslant T}\|u(\cdot,t)\|_{W_\infty^2}\leqslant C, \tag{42}$$

where constant C is independent of λ.

IV. SOLUTION OF THE HASEGAWA–MIMA EQUATION

The proof of Theorem 1: Using Lemmas 4 and 6, let $\lambda\to 0$. We then have that there exists a global solution u of the problem (1) and (2) such that $u\in L^\infty([0,T];H^m(R^2))$. Employing (3), we get $u_t\in L^\infty([0,T];H^{m-1}(R^2))$. Repeating the same procedure as that produced in the proof of Lemma 5, we can obtain that the regular solution of problem (1) and (2) is unique. Theorem 1 is proved.

The proof of Theorem 2: Using Lemma 5, let $\lambda\to 0$. We then have that there exists a global solution u of the problem (1) and (2) such that $u\in L^\infty([0,T];H^2(R^2))$. Employing (3), we get $u_t\in L^\infty([0,T];H^1(R^2))$. If $u_0\in H^2(R^2)\cap W_\infty^2(R^2)$, repeat the same procedure as that produced in the proof of Lemma 5. We can then obtain that the weak solution of problem (1) and (2) is unique. Theorem 2 is proved.

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Eigenvalue distribution of large weighted random graphs

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We study eigenvalue distribution of the adjacency matrix $A^{(N,p)}$ of weighted random graphs $\Gamma=\Gamma_{N,p}$. We assume that the graphs have N vertices and the average number of edges attached to one vertex is p. To each edge of the graph e_{ij} we assign a weight given by a random variable a_{ij} with zero mathematical expectation and all moments finite. In the first part of the paper, we consider the moments of normalized eigenvalue counting function $\sigma_{N,p}$ of $A^{(N,p)}$. Assuming all moments of a finite, we obtain recurrent relations that determine the moments of the limiting measure $\sigma_p=\lim_{N\to\infty}\sigma_{N,p}$. The method developed is applied to the Laplace operator Δ_Γ closely related with $A^{(N,p)}$. Using the recurrent relations, we analyze the form of σ_p for the both of random matrix families. In the second part of the paper we consider the resolvents $G^{(A,\Delta)}(z)$ of $A^{(N,p)}$ and Δ_Γ of $\Gamma_{N,p}$ and study the functions $f_N^{(A,\Delta)}(z,u)=(1/N)\,\Sigma_{k=1}^N \exp\{-uG_{kk}^{(A,\Delta)}(z)\}$ in the limit $N\to\infty$. We derive closed equations that uniquely determine the limiting functions $f^{(A,\Delta)}(z,u)$. These equations allow us to prove the existence of the limiting σ_p for adjacency matrix and the Laplace operator under a rather weak condition that only the fourth moment of a_{ij} is finite. Besides, equations for $f^{(A,\Delta)}(z,u)$ give us the asymptotic expansions for the Stieltjes transform of the limiting σ_p with respect to z^{-k} and p^k. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1667610]

I. INTRODUCTION

The spectral theory of graphs is an actively developing field of mathematics involving a variety of methods and deep results (see Refs. 5, 6, and 11). Given a graph with N vertices, one can associate with it many different matrices, but the most studied are the adjacency matrix and the Laplacian matrix of the graph. Commonly, the set of N eigenvalues of the adjacency matrix is referred to as the spectrum of the graph. In these studies, the dimension of the matrix N is usually regarded as a fixed parameter. The spectra of infinite graphs is considered in certain particular cases of graphs having a certain regular structure (see, for example, Ref. 12).

Another large class of graphs, where the limiting transition $N\to\infty$ provides a natural approximation, is represented by random graphs.[4,13] In this branch, geometrical and topological properties of graphs are studied for a wide variety of random graph ensembles. One of the classes of the prime reference is the *binomial random graph* originating by P. Erdős (see, e.g., Ref. 13). Given a number $p_N\in(0,1)$, this family of graphs $\mathbf{G}(N,p_N)$ is defined by taking as Ω the set of all graphs on N vertices with the probability

$$P(G)=p_N^{e(G)}(1-p_N)^{\binom{N}{2}-e(G)}, \tag{1.1}$$

where $e(G)$ is the number of edges of G. Most of the random graphs studies are devoted to the cases where $p_N\to 0$ as $N\to\infty$.

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Intersection of these two branches of the theory of graphs contains the spectral theory of random graphs that is still poorly explored. However, a number of powerful tools can be employed here because the ensemble of random symmetric $N\times N$ adjacency matrices A_N is a particular representative of the random matrix theory, where the limiting transition $N\to\infty$ has been intensively studied during half of century since the pioneering works by E. Wigner.[22] Initiated by theoretical physics applications, the spectral theory of random matrices has revealed deep nontrivial links with many fields of mathematics.

Spectral properties of random matrices corresponding to (1.1) were examined in the limit $N\to\infty$ both in numerical and theoretical physics studies.[7–9,18,20,21] There are two major asymptotic regimes: $p_N\gg 1/N$ and $p_N=O(1/N)$ and corresponding models can be called the *dilute random matrices* and *sparse random matrices*, respectively. The first studies of spectral properties of sparse and dilute random matrices in the physical literature are related to Refs. 20, 21, and 18, where equations for the limiting density of states of sparse random matrices were derived. In Refs. 18 and 10 a number of important results on the universality of the correlation functions and the Anderson localization transition were obtained. Unfortunately, all these results were obtained with nonrigorous replica and supersymmetry methods.

On a mathematical level of rigour, the eigenvalue distribution of dilute random matrices was studied in Ref. 16. It was shown that the normalized eigenvalue counting function of

$$\frac{1}{\sqrt{Np_N}}A_{N,p_N} \tag{1.2}$$

converges in the limit $N,p_N\to\infty$ to the distribution of explicit form known as the semicircle or Wigner law.[22] The moments of this distribution verify the well-known recurrent relation for the Catalan numbers and can be found explicitly. Therefore, one can say that the dilute random matrices represent explicitly solvable model (see also Refs. 20 and 21).

In the series of papers in Refs. 2–4 and simultaneously in Ref. 15, the adjacency matrix and the Laplace matrix of random graphs (1.1) with $p_N=pN$ were studied. It was shown that this sparse random matrix ensemble can also be viewed as the explicitly solvable model. In particular, one can derive recurrent relations that determine the moments of the limiting eigenvalue distribution of $A_{N,pN}$, $N\to\infty$, depending on given value of p.

In the present paper we generalize the results of Refs. 3 and 15 to the case of weighted random graphs. We study also the resolvent of the adjacency matrix and the Laplace operator of large weighted random graphs and derive rigorously equations for the Stieltjes transform $g(z)$ of the limiting eigenvalue distribution, obtained initially in Refs. 20, 21, and 18 by using the replica and the supersymmetry approaches. We stress that our approach allows us to prove the existence of the limiting eigenvalue distribution under rather weak conditions, when only the fourth moment of a_{ij} is required to be bounded. Using our results it is not difficult to obtain the asymptotic expansions for $g(z)$ with respect to z^{-k}. Since it is well known that the coefficients of this expansion are the moments of the limiting IDS, we rediscover the recurrent formulas for the moments. Besides, constructing the asymptotic expansion of $g(z)$ with respect to p^k, it is easy to show that this expansion is convergent for $p<1$. Since in the case $a_{ij}=1$ the coefficients of this expansion are the rational functions on z, we can conclude that the limiting spectrum is pure point and consists of the spectra of finite blocks only.

II. MAIN RESULTS

Let $\mathcal{V}_N$ denotes the set of N vertices $v_1,v_2,\ldots,v_N$. We define the set $\mathcal{F}_{\mathcal{V}_N}=\mathcal{V}_N\to\mathbf{R}$ of all real functions $f=(f(v_1),f(v_2),\ldots,f(v_N))$. Let us assume that each pair of vertices of $\mathcal{V}_N$ is either connected by one nonoriented edge or not connected. Let us denote by E_N the set of the edges and by $\Gamma_N=(\mathcal{V}_N,E_N)$ the corresponding graph.

Assume that each edge $e=(v_i,v_j)\in E_N$ is assigned by the real weight $\xi(e)$. Then one can define a linear operator $\Delta_\Gamma^{(\xi)}:\mathcal{F}_{\mathcal{V}_N}\to\mathcal{F}_{\mathcal{V}_N}$ by the relation

$$\Delta_\Gamma^{(\xi)}(f(v_i))=\sum_{j:v_j\sim v_i}\xi(v_i,v_j)\cdot[f(v_i)-f(v_j)], \tag{2.1}$$

where the sum goes over all vertices v_j adjacent to given v_i. One can consider the operator $\Delta_\Gamma^{(\xi)}$ as a generalization of the discrete analog of the Laplace operator on the graph Γ_N.

Clearly, $\Delta_\Gamma^{(\xi)}$ is a real symmetric $N\times N$ matrix that can be represented in the form

$$\Delta_\Gamma^{(\xi)}=B^{(N,\xi)}-A^{(N,\xi)},$$

where $A^{(N,\xi)}$ is a weighted adjacency matrix of Γ_N,

$$A_{ij}^{(N,\xi)}=\begin{cases}\xi(v_i,v_j), & \text{if } v_i\sim v_j,\\ 0, & \text{if } v_i\not\sim v_j,\end{cases} \tag{2.2}$$

and $B^{(N,\xi)}$ is a diagonal matrix

$$B_{ii}^{(N,\xi)}=\sum_{j:v_j\sim v_i}\xi(v_i,v_j).$$

Note that $A_{ii}^{(N,\xi)}=0$ and

$$\Delta_\Gamma^{(\xi)}=\mathrm{diag}[(MA^{(N,\xi)})]-A^{(N,\xi)}, \tag{2.3}$$

where

$$M_{ij}=1-\delta_{ij}=\begin{cases}0, & \text{if } i=j,\\ 1, & \text{if } i\neq j.\end{cases}$$

The set of eigenvalues $\lambda_1\leqslant\cdots\leqslant\lambda_N$ of $A^{(N,\xi)}$ is referred to as the spectrum of the graph Γ.

With these definitions in hand, we can introduce the randomly weighted adjacency matrix of random binomial graphs. In this case the weights ξ are represented by the following family of random variables. Let $\Xi=\{a_{ij},\ \ i\leqslant j,\ \ i,j\in\mathbf{N}\}$ be the set of jointly independent identically distributed (i.i.d.) random variables defined on the same probability space and possessing the moments

$$\mathbf{E}a_{ij}^k=X_k<\infty\quad\forall\ \ i,j,k\in\mathbf{N}, \tag{2.4}$$

where $\mathbf{E}$ denotes the mathematical expectation corresponding to Ξ. We set $a_{ji}=a_{ij}$ for $i\leqslant j$.

Given $0<p\leqslant N$, let us define the family $D_N^{(p)}=\{d_{ij}^{(N,p)},\ \ i\leqslant j,\ \ i,j\in\overline{1,\ N}\}$ of jointly independent random variables

$$d_{ij}^{(N,p)}=\begin{cases}\dfrac{1}{\sqrt{p}}, & \text{with probability } p/N,\\ 0, & \text{with probability } 1-p/N.\end{cases} \tag{2.5}$$

We set $d_{ji}=d_{ij}$ and assume that $\Lambda_N^{(p)}$ is independent of Ξ.

Now one can consider the real symmetric matrix $A^{(N,p)}(\omega)$,

$$[A^{(N,p)}]_{ij}=a_{ij}d_{ij}^{(N,p)}, \tag{2.6}$$

that has N real eigenvalues $\lambda_1^{(N,p)}\leqslant\lambda_2^{(N,p)}\leqslant\cdots\leqslant\lambda_N^{(N,p)}$.

The normalized eigenvalue counting function [or integrated density of states (IDS)] of A is determined by the formula

$$\sigma(\lambda;A^{(N,p)})=\frac{\sharp\{j:\lambda_j^{(N,p)}<\lambda\}}{N}.$$

Similarly we define $\sigma(\lambda;\Delta_\Gamma^{(\xi)})$.

In this paper we study the normalized eigenvalue counting functions by two complementary approaches: the moments and the resolvent techniques. Corresponding results are represented in the following two subsections.

A. Moment relations approach

The first group of results concerns the averaged moments

$$M_k^{(N,p)}=\mathbf{E}\left\{\int \lambda^k d\sigma(\lambda;A^{(N,p)})\right\}.$$

Theorem 1: *Assuming conditions (2.4), there exist limits*

$$\lim_{N\to\infty} M_s^{(N,p)}=\begin{cases} m_k^{(p)}=\sum_{i=0}^{k} S(k,i), & if\ \ s=2k,\\ 0, & if\ \ s=2k-1,\end{cases} \tag{2.7}$$

where numbers $\mathrm{S}(k,i)$ *are determined by the system of recurrent relations*

$$\mathrm{S}(l,r)=\sum_{f=1}^{r}\binom{r-1}{f-1}\cdot\frac{X_{2f}}{p^{f-1}}\cdot\sum_{u=0}^{l-r}\mathrm{S}(l-u-f,r-f)\cdot\sum_{v=0}^{u}\binom{f+v-1}{f-1}\cdot\mathrm{S}(u,v) \tag{2.8}$$

with the initial condition $S(l,0)=\delta_{l,0}$.

The next theorem deals with the moments

$$L_s^{(N,p)}=\mathbf{E}\left\{\int \lambda^s d\sigma(\lambda;\Delta_\Gamma)\right\}.$$

Theorem 2: *Assume that (2.4) holds. Then, given* $s\in\mathbf{N}$, *there exists the limit*

$$\lim_{N\to\infty} L_s^{(N,p)}=l_s^{(p)}=\sum_{i=0}^{s}\hat{\mathrm{S}}(s,i), \tag{2.9}$$

where numbers $\hat{\mathrm{S}}(s,i)$ *are determined by the system of recurrent relations*

$$\hat{\mathrm{S}}(l,r_1)=\sum_{g_1=1}^{r_1}\binom{r_1-1}{g_1-1}\cdot\left(\hat{\mathrm{S}}(l-g_1,r_1-g_1)\cdot\frac{X_{g_1}}{p^{g_1/2-1}}+\sum_{d=r_1-g_1}^{l-r_1}\hat{\mathrm{S}}(d,r_1-g_1)\cdot\sum_{g_2=1}^{l-d-g_1}\binom{g_1+g_2-1}{g_1-1}\right.$$
$$\left.\cdot\frac{X_{g_1+g_2}}{p^{(g_1+g_2)/2-1}}\sum_{r_2=1}^{l-d-g_1-g_2}\binom{r_2+g_2-1}{g_2-1}\cdot\hat{\mathrm{S}}(l-d-g_1-g_2,r_2)\right) \tag{2.10}$$

with the initial condition

$$\hat{\mathrm{S}}(l,0)=\delta_{l,0}.$$

We discuss these results later. Let us only note that if $a_{ij}\equiv 1$ and $p=1$, then $A^{(N,1)}$ becomes exactly the adjacency matrix of Γ and $\Delta_\Gamma^{(a)}$ takes the form of the Laplace operator on the graph. In this case formula (2.8) is reduced to

$$\mathrm{S}(l,r)=\sum_{f=1}^{r}\binom{r-1}{f-1}\cdot\sum_{u=0}^{l-r}\mathrm{S}(l-u-f,r-f)\cdot\sum_{v=0}^{u}\binom{f+v-1}{f-1}\cdot\mathrm{S}(u,v)\,. \tag{2.11}$$

This system of recurrent relations is obtained for the first time in Ref. 15. It is simpler than that derived in Ref. 2 to determine $m_k^{(1)}$ in (2.7). The difference is that our system (2.8) has one variable of summation less than the system of Ref. 2. We explain this difference at the end of Sec. IV.

In the case $a_{ij}\equiv 1$ and $p=1$ formulas (2.10) reduce to

$$\hat{\mathrm{S}}(l,r_1)=\sum_{g_1=1}^{r_1}\binom{r_1-1}{g_1-1}\cdot\Bigg(\hat{\mathrm{S}}(l-g_1,r_1-g_1)+\sum_{d=r_1-g_1}^{l-r_1}\hat{\mathrm{S}}(d,r_1-g_1)\cdot\sum_{g_2=1}^{l-d-g_1}\binom{g_1+g_2-1}{g_1-1}\cdot\sum_{r_2=1}^{l-d-g_1-g_2}\binom{r_2+g_2-1}{g_2-1}\cdot\hat{\mathrm{S}}(l-d-g_1-g_2,r_2)\Bigg).$$

B. Resolvent approach

The resolvent approach is a powerful tool of the spectral theory in general and the spectral theory of random matrices also. In particular, it allows us to simplify and generalize the pioneer method of Wigner[22] (based on the analysis of the moments of σ) used to study the IDS of the ensemble with independent Gaussian entries. The resolvent approach produces also a lot of new results (see, e.g., Refs. 16 and 19, which are review papers, and references therein). It is well known that the trace of the resolvent is the Stiltjes transform $g_N(z)$ of the normalized counting function of the matrix. Since the Stiltjes transform uniquely determines the measure, the proof of the existence of the limiting IDS is equivalent to the proof of the existence of the limit $\lim_{N\to\infty}g_N(z)=g(z)$. Besides, the equations for $g(z)$ give complete information about the limiting IDS.

For any z: $\Re z>0$ consider the function $f_N(u,z):\mathbf{R}_+\to\mathbf{C}$:

$$f_N(u,z)=\frac{1}{N}\sum_{k=1}^{N}e^{-ua_k^2G_{kk}^{(N,p)}(z)},\quad G_{kk}^{(N,p)}(z)=(z-iA^{(N,p)})_{kk}^{-1}, \tag{2.12}$$

where $\{a_i\}_{i=1}^{\infty}$ is a family of i.i.d. random variables which do not depend on $\{a_{i,j}\}_{i<j}^{\infty}$ and have the same probability distribution as $a_{1,2}$.

Theorem 3: *Assume that* $\mu(a)=\mathbf{E}\{\theta(a-a_{i,j})\}$, *the probability distribution of* $a_{i,j}$, *possesses the property*

$$\int a^4d\mu(a)=X_4<\infty. \tag{2.13}$$

Then (i) the variance of the function $f_N(u,z)$ *defined by (2.12) vanishes in the limit* $N\to\infty$:

$$\lim_{N\to\infty}\mathbf{E}\{|f_N(u,z)-\mathbf{E}\{f_N(u,z)\}|^2\}=0; \tag{2.14}$$

(ii) there exists the limit

$$\lim_{N\to\infty}\mathbf{E}\{f_N(u,z)\}=f(u,z); \tag{2.15}$$

and (iii) if we consider the class $\mathcal{C}$ *of functions which are analytic with respect to* z: $\Re z>0$ *and for any fixed* z: $\Re z>0$ *possessing the norm*

$$\|f(u,z)\| = \max_{u>0} \frac{|f(u,z)|}{\sqrt{1+u}}, \tag{2.16}$$

then the limiting function is the unique solution in $\mathcal{C}$ of the functional equation

$$f(u,z) = 1 - u^{1/2} e^{-p} \int |a| d\mu(a) \int_0^\infty dv \, \frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}} \exp\{-zv + pf(v/p,z)\}, \tag{2.17}$$

where $\mathcal{J}_1(\zeta)$ is the Bessel function

$$\mathcal{J}_1(\zeta) = \frac{\zeta}{2} \sum_{k=0}^{\infty} \frac{(-\zeta^2/4)^k}{k!(k+1)!}. \tag{2.18}$$

It is easy to see that Eq. (2.17) coincides with that obtained in Refs. 20 and 18 by the replica trick and supersymmetry approach, respectively, by using the assumption that the solution of the problem is replica symmetric (or an equivalent assumption for the saddle point method). Our proof is rigorous and it needs no additional assumption.

One can easily see that

$$-\frac{\partial}{\partial u} f_N(u,z)\bigg|_{u=0} = \frac{X_2}{N} \sum_{k=1}^{N} \mathbf{E}\{G_{kk}^{(N,p)}(z)\} = X_2 \mathbf{E}\{i g_{N,p}(-iz)\},$$

where $g_{N,p}(z)$ is the Stieltjes transform of the normalized counting function $\sigma(\lambda, A^{(N,p)})$:

$$g_{N,p}(z) = \int \frac{d\sigma(\lambda, A^{(N,p)})}{\lambda - z}.$$

Hence, Theorem 3 implies that for any z: $\Im z \neq 0$

$$\lim_{N\to\infty} \mathbf{E}\{|g_{N,p}(z) - \mathbf{E}\{g_{N,p}(z)\}|^2\} = 0,$$

i.e., the fluctuations of $g_{N,p}(z)$ vanish in the limit $N \to \infty$. And (2.15) implies that

$$g(z) = \lim_{N\to\infty} \mathbf{E}\{g_{N,p}(z)\} = -X_2^{-1} \frac{\partial}{\partial u} f(u,z)\bigg|_{u=0}. \tag{2.19}$$

Thus, Theorem 3 states that under condition (2.13) there exists the weak limit $\sigma(\lambda, A)$ of the normalized counting measure $\sigma(\lambda, A^{(N,p)})$ and the Stieltjes transform $g_p(-iz)$ can be obtained as the first derivative of the solution of (2.17).

If the random variables $\{a_{i,j}\}$ possess the $2m$th moments, then on the basis of (2.17) it is easy to construct an asymptotic expansion of the function $f(u,z)$ in z^{-k} up to z^{-2m}:

$$f(u,z) = \sum_{k=0}^{2m} z^{-k} P_k(u) + o(z^{-2m}), \quad z \to \infty,$$

where $P_k(u)$ are some polynomials. Since for any polynomial $P(u)$

$$u^{1/2} e^{-p} \int |a| d\mu(a) \int_0^\infty dv \, \frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}} \exp\{-zv\} P(v) = O(z^{-1}),$$

this expansion gives us recurrent formulas which express the coefficients of $P_k(u)$ via the coefficients of $P_{k-1}(u),\dots,P_1(u)$. By (2.19) it is evident that the coefficient c_{k1} of $P_k(u)$ near u is the kth coefficient of the expansion of $g_p(-iz)$, in z^{-k}. So, $c_{k1}=(-i)^k M_k$, where M_k is the kth moment of the limiting measure $\sigma(\lambda)$.

Similarly, one can construct an expansion of $g(z)$ with respect to p^k. To this end it is more convenient to study the case when $a_{ij}=1$ and $d_{ij}=0,1$ with probabilities $1-p/N$ and p/N, respectively. It is equivalent to the change of variables $z\to zp^{-1/2}$, $u\to up^{-1/2}$. Then we get the equation

$$\tilde f(u,z)=1-u^{1/2}e^{-p}\int_0^\infty dv\,\frac{\mathcal{J}_1(2\sqrt{uv})}{\sqrt{v}}\cdot\exp\{-zv+p\tilde f(v,z)\}. \tag{2.20}$$

Let us seek the expansion of the form $\tilde f(u,z)=1+\Sigma p^k f_k(u,z)$. Since on the r.h.s. of (2.20) we have the exponent of $p(\tilde f(u,z)-1)$, it is evident that (2.20) gives us the recurrent formula for $f_k(u,z)$ and $f_k(u,z)$ is a linear combination of the functions $e^{-uR_{k,l}(z)}$ $(l=1,\dots,k!)$ with $R_{k,l}(z)$ being rational functions of z. It is easy to prove that the expansion is convergent, if $p<1$. Therefore we can differentiate it with respect to u. Hence, for the function $\tilde g(z)$ defined as in Remark 1, we get the convergent expansion $\tilde g(z)=\Sigma p^k\tilde R_k(z)$, where $\tilde R_k(z)$ are the rational functions of z. Thus, we can state that for $p<1$ the spectrum of the adjacency matrix consists only from the spectrum of finite graphs.

Now let us study the IDS of the Laplace operator of the random graph. To this end for any z: $\Re z>0$ define the function $f_N^{(\Delta)}(u,z):\mathbf{R}_+\to\mathbf{C}$:

$$f_N^{(\Delta)}(u,z)=\frac{1}{N}\sum_{k=1}^N e^{-iua_k-ua_k^2G_{kk}^{(\Delta,N,p)}(z)},\quad G_{kk}^{(\Delta,N,p)}(z)=(z-iL^{(N,p)})_{kk}^{-1}, \tag{2.21}$$

where $\{a_i\}_{i=1}^\infty$ are defined by the same way as in (2.12).

Theorem 4: *Let the distribution of $a_{j,k}$ satisfy condition (2.13). Then*

(i) fluctuations of the function $f_N^{(\Delta)}(u,z)$ defined by (2.21) vanish in the limit $N\to\infty$:

$$\lim_{N\to\infty}\mathbf{E}\{|f_N^{(\Delta)}(u,z)-\mathbf{E}\{f_N^{(\Delta)}(u,z)\}|^2\}=0, \tag{2.22}$$

(ii) there exists the limit

$$\lim_{N\to\infty}\mathbf{E}\{f_N^{(\Delta)}(u,z)\}=f^{(\Delta)}(u,z), \tag{2.23}$$

and (iii) the limiting function is the unique solution in the class $\mathcal{C}$ defined in Theorem 3 of the functional equation

$$f^{(\Delta)}(u,z)=\hat\mu(-u)-u^{1/2}e^{-p}\int|a|e^{-iau}d\mu(a)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}\exp\{-zv+pf^{(\Delta)}(v/p,z)\}, \tag{2.24}$$

where $\hat\mu(u)=\int e^{iua}d\mu(a)$ is the Fourier transform of the measure $\mu(a)$, defined in Theorem 3.

III. MOMENTS AND TREES

In this section we give an outlook of the method of computing moments. Rigorous description is given in the next section.

To study the mathematical expectation

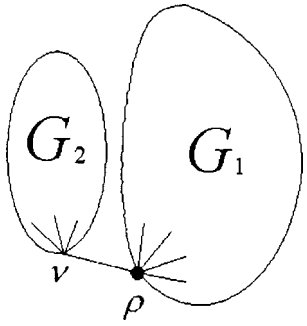

FIG. 1. Decomposition of τ_m by the first edge (ρ, ν).

$$\mathbf{E}\frac{1}{N}\mathrm{Tr}(\mathrm{A}^{(N,p)})^k=\frac{1}{N}\sum_{i_l=1}^{N}\mathbf{E}\{A_{i_1i_2}^{(N,p)}A_{i_2i_3}^{(N,p)}\cdots A_{i_ki_1}^{(N,p)}\}, \tag{3.1}$$

we give a further development to the method originated by E. Wigner (see, e.g., Ref. 22). In this approach the set of variables $I_k=\{i_1,i_2,\ldots,i_k,i_1\}$, $i_l\in\overline{1,\ N}$, is regarded as a set of trajectories (walks) W_k of k steps. Each walk provides a contribution $\mathbf{E}\{A_{i_1i_2}^{(N,p)}A_{i_2i_3}^{(N,p)}\cdots A_{i_ki_1}^{(N,p)}\}$. This mathematical expectation is nonzero only when each step (i_j,i_{j+1}) appears an even number of times in this walk W_k. The order and the number of repetitions of the steps leads to partition of the set $\{W_k\}$ of the walks into the classes of equivalence.

In the case of the Wigner ensemble $A^{(N,N)}$, the classes of equivalence were labeled by the plane rooted trees τ_l of l edges for $k=2l$. Such a tree can be run over by $2l$ steps starting and finishing at the root and passing each edge two times exactly (there and back). This path is made in the lexicographical order. This means that each time when there is a choice where to go, the most left edge is passed. The set T_l of all trees τ_l contains $C_l=(2l)!/l!(l+1)!$ elements.

The situation is more delicate in the case of dilute matrices (2.6), when p is fixed and $N\to\infty$. In Ref. 14 it is shown that the leading contribution to (3.1) in this limit is provided by the walks $I_k, k=2l$, that fall into the classes of equivalence described as follows.

We consider an element $\tau_m\in T_m, m\leqslant l$, and construct a path of $2l$ steps over this tree. Each edge is passed even number of times. If $m<l$, then there exist one or several edges passed an even number of times, which is greater than 2. This path is made in the lexicographical order that chooses the most left edge among those that are yet not passed. The number of such paths and the corresponding contribution were estimated in Ref. 14.

The case of a nonweighted adjacency matrix and corresponding Laplace operator is considered in Refs. 2 and 15, where these paths were computed exactly and recurrent relations for their number were obtained.

In the present paper we develop the method to compute these paths and corresponding contributions in the case of weighted matrices. It is similar to the method of decomposition of trees by one edge that is a well-known combinatorial tool to obtain recurrent relations needed.

Let us briefly describe our method. Consider a tree τ_m with m edges and the root ρ and denote by (ρ,ν) the edge that is passed first. If one removes this edge, one gets two subtrees G_2 and G_1 (see Fig. 1).

Denote by f the number of passages $\rho\to\nu$. Then the path over the tree τ_m is described as follows: after the first passage $\rho\to\nu$ one enters the tree G_2 and goes over its edges. Each time when one gets into the vertex ν, there is a choice of where to go: either to the leave G_u and enter the subtree G_1 by $\nu\to\rho$, or to continue the path over G_2. It is clear that the paths over the subtrees G_2 and G_1 are performed independently. More precisely, when leaving the subtree G_1, one keeps the information about its part already passed. Returning back to it by the passage $\nu\to\rho$, we continue this path with no regard to what part of the path over G_1 is performed. The

number of passages f over the edge (ρ,ν) in direction $(\overrightarrow{\rho,\nu})$ determines the weight factor $\mathbf{E}a^{2f}=X_{2f}$.

This splitting of trees (and paths) in two parts leads to the recurrent relations for the number of the paths and corresponding contributions.

Certainly this brief presentation does not reflect all of the details of the procedure. Moreover, in the rigorous proof we study the classes of walks W_k directly and the trees arise as somehow supplementary objects. We used them here as more visual illustrations than the walks.

IV. PROOF OF THEOREM 1

A. Walks and contributions

Using independence of families Ξ and $\Lambda_N^{(p)}$, we have

$$\begin{aligned}
M_k^{(N,p)} &= \int \mathbf{E}\{\lambda^k d\sigma_{A^{(N,p)}}\} \\
&= \mathbf{E}\left(\frac{1}{N}\sum_{i=1}^{N}[\lambda_i^{(N,p)}]^k\right) \\
&= \frac{1}{N}\mathbf{E}(Tr[A^{(N,p)}]^k) \\
&= \frac{1}{N}\sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\cdots\sum_{j_k=1}^{N}\mathbf{E}(A_{j_1,j_2}^{(N,p)}A_{j_2,j_3}^{(N,p)}\cdots A_{j_k,j_1}^{(N,p)}) \\
&= \frac{1}{N}\sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\cdots\sum_{j_k=1}^{N}\mathbf{E}(a_{j_1,j_2}a_{j_2,j_3}\cdots a_{j_k,j_1})\cdot\mathbf{E}(d_{j_1,j_2}^{(N,p)}d_{j_2,j_3}^{(N,p)}\cdots d_{j_k,j_1}^{(N,p)}). \qquad (4.1)
\end{aligned}$$

Consider $W_k^{(N)}$ the set of closed walks of k steps over the set $\overline{1,\ N}$:

$$W_k^{(N)}=\{w=(w_1,w_2,\ldots,w_k,w_{k+1}=w_1):\forall i\in\overline{1,\ k+1}\quad w_i\in\overline{1,\ N}\}.$$

For $w\in W_k^{(N)}$ let us denote $a(w)=\Pi_{i=1}^k a_{w_i,w_{i+1}}$ and $d^{(N,p)}(w)=\Pi_{i=1}^k d_{w_i,w_{i+1}}^{(N,p)}$. Then we have

$$M_k^{(N,p)}=\frac{1}{N}\sum_{w\in W_k^{(N)}}\mathbf{E}a(w)\cdot\mathbf{E}d^{(N,p)}(w). \qquad (4.2)$$

Let $w\in W_k^{(N)}$ and $f,g\in\overline{1,\ N}$. Denote by $n_w(f,g)$ the number of steps $f\to g$ and $g\to f$:

$$n_w(f,g)=\sharp\{i\in\overline{1,k}:\ (w_i=f\wedge w_{i+1}=g)\vee(w_i=g\wedge w_{i+1}=f)\}.$$

Then

$$\mathbf{E}a(w)=\prod_{f=1}^{N}\prod_{g=f}^{N}X_{n_w(f,g)}.$$

Given $w\in W_k^{(N)}$, let us define the sets $V_w=\cup_{i=1}^k\{w_i\}$ and $E_w=\cup_{i=1}^k\{(w_i,w_{i+1})\}$, where (w_i,w_{i+1}) is a nonordered pair. It is easy to see that $G_w=(V_w,E_w)$ is a simple nonoriented graph and the walk w covers the graph G_w. Let us call G_w the skeleton of walk w. We denote by $n_w(e)$ the number of passages of the edge e by the walk w in direct and inverse directions. For $(w_j,w_{j+1})=e_j\in E_w$ let us denote $a_{e_j}=a_{w_j,w_{j+1}}=a_{w_{j+1},w_j}$. Then we obtain

$$\mathbf{E}a(w)=\prod_{e\in E_w}\mathbf{E}a_e^{n_w(e)}=\prod_{e\in E_w}X_{n_w(e)}.$$

Similarly we can write

$$\mathbf{E}d^{(N,p)}(w)=\prod_{e\in E_w}\mathbf{E}([d_e^{(N,p)}]^{n_w(e)})=\prod_{e\in E_w}\frac{1}{N\cdot p^{n_w(e)/2-1}}.$$

Then, we can rewrite (4.2) in the form

$$M_k^{(N,p)}=\frac{1}{N}\sum_{w\in W_k^{(N)}}\prod_{e\in E_w}\frac{X_{n_w(e)}}{N\cdot p^{n_w(e)/2-1}}=\sum_{w\in W_k^{(N)}}\left(\frac{1}{N^{|E_w|+1}\cdot p^{k/2-|E_w|}}\prod_{e\in E_w}X_{n_w(e)}\right)=\sum_{w\in W_k^{(N)}}\theta(w), \tag{4.3}$$

where $\theta(w)$ is the contribution of the walk w to the mathematical expectation of the corresponding moment. To perform the limiting transition $N\to\infty$ it is natural to separate W_k^N into classes of equivalence. Walks $w^{(1)}$ and $w^{(2)}$ are equivalent, $w^{(1)}\sim w^{(2)}$, if and only if there exists a bijection f between the sets of vertices $V_w^{(1)}$ and $V_w^{(2)}$ such that for $i=1,2,\ldots,k$, $w_i^{(2)}=f(w_i^{(1)})$,

$$w^{(1)}\sim w^{(2)}\ \Leftrightarrow\ \exists f:\ V_w^{(1)}\overset{bij}{\to}V_w^{(2)}:\ \forall\ \ i\in\overline{1,\ k+1}\quad w_i^{(2)}=f(w_i^{(1)}).$$

Let us denote by $[w]$ the class of equivalence of walk w and by $C_k^{(N)}$ the set of such classes. It is obvious that if two walks $w^{(1)}$ and $w^{(2)}$ are equivalent, then their contributions are equal:

$$w^{(1)}\sim w^{(2)}\ \Rightarrow\theta(w^{(1)})=\theta(w^{(2)}).$$

Cardinality of the class of equivalence $[w]$ is equal the number of all mappings $f:V_w\to R_f\subset\overline{1,\ N}$ i.e., $N\cdot(N-1)\cdot\cdots\cdot(N-|V_w|+1)$. Then we can rewrite (4.3) in the form

$$\begin{aligned}M_k^{(N,p)}&=\sum_{w\in W_k^{(N)}}\left(\frac{1}{N^{|E_w|+1}\cdot p^{k/2-|E_w|}}\prod_{e\in E_w}X_{n_w(e)}\right)\\&=\sum_{[w]\in CW_k^{(N)}}\left(\frac{N\cdot(N-1)\cdot\cdots\cdot(N-|V_w|+1)}{N^{|E_w|+1}\cdot p^{k/2-|E_w|}}\prod_{e\in E_w}X_{n_w(e)}\right)\\&=\sum_{[w]\in CW_k^{(N)}}\hat{\theta}([w]).\end{aligned} \tag{4.4}$$

B. Minimal and essential walks

To consider the set $C_k^{(N)}$, it is convenient to relate a given class of equivalence $[w]$ with one particular walk from this class. More precisely, we give the rule to determine this walk that we will call the minimal walk.

Definition 1: The walk w is a minimal walk, if w_1 (the root of walk) has the number 1 and the number of each new vertex is equal to the number of all already passed vertices plus 1.

Example 1: The sequences (1,2,1,2,3,1,4,2,1,4,3,1) and (1,2,3,2,4,2,3,2,1,2,4,1,5,1) represent the minimal walks.

Let us denote the set of all minimal walks of $W_k^{(N)}$ by $MW_k^{(N)}$. It is clear that there is only one minimal walk at each class of equivalence and vice versa. Therefore we can rewrite (4.4) in the form

$$M_k^{(N,p)}=\sum_{w\in MW_k^{(N)}}\left(\frac{N\cdot(N-1)\cdot\cdots\cdot(N-|V_w|+1)}{N^{|E_w|+1}\cdot p^{k/2-|E_w|}}\prod_{e\in E_w}X_{n_w(e)}\right)=\sum_{w\in MW_k^{(N)}}\hat{\theta}([w]). \tag{4.5}$$

Walk w of $W_k^{(N)}$ has at least k vertices. Hence, $MW_k^{(1)}\subset MW_k^{(2)}\subset\cdots\subset MW_k^{(i)}\subset\cdots\subset MW_k^{(k)}=MW_k^{(k)}=\cdots$. It is natural to denote $MW_k=MW_k^{(k)}$. Then (4.5) can be written as

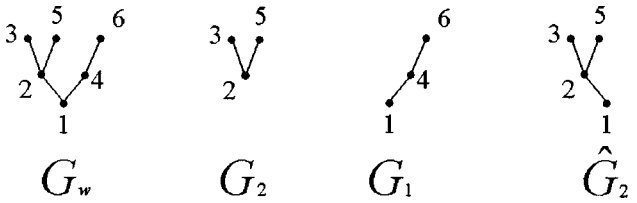

FIG. 2. Examples of G_2, G_1, $\hat{G}_2$.

$$
\begin{aligned}
m_k^{(p)} &= \lim_{N\to\infty} M_k^{(N,p)} \\
&= \lim_{N\to\infty} \sum_{w\in MW_k} \left(\frac{N\cdot(N-1)\cdot\cdots\cdot(N-|V_w|+1)}{N^{|E_w|+1}\cdot p^{k/2-|E_w|}} \prod_{e\in E_w} X_{n_w(e)} \right) \\
&= \lim_{N\to\infty} \sum_{w\in MW_k} \left(N^{|V_w|-|E_w|-1} \prod_{e\in E_w} \frac{X_{n_w(e)}}{p^{k/2-1}} \right). \qquad (4.6)
\end{aligned}
$$

The set MW_k is finite. Regarding this and (4.6), we conclude that the minimal walk w has nonvanishing contribution, if $|V_w|-|E_w|-1\geqslant 0$. But for each simple connected graph $G=(V,E)$, $|V_w|\leqslant|E_w|+1$, and the equality takes place if and only if the graph G is a tree.

Definition 2: The minimal walk w is an essential walk, if its contribution in the limit $N\to\infty$ is not zero.

Clearly, each essential walk is a minimal walk that has a tree as a skeleton and vice versa. Then the number of passages of each edge e belonging to the essential walk w is even. Hence, the limiting mathematical expectation $m_k^{(p)}$ depends only on the even moments of random variable of a. It is clear that the limiting mathematical expectation $\lim_{N\to\infty} M_{2s+1}^{(N,p)}$ is equal to zero.

C. First edge decomposition of essential walks

Let us start with necessary definitions. The first vertex $w_1=1$ of the essential walk w is called the root of the walk. We denote it by ρ. Let us denote the second vertex $w_2=2$ of the essential walk w by ν. We denote by l half of walk's length and by r the number of steps of w starting from root ρ. In Sec. III we explained that we derive the recurrent relations by splitting of the walk (or of the tree) into two parts. To describe this procedure, it is convenient to consider the set of the essential walks of length $2l$ such that they have r steps starting from the root ρ. We denote this set by $\Lambda(l,r)$. One can see that this description is exact, in the sense that it is minimal and gives complete description of the walks we need. Denote by $S(l,r)$ the sum of contributions of the walk of $\Lambda(l,r)$. Let us remove the edge $(\rho,\nu)=(1,2)$ from G_w and denote by $\hat{G}_w$ the graph obtained. The graph $\hat{G}_w$ has two components. Denote the component that contains the vertex ν by G_2 and the component containing the root ρ by G_1. Add the edge (ρ,ν) to the edge set of the tree G_2. Denote the result of this operation by $\hat{G}_2$. In Fig. 2 one can see examples of G_2, G_1, $\hat{G}_2$. Denote by u the half of the walk's length over the tree G_2 and by f the number of steps (ρ,ν) in the walk w. It is clear that the following inequalities hold for all essential walks (except the walk of length zero): $1\leqslant f\leqslant r$, $r+u\leqslant l$. Let us denote by $\Lambda_1(l,r,u,f)$ the set of the essential walks with fixed parameters l, r, u, f and by $S_1(l,r,u,f)$ the sum of contributions of the walks of $\Lambda_1(l,r,u,f)$. Denote by $\Lambda_2(l,r)$ the set of the essential walks of $\Lambda(l,r)$ such that their skeleton has only one edge attached the root ρ. Also we denote by $S_2(l,r)$ the sum of contributions of the walk of $\Lambda_2(l,r)$. Now we can formulate the first lemma of decomposition. It allows express S as a function of the S, S_2.

Lemma 1 (First decomposition lemma): The following relation holds,

$$
\mathrm{S}(l,r)=\sum_{f=1}^{r}\sum_{u=0}^{l-r}\mathrm{S}_1(l,r,u,f), \qquad (4.7)
$$

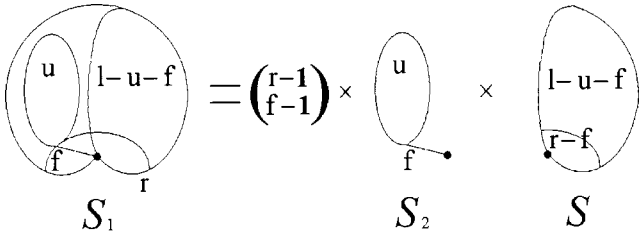

FIG. 3. Decomposition of Λ_1.

where

$$S_1(l,r,u,f)=\binom{r-1}{f-1}\cdot S_2(f+u,f)\cdot S(l-u-f,r-f). \tag{4.8}$$

Proof: The first equality is obvious. The second equality follows from the bijection

$$\Lambda_1(l,r,u,f)\overset{bij}{\to}\Lambda_2(f+u,f)\times\Lambda(l-u-f,r-f)\times\Theta_1(r,f), \tag{4.9}$$

where $\Theta_1(r,f)$ is the set of sequences of 0 and 1 of length r such that there are exactly f symbols 1 in the sequence and the first symbol is 1. Equality (4.8) is illustrated by Fig. 3.

Let us construct this mapping F. Regarding one particular essential walk w of $\Lambda_1(l,r,u,f)$, we consider the first edge e_1 of the graph G_w and separate w in two parts, the left and the right ones with respect to this edge e_1. Then we add a special code that determines the transitions from the left part to the right one and back through the root ρ. Obviously these two parts are walks, but not necessarily minimal walks. Then we minimize these walks. This decomposition is constructed by the following algorithm. We run over w and simultaneously draw the left part, the right part, and the code. If the current step belongs to G_1, we add it to the first part, otherwise we add this step to the second part. The code is constructed as follows. Each time the walk leaves the root the sequence is enlarged by one symbol. If the current step is (ρ,ν) and "0" otherwise, this symbol is "1." It is clear that the first element of the sequence is "1," the number of signs "1" is equal to f, and the full length of the sequence is r. Now we minimize the left and the right parts. Thus, we have constructed the decomposition of the essential walk w and the mapping F.

Example 2: For $w=(1,2,1,2,3,2,1,4,1,2,5,2,1,4,6,4,1,2,5,2,3,2,3,2,1,4,1)$ the left part, the right one, and the code are $(1,2,1,2,3,2,1,2,4,2,1,2,4,2,3,2,3,2,1)$, $(1,2,1,2,3,2,1,2,1)$, $(1,1,0,1,0,1,0)$, respectively.

Let us denote the left part by $(w^{(f)})$ and the right part by $(w^{(s)})$. These parts are really walks with the root ρ. For each edge e in the tree $\hat{G}_2$ the number of passages of e of the essential walk w is equal to the corresponding number of passages of e of the left part $(w^{(f)})$. Also for each edge e belonging to the tree G_1 the number of passages of e of essential walk w is equal to the corresponding number of passages of e of the right part $(w^{(s)})$. The weight of the essential walk is multiplicative with respect to edges. Then the weight of the essential walk w is equal to the product of weights of left and right parts. The walk of zero length has unit weight. Combining this with (4.9), we obtain

$$S_1(l,r,u,f)=|\Theta_1(r,f)|\cdot S_2(f+u,f)\cdot S(l-u-f,r-f). \tag{4.10}$$

Taking into account that $|\Theta_1(r,f)|=\binom{r-1}{f-1}$, we derive from (4.10) (4.8).

Now let us prove that for any given elements $w^{(f)}$ of $\Lambda_2(f+u,f)$, $w^{(s)}$ of $\Lambda(l-u-f,r-f)$, and the sequence $\theta\in\Theta_1(r,f)$, one can construct one and only one element w of $\Lambda_1(l,r,u,f)$. We do this with the following gathering algorithm. We go along either $w^{(f)}$ or $w^{(s)}$ and simultaneously draw the walk w. The switch from $w^{(f)}$ to $w^{(s)}$ and back is governed by the

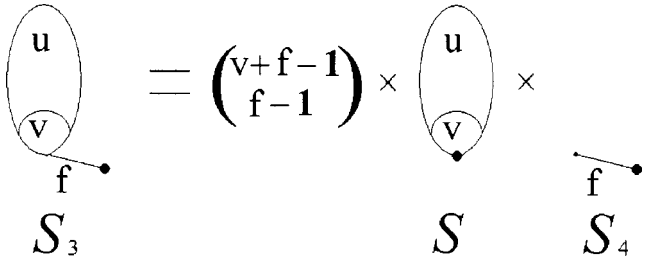

FIG. 4. Decomposition of Λ_3.

code sequence θ. In fact, this procedure is inverse to the decomposition procedure described above up to the fact that $w^{(s)}$ is minimal. This difficulty can be easily resolved, for example, by coloring vertices of $w^{(f)}$ and $w^{(s)}$ in red and blue colors, respectively. Certainly, the common root of $w^{(f)}$ and $w^{(s)}$ has only one color. To illustrate the gathering procedures we give the following example.

Example 3: For $w^{(f)}=(1,2,1,2,3,2,1,2,4,2,1,2,4,2,3,2,3,2,1)$, $w^{(s)}=(1,2,1,2,3,2,1,2,1)$, $\theta=(1,1,0,1,0,1,0)$ the gathering procedure gives $w=(1,2,1,2,3,2,1,4,1,2,5,2,1,4,6,4,1,2,5,2,3,2,3,2,1,4,1)$.

It is clear that the decomposition and gathering are injective mappings. Their domains are finite sets, and therefore the corresponding mapping (4.9) is bijective. This completes the proof of Lemma 1. ■

To formulate Lemma 2, let us give necessary definitions. We denote by v the number of steps starting from the root ρ except the step $(\widetilde{\rho,\nu})$ and by $\Lambda_3(u+f,f,v)$ the set of essential walks of $\Lambda_2(u+f,f)$ with fixed parameter v. Also we denote by $S_3(u+f,f,v)$ the sum of weights of walks of $\Lambda_3(u+f,f,v)$. Let us denote by $G_{1,2}$ the graph consisting of only one edge (ρ,ν) and by $\Lambda_4(f)$ the set of essential walks of length $2f$ such that their skeleton coincides with the graph $G_{1,2}$. It is clear that $\Lambda_4(f)$ consists of only the one walk (1,2,1,2,...,2,1) of weight X_{2f}/p^{f-1}. The previous lemma allows us to express S_2 as a function of S. The next lemma allows us to express S_2 as a function of S. Thus, two lemmas allow us to express S as a function of S.

Lemma 2 (Second decomposition lemma):

$$S_2(f+u,f)=\sum_{v=0}^{u} S_3(f+u,f,v), \tag{4.11}$$

$$S_3(f+u,f,v)=\binom{f+v-1}{f-1}\cdot\frac{X_{2f}}{p^{f-1}}\cdot S(u,v). \tag{4.12}$$

The first equality is trivial, the second one follows from the bijection

$$\Lambda_3(f+u,f,v)\overset{bij}{\to}\Lambda_4(u,v)\times\Lambda_4(f)\times\Theta_2(f+v,f), \tag{4.13}$$

where $\Theta_2(f+v,f)$ is the set of sequences of 0 and 1 of length $f+v$ such that there are exactly f symbols 1 in the sequence and the last symbol of it is 1. The proof is analogous to the proof of the first decomposition lemma. Equality (4.12) is illustrated by Fig. 4.

D. Recurrent relations for S

Combining these two decomposition lemmas and changing the order of summation, we get the recurrent relations

$$S(l,r)=\sum_{f=1}^{r}\binom{r-1}{f-1}\cdot\frac{X_{2f}}{p^{f-1}}\cdot\sum_{u=0}^{l-r} S(l-u-f,r-f)\cdot\sum_{v=0}^{u}\binom{f+v-1}{f-1}\cdot S(u,v),$$

with the initial condition $\mathrm{S}(l,0)=\delta_l$. This gives (2.8).

Using this system of recurrent relations, one can obtain information about limiting σ. For example, one can observe that the support of the limiting measure σ is unbounded even when the support of the distribution of $\{a_{i,j}\}$ is finite. This fact follows from inequality

$$M_{4k}\geqslant(\mathrm{C}\cdot k)^k, \tag{4.14}$$

where C is a constant. To explain (4.14), let us denote by Ψ the set of essential walks of length $4k$ such that the root ρ belongs to each of the edges of the skeleton and each edge is passed four times. The weight of the essential walk of Ψ is equal to $(X_4/p)^k$. The cardinality of Ψ equals $(2k-1)!!$. This implies (4.14).

Finally, let us note that using the technique developed, one can derive recurrent relations that determine the coefficients of $1/p$-expansion of $m_l^{(p)}$:

$$m_l^{(p)}=\sum_{i=0}^{l-1}\left(\sum_{r=0}^{l}\mathrm{S}(l,r,i)\right)\cdot\frac{1}{p^{\overline{i}}}. \tag{4.15}$$

Then we get

$$\begin{aligned}\mathrm{S}(l,r,i)=&\sum_{f=1}^{r}\binom{r-1}{f-1}\cdot X_{2\,f}\cdot\sum_{u=0}^{l-r}\sum_{j=0}^{(l-u-f-1)\cdot(1-\delta_{l-u-f})}\mathrm{S}(l-u-f,r-f,j)\\&\cdot\sum_{v=0}^{u}\binom{f+v-1}{f-1}\cdot\mathrm{S}(u,v,i-f-j+1)\end{aligned} \tag{4.16}$$

with the initial condition $S(l,0,i)=\delta_l\cdot\delta_i$. We do not explain the detail of this derivation. Similar formulas are obtained in Ref. 2. The difference is that in Ref. 2 matrices are not normalized by $1/\sqrt{p}$. This leads to expressions for $1/p$-terms different from our (4.16). Relations (4.12) provide more information about the properties of $m_l^{(p)}$ than relations (2.8). As the result, (4.13) are more cumbersome than (2.8).

V. LAPLACE OPERATOR

Regarding the Laplace operator, we have to modify our method. In this case the random variable Δ_{ii} is given by the sum of A_{ij} and therefore is dependent on random variables a_{ij}. Each of the nondiagonal entries differs from the corresponding entry of the weighted adjacency matrix by the sign only. Each diagonal entry of $\Delta_\Gamma^{(\xi)}$ equals the sum of all entries of the same line of the corresponding weighted adjacency matrix. Taking into account this observation one can write

$$\begin{aligned}L_s^{(N,p)}&=\mathbf{E}\left\{\int\lambda^s d\sigma(\lambda;\Delta_\Gamma)\right\}\\&=\mathbf{E}\frac{1}{N}\mathrm{Tr}[\Delta_\Gamma]^s\\&=\mathbf{E}\frac{1}{N}\mathrm{Tr}[B-A]^s\\&=\sum_{i\in\overline{1,N}^s}\sum_{b\in\{0,1\}^s}\mathbf{E}(K_{i_1i_2}^{(b_1)}\cdot K_{i_2i_3}^{(b_2)}\cdot\cdots\cdot K_{i_si_1}^{(b_s)}),\end{aligned} \tag{5.1}$$

where $K_{ij}^{(0)}=-A_{ij}$, $K_{ij}^{(1)}=B_{ij}$. Let us introduce the symbol

$$M_{ij}=1-\delta_{ij}=\begin{cases}0, & \text{if } i=j,\\ 1, & \text{if } i\neq j.\end{cases}$$

then B can be rewritten in the form

$$B_{ij}=\begin{cases}0, & \text{if } i\neq j,\\ \sum_{l=1}^{N} A_{il}\cdot M_{li}, & \text{if } i=j.\end{cases} \tag{5.2}$$

Given numbers $b_1,b_2,\ldots,b_s$, we substitute (5.2) into (5.1) and change the order of sums over l's and $\mathbf{E}\{\cdot\}$ and observe that the mathematical expectation depends on the product of A's only. The difference between this representation and that of (4.1) is that the moment $L_s^{(N,p)}$ is expressed as the sum of weights of closed walks of s steps. A step can be usual or special (double). Let us explain the nature of the special step that corresponds to the factor $A_{ij}\cdot M_{ji}$. We denote it by an arrow from i to j. To turn back to the walk we add the step $(\overrightarrow{j,i})$ which is represented by M_{ji}. This step can be regarded as the imaginary one because it does not contribute to the length of the walk and to the weight (mathematical expectation) of the walk. In the figures we denote the special step corresponding to the factor $A_{ij}\cdot M_{ji}$ by an arrow from i to j.

As before, we determine the classes of equivalence of the walks, the minimal walks, and the essential walks. In the case of Δ_Γ the essential walks are the minimal walks that have a tree as a skeleton. Each of the usual steps $(\overrightarrow{j,k})$ of the essential walk corresponds to one usual step $(\overrightarrow{k,j})$ only. Then, if there are b usual steps $(\overrightarrow{j,k})$, c special steps $(\overrightarrow{j,k})$, and d special steps $(\overrightarrow{k,j})$, then the edge (k,j) has the weight $(-1)^{2b}\cdot X_{2b+c+d}=X_{2b+c+d}$.

Let us give necessary definitions and formulate two analogs of the decomposition lemmas. Denote by l the number of usual and special steps of the essential walk w, by r_1 the number of steps starting from the root ρ and by f the number of usual and special steps $(\overrightarrow{\rho,\nu})$. We denote by $\hat{\Lambda}(l,r_1)$ the set of the essential walks of l steps such that they have r_1 steps starting from the root ρ and by $\hat{\mathrm{S}}(l,r_1)$ the sum of contributions of the walk of $\hat{\Lambda}(l,r_1)$. Let d be the length of the walk over the tree G_1. Denote by $\hat{\Lambda}_1(l,r_1,d,f)$ the set of essential walks with fixed parameters l, r_1, d, and f and by $\hat{\mathrm{S}}_1(l,r_1,d,f)$ the sum of weights of walks of $\hat{\Lambda}_1(l,r_1,d,f)$. Let us denote by $\hat{\Lambda}_2(l,r_1)$ the set of essential walks of $\hat{\Lambda}(l,r_1)$ such that their skeleton has only one edge attached to the root ρ and by $\hat{\mathrm{S}}_2(l,r_1)$ the sum of contributions of the walks of $\hat{\Lambda}_2(l,r_1)$.

Lemma 3 (Third decomposition lemma):

$$\hat{\mathrm{S}}(l,r_1)=\sum_{f=1}^{r_1}\sum_{d=0}^{l-f}\hat{\mathrm{S}}_1(l,r_1,d,f), \tag{5.3}$$

$$\hat{\mathrm{S}}_1(l,r_1,d,f)=\binom{r_1-1}{f-1}\cdot\hat{\mathrm{S}}_2(l-d,f)\cdot\hat{\mathrm{S}}(d,r_1-f). \tag{5.4}$$

The first equality is trivial and the second one follows from the bijection

$$\hat{\Lambda}_1(l,r_1,d,f)\overset{bij}{\to}\hat{\Lambda}_2(l-d,f)\times\hat{\Lambda}(d,r_1-f)\times\Theta_1(r_1,f). \tag{5.5}$$

The proof is analogous to the proof of the first decomposition lemma. Equality (5.4) is illustrated by Fig. 5.

To formulate the fourth decomposition lemma, let us give necessary definitions. We denote by r_2 the number of steps starting from the root ρ [excepting the usual and special steps $(\overrightarrow{\rho,\nu})$], by n the number of usual steps $(\overrightarrow{\rho,\nu})$, by f_1 the number of special steps $(\overrightarrow{\rho,\nu})$ and by f_2 the number of special steps $(\overrightarrow{\nu,\rho})$. Denote by $\hat{\Lambda}_3(l,n,f_1,f_2,r_2)$ the set of essential walks with fixed parameters l, n, f_1, f_2, r_2 such that their skeletons have only one edge attached to the root ρ. Let

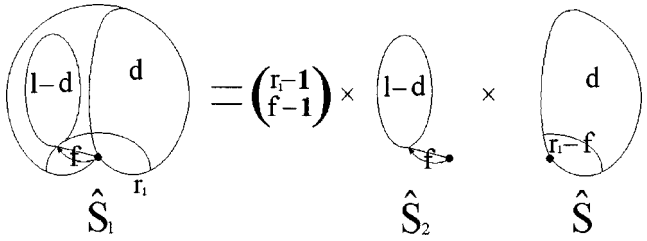

FIG. 5. Decomposition of $\hat{\Lambda}_1$.

$\hat{S}_3(l,n,f_1,f_2,r_2)$ be the sum of weights of walks of $\hat{\Lambda}_3(l,n,f_1,f_2,r_2)$. Denote by $\hat{\Lambda}_4(n,f_1,f_2)$ the set of essential walks of length $2n+f_1+f_2$ with fixed parameters n, f_1, f_2 such that their skeletons coincide with the graph $G_{1,2}$. It is not hard to see that for the case $n\geqslant 1$ one has the equality $|\hat{\Lambda}_4(n,f_1,f_2)|=\binom{n+f_1}{n}\cdot\binom{n+f_2-1}{n-1}$. It is clear that each of the walks of $\hat{\Lambda}_4(n,f_1,f_2)$ has the weight $X_{2n+f_1+f_2}/p^{n+f_1/2+f_2/2-1}$.

Lemma 4 (Fourth decomposition lemma):

$$\hat{S}_2(l,r_1,d,f)=\sum_{n=0}^{\min\{[(l-d)/2)],f\}}\ \sum_{f_2=0}^{l-d-f-n}\ \sum_{r_2=0}^{l-d-f-n-f_2}\hat{S}_3(l-d,n,f-n,f_2,r_2), \tag{5.6}$$

$$\hat{S}_3(l-d,n,f_1,f_2,r_2)=\begin{cases}\binom{n+f_2+r_2-1}{r_2}\cdot\binom{n+f_1}{n}\cdot\binom{n+f_2-1}{n-1}\cdot\hat{S}(l-d-n-f-f_2,r_2), & \text{if } n\geqslant 1,\\ \delta_{l-d-f_1}\delta_{f_2}\delta_{r_2}\dfrac{X_{2n+f_1+f_2}}{p^{n+f_1/2+f_2/2-1}}, & \text{if } n=0.\end{cases} \tag{5.7}$$

The first equality is trivial and the second one follows from the bijection

$$\hat{\Lambda}_2(l-d,n,f_1,f_2,r_2)\overset{bij}{\to}\hat{\Lambda}(l-d-2n-f_1-f_2,r_2)\times\hat{\Lambda}_3(n,f_1,f_2)\times\Theta_2(n+f_2+r_2,n+f_2). \tag{5.8}$$

The proof is analogous to the proof of the first decomposition lemma. Equation (5.7) is illustrated by Fig. 6.

Combining these two lemmas, we get an expression for $\hat{S}$. This expression is the sum over all admissible values of f,d,n,f_2,r_2. Let us change the order of summation. On the one hand, the number n of usual steps $(\overrightarrow{\rho,\nu})$ is not greater than the number f of all steps $(\overrightarrow{\rho,\nu})$; on the other hand, the inequality $2n+f_1\leqslant l$ holds because each of the usual steps $(\overrightarrow{\rho,\nu})$ corresponds to the step

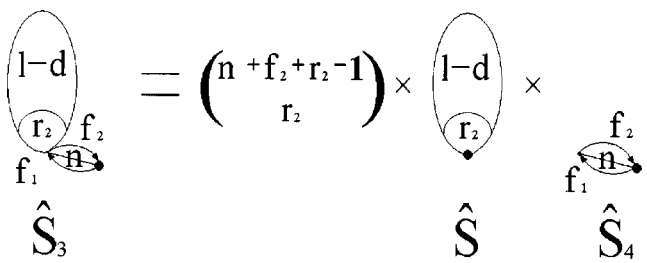

FIG. 6. Decomposition of $\hat{\Lambda}_3$.

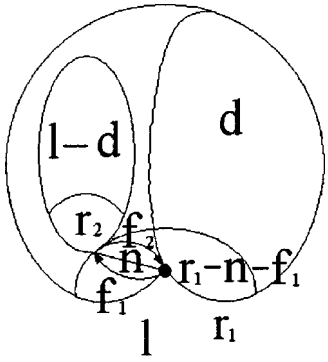

FIG. 7. Relations between parameters.

$(\overrightarrow{\nu,\rho})$. Then $n\leqslant\min(r_1,l-r_1)$. The number f_1 of special steps $(\overrightarrow{\rho,\nu})$ is not greater than the number r_1 of all steps starting from the root ρ minus the number n of usual steps $(\overrightarrow{\rho,\nu})$. Then f_1 changes from 0 to r_1-n. Now there are only $l-r_1-n$ free steps. Then the number f_2 of special steps $(\overrightarrow{\nu,\rho})$ can be changed from 0 to $l-r_1-n$. Now it remains $l-r_1-n-f_2$ free steps. The walk's length d over the tree G_1 is not less than the number r_1 of steps starting from the root ρ minus the number $n+f_1$ of steps $(\overrightarrow{\rho,\nu})$. Then $r_1-f_1-n\leqslant d\leqslant l-r_1-n-f_2$. Now there are only $l-d-2n-f_1-f_2$ free steps. In the case $n=0$, the expression is simplified to $\Sigma_{f_1=1}^{r_1}C_{r_1-1}^{f_1-1}\cdot\hat{\mathrm{S}}(l-f_1,r_1-f_1)$. The relations described above are illustrated by Fig. 7:

$$\begin{aligned}\hat{\mathrm{S}}(l,r_1)=&\sum_{n=1}^{\min(r_1,\,l-r_1)}\sum_{f_1=0}^{r_1-n}\binom{n+f_1}{n}\binom{r_1-1}{n+f_1-1}\cdot\sum_{f_2=0}^{l-r_1-n}\binom{n+f_2-1}{n-1}\cdot\frac{X_{(2n+f_1+f_2)}}{p^{(2n+f_1+f_2)/2-1}}\\&\times\sum_{d=r_1-f_1-n}^{l-r_1-n-f_2}\hat{\mathrm{S}}(d,r_1-n-f_1)\cdot\sum_{r_2=0}^{l-d-2n-f_1-f_2}\binom{r_2+f_2+n-1}{r_2}\cdot\hat{\mathrm{S}}(l-d-2n-f_1-f_2,r_2)\\&+\sum_{f_1=1}^{r_1}\binom{r_1-1}{f_1-1}\cdot\hat{\mathrm{S}}(l-f_1,r_1-f_1)\end{aligned}\tag{5.9}$$

with the initial condition

$$\hat{\mathrm{S}}(l,0)=\delta_{l,0}.$$

Let us denote $g_1=f_1+n$, and $g_2=f_2+n$. Using the identity $\Sigma_{n=1}^{\min\{g_1,g_2\}}\binom{g_1}{n}\cdot\binom{g_2-1}{n-1}=\binom{g_1+g_2-1}{g_1-1}$ and (5.9), we get

$$\begin{aligned}\hat{\mathrm{S}}(l,r_1)=&\sum_{g_1=1}^{r_1}\binom{r_1-1}{g_1-1}\cdot\Bigg(\hat{\mathrm{S}}(l-g_1,r_1-g_1)\cdot\frac{X_{g_1}}{p^{g_1/2-1}}+\sum_{d=r_1-g_1}^{l-r_1}\hat{\mathrm{S}}(d,r_1-g_1)\\&\cdot\sum_{g_2=1}^{l-d-g_1}\binom{g_1+g_2-1}{g_1-1}\cdot\frac{X_{g_1+g_2}}{p^{(g_1+g_2)/2-1}}\sum_{r_2=1}^{l-d-g_1-g_2}\binom{r_2+g_2-1}{g_2-1}\cdot\hat{\mathrm{S}}(l-d-g_1-g_2,r_2)\Bigg).\end{aligned}$$

If $a_{ij}\equiv1$ and $p=1$, we obtain

$$\hat{\mathrm{S}}(l,r_1)=\sum_{g_1=1}^{r_1}\binom{r_1-1}{g_1-1}\cdot\Bigg(\hat{\mathrm{S}}(l-g_1,r_1-g_1)+\sum_{d=r_1-g_1}^{l-r_1}\hat{\mathrm{S}}(d,r_1-g_1)\cdot\sum_{g_2=1}^{l-d-g_1}\binom{g_1+g_2-1}{g_1-1}$$
$$\cdot\sum_{r_2=1}^{l-d-g_1-g_2}\binom{r_2+g_2-1}{g_2-1}\cdot\hat{\mathrm{S}}(l-d-g_1-g_2,r_2)\Bigg).$$

If we want to find the coefficients of $1/p$-expansion of $l_k^{(p)}$,

$$l_k^{(p)}=\sum_{i=-k}^{k-2}\Bigg(\sum_{r_1=0}^{k}\hat{\mathrm{S}}(k,r_1,i)\Bigg)\cdot\frac{1}{p^{i/2}},\tag{5.10}$$

we can apply the method described above. Then after some calculations we get the following recurrent relations:

$$\hat{\mathrm{S}}(k,r_1,i)=\sum_{g_1=1}^{r_1}\binom{r_1-1}{g_1-1}\cdot\Bigg(\hat{\mathrm{S}}(k-g_1,r_1-g_1,i+2-g_1)\cdot X_{g_1}+\sum_{d=r_1-g_1}^{k-r_1}\sum_{j=-d}^{d-2\cdot(1-\delta_d)}\hat{\mathrm{S}}(d,r_1-g_1,j)$$
$$\cdot\sum_{g_2=1}^{k-d-g_1}\binom{g_1+g_2-1}{g_1-1}\cdot\frac{X_{g_1+g_2}}{p^{(g_1+g_2)/2-1}}\cdot\sum_{r_2=1}^{k-d-g_1-g_2}\binom{r_2+g_2-1}{g_2-1}$$
$$\cdot\hat{\mathrm{S}}(k-d-g_1-g_2,r_2,i+2-g_1-g_2-j)\Bigg)\tag{5.11}$$

with the initial condition $\hat{\mathrm{S}}(l,0,i)=\delta_{l,0}\cdot\delta_{i,0}$.

Similar formulas are obtained in Ref. 2. The difference is that in Ref. 2 matrices are not normalized by $1/\sqrt{p}$. This leads to expressions for $1/p$-terms different from our (5.11).

In conclusion, let us discuss the limiting transition $p\to\infty$ in (2.8) and (2.10). Regarding the first sum of the relation for the limiting moments of the adjacency matrix (2.8), one can easily observe that the terms with $f>1$ vanish in the limit of infinite p. Then gathering (2.8) with (2.7) leads to the recurrent relations

$$m_k=X_2\sum_{u=0}^{k-1}m_{k-1-u}m_u$$

that certainly determine the semicircle law.[22]

Let us turn to the Laplace case. In general, it is impossible to pass to the limit $p\to\infty$ in relations (2.10) because there is the term of the order $p^{1/2}$. However, if one passes to the case of random variables a with zero mean value, $X_1=0$, then the limit $p\to\infty$ leads to the following recurrent relations:

$$\hat{\mathrm{S}}(l,r_1)=X_2\cdot\Bigg((r_1-1)\cdot\hat{\mathrm{S}}(l-2,r_1-2)+\sum_{d=r_1-1}^{l-r_1}\hat{\mathrm{S}}(d,r_1-1)\cdot\sum_{r_2=1}^{l-d-2}\hat{\mathrm{S}}(l-d-2,r_2)\Bigg)\tag{5.12}$$

with the initial condition $\hat{\mathrm{S}}(l,0)=\delta_{l,0}$.

These recurrent relations obviously differ from those for the semicircle law. Using the resolvent approach, we show at the end of Sec. 6 that the limiting moments

$$l_s=\lim_{p\to\infty}l_s^{(p)}=\sum_{i=0}^{s}\hat{S}(s,i)$$

determine the distribution known as the deformed semicircle law (see Ref. 16).

VI. PROOFS OF THEOREMS 3 AND 4

Proof of Theorem 3: It is easy to see that $G_{11}^{(N,p)}(z)$ can be represented in the form

$$G_{11}^{(N,p)}(z)=\left(z+\sum_{j,k=2}^{N} \widetilde{G}_{jk}^{(N-1,p)} A_{1j}^{(N,p)} A_{1k}^{(N,p)} \right)^{-1}, \tag{6.1}$$

where the matrix $\{\widetilde{G}_{ij}^{(N-1,p)}(z)\}_{i,j=2}^{N}$ is the resolvent of the matrix $i\widetilde{A}^{(N-1,p)}$, which can be obtained from $A^{(N,p)}$ if we replace $\{A_{1j}^{(N,p)}\}_{j=2}^{N}$, $\{A_{j1}^{(N,p)}\}_{i=2}^{N}$ by zeros. We remark here that in order to simplify formulas in this section we assume that $A_{jj}^{(N,p)}=0$. The general case can be studied in the same way. Let us use the formula (see Ref. 1)

$$e^{-ua^2R}=1-u^{1/2}|a|\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}\exp\{-R^{-1}v\}, \tag{6.2}$$

which is valid for any $u\geqslant 0$, $\Re R>0$. Then, on the basis of (6.1), we get

$$\exp\{-ua_1^2G_{11}^{(N,p)}\}=1-u^{1/2}|a_1|\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a_1|\sqrt{uv})}{\sqrt{v}}\exp\left\{-zv-v\sum_{j,k=2}^{N}\widetilde{G}_{ij}^{(N-1,p)}A_{1i}^{(N,p)}A_{1j}^{(N,p)}\right\}. \tag{6.3}$$

Denote

$$\widetilde{R}_N=\sum_{j\neq k}\widetilde{G}_{jk}^{(N-1,p)}A_{1j}^{(N,p)}A_{1k}^{(N,p)}. \tag{6.4}$$

One can see easily that

$$\mathbf{E}\{|\widetilde{R}_N|^2\}\leqslant 2\,\frac{X_2^2}{N|\Re z|^2}+\frac{p^2X_1^4}{N^2|\Re z|^2}+\frac{pX_1^2X_2}{N^2|\Re z|^2}. \tag{6.5}$$

Indeed,

$$\begin{aligned}\mathbf{E}\{|\widetilde{R}_N|^2\}=&\sum_{j_1\neq j_2\neq k_1\neq k_2}\mathbf{E}\{G_{j_1k_1}^{(N-1,p)}\overline{\widetilde{G}_{j_2k_2}^{(N-1,p)}}A_{1j_1}^{(N,p)}A_{1j_2}^{(N,p)}A_{1k_1}^{(N,p)}A_{1k_2}^{(N,p)}\}\\&+4\sum_{j,k_1\neq k_2}\mathbf{E}\{\widetilde{G}_{jk_1}^{(N-1,p)}\overline{\widetilde{G}_{jk_2}^{(N-1,p)}}|A_{1j}^{(N,p)}|^2A_{1k_1}^{(N,p)}A_{1k_2}^{(N,p)}\}\\&+2\sum_{j\neq k}\mathbf{E}\{\widetilde{G}_{jk}^{(N-1,p)}\overline{\widetilde{G}_{jk}^{(N-1,p)}}|A_{1j}^{(N,p)}|^2|A_{1k}^{(N,p)}|^2\}=I+4II+2III.\end{aligned} \tag{6.6}$$

Averaging with respect to $\{A_{1,i}^{(N,p)}\}_{i=2}^{N}$ and using the fact that $\{\widetilde{G}_{ij}^{(N-1,p)}(z)\}_{i,j=2}^{N}$ do not depend on $A_{1,i}^{(N,p)}$, we obtain

$$I\leqslant X_1^4\frac{p^2}{N^2}\mathbf{E}\left\{\left|N^{-1}\sum_{j,k}(z-i\widetilde{A}^{(N-1,p)})_{jk}^{-1}\right|^2\right\}\leqslant\frac{p^2X_1^4}{N^2|\Re z|^2},$$

$$II\leqslant X_1^2X_2\frac{p}{N^3}\sum_{k_1\neq k_2}\mathbf{E}\{[(z-i\widetilde{A}^{(N-1,p)})(\overline{z}+i\widetilde{A}^{(N-1,p)})]_{k_1k_2}^{-1}\}\leqslant\frac{pX_1^2X_2}{N^2|\Re z|^2},$$

$$III\leqslant\frac{X_2^2}{N^2}\sum_{k}\mathbf{E}\{[(z-i\widetilde{A}^{(N-1,p)})(\overline{z}+i\widetilde{A}^{(N-1,p)})]_{kk}^{-1}\}\leqslant\frac{X_2^2}{N|\Re z|^2}.$$

Besides, since evidently

$$\Re\left\{\sum \widetilde{G}_{ij}^{(N-1,p)}A_{1i}^{(N,p)}A_{1j}^{(N,p)}\right\}\geqslant 0,\quad \Re\left\{\sum \widetilde{G}_{jj}^{(N-1,p)}\left|A_{jj}^{(N,p)}\right|^2\right\}\geqslant 0,$$

the inequality $|e^{-z_1}-e^{-z_2}|\leqslant|z_1-z_2|$ (valid for $\Re z_1,\Re z_2\geqslant 0$) and (6.3) imply

$$\exp\{-ua_1^2G_{11}^{(N,p)}\}=1-u^{1/2}|a_1|\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a_1|\sqrt{uv})}{\sqrt{v}}\times\exp\left\{-zv-v\sum \widetilde{G}_{ij}^{(N-1,p)}|A_{1j}^{(N,p)}|^2\right\}+\tilde{r}_N(u),\tag{6.7}$$

where

$$|\tilde{r}_N(u)|\leqslant|\widetilde{R}_N|u^{1/2}|a_1|\int_0^\infty dv\left|\frac{\mathcal{J}_1(2|a_1|\sqrt{uv})}{\sqrt{v}}e^{-zv}\right|\leqslant C|\widetilde{R}_N|u^{1/2}|a_1||\Re z|^{-3/2}.$$

Here and below we denote by C some constants (different in different formulas), which do not depend on N,z,p. Taking into account (6.5), we get

$$\mathbf{E}\{|\tilde{r}_N(u)|^2\}\leqslant\frac{Cup}{N|\Re z|^3}.\tag{6.8}$$

Averaging with respect to a_1 and $\{A_{1,i}^{(N,p)}\}_{i=2}^N$ we obtain

$$\begin{aligned}\mathbf{E}\{\exp\{-ua_1^2G_{11}^{(N,p)}\}\}&=1-u^{1/2}\int d\mu(a_1)|a_1|\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a_1|\sqrt{uv})}{\sqrt{v}}\\&\quad\times\mathbf{E}\left\{\exp\left\{-zv-v\sum_{j=2}^N \widetilde{G}_{jj}^{(N-1,p)}|A_{1j}^{(N,p)}|^2\right\}\right\}+r_N(u),\\ r_N(u)&\leqslant\frac{C(up)^{1/2}}{N^{1/2}|\Re z|^{3/2}}.\end{aligned}\tag{6.9}$$

Taking into account that $\{\widetilde{G}_{ij}^{(N-1,p)}(z)\}_{i,j=2}^N$ do not depend on $A_{1,i}^{(N,p)}$, we obtain

$$\begin{aligned}\mathbf{E}\left\{\exp\left\{-v\sum G_{jj}^{(N-1,p)}|A_{1j}^{(N,p)}|^2\right\}\right\}&=\mathbf{E}\left\{\prod_{j=2}^N\left(\left(1-\frac{p}{N}\right)+\frac{p}{N}e^{-va_{1j}^2\widetilde{G}_{jj}^{(N-1,p)}/p}\right)\right\}\\&=e^{-p}\mathbf{E}\{\exp\{p\widetilde{f}_{N-1}(v/p,z)\}\}+R_N(v),\\ |R_N(v)|&\leqslant\frac{Cp^2}{N}.\end{aligned}\tag{6.10}$$

Let us prove that $\widetilde{f}_{N-1}(v/p,z)=(1/N)\,\Sigma e^{-va_{1j}^2\widetilde{G}_{jj}^{(N-1,p)}/p}$ can be replaced by $f_N(v/p,z)$. To this end consider the matrices $A^{(N,p)}(t)=(1-t)A^{(N,p)}+t\tilde{A}^{(N-1,p)}$, $G(t,z)=(z-iA^{(N,p)}(t))^{-1}$ and the function

$$f_N(u,z,t)=\frac{1}{N}\sum_{i=1}^N e^{-ua_i^2G_{ii}(t,z)}.\tag{6.11}$$

It is easy to see that

$$\left|\widetilde{f}_{N-1}(u,z)-f_N(u,z)+\frac{1}{Nz}\right|=\left|\frac{1}{Nz}+\frac{1}{N}\sum_{i=2}^{N}e^{-ua_i^2\widetilde{G}_{ii}^{(N-1,p)}(z)}-\frac{1}{N}\sum_{i=1}^{N}e^{-ua_i^2G_{ii}(z)}\right|$$

$$=|f_N(u,z,1)-f_N(u,z,0)|$$

$$=\left|\int_0^1 dt\,\frac{d}{dt}f_N(u,z,t)\right|$$

$$=2\left|\int_0^1 dt\,\frac{u}{N}\sum_{i=2}^{N}a_i^2G_{ij}(z,t)A_{j1}^{(N,p)}G_{1i}(z,t)e^{-ua_i^2G_{ii}(z,t)}\right|$$

$$\leqslant 2\,\frac{u}{N|\Re z|^2}\left[\sum_{j=2}^{N}|a_i|^4\right]^{1/2}\left[\sum_{j=2}^{N}|A_{j1}^{(N,p)}|^2\right]^{1/2}, \tag{6.12}$$

where we have used that $\|G(t,z)\|\leqslant|\Re z|^{-1}$. Therefore, for any $u\in\mathbf{R}$,

$$\mathbf{E}\{|\widetilde{f}_{N-1}(u,z)-f_N(u,z)|^2\}\leqslant\frac{u^2X_4^{1/2}X_2^{1/2}}{|\Re z|^4N}+\frac{1}{N^2|z|^2}. \tag{6.13}$$

Hence, (6.9) and (6.10) could be rewritten as

$$\mathbf{E}\{f_N(u,z)\}=1-u^{1/2}e^{-p}\int|a_1|d\mu(a_1)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a_1|\sqrt{uv})}{\sqrt{v}}e^{-zv}\mathbf{E}\{e^{pf_N(v/p,z)}\}+r_N'(v),$$

$$\mathbf{E}\{|r_N'^2(u)|\}\leqslant\frac{Cp^2u}{|\Re z|^4N}. \tag{6.14}$$

Now let us prove (2.14). Denote

$$\delta_N(z,u)=f_N(z,u)-\mathbf{E}\{f_N(z,u)\}$$

and observe that due to the symmetry of the problem

$$\mathbf{E}\{\delta_N^2(z,u)\}=\frac{N-1}{N}(\mathbf{E}\{e^{-ua_1^2G_{11}(z)}e^{-ua_2^2G_{22}(z)}\}-\mathbf{E}\{e^{-ua_1^2G_{11}(z)}\}\mathbf{E}\{e^{-ua_2^2G_{22}(z)}\})+O(N^{-1}). \tag{6.15}$$

We shall use the formulas [cf. (6.1)]

$$G_{\ell\ell}^{(N,p)}=\left[\left(z+\sum_{j,k=3}^{N}\widetilde{G}_{jk}^{(N-2,p)}A_{\ell j}^{(N,p)}A_{\ell k}^{(N,p)}\right)-\left(\sum_{j,k=3}^{N}\widetilde{G}_{jk}^{(N-2,p)}A_{1j}^{(N,p)}A_{2k}^{(N,p)}\right)^2\right.$$

$$\left.\times\left(z+\sum_{j,k=3}^{N}\widetilde{G}_{jk}^{(N-2,p)}A_{\underline{\ell},j}^{(N,p)}A_{\underline{\ell}k}^{(N,p)}\right)^{-1}\right]^{-1}. \tag{6.16}$$

Here $\ell=1,2$, $\underline{\ell}=3-\ell$ and $\widetilde{G}^{(N-2,p)}=(z-i\widetilde{A}^{(N-2,p)})^{-1}$, where $\widetilde{A}^{(N-2,p)}$ can be obtained from $A^{(N,p)}$ by replacing $A_{1j}^{(N,p)},A_{2j}^{(N,p)}$ $A_{j1}^{(N,p)},A_{j2}^{(N,p)}$ $(j=3,\ldots,N)$ by zeros. Similarly to (6.5), one can get that

$$\mathbf{E}\left\{\left|\sum\widetilde{G}_{jk}^{(N-2,p)}A_{1j}^{(N,p)}A_{2k}^{(N,p)}\right|^2\right\}\leqslant\frac{Cp}{N|\Re z|^2},\quad\mathbf{E}\left\{\left|\sum_{j\neq k}\widetilde{G}_{jk}^{(N-2,p)}A_{\ell j}^{(N,p)}A_{\ell k}^{(N,p)}\right|^2\right\}\leqslant\frac{Cp}{N|\Re z|^2}.$$

Hence, using (6.2), similarly to (6.3)–(6.6), we get

$$\mathbf{E}\{e^{-ua_1^2G_{11}^{(N,p)}}e^{-ua_2^2G_{22}^{(N,p)}}\}-\mathbf{E}\{e^{-ua_1^2G_{11}^{(N,p)}}\}\mathbf{E}\{e^{-ua_2^2G_{22}^{(N,p)}}\}$$
$$=ue^{-2p}\int|a_1||a_2|d\mu(a_1)d\mu(a_2)\int_0^\infty\int_0^\infty dv_1dv_2\frac{\mathcal{J}_1(2|a_1|\sqrt{uv_1})\mathcal{J}_1(2|a_2|\sqrt{uv_2})}{\sqrt{v_1v_2}}e^{-zv_1-zv_2}$$
$$\times[\mathbf{E}\{e^{p\tilde{f}_{N-2}(v_1/p,z)}e^{p\tilde{f}_{N-2}(v_2/p,z)}\}-\mathbf{E}\{e^{p\tilde{f}_{N-2}(v_1/p,z)}\}\mathbf{E}\{e^{p\tilde{f}_{N-2}(v_2/p,z)}\}]+\tilde{r}_N(u), \tag{6.17}$$
$$\mathbf{E}\{|\tilde{r}_N(u)|\}\leq\frac{Cp}{N|\Re z|^2}.$$

By the same way as in (6.11)–(6.13) it is easy to prove that the estimate (6.13) remains valid if we replace $\tilde{f}_{N-1}(u,z)$ by $\tilde{f}_{N-2}(u,z)$. Thus inequalities (6.17) remain valid if we replace $\tilde{f}_{N-2}(u,z)$ by $f_N(u,z)$ on the r.h.s. of (6.17).

Besides, since

$$|f_N(v,z)|\leq\max_i e^{-ua_i^2\Re G_{ii}^{(N,p)}}\leq 1, \tag{6.18}$$

we have the bound

$$|\mathbf{E}\{e^{pf_N(v_1/p,z)}e^{pf_N(v_2/p,z)}\}-\mathbf{E}\{e^{pf_N(v_1/p,z)}\}\mathbf{E}\{e^{pf_N(v_2/p,z)}\}|$$
$$\leq 4e^{2p}p^2(\mathbf{E}\{|\delta_N(v_1/p,z)|^2\}+\mathbf{E}\{|\delta_N(v_2/p,z)|^2\}). \tag{6.19}$$

Let us take the norm (2.16) and consider the Banach space $\mathcal{B}$ of all the functions $\phi:\mathbf{R}_+\to\mathbf{C}$ which possess this norm. Consider $\phi_z(u)=\delta_N(u,z)$.

Then, using (6.19) and the inequality $|\mathcal{J}_1(x)|\leq 1$ (see Ref. 1), on the basis of (6.15)–(6.18) we get

$$\mathbf{E}\{\|\delta_N(u,z)\|^2\}\leq\frac{8X_2e^{2p}p^2\pi}{|\Re z|}\left(1+\frac{1}{2p|\Re z|}\right)\mathbf{E}\{\|\delta_N(u,z)\|^2\}+\frac{C}{N}. \tag{6.20}$$

Hence, it is evident that there exists $M>0$, such that for any $z:\Re z>M$

$$\mathbf{E}\{\|\delta_N(u,z)\|^2\}\leq\frac{C}{N}. \tag{6.21}$$

Thus, for any $z:\Re z>M$, Eq. (6.14) can be rewritten in the form

$$\mathbf{E}\{f_N(u,z)\}=1-u^{1/2}e^{-p}\int|a|d\mu(a)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}e^{-zv}e^{p\mathbf{E}\{f_N(v/p,z)\}}+\tilde{r}'_N(u),$$
$$\mathbf{E}\{|\tilde{r}'^2_N(u)|\}\leq\frac{Cp^2u}{N}. \tag{6.22}$$

Define the operator $F_z:\mathcal{B}\to\mathcal{B}$ of the form

$$F_z(\phi)(u)=1-u^{1/2}e^{-p}\int|a|d\mu(a)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}e^{-zv}e^{p\phi(v/p)}. \tag{6.23}$$

Then for any ϕ_1, ϕ_2 $\|\phi_{1,2}\|\leq 1$

$$\|F_z(\phi_1)-F_z(\phi_2)\|\leqslant X_2^{1/2}\int_0^\infty \frac{dv}{\sqrt{v}}e^{-|\Re z|v}e^{v^{1/2}/p^{1/2}}\|\phi_1-\phi_2\|\leqslant \frac{2X_2^{1/2}\sqrt{\pi}e^{1/4p|\Re z|}}{|2\Re z|^{1/2}}\|\phi_1-\phi_2\|.$$

Hence, there exists $M_1>0$, such that for all $z:\Re z>M_1$

$$\|F_z(\phi_1)-F_z(\phi_2)\|\leqslant \tfrac{1}{2}\|\phi_1-\phi_2\|.$$

Thus, if we denote by $B_{0,1}=\{\phi:\|\phi\|\leqslant 1\}$ the ball of radius 1 centered in the origin, then we obtain that $F_z:B_{0,1}\to B_{0,1}$ and the restriction F_z on $B_{0,1}$ is a contraction. Therefore, there exists the unique fixed point $f(u,z)$ of the mapping $F_z:B_{0,1}\to B_{0,1}$ which is a solution of (2.17), and $\mathbf{E}\{f_N(u,z)\}\to f(u,z)$, as $N\to\infty$. But since $\mathbf{E}\{f_N(u,z)\}$ for any z: $\Re z>0$ is an analytical function, the uniqueness theorem of complex analysis guarantees that Eq. (2.17) has a solution for any $z:\Re z>0$ and $\mathbf{E}\{f_N(u,z)\}\to f(u,z)$, as $N\to\infty$.

Similarly, since $\delta_N(u,z)$ is a bounded analytical function, $\mathbf{E}\{\|\delta_N(u,z)\|^2\}\to 0$ $(N\to\infty)$ implies that $\mathbf{E}\{\|\delta_N(u,z)\|^2\}\to 0$ for any $z:\Re z>0$.

Proof of Theorem 4: The proof of Theorem 4 repeats almost literally the proof of Theorem 3. We use the formula [cf. (6.3)]

$$G_{11}^{(\Delta,N,p)}(z)=\left(z+i\sum_{j=2}^N A_{1j}^{(N,p)}+\sum_{j,k=2}^N \tilde{G}_{jk}^{(\Delta,N-1,p)}A_{1j}^{(N,p)}A_{1k}^{(N,p)}\right)^{-1}, \tag{6.24}$$

where $\{\tilde{G}_{ij}^{(\Delta,N-1,p)}(z)\}_{i,j=2}^N$ is the resolvent of the matrix $i\Delta^{(N-1,p)}$, obtained from $\Delta^{(N,p)}$ by replacing $\{A_{1j}^{(N,p)}\}_{j=2}^N$ $\{A_{j1}^{(N,p)}\}_{j=2}^N$ with zeros. Then, similarly to (6.2)–(6.22) we obtain

$$\mathbf{E}\{f_N^{(\Delta)}(u,z)\}=\hat{\mu}(-u)-u^{1/2}e^{-p}\int |a|e^{iua}d\mu(a)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}e^{-zv}e^{p\mathbf{E}\{f_N^{(\Delta)}(v/p,z)\}}$$

$$+\tilde{r}_N'(u),\quad \mathbf{E}\{|\tilde{r}_N'^2(u)|\}\leqslant\frac{Cp^2u}{N}. \tag{6.25}$$

Then we consider the Banach space $\mathcal{B}$ with the norm (2.16) and the operator $F_z^{(\Delta)}:\mathcal{B}\to\mathcal{B}$ of the form

$$F_z^{(\Delta)}(\phi)(u)=\hat{\mu}(-u)-u^{1/2}e^{-p}\int |a|e^{iua}d\mu(a)\int_0^\infty dv\,\frac{\mathcal{J}_1(2|a|\sqrt{uv})}{\sqrt{v}}e^{-zv}\cdot e^{p\phi(v/p)}. \tag{6.26}$$

It is easy to see that there exists $M_1>0$, such that for any $z:\Re z>M_1$ the operator $F_z^{(\Delta)}:B_{0,1}\to B_{0,1}$ and its restriction to $B_{0,1}$ is a contraction.

Hence, there exists the unique fixed point $f^{(\Delta)}(u,z)$, which is a solution of (2.24), and $\mathbf{E}\{f_N^{(\Delta)}(u,z)\}\to f^{(\Delta)}(u,z)$, as $N\to\infty$. Similarly to Theorem 3 the statement of Theorem 4 can be derived from this fact.

In conclusion let us discuss the limiting transition $p\to\infty$. Assume that $X_1=0$. Then in the case of the adjacency matrix, by using formula (6.1) we can write

$$G_{11}^{(N,p)}(z)=\left(z+\sum_{j=2}^N \tilde{G}_{jj}^{(N-1,p)}\frac{X_2}{N}+\tilde{R}_N+R_p\right)^{-1}, \tag{6.27}$$

where $\tilde{R}_N$ is defined by (6.4) and

$$R_p=\sum_{j,k=2}^N \tilde{G}_{jj}^{(N-1,p)}(A_{1,j}^2-\mathbf{E}\{A_{1,j}^2\}).$$

Then, since $X_1=0$, in view of (6.5) $\mathbf{E}\{|\tilde{R}_N|^2\}\to 0$, as $N\to\infty$ and

$$\mathbf{E}\{|R_p|^2\}\leqslant\sum_{j=2}^{N}|\tilde{G}_{jj}^{(N-1,p)}|^2\frac{X_4}{Np}+O(|\Re z|^{-2}N^{-1})=O(|\Re z|^{-2}p^{-1})+O(|\Re z|^{-2}N^{-1}).$$

Besides, similarly to the above consideration, it is easy to conclude that

$$\mathbf{E}\{|N^{-1}\mathrm{Tr}\ \tilde{G}^{(N-1,p)}-N^{-1}\mathrm{Tr}\ G^{(N,p)}|^2\}\to 0,$$

$$\mathbf{E}\{|N^{-1}\mathrm{Tr}\ G^{(N,p)}-\mathbf{E}\{N^{-1}\mathrm{Tr}\ G^{(N,p)}\}|^2\}\to 0,\quad N\to\infty.$$

We remark also that this self-averaging property can be obtained directly from Theorem 3 (see Sec. 2.2).

Thus, we get that if $g_{N,p}(z)=N^{-1}\mathrm{Tr}\ (A^{(N,p)}-z)^{-1}$, then

$$\mathbf{E}\{ig_{N,p}(-iz)\}=(z+X_2\mathbf{E}\{ig_{N,p}(-iz)\})^{-1}+o(1).$$

Similarly to the proof of Theorem 3, we conclude that for $|\Re z|$ large enough $\mathbf{E}\{g_{N,p}(-iz)\}\to g(-iz)$, as $N,p\to\infty$, where $g(z)$ is the solution of the equation

$$g(z)=(X_2g(z)-z)^{-1},$$

satisfying condition $\Re g(z)\Re z>0$. So we have got once more the result of Ref. 16 that if $X_1=0$ and $N,p\to\infty$, then the IDS of $A^{(N,p)}$ tends to the Wigner semicircle law.

By the same way, using formula (6.24), we get for the $G^{(\Delta,N,p)}(z)$

$$G_{11}^{(\Delta,N,p)}(z)=\left(z+i\sum_{j=2}^{N}A_{1j}^{(N,p)}+\frac{X_2}{N}\mathbf{E}\{\mathrm{Tr}\ G^{(\Delta,N,p)}(z)\}\right)^{-1}+O(|\Re z|^{-2}p^{-1})+O(|\Re z|^{-2}N^{-1}).\tag{6.28}$$

Thus, since $\Sigma_{j=2}^{N}A_{1j}^{(N,p)}$ converge in distribution as $N,p\to\infty$ to the Gaussian random variable with zero mean and the variance X_2, we get from (6.28) the equation

$$\mathbf{E}\{ig_{N,p}^{(\Delta)}(-iz)\}=\int\frac{e^{-v^2/2}dv}{\sqrt{2\pi}}(z+iv+\mathbf{E}\{ig_{N,p}^{(\Delta)}(-iz)\})^{-1}$$

and so we conclude that there exists

$$\lim_{N,p\to\infty}\mathbf{E}\{ig_{N,p}^{(\Delta)}(iz)\}=ig^{(\Delta)}(iz),$$

where $ig^{(\Delta)}(iz)$ is defined by the equation

$$g^{(\Delta)}(-iz)=\int\frac{e^{-v^2/2}dv}{\sqrt{2\pi}}(iz-v-X_2g_{N,p}^{(\Delta)}(-iz))^{-1}\tag{6.29}$$

and the condition $\Re g(z)\Re z>0$. The last equation determines the Stieltjes transform of the deformed Wigner law (see Ref. 16). The semicircle distribution is ''deformed'' by the normal one and this makes the support of the corresponding IDS to be infinite. The moments of this deformed Wigner law are determined by relations (5.12).

Regarding the matrix of the Laplace operator (2.3), it is easy to explain the result (6.29). The diagonal term B of (2.3) is given by the sum of approximately p independent random variables a and this sum is normalized by $\sqrt{p}$. So, if the mathematical expectation of a equals to zero, the order of magnitude of the diagonal term of (2.3) remains finite as $p\to\infty$ and this equalizes it with

the matrix $A^{(N,p)}$. Since the elements of these random matrices A and B become statistically independent in the limit $p \to \infty$, the limiting IDS results in the semicircle law given by A deformed by the normal distribution provided by B.

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The determination of all syzygies for the dependent polynomial invariants of the Riemann tensor. I. Pure Ricci and pure Weyl invariants

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In this paper, we shall consider all pure Ricci and pure Weyl scalar invariants of any degree, in a four-dimensional Lorentzian space. We present a general graph-theoretic based reduction algorithm which decomposes, using syzygies, any pure invariant in terms of the independent base invariants $\{r_1,r_2,r_3\}$ or $\{w_1,w_2\}$ [E. Zakhary and J. Carminati, J. Math. Phys. **42**, 1474 (2001)]. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1646431]

I. INTRODUCTION

In recent years, there has been a considerable resurgence of interest into the classic problem of determining a complete[1] set of polynomial invariants of the Riemann tensor in a four-dimensional Lorentzian space.[2–19] Apart from being important in the classification of the Riemann tensor and in general the equivalence problem, the invariants also play a crucial role in revealing interesting geometrical properties of space–time.

Recall that an invariant of a set of tensors in n dimensions is classically defined to be a polynomial function of the components of those tensors that is invariant under some group of transformations [in our case, the Lorentz Group or SO(1,3)] of the tensors. A *complete set*, $I=\{I_1,I_2,\ldots,I_n\}$, of invariants is one having the property that any polynomial invariant can be expressed as a *polynomial* in $I_1,I_2,\ldots,I_n$, and no invariant in the set can be so expressed in terms of the remaining I_i. Note that an *algebraically independent* set of invariants, $\{I_1,I_2,\ldots,I_n\}$, is one for which an algebraic function, f, such that $f(I_1,I_2,\ldots,I_n)=0$ implies that $f\equiv 0$. The main theorems of invariant theory are the following.[6,20]

First fundamental theorem: *Any polynomial invariant of a set of tensors can be expressed as a linear combination of complete contractions of products of those tensors, together with the metric or* $\epsilon_{j_1\ldots j_n}$.

Second fundamental theorem: *Any identity between the invariants of a set of tensors in n dimensions can be obtained as a consequence of the fact that skew-symmetrizing over* $n+1$ *indices will annihilate any tensor*.

Recently, Sneddon[7] has determined a complete set of invariants, K, using matrix theory. The set K consists of 38 real invariants of maximum degree 12. Hence, due to their high degree and complexity, their usefulness would tend to be rather limited. To arrive at a more ''manageable'' set, the concept of algebraic independence was introduced and this reduced the number of invariants to 18 with maximum degree 6.[11–13] However, despite these contributions to the classic problem, the explicit relationships between dependent and independent invariants via syzygies[21] are still not completely understood. Indeed apart from a few special ''exact'' identities, the best that has been achieved so far is a numerical procedure leading to approximate relations.[6]

In this paper we intend to address this problem for the pure Weyl and pure Ricci invariants. We denote the sets of pure Weyl and pure Ricci invariants as $\mathcal{W}$ and $\mathcal{R}$, respectively. In the SL(2,C) representation, these polynomial invariants can be equivalently defined as complete contractions of arbitrary products of either Ψ_{ABCD} or $\Phi_{AB\dot{A}\dot{B}}$, but not both. Initially, we consider the sets of pure Weyl and Ricci invariants, $\hat{\mathcal{W}}$ and $\hat{\mathcal{R}}$, where there is an even number of index

contractions between any pair of spinors. We derive the general expression for the syzygies relating any invariant within $\hat{\mathcal{R}}$ or $\hat{\mathcal{W}}$ to the invariants $\{r_1,r_2,r_3\}$ or $\{w_1,w_2\}$,[11] respectively. Furthermore, we introduce a graph-theoretical approach to establish that any pure invariant outside $\hat{\mathcal{W}}$ and $\hat{\mathcal{R}}$ is expressible as a polynomial syzygy of the invariants within these sets. This, in part, answers the question partially alluded to by Bonanos.[3,22] We shall then present a general reduction algorithm which decomposes using syzygies, any pure invariant in terms of $\{r_1,r_2,r_3\}$ and $\{w_1,w_2\}$.

II. GRAPHICAL REPRESENTATION OF THE INVARIANTS

We introduce a graphical notation, where any pure invariant may be represented as a directed multigraph. We shall call the ''lines'' in a directed graph *arcs*, and their undirected counterparts *edges*.

Definition 1: We associate a unique directed multigraph G_N with each pure Weyl invariant N. The directed multigraph G_N consists of a vertex set $V=\{v_1,v_2,\ldots,v_n\}$, where each element of V is uniquely associated with each Weyl spinor, an arc set $E=V\times V$, and a function m: $V\times V\rightarrow\{0,1,2,3,4\}$. The multiplicity $m(v_j,v_k)$ of the arc $(v_j,v_k)\in E$ is the number of contractions between lower indices on the spinor v_j and upper indices on the spinor v_k.

It follows from this definition that the *underlying undirected graph* of G_N, which is obtained by deleting all directions from the arcs of G_N, must be a 4-regular multigraph. Reversing the direction of one arc is equivalent to raising the lower index and dropping the upper index in a pair of contracted indices, and has the effect of changing the overall sign of the invariant. For clarity, we shall, where required, use the subscript G_N to denote the multiplicity of the arc (v_j,v_k) in the specific graph G_N as $m_{G_N}(v_j,v_k)$.

We must first address the matter of conflicting definitions of degree. Each vertex in the underlying undirected graph of G_N is adjacent to four edges. In graph theoretic terms, the degree of each vertex in this underlying graph is therefore four. However, the degree of the polynomial invariant N is equivalent to the order (number of vertices) of its associated graph, G_N. We will use the phrase polynomial degree when referring to degree in the latter context.

We describe N as being connected if and only if G_N is a connected graph, otherwise we say N is disconnected. If G_N is disconnected, its components (connected subgraphs) would correspond to the connected factors of the disconnected invariant, N.

For the pure Weyl invariant, N, we define the $n\times n$ matrix, $A(G_N)$ to be the adjacency matrix of G_N, where its vertex set $V(G_N)$ possesses n vertices corresponding to the n Weyl spinors contracted to form N. Each element a_{jk} of $A(G_N)$,

$$A(G_N)=[a_{jk}],$$

$$a_{jk}=m(v_j,v_k),\quad j,k=1,2,\ldots,n \tag{1}$$

is equivalent to the multiplicity of the arc from vertex v_j to vertex v_k. The sum of the entries in row j corresponds to the outdegree of v_j, whereas the sum of the entries in column k corresponds to the indegree of v_k. Loops, which are arcs leaving and entering the same vertex, would actually correspond to contraction within a single Weyl spinor and the resulting invariant will be identically zero. Hence, we can assume that no loops are present in the graphs and $a_{jj}=m(v_j,v_j)=0$ without loss of generality. Since the sum of the outdegree and the indegree at each vertex must be four, the following condition holds:

$$\sum_{k=1}^{n}(a_{jk}+a_{kj})=4,\quad j=1,2,\ldots,n.$$

Three examples of graphical representations of fifth-degree (polynomial), pure Weyl invariants are depicted in Fig. 1.

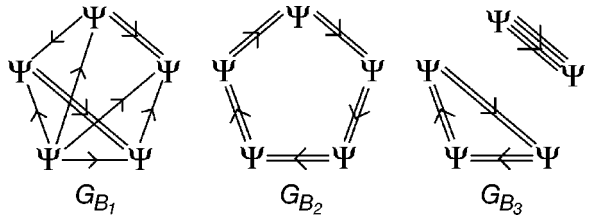

FIG. 1. Graphical representations of three pure Weyl invariants.

Graphs G_{B_1}, G_{B_2}, and G_{B_3} represent the invariants $B_1=\Psi_{AB}{}^{C}{}_{D}\Psi^{ABEF}\Psi_{E}{}^{GHJ}\times\Psi_{FCJK}\Psi^{D}{}_{GH}{}^{K}$, $B_2=\Psi_{AB}{}^{CD}\Psi_{CD}{}^{EF}\Psi_{EF}{}^{GH}\Psi_{GH}{}^{JK}\Psi_{JK}{}^{AB}$, and $B_3=\Psi_{ABCD}\Psi^{ABCD}\Psi_{EF}{}^{GH}\times\Psi_{GH}{}^{IJ}\Psi_{IJ}{}^{EF}$, and are associated with the matrices:

$$A(G_{B_1})=\begin{bmatrix}0&2&0&0&1\\0&0&0&0&0\\0&1&0&0&0\\1&1&1&0&1\\0&0&2&0&0\end{bmatrix},\quad A(G_{B_2})=\begin{bmatrix}0&2&0&0&0\\0&0&2&0&0\\0&0&0&2&0\\0&0&0&0&2\\2&0&0&0&0\end{bmatrix},$$

$$A(G_{B_3})=\begin{bmatrix}0&4&0&0&0\\0&0&0&0&0\\0&0&0&2&0\\0&0&0&0&2\\0&0&2&0&0\end{bmatrix}.$$

Invariants B_1 and B_2 are connected, whereas invariant B_3 is disconnected, and possesses two connected factors of lower polynomial degree: $\Psi_{ABCD}\Psi^{ABCD}$ and $\Psi_{EF}{}^{GH}\Psi_{GH}{}^{IJ}\Psi_{IJ}{}^{EF}$.

A directed multigraph G is *oriented* iff $m(v_j,v_k)=0$ whenever $m(v_k,v_j)\neq 0$ for $j\neq k$. It will be convenient for us to work with the oriented directed multigraph $G_{N'}$, which is formed by reversing the directions of edges of G_N as necessary to satisfy the above condition. $A(G_{N'})$ can be formed from $A(G_N)$ as follows:

$$A(G_{N'})=[a'_{jk}],\quad j,k=1,2,\ldots,n,$$

where

$$a'_{jk}=\begin{cases}a_{jk}+a_{kj}, & j<k,\\ 0, & j\geqslant k.\end{cases}\tag{2}$$

The invariant N is equivalent to its oriented form N' up to a sign; the exact relationship being given by

$$N'=(-1)^{\sigma}N,\tag{3}$$

where

$$\sigma=\sum_{j>k}a_{jk},$$

σ being the number of arcs that have been reversed.

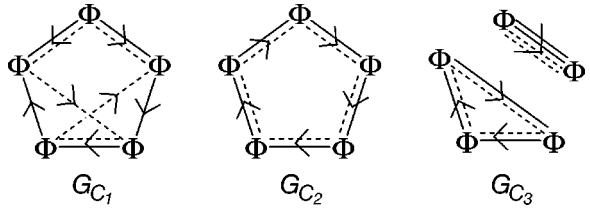

FIG. 2. Graphical representations of three pure Ricci invariants.

The graphical representation of the Ricci invariants is defined in a similar fashion to that of the Weyl invariants.

Definition 2: We associate a unique directed multigraph G_N, with each pure Ricci invariant N. The directed multigraph G_N consists of a vertex set $V=\{v_1,v_2,\ldots,v_n\}$, where each element of V is uniquely associated with each Ricci spinor, an arc set $E=V\times V$, and two functions: $m^S:V\times V\to\{0,1,2\}$, *and* $m^D:V\times V\to\{0,1,2\}$. *Each arc* $(v_j,v_k)\in E$ *is associated with two multiplicities: the number of contractions between lower undotted indices on the spinor* v_j *and upper undotted indices on the spinor* v_k *is* $m^S(v_j,v_k)$, *whereas the number of contractions between lower dotted indices on the spinor* v_j *and upper dotted indices on the spinor* v_k *is* $m^D(v_j,v_k)$.

The graph G_N possesses two distinct types of arcs. Solid arcs correspond to contractions between undotted indices and dashed arcs correspond to contractions between dotted indices. The multiplicities of the solid and dashed arcs (v_j,v_k) are $m^S(v_j,v_k)$ and $m^D(v_j,v_k)$, respectively. We associate with each type of arc an *arc characteristic*, ϖ which is 1 for a solid arc and i for a dashed arc. The total multiplicity between v_j and v_k, $m(v_j,v_k)$ is therefore defined as follows:

$$m(v_j,v_k)=m^S(v_j,v_k)+im^D(v_j,v_k). \tag{4}$$

An analogous distinction between irreducible and reducible invariants can also be made for these invariants. Three examples of graphical representations of fifth-degree, pure Ricci invariants are depicted in Fig. 2. Graphs G_{C_1}, G_{C_2}, and G_{C_3} represent the invariants $C_1=\Phi_{AB\dot{A}\dot{B}}\Phi^{A}{}_{C}{}^{\dot{A}\dot{C}}\Phi^{C}{}_{D}{}^{\dot{D}}{}_{\dot{D}}{}^{\dot{E}}\Phi^{D}{}_{E}{}^{\dot{C}}{}_{\dot{C}}{}^{\dot{D}}\Phi^{BE\dot{B}}{}_{\dot{E}}$, $C_2=\Phi_{A}{}^{B}{}_{\dot{A}}{}^{\dot{B}}\Phi_{B}{}^{C}{}_{\dot{B}}{}^{\dot{C}}\Phi_{C}{}^{D}{}_{\dot{C}}{}^{\dot{D}}\Phi_{D}{}^{E}{}_{\dot{D}}{}^{\dot{E}}\Phi_{E}{}^{A}{}_{\dot{E}}{}^{\dot{A}}$, and $C_3=\Phi_{AB\dot{A}\dot{B}}\Phi^{AB\dot{A}\dot{B}}\Phi_{E}{}^{F}{}_{\dot{E}}{}^{\dot{F}}\Phi_{F}{}^{G}{}_{\dot{F}}{}^{\dot{G}}\Phi_{G}{}^{E}{}_{\dot{G}}{}^{\dot{E}}$. Invariants C_1 and C_2 are connected, whereas invariant C_3 is disconnected, and possesses two connected factors of lower degree: $\Phi_{AB\dot{A}\dot{B}}\Phi^{AB\dot{A}\dot{B}}$ and $\Phi_{E}{}^{F}{}_{\dot{E}}{}^{\dot{F}}\Phi_{F}{}^{G}{}_{\dot{F}}{}^{\dot{G}}\Phi_{G}{}^{E}{}_{\dot{G}}{}^{\dot{E}}$. As in the case for the pure Weyl invariants, reversing the direction of any one arc has the effect of changing the overall sign of the invariant.

For the pure Ricci invariants, applying the definition of $m(v_j,v_k)$ in Eq. (4) to the adjacency matrix definition in Eq. (1) introduces a generalized adjacency matrix consisting of complex entries a_{jk}.

The invariants C_1, C_2, and C_3 in Fig 2. are thus associated with the matrices:

$$A(G_{C_1})=\begin{bmatrix} 0 & 1+i & 0 & 0 & 1+i \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1+i & 0 \\ 0 & i & 0 & 0 & 1 \\ 0 & 0 & i & 0 & 0 \end{bmatrix},$$

$$A(G_{C_2})=\begin{bmatrix} 0 & 1+i & 0 & 0 & 0 \\ 0 & 0 & 1+i & 0 & 0 \\ 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 1+i \\ 1+i & 0 & 0 & 0 & 0 \end{bmatrix},$$

FIG. 3. The graphs corresponding to a pure Ricci invariant and its conjugate.

$$A(G_{C_3})=\begin{bmatrix} 0 & 2+2i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 1+i \\ 0 & 0 & 1+i & 0 & 0 \end{bmatrix}.$$

The sum of the real parts of the entries in row j corresponds to the solid-arc outdegree of v_j, whereas the sum of the real parts of the entries in column k corresponds to the solid-arc indegree of v_k. An analogous condition relating the imaginary parts of the matrix entries and the dashed arcs holds. Also, loops are assumed not to be present in these graphs, and consequently $a_{jj}=0$. Since the sum of the outdegree and the indegree at each vertex must be two for both types of arc, the following condition holds:

$$\sum_{k=1}^{n}(a_{jk}+a_{kj})=2+2i, \quad j=1,2,\ldots,n.$$

Equation (4) allows us to directly extend the definition of orientedness to the graphs associated with pure Ricci invariants: G_N is *oriented* iff $m(v_j,v_k)=0$ whenever $m(v_k,v_j)\neq 0$ for $j\neq k$. Given a pure Ricci invariant N, its oriented form N' satisfies the conditions in Eqs. (2) and (3), where the number σ of arcs reversed to form N' from N is given by

$$\sigma=\sum_{j>k}(x_{jk}+y_{jk}),$$

where $a_{jk}=x_{jk}+iy_{jk}$.

When dealing with the pure Ricci invariants, it will be useful to consider the graphical representation of the conjugate of an invariant. Given some pure Ricci invariant N, the graph $G_{\bar{N}}$ associated with its conjugate $\bar{N}$ is obtained from G_N simply by replacing all solid arcs with dashed arcs, and all dashed arcs with solid arcs. Since $\Phi_{AB\dot{A}\dot{B}}$ is Hermitian, all pure Ricci invariants are real quantities.

For example, the graph G_H associated with the pure Ricci invariant H is given in Fig. 3. The aforementioned interchange of solid and dashed arcs will provide the graph, $G_{\bar{H}}$ associated with the conjugate of H, which is equal to H itself.

III. THE PURE WEYL INVARIANTS

A. Properties of the set $\hat{\mathcal{W}}$

The set $\hat{\mathcal{W}}\subset\mathcal{W}$ is defined to be the set of all pure Weyl invariants such that all contractions between Weyl spinors occur pairwise, and the contractions belonging to each pair have the same direction, i.e., are both from lower indices to upper indices or vice versa. Thus, a pure Weyl invariant, N, is a member of the set $\hat{\mathcal{W}}$ iff every arc in G_N is of even multiplicity, i.e., $A(G_N)$ contains no odd integer elements. In Fig. 1, the invariant corresponding to B_1 does not belong to $\hat{\mathcal{W}}$, whereas the invariants corresponding to B_2 and B_3 are members of $\hat{\mathcal{W}}$.

Consider the set $\hat{\mathcal{W}}^c \subset \hat{\mathcal{W}}$, which consists of the connected invariants within $\hat{\mathcal{W}}$.

Lemma 1: All elements of $\hat{\mathcal{W}}$ are either elements of $\hat{\mathcal{W}}^c$, or are expressible as products of elements of $\hat{\mathcal{W}}^c$.

Proof: Obvious. ■

Lemma 2: For every integer $n \geqslant 2$, there exists a unique element of $\hat{\mathcal{W}}^c$, with polynomial degree n. We denote this element as $\hat{\mathcal{W}}^c(n)$.

Proof: The cases where the polynomial degree is 2 or 3 are trivial. Consider a *connected* directed multigraph G possessing $n>3$ vertices and a 4-regular underlying graph. We require that every arc be of even multiplicity, and arcs of multiplicity four, which would result in a disconnected graph, are not permitted. Therefore, G possesses n distinct arcs, and each arc must be of multiplicity two. Since graphs possessing loops are disregarded, it also follows that each vertex in G is incident with two distinct arcs. By appealing to elementary graph theory, which states that a graph is a n-cycle iff it is a connected 2-regular graph possessing n vertices, we conclude that G is a n-cycle with each edge replaced by an arc of multiplicity two. Given any two such directed multigraphs, we can transform one into the other by reorienting its arcs; i.e., their associated invariants are identical up to a sign. Given that all arcs in G are of multiplicity two, this transformation will leave the sign of its associated invariant unchanged. Hence for each n, there must be a unique invariant belonging to $\hat{\mathcal{W}}^c$. ■

We shall now construct the general formula relating any invariant in $\hat{\mathcal{W}}$ to the invariants w_1 and w_2. We begin by considering the members of $\hat{\mathcal{W}}^c$ in the standard canonical frame, where $\Psi_1=\Psi_3=0$. We construct the spinor ${}^n\Omega_{AB}{}^{CD}$ *via* consecutive pairwise contractions of n Weyl spinors and collect its dyad expansion as follows:

$$
\begin{aligned}
{}^n\Omega_{AB}{}^{CD} &= \underbrace{\Psi_{ABXY}\,\Psi^{XY}{}_{ZT}\,\Psi^{ZT}{}_{EF}\cdots\Psi^{GHCD}}_{n \text{ factors, } n\geq 2} \\
&= {}^nP_0\,\iota_A\,\iota_B\,\iota^C\iota^D + {}^nP_{2s}(o_A\,o_B\,\iota^C\iota^D + o^C o^D\,\iota_A\,\iota_B) \\
&\quad + {}^nP_{2a}(o_A\,o^C\,\iota_B\,\iota^D + o_A\,o^D\,\iota_B\,\iota^C + o_B\,o^C\,\iota_A\,\iota^D + o_B\,o^D\,\iota_A\,\iota^C) \\
&\quad + {}^nP_4 o_A\,o_B\,o^C o^D.
\end{aligned}
$$

It is straightforward to show that the coefficients ${}^nP_0$, ${}^nP_{2s}$, ${}^nP_{2a}$, and ${}^nP_4$ obey the following recursion relations:

$$
\begin{aligned}
{}^nP_0 &= {}^{n-1}P_0\Psi_2 + {}^{n-1}P_{2s}\Psi_0, \\
{}^nP_{2s} &= {}^{n-1}P_{2s}\Psi_2 + {}^{n-1}P_4\Psi_0, \\
{}^nP_{2a} &= -2({}^{n-1}P_{2a}\Psi_2), \\
{}^nP_4 &= {}^{n-1}P_4\Psi_2 + {}^{n-1}P_{2s}\Psi_4,
\end{aligned}
\tag{5}
$$

where

$$
{}^1P_0=\Psi_0, \quad {}^1P_{2s}={}^1P_{2a}=\Psi_2, \quad {}^1P_4=\Psi_4.
$$

From these recursion relations, we derive the following expressions for the coefficients:

$$
{}^nP_{2s} = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} (\Psi_0\Psi_4)^k\,\Psi_2{}^{n-2k},
$$

$$
{}^nP_{2a} = (-2)^{n-1}\,\Psi_2^n,
$$

$$
{}^nP_0 = \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \binom{n}{2k+1} \Psi_0 (\Psi_0\Psi_4)^k\,\Psi_2{}^{n-2k-1},
$$

$$ {}^{n}P_4 = \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \binom{n}{2k+1} \Psi_4 (\Psi_0 \Psi_4)^k \Psi_2^{\,n-2k-1}. $$

Since $\hat{\mathcal{W}}^c(n)$ is the trace of ${}^{n}\Omega_{AB}{}^{CD}$, it follows that the formula for $\hat{\mathcal{W}}^c(n)$ in the standard canonical frame, in terms of the Weyl curvature components, is

$$ \hat{\mathcal{W}}^c(n) = {}^{n}\Omega_{AB}{}^{AB} = 2({}^{n}P_{2s} - {}^{n}P_{2a}) = (-2\Psi_2)^n + 2\sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} (\Psi_0 \Psi_4)^k \Psi_2^{\,n-2k}. $$

The following general syzygy relation can be derived from Eq. (5):

$$ \hat{\mathcal{W}}^c(n) = \tilde{w}_1 \hat{\mathcal{W}}^c(n-2) + \tilde{w}_2 \hat{\mathcal{W}}^c(n-3), \quad n>3, \quad \hat{\mathcal{W}}^c(1) = 0, \tag{6} $$

where

$$ \tilde{w}_1 = \frac{\hat{\mathcal{W}}^c(2)}{2} = \frac{1}{2} \Psi_{ABCD} \Psi^{ABCD} = 3 w_1 $$

and

$$ \tilde{w}_2 = \frac{\hat{\mathcal{W}}^c(3)}{3} = \frac{1}{3} \Psi_{AB}{}^{CD} \Psi_{CD}{}^{EF} \Psi_{EF}{}^{AB} = 2 w_2 . $$

All invariants belonging to $\hat{\mathcal{W}}^c$ in an arbitrary frame can therefore be expressed as a polynomial function of the Weyl invariants w_1 and w_2,

$$ \hat{\mathcal{W}}^c(n) = n \sum_{2p+3q=n} \frac{(p+q-1)!}{p!\,q!} \tilde{w}_1^p \tilde{w}_2^q . $$

Hence, as a consequence of Lemmas 1 and 2 and this relation for $\hat{\mathcal{W}}^c(n)$, we can express any invariant within $\hat{\mathcal{W}}$ as a polynomial function of w_1 and w_2.

B. Invariants outside $\hat{\mathcal{W}}$

The pure Weyl invariants outside $\hat{\mathcal{W}}$ are associated with graphs that possess arcs of odd multiplicity. If we can express these invariants as polynomials of invariants belonging to $\hat{\mathcal{W}}$, we will have found the syzygies relating these invariants to w_1 and w_2. As a consequence of the second fundamental theorem, any polynomial syzygy relating the invariants outside $\hat{\mathcal{W}}$ to the invariants inside $\hat{\mathcal{W}}$ must be a consequence of the following identity:

$$ 3\varepsilon_{A[B}\varepsilon_{CD]} = \varepsilon_{AB}\varepsilon_{CD} + \varepsilon_{AC}\varepsilon_{DB} + \varepsilon_{AD}\varepsilon_{BC} \equiv 0, $$

which may be rewritten as

$$ \varepsilon_{AB}\varepsilon^{CD} = \delta_A^C \delta_B^D - \delta_A^D \delta_B^C . \tag{7} $$

Contracting the identity in Eq. (7) with $\Psi^A{}_{FGH}\Psi^{BJKL}\Psi_{CSTU}\Psi_D{}^{XYZ}$ leads to the following identity which transforms a pair of contractions spanning four distinct Weyl spinors:

$$ \Psi_{CSTU}\Psi^C{}_{FGH}\Psi_D{}^{XYZ}\Psi^{DJKL} = \Psi_{CSTU}\Psi^D{}_{FGH}\Psi_D{}^{XYZ}\Psi^{CJKL} + \Psi_{CSTU}\Psi_{BFGH}\Psi^{CXYZ}\Psi^{BJKL}. \tag{8} $$

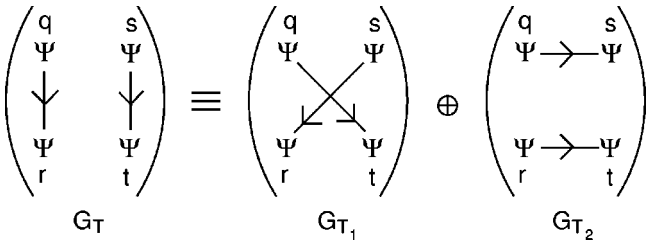

FIG. 4. The identity in Eq. (8) expressed in graphical notation.

In graphical notation, this identity is represented by transforming a pair of arcs spanning four distinct vertices (Fig. 4). The contracted spinor associated with the graph on the left-hand side (LHS) of the equation is the sum of the two contracted spinors associated with the two graphs on the right-hand side (RHS) of the equation, i.e., $T=T_1+T_2$. The vertices labeled q, r, s, and t correspond to the first, second, third, and fourth spinor in each term in Eq. (8), respectively.

In the graphical representation, we shall use the symbol $\oplus$ to denote addition of the associated spinors of two graphs. As expected, these edge transformations preserve the degree of each vertex. Contracting Eq. (7) (or its conjugate) with appropriate products of four Ricci spinors will provide the Ricci identities analogous to the Weyl identity in Eq. (8) where either a pair of solid arcs, or a pair of dashed arcs, are transformed. From now on, we shall simply refer to the graphical forms of these identities arising from Eq. (7) (or its conjugate) as ''the identity.'' The arc transformations in the graphical Ricci identities directly resemble those of the Weyl identity depicted in Fig. 4. Note that if the pair of contractions transformed do not span four distinct spinors, Eq. (7) results in a trivial identity.

We can establish the following properties of $G_{N'}$.

Lemma 3: The total number of arcs of odd multiplicity incident with each vertex of $G_{N'}$ is even (or zero).

Proof: This immediately follows from the fact that $G_{N'}$ is oriented and every vertex in the underlying undirected graph of $G_{N'}$ is of degree four. ■

Lemma 4: For any pure Weyl invariant $N \notin \hat{\mathcal{W}}$, the number of distinct arcs of odd multiplicity in $G_{N'}$ is even, and greater than or equal to four.

Proof: By elementary graph theory, if $G_{N'}$ possesses n vertices, the sum of all arc multiplicities in $G_{N'}$ will be $2n$. Since the sum of all even arc multiplicities is even, it follows that there must be an even number of odd multiplicities. Suppose we had some $G_{N'}$ possessing only two arcs of odd multiplicity. By Lemma 3, it follows that both these arcs must connect one pair of vertices v_j and v_k, where both $m(v_j,v_k)$ and $m(v_k,v_j)$ are odd. This contradicts the fact that $G_{N'}$ is oriented. Thus, if $N \notin \hat{\mathcal{W}}$, the minimum number of arcs of odd multiplicity in $G_{N'}$ is four. ■

We now intend to focus on the arcs of odd multiplicity in $G_{N'}$, and apply the arc transformations in the identity to pair up these arcs. Consider the subgraph, $S_{N'}$, of the oriented directed graph, $G_{N'}$ where $m_{S_{N'}}(v_j,v_k)=1$ iff $m_{G_{N'}}(v_j,v_k)$ is odd, and $m_{S_{N'}}(v_j,v_k)=0$ otherwise. Recall that the union of two graphs is defined such that $V(G_1 \cup G_2)=V(G_1)\cup V(G_2)$ and $E(G_1 \cup G_2)=E(G_1)\cup E(G_2)$. Thus, $G_{N'}$ may be considered as the union of two edge-disjoint subgraphs, $S_{N'}$, and $G^S_{N'}$, which contains the arcs of even multiplicity in $G_{N'}$,

$$G_{N'}=S_{N'}\cup G^S_{N'}, \tag{9}$$

and where the adjacency matrices of these three graphs are related as follows:

$$A(G_{N'})=A(S_{N'})+A(G^S_{N'}). \tag{10}$$

The elements of $A(S_{N'})$ and $A(G^S_{N'})$ may be obtained directly from the elements a'_{jk} of $A(G_{N'})$, in the following manner:

$$A(S_{N'}) = [a'_{jk} \bmod 2],$$

$$A(G^S_{N'}) = [a'_{jk} - (a'_{jk} \bmod 2)]. \tag{11}$$

We can now state our main theorem.

Theorem 1: *For any pure Weyl invariant $N \notin \hat{\mathcal{W}}$, $S_{N'}$ is expressible, using the identity, as a finite sum of graphs consisting only of arcs of even multiplicity, $\tilde{S}_j$,*

$$S_{N'} \equiv \bigoplus_{j=1}^{n} c_j \tilde{S}_j, \tag{12}$$

where the coefficients c_j are rational numbers.

The graph $G_{N'}$ may then be expressed as

$$G_{N'} \equiv \bigoplus_{j=1}^{n} c_j G_{X_j},$$

where

$$G_{X_j} = G^S_{N'} \cup \tilde{S}_j. \tag{13}$$

The invariant N' then obeys the following identity:

$$N' = \sum_{j=1}^{n} c_j X_j, \tag{14}$$

where $X_j \in \hat{\mathcal{W}}$, $j = 1,2,\ldots,n$.

Proof: It immediately follows from Lemmas 3 and 4 that $S_{N'}$ possesses an even number of arcs and each of its connected components of its underlying undirected graph is Eulerian. For the purpose of proving this theorem, we reorient the arcs of $S_{N'}$ to form a digraph $S_{N''}$ such that each

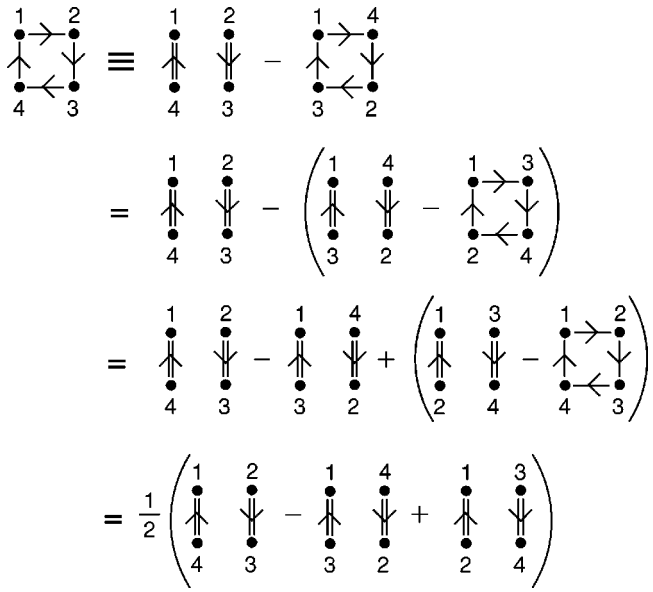

FIG. 5. Complete decomposition of a 4-circuit into graphs consisting solely of arcs of even multiplicity.

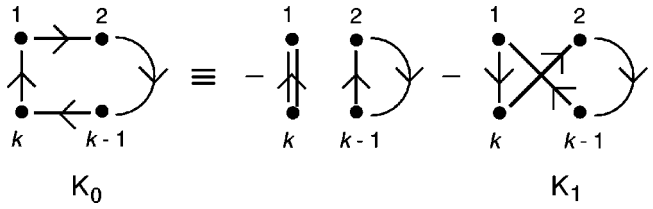

FIG. 6. First stage in the decomposition of a k-circuit.

component of $S_{N''}$ has a (directed) Euler circuit. If the number of arcs reoriented is σ', then the invariant N'' corresponding to the graph $G^S_{N'} \cup S_{N''}$ is equivalent to $(-1)^{\sigma'} N'$; and the original invariant N is given by $(-1)^{\sigma+\sigma'} N''$. For convenience, we shall use the term k-circuit to mean a circuit of length k.

Case 1: $S_{N''}$ is connected.

In this case $S_{N''}$ possesses a Eulerian circuit of even length; the smallest possible circuit consists of four edges. Consider the simplest case where $S_{N''}$ is a 4-circuit. As Fig. 5 shows, application of the identity relates this circuit to two new graphs: one of which possesses paired edges and the other being a new 4-circuit.[23] This new circuit can be decomposed in a similar fashion, and ultimately we return to the original 4-circuit, with opposite sign. We can then solve for an expression relating $S_{N''}$ to graphs where all vertices are paired, and by taking the union of all terms in this expression with $G^S_{N'}$, it can be used to construct the polynomial syzygy relating N to invariants within $\hat{\mathcal{W}}$ according to Eqs. (13) and (14).

Next, we establish that when $S_{N''}$ possesses an Euler circuit of length $k \geqslant 6$, where k is even, it is expressible entirely in terms of $(k-2)$-circuits modulo the identity. We begin by denoting the Euler circuit of $S_{N''}$ as K_0, and sequentially label each vertex as shown in Fig. 6. The curved arrow in K_0 corresponds to a directed path of length $k-3$. Applying the arc transformation of Fig. 4 on the arcs $(1,2)$ and $(k-1,k)$, depicted in bold, and reorienting the direction of various arcs and changing signs appropriately result in the identity shown in Fig. 6. This expresses K_0 in terms of a $(k-2)$-circuit (the remaining two edges may be oriented to form an edge of multiplicity two), and a new k-circuit, denoted K_1. It will be convenient to represent these k-circuits as their vertex sequences, where we adopt the convention that each sequence begins and ends at the vertex labeled 1. We omit the final 1 in the sequence, as it is understood to be present. Thus, we represent the circuit K_0 as $(1,2,3,\ldots,k-2,k-1,k)$, and K_1 as $(1,k,2,\ldots,k-3,k-2,k-1)$.

We subsequently transform the arcs $(1,k)$ and $(k-2,k-1)$ in K_1 to produce another $(k-2)$-circuit, and K_2, which is a k-circuit possessing the vertex sequence $(1,k-1,k,\ldots k-4,k-3,k-2)$ (Fig. 7). Note that the arcs transformed in K_1 are distinct from the arcs formed from the transformation of K_0 in the previous step, i.e., $(k,2)$ and $(k-1,1)$. This is necessary to ensure that we do not derive trivial relationships such as $0=0$. Hence, we shall always choose to transform two arcs in the k-circuits such that the first arc connects the first two vertices in the vertex sequences, and the second arc connects the last two vertices in the vertex sequences.

At each step, the k-circuit is expressed as a $(k-2)$-circuit, together with a new k-circuit with opposite sign. After n steps following this procedure, we obtain an expression for K_0 which is the

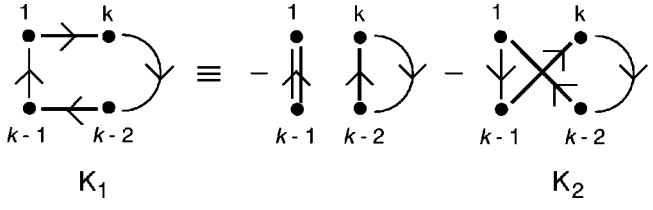

FIG. 7. Second stage in the decomposition of a k-circuit.

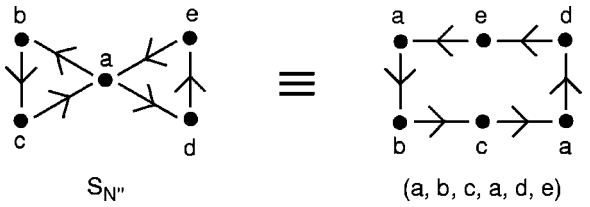

FIG. 8. Expression of an unpaired subgraph possessing a vertex of degree four as an equivalent vertex sequence.

sum of n terms associated with $(k-2)$-circuits, and $(-1)^n K_n$. The vertex sequence of K_{n+1} can be obtained by applying the permutation

$$\begin{pmatrix} 1 & 2 & 3 & 4 & \cdots & k-3 & k-2 & k-1 & k \\ 1 & k & 2 & 3 & \cdots & k-4 & k-3 & k-2 & k-1 \end{pmatrix} \tag{15}$$

on the vertex sequence of K_n. This permutation is of order $k-1$, therefore $K_{k-1} \equiv K_0$, and since $k-1$ is odd, we will return to the original circuit with opposite sign after $k-1$ steps. We are thus able to solve for K_0 to obtain an equivalent expression entirely in terms of $(k-2)$-circuits after $k-1$ steps.

Repeating this procedure with each of these $(k-2)$-circuits will then result in an expression for K_0 entirely in terms of $(k-4)$-circuits. Further repetition of this process will successively reduce the lengths of the circuits by two, and we eventually express K_0 in terms of 4-circuits. By Fig. 5, we can then express K_0 as a finite sum of graphs which only possess arcs of even multiplicity.

In the above discussion all vertices in the circuit have been labeled as distinct. This would correspond to the case where all vertices in the underlying graph of $S_{N''}$ are of degree two. In the event that vertices of degree four are present in the underlying graph of $S_{N''}$, these vertices will occur twice in the vertex sequence of a Eulerian circuit of $S_{N''}$. For example, if $S_{N''}$ is the graph in Fig. 8, then it corresponds to the vertex sequence (a,b,c,a,d,e).

This Eulerian circuit is still of even length, and despite the fact that vertex a appears twice in the vertex sequence, we may decompose it in the manner described above to ultimately pair all the arcs in $S_{N''}$. Owing to the vertex repetition in the vertex sequence, graphs possessing loops will be formed during this decomposition. In the vertex sequence representation, these would correspond to sequences with identical vertices next to each other. Whenever such graphs are formed, they ultimately correspond to expressions possessing spinors of the form $\Psi_A{}^{AXY}$ or $\Psi_{AB}{}^{AB}$. These expressions are identically zero and thus at any stage of the decomposition, graphs possessing loops may be removed from the sum in Eq. (12) as they are formed.

Case 2: $S_{N''}$ is disconnected.

Suppose that $S_{N''}$ consists of two disjoint circuits of length m and n, respectively. By Lemmas 3 and 4, $m+n$ must be even. By transforming a pair of arcs such that one arc comes from each circuit, $S_{N''}$ may be expressed in terms of graphs consisting of single circuits of length $m+n$, reducing the problem to Case 1 (Fig. 9). The extension of this result to three or more disjoint cycles is obvious.

We have established that using the arc transformation of Fig. 4, the subgraph $S_{N''}$ may be expressed equivalently as the sum of graphs consisting solely of arcs of multiplicity two, and we

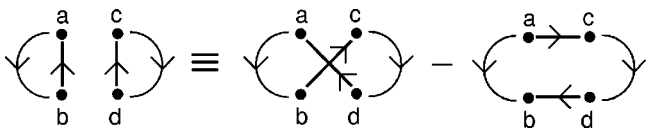

FIG. 9. Expression of two disjoint unpaired subgraphs of length m and n in terms of single circuits of length $m+n$.

get the corresponding decomposition of $S_{N'}$ [Eq. (12)] by multiplying both sides of this equation by $(-1)^{\sigma'}$. Taking the union of both sides of Eq. (12) with $G^S_{N'}$ will therefore provide the decomposition of $G_{N'}$ in terms of graphs consisting solely of arcs of even multiplicity [Eq. (13)]. The associated invariant identity then expresses N' as a polynomial of invariants within $\hat{\mathcal{W}}$ [Eq. (14)]. ■

In the preceding section it was established that every invariant within $\hat{\mathcal{W}}$ is expressible as a polynomial function of the base invariants w_1 and w_2. *Hence it follows from Theorem 1 that any pure Weyl invariant is expressible as a polynomial function of the base invariants* w_1 *and* w_2.

IV. THE PURE RICCI INVARIANTS

A. Properties of the set $\hat{\mathcal{R}}$

We define the set $\hat{\mathcal{R}} \subset \mathcal{R}$ to be the set of all pure Ricci invariants such that consecutive contractions between spinors also occur pairwise, where each pair of contractions consists of one contraction between a pair of undotted indices, and one contraction between a pair of dotted indices, such that both of these contractions are in the same direction. For convenience, we will call such a pair of contractions a *couple*, and any arc not belonging to a couple is said to be uncoupled. If $N \in \hat{\mathcal{R}}$, then all of the elements of its associated adjacency matrix, $A(G_N)$ satisfy the condition $x_{jk}=y_{jk}$, and every element of $A(G_N)$ is an integral multiple of $1+i$. In Fig. 2, the invariant corresponding to C_1 does not belong to $\hat{\mathcal{R}}$, whereas the invariants corresponding to C_2 and C_3 are members of $\hat{\mathcal{R}}$. In terms of the graphical representation adopted here, if $N \in \hat{\mathcal{R}}$, then the arcs of G_N are paired such that $\forall (v_j, v_k) \in E(G_N)$, $m^S(v_j, v_k) = m^D(v_j, v_k)$.

Let $\hat{\mathcal{R}}^c$, $\hat{\mathcal{R}}^c \subset \hat{\mathcal{R}}$, denote the set of all connected invariants within $\hat{\mathcal{R}}$. We can establish two properties of this set.

Lemma 5: All elements of $\hat{\mathcal{R}}$ *are either elements of* $\hat{\mathcal{R}}^c$, *or are expressible as products of elements of* $\hat{\mathcal{R}}^c$.

Proof: Obvious. ■

Lemma 6: For every integer $n \geqslant 2$, *there exists a unique element of* $\hat{\mathcal{R}}^c$ *with polynomial degree* n. *We denote this element as* $\hat{\mathcal{R}}^c(n)$.

Proof: This is obviously true for $n=2,3$. Consider a *connected* directed multigraph G possessing $n>3$ vertices. We require that every vertex in the underlying graph of G be adjacent to two solid edges and two dashed edges, and that arcs are paired in couples, resulting in equal multiplicities of solid and dashed arcs between any given pair of vertices (v_j, v_k). The presence of two such couples between a pair of vertices would result in a disconnected graph, hence there is at most one couple between every pair of vertices. Therefore, G possesses n distinct couples. Since graphs possessing loops are disregarded, it also follows that each vertex in G is adjacent to two distinct couples. By appealing to elementary graph theory, which states that a graph is a n-cycle iff it is a connected 2-regular graph possessing n vertices, we conclude that G is a n-cycle with each edge replaced by a couple. Given any two such directed multigraphs, we can transform one into the other by reversing the directions of couples. This transformation reverses the direction of an even number of arcs and will leave the sign of its associated invariant unchanged. Hence there must be a unique invariant belonging to $\hat{\mathcal{R}}^c$ for each n. ■

We begin the construction of the general formula relating the invariants in $\hat{\mathcal{R}}$ to the invariants r_1, r_2, and r_3 by considering the members of $\hat{\mathcal{R}}^c$ in the standard canonical frame, where $\Phi_{10} = \Phi_{01} = \Phi_{21} = \Phi_{12} = 0$. The spinor ${}^n\chi_A{}^Y{}_{\dot{A}}{}^{\dot{Y}}$, which is constructed *via* consecutive couple-by-couple contractions of n Ricci spinors ($n \geqslant 2$), may be written as

$$
\begin{aligned}
{}^{n}\chi_{A}{}^{Y}{}_{\dot{A}}{}^{\dot{Y}} &= \underbrace{\Phi_{AB\dot{A}\dot{B}}\,\Phi^{B}{}_{C}{}^{\dot{B}}{}_{\dot{C}}\,\Phi^{C}{}_{D}{}^{\dot{C}}{}_{\dot{D}}\,\Phi^{D}{}_{E}{}^{\dot{D}}{}_{\dot{E}}\cdots\Phi^{XY\dot{X}\dot{Y}}}_{n\ \text{factors},\ n\geqslant 2}\\
&= {}^{n}Q_{00}\,\iota_{A}\,\iota^{Y}\bar{\iota}_{\dot{A}}\bar{\iota}^{\dot{Y}} + {}^{n}Q_{11s}(o_{A}\,\iota^{Y}\bar{o}_{\dot{A}}\bar{\iota}^{\dot{Y}} + o^{Y}\iota_{A}\bar{o}^{\dot{Y}}\bar{\iota}_{\dot{A}})\\
&\quad + {}^{n}Q_{11a}(o_{A}\,\iota^{Y}\bar{o}^{\dot{Y}}\bar{\iota}_{\dot{A}} + o^{Y}\iota_{A}\bar{o}_{\dot{A}}\bar{\iota}^{\dot{Y}}) + {}^{n}Q_{20}\,o_{A}\,o^{Y}\bar{\iota}_{\dot{A}}\bar{\iota}^{\dot{Y}}\\
&\quad + {}^{n}Q_{02}\,\iota_{A}\,\iota^{Y}\bar{o}_{\dot{A}}\bar{o}^{\dot{Y}} + {}^{n}Q_{22}\,o_{A}\,o^{Y}\bar{o}_{\dot{A}}\bar{o}^{\dot{Y}}.
\end{aligned}
$$

It can be shown that the coefficients ${}^{n}Q_{00}$, ${}^{n}Q_{11s}$, ${}^{n}Q_{11a}$, ${}^{n}Q_{20}$, ${}^{n}Q_{02}$, and ${}^{n}Q_{22}$ obey the following recursion relations:

$$
\begin{aligned}
{}^{n}Q_{00} &= {}^{n-1}Q_{00}\Phi_{11} + {}^{n-1}Q_{11s}\Phi_{00},\\
{}^{n}Q_{11s} &= {}^{n-1}Q_{11s}\Phi_{11} + {}^{n-1}Q_{00}\Phi_{22},\\
{}^{n}Q_{11a} &= -\,{}^{n-1}Q_{11a}\Phi_{11} - {}^{n-1}Q_{02}\Phi_{20},\\
{}^{n}Q_{20} &= -\,{}^{n-1}Q_{20}\Phi_{11} - {}^{n-1}Q_{11a}\Phi_{20},\\
{}^{n}Q_{02} &= -\,{}^{n-1}Q_{02}\Phi_{11} - {}^{n-1}Q_{11a}\Phi_{02},\\
{}^{n}Q_{22} &= {}^{n-1}Q_{22}\Phi_{11} + {}^{n-1}Q_{11s}\Phi_{22},
\end{aligned}
\tag{16}
$$

where

$$
{}^{1}Q_{00} = \Phi_{00},\quad {}^{1}Q_{11s} = {}^{1}Q_{11a} = \Phi_{11},\quad {}^{1}Q_{20} = \Phi_{20},\quad {}^{1}Q_{02} = \Phi_{02},\quad {}^{1}Q_{22} = \Phi_{22}.
$$

The following expressions for the coefficients can be derived using these recursion relations:

$$
{}^{n}Q_{00} = \sum_{j=0}^{\lfloor (n-1)/2\rfloor}\binom{n}{2j+1}\Phi_{00}\,(\Phi_{00}\Phi_{22})^{j}\,\Phi_{11}^{n-2j-1},
$$

$$
{}^{n}Q_{11s} = \sum_{j=0}^{\lfloor n/2\rfloor}\binom{n}{2j}\,(\Phi_{00}\Phi_{22})^{j}\,\Phi_{11}^{n-2j},
$$

$$
{}^{n}Q_{11a} = (-1)^{n+1}\sum_{j=0}^{\lfloor n/2\rfloor}\binom{n}{2j}\,(\Phi_{20}\Phi_{02})^{j}\,\Phi_{11}^{n-2j},
$$

$$
{}^{n}Q_{20} = (-1)^{n+1}\sum_{j=0}^{\lfloor (n-1)/2\rfloor}\binom{n}{2j+1}\Phi_{20}\,(\Phi_{20}\Phi_{02})^{j}\,\Phi_{11}^{n-2j-1},
$$

$$
{}^{n}Q_{02} = (-1)^{n+1}\sum_{j=0}^{\lfloor (n-1)/2\rfloor}\binom{n}{2j+1}\Phi_{02}\,(\Phi_{20}\Phi_{02})^{j}\,\Phi_{11}^{n-2j-1},
$$

$$
{}^{n}Q_{22} = \sum_{j=0}^{\lfloor (n-1)/2\rfloor}\binom{n}{2j+1}\Phi_{22}\,(\Phi_{00}\Phi_{22})^{j}\,\Phi_{11}^{n-2j-1}.
$$

The nth degree invariant $\hat{\mathcal{R}}^{c}(n)$ is the trace of ${}^{n}\chi_{A}{}^{Y}{}_{\dot{A}}{}^{\dot{Y}}$. We can therefore express the invariants in $\hat{\mathcal{R}}^{c}$, in the standard canonical frame, in terms of the Ricci curvature components,

$$ {}^{n}\chi_{A}{}^{A}{}_{\dot{A}}{}^{\dot{A}}=2({}^{n}Q_{11s}-{}^{n}Q_{11a})=2\sum_{j=0}^{\lfloor n/2\rfloor}\binom{n}{2j}((\Phi_{00}\Phi_{22})^{j}+(-1)^{n}(\Phi_{20}\Phi_{02})^{j})\,\Phi_{11}^{n-2j}. $$

The following general syzygy relation can be derived from Eqs. (16):

$$ \hat{\mathcal{R}}^{c}(n)=\tilde{r}_{1}\hat{\mathcal{R}}^{c}(n-2)+\tilde{r}_{2}\hat{\mathcal{R}}^{c}(n-3)+\tilde{r}_{3}\hat{\mathcal{R}}^{c}(n-4),\quad n>4,\quad \hat{\mathcal{R}}^{c}(1)=0, \tag{17} $$

where

$$ \tilde{r}_{1}=\frac{\hat{\mathcal{R}}^{c}(2)}{2}=\frac{1}{2}\Phi_{AB\dot{A}\dot{B}}\Phi^{AB\dot{A}\dot{B}}=\frac{3}{2}r_{1}, $$

$$ \tilde{r}_{2}=\frac{\hat{\mathcal{R}}^{c}(3)}{3}=\frac{1}{3}\Phi_{AB\dot{A}\dot{B}}\Phi^{BC\dot{B}\dot{C}}\Phi^{A}{}_{C}{}^{\dot{A}}{}_{\dot{A}}=r_{2}, $$

$$ \tilde{r}_{3}=\frac{2\hat{\mathcal{R}}^{c}(4)-[\hat{\mathcal{R}}^{c}(2)]^{2}}{8}=\frac{1}{4}[\Phi_{AB\dot{A}\dot{B}}\Phi^{BC\dot{B}\dot{C}}\Phi_{CD\dot{C}\dot{D}}\Phi^{DA\dot{D}\dot{A}}-2\tilde{r}_{1}^{2}]=\frac{3}{16}(4r_{3}-3r_{1}^{2}). $$

All invariants belonging to $\hat{\mathcal{R}}^{c}$ in an arbitrary frame can therefore be expressed as a polynomial function of the pure Ricci invariants r_1, r_2, and r_3, as follows:

$$ \hat{\mathcal{R}}^{c}(n)=n\sum_{2p+3q+4r=n}\frac{(p+q+r-1)!}{p!q!r!}\tilde{r}_{1}^{p}\tilde{r}_{2}^{q}\tilde{r}_{3}^{r}. $$

Thus, as a consequence of Lemmas 5 and 6 and this relation for $\hat{\mathcal{R}}^{c}(n)$, we can express any invariant within $\hat{\mathcal{R}}$ as a polynomial function of r_1, r_2, and r_3.

B. Invariants outside $\hat{\mathcal{R}}$

If the pure Ricci invariant $N\notin\hat{\mathcal{R}}$, then G_N possesses uncoupled arcs. In order to relate N to the invariants within $\hat{\mathcal{R}}$, we need to apply the identity to G_N to form couples from the uncoupled arcs. In this case, the identity is applied to transform either two solid arcs spanning four distinct vertices, or two dashed arcs spanning four distinct vertices.

The graph $G_{N'}$ satisfies the following properties.

Lemma 7: For each vertex of $G_{N'}$, the total number of uncoupled arcs incident with it is even (or zero), and these uncoupled arcs consist of an equal number of solid and dashed arcs.

Proof: Each vertex of $G_{N'}$ is incident with two solid arcs and two dashed arcs. Removing couples incident with a vertex will leave behind an equal number of uncoupled solid arcs and uncoupled dashed arcs incident with this vertex. ■

Lemma 8: For any pure Ricci invariant $N\notin\hat{\mathcal{R}}$, the total number of distinct uncoupled arcs in $G_{N'}$ is even, and greater than or equal to four. These uncoupled arcs consist of an equal number of solid and dashed arcs.

Proof: If $G_{N'}$ possesses n vertices, the sum of all solid arc multiplicities in $G_{N'}$ will be n, and the sum of all dashed arc multiplicities in $G_{N'}$ will be n. Since each couple consists of one solid and one dashed arc, it follows that there must be an equal number of solid and dashed uncoupled arcs in $G_{N'}$. Suppose we had some $G_{N'}$ possessing only two uncoupled arcs. By Lemma 7, it follows that both these arcs must connect one pair of vertices v_j and v_k, where $m^{S}(v_j,v_k)=m^{D}(v_k,v_j)=1$, or $m^{D}(v_j,v_k)=m^{S}(v_k,v_j)=1$. This contradicts the fact that $G_{N'}$ is oriented. Thus, if $N\notin\hat{\mathcal{R}}$, the minimum number of uncoupled arcs in $G_{N'}$ is four. ■

We construct the unpaired subgraph $S_{N'}$ of $G_{N'}$ by removing couples from $G_{N'}$. We define the relative arc abundance between a pair of vertices v_j,v_k as the function δ: $(v_j,v_k)\rightarrow\{-2,-1,0,1,2\}$ where $\delta(v_j,v_k)=m^{S}_{G_{N'}}(v_j,v_k)-m^{D}_{G_{N'}}(v_j,v_k)$. If $\delta(v_j,v_k)>0$ then $m^{S}_{S_{N'}}(v_j,v_k)$

$=\delta(v_j,v_k)$ and $m^D_{S_{N'}}(v_j,v_k)=0$. However, if $\delta(v_j,v_k)<0$ then $m^D_{S_{N'}}(v_j,v_k)=-\delta(v_j,v_k)$ and $m^S_{S_{N'}}(v_j,v_k)=0$. Finally, if $\delta(v_j,v_k)=0$ then $m^S_{S_{N'}}(v_j,v_k)=m^D_{S_{N'}}(v_j,v_k)=0$.

As an immediate consequence of Lemma 8, the relative arc abundance function satisfies the following global property:

$$\sum_{V(G_{N'})}\delta(v_j,v_k)=0.$$

As in the case of the pure Weyl invariants, $G_{N'}$ may be considered to be the union of two edge-disjoint subgraphs [Eq. (9)]: $S_{N'}$, and $G^S_{N'}$, where $G^S_{N'}$ contains all of the couples present in $G_{N'}$. The adjacency matrices of these three graphs also satisfy the condition in Eq. (10), and the elements of $A(S_{N'})$ and $A(G^S_{N'})$ are related to the elements of $A(G_{N'})$, a'_{jk} in the following manner:

$$A(S_{N'})=[\eta_{jk}],$$

$$A(G^S_{N'})=[a'_{jk}-\eta_{jk}],$$

where

$$\eta_{jk}=\begin{cases}\delta(v_j,v_k), & \delta(v_j,v_k)\geqslant 0,\\ -i\,\delta(v_j,v_k), & \delta(v_j,v_k)<0.\end{cases} \tag{18}$$

Every nonzero entry in $A(S_{N'})$ is either real or imaginary. We will make use of the following property of $S_{N'}$.

Lemma 9: The arcs in $S_{N'}$ may be reoriented to form $S_{N''}$, such that each component of $S_{N''}$ is a single directed Euler circuit consisting of alternating solid and dashed arcs.

Proof: Suppose $S_{N'}$ is connected. Lemma 8 requires that $S_{N'}$ possesses an even number of arcs. It also follows from Lemma 7 that each vertex of its underlying undirected graph U_S is incident with an equal number of solid and dashed edges. We begin by constructing an alternating path in the following manner. We start at vertex v_a in U_S and take any edge incident with v_a. If we approach a vertex v_b via a solid edge, the number of unused dashed edges incident with v_b will exceed the number of unused solid edges incident with v_b by one. Similarly, if we approach v_b via a dashed edge, the number of unused solid edges incident with v_b will exceed the number of unused dashed edges incident with v_b by one. Hence at any vertex we come to, we can always leave by an unused edge of different type. Since U_S is finite, we will eventually return to v_a, approaching it via an edge of different type from the edge we used to leave it in the first place. Hence it follows that any vertex in U_S lies on a circuit consisting of alternating solid and dashed edges.

Let C be the longest such circuit in U_S. If C contains every edge in U_S then it is a Euler circuit and the lemma is true. Otherwise, if C does not contain every edge in U_S, we subtract the edges of C from U_S to give U_{S-C}. Each vertex in U_{S-C} must be incident with an equal number of solid and dashed edges. Since U_S is connected, C and U_{S-C} must have a vertex V in common. It follows from the previous paragraph that V must lie on a circuit C_1 consisting of alternating solid and dashed edges in the component of U_{S-C} containing V. Given the circuit C $(\ldots v_e,V,v_f,\ldots)$ and the circuit C_1 $(\ldots v_s,V,v_t,\ldots)$, where, without loss of generality, we assume the edges (v_e,V) and (v_s,V) are solid and the edges (V,v_f) and (V,v_t) are dashed, we can construct an alternating circuit C_2 $(\ldots v_e,V,v_t,\ldots v_s,V,v_f,\ldots)$. Thus, C_2 is longer than C, which contradicts the assumption that C is the longest circuit in U_S. Hence, the longest such C must contain every edge in U_S and be a Euler circuit. We can subsequently reorient the arcs in $S_{N'}$ to form a directed alternating Euler circuit.

If $S_{N'}$ is not connected, we first remove any isolated vertices present in $S_{N'}$, as these are components of $S_{N'}$ that do not possess any arcs. We can then apply the above argument individu-

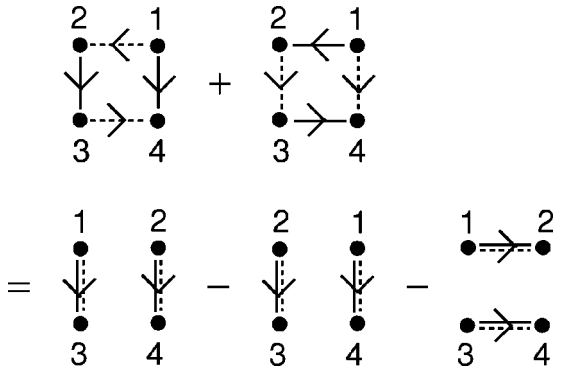

FIG. 10. Decomposition of an alternating 4-circuit into couples.

ally to each of the remaining connected components to show that each component may be reoriented as required. ■

We can now state the main result of this section.

Theorem 2: *For any pure Ricci invariant $N \notin \hat{\mathcal{R}}$, the sum $S_{N'} \oplus \overline{S_{N'}}$ is expressible, using the identity, as a finite sum of graphs consisting only of couples, $\tilde{S}_j$,*

$$S_{N'} \oplus \overline{S_{N'}} \equiv \overset{n}{\underset{j=1}{\oplus}} c_j \tilde{S}_j , \tag{19}$$

where $\overline{S_{N'}}$ is the graph $S_{N'}$ with solid arcs replaced by dashed arcs and dashed arcs replaced by solid arcs, and the coefficients c_j are rational numbers.

The sum $G_{N'} \oplus G_{\overline{N'}}$ may then be expressed as

$$G_{N'} \oplus G_{\overline{N'}} \equiv \overset{n}{\underset{j=1}{\oplus}} c_j G_{X_j},$$

where

$$G_{X_j} = G^S_{N'} \cup \tilde{S}_j , \tag{20}$$

and it follows that the invariant N' is given by

$$2N' = \sum_{j=1}^{n} c_j X_j , \tag{21}$$

where $X_j \in \hat{\mathcal{R}}$, $j = 1,2,\ldots,n$

Proof: We first orient $S_{N'}$ to obtain $S_{N''}$, and let σ' be the total number of arcs reoriented. Then, the invariant N'' corresponding to the graph $G^S_{N'} \cup S_{N''}$ is equal to $(-1)^{\sigma'} N'$. Therefore, $N = (-1)^{\sigma+\sigma'} N''$.

Case 1: $S_{N''}$ is connected.

By Lemmas 8 and 9, $S_{N''}$ consists of a single Eulerian circuit which is alternating, i.e., it consists of alternating solid and dashed arcs and has an even number of arcs. The smallest such circuit possible consists of four arcs.

Consider the simplest case where $S_{N''}$ is an alternating 4-circuit. Performing arc transformations analogous to those shown in Fig. 4 results in an identity whereby the sum of $S_{N''}$ and its "conjugate," $\overline{S_{N''}}$ is expressed in terms of graphs consisting entirely of couples (Fig. 10).

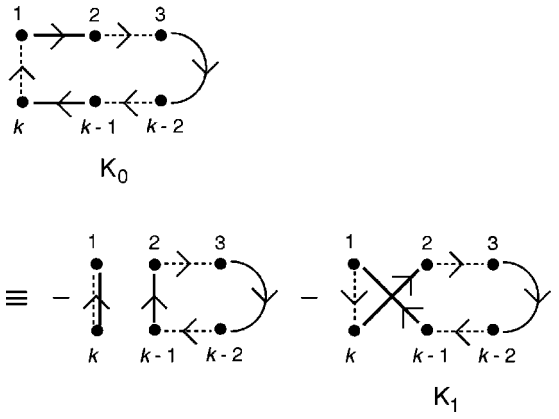

FIG. 11. First stage of the decomposition of an alternating k-circuit.

Taking the union of the left-hand side of Eq. (19) with $G^S_{N'}$ gives the sum $(G^S_{N'} \cup S_{N''}) \oplus (G^S_{N'} \cup \overline{S_{N''}})$. The first term is simply $G_{N''}$ the graph associated with N''. The graph $G^S_{N'}$ consists solely of couples, and is therefore invariant under the interchange of solid and dashed arcs. Hence, $G^S_{N'} \cup \overline{S_{N''}}$ is the graph $G_{N''}$ with solid and dashed arcs interchanged, and is hence associated with $\overline{N''}$, which is equivalent to N''. Taking the union of the right-hand side with $G^S_{N'}$ results in graphs consisting solely of coupled arcs. Hence, in this case, N'' can be expressed entirely in terms of invariants belonging to $\hat{\mathcal{R}}$. We emphasize that while $S_{N''}$ and its "conjugate" (solid–dashed arc interchange) $\overline{S_{N''}}$ are distinct graphs, their respective unions with $G^S_{N'}$ are associated with the same pure Ricci invariant owing to the fact that pure Ricci invariants are real.

Next, we extend this to show that when $S_{N''}$ is an alternating k-circuit, where k is even and $k \geqslant 6$, the sum $S_{N''} \oplus \overline{S_{N''}}$ is expressible entirely in terms of alternating $(k-2)$-circuits modulo the identity. Following what was done in the preceding section, we denote $S_{N''}$ as K_0 and represent it as the vertex sequence $(1,2,3,\ldots,k-2,k-1,k)$. Applying the identity on the solid arcs $(1,2)$ and $(k-1,k)$, depicted in bold, and reorienting the direction of various arcs and changing signs appropriately result in an expression for K_0 in terms of an alternating $(k-2)$-circuit and a new alternating k-circuit, K_1, possessing the vertex sequence $(1,k,2,\ldots,k-3,k-2,k-1)$ (Fig. 11).

The subsequent transformation of the dashed arcs $(1,k)$ and $(k-2,k-1)$ in K_1 produces another alternating $(k-2)$-circuit, and K_2, which is an alternating k-circuit which possesses the vertex sequence $(1,k-1,k,\ldots k-4,k-3,k-2)$ (Fig. 12). As before, we always choose to transform two arcs in the circuit such that the first arc connects the first two vertices in the vertex

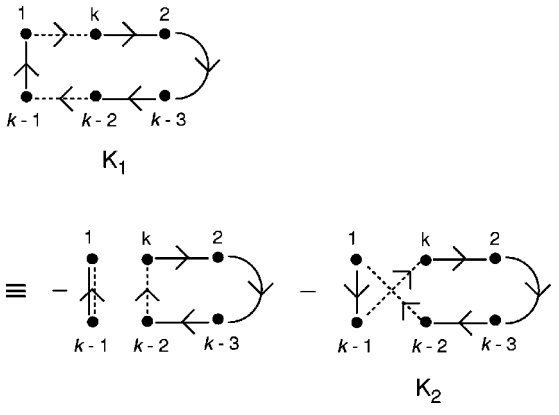

FIG. 12. Second stage of the decomposition of an alternating k-circuit.

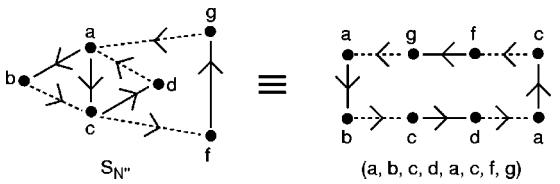

FIG. 13. Expression of a Ricci unpaired subgraph possessing a vertex of degree four as an equivalent vertex sequence.

sequence, and the second arc connects the last two vertices in the vertex sequence. For example, the arcs transformed in $K_0=(1,2,3,\ldots,k-2,k-1,k)$ were the solid arcs $(1,2)$ and $(k-1,k)$. This leads to $K_1=(1,k,2,\ldots,k-3,k-2,k-1)$, and the dashed arcs $(1,k)$ and $(k-2,k-1)$ are chosen from it for the next transformation. Thus, in the alternating circuit K_j, the pair of chosen vertices will be solid or dashed when j is even or odd, respectively.

After n applications of this procedure, we obtain an expression for K_0 which is the sum of n terms associated with $(k-2)$-circuits and $(-1)^n K_n$. The vertex sequence of K_{n+1} can be obtained by applying the permutation (15) on the vertex sequence of K_n and interchanging solid arcs with dashed arcs. For example, $K_0=(1,2,3,\ldots,k-2,k-1,k)$ and its first arc $(1,2)$ is solid. Applying permutation (15) on its vertex sequence and interchanging solid and dashed arcs give $K_1=(1,k,2,\ldots,k-3,k-2,k-1)$ with a dashed first arc $(1,k)$. Permutation (15) is of order $k-1$, therefore the vertex sequence of K_{k-1} will be identical to the vertex sequence of K_0, namely $(1,2,3,\ldots,k-2,k-1,k)$. However, since $k-1$ is odd, K_{k-1} will possess solid arcs between the vertices where K_0 possesses dashed arcs and vice versa. Thus $K_{k-1}\equiv\overline{K_0}$ and we are able to express the sum $K_0+\overline{K_0}$ entirely in terms of alternating $(k-2)$-circuits after $k-1$ steps.

Repeating this procedure with each of these alternating $(k-2)$-circuits leads to the fact that the sum of each $(k-2)$-circuit and its conjugate is expressible entirely in terms of alternating $(k-4)$-circuits. Thus $K_0+\overline{K_0}$ is expressible entirely in this form. Further repetition of this process will successively reduce the lengths of the circuits by two at each stage, and we eventually express $K_0+\overline{K_0}$ in terms of alternating 4-circuits. By Fig. 10, we can then express $K_0+\overline{K_0}$ as a finite sum of graphs which only possess coupled arcs.

In the event that vertices of degree four are present in the underlying graph of K_0, these vertices will occur twice in the vertex sequence of K_0. For example, the graph $S_{N''}$ in Fig. 13 corresponds to the vertex sequence (a,b,c,d,a,c,f,g). We can still decompose K_0 in the above manner, noting that whenever graphs with loops are formed by the arc transformations, they ultimately correspond to expressions possessing spinors of the form $\Phi_{A}{}^{A}{}_{B}{}^{\dot{C}}$, $\Phi_{B}{}^{C}{}_{A}{}^{\dot{A}}$ or $\Phi_{A}{}^{A}{}_{A}{}^{\dot{A}}$. These expressions are identically zero and thus at any stage of the decomposition, graphs possessing loops may be removed from the sum in Eq. (19) as they are formed.

Case 2: $S_{N''}$ is disconnected.

This reduces to Case 1 in a similar fashion to the pure Weyl invariants.

We have shown that the sum $S_{N''}\oplus\overline{S_{N''}}$ may be expressed equivalently as the sum of graphs consisting solely of couples via the application of the identity in Fig. 4. Multiplying both sides of this equation by $(-1)^{\sigma'}$ provides corresponding decomposition of $S_{N'}\oplus\overline{S_{N'}}$ [Eq. (19)]. Taking the union of both sides of Eq. (19) with $G^{S}_{N'}$ will therefore provide the decomposition of $G_{N'}\oplus G_{\overline{N'}}$ in terms of graphs consisting solely of couples [Eq. (20)]. The associated invariant identity, and the fact that $\overline{N'}=N'$, finally provides the expression for N' as a polynomial of invariants within $\hat{\mathcal{R}}$ [Eq. (21)]. ■

In the preceding section we established that every invariant within $\hat{\mathcal{R}}$ is expressible as a polynomial function of the base invariants r_1, r_2, and r_3. *It therefore follows from this theorem that any pure Ricci invariant is expressible as a polynomial function of the base invariants r_1, r_2, and r_3.*

V. COMPUTER IMPLEMENTATION

The proofs of Theorems 1 and 2 are constructive and provide general algorithms for the decomposition of any pure Weyl or Ricci invariant into a polynomial function of the basis invariants $\{w_1,w_2\}$ and $\{r_1,r_2,r_3\}$. The pure invariant N is provided as input in the form of its associated oriented matrix $A(G_{N'})$. It will be clear from the nature of the matrix entries (real or complex) whether the invariant is a pure Weyl or pure Ricci invariant. The matrices $A(S_{N'})$ and $A(G^S_{N'})$ are obtained from $A(G_{N'})$ using Eqs. (11) or (18). $A(S_{N'})$ is analyzed to determine whether $S_{N'}$ is connected, and if it is not connected, transformations are made to express $S_{N'}$ in terms of connected graphs (Case 2 of Theorems 1 and 2). These graphs are reoriented to form directed circuits while keeping track of any necessary sign changes. Each circuit is expressed as a vertex sequence.

We shall provide the decomposition algorithm in terms of vertex sequences because this construction, which we use in the proof of the syzygy theorems, assures us that the decomposition process will terminate, and not give a trivial relation. We start by denoting each oriented circuit as a list containing a multiplicative factor associated to that particular circuit and a second list corresponding to the vertex sequence of the circuit. For example, if $S_{N''}$ is a single connected k-circuit, it shall be denoted as $[1,[1,2,3,\ldots,k-2,k-1,k]]$, where the multiplicative factor is initially set as 1.

Transformation in the manner depicted by Fig. 6 and suitable arc reorientations will result in this particular circuit being expressed as the sum of two graphs:

$$[+1,[k,1],[2,3,\ldots,k-2,k-1]] \quad \text{and} \quad [-1,[1,k,2,\ldots,k-3,k-2,k-1]].$$

The first graph possesses two subgraphs: a 2-circuit connecting the kth and first vertices in the original sequence, and a $(k-2)$-circuit connecting the middle $k-2$ vertices in the original sequence. The 2-circuit $[k,1]$ may be considered to be, after reversing one edge and changing sign, an edge of multiplicity two between k and 1 in the case of the Weyl invariants, and a couple between k and 1 in the case of the Ricci invariants. The second graph is a k-circuit, and the vertex sequence of this k-circuit is obtained by applying the permutation (15) on the original vertex sequence (Fig. 6).

After $k-1$ successive transformations of the residual k-circuit, the original graph is expressed as the sum of the negative of the original k-circuit (or its ''conjugate'' in the case of the pure Ricci invariants) and $k-1$ terms, each containing an arc of multiplicity two (or a couple) and a $(k-2)$-circuit. We can thus solve for the original k-circuit, causing the multiplicative factors associated with the $(k-2)$-circuits to halve. Each $(k-2)$-circuit is passed to the reduction algorithm again and the reduction occurs recursively until the original circuit is expressed entirely in terms of 2-circuits. Each 2-circuit $[a,b]$ is transformed into arcs of even multiplicity (or couples) $\{a,b\}$ by reorienting one arc in each 2-circuit and changing sign appropriately, i.e, $[c,[a,b],\ldots]=[-c,\{a,b\},\ldots]$. Each graph consisting solely of even multiplicity arcs or couples is subsequently translated back into matrix form and added to $G^S_{N'}$ to obtain each term in the syzygy of N' as per Eqs. (13) and (14), or (20) and (21).

For example, consider the case where $S_{N'}$ is a single Eulerian 6-circuit, originating from a pure Weyl invariant. We represent $S_{N'}$ as $[1,[1,2,3,4,5,6]]$. Transforming the 6-circuit five times and solving for $S_{N'}$ gives the following decomposition of $S_{N'}$ into 2-circuits and 4-circuits. Figure 14 depicts this stage of the decomposition,

$$\begin{aligned} S_{N'}=&[\tfrac{1}{2},[6,1],[2,3,4,5]]+[-\tfrac{1}{2},[5,1],[6,2,3,4]]+[\tfrac{1}{2},[4,1],[5,6,2,3]] \\ &+[-\tfrac{1}{2},[3,1],[4,5,6,2]]+[\tfrac{1}{2},[2,1],[3,4,5,6]]. \end{aligned} \tag{22}$$

Each 4-circuit is expressible via the reduction algorithm as three terms involving solely 2-circuits. Therefore $S_{N'}$ is equivalent to the following expansion:

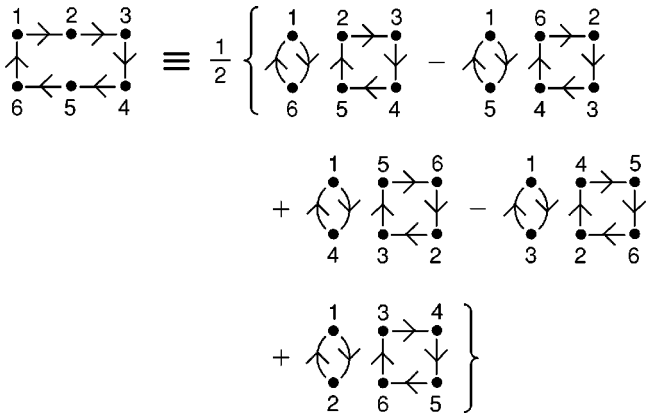

FIG. 14. Decomposition of a 6-circuit into 4-circuits and 2-circuits.

$$
\begin{aligned}
S_{N'} = {} & [\tfrac{1}{4},[6,1],[5,2],[3,4]] + [-\tfrac{1}{4},[6,1],[4,2],[5,3]] + [\tfrac{1}{4},[6,1],[3,2],[4,5]] \\
& + [-\tfrac{1}{4},[5,1],[4,6],[2,3]] + [\tfrac{1}{4},[5,1],[3,6],[4,2]] + [-\tfrac{1}{4},[5,1],[2,6],[3,4]] \\
& + [\tfrac{1}{4},[4,1],[3,5],[6,2]] + [-\tfrac{1}{4},[4,1],[2,5],[3,6]] + [\tfrac{1}{4},[4,1],[6,5],[2,3]] \\
& + [-\tfrac{1}{4},[3,1],[2,4],[5,6]] + [\tfrac{1}{4},[3,1],[6,4],[2,5]] + [-\tfrac{1}{4},[3,1],[5,4],[6,2]] \\
& + [\tfrac{1}{4},[2,1],[6,3],[4,5]] + [-\tfrac{1}{4},[2,1],[5,3],[6,4]] + [\tfrac{1}{4},[2,1],[4,3],[5,6]]. \qquad (23)
\end{aligned}
$$

Each 2-circuit may then be converted into an arc of multiplicity two by reorienting one arc in each circuit as described previously. Therefore,

$$
\begin{aligned}
S_{N'} = {} & [-\tfrac{1}{4},\{6,1\},\{5,2\},\{3,4\}] + [\tfrac{1}{4},\{6,1\},\{4,2\},\{5,3\}] + [-\tfrac{1}{4},\{6,1\},\{3,2\},\{4,5\}] \\
& + [\tfrac{1}{4},\{5,1\},\{4,6\},\{2,3\}] + [-\tfrac{1}{4},\{5,1\},\{3,6\},\{4,2\}] + [\tfrac{1}{4},\{5,1\},\{2,6\},\{3,4\}] \\
& + [-\tfrac{1}{4},\{4,1\},\{3,5\},\{6,2\}] + [\tfrac{1}{4},\{4,1\},\{2,5\},\{3,6\}] + [-\tfrac{1}{4},\{4,1\},\{6,5\},\{2,3\}] \\
& + [\tfrac{1}{4},\{3,1\},\{2,4\},\{5,6\}] + [-\tfrac{1}{4},\{3,1\},\{6,4\},\{2,5\}] + [\tfrac{1}{4},\{3,1\},\{5,4\},\{6,2\}] \\
& + [-\tfrac{1}{4},\{2,1\},\{6,3\},\{4,5\}] + [\tfrac{1}{4},\{2,1\},\{5,3\},\{6,4\}] + [-\tfrac{1}{4},\{2,1\},\{4,3\},\{5,6\}]. \qquad (24)
\end{aligned}
$$

Taking the union of this expression with $G^S_{N'}$ then gives the expression relating $G_{N'}$ to 15 graphs possessing only arcs of even multiplicity. This expression can be immediately converted into the identity relating N' to invariants within $\hat{\mathcal{W}}$, and from there, to the base invariants w_1 and w_2.

In the event that $S_{N'}$ is a single oriented alternating circuit of length six, originating from a pure Ricci invariant, the decomposition occurs in a very similar fashion. Applying the decomposition as detailed in Theorem 2 expresses the sum $S_{N'} \oplus \overline{S_{N'}}$ as the sum of five terms, each consisting of a 2-circuit and a 4-circuit. Since both $S_{N'}$ and $\overline{S_{N'}}$ correspond to the same invariant N' after taking their unions with $G^S_{N'}$ (see the proof of Theorem 2), we can associate $S_{N'} \oplus \overline{S_{N'}}$ with $2N'$, resulting in the validity of the application of the identity in Eq. (22) to this case. Extending this argument yields the result that Eqs. (23) and (24), also apply in the pure Ricci case. Equation (24) thus leads to the syzygy relating N' to the invariants within $\hat{\mathcal{R}}$, and, from there, to r_1, r_2, and r_3. Examples of this decomposition process for both pure Weyl and Ricci invariants are given in the Appendix.

It should be noted that the arc transformation in Fig. 4 (or its dashed arc form) also corresponds to well-defined operations on the elements of the matrix representations of these graphs, i.e., the elements of the matrices $A(G_{N_1})=[b_{jk}]$ and $A(G_{N_2})=[c_{jk}]$ corresponding to the graphs G_{N_1} and G_{N_2} obtained via operating on arcs (q,r) and (s,t) in $G_{N'}$, are equal to the matrix elements of $A(G_{N'})=[a_{jk}]$ with the exception of the following:

$$b_{qr}=c_{qr}=a_{qr}-\varpi, \quad b_{st}=c_{st}=a_{st}-\varpi,$$
$$b_{qt}=a_{qt}+\varpi, \quad b_{sr}=a_{sr}+\varpi,$$
$$c_{qs}=a_{qs}+\varpi, \quad c_{rt}=a_{rt}+\varpi, \tag{25}$$

where ϖ is the arc-characteristic of the two arcs being transformed. We note that the transformation can only occur between two arcs of the same type, and hence produces new arcs with the same characteristic. It follows that each transformation as described above has a unique characteristic, ϖ. Owing to the trace-free character of Ricci and Weyl spinors, if at any stage of the decomposition a matrix with a nonzero trace is formed, we can just remove this matrix from the sum, and proceed as usual.

VI. SUMMARY AND CONCLUDING REMARKS

In this paper, we have introduced a radically new approach to the classical problem of determining an independent set of polynomial invariants of the Riemann tensor. It is already well known that $\{w_1,w_2\}$ and $\{r_1,r_2,r_3\}$ form complete sets for the pure Weyl and Ricci invariants, respectively. However, our work builds on this knowledge by providing explicit formulas relating invariants within the special families $\hat{\mathcal{W}}$ and $\hat{\mathcal{R}}$ of pure Weyl and Ricci invariants to these sets, and subsequently proving constructively that all other invariants may be related to these families. We can therefore now explicitly construct the polynomial syzygies relating any pure invariant to members of the aforementioned complete sets.

We have laid down a fundamental framework that intimately links spinors to graphs. It is within this graph-theoretic setting that the construction of invariants becomes quite transparent and readily leads to algorithms which may be easily implemented on a computer. Our application of this formalism has thus far been limited to the pure Weyl and pure Ricci invariants. However, this approach is readily extendable to the mixed invariants. Work in this direction is currently in progress and our results thus far look quite promising. This work will be reported in a subsequent paper. Finally, we hope that the formulation established in this paper may well prove to be of broader interest generally.

APPENDIX

Example 1: $N'=\Psi_{ABCD}\Psi^{A}{}_{EFG}\Psi^{BEF}{}_{H}\Psi^{H}{}_{JKL}\Psi^{JKL}{}_{M}\Psi^{CDGM}$.

The graph $G_{N'}$ associated with N' is shown in Fig. 15. The vertices of $G_{N'}$ are labeled as a necessary step for the construction of its associated matrix $A(G_{N'})$. All matrices in this example are with respect to the vertex ordering $\{a,b,c,d,e,f\}$,

$$A(G_{N'})=\begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

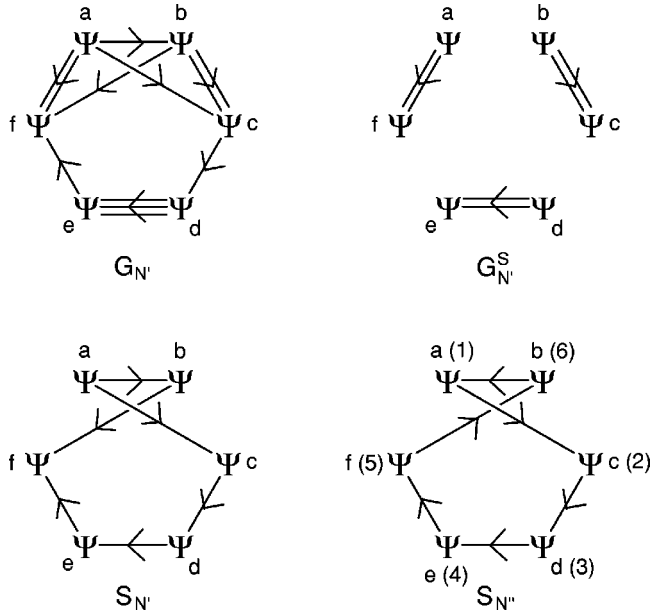

FIG. 15. Graphs associated with the decomposition process in Example 1.

The arc set of $G_{N'}$ is partitioned to give two subgraphs: $G^S_{N'}$ and $S_{N'}$, and their associated matrices $A(G^S_{N'})$ and $A(S_{N'})$ are related to $A(G_{N'})$ via Eq. (11),

$$A(G^S_{N'})=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad A(S_{N'})=\begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

As expected, the arcs in $S_{N'}$ may be reoriented to form an Eulerian circuit. Reorienting the two arcs (a,b) and (b,f) in $S_{N'}$ allows us to form the 6-circuit $S_{N''}$. This circuit can be expressed as a vertex sequence of the form introduced in the computer implementation section by making the identification $\{1=a,2=c,3=d,4=e,5=f,6=b\}$. In this notation, $S_{N''}=[1,[1,2,3,4,5,6]]$. Since an even number of arcs were reoriented to form $S_{N''}$ from $S_{N'}$, the invariant, N'' associated with $(S_{N''}\cup G^S_{N'})$ will be identically equal to N'.

Equation (24) provides the decomposition of $S_{N''}$ in terms of graphs consisting solely of arcs of multiplicity two. Taking the union of this equation with $G^S_{N'}$ will give the relationship between N' and the invariants within $\hat{\mathcal{W}}$. This may be practically achieved by constructing an appropriate matrix and adding it to $A(G^S_{N'})$. For example, the first term in Eq. (24), $\tilde{S}_1=[-\frac{1}{4}, \{6,1\},\{5,2\},\{3,4\}]$ will be associated with the matrix $A(\tilde{S}_1)$ corresponding to edges of multiplicity two between the three pairs of vertices $\{b,a\}$, $\{f,c\}$, and $\{d,e\}$. The precise directions of these arcs of multiplicity two are not important, because changing the direction of any arc of multiplicity two will leave the original invariant unchanged. Therefore, we can reorient these arcs of multiplicity two as necessary to form upper triangular matrices, which is a condition for the orientedness of the graphs,

$$A(\tilde{S}_1)=\begin{bmatrix}0&2&0&0&0&0\\0&0&0&0&0&0\\0&0&0&0&0&2\\0&0&0&0&2&0\\0&0&0&0&0&0\\0&0&0&0&0&0\end{bmatrix}.$$

Thus, the first term in the syzygy, G_{X_1} will be associated with the matrix

$$A(G_{X_1})=A(G^S_{N'})+A(\tilde{S}_1)=\begin{bmatrix}0&2&0&0&0&2\\0&0&2&0&0&0\\0&0&0&0&0&2\\0&0&0&0&4&0\\0&0&0&0&0&0\\0&0&0&0&0&0\end{bmatrix}.$$

Hence, from the matrix, it can be determined that the first term X_1, in the syzygy relating N' to the invariants within $\hat{\mathcal{W}}$, is equivalent to $-\frac{1}{4}\hat{\mathcal{W}}^c(2)\hat{\mathcal{W}}^c(4)$. After doing the same for the remaining terms in Eq. (24), and cancellation of like terms with opposite signs, the following expression for N' is obtained:

$$N'=\tfrac{1}{4}[\hat{\mathcal{W}}^c(2)]^3-\tfrac{1}{2}\hat{\mathcal{W}}^c(2)\hat{\mathcal{W}}^c(4)=2\tilde{w}_1^3-2\tilde{w}_1^3=0.$$

Example 2: $N'=\Psi_{ABCD}\Psi^{ABC}{}_E\Psi^E{}_{FGH}\Psi^F{}_{JKL}\Psi^{JK}{}_{MN}\Psi^{DMN}{}_P\Psi^{GHLP}$.

The graph $G_{N'}$ is drawn and its vertices labeled as shown in Fig. 16. The matrices are constructed with respect to the ordering $\{a,b,c,d,e,f,g\}$.

Partitioning the arc set of $G_{N'}$ as previously described gives the graphs $G^S_{N'}$ and $S_{N'}$, where

$$A(G^S_{N'})=\begin{bmatrix}0&2&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&2\\0&0&0&0&2&0&0\\0&0&0&0&0&2&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\end{bmatrix},\quad A(S_{N'})=\begin{bmatrix}0&1&0&0&0&1&0\\0&0&1&0&0&0&0\\0&0&0&1&0&0&0\\0&0&0&0&0&0&1\\0&0&0&0&0&0&0\\0&0&0&0&0&0&1\\0&0&0&0&0&0&0\end{bmatrix}.$$

Reorienting the two arcs (a,f) and (f,g) and removing the isolated vertex e transforms $S_{N'}$ into $S_{N''}$, which can be expressed in vertex sequence notation as [1,[1,2,3,4,5,6]] after making the identification $\{1=a,2=b,3=c,4=d,5=g,6=f\}$. The invariant N'' corresponding to $(S_{N''}\cup G^S_{N'})$ is equal to N' as an even number of arcs were reoriented. Taking the union of Eq. (24) with $G^S_{N'}$ then gives the syzygy relating N' to invariants within $\hat{\mathcal{W}}$, and from there, to w_1 and w_2.

Following the procedure described in the previous example gives the following expression for N':

$$N'=\tfrac{1}{4}[\hat{\mathcal{W}}^c(2)]^2\hat{\mathcal{W}}^c(3)-\tfrac{1}{2}\hat{\mathcal{W}}^c(2)\hat{\mathcal{W}}^c(5)=-2\tilde{w}_1^2\tilde{w}_2=-36w_1^2w_2.$$

Example 3: $N'=\Phi_{AB\dot{A}\dot{B}}\Phi_{CD}{}^{\dot{A}}{}_{\dot{C}}\Phi^D{}_E{}^{\dot{B}}{}_{\dot{E}}\Phi^A{}_{FD\dot{F}}\Phi^B{}_G{}^{\dot{D}}{}_{\dot{G}}\Phi^E{}_H{}^{\dot{E}}{}_{\dot{H}}\Phi^{GH\dot{G}\dot{H}}\Phi^{CF\dot{C}\dot{F}}$.

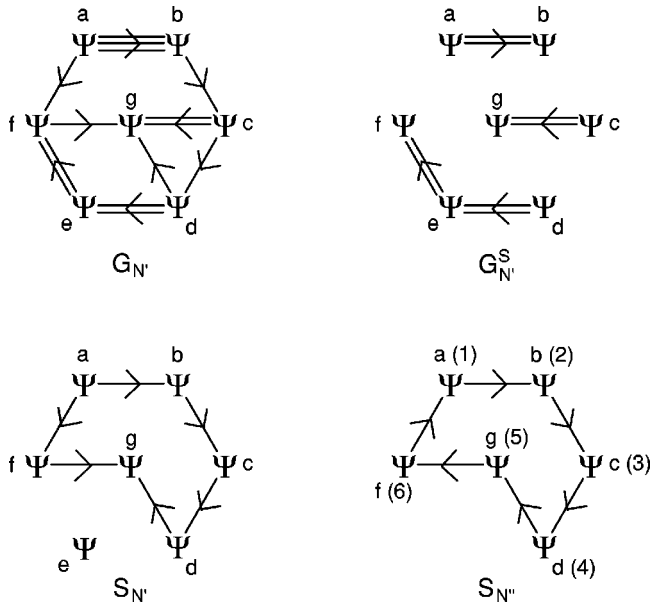

FIG. 16. Graphs associated with the decomposition process in Example 2.

The graph $G_{N'}$ is drawn and its vertices labeled as shown in Fig. 17. The matrices are constructed with respect to the ordering $\{a,b,c,d,e,x,y,z\}$.

Partitioning the arc set of $G_{N'}$ as previously described gives the graphs $G^S_{N'}$ and $S_{N'}$, where

$$A(G^S_{N'})=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+i \\ 0 & 0 & 0 & 0 & 0 & 1+i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+i \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$A(S_{N'})=\begin{bmatrix} 0 & i & i & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Reorienting the two edges (a,c) and (a,e) and removing all isolated vertices transforms $S_{N'}$ into $S_{N''}$, which can be expressed in vertex sequence notation as [1,[1,2,3,4,5,6]] after making the identification $\{1=a,2=b,3=c,4=a,5=d,6=e\}$. The invariant $(S_{N''}\cup G^S_{N'})$ is equal to N' as an even number of edges were reoriented. Note that the degree-4 vertex a is represented twice in

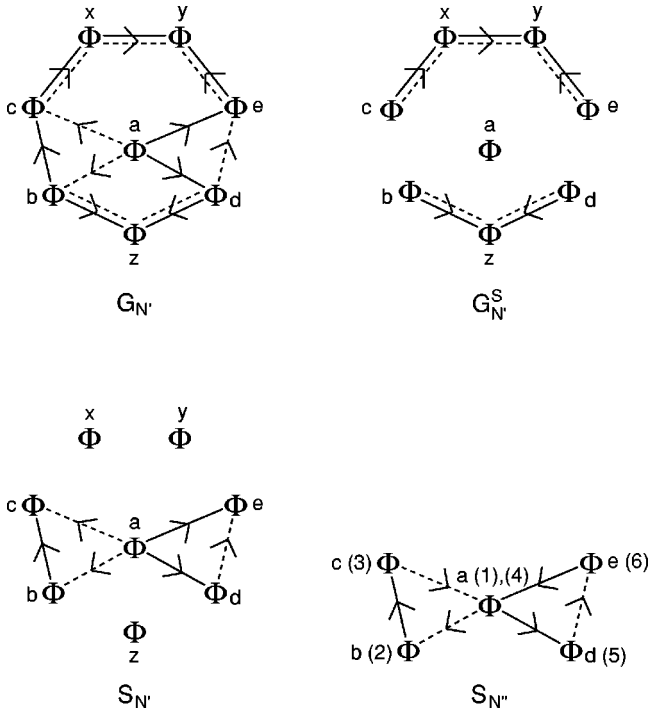

FIG. 17. Graphs associated with the decomposition process in Example 3.

this sequence; the labels 4 and 1 both represent the same vertex, a. The decomposition of Eqs. (22)–(24) are still valid, however, any terms in these equations that have vertex 4 adjacent to vertex 1 within the same circuit can be immediately disregarded as they ultimately correspond to graphs with loops at vertex a and are therefore associated with invariants which are identically zero. As a consequence, we only need to consider 12 terms in Eq. (24) in this case. The first term in Eq. (24), $\tilde{S}_1=[-\frac{1}{4},\{6,1\},\{5,2\},\{3,4\}]$ will be associated with the matrix corresponding to couples between the three pairs of vertices $\{e,a\}$, $\{d,b\}$, and $\{c,a\}$. The precise direction of these couples are not important, because changing the direction of any couple will leave the original invariant unchanged. Therefore, we are able to reorient these couples as necessary to form upper-triangular matrices,

$$A(\tilde{S}_1)=\begin{bmatrix} 0 & 0 & 1+i & 0 & 1+i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Thus, the first term in the syzygy, G_{X_1} will be associated with the matrix,

$$A(G_{X_1})=A(G^S_{N'})+A(\tilde{S}_1)=\begin{bmatrix} 0 & 0 & 1+i & 0 & 1+i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+i & 0 & 0 & 0 & 1+i \\ 0 & 0 & 0 & 0 & 0 & 1+i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+i \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Hence, it follows that the first term, X_1, in the syzygy relating N' to the invariants within $\hat{\mathcal{R}}$ is $-\frac{1}{4}\hat{\mathcal{R}}^c(3)\hat{\mathcal{R}}^c(5)$. Doing the same for the remaining terms in Eq. (24) then gives the syzygy relating N' to invariants within $\hat{\mathcal{R}}$, and, from there, to r_1, r_2, and r_3. Following this procedure yields

$$N'=\hat{\mathcal{R}}^c(8)-\tfrac{1}{2}\{\hat{\mathcal{R}}^c(3)\hat{\mathcal{R}}^c(5)+[\hat{\mathcal{R}}^c(4)]^2\}=\tfrac{1}{2}\tilde{r}_2^2\tilde{r}_1-4\tilde{r}_3^2=\tfrac{3}{64}(16r_2^2r_1-48r_3^2+72r_1^2r_3-27r_1^4).$$

[1] The classic problem involves "polynomial" completeness whereas recently the idea of algebraic completeness was introduced (see Ref. 11).
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[21] We use the term "syzygy," in a broader sense, to refer to any polynomial relationship between invariants.
[22] It may be possible to prove Bonanos' conjecture using rotor calculus, however, no evidence of this appears in the literature [G. E. Sneddon (private communication)].
[23] The equivalence stated in this diagram is understood as equality modulo union with $G^S_{N'}$. Also, for convenience, we have abbreviated $\oplus$ as $+$ and $A\oplus[(-1)\times B]$ as $A-B$.

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An inverse problem in coupled mode theory

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We study an inverse problem for the Zakharov–Shabat system which is motivated by an application to the design of co-directional couplers with prescribed response properties. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1645977]

I. STATEMENT OF DIRECT AND INVERSE PROBLEM

In this paper we are interested in an inverse problem for a system of ordinary differential equations which arises in the design of optical fiber devices. In the direct problem, we are given a coupling coefficient $q(x)$, which is a bounded, complex valued function on $[0,X]$. For any $k \in \mathbb{C}$ and $x \in [0,X]$ let $A=A(x,k), B=B(x,k)$ denote the solution of

$$\frac{\partial A}{\partial x} = ikA + q^*B, \quad \frac{\partial B}{\partial x} = -ikB \pm qA, \tag{1.1}$$

with initial conditions

$$A(0,k)=1, \quad B(0,k)=0. \tag{1.2}$$

The corresponding inverse problem is to determine $q(x)$ on $[0,X]$ given the scattering data,

$$\{B(X,k): k \in \mathbb{R}\}. \tag{1.3}$$

A closely related problem is the system (1.1) with boundary conditions

$$A(0,k)=1, \quad B(X,k)=0, \tag{1.4}$$

in which case the data for the inverse problem is

$$\{B(0,k): k \in \mathbb{R}\}. \tag{1.5}$$

For convenience of reference, let us refer to (1.1)–(1.2)–(1.3) as $\mathbf{P1}_{\pm}$ and (1.1)–(1.4)–(1.5) as $\mathbf{P2}_{\pm}$. [$\pm$ refers to the sign in the second equation of (1.1). Here and elsewhere when the symbols $\pm$ and $\mp$ are used it is understood that the top sign pertains to (1.1) in the $+q$ case and the lower sign to the $-q$ case.] Below we will say more about the distinctions among these four cases.

The system (1.1) is often referred to as the Zakharov–Shabat system, following the original work of Zakharov and Shabat[23] showing that the Cauchy problem for the cubic Schrödinger equation,

$$i\Psi_t = \Psi_{xx} \mp \Psi^2\Psi^*, \tag{1.6}$$

can be solved by means of an inverse scattering transform based on $\mathbf{P2}_{\pm}$. In Ref. 23 the spatial domain $[0,X]$ is replaced by $\mathbb{R}$, but if q in $\mathbf{P2}_{\pm}$ is extended to be 0 outside of $[0,X]$ then the problem coincides with that of Ref. 23. This theory has been elaborated in many books and papers; see, e.g., Refs. 1, 5, 20, 23, 24. See also Ref. 3 for a generalization of the $+q$ case to a $2N$ component system. The system (1.1) also arises in the description of the propagation of coupled

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modes of electromagnetic waves in a waveguide. When the coefficient in the second equation is $+q$ one has the so-called contra-directional case, while $-q$ is the co-directional case. We mention also that (1.1) is related by a simple change of variables to the Dirac system for which direct and inverse scattering theory is of interest; see, for example, Refs. 6, 12.

The main motivation for the study of $\mathbf{P1}_-$ is the works,[11,13] in which this problem arises in connection with the design of optical fiber devices with certain prescribed properties. In this paper we will allow both choices of sign in (1.1) since it seems to be conventional in the literature to do so, and is of mathematical interest, but we do not know of any specific application for $\mathbf{P1}_+$. Problem $\mathbf{P2}_\pm$ has arisen in a larger number of recent works concerned with the design of fiber gratings (e.g., Refs. 9, 15, 19, 20, 22; see also Ref. 17 for a corresponding time domain problem), the $+$ sign being usually the physically significant case here. As mentioned above, $\mathbf{P2}_\pm$ is by now fairly well understood from a theoretical point of view—these papers are more concerned with computational issues.

Let us emphasize, however, that in the sort of application just mentioned, the questions of ultimate importance have to do with the *design* of the coupling coefficient q rather than *reconstruction* of q. The literature on inverse scattering is concerned almost entirely with reconstruction, so that uniqueness of solutions and, to a somewhat lesser extent, characterization of the data for which a solution exists, are the principal concerns. By contrast in a design problem we seek to choose a coefficient q so as to obtain a physical system with prescribed properties, and in many cases these are idealized properties which are not physically realizable. [For example, $B(X,k) \equiv 0$ outside of some k interval.] From the mathematical point of view it means we are given data for which no solution exists, and we attempt to find a solution anyway—or, less facetiously, obtain an ''optimal'' solution in some sense. There seems to be very little mathematical analysis of the design problem from this point of view (see, e.g., Ref. 10 for some such work), even for the simpler case of Schrödinger scattering and none will be given in this paper either. However we do believe this is an important problem for future investigation, and that the material in this paper on the reconstruction problem for $\mathbf{P1}_\pm$ will be useful for that.

To conclude this Introduction we discuss the difference in character between problems $\mathbf{P1}_\pm$ and $\mathbf{P2}_\pm$, due to the different side conditions. In certain cases (see Sec. III) there is an exact correspondence to an inverse scattering problem for a potential $V(x)$ in the more familiar Schrödinger equation. The case of $\mathbf{P2}_\pm$ corresponds to data being $L(k)$, the left hand reflection coefficient (see below for a review of the definitions) whereas in the case of $\mathbf{P1}_\pm$ the data amounts to $L(k)/T(k)$, the ratio of the reflection coefficient to the transmission coefficient. The use of L/T as basic scattering data, in the case of a real V, has appeared in a few previous papers (Refs. 16, 18), but usually in a somewhat artificial way. Here it seems that there is a clear physical motivation. In the Schrödinger scattering case it is not difficult to show that L/T uniquely determines L and hence the potential, at least if there are no bound states (see Ref. 4 for a careful study of multiplicity results when bound states are allowed), and we will derive the analogous result for $\mathbf{P1}_\pm$. The proof relies on analytic continuation, and thus does not immediately show how known numerical techniques for $\mathbf{P2}_\pm$ could be adapted to $\mathbf{P1}_\pm$. From another point of view the inverse problem $\mathbf{P2}_\pm$ is ''local in depth,'' whereas $\mathbf{P1}_\pm$ is not, meaning that layer stripping type methods cannot be used, at least in any direct way. One alternative computational approach, somewhat analogous to Ref. 18, will be discussed in Sec. VII.

II. CONSERVATION OF ENERGY AND BOUND STATES

Clearly a solution of (1.1), (1.2) exists on $[0,X]$ for any $k \in \mathbb{C}$. Extending q by zero for $x \notin [0,X]$ we may assume when convenient that $A(x,k), B(x,k)$ are defined for all $x \in \mathbb{R}, k \in \mathbb{C}$. If we let

$$E(x,k) = (|A(x,k)|^2 \mp |B(x,k)|^2), \tag{2.1}$$

then a simple calculation gives

$$\frac{\partial E}{\partial x} = i(k-k^*)(|A(x,k)|^2 \pm |B(x,k)|^2). \tag{2.2}$$

In particular for $k \in \mathbb{R}$,

$$|A(X,k)|^2 \mp |B(X,k)|^2 \equiv 1. \tag{2.3}$$

A bound state of (1.1) is a nonzero solution of (1.1) for some fixed $k \in \mathbb{C}$ with $A(\cdot,k), B(\cdot,k) \in L^2(\mathbb{R})$. Such solutions are impossible in the $+q$ case of (1.1) since by (2.2) and the fact that E must be exponentially decaying at $\pm\infty$ we must have $\operatorname{Im} k \neq 0$ and

$$0 = \int_{-\infty}^{\infty} \frac{\partial E}{\partial x}(x,k)\, dx = i(k-k^*) \int_{-\infty}^{\infty} (|A(x,k)|^2 + |B(x,k)|^2)\, dx. \tag{2.4}$$

In the $-q$ case bound states may exist, although only for sufficiently large q. This is in contrast to the standard Schrödinger scattering case in which any potential $V(x) \leqslant 0, V(x) \not\equiv 0$ has at least one bound state. As is well known, it is the existence of such bound states which give rise to the existence of solitary wave solutions of the cubic Schrödinger equation (1.6).

It is easy to check that if $\operatorname{Im} k < 0$ and $A(X,k) = 0$ then both components are either identically zero or exponentially decaying at both $\pm\infty$, hence $\{A(x,k), B(x,k)\}$ is a bound state.

III. RELATION TO OTHER FORMS OF SCATTERING DATA

Consider the special case that $\pm q = q^*$, i.e., q is real in the $+q$ case or imaginary in the $-q$ case. If we set $\psi = A + B$ then straightforward computation gives

$$\psi'' + (k^2 - V(x))\psi = 0, \tag{3.1}$$

where $V = \pm q' + q^2$, a Schrödinger equation with (possibly complex) potential V.

Proceeding as in the case of a real potential (e.g., Refs. 5, 7, 8) we introduce the standard fundamental set of solutions ψ_-, ψ_+ of (3.1) which satisfy

$$\psi_-(x,k) = \begin{cases} e^{ikx} + L(k)e^{-ikx}, & x < 0, \\ T(k)e^{ikx}, & x > X; \end{cases} \tag{3.2}$$

$$\psi_+(x,k) = \begin{cases} T(k)e^{-ikx}, & x < 0, \\ e^{-ikx} + R(k)e^{ikx}, & x > X; \end{cases} \tag{3.3}$$

where L, R are left and right hand reflection coefficients and T is the transmission coefficient. (It may be checked that even in the case of complex V, the left and right transmission coefficients coincide.)

From (1.2) we clearly have

$$A(x,k) = e^{ikx}, \quad B(x,k) = 0, \quad x < 0, \tag{3.4}$$

and

$$B(x,k) = B(X,k)e^{-ik(x-X)}, \quad A(x,k) = A(X,k)e^{ik(x-X)}, \quad x > X. \tag{3.5}$$

From (3.4) it follows that

$$\psi(x,k) = \psi_-(x,k) - \frac{L(k)}{T(k)}\psi_+(x,k), \tag{3.6}$$

so that

$$\psi(x,k)=\left(T(k)-\frac{L(k)R(k)}{T(k)}\right)e^{ikx}-\frac{L(k)}{T(k)}e^{-ikx},\quad x>X. \tag{3.7}$$

From this and (3.5) then

$$A(X,k)=e^{ikX}\left(T(k)-\frac{L(k)R(k)}{T(k)}\right),\quad B(X,k)=-e^{-ikX}\frac{L(k)}{T(k)}. \tag{3.8}$$

At least in the case of real q, the expression for $A(X,k)$ can be further simplified, using standard identities for Schrödinger scattering, to

$$A(X,k)=\frac{e^{ikX}}{T(k)^*},\quad k\in\mathbb{R}. \tag{3.9}$$

The inverse problem $\mathbf{P1}_{\pm}$ thus corresponds, in such a case, to Schrödinger inverse scattering in which the available data is the ratio L/T of a reflection and transmission coefficient. By comparison, the data for problem $\mathbf{P2}_{\pm}$ would be simply $L(k)$, by a similar calculation, and so amounts to a familiar problem. It is well known (e.g., Refs. 5, 7, 8) that a real V is uniquely determined by $L(k)$ if no bound states are present.

IV. UNIQUENESS

In the Schrödinger scattering case, when V has no bound states it is not hard to see that L/T uniquely determines L and hence V. Uniqueness for $\mathbf{P1}_{\pm}$ amounts to essentially the same thing for the system (1.1).

Theorem 1: *There is at most one solution of* $\mathbf{P1}_{+}$, *and the same is true of* $\mathbf{P1}_{-}$ *if there are no bound states*.

Proof: First note from (2.3) that $|A(X,k)|$ is known from the data, and it is not hard to check that

$$A(X,k)=a^*(k^*)e^{ikX}, \tag{4.1}$$

where $a(k)$ is defined in Eq. (1.3.3a) in Ref. 1 (again with the understanding that q has been extended by zero outside of $[0,X]$). The function a is entire and $a(k)\to 1$ as $|k|\to\infty$ in the upper half plane.

Recall from Sec. II that there can be no bound states in the case of $\mathbf{P1}_{+}$, and the same is true in the case of $\mathbf{P1}_{-}$ by hypothesis. From the last remark in Sec. II it follows that $A(X,k)$ has no zeros in the lower half of the complex plane. Thus $g(k):=\log(A(X,k)e^{-ikX})$ is analytic in the lower half plane and tends to zero as $|k|\to\infty$. It follows by the usual Hilbert transform relation that the imaginary part of g on the real axis is uniquely determined by its real part, that is to say, the phase of $A(X,k)$ may be determined from $|A(X,k)|$, and so $A(X,k)$ is itself known. Finally one may check that

$$\{A(X-x,-k)/A(X,-k),-B(X-x,-k)/A(X,-k)\} \tag{4.2}$$

is a solution pair of (1.1) with $q(x)$ replaced by $q(x-X)$, satisfying side conditions (1.4) and having known scattering data (1.5). Thus q is uniquely determined according to the standard results about problems $\mathbf{P2}_{\pm}$. □

In the Schrödinger scattering case it is known (e.g., Theorem 2.3 of Ref. 18) that L/T does not uniquely determine the potential in the presence of bound states, hence we expect that the ''no bound state'' hypothesis in the case of $\mathbf{P1}_{-}$ cannot be dispensed with. Numerical examples (see Sec. VII below) also indicate this quite clearly. On the other hand in the more conventional case of Schrödinger scattering with data L, even though bound state data is needed in general to

uniquely determine a potential, this is not the case if V is known to be supported in a half line (Refs. 2, 14), i.e., $L(k)$ alone suffices to determine V in such a case. We conjecture that the same is true for $\mathbf{P2}_-$.

V. TIME DOMAIN PROBLEM

It is well known that problem $\mathbf{P2}_\pm$ can be analyzed in terms of an associated hyperbolic ''time domain'' problem, which is recalled in (6.2) below; see, e.g., Refs. 9, 17, 19, 20. Here we derive a corresponding hyperbolic problem (5.15) for $\mathbf{P1}_\pm$. We remark that in the case of $\mathbf{P2}_\pm$ the derivation of (6.2) requires an assumption that there be no bound states, but this hypothesis is not needed in the case of (5.15).

Let $\{a(x,t),b(x,t)\}$ denote solutions of the hyperbolic problem in $\mathbb{R}^2$,

$$a_t+a_x=q^*(x)b, \quad b_t-b_x=\mp q(x)a, \tag{5.1}$$

$$a(0,t)=\delta(t), \quad b(0,t)=0. \tag{5.2}$$

Regarding this as an evolution equation in the space variable x we see by the standard domain of dependence considerations that the support of the solution is in the triangle $\{(x,t):|t|\leqslant x<X\}$. Taking the Fourier transform in t, using the convention

$$\hat{f}(k)=\int_{-\infty}^{\infty} f(t)e^{ikt}\,dt, \tag{5.3}$$

we find that

$$-ik\hat{a}+\hat{a}_x=q^*\hat{b}, \quad -ik\hat{b}-\hat{b}_x=\mp q\hat{a} \tag{5.4}$$

and

$$\hat{a}(0,k)=1, \quad \hat{b}(0,k)=0. \tag{5.5}$$

That is to say $A(x,k)=\hat{a}(x,k), B(x,k)=\hat{b}(x,k)$ is the solution of (1.1), (1.2), since the solution is unique.

By a standard propagation of singularity (geometric optics) arguments, we may obtain equivalent characteristic boundary conditions for a,b. The solution with $q\equiv 0$ is $a(x,t)=\delta(x-t), b(x,t)=0$, thus near the characteristic $t=x$ we should have

$$a(x,t)=\delta(x-t)+\alpha(x)H(x-t)+ \text{ smoother terms}, \tag{5.6}$$

$$b(x,t)=\beta(x)H(x-t)+ \text{ smoother terms}, \tag{5.7}$$

where H denotes the unit step function and α, β are transport coefficients to be determined. Inserting these expansions into (5.1) and matching the coefficients of the most singular terms we get

$$\alpha(x)=\pm\frac{1}{2}\int_0^x |q(s)|^2\,ds, \quad \beta(x)=\pm\frac{1}{2}q(x). \tag{5.8}$$

When we carry out a similar calculation on the lower characteristic $t=-x$, substituting

$$a(x,t)=\alpha(x)H(x+t)+ \text{ smoother terms}, \tag{5.9}$$

$$b(x,t)=\beta(x)H(x+t)+ \text{ smoother terms}, \tag{5.10}$$

the relations

$$\alpha(x)=0, \quad -\beta'(x)=\mp q(x)\alpha(x) \tag{5.11}$$

are obtained. Thus

$$\alpha(x)=0, \quad \beta(x)=\beta(0), \tag{5.12}$$

and the continuity of a,b from inside the cone $|t|<x$ then gives

$$\beta(0)=\pm\tfrac{1}{2}q(0). \tag{5.13}$$

Note that

$$A(X,k)=\int_{-X}^{X}a(X,t)e^{ikt}\,dt, \quad B(X,k)=\int_{-X}^{X}b(X,t)e^{ikt}\,dt, \tag{5.14}$$

from which it follows that $A(X,\cdot),B(X,\cdot)$ are bandlimited functions, hence uniquely determined by appropriate sampling.

We may now reformulate the inverse problem $\mathbf{P1}_{\pm}$ as an overdetermined boundary value problem: If $B(X,k)$ is the data corresponding to q then there exist $\{a(x,t),b(x,t)\}$ such that

$$a_t+a_x=q^*(x)b, \quad b_t-b_x=\mp q(x)a, \quad |t|<x<X, \tag{5.15a}$$

$$b(x,x)=\pm\frac{1}{2}q(x), \quad 0<x<X, \tag{5.15b}$$

$$a(x,-x)=0, \quad 0<x<X, \tag{5.15c}$$

$$b(X,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}B(X,k)e^{-ikt}\,dk, \quad |t|<X. \tag{5.15d}$$

Note that the additional characteristic boundary conditions,

$$a(x,x)=\pm\frac{1}{2}\int_{0}^{x}|q(s)|^2\,ds, \quad b(x,-x)=\pm\frac{1}{2}q(0), \quad 0<x<X, \tag{5.16}$$

follow from (5.15), consistently with the expressions for $\alpha(x)$ in (5.8) and $\beta(x)$ in (5.12).

VI. NONLINEAR PLANCHEREL IDENTITY

In the context of inverse scattering for the Helmholtz equation, Sylvester, Winebrenner, and Gylys-Colwell[21] discovered an interesting identity relating the L^2 norm of the coefficient to a certain nonlinear functional of the scattering data. It was referred to as a nonlinear Plancherel identity because in the weak scattering limit, the coefficient to data mapping becomes the Fourier transform, and so the identity in question goes over to the classical Plancherel equality. In this section we will state and prove an analogous property for the inverse scattering problem $\mathbf{P1}_{\pm}$. For the proof we will need a corresponding result for $\mathbf{P2}_{\pm}$, which as far as we know is also new, although the proof follows closely the pattern of Ref. 21.

Before proceeding let us note that if we set $R(x,k)=B(x,k)/A(x,k)$ then it is easy to check that R satisfies the Riccati type equation,

$$\frac{\partial R}{\partial x}=-2ikR(x,k)-q^*(x)R(x,k)^2\pm q(x), \tag{6.1}$$

at least provided that $A(x,k)\neq 0$. Numerical methods for $\mathbf{P2}_{\pm}$ have been developed which exploit (6.1) and the fact that $R(0,k),R(X,k)$ are known from the data and side conditions (Refs. 9, 19). For $\mathbf{P1}_{\pm}$, however, we only know that $R(0,k)=0$ and have no explicit way to obtain $R(X,k)$.

We also will make use of the analog of (5.15) for $\mathbf{P2}_{\pm}$ which is the following: If $B(0,k)$ is the data corresponding to q there exists $\{a(x,t),b(x,t)\}$ such that

$$a_t+a_x=q^*(x)b, \quad b_t-b_x=\mp q(x)a, \quad 0<x<t, \tag{6.2a}$$

$$b(x,x)=\mp\frac{1}{2}q(x), \quad x>0, \tag{6.2b}$$

$$a(0,t)=0, \quad t>0, \tag{6.2c}$$

$$b(0,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}B(0,k)e^{-ikt}\,dk, \quad t>0. \tag{6.2d}$$

Here we are again regarding $q(x)$ as defined to be zero outside of $[0,X]$. In the case of $\mathbf{P2}_{-}$ we must assume in addition that no bound states exist, so that $b(0,t)$ is Fourier transformable with respect to time. This solution corresponds to (5.1) with side conditions

$$a(x,t)=\delta(x-t), \quad b(x,t)=0, \quad t<0, \tag{6.3}$$

and may be derived in a manner analogous to (5.15). See also Refs. 17, 20 for more about (6.2). In particular $\{a,b\}$ may be viewed as a solution of (6.2a) for all t, which is zero for $t<x$. Since $b(0,t)=0$ for $t<0$ it follows that $B(0,k)$ is analytic in the upper half of the complex plane.

Theorem 2: *In the case of problem* $\mathbf{P2}_{+}$ *we have*

$$-\int_{-\infty}^{\infty}\log(1-|B(0,k)|^2)\,dk=\pi\int_0^X|q(x)|^2\,dx, \tag{6.4}$$

and in the case of problem $\mathbf{P1}_{+}$ *we have*

$$\int_{-\infty}^{\infty}\log(1+|B(X,k)|^2)\,dk=\pi\int_0^X|q(x)|^2\,dx. \tag{6.5}$$

Proof: First consider the case of $\mathbf{P2}_{+}$. Note from (2.1), (2.2) that $|A(x,k)|^2-|B(x,k)|^2$ is equal to the constant $|A(X,k)|^2$ for real k; hence $A(x,k)=0$ is impossible for $k\in\mathbb{R}$ or $x\in[0,X]$. Now multiply (6.1) by $R(x,k)^*$ to get

$$R(x,k)^*\frac{\partial R}{\partial x}(x,k)=-2ik|R(x,k)|^2-q^*(x)R(x,k)|R(x,k)|^2+q(x)R(x,k)^*. \tag{6.6}$$

Taking the real part of this identity gives

$$\frac{\partial}{\partial x}|R(x,k)|^2=2(1-|R(x,k)|^2)\,\mathrm{Re}\,(q^*(x)R(x,k)) \tag{6.7}$$

or

$$-\frac{\partial}{\partial x}\log(1-|R(x,k)|^2)=2\,\mathrm{Re}\,(q^*(x)R(x,k)). \tag{6.8}$$

We next claim that

$$\int_{-\infty}^{\infty} R(x,k)\,dk = -\frac{\pi}{2} q(x), \quad 0 \leqslant x \leqslant X. \tag{6.9}$$

Given this, we integrate both sides of (6.8) with respect to k to get

$$\frac{\partial}{\partial x} \int_{-\infty}^{\infty} \log(1-|R(x,k)|^2)\,dk = \pi |q(x)|^2. \tag{6.10}$$

Finally integrate with respect to x from 0 to X, using the fact that $R(0,k)=B(0,k)$, $R(X,k)=0$ to obtain (6.4).

To verify the claim (6.9), consider first the case $x=0$ in which case $R(0,k)=B(0,k)$, the Fourier transform of $b(0,t)$. Since $b(0,0+)=\lim_{t\to 0+} b(0,t) = -q(0)/2$ and $b(0,0-) = \lim_{t\to 0-} b(0,t)=0$, it follows that $1/2\pi \int_{-\infty}^{\infty} B(0,k)$; the inverse Fourier transform of $B(0,k)$ evaluated at $t=0$ is the average of the one sided limits of $b(0,t)$, i.e.,

$$\int_{-\infty}^{\infty} R(0,k)\,dk = \int_{-\infty}^{\infty} B(0,k) = 2\pi\left(-\frac{q(0)}{4}\right), \tag{6.11}$$

which is the required result.

Now for any fixed $x_0 \in [0,X]$ it is not hard to check that $R(x_0,k)=\tilde{B}(x_0,k)$ where $\tilde{A},\tilde{B}$ solves

$$\tilde{A}' = ikA + q^*\tilde{B}, \quad \tilde{B}' = -ikB + q\tilde{A}, \quad x_0 < x < X, \tag{6.12}$$

$$\tilde{A}(x_0,k)=1, \quad \tilde{B}(X,k)=0. \tag{6.13}$$

The argument in the previous paragraph shows that $\int_{-\infty}^{\infty} \tilde{B}(x_0,k)\,dk = -(\pi/2)\,q(x_0)$ and so (6.9) follows for all $x \in [0,X]$.

In the case of problem $\mathbf{P1}_+$, if $A(x,k),B(X,k)$ is the solution of (1.1), (1.2), and

$$A_1(x,k) = \frac{A(X-x,-k)}{A(X,-k)}, \quad B_1(x,k) = -\frac{B(X-x,-k)}{A(X,-k)}; \tag{6.14}$$

then one easily checks that $A_1(x,k),B_1(x,k)$ satisfies (1.1), (1.4) with coefficient $q(x)$ replaced by $q_1(x)=q(X-x)$. From the first part of the proof it then follows that

$$\begin{aligned}
\pi \int_0^X |q(x)|^2\,dx &= \pi \int_0^X |q_1(x)|^2\,dx \\
&= -\int_{-\infty}^{\infty} \log(1-|B_1(0,k)|^2)dk \\
&= -\int_{-\infty}^{\infty} \log(1-|R(X,k)|^2)dk \\
&= -\int_{-\infty}^{\infty} \log\left(\frac{1}{1+|B(X,k)|^2}\right)dk,
\end{aligned} \tag{6.15}$$

where in the last equality we used the conservation property (2.3). The conclusion (6.5) follows.□

Using the elementary inequalities $\log(1+r) \leqslant r, r \geqslant 0$ and $r \leqslant -\log(1-r)$ for $0 \leqslant r \leqslant 1$ and the fact that $|B(0,k)| \leqslant 1$ in $\mathbf{P2}_+$ we obtain the immediate corollaries,

$$\int_{-\infty}^{\infty} |B(X,k)|^2\,dk \geqslant \pi \int_0^X |q(x)|^2\,dx, \tag{6.16}$$

in the case of $\mathbf{P2}_+$ and

$$\int_{-\infty}^{\infty} |B(0,k)|^2\, dk \leqslant \pi \int_0^X |q(x)|^2\, dx, \tag{6.17}$$

in the case of $\mathbf{P1}_+$.

Similar properties can be proved for problems $\mathbf{P1}_-$, $\mathbf{P2}_-$ with further restrictions.

Theorem 3: *Assume that there are no bound states and that* $A(x,k) \neq 0$ *for* $x \in [0,X]$ *and* $k \in \mathbb{R}$. *Then in the case of problem* $\mathbf{P2}_-$ *we have*

$$\int_{-\infty}^{\infty} |B(0,k)|^2\, dk \geqslant \int_{-\infty}^{\infty} \log(1+|B(0,k)|^2)\, dk = \pi \int_0^X |q(x)|^2\, dx, \tag{6.18}$$

and in the case of problem $\mathbf{P1}_-$ *we have*

$$\int_{-\infty}^{\infty} |B(X,k)|^2\, dk \leqslant -\int_{-\infty}^{\infty} \log(1-|B(X,k)|^2)\, dk = \pi \int_0^X |q(x)|^2\, dx. \tag{6.19}$$

VII. CONSTRUCTIVE METHODS

A simple approximate solution for $\mathbf{P2}_\pm$ which may nevertheless be quite accurate for sufficiently small q's is the Born approximation. If we replace q by $q_0 + \epsilon q_1$ with corresponding solutions $A_0 + \epsilon A_1, B_0 + \epsilon B_1$ and match powers of ϵ we get $A_0(x,k) = e^{ikx}, B_0(x,k) = 0$ and

$$B_1' + ikB_1 = \pm q(x) e^{ikx}. \tag{7.1}$$

Solving with $B_1(0,k) = 0$ leads to

$$B_1(X,k) = \pm e^{-ikX} \int_0^X q(s) e^{2iks}\, ds, \tag{7.2}$$

and so by Fourier inversion,

$$q(x) \approx \pm \frac{1}{\pi} \int_{-\infty}^{\infty} B(X,k) e^{-ik(2x-X)}\, dk. \tag{7.3}$$

The same result may be obtained by ignoring the quadratic term in (6.1), or from (5.15) as explained below. This formula is exploited in Ref. 11 (also Ref. 22 in the case of $\mathbf{P2}_\pm$). An improved method based on the calculation of transfer matrices for piecewise constant q is presented in Ref. 13.

Several types of exact methods may be derived by first transforming the data for $\mathbf{P1}_\pm$ to that of $\mathbf{P2}_\pm$, in the manner indicated by the proof of the uniqueness result Theorem 1. From the data and (2.3) one may obtain $|A(X,k)|$; a Hilbert transform calculation of $\log|A(X,k)|$ then yields $A(X,k)$ from which we obtain data for a reflected version of $\mathbf{P2}_\pm$, according to (4.2). One can then proceed to use one of the methods which have been developed for a numerical solution of $\mathbf{P2}_\pm$, e.g., Refs. 9, 15, 19, 20. For this transformation it is necessary to assume that there are no bound states. Furthermore the Hilbert transform step may present numerical difficulties if $B(X,k)$ is known only on a coarse grid of k values, whereas coarse sampling need not in itself be a problem due to the bandlimitation property of $B(X,k)$ discussed above.

A final possibility for an exact method which we discuss in more detail is based on the equivalent time domain problem (5.15). Let us define the mapping $q \mapsto \Lambda(q)$ by $\Lambda(q)(t) = b(X,t), |t| < 1$ where $\{a(x,t), b(x,t)\}$ is the solution pair of the well-posed characteristic boundary value problem, (5.15a)–(5.15c). We may then attempt to obtain q as the solution of the nonlinear operator equation,

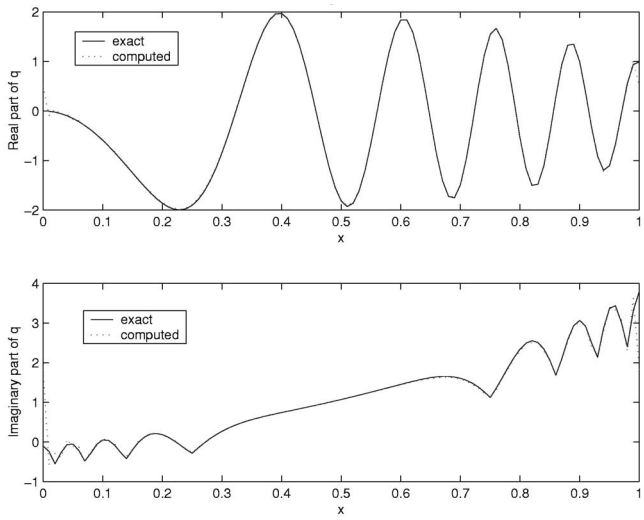

FIG. 1. Reconstruction of real and imaginary parts of smaller coupling coefficient $q(x)$ in **P1**$_-$ by the iteration scheme (7.8).

$$\Lambda(q)=g, \tag{7.4}$$

where $g(t)=b(X,t)$ is known from the given data. Recalling that $b(X,t)$ has support in $[-X,X]$ it follows from (5.14) that we may represent g as a Fourier series,

$$b(X,t)=\frac{1}{2X}\sum_{n=-\infty}^{\infty} B\left(X,\frac{n\pi}{X}\right)e^{-in\pi t/X}, \tag{7.5}$$

involving only sampled values of $B(X,k)$. Of course in theory $b(X,t)$ is uniquely determined by the data $\{B(X,k_n)\}_{n=1}^{\infty}$ where k_n is any sequence with a finite limit point, or a sequence tending to $\pm\infty$ with an appropriate asymptotic spacing. The coefficients in (7.5) will typically decay at a rate $O(1/n)$ and no faster, unless additional smoothness assumptions are made on q (or more presicely on the X periodic extension of q).

A simple iterative scheme is the Newton–Kantorovich method,

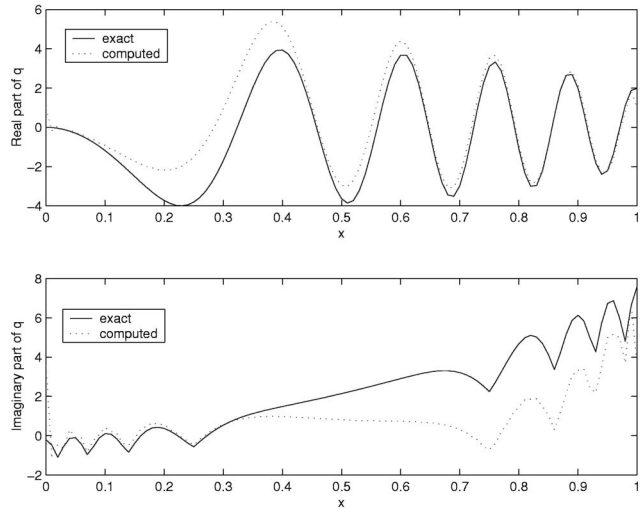

FIG. 2. Reconstruction of real and imaginary parts of larger coupling coefficient $q(x)$ in **P1**$_-$ by the iteration scheme (7.8).

$$q_{n+1}=q_n-D\Lambda(0)^{-1}(\Lambda(q_n)-g), \tag{7.6}$$

where the Fréchet derivative $D\Lambda(0)$ is easily found to be

$$D\Lambda(0)\zeta(t)=\pm\frac{1}{2}\zeta\left(\frac{X+t}{2}\right). \tag{7.7}$$

The resulting scheme is thus explicitly

$$q_{n+1}(x)=q_n(x)\pm 2g(2x-X)\mp 2\Lambda(q_n)(2x-X), \tag{7.8}$$

initialized, for example, by $q_0(x)=0$, in which case $q_1(x)=D\Lambda(0)^{-1}g(x)=\pm 2g(2x-X)$ is the same as the Born approximation mentioned above, which could also be used as the initial guess.

If the coupling coefficient q is sufficiently small then convergence of q_n to q in $L^2(0,X)$ can be shown, essentially by the inverse function theorem and the fact that Λ can be shown to have suitable differentiability properties. The proof is very similar, e.g., to that of Corollary 3.1 of Ref. 18.

In general the scheme is not globally convergent. In the case of $\mathbf{P1}_+$ the inverse problem has a unique solution which must also be the unique solution of $\Lambda(q)=g$, so if the sequence q_n converges at all then it must be to the solution q. In the case of $\mathbf{P1}_-$ the solution is not unique in general, so the sequence q_n may converge to some other solution of the inverse problem.

In Fig. 1 a reconstruction is displayed together with the exact coupling coefficient for $\mathbf{P1}_-$. In this example $X=1$, and the data $B(1,n\pi)$ is used for $|n|\leqslant 50$ to approximate $b(1,t)$ using (7.5). The direct problem (1.1)–(1.2) was solved using ode45 in MATLAB, and the time domain map Λ was approximated by means of a straightforward finite difference scheme in characteristic coordinates, with grid size extrapolation to improve the accuracy. The relative error in q is about 15%, but essentially all of this may be attributed to the error in $b(1,t)$ due to the truncation error in (7.5). That is to say, if we used more (or fewer) terms we will always find that the relative error in the computed q is comparable to the relative error in $b(1,t)$. The results are very similar if we repeat the calculation for $\mathbf{P1}_+$.

For a second example we replace q in the previous case by $2q$. We now find that the sequence q_n does not converge at all in the case of $\mathbf{P1}_+$, while in the case of $\mathbf{P1}_-$ the sequence converges, but to a different solution displayed in Fig. 2, consistent with the earlier discussion of nonuniqueness. It seems clear that some alternative optimization approach could be used to obtain the original q, provided a sufficiently accurate initial guess were available. We note that in the first example the identity (6.19) is satisfied, while in the second example it is satisfied by the computed $q(x)$, not by the original q, leading one to surmise that the result of the computational method just described will be the unique choice of q with the prescribed data (1.3) but with no bound states.

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Comment on "Two-dimensional, highly directive currents on large circular loops" [J. Math. Phys. 41, 6130 (2000)]

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Margetis and Fikioris, apparently unaware of the earlier results available in the literature, used an elaborate Mellin transform technique to obtain an asymptotic approximation for a particular case of a Bessel function integral. Here, the earlier, more general results are pointed out. © *2004 American Institute of Physics.*
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In Sec. III of a recent paper, Margetis and Fikioris[1] use the Mellin transform technique to obtain an asymptotic expansion up to the order $O(\lambda^{-7/2})$ for the particular case $\mu=\nu=0$ of the integral

$$I(\lambda)=\int_0^{\pi/2} J_\mu(\lambda \sin\theta) J_\nu(\lambda \sin\theta) d\theta, \tag{1}$$

where J_μ is the μth-order Bessel function of the first kind and λ is a large parameter tending to infinity. Their application of this technique, which is elaborated in Ref. 13 of their paper,[1] differs in many technical details from the earlier work (see below), where the Mellin transforms were applied to more general cases of integral (1). A major difference that should be noted here is a clever use by Margetis and Fikioris[1] of an integration path in the complex θ-plane in order to obtain the contributions oscillatory in λ, which arise from the upper limit of integration in (1).

An asymptotic expansion of integral (1) up to the order $O(\lambda^{-3/2})$ for the particular $\mu=\nu=0$ case was originally obtained by Stoyanov and Farrell[2] by a straightforward method based on a heuristic approach. Referring to their paper,[2] Margetis and Fikioris[1] remark that "These authors calculate only the first three terms of the asymptotic expansion [...]. Their method does not make use of the Mellin transform technique." We point out that the Mellin transform technique was previously used by Wong[3,4] to obtain the asymptotic expansion up to the order $O(\lambda^{-3})$ for a more general case $\mu=\nu>-1/2$ of integral (1). Then, Stoyanov, Farrell, and Bird[5] used both the straightforward method originally introduced in Ref. 2 and the Mellin-transform technique with certain simplifications and modifications to obtain the asymptotic expansions to the same order for the general case $\mathrm{Re}(\mu+\nu)>-1$ of integral (1), as well as for another, Hankel-type integral. Furthermore, the complete (i.e., infinite) asymptotic expansions for the two integrals treated in Ref. 5 have also been obtained by Stoyanov, Farrell, and Bird[6] by using the generalized hypergeometric and Meijer functions.

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Supersymmetric exact sequence, heat kernel and super Korteweg–de Vries hierarchy

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We introduce the free $N=1$ supersymmetric derivation ring and prove the existence of an exact sequence of supersymmetric rings and linear transformations. We apply necessary and sufficient conditions arising from this exact supersymmetric sequence to obtain the essential relations between conserved quantities, gradients and the $N=1$ super Korteweg–de Vries (KdV) hierarchy. We combine this algebraic approach with an analytic analysis of the super heat operator. We obtain the explicit expression for the Green's function of the super heat operator in terms of a series expansion and discuss its properties. The expansion is convergent under the assumption of bounded bosonic and fermionic potentials. We show that the asymptotic expansion when $t\to 0^+$ of the Green's function for the superheat operator evaluated over its diagonal generates all the members of the $N=1$ super KdV hierarchy. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1650047]

I. INTRODUCTION

The analysis of supersymmetric quantum problems has been recently considered in several relevant physical contexts. At very high energies one way of studying the M-theory, which has been proposed as a theory of unification of all known interactions in nature, is through Matrix models describing supersymmetric quantum problems. The supersymmetry is one of the relevant ingredients of these models. In particular the presence of supersymmetry may change completely the spectrum of the quantum Hamiltonian. The bosonic Hamiltonian in the case of the $D=11$ supermembrane, with Minkowski target space, has a discrete spectrum while its supersymmetric extension has a continuous spectrum. Moreover in that case the Green's function does not admit a representation in terms of the Feynman path integral since the potential is not bounded from below in some directions in spite of the fact that the SUSY Hamiltonian is nonnegative. These systems are very closely related to certain supersymmetric integrable systems. These models in themselves are a great help in understanding integrable systems. The $N=1,2$ supersymmetric extensions of the Korteweg–de Vries (KdV) equations were found several years ago,[1–4] while $N=3$ and $N=4$ have been considered more recently in Refs. 5, 6, 7. The bi-Hamiltonian structure of the super KdV equations was studied in Refs. 8, 9. For a review of $N=1$ and $N=2$ super KdV equations see Ref. 10. Extensions of the supersymmetric model have been proposed in Ref. 11.

In the first part of this work we focus on the algebraic structure of $N=1$ supersymmetric

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models. We introduce the ''Free SUSY derivation ring on a single fermionic generator'' which contains a parity automorphism, a canonical superderivation and a supersymmetric gradient operator. We established an exact sequence of SUSY rings and linear transformations. Several of these relations were already known in the literature.[2,12] This is a general algebraic construction valid for one-dimensional supersymmetric models. Using necessary and sufficient conditions arising from the exact sequence we obtain the essential relations between conserved quantities, gradients and the $N=1$ SKdV hierarchy. In the second part of this work we use the exact sequence together with an analytic analysis of the super heat kernel to show that the asymptotic expansion when $t\to 0^+$ of the Green's function for the superheat operator, evaluated over its diagonal, generates all the left hand members of the SKdV hierarchy. Using the symmetry properties of that Green's function we obtain an iterative procedure to obtain all the gradients and members of the SKdV hierarchy. The algebraic approach arising from the exact SUSY sequence together with the analytic approach arising from the analysis of the Green's function of the super heat operator combine to give a satisfactory description of the SKdV hierarchy.

II. THE FREE SUPERSYMMETRIC DERIVATION RING ON A SINGLE FERMIONIC GENERATOR

A. Definitions

A ring $\mathcal{A}$ is associative but not necesarily commutative. It is ''oriented'' when there is given a ring automorphism $P:\mathcal{A}\to\mathcal{A}$ satisfying $P^2=I$, as well as $P(f+g)=Pf+Pg$ and $P(fg)=(Pf)(Pg)$. An element f of $\mathcal{A}$ is ''oriented'' when $Pf=\pm f$, f being called ''bosonic'' when $Pf=f$ and ''fermionic'' when $Pf=-f$. The oriented ring $(\mathcal{A},P)$ is said to be ''commutative'' when

$$fg=gf(-1)^{\sigma\tau}$$

wherever $f,g\in\mathcal{A}$ satisfy $Pf=(-1)^{\sigma}f$, $Pg=(-1)^{\tau}g$. In this situation the commutation formula,

$$uf=f(P^{\sigma}u),$$

holds for all $u\in\mathcal{A}$, given that $Pf=(-1)^{\sigma}f$; this follows from $u=u_0+u_1=\text{boson}+\text{fermion}$. A linear map $D:\mathcal{A}\to\mathcal{A}$ is called an ''ordinary derivation'' when

$$DP=PD,$$

$$D(uv)=(Du)v+u(Dv),$$

for all $u,v\in\mathcal{A}$, and is called a ''superderivation'' when

$$DP=-PD,$$

$$D(uv)=(Du)v+(Pu)(Dv).$$

The two definitions may be combined by saying that $\Pi(D)=(-1)^{\delta}$ when

$$DP=(-1)^{\delta}PD,$$

$$D(uv)=(Du)v+(P^{\delta}u)Dv.$$

Then, if $(\mathcal{A},P)$ is commutative and f satisfies $Pf=(-1)^{\sigma}f$, the product fD will also be a derivation, with

$$\Pi(fD)=(-1)^{\sigma+\delta}.$$

Thus a fermionic f times a bosonic D will be a fermionic fD, and similarly for the other three cases.

B. Construction of the ring $\mathcal{A}$

We may begin with the commutative ring $\mathcal{B}$ of all polynomials in the commuting letters $b_2, b_4, b_6, \ldots$. The ordinary derivations $\partial/\partial b_n : \mathcal{B} \to \mathcal{B}$ all commute, as n runs through even positive integers. Then $\mathcal{A}$ is the supersymmetric extension of $\mathcal{B}$, constructed as follows. Let $\mathbb{M} = \{1,3,5,\ldots\}$ be the set of all positive odd numbers, and let $2^{\mathbb{M}} = \{\phi, 1, 3, 13, \ldots\}$ be the collection of all finite subsets of $\mathbb{M}$, including the empty set ϕ. Then $\mathcal{A}$ is to consist of all finitely supported functions $f : 2^{\mathbb{M}} \to \mathcal{B}$. The product of two elements f and g, evaluated at a finite subset $E \subset \mathbb{M}$, is defined to be

$$(fg)(E) = \sum_{A \cup B = E} f(A) g(B) \varepsilon(A,B).$$

Here the function $\varepsilon : 2^{\mathbb{M}} \times 2^{\mathbb{M}} \to \{-1,0,1\}$ is defined to be

$$\varepsilon(A,B) = \prod_{a \in A} \prod_{b \in B} \varepsilon(a,b),$$

where $\varepsilon : \mathbb{M} \times \mathbb{M} \to \{-1,0,1\}$ is defined by

$$\varepsilon(a,b) = \begin{cases} 1, & a < b, \\ 0, & a = b, \\ -1, & a > b. \end{cases}$$

If the number of elements in E is $|E|$, then the above sum has $2^{|E|}$ terms, since $\varepsilon(A,B) \neq 0$ only occurs when A and B are disjoint. The parity automorphism $P : \mathcal{A} \to \mathcal{A}$ is given by $(Pf)(E) = f(E)(-1)^{|E|}$.

The easy formula $\varepsilon(A,B) = \varepsilon(B,A)(-1)^{|A||B|}$ makes it clear that $(\mathcal{A}, P)$ is commutative.

When $B, C \subset \mathbb{M}$ are disjoint, one has $\varepsilon(A, B \cup C) = \varepsilon(A,B)\varepsilon(A,C)$. This shows that the product operation is associative, the value of $(fg)h = f(gh)$ on $E \subset \mathbb{M}$ being given by

$$\sum_{A \cup B \cup C = E} f(A) g(B) h(C) \varepsilon(A,B) \varepsilon(A,C) \varepsilon(B,C).$$

This completes the construction of the oriented ring $(\mathcal{A}, P)$. The generating elements $a_1, a_2, a_3, \ldots \in \mathcal{A}$ are now to be identified.

The inclusion $\mathcal{B} \subset \mathcal{A}$ is realized by associating each $b \in \mathcal{B}$ with that function $2^{\mathbb{M}} \to \mathcal{B}$ which sends the empty set ϕ to b, and everything else to zero. Thus, for m even, $a_m(\phi) = b_m$ and $a_m(E) = 0$ for all nonempty $E \subset \mathbb{M}$.

When p is an odd positive integer, $a_p : 2^{\mathbb{M}} \to \mathcal{B}$ is defined by $a_p(p) = 1 \in \mathcal{B}$ and $a_p(E) = 0$ for all other finite subsets of $\mathbb{M}$.

This gives us $\{a_1, a_2, a_3, \ldots\} \subset \mathcal{A}$.

Evidently $Pa_n = (-1)^n a_n$. Further, if $1 \leqslant p_1 < p_2 < \cdots < p_n$ are odd, the product $a_{p_1} a_{p_2} \cdots a_{p_m} \in \mathcal{A}$ takes the value $+1$ on the subset $\{p_1, p_2, \ldots, p_n\} \subset \mathbb{M}$ and zero everywhere else. Therefore every element of $\mathcal{A}$ may be written as a finite polynomial in the elements $a_1, a_2, a_3, \ldots$.

C. Derivations of $\mathcal{A}$

The fundamental superderivation of $\mathcal{A}$ is defined by

$$D=a_2\frac{\partial}{\partial a_1}+a_3\frac{\partial}{\partial a_2}+a_4\frac{\partial}{\partial a_3}+\cdots.$$

It sends $a_1\to a_2\to a_3\to\cdots$, exchanging bosons and fermions. This suggests that $(\mathcal{A},P,D)$ is in some sense the natural model of an oriented superderivation ring generated by a single fermion a_1.

The square of a superderivation is an ordinary derivation. Thus D^2 restricted to $\mathcal{B}\subset\mathcal{A}$ sends $a_2\to a_4\to a_6\to\cdots$, and the pair $(\mathcal{B},D^2)$ can be called the free bosonic derivation ring on a single generator.

The inclusions $D\mathcal{A}_n\subset\mathcal{A}_n$ which follow from $DE=ED$ will be used later in the proofs of the exact sequence.

D. The supersymmetric gradient operator

Given $h\in\mathcal{A}$ we ask whether $f\subset\mathcal{A}$ exists with $h=Df$. A linear operator $M:\mathcal{A}\to\mathcal{A}$ with $MD=0$ would give at least a necessary condition.

In analogy with the bosonic case, for which it is known the gradient operator M, it can be found that the SUSY M operator has the expression

$$M=\frac{\partial}{\partial a_1}+D\frac{\partial}{\partial a_2}-D^2\frac{\partial}{\partial a_3}-D^3\frac{\partial}{\partial a_4}+D^4\frac{\partial}{\partial a_5}+\cdots.$$

It is a linear operator sending $\mathcal{A}$ into itself, and we have seen that the equation $Mh=0$ is a necessary condition for the existence of $f\in\mathcal{A}$ with $Df=h$.

Later it will be shown that the condition $Mh=0$ is also sufficient. (With respect to parity we note that $PM=-MP$.)

E. Operators and adjoints

Given $(\mathcal{A},P,D)$ as constructed: a ''differential operator'' is a linear map of $\mathcal{A}$ into itself having the form

$$L=\sum_0^N l_nD^n,$$

with coefficients $l_n\in\mathcal{A}$. L is the identically zero map $\mathcal{A}\to\mathcal{A}$ if and only if all the coefficients are zero.

Then $\mathcal{O}_p\mathcal{A}$ is defined to be the set of all differential operators. It is an associative ring: the composition of two operators has the same form, because $D_n(fI)$ can be expanded as a finite sum $\Sigma_{r=0}^n g_rD^r$, by using the defining property of D on products of elements of $\mathcal{A}$.

Composing L with the parity automorphism $P:\mathcal{A}\to\mathcal{A}$ we find that

$$PLP=\sum_0^N (Pl_n)(-D)^n.$$

Therefore $O_p\mathcal{A}$ is also an oriented ring, its parity automorphism given by $L\to PLP$. As before, L can be called ''oriented'' if $PL=\pm LP$, ''fermionic'' in one case and ''bosonic'' in the other.

We now ask how to integrate by parts in $\mathcal{A}$. Suppose $u,v\in\mathcal{A}$ are oriented elements with $Pu=u(-1)^\alpha, Pv=v(-1)^\beta$. Starting with $D\in\mathcal{O}_p$, we compute

$$\begin{aligned} D(uv) &= (Du)v + (-1)^{\alpha} u(Dv) \\ &= (Du)v + (-1)^{\alpha}(Dv)u(-1)^{\alpha(\beta+1)} \\ &= (Du)v + (Dv)u(-1)^{\alpha\beta}. \end{aligned}$$

This can be written as $(Du)v \equiv (-Dv)u(-1)^{\alpha\beta}$ if the congruence notation $f \equiv g$ in $\mathcal{A}$ is defined to mean that $f - g = Dh$ for some $h \in \mathcal{A}$.

More generally, L and $L^* \in \mathcal{O}_p\mathcal{A}$ may be said to be "mutually adjoint" if

$$(Lu)v \equiv (L^*v)u(-1)^{\alpha\beta},$$

for all oriented u, v as above. Thus, $D^* = -D$, while a zeroth order operator $l_0 I$ is its own adjoint.

The uniqueness of the adjoint operator is argued as follows: if $L = 0$ then every $h = L^*v$ satisfies $hu \equiv 0$ for all $u \in \mathcal{A}$. However, it can be shown that for any nonzero $h \in \mathcal{A}$ there exist u such that hu cannot be of the form Df for any $f \in \mathcal{A}$.

Consequently, $L = 0$ in $\mathcal{O}_p\mathcal{A}$ implies that all $L^*v = 0$ in $\mathcal{A}$, and hence $L^* = 0$ in $\mathcal{O}_p\mathcal{A}$. This shows that any $L \in \mathcal{O}_p\mathcal{A}$ can have at most one adjoint $L^* \in \mathcal{O}_p\mathcal{A}$, and furthermore that $(L^*)^* = L$.

The commutation of the constructions $L \to PLP$ and $L \to L^*$ is shown by applying P to the congruence,

$$(LPu)Pv \equiv (L^*Pv)Pu(-1)^{\alpha\beta}.$$

Thus if L has an adjoint then so does PLP, and

$$(PLP)^* = PL^*P.$$

The existence of adjoints for all differential operators must now be shown.

Proposition: Suppose $K, L \in \mathcal{O}_p\mathcal{A}$ have adjoints, and that $PKP = K(-1)^{\kappa}, PLP = L(-1)^{\lambda}$. Then KL has an adjoint, and it is given by

$$(KL)^* = L^*K^*(-1)^{\kappa\lambda}.$$

The proposition generalizes inmediately to finite products of operators $L_1 L_2 \cdots L_m$ in which each L_k has an adjoint and is oriented with $PL_kP = L_k(-1)^{\lambda_k}$. Then

$$(L_1 L_2 \cdots L_m)^* = (L_m^* L_{m-1}^* \cdots L_1^*)(-1)^{\mu},$$

$$\mu = \sum_{1 \le i < j \le m} \lambda_i \lambda_j .$$

Thus lD^k, when $Pl = \pm l$, has an adjoint $\pm D^k(lI)$, the sign depending on k and the parity of l. This proves that every $L \in \mathcal{O}_p\mathcal{A}$ possesses a unique adjoint $L^* \in \mathcal{O}_p\mathcal{A}$, the bijection $L \leftrightarrow L^*$ satisfying $(L^*)^* = L$.

We conclude by computing the adjoint of $D^p l D^q, p + q = m$. If $Pl = -l$ then all the $m+1$ exponents are $+1$ and $\mu = m(m+1)/2$.

Then

$$\begin{aligned} (D^p l D^q)^* &= (-D)^q l (-D)^p (-1)^{m(m+1)/2} \\ &= D^q l D^p (-1)^{m + m(m+1)/2} \\ &= D^q (P^m l) D^p (-1)^{m(m+1)/2}. \end{aligned}$$

On the other hand, if $Pl = +l$ then all but one of the exponents $\lambda_1, \ldots, \lambda_{m+1}$ is $+1$, the remaining exponent being zero. Then

$$(D^p l D^q)^* = (-D)^q l (-D)^p (-1)^{m(m-1)/2}$$
$$= D^q l D^p (-1)^{m(m+1)/2}$$
$$= D^q (P^m l) D^p (-1)^{m(m+1)/2}.$$

But every $l \in \mathcal{A}$ is uniquely the sum of a boson and a fermion. Therefore, for any $l \in \mathcal{A}$ and any nonnegative integers p and q, the adjoint of $D^p l D^q \in \mathcal{O}_p \mathcal{A}$ is given by

$$(D^p l D^q)^* = D^q (P^m l) D^p (-1)^{m(m+1)/2},$$

where $p+q=m$.

F. Frechet derivative

The construction of the Frechet derivative operator gives a linear map $\mathcal{A} \to \mathcal{A}$, sending $f \to L_f$. Given $f(a_1, a_2, \ldots, a_n)$ an element of $\mathcal{A}$, the action of L_f on a fermionic element $v \in \mathcal{A}, Pv = -v$, may be defined by

$$L_f v = \frac{d}{d\epsilon}\bigg|^{\epsilon=0} f(a_1 + \epsilon v, a_2 + \epsilon D v, \ldots, a_n + \epsilon D^{n-1} v).$$

The coefficients of L_f are obtained as follows. If q is odd and $f = g a_q h$ with g and h independent of a_q, we have $(\partial/\partial a_q) f = (Pg)h$, while $g(D^{q-1}v)h = g(Ph)(D^{q-1}v)$ since $D^{q-1}v$ is fermionic. Therefore $D^{q-1}v$ is multiplied on the left by $(P(\partial/\partial a_q) f)$. If m is even then $\partial/\partial a_m$ is an ordinary derivation and $D^{m-1}v$ is bosonic. In this case there is no anticommutation, and $D^{m-1}v$ is multiplied on the left by $\partial f/\partial a_m$. Combining these two cases, we obtain the general formula

$$L_f = \sum_{n=1}^{\infty} \left(P^n \frac{\partial f}{\partial a_n} \right) D^{n-1},$$

which gives the Frechet derivative operator $L_f \in \mathcal{O}_p \mathcal{A}$ for any $f \in \mathcal{A}$.

Applying L_f to the generating element $a_1 \in \mathcal{A}$ we get

$$L_f a_1 = \sum_{n=1}^{\infty} \left(P^n \frac{\partial f}{\partial a_n} \right) a_n.$$

But $h a_n = a_n (P^n h)$ for all $h \in \mathcal{A}$. Hence $L_f a_1 = Ef$, connecting L_f to the Euler operator E.

The adjoint operator to L_f may be written down using the results of the previous section:

$$L_f^* = \sum_{n=1}^{\infty} (-1)^{n(n-1)/2} D^{n-1} \left(\left(P \frac{\partial f}{\partial a_n} I \right) \right).$$

Applying the operator parity automorphism $K \to PKP$ we get

$$P L_f^* P = \sum_{n=1}^{\infty} (-1) \frac{n(n-1)}{2} (-D)^{n-1} \left(\frac{\partial f}{\partial a_n} I \right).$$

The coefficient of the identity operator is readily accessible since

$$D^{n-1} \left(\frac{\partial f}{\partial a_n} I \right) = \left(D^{n-1} \frac{\partial f}{\partial a_n} \right) I + (?) D + \cdots.$$

After checking the $\pm$ signs we see that this coefficient is just the supersymmetric gradient Mf of f: thus

$$L_f^* = (PMf)I + (?)D + \cdots .$$

Going back to the equation $Mh=0$, we see that this condition would imply the existence of $K \in \mathcal{O}_p\mathcal{A}$ satisfying $L_h^* = KD$ and hence also $L_h = \pm DK^*$ if h is oriented. Applying this operator equation to the generating element $a_1 \in \mathcal{A}$, we find that $Eh = Df$ for some $f \in \mathcal{A}$.

Thus $Mh=0$ implies $h \equiv 0$, at least when h is oriented and $Eh = nh, n>0$. But the two extra conditions are no obstacle.

Proposition: Given $h \in \mathcal{A}$, with a zero constant term. Then $Mh=0$ if and only if $h = Df$ for some $f \in \mathcal{A}$.

Proof: The equation $PM = -MP$ shows that $h \pm Ph$ also has a zero gradient. Replacing h by either summand in $h = boson + fermion$, we may suppose that h is oriented. The presentation,

$$\mathcal{A} = \mathcal{A}_0 \oplus \mathcal{A}_1 \oplus \mathcal{A}_2 \oplus \cdots ,$$

by eigenspaces of the Euler operator permits h to be written as $h = h_0 + h_1 + h_2 + \cdots$, in which $h_0 = 0$ by hypothesis. Then, since $M\mathcal{A}_n \subset \mathcal{A}_{n-1}$ the condition $Mh=0$ implies $Mh_n = 0$ for all $n \geqslant 1$.

By what was said earlier, there exist f_n with $Df_n = Eh_n = nh_n$. Therefore $h = D(f_1 + \frac{1}{2}f_2 + \frac{1}{3}f_3 + \cdots)$ and the proof is complete.

In the next section we will need to know the interaction between the $f \to L_f$ construction and the parity automorphism $P: \mathcal{A} \to \mathcal{A}$. The formula $L_{Pf} = -PL_fP$ is easily verified by

$$\left(P^n \frac{\partial}{\partial a_n} Pf \right) D^{n-1} = (-1)^n \left(P^{n+1} \frac{\partial f}{\partial a_n} \right) D^{n-1}$$

$$= -\left(P\left(P^n \frac{\partial f}{\partial a_n} \right) \right) (-D)^{n-1}.$$

G. Gradients and operators

We wish to determine which elements $g \in \mathcal{A}$ are of the form Mh for some $h \in \mathcal{A}$: in the applications this asks which g are gradients of possible conserved quantities. Here are two facts, that can be proven easily.

(i) For any $f \in \mathcal{A}$, the Frechet derivative operators of f and of Df are connected by the equation

$$L_{Df} = DL_f .$$

(ii) When $g = Mh$, the Frechet derivative operator of g is antisymmetric:

$$L_g^* = -L_g .$$

Evidently the second fact gives a necessary condition for g to be a gradient. But it is also sufficient.

Proposition: Given $g \in \mathcal{A}$. The antisymmetry equation $L_g^* = -L_g$ in $\mathcal{O}_p\mathcal{A}$ is necessary and sufficient for the existence of h with $Mh = g$.

Proof: Suppose first that g is oriented and satisfies $Eg = ng, n \geqslant 0$, as well as the hypothesis $L_g^* = -L_g$. If $Pg = g(-1)^\nu$, then the Frechet derivative operator of element $h = a_1 g$ is given by

$$L_h = (Pg)I + \sum_{n=1}^{\infty} \left(P^n (-1)^n a_1 \frac{\partial g}{\partial a_n} \right) D^{n-1}$$

$$= (Pg)I + a_1 L_g .$$

From $L_{Pg}=-PL_gP$ we see that L_g has orientation opposite to that of g, that is, $PL_gP=L_g(-1)^{\nu+1}$. This permits the adjoint of L_h to be calculated as

$$L_h^*=(Pg)I+L_g^*(a_1I)(-1)^{\nu+1}$$
$$=(-1)^{\nu}\{gI+L_g(a_1I)\}.$$

This shows that $(-1)^{\nu}L_h^*=(g+Eg)+(?)D+\cdots$.

But it was seen before that $L_h^*=(PMh)I+(?)D+\cdots$. Observing $PM=-MP$ and $Ph=h(-1)^{\nu+1}$, we conclude that $M(a_1g)=g+Eg=(n+1)g$ in consequence of three assumptions made at the beginning of this proof. Returning now to the general case, we note that operator adjoints, Frechet derivative operators, and the parity automorphism are interconnected by

$$(PL_gP)^*=PL_g^*P=L_{Pg}=-PL_gP.$$

Thus, if $g\in\mathcal{A}$ has an antisymmetric Frechet derivative operator then so do Pg and $g\pm Pg$. Hence it suffices to treat only the case of oriented g. Expanding $g=g_0+g_1+g_2+\cdots$ by homogeneous components in $\mathcal{A}_0\oplus\mathcal{A}_1\oplus\cdots$, we observe that the coefficients of L_{g_n} and $L_{g_n}^*$ fall within $\mathcal{A}_{n-1}$. Therefore the antisymmetry of L_g implies the antisymmetry of all the L_{g_n}. From what was said before $g=Mh$ with $h=a_1(g_0+\frac{1}{2}g_1+\frac{1}{3}g_2+\cdots)$.

This completes the proof.

H. Summary: the exact sequence

A ring $\mathcal{A}$, the "free SUSY derivation ring on a single fermionic generator" has been constructed. It has a parity automorphism P, a canonical superderivation D, and a SUSY gradient operator M.

Necessary and sufficient conditions have been given for recognizing which elements of $\mathcal{A}$ are derivatives and which are gradients. In terms of the SUSY gradient operator M, the Frechet derivative operator L_g, and the operator adjoint construction $L\to L^*$, these conditions are expressed by the following exact sequence of rings and linear transformations:

$$\begin{array}{llll} O_p\mathcal{A}\leftarrow & \mathcal{A}\leftarrow & \mathcal{A}\leftarrow & \mathcal{A}\leftarrow\mathbb{R}\leftarrow 0 \\ & & Df\leftarrow & f \\ & Mh\leftarrow & h & \\ L_g+L_g^*\leftarrow & g. & & \end{array}$$

The sequence is exact in that the kernals of the outgoing transformations coincide with the images of the incoming transformations.

III. THE SUSY HEAT OPERATOR

The ordinary heat equation with potential $u(x)$ and temperature function $f(x,t)$ is

$$L_uf=0,\quad L_u=\frac{\partial}{\partial t}-\Delta+u(x).$$

Its Green's function evaluated at a field point $p=(x,t)$ and source point $q=(x',0)$ may be written as $G(p,q)=\mathcal{G}_t(x,x')$. For fixed x' and variable x and t it satisfies the above heat equation with initial value

$$\lim_{t\downarrow 0}\quad \mathcal{G}_t(x,x')=\delta(x-x').$$

When the potential is zero the Green's function is

$$g_t(x-x')\equiv g(x-x',t)=\frac{1}{\sqrt{4\pi t}}\exp\left(-\frac{(x-x')^2}{4t}\right).$$

It has the basic properties

$$\text{(i)}\quad g_t(x-x')>0;$$

$$\text{(ii)}\quad \int_{\mathbb{R}^n} g_t(x-x')dx=1;$$

$$\text{(iii)}\quad g_{t+s}(x-x')=\int_{\mathbb{R}^n} g_s(y-x')g_t(x-y)dy. \tag{1}$$

These properties allow the definition of the conditional Wiener measure, which may be used to express the Green's function $\mathcal{G}_t(x,x')$ of the operator L_u by the Feyman–Kac formula,[13] when the potential $u(x)$ is real and bounded from below.

For bounded potentials the Green's function admits an asymptotic expansion,

$$\mathcal{G}_t(x,x')=g(x-x',t)\sum_{n=0}^{\infty}\frac{1}{n!}a_n(x,x')t^n,$$

in which the coefficients $a_n(x,x')$ are determined recursively by $a_0(x,x')=1$,

$$(n+(x-x')\partial_x)a_n(x,x')=(\partial_x^2+u(x))a_{n-1}(x,x').$$

On the diagonal $x=x'$, one has

$$a_n(x,x)=g_n(u(x),u'(x),\ldots),$$

a finite polynomial in the potential function $u(x)$ and its derivatives.

Then the equations of the KdV hierarchy,[14] for unknown functions $w(x,t)$, are

$$w_t=\frac{\partial}{\partial x}g_n(w,w_x,w_{xx},\ldots).$$

We now present a supersymmetric extension of this construction. The potential and the temperature function now have their values in an exterior algebra Λ, also called a Grassmann algebra.

If anticommuting generators of Λ are written as $\theta,\theta_2,\theta_3,\ldots,\theta_m$ then every element of Λ has a unique presentation,

$$\Phi=\xi+\theta u,$$

where ξ and u are in the subalgebra of Λ generated by $\theta_2,\theta_3,\ldots,\theta_m$. Then, defining $\partial_\theta\Phi=u$, we obtain a superderivation $\partial_\theta:\Lambda\to\Lambda$, that is,

$$\partial_\theta(\Phi_1\Phi_2)=(\partial_\theta\Phi_1)\Phi_2+\overline{\Phi}_1(\partial_\theta\Phi_2),$$

where $\Phi\to\overline{\Phi}$ is the parity automorphism of Λ.

The operator $D=\partial_\theta+\theta\partial_x$ then acts on "superfields," that is, on differentiable functions $\mathbb{R}\to\Lambda$. Using Φ_1 and Φ_2 to designate superfields, one can check

$$D(\Phi_1\Phi_2)=(D\Phi_1)\Phi_2+\overline{\Phi}_1(D\Phi_2),$$

$$D^2=\partial_x.$$

It will be assumed that the potential Φ is fermionic: $\overline{\Phi}=-\Phi$ meaning that $\overline{\xi}=-\xi$ and $\overline{u}=u$.

If we take the dimension of x to be 1:

$$[x]=1,$$

then one must have

$$[\theta]=\tfrac{1}{2},$$

$$[D]=-\tfrac{1}{2};$$

consequently,

$$[u]=-2,$$

$$[\Phi]=[\xi]=-\tfrac{3}{2}.$$

The most general supersymmetric extension of L_u, assuming positive powers of D, becomes then

$$\mathbf{L}=\frac{\partial}{\partial t}-(D^4-D\Phi+\lambda\Phi D),$$

where λ is a constant, dimensionless parameter.

When the superpotential Φ is zero, it reduces to the heat operator, while if $\xi=0$ and $\theta=0$ it reduces to L_u.

The parameter λ already appeared in the analysis of Mathieu[1] for all supersymmetric extensions of the KdV equation. The case $\lambda=1$ was related to the integrable supersymmetric extension of the KdV equation. We will consider in what follows $\lambda=1$.

There are two supersymmetric extensions of $\delta(x-x')$.

$\delta(x-x')\delta(\theta-\theta')$ and $\delta(x-x'-\theta\theta')=\delta(x-x')-\theta\theta'\delta'(x-x')$ are both invariants under the supersymmetric transformations,

$$x\to x+\theta\eta,\quad \theta\to\theta+\eta,$$

$$x'\to x'+\theta'\eta,\quad \theta'\to\theta'+\eta. \tag{2}$$

We may then consider two Green's functions according to each possible initial condition. We will denote the corresponding Green's function by $\mathbf{K}_t(x,x',\theta,\theta')$ and $\mathbf{G}_t(x,x',\theta,\theta')$, respectively.

The Green's function for the potential Φ, as a function of the source point $q=(x',0)$ and field point $p=(x,t)$, is to be a function $\mathbf{K}_t(x,x',\theta,\theta')$, $\mathbf{G}_t(x,x',\theta,\theta')$ having values in Λ and satisfying $\mathbf{L}\mathbf{K}_t=0$,$\mathbf{L}\mathbf{G}_t=0$ when $t>0$, while $\lim_{t\downarrow 0}\mathbf{K}_t=\delta(x-x')\delta(\theta-\theta')$, $\lim_{t\downarrow 0}\mathbf{G}_t=\delta(x-x')-\theta\theta'\delta'(x-x')$.

$\mathbf{K}_t$ and $\mathbf{G}_t$ are related by

$$-D'\mathbf{K}_t=\mathbf{G}_t,$$

in which

$$D'=\frac{\partial}{\partial\theta'}+\theta'\frac{\partial}{\partial x'}$$

is the superderivative with respect to (x',θ').

The Green's function $\mathbf{K}_t$ may then be expressed as

$$\mathbf{K}_t(x,x';\theta,\theta')=\mathcal{K}_t(x-x',\theta-\theta')-\langle\tilde{D}[\Phi(\tilde{x},\tilde{\theta})\mathcal{K}_{\tilde{t}}(\tilde{x}-x',\tilde{\theta}-\theta')]\mathcal{K}_{t-\tilde{t}}(x-\tilde{x},\theta-\tilde{\theta})\rangle_{\tilde{x},\tilde{t},\tilde{\theta}}$$
$$+\langle\langle\tilde{D}[\Phi(\tilde{x},\tilde{\theta})\mathcal{K}_{\tilde{t}}(\tilde{x}-x',\tilde{\theta}-\theta')]\tilde{\tilde{D}}[\Phi(\tilde{\tilde{x}},\tilde{\tilde{\theta}})\mathcal{K}_{\tilde{\tilde{t}}-\tilde{t}}(\tilde{\tilde{x}}-\tilde{x},\tilde{\tilde{\theta}}-\tilde{\theta})]$$
$$\times\mathcal{K}_{t-\tilde{\tilde{t}}}(x-\tilde{\tilde{x}},\theta-\tilde{\tilde{\theta}})\rangle_{\tilde{x},\tilde{t},\tilde{\theta}}\rangle_{\tilde{\tilde{x}},\tilde{\tilde{t}},\tilde{\tilde{\theta}}}-\cdots,$$

where

$$\mathcal{K}_t(x-x',\theta-\theta')=g_t(x-x')(\theta-\theta'),$$

$$0<\tilde{t}<\tilde{\tilde{t}}<\cdots<t,$$

$$\tilde{D}=\tilde{\theta}\frac{\partial}{\partial\tilde{x}}+\frac{\partial}{\partial\tilde{\theta}},$$

and

$$\langle\cdot\rangle_{\tilde{x},\tilde{t},\tilde{\theta}}=\int\frac{\partial}{\partial\tilde{\theta}}(\cdot)|_{\tilde{\theta}=0}\,d\tilde{x}\,d\tilde{t}.$$

The integration on $\tilde{x}$ is over $\mathbb{R}$, the integration on the $\tilde{t}$ variable is according to the above ordering while the integration on the odd coordinate means $[\partial/\partial\tilde{\theta}]_{\tilde{\theta}=0}$ and it must be performed in the order indicated in our formula. We will show that this series expansion is convergent, under the assumption of bounded potentials.

The generic term of the expansion may be constructed from the previous one replacing $\mathcal{K}_{t-\tilde{\tilde{t}}}(x-\tilde{\tilde{x}},\theta-\tilde{\tilde{\theta}})$ by $\hat{D}[\Phi(\hat{x},\hat{\theta})\mathcal{K}_{\hat{t}-\tilde{\tilde{t}}}(\hat{x}-\tilde{\tilde{x}},\hat{\theta}-\tilde{\tilde{\theta}})]\mathcal{K}_{t-\hat{t}}(x-\hat{x},\theta-\hat{\theta})$ and performing an overall integration on $\hat{x},\hat{\theta},\hat{t}$ where this point is an intermediate one with $\tilde{\tilde{t}}<\hat{t}<t$.

The explicit expansion for $\mathbf{G}_t$ turns out to be, after some calculations,

$$\mathbf{G}_t(x,x';\theta,\theta')=g_t(x-x'-\theta\theta')-\langle\Phi(\tilde{x},\tilde{\theta})g_{\tilde{t}}(\tilde{x}-x'-\tilde{\theta}\theta')g_{t-\tilde{t}}(x-\tilde{x}-\theta\tilde{\theta})\rangle_{\tilde{x},\tilde{t},\tilde{\theta}}$$
$$+\langle\langle\Phi(\tilde{x},\tilde{\theta})g_{\tilde{t}}(\tilde{x}-x'-\tilde{\theta}\theta')\Phi(\tilde{\tilde{x}},\tilde{\tilde{\theta}})g_{\tilde{\tilde{t}}-\tilde{t}}(\tilde{\tilde{x}}-\tilde{x}-\tilde{\tilde{\theta}}\tilde{\theta})g_{t-\tilde{\tilde{t}}}(x-\tilde{\tilde{x}}-\theta\tilde{\tilde{\theta}})\rangle_{\tilde{x},\tilde{t},\tilde{\theta}}\rangle_{\tilde{\tilde{x}},\tilde{\tilde{t}},\tilde{\tilde{\theta}}}$$
$$-\cdots.$$

The generic term of the expansion may be constructed from the previous one replacing $g_{t-\tilde{\tilde{t}}}(x-\tilde{\tilde{x}}-\theta\tilde{\tilde{\theta}})$ by $\Phi(\hat{x},\hat{\theta})g_{\hat{t}-\tilde{\tilde{t}}}(\hat{x}-\tilde{\tilde{x}}-\hat{\theta}\tilde{\tilde{\theta}})g_{t-\hat{t}}(x-\hat{x}-\theta\hat{\theta})$ and performing an overall integration on $\hat{x},\hat{\theta},\hat{t}$ where this point is an intermediate one with $\tilde{\tilde{t}}<\hat{t}<t$.

In the bosonic limit, when $\xi(x)=0$ and $\theta=\theta'=0$, the integration on the odd variables $\tilde{\theta}$ becomes straightforward and the formula reduces to

$$\mathbf{G}_t(x,x';0,0)|_{\xi=0}=g_t(x-x')-\langle u(\tilde{x})g_{\tilde{t}}(\tilde{x}-x')g_{t-\tilde{t}}(x-\tilde{x})\rangle_{\tilde{x},\tilde{t}}$$
$$+\langle\langle u(\tilde{x})g_{\tilde{t}}(\tilde{x}-x')u(\tilde{\tilde{x}})g_{\tilde{\tilde{t}}-\tilde{t}}(\tilde{\tilde{x}}-\tilde{x})g_{t-\tilde{\tilde{t}}}(x-\tilde{\tilde{x}})\rangle_{\tilde{x},\tilde{t}}\rangle_{\tilde{\tilde{x}},\tilde{\tilde{t}}}-\cdots.$$

This is exactly the Green's function $\mathcal{G}$ for the operator $L_u=\partial_t-\Delta-u(x)$. If we assume $u(x)$ to be bounded and continuous:

$$|u(x)|<M,$$

it then follows, using the semigroup property for the Green's function, that

$$|\mathcal{G}_t(x,x')| < e^{tM} g_t(x-x').$$

It may also be shown that the convergent expansion for $\mathcal{G}_t(x,x')$ is equal to the Feynman–Kac formula,

$$\mathcal{G}_t(x,x') = \int dW_t(x,x') \exp\left(- \int_{-t/2}^{+t/2} u(x(s)) ds \right),$$

where $dW_t(x,x')$ denotes the Wiener measure for the continuous paths between x' and x. When $u(x)$ is real and bounded both formulas are exactly the same. However, the Feynman–Kac formula may be established even when $u(x)$ is bounded from below and $\Delta + u(x)$ is (essentially) self-adjoint, while the expansion in terms of the potential is valid when u is bounded without assuming the self-adjoint property of the operator.

$\mathcal{G}_t(x,x')$ is positive. This property arises directly from the Feynman–Kac formula.

It also satisfies

$$\mathcal{G}_t(x,x') = \mathcal{G}_t(x',x),$$

under the interchange of the positions of the field point and the source one.

In the next section we will analyze these properties for the supersymmetric extensions we are considering.

IV. THE SUSY GREEN'S FUNCTION AND THE SKdV HIERARCHY

The Green's function $\mathbf{G}_t$ depends on x, θ and x', θ' and on the components of the superpotential u and ξ. In order to analyze the transformation law, under supersymmetry, of $\mathbf{G}_t$ we will write explicitly its dependence on u and ξ, $\mathbf{G}_t(x,x';\theta,\theta';u,\xi)$. Under the supersymmetric transformations:

$$x \to x + \delta x = x - \eta\theta,$$

$$\theta \to \theta + \delta\theta = \theta + \eta,$$

$$\Phi \to \Phi + \delta\Phi = \Phi - \eta u(x) + \eta\theta\xi'(x),$$

the components of Φ transforms as

$$u \to u + \delta u = u - \eta\xi',$$

$$\xi \to \xi + \delta\xi = \xi - \eta u.$$

$\mathbf{G}_t$ is then invariant under these transformations. That is,

$$\mathbf{G}_t(x+\delta x, x'+\delta x'; \theta+\delta\theta, \theta'+\delta\theta'; u+\delta u, \xi+\delta\xi) = \mathbf{G}_t(x,x';\theta,\theta';u,\xi). \tag{3}$$

To show this invariance property of $\mathbf{G}_t$ we notice that

$$(\Phi + \delta\Phi)(\tilde{x},\tilde{\theta}) = \Phi(\tilde{x} - \delta\tilde{x}, \tilde{\theta} - \delta\tilde{\theta}).$$

We then evaluate the left hand member of (3) using the previous expansion formula and perform a change of variable at each intermediate point $\tilde{x},\tilde{\theta}$:

$$\tilde{x} \to \tilde{x}_1 = \tilde{x} - \delta\tilde{x},$$

$$\tilde{\theta} \to \tilde{\theta}_1 = \tilde{\theta} - \delta\tilde{\theta},$$

with a Jacobian equal to 1.

We then use the property that the combination $(\tilde{\tilde{x}}-\tilde{x}-\tilde{\tilde{\theta}}\tilde{\theta})$ is invariant under this change of coordinates. We end up with the relation (3).

The other symmetry of the SUSY Green's function $\mathbf{G}_t$ is

$$\mathbf{G}_t(x,x';\theta,\theta';u,\xi)=\mathbf{G}_t(x,x';\theta',\theta;u,\xi). \tag{4}$$

It follows by performing changes of variables on the time arguments at each integrand on each term of the expansion. In terms of the components of $\mathbf{G}_t$ it means

$$\mathbf{G}_t(x,x';\theta,\theta')=A_t(x,x')+\theta' B_t(x,x')+\theta C_t(x,x')+\theta\theta' D_t(x,x'),$$

$$A_t(x,x')=A_t(x',x),$$

$$B_t(x,x')=C_t(x',x),$$

$$D_t(x,x')=-D_t(x',x).$$

We will now evaluate $\mathbf{G}_t$ by performing all integrations on the odd variables. We start evaluating $\mathbf{G}_t(x,x';0,0;u,\xi)$. We denote

$$\tilde{x},\tilde{t}\Rightarrow\tilde{\tilde{x}},\tilde{\tilde{t}}=\mathcal{G}^{\tilde{}}_{\tilde{t}-\tilde{t}}(\tilde{\tilde{x}},\tilde{x}),\ \text{the bosonic propagator;}$$

$$\tilde{x},\tilde{t}\rightsquigarrow\tilde{\tilde{x}},\tilde{\tilde{t}}=-\frac{1}{2}\frac{(\tilde{\tilde{x}}-\tilde{x})}{(\tilde{\tilde{t}}-\tilde{t})}g^{\tilde{}}_{\tilde{t}-\tilde{t}}(\tilde{\tilde{x}}-\tilde{x});\ \text{the fermionic propagator.}$$

An arrow followed by a vertex $\xi(\tilde{\tilde{x}})$ denotes multiplication of the propagator by the vertex and integration on the corresponding coordinates $\tilde{\tilde{x}},\tilde{\tilde{t}}$.

The Green's function at $\theta=\theta'=0$ may then be expressed by

$$\mathbf{G}_t(x,x';0,0;u,\xi)=x',t'\Rightarrow x,t+x',t'\Rightarrow\xi\rightsquigarrow\xi\Rightarrow x,t+x',t'\Rightarrow\xi\rightsquigarrow\xi\Rightarrow\xi\rightsquigarrow\xi\Rightarrow x,t$$
$$+x',t'\Rightarrow\xi\rightsquigarrow\xi\Rightarrow\xi\rightsquigarrow\xi\Rightarrow\xi\rightsquigarrow\xi\Rightarrow x,t+\cdots.$$

It can be shown that this expansion on the fermionic vertex ξ is convergent provided $u(x)$ is bounded and $\xi(x)$ is bounded in the following sense. It is possible to express the product

$$\xi(\tilde{\tilde{x}})\xi(\tilde{\tilde{x}})=\frac{1}{2}(x-\tilde{\tilde{x}})f(\tilde{\tilde{x}},\tilde{x}), \tag{5}$$

since the left hand member is antisymmetric on $\tilde{x}\leftrightarrow\tilde{\tilde{x}}$. We assume then that

$$|u(x)|<M,$$

$$f(\tilde{\tilde{x}},\tilde{x})<M^2. \tag{6}$$

The square arises from dimensional arguments. In fact, let us remember that $[\xi]=-3/2$ and $[u]=-2$ and hence $[f]$ must be -4. After replacing (5) in the expression of $\mathbf{G}_t(x,x';0,0;u,\xi)$, the contributions of the fermionic propagator times the fermionic vertices may be worked out in terms of derivatives of g_t. One may then use (6) and the semigroup properties for g_t to obtain a bound for the series expansion of $\mathbf{G}_t(x,x';0,0;u,\xi)$.

The complete expression for $\mathbf{G}_t(x,x';\theta,\theta')$, expressed in terms of its value at $\theta=\theta'=0$, is the following:

$$\mathbf{G}_t(x,x';\theta,\theta')=\mathbf{G}_t(x,x',0,0)-\theta\langle\mathbf{G}_{t-t'}^{\sim}(\tilde{x},x',0,0)\xi(\tilde{x})g'_{t-\tilde{t}}(x-\tilde{x})\rangle_{\tilde{x},\tilde{t}}$$
$$+\theta'\langle\xi(\tilde{x})g'_{t-t'}(\tilde{x}-x')\mathbf{G}_{t-\tilde{t}}(x,\tilde{x},0,0)\rangle_{\tilde{x},\tilde{t}}$$
$$-\theta\theta'\langle\langle\xi(\tilde{x})g'_{t-t'}(\tilde{x}-x')\mathbf{G}_{\tilde{t}-\tilde{t}}^{\tilde{}}(\tilde{\tilde{x}},\tilde{x};0,0)\xi(\tilde{\tilde{x}})g'_{t-\tilde{t}}(x-\tilde{\tilde{x}})\rangle_{\tilde{x},\tilde{t}}\rangle_{\tilde{\tilde{x}},\tilde{\tilde{t}}}.$$

Just as in the bosonic case, $\mathbf{G}_t$ possesses an asymptotic expansion:

$$\mathbf{G}_t(x,x',\theta,\theta')=g_t(x-x'-\theta\theta')\sum_{k=0}^{\infty}\frac{t^k}{k!}\Gamma_k(x,x'),$$

in which each term has the form

$$\Gamma_k(x,x')=A_k(x,x')+\theta B_k(x,x')+\theta' C_k(x,x')+\theta\theta' D_k(x,x').$$

The approximation of $\mathbf{G}_t$ by its asymptotic expansion proves that A_k, B_k, C_k, D_k have the same x,x' symmetry as noted before. As before, Γ_k is constructed from the potential $\Phi(x)=\xi(x)+\theta u(x)$ by an iterative procedure starting with $\Gamma_0(x,x')=1$.

Formally equating x with x' and θ with θ' we define

$$g_k(x)=A_k(x,x)+2\theta B(x,x).$$

This must be a polynomial in $\xi(x)$, $u(x)$, and their derivatives. But it turns out to be expressible as a polynomial in $\Phi=\xi+\theta u, D\Phi=u+\theta\partial_x\xi, D^2\Phi=\partial_x\xi+\theta\partial_x u,\ldots$.

These polynomials can be seen as elements of the free supersymmetric derivation ring on a single fermionic generator, but in the notation $\Phi=a_1, D\Phi=a_2,\ldots$.

The first few such polynomials are

$$g_2=-a_2,$$

$$g_6=-a_6+3a_2^2-2a_1a_3,$$

$$g_{10}=(-a_{10}+10a_2a_6+5a_4^2-10a_2)^3-(4a_1a_7+a_3a_5-15a_1a_2a_3).$$

They have been shown to be gradients of conserved quantities of the SKdV[1] equation, whose unknown function $\Omega(x,t)$ is to satisfy

$$\Omega_t=-D^6\Omega+3\Omega(D^3\Omega)+3((D\Omega)(D^2\Omega)).$$

The symmetry of the asymptotic Green's function permits the derivation, after several calculations, of the recursive algorithm,

$$D^2g_{n+4}=(D^6+2a_1D^3-4a_2D^2+a_3D-2a_4I)g_n-a_1l_n,$$

$$D^2l_n=-a_2Dg_n+a_3g_n.$$

The members of the super KdV hierarchy are then given by Mg_n with

$$M=D^5-3a_1D^2-a_2D-2a_3I.$$

In particular Mg_2 is the super KdV equation of Mathieu,[1] the same one appearing above.

One may use necessary and sufficient conditions arising from the exact sequence established in Sec. II to show g_n are the gradients of conserved quantities of the SKdV hierarchy.

V. CONCLUSIONS

We introduced the free $N=1$ supersymmetric derivation ring. We established the exact sequence of supersymmetric rings and linear transformations:

$$\begin{array}{llll} O_p\mathcal{A}\leftarrow & \mathcal{A}\leftarrow & \mathcal{A}\leftarrow & \mathcal{A}\leftarrow\mathbb{R}\leftarrow 0 \\ & & Df\leftarrow & f \\ & Mh\leftarrow & h & \\ L_g+L_g^*\leftarrow & g. & & \end{array}$$

Several of these relations were already known in the literature.[2,12]

We used necessary and sufficient conditions arising from this exact sequence to obtain the essential relations between conserved quantities, gradients, and the $N=1$ super KdV hierarchy. We combine these algebraic conditions together with an analytical analysis of the superheat operator,

$$\mathbf{L}=\frac{\partial}{\partial t}-(D^4-D\Phi+\Phi D).$$

We found an explicit series expansion for the Green's function of the superheat operator and discussed its properties. The expansion is convergent under the assumption of bounded bosonic and fermionic potentials as established in Sec. IV. This analysis may be relevant since there is no rigorous Feynman–Kac formula for the fermionic case.

Finally we show that the asymptotic expansion when $t\rightarrow 0^+$ of the Green's function of $\mathbf{L}$, evaluated over its diagonal, generates all the members of the $N=1$ super KdV hierarchy.

The exact sequence of SUSY rings and linear transformations may also be constructed with $N>1$ SUSY generators; we hope to discuss this extension elsewhere. We expect that the algebraic construction established in the first part of this work may have a natural extension for more general finite-dimensional quantum systems. This would be of great help in understanding, for example, the quantum behavior of the supermembrane and super D-brane theories.[15–17]

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The Günther's formalism in classical field theory: momentum map and reduction

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The polysymplectic formalism in local field theory, developed by Günther [J. Diff. Geom. **25**, 23 (1987)], is revised. A new approach and new results on momentum maps and reduction are given. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Günther's paper[1] gives a geometric Hamiltonian formalism for field theories. The crucial device is the introduction of a vector-valued generalization of a symplectic form, called a polysymplectic form. One of the advantages of this formalism is that one only needs the tangent and cotangent bundle of a manifold to develop it.

In this paper our purpose is, first, to clarify the Günther's formalism, second, give new results on momentum maps and reduction for this formalism.

We describe his polysymplectic formalism using a standard notation as that in the Abraham–Marsden[2] book. We show that the polysymplectic structures used by Günther to develop his formalism could be replaced by the k-symplectic structures defined by Awane.[3–5] So this formalism could be called the k-symplectic formalism.

We believe that this clarifies Günther's paper.[1] We present new examples of the formalism, new results about momentum maps, and we extend the reduction procedures by Marsden and Weinstein and Kostant-Souriau to polysymplectic manifolds.

Let us remark here that the polysymplectic formalism developed by Sardanashvily and co-workers,[6,7] based on a vector valued form on some associated fiber bundle, is a different description of classical field theories of first order than the polysymplectic formalism proposed by Günther.

In Secs. II–IV we develop the Günther's formalism: in Sec. II the field theoretic phase space is introduced as the Whitney sum $(T^1_k)^*Q$ of k-copies of the cotangent bundle T^*Q of a manifold Q. This space is the canonical example of polysymplectic manifold. A particular case of polysymplectic manifolds are the k-symplectic manifolds (see Refs. 3–5, 8, and 9).

The field theoretic state space is introduced in Sec. II as the Whitney sum T^1_kQ of k-copies of the tangent bundle TQ of a manifold Q. This manifold has a canonical k-tangent structure defined by k tensor fields of type (1, 1) satisfying certain algebraic properties. The k-tangent manifolds were introduced by de León *et al.*,[10,11] and they generalize the tangent manifolds (see Refs. 12–17).

Section III is devoted to give a geometric interpretation of the second order partial differential equations. Here we show that these equations can be characterized using the canonical k-tangent structure of T^1_kQ, which generalizes the case of Classical Mechanics.

Hamiltonian and Lagrangian formalisms are developed in Sec. IV. We present two new ex-

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amples, the electrostatic equations as an example of the Hamiltonian formalism, and the theory of a vibrating string as an example of the Lagrangian formalism.

We prove that the Lagrangian formalism can be developed using the canonical k-tangent structure of T^1_kQ, or the Legendre transformation by Günther.[1]

A natural extension of these formalisms is the geometric description of first order classical field theories given in terms of k-cosymplectic manifolds. This description can be found in Refs. 18 and 19.

In Sec. V we discuss symmetries and conservation laws of classical field theories in terms of momentum maps generalizing the concept of momentum map in mechanics. Some results on conservation laws and a Noether theorem obtained by Günther[1] are recalled. We extend the results about momentum maps in T^*Q and TQ, to the polysymplectic manifolds $(T^1_k)^*Q$ and T^1_kQ. In fact we show that the conservation law, given in Theorem 4.2.2 of Abraham–Marsden,[2] for a symplectic manifold, can be extended to $(T^1_k)^*Q$. We also present a generalized Noether theorem on T^1_kQ, which is a generalization of Corollary 4.2.14 by Abraham–Marsden.[2]

Reduction for symplectic manifolds is generalized to the polysymplectic structures in Sec. VI. So, we obtain "the reduced phase space" M_μ of a polysymplectic manifold, we give an explicit realization of M_μ for $M=(T^1_k)^*Q$, and we reduce the Hamiltonian $H:(T^1_k)^*Q\to\mathbb{R}$ to M_μ. An example of reduction for the left action of G on $(T^1_k)^*G$, where G is a Lie group, is presented. We study the particular case $G=\mathrm{SO}(3)\overset{k}{\times}\cdots\times\mathrm{SO}(3)$.

Finally, let us remark that the reduction problem was also discussed in the different frameworks of the classical field theory, the GIMMSY[20] paper is probably the most ambitious program to develop full description of the reduction theory, not only on the finite dimensional setting by the multisymplectic form, but also on the infinite dimensional setting of the associated Cauchy space.

II. POLYSYMPLECTIC MANIFOLDS

A. The cotangent bundle of k^1-covelocities of a manifold

Let Q be a differentiable manifold of dimension n, $\tau_Q:TQ\to Q$ its tangent bundle and $\tau^*_Q:T^*Q\to Q$ its cotangent bundle. Let us denote by $(T^1_k)^*Q=T^*Q\overset{k}{\oplus}\cdots\oplus T^*Q$ the Whitney sum of k copies of T^*Q, with projection map $\tau^*:(T^1_k)^*Q\to Q$, $\tau^*(\alpha_1(q),\ldots,\alpha_k(q))=q$.

$(T^1_k)^*Q$ can be canonically identified with the vector bundle $J^1(Q,\mathbb{R}^k)_0$ of k^1-covelocities of the manifold Q, the manifold of 1-jets of maps with target at $0\in\mathbb{R}^k$ and projection map $\tau^*:J^1(Q,\mathbb{R}^k)_0\to Q$, $\tau(j^1_{q,0}\sigma)=q$, say,

$$J^1(Q,\mathbb{R}^k)_0\equiv T^*Q\overset{k}{\oplus}\cdots\oplus T^*Q,$$

$$j^1_{q,0}\sigma\equiv(\mathrm{d}\sigma^1(q),\ldots,\mathrm{d}\sigma^k(q)),$$

where $\sigma^A=\pi_A\circ\sigma:Q\to\mathbb{R}$ is the Ath component of σ, and $\pi_A:\mathbb{R}^k\to\mathbb{R}$ is the canonical projection $1\leqslant A\leqslant k$. For this reason we shall also call to $(T^1_k)^*Q$ *the bundle of k^1-covelocities of the manifold Q*.

If (q^i) are local coordinates on $U\subseteq Q$, then the induced local coordinates (q^i,p_i), $1\leqslant i\leqslant n$, on $T^*U=(\tau^*_Q)^{-1}(U)$, are given by

$$q^i(\alpha_q)=q^i(q),\quad p_i(\alpha_q)=\alpha_q\left(\frac{\partial}{\partial q^i}(q)\right),\tag{1}$$

and the induced local coordinates (q^i,p^A_i), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, on $(T^1_k)^*U=(\tau^*)^{-1}(U)$ are given by

$$q^i(\alpha_1(q),\ldots,\alpha_k(q))=q^i(q),\quad p^A_i(\alpha_1(q),\ldots,\alpha_k(q))=\alpha_A(q)\left(\frac{\partial}{\partial q^i}(q)\right).$$

Let us denote by $\{r_1,\ldots,r_k\}$ the canonical basis of $\mathbb{R}^k$.

Definition II.1 (Günther[1]): A closed nondegenerate $\mathbb{R}^k$-valued 2-form,

$$\overline{\omega}=\sum_{A=1}^{k}\omega_A\otimes r_A,$$

on a manifold M of dimension N is called a polysymplectic form. *The pair $(M,\overline{\omega})$ is called a* polysymplectic manifold.

We shall introduce now the *canonical polysymplectic structure* on $(T^1_k)^*Q$. The canonical polysymplectic structure $\overline{\omega}=\Sigma^k_{A=1}(\omega_0)_A\otimes r_A$, on $(T^1_k)^*Q$ is defined by

$$(\omega_0)_A=(\tau^*_A)^*(\omega_0),\quad 1\leqslant A\leqslant k,$$

where $\tau^*_A:(T^1_k)^*Q\to T^*Q$ is the projection on the Ath-copy T^*Q of $(T^1_k)^*Q$, and $\omega_0=-\mathrm{d}\theta_0$ is the canonical symplectic structure of T^*Q, being θ_0 the Liouville 1-form defined by

$$\theta_0(\alpha_q)(\tilde{X}_{\alpha_q})=\alpha_q((\tau^*_Q)_*(\alpha_q)(\tilde{X}_{\alpha_q})),\quad \alpha_q\in T^*Q,\ \tilde{X}_{\alpha_q}\in T_{\alpha_q}(T^*Q).$$

One can also define the 2-forms $(\omega_0)_A$ by $(\omega_0)_A=-d(\theta_0)_A$ where $(\theta_0)_A=(\tau^*_A)^*\theta_0$. Thus the canonical symplectic structure on T^*Q is locally given by

$$\omega_0=-\mathrm{d}\theta_0=-d(p_i\,\mathrm{d}q^i)=\mathrm{d}q^i\wedge\mathrm{d}p_i,\tag{2}$$

and the canonical polysymplectic structure $((\omega_0)_1,\ldots,\omega_0)_k)$ on $(T^1_k)^*Q$ is locally given by

$$(\omega_0)_A=-d(\theta_0)_A=-d(p^A_i\,\mathrm{d}q^i)=\mathrm{d}q^i\wedge\mathrm{d}p^A_i.\tag{3}$$

Definition II.2 (Günther[1]): A polysymplectic form $\overline{\omega}$ on a manifold M is called standard *iff for every point of M there exists a local coordinates system such that ω_A is written locally as in (3).*

So the canonical polysymplectic form $\overline{\omega}$ on $(T^1_k)^*Q$ is standard.

B. The tangent bundle of k^1-velocities of a manifold

For an arbitrary manifold Q, let us denote by T^1_kQ the Whitney sum $TQ\overset{k}{\oplus\cdots\oplus}TQ$ of k copies of TQ, with projection $\tau:T^1_kQ\to Q$, $\tau(v_1(q),\ldots,v_k(q))=q$.

T^1_kQ can be identified with the manifold $J^1_0(\mathbb{R}^k,Q)$ of the k^1-velocities of Q, that is, 1-jets of maps with source at $0\in\mathbb{R}^k$ and with projection map $\tau:T^1_kQ\to Q$, $\tau(j^1_{0,q}\sigma)=\sigma(0)=q$, say

$$J^1_0(\mathbb{R}^k,Q)\equiv TQ\overset{k}{\oplus\cdots\oplus}TQ,$$

$$j^1_{0,q}\sigma\equiv(v_1(q),\ldots,v_k(q)),$$

where $q=\sigma(0)$ and $v_A=\sigma_*(0)[(\partial/\partial t^A)(0)]$.

So we shall call T^1_kQ *the tangent bundle of k^1-covelocities of Q*. If (q^i) are local coordinates on $U\subseteq Q$ then the induced local coordinates (q^i,v^i), $1\leqslant i\leqslant n$, on $TU=\tau_Q^{-1}(U)$ are given by

$$q^i(v_q)=q^i(q),\quad v^i(v_q)=v_q(q^i),$$

and the induced local coordinates (q^i,v^i_A), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, on $T^1_kU=\tau^{-1}(U)$ are given by

$$q^i(v_1(q),\ldots,v_k(q))=q^i(q),\quad v^i_A(v_1(q),\ldots,v_k(q))=v_A(q)(q^i).$$

We shall introduce now the *canonical k-tangent structure* on T^1_kQ.

Definition II.3: For a vector X_q at Q, and for $A=1,\ldots,k$, we define its vertical A-lift $(X_q)^A$ as the vector on T^1_kQ given by

$$(X_q)^A(v_1(q),\ldots,v_k(q))=\frac{d}{ds}(v_1(q),\ldots,v_{A-1}(q),v_A(q)+sX_q,v_{A+1}(q),\ldots,v_k(q))_{|_{s=0}}$$

for all points $(v_1(q),\ldots,v_k(q))\in T_k^1Q$.

In local coordinates we have

$$(X_q)^A=a^i\frac{\partial}{\partial v_A^i} \tag{4}$$

for a vector $X_q=a^i(\partial/\partial q^i)$.

The *canonical k-tangent structure* on T_k^1Q is the set $(S^1,\ldots,S^k)$ of tensor fields of type (1, 1) defined by

$$S^A(v)(Z_v)=(\tau_*(v)(Z_v))^A,\quad \text{for all } Z_v\in T_v(T_k^1Q),\quad v=(v_1(q),\ldots,v_k(q)),$$

for each $A=1,\ldots,k$.

From (4) we have in local coordinates

$$S^A=\frac{\partial}{\partial v_A^i}\otimes dq^i. \tag{5}$$

The tensors S^A can be regarded as the $(0,\ldots,0,\overset{A}{1},0,\ldots,0)$-lift of the identity tensor on Q to T_k^1Q defined by Morimoto.[21]

Remark II.1: The k-tangent manifolds were introduced as a generalization of the tangent manifolds by de León *et al.*[10,11] The canonical model of these manifolds is T_k^1Q with the structure given by $(S^1,\ldots,S^k)$.

To develop later the Lagrangian formalism, we shall construct now a polysymplectic structure on T_k^1Q, for each regular Lagrangian $L:T_k^1Q\to\mathbb{R}$, using its canonical k-tangent structure.

Definition II.4: A Lagrangian $L:T_k^1Q\to\mathbb{R}$ *is called regular if and only if*

$$\det\left(\frac{\partial^2L}{\partial v_A^i\partial v_B^j}\right)\neq 0,\quad 1\leqslant i,j\leqslant n,\quad 1\leqslant A,B\leqslant k. \tag{6}$$

Let us consider the 1-forms $(\theta_L)_A=dL\circ S^A$, $1\leqslant A\leqslant k$. In a local coordinates system (q^i,v_A^i) we have

$$(\theta_L)_A=\frac{\partial L}{\partial v_A^i}dq^i,\quad 1\leqslant A\leqslant k. \tag{7}$$

Introducing the following 2-forms $(\omega_L)_A=-d(\theta_L)_A$, $1\leqslant A\leqslant k$, one can easily prove the following proposition.

Proposition II.1: $L:T_k^1Q\to\mathbb{R}$ *is a regular Lagrangian if and only if* $((\omega_L)_1,\ldots,(\omega_L)_k)$ *is a polysymplectic structure on* T_k^1Q. ■

This polysymplectic structure, associated to L, was also introduced by Günther[1] using the Legendre transformation.

The Legendre map $FL:T_k^1Q\to(T_k^1)^*Q$, was introduced by Günther,[1] and we rewrite it as follows: if $(v_1(q),\ldots,v_k(q))\in(T_k^1)_qQ$,

$$[FL(v_1(q),\ldots,v_k(q))]^A(w_q)=\frac{d}{ds}L(v_1(q),\ldots,v_A(q)+sw_q,\ldots,v_k(q))_{|s=0},$$

for each $A=1,\ldots,k$. We deduce that FL is locally given by

$$(q^i, v^i_A) \to \left(q^i, \frac{\partial L}{\partial v^i_A} \right). \tag{8}$$

In fact, from (7) and (8), we easily obtain the following Lemma.

Lemma II.1: For every $1 \leqslant A \leqslant k$, $(\omega_L)_A = (FL)^*(\omega_0)_A$, *where* $(\omega_0)_1, \ldots, (\omega_0)_k$ *are the 2-forms of the canonical polysymplectic structure.* ■

Then, from (8) we obtain the following.

Proposition II.2: Let L be a Lagrangian. The following conditions are equivalent: (1) L is regular, (2) FL is a local diffeomorphism. (3) $((\omega_L)_1, \ldots, (\omega_L)_k)$ *is a polysymplectic structure on* $T^1_k Q$. ■

III. SECOND ORDER PARTIAL DIFFERENTIAL EQUATIONS ON $T^1_k Q$

A. *k*-vector fields

Let M be an arbitrary manifold and $\tau: T^1_k M \to M$ its tangent bundle of k^1-velocities.

Definition III.1: A section $X: M \to T^1_k M$ *of the projection* τ *will be called a* k-vector field *on* M.

Since $T^1_k M$ is the Whitney sum $TM \overset{k}{\oplus \cdots \oplus} TM$ of k copies of TM, we deduce that a k-vector field X defines a family of k-vector fields $X_1, \ldots, X_k$ on M by projecting X onto every factor.

Definition III.2: An integral section of the k-vector field $(X_1, \ldots, X_k)$ *passing through a point* $x \in M$ *on* M *is a map* $\phi: U_0 \subset \mathbb{R}^k \to M$, *defined on some neighborhood* U_0 *of* $0 \in \mathbb{R}^k$, *such that*

$$\phi(0) = x, \quad \phi_*(t)\left(\frac{\partial}{\partial t^A}(t) \right) = X_A(\phi(t)) \quad \textit{for all } t \in U_0, \quad 1 \leqslant A \leqslant k, \tag{9}$$

or equivalently, ϕ *satisfies* $X \circ \phi = \phi^{(1)}$, *where* $\phi^{(1)}$ *is the first prolongation of* ϕ *defined by*

$$\phi^{(1)}: U_0 \subset \mathbb{R}^k \to T^1_k M,$$

$$t \to \phi^{(1)}(t) = j^1_0 \phi_t, \quad \phi_t(\overline{t}) = \phi(\overline{t} + t),$$

for all $\overline{t}, t \in \mathbb{R}^k$ *such that* $\overline{t} + t \in U_0$.

In local coordinates,

$$\phi^{(1)}(t^1, \ldots, t^k) = \left(\phi^i(t^1, \ldots, t^k), \frac{\partial \phi^i}{\partial t^A}(t^1, \ldots, t^k) \right), \quad 1 \leqslant A \leqslant k, \ 1 \leqslant i \leqslant n. \tag{10}$$

We say that a k-vector field $(X_1, \ldots, X_k)$ on M is integrable if there is an integral section passing through each point of M.

Remark III.1: Let us consider the trivial bundle $\pi: E = \mathbb{R}^k \times M \to \mathbb{R}^k$. A jet field γ on π (see Ref. 22) is a section of the projection $\pi_{1,0}: J^1\pi \equiv \mathbb{R}^k \times T^1_k M \to E \equiv \mathbb{R}^k \times M$. If we identify each k-vector field X on M with the jet field $\gamma = (id_{R^k}, X)$, that is $\gamma(t,q) = (t, X_1(q), \ldots, X_k(q))$, then the integral sections of the jet field γ correspond to the *solutions* of the k-vector field X.

We remark that if ϕ is an integral section of a k-vector field $(X_1, \ldots, X_k)$ then each curve on M defined by $\phi_A = \phi \circ h_A$, where $h_A: \mathbb{R} \to \mathbb{R}^k$ is the natural inclusion $h_A(s) = (0, \ldots, \overset{A}{0}, s, 0, \ldots, 0)$, is an integral curve of the vector field X_A on M, with $1 \leqslant A \leqslant k$.

B. Second order partial differential equations on $T^1_k Q$

The aim of this section is to characterize the integrable k-vector fields on $T^1_k Q$ such that their integral sections are canonical prolongations of maps from $\mathbb{R}^k$ to Q.

Definition III.3: A k-vector field on T^1_kQ, that is, a section $\xi\equiv(\xi_1,\ldots,\xi_k):T^1_kQ\to T^1_k(T^1_kQ)$ of the projection $\tau_{T^1_kQ}:T^1_k(T^1_kQ)\to T^1_kQ$, is a second order partial differential equation (SOPDE) *if and only if it is also a section of the vector bundle $T^1_k(\tau):T^1_k(T^1_kQ)\to T^1_kQ$, where $T^1_k(\tau)$ is defined by $T^1_k(\tau)(j^1_0\sigma)=j^1_0(\tau\circ\sigma)$.*

From a direct computation in local coordintes we obtain that the local expression of a SOPDE ξ is

$$\xi_A(q^j,v^j_C)=v^i_A\frac{\partial}{\partial q^i}+(\xi_A)^i_B(q^j,v^j_C)\frac{\partial}{\partial v^i_B},\quad 1\leqslant A\leqslant k. \tag{11}$$

From (9), (10), and (11) we deduce the following proposition.

Proposition III.1: Let ξ be an integrable k-vector field on T^1_kQ. The necessary and sufficient condition for ξ to be a second order partial differential equation is that its integral sections are first prolongations $\phi^{(1)}$ of maps $\phi:\mathbb{R}^k\to Q$. That is

$$\xi_A(\phi^{(1)}(t))=(\phi^{(1)})_*(t)\left(\frac{\partial}{\partial t^A}(t)\right),$$

for all $A=1,\ldots,k$. These maps ϕ will be called solutions of the SOPDE ξ.

From (10) and (11) we have the following.

Proposition III.2: $\phi:\mathbb{R}^k\to Q$ is a solution of the SOPDE $\xi=(\xi_1,\ldots,\xi_k)$, locally given by (11), if and only if

$$\frac{\partial^2\phi^i}{\partial t^A\partial t^B}(t)=(\xi_A)^i_B(\phi^{(1)}(t)).$$

If $\xi:T^1_kQ\to T^1_k(T^1_kQ)$ is an integrable SOPDE, then for all integral sections $\sigma:U\subset\mathbb{R}^k\to T^1_kQ$ we have $(\tau\circ\sigma)^{(1)}=\sigma$, where $\tau:T^1_kQ\to Q$ is the canonical projection.

Now we show how to characterize the SOPDE's using the canonical k-tangent structure of T^1_kQ.

Definition III.4: The Liouville vector field C on T^1_kQ is the infinitesimal generator of the following flow:

$$\mathbb{R}\times T^1_kQ\to T^1_kQ,$$

$$(s,(v_1(q),\ldots,v_k(q)))\to(e^s v_1(q),\ldots,e^s v_k(q)),$$

and in local coordinates has the form

$$C=\sum_{i,B} v^i_B\frac{\partial}{\partial v^i_B}. \tag{12}$$

We can write $C=C_1+\cdots+C_k$ where C_A are the canonical vector fields on T^1_kQ given by the following flows:

$$\mathbb{R}\times T^1_kQ\to T^1_kQ,$$

$$(s,(v_1(q),\ldots,v_k(q)))\to(v_1(q),\ldots,v_{A-1}(q),e^s v_A(q),v_{A+1}(q),\ldots,v_k(q)).$$

In local coordinates,

$$C_A=\sum_i v^i_A\frac{\partial}{\partial v^i_A}. \tag{13}$$

From (5), (11), (12), and (13) we deduce the following.

Proposition III.3: A k-vector field $\xi=(\xi_1,\ldots,\xi_k)$ *on* T^1_kQ *is a SOPDE if and only if* $S^A(\xi_A)=C_A$, *for all* $1\leqslant A\leqslant k$, *where* $(S^1,\ldots,S^k)$ *is the canonical k-tangent structure on* T^1_kQ.

IV. HAMILTONIAN AND LAGRANGIAN FORMALISMS

A. Hamiltonian formalism

We recall the Hamilton formalism developed by Günther[1] using polysymplectic structures, showing that the role played by symplectic manifolds in classical mechanics is here played by the polysymplectic manifolds.

Let $(M,\omega_A,1\leqslant A\leqslant k)$ be a polysymplectic manifold and let us consider the vector bundle morphism $\Omega^\sharp$ defined by

$$\begin{aligned}&\Omega^\sharp:\quad T^1_kM\to T^*M,\\ &(X_1,\ldots,X_k)\to\Omega^\sharp(X_1,\ldots,X_k)=\sum_{A=1}^{k}\imath_{X_A}\omega_A\,.\end{aligned}\tag{14}$$

Definition IV.1: Let $H:M\to\mathbb{R}$ *be a function on M. Any k-vector field* $(X_1,\ldots,X_k)$ *on M such that*

$$\Omega^\sharp(X_1,\ldots,X_k)=\mathrm{d}H\tag{15}$$

will be called an evolution k-vector field on M associated with the Hamiltonian function H.

It should be noticed that in general the solution to the above equation is not unique. In fact the solutions are given by $(X_1,\ldots,X_k)+(\ker\Omega^\sharp)$.

If M is a standard manifold we have coordinates (q^i,p^A_i) on M. Then from Definition III.2, (14) and (15) we deduce the following.

Proposition IV.1: If $(X_1,\ldots,X_k)$ *is an integrable evolution k-vector field associated to H, then its integral sections* $\phi(t^B)\equiv(\phi^i(t^B),\phi^A_i(t^B))$ *are solutions of the Hamilton field equations corresponding to H,*

$$\frac{\partial H}{\partial q^i}=-\sum_{A=1}^{k}\frac{\partial\phi^A_i}{\partial t^A},\quad \frac{\partial H}{\partial p^A_i}=\frac{\partial\phi^i}{\partial t^A},\quad 1\leqslant i\leqslant n,\quad 1\leqslant A\leqslant k.\tag{16}$$

Remark IV.1: The *k*-symplectic manifolds were introduced in Awane[3–5] and they coincide with the *standard polysymplectic* manifolds. In the Hamiltonian formalism Günther uses a standard polysymplectic manifold in order to have local coordinates (q^i,p^A_i), which is equivalent to consider a *k*-symplectic manifold. We explain this now.

Definition IV.2 (Awane[3]): A k-symplectic structure on a manifold M of dimension $N=n+kn$ *is a family* $(\omega_A,V;1\leqslant A\leqslant k)$, *where each* ω_A *is a closed 2-form and V is an integrable nk-dimensional distribution on M such that*

$$(i)\quad \omega_{A_{]V\times V}}=0,\quad (ii)\quad \bigcap_{A=1}^{k}\ker\omega_A=\{0\}.$$

In this case (M,ω_A,V) *is called a k-symplectic manifold.*

Theorem IV.1 *(Awane[3]): Let* $(\omega_A,V;1\leqslant A\leqslant k)$ *be a k-symplectic structure on M. About every point of M we can find a local coordinate system* (q^i,p^A_i), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, *such that*

$$\omega_A=\mathrm{d}q^i\wedge\mathrm{d}p^A_i,\quad 1\leqslant A\leqslant k.\tag{17}$$

The canonical model of *k*-symplectic manifolds is also $(T^1_k)^*Q$ and the canonical *k*-symplectic structure $(\omega_A,V;1\leqslant A\leqslant k)$, on $(T^1_k)^*Q$ is given by

$$\omega_A=(\omega_0)_A=(\tau_A^*)^*(\omega_0),\quad V(j^1_{q,0}\sigma)=\ker(\tau^*)_*(j^1_{q,0}\sigma).$$

Therefore, the 2-forms of the canonical polysymplectic structure and the canonical k-symplectic structure on $(T^1_k)^*Q$ coincide.

From (17) we know that the standard polysymplectic structures and the k-symplectic structures coincide. Indeed, if $\overline{\omega}=\Sigma_{A=1}^k\omega_A\otimes r_A$ is a standard polysymplectic structure on M, given a local adapted coordinate system (q^i,p_i^A) we can define, locally, the distribution V, of dimension nk, by $\mathrm{d}q^1=\cdots=\mathrm{d}q^n=0$. Then, $(\omega_1,\ldots,\omega_k,V)$ is a k-symplectic structure on M.

For this reason, the Günther's formalism, called polysymplectic formalism, could be called k-symplectic formalism.

Example IV.1: We shall use the above formalism to obtain an intrinsic version for the electrostatic equations. Consider $\mathbb{R}^3$ with a metric g with components g_{ij}. Let $\sigma:\mathbb{R}^3\to\mathbb{R}$ be the electric potential and $P=(P_1,P_2,P_3):\mathbb{R}^3\to\mathbb{R}^3$ the electric field. Denote by (t^1,t^2,t^3) the standard coordinates on $\mathbb{R}^3$, and set $\sqrt{g}=\sqrt{\det g_{ij}}$. By $r(t)$ we denote the scalar function which gives the density of electric charge on $\mathbb{R}^3$.

In this example we suppose that $r(t)$ is constant $r(t)=r$, that is, the distribution of the electric charge is constant on $\mathbb{R}^3$, and that the metric g on $\mathbb{R}^3$ is the Euclidean metric.

Let us consider on $M=(T^1_3)^*\mathbb{R}$ the canonical polysymplectic structure $((\omega_0)_1,(\omega_0)_2,(\omega_0)_3)$. We denote by (q,p^1,p^2,p^3) the local coordinates on $(T^1_3)^*\mathbb{R}$ induced by the standard coordinate (q) on $\mathbb{R}$, and define a Hamiltonian function $H:(T^1_3)^*\mathbb{R}\to\mathbb{R}$ by

$$H(q,p^1,p^2,p^3)=4\pi rq+\frac{1}{2}\sum_{A=1}^{3}(p^A)^2.$$

Consider the equation

$$\Omega^\sharp(X_1,X_2,X_3)=\sum_{A=1}^{3}\imath_{X_A}(\omega_0)_A=\mathrm{d}H, \tag{18}$$

where (X_1,X_2,X_3) is a 3-vector field on $(T^1_3)^*\mathbb{R}$.

Let $\phi:\mathbb{R}^3\to(T^1_3)^*\mathbb{R},\phi(t)=(\psi(t),\psi^1(t),\psi^2(t),\psi^3(t))$ be an integral section of an evolution 3-vector field which is a solution of (18). Then we obtain

$$4\pi r=-\left(\frac{\partial\psi^1}{\partial t^1}+\frac{\partial\psi^2}{\partial t^2}+\frac{\partial\psi^3}{\partial t^3}\right),\quad \psi^A=\frac{\partial\psi}{\partial t^A},\quad 1\leqslant A\leqslant 3,$$

which are the electrostatic equations, and then the components $\psi(t)$ and $(\psi^1(t),\psi^2(t),\psi^3(t))$ of ϕ are the electric potential σ and the electric field $P=(P_1,P_2,P_3)$ on $\mathbb{R}^3$, respectively. So Eq. (18) is a geometric version of the electrostatic equations.

B. Lagrangian formalism

In classical mechanics the symplectic structure of Hamiltonian theory and the tangent structure of Lagrangian theory play complementary roles (see Refs. 13, 15, and 16).

In this section, we recall the Lagrangian formalism developed by Günther[1] using the polysymplectic structures. Here we can see how the polysymplectic structures and the k-tangent structures play also a complementary role in field theory.

Given a Lagrangian function of the form $L=L(q^i,v^i_A)$ one obtains, by using a variational principle, the *generalized Euler–Lagrange equations* for L:

$$\sum_{A=1}^{k}\frac{d}{\mathrm{d}t^A}\left(\frac{\partial L}{\partial v^i_A}\right)-\frac{\partial L}{\partial q^i}=0,\quad v^i_A=\frac{\partial q^i}{\partial t^A}. \tag{19}$$

Let $L:T^1_kQ\to\mathbb{R}$ be a regular Lagrangian and let us consider the polysymplectic structure $((\omega_L)_1,\ldots,(\omega_L)_k)$ on T^1_kQ defined by L. Let us observe that when L is regular then $((\omega_L)_1,\ldots,(\omega_L)_k,V)$ is a k-symplectic structure on T^1_kQ.

Let $\Omega_L^\sharp:T^1_k(T^1_kQ)\to T^*(T^1_kQ)$ be the morphism defined by $((\omega_L)_1,\ldots,(\omega_L)_k)$ as in (14), we can set the following equation:

$$\Omega_L^\sharp(X_1,\ldots,X_k)=\mathrm{d}E_L, \tag{20}$$

where $E_L=C(L)-L$, and C is the Liouville vector field on T^1_kQ.

Proposition IV.2: Let L be a regular Lagrangian. If $\xi=(\xi_1,\ldots,\xi_k)$ is a solution of (20) then it is a SOPDE. Moeover if ξ is integrable then the solutions of ξ are solutions of the Euler–Lagrange equations (19).

Proof: It is a direct computation in local coordinates using (6), (7), (11), and (12). ■

Example IV.2: In this example we consider the theory of a vibrating string. Coordinates (t^1,t^2) are interpreted as the time and the distance along the string, respectively. If $\phi(t^1,t^2)$ denotes the displacement of each point of the string as function of the time t^1 and the position t^2, the motion equations are

$$\sigma\frac{\partial^2\phi}{\partial(t^1)^2}-\tau\frac{\partial^2\phi}{\partial(t^2)^2}=0, \tag{21}$$

where σ and τ are certain constants of the mechanical system.

We shall show that the equations (21) can be described as the Euler–Lagrange equations associated to a Lagrangian L defined on the jet bundle T^1_kQ with $Q=\mathbb{R}$ and $k=2$. Let us denote by (x,v_1,v_2) the coordinates of $T^1_2\mathbb{R}$ and consider the Lagrangian

$$L:\quad T^1_2\mathbb{R}\to\mathbb{R},$$

$$(x,v_1,v_2)\to\tfrac{1}{2}(\sigma v_1^2-\tau v_2^2).$$

Since L is regular there exists a polysymplectic structure, $((\omega_L)_1,(\omega_L)_2)$, associated to L given in local coordinates by $(\omega_L)_1=\sigma\ \mathrm{d}v_1\wedge\mathrm{d}x$, $(\omega_L)_2=-\tau\,\mathrm{d}v_2\wedge\mathrm{d}x$.

The energy $E_L=C(L)-L$ is locally given by $E_L=\frac{1}{2}(\sigma v_1^2-\tau v_2^2)$ and

$$\mathrm{d}E_L=\sigma v_1\,\mathrm{d}v_1-\tau v_2\,\mathrm{d}v_2. \tag{22}$$

Now we consider the map $\Omega_L^\sharp:T^1_2(T^1_2\mathbb{R})\to T^*(T^1_2\mathbb{R})$, and let us suppose that there exists (ξ_1,ξ_2) solution of the equation

$$\Omega_L^\sharp(\xi_1,\xi_2)=\imath_{X_1}(\omega_L)_1+\imath_{X_2}(\omega_L)_2=\mathrm{d}E_L, \tag{23}$$

then, from Proposition IV.2 we know that (ξ_1,ξ_2) is a SOPDE. Let us suppose that $(\xi_1,\xi_2)\in T^1_2(T^1_2\mathbb{R})$ are locally given by

$$\xi_A=v_A\frac{\partial}{\partial x}+(\xi_A)_1\frac{\partial}{\partial v_1}+(\xi_A)_2\frac{\partial}{\partial v_2},\quad 1\leqslant A\leqslant 2, \tag{24}$$

thus, if (ξ_1,ξ_2) is a solution of $\Omega_L^\sharp(\xi_1,\xi_2)=\mathrm{d}E_L$, from (22) and (24) we have

$$\sigma(\xi_1)_1-\tau(\xi_2)_2=0. \tag{25}$$

If $\phi:\mathbb{R}^2\to\mathbb{R}$, $\phi=\phi(t_1,t_2)$ is a solution of $\xi=(\xi_1,\xi_2)$, then from Proposition III.2 and (25) we obtain

$$0=\sigma(\xi_1)_1-\tau(\xi_2)_2=\sigma\frac{\partial\phi}{\partial t_1^2}-\tau\frac{\partial\phi}{\partial t_2^2},$$

thus equation (23) is a geometric version for the equations (21).

V. THE MOMENTUM MAP

Let G be a Lie group and $\mathcal{G}$ its Lie algebra. We shall use the notations $\mathcal{G}^k=\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G}$ and $\mathcal{G}^k{}^*=(\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G})^*$.

The adjoint representation $\mathrm{Ad}:G\to\mathrm{Aut}(\mathcal{G})$ induces, for any $g\in G$, the map $\mathrm{Ad}_g^k:\mathcal{G}^k\to\mathcal{G}^k$ defined by

$$\mathrm{Ad}_g^k(\xi_1,\ldots,\xi_k)=(\mathrm{Ad}_g\xi_1,\ldots,\mathrm{Ad}_g\xi_k),\quad(\xi_1,\ldots,\xi_k)\in\mathcal{G}^k,$$

and thus an action $\Phi:G\times\mathcal{G}^k\to\mathcal{G}^k$, defined by

$$\Phi(g,\eta)=\mathrm{Ad}_g^k(\eta),\quad g\in G,\quad \eta=(\eta_1,\ldots,\eta_k)\in\mathcal{G}^k,$$

and we shall call it the *k-adjoint action* of G on $\mathcal{G}^k$.

The representation $\mathrm{Ad}^k:G\to\mathrm{Aut}(\mathcal{G}^k)$, $g\to\mathrm{Ad}_g^k$, induces $\mathrm{ad}^k=(\mathrm{Ad}^k)_*(e):\mathcal{G}\to\mathrm{End}(\mathcal{G}^k)$, which is given by

$$\mathrm{ad}_\xi^k(\xi_1,\ldots,\xi_k)=(\mathrm{ad}_\xi\xi_1,\ldots,\mathrm{ad}_\xi\xi_k),\quad \xi\in\mathcal{G},(\xi_1,\ldots,\xi_k)\in\mathcal{G}^k,$$

where $\mathrm{ad}_\xi\xi_A=[\xi,\xi_A]$.

Now, for any $g\in G$ we define $\mathrm{Ad}_g^k{}^*:\mathcal{G}^k{}^*\to\mathcal{G}^k{}^*$ by

$$\mathrm{Ad}_g^k{}^*(\mu)=\mu\circ\mathrm{Ad}_g^k,\quad \mu\in\mathcal{G}^k{}^*,$$

and we define *k-coadjoint action* $\Phi:G\times\mathcal{G}^k{}^*\to\mathcal{G}^k{}^*$ by

$$\Phi(g,\mu)=\mathrm{Ad}_{g^{-1}}^k{}^*(\mu),\quad g\in G,\quad \mu\in\mathcal{G}^k{}^*. \tag{26}$$

The representation $\mathrm{Ad}^k{}^*:G\to\mathrm{Aut}(\mathcal{G}^k{}^*)$, $g\to\mathrm{Ad}_g^k{}^*$, induces $\mathrm{ad}^k{}^*=(\mathrm{Ad}^k{}^*)_*(e):\mathcal{G}\to\mathrm{End}(\mathcal{G}^k{}^*)$, given by

$$(\mathrm{ad}_\xi^k{}^*(\alpha))(\xi_1,\ldots,\xi_k)=(\alpha\circ\mathrm{ad}_\xi^k)(\xi_1,\ldots,\xi_k),\quad \alpha\in\mathcal{G}^k{}^*,(\xi_1,\ldots,\xi_k)\in\mathcal{G}^k.$$

Definition V.1: Let $(M,\omega_1,\ldots,\omega_k)$ be a polysymplectic manifold. An action $\Phi:G\times M\to M$ of the Lie group G on M, is called polysymplectic if $\Phi_g^*\omega_A=\omega_A$ for all $g\in G$ and all $A=1,\ldots,k$.

If $\mathcal{G}=T_eG$ is the Lie algebra of the Lie group G, then for any $\xi\in\mathcal{G}$ we consider the fundamental vector field ξ_M defined by

$$\xi_M(x)=(\Phi_x)_*(e)(\xi)=\frac{d}{\mathrm{d}s}\Phi(\exp s\xi,x)_{|s=0},\quad x\in M.$$

Definition V.2: Let (M,ω) be a symplectic manifold with a symplectic action $\Psi:G\times M\to M$. The map $J:M\to\mathcal{G}^*$ is said to be a momentum map for the action Ψ if

$$i_{\xi_M}\omega=\mathrm{d}\hat{J}(\xi),\quad \textit{for all}\quad \xi\in\mathcal{G}, \tag{27}$$

where $\hat{J}(\xi):M\to\mathbb{R}$ is the map defined by $\hat{J}(\xi)(x)=J(x)(\xi)$, $x\in M$.

Taking into account (14) we introduce the following definition.

Definition V.3: Let $(M,\omega_1,\ldots,\omega_k)$ be a polysymplectic manifold. The map $J:M\to\mathcal{G}^k{}^*$ is said to be a momentum map for the action Φ if

$$\sum_{A=1}^{k} i_{(\xi_A)_M}\omega_A = \mathrm{d}\hat{J}(\xi_1,\ldots,\xi_k), \quad \textit{for all } (\xi_1,\ldots,\xi_k)\in \mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G}, \tag{28}$$

where $\hat{J}(\xi_1,\ldots,\xi_k):M\to\mathbb{R}$ *is the map defined by*

$$\hat{J}(\xi_1,\ldots,\xi_k)(x) = J(x)(\xi_1,\ldots,\xi_k), \quad x\in M.$$

Our definition of momentum map coincides with the definition given by Günther[1] in Remark 6.6. Let us observe that if J is a momentum map

$$d(\hat{J}(0,\ldots,\overset{A}{0},\xi,0,\ldots,0)) = i_{\xi_M}\omega_A \quad , \forall \xi\in\mathcal{G}, \ \ 1\leqslant A\leqslant k. \tag{29}$$

Definition V.4: A momentum map $J:M\to(\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G})^*$ *is called* $\mathrm{Ad}^{k}{}^*$*-equivariant if*

$$J(\Phi_g(x)) = \mathrm{Ad}^{k*}_{g^{-1}}J(x) \quad , \forall g\in G, x\in M. \tag{30}$$

In the following theorem, we resume Theorem 6.2, Proposition 6.8, and Theorem 6.10 of Günther,[1] given by (i), (ii), and (iii), respectively.

Theorem V.1: *Let* Φ *be a polysymplectic action of* G *on* M*. Let* H *be a* G*-invariant Hamiltonian function, and let* $\phi:U\to M$ *be an integral section of a evolution* k*-vector field* $((X_H)_1,\ldots,(X_H)_k)$ *associated with the Hamiltonian function* H*.*

(i) Let us suppose that Φ *is a strongly polysymplectic action, which means*

$$i_{\xi_M}\omega_A = \mathrm{d}F^A_\xi, \quad \textit{for all } \xi\in\mathcal{G}, \quad 1\leqslant A\leqslant k, \tag{31}$$

for some function $F_\xi:M\to\mathbb{R}^k$*. Then Trace* $d(F_\xi\circ\phi)=0$*, that is*

$$\sum_{A=1}^{k} d(F^A_\xi\circ\phi)(t)\left(\frac{\partial}{\partial t^A}(t)\right) = 0.$$

(ii) Let us suppose that Φ *has momentum map* J*. Then Trace* $d(P\circ\phi)=0$*, that is*

$$\sum_{A=1}^{k} d(P^A\circ\phi)(t)\left(\frac{\partial}{\partial t^A}(t)\right) = 0,$$

where $P^A = \hat{J}(0,\ldots,\overset{A}{0},\xi,0,\ldots,0):M\to\mathbb{R}$ *for all* $\xi\in\mathcal{G}$*.*

(iii) Let us assume that $\Omega = -d\theta$ *and* θ *are* G*-invariant. Then Trace* $d(\theta(\xi_M)\circ\phi)=0$*, that is*

$$\sum_{A=1}^{k} d(\theta^A(\xi_M)\circ\phi)(t)\left(\frac{\partial}{\partial t^A}(t)\right) = 0, \quad \textit{for all } \xi\in\mathcal{G}.$$

Proof: It is a consequence of (9), (14), (28), (31) and the fact that H is G-invariant. ■

Günther[1] remarks that (i) and (ii) are a version of the classical Noether theorem, which says that the infinitesimal generators of canonical transformations induce conserved currents; (iii) is the usual version of the field theoretic Noether theorem.

The following theorem, which generalizes the Theorem 4.2.10 in Abraham–Marsden,[2] will allow us to construct momentum maps for the manifolds $(T^1_k)^*Q$ and T^1_kQ. It is equivalent to the Proposition 6.9 in Günther.[1]

Theorem V.2: *Let Φ be a polysymplectic action of the Lie group G on the polysymplectic manifold $(M,\omega_1,\ldots,\omega_k)$. If we assume that the polysymplectic structure ω_A is exact, that is $\omega_A=-\mathrm{d}\theta_A$, and the action leaves each θ_A invariant, that is $\Phi_g^*\theta_A=\theta_A$ for all $g\in G$, then $J:M\to(\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G})^*$ defined by*

$$J(x)(\xi_1,\ldots,\xi_k)=\sum_{A=1}^{k}(\theta_A)(x)((\xi_A)_M(x)),\quad x\in M,(\xi_1,\ldots,\xi_k)\in\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G},\tag{32}$$

is an $\mathrm{Ad}^k{}^*$-equivariant momentum map for the action Φ.

Proof: Since $\mathcal{L}_{(\xi_A)_M}\theta^A=0$ we obtain $i_{(\xi_A)_M}\mathrm{d}\theta_A=-d(\theta_A(\xi_A)_M)$, and from (28) we obtain (32). To prove $\mathrm{Ad}^k{}^*$-equivariance we must show that

$$\hat{J}(\xi_1,\ldots,\xi_k)(\Phi_g(x))=\mathrm{Ad}^{k*}_{g^{-1}}J(x)(\xi_1,\ldots,\xi_k)=J(x)(\mathrm{Ad}_{g^{-1}}\xi_1,\ldots,\mathrm{Ad}_{g^{-1}}\xi_k),$$

that is,

$$\sum_{A=1}^{k}\theta_A((\xi_A)_M)(\Phi_g(x))=\sum_{A=1}^{k}\theta_A(x)((\mathrm{Ad}_{g^{-1}}\xi_A)_M(x)).$$

But this follows immediately from the identity $(\mathrm{Ad}_{g^{-1}}\xi)_M=(\Phi_g)^*\xi_M$, $\xi\in\mathcal{G}$, together with the invariance of each θ_A under Φ_g. ∎

Now, following Abraham–Marsden,[2] we extend the results about momentum maps in T^*Q and TQ, to the polysymplectic manifolds $(T^1_k)^*Q$ and T^1_kQ.

If $f:Q\to Q$, is a diffeomorphism then we can define the diffeomorphism $T^k{}^*f:(T^1_k)^*Q\to(T^1_k)^*Q$, by

$$T^k{}^*f(\alpha_1(q),\ldots,\alpha_k(q))=(\alpha_1(q)\circ f_*(f^{-1}(q)),\ldots,\alpha_k(q)\circ f_*(f^{-1}(q))).$$

Proposition V.1: For any diffeomorphism $f:Q\to Q$ we have $(T^k{}^*f)^*(\theta_0)_A=(\theta_0)_A$ and $(T^k{}^*f)^*(\omega_0)_A=(\omega_0)_A$, where $(\omega_0)_A=-d(\theta_0)_A$, $1\leqslant A\leqslant k$, is the canonical polysymplectic structure on $(T^1_k)^*Q$.

Proof: Analogous to the proof of Theorem 4.2.10 in Abraham–Marsden,[2]

$$(T^k{}^*f)^*(\theta_0)_A=(\tau_A^*\circ T^k{}^*f)^*\theta_0=(T^*f\circ\tau_A^*)^*\theta_0=((\tau_A^*)^*\circ(T^*f)^*)\theta_0=(\tau_A^*)^*\theta_0=(\theta_0)_A.$$

∎

An action $\Phi:G\times Q\to Q$ can be lifted to an action $\Phi^{T^*}:G\times(T^1_k)^*Q\to(T^1_k)^*Q$ defining

$$\Phi^{T^*}(g,(\alpha_1(q),\ldots,\alpha_k(q)))=(\alpha_1(q)\circ(\Phi_{g^{-1}})_*(\Phi_g(q)),\ldots,\alpha_k(q)\circ(\Phi_{g^{-1}})_*(\Phi_g(q))).\tag{33}$$

Let us observe that $(\Phi^{T^*})_g=T^k{}^*\Phi_{g^{-1}}$, then from Proposition V.1 and Theorem V.2, we obtain the following.

Corollary V.1: (i) If Φ is an action of G on Q then Φ^{T^*} is a polysymplectic action of G on $(T^1_k)^*Q$.

(ii) Φ^{T^*} has an $\mathrm{Ad}^k{}^*$-equivariant momentum map $J:(T^1_k)^*Q\to(\mathcal{G}\times\overset{k}{\cdots}\times\mathcal{G})^*$ given by

$$J(u)(\xi_1,\ldots,\xi_k)=\sum_{A=1}^{k}(\theta_0)_A(u)(\xi_{(T^1_k)^*Q}(u))=\sum_{A=1}^{k}\alpha_A(q)((\xi_A)_Q(q)),\tag{34}$$

where $u=(\alpha_1(q),\ldots,\alpha_k(q))$.

Proof: (i) It is a consequence of Proposition V.1.

(ii) It is a consequence of Theorem V.2 and the following identity:

$$(\theta_0)_A(u)((\xi_A)_{(T^1_k)^*Q}(u)) = ((\tau_A^*)^*\theta_0)(u)(\xi_A)_{(T^1_k)^*Q}(u)$$
$$= \theta_0(\tau_A^*(u))((\tau_A^*)_*(u)(\xi_A)_{(T^1_k)^*Q}(u))$$
$$= \tau_A^*(u)((\tau_Q^*\circ\tau_A^*)_*(u)(\xi_{(T^1_k)^*Q}(u))) = \alpha_A(q)((\xi_A)_Q(q)),$$

where in the last identity we have used that $\tau_Q^*\circ\tau_A^* = \tau^*$ and $(\tau^*)_*(\xi_{(T^1_k)^*Q}) = \xi_Q\circ\tau^*$. ■

When the manifold M is $(T^1_k)^*Q$ and we have a momentum map J on $(T^1_k)^*Q$, then for each fixed $A=1,\ldots,k$, we can define the map $J_A: T^*Q\to\mathcal{G}^*$ by

$$J_A(\alpha_q)(\xi) = J(0,\ldots,0,\overset{A}{\alpha_q},0,\ldots,0)(0,\ldots,0,\overset{A}{\xi},0,\ldots,0)\,, \tag{35}$$

where α_q and ξ are in the Ath position, $q\in Q$.

If we denote by $i_A: T^*Q\to(T^1_k)^*Q$ the inclusion map $\alpha_q\to(0,\ldots,0,\overset{A}{\alpha_q},0,\ldots,0)$ then

$$\hat{J}_A(\xi)(\alpha_q) = \hat{J}(0,\ldots,0,\overset{A}{\xi},0,\ldots,0)(0,\ldots,0,\overset{A}{\alpha_q},0,\ldots,0) = (\hat{J}(0,\ldots,0,\overset{A}{\xi},0,\ldots,0)\circ i_A)(\alpha_q)\,.$$

Lemma V.1: J_A is a momentum map on T^*Q.

Proof: For any $\xi\in\mathcal{G}$, $\alpha_q\in T^*Q$, $v_{\alpha_q}\in T_{\alpha_q}(T^*Q)$, we have

$$\mathrm{d}\hat{J}_A(\xi)(\alpha_q)(v_{\alpha_q}) = [\mathrm{d}\hat{J}(0,\ldots,0,\overset{A}{\xi},0,\ldots,0)(i_A(\alpha_q))\circ\mathrm{d}i_A(\alpha_q)](v_{\alpha_q})$$
$$= (i_{\xi_{(T^1_k)^*Q}}\omega_A)(i_A(\alpha_q))[(i_A)_*(\alpha_q)(v_{\alpha_q})]$$
$$= (i_{\xi_{(T^1_k)^*Q}}(\tau_A^*)^*\omega_0)(i_A(\alpha_q))[(i_A)_*(\alpha_q)(v_{\alpha_q})]$$
$$= \omega_0(\tau_A^*(i_A(\alpha_q)))\,((\tau_A^*)_*(i_A(\alpha_q))(\xi_{(T^1_k)^*Q}(i_A(\alpha_q))),(\tau_A^*\circ i_A)_*(\alpha_q)(v_{\alpha_q}))$$
$$= \omega_0(\alpha_q)\,(\xi_{T^*Q}(\alpha_q),v_{\alpha_q})\,.$$

We have used that $(\tau_A^*)_*(\xi_{(T^1_k)^*Q}) = \xi_{T^*Q}\circ\tau_A^*$, which holds from $\tau_A^*\circ\Phi^{T^*}_{(\alpha_1,\ldots,\alpha_k)} = \Psi_{\alpha_A}\circ\tau_A^*$ where $\Psi: G\times T^*Q\to T^*Q$ is the canonical action induced by the action $\Phi: G\times Q\to Q$. ■

The conservation law given in Theorem 4.2.2 in Abraham–Marsden[2] for a symplectic manifold can be extended in the following way to $(T^1_k)^*Q$.

Proposition V.2: Let Φ be an action of G on Q, Ψ^{T^*} the induced action of G on T^*Q, and Φ^{T^*} the induced action of G on $(T^1_k)^*Q$.

Let J be the $\mathrm{Ad}^k{}^*$-equivariant momentum map given in (34) and let J_Q be one of the momentum maps on T^*Q induced by J.

If X is a vector field on $(T^1_k)^*Q$, then we have the following.

(i) J is an integral for X if and only if J_Q is an integral for all $(\tau_A^*)_*X$, $1\leqslant A\leqslant k$.

(ii) If $\phi:\mathbb{R}^k\to(T^1_k)^*Q$ is an integral section of an integrable evolution k-vector field $((X_H)_1,\ldots,(X_H)_k)$ and J is an integral for all $(X_H)_A$, then J is constant along ϕ.

Proof: (i) From (28) and the identities

$$i_{\xi_{T^*Q}}\omega_0 = \mathrm{d}\hat{J}_Q(\xi)\,,\quad \forall\,\xi\in\mathcal{G},\quad \omega_A = (\tau_A^*)^*\omega_0\,,\quad (\tau_A^*)_*(\xi_A)_{(T^1_k)^*Q} = (\xi_A)_{T^*Q}\circ\tau_A^*\,, \tag{36}$$

$$\hat{J}(\xi_1,\ldots,\xi_k) = \sum_{A=1}^{k}\hat{J}(0,\ldots,0,\overset{A}{\xi_A},0,\ldots,0)\,, \tag{37}$$

we deduce

$$\mathrm{d}\hat{J}(\xi_1,\ldots,\xi_k)(X)=\sum_{B=1}^{k} d(\hat{J}_Q(\xi_B)\circ\tau_B^*)(X). \tag{38}$$

Let us suppose that J is an integral of X. So, taking $\xi_A=\xi$ and $\xi_B=0$ for all $B\neq A$ we obtain from (38) $\mathrm{d}\hat{J}_Q((\tau_A^*)_*X)=0$, for each A, $1\leqslant A\leqslant k$. Therefore J_Q is an integral for $(\tau_A^*)_*X$, $A=1,\ldots,k$.

Now let us suppose that J_Q is an integral for all $(\tau_A^*)_*X$, then from (38) we deduce that J is an integral for X.

(ii) By Definition III.2 we have

$$0=(X_H)_A(\phi(t))(\hat{J}(\xi_1,\ldots,\xi_k))=\frac{\partial}{\partial t^A}(t)(\hat{J}(\xi_1,\ldots,\xi_k)\circ\phi).$$

■

A generalized Noether theorem, which is a generalization of Corollary 4.2.14 in Abraham–Marsden[2] is the following.

Corollary V.2: Let G act on Q by $\Phi:G\times Q\to Q$ and let Φ^T denote the k-tangent action $\Phi^T:G\times T_k^1Q\to T_k^1Q$, defined by

$$\Phi^T(g,v_1(q),\ldots,v_k(q))=((\Phi_g)_*(q)(v_1(q)),\ldots,(\Phi_g)_*(q)(v_k(q)))$$

for all $(v_1(q),\ldots,v_k(q))\in T_k^1Q$, $q\in Q$, $g\in G$.

Let L be a regular Lagrangian on T_k^1Q with $(\theta_L)_A=(FL)^*(\theta_0)_A$, as usually. If we suppose that L is invariant under the action Φ^T, that is $L\circ\Phi_g^T=L$, for all $g\in G$, then we have the following.

(i) $(\Phi_g^T)^*(\theta_L)_A=(\theta_L)_A$, for all $g\in G$, $A=1,\ldots,k$;

(ii) the momentum map $J:T_k^1Q\to(\overset{k}{\mathcal{G}\times\cdots\times\mathcal{G}})^*$ for the action Φ^T is given by

$$J(u)(\xi_1,\ldots,\xi_k)=\sum_{A=1}^{k}\tau_A^*(FL(u))((\xi_A)_Q(q)), \tag{39}$$

and it is $\mathrm{Ad}^k{}^*$-equivariant.

Proof: (i) Using the definition of FL and the invariance of L under the action Φ^T we obtain $FL\circ\Phi_g^T=\Phi_g^{T^*}\circ FL$. Then, from Corollary V.1 and since $FL\circ\Phi_g^T=\Phi_g^{T*}\circ FL$ we obtain easily that $(\Phi_g^T)^*(\theta_L)_A=(\theta_L)_A$.

(ii) It is a consequence of Theorem V.2 and the fact that

$$(\theta_L)_A(u)(\xi_A)_{T_k^1Q}(u)=\tau_A^*(FL(u))((\xi_A)_Q(\tau^*(u))),$$

which can be obtained as follows:

$$\begin{aligned}(\theta_L)_A(u)(\xi_A)_{T_k^1Q}(u)&=((FL)^*(\theta_0)_A)(u)((\xi_A)_{T_k^1Q}(u))\\&=(\tau_A^*)^*\theta_0(FL(u))((FL)_*(u)(\xi_A)_{T_k^1Q}(u))\\&=\theta_0(\tau_A^*(FL(u)))((\tau_A^*\circ FL)_*(u)(\xi_A)_{T_k^1Q}(u))\\&=\tau_A^*(FL(u))((\tau_Q^*\circ\tau_A^*\circ FL)_*(u)(\xi_{T_k^1Q}(u)))\\&=\tau_A^*(FL(u))(\xi_A)_Q(\tau^*(u)),\end{aligned}$$

where in the last identity we have used that $\tau_Q^*\circ\tau_A^*\circ FL=\tau_Q$ and $(\tau_Q)_*(\xi_A)_{T_k^1Q}=\xi_Q$. ■

Example V.1: Let us consider any Riemannian metric $g=\langle\,,\rangle$ on a manifold Q. The Lagrangian $L=\frac{1}{2}g_{ij}(q)v_A^i v_B^j$ on T_k^1Q is regular and the Legendre tranformation $FL:T_k^1Q\to(T_k^1)^*Q$ is locally given by $(q^i,v_A^i)\to(q^i,p_i^A=g_{ij}(q)v_A^j)$. Then working on T_k^1Q, Corollary V.2 gives the momentum map

$$J(u)(\xi_1,\ldots,\xi_k)=\sum_{A=1}^{k}\tau_A^*(FL(u))(\xi_A(q))=\sum_{A=1}^{k}g(q)(v_A(q),\xi_A(q)) \tag{40}$$

for all $u=(v_1(q),\ldots,v_k(q))\in T_k^1Q$.

VI. REDUCTION

Let $(M,\omega_1,\ldots,\omega_k)$ be a polysymplectic manifold and $\Phi:G\times M\to M$ a polysymplectic action of the Lie group G on M. If $\mathcal{G}$ is the Lie algebra of G we have

$$T_p(Gp)=\{\xi_M(p)\,|\,\xi\in\mathcal{G}\},\quad \forall p\in M, \tag{41}$$

where Gp is the orbit of p and ξ_M is the fundamental vector field of M, under Φ, corresponding to ξ.

Let us assume that this action has an Ad^k*-equivariant momentum map $J:M\to\mathcal{G}^k*$. For $\mu\in\mathcal{G}^k*$, we denote by $G_\mu=\{g\in G\,|\,\mathrm{Ad}^{k*}_{g^{-1}}(\mu)=\mu\}$ the isotropy subgroup of G under the k-coadjoint action. The orbit space $M_\mu=J^{-1}(\mu)/G_\mu$ is well defined. If $\mu\in\mathcal{G}^k*$ is a regular value of J, then $J^{-1}(\mu)$ is a submanifold of M and if we assume that G_μ acts freely and properly on $J^{-1}(\mu)$ then we know that M_μ is a manifold, being the canonical projection $\pi_\mu:J^{-1}(\mu)\to M_\mu$ a submersion.

For the proof of the next theorem (which generalizes the Theorem 4.3.1 in Ref. 2) it is important to find next result.

Lemma VI.1: Under the conditions above, for any $p\in J^{-1}(\mu)$, we have the following:

(i) $T_p(G_\mu p)=T_p(Gp)\cap T_p(J^{-1}(\mu))$;

(ii) $T_p(J^{-1}(\mu))$ is the $(\Sigma_{A=1}^k\omega_A\otimes r^A)$-orthogonal complement of $T_p(Gp)$.

Proof: The proof of assertion (i) is exactly the same as that in Lemma 4.3.2 in Abraham–Marsden.[2] The assertion (ii) is an immediate consequence of (28) and the identity $T_p(J^{-1}(\mu))=ker\,J_*(p)$. ■

Theorem VI.1: *Let $(M,\omega_1,\ldots,\omega_k)$ be a polysymplectic manifold on which the Lie group acts polysymplectically and let $J:M\to\mathcal{G}^k*$ be an Ad^k*-equivariant momentum map for this action. Assume that $\mu\in\mathcal{G}^k*$ is a regular value of J and that the isotropy group G_μ, under the Ad^k* action on $\mathcal{G}^k*$, acts freely and properly on $J^{-1}(\mu)$. Then $M_\mu=J^{-1}(\mu)/G_\mu$ has a unique polysymplectic structure $((\omega_\mu)_1,\ldots,(\omega_\mu)_k)$ with the property*

$$\pi_\mu^*(\omega_\mu)_A=i_\mu^*\omega_A,\quad \forall A=1,\ldots,k,$$

where $\pi_\mu:J^{-1}(\mu)\to M_\mu$ is the canonical projection and $i_\mu:J^{-1}(\mu)\to M$ is the inclusion.

Proof: We define $(\omega_\mu)_A$ by

$$((\omega_\mu)_A([v],[w])=\omega_A(v,w),\quad \forall v,w\in T_p(J^{-1}(\mu)),$$

where $[v]=(\pi_\mu)_*(p)(v)$ and $[w]=(\pi_\mu)_*(p)(w)$. Since π_μ and $(\pi_\mu)_*$ are surjective the 2-forms $(\omega_\mu)_A$, $A=1,\ldots,k$ are unique.

From (ii) in Lemma VI.1 we deduce that $\omega_A(\xi_M,v)=0$ for all $v\in T_p(J^{-1}(\mu))$, therefore since $T_{[p]}(J^{-1}(\mu)/G_\mu)=T_p(J^{-1}(\mu))/T_p(G_\mu p)$ we deduce from (41) that $(\omega_\mu)_A$ is well defined. The assertion $\pi_\mu^*(\omega_\mu)_A=i_\mu^*\omega_A$ is evident, from it one obtains that $(\pi_\mu)^*(d(\omega_\mu)_A)=0$, and since π_μ and $(\pi_\mu)_*$ are surjective then $d(\omega_\mu)_A=0$.

For nondegeneracy of $((\omega_\mu)_1,\ldots,(\omega_\mu)_k)$, suppose

$$\sum_{A=1}^{k} (\omega_\mu)_A([v],[w])=0, \quad \text{for all } w\in T_pJ^{-1}(\mu),$$

hence $\omega_A(v,w)=0$ for all $w\in T_p(J^{-1}(\mu))$ and for all $A\in\{1,\ldots,k\}$. Now using (ii) of Lemma VI.1 we deduce that $v\in T_p(Gp)$ and from (i) of the same Lemma we obtain that $v\in T_p(G_\mu p)$. Therefore $[v]=0$ since $T_{[p]}(J^{-1}(\mu)/G_\mu)=T_p(J^{-1}(\mu))/T_p(G_\mu p)$. ■

Theorem VI.2: *Let us consider $M=(T^1_k)^*Q$ with the canonical polysymplectic structure. Let Φ^{T^*} be the polysymplectic action (33) on M and J the momentum map given by (34).*

Under the assumptions of the Theorem VI.1, if $H:(T^1_k)^*Q\to\mathbb{R}$ is a Hamiltonian such that

(a) H is invariant under the action Φ^{T^*}

(b) there exists an evolution k-vector field $((X_H)_1,\ldots,(X_H)_k)$ associated with H which are invariant

$$(\Phi^{T^*}_g)_*(X_H)_A=(X_H)_A, \quad \forall A=1,\ldots,k, \ \ \forall g\in G_\mu \tag{42}$$

and

$$J \text{ is an integral for all } (X_H)_A, \quad A=1,\ldots,k, \tag{43}$$

then we have the following.

(i) For each $A=1,\ldots,k$, the flow F^A_t of $(X_H)_A$ leaves $J^{-1}(\mu)$ invariant and commutes with the action of G_μ on $J^{-1}(\mu)$, and so it induces canonically a flow H^A_t on M_μ satisfying $\pi_\mu\circ F^A_t=H^A_t\circ\pi_\mu$.

(ii) If Y_A is the generator of H^A_t, then $(Y_1,\ldots,Y_k)$ is an evolution k-vector field on M_μ associated with a Hamiltonian function $H_\mu:M_\mu\to\mathbb{R}$ satisfying $H_\mu\circ\pi_\mu=H\circ i_\mu$. Such H_μ is called the reduced Hamiltonian.

Proof: (i) From (43), for each $A=1,\ldots,k$ and each $\alpha\in J^{-1}(\mu)$, we have $J(F^A_t(\alpha))=J(\alpha)=\mu$, $A=1,\ldots,k$, and then $F^A_{t\,|J^{-1}(\mu)}:J^{-1}(\mu)\to J^{-1}(\mu)$.

From (42) we deduce that $F^A_t\circ\Phi^{T^*}_g=\Phi^{T^*}_g\circ F^A_t$, for all $g\in G_\mu$, $A=1,\ldots,k$. This property lets us define an induced flow H^A_t on M_μ, for each $A=1,\ldots,k$, by $H^A_t([\alpha])=[F^A_t(\alpha)]$, $[\alpha]\in M_\mu$. Now the identity $\pi_\mu\circ F^A_t=H^A_t\circ\pi_\mu$, is obvious for all $A=1,\ldots,k$.

(ii) Since H is invariant under the action of G, we can define the function $H_\mu:M_\mu\to\mathbb{R}$ by $H_\mu([\alpha])=H(\alpha)$, for all $[\alpha]\in M_\mu$. So, we have

$$H_\mu\circ\pi_\mu=H\circ i_\mu. \tag{44}$$

Since $\pi_\mu\circ F^A_t=H^A_t\circ\pi_\mu$, we have

$$(\pi_\mu)_*\circ(X_H)_A=Y_A\circ\pi_\mu, \quad 1\leqslant A\leqslant k. \tag{45}$$

Using $i^*_\mu\omega_A=\pi^*_\mu(\omega_\mu)_A$, (44) and (45), one easily proves that $\mathrm{d}H_\mu=\Sigma^k_{A=1}i_{Y_A}(\omega_\mu)_A$, that is, $(Y_1,\ldots,Y_k)$ is an evolution k-vector field on M_μ associated with the reduced Hamiltonian function H_μ. ■

Remark VI.1: If each flow F^A_t preserves ω_A, that is $(F^A_t)^*\omega_A=\omega_A$, for all $A=1,\ldots,k$, then each flow H^A_t preserves $(\omega_\mu)_A$, that is $(H^A_t)^*(\omega_\mu)_A=(\omega_\mu)_A$, for all $A=1,\ldots,k$.

Indeed, from the fact

$$\begin{aligned}\pi^*_\mu(H^A_t)^*(\omega_\mu)_A&=(H^A_t\circ\pi_\mu)^*(\omega_\mu)_A\\&=(\pi_\mu\circ F^A_t)^*(\omega_\mu)_A=(F^A_t)^*\pi^*_\mu(\omega_\mu)_A=(F^A_t)^*i^*_\mu\omega_A=i^*_\mu\omega_A=\pi^*_\mu(\omega_\mu)_A\end{aligned}$$

and taking into account that π^*_μ is a surjective submersion, we obtain the assertion.

Next, we shall show that in the case of $M=(T^1_k)^*Q$, the reduced manifold M_μ is in fact the k-cotangent bundle $(T^1_k)^*(Q/G_\mu)$ of the manifold $Q_\mu=Q/G_\mu$ if $\mathcal{G}=\mathcal{G}_\mu$ where $\mu\in\mathcal{G}^{k*}$ is a regular value of J.

Theorem VI.3: *Let G act on Q and hence on $(T^1_k)^*Q$ as in (33) and let J be the Ad^{k*}-equivariant momentum map defined in (34). We suppose that all conditions from hypothesis of the Theorem VI.1 hold and that G_μ acts freely and properly on Q. Additionally, we assume that there exist G_μ-equivariant 1-forms $(\alpha_\mu)_1,\ldots,(\alpha_\mu)_k$ on Q, such that $((\alpha_\mu)_1,\ldots,(\alpha_\mu)_k)\in J^{-1}(\mu)$ and we define on $(T^1_k)^*Q$ the polysymplectic structure*

$$(\Omega_\mu)_A=(\omega_0)_A-(\tau_Q^*)^*d(\alpha_\mu)_A,\quad A=1,\ldots,k,$$

where $\tau_Q^*:(T^1_k)^*Q\to Q$ is the canonical projection, which allow us to consider on $(T^1_k)^*Q_\mu$ the corresponding induced polysymplectic structure.

Then there is an induced polysymplectic embedding $\Phi_\mu:M_\mu\to(T^1_k)^*Q_\mu$ onto a subbundle over Q_μ and this map Φ_μ is a diffeomorphism if and only if $\mathcal{G}=\mathcal{G}_\mu$.

Proof: Since $T^*Q_\mu=F_\mu/G_\mu$ where $F_\mu=\{\alpha_q\in T^*Q\mid\alpha_q(\xi_Q(q))=0,\forall\xi\in\mathcal{G}_\mu\}$, we have

$$(T^1_k)^*Q_\mu=(F_\mu/G_\mu)\overset{k}{\oplus\cdots\oplus}(F_\mu/G_\mu)=(F_\mu\overset{k}{\oplus\cdots\oplus}F_\mu)/G_\mu,$$

where

$$F_\mu\overset{k}{\oplus\cdots\oplus}F_\mu=\{(\alpha_1(q),\ldots,\alpha_k(q))\in(T^1_k)^*Q\mid\alpha_A(q)(\xi_Q(q))=0,\forall\xi\in\mathcal{G}_\mu,A=1,\ldots,k\}.$$

On the other hand,

$$J^{-1}(\mu)=\left\{(\alpha_1(q),\ldots,\alpha_k(q))\in(T^1_k)^*Q\,\middle|\,\sum_{A=1}^{k}\alpha_A(q)((\xi_A)_Q(q))=\mu(\xi_1,\ldots,\xi_k),\forall\xi_1,\ldots,\xi_k\in\mathcal{G}\right\},$$

and we define $\Psi_\mu:J^{-1}(\mu)\to F_\mu\overset{k}{\oplus\cdots\oplus}F_\mu$ by

$$\Psi_\mu(\alpha_1(q),\ldots,\alpha_k(q))=(\alpha_1(q)-(\alpha_\mu)_1(q),\ldots,\alpha_k(q)-(\alpha_\mu)_k(q)).$$

Since $(\alpha_1(q),\ldots,\alpha_k(q)),(\underset{A}{(\alpha_\mu)_1}(q),\ldots,(\alpha_\mu)_k(q))\in J^{-1}(\mu)$, we have that $(\alpha_\mu)_A(q)(\xi_Q(q))=\alpha_A(q)(\xi_Q(q))=\mu(0,\ldots,0,\xi,0,\ldots,0)$ for each $A=1,\ldots,k$, and therefore Ψ_μ is well defined.

The map Ψ_μ is a translation in each component and it is polysymplectic, that is, for any $A=1,\ldots,k$, we have

$$\Psi_\mu^*((\Omega_\mu)_{A|F_\mu\overset{k}{\oplus\cdots\oplus}F_\mu})=(\omega_0)_{A|J^{-1}(\mu)}.$$

In fact, a simple computation shows that $\Psi_\mu^*((\theta_0)_A)+(\tau_Q^*)^*(\alpha_\mu)_A=(\theta_0)_{A|J^{-1}(\mu)}$. Also, Ψ_μ is an embedding (if and only if $\mathcal{G}=\mathcal{G}_\mu$).

Since $(\alpha_\mu)_1,\ldots,(\alpha_\mu)_k$ are G_μ-equivariant and as a consequence of definition of Φ^{T^*}, the map Ψ_μ passes to the quotient defining

$$\Phi_\mu:M_\mu\equiv J^{-1}(\mu)/G_\mu\to(T^1_k)^*Q_\mu\equiv(F_\mu/G_\mu)\overset{k}{\oplus\cdots\oplus}(F_\mu/G_\mu)$$

by

$$\Phi_\mu([\alpha_1(q),\ldots,\alpha_k(q)])=([\alpha_1(q)-(\alpha_\mu)_1(q)],\ldots,[\alpha_k(q)-(\alpha_\mu)_k(q)]).$$

Clearly Φ_μ is an embedding (and onto if and only if $\mathcal{G}=\mathcal{G}_\mu$). The induced polysymplectic

structure $((\tilde{\Omega}_\mu)_A, 1\leqslant A\leqslant k)$ on $(T^1_k)^*Q_\mu$ defined by the polysymplectic structure $((\Omega_\mu)_A, 1\leqslant A\leqslant k)$ on $(T^1_k)^*Q$ allow us to consider the polysymplectic structure $(\Phi^*_\mu(\tilde{\Omega}_\mu)_A, 1\leqslant A\leqslant k)$ on M_μ. It is easy to see that $\pi^*_\mu(\Phi^*_\mu(\tilde{\Omega}_\mu)_A)=i^*_\mu\omega_A$ and from unicity of Theorem VI.1 it follows that Φ_μ is polysymplectic. ■

Example of reduction: Let G be a Lie group and denote by $\Lambda: G\times G\to G$ the action of G on itself by left translations, that is, $\Lambda_g=L_g$ for all $g\in G$. Let Λ^{T^*} be the induced action on $(T^1_k)^*G$ defined in (33). Since $\xi_G(g)=(R_g)_*(e)(\xi)$ for any $\xi\in\mathcal{G}$ and for any $g\in G$, from (34) we know that the momentum map $J:(T^1_k)^*G\to\mathcal{G}^{k*}$ of this action is

$$J(\alpha_1(g),\ldots,\alpha_k(g))(\xi_1,\ldots,\xi_k)=\sum_{A=1}^{k}\alpha_A(g)((\xi_A)_G(g))=\sum_{A=1}^{k}\alpha_A(g)((R_g)_*(e)\xi_A),$$

and then $J^{-1}(\mu)$ is given by

$$\left\{(\alpha_1(g),\ldots,\alpha_k(g))\in(T^1_k)^*G\,\middle|\,\sum_{A=1}^{k}\alpha_A(g)((R_g)_*(e)\xi_A)=\mu(\xi_1,\ldots,\xi_k),\ \forall\xi_1,\ldots,\xi_k\in\mathcal{G}\right\},$$

for any $\mu\in\mathcal{G}^{k*}$ (each $\mu\in\mathcal{G}^{k*}$ is a regular value of J).

If we consider, for each $A=1,\ldots,k$ the right-invariant 1-form $(\alpha_\mu)_A$, defined by

$$(\alpha_\mu)_A(g)=\mu\circ i_A\circ(R_{g^{-1}})_*(g),\quad \forall g\in G,$$

where $i_A:\mathcal{G}\to\mathcal{G}^k$ is the natural inclusion, $i_A(\xi)=(0,\ldots,0,\overset{A}{\xi},0,\ldots,0)$, then

$$J^{-1}(\mu)=\{((\alpha_\mu)_1(g),\ldots,(\alpha_\mu)_k(g))\,|\,g\in G\}\tag{46}$$

and therefore $J^{-1}(\mu)$ can be identified with G.

By a direct computation it is easy to see that

$$G_\mu=\{g\in G\,|\,(L_g)^*(\alpha_\mu)_A=(\alpha_\mu)_A,\ \forall A=1,\ldots,k\},$$

which means that G_μ acts on $J^{-1}(\mu)$ by left translations.

Thus $J^{-1}(\mu)/G_\mu\equiv G/G_\mu\equiv G\cdot\mu\subset\mathcal{G}^{k*}$, that is, the reduced phase space is naturally identifiable with the orbit of μ in $\mathcal{G}^{k*}$ under the k-coadjoint action, from which we deduce (using Theorem VI.1) that $G\cdot\mu$ is a polysymplectic manifold. For $k=1$ this is the statement of the Kirillov–Konstant–Souriau theorem.

Now, we want to compute explicitly the polysymplectic structure $((\omega_\mu)_A, 1\leqslant A\leqslant k)$ on $G\cdot\mu$. Let $\rho: J^{-1}(\mu)\to G\cdot\mu$ be the map given by $((\alpha_\mu)_1(g),\ldots,(\alpha_\mu)_k(g))\to \mathrm{Ad}^{k*}_{g^{-1}}(\mu)$ so that from Theorem VI.1 $\rho^*(\omega_\mu)_A=i^*_\mu(\omega_0)_A$, for all $1\leqslant A\leqslant k$, where $((\omega_0)_A, 1\leqslant A\leqslant k)$ is the canonical polysymplectic structure on $(T^1_k)^*G$ and $i_\mu: J^{-1}(\mu)\to(T^1_k)^*G$ is the natural inclusion.

First we compute $i^*_\mu(\omega_0)_A$. Let us observe that

$$T_{\alpha_\mu(g)}J^{-1}(\mu)=\{(\alpha_\mu\circ R_g)_*(e)(\xi)\,|\,\xi\in\mathcal{G}\},$$

because $J^{-1}(\mu)$ is the graph of $\alpha_\mu: G\to J^{-1}(\mu)$, $\alpha_\mu(g)=((\alpha_\mu)_1(g),\ldots,(\alpha_\mu)_k(g))$. Then

$$\begin{aligned}
&i^*_\mu(\omega_0)_A(\alpha_\mu(g))((\alpha_\mu)_*(g)((R_g)_*(e)(\xi)),(\alpha_\mu)_*(g)((R_g)_*(e)(\eta)))\\
&\quad=((\alpha_\mu)_A)^*\ \omega_0\ (g)((R_g)_*(e)(\xi),(R_g)_*(e)(\eta))\\
&\quad=-d(\alpha_\mu)_A(g)((R_g)_*(e)(\xi),(R_g)_*(e)(\eta))\\
&\quad=-d(\alpha_\mu)_A(\tilde{X}_\xi,\tilde{X}_\eta)(g)=(\alpha_\mu)_A([\tilde{X}_\xi,\tilde{X}_\eta])(g)=-(\alpha_\mu)_A(\tilde{X}_{[\xi,\eta]})(g)=-(\mu\circ i_A)([\xi,\eta]),
\end{aligned}\tag{47}$$

where $\tilde{X}_\xi$, $\tilde{X}_\eta$ are the right invariant vector fields corresponding to $\xi, \eta \in \mathcal{G}$, respectively.

On the other hand, we obtain by a direct computation

$$\rho^*(\omega_\mu)_A(\alpha_\mu(g))((\alpha_\mu)_*(g)((R_g)_*(e)(\xi)),(\alpha_\mu)_*(g)((R_g)_*(e)(\eta)))$$
$$=(\omega_\mu)_A(\mathrm{Ad}^{k*}_{g^{-1}}\mu)((\mathrm{Ad}_g\xi)_{\mathcal{G}^k*}(\mathrm{Ad}^{k*}_{g^{-1}}\mu),(\mathrm{Ad}_g\eta)_{\mathcal{G}^k*}(\mathrm{Ad}^{k*}_{g^{-1}}\mu)). \tag{48}$$

Therefore, from (47) and (48) we have

$$(\omega_\mu)_A(\mathrm{Ad}^{k*}_{g^{-1}}\mu)(\xi_{\mathcal{G}^k*}(\mathrm{Ad}^{k*}_{g^{-1}}\mu),\eta_{\mathcal{G}^k*}(\mathrm{Ad}^{k*}_{g^{-1}}\mu))=-(\mathrm{Ad}^*_{g^{-1}}(\mu\circ i_A))([\xi,\eta]), \tag{49}$$

for any element $\mathrm{Ad}^{k*}_{g^{-1}}\mu \in G\cdot\mu$.

Remark VI.2: Let us observe that the forms of the polysymplectic structure $((\omega_\mu)_A, 1\leqslant A \leqslant k)$ on $G\cdot\mu$ coincides with the forms obtained by Awane.[4,5]

Example VI.1: Now we will describe the reduction in the case $G=\mathrm{SO}(3)\times\overset{k}{\cdots}\times\mathrm{SO}(3)$.

A basis for the Lie algebra so(3) of the Lie group SO(3) is

$$E_1=\begin{pmatrix}0&0&0\\0&0&-1\\0&1&0\end{pmatrix},\quad E_2=\begin{pmatrix}0&0&1\\0&0&0\\-1&0&0\end{pmatrix},\quad E_3=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix}.$$

The map $j:\mathbb{R}^3\to\mathrm{so}(3):x=x_1e_1+x_2e_2+x_3e_3\mapsto X=x_1E_1+x_2E_2+x_3E_3$ is an isomorphism of the Lie algebras $(\mathbb{R}^3,\times)$ and $(\mathrm{so}(3),[\,,\,])$ where $\times$ denotes the vectorial product. With this isomorphism the action of so(3) on $\mathbb{R}^3$ is given by

$$j(x)\,y=\begin{pmatrix}0&-x_3&x_2\\x_3&0&-x_1\\-x_2&x_1&0\end{pmatrix}\begin{pmatrix}y_1\\y_2\\y_3\end{pmatrix}=x\times y\,. \tag{50}$$

The isomorphism $\kappa:\mathbb{R}^3\to\mathrm{so}(3)^*$ is given by $\kappa(x)=x_1E^1+x_2E^2+x_3E^3$ and so

$$\kappa(x)(j(y))=\langle x,y\rangle\,, \tag{51}$$

where E^1,E^2,E^3 is the dual basis of E_1,E_2,E_3.

It is well known that, the adjoint representation $\mathrm{Ad}:\mathrm{SO}(3)\to\mathrm{Aut}(\mathrm{so}(3))$ is given by

$$\mathrm{Ad}_A(j(x))=j(Ax)\,. \tag{52}$$

Thus, the adjoint representation $\mathrm{Ad}:\mathrm{SO}(3)\times\overset{k}{\cdots}\times\mathrm{SO}(3)\to\mathrm{Aut}(\mathrm{so}(3)^*\oplus\overset{k}{\cdots}\oplus\mathrm{so}(3)^*)$ is given by

$$\mathrm{Ad}_{(A_1,\ldots,A_k)}(j(x_1),\ldots,j(x_k))=(j(A_1x_1),\ldots,j(A_kx_k))\,, \tag{53}$$

where $(A_1,\ldots,A_k)\in\mathrm{SO}(3)\times\overset{k}{\cdots}\times\mathrm{SO}(3)$, $(x_1,\ldots,x_k)\in\mathbb{R}^3\times\overset{k}{\cdots}\times\mathbb{R}^3$.

We shall use the following isomorphisms:

$$\mathrm{so}(3)^*\oplus\overset{k}{\cdots}\oplus\mathrm{so}(3)^*\overset{F}{\to}(\mathrm{so}(3)\times\overset{k}{\cdots}\times\mathrm{so}(3))^*,$$

$$(\alpha_1,\ldots,\alpha_k)\to F(\alpha_1,\ldots,\alpha_k),$$

where $F(\alpha_1,\ldots,\alpha_k)(X_1,\ldots,X_k)=\Sigma_{i=1}^k\alpha_i(X_i)$, and

$$(\mathrm{so}(3)\times\overset{k}{\cdots}\times\mathrm{so}(3))^*\overset{F^{-1}}{\to}\mathrm{so}(3)^*\oplus\overset{k}{\cdots}\oplus\mathrm{so}(3)^*,$$

$$\mu \to F^{-1}(\mu) = (\mu \circ i_1, \ldots, \mu \circ i_k),$$

where $i_j(X) = (0,\ldots,0,\overset{j}{X},0,\ldots,0)$.

From (51) we have

$$F(\kappa(x_1),\ldots,\kappa(x_k))(j(y_1),\ldots,j(y_k)) = \sum_{\alpha=1}^{k} \langle x_\alpha, y_\alpha \rangle . \tag{54}$$

Let us denote by $G = \mathrm{SO}(3) \overset{k}{\times \cdots \times} \mathrm{SO}(3)$ and by $\mathcal{G} = \mathrm{so}(3) \overset{k}{\oplus \cdots \oplus} \mathrm{so}(3)$ its Lie algebra. Now we shall describe the k-coadjoint orbit of

$$\mu \in \mathcal{G}^{k*} = ((\mathrm{so}(3) \overset{k}{\oplus \cdots \oplus} \mathrm{so}(3)) \overset{k}{\times \cdots \times} (\mathrm{so}(3) \overset{k}{\oplus \cdots \oplus} \mathrm{so}(3)))^* .$$

Let $\mu : \mathcal{G} \overset{k}{\times \cdots \times} \mathcal{G} \to \mathbb{R}$ be an element of $\mathcal{G}^{k*}$. We define $\mu_\alpha \in \mathcal{G}^*$ by $\mu_\alpha = \mu \circ i_\alpha$ where $i_\alpha : \mathcal{G} \to \mathcal{G} \overset{k}{\times \cdots \times} \mathcal{G}$ is the inclusion in the α-factor, that is, $i_\alpha(X_1,\ldots,X_k) = (0,\ldots,0,(X_1,\ldots,X_k),0,\ldots,0)$.

Let $(\hat{\mu}_\alpha)_\beta \in \mathbb{R}^3$ such that $\mu_\alpha = F(\kappa((\hat{\mu}_\alpha)_1),\ldots,\kappa((\hat{\mu}_\alpha)_k))$. Then from (26), (52), and (54) the k-coadjoint action is given by

$$\Phi((A_1,\ldots,A_k),\mu) = \mathrm{Ad}^{k*}_{(A_1^{-1},\ldots,A_k^{-1})}(\mu) = \sum_{\alpha,\beta}^{k} \langle A_\beta(\hat{\mu}_\alpha)_\beta, j^{-1}(-) \rangle . \tag{55}$$

Thus, using the above identifications, from (55) we deduce that the k-coadjoint action

$$\Phi : G \times (\mathcal{G} \overset{k}{\times \cdots \times} \mathcal{G})^* \to (\mathcal{G} \overset{k}{\times \cdots \times} \mathcal{G})^*$$

with $G = \mathrm{SO}(3) \overset{k}{\times \cdots \times} \mathrm{SO}(3)$ and $\mathcal{G} = \mathrm{so}(3) \overset{k}{\oplus \cdots \oplus} \mathrm{so}(3)$, can be identified with the natural action

$$\Phi : G \times (\mathbb{R}^3 \overset{k}{\times \cdots \times} \mathbb{R}^3) \overset{k}{\times \cdots \times} (\mathbb{R}^3 \overset{k}{\times \cdots \times} \mathbb{R}^3) \to (\mathbb{R}^3 \overset{k}{\times \cdots \times} \mathbb{R}^3) \overset{k}{\times \cdots \times} (\mathbb{R}^3 \overset{k}{\times \cdots \times} \mathbb{R}^3),$$

$$\begin{aligned} &\Phi((A_1,\ldots,A_k),((x_1)_1,\ldots,(x_1)_k),\ldots,((x_k)_1,\ldots,(x_k)_k)) \\ &\quad = ((A_1(x_1)_1,\ldots,A_k(x_1)_k),\ldots,(A_1(x_k)_1,\ldots,A_k(x_k)_k)) . \end{aligned}$$

Then, the k-coadjoint orbit $(\mathrm{SO}(3) \overset{k}{\times \cdots \times} \mathrm{SO}(3)) \cdot \mu$ of μ is

$$\begin{aligned} &\{((A_1(\hat{\mu}_1)_1,\ldots,A_k(\hat{\mu}_1)_k),\ldots,(A_1(\hat{\mu}_k)_1,\ldots,A_k(\hat{\mu}_k)_k)) \mid A_\alpha \in \mathrm{SO}(3),\ \alpha = 1,\ldots,k\} \subset \mathbb{S}^2(\|(\hat{\mu}_1)_1\|) \\ &\quad \times \cdots \times \mathbb{S}^2(\|(\hat{\mu}_1)_k\|) \overset{k}{\times \cdots \times} \mathbb{S}^2(\|(\hat{\mu}_k)_1\|) \times \cdots \times \mathbb{S}^2(\|(\hat{\mu}_k)_k\|), \end{aligned}$$

where $\mathbb{S}^2(\|(\hat{\mu}_\alpha)_\beta\|)$ is the sphere of radius $\|(\hat{\mu}_\alpha)_\beta\|$ in $\mathbb{R}^3$, $\alpha,\beta = 1,\ldots,k$. Obviously each orbit is diffeomorphic to $\mathbb{S}^2 \overset{k}{\times \cdots \times} \mathbb{S}^2$.

From the example of reduction above we know that the orbit $(\mathrm{SO}(3) \overset{k}{\times \cdots \times} \mathrm{SO}(3)) \cdot \mu$ is a polysymplectic manifold. From (49) and (52) we obtain the polysymplectic structure of $G \cdot \mu$: if $\mathbf{A} \equiv (A_1,\ldots,A_k) \in G$, $\mathbf{X} = (X_1,\ldots X_k), \mathbf{Y} = (Y_1,\ldots Y_k) \in \mathcal{G}$, the polysymplectic structure is given by

$$(\omega_\mu)_\alpha(\mathbf{A}\cdot\mu)(\mathbf{X}_{\mathcal{G}^{k*}}(\mathbf{A}\cdot\mu), \mathbf{Y}_{\mathcal{G}^{k*}}(\mathbf{A}\cdot\mu)) = -\sum_{\beta=1}^{k} \langle A_\beta(\hat{\mu}_\alpha)_\beta, x_\beta \times y_\beta \rangle , \quad \alpha = 1,\ldots,k,$$

where $j(x_\beta) = X_\beta, j(y_\beta) = Y_\beta$. In fact we have

$$
\begin{aligned}
&(\omega_\mu)_\alpha((A_1,\ldots,A_k)\cdot\mu)(\mathbf{X}_{\mathcal{G}^k*}((A_1,\ldots,A_k)\cdot\mu),\mathbf{Y}_{\mathcal{G}^k*}((A_1,\ldots,A_k)\cdot\mu))\\
&\quad=-\mathrm{Ad}^*_{(A_1,\ldots,A_k)^{-1}}(\mu\circ i_\alpha)([(X_1,\ldots,X_k),(Y_1,\ldots,Y_k)])\\
&\quad=-\mathrm{Ad}^*_{(A_1,\ldots,A_k)^{-1}}(\mu\circ i_\alpha)([X_1,Y_1],\ldots,[X_k,Y_k])\\
&\quad=-((\mu\circ i_\alpha)\circ\mathrm{Ad}_{(A_1,\ldots,A_k)^{-1}})(j(x_1\times y_1),\ldots,j(x_k\times y_k))\\
&\quad=-(\mu\circ i_\alpha)(j(A_1^{-1}(x_1\times y_1)),\ldots,j(A_k^{-1}(x_k\times y_k)))\\
&\quad=-F(\kappa((\hat\mu_\alpha)_1),\ldots\kappa((\hat\mu_\alpha)_k))(j(A_1^{-1}(x_1\times y_1)),\ldots,j(A_k^{-1}(x_k\times y_k)))\\
&\quad=-\sum_{\beta=1}^{k}\langle(\hat\mu_\alpha)_\beta,(A_\beta)^{-1}(x_\beta\times y_\beta)\rangle=-\sum_{\beta=1}^{k}\langle A_\beta(\hat\mu_\alpha)_\beta,x_\beta\times y_\beta\rangle,
\end{aligned}
$$

where the Lie bracket $[X,Y]$ in so(3) is identified with the vectorial product $x\times y$ in $\mathbb{R}^3$.

In the case $k=1$, it is well known that the coadjoint orbit $\mathrm{SO}(3)\cdot\mu\subset\mathrm{so}(3)^*\simeq\mathbb{R}^3$ is the sphere $\mathbb{S}^2(\|\mu\|)$ of radius $\|\mu\|$ and the symplectic structure is

$$
\omega_\mu(A\cdot\mu)(X_{\mathcal{G}*}(A\cdot\mu),Y_{\mathcal{G}*}(A\cdot\mu))=-\langle A\hat\mu,x\times y\rangle,\quad \kappa(\hat\mu)=\mu\ ,
$$

that is, the area element given by the normal vector $A\hat\mu$ applied to the tangent vectors x and y. (Also see Refs. 23–31.)

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Two new types of quantum states generated via higher powers of Bogoliubov's transformation

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By applying higher powers of Bogoliubov's transformation operator $b^\dagger = \nu^* a + \mu^* a^\dagger$ to the even and odd coherent states we construct mathematically two new types of quantum states. Various special functions and mathematical formulations are used to obtain the matrix elements for the states in the coherent state representation. The nonclassical nature of these states is found to be related to their quantum coherence in phase space. The interference effects can also be regarded as a consequence of the oscillatory behavior of the special functions in the structure of the states. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1688434]

I. INTRODUCTION

Since the even and odd coherent states were proposed by Dodonov *et al.* in 1974[1] and Hillery in 1987[2] for a single mode field they have attracted considerable attention in quantum optics. The quantum properties of these states have been studied in detail,[3,4] and various schemes for their realization have been proposed.[5–8] In addition, multimode even and odd coherent fields[9] as well as certain excited states related to the even and odd states[10] have been investigated as important types of nonclassical fields. In recent years the possible application of similar superpositions of even and odd states have been proposed as quantum entangled states which may be used to realize quantum teleportation.[11,12]

Through a new mathematical formulation we define two general classes of quantum states which are broader than the even/odd coherent states[1,2] and the excited even/odd coherent states.[10] They are generated by m-fold application of Bogoliubov's transformation operator $b^\dagger$, also known as the pseudocreation operator, on the even/odd coherent states to obtain what we call, respectively, the generalized excited even/odd coherent states. It is our purpose to construct these states in the coherent state representation which can describe the relationship and properties of these states. We also examine the nonclassical behavior of several quasiprobability distributions, and the influence of the phase relation between two parameters μ and ν on the probability distributions of these nonclassical fields. Our results show that these states are in fact two new general classes of quantum states which exhibit remarkable nonclassical characteristics different from previously known states.[1,2,10,13–15]

II. REPRESENTATIONS OF TWO NEW CLASSES OF QUANTUM STATES

We consider a single mode of the field described in terms of the boson annihilation and creation operators a and $a^\dagger$. The even $|\alpha\rangle_E$ and odd $|\alpha\rangle_O$ coherent states can be defined as the eigenstates of the double-annihilation operator aa,

$$aa|\alpha\rangle_{E(O)} = \alpha^2 |\alpha\rangle_{E(O)}, \tag{1}$$

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and may be written explicitly as

$$|\alpha\rangle_E=\frac{1}{\sqrt{\cosh(|\alpha|)^2}}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{\sqrt{(2n)!}}|2n\rangle, \tag{2}$$

$$|\alpha\rangle_O=\frac{1}{\sqrt{\sinh(|\alpha|)^2}}\sum_{n=0}^{\infty}\frac{\alpha^{2n+1}}{\sqrt{(2n+1)!}}|2n+1\rangle. \tag{3}$$

The even/odd coherent states can also be written as the superposition of two coherent states $|\alpha\rangle$ and $|-\alpha\rangle$, which have the form

$$|\alpha\rangle_E=\tfrac{1}{2}\exp(\tfrac{1}{2}|\alpha|^2)[\cosh|\alpha|^2]^{-1/2}(|\alpha\rangle+|-\alpha\rangle), \tag{4}$$

$$|\alpha\rangle_O=\tfrac{1}{2}\exp(\tfrac{1}{2}|\alpha|^2)[\sinh|\alpha|^2]^{-1/2}(|\alpha\rangle-|-\alpha\rangle), \tag{5}$$

where $|\pm\alpha\rangle$ is a coherent state. We now make use of a linear transformation of the annihilation and creation operators or the Bogoliubov transformation operator b, defined by

$$b=b(\mu,\nu)=\mu a+\nu a^{\dagger}, \tag{6}$$

where the complex parameters μ and ν obey $|\mu|^2-|\nu|^2=1$, $\mu,\nu\in C$. The basic operators b and $b^{\dagger}$ satisfy the same canonical commutation relation as $a,a^{\dagger}$, i.e.,

$$[b(\mu,\nu),b^{\dagger}(\mu^*,\nu^*)]=1. \tag{7}$$

This transformation operator b was first used by Bogoliubov in solid state physics[16] and later by Yuen to derive his two-photon coherent states.[14] Its Hermitian adjoint operator $b^{\dagger}(\mu^*,\nu^*)$ is

$$b^{\dagger}(\mu^*,\nu^*)=\nu^* a+\mu^* a^{\dagger}. \tag{8}$$

We now apply the Bogoliubov operator $b^{\dagger}(\mu^*,\nu^*)$ m-times to the even/odd coherent states[1,2] based on the above representation and obtain two new types of quantum states, the generalized excited even coherent states $|\alpha,m,\mu,\nu\rangle_E$ (GEECS) and the generalized excited odd coherent states $|\alpha,m,\mu,\nu\rangle_O$ (GEOCS). They may be written, respectively, as

$$|\alpha,m,\mu,\nu\rangle_E=N_E^{1/2}b^{\dagger m}|\alpha\rangle_E \tag{9}$$

and

$$|\alpha,m,\mu,\nu\rangle_O=N_O^{1/2}b^{\dagger m}|\alpha\rangle_O, \tag{10}$$

where m is a non-negative integer, and $N_E^{1/2}$ and $N_O^{1/2}$ are normalization constants.

In order to examine the properties of the generalized excited even/odd coherent states, we need to obtain the matrix elements based on the coherent state representations of Eqs. (9) and (10). The general matrix elements $A_{\lambda,\rho}^{n,m}(\alpha^*,\beta)$ and $B_{\lambda,\rho}^{n,m}(\alpha^*,-\beta)$ can be defined as

$$A_{\lambda,\rho}^{n,m}(\alpha^*,\beta)=\langle\alpha|b^n a^{\lambda}a^{\dagger\rho}b^{\dagger m}|\beta\rangle, \tag{11}$$

$$B_{\lambda,\rho}^{n,m}(\alpha^*,-\beta)=\langle\alpha|b^n a^{\lambda}a^{\dagger\rho}b^{\dagger m}|-\beta\rangle. \tag{12}$$

To calculate the matrix elements we need to employ the mathematical formulas of Refs. 10, 15, and 17, so from Eqs. (6), (7), and (8) we have

$$b^{\dagger m}(\mu^*,\nu^*)=[\nu^* a+\mu^* a^\dagger]^m=\sum_{k=0}^{[m/2]}\sum_{M=0}^{m-2k} d^m_{M,m-2k-M}(\mu^*,\nu^*)a^{\dagger M}a^{m-2k-M}, \tag{13}$$

where $d^m_{M,N}(\mu^*,\nu^*)$ is a c-number factor defined by

$$d^m_{M,N}(\mu^*,\nu^*)=\frac{m!}{M!N!(m-M-N)!!}(\nu^*)^{1/2(m-M+N)}(\mu^*)^{1/2(m+M-N)}. \tag{14}$$

We thus have

$$\begin{aligned}A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)&=\langle\alpha|b^n a^\lambda a^{\dagger\rho}b^{\dagger m}|\beta\rangle\\&=\sum_{M,N}^{m}\sum_{K,L}^{n} d^m_{M,N}(\mu^*,\nu^*)d^n_{K,L}(\mu,\nu)\alpha^{*L}\beta^N\langle\alpha|a^{(K+\lambda)}a^{\dagger(M+\rho)}|\beta\rangle,\end{aligned} \tag{15}$$

$$\begin{aligned}B^{n,m}_{\lambda,\rho}(\alpha^*,-\beta)&=\langle\alpha|b^n a^\lambda a^{\dagger\rho}b^{\dagger m}|-\beta\rangle\\&=\sum_{M,N}^{m}\sum_{K,L}^{n} d^m_{M,N}(\mu^*,\nu^*)d^n_{K,L}(\mu,\nu)\alpha^{*L}(-\beta)^N\langle\alpha|a^{(K+\lambda)}a^{\dagger(M+\rho)}|-\beta\rangle.\end{aligned} \tag{16}$$

We now calculate the matrix elements explicitly. To do this, we set

$$G^{M+\rho}_{K+\lambda}(\alpha^*,\beta,-\alpha^*\beta)=\langle\alpha|\beta\rangle F^{M+\rho}_{K+\lambda}(\alpha^*,\beta,-\alpha^*\beta), \tag{17}$$

where

$$F^{M+\rho}_{K+\lambda}(\alpha^*,\beta,-\alpha^*\beta)=\begin{cases}\beta^{[(K+\lambda)-(M+\rho)]}(M+\rho)!L^{[(K+\lambda)-(M+\rho)]}_{(M+\rho)}(-\alpha^*\beta),\\ \qquad (k+\lambda)\geqslant(m+\rho),\\ \alpha^{*[(M+\rho)-(K+\lambda)]}(K+\lambda)!L^{[(M+\rho)-(K+\lambda)]}_{(K+\lambda)}(-\alpha^*\beta),\\ \qquad (k+\lambda)\leqslant(m+\rho).\end{cases} \tag{18}$$

In deriving (13)–(16) we have employed the associated Laguerre polynomial $L^{(k)}_m(x)$ and the normally ordered expression of the operator

$$L^{(k)}_m(x)=\sum_{n=0}\frac{(m+k)!(-x)^n}{(m-n)!n!(n+k)!}\quad(k>-1), \tag{19}$$

$$a^n a^{\dagger m}=\begin{cases}n!m!\sum_{l=0}^{m}\dfrac{a^{\dagger l}a^{l+n-m}}{(m-l)!l!(l+n-m)!}, & n\geqslant m,\\ n!m!\sum_{l=0}^{m}\dfrac{a^{\dagger(l+m-n)}a^l}{(m-l)!l!(l+m-n)!}, & n\leqslant m.\end{cases} \tag{20}$$

To determine the upper and lower limits of the fourfold summation $\Sigma^m_{M,N}\Sigma^n_{K,L}$ we use Eq. (14) to find the optimum values of M and N. It is easy to see that for any numbers r and k we may choose N to be

$$N=m-M-2r=\begin{cases}2k-2r & \text{when } m-\mathrm{M} \text{ is even},\\ (2k+1)-2r & \text{when } m-\mathrm{M} \text{ is odd}.\end{cases} \tag{21}$$

If we select $r=0$ then N is a series of non-negative integers $2k+1,2k,2k-1,\ldots,2,1,0$. This shows that the even and odd numbers appear alternately, and the upper limit of M is $2k+1$ or $2k$,

$$M=\begin{cases} m-2k, & k=0,1,2,\ldots\ [m/2], \\ m-(2k+1), & k=0,1,2,\ldots\ [(m-1)/2]. \end{cases} \tag{22}$$

Similarly, when K is even or odd, we have

$$L=\begin{cases} 2k-2r & \text{when } n-K \text{ is even}, \\ (2k+1)-2r & \text{when } n-K \text{ is odd}, \end{cases} \tag{23}$$

and so

$$K=\begin{cases} n-2k, & k=0,1,2,\ldots\ [n/2], \\ n-(2k+1), & k=0,1,2,\ldots\ [(n-1)/2]. \end{cases} \tag{24}$$

Furthermore, we can rewrite the matrix element $A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)$ of Eq. (15) as the sum of an even and odd term,

$$\begin{aligned} \langle\alpha|b^n a^\lambda a^{\dagger\rho} b^{\dagger m}|\beta\rangle &= \sum_{M,N}^{m}\sum_{K,L}^{n} d^m_{M,N}(\mu^*,\nu^*) d^n_{K,L}(\mu,\nu)\alpha^{*L}\beta^N \langle\alpha|a^{(K+\lambda)}a^{\dagger(M+\rho)}|\beta\rangle \\ &= g_{2k}+g_{2k+1}. \end{aligned} \tag{25}$$

Next we note that after inserting Eqs. (21)–(24) into (14) we obtain

$$\begin{aligned} g_{2k} &= \sum_{k=0}^{[m/2]}\sum_{r=0}^{k} \frac{G^{m-2k+\rho}_{K+\lambda} m!\,\mu^{*(m-2k+r)}\nu^{*(2k-r)}\beta^{(2k-2r)}}{(m-2k)!(2k-2r)!(2r)!!} \\ &\quad\times \sum_{k=0}^{[n/2]}\sum_{r=0}^{k} \frac{n!\,\mu^{(n-2k+r)}\nu^{(2k-r)}\alpha^{*(2k-2r)}}{(n-2k)!(2k-2r)!(2r)!!} \\ &= \mu^{*m}\sum_{k=0}^{[m/2]} \frac{G^{m-2k+\rho}_{K+\lambda} m!}{(m-2k)!(2k)!}\left(i\sqrt{\frac{\nu^*}{\mu^*}}\right)^{2k} H_{2k}\left(i\sqrt{\frac{\nu^*}{\mu^*}}\beta\right) \\ &\quad\times \mu^{n}\sum_{k=0}^{[n/2]} \frac{G^{n-2k+\rho}_{K+\lambda} n!}{(n-2k)!(2k)!}\left(i\sqrt{\frac{\nu}{\mu}}\right)^{2k} H_{2k}\left(i\sqrt{\frac{\nu}{\mu}}\alpha^*\right) \end{aligned} \tag{26}$$

and

$$\begin{aligned} g_{2k+1} &= \sum_{k=0}^{[(m-1)/2]}\sum_{r=0}^{k} \frac{G^{m-(2k+1)+\rho}_{K+\lambda} m!\,\mu^{*[m-(2k+1)+r]}\nu^{*[(2k+1)-r]}\beta^{[(2k+1)-2r]}}{[m-(2k+1)]![(2k+1)-2r]!(2r)!!} \\ &\quad\times \sum_{k=0}^{[(n-1)/2]}\sum_{r=0}^{k} \frac{n!\,\mu^{[n-(2k+1)+r]}\nu^{[(2k+1)-r]}\alpha^{*[(2k+1)-2r]}}{[n-(2k+1)]![(2k+1)-2r]!(2r)!!} \\ &= \mu^{*m}\sum_{k=0}^{[(m-1)/2]} \frac{G^{m-(2k+1)+\rho}_{K+\lambda} m!}{[m-(2k+1)]!(2k+1)!}\left(i\sqrt{\frac{\nu^*}{\mu^*}}\right)^{2k+1} H_{2k+!}\left(i\sqrt{\frac{\nu^*}{\mu^*}}\beta\right) \\ &\quad\times \mu^{n}\sum_{k=0}^{[(n-1)/2]} \frac{G^{n-(2k+1)+\rho}_{K+\lambda} n!}{[n-(2k+1)]!(2k+1)!}\left(i\sqrt{\frac{\nu}{\mu}}\right)^{2k+1} H_{2k+1}\left(i\sqrt{\frac{\nu}{\mu}}\alpha^*\right). \end{aligned} \tag{27}$$

In deriving (26) and (27) we have used the even and odd order Hermite polynomials

$$H_{2k}(x)=(2k)!\sum_{r=0}^{k}\frac{(-1)^r x^{2k-2r}}{(2k-2r)!(2r)!!}, \tag{28}$$

$$H_{2k+1}(x)=(2k+1)!\sum_{r=0}^{k}\frac{(-1)^r x^{(2k+1)-2r}}{[(2k+1)-2r]!(2r)!!}. \tag{29}$$

In Eqs. (26)–(27), we should take note of the range of m and n. It can be proved that, no matter whether m and n are even or odd, we always have $g_{2k}=g_{2k+1}$ for $k=[m/2],[(m-1)/2]$ (or $[n/2],[(n-1)/2]$). We now rewrite the upper and lower limits of M by replacing $2k$ [or $(2k+1)$] with s and of K by replacing $2k$ [or $(2k+1)$] with t, so that

$$A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)=\langle\alpha|\beta\rangle\sum_{s=0}^{m}\sum_{t=0}^{n}F^{m+\rho-s}_{n+\lambda-t}(\beta,\alpha^*,-\alpha^*\beta)R^m_s(\mu^*,\nu^*,\beta)S^n_t(\mu,\nu,\alpha^*), \tag{30}$$

$$B^{n,m}_{\lambda,\rho}(\alpha^*,-\beta)=\langle\alpha|-\beta\rangle\sum_{s=0}^{m}\sum_{t=0}^{n}F^{m+\rho-s}_{n+\lambda-t}(-\beta,\alpha^*,\alpha^*\beta)R^m_s(\mu^*,\nu^*,-\beta)S^n_t(\mu,\nu,\alpha^*), \tag{31}$$

where

$$F^p_q(\beta,\alpha^*,-\alpha^*\beta)=\begin{cases}p!\beta^{(q-p)}L_p^{(q-p)}(-\alpha^*\beta), & q\geqslant p,\\ q!\alpha^{*(p-q)}L_q^{(p-q)}(-\alpha^*\beta), & q\leqslant p,\end{cases} \tag{32}$$

$$R^m_s(\mu^*,\nu^*,\beta)=\mu^{*m}\binom{m}{s}\left(i\sqrt{\frac{\nu^*}{\mu^*}}\right)^s H_s\left(\frac{1}{i}\sqrt{\frac{\nu^*}{\mu^*}}\beta\right), \tag{33}$$

$$S^n_t(\mu,\nu,\alpha^*)=\mu^n\binom{n}{t}\left(i\sqrt{\frac{\nu}{\mu}}\right)^t H_t\left(\frac{1}{i}\sqrt{\frac{\nu}{\mu}}\alpha^*\right). \tag{34}$$

In order to solve the matrix element equations (30) and (31) by means of a general approach, we modify the elements by replacing α^* with $-\alpha^*$ and β with $-\beta$. We can show the following:

(i) when $(n+\lambda)-(m+\rho)$ is even,

$$\begin{aligned}A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)&=A^{n,m}_{\lambda,\rho}(-\alpha^*,-\beta),\\ B^{n,m}_{\lambda,\rho}(\alpha^*,-\beta)&=B^{n,m}_{\lambda,\rho}(-\alpha^*,\beta);\end{aligned} \tag{35}$$

(ii) when $(n+\lambda)-(m+\rho)$ is odd,

$$\begin{aligned}A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)&=-A^{n,m}_{\lambda,\rho}(-\alpha^*,-\beta),\\ B^{n,m}_{\lambda,\rho}(\alpha^*,-\beta)&=-B^{n,m}_{\lambda,\rho}(-\alpha^*,\beta).\end{aligned} \tag{36}$$

The normalization constants N_E and N_O in Eqs. (9) and (10) can thus be readily obtained in the coherent state representation when $m=n$, $\alpha=\beta$, and $\lambda=\rho=0$,

$$N_E={}_E\langle\alpha|b^m b^{\dagger m}|\alpha\rangle_E=\frac{\exp(|\alpha|^2)[A^m(\alpha)+B^m(\alpha)]}{2\cosh(|\alpha|^2)}, \tag{37}$$

$$N_O={}_O\langle\alpha|b^m b^{\dagger m}|\alpha\rangle_O=\frac{\exp(|\alpha|^2)[A^m(\alpha)-B^m(\alpha)]}{2\sinh(|\alpha|^2)}. \tag{38}$$

We note here that $J^m_{\lambda,\rho}(\alpha)$ and $K^m_{\lambda,\rho}(\alpha)$ are related by a set of the sum of the matrix elements $A^m_{\lambda,\rho}(\alpha^*,\alpha)$ and $B^m_{\lambda,\rho}(\alpha^*,-\alpha)$,

$$J^{m}_{\lambda,\rho}(\alpha)=J^{m,m}_{\lambda,\rho}(\alpha^*,\alpha)=A^{m,m}_{\lambda,\rho}(\alpha^*,\alpha)+B^{m,m}_{\lambda,\rho}(\alpha^*,-\alpha), \tag{39}$$

$$K^{m}_{\lambda,\rho}(\alpha)=K^{m,m}_{\lambda,\rho}(\alpha^*,\alpha)=A^{m,m}_{\lambda,\rho}(\alpha^*,\alpha)-B^{m,m}_{\lambda,\rho}(\alpha^*,-\alpha), \tag{40}$$

$$J^{m}(\alpha)=A^{m}(\alpha)+B^{m}(\alpha), K^{m}(\alpha)=A^{m}(\alpha)-B^{m}(\alpha), \tag{41}$$

where λ and ρ are non-negative integers.

III. QUASIPROBABILITY FUNCTION OF THE QUANTUM STATES

We shall use the general matrix elements $A^{n,m}_{\lambda,\rho}(\alpha^*,\beta)$, $B^{n,m}_{\lambda,\rho}(\alpha^*,-\beta)$, $A^{n,m}_{\lambda,\rho}(-\alpha^*,-\beta)$, and $B^{n,m}_{\lambda,\rho}(-\alpha^*,\beta)$ defined above, and calculate the quantum statistical properties of these new types of quantum states. It is well known that the quasiprobability distribution functions are extremely useful in the mathematical description of quantum mechanical systems.[13,18–20] They include the P function, Q function, and Wigner function, which are all closely related to the quantum statistical behavior of a microscopic system. Our results are expected to give distribution functions characteristic of quantum fields.[21] To this purpose we first consider the fact that the P, Q, and W functions may be obtained in the integral form of the density matrix $\rho=(1/\pi)\int P(z)|z\rangle\langle z|\mathrm{d}^2z$, where $|z\rangle$ is the coherent state. We have thus established the relationship between the matrix and the mathematical structure of the GEECS and GEOCS in the coherent state space.

A. *P* function representation

To determine the P distribution of the $|\alpha,m,\mu,\nu\rangle_{E(O)}$ state it is customary to use the Glauber–Sudarshan representation, so the density matrix is

$$\rho=|\alpha,m,\mu,\nu\rangle_{E(O)(O)E}\langle\alpha,m,\mu,\nu|=\int P_{GEE(GEO)}(z)|z\rangle\langle z|\mathrm{d}^2z. \tag{42}$$

By the double-Fourier transform[22] we have

$$P_{GEE(GEO)}(z)=\frac{e^{|z|^2}}{\pi^2}\int \mathrm{d}^2\beta\langle-\beta|\alpha,m,\mu,\nu\rangle_{E(O)(O)E}\langle\alpha,m,\mu,\nu|\beta\rangle\times\exp[z\beta^*-z^*\beta], \tag{43}$$

where $[z\beta^*-z^*\beta]$ is an imaginary variable which is known to be integrable and satisfies

$$\int \mathrm{d}^2\beta\exp[\pm(z\beta^*-z^*\beta)]=\pi^2\delta^2(z). \tag{44}$$

We thus have

$$P_{GEE}(\alpha,z)=\frac{e^{|z|^2-|\alpha|^2}}{J^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R^m_s(\mu^*,\nu^*,\alpha)S^n_t(\mu,\nu,\alpha^*)\frac{\partial^{(2m-s-t)}}{\partial z^{(m-s)}\partial z^{*(m-t)}}\{(-1)^{s+t}\delta^2(z-\alpha)$$
$$+\delta^2(z+\alpha)+(-1)^s\delta(z-\alpha)\delta(z+\alpha)^*+(-1)^t\delta(z+\alpha)\delta(z-\alpha)^*\}, \tag{45}$$

$$P_{GEO}(\alpha,z)=\frac{e^{|z|^2-|\alpha|^2}}{k^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R^m_s(\mu^*,\nu^*,\alpha)S^n_t(\mu,\nu,\alpha^*)\frac{\partial^{(2m-s-t)}}{\partial z^{(m-s)}\partial z^{*(m-t)}}\{(-1)^{s+t}\delta^2(z-\alpha)$$
$$+\delta^2(z+\alpha)-(-1)^s\delta(z-\alpha)\delta(z+\alpha)^*-(-1)^t\delta(z+\alpha)\delta(z-\alpha)^*\}. \tag{46}$$

In deriving (45) and (46), we have utilized Eqs. (33) and (34), and the relationship

$$R^m_s(\mu^*,\nu^*,-\alpha)=(-1)^sR^m_s(\mu^*,\nu^*,\alpha),$$
$$S^m_t(\mu,\nu,-\alpha^*)=(-1)^tS^m_t(\mu,\nu,\alpha^*), \tag{47}$$

which can be easily proved for $\alpha=-\alpha$, $\alpha^*=-\alpha^*$. From the double δ-function we see that $P_{GEE}(\alpha,z)$ and $P_{GEO}(\alpha,z)$ are extremely singular, which is a characteristic typical of nonclassical states. In particular, for the parameter values $\nu=0$ and $\mu=1$, the distribution functions $P_{GEE}(\alpha,z)$ and $P_{GEO}(\alpha,z)$ reduce to $P_{EE}(\alpha,z)$ and $P_{EO}(\alpha,z)$, which are the P functions of the excited even/odd coherent states from previously known states.[10]

B. *Q* function representation

The quasiprobability Q function, also known as the Husimi function, is given in the diagonal element of the density matrix ρ associated with the GEECS and GEOCS states,

$$Q_{GEE}(\alpha,z)=\frac{1}{\pi J^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R_s^m(\mu^*,\nu^*,\alpha)S_t^m(\mu,\nu,\alpha^*)z^{*(m-s)}z^{(m-t)}$$
$$\times\{\exp[-|z-\alpha|^2]+(-1)^{s+t}\exp[-|z+\alpha|^2]+(-1)^t$$
$$\times\exp[-z^*(z-\alpha)-\alpha^*(z+\alpha)]+(-1)^s\exp[-z^*(z+\alpha)+\alpha^*(z-\alpha)]\}, \tag{48}$$

$$Q_{GEO}(\alpha,z)=\frac{1}{\pi K^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R_s^m(\mu^*,\nu^*,\alpha)S_t^m(\mu,\nu,\alpha^*)z^{*(m-s)}z^{(m-t)}$$
$$\times\{\exp[-|z-\alpha|^2]+(-1)^{s+t}\exp[-|z+\alpha|^2]-(-1)^t$$
$$\times\exp[-z^*(z-\alpha)-\alpha^*(z+\alpha)]-(-1)^s\exp[-z^*(z+\alpha)+\alpha^*(z-\alpha)]\}. \tag{49}$$

Because the GEECS and GEOCS are superpositions of the coherent states $|\alpha\rangle$ and $|-\alpha\rangle$, a three-dimensional plot in phase space with respect to the complex number $z=x+iy$ of their $Q_{GEE}(\alpha,z)$ and $Q_{GEO}(\alpha,z)$ functions displays two peaks when $\arg\nu=\arg\mu$, $\arg\nu=-\arg\mu$, and $\alpha=\alpha_1+i\alpha_2$. Figures 1(a) and 1(b) show the $Q_{GEE}(\alpha,z)$ and $Q_{GEO}(\alpha,z)$ distributions, which can be seen even more clearly by projecting symmetrically about x onto a two-dimensional complex plane. However, we observe that for a given μ, ν, and m the functions $Q_{GEE}(\alpha,z)$ and $Q_{GEO}(\alpha,z)$ for a Schrödinger-cat-like state can be analytically derived from the definitions in (9) and (10). We see from Fig. 1(a) that $Q_{GEE}(\alpha,z)$ has two split peaks which then move in opposite directions with appropriate choices of μ and ν when m and $|\alpha|$ are fixed, and as the parameter ν increases ($\nu=-0.4,-0.6$, and -1), oscillations appear between the two peaks. As the value of ν increases, the oscillations become more pronounced and the peaks smaller. In Fig. 1(b) for the function $Q_{GEO}(\alpha,z)$, as the degree of excitation m increases the two peaks move in opposite directions while their height decreases and their distance becomes wider for $\nu=-0.8$ ($m=0,2$, and 4, respectively). No matter how the parameters ν, μ, and m are chosen for $\arg\alpha=\pi/2$, the $Q_{GEE}(\alpha,z)$ and $Q_{GEO}(\alpha,z)$ functions always exhibit some oscillatory behavior. This is related to the negative parts of the Wigner function since the Q function can be regarded as a smoothed Wigner function.

C. Wigner function representation

The Wigner function is also a useful measure for studying the nonclassical features of quantum states. The form through the density operator associated with the coherent state representation is given by

$$W(z)=\frac{2e^{2|z|^2}}{\pi^2}\int d^2\langle-\beta|\rho|\beta\rangle\exp[2(z\beta^*-z^*\beta)]. \tag{50}$$

Because the above case is an imaginary variable transformation in the complex plane, we can use integration and Leibnitz's formulas,

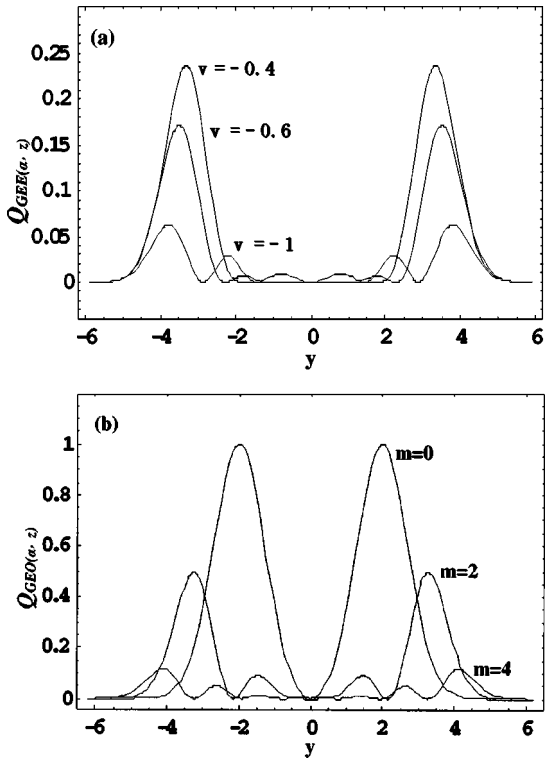

FIG. 1. The Q function of $Q_{GEE}(\alpha,z)$ and $Q_{GEO}(\alpha,z)$ in the case of $\alpha_1=0$, $\alpha_2=2$, $\arg\nu=\arg\mu$, for (a) $m=3$, $\nu=-0.4,-0.6,-1$ and (b) $\nu=-0.8$, $m=0,2,4$.

$$\int \frac{\mathrm{d}^2\beta}{\pi}[\zeta|\beta|^2+\xi^*|\beta|+\eta\beta^*]=\left(-\frac{1}{\zeta}\right)\exp\left(-\frac{\xi\eta}{\zeta}\right) \quad (\zeta\geqslant -1) \tag{51}$$

and

$$\left(\frac{\partial^{2n}}{\partial\xi^{*n}\partial\xi^n}\right)e^{-\xi^*\xi}=(-1)^n n!\,e^{-\xi^*\xi}L_n(-|\xi|^2). \tag{52}$$

From Eq. (50) and after performing a two-dimensional Fourier transformation, the $W_{GEE}(\alpha,z)$ and $W_{GEO}(\alpha,z)$ functions can be expressed in the following form:

$$\begin{aligned}W_{GEE}(\alpha,z)=&\frac{2e^{2|z|^2-|\alpha|^2}}{\pi J^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R_s^m(\mu^*,\nu^*,\alpha)S_t^n(\mu,\nu,\alpha^*)\\&\times\{\exp[|\xi|^2]G_{m-t}^{m-s}[\xi^*,\xi,|\xi|^2]+(-1)^{s+t}\exp[|\eta|^2]G_{m-t}^{m-s}[\eta^*,\eta,|\eta|^2]+(-1)^t\\&\times\exp[-\eta^*\xi]G_{m-t}^{m-s}[\eta^*,\xi,\eta^*\xi]+(-1)^s\exp[-\xi^*\eta]G_{m-t}^{m-s}[\xi^*,\eta,\xi^*\eta]\},\end{aligned} \tag{53}$$

$$\begin{aligned}W_{GEO}(\alpha,z)=&\frac{2e^{2|z|^2-|\alpha|^2}}{\pi K^m(\alpha)}\sum_{s=0}^{m}\sum_{t=0}^{m}R_s^m(\mu^*,\nu^*,\alpha)S_t^n(\mu,\nu,\alpha^*)\\&\times\{\exp[|\xi|^2]G_{m-t}^{m-s}[\xi^*,\xi,|\xi|^2]+(-1)^{s+t}\exp[|\eta|^2]G_{m-t}^{m-s}[\eta^*,\eta,|\eta|^2]-(-1)^t\\&\times\exp[-\eta^*\xi]G_{m-t}^{m-s}[\eta^*,\xi,\eta^*\xi]-(-1)^s\exp[-\xi^*\eta]G_{m-t}^{m-s}[\xi^*,\eta,\xi^*\eta]\},\end{aligned} \tag{54}$$

where $\xi=2z-\alpha$, $\eta=2z+\alpha$, and

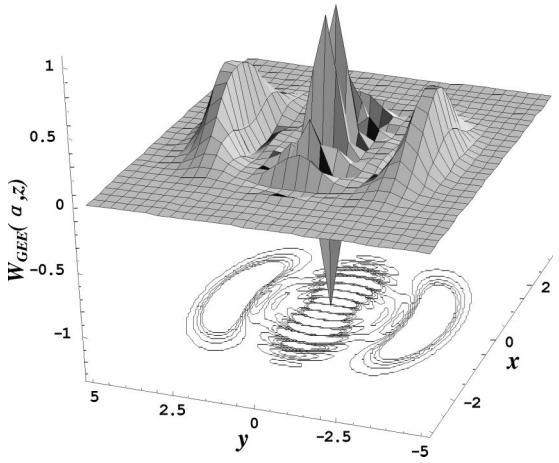

FIG. 2. The Wigner function $W_{GEE}(\alpha,z)$ in the case of $\alpha_1=0$, $\alpha_2=2$, $\nu=-0.1$, $\arg\nu=\arg\mu$ for $m=3$.

$$G_q^p(\xi,\eta^*,\eta^*\xi)=\begin{cases}(-1)^p p!\,\xi^{(q-p)}L_p^{(q-p)}(\eta^*\xi), & q\geqslant p,\\ (-1)^q q!\,\eta^{*(p-q)}L_q^{(p-q)}(\eta^*\xi), & q\leqslant p.\end{cases} \tag{55}$$

Exact analytical expressions for the generalized excited even/odd coherent states when ν, μ, and m are varied can be obtained from expressions (53) and (54). Let us look at the special case of $\arg\alpha=\arg(\alpha_1+i\alpha_2)=\pi/2$, i.e., corresponding to $\alpha_1=0,\alpha_2=2$. The nonclassical properties of the GEECS and GEOCS can be seen even more clearly by projecting the three-dimensional plots of $W_{GEE}(\alpha,z)$ and $W_{GEO}(\alpha,z)$ onto the two-dimensional (x,y) plane. Figures 2 and 3 show the distributions of the $W_{GEE}(\alpha,z)$ and $W_{GEO}(\alpha,z)$ contours for different values of ν, μ, m, and $|\alpha|$. We see that $W_{GEE}(\alpha,z)$ is a function of a complex number $z=x+iy$ when $\arg\nu=\arg\mu$. As the degree of excitation increases ($m>1$) the peak of the $W_{GEE}(\alpha,z)$ function begins to split into two peaks, which then move in opposite directions when $\nu=-0.1$ and $m=2$, as can be seen in Fig. 2. For the GEOCS state in Fig. 3, the $W_{GEO}(\alpha,z)$ function also splits into two peaks when m and $|\alpha|$ are fixed, and the distance between them increases as ν becomes more negative. Both sets of contours are symmetrical about the $y=0$ plane, exhibiting the two mirror-symmetrical Gaussian hills of the Wigner function distributions and reflecting the superposition of the Schrödinger cat-like state. At the center where the two peaks split there are marked oscillations. We see that the

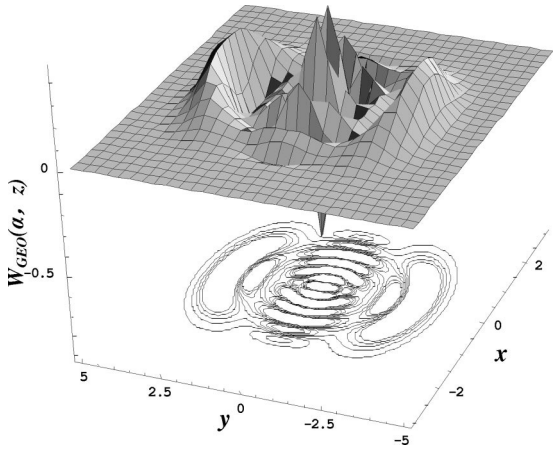

FIG. 3. The Wigner function $W_{GEO}(\alpha,z)$ in the case of $\alpha_1=0$, $\alpha_2=2$, $m=2$, $\arg\nu=\arg\mu$ for $\nu=-0.5$.

greater the value of m for the GEECS, the stronger the oscillation between the two highest peaks. On the other hand, the GEOCS state is also greatly affected by changes in ν and μ.

IV. CONCLUSION

By means of specific mathematical procedures we have obtained two new classes of quantum states in the coherent state representation. The general expressions for these states reduce to previously known quantum states for special values of the parameters given. For example, when $\nu=0$ and $\mu=1$, they reduce to the excited even/odd coherent states,[10] which further reduce to the even/odd coherent states when $m=0$.[1,2] Through numerical computation of various quantum properties, i.e., the P function, Q function, and Wigner function, we find that these new states exhibit highly nonclassical characteristics. The quantum interference patterns are very pronounced and narrow, while parts of the central region of the Wigner function are negative. It is obvious that these results all deviate considerably from a Gaussian distribution. The oscillatory behavior of the states is due to the structure of their formulation; since they are superpositions of the coherent states $|\alpha\rangle$ and $|-\alpha\rangle$ their probability distributions undergo destructive or constructive interference. We can also see that the interference effects are a consequence of the oscillatory nature of the associated Laguerre and Hermite polynomials, and the exponential factors which make up the functions $R_s^m(\mu^*,\nu^*,\beta), S_t^n(\mu,\nu,\alpha^*)$, and $G_q^p(\eta^*,\xi,\eta^*\xi)$ in the Wigner function.

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Interior structural bifurcation and separation of 2D incompressible flows

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We study transitions in the topological structure of a family of divergence-free vector fields $u(\cdot,t)$ near an interior point. It is shown that structural bifurcation occurs at t_0 if $u(\cdot,t_0)$ has an isolated degenerate singular point $x_0 \in \mathring{M}$ with zero index and nonzero Jacobian at x_0, and with nonzero acceleration in the direction normal to the (unique) eigenspace of the Jacobian. This result is carried out by analyzing the orbit structure of u near such an isolated degenerate interior singular point of $u(\cdot,t_0)$. Applications to typical interior separation phenomena in two-dimensional fluid flows are addressed as well. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1689005]

I. INTRODUCTION

The main objective of this paper is to derive a rigorous kinematic theory for the typical interior separation phenomena in two-dimensional fluid flows. This is part of a research program on the use of topological ideas to study the spatial–temporal structure of 2D incompressible fluid flows in physical space, along with its stability and bifurcations. This program consists of research in two areas: (a) the study of the topological structure of divergence-free vector fields, and its evolution in time or with respect to an arbitrary parameter, and (b) the study of the structure and evolution of velocity fields for 2D incompressible fluid flows governed by a class of equations that comprises the Navier–Stokes equations, the Euler equations, and the quasigeostrophic equations of rotating flows. The objectives of this research program are consistent with the program by Newton and his collaborators, using in particular the vorticity in their analysis; see Ref. 6 and the reference therein.

In this paper, we address structural bifurcation for a family of divergence-free vector fields $u(\cdot,t)$ near an interior point. Structural bifurcation near boundary singular points was carried out by the authors in collaboration with Michael Ghil, leading to a rigorous characterization for boundary layer separation for 2D incompressible fluid flows; see Refs. 2 and 3 and the survey article[5] for details.

More precisely, we shall show that structural bifurcation occurs at t_0 if $u(\cdot,t_0)$ has an isolated degenerate singular point $x_0 \in \mathring{M}$ with zero index and nonzero Jacobian at x_0, and with nonzero acceleration in the direction normal to the (unique) eigenspace of the Jacobian.

Technically speaking, the main results are carried out by analyzing the orbit structure of u near such an isolated degenerate interior singular point of $u(\cdot,t_0)$. We now summarize the analysis. For this purpose, we consider the Taylor expansion of the divergence-free vector fields $u(\cdot,t)$ at t_0 $(0<t_0<T)$

$$u(x,t)=u^0(x)+(t-t_0)u^1(x)+o(|t-t_0|),$$

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$$u^0(x)=u(x,t_0),$$

$$u^1(x)=\frac{\partial}{\partial t}u(x,t_0).$$

First we observe by the structural stability theorem, Theorem 2.4, that structural bifurcation can only occur near a degenerate singular point x_0, i.e., the determinant of the Jacobian of u at x_0 is zero: $\det Du(x_0)=0$. Generically, we only have to examine then the case where Jacobian itself is not zero: $Du(x_0)\neq 0$; see Theorem 5.5.

Second, further analysis shows that a degenerate singular point $x_0\in\mathring{M}$ of $u\in D^r(TM)$ $(r\geqslant 1)$ with nonzero Jacobian $Du(x_0)\neq 0$ can only be one of the three cases:

(1) a degenerate center,
(2) a degenerate saddle such that the four orbits connected to x_0 are tangent to each other at x_0, and
(3) a point with $\mathrm{ind}(u,x_0)=0$ such that the angle between the two orbits connected to x_0 is zero.

Again, the genericity result given in Theorem 5.5 shows that we only have to consider the structural bifurcation in the third case, i.e., near an interior degenerate singular point such that $\mathrm{ind}(u,x_0)=0$ and the angle between the two orbits connected to x_0 is zero.

Third, when $Du(x_0)\neq 0$ but $\det Du(x_0)=0$, there is a unique eigendirection of $Du(x_0)$ corresponding to the zero eigenvalue. Let e_1 be the eigenvector, and e_2 is orthogonal to e_1. Then we are able to derive the main theorems of this paper, Theorems 4.4 and 4.5. In addition to detailed characterization of the structural transition near the bifurcation point, in particular, we are able to show that structural bifurcation occurs at (t_0,x_0) if x_0 is an isolated degenerate singular point of $u^0(x)$, and

$$\mathrm{ind}(u^0,x_0)=0,$$

$$Du^0(x_0)\neq 0,$$

$$u^1(x_0)\cdot e_2\neq 0.$$

Fourth, the bifurcation obtained in these two theorems corresponds directly to typical interior separation phenomena in two-dimensional fluid flows, and is generic; see Theorems 5.2 and 5.5.

The paper is organized as follows. In Sec. II, we recall some preliminaries, including a structural stability theorem, and a singularity classification theory for 2D divergence-free vector fields. Section III classifies interior degenerate singular points, and identifies some useful and easy to verify kinematic conditions. Section IV states and proves the main structural bifurcation theorems. Genericity and connections to interior separation phenomena of fluid flows are given in Sec. V.

II. PRELIMINARIES

We first recall some basic facts and definitions on structural stability and bifurcation of divergence-free vector fields. Let $M\subset\mathbb{R}^2$ be a closed and bounded domain with C^r $(r\geqslant 1)$ boundary ∂M. Let TM be the tangent bundle of M, and $C^r(TM)$ be the space of all C^r vector fields on M. Let

$$D^r(TM)=\{v\in C^r(TM)\,|\,v_n|_{\partial M}=0,\ \mathrm{div}\,v=0\},$$

where n is the unit outward normal vector on ∂M and $v_n=v\cdot n$.

The structural stability theorems of divergence-free vector fields with various boundary conditions, obtained by the authors in Ref. 4, are useful in the study of structural bifurcation. Here, we only introduce the structural stability theorem in $D^r(TM)$ (for divergence-free vector fields with no-normal flows).

Definition 2.1: Two vector fields $u,v \in D^r(TM)$ are called topologically equivalent in $D^r(TM)$ if there exists a homeomorphism of $\varphi: M \to M$, which maps orbits of u to orbits of v and preserves their orientation.

Definition 2.2: A vector field $v \in$ is called structurally stable in $D^r(TM)$ if there exists a neighborhood $\mathcal{O} \subset D^r(TM)$ of v such that for any $u \in \mathcal{O}$, u and v are topologically equivalent.

Definition 2.3: Let $u \in C^1([0,T], D^r(TM))$. We say that $u(x,t)$ has a bifurcation in its local structure in a neighborhood $U \subset M$ of x_0 at t_0 $(0<t_0<T)$ if, for any $t^- < t_0$ and $t_0 < t^+$ with t^- and t^+ sufficiently close to t_0, the vector fields $u(\cdot,t^-)$ and $u(\cdot,t^+)$ are not topologically equivalent locally in $U \subset M$, and we say that $u(\cdot,t)$ has a bifurcation at t_0 in its global structure if $U = M$.

A point $p \in M$ is called a singular point of $u \in D^r(TM)$ if $u(p)=0$; a singular point p of u is called nondegenerate if the Jacobian matrix $Du(p)$ is invertible; u is called regular if all singular points are nondegenerate. Then the following theorem provides necessary and sufficient conditions for structural stability of a divergence-free vector field in $D^r(TM)$.

Theorem 2.4 (Ma and Wang[4]): *A divergence-free vector field $u \in D^r(TM)$ $(r \geqslant 1)$ is structurally stable in $D^r(TM)$ if and only if*

(1) u is regular;
(2) all interior saddle points of u are self-connected; and
(3) each saddle point of u on ∂M is connected only to saddle points on the same connected component of ∂M.

Moreover, the set of all structurally stable vector fields is open and dense in $D^r(TM)$.

From the above definitions and the structural stability theorem, the local structural bifurcation can only occur at degenerate singularity points. For bifurcation near boundary points, we refer the interested reader to Ref. 2. Here in this paper we address the bifurcation near an interior singular point.

For this purpose, let $p \in M$ be an isolated singular point of $v \in C_n^r(TM)$; then

$$\mathrm{ind}(v,p) = \deg(v,p),$$

where $\deg(v,p)$ is the Brouwer degree of v at p.

Let $p \in \partial M$ be an isolated singular point of v, and $\tilde{M} \subset \mathbb{R}^2$ be an extension of M, i.e., $M \subset \tilde{M}$ such that $p \in \tilde{M}$ is an interior point of $\tilde{M}$. In a neighborhood of p in $\tilde{M}$, v can be extended by reflection to $\tilde{v}$ such that p is an interior singular point of $\tilde{v}$, thanks to the no-normal flow condition, i.e., $v \cdot n|_{\partial M} = 0$. Then we define the index of v at $p \in \partial M$ by

$$\mathrm{ind}(v,p) = \tfrac{1}{2}\,\mathrm{ind}(\tilde{v},p).$$

Let $p \in M$ be an isolated singular point of $v \in C_n^r(TM)$. An orbit γ of v is said to be a stable orbit (respectively, an unstable orbit) connected to p, if the limit set $\omega(x)=p$ [respectively, $\alpha(x)=p$] for $x \in \gamma$.

Theorem 2.5 (Ref. 2): *Let $p \in M$ be an isolated singular point of $v \in D^r(TM)$, $r \geqslant 1$. Then p is connected only to a finite number of orbits and the stable and unstable orbits connected to p alternate when tracing a closed curve around p. Furthermore,*

(1) when $p \in \mathring{M}$, p has $2n$ $(n \geqslant 0)$ orbits, n of which are stable, and the other n unstable, while the index of p is

$$\mathrm{ind}(v,p) = 1 - n,$$

(2) when $p \in \partial M$, p has $n+2$ $(n \geqslant 2)$ orbits, two of which are on the boundary ∂M, and the index of p is

$$\mathrm{ind}(v,p) = -\frac{n}{2}.$$

III. INTERIOR DEGENERATE SINGULARITIES

A. Characterization of degenerate singularities with nonzero Jacobian

The structural stability theorem (Theorem 2.4) suggests studying the structure of divergence-free vector fields near degenerate singular points. To this end, we now introduce some lemmas characterizing degenerate interior singularities with nonzero Jacobians, which are useful for studying interior structural bifurcation.

Lemma 3.1: Let $u \in D^r(TM)$ $(r \geqslant 1)$, and $x_0 \in \mathring{M}$ be an isolated singular point of u. If the index $\mathrm{ind}(u,x_0) \neq 1,0,-1$, *then the Jacobian matrix*

$$Du(x_0) = 0. \tag{3.1}$$

Proof: By Theorem 2.5, the index of an interior singular point of a divergence-free vector field is determined by the $2n$ $(n \geqslant 0)$ orbits connected to x_0, i.e., $\mathrm{ind}(u,x_0) = 1-n$. Hence, by assumption, $n \geqslant 3$.

Let γ be an orbit of u connected to x_0. Let (x_1,x_2) be the orthogonal coordinate system with x_0 as its origin, and with its x_1-axis tangent to γ at x_0. Then u can be expressed locally by

$$\begin{aligned} u(x) &= \begin{pmatrix} a & b \\ c & -a \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + o(|x|), \\ Du(x_0) &= Du(0) = \begin{pmatrix} a & b \\ c & -a \end{pmatrix}. \end{aligned} \tag{3.2}$$

We shall prove that $a = b = c = 0$ in several steps as follows.

Step 1: We show that $a = c = 0$. By definition, the x_1-axis is tangent to γ at $x_0 = 0$, which yields

$$\lim_{\substack{x \in \gamma \\ x \to 0}} \frac{u_2(x)}{u_1(x)} = 0. \tag{3.3}$$

In addition, for $(x_1,x_2) \in \gamma$, $x_2 = o(|x_1|)$. Hence, we infer from (3.2) and (3.3) that

$$\lim_{\substack{x \in \gamma \\ x \to 0}} \frac{u_2(x)}{u_1(x)} = \lim_{\substack{x \in \gamma \\ x \to 0}} \frac{cx_1 - ax_2 + o(|x|)}{ax_1 + bx_2 + o(|x|)} = \lim_{\substack{x \in \gamma \\ x_1 \to 0}} \frac{cx_1 + o(|x_1|)}{ax_1 + o(|x_1|)} = \frac{c}{a} = 0.$$

Hence $c = 0$. By $\mathrm{ind}(u,x_0) \neq 1,-1$, the singular point x_0 of u is degenerate. Therefore $c = 0$ implies that $a = 0$.

Hence when $\mathrm{ind}(u,x_0) \neq 1,-1$, u can be expressed near $x_0 = 0$ as

$$\begin{aligned} u_1(x) &= bx_2 + o(|x|), \\ u_2(x) &= o(|x|). \end{aligned} \tag{3.4}$$

Step 2: Consider the case where there is another orbit γ_1 of u connected to x_0, and the angle between γ_1 and γ is θ different from 0 and π. Then by (3.4) we deduce that

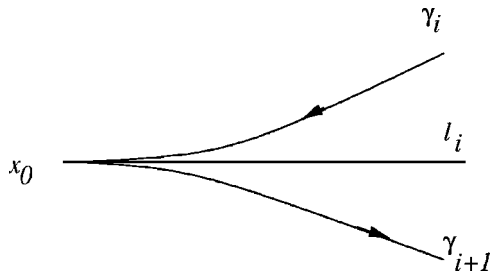

FIG. 1. Sketch illustrating the proof of Lemma 3.1.

$$\lim_{\substack{x\in\gamma_1\\ x\to 0}}\frac{u_2(x)}{u_1(x)}=\lim_{\substack{x\in\gamma_1\\ x\to 0}}\frac{o(|x|)}{bx_2+o(|x|)}=\tan\theta\neq 0$$

which yields that $b=0$. Hence (3.1) holds true in this case.

Step 3: Consider the case where all orbits connected to x_0 are tangent to γ at x_0. Let $O\in M$ be a sufficiently small neighborhood of x_0, F_i $(1\leqslant i\leqslant 2n)$ be the domains in O enclosed by the orbits connected to x_0, and the θ_i be the angle of the boundary of F_i at x_0. It is easy to see that in each F_i with $\theta_i=0$, there exists at least a curvilinear segment ℓ_i, with x_0 being its end point, such that $u_1(x)=0$, $x\in\ell_i$ (see Fig. 1). Hence, there are at least $2(n-1)$ curvilinear segments in O with x_0 as their common end point where $u_1=0$. On the other hand, by the implicit function theorem, if $b\neq 0$ in (3.4), then there is a unique curve $L\subset O$ with $x_0\in L$ such that $u_1(x)=0$, $x\in L$, i.e., there are only two line segments $L=\ell_1\cup\ell_2$ in O along which $u_1=0$; hence if $n\geqslant 3$ it follows that $b=0$ and (3.1) holds true.

This completes the proof of this lemma. □

Lemma 3.2: Let $u\in D^r(TM)$ $(r\geqslant 1)$, and $x_0\in\mathring{M}$ be an isolated singular point of u. If the index $\mathrm{ind}(u,x_0)=0$, *and the angle θ between the two orbits connected to x_0 is different from* 0, *then (3.1) holds true.*

Proof: By Step 2 in the proof of Lemma 3.1, it suffices to prove (3.1) when $\theta=\pi$. In this case the two orbits γ_1 and γ_2 connected to x_0 form a curve Γ with the x_1-axis tangent to Γ at x_0. By Theorem 2.5, it is obvious that for any $x_2>0$ sufficiently small, we have

$$\mathrm{sign}\,u_1(0,x_2)=\mathrm{sign}\,u_1(0,-x_2),$$

which, together with (3.4), yields that $b=0$. This proof is complete. □

From Lemma 3.1, we see that a degenerate singular point $x_0\in\mathring{M}$ of $u\in D^r(TM)$ $(r\geqslant 1)$ with nonzero Jacobian $Du(x_0)\neq 0$ can only be one of the three cases:

(1) a degenerate center;
(2) a degenerate saddle such that the four orbits connected to x_0 are tangent to each other at x_0; and
(3) a point with $\mathrm{ind}(u,x_0)=0$ such that the angle between the two orbits connected to x_0 is zero.

We now take a further examination of these cases.

Let $x_0\in\mathring{M}$ be an isolated degenerate singular point of $u\in D^r(TM)$ $(r\geqslant 1)$ with nonzero Jacobian, $Du(x_0)\neq 0$. Since $Du(x_0)$ is a degenerate matrix, $Du(x)$ has an eigenvector e_1 satisfying

$$Du(x_0)e_1=0,\quad |e_1|=1. \tag{3.5}$$

Let e_2 be a unit vector, which is orthogonal to e_1, and satisfies that

$$Du(x_0)e_2=\alpha e_1, \tag{3.6}$$

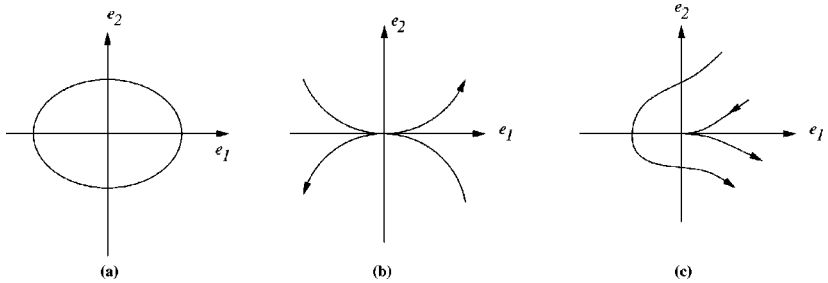

FIG. 2. (a) The case with index 1, (b) the case with index -1, and (c) the case with index 0.

for some constant $\alpha \neq 0$.

For simplicity, we always take the orthogonal coordinate system (x_1, x_2) with the origin at x_0, x_1-axis and x_2-axis pointing, respectively, in the e_1 and e_2 directions. In this case, the matrix $Du(x_0)$ and the vectors e_1, e_2 can be written as follows:

$$Du(x_0) = Du(0) = \begin{pmatrix} 0 & \alpha \\ 0 & 0 \end{pmatrix}, \quad \alpha \neq 0,$$
$$e_1 = (1,0), \quad e_2 = (0,1). \tag{3.7}$$

Geometrically, e_1 and e_2 can be illustrated as in Fig. 2.

B. Index and kinematic conditions

We now make connections between the index of u at x_0 and different orders of u in its Taylor expansion near x_0. Let $x_0 \in \mathring{M}$ be an isolated degenerate singular point of u, and

$$Du(x_0) \neq 0, \tag{3.8}$$

$$\frac{\partial^m (u(x_0) \cdot e_2)}{\partial e_1^m} \begin{cases} = 0, & 1 \leqslant m < n, \\ \neq 0, & m = n. \end{cases} \tag{3.9}$$

Under the conditions (3.8) and (3.9), the vector field $u(x)$ has the Taylor expansion, by (3.7), as follows:

$$u(x) = \begin{cases} \alpha x_2 + f(x_1) + x_2 g_1(x), \\ \beta x_1^n - x_2 f'(x_1) + x_2^2 g_2(x) + o(|x_1|^n), \end{cases} \tag{3.10}$$

where $\alpha, \beta \neq 0$, $f(x_1) = o(|x_1|)$, and $g_i(0) = 0$ $(i = 1,2)$. Let $k = \deg f$ be defined by

$$\lim_{z \to 0} \frac{f(z)}{z^k} = \lambda \neq 0, \quad k \leqslant \infty.$$

Lemma 3.3: Let $x_0 \in \mathring{M}$ be an isolated degenerate singular point of u satisfying (3.8) and (3.9).

(1) If $2k > n+1$, then

$$\operatorname{ind}(u, x_0) = \begin{cases} 0, & \text{as } n = \text{even}, \\ -1, & \text{as } n = \text{odd and } \alpha \cdot \beta > 0 \text{ in (3.10)}, \\ 1, & \text{as } n = \text{odd and } \alpha \cdot \beta < 0. \end{cases}$$

(2) If either $2k < n+1$, or $2k = n+1$ and $\alpha\beta \neq -k\lambda^2$, then $\operatorname{ind}(u, x_0) = -1$.

Proof: Proof of Assertion (1). Let

$$u_t(x)=\begin{cases}\alpha x_2+t[f(x_1)+x_2g_1(x)],\\ \beta x_1^n+t[-x_2f'(x_1)+x_2^2g_2(x)+o(|x_1|^n)],\end{cases}$$

where $0\leqslant t\leqslant 1$. Since $2k-1>n$, it is easy to see that there exists a neighborhood $U\subset M$ of x_0 $(=0)$, such that $u_t(x)$ has only a singular point $x=0$ in U for all $t\in[0,1]$. By the homotopy invariance of the index, we derive that

$$\mathrm{ind}(u_0,x_0)=\mathrm{ind}(u_1,x_0)=\mathrm{ind}(u,x_0). \tag{3.11}$$

In a neighborhood of $x=0$, orbits of $u_0=(\alpha x_2,\beta x_1^n)$ are given by the following equations:

$$\frac{\alpha}{2}x_2^2-\frac{\beta}{n+1}x_1^{n+1}=C,\quad 0\leqslant|C|<\delta. \tag{3.12}$$

Obviously, we can see from (3.12) that if $n=$ even, the flow of u_0 in a neighborhood of $x=0$ is as shown in Fig. 2(c). If $n=$ odd, when $\alpha\cdot\beta>0$ (respectively, $\alpha\cdot\beta<0$) the flows of u_0 looks as shown in Fig. 2(b) [respectively, as shown in Fig. 2(a)]. Thus, we derive from (3.11) this claim.

Proof of assertion (2): We take $\varepsilon>0$ sufficiently small, and consider singular points of the following vector field near $x=0$:

$$u_\varepsilon=\begin{cases}\alpha x_2+f(x_1)+x_2g_1(x),\\ \beta x_1^n-x_2f'(x_1)+x_2^2g_2(x)+o(|x_1|^n)-\varepsilon.\end{cases}$$

By assumption, f can be expressed near $x=0$ by

$$f(x_1)=\lambda x_1^k+o(|x_1|^k),\quad \lambda\neq 0,\ 1<k\leqslant\frac{n+1}{2}.$$

Thus, singular points of u_ε in a small neighborhood of $x=0$ satisfy the equation below

$$\begin{aligned}x_2&=-\frac{\lambda}{\alpha}x_1^k+o(|x_1|^k),\\ \beta x_1^n&+\frac{1}{\alpha}k\lambda^2x_1^{2k-1}=\varepsilon+o(|x_1|^{2k-1}).\end{aligned} \tag{3.13}$$

Obviously, when $2k-1<n$, or $2k-1=n$ and $\alpha\beta\neq-k\lambda^2$, (3.13) has a unique solution

$$x_\varepsilon\sim\left(C\varepsilon^{1/(2k-1)},-\frac{\lambda}{\alpha}C^k\varepsilon^{k/(2k-1)}\right),$$

where

$$C=\begin{cases}\alpha k^{-1}\lambda^{-2},\quad \text{as } 2k-1<n,\\ \alpha(\alpha\beta+\lambda^2)^{-1},\quad \text{as } 2k-1=n \text{ and } \alpha\beta\neq k\lambda^2.\end{cases}$$

It is easy to check that

$$\mathrm{sign}\det Du_\varepsilon(x_\varepsilon)=-1, \tag{3.14}$$

for any $\varepsilon>0$ sufficiently small. By the invariance of index sums in a small domain with a perturbation we refer from (3.14) that $\mathrm{ind}(u,x_0)=-1$. The proof of this lemma is complete. □

IV. STRUCTURAL BIFURCATION NEAR INTERIOR SINGULAR POINTS WITH INDEX ZERO

A. Main theorems

Let $u \in C^1([0,T],D^r(TM))$ $(r \geqslant 1)$ be a one-parameter family of divergence-free vector fields. We consider the Taylor expansion of $u(x,t)$ at t_0 $(0<t_0<T)$,

$$u(x,t)=u^0(x)+(t-t_0)u^1(x)+o(|t-t_0|),$$

$$u^0(x)=u(x,t_0), \tag{4.1}$$

$$u^1(x)=\frac{\partial}{\partial t}u(x,t_0).$$

We start with the following assumptions for the structural bifurcation.

Assumption (H_1)*:* Let $x_0 \in \mathring{M}$ be an isolated degenerate singular point of $u^0(x)$. Suppose that

$$\mathrm{ind}(u^0,x_0)=0, \tag{4.2}$$

$$Du^0(x_0)\neq 0, \tag{4.3}$$

$$u^1(x_0)\cdot e_2 \neq 0, \tag{4.4}$$

where e_2 is the unit vector defined as in (3.6).

Assumption (H_2)*:* Under the conditions of Assumption (H_1), we also assume that $u^0 \in C^n$ near $x_0 \in \mathring{M}$ for some $n \geqslant 2$, and

$$\frac{\partial^k (u^0(x_0)\cdot e_2)}{\partial e_1^k}\begin{cases} =0, & \text{for } 1\leqslant k<n=\text{even},\\ \neq 0, & \text{for } k=n=\text{even}. \end{cases} \tag{4.5}$$

Remark 4.1: The conditions (4.2) and (4.3) imply by Lemma 3.2 that the flows of u^0 near x_0 is as shown in Fig. 2(c), i.e., both orbits of u^0 connected to x_0 are tangent to each other at x_0, and the eigenvector e_1 of $Du(x_0)$ is their common tangent vector. We shall see later that the conditions (4.2) and (4.3) are generic for the interior structural bifurcation.

Remark 4.2: In view of fluid mechanics applications, condition (4.4) is equivalent to nonzero acceleration of the flow in the orthogonal direction to the eigenvector e_1 of $Du(x_0)$. This is a natural condition for the structural bifurcation.

Remark 4.3: Condition (4.5) is a technical condition, which by Lemma 3.3 ensures the regularity of the bifurcated singular points of $u(x,t)$ from (x_0,t_0). In addition, from (3.7) we can see that the integer number n satisfying (4.5) must be $n \geqslant 2$.

The interior structural bifurcation of $u(x,t)$ near a singular point with index zero is described by the following theorems.

Theorem 4.4: *Let* $u \in C^1([0,T],D^r(TM))$ $(r \geqslant 1)$ *satisfy Assumption* (H_1)*. Then*

(1) the vector field u has a bifurcation in its local structure at (x_0,t_0)*. More precisely,* $u(x,t)$ *has no singular point in a small neighborhood of* x_0 *for any* $t<t_0$ *(or* $t>t_0$*) sufficiently close to* t_0*, and* $u(x,t)$ *bifurcates at least two singular points from* x_0 *as* $t>t_0$ *(or* $t<t_0$*), and*

(2) if $x_0 \in \mathring{M}$ *is a unique singular point with index zero of* u^0*, then* $u(x,t)$ *has a bifurcation in its global structure at* $t=t_0$*.*

Theorem 4.5: *Let* $u \in C^1([0,T],D^r(TM))$ $(r \geqslant 1)$ *satisfy Assumption* (H_2)*. Then,* $u(x,t)$ *bifurcates from* (x_0,t_0) *exactly two nondegenerate singular points, one of which is a center and another is a saddle.*

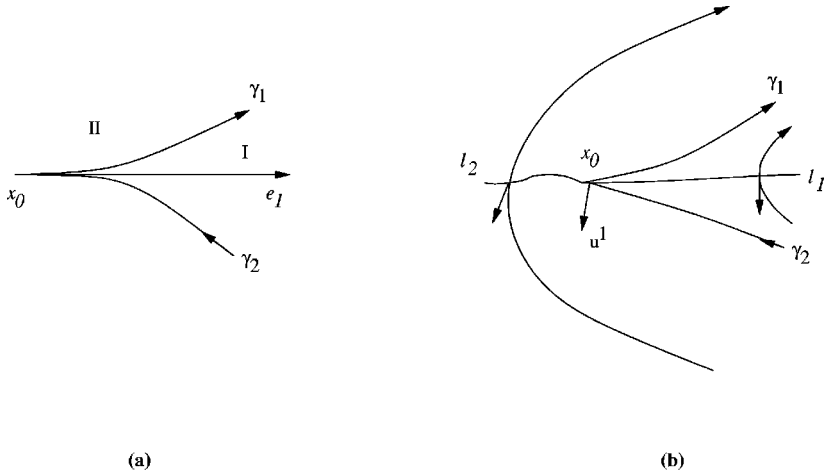

FIG. 3. Sketch illustrating the proof of Theorem 4.4.

Remark 4.6: Both Theorems 4.4 and 4.5 study structural bifurcation of u near an interior point x_0 with $\mathrm{ind}(u^0,x_0)=0$. When $\mathrm{ind}(u^0,x_0)$ is different from zero, interior structural bifurcation may not occur as we shall see in Examples 5.6 and 5.7. In addition, Theorem 5.5 shows that the bifurcation given in Theorems 4.4 and 4.4 is generic.

This is quite different from the structural bifurcation near a boundary singular point; see Refs. 2 and 3. We have shown in Refs. 2 and 3 that under suitable necessary conditions, $u(x,t)$ will always be a structural bifurcation near a boundary singular point with index different from $-1/2$. Reference 2 considers vector fields with free-slip boundary conditions, while Ref. 3 deals with vector fields with Dirichlet boundary conditions, which is related to boundary layer separation problems in viscous fluid flows.

B. Proof of Theorem 4.4

To investigate the structural bifurcation of $u(x,t)$ at t_0, by the Taylor expansion (4.1) and condition (4.4) it suffices to consider only the topological structure of the first-order approximation $u^0 \pm \varepsilon u^1$ of (4.1) for $\varepsilon>0$ sufficiently small.

By Lemma 3.2, let γ_1 and γ_2 be the two orbits of $u^0(x)$ connected to $x_0 \in \mathring{M}$. The eigenvector e_1 of $Du^0(x_0)$ is a common tangent vector of γ_1 and γ_2 at x_0 [see Fig. 3(a)].

Both orbits γ_1 and γ_2 divide a neighborhood of x_0 into open domains I and II as shown in Fig. 3(a). Since the angles between e_1 and the vectors of u^0 on γ_1 and γ_2 vary from 0 to π, and by assumption that angle θ between e_1 with $u^1(x_0)$ satisfies $0<\theta<\pi$, there exist curves ℓ_1 in domain I and curve ℓ_2 in domain II connected to x_0, such that u^1 are parallel to u^0 on ℓ_1 and ℓ_2 [see Fig. 3(b)]. Obviously the singular points of $u^0 \pm \varepsilon u^1$ are only on the curves as ℓ_1 and ℓ_2. Without loss of generality, we assume that u^0 and u^1 have a reverse orientation on ℓ_1 and ℓ_2, i.e., u^0 and $-\varepsilon u^1$ have the same orientation on ℓ_1 and ℓ_2. By condition (4.4) it follows that $u^0 - \varepsilon u^1$ has no singular points in ℓ_1 and ℓ_2, and therefore has no singular points in a neighborhood of x_0. Because $x_0 \in \mathring{M}$ is an isolated singular point of u^0, the values $|u^0(x)|$ are variant from 0 to a $\delta>0$ sufficiently small on ℓ_1 and ℓ_2, i.e.,

$$0<|u^0(x)|<\delta \quad \forall\ x \in \ell_1 \cup \ell_2,$$
$$\sup_{\ell_1 \cup \ell_2}|u^0|=\delta, \quad \inf_{\ell_1 \cup \ell_2}|u^0|=0. \tag{4.6}$$

It follows from (4.6) that there is an $\varepsilon_0>0$ sufficiently small such that for any $0<\varepsilon<\varepsilon_0$ the vector field $u^0+\varepsilon u^1$ has at least a singular point on each of ℓ_1 and ℓ_2, i.e., $u^0+\varepsilon u^1$ has at least two singular points near x_0. Thus, $u^0+\varepsilon u^1$ and $u^0-\varepsilon u^1$ are not topologically equivalent in a neighborhood of x_0. The first assertion is proved.

Obviously, if x_0 is a unique singular point of $u^0(x)$ with index zero, then $u^0+\varepsilon u^1$ and $u^0-\varepsilon u^1$ are not topologically equivalent on M. Hence, $u(x,t)$ has a globally structural bifurcation at $t=t_0$. This theorem is proved. □

C. Proof of Theorem 4.5

By Assumption (H_2) and Lemma 3.3 the vector field $u^0(x)$ has the Taylor expansion at x_0 $(x=0)$ as follows:

$$u^0(x)=\begin{cases}\alpha x_2+f(x_1)+x_2g_1(x),\\ \beta x_1^{2m}-x_2f'(x_1)+x_2g_2(x)+o(|x_1|^{2m}),\end{cases} \tag{4.7}$$

where $\alpha\neq 0$, $\beta\neq 0$, and

$$\begin{aligned} &f(x_1)=o(|x_1|^{m+1/2}),\\ &f'(x_1)=o(|x_1|^{m-1/2}),\\ &g_i(0)=0 \quad (i=1,2).\end{aligned} \tag{4.8}$$

By (4.4), we have

$$u^1(x)=\begin{cases}\lambda_1+h_1(x),\\ \lambda_2+h_2(x),\end{cases} \tag{4.9}$$

where $\lambda_2\neq 0$ and $h_i(x)=O(|x|)$, $i=1,2$.

By Theorem 4.4, one of $u^0\pm\varepsilon u^1$ has no singular points, and another has at least two singular points near x_0 for all $\varepsilon>0$ sufficiently small. We assume that $u^0-\varepsilon u^1$ has singular points, i.e., $\beta>0$ in (4.7) and $\lambda_2>0$ in (4.9). We need to prove that the equations below have exactly two solutions

$$\alpha x_2+x_2g_1(x)=\lambda_1\varepsilon+\varepsilon h_1(x)-f(x_1), \tag{4.10}$$

$$\beta x_1^{2m}-x_2f'(x_1)+x_2^2g_2(x)=o(|x_1|^{2m})=\lambda_2\varepsilon+\varepsilon h_2(x). \tag{4.11}$$

By the implicit function theorem, we derive from (4.8) and (4.10) that

$$\begin{aligned} &x_2=\alpha^{-1}\lambda_1\varepsilon-f(x_1)+G(\varepsilon,x_1),\\ &G(\varepsilon,x_1)=o(|\varepsilon|,|x_1|^{m+1/2}).\end{aligned} \tag{4.12}$$

Setting (4.12) in (4.11), we get the algebraic equation

$$\beta x_1^{2m}=\lambda_2\varepsilon+\alpha^{-1}\lambda_1\varepsilon f'(x_1)+\varepsilon\cdot O(|x|)+o(|\varepsilon|,|x_1|^{2m}), \tag{4.13}$$

where $\beta,\lambda_2>0$. It is clear that for any $\varepsilon>0$ sufficiently small, the equation (4.13) has exactly two solutions

$$x_1=\pm(\beta^{-1}\lambda_2)^{1/2m}\varepsilon^{1/2m}+o(\varepsilon^{1/2m}).$$

Thus, we deduce that the vector field $u^0-\varepsilon u^1$ has exactly two singular points $x(\varepsilon)=(x_1(\varepsilon),x_2(\varepsilon))$ as follows:

$$x_1^{\pm}(\varepsilon)=\pm(\beta^{-1}\lambda_2)^{1/2m}\varepsilon^{1/2m}+o(\varepsilon^{1/2m}),$$
$$x_2^{\pm}(\varepsilon)=\alpha^{-1}\lambda_1\varepsilon+o(\varepsilon,|x_1^{\pm}|^{m+1/2}). \tag{4.14}$$

Finally, we shall show that $x^{\pm}(\varepsilon)$ are nondegenerate for all $\varepsilon>0$ sufficiently small. By $\operatorname{div} u=0$, we have

$$\begin{aligned}\det D(u^0-\varepsilon u^1)_{x=x(\varepsilon)}&=-\left(\frac{\partial}{\partial x_1}(u_1^0-\varepsilon u_1^1)\right)^2-\frac{\partial}{\partial x_2}(u_1^0-\varepsilon u_1^1)\cdot\frac{\partial}{\partial x_1}(u_2^0-\varepsilon u_2^1)\\&=[\text{by (4.8) and (4.14)}]\\&=\pm 2m\alpha\beta(\beta^{-1}\lambda_2)^{(2m-1)/2m}\varepsilon^{(2m-1)/2m}+o(\varepsilon^{(2m-1)/2m}),\end{aligned}$$

which yields that

$$\det D(u^0-\varepsilon u^1)\begin{cases}>0, & \text{as } x=x^-,\\ <0, & \text{as } x=x^+.\end{cases}$$

Thus, we prove that $u^0-\varepsilon u^1$ has exactly two singular points x^+ and x^- for any $\varepsilon>0$ sufficiently small, and x^- is a center, x^+ is a saddle, which are nondegenerate. This proof is complete. □

V. APPLICATIONS TO INTERIOR SEPARATION OF FLUID FLOWS

A. Interior separation of fluid flows

We start with a typical example, illustrating how structural bifurcation occurs in the interior of fluid flows.

Let $u\in C^1([0,T],D^r(TM))$, and $x_0\in\mathring{M}$ be an isolated singular point of $u^0(x)=u(x,t_0)$, $0<t_0<T$.

Example 5.1: Consider the case where the index of $u^0(x)$ at the singular point $x_0\in\mathring{M}$ is zero, and the Jacobian matrix at x_0 is nonzero, i.e.,

$$\operatorname{ind}(u^0,x_0)=0,\quad Du^0(x_0)\neq 0.$$

The structural bifurcation occurs as shown in Fig. 4, which corresponds to interior separation phenomena in fluid mechanics.

When $t=t_0-\varepsilon$ with $\varepsilon>0$ small, the flow of $u(x,t_0-\varepsilon)$ given by Fig. 4(a) exhibits no singular points in a neighborhood of x_0. At $t=t_0$, $u^0=u(x,t_0)$ is given by Fig. 4(b), which has an isolated singular point $x_0\in\mathring{M}$ with index zero. When $t=t_0+\varepsilon$ for $\varepsilon>0$ small, $u(x,t_0+\varepsilon)$ is given by either Fig. 4(c) or Fig. 4(c′) or even more complicated circulation patterns in the back flow region. As we shall see in Theorem 5.5, the flow pattern given by Fig. 4(c) is generic. In other words, the flow transition from Fig. 4(a), to Fig. 4(b), and then to Fig. 4(c), or vice versa, is in general the pattern transition obtained both experimentally and numerically. For instance, in the axisymmetric plume shown Fig. 5, which is reproduced from Ref. 1, the three ''bubbles'' were caused by interior separation as described here.

We now address interior flow separation from a rigorous analysis point of view.

Theorem 5.2: *Let $u\in C^1([0,T],D^1(TM))$ satisfy Assumption (H_1). Then*

(1) there must be some centers of u separated from $x_0\in\mathring{M}$ as shown schematically in either Fig. 4(c) or Fig. 4(c′);
(2) the centers (back flows) are enclosed by a closed orbit line $\gamma(t)$ consisting of orbits of $u(\cdot,t)$, and $\gamma(t)$ converges/shrinks to x_0 as $t\to t_0$; and
(3) if Assumption (H_2) is satisfied, then the center separated from $x_0\in\mathring{M}$ is unique, as shown in Fig. 4(c).

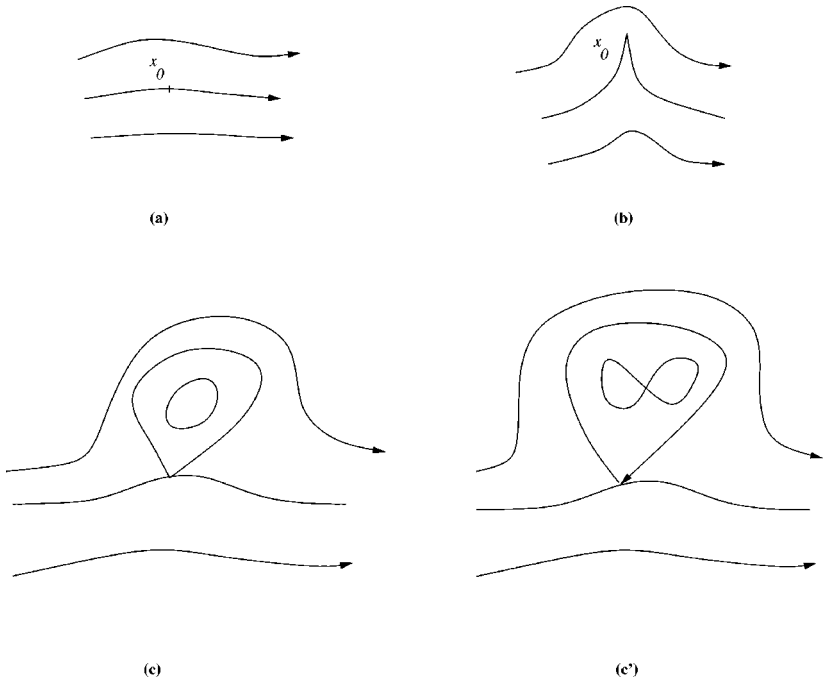

FIG. 4. Schematic of structural bifurcation for the case index $(u^0, x_0) = 0$, a typical case in fluid flows.

The centers in Figs. 4(c) and 4(c′) correspond, in a real fluid, to isolated vortices or, in the case of figure-eight ones, to pairs of co-rotating vortices. This theorem is a direct corollary of Theorems 4.4 and 4.5 and a stability lemma of extended orbits.

We now introduce this stability lemma.

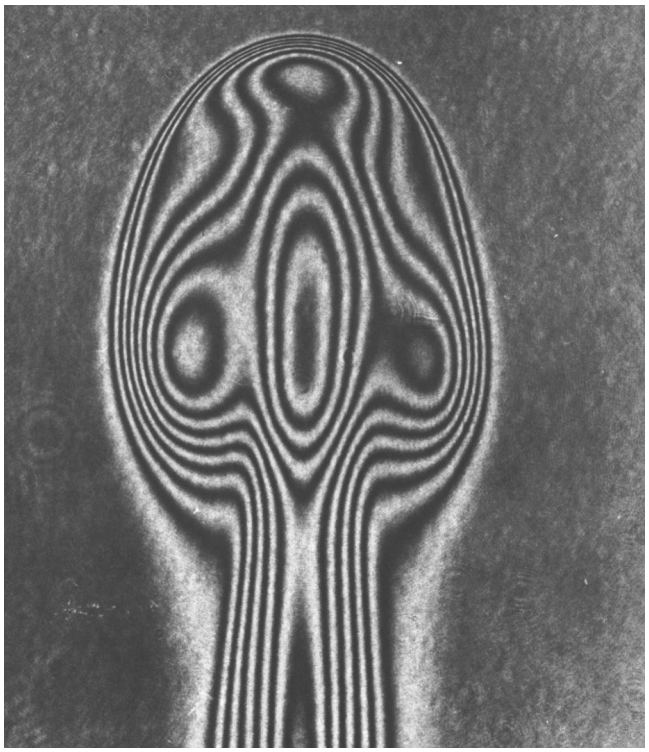

FIG. 5. The three ''bubbles'' in the axis symmetric plume, generated by interior bifurcations, reproduced from Ref. 1.

Definition 5.3: Let $v \in C^r(TM)$ be a vector field. A curve $\gamma \subset M$ is called an extended orbit of v, if

(i) it is a union of curves

$$\gamma = \bigcup_{i=1} \gamma_i;$$

(ii) either γ_i is an orbit of v, or γ_i consists of both orbits and singular points of v, and

(iii) if γ_i and γ_{i+1} are orbits of v, then the ω-limit set of γ_i is the α-limit set of γ_{i+1},

$$\omega(\gamma_i) = \alpha(\gamma_{i+1}),$$

namely, the end points of γ_i are singular points of v, and the starting end point of γ_{i+1} is the finishing end point of γ_i.

The point $\varphi_1 = \alpha(\gamma_1)$ is called the starting point of the extended orbit γ.

We have the following stability lemma for extended orbits. The result of this lemma has been proved by Ma and Wang[4] in Step 2 of the proof of Lemma 4.5 in their paper. This lemma is quite useful in analyzing the orbits of families of vector fields, and thus in solving some problems in 2D incompressible fluid flows. Here we only state the result.

Lemma 5.4: (stability of extended orbits, Ref. 4) Let $v^n \in C^r(TM)$ be a sequence of vector fields with $\lim_{n\to\infty} v^n = v \in C^r(TM)$. Suppose that $\gamma^n \subset M$ is an extended orbit of v^n and the starting points p_1^n of γ^n converge to p_1. Then the extended orbits γ^n of v^n converge to an extended orbit γ of v with starting point p_1.

B. Genericity of structural bifurcation with index zero

In the following, we shall show that the type of structural bifurcation as shown in Fig. 4(c), i.e., one center interior separation, is generic in the interior structural bifurcation. This is remarkably different from the structural bifurcation near the boundary.[2,3,5] It also explains why interior separation to multiple centers and the interior flow separation from the singularities with nonzero index are seldom observed in fluid motions.

Let $x_0 \in \mathring{M}$ and $0 < t_0 < T$ be given. We define a topological space $B \subset C^1([0,T], D^2(TM))$ as follows:

$$B = \{u \in C^1([0,T], D^2(TM)) \,|\, u^0(x_0) = 0, \det Du^0(x_0) = 0, u^0 = u(\cdot, t_0)\}$$

with the topology of $C^1([0,T], D^2(TM))$. Obviously, the space B contains all vector fields in $C^1([0,T], D^2(TM))$, which have a bifurcation in their local structure at (x_0, t_0). It is easy to see that the set

$$B_0 = \left\{ u \in B \;\middle|\; Du^0(x_0) \neq 0,\ \frac{\partial^2 (u^0(x_0) \cdot e_2)}{\partial e_1^2} \neq 0,\ u^1(x_0) \cdot e_2 \neq 0 \right\}$$

is open and dense in B, where e_1 and e_2 are as in (3.5) and (3.6), and $u^1(x) = (\partial/\partial t)\, u(x, t_0)$. From Lemma 3.3, it immediately follows the following genericity theorem of structural bifurcation.

Theorem 5.5 (Genericity of structural bifurcation): *For any $u \in B_0$, u has a bifurcation in its local structure at (x_0, t_0). More precisely, u bifurcates from (x_0, t_0) exactly two nondegenerate singular points, one of which is a center and another is a saddle, as shown in Figs. 4(a)–4(c). Moreover, the set B_0 is open and dense in the topological space B, which contains all vector fields in $C^1([0,T], D^2(TM))$ having a locally structural bifurcation at (x_0, t_0).*

Proof: If $u \in B_0$, then $u^0 \in D^2(TM)$, and u^0 has the Taylor expansion (3.10) with $n = 2$, and

$$\deg f = k \geqslant 2 \quad [\text{by } f \in C^2 \text{ and } f(z) = o(|z|)].$$

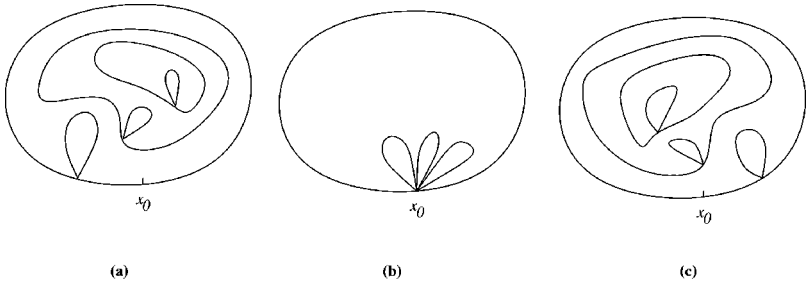

FIG. 6. Schemaatic phase diagrams, showing no structural bifurcation, as explained in Example 5.6.

Hence, by Lemma 3.3, we have

$$\mathrm{ind}(u^0,x_0)=0.$$

Then this theorem follows from Theorems 4.4–4.5. The proof is complete. □

C. Examples of no structural bifurcation

We know that for a locally structurally stable singular point of a vector field $v\in D^r(TM)$, its index obeys

$$\mathrm{ind}(v,x_0)=\begin{cases}-\frac{1}{2}, & x_0\in\partial M,\\ -1 \text{ or } +1, & x\in\mathring{M}.\end{cases}$$

For a vector field $u(x,t)=u^0(x)+(t-t_0)u^1(x)+o(|t-t_0|)$ the structural bifurcation theorem given in Ref. 2 amounts to saying that if x_0 is a boundary singular point with $\mathrm{ind}(u^0,x_0)\neq-\frac{1}{2}$ and $u^1(x_0)\neq 0$ for $x_0\in\partial M$, then $u(x,t)$ has a bifurcation in its local structure at (x_0,t_0). However, for an interior singular point $x_0\in\mathring{M}$ of u^0 with $\mathrm{ind}(u^0,x_0)\neq 1$ or -1, the vector field $u(x,t)$ may have no structural bifurcation near (x_0,t_0). In the following, we give two examples to show this.

Example 5.6: Figures 6(a)–6(c) illustrates a structural evolution of a vector field $u(x,t)$ near $x_0\in\mathring{M}$ as time t crosses t_0, where $\mathrm{ind}(u^0,x_0)=-n$ $(n>1)$, $u^0=u(x,t_0)$, and $u^1(x_0)=(\partial/\partial t)\,u(x_0,t)\neq 0$.

In Fig. 6, we see that the vector fields $u(x,t_0-\varepsilon)$ given by (a) and $u(x,t_0-\varepsilon)$ given by (c) are topologically equivalent for all $\varepsilon>0$ small. Hence, $u(x,t)$ has no structural bifurcation at (x_0,t_0).

Example 5.7: Let $\mathrm{ind}(u^0,x_0)=0$, and $Du^0(x_0)=0$, and the structure of u^0 near x_0 is illustrated by Fig. 7(a).

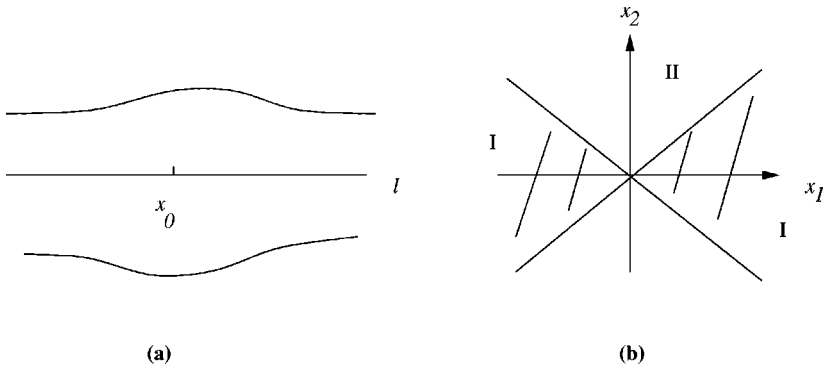

FIG. 7. Sketch showing no bifurcation given in Example 5.7.

Let the x_1-axis of the coordinate system in Fig. 7(b) be tangent to the orbit line ℓ in (a) at x_0. The angles between $u^0(x)$ and the x_1-axis near x_0 vary in the shadow domain I in (b). Hence if the angle between $u^1(x_0)$ and the x_1-axis is in the domain II in (b), then $u^1(x)$ is transversal to $u^0(x)$ near x_0, which implies that the vector field $u(x,t)=u^0(x)+(t-t_0)u^1+o(|t-t_0|^2)$ has no structural bifurcation near (x_0,t_0).

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On the exterior structure of graphs*

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After a detailed *ab initio* description of the exterior structure of graphs as handled by Connes and Kreimer in their work on renormalization (illustrated by the example of the ϕ^3 model in six dimensions) we spell out in detail their study of the Lie algebra of infinitesimal characters and of the group of characters of the Hopf algebra of Feynman graphs. © *2004 American Institute of Physics.*
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I. INTRODUCTION

These notes are a comment on basic aspects of the Connes–Kreimer work[1] describing renormalization in terms of a Hopf algebra **H** of Feynman graphs. They consign our effort to understand the central, but in Ref. 1 somewhat periferally treated notion of ''exterior structure of graphs,'' we offer them as an aid to comprehension providing missing or understressed details. Prior to the exterior structure, the somewhat involved recipe for the Hopf coproduct is spelled out in detail.

As an application we give detailed descriptions of the Lie algebra **L** of infinitesimal characters of **H** (as the semidirect product of its Lie subalgebra $\mathbf{L}_c$ by its Abelian ideal $\mathbf{L}_0$), and of the group **G** of characters of **H** (as the semidirect product of its subgroup $\mathbf{G}_c$ by its Abelian normal subgroup $\mathbf{G}_0$).

As in Ref. 1 we discuss the case of the ϕ^3 model $d=6$ with Lagrangian

$$L=\tfrac{1}{2}(\partial\phi)^2+\tfrac{1}{2}m^2\phi^2+g_{\mathrm{dim}}\phi^3 \quad (g_{\mathrm{dim}}=\mu^{3-d/2}g). \tag{$*$}$$

II. NAKED GRAPHS

(i) A *naked graph* Γ is a (nonvoid) set of *lines* and *vertices*, where each vertex touches at least one line and each line touches at least one vertex. There are thus two kinds of lines: indeed a line

(1) either touches two vertices (*internal lines*), or
(2) touches one vertex at one of its extremities (*external lines*).

(ii) In the case of the model (*) above a vertex [generally one has as many types of vertices as there are terms in the Lagrangian, each term yielding one type of vertex]

(1) either touches three lines (*three-vertices*): then drawn as ⅄ (standing for $g_{\mathrm{dim}}\phi^3$), or
(2) touches two lines (*two-vertices*), of either the kind $\overset{\times}{\underset{(0)}{\text{-}\,\text{-}}}$, or the kind $\overset{\times}{\underset{(1)}{\text{-}\,\text{-}}}$ [standing, respectively, for $m^2\phi^2$ and $\partial\phi)^2$].

(iii) We consider only naked graphs with $N\geqslant 2$ external lines. We discard the *vacuum-graphs* ($N=0$) and the *tadpoles* (N=1).

(iv) We retain only 1PI (*one-particle-irreducible*) naked graphs, namely,

(1) connected,

*Dedicated to Rudolf Haag on his eightieth birthday.
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(2) which cannot be disconnected by cutting one interior line [Observe that an exterior line of a 1PI graph cannot touch a two-vertex. The graphs $\overset{\text{-}\times\text{-}}{(0)}$, $\overset{\text{-}\times\text{-}}{(1)}$, and $\curlywedge$ are not disconnectable by cutting an interior line, they have to be explicitly discarded.],
(3) having at least one loop (this discards the graphs $\overset{\text{-}\times\text{-}}{(0)}$ or $\overset{\text{-}\times\text{-}}{(1)}$ and $\curlywedge$).

(v) Terminology and notation: the set of 1PI naked graphs is as follows the union $\mathbb{V}\cup\mathbb{S}$:

(1) the 1PI naked graphs with $N>2$ external lines are called *N-vertex graphs*. Their set is denoted by $\mathbb{V}_N$ with $\mathbb{V}=\cup_{N>2}\mathbb{V}_N$.
(2) the 1PI naked graph with two external lines are called *self-energy graphs*. Their set is denoted by $\mathbb{S}$.

(vi) A special role will be played by the superficially divergent graphs, whose set is $\mathbb{V}_3\cup\mathbb{S}$ in the case of our model (*).

III. DRESSED GRAPHS

(i) For the 1PI graph with $N\geqslant 2$ external lines we set

$$E_\Gamma=\{(p_1,\ldots,p_N)\in\mathbb{R}^n;p_1+\cdots+p_N=0\} \tag{1}$$

and select appropriate sets $S(E_\Gamma)$ of test functions and dual set $S'(E_\Gamma)$ of distributions. [For $\Gamma\in\mathbb{V}_3$, respectively, $\Gamma\in\mathbb{S}$, $S(E_\Gamma)$ should contain the constants, respectively, the constants and the function p^2.] A *dressed graph* is a couple (Γ,σ), $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $\sigma\in S'(E_\Gamma)$ linear in its *external structure* σ. For a fixed $\Gamma\in\mathbb{V}\cup\mathbb{S}$ we identify the vector spaces $(\Gamma,S'(E_\Gamma))$ and $S'(E_\Gamma)$.

(ii) For $\Gamma\in\mathbb{V}_3$ with $\phi_0(p)=1$, $p\in E_\Gamma$, we constrain $\sigma_0\in S'(E_\Gamma)$ as follows [this specifies σ_0 up to a choice depending on the type of theory at hand; we then set $\Gamma_{(0)}=(\Gamma,\sigma_0)$]:

$$\langle\sigma_0,\phi_0\rangle=1 \tag{2}$$

yielding the codimension-1 annihilator: with associated dual direct splitting

$$S(E_\Gamma)_0=\{\mathrm{f}\in S(E_\Gamma);\langle\sigma_0,f\rangle=0\}, \tag{3}$$

$$\begin{cases} S(E_\Gamma)=\mathbb{C}\phi_0\oplus S(E_\Gamma)_0, \\ S'(E_\Gamma)=\mathbb{C}\sigma_0\oplus\phi_0^\perp. \end{cases} \tag{4}$$

[A *dual direct splitting* of a pair (Σ,V) of vector spaces in separating duality $\langle\cdot,\cdot\rangle$ is a pair of direct splittings

$$\begin{cases} V=U\oplus W, \\ \Sigma=\Theta\oplus\Psi \end{cases}$$

such that the pairs (Θ,U) and (Ψ,V) are both in separating duality, and one has $\langle\Theta\oplus 0,0\oplus W\rangle=\langle 0\oplus\Psi,\mathrm{U}\oplus 0\rangle=0$. Observe that the described situation follows from the latter requirement if the pairs (Σ,V) and (Θ,U) are both in separating duality.]

(iii) For $\Gamma\in\mathbb{S}$, with $\phi_0(p)=m^2$, $\phi_1(p)=p^2$, $p\in E_\Gamma$, we specify as follows σ_0, $\sigma_1\in S'(E_\Gamma)$:

$$\begin{cases}\langle\sigma_0,\phi_0\rangle=1 \\ \langle\sigma_0,\phi_1\rangle=0,\end{cases}\quad\begin{cases}\langle\sigma_1,\phi_0\rangle=0 \\ \langle\sigma_1,\phi_1\rangle=1,\end{cases} \tag{5}$$

yielding the codimension-2 annihilator and associated dual direct splitting

$$S(E_\Gamma)_0=\{f\in(S(E_\Gamma);\langle\sigma_0,f\rangle=\langle\sigma_1,f\rangle=0\}, \tag{6}$$

$$\begin{cases} S(E_\Gamma)=\mathbb{C}\phi_0+\mathbb{C}\phi_1 \quad \oplus \quad S(E_\Gamma)_0, \\ S'(E_\Gamma)=\mathbb{C}\sigma_0+\mathbb{C}\sigma_1 \quad \oplus \quad \mathbb{C}\phi_0^\perp\cap\mathbb{C}\phi_1^\perp. \end{cases} \tag{7}$$

[(5) specifies σ_0 and σ_1 up to a choice depending on the type of theory at hand. We set $\Gamma_{(0)}=(\Gamma,\sigma_0)$, $\Gamma_{(1)}=(\Gamma,\sigma_1)$. Note that we chose our notational conventions in such a way that the cases $\Gamma\in\mathbb{V}_3$ and $\Gamma\in\mathbb{S}$ differ merely in that the index i has the single value 0 for $\mathbb{V}_3$, and ranges over $\{0,1\}$ for $\mathbb{S}$.]

IV. THE HOPF ALGEBRA H

We wrote this paper so that the hurried reader can skip this section at first reading.

(i) As an algebra **H** is the symmetric (i.e., polynomial) algebra

$$\mathbf{H}=\oplus_{n\in\mathbb{N}}\mathbf{V}^{\vee n}=\mathbb{C}\mathbb{1}+\oplus_{n\geqslant 1}\mathbf{V}^{\vee n} \tag{8}$$

over the vector space

$$\mathbf{V}=\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}S'(E_\Gamma) \quad \text{(finite direct sums)} \tag{9}$$

of finite direct sums $\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}(\Gamma,\sigma)$ of dressed 1PI graphs (Γ,σ), $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $\sigma\in S'(E_\Gamma)$. [Note that **V** is in separating duality with $\mathbf{V}'=\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}S(E_\Gamma)$ consisting of finite direct sums of pairs (Γ,f), $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $f\in S(E_\Gamma)$, the duality being specified by $\langle(\Gamma,f),(\Gamma',\sigma)\rangle=\delta_{\Gamma\Gamma'}\langle\sigma,f\rangle$. We shall write $(\Gamma,\phi_i)=\Gamma^{(i)}$, $i=0$ if $\Gamma\in\mathbb{V}$, $i=0$ or 1 if $\Gamma\in\mathbb{S}$.]

(ii) Counit ϵ: linear multiplicative s.t. $\epsilon(\lambda\mathbb{1})=\lambda$, $\lambda\in\mathbb{C}$, and Ker $\epsilon=\mathbf{H}^+=\oplus_{n\geqslant 1}\mathbf{V}^{\wedge n}$.

(iii) Coproduct Δ: it suffices to specify Δ σ-linearly on all symbols (Γ,σ), $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $\sigma\in(S'(E_\Gamma)$. Denoting by $\underline{\Gamma}$, γ the vacuum graphs obtained from the naked graph Γ, γ by removing all its (open) external lines we define a *subgraph* γ of Γ (consisting of some vertices of Γ and the lines touching them) as *admissible* whenever

(1) $\gamma\in\mathbb{V}_3\cup\mathbb{S}$ ($\Leftrightarrow\gamma$ is superficially divergent),
(2) $\gamma\underset{\neq}{\subset}\underline{\Gamma}$,
(3) γ is obtained from γ by adding to it all lines of Γ (interior and exterior) touching it. The dressed graphs $\gamma_{(i)}$, $i=0$ or 0,1, are then those in III(ii), respectively, (iii). We then specify the linear multiplicative coproduct Δ by asking $\Delta\mathbb{1}=\mathbb{1}\otimes\mathbb{1}$ and

$$\Delta(\Gamma,\sigma)=(\Gamma,\sigma)\otimes\mathbb{1}+\mathbb{1}\otimes(\Gamma,\sigma)+\Delta'(\Gamma,\sigma), \quad (\Gamma,\sigma)\in\mathbf{V}, \tag{10}$$

with

$$\Delta'(\Gamma,\sigma)=\Sigma\Pi\gamma_{(i)}\otimes(\Gamma/\Pi\gamma_{(i)},\sigma) \tag{11}$$

the sum being over all products $\Pi\gamma_{(i)}$ s.t.

(1) all factors γ are admissible, the mutual intersections of the corresponding γ being all void (the γ themselves may intersect),
(2) the sum is over all combinations of indices.

The graph $\Gamma/\Pi\gamma_{(i)}$ is obtained by replacing in Γ each $\gamma_{(i)}$ by the vertex with label (i).

These requirements yield an $\mathbb{N}$-graded connected bialgebra for the grading defined by the number of loops ($\geqslant 1$, cf. Ref. 2, (iv)), hence a Hopf algebra by Ref. 2 Proposition 2.7, moreover a CMK Hopf algebra in the sense of Ref. 2 Definition 3.1 suitably generalized. [The definition of CMK-algebras in Ref. 2 **3** should be altered to accommodate graphs with exterior structure: replace the basis $\{x_i\}$ of **V** by a direct sum $\mathbf{V}=\oplus_i X_i$ (in our case $\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}S'(E_\Gamma)$).]

V. THE LIE ALGEBRA L

At the cost of some duplication we wrote this section in a manner independent of the preceding one. The notion of CMK algebra should be adapted to our situation as we just mentioned.

Since **H** is a CMK Hopf algebra its Lie algebra of algebraic infinitesimal characters is the algebraic dual of $\mathbf{V}=\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}S'(\mathrm{E}_\Gamma)$, cf. Ref. 2 Proposition 3.3. In order to deal with a reasonable topological dual **L** of **V** we *define* **L** as the above subset $\mathbf{V}'$:

$$\mathbf{L}\cong\mathbf{V}'=\oplus_{\Gamma\in\mathbb{V}\cup\mathbb{S}}S(E_\Gamma)\quad(\text{finite direct sums of elements }(\Gamma,f)\in\mathbf{L},f\in S(E_\Gamma)),\tag{12a}$$

the linear form (Γ,f), $\mathrm{f}\in S(E_\Gamma)$ (vanishing on $\mathbb{C}\mathbb{1}\cup(\oplus_{\mathrm{n}\geqslant 2}\mathbf{V}^{\vee n})$ taking on **V** the values:

$$\langle(\Gamma,f),(\Gamma',\sigma)\rangle=\delta_{\Gamma\Gamma'}\langle\sigma,f\rangle,\quad(\Gamma',\sigma)\in\mathbf{V},\sigma\in S(E_{\Gamma'}).\tag{12b}$$

This choice will actually ensure that $[Z_1{*}Z_2]\in\mathbf{L}$ for Z_1, $Z_2\in\mathbf{L}$ as shown by the computation of the Lie bracket $[Z_1{*}Z_2]=Z_1{*}Z_2-Z_2{*}Z_1$, Z_1, $Z_2\in\mathbf{L}$, to which we now proceed. Since the elements of **L** are concentrated in polynomial grade one, computing $\langle Z_1{*}Z_2,x\rangle=\langle Z_1\otimes Z_2,\Delta' x\rangle$ for Z_1, $Z_2\in\mathbf{L}$, $x\in\mathbf{H}^{\wedge|}=\mathbf{V}$, involves the special case of Δ' in (11) where all products Π figuring there have only one factor: Δ' is then replaced by a reduced algorithm Δ'_{r} which we now describe *ab initio*: one has for $\Gamma\in\mathbb{V}\cup\mathbb{S}$:[3]

$$\Delta'_r(\Gamma,\sigma)=\sum_{\gamma\ll\Gamma}\sum_i\ \gamma_{(i)}\otimes(\Gamma/\gamma_{(i)},\sigma).\tag{13a}$$

(i) Recall that a subgraph $\gamma\subset\Gamma$ of $\Gamma\in\mathbb{V}\cup\mathbb{S}$ is *admissible* (notation $\gamma\ll\Gamma$) whenever

(a) $\gamma\in\mathbb{V}_3\cup\mathbb{S}$ ($\Leftrightarrow\gamma$ is superficially divergent),
(b) $\gamma\subsetneqq\Gamma$
(c) γ is obtained from γ by adding to it all the open lines of Γ (interior and exterior) which it touches.

The dressed graphs $\gamma_{(i)}$, $i=0$ or 0, 1, are then those encountered above.

(ii) The graph $\Gamma/\gamma_{(i)}$ obtained by replacing γ

(1) by $\curlywedge$ if γ is a 3-vertex graph (we might then as well write Γ/γ),
(2) by $\overset{\text{-}\times\text{-}}{(i)}$, $i=1$ or 2, if γ is a self-energy graph.

If we separate the contributions of 3-vertex and self-energy graphs, (13a) reads

$$\Delta'_r(\Gamma,\sigma)=\sum_{\gamma\ll\Gamma,\,\gamma\in\mathbb{V}_3}\gamma_{(0)}\otimes(\Gamma/\gamma,\sigma)+\sum_{\gamma\ll\Gamma,\,\gamma\in\mathbb{S}}\sum_{i=1,2}\gamma_{(i)}\otimes(\Gamma/\gamma_{(i)},\sigma).\tag{13b}$$

We have now owing to (13a) and (12b) for $Z_1=(\Gamma_1,f_1)$, $Z_2=(\Gamma_2,\mathrm{f}_2)\in\mathbf{L}$, $(\Gamma,\sigma)\in\mathbf{V}$, Γ_1, Γ_2, $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $f_1\in S(\mathrm{E}_{\Gamma_1})f_2\in S(\mathrm{E}_{\Gamma_2})$, $\sigma\in S'(E_\Gamma)$:

$$\langle Z_1{*}Z_2,(\Gamma,\sigma)\rangle=\langle Z_1\otimes Z_2,(\Delta'_{\mathrm{r}}(\Gamma,\sigma)\rangle=\sum_{\gamma\ll\Gamma}\sum_i\ \delta_{\Gamma_1\gamma}\langle\sigma_i,f_1\rangle\delta_{\Gamma_2\Gamma/\gamma_{(i)}}\langle\sigma,f_2\rangle,\tag{14}$$

which, introducing the notation:

$$n_i(\Gamma_1,\Gamma_2;\Gamma)=\#\{\gamma\subset\Gamma\ \text{ admissible};\gamma\cong\Gamma_1\ \text{ and }\Gamma/\gamma_{(\mathrm{i})}\cong\Gamma_2\},\quad\Gamma_1,\Gamma_2,\Gamma\in\mathbb{V}\cup\mathbb{S},\tag{15}$$

is turned into

$$\langle Z_1 * Z_2, (\Gamma,\sigma)\rangle = \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)\langle \sigma_i f_1\rangle\langle \sigma, f_2\rangle = \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)\langle \sigma_i, f_1\rangle\langle (\Gamma,f_2),(\Gamma,\sigma)\rangle. \tag{16a}$$

In other terms one has in restriction to **V**:

$$Z_1 * Z_2|_{\mathbf{V}} = \sum_{\Gamma\in\mathbb{V}\cup\mathbb{S}} \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)\langle \sigma_i, f_1\rangle(\Gamma,f_2). \tag{16b}$$

Note that nonvanishing of $n_i(\Gamma_1,\Gamma_2;\Gamma)$ requires the two facts:

$$\Gamma_1 \in \mathbb{V}_3\cup\mathbb{S} \quad (\Leftrightarrow \Gamma_1 \text{ is superficially divergent}), \tag{$*_1$}$$

$$\Gamma \text{ and } \Gamma_2 \text{ have the same external lines.} \tag{$*_2$}$$

From (16a) follows

$$[Z_1 * Z_2] = \sum_{\Gamma\in\mathbb{V}\cup\mathbb{S}} \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)\langle \sigma_i, f_1\rangle(\Gamma,f_2) - \sum_{\Gamma'\in\mathbb{V}\cup\mathbb{S}} \sum_i n_i(\Gamma_2,\Gamma_1;\Gamma')\langle \sigma_i, f_2\rangle(\Gamma',f_1)] \tag{17}$$

the bracket $[Z_1 * Z_2]$ thus belongs actually to **L**.

Consider now the subspace $\mathbf{L}_0$ of **L** spanned by the annihilator (3) and (6), recalled to be

$$S(E_\Gamma)_0 = \{f\in(S(E_\Gamma) \text{ s.t. } \begin{cases} \langle \sigma_0, f\rangle = 0\} & \text{if } \Gamma\in\mathbb{V}_3 \\ \langle \sigma_0, f\rangle = \langle \sigma_1, f\rangle = 0 & \text{if } \Gamma\in\mathbb{S}\end{cases}, \tag{18}$$

together with the (Γ,f), $\Gamma\in\cup_{n>3}\mathbb{V}_n$, $f\in(S(E_\Gamma)$; and further the subspace $\mathbf{L}_c$ of **L** spanned by the (Γ,f), $\Gamma\in\mathbb{V}_3\cup\mathbb{S}$, $f\in(E_\Gamma)_c$=linear span of

$$\begin{cases} \phi_0 = 0 & \text{if } \Gamma\in\mathbb{V}_3 \\ \phi_0 \text{ and } \phi_1 & \text{if } \Gamma\in\mathbb{S}^{\cdot}\end{cases}$$

Those definitions are subsumed by the dual direct splitting

$$\begin{cases} \mathbf{V} = \mathbf{V}_c = \text{lin}\{(\Gamma,\sigma_i),\Gamma\in\mathbb{V}_3\cup\mathbb{S}\} & \oplus & \mathbf{L}_c^{\perp} \\ \mathbf{L} = \mathbf{L}_c = \text{lin}\{(\Gamma,\phi_i),\Gamma\in\mathbb{V}_3\cup\mathbb{S}\} & \oplus & \mathbf{L}_0 = \text{lin}\{(\Gamma,f),\Gamma\in\mathbb{V}_3\cup\mathbb{S}, f\in S(E_\Gamma)_0\} \\ & & \quad + \text{lin}\{(\Gamma,f),\Gamma\in\cup_{n>3}\mathbb{V}_n, f\in S(E_\Gamma)\} \end{cases} \tag{19}$$

Lemma 1: (i) One has $\mathbf{L}_0 * \mathbf{L}|_{\mathbf{V}} = 0$, thus $[\mathbf{L}_0 * \mathbf{L}_0]$ vanishes: $\mathbf{L}_0$ is an Abelian Lie subalgebra of **L**.

(ii) One has $[\mathbf{L} * \mathbf{L}_0] \subset \mathbf{L}_0$: $\mathbf{L}_0$ is a Lie ideal of **L**.

(iii) One has $[\mathbf{L}_c * \mathbf{L}_c] \subset \mathbf{L}_c$: $\mathbf{L}_c$ is a Lie subalgebra of **L**.

Proof: (i) If $Z_1\in\mathbf{L}_0$ in (16a) one has $\Gamma_1\in\mathbb{V}_3\cup\mathbb{S}$ by ($*_1$), Γ_1 thus lies in the first summand of $\mathbf{L}_0$ in (19) whence $f_1\in S(E_\Gamma)_0$, thus by (18) the vanishing of $\langle \sigma_i, f_1\rangle$ right-hand side of (16b).

(ii) By (i) (17) reads for $Z_1\in\mathbf{L}$ and $Z_2\in\mathbf{L}_0$:

$$[Z_1 * Z_2] = \sum_{\Gamma\in\mathbb{V}\cup\mathbb{S}} \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)\langle \sigma_i, f_1\rangle(\Gamma,f_2), \tag{20}$$

which, owing to ($*_2$), belongs to $\mathbf{L}_0$.

(iii) We make Z_1, $Z_2\in\mathbf{L}_c$ in (17), then Γ_1, $\Gamma_2\in\mathbb{V}_3\cup\mathbb{S}$ by (19). Now ($*_2$) says that Γ, respectively, Γ', have the same external lines as Γ_2, respectively, Γ_1, they thus both belong to $\mathbb{V}_3\cup\mathbb{S}$ hence the right-hand side of (17) belongs to $\mathbf{L}_c$.

The next theorem describes the structure of $\mathbf{L}$ by first stating how $\mathbf{L}$ is built up from $\mathbf{L}_c$ and $\mathbf{L}_0$ (moral of the preceding Lemma); and then formulating the Lie bracket of $\mathbf{L}_c$ (for that matter its pre-Lie product) in terms of ''grafting the graph of the first factor at the vertices of the second''—a basic algorithm aspect of the theory.

Theorem A: (i) The Lie algebra $\mathbf{L}$ is the semidirect product of its subalgebra $\mathbf{L}_c$ by its Abelian ideal $\mathbf{L}_0$ (cf. Appendix B):

$$\mathbf{L}=\mathbf{L}_c \ltimes \mathbf{L}_0 . \tag{21}$$

(ii) After regauging as follows the basis of $\mathbf{L}_c$:

$$\Gamma^{(i)} \to \Gamma'^{(i)} = S(\Gamma)\Gamma^{(i)}, \quad \Gamma^{(i)}=(\Gamma,\phi_i)\in \mathbf{L}_c , \tag{22}$$

where $S(\Gamma)$ is the number of automorphisms of the naked graph Γ [mappings of the naked graph onto itself which do not change it] we have

$$[\Gamma_1'^{(i)} * \Gamma_2'^{(j)}] = \sum_v (\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(\mathrm{j})} - \sum_v (\Gamma_2'^{(j)} \circ_v \Gamma_1')^{(i)}, \quad \Gamma_1'^{(i)},\ \Gamma_2'^{(j)} \in \mathbf{L}_c , \tag{23a}$$

in fact separately

$$\Gamma_1'^{(i)} * \Gamma_2'^{(j)}|_{\mathrm{v}} = \sum_v (\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(j)}, \quad \Gamma_1'^{(i)},\ \Gamma_2'^{(j)} \in \mathbf{L}_c , \tag{23b}$$

a sum over vertices v of Γ_2', where the notation $(\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(j)}$ stands for *grafting* $\Gamma_1'^{(i)}$ *on* Γ_2' *at* v, namely:

(1) if $\Gamma^{(i)}=\Gamma^{(0)}=(\Gamma_1,\phi_0)$ with $\Gamma_1 \in \mathbb{V}_3$, the sum is over the three-vertices v of Γ_2, with the dressed graph $(\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(j)}$ obtained by replacing the vertex $v=$  by the naked graph $\Gamma_1=$  (for an arbitrary order of the legs of both objects),

(2) if $\Gamma^{(i)}=\Gamma^{(0)}=(\Gamma_1,\phi_0)$ with $\Gamma_1 \in \mathbb{S}$, the sum is over the two-vertices v of Γ_2 of the type $\overset{\times}{\underset{(0)}{\cdot\!\cdot}}$, with the dressed graph $(\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(j)}$ obtained by replacing the vertex $v=\overset{\times}{\underset{(0)}{\cdot\!\cdot}}$ by the naked graph $\Gamma_1=$  (for an arbitrary order of the legs of both objects),

(3) if $\Gamma^{(i)}=\Gamma^{(1)}=(\Gamma_1,\phi_1)$ with $\Gamma_1 \in \mathbb{S}$, the sum is over the two-vertices v of Γ_2 of the type $\overset{\times}{\underset{(1)}{\cdot\!\cdot}}$, with the dressed graph $(\Gamma_1'^{(i)} \circ_v \Gamma_2')^{(j)}$ obtained by replacing the vertex $v=\overset{\times}{\underset{(1)}{\cdot\!\cdot}}$ by the naked graph $\Gamma_1=$  (for an arbitrary order of the legs of both objects).

Summarizing this somewhat lenghty recipe: (23b) is a sum over vertices v of $\Gamma_2'^{(j)}$ ''of type $\Gamma_1'^{(i)}$'' by graphs replacing these vertices (irrespective of the order of legs) by the naked graph Γ_1. In conformity with $(*_2)$ all those graphs have the same exterior structure as Γ_2. Convention (22) aims at getting a sum (23b) without coefficients.

Proof: (i) Indeed $\mathbf{L}$ is the direct sum $\mathbf{L}_c \oplus \mathbf{L}_0$ of the subalgebra $\mathbf{L}_c$ and the ideal $\mathbf{L}_0$ (cf. Appendix B).

(ii) Check of (23b): let $\Gamma_1^{(i)}$, $\Gamma_2^{(j)} \in \mathbf{L}_c$ with $\Gamma_1'^{(i)}$, $\Gamma_2'^{(j)}$ as in (22): we have by (16b) owing to $(*_1)$:

$$\Gamma_1^{(i)} * \Gamma_2^{(j)}|_{\mathrm{v}} = \sum_{\Gamma \in \mathbb{V}_3 \cup \mathbb{S}} \sum_i n_k(\Gamma_1,\Gamma_2;\Gamma)\,\delta_{ki}(\Gamma,\phi_j) = \sum_{\Gamma \in \mathbb{V}_3 \cup \mathbb{S}} \sum_i n_i(\Gamma_1,\Gamma_2;\Gamma)(\Gamma,\phi_j),$$

where $\Gamma_1 \cong \gamma$ whilst $\Gamma_2 \cong \Gamma/\gamma_{(i)}$ for $\gamma \subset \Gamma$ admissible, i.e., $(\Gamma,\phi_{\mathrm{j}})$ is a multiple of $(\Gamma_1'^{(i)} \circ_{\mathrm{v}} \Gamma_2')^{(j)}$: we have to find which multiple. Now from the definition (15) of $n_i(\Gamma_1,\Gamma_2;\Gamma)$ follows that $S(\Gamma_1)S(\Gamma_2)n_i(\Gamma_1,\Gamma_2;\Gamma)$ is the number $S(\Gamma)$ of automorphisms of the naked graph Γ. Equation (16a) is thus turned into (23b).

VI. THE GROUP G

Call $\mathbf{G}$ the group of continuous characters of $\mathbf{H}$, viz., the subgroup of its algebraic characters χ (cf. Ref. 2, Definition 12, Proposition 13) for which $\langle\chi,(\Gamma,\sigma)\rangle$, $\Gamma\in\mathbb{V}\cup\mathbb{S}$, $\sigma\in S'(E_\Gamma)$ is continuous in σ. By multiplicativity $\chi\in\mathbf{G}$ is uniquely determined by its restriction $\chi|_{\mathbf{V}'}$ each continuous linear form of $\mathbf{V}$ being the restriction of a unique $\chi\in\mathbf{G}$ (its "multiplicative extension": the restriction $\chi\to\chi|_{\mathbf{V}}$ and the multiplicative extension $\chi|_{\mathbf{V}}\to\chi$ are inverse of each other). We will accordingly handle the elements $\chi\in\mathbf{G}$ by handling their restrictions $\chi|_{\mathbf{V}}$. Recall that the product of $\mathbf{G}$ is the convolution product $*$ (under which $\mathbf{G}$ is closed), hence that its unit element is the counit ϵ of $\mathbf{H}$.

Call $\mathbf{H}_c$ the smallest subalgebra of $\mathbf{H}$ containing the (Γ,σ_i), $\Gamma\in\mathbb{V}_3\cup\mathbb{S}$, $i=0$ for $\Gamma\in\mathbb{V}_3$, $i=0$ or 1 for $\Gamma\in\mathbb{S}$ (equivalently $\mathbf{H}_c=\mathbb{C}1+\oplus_{n\geqslant 1}\mathbf{V}_c^{\vee n}$). Definitions (10) and (11) of the coproduct of $\mathbf{H}$ implying the inclusion $\Delta\mathbf{V}_c\subset\mathbf{H}_c\otimes\mathbf{H}_c$, hence $\Delta\mathbf{H}_c\subset\mathbf{H}_c\otimes\mathbf{H}_c$ by the multiplicativity of Δ, $\mathbf{H}_c$ is a Hopf subalgebra of $\mathbf{H}$ whose counit is the restriction $\epsilon|_{\mathbf{H}_c}$.

Denoting by $\mathbf{G}_c$ the subgroup of algebraic characters of $\mathbf{H}_c$ continuous for the topology of the exterior structure, the restriction ρ to $\mathbf{H}_c$ of the characters of $\mathbf{G}$:

$$\rho\chi=\chi|_{\mathbf{H}_c},\quad \chi\in\mathbf{G} \tag{24}$$

is a group homomorphism: $\mathbf{G}\to\mathbf{G}_c$ whose kernel $\mathbf{G}_0$ is the normal subgroup of $\mathbf{G}$ consisting of the $\chi\in\mathbf{G}$ restricting on $\mathbf{H}_c$ to the unit character, viz., the counit $\epsilon|_{\mathbf{H}_c}$ of $\mathbf{H}_c$. Since ϵ is multiplicative, a $\chi\in\mathbf{G}$ belongs to $\mathbf{G}_0$ iff $\chi|_{\mathbf{V}_c}$ coincides with $\epsilon|_{\mathbf{V}_c}=0$:

$$\mathbf{G}_0=\{\chi\in\mathbf{G};\chi|_{\mathbf{H}_c}=\epsilon|_{\mathbf{H}_c}\}=\{\chi\in\mathbf{G};\chi\ \text{vanishes on}\ \mathbf{V}_c\}. \tag{25}$$

Lemma 2: (i) $\mathbf{G}_0$ is an Abelian normal subgroup of $\mathbf{G}$.
(ii) Defining ρ': $\mathbf{G}_c\to\mathbf{G}$ by

$$\rho'\psi(\text{abbreviated}\ \tilde{\psi})=\begin{cases}\psi & \text{on}\ \mathbf{V}_c\\ 0 & \text{on}\ \mathbf{L}_c^{\perp},\end{cases}\quad \psi\in\mathbf{G}_c, \tag{26}$$

yields the lift of a split exact sequence of group homomorphisms:

$$1\to\mathbf{G}_0\to\mathbf{G}\underset{\rho'}{\overset{\rho}{\leftrightarrows}}\mathbf{G}_c\to 1, \tag{27a}$$

that is ρ' is a group homomorphism fulfilling:

$$\rho\circ\rho'=\mathrm{id}_{\mathbf{G}_c}. \tag{27b}$$

Proof: (i) We noted that $\mathbf{G}_0$ is normal. Proof that $\mathbf{G}_0$ is Abelian: let χ_0, $\chi_0'\in\mathbf{G}_0$, we have for all dressed graphs (Γ,σ), using (25) and the fact that (10), (11) imply $\Delta'(\Gamma,\sigma)\in\mathbf{H}_c\otimes\mathbf{H}$:

$$\langle\chi_0*\chi_0',(\Gamma,\sigma)\rangle=\langle\chi_0\otimes\chi_0',\Delta(\Gamma,\sigma)\rangle=\langle\chi_0\otimes\chi_0',(\Gamma,\sigma)\otimes 1+1\otimes(\Gamma,\sigma)+\Delta'(\Gamma,\sigma)\rangle$$

$$=\langle\chi_0,(\Gamma,\sigma)\rangle+\langle\chi_0',(\Gamma,\sigma)\rangle+\langle\chi_0\otimes\chi_0',\Delta'(\Gamma,\sigma)\rangle=\langle\chi(\Gamma,\sigma)\rangle+\langle\chi',(\Gamma,\sigma)\rangle.$$

(ii) It suffices to check (27) which is obvious from (26).

Theorem B: (i) $\mathbf{G}$ is the semi-direct product [One has to make a choice of the order of factors in the definition of the semidirect product of groups. This choice is adapted to the order of factors in the definition of the semidirect product of Lie algebra in Theorem A above—changing to the opposite order of factors follows from a trivial calculation.] of its subgroups $\rho'\mathbf{G}_c\cong\mathbf{G}_c$ and $\mathbf{G}_0$: we have $\rho'\mathbf{G}_c\cap\mathbf{G}_0=\{\epsilon\}$ and $\mathbf{G}=\rho'\mathbf{G}_c*\mathbf{G}_0$. Consequently each $\chi\in\mathbf{G}$ is uniquely written as a product

$$\chi=\tilde{\psi}*\chi_0 \quad \text{with} \quad \tilde{\psi}=\rho'\psi\in\rho'\mathbf{G}_c(\psi\in\rho\mathbf{G}_c), \quad \text{and} \quad \chi_0\in\mathbf{G}_0, \tag{28a}$$

specifically

$$\tilde{\psi}=(\rho'\circ\rho)\chi \quad (\psi=\rho\chi) \quad \text{and} \quad \chi_0=[(\rho'\circ\rho)\chi]^{-1}*\chi. \tag{28b}$$

(ii) The product in $\mathbf{G}$ then reads

$$(\tilde{\psi}*\chi_0)*(\tilde{\psi}'*\chi_0')=(\tilde{\psi}*\tilde{\psi}')*[(\mathrm{ad}\,\tilde{\psi}'^{-1}(\chi_0))*\chi_0'], \tag{29a}$$

where

$$\mathrm{ad}\,\chi(\chi_0)=\chi*\chi_0*\chi^{-1}\in\mathbf{G}_0, \quad \chi_0\in\mathbf{G}_0, \ \chi\in\mathbf{G}, \tag{29b}$$

yields a group homomorphism [Trivial on $\mathbf{G}_0$, its interesting part is its restriction to $\rho'\mathbf{G}_c$, cf. (29a).] ad: $\mathbf{G}\to\mathrm{Aut}\,\mathbf{G}_0$ into the automorphism group of $\mathbf{G}_0$.

(iii) $\mathrm{ad}(\rho'\mathbf{G}_c)$ acts as follows: one has with the sum as specified in (11) for $\tilde{\psi}\in\rho'\psi$, $\psi\in\mathbf{G}_c$, $\chi_0\in\mathbf{G}_0$:

$$\langle\mathrm{ad}\,\tilde{\psi}(\chi_0),(\Gamma,\sigma)\rangle=\langle\chi_0,(\Gamma,\sigma)\rangle+\Sigma\langle\psi,\Pi\gamma_{(i)}\rangle\langle\chi_0,(\Gamma/\Pi\gamma_{(i)},\sigma)\rangle, \quad \Gamma\in\mathbb{V}\cup\mathbb{S}, \ \sigma\in S'(E_\Gamma). \tag{30}$$

Proof: (i) Check of $\rho'\mathbf{G}_c\cap\mathbf{G}_0=\{\epsilon\}$: if $\psi\in\mathbf{G}_c$ fulfills $\rho'\psi\in\mathbf{G}_0$ we have using (27b) $(\rho\circ\rho')\psi=\psi=\epsilon_c$, thus $\rho'\psi=\epsilon$ since ρ' is a homomorphism of groups.

Uniqueness of the decomposition (28a), (28b):

$$\rho'\psi*\chi_0=\rho'\psi'*\chi_0' \ \text{ implies } \ (\rho'\psi)^{-1}*\rho'\psi'=\chi_0*(\chi_0')^{-1}\in\rho'\mathbf{G}_c\cap\mathbf{G}_0=\{\epsilon\}.$$

Existence of the decomposition (28a), (28b):

(1) one has $\chi_0\in\mathbf{G}_0$, indeed by (27b) $\rho\chi_0=[(\rho\circ\rho'\circ\rho)\chi]^{-1}*\rho\chi=(\rho\chi)*(\rho\chi)^{-1}=\epsilon$,
(2) one has (28a), indeed $\rho'\psi*\chi_0=(\rho'\circ\rho)\chi*\chi_0=(\rho'\circ\rho)\chi*[(\rho'\circ\rho)\chi]^{-1}*\chi=\chi$.

(ii) Check of (29a): we have: $\tilde{\psi}*\chi_0*\tilde{\psi}'*\chi_0'=\tilde{\psi}*\tilde{\psi}'*\tilde{\psi}'^{-1}*\chi_0*\tilde{\psi}'*\chi_0'$.

(iii) First notice that (30) makes sense, $\langle\psi,\Pi\gamma_{(i)}\rangle$ denoting the value of $\Pi\gamma_{(i)}\in\mathbf{H}_c$ for $\psi\in\mathbf{G}_c$. We check (30) separately for (Γ,σ) in the complementary subspaces $\mathbf{V}_c$ and $\mathbf{L}_c^\perp$, cf. (19).

For $(\Gamma,\sigma)\in\mathbf{V}_c$, $\langle\mathrm{ad}\,\tilde{\psi}(\chi_0),(\Gamma,\sigma)\rangle$ and $\langle\chi_0,(\Gamma,\sigma)\rangle$ vanish by (25): indeed $\chi_0\in\mathbf{G}_0$ by assumption whence $\mathrm{ad}\,\tilde{\psi}(\chi_0)\in\mathbf{G}_0$ by normality of $\mathbf{G}_0$; furthermore $\langle\chi_0,(\Gamma/\Pi\gamma_{(i)},\sigma)\rangle$ vanishes by (25) because $(\Gamma/\Pi\gamma_{(i)},\sigma)\in\mathbf{V}_c$ has the exterior structure σ.

Assume now $(\Gamma,\sigma)\in\mathbf{L}_c^\perp$, our assumption $\tilde{\psi}\in\rho'\psi$, $\psi\in\mathbf{G}_c$, entailing $\tilde{\psi}|_{\mathbf{V}}\in\mathbf{L}_c$. Recalling

$$\Delta'(\Gamma,\sigma)=\Sigma\Pi\gamma_{(i)}\otimes(\Gamma/\Pi\gamma_{(i)},\sigma)\in\mathbf{H}_c\otimes\mathbf{V}_c, \tag{11}$$

for convenience, we compute the left-hand side of (30):

$$\begin{aligned}\langle\mathrm{ad}\,\tilde{\psi}(\chi_0),(\Gamma,\sigma)\rangle&=\langle\tilde{\psi}*\chi_0*\tilde{\psi}^{-1},(\Gamma,\sigma)\rangle=\langle(\psi*\chi_0)\otimes\tilde{\psi}^{-1},\Delta(\Gamma,\sigma)\rangle\\&=\langle(\tilde{\psi}*\chi_0)\otimes\tilde{\psi}^{-1},(\Gamma,\sigma)\otimes\mathbb{1}+\mathbb{1}\otimes(\Gamma,\sigma)+\Delta'(\Gamma,\sigma)\rangle\\&=\langle\tilde{\psi}*\chi_0,(\Gamma,\sigma)\rangle+\langle\tilde{\psi}^{-1},(\Gamma,\sigma)\rangle+\langle\psi*\chi_0,\Delta'(\Gamma,\sigma)\rangle.\end{aligned}$$

Now $\langle\tilde{\psi}^{-1},(\Gamma,\sigma)\rangle=0$ since $\tilde{\psi}^{-1}|_{\mathbf{V}}\in\mathbf{L}_c$. And $\langle\tilde{\psi}*\chi_0,\Delta'(\Gamma,\sigma)\rangle=0$ by (25) and (11), we are thus left with

$$\begin{aligned}\langle\tilde{\psi}*\chi_0,(\Gamma,\sigma)\rangle&=\langle\tilde{\psi}\otimes\chi_0,\Delta(\Gamma,\sigma)\rangle\\&=\langle\tilde{\psi}\otimes\chi_0,(\Gamma,\sigma)\otimes\mathbb{1}+\mathbb{1}\otimes(\Gamma,\sigma)+\Delta'(\Gamma,\sigma)\rangle\\&=\langle\tilde{\psi},(\Gamma,\sigma)\rangle+\langle\chi_0,(\Gamma,\sigma)\rangle+\langle\tilde{\psi}\otimes\chi_0,\Delta'(\Gamma,\sigma)\rangle\\&=\langle\chi_0,(\Gamma,\sigma)\rangle+\langle\tilde{\psi}\otimes\chi_0,\Delta'(\Gamma,\sigma)\rangle,\end{aligned}$$

because, as above, $\langle\tilde{\psi},(\Gamma,\sigma)\rangle=0$, since $\tilde{\psi}|_{\mathbf{V}}\in\mathbf{L}_c$. Plugging in (11) we finally get

$$\langle\tilde{\psi}*\chi_0,\Delta'(\Gamma,\sigma)\rangle=\langle\tilde{\psi},\Sigma\Pi\gamma_{(i)}\rangle+\chi_0,(\Gamma/\Pi\gamma_{(i)},\sigma),$$

where the first term can be written as in (30) in view of (27a).

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APPENDIX A: THE AUGMENTATION IDEAL

Here is a more synthetic version of results scattered in Ref. 2.

Proposition: Let $\mathbf{H}(\wedge,\mathbb{1}=e1,\Delta,\epsilon)=\oplus_{n\in\mathbb{N}}\mathbf{H}^n$, $\mathbf{H}^n=\{h\in\mathbf{H},Yh=nh\}$, *be an* $\mathbb{N}$*-graded connected Hopf algebra* (i.e., $\mathbf{H}^0=\mathbb{C}\mathbb{1}$) *with augmentation ideal* $\mathbf{H}^+=\mathrm{Ker}\,\epsilon$ *and assume in addition that* $\mathbf{H}=\oplus_{n\in\mathbb{N}}\mathbf{V}^{\vee n}$, $\mathbf{V}$ *is a linear subspace of* $\mathbf{H}^+$ *spanned by Y-homogeneous elements. We have*:

$$\mathbf{H}=\mathbb{C}\mathbb{1}\oplus\mathbf{H}^+,\tag{A1}$$

$$\mathbf{H}^+=\oplus_{n\geqslant 1}\mathbf{H}^n,\tag{A2}$$

$$\mathbf{H}^+=\oplus_{n\geqslant 1}\mathbf{V}^{\vee n}.\tag{A3}$$

Subsuming we have the threefold equation

$$\mathbf{H}=\mathbb{C}\mathbb{1}\oplus\begin{Bmatrix}\mathbf{H}^+\\ H_{n\epsilon 1}\mathbf{H}^n\\ H_{n\epsilon 1}\mathbf{V}^{\Delta n}.\end{Bmatrix}\tag{A4}$$

Proof: (A1) holds for arbitrary Hopf algebras for which $e\epsilon$ is an idempotent with image $\mathbb{C}\mathbb{1}$ and kernel $\mathbf{H}^+=\mathrm{Ker}\,\epsilon$, indeed one has for $h\in\mathbf{H}$: $e\epsilon(e\epsilon h)=e\epsilon(\epsilon(h)\mathbb{1})=e(\epsilon(h))=e\epsilon h$ with $\mathrm{Im}\,e\epsilon=\mathbb{C}\mathbb{1}$ since $e\epsilon(h)=\epsilon(h)\mathbb{1}$ and $e\epsilon(\mathbb{1})=e1=\mathbb{1}$; and with $\mathrm{Ker}\,e\epsilon=\mathbf{H}^+$ since $e\epsilon(h)=\epsilon(h)\mathbb{1}=0$ holds iff $\epsilon(h)=0$.

(A2) is a property of $\mathbb{N}$-graded connected Hopf algebras: check of $\supset$: since $\epsilon\circ Y=0$ (cf. Ref. 2, **2.2** (ii)) for $h\in\mathbf{H}^n$, $\geqslant 1$, $0=\epsilon(Yh)=n\epsilon(h)$ implies $\epsilon(h)=0$. Check of $\subset$: let $h\in\mathbf{H}^+$: by connectivity $h=\lambda\mathbb{1}+h'$ with, $\lambda\in\mathbb{C}$ and $h'\in\oplus_{n\geqslant 1}\mathbf{H}^n$. Hence $\epsilon(h)=0=\lambda+\epsilon(h')=\lambda$ by what precedes, thus $h=h'\in\oplus_{n\geqslant 1}\mathbf{H}^n$.

(A3): check of $\supset$: by definition $\mathbf{V}\subset\mathbf{H}^+$. Hence $\mathbf{V}^{\vee n}\subset\mathbf{H}^{+\vee n}\subset\mathbf{H}^+$. Check of $\subset$: by definition each $h\in\mathbf{H}$ is of the form $h=\lambda\mathbb{1}+h''$, $\lambda\in\mathbb{C}$, $h''\in\oplus_{n\geqslant 1}\mathbf{V}^{\vee n}$. If $h\in\mathbf{H}^+\epsilon(h)=\lambda+0$, hence $\lambda=0$, $h\in\oplus_{n\geqslant 1}\mathbf{V}^{\vee n}$.

APPENDIX B: SEMIDIRECT PRODUCT OF LIE ALGEBRAS

In what follows the ground field is $\mathbb{C}$, or, for that matter, any field of characteristic zero.

Definition-Lemma: Let $\mathbf{L}'$ and $\mathbf{J}$ be two Lie algebras. The *semidirect product* $\mathbf{L}$ *of* $\mathbf{L}'$ *by* $\mathbf{J}$ (denoted by $\mathbf{L}=\mathbf{L}'\ltimes\mathbf{J}$) is defined either as

(i) the vector space $\mathbf{L}'\oplus\mathbf{J}$ with Lie bracket given as follows in terms of the Lie brackets of $\mathbf{L}'$ and $\mathbf{J}$: with $x,y\in\mathbf{L}'$, $j,k\in\mathbf{J}$:

(1) $[x\oplus 0,y\oplus 0]=[x,y]\oplus 0$, $x,y\in\mathbf{L}'$,
(2) $[0\oplus \mathrm{j},0\oplus \mathrm{k}]=0\oplus[j,k]$, $j,k\in\mathbf{J}$,
(3) $[x\oplus 0,0\oplus j]=-[0\oplus j,x\oplus 0]=0\oplus\theta(x)j$, $x\in\mathbf{L}'$, $j\in\mathbf{J}$,

where θ is a Lie algebra homomorphism from $\mathbf{L}'$ to the Lie algebra of derivations of $\mathbf{J}$.

(ia) *This defines a Lie algebra* $\mathbf{L}$.

(ii) the Lie algebra $\mathbf{L}=\mathbf{L}'\oplus\mathbf{J}$ where $\mathbf{L}'$ is a Lie subalgebra and $\mathbf{J}$ is a Lie ideal.

Proof: Check of (ia) from (i): antisymmetry of the Lie bracket is obvious. The Jacobi identify $J(X,Y,Z)=[X,[Y,Z]]+[Y,[Z,X]]+[Z,[X,Y]]=0$ is checked as follows: with $x,y,z\in\mathbf{L}'$, $j,k,l\in\mathbf{J}$:

$$J(x\oplus 0,y\oplus 0,z\oplus 0)=0\Leftarrow\mathbf{L}' \text{ is a Lie algebra: indeed one has}$$

$$[x\oplus 0,[y\oplus 0,z\oplus 0]]=[x\oplus 0,[y,z]\oplus 0]=[x,[y,z]]\oplus 0$$

$$J(0\oplus j,0\oplus k,0\oplus l)=0\Leftarrow\mathbf{J} \text{ is a Lie algebra: indeed one has}$$

$$[0\oplus j,[0\oplus k,0\oplus l]=[0\oplus j,0\oplus[k,l]=0\oplus[j,[k,l]$$

$$J(0\oplus j,y\oplus 0,z\oplus 0)=0\Leftarrow\theta([y,z])=\theta(y)\theta(z)-\theta(z)\theta(y)\text{: indeed one has}$$

$$[0\oplus j,[y\oplus 0,z\oplus 0]]+[y\oplus 0[z\oplus 0,0\oplus j]]+[z\oplus 0,[0\oplus j,y\oplus 0]]$$

$$=[0\oplus j,[y,z]]\oplus 0]+[y\oplus 0,0\oplus\theta(x)j]-[z\oplus 0,0\oplus\theta(y)j]$$

$$=-0\oplus\theta([y,z])j+0\oplus\theta(y)\theta(z)j-0\oplus\theta(z)\theta(y)j$$

$$=-0\oplus(-\theta([y,z]+\theta(y)\theta(z)-\theta(z)\theta(y))j$$

$$J(0\oplus j,0\oplus k,z\oplus 0)=0\Leftarrow\theta(z) \text{ is a derivation of } \mathbf{J} \text{ indeed one has}$$

$$[0\oplus j,[0\oplus k,z\oplus 0]]+[0\oplus k,[z\oplus 0,0\oplus j]]+[z\oplus 0,[0\oplus j,0\oplus k]]$$

$$=-[0\oplus j,0\oplus\theta(z)k]+[0\oplus k,0\oplus\theta(z)j]+[z\oplus 0,0\oplus[j,k]]$$

$$=-0\oplus[j,\theta(z)k]+0\oplus[k,\theta(z)j]+0\oplus\theta(z)[j,k]$$

$$=0\oplus(\theta(z)[j,k]-[\theta(z)j,k]-[j,\theta(z)k])$$

Implication $(i)\Rightarrow(ii)$: obvious.

Implication (ii)⇒(i): (1) respectively, (2) are the definition of the brackets of the Lie subalgebras $\mathbf{L}'$ respectively $\mathbf{J}$. the first equation (3) is obvious, the second arises from the fact that $\mathbf{J}$ is a Lie ideal, with $\theta(x)$ depending linearly on x. The fact that $\theta(x)$ is a derivation of $\mathbf{J}$, and that θ a Lie-algebra map results from former arguments in the reversed direction.

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Geodesic distances on density matrices

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We find an upper bound for geodesic distances associated to monotone Riemannian metrics on positive definite matrices and density matrices. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1689000]

I. INTRODUCTION

The notion and importance of Fisher information is well established in statistics and probability theory. As a measure of distinguishability of probability densities, the Fisher information was used by Rao to define a Riemannian metric on probability spaces. On the simplex of probability vectors $\mathcal{P}_n=\{p=(p_1,\ldots,p_n),\ \Sigma_i p_i=1, p_i>0, i=1,\ldots,n\}$, this is the unique metric contracting under Markovian mappings, by the Chentsov uniqueness theorem. On $\mathcal{P}_n$, the Fisher metric is

$$\lambda_p(x,y)=\sum_i p_i^{-1}x_i y_i, \quad x,y\in T_p\mathcal{P}_n.$$

The geometry of $\mathcal{P}_n$ with this metric is quite simple. By

$$p\mapsto 2(\sqrt{p_1},\ldots,\sqrt{p_n}), \tag{1}$$

it is isometric with an open subset in the sphere of radius 2 in $\mathbb{R}^n$.[5] The metric can be extended to the set $\mathcal{M}_n=\{p=(p_1,\ldots,p_n),\ p_i>0\}$ of all finite (strictly positive) measures on the set $\{1,\ldots,n\}$. Using the isometry (1) and elementary geometry in R^n, we may compute the geodesic distance for the Fisher metric in $\mathcal{P}_n$ and $\mathcal{M}_n$:

$$D(p,q)=2\arccos\left(\sum_i \sqrt{p_i}\sqrt{q_i}\right), \quad p,q\in\mathcal{P}_n$$

(the Bhattacharya distance) and

$$d(p,q)=2\left(\sum_i (\sqrt{p_i}-\sqrt{q_i})^2\right)^{1/2}, \quad p,q\in\mathcal{M}_n.$$

The last expression is related to the Hellinger distance $H(p,q)$ by $d(p,q)=\sqrt{2H(p,q)}$. The Hellinger distance belongs to the family of Cziszár's f-divergences

$$D_f(p,q)=\int f(q/p)dp.$$

Here f is a convex function. As it was shown in Ref. 1, the metric given by the Hessian of f-divergence is a constant multiple of the Fisher metric.

In the case of a quantum system, the situation becomes more complicated. In the simplest case, the states of the system are represented by density matrices. In analogy with manifolds of classical probability densities, a quantum version of the Fisher information metric must be de-

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creasing under stochastic maps. Contrary to the classical case, this monotonicity condition does not specify the metric uniquely. In fact, it was shown by Petz that the monotone metrics can be labeled by operator-monotone functions.

As it was mentioned in Ref. 5, there is no general formula for geodesic path and distance for monotone metrics. Explicit expressions are known only in two particular cases, namely the Bures metric and the Wigner–Yanase metric. In the present paper, we find an upper bound for the geodesic distances for all monotone metrics. This is done in a simple way: Following Uhlmann,[18,19] we obtain the Bures geodesics from certain purifying lifts of curves of density matrices and then make use of a duality relation between the smallest (Bures) and the largest (RLD) of monotone metrics. It is also shown that this upper bound is related to a particular noncommutative version of the Hellinger distance.

II. THE MANIFOLD AND MONOTONE METRICS

Let M_n be the algebra of n by n complex matrices. The set of faithful positive linear functionals on M_n is identified with the cone of positive definite matrices. This set, with the differentiable manifold structure inherited from M_n, will be denoted by $\mathcal{M}$. Let $\mathcal{D}\subset\mathcal{M}$ denote the submanifold of density matrices in $\mathcal{M}$, that is,

$$\mathcal{D}=\{\rho\in\mathcal{M}:\mathrm{Tr}\,\rho=1\}.$$

The tangent space to $\mathcal{M}$ at $\rho\in\mathcal{M}$ is $T_\rho\mathcal{M}=\{x\in M_n:x=x^*\}$. If $\rho\in\mathcal{D}$, then the tangent space $T_\rho\mathcal{D}$ is the subspace of traceless matrices in $T_\rho\mathcal{M}$.

Let λ be a Riemannian metric on $\mathcal{M}$. Then we will say that λ is a monotone metric if

$$\lambda_{T(\rho)}(T(h),T(h))\leqslant\lambda_\rho(h,h),\quad \rho\in\mathcal{M},\ \ h\in T_\rho\mathcal{M},$$

for all completely positive trace preserving maps T. It is an important result of Petz[16] that a Riemannian metric is monotone if and only if it has the form

$$\lambda_\rho(h,k)=\mathrm{Tr}\,hJ_\rho(k),$$

where J_ρ is given by the operator mean

$$J_\rho=R_\rho^{-1}[f(L_\rho/R_\rho)]^{-1}. \tag{2}$$

Here L_ρ and R_ρ are the left and the right multiplication operators and $f:(0,\infty)\to\mathbb{R}$ is an operator monotone function which is symmetric, that is, $f(t)=tf(t^{-1})$. It is immediate from (2) that under the normalization $f(1)=1$, any monotone metric is equal to the Fisher metric on commutative submanifolds. Moreover, we have

$$\frac{2t}{1+t}\leqslant f(t)\leqslant\frac{1+t}{2}$$

for all symmetric normalized operator monotone functions.[12] Accordingly, there is a greatest and a smallest element in the set of monotone metrics.

The smallest monotone metric is obtained for $f(t)=(1+t)/2$. It is called the Bures metric because it is related to the Bures distance (see also Sec. IV). The operator

$$J_\rho(h)=g,\quad \rho g+g\rho=2h,$$

is the symmetric logarithmic derivative (see Refs. 9, 18, and 2).

The greatest monotone metric corresponds to the function $f(t)=2t/(1+t)$. In this case J_ρ is the right logarithmic derivative (RLD)

$$J_\rho(h)=\tfrac{1}{2}(\rho^{-1}h+h\rho^{-1})$$

(see Refs. 9, 16, and 17). More examples of monotone metrics can be found in Sec. V.

III. STANDARD REPRESENTATION AND MONOTONE METRICS

The standard representation of the algebra M_n is obtained if M_n is endowed with the Hilbert–Schmidt inner product

$$\langle x,y\rangle=\mathrm{Tr}\,x^*y.$$

Let us denote the resulting Hilbert space by H. Then M_n is represented on H by

$$\phi:M_n\to\mathcal{B}(H),\quad a\mapsto L_a,$$

where L_a is the left multiplication operator $L_aw=aw$, $w\in H$. Each element ρ in $\mathcal{M}$ has a vector representative, or purification, w in H, such that

$$\mathrm{Tr}\,\rho a=\langle w,L_aw\rangle\quad\forall a\in M_n.$$

Then $w\in H$ is a vector representative of $\rho\in\mathcal{M}$ if and only if $\rho=ww^*$.

Let ρ_t, $t\in I$, be a smooth curve in $\mathcal{M}$. A curve w_t in H, such that w_t is a vector representative of ρ_t for all $t\in I$, is called a lift of ρ_t. In this case, the tangent vectors are related by

$$\dot\rho_t=\dot w_tw_t^*+w_t\dot w_t^*. \tag{3}$$

Let us denote the corresponding projection of the tangent spaces $T_wH\to T_{ww^*}\mathcal{M}$ by Π.

Let $w_0w_0^*=\rho_0$. There are many lifts of ρ_t through w_0. Among such lifts, there is a unique lift with minimal Hilbert space length

$$l_H(w_t)=\int_I\sqrt{\langle\dot w_t,\dot w_t\rangle}dt.$$

It will be called the horizontal lift.

The horizontal lift was introduced in Refs. 18 and 19, where the geometric phase was extended to mixed states. It was shown that the above minimalization problem leads to the condition

$$w_t^*\dot w_t=\dot w_t^*w_t \tag{4}$$

for all t. The curves w_t in H, satisfying this condition, are called horizontal curves. The tangent vectors to horizontal curves at $w\in H$ form a real vector subspace $H_w=\{gw,\ g=g^*\}$. Let H_w be endowed with the inner product $\mathrm{Re}\langle\cdot,\cdot\rangle$. Then it is a real Hilbert space, called the horizontal subspace. For each $h\in T_{ww^*}\mathcal{M}$, there is a unique element $\hat h$ in H_w satisfying $h=\Pi(\hat h)$. It follows that the inner product in H_w can be projected onto $T_{ww^*}\mathcal{M}$. As it turns out, this projection defines a Riemannian metric on $\mathcal{M}$. Moreover,

$$4\,\mathrm{Re}\,\langle\hat h,\hat k\rangle=2\,\mathrm{Tr}\,h(L_\rho+R_\rho)^{-1}(k),\quad h,k\in T_\rho\mathcal{M}, \tag{5}$$

is exactly the Bures metric.

The commutant of $\phi(M_n)$ is the algebra of right multiplication operators $R_aw=wa$, $a\in M_n$, on H. For each $\sigma\in\mathcal{M}$, there is an element $w\in H$ such that

$$\langle w,R_aw\rangle=\mathrm{Tr}\,\sigma a.$$

This element is given by $\sigma=w^*w$. For each curve σ_t in $\mathcal{M}$, let us consider the curves w_t in H satisfying $w_t^*w_t=\sigma_t$. The tangent vectors of such curves satisfy $\dot{\sigma}_t=\tilde{\Pi}(\dot{w}_t)$, where $\tilde{\Pi}:T_wH \to T_{w^*w}\mathcal{M}$ is given by

$$\tilde{\Pi}(x)=x^*w+w^*x.$$

We may now proceed exactly as before, choosing for each σ_t the shortest of these curves. It is quite clear that w_t is the shortest curve if and only if w_t^* is horizontal; equivalently, $\dot{w}_t\in\tilde{H}_{w_t}$ $:=\{w_tg,\ g=g^*\}$ for all t. Moreover, we have

$$x\in H_w\Leftrightarrow x^*\in\tilde{H}_{w^*}. \tag{6}$$

If we now project the real Hilbert space structure from $\tilde{H}_w$ to $T_{w^*w}\mathcal{M}$, using the projection $\tilde{\Pi}$, we will, of course, get the Bures metric again. On the other hand, it is easy to see that for each ρ $=ww^*$ and $h\in T_\rho\mathcal{M}$, $\tilde{h}:=\frac{1}{2}h(w^*)^{-1}$ is the unique element in $\tilde{H}_w$ satisfying $h=\Pi(\tilde{h})$. We may therefore define

$$\lambda_\rho(h,k):=4\ \mathrm{Re}\langle\tilde{h},\tilde{k}\rangle=\tfrac{1}{2}\mathrm{Tr}\,\rho^{-1}(hk+kh), \tag{7}$$

which is the RLD metric. This shows that there is a duality relation between the Bures metric and RLD (see also Refs. 14 and 10).

IV. THE GEODESIC DISTANCES

Let λ be a Riemannian metric on $\mathcal{M}$. A curve ρ_t, $t\in[0,1]$, is a geodesic path in $\mathcal{M}$ if its length

$$l_\lambda(\rho_t)=\int_0^1\sqrt{\lambda_{\rho_t}(\dot{\rho}_t,\dot{\rho}_t)}dt$$

is the minimum of lengths of all curves connecting ρ_0 and ρ_1. This length is then the geodesic distance of ρ_0 and ρ_1. Let us denote by d_λ the geodesic distance for the metric λ in $\mathcal{M}$ and by D_λ the geodesic distance in $\mathcal{D}$.

For the Bures metric, the geodesic paths and distances were obtained by Uhlmann[18,19] as follows. Let ρ_0 and ρ_1 be two elements in $\mathcal{M}$ and let ρ_t be a curve connecting them. If w_t is the horizontal lift of ρ_t, then by (5)

$$l_{\mathrm{Bures}}(\rho_t)=2l_H(w_t),$$

hence minimizing the Bures length means minimizing the Hilbert space length of horizontal lifts of curves connecting ρ_0 and ρ_1. From the definition of horizontality, this minimum is attained at the line segment $w_t=tw_1+(1-t)w_0$, such that $\|w_0-w_1\|$ is minimal over $w_0w_0^*=\rho_0$, $w_1w_1^*$ $=\rho_1$. This happens if and only if w_1 and w_0 are parallel amplitudes, that is, these satisfy Uhlmann's parallelity condition

$$w_1^*w_0\geqslant 0. \tag{8}$$

For each w_0 there is a unique w_1 parallel to w_0, given by[19]

$$w_1=\rho_0^{-1/2}(\rho_0^{1/2}\rho_1\rho_0^{1/2})^{1/2}\rho_0^{-1/2}w_0.$$

The geodesic path in $\mathcal{M}$, connecting ρ_0 and ρ_1, is then

$$\rho_t=(tw_1+(1-t)w_0)(tw_1+(1-t)w_0)^*,$$

and the geodesic distance is

$$d_{\mathrm{Bures}}(\rho_0,\rho_1)=2\|w_0-w_1\|=2\sqrt{\mathrm{Tr}\,\rho_0+\mathrm{Tr}\,\rho_1-2\mathrm{Tr}\,(\rho_0^{1/2}\rho_1\rho_0^{1/2})^{1/2}}.$$

This is called the Bures distance.

Let ρ_t now be a curve in $\mathcal{D}$. Then all lifts of ρ_t are curves on the unit sphere S in H. If w_0, $w_1\in S$, the shortest curve connecting them lies on the large circle in S through them. The length of such arcs for $w_0w_0^*=\rho_0$ and $w_1w_1^*=\rho_1$ is minimal if w_0 and w_1 are parallel amplitudes and, by definition, in this case the arc is also horizontal. Hence, the Bures geodesic in $\mathcal{D}$ is

$$\rho_t=\frac{(w_0+(1-t)w_1)(tw_0+(1-t)w_1)^*}{\|tw_0+(1-t)w_1)\|^2}$$

for parallel amplitudes w_0 and w_1 and the Bures distance

$$D_{\mathrm{Bures}}(\rho_0,\rho_1)=2\arccos\mathrm{Tr}\,w_0w_1^*=2\arccos\mathrm{Tr}\,(\rho_0^{1/2}\rho_1\rho_0^{1/2})^{1/2}.$$

The duality of the Bures and RLD metrics leads to the following upper bound for the RLD geodesic distance.

Proposition 4.1: Let $\rho_0,\ \rho_1\in\mathcal{M}$. *Then*

$$d_{\mathrm{RLD}}(\rho_0,\rho_1)\leqslant d_{\mathrm{Bures}}(\rho_0,\rho_0^{-1/2}(\rho_0\#\rho_1)^2\rho_0^{-1/2}),$$

where

$$\rho_0\#\rho_1=\rho_0^{1/2}(\rho_0^{-1/2}\rho_1\rho_0^{-1/2})^{1/2}\rho_0^{1/2}$$

is the geometric mean. If ρ_0 and ρ_1 are in $\mathcal{D}$, the same holds for geodesic distances D_{RLD} and D_{Bures}.

Proof: Let $w_0=\rho_0^{1/2}$ and let $w\in H$ be such that w_0 and w satisfy the parallelity condition (8). Then the curve $w_t=tw+(1-t)w_0$ is the horizontal lift of the Bures geodesic connecting ρ_0 and ww^*, in particular, $\dot{w}_t\in H_{w_t}$ for all t. Then w_t^* is a lift of a curve ρ_t in $\mathcal{M}$, connecting ρ_0 and w^*w and by (6), $\dot{w}_t^*\in\tilde{H}_{w_t^*}$. Consequently, by (7),

$$d_{\mathrm{RLD}}(\rho_0,w^*w)\leqslant l_{\mathrm{RLD}}(\rho_t)=2\|w^*-w_0^*\|=2\|w-w_0\|=d_{\mathrm{Bures}}(\rho_0,ww^*).$$

From the parallelity condition, $w=qw_0$ for some $q=q^*>0$. Let us choose w such that

$$\rho_1=w^*w=\rho_0^{1/2}q^2\rho_0^{1/2}.$$

Then $q=(\rho_0^{-1/2}\rho_1\rho_0^{-1/2})^{1/2}$ and

$$ww^*=\rho_0^{-1/2}(\rho_0\#\rho_1)^2\rho_0^{-1/2}.$$

The statement for distances in $\mathcal{D}$ is proved exactly the same way. □

Remark 4.1: Let w_0, w and q be as in the proof of the previous proposition. Then we have

$$\|w_0-w\|^2=\mathrm{Tr}\,\rho_0+\mathrm{Tr}\,\rho_1-2\mathrm{Tr}\,\rho_0q$$

and

$$d_{\mathrm{Bures}}(\rho_0,\rho_0^{-1/2}(\rho_1\#\rho_0)^2\rho_0^{-1/2})=2\sqrt{\mathrm{Tr}\,\rho_0+\mathrm{Tr}\,\rho_1-2\mathrm{Tr}\,\rho_0\#\rho_1}\tag{9}$$

so that ρ_0 and ρ_1 can be exchanged.

Remark 4.2: Let $\rho_t = w_t^* w_t$ and q be as in the proof of Proposition 4.1. Then, in general, ρ_t is not the RLD geodesic. Indeed, it can be easily computed that for the RLD metric, the geodesic equation reads

$$\ddot{\rho}_t + \frac{1}{L_{\rho_t} + R_{\rho_t}}(\dot{\rho}_t^2) - \dot{\rho}_t \rho_t^{-1} \dot{\rho}_t = a(t)\dot{\rho}_t,$$

where a is a smooth function $a: I \to \mathbb{R}$ (see also Ref. 3). We have

$$\rho_t = w_t^* w_t = \rho_0^{1/2}(1 + t(q-1))^2 \rho_0^{1/2}.$$

It can be shown by direct computation that the geodesic equation is satisfied if and only if

$$q(\rho_0 q - q\rho_0) = (\rho_0 q - q\rho_0)q,$$

which, for self-adjoint operators, implies $q\rho_0 = \rho_0 q$. It follows that the inequality in Proposition 4.1 is strict, unless ρ_0 and ρ_1 commute. In that case, the geodesic distances are the same for all monotone metrics.

In Ref. 17, a class of generalized relative entropies

$$H_g(\rho_0, \rho_1) = \operatorname{Tr} \rho_0 g(\rho_0^{-1/2} \rho_1 \rho_0^{-1/2})$$

was introduced; here g is an operator convex function. This is a noncommutative version of the f-divergence. It was shown in Ref. 17 that the generalized entropy H_g leads to a constant multiple of the RLD metric for infinitesimaly close elements in $\mathcal{D}$.

It is easy to see that the right hand side of (9) is equal to $\sqrt{2H_{g_0}(\rho_0, \rho_1)}$, where

$$g_0(t) = 2 + 2t - 4t^{1/2}. \tag{10}$$

Note that on commuting elements, H_{g_0} is equal to the Hellinger distance.

By maximality of the RLD metric, we obtain the following.

Corollary 4.1: Let $\rho_0, \rho_1 \in \mathcal{M}$ and let λ be a monotone metric. Then

$$d_{\text{Bures}}(\rho_0, \rho_1) \leq d_\lambda(\rho_0, \rho_1) \leq \sqrt{2H_{g_0}(\rho_0, \rho_1)} < 2\sqrt{\operatorname{Tr}\rho_0 + \operatorname{Tr}\rho_1}.$$

If $\rho_0,\ \rho_1 \in \mathcal{D}$, then

$$2 \arccos \operatorname{Tr}(\rho_0^{1/2} \rho_1 \rho_0^{1/2})^{1/2} \leq D_\lambda(\rho_0, \rho_1) \leq 2 \arccos \operatorname{Tr} \rho_0 \# \rho_1 < \pi.$$

V. THE WYD METRICS

The Wigner–Yanase–Dyson (WYD) metrics are defined by

$$\lambda_\rho^\alpha(h,k) = \frac{\partial^2}{\partial t \partial s} \operatorname{Tr} f_\alpha(\rho + th) f_{-\alpha}(\rho + sk)\big|_{s,t=0},$$

where

$$f_\alpha(x) = \begin{cases} \dfrac{2}{1-\alpha} x^{(1-\alpha)/2}, & \alpha \neq 1, \\ \log(x), & \alpha = 1. \end{cases}$$

As it was shown in Ref. 8, these metrics are monotone for $\alpha\in[-3,3]$. The family of WYD metrics is important in quantum information geometry (see Refs. 7, 11, and 6). As special cases, for $\alpha=\pm1$, we get the well known Bogoljubov–Kubo–Mori metric and for $\alpha=\pm3$ we get the RLD metric.

The smallest in this family is the Wigner–Yanase (WY) metric, obtained for $\alpha=0$. The WY metric has the form

$$\lambda_\rho(h,k)=4\,\mathrm{Tr}\,h(\sqrt{L_\rho}+\sqrt{R_\rho})^{-2}(k).$$

The corresponding geodesic path and distance was computed in Ref. 5, using a noncommutative version of the square root map (1) and a pullback technique. We will show that these can also be easily obtained using a similar method as in the Bures case.

Let ρ_t be a curve in $\mathcal{M}$. Among its lifts $w_tw_t^*=\rho_t$, we will again choose a horizontal one. In this case, the lift w_t is horizontal if it is contained in the natural positive cone at w_0, that is, if $w_t=\rho_t^{1/2}u_0$ for all t. In this case, the horizontal subspace is $H_w^0=\{gu,\ g=g^*\}$, where $w=\rho^{1/2}u$ is the polar decomposition of w. Each tangent vector $h\in T_{ww^*}\mathcal{M}$ has a unique horizontal lift $h^0=gu\in H_w^0$, such that $h=\Pi(h^0)=g\rho^{1/2}+\rho^{1/2}g$. The induced metric

$$\lambda_\rho(h,k)=4\,\mathrm{Re}\langle h^0,k^0\rangle=4\,\mathrm{Tr}\,h(L_\rho^{1/2}+R_\rho^{1/2})^{-2}(k)$$

is the WY metric. Note that in this case $x\in H_w^0$ if and only if $x^*\in H_{w^*}^0$, so that the WY metric is self-dual, in the sense mentioned in Sec. III. Let us also remark that it is possible to obtain all the monotone metrics in a similar manner (see Refs. 4 and 10).

Now let ρ_0 and ρ_1 be in $\mathcal{M}$ and let ρ_t be a curve connecting them. Again, the WY length of ρ_t is twice the Hilbert space length of its horizontal lift $w_t=\rho_t^{1/2}u_0$. Therefore, ρ_t is the geodesic path if $w_t=t\rho_1^{1/2}u_0+(1-t)\rho_0^{1/2}u_0$, that is,

$$\rho_t=(t\rho_1^{1/2}+(1-t)\rho_0^{1/2})^2$$

and the geodesic distance is

$$d_{\mathrm{WY}}(\rho_0,\rho_1)=2\|\rho_0^{1/2}-\rho_1^{1/2}\|=2\sqrt{\mathrm{Tr}\,\rho_0+\mathrm{Tr}\,\rho_1-2\,\mathrm{Tr}\,\rho_0^{1/2}\rho_1^{1/2}}.$$

Similarly, if $\rho_0,\ \rho_1\in\mathcal{D}$, then ρ_t is a geodesic path if and only if w_t lies on the large circle connecting $\rho_0^{1/2}u_0$ and $\rho_1^{1/2}u_0$. Hence

$$\rho_t=\frac{(t\rho_1^{1/2}+(1-t)\rho_0^{1/2})^2}{\|t\rho_1^{1/2}+(1-t)\rho_0^{1/2}\|^2}$$

and

$$D_{\mathrm{WY}}(\rho_0,\rho_1)=2\arccos\mathrm{Tr}\,\rho_0^{1/2}\rho_1^{1/2}.$$

Let us denote by $\Delta_{\sigma,\rho}=L_\sigma R_\rho^{-1}$ the relative modular operator. In Ref. 15, a class of quasi-entropies was introduced by

$$S_g(\rho,\sigma)=\mathrm{Tr}\,\rho^{1/2}g(\Delta_{\sigma,\rho})(\rho^{1/2}),$$

where g is an operator convex function. This is another quantum version of the f-divergences. It is easy to see that

$$d_{WY}(\rho_0,\rho_1)=\sqrt{2S_{g_0}(\rho_0,\rho_1)},\tag{11}$$

where g_0 is given by (10). It was proved in Ref. 13 that each monotone metric can be obtained as the Hessian of S_g for a suitable operator convex function g. The choice $g=g_0$ leads to the WY metric.

From the previous section and the fact that the WY metric is the least element in the family of WYD metrics, we obtain the following.

Corollary 5.1: Let λ *be a WYD metric and* $\rho_0,\rho_1\in\mathcal{M}$. *Then*

$$\sqrt{2S_{g_0}(\rho_0,\rho_1)}=d_{\mathrm{WY}}(\rho_0,\rho_1)\leq d_\lambda(\rho_0,\rho_1)\leq\sqrt{2H_{g_0}(\rho_0,\rho_1)},$$

where $g_0(t)=2+2t-4t^{1/2}$. If $\rho_0,\rho_1\in\mathcal{D}$, *then*

$$2\arccos\mathrm{Tr}\,\rho_0^{1/2}\rho_1^{1/2}\leq D_\lambda(\rho_0,\rho_1)\leq 2\arccos\mathrm{Tr}\,\rho_0\#\rho_1.$$

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Locality and orthomodular structure of compound systems

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A P-lattice is defined as a σ-complete, orthomodular atomic lattice $\mathcal{L}$ which is formed by the set of propositions of a physical system. A composition of physical systems in the framework of P-lattices is considered and some notions of locality are given. It is shown that the following statements about compound systems are equivalent. (a) All atoms of a compound system are reducible to those of its subsystems. (b) All pure states of a compound system are separable into those of its subsystems. (c) A compound system has statistical property independence. (d) At least one of the subsystems is classical. (e) Bell-type inequalities hold. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1690490]

I. INTRODUCTION

According to so-called logico-algebraic approaches to physics, one of the differences between classical and quantum mechanics is in whether distributive law holds in their propositional structures; the lattices of observational propositions in classical mechanics are distributive and those in quantum mechanics are not (see, e.g., Ref. 1).

On the other hand, Bell[2] found another difference. He showed that stochastic inequalities following from a kind of locality condition, which holds for classical mechanics, can be violated by quantum mechanical predictions. According to experimental results and philosophical discussions, one must recognize some nonlocality in quantum mechanics (henceforce *Bell-type arguments*).

The questions now arise: Is there any relation between the two new features of quantum mechanics, i.e., nondistributivity and nonlocality? For example, could the nondistributive propositional structure of a compound system imply the nonlocal feature of the system? Or, would these features merely tell how large the differences between classical and quantum picture of reality are? Studies which have been made on the matter can be divided into two groups: One group, which focuses on the role of joint probabilities in the Bell-type arguments, studies connections between propositional structures and certain stochastic inequalities for them.[3–6] The other group, which focuses on the role of locality in the Bell-type arguments, formulates locality conditions for propositional structures and studies connections between nonlocality and nondistributivity.[7–13]

However, very few attempts[14] have been made to unify the two ways. What seems to be lacking is a logical and conceptual clarification of notions such as ''classicality'' and ''locality'' in the Bell-type arguments. The purpose of this article is to clarify these notions within a lattice-theoretical approach, and to establish the logical connections among propositional structures of sub- and compound systems, locality conditions and Bell-type inequalities.

II. PROPOSITIONAL STRUCTURES OF PHYSICAL SYSTEMS

Presupposing definitions of standard lattice-theoretical notions (see, e.g., Ref. 15), let us begin with basic definitions and notations for our arguments (see also Ref. 10).

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A *P-lattice* is a σ-complete, orthomodular atomic lattice $\mathcal{L}$ which is formed by the set of propositions of a physical system.[16] A distributive P-lattice is called *classical*, which is isomorphic to the Borel σ-field of some phase space in classical mechanics. An irreducible P-lattice is called *quantum*, which is isomorphic to the lattice of all closed subspaces of some Hilbert space.

For notation, $(a,b)\,\mathsf{C}$ denotes that elements $a,b\in\mathcal{L}$ commute with each other, $\mathcal{C}(\mathcal{L})$ stands for the center of $\mathcal{L}$, and $\mathcal{A}(\mathcal{L})$ for the set of all atoms of $\mathcal{L}$.

A σ-additive probability measure m on a P-lattice $\mathcal{L}$ is called a *state*, and the set of states is denoted by $\mathcal{M}$. The set $\mathcal{M}$ is σ-convex. An element of the extremal subset $\mathcal{M}_p$ of $\mathcal{M}$ is called a *pure state*. Further, we shall suppose the Jauch–Piron condition for pure states, i.e., $m(a)=1=m(b)$ imply $m(a\wedge b)=1$ for any $m\in\mathcal{M}_p$.

A pair $(\mathcal{L},\mathcal{M}_p)$ of a P-lattice $\mathcal{L}$ and a set $\mathcal{M}_p$ of pure states on $\mathcal{L}$ is called *complete* if there is a bijective correspondence between $\mathcal{A}(\mathcal{L})$ and $\mathcal{M}_p$ such that $m(x)=1$ for all $x\in\mathcal{A}(\mathcal{L})$ and all $m\in\mathcal{M}_p$. A complete pair $(\mathcal{L},\mathcal{M}_p)$ is called a *physical system*. We shall say that a physical system is *classical* (resp. *quantum*) if the P-lattice is classical (resp. quantum).

Let $\mathcal{S}$ be a set of pure states on a P-lattice $\mathcal{L}$. We say that a state m is the *superposition* of the states in $\mathcal{S}$ if

$$\mathcal{S}(a)=1\ \ [\text{i.e., } s(a)=1\ \ \text{for}\ \ \forall s\in\mathcal{S}]\Rightarrow m(a)=1\,\text{for}\ \ \forall a\in\mathcal{L}.$$

If $(\mathcal{L},\mathcal{M}_p)$ is a physical system, we put $\overline{\mathcal{S}}=\{m\in\mathcal{M}_p|\mathcal{S}(a)=1\Rightarrow m(a)=1\}$ for any $\mathcal{S}\subseteq\mathcal{M}_p$.

In the following sections, we prove some theorems. For their proofs, we shall appeal frequently to the following two theorems:

Theorem 1 (e.g., Ref. 17, Lemma 3.10): *Let $\mathcal{L}$ be a σ-complete orthomodular lattice, and let $a,b_1,b_2,\ldots$ be elements of $\mathcal{L}$. If $(a,b_i)\,\mathsf{C}$ for all i, then $(a,b_i^{\perp})\,\mathsf{C}$, $(a,\vee b_i)\,\mathsf{C}$ and $(a,\wedge b_i)\,\mathsf{C}$.*

Theorem 2 [Foulis–Holland (e.g., Ref. 18, Theorem 3)]: *Let $\mathcal{L}$ be an orthomodular lattice, and let a,b,c be elements of $\mathcal{L}$. If one of them commutes with the other two, then triple (a,b,c) is distributive.*

III. DESCRIPTIONS OF COMPOUND SYSTEMS

Over the last few decades, a considerable number of studies have been made on the description of compound systems in lattice-theoretical approaches. Unfortunately, there is a well-known open problem in the case of compound systems consisting of two quantum subsystems.[7–12,19] However, our purposes are not to deal with the problem but to consider some properties in compound systems if such a description is possible. With this problem in mind, let us now turn to our task.

We shall be almost exclusively concerned with a compound system S consisting of two subsystems S_1 and S_2. Let us state how to describe the situation in terms of P-lattices. By using P-lattices $\mathcal{L}_i$ associated with subsystems S_i $(i=1,2)$, we define a P-lattice associated with the compound system S as follows.[10,13]

Definition 1: Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be P-lattices. A P-lattice $\mathcal{L}$ is called a compound P-lattice if

(i) *there exist two injective σ-orthohomomorphisms $h_i:\mathcal{L}_i\to\mathcal{L}(i=1,2)$,*
(ii) *$h_1(p)\wedge h_2(q)\in\mathcal{A}(\mathcal{L})$ for every $p\in\mathcal{A}(\mathcal{L}_1)$, $q\in\mathcal{A}(\mathcal{L}_2)$,*
(iii) *$(h_1(a),h_2(b))\,\mathsf{C}$ for every $a\in\mathcal{L}_1$, $b\in\mathcal{L}_2$, and*
(iv) *$h_1(\mathcal{L}_1)\cup h_2(\mathcal{L}_2)$ generates $\mathcal{L}$.*

Further, by using physical systems $(\mathcal{L}_i,\mathcal{M}_{p_i})$ associated with S_i $(i=1,2)$, we define a physical system associated with S as follows.[10]

Definition 2: Let $(\mathcal{L}_1,\mathcal{M}_{p_1})$ and $(\mathcal{L}_2,\mathcal{M}_{p_2})$ be physical systems. We say that a physical system $(\mathcal{L},\mathcal{M}_p)$ is a compound physical system of $(\mathcal{L}_1,\mathcal{M}_{p_1})$ and $(\mathcal{L}_2,\mathcal{M}_{p_2})$ if there exist mappings α,β such that

(i) $\alpha:\mathcal{L}_1\times\mathcal{L}_2\to\mathcal{L}$, $\beta:\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}\to\mathcal{M}_p$,
$$\beta(m_1,m_2)(\alpha(a_1,a_2))=m_1(a_1)m_2(a_2) \quad \text{for} \quad a_i\in\mathcal{L}_i, m_i\in\mathcal{M}_{p_i}(i=1,2),$$
(ii) $\{m\in\mathcal{M}_p|m(a)=1\}=\overline{\{\beta(m_1,m_2)|\beta(m_1,m_2)(a)=1\}}$ *for* $a\in\mathcal{L}$ *of the form*
$$a=\wedge_{k=1}^{N}\alpha(a_1^k,a_2^k), \quad a_i^k\in\mathcal{L}_i \quad (i=1,2) \quad \textit{or}$$
$$a=\alpha(a_1,I_2)^{\perp}, \quad a_1\in\mathcal{L}_1 \quad \textit{or} \quad a=\alpha(I_1,a_2)^{\perp}, \quad a_2\in\mathcal{L}_2,$$
(iii) $\alpha[\mathcal{L}_1\times\mathcal{L}_2]$ *generates* $\mathcal{L}$, *and*
(iv) $\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]=\mathcal{M}_p$.

A connection between compound P-lattices and compound physical systems is given by the following theorem.

Theorem 3 (Ref. 10, Theorem 4): *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *Let us put*
$$h_1:\mathcal{L}_1\to\mathcal{L} \ , \ a_1\mapsto\alpha(a_1,I_2), \quad h_2:\mathcal{L}_2\to\mathcal{L} \ , \ a_2\mapsto\alpha(I_1,a_2).$$
Then $\mathcal{L}$ *is a compound P-lattice of* $\mathcal{L}_1$ *and* $\mathcal{L}_2$.

From these definitions, the following expected results are obtained. (For similar result in other schemes, see Ref. 11.)

Theorem 4 (Ref. 20, Corollaries 1 and 2): *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$.

(i) $\mathcal{L}$ *is distributive if and only if both* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *are distributive.*
(ii) $\mathcal{L}$ *is irreducible if and only if both* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *are irreducible.*

This theorem seems to assure that Definitions 1 and 2 grasp the notion of composition which classical and quantum mechanics have in common.

IV. SUFFICIENT CONDITIONS FOR BELL-TYPE INEQUALITIES

In this section, we shall consider some important notions concerning Bell-type arguments, and examine connections among them. Furthermore, we shall show that these notions are sufficient conditions for deriving Bell-type inequalities mentioned later. Let us begin with some definitions.

Definition 3: Let $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$.

(1) We say that $(\mathcal{L},\mathcal{M}_p)$ *has property reducibility if the set of all atoms of* $\mathcal{L}$ *is of the form*
$$\mathcal{A}(\mathcal{L})=\{h_1(q_1)\wedge h_2(q_2)|q_1\in\mathcal{A}(\mathcal{L}_1),q_2\in\mathcal{A}(\mathcal{L}_2)\}.$$
(2) We say that $(\mathcal{L},\mathcal{M}_p)$ *has state separability if the set of all pure states on* $\mathcal{L}$ *is of the form*
$$\mathcal{M}_p=\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}].$$

Intuitively, the property reducibility means that all physical properties of a whole system are merely the sum of, or are supervenient on, those of its subsystems. (We say that there exists a *holistic property* in a compound physical system, if it does not have property reducibility.) The state separability reflects a notion that spatially separated systems always possess states of their own, which determine the state assigned to the compound system. (We say that there exists a *nonseparable state* in a compound physical system, if it does not have state separability.)

Remark that from a philosophical point of view, the notions of reducibility and separability should be distinguished from each other as Healey[21] pointed out; that is, while the term ''reducibility'' is used to describe part-whole relations, the term ''separability'' is based on spatio-temporal relations. However, we shall identify these notions by virtue of the following theorem.

Theorem 5: *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *The following statements are equivalent.*

(a) $(\mathcal{L},\mathcal{M}_p)$ *has property reducibility.*
(b) $(\mathcal{L},\mathcal{M}_p)$ *has state separability.*

Proof: [(a)⇒(b)]: Since $(\mathcal{L},\mathcal{M}_p)$ is complete, there is an atom $a\in\mathcal{A}(\mathcal{L})$ such that $m(a)=1$ for any $m\in\mathcal{M}_p=\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$. From (a), there exist $x\in\mathcal{A}(\mathcal{L}_1)$ and $y\in\mathcal{A}(\mathcal{L}_2)$ such that $a=h_1(x)\wedge h_2(y)=\alpha(x,I_2)\wedge\alpha(I_1,y)=\alpha(x,y)$ (where last equality is due to Proposition 2 of Ref. 10). Further, there exist $m_1\in\mathcal{M}_{p_1}$ and $m_2\in\mathcal{M}_{p_2}$ such that $m_1(x)=1$ and $m_2(y)=1$, and we have

$$m(\alpha(x,y))=1=m_1(x)m_2(y)=\beta(m_1,m_2)(\alpha(x,y)).$$

Then we get $m=\beta(m_1,m_2)\in\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$, and hence $\overline{\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]}\subseteq\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$. It is obvious by definition that the opposite inclusion holds. As a result we have $\overline{\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]}=\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$.

[(b)⇒(a)]: There exist $m_1\in\mathcal{M}_{p_1}$ and $m_2\in\mathcal{M}_{p_2}$ such that $m=\beta(m_1,m_2)$ for any $m\in\mathcal{M}_p=\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$. Further, there exist $x\in\mathcal{A}(\mathcal{L}_1)$ and $y\in\mathcal{A}(\mathcal{L}_2)$ such that $m_1(x)=1$ and $m_2(y)=1$ for m_1 and m_2. Then we have

$$1=m_1(x)m_2(y)=\beta(m_1,m_2)(\alpha(x,y))=m(\alpha(x,y)),$$

which means that an atom corresponding to $m\in\mathcal{M}_p$ is of the form $\alpha(x,y)=h_1(x)\wedge h_2(y)$. Therefore we get $\mathcal{A}(\mathcal{L})=\{h_1(q_1)\wedge h_2(q_2)|q_1\in\mathcal{A}(\mathcal{L}_1),q_2\in\mathcal{A}(\mathcal{L}_2)\}$. □

As a consequence, we shall simply say in the following argument that $(\mathcal{L},\mathcal{M}_p)$ has *separability* if it has one (hence both) of these features.

An implication of having separability is shown in the following theorem, which has been given by Pykacz and Santos.[14] (Their scheme is slightly different from ours, but the method of their proof can be applied to ours.)

Theorem 6 (Ref. 14, Theorem 2): *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *If* $(\mathcal{L},\mathcal{M}_p)$ *has state separability, the following Clauser–Horne version of Bell's inequalities,*

$$\begin{aligned}&m(\,h_1(a)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(d)\,)\\&\quad-m(\,h_1(a)\wedge h_2(d)\,)-m(\,h_1(c)\,)-m(\,h_2(b)\,)\leqslant 0,\end{aligned}\tag{1}$$

holds for any $m\in\mathcal{M}_p$ *and for any quadruple* $(h_1(a),h_2(b),h_1(c),h_2(d))$, *where* $a,c\in\mathcal{L}_1$ *and* $b,d\in\mathcal{L}_2$.

Let us suppose that the inequalities (1) are violated in some compound physical system. Then, Theorem 6 tells us that such a system cannot have separability. That is, such a system is either (i) that there is an atomic property which cannot be reducible to the properties possessed by its subsystems, or (ii) that the subsystems do merely not possess any of thier own properties. This seems to be the reason that violations of Bell's inequalities in quantum mechanics have been regarded as problematic.

So far, we have seen a connection between separability and Bell-type inequalities. Recall that, for example, the property reducibility is a restriction on the set of all atoms of a compound physical system. The questions now arise: For what structure is such a restriction permitted? Or, more directly, *from what structure are Bell-type inequalities derived?* As for the former question, the following theorem has been proved by the author.[13]

Theorem 7 (Ref. 13, Corollary): *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *The statement* (a) *in Theorem 5 is equivalent to the following statement.*
(c) At least one of $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *is distributive.*

Consequently, we can see that the statements (a), (b) and (c) are equivalent. Finally, with the aid of Theorem 6, we can show a new connection among propositional structures of sub- and compound system and Bell-type inequalities.

Theorem 8: *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *If at least one of* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *is distributive, the Clauser–Horne version of Bell's inequalities (1) hold for any* $m\in\mathcal{M}_p$ *and for any quadruple* $(h_1(a),h_2(b),h_1(c),h_2(d))$, *where* $a,c\in\mathcal{L}_1$ *and* $b,d\in\mathcal{L}_2$.

It should be noticed that there are seemingly no locality conditions in the statement of Theorem 8.

V. A NECESSARY CONDITION FOR BELL-TYPE INEQUALITIES

In the previous section, we considered a question such that: From what structure are Bell-type inequalities derived? And we answered the question by establishing Theorem 8. Now we must ask the converse question, to which little attention has been given: *What structure do Bell-type inequalities imply?* More accurately, *what structure does the compound physical system have if Bell-type inequalities always hold for the system?* In this section, we shall try to answer the question.

The following lemma is helpful for our purpose.

Lemma 1: Let $(\mathcal{L},\mathcal{M}_p)$ *be a physical system such that* $\mathcal{L}$ *is nondistributive. Then, for any distinct atoms* $x,y\in\mathcal{A}(\mathcal{L})$ *such that* x *is not orthogonal to* y,

$$m(x)=1 \quad\Rightarrow\quad m(y)\neq 0,1 \quad \text{for} \quad m\in\mathcal{M}_p.$$

Proof: Suppose that $m(x)=1$.

(i) In the case of $m(y)=1$:
Due to the Jauch–Piron condition, we have $m(x\wedge y)=1$. On the other hand, since x and y are distinct atoms, it follows that $x\wedge y=\varnothing$ so that $m(x\wedge y)=0$, which is a contradiction.

(ii) In the case of $m(y)=0$:
$$1=m(x)\leqslant m(x\vee y)=m(\{(x\vee y)\wedge y^{\perp}\}\vee y)=m((x\vee y)\wedge y^{\perp})+m(y)=m((x\vee y)\wedge y^{\perp}).$$
Hence $m((x\vee y)\wedge y^{\perp})=1$. Due to the Jauch–Piron condition and due to the fact that $x\wedge y^{\perp}=\varnothing$, it follows that $1=m(\{(x\vee y)\wedge y^{\perp}\}\wedge x)=m(\varnothing)=0$, which is a contradiction.

So we conclude that $m(y)\neq 0,1$. □

We shall now answer the question mentioned above. The following theorem, which is the converse of Theorem 8, is also true.

Theorem 9: *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *If the following Clauser–Horne version of Bell's inequalities*

$$m(\,h_1(a)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(d)\,)$$
$$-m(\,h_1(a)\wedge h_2(d)\,)-m(\,h_1(c)\,)-m(\,h_2(b)\,)\leqslant 0$$

holds for any $m\in\mathcal{M}_p$ *and for any quadruple* $(h_1(a),h_2(b),h_1(c),h_2(d))$, *where* $a,c\in\mathcal{L}_1$ *and* $b,d\in\mathcal{L}_2$, *then at least one of* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *is distributive.*

Proof: Suppose that both $\mathcal{L}_1$ and $\mathcal{L}_2$ are nondistributive. Then we can choose distinct atoms $a,a',c,c'\in\mathcal{A}(\mathcal{L}_1)$ such that $a\perp a'$, $c\perp c'$ and $a\vee a'=c\vee c'$. Similarly, choose distinct $b,b',d,d'\in\mathcal{A}(\mathcal{L}_2)$ such that $b\perp b'$, $d\perp d'$ and $b\vee b'=d\vee d'$. Let X denote $a\vee a'$ and Y denote $b\vee b'$. It is easily seen that

$$(h_1(a)\wedge h_2(b))\vee(h_1(a)\wedge h_2(b'))\vee(h_1(a')\wedge h_2(b))\vee(h_1(a')\wedge h_2(b'))=h_1(X)\wedge h_2(Y).$$

Therefore, it follows that $\dim(h_1(X)\wedge h_2(Y))=4$. [Remark that by definition, for example, $h_1(a)\neq h_2(b)$.]

First, we shall show that $\Gamma:=(h_1(c')\vee h_2(d))\wedge(h_1(a)\vee h_2(b'))\wedge(h_1(a')\vee h_2(d'))$ is not a null element $\varnothing$. If $\Gamma=\varnothing$, then

$$h_1(X)\wedge h_2(Y)=h_1(X)\wedge h_2(Y)\wedge\Gamma^{\perp}$$
$$=h_1(X)\wedge h_2(Y)\wedge[(h_1(c')^{\perp}\wedge h_2(d)^{\perp})\vee(h_1(a)^{\perp}\wedge h_2(b')^{\perp})\vee(h_1(a')^{\perp}\wedge h_2(d')^{\perp})]. \tag{2}$$

Due to Theorem 1, $h_1(X)\wedge h_2(Y)$ commutes with $h_1(c')^{\perp}\wedge h_2(d)^{\perp}$, $h_1(a)^{\perp}\wedge h_2(b')^{\perp}$ and $h_1(a')^{\perp}\wedge h_2(d')^{\perp}$. Hence (2) reduces to

$$(h_1(c)\wedge h_2(d'))\vee(h_1(a')\wedge h_2(b))\vee(h_1(a)\wedge h_2(d)). \tag{3}$$

Since the element (3) is a join of three atoms, its dimension is less than or equal to 3, which contradicts with $\dim(h_1(X)\wedge h_2(Y))=4$. So we conclude that $\Gamma\neq\varnothing$. By atomicity of $\mathcal{L}$, there exists an atom q such that $q\leqslant\Gamma$. It follows that $q\leqslant\Gamma\leqslant(h_1(c')\vee h_2(d))\wedge(h_1(a')\vee h_2(d'))$. By using the fact that $h_2(d)$ commutes with $h_1(c')$ and $h_1(a')\vee h_2(d')$ (due to Theorem 1) and by applying Foulis–Holland's theorem, we have

$$q\leqslant(h_1(c')\vee h_2(d))\wedge(h_1(a')\vee h_2(d'))$$
$$=[h_1(c')\wedge(h_1(a')\vee h_2(d'))]\vee[h_2(d)\wedge(h_1(a')\vee h_2(d'))]$$
$$=(h_1(c')\wedge h_2(d'))\vee(h_1(a')\wedge h_2(d))\leqslant h_1(X)\wedge h_2(Y).$$

Second, we shall consider a pure state m such that $m(q)=1$. Since

$$q\leqslant h_1(c')\vee h_2(d),\ h_1(a)\vee h_2(b'),\ h_1(a')\vee h_2(d'),$$

we have

$$1=m(h_1(c')\vee h_2(d))=m(h_1(a)\vee h_2(b'))=m(h_1(a')\vee h_2(d')),$$

or, equivalently, we have

$$0=m(h_1(c')^{\perp}\wedge h_2(d)^{\perp})=m(h_1(a)^{\perp}\wedge h_2(b')^{\perp})=m(h_1(a')^{\perp}\wedge h_2(d')^{\perp}).$$

Since $X\wedge c^{\perp}=c'\leqslant c^{\perp}$, i.e., $c\leqslant c'^{\perp}$ so that $h_1(c)\wedge h_2(d)^{\perp}\leqslant h_1(c'^{\perp})\wedge h_2(d)^{\perp}=h_1(c')^{\perp}\wedge h_2(d)^{\perp}$, we obtain $m(h_1(c)\wedge h_2(d)^{\perp})=0$. Similarly, we obtain

$$m(h_1(a)^{\perp}\wedge h_2(b))=m(h_1(a)\wedge h_2(d))=0. \tag{4}$$

Hence we have

$$m(h_1(c))=m(h_1(c)\wedge h_2(d))+m(h_1(c)\wedge h_2(d)^{\perp})=m(h_1(c)\wedge h_2(d)), \tag{5}$$

$$m(h_2(b))=m(h_1(a)\wedge h_2(b))+m(h_1(a)^{\perp}\wedge h_2(b))=m(h_1(a)\wedge h_2(b)). \tag{6}$$

Third, we shall show that q is not orthogonal to $h_1(c)\wedge h_2(b)$. Since $q\leqslant h_1(X)\wedge h_2(Y)$, it follows that

$$q\wedge(h_1(c)\wedge h_2(b))^{\perp}=q\wedge h_1(X)\wedge h_2(Y)\wedge(h_1(c)\wedge h_2(b))^{\perp}$$
$$=q\wedge[(h_1(c')\wedge h_2(Y))\vee(h_1(X)\wedge h_2(b'))]$$
$$\leqslant\Gamma\wedge[(h_1(c')\wedge h_2(Y))\vee(h_1(X)\wedge h_2(b'))]$$
$$=(h_1(c')\vee h_2(d))\wedge(h_1(a)\vee h_2(b'))\wedge(h_1(a')\vee h_2(d'))$$
$$\wedge[(h_1(c')\wedge h_2(Y))\vee(h_1(X)\wedge h_2(b'))]. \tag{7}$$

By using Theorem 1, it follows that $h_1(c')\wedge h_2(Y)$ commutes with $h_1(c')\vee h_2(d)$ and $h_1(X)\wedge h_2(b')$. Then, by applying Foulis–Holland's theorem, we can see

$$\begin{aligned}&(h_1(c')\vee h_2(d))\wedge[(h_1(c')\wedge h_2(Y))\vee(h_1(X)\wedge h_2(b'))]\\&\quad=[(h_1(c')\vee h_2(d))\wedge(h_1(c')\wedge h_2(Y))]\vee[(h_1(c')\vee h_2(d))\wedge(h_1(X)\wedge h_2(b'))]\\&\quad=(h_1(c')\wedge h_2(Y))\vee[(h_1(c')\wedge h_1(X)\wedge h_2(b'))\vee(h_2(d)\wedge h_1(X)\wedge h_2(b'))]\\&\quad=(h_1(c')\wedge h_2(Y))\vee(h_1(c')\wedge h_2(b'))=h_1(c')\wedge h_2(Y).\end{aligned}\tag{8}$$

Therefore, by applications of Foulis–Holland's theorem, the right-hand side of (7) reduces to

$$\begin{aligned}&h_1(c')\wedge h_2(Y)\wedge(h_1(a)\vee h_2(b'))\wedge(h_1(a')\vee h_2(d'))\\&\quad=[(h_1(c')\wedge h_2(Y)\wedge h_1(a))\vee(h_1(c')\wedge h_2(Y)\wedge h_2(b'))]\wedge(h_1(a')\vee h_2(d'))\\&\quad=h_1(c')\wedge h_2(b')\wedge(h_1(a')\vee h_2(d'))\\&\quad=h_1(c')\wedge[(h_1(a')\wedge h_2(b'))\vee(h_2(b')\wedge h_2(d'))]=h_1(c')\wedge h_1(a')\wedge h_2(b')=\varnothing.\end{aligned}$$

Hence we conclude that $q\wedge(h_1(c)\wedge h_2(b))^{\perp}=\varnothing$, i.e., the atom q is not orthogonal to $h_1(c)\wedge h_2(b)$. By virtue of Lemma 1, we obtain

$$m(h_1(c)\wedge h_2(b))\neq 0.\tag{9}$$

Finally, we shall show that our supposition for $\mathcal{L}_1$ and $\mathcal{L}_2$ leads to a contradiction. By the premise of the theorem, the following inequality,

$$\begin{aligned}&m(h_1(a)\wedge h_2(b))+m(h_1(c)\wedge h_2(b))+m(h_1(c)\wedge h_2(d))\\&\quad-m(h_1(a)\wedge h_2(d))-m(h_1(c))-m(h_2(b))\leqslant 0,\end{aligned}\tag{10}$$

holds for our choice of a,b,c,d and m. From (5) and (6), this inequality reduces to

$$m(h_1(c)\wedge h_2(b))\leqslant m(h_1(a)\wedge h_2(d)).\tag{11}$$

However, it follows from (4) that $m(h_1(c)\wedge h_2(b))=0$, which contradicts with (9). Therefore, we conclude that at least one of $\mathcal{L}_1$ and $\mathcal{L}_2$ must be distributive. □

We would like to add one to our results. The following notion often appears in Bell-type arguments.

Definition 4: Let $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *We say that* $(\mathcal{L},\mathcal{M}_p)$ *has statistical property independence if for any state* $m\in\mathcal{M}_p$ *and for any* $x\in\mathcal{L}_1$ *and* $y\in\mathcal{L}_2$ *it holds that*

$$m(h_1(x)\wedge h_2(y))=m(h_1(x))\,m(h_2(y)).$$

Further, we say that there exists a *nonlocal correlation* in a compound physical system, if it does not have statistical property independence. The following theorem can be obtained.

Theorem 10: *Let* $(\mathcal{L},\mathcal{M}_p)$ *be a compound physical system of* $(\mathcal{L}_1,\mathcal{M}_{p_1})$ *and* $(\mathcal{L}_2,\mathcal{M}_{p_2})$. *The statement* (b) *in Theorem 5 is equivalent to the following statement.*

(d) $(\mathcal{L},\mathcal{M}_p)$ *has statistical property independence.*

Proof: [(b)⇒(d)]: Since there exist some $m_1\in\mathcal{M}_{p_1}$ and $m_2\in\mathcal{M}_{p_2}$ for any state $m\in\beta[\mathcal{M}_{p_1}\times\mathcal{M}_{p_2}]$, it follows that for any $x\in\mathcal{L}_1$ and $y\in\mathcal{L}_2$

TABLE I. $(\mathcal{L}_1,\mathcal{M}_{p_1})$ and $(\mathcal{L}_2,\mathcal{M}_{p_2})$ are physical systems respectively associated with systems S_1 and S_2. $(\mathcal{L},\mathcal{M}_p)$ is the compound physical system of them. This table shows connections among features of $\mathcal{L}_1$ and $\mathcal{L}_2$, those of $(\mathcal{L},\mathcal{M}_p)$ and the Clauser-Horne version of Bell's inequalities (12).

$\mathcal{L}_1$	$\mathcal{L}_2$	Properties of $(\mathcal{L},\mathcal{M}_p)$	Bell-type inequalities (12)
Distributive	Distributive	Distributive and separable	○
Either (not both) distributive		Nondistributive and separable	○
Nondistributive	Nondistributive	Nondistributive and nonseparable	×

$$m(h_1(x)\wedge h_2(y))=\beta(m_1,m_2)(\alpha(x,y))=m_1(x)m_2(y)=m_1(x)m_2(I_2)m_1(I_1)m_2(y)$$
$$=\beta(m_1,m_2)(\alpha(x,I_2))\,\beta(m_1,m_2)(\alpha(I_1,y))=m(h_1(x))\,m(h_2(y)),$$

which shows that $(\mathcal{L},\mathcal{M}_p)$ has statistical property independence.

[(d)⇒(b)]: Suppose that $(\mathcal{L},\mathcal{M}_p)$ has statistical property independence. Then, by virtue of Theorem 2 of Ref. 14, it follows that the Clauser–Horne version of Bell's inequalities (1) holds for any $m\in\mathcal{M}_p$ and for any $a,c\in\mathcal{L}_1$ and $b,d\in\mathcal{L}_2$. Due to Theorem 9, we conclude that at least one of $\mathcal{L}_1$ and $\mathcal{L}_2$ is distributive. This statement is equivalent to the statement (b) by Theorem 5 and 7. □

VI. CONCLUDING REMARKS

In summary, we have the following results.

Corollary: Let $(\mathcal{L},\mathcal{M}_p)$ be a compound physical system of $(\mathcal{L}_1,\mathcal{M}_{p_1})$ and $(\mathcal{L}_2,\mathcal{M}_{p_2})$. The following statements are equivalent.

(a) $(\mathcal{L},\mathcal{M}_p)$ has property reducibility.
(b) $(\mathcal{L},\mathcal{M}_p)$ has state separability.
(c) At least one of $\mathcal{L}_1$ and $\mathcal{L}_2$ is distributive.
(d) $(\mathcal{L},\mathcal{M}_p)$ has statistical property independence.
(e) The Clauser–Horne version of Bell's inequalities

$$m(\,h_1(a)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(b)\,)+m(\,h_1(c)\wedge h_2(d)\,)$$
$$m(\,h_1(a)\wedge h_2(d)\,)-m(\,h_1(c)\,)-m(\,h_2(b)\,)\leqslant 0 \tag{12}$$

hold for any $m\in\mathcal{M}_p$ and for any $a,\ c\in\mathcal{L}_1$ and $b,\ d\in\mathcal{L}_2$.

Or, equivalently, we have the following.

Corollary: Let $(\mathcal{L},\mathcal{M}_p)$ be a compound physical system of $(\mathcal{L}_1,\mathcal{M}_{p_1})$ and $(\mathcal{L}_2,\mathcal{M}_{p_2})$. The following statements are equivalent.
(a′) There exists a holistic property in $(\mathcal{L},\mathcal{M}_p)$.
(b′) There exists a nonseparable state in $(\mathcal{L},\mathcal{M}_p)$.
(c′) Both $\mathcal{L}_1$ and $\mathcal{L}_2$ are nondistributive.
(d′) There exists a nonlocal correlation in $(\mathcal{L},\mathcal{M}_p)$.
(e′) The Clauser–Horne version of Bell's inequalities (12) violate for some $m\in\mathcal{M}_p$ and for some $a,c\in\mathcal{L}_1$ and $b,d\in\mathcal{L}_2$.

The connections among distributivity of P-lattices, the separability and the Bell-type inequalities (12) are summarized as in Table I.

In conclusion, we would like to state the following two points.

(I) According to Pykacz and Santos,[14] it has been an open question whether Gisin's result[22] within the usual Hilbert-space formalism for quantum mechanics, which has shown that for any entangled state there are projectors violating Bell's inequalities, could be also obtained within lattice-theoretical approaches. Now, our results partially answer the question. That is, it follows

from our results that if the system has nonseparable states, there exists at least one pair of a state and elements violating Bell-type inequalities (12). Remark that it is still an open question whether for *any* nonseparable state there are elements violating inequalities (12).

(II) It is important to distinguish two type of nondistributivity (nonclassicality) of compound physical systems; one results from the case where only one of $\mathcal{L}_1$ and $\mathcal{L}_2$ is nonclassical. Another results from the case where both $\mathcal{L}_1$ and $\mathcal{L}_2$ are nonclassical. Only for the latter case the Bell-type inequalities (12) can be violated (see Table I). Therefore, *nonclassicality of a compound physical system by itself has nothing to do with whether Bell-type inequalities for the system are violated or not*. In order to see the relation, we need to refer to a whole construction of the system.

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Anisotropic scattering kernel: Generalized and modified Maxwell boundary conditions

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This article presents a model of a scattering kernel of boundary conditions for the Boltzmann equation. The proposed scattering kernel is based on an anisotropic accommodation argument. Three parameters equal to the momentum accommodation coefficients are shown as characterizing the influence of each direction. First the new scattering kernel is derived from a phenomenological criticism of the first form of the scattering kernel proposed by Maxwell; then the same result is established from an analytic approach based on the spectral nature of the linear integral operator associated to the scattering kernel problem. As a result, the model provides a correct form of scattering kernel to handle the influence of each direction in particle collisions with the wall. Finally independent accommodation of each internal mode is added to extend the model to the case of polyatomic gases. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1690491]

I. INTRODUCTION

The problem of writing good boundary conditions for the Boltzmann equation in rarefied gas flows is to find an operator called the scattering kernel in kinetic theory. The first known scattering kernel was proposed by Maxwell and is based on phenomenological argument.[1] However, in various situations this kernel fails to reproduce correctly the phenomena occurring at the wall.[2,3] Indeed the Maxwell boundary condition corresponds to an isotropic conception of the reflection at the wall; so, in this approach, the three velocity components are considered as equivalent in the accommodation process.

Another class of scattering kernel is the CL (*Cercignani–Lampis*) model by Cercignani *et al.*[3,4] The authors extend the research to a more general field of operators and obtain a more flexible model. However, as is well-known, this class of scattering kernels is not totally efficient to describe physically gas behavior close to the wall.[4] Moreover, some results in particle simulation of rarefied gas flows seem to show that none of the existing models of the scattering kernel can reproduce all the features of the real gas dynamics.[5]

Generally the existing models of the scattering kernel do not describe the interplay between the different degrees of freedom (i.e., the three velocity components of the particle and its internal energy modes) in interaction with the wall.[5] This would explain the partial inefficiency of these models to reproduce the behavior of high speed nonequilibrium flows near the wall. The main purpose of this article is to propose a new model of scattering kernel by considering more possible reflection types of particles at the wall. In this way we attempt to eliminate any isotropic character of momentum accommodation in the velocity reflection process, and we introduce three coefficients to take into account the influence of the velocity directions.

From Sec. II to Sec. VI, we consider only unstructured atom-like molecules. In Sec. II the basic conditions required for a scattering kernel are briefly analyzed and discussed. In Sec. III the Maxwell phenomenological argument is recalled and we present the new model. In Sec. IV we

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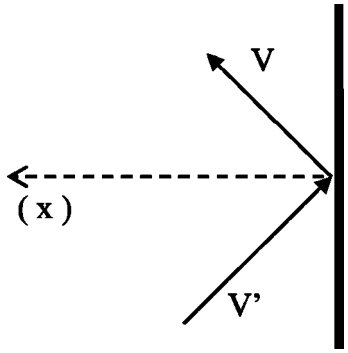

FIG. 1. Particle hitting the wall.

develop a consistent analytical approach to build the new scattering kernel. In Sec. V the coefficients introduced in the modeling are shown to equal the well known momentum accommodation coefficients. Finally, in Sec. VI the new kernel is involved in a more complete model characterizing molecules with internal modes by using a phenomenological derivation.

II. CONDITIONS REQUIRED FOR THE SCATTERING KERNELS

Let us consider a particle hitting the wall, as shown in Fig. 1. V' is the velocity of the impinging gas particle referred to the wall, $V'=(V'_x,V'_y,V'_z)\in\{\Omega'=\mathbb{R}_-\times\mathbb{R}\times\mathbb{R}\}$ and V is the velocity of the reflected one referred to the wall, $V=(V_x,V_y,V_z)\in\{\Omega=\mathbb{R}_+\times\mathbb{R}\times\mathbb{R}\}$. These velocities reduce to peculiar velocities when the slip velocity at the wall is neglected. V_R is defined as $V_R=(-V_x,V_y,V_z)$.

The kernel, $B(V',V)$, is the density of probability that a molecule impinging the wall at any point X of the wall with velocity V' is reflected at the same point with velocity V. This kernel, which turns the impinging particles at the wall into reflected ones, must satisfy some basic physical conditions. The least obvious of them is the reciprocity relation. This relation is a necessary condition for a good scattering kernel in the kinetic theory of gases.[6,7]

According to the scattering kernel probability density property, kernel $B(V',V)$ must satisfy

$$B(V',V)\geqslant 0 \quad , \tag{1}$$

and also the normalization condition

$$\int_\Omega B(V',V)d_V=1. \tag{2}$$

Finally, the balance of particles hitting the wall at position X and reflected with velocity V at a given time may be written[8]

$$V_x f(V)=\int_{\Omega'}|V'_x|f(V')B(V',V)d_{V'}, \tag{3}$$

where $f(V)$ is the gas particle distribution function given by the Boltzmann equation.

In the thermodynamic equilibrium state between the gas and the wall at the same temperature, the time reversibility assumption of the thermodynamic equilibrium state may be formulated as follows:[3,7,9] the number of gas particles which hit the wall during time t, with velocity V', and reflect with velocity V at position X of the wall, is equal to the number of particles with incident velocity $-V$ reflected with velocity $-V'$ at the same time t, at the same position X of the wall. This may be written

$$|V'_x| f_0(V') B(V', V) = |V_x| f_0(-V) B(-V, -V'), \tag{4}$$

where $f_0(V) = n/(C_w\sqrt{\pi})^3 e^{-\|V\|^2/C_w^2}$ is the Maxwellian distribution function of the gas in equilibrium state at the temperature of the wall. $C_w^2 = 2kT_w/m$, where T_w is the wall temperature, k is the Boltzmann constant, m is the molecular mass of gaseous particles and n is their numerical density. The time reversibility assumption means that all detailed balancing of energy exchange between the gas and the wall in the thermodynamic equilibrium state at any time t is equal to zero. This state of thermodynamic equilibrium between the gas and the wall at the same temperature is a reference state. Owing to this fact, any scattering kernel in kinetic theory must be validated by the property (4), called the reciprocity relation.

Note that the normalization condition (2) is equivalent to

$$\int_{\Omega'} B(-V, -V'_R) d_{V'} = 1.$$

From this remark, the reciprocity relation also leads to

$$\int_{\Omega'} |V'_x| f_0(V') B(V'_R, V) d_{V'} = |V_x| f_0(-V). \tag{4'}$$

It is also necessary to note that the required conditions formulated above characterize a physical situation at the wall involving the conservation of the particle flux and then a binary and short interaction between the solid atoms and gaseous particles.[9] So the model presented here excludes the gas dissociation and various steps involved in catalysis (chemical reaction at the wall, adsorption, etc.).

III. PHENOMENOLOGICAL APPROACH TO SCATTERING KERNELS

A. Maxwell scattering kernel

The first form of the scattering kernel proposed by Maxwell is given by

$$B_M(V', V) = (1-\alpha)\,\delta(V - V'_R) + \alpha \frac{2}{C_w^4 \pi} V_x e^{-\|V\|^2/C_w^2}. \tag{5}$$

$B_M(V', V)$ is a linear combination of two elementary kernels: the Dirac function for the specular reflection part and the exponential function for the diffuse reflection part at temperature T_w of the wall; α, called the accommodation coefficient, represents the weight of the diffusion in the gas collision process at the wall.

Before writing this scattering kernel Maxwell made several phenomenological comments on the nature of the surface in contact with the gas, which can be found in the appendix of Ref. 1. First, he assumed the surface to be a ''perfectly elastic smooth surface.'' Then each molecule striking the surface had its normal component reversed while the other components were not altered by the impact; the scattering kernel in this case was simply given by $\delta(V - V'_R)$. Second, he assumed the surface to be a perfectly absorbing surface so that each particle hitting the wall was absorbed before being reemitted, and the velocity of each reemitted particle was oriented from the surface towards the gas. But the probability of any particular magnitude and direction of its velocity would be the same as in a gas at rest in the thermal equilibrium state at the temperature of the wall; in this case, this led to the diffusive scattering kernel given by $(2/C_w^4\pi)\, V_x e^{-\|V\|^2/C_w^2}$.

Finally, Maxwell decided to consider the real reflecting surfaces as an intermediate surface between these two extreme perfect surfaces and then proposed the linear combination (5).

In our view, the scattering process on a real surface must be more complicated than those described by the sum of the scattering kernels of the two extreme perfect surfaces. It is easily seen that the two elementary scattering kernels written for the two perfect surfaces are isotropic ones;

this is reasonable for these two types of perfect surfaces. Then, using a linear combination of these two elementary scattering kernels, the result will still be an isotropic one, but we cannot be sure that a scattering kernel characterizing any real surface is an isotropic one. Moreover, in the kernel (5), the weight of the diffusion in any direction is represented by the same coefficient α: this description cannot be considered as correct, as pointed out by various authors.[2,10]

B. Our scattering kernel proposal

In order to write a general scattering kernel for any kind of real surface, we return to the investigation of various possible types of accommodation which can occur during a particle collision with the wall. Then we have to consider a more general type of accommodation than the isotropic one, in which of course the normal component of the incoming particle velocity must be reversed during the collision. We can thus assume elementary processes where diffusive and specular reflection are mixed: each of the velocity components can be altered or not by the wall independently of others. This argument leads us to consider the eight elementary operators listed below:

$$B_0(V',V)=\delta(V_x+V_x')\,\delta(V_y-V_y')\,\delta(V_z-V_z'), \tag{6a}$$

$$B_{yz}(V',V)=\frac{1}{\pi C_w^2}\,\delta(V_x+V_x')e^{-V_y^2/C_w^2}e^{-V_z^2/C_w^2},$$

$$B_{xz}(V',V)=\frac{2}{C_w^3\sqrt{\pi}}V_x\delta(V_y-V_y')e^{-V_x^2/C_w^2}e^{-V_z^2/C_w^2},$$

$$B_{xy}(V',V)=\frac{2}{C_w^3\sqrt{\pi}}V_x\delta(V_z-V_z')e^{-V_x^2/C_w^2}e^{-V_y^2/C_w^2},$$

$$B_{xyz}(V',V)=\frac{2}{\pi C_w^4}V_x e^{-V_x^2/C_w^2}e^{-V_y^2/C_w^2}e^{-V_z^2/C_w^2}, \tag{6b}$$

$$B_z(V',V)=\frac{1}{C_w\sqrt{\pi}}\,\delta(V_x+V_x')\,\delta(V_y-V_y')e^{-V_z^2/C_w^2},$$

$$B_y(V',V)=\frac{1}{C_w\sqrt{\pi}}\,\delta(V_x+V_x')\,\delta(V_z-V_z')e^{-V_y^2/C_w^2},$$

$$B_x(V',V)=\frac{2}{C_w^2}V_x\delta(V_y-V_y')\,\delta(V_z-V_z')e^{-V_x^2/C_w^2}.$$

It is easy to show that each of these elementary kernels satisfies positivity and normalization conditions. These kernels also satisfy the reciprocity relation (more details are given in Appendix A). The coefficients appearing in front of each operator are normalizing coefficients obtained by calculating $\int_\Omega B_\kappa(V',V)d_V$.

Each of these elementary kernels represents a particular possible situation of accommodation. Then the complete scattering kernel will be a linear combination of the elementary kernels in which the combination coefficients will represent the weight of each kind of accommodation at the wall. This complete scattering kernel may be written

$$B(V',V)=\sum_\kappa \mu_\kappa B_\kappa(V',V), \tag{7}$$

with

$$\sum_{\kappa} \mu_{\kappa} = 1. \tag{8}$$

If we introduce three coefficients, α_j $(j=1,2,3)$ satisfying $\alpha_j \in [0,1]$, to quantify the influence of each direction in a particle accommodation process by the wall, and taking into account condition (8), the coefficients μ_{κ} may be written

$$\begin{gathered}\mu_{xz} = \alpha_x \alpha_z (1-\alpha_y), \quad \mu_{xy} = \alpha_x \alpha_y (1-\alpha_z), \quad \mu_{yz} = \alpha_y \alpha_z (1-\alpha_x), \\ \mu_x = \alpha_x (1-\alpha_y)(1-\alpha_z), \quad \mu_{xyz} = \alpha_x \alpha_y \alpha_z, \quad \mu_0 = (1-\alpha_x)(1-\alpha_y)(1-\alpha_z), \\ \mu_y = \alpha_y (1-\alpha_x)(1-\alpha_z), \quad \mu_z = \alpha_z (1-\alpha_x)(1-\alpha_y).\end{gathered} \tag{9}$$

According to this last relationship, the complete scattering kernel (7) satisfies the positivity and the normalization properties. It obviously satisfies the reciprocity relation since the elementary kernels satisfy it.

It is clear that neglecting the elementary kernels with incomplete diffusion or incomplete specular reflection in the full scattering kernel (7), the result reduces to the sum of the kernels (6a) and (6b) which represents the Maxwell scattering kernel. Moreover, it is easy to show that the Maxwell boundary conditions give satisfactory results for values of α close to 1: indeed, if the gas is in a state very close to thermodynamic equilibrium at the temperature of the wall, the most important reflection is the reflection with complete accommodation in all directions.

In the following section, an analytical method to build the complete scattering kernel (7) is presented.

IV. ANALYTICAL FORMULATION OF THE NEW SCATTERING KERNEL

Let us consider the problem of finding operator $B(V',V)$, satisfying the conditions listed in Sec. II, and let us write the transformation

$$K(V,V') = [|V_x'| f_0(V')]^{1/2} [|V_x| f_0(V)]^{-1/2} B(V_R', V). \tag{10}$$

Since $f_0(V)$ is a known function, the problem of finding $B(V',V)$ is equivalent to finding $K(V,V')$. Instead of studying the problem in $K(V,V')$, we can study the linear integral associated operator A defined by the relation

$$A(\psi) = \int_{\Omega'} K(V,V') \psi(V') d_{V'}. \tag{11}$$

This integral operator is defined in the Hilbert space of square summable functions of V noted $L^2(\Omega)$ [i.e., $\psi(V) \in L^2(\Omega)$], where the scalar product is defined as follows:

$$\langle \psi, \varphi \rangle = \int_{\Omega} \psi(V) \varphi(V) d_V.$$

Therefore, the problem is reduced to an eigenvalue problem, and then to discussing the spectral nature of operator A.

It is to be noted that the above formulation of the scattering kernel problem, through the transformation (10), is especially convenient to solve the linearized form of the Boltzman equation (LBE).[11,12]

Assuming that the operator A has a purely discrete spectrum, its kernel $K(V,V')$ can be written

$$K(V,V')=\sum_{n=0}^{\infty}\lambda^n\psi^n(V)\psi^n(V'), \tag{12}$$

where $\psi^n(V)\in L^2(\Omega)$ is an eigenfunction of the operator A and λ^n is its corresponding eigenvalue. According to positivity and normalization conditions required in $B(V',V)$, the operator A must be non-negative and its eigenvalues satisfy $\lambda^n\in[0,1]$ for any $n\in\mathbb{N}$.

From now the eigenfunction $\psi^n(V)$ is assumed to be in the form

$$\psi_r(V_x)\psi_l(V_y)\psi_m(V_z)=\prod_{j=1}^{3}\psi_{k_j}(V_j).$$

Since the eigenfunction $\psi^n(V)$ is a square summable function, we have $\psi_{k_j}(V_j)\in L^2(\Omega_j)$, where Ω_j denotes the scalar space associated to V_j. Moreover, the family of the function set $\psi_{k_j}(V_j)$, $k_j\in\mathbb{N}$, must be a function basis of the Hilbert space $L^2(\Omega_j)$ [note that this assumption will lead immediately to the coming property (16)]. The eigenvalues of operator A become λ_{rlm}, and we can assume $\lambda_{rlm}=\lambda_r\lambda_l\lambda_m$, in respect to the respective scalar products in the different Hilbert spaces $L^2(\Omega_j)$ and $L^2(\Omega)$. Finally, the expression (12) can be replaced by

$$K(V,V')=\sum_{r,l,m}\lambda_r\lambda_l\lambda_m\psi_r(V_x)\psi_l(V_y)\psi_m(V_z)\psi_r(V_x')\psi_l(V_y')\psi_m(V_z'). \tag{13}$$

The sum in the right member of (13) can be written as the product of three infinite sums:

$$K(V,V')=\prod_{j=1}^{3}\sum_{k=0}^{\infty}\lambda_{k_j}\psi_{k_j}(V_j)\psi_{k_j}(V_j'). \tag{14}$$

Let us put

$$\psi_{0_x}(V_x)=\frac{\sqrt{2}}{C_w}|V_x|^{1/2}e^{-V_x^2/2C_w^2},$$

$$\psi_{0_y}(V_y)=(C_w\sqrt{\pi})^{-1/2}e^{-V_y^2/2C_w^2},$$

$$\psi_{0_z}(V_z)=(C_w\sqrt{\pi})^{-1/2}e^{-V_z^2/2C_w^2}.$$

Each of $\psi_{0_j}(V_j)$ functions satisfies

$$\|\psi_{0_j}(V_j)\|_j^2=\int_{\Omega_j}[\psi_{0_j}(V_j)]^2dV_j=1.$$

From the relation $(4')$, it may be deduced that the function $\psi^0(V)=\psi_{0_x}(V_x)\psi_{0_y}(V_y)\psi_{0_z}(V_z)$ is an eigenfunction of operator A, associated to eigenvalue $\lambda_{0_x}\lambda_{0_y}\lambda_{0_z}=1$ (see demonstration in Appendix B). This first eigenfunction takes an important part in the solution of the problem because it corresponds to the maximal eigenvalue of A, and so leads to an equilibrium state. Indeed, in the equilibrium state between the gas and the wall, the most physically convenient scattering kernel is the complete accommodation kernel, which is assigned here to $\psi^0(V)$. Therefore any good model of a scattering kernel must converge to this equilibrium scattering kernel. This point matches the basic assumption founding the reciprocity relation which is that any scattering kernel must be valid when a thermodynamic equilibrium exists between the gas and the wall.

In agreement with the concept of three distinguishable degrees of freedom in the reflection process, we introduce three coefficients α_j, related to the set of eigenvalues by $\lambda_{0_j}=1$ and $\lambda_{k_j}=(1-\alpha_j)$ for $k\neq 0$ with $\alpha_j\in[0,1]$; relation (14) becomes

$$K(V,V')=\prod_{j=1}^{3}\left(\psi_{0_j}(V_j)\psi_{0_j}(V_j')+(1-\alpha_j)\sum_{k=1}^{\infty}\psi_{k_j}(V_j)\psi_{k_j}(V_j')\right), \tag{15}$$

which may be rewritten

$$K(V,V')=\prod_{j=1}^{3}\left(\alpha_j\psi_{0_j}(V_j)\psi_{0_j}(V_j')+(1-\alpha_j)\sum_{k=0}^{\infty}\psi_{k_j}(V_j)\psi_{k_j}(V_j')\right).$$

Finally, by using the following property,

$$\sum_{k=0}^{\infty}\psi_{k_j}(V_j)\psi_{k_j}(V_j')=\delta(V_j-V_j'), \tag{16}$$

we obtain the result

$$K(V,V')=\prod_{j=1}^{3}\left(\alpha_j\psi_{0_j}(V_j)\psi_{0_j}(V_j')+(1-\alpha_j)\,\delta(V_j-V_j')\right). \tag{17}$$

By developing the product (17) we obtain $K(V,V')$ as a sum of elementary operators as follows:

$$K(V,V')=\sum_{\kappa}\mu_\kappa K_\kappa(V,V'), \tag{18}$$

where μ_κ is given again by the relations (9) of Sec. III, and where the elementary operators $K_\kappa(V,V')$ are written below:

$$\begin{aligned}
K_0(V,V')&=\delta(V_x-V_x')\,\delta(V_y-V_y')\,\delta(V_z-V_z'),\\
K_{yz}(V,V')&=\frac{1}{\pi C_w^2}\,\delta(V_x-V_x')e^{-V_y^2/2C_w^2}e^{-V_z^2/2C_w^2}e^{-V_y'^2/2C_w^2}e^{-V_z'^2/2C_w^2},\\
K_{xz}(V,V')&=\frac{2}{C_w^3\sqrt{\pi}}|V_xV_x'|^{1/2}\delta(V_y-V_y')e^{-V_x^2/2C_w^2}e^{-V_z^2/2C_w^2}e^{-V_x'^2/2C_w^2}e^{-V_z'^2/2C_w^2},\\
K_{xy}(V,V')&=\frac{2}{C_w^3\sqrt{\pi}}|V_xV_x'|^{1/2}\delta(V_z-V_z')e^{-V_x^2/2C_w^2}e^{-V_y^2/2C_w^2}e^{-V_x'^2/2C_w^2}e^{-V_y'^2/2C_w^2},\\
K_{xyz}(V,V')&=\frac{2}{\pi C_w^4}|V_xV_x'|^{1/2}e^{-V_x^2/2C_w^2}e^{-V_y^2/2C_w^2}e^{-V_z^2/2C_w^2}e^{-V_x'^2/2C_w^2}e^{-V_y'^2/2C_w^2}e^{-V_z'^2/2C_w^2},\\
K_z(V,V')&=\frac{1}{C_w\sqrt{\pi}}\,\delta(V_x-V_x')\,\delta(V_y-V_y')e^{-V_z^2/C_w^2}e^{-V_z'^2/C_w^2},\\
K_y(V,V')&=\frac{1}{C_w\sqrt{\pi}}\,\delta(V_x-V_x')\,\delta(V_z-V_z')e^{-V_y^2/2C_w^2}e^{-V_y'^2/2C_w^2},
\end{aligned} \tag{19}$$

$$K_x(V,V')=\frac{2}{C_w^2}|V_xV_x'|^{1/2}\delta(V_y-V_y')\,\delta(V_z-V_z')e^{-V_x^2/2C_w^2}e^{-V_x'^2/2C_w^2}.$$

It is easy to verify that the elementary operators $K_\kappa(V,V')$ given above correspond to the elementary kernels $B_\kappa(V',V)$ given in Sec. III, through transformation (10); so the complete operator $K(V,V')$ obtained from relation (18) corresponds exactly to the scattering kernel given by relation (7).

Referring now directly to Eqs. (15) and (13), it is clear that our choice corresponds to a spectral expansion of $K(V,V')$ involving eight different eigenvalues, namely, 1, $(1-\alpha_x)$, $(1-\alpha_y)$, $(1-\alpha_z)$, $(1-\alpha_x)(1-\alpha_y)$, $(1-\alpha_x)(1-\alpha_z)$, $(1-\alpha_y)(1-\alpha_z)$,$(1-\alpha_x)(1-\alpha_y)\times(1-\alpha_z)$. Of course this choice also corresponds to a degeneracy of the eigenfunction space associated to each eigenvalue, except for the maximum eigenvalue; therefore, as shown above, it is not necessary to specify the eigenfunctions.

As is well known, the classical CL model and its extensions by Lord[13,14] to polyatomic molecules are derived from another procedure based on a more general relation:[12]

$$K(V,V')=\sum_{n,m=0}^{\infty}\lambda^{nm}\varphi^n(V)\varphi^m(V'), \tag{20}$$

where the φ^k function is specified. As it can be seen, kernels built on this general form could not automatically insure the properties listed above for good scattering kernels (i.e., positivity, normalization, and reciprocity properties).[12] Moreover, in these CL scattering kernel models the normal and the tangential components of the velocity of the molecule colliding with the wall are considered as independent, and then the scattering kernel is written separately in normal and tangential parts. This aspect of the CL models was recently criticized as not allowing interplay between the various components of the impinging particle velocity.[5]

V. RELATIONS WITH ACCOMMODATION COEFFICIENTS

In this section the physical meaning of the parameters involved in the kernel is clarified. So doing, we prove that the α_j coefficients respectively equal the accommodation coefficients β_j of the momentum components.

First μ_κ may be easily shown to represent the weight of particles reflected according to the process κ in the flux of reflected particles. This property appears obvious when integrating the two members of Eq. (3) over the reflected velocity range, using $B(V',V)$ expressions given in relations (7) and (9). Moreover, the scattering is built using three independent coefficients α_j: then it can be seen that taking into account condition (8), the μ_κ coefficients are necessarily given by relations (9).

On the other hand, the momentum accommodation coefficients β_j are defined as[9]

$$\beta_j=\frac{\Phi_j^- -\Phi_j^+}{\Phi_j^- -\Phi_j^e}. \tag{21}$$

where Φ_j^- is the incoming flux at the wall of the momentum j component, Φ_j^+ is the corresponding reflected flux, and Φ_j^e is the reflected flux in the hypothetical situation of perfect accommodation to the wall. These various momentum fluxes may be written for each component:

$$\Phi_j^-=\int_{\Omega'}m|V_x'|V_j'f^-(V')d_{V'},$$
$$\Phi_j^+=\int_{\Omega}m|V_x|V_jf^+(V)d_V, \tag{22}$$

where $f^-(V)$ and $f^+(V)$ are respectively the incident and the reflected distribution function. Remembering that $f^+(V)$ is given by (3) and using expression (7) of $B(V',V)$, Φ_j^+ is written

$$\Phi_j^+ = \int_{\Omega'} m|V_x'| f^-(V') \sum_\kappa \mu_\kappa \left(\int_\Omega V_j B_\kappa(V',V) d_V \right) d_{V'} . \tag{23}$$

And Φ_j^e for total perfect accommodation (i.e., $\alpha_x = \alpha_x = \alpha_x = 1$) is written

$$\Phi_j^e = \int_{\Omega'} m|V_x'| f^-(V') \left(\int_\Omega V_j B_{xyz}(V',V) d_V \right) d_{V'} . \tag{24}$$

A. Calculation of β_y and β_z

First the case $V_j = V_y$ is dealt with.

According to the expression of $B_{xyz}(V',V)$, $V_y B_{xyz}(V',V)$ is an odd function of the V_y component, therefore,

$$\int_\Omega V_y B_{xyz}(V',V) d_V = 0$$

and then $\Phi^e = 0$, so we can write

$$\beta_y = 1 - \frac{\Phi_y^+}{\Phi_y^-}.$$

On the other hand, looking at relation (23), the contribution of each partial kernel $B_\kappa(V',V)$ in Φ_y^+ expression can be estimated separately by

$$\int_\Omega V_y B_\kappa(V',V) d_V .$$

Each of these partial integrals can be calculated easily and give for any κ either 0 or V_y'. As a result we obtain

$$\sum_\kappa \mu_\kappa \int_\Omega V_y B_\kappa(V',V) d_V = V_y'(\mu_0 + \mu_x + \mu_z + \mu_{xz}),$$

and

$$\Phi_j^+ = (\mu_0 + \mu_x + \mu_z + \mu_{xz}) \Phi_j^- .$$

It results directly that

$$\beta_y = 1 - (\mu_0 + \mu_x + \mu_z + \mu_{xz}),$$

which, according to the normalization condition (8), is also equal to

$$\beta_y = \mu_y + \mu_{xy} + \mu_{yz} + \mu_{xyz} . \tag{25}$$

Similarly we obtain for β_z

$$\beta_z = \mu_z + \mu_{xz} + \mu_{yz} + \mu_{xyz} . \tag{26}$$

By using the μ_κ expressions given by relations (9), Eqs. (25) and (26) lead to

$$\beta_y = \alpha_y \tag{27}$$

and

$$\beta_z = \alpha_z. \tag{28}$$

B. Calculation of β_x

Now $V_j = V_x$ is considered.

Using the same definition of the various fluxes with respect to the sign of the incident flux, we can write

$$\Phi_x^- = \int_{\Omega'} m V_x'^2 f^-(V') d_{V'}. \tag{29}$$

The calculation of the partial integrals involved in relation (23),

$$\int_\Omega V_x B_\kappa(V', V) d_V,$$

gives in this case either $-V_x'$ or $C_w\sqrt{\pi}/2$ for any κ. As a result we obtain

$$\sum_\kappa \mu_\kappa \int_\Omega V_x B_\kappa(V', V) d_V = -V_x'(\mu_0 + \mu_y + \mu_z + \mu_{yz}) + \frac{C_w\sqrt{\pi}}{2}(\mu x + \mu_{xy} + \mu_{xz} + \mu_{xyz}).$$

Using the flux expressions (29) and (23), this result leads to

$$\Phi_x^- - \Phi_x^+ = (1 - (\mu_0 + \mu_y + \mu_z + \mu_{yz}))\Phi_x^- - \frac{C_w\sqrt{\pi}}{2}(\mu_x + \mu_{xy} + \mu_{xz} + \mu_{xyz}) \int_{\Omega'} m|V_x'| f^-(V') d_{V'}.$$

We also have

$$\int_\Omega V_x B_{xyz}(V', V) d_V = \frac{C_w\sqrt{\pi}}{2}$$

and so

$$\Phi_x^- - \Phi_x^e = \Phi_x^- - \frac{C_w\sqrt{\pi}}{2} \int_{\Omega'} m|V_x'| f^-(V') d_{V'}.$$

Consequently, remembering condition (8), it results that

$$\beta_x = \mu_x + \mu_{xy} + \mu_{xz} + \mu_{xyz}. \tag{30}$$

Replacing μ_κ by relations (9) once more, the result shows

$$\beta_x = \alpha_x.$$

The classical Maxwell model predicted the same value of the various accommodation coefficients.[9] However it is well-known, notably from the measurements of accommodation coefficients by various procedures,[15–17] that these coefficients do not have the same value; and this description of equivalent accommodation is not physically consistent.[18] In the new model we can see that the three parameters introduced in the theoretical modelling equal the three accommodation coefficients of momentum component fluxes which are basically different.

VI. EXTENSION OF THE NEW MODEL TO POLYATOMIC GASES

In polyatomic gases the internal state of a molecule is characterized by the rotational and vibrational energies, E_{ir} and E_{iv}, and depends on quantum numbers ir and iv. In addition, because of the degeneracy of rotational levels, a weight factor ($g_{ir}=2ir+1$) is involved in the distribution function expression. The distribution functions of impinging and emerging particles are linked by the following relation [generalizing relation (3)]:[9,19]

$$V_x f_i^+(V,E_{ir},g_{ir},E_{iv}) = \sum_{ir',iv'} \int_{\Omega'} |V_x'| f^-(V',E_{ir'},g_{ir'},E_{iv'}) P_G(V',E_{ir'},g_{ir'},E_{iv'},V,E_{ir},g_{ir},E_{iv}) d_{V'}, \tag{31}$$

where $P_G(V',E_{ir'},g_{ir'},E_{iv'},V,E_{ir},g_{ir},E_{iv})$ is the generalized scattering kernel for molecules considered with internal modes. Of course normalization and non-negative conditions are easily generalized to

$$\sum_{ir,iv} \int_{\Omega} P_G(V',E_{ir'},g_{ir'},E_{iv'},V,E_{ir},g_{ir},E_{iv}) d_V = 1 \tag{32}$$

and

$$P_G(V',E_{ir'},g_{ir'},E_{iv'},V,E_{ir},g_{ir},E_{iv}) \geqslant 0. \tag{33}$$

Furthermore, for the reciprocity condition, we admit the form given by Kuscer[9] which, excluding external magnetic fields, assumes the form

$$\begin{aligned} &|V_x'| e^{-\|V'\|^2/C_w^2} e^{-\varepsilon_{ir'}} e^{-\varepsilon_{iv'}} (2ir'+1) P_G(V',E_{ir'},E_{iv'},V,E_{ir},E_{iv}) \\ &\quad = V_x e^{-\|V\|^2/C_w^2} e^{-\varepsilon_{ir}} e^{-\varepsilon_{iv}} (2ir+1) P_G(-V,E_{ir},E_{iv},-V',E_{ir'},E_{iv'}), \end{aligned} \tag{34}$$

with

$$\varepsilon_{ir} = \frac{E_{ir}}{kT_w}, \quad \varepsilon_{iv} = \frac{E_{iv}}{kT_w}. \tag{35}$$

Reference 19 presents, phenomenologically, a scattering kernel P characterizing the interaction of diatomic molecules with internal modes at the wall (this kernel P is recalled in Appendix C). In kernel P the translation mode was taken as a whole (without interplay between the three translational degrees of freedom), so, when applied to unstructured molecules, P reduced to a classical Maxwell kernel. Nevertheless, a partial accommodation concept was employed in the P derivation allowing different accommodations of the various modes (translation, rotation, vibration). In fact, this concept was analogous to those used in the new model to disconnect the three translation degrees in the accommodation process. From Ref. 19, P may be immediately rewritten:

$$\begin{aligned} P = &\left((1-\alpha_\theta)\delta(V-V_R') + \alpha_\theta \frac{2}{C_w^4 \pi} V_x e^{-V^2/C_w^2} \right) ((1-\alpha_r)(1-\alpha_v)\tilde{P}_0 + \alpha_v(1-\alpha_r)\tilde{P}_v \\ &+ \alpha_r(1-\alpha_v)\tilde{P}_r + \alpha_v\alpha_r\tilde{P}_{rv}), \end{aligned} \tag{36}$$

where α_θ, α_v and α_r are real parameters independent of the microscopic state of the molecules and are considered in [0,1], and

$$\tilde{P}_0=\delta(E_{ir'}-E_{ir})\,\delta(E_{iv'}-E_{iv})\ , \quad \tilde{P}_{rv}=\frac{e^{-\varepsilon_{ir}}}{Q_r}(2i_r+1)\,\frac{e^{-\varepsilon_{iv}}}{Q_v},$$

$$\tilde{P}_v=\delta(E_{ir'}-E_{ir})\,\frac{e^{-\varepsilon_{iv}}}{Q_v}\ , \quad \tilde{P}_r=\frac{e^{-\varepsilon_{ir}}}{Q_r}(2ir+1)\,\delta(E_{iv'}-E_{iv}).$$

The quantities Q_v and Q_r involved in $\tilde{P}_\chi$ $(\chi=v,r,rv)$ are the partition functions defined at the wall temperature:

$$Q_r=\sum_{iv}\ (2ir+1)e^{-\varepsilon_{ir}}\ , \quad Q_v=\sum_{iv}\ e^{-\varepsilon_{iv}}.$$

Now, in operator P in (36), let us replace the first parenthesis corresponding to the classical Maxwell scattering kernel by the new kernel proposed in relation (7) and (9). So a general scattering kernel is obtain in the form

$$P_G=\left(\sum_\kappa\ \mu_\kappa^* B_\kappa(V',V)\right)((1-\alpha_r)(1-\alpha_v)\tilde{P}_0+\alpha_v(1-\alpha_r)\tilde{P}_v+\alpha_r(1-\alpha_v)\tilde{P}_r+\alpha_v\alpha_r\tilde{P}_{rv}), \tag{37}$$

where the μ_κ^* are expressed by relations (9) using the directional parameters α_x^*, α_y^*, and α_z^*. The superscript $(*)$ is used to indicate that the physical meaning of the three parameters is not yet shown in the polyatomic modeling frame.

Considering the properties of its parts, P_G visibly satisfies the normalization and nonnegativity conditions. Furthermore, P_G is a sum of partial operators assuming the factorized form $\tilde{P}_\chi B_\kappa$ (where χ refers to the internal accommodation process). It is clear that the B_κ satisfying condition (4) implies that $\tilde{P}_\chi B_\kappa$ satisfies the generalized reciprocity condition (34). Consequently, P_G also satisfies (34) as a linear combination of $\tilde{P}_j B_\kappa$ terms. So a good anisotropic scattering kernel P_G has been obtained phenomenologically.

Furthermore, in relation (37) the part in the first parenthesis of the second member concerns the translation mode. Introducing into it α_θ defined as $\alpha_\theta=1-\mu_0^*=\Sigma_{\kappa\neq 0}\mu_\kappa^*$, this part assumes the form

$$P_G=(1-\alpha_\theta)\,\delta(V-V_R')+\alpha_\theta\sum_{\kappa\neq 0}\ \lambda_\kappa^* B_\kappa(V',V), \tag{38}$$

where

$$\lambda_\kappa^*=\frac{\mu_\kappa^*}{\alpha_\theta}, \quad \sum_{\kappa\neq 0}\ \lambda_\kappa^*=1. \tag{39}$$

In this last form the complete specular reflection appears separately from all the processes in which partial or complete accommodation occurs.

Integrating on velocity and summing over quantum numbers on the left and right sides of Eq. (31), it is easily shown that μ_κ^* represents (as μ_κ for the unstructured molecules) the part of the particle flux reflected according to the directional process κ. The analytical systematic derivation of P_G and further physical interpretation of α_x^*, α_y^*, α_z^*, α_v, α_r, and α_θ will be presented in a subsequent study.

Regarding now the process from the point of view of energy transfer, the comments given in Ref. 19 can be extended. The thermal kinetic energy of the particle flow may be exchanged in collisions at the wall: at the statistical level the specular kernels reflect the effect of elastic collisions at the wall for the translational mode, while diffusive kernels represent the effects of inelastic collisions for this same mode. In the present model the influence of these inelastic

collisions is considered independently for each translational degree (i.e., for each direction). Statistically the scattered distribution function is no longer accommodated in the same way according to the normal and tangential directions: and on the microscopic level this means that the kinetic energy transfers of an impinging molecule change according to its velocity direction with respect to the wall.

In the same manner the three energy modes may interplay when exchanging energy at the wall, and, so, in operators $\tilde{P}_0$, $\tilde{P}_r$, $\tilde{P}_v$, and $\tilde{P}_{rv}$ the effects of elastic or inelastic collisions for each internal mode appear independently.

VII. DISCUSSION

The new model proposed in this article presents many aspects which allow realistic gas surface interactions to be described. First, the model takes into account the anisotropic effects in the interacting process at the wall. This anisotropic character of the surface derives basically from its physical properties and/or from its suitable treatment. Consequently the real physical properties of the wall are embedded in the three accommodation coefficients of the momentum components. Existing models rarely involve three directional parameters as the present model does: the former approaches using a three parameter representation[2,20] are based on the suggestion of a shifted Maxwellian to describe the reemitted distribution function of a monatomic gas from a solid surface and the parameters are arbitrary constants.[21] Here the new model gives an anisotropic description of the interaction in the sense employed by Kuscer[9] i.e., the new kernel operator is no longer invariant under rotation about the normal axis at the solid surface; moreover, in the new model the parameters are shown to be the accommodation coefficients themselves so it is possible to relate them to physical measurements.[15–18,22] In addition, in polyatomic cases, the present model allows independent accommodation processes at the wall for the various energy modes which seems a realistic description if, for example, the very different situations occurring at the wall for vibrational or translational accommodation are kept in mind.[23,24] Then, it is to be noted that the present model also appears as an improvement with respect to two well-known criticisms opposed to the methods based on the scattering kernel concept. The first criticism formulated by Cercignani[3] concerns the Maxwellian-type kernel: for a given monochromatic beam this model predicts a sharp maximum in the number of molecules at the angle corresponding to specular reflection, which is contradicted by experiments;[25] it is clear that this maximum is smoothed in the new model [see relation (38)]. The second criticism recently formulated by Bruno *et al.*,[5] is not completely justified because it is based, in a part, on studies of reactive or dissociated flows, and, as is well-known, the scattering kernel modeling cannot give correct results in such a case because of the assumption of the wall impermeability involved in it. But, on the other hand, the comments of the authors requiring the introduction of interplay between the velocity directions and the various energy modes is, in our opinion, completely justified. In the present model, precisely such an interplay is present, and the separating procedure of velocity components, which appears in the CL models[3] (also when extended to internal modes[13,14,26]) is not employed here.

A final argument in defense of the new model is its simplicity: as seen above the physical interpretation of the various parts of the kernel is straightforward. Moreover, the model is easy-to-use: first the calculations are simplified because the kernel only depends on the reflected microscopic space parameters; then, from the account of different kinds of accommodation of the moment components a preponderant weight can be given to a particular accommodation process, so the model may be easily simplified according to the geometrical symmetry or the physical conditions of the problem.

VIII. CONCLUDING REMARKS

We have derived an anisotropic model of a scattering kernel. For the unstructured molecules, three directional parameters involved in the model have been shown to be equal to the accommodation coefficients of the fluxes of the momentum components at the wall.

We have also extended the new model to polyatomic structured molecules. In this domain only a phenomenological derivation has been presented. The corresponding analytical method and further calculations to relate parameters α_x^*, α_y^*, α_z^*, α_v, α_r, α_θ to the accommodation coefficients β_j of momentum fluxes and to accommodation coefficients of the energy fluxes will be presented in a subsequent study. These relationships are not expected to be very simple, especially because the constant parameters introduced in the model refer to direct exchanges between each molecular mode and the wall, while the energy accommodation coefficients involve direct exchange with the wall for each mode and also intermode exchanges. Finally, even if not yet confirmed in applications, many arguments have been developed, showing the consistency, physical pertinence and usefulness of the new scattering kernel.

APPENDIX A: $B_\kappa(V',V)$ SATISFIES THE RECIPROCITY RELATION

The property for operator B_{zy} is demonstrated. For the rest of the operators the demonstrations are similar:

$$|V_x'| f_0(V') B_{zy}(V',V) = |V_x'| \frac{n}{(C_w\sqrt{\pi})^3} e^{-\|V'\|^2/C_w^2} \frac{1}{\pi C_w^2} \delta(V_x + V_x') e^{-V_y^2/C_w^2} e^{-V_z^2/C_w^2},$$

and

$$|V_x| f_0(-V) B_{zy}(-V,-V') = |V_x| \frac{n}{(C_w\sqrt{\pi})^3} e^{-\|V\|^2/C_w^2} \frac{1}{\pi C_w^2} \delta(V_x + V_x') e^{-V_y'^2/C_w^2} e^{-V_z'^2/C_w^2}.$$

In these two expressions, there appear the same terms in y and z; the full equality of both the expressions comes from the property of the Dirac function.

APPENDIX B: ψ^0 AS AN EIGENFUNCTION OF OPERATOR A

$$A(\psi^0) = \int_{\Omega'} [|V_x'| f_0(V')]^{1/2} [|V_x| f_0(V)]^{-1/2} B(V_R', V) \psi^0(V') dV'.$$

Replacing ψ^0 and $f_0(V)$ by their expression in this integral: $\psi^0 = (\sqrt{2}/C_w^2\sqrt{\pi})\,|V_x|^{1/2} e^{-\|V\|^2/2C_w^2}$ and $f_0(V) = (n/(C_w\sqrt{\pi})^3)\, e^{-\|V\|^2/C_w^2}$, it is found

$$A(\psi^0) = \frac{\sqrt{2}}{C_w^2\sqrt{\pi}} \int_{\Omega'} |V_x|^{-1/2} |V_x'| e^{\|V\|^2/2C_w^2} e^{-\|V'\|^2/C_w^2} B(V_R', V) dV'.$$

The reciprocity relation $(4')$ leads to

$$\int_{\Omega'} |V_x'| e^{-\|V'\|^2/C_w^2} B(V_R', V) dV' = |V_x| e^{-\|V\|^2/C_w^2},$$

and, consequently,

$$A(\psi^0) = \frac{\sqrt{2}}{C_w^2\sqrt{\pi}} |V_x|^{1/2} e^{-\|V\|^2/2C_w^2} = \psi^0.$$

APPENDIX C: KERNEL OPERATOR OF REF. 19

The full scattering kernel of Ref. 19 is given by

$$P=(1-\alpha_\theta)(1-\alpha_r)(1-\alpha_v)P_1+(1-\alpha_\theta)(1-\alpha_r)\alpha_v P_2+(1-\alpha_\theta)\alpha_r(1-\alpha_v)P_3+(1-\alpha_\theta)$$
$$\times\alpha_r\alpha_v P_4+\alpha_\theta(1-\alpha_r)(1-\alpha_v)P_5+\alpha_\theta\alpha_r(1-\alpha_v)P_6+\alpha_\theta(1-\alpha_r)\alpha_v P_7+\alpha_\theta\alpha_r\alpha_v P_8,$$

where $\alpha_\theta,\alpha_r,\alpha_v$ are real parameters independent of the microscopic state of the molecules. The specular operators with elastic and inelastic parts for each internal mode are given by

$$P_1=\delta(V'-V_R)\quad\delta(E'_{ir}-E_r)\,\delta(E'_{iv}-E_v),$$

$$P_2=\delta(V'-V_R)\quad\delta(E'_{ir}-E_r)\,\frac{e^{-\varepsilon_{iv,w}}}{Q_{v,w}},$$

$$P_3=\delta(V'-V_R)\,\frac{e^{-\varepsilon_{ir,w}}}{Q_{r,w}}(2ir+1)\,\delta(E'_{iv}-E_v),$$

$$P_4=\delta(V'-V_R)\,\frac{e^{-\varepsilon_{ir,w}}}{Q_{r,w}}(2ir+1)\,\frac{e^{-\varepsilon_{iv,w}}}{Q_{v,w}}.$$

The diffusive operators with elastic and inelastic parts, for each internal mode, are given by

$$P_5=\frac{2}{\pi C_w^4}V_x e^{-v_w^2}\delta(E_{ir}-E'_{ir})\,\delta(E_{iv}-E'_{iv}),$$

$$P_6=\frac{2}{\pi C_w^4}V_x e^{-v_w^2}\frac{e^{-\varepsilon_{ir,w}}}{Q_{r,w}}(2ir+1)\,\delta(E_{iv}-E'_{iv}),$$

$$P_7=\frac{2}{\pi C_w^4}V_x e^{-v_w^2}\delta(E_{ir}-E'_{ir})\,\frac{e^{-\varepsilon_{iv,w}}}{Q_{v,w}},$$

$$P_8=\frac{2}{\pi C_w^4}V_x e^{-v_w^2}\frac{e^{-\varepsilon_{ir,w}}}{Q_{r,w}}(2ir+1)\,\frac{e^{-\varepsilon_{iv,w}}}{Q_{v,w}},$$

with

$$\frac{1}{C_w^4}=\left(\frac{m}{2kT_w}\right)^2.$$

In Ref. 19, E_r and E_v defined as mean energy per molecule have been used by error. The correct parameters to use anywhere in this reference are E_{ir} and E_{iv}.

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On the discrete spectrum of non-self-adjoint Schrödinger differential equation with an operator coefficient

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We study the discrete part of spectrum of a singular non-self-adjoint second-order differential equation on a semiaxis with an operator coefficient. Its boundedness is proved. The result is applied to the Schrödinger boundary value problem $-\Delta u + q(x)u = \lambda^2 u$, $u|_{\partial D} = 0$, with a complex potential $q(x)$ in an angular domain. [DOI: 10.1063/1.1695446]

I. INTRODUCTION

As is known, the Schrödinger problem with a complex potential appeared in the theory of quantum mechanical systems with dissipative energy (see Refs. 1 and 9). As for non-self-adjoint operators, they arose, in general, of studying nonclosed physical systems (see Refs. 5 and 9; for details we refer to Refs. 4 and 6). In this paper we study the discrete part of spectrum of the non-self-adjoint operator L_α, generated in the Hilbert space $L_2((0,\infty),l_2)$ by the expression

$$L_\alpha u = -\frac{d^2u}{dx^2} + \frac{\beta(\alpha)}{x^2}u + Q(x)u$$

and the boundary condition

$$u(0) = 0,$$

where

$$\beta(\alpha) = \left\{\left(\left(\frac{k\pi}{\alpha}\right)^2 - \frac{1}{4}\right)\delta_{kj}\right\}, \quad k,j = 1,2,..., \quad Q(x) = \{q_{jk}(x)\}_{j,k=1}^{\infty},$$

$v_k = k\pi/\alpha \notin Z$ $(k = 1,2,...)$, $q_{jk}(x) = q_{kj}(x)$ is a complex-valued function, $Q(x)$, $x \in [0,\infty)$, is an l_2-valued function such that $\|Q(x)\| \leqslant Ce^{-\epsilon x}$ with some $\epsilon > 0$ [$\|Q(x)\|$ denotes the norm of the operator $Q(x)$ acting in the space l_2].

In the case where $\beta(\alpha) = \{l(l+1)\delta_{lj}\}$, $l = 0,1,2,...$, the spectrum of L_α was investigated, and the expansions in its eigenfunctions were obtained (see Ref. 7). Using the general spectral theory of self-adjoint operators, the expansions in eigenvectors of L_α were studied in Ref. 3 for $q_{kj}(x) = \overline{q}_{jk}(x)$, $\beta(\alpha) = \{l_j(l_j+1)\delta_{jk}\}$, where the numbers $l_j \geqslant 0$ are such that $\lim_{j\to\infty} l_j = \infty$. In this case the operator L_α is self-adjoint in the space $L_2((0,\infty),l_2)$. But in the situation under consideration L_α is non-self-adjoint, and there is no a general theory to investigate its spectrum. Therefore we start from studying the characteristic properties of L_α.

In what follows we denote by $L_{2,\epsilon}((0,\infty),l_2)$ the set of l_2-valued vector functions $f(x) = (f_1(x),f_2(x),\ldots,f_n(x),\ldots)$, strongly measurable on $[0,\infty)$ and satisfying the condition

$$\int_0^\infty \|f(x)\|^2 e^{-\epsilon x}dx=\int_0^\infty \sum_{j=1}^\infty |f_j(x)|^2 e^{-\epsilon x}dx<\infty.$$

The set $L_{2,\epsilon}=L_{2,\epsilon}((0,\infty),l_2)$ is a separable Hilbert space with respect to the inner product

$$(f,g)=\int_0^\infty (f(x),g(x))^2 e^{-\epsilon x}dx$$

[here $(f(x),g(x))$ denotes the inner product in l_2]. We also set $L_{2,0}((0,\infty),l_2)=L_2((0,\infty),l_2)$.

II. INVESTIGATION OF THE DISCRETE PART OF SPECTRUM

Let L_0 be the operator defined in $L_2((0,\infty),l_2)$ by the differential expression

$$L_0u=-\frac{d^2u}{dx^2}+\frac{\beta(\alpha)}{x^2}u$$

and the boundary condition

$$u(0)=0.$$

It is obvious that the operator L_0 is self-adjoint.

By $G_\alpha(\tau,t,\lambda)$ we mean the resolvent kernel of the operator L_α:

$$G_\alpha(\tau,t,\lambda)=\frac{\pi}{2i}\sqrt{\tau t}\times\begin{cases}\{J_{v_k}(\lambda t)H_{v_k}^{(1)}(\lambda\tau)\delta_{kj}\} & \text{if } \tau>t\\ \{J_{v_k}(\lambda\tau)H_{v_k}^{(1)}(\lambda t)\delta_{kj}\} & \text{if } \tau\leqslant t,\end{cases}$$

where $J_v(x)$ and $H_v^{(1)}(x)$ are the Bessel and Hankel functions of the first kind, respectively. If we apply $(L_0-\lambda^2)^{-1}$ to both sides of the equation $L_\alpha u=\lambda^2 u$, we will get

$$u(\tau,\lambda)=\int_0^\infty G_\alpha(\tau,t,\lambda)Q(t)u(t,\lambda)dt. \tag{2.1}$$

Evidently that the set of λ for which Eq. (2.1) has a nontrivial solution coincides with the eigenvalue set of the equation $L_\alpha u=\lambda^2 u$. Since $G_\alpha(\tau,t,\lambda)$ is a diagonal matrix,

$$\|G_\alpha(\tau,t,\lambda)\|_{l_2}=\frac{\pi}{2}\max_{v_k}\sqrt{\tau t}|J_{v_k}(\lambda t)H_{v_k}^{(1)}(\lambda\tau)|.$$

It follows from Ref. 2 that

$$\sqrt{\tau t}J_{v+n}(\lambda t)H_{v+n}^{(1)}(\lambda\tau)=\frac{n!\Gamma(v)\lambda^v 2^{v-1}}{\pi\Gamma(n+2v)}(\tau t)^{v+(1/2)}\int_{-1}^1\frac{H_v^{(1)}(\lambda\sqrt{\tau^2+t^2-2\tau ts})}{(\sqrt{\tau^2+t^2-2\tau ts})}\times C_n^v(s)(1-s^2)^{v-(1/2)}ds, \tag{2.2}$$

where $C_n^v(s)$ is the Gegenbauer function,[12] and if $\operatorname{Re} v>-\frac{1}{2}$, $-(\pi/2)<\arg\lambda<3\pi/2$, $x>0$, then

$$H_v^{(1)}(\lambda x)=\frac{x^v e^{i(\lambda v-(\pi/2)v-(\pi/4))}}{\Gamma\left(v+\frac{1}{2}\right)}\int_0^\infty\left(1+\frac{it}{2\lambda}\right)^{v-(1/2)}t^{v-(1/2)}e^{-xt}dt. \tag{2.3}$$

Let us estimate $\sqrt{\tau t}J_{v+n}(\lambda t)H_{v+n}^{(1)}(\lambda\tau)$ when $0<v\leqslant 1/2$.

Taking into account that for each $\lambda\in(-(\pi/2)<\arg\lambda<(3\pi/2))$ there exists a positive number β such that $|2\lambda+it|\geqslant\beta$ and $|2\lambda+it|^{\upsilon-(1/2)}\leqslant\beta^{\upsilon-(1/2)}$ as $0<\upsilon\leqslant 1/2$, we obtain from (2.3) the inequality

$$|H_{\upsilon}^{(1)}(\lambda x)|\leqslant C_1\frac{x^{\upsilon}}{\sqrt{|\lambda|}}e^{-(\operatorname{Im}\lambda)x}\frac{1}{|\lambda|^{\upsilon-(1/2)}}\int_0^{\infty}t^{\upsilon-(1/2)}e^{-xt}dt=C_2\frac{e^{-\operatorname{Im}\lambda x}}{|\lambda|^{\upsilon}\sqrt{x}},\quad \tau\leqslant t,$$

where C_1 and C_2 are some constants, whence

$$\begin{aligned}&\sqrt{\tau t}|J_{\upsilon+n}(\lambda\tau)H_{\upsilon+n}^{(1)}(\lambda t)|\\&\quad\leqslant\frac{Cn!\Gamma(\upsilon)(\tau t)^{\upsilon+1/2}}{\Gamma(n+2\upsilon)}e^{-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|}\int_0^{\infty}\frac{C_n^{\upsilon}(\cos\gamma)(\sin\gamma)^{2\upsilon}}{(1-\cos\gamma)^{\upsilon/2+1/4}\tau^{\upsilon+1/2}}d\gamma,\quad \tau\leqslant t.\end{aligned}\tag{2.4}$$

Since for large n,

$$|C_n^{\upsilon}(\cos\gamma)|\leqslant\frac{C\Gamma(n+2\upsilon)}{\sqrt{n}\Gamma(2\upsilon)\Gamma(n+\upsilon+1/2)(\sin\gamma)^{\upsilon}}$$

(see Ref. 12), inequality (2.4) implies the estimate

$$\begin{aligned}|\sqrt{\tau t}J_{\upsilon+n}(\lambda\tau)H_{\upsilon+n}^{(1)}(\lambda t)|&\leqslant\frac{Cn!t^{\upsilon+1/2}}{\sqrt{n}\Gamma(n+\upsilon+1/2)}\int_0^{\pi}\frac{\sin^{\upsilon}\alpha}{(1-\cos\alpha)^{\upsilon/2+1/4}}d\alpha\\&=C_1\frac{t^{\upsilon+(1/2)}}{n^{\upsilon}}e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}.\end{aligned}$$

In the same way, we obtain

$$\sqrt{\tau t}|J_{\upsilon+n}(\lambda t)H_{\upsilon+n}^{(1)}(\lambda\tau)|\leqslant C\frac{t^{\upsilon+(1/2)}}{n^{\upsilon}}e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\quad\text{as}\quad\tau\geqslant t.$$

So, if n is large, the estimate

$$\forall\tau\in[0,\infty),\quad\forall t\in[0,\infty),$$

$$\sqrt{\tau t}|J_{\upsilon+n}(\lambda x_<)H_{\upsilon+n}^{(1)}(\lambda x_>)|\leqslant C\frac{1}{n^{\upsilon}}(\tau^{\upsilon+(1/2)}+t^{\upsilon+(1/2)})e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\tag{2.5}$$

is valid, where $x_<=\min(\tau,t)$, $x_>=\max(\tau,t)$.

If we let $\upsilon\to 0$, then, as is known from Ref. 2,

$$C_n^{\upsilon}(\cos\gamma)\sim\frac{\Gamma(n+2\upsilon)\Gamma(\upsilon+\frac{1}{2})}{\sqrt{n\pi}\Gamma(2\upsilon)\Gamma(n+\upsilon+\frac{1}{2})}\left\{\frac{\cos[(n+\upsilon)\gamma-\frac{1}{2}\gamma\pi]}{(\sin\gamma)^{\upsilon}}+O(n^{-(3/2)})\right\}\quad\text{as}\quad n\to\infty.$$

Therefore for $\tau<t$ and $\upsilon\to 0$, we have

$$\sqrt{\tau t}J_{v+n}(\lambda\tau)H^{(1)}_{v+n}(\lambda t)\sim C\frac{\lambda^v\Gamma(n+1)(\tau t)^{v+(1/2)}}{\sqrt{n}\Gamma\left(n+v+\frac{1}{2}\right)}\int_0^\pi\frac{H^{(1)}_v(\lambda\sqrt{\tau^2+t^2-2\tau t\gamma})}{(\sqrt{\tau^2+t^2-2\tau+\gamma})^v}\cos n\gamma d\gamma$$

$$\sim Ct^{v+(1/2)}e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\int_0^\pi\lambda^v\tau^{v+(1/2)}$$

$$\times e^{(\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\frac{H^{(1)}_v(\lambda\sqrt{\tau^2+t^2-2\tau t\gamma})}{(\sqrt{\tau^2+t^2-2\tau+\gamma})^v}(\sin\gamma)^v\cos n\gamma d\gamma. \tag{2.6}$$

Since

$$\left|\lambda^v(\tau t)^{v+(1/2)}e^{(\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\frac{H^{(1)}_v(\lambda\sqrt{\tau^2+t^2-2\tau t\gamma})}{(\sqrt{\tau^2+t^2-2\tau+\gamma})^v}(\sin\gamma)^v\right|\leqslant\frac{C}{(1-\cos\gamma)^{1/4}},$$

and

$$\int_0^\pi\frac{d\alpha}{(1-\cos\alpha)^{1/4}}<\infty,$$

the coefficient of $\cos n\gamma$ in (2.6) is absolutely integrable. By the Riemann–Lebesgue Lemma,

$$\sqrt{\tau t}|J_{v+n}(\lambda\tau)H^{(1)}_{v+n}(\lambda t)|=o(1)t^{v+(1/2)}e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}, \tag{2.7}$$

where $o(1)\to 0$ as $n\to\infty$.

A similar argument yields

$$\sqrt{\tau t}|J_{v+n}(\lambda\tau)H^{(1)}_{v+n}(\lambda t)|=o(1)\tau^{v+(1/2)}e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}\quad\text{as}\quad\tau<t. \tag{2.8}$$

Formulas (2.5), (2.7), and (2.8) imply that

$$\sqrt{\tau t}|J_{v+n}(\lambda\tau)H^{(1)}_{v+n}(\lambda t)|=(\tau^{v+1/2}+t^{v+1/2})o(1)e^{(-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|)}, \tag{2.9}$$

where $\lim_{n\to\infty}o(1)=0$ and $0\leqslant\tau,\ t<\infty$.

Analogously, it can be shown that (2.9) holds if $\frac{1}{2}<v<1$.

One can see from estimate (2.9) that for all τ and t, the diagonal entries of the matrix $G_\alpha(\tau,t,\lambda)$ become vanishingly small with $n\to\infty$. In view of (2.2), the function $G_\alpha(\tau,t,\lambda)$, whose values are operators in l_2, is an analytic function of λ in the domain $-(\pi/2)<\arg\lambda<(3\pi/2)$. We summarize the above assertions in the following lemma:

Lemma: For all τ and t, and $-(\pi/2)<\arg\lambda<(3\pi/2)$, the matrix $G_\alpha(\tau,t,\lambda)$ is a compact operator in l_2. If we fix τ and t, then $G_\alpha(\tau,t,\lambda)$ is an analytic operator function of λ in the domain $-(\pi/2)<\arg\lambda<(3\pi/2)$.

Let

$$S_\epsilon=\left\{\lambda\in C:-\frac{\pi}{2}<\arg\lambda<\frac{3\pi}{2},\operatorname{Im}\lambda>-\frac{\epsilon}{2}\right\}.$$

The following theorem holds:

Theorem 1: If $\lambda\in S_\epsilon$, then the integral operator on the right-hand side of (2.1) is compact in $L_{2,\epsilon}((0,\infty),l_2)$.

Proof: First of all we note that the operator $G_\alpha(\tau,t,\lambda)Q(t)$ is compact as a product of the compact operator G_α and the bounded operator Q acting in l_2. By (2.9), under the conditions on $Q(x)$ the inequality

$$\|G_\alpha(\tau,t,\lambda)Q(t)\| \leqslant C \max_{\tau,t}(\tau^{\nu+1/2}+t^{\nu+1/2})e^{-\operatorname{Im}\lambda|\tau-\operatorname{sign}(\operatorname{Im}\lambda)t|}e^{-\epsilon t} \tag{2.10}$$

is fulfilled.

Denote by E_N the infinite diagonal matrix whose first N entries on the main diagonal are 1 and all the rest are equal to 0. It follows from (2.10) that the kernel

$$A_N(\tau,t,\lambda)=G_\alpha(\tau,t,\lambda)E_NQ(t)E_N$$

is of Hilbert–Schmidt-type in $L_{2,\epsilon}((0,\infty),l_2)$ as $\lambda\in S_\epsilon$.

If $\lambda\in S_\epsilon$, then the sequence of kernels A_N converges to $G_\alpha(\tau,t,\lambda)$ $(N\to\infty)$ in the norm of an operator in $L_{2,\epsilon}(0,\infty;l_2)$. Since a limit of a sequence of compact operators is a compact operator, the proof is complete.

Let us consider the following integral equation:

$$u(t)=v(t)-\int_0^\infty G_\alpha(\tau,t,\lambda)Q(t)u(t)dt, \tag{2.11}$$

where $v(\tau)\in L_{2,\epsilon}((0,\infty),l_2)$ and $u(\tau)\in L_{2,\epsilon}((0,\infty),l_2)$ are a known and unknown vector-valued functions, respectively.

Theorem 2: Equation (2.9) is solvable in $L_{2,\epsilon}((0,\infty),l_2)$ for all $\lambda\in S_\epsilon$ except for at most a countable set of points from this set. If there exists infinitely many points λ for which this equation is not solvable, then the limit points of such λ belong to the boundary of S_ϵ.

Proof: The integral equation (2.9) may be written in the form

$$u=v-A(\lambda)u. \tag{2.12}$$

By Lemma and Theorem 1, $A(\lambda)$ is an analytic function of $\lambda\in S_\epsilon$, whose values are compact operators in l_2.

As is done in Ref. 8, it can be shown that Eq. (2.10) has a unique solution for $\lambda\in S_\epsilon$ with large $|\lambda|$. It follows from the Gohberg theorem (see Ref. 10, Chap. I, Theorem 5.1) that the number of points, at which the operator $I-A(\lambda)$ has no inverse, is not greater than countable, and if there exists infinitely many such points, their limit points belong to the boundary of S_ϵ. This completes the proof of the theorem.

Theorem 3: The number $\lambda^2(\operatorname{Im}\lambda>0)$ is an eigenvalue of the operator L_α if and only if Eq. (2.1) has no nontrivial solutions in $L_{2,\epsilon}((0,\infty),l_2)$.

Proof: Assume that $\lambda^2(\operatorname{Im}\lambda>0)$ is an eigenvalue of L_α, and $u(\tau,\lambda)$ is the corresponding eigenfunction. Then $u(\tau,\lambda)$ satisfies (2.1). Since $u(\tau,\lambda)\in L_2((0,\infty),l_2)$, we have $u(\tau,\lambda)\in L_{2,\epsilon}((0,\infty),l_2)$. This shows that the sufficiency is fulfilled.

To prove the necessity, suppose that the vector-valued function $u(\tau,\lambda)\in L_{2,\epsilon}(0,\infty;l_2)$ satisfies Eq. (2.1). Then $Q(t)u(t,\tau)$ belongs to $L_2((0,\infty),l_2)$. Since $G_\alpha(t,\tau,\lambda)$ is the resolvent kernel of the self-adjoint operator L_0, $u(\tau,\lambda)\in L_2(0,\infty;l_2)$.

Applying the expression

$$-\frac{d^2}{d\tau^2}+\frac{B(\alpha)}{\tau^2}-\lambda^2$$

to both sides of (2.1) makes sure that

$$-\frac{d^2u}{d\tau^2}+\frac{B(\alpha)u}{\tau^2}+Q(\tau)u=\lambda^2u.$$

As is seen from (2.1), the boundary condition $u(0)=0$ is satisfied, too. So, the number λ^2 is an eigenvalue of the operator L_α, which is what had to be proved.

In Ref. 11 (see also Ref. 3), it was shown that the operator L_α has no positive eigenvalues. Using Theorems 2 and 3, we arrive at the following result:

Theorem 4: The discrete part of spectrum of L_α forms a bounded set. If this set is infinite then it has only one limit point which is equal to zero.

Example: Let D be an angular domain in the plane $x=(x_1,x_2)$ with center at zero and angle α. Moreover, α is chosen in the way that $v_k=(k\pi/\alpha)\notin Z\ (n=1,2,...)$. In the space $L_2(D)$ we consider the operator L generated by the Schrödinger differential expression

$$Lu=-\Delta u+q(x)u$$

and the boundary condition $u|_{\partial D}=0$. We assume also that the condition $|q(x)|\leqslant ce^{-\epsilon|x|}$, $\epsilon>0$, is satisfied.

Let $\phi_n(\varphi)=\sqrt{(2/\alpha)}\sin(\pi n/\alpha)\varphi$. The functions $\{\phi_n(\varphi)\}_{n=1}^{\infty}$ form a complete orthonormal system in $L_2(0,\alpha)$. We look for a solution of the equation $Lu=\lambda^2u$ in polar coordinates so that

$$u(x,\lambda)=\sum_{j=1}^{\infty}\frac{1}{\sqrt{r}}u_j(r,\lambda)\phi_j(\varphi)\quad(r=|x|).$$

Then determination of the eigenvalues of the operator L is reduced to finding those of the operator L_α. As a result, we can state that the eigenvalues of the non-self-adjoint operator L form a bounded set, and if this set has a limit point, then this limit point is equal to zero.

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On diffusion dynamics for continuous systems with singular superstable interaction

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We consider the time evolution of states for continuous infinite particle systems which corresponds to nonequilibrium diffusion dynamics. For initial states μ_0 which are perturbations of the equilibrium we obtain a bound for finite volume nonequilibrium correlation functions and their continuity in time uniformly in volume for any finite time interval. This gives the possibility to construct the time evolution of correlation functions and corresponding states in the thermodynamic limit. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1690489]

I. INTRODUCTION

A diffusion of an interacting infinite particle system can be described by an infinite system of stochastic differential equations of the so-called gradient type:

$$dx_i(t) = -\sum_{j,i\neq j} \nabla\phi(x_i(t)-x_j(t))dt + \sqrt{\frac{2}{\beta}}\quad dw_i(t). \tag{1.1}$$

Here $\phi:\mathbb{R}^d\backslash\{0\}\to\mathbb{R}$ $(\phi(x)=\phi(-x))$ is an interaction potential, $w_i(t)$ are independent standard Wiener processes in $\mathbb{R}^d$ and the parameter $\beta>0$ is the inverse temperature of the system. The physical background and motivation can be found in the article by Spohn[1] and references therein. The set of positions $\{x_i\}_{i\in\mathbb{N}}$ of identical particles is a locally finite subset in $\mathbb{R}^d$ and the set of all such subsets is the *configuration space* Γ:

$$\Gamma := \{\gamma\subset\mathbb{R}^d \quad | \quad |\gamma\cap K|<\infty \quad \textit{for any compact} \quad K\subset\mathbb{R}^d\},$$

where $|A|$ is the cardinality of A. Heuristically, any Gibbs measure μ on Γ corresponding to the interaction ϕ and the inverse temperature β is a stationary measure of the Markov process defined by (1.1). The corresponding Markov generator can be calculated by Ito's formula and defined in $L^2(\Gamma,\mu)$ on some domain of smooth cylinder functions F by the following expression:

$$(HF)(\gamma) = \sum_{x\in\gamma}\left(-\frac{1}{\beta}\Delta_x + \nabla_x U_\phi(\gamma)\cdot\nabla_x\right)F(\gamma), \tag{1.2}$$

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where

$$U_\phi(\gamma)=\sum_{\{x,y\}\subset\gamma}\phi(x-y),\quad \nabla_x U_\phi(\gamma)=\sum_{y\in\gamma\setminus x}\nabla\phi(x-y),\quad x\in\gamma. \tag{1.3}$$

Under some natural restrictions on the class of interaction potentials ϕ the generator H has a self-adjoint extension in $L^2(\Gamma,\mu)$ (see Ref. 2).

A rigorous study of (1.1) has been initiated by Lang[3] who has proved the existence of the so-called equilibrium stochastic dynamics which corresponds to (1.1) for a superstable, three times continuously differentiable potential with finite range. In more recent works by Osada,[4] Yoshida[5] and Albeverio *et al.*[2] the equilibrium stochastic dynamics was constructed by Dirichlet form methods for a wide class of potentials ϕ. The existence of the nonequilibrium dynamics was proved by Rost[6] and Lippner[7] in the one-dimensional case and by Fritz[8] for smooth superstable finite range potentials in the case $d\leqslant 4$.

To construct the nonequilibrium dynamics one can consider the corresponding semigroup $T_t=e^{-t\tilde{H}}$ on some class $\mathcal{F}(\Gamma)$ of observables $F:\Gamma\to\mathbb{R}$ defined by the Kolmogorov equation

$$\frac{\partial F_t}{\partial t}=-\tilde{H}F_t,\quad F_0\in\mathcal{F}(\Gamma), \tag{1.4}$$

where $\tilde{H}$ is the Friedrichs extension of H on $L^2(\Gamma,\mu)$ for some fixed Gibbs measure μ. On the other hand, instead of the evolution of observables one can consider the evolution of states, i.e., the evolution of probability measures on Γ. Such evolution is defined by the adjoint semigroup via the following equation:

$$\frac{d}{dt}\mu_t=-H^*\mu_t. \tag{1.5}$$

In the case of a finite particle system this equation can be rewritten in terms of the densities $\mathcal{D}(t,\gamma)$ w.r.t. Lebesgue measure $d\gamma=dx_1\cdots dx_N$ ($|\gamma|=N<\infty$). Then (1.5) is, sometimes, called the generalized Smoluchowski equation (see, e.g., Ref. 9).

For infinite particle systems initial states μ_0 are not absolutely continuous w.r.t. any standard measure and the time evolution of densities has no rigorous sense. Below we consider an alternative approach in terms of correlation functions which correspond to the states of the system. To define these correlation functions we introduce the space of *finite configurations* Γ_0:

$$\Gamma_0:=\bigcup_{n\in\mathbb{N}_0}\Gamma^{(n)},\quad \Gamma^{(n)}:=\{\gamma\in\Gamma\ \mid\ |\gamma|=n\},\quad \mathbb{N}_0=\mathbb{N}\cup\{0\}. \tag{1.6}$$

Γ_0 is naturally equipped with the Borel σ-algebra $\mathfrak{B}(\Gamma_0)$ given by the disjoint union of the measurable spaces $(\Gamma^{(n)},\mathfrak{B}(\Gamma^{(n)}))$. For any bounded $Y\in\mathfrak{B}(\mathbb{R}^d)$ the topology of

$$\Gamma_Y^{(n)}:=\{\gamma\in\Gamma\ \mid\ \gamma\cap(\mathbb{R}^d\setminus Y)=\varnothing,\ |\gamma|=n\}$$

is induced by the bijection between $\Gamma_Y^{(n)}$ and the symmetrization $\tilde{Y}^n/S_n$ of $\tilde{Y}^n$ (see Ref. 10 for details), where S_n is the permutation group over $\{1,\ldots,n\}$,

$$\tilde{Y}^n:=\{(x_1,\ldots,x_n)\ \mid\ x_i\in Y,\ x_i\neq x_j, i\neq j\},$$

and we denote by $\Gamma_Y=\cup_{n=0}^\infty\Gamma_Y^{(n)}$ the set of configurations in Y.

Starting with an intensity measure $\sigma=zdx$ ($z>0$) on $\mathfrak{B}(\mathbb{R}^d)$ we introduce the product-measure $\sigma^{\otimes n}$ on $(\mathbb{R}^d,\mathfrak{B}(\mathbb{R}^{dn}))$ and denote $\sigma^{(n)}:=\sigma^{\otimes n}\circ(s_n)^{-1}$, where s_n is the map $s_n:\mathbb{R}^{dn}\ni(x_1,\ldots,x_n)\mapsto\{x_1,\ldots,x_n\}\in\Gamma^{(n)}$. The Lebesgue–Poisson measure λ_σ on $\mathfrak{B}(\Gamma_0)$ is defined by the formula

$$\lambda_\sigma := \sum_{n\geqslant 0} \frac{1}{n!}\sigma^{(n)}. \tag{1.7}$$

Definition 1.1: Let $G:\Gamma_0\to\mathbb{R}$ *be a measurable function with local support [i.e., there exists a bounded* $\Lambda\in\mathfrak{B}(\mathbb{R}^d)$ *such that* $G\restriction(\Gamma_0\setminus\Gamma_\Lambda)=0$*]. Define the function* KG: $\Gamma\to\mathbb{R}$ *as*

$$(KG)(\gamma) := \sum_{\eta\Subset\gamma} G(\eta). \tag{1.8}$$

The summation in (1.8) is taken over all finite subconfigurations $\eta\subset\gamma$.

Remark 1.1: Functions on Γ can be considered as *observables* of our infinite particle system, and functions on Γ_0 can be interpreted as *quasi-observables*. The mapping (1.8) was introduced by Lenard[11] in order to give an abstract definition of the correlation functions in classical statistical mechanics. For a detailed study of properties of the K-transform in the framework of harmonic analysis on configuration spaces we refer to Refs. 12–14.

For a given probability measure μ on $\mathfrak{B}(\Gamma)$ one can define the correlation measure ρ_μ on $\mathfrak{B}(\Gamma_0)$ by

$$\rho_\mu(A) := \int_\Gamma (K\mathbb{1}_A)(\gamma)\mu(d\gamma), \tag{1.9}$$

where $\mathbb{1}_A$ is the indicator function of a set $A\in\mathfrak{B}(\Gamma_0)$. Assuming that ρ_μ is absolutely continuous w.r.t. λ_σ we can define the correlation functional

$$k(\eta) = k_\mu(\eta) := \frac{d\rho_\mu}{d\lambda_\sigma}(\eta). \tag{1.10}$$

In statistical physics it is useful to work with the corresponding family of correlation functions

$$k^{(n)} := k\restriction\Gamma^{(n)}, \quad n\geqslant 0. \tag{1.11}$$

Under certain general conditions on the interaction potential the correlation functions $k^{(n)} = k^{(n)}(x_1,\ldots,x_n) := k^{(n)}(x)_n$ are bounded measurable functions on some Banach space (for example, E_ξ in Ref. 15). For any $G\in L^1(\Gamma_0,\rho_\mu)$ the following formula is true (see Ref. 12 for details):

$$\int_\Gamma (KG)(\gamma)\mu(d\gamma) = \int_{\Gamma_0} G(\eta)\rho_\mu(d\eta) = \int_{\Gamma_0} G(\eta)k(\eta)\lambda_\sigma(d\eta). \tag{1.12}$$

To construct the dynamics for correlation functions, let us consider the K-transform of the generator H which is defined by

$$\hat{H} = K^{-1}HK \tag{1.13}$$

on a proper set $\mathcal{F}_0(\Gamma_0)$ of functions on Γ_0 (quasi-observables). The corresponding evolution of quasi-observables is given then by the following equation:

$$\frac{\partial G_t}{\partial t} = -\hat{H}G_t, \quad G_0\in\mathcal{F}_0(\Gamma_0). \tag{1.14}$$

We can define the time evolution of correlation functions via the duality relation:

$$\int_{\Gamma_0} G_t(\eta)k_0(\eta)\lambda_\sigma(d\eta) = \int_{\Gamma_0} G_0(\eta)k_t(\eta)\lambda_\sigma(d\eta). \tag{1.15}$$

Then the adjoint operator $(\hat{H})^* =: H_B$ in $L^2(\Gamma_0, \lambda_\sigma)$ is the generator of the evolution semigroup for the correlation functional, i.e.,

$$\frac{\partial}{\partial t} k_t = -H_B k_t . \tag{1.16}$$

Using (1.2) and (1.13)–(1.15) we can show that (1.16) has the following form (see Ref. 14):

$$\frac{\partial}{\partial t} k_t(\eta) = \sum_{x \in \eta} \nabla_x \left[\frac{1}{\beta} \nabla_x k_t(\eta) + \nabla_x U_\phi(\eta) k_t(\eta) + \int dx' \nabla \phi(x - x') k_t(x' \cup \eta) \right], \quad \eta \in \Gamma_0 . \tag{1.17}$$

In terms of the correlation functions this equation has the following hierarchical structure:

$$\frac{\partial}{\partial t} k_t^{(m)}(x)_m = \frac{1}{\beta} \sum_{j=1}^{m} \Delta_{x_j} k_t^{(m)}(x)_m + \sum_{j=1}^{m} \sum_{k \neq j}^{m} ((\nabla \phi)(x_j - x_k) \nabla_{x_j} + (\Delta \phi)(x_j - x_k)) k_t^{(m)}(x)_m$$
$$+ \sum_{j=1}^{m} \int_{\mathbb{R}^d} dx' [(\nabla \phi)(x_j - x') \nabla_{x_j} + (\Delta \phi)(x_j - x')] k_t^{(m+1)}((x)_m, x') . \tag{1.18}$$

This equation appeared for the first time on a heuristic level in Ref. 16. In the present context the hierarchy (1.16)–(1.18) is a direct consequence of the Kolmogorov equation (1.4). It is called sometimes the Bogoliubov diffusion hierarchy and it is analogous to the BBGKY hierarchy for Hamiltonian dynamics. Note that some approaches to investigating this chain of equations in the case of a smooth interaction potential ϕ were proposed in Refs. 17–20.

The problem of existence of solutions of hierarchy (1.18) is additionally complicated by the fact that one should check that the obtained solution k_t corresponds to some state μ_t. Otherwise we cannot prove that we construct the evolution of some initial state μ_0. This problem was not discussed in Refs. 17–20. More precisely, for regular types of interaction potentials, low particle density and sufficiently small interval of time evolution the solution of the diffusion hierarchy (1.18) in the thermodynamic limit was obtained without any analysis of the existence of the dynamics for the corresponding states. In this article we obtain the existence of state μ_t using a general theorem about the connection between states and positive-definiteness of the corresponding correlations functions.[14,21]

Remark 1.2: Note that in theoretical physics a hierarchical system of equations is accepted very often as the definition of the dynamics of an infinite particle system. Such situation takes place, e.g., in Hamiltonian dynamics where the BBGKY hierarchy is considered as the definition of the evolution. Let us mention that, in general, connections between the BBGKY hierarchy approach and the state evolution are not investigated enough as pointed out in Ref. 22, Sec. 3.3. From the physical point of view the property of positivity for correlation functions is very important. But it is not enough to reconstruct the corresponding state.[11] A constructive condition which guarantees such reconstruction was proposed in Ref. 12 (see also Ref. 21). This is the positive-definiteness of the sequence of correlation functions [see below (2.25)–(2.27)]. The situation is the same as in the classical problem of momentum (see, e.g., Ref. 23). From this point of view many results on existence of solutions of the BBGKY hierarchy (see, e.g., Refs. 24 and 25) should be completed by a proof for the existence of the dynamics of states for every particular class of models, as it has been done for stationary solutions in Ref. 26 and for the one-dimensional nonstationary case in Ref. 27.

In this article we consider some class of singular superstable interactions (see Sec. III). Our main strategy is based on a construction of the semigroup p_B^t which corresponds to the evolution equation (1.16). For appropriate initial data k_0 it provides a global solution to the diffusion hierarchy (1.16)–(1.18):

$$k_t(\eta)=(p_B^t k_0)(\eta). \tag{1.19}$$

We obtain an expression for the operator p_B^t which can be easily defined on the Banach space $L^1_\beta(\Gamma_0,\lambda_{\xi\sigma})$ of $\lambda_{\xi\sigma}$-integrable functionals for some appropriate weight ξ (see Sec. II). But for most cases, which are interesting from a physical point of view, the correlation functionals of initial particle distributions do not belong to $L^1_\beta(\Gamma_0,\lambda_{\xi\sigma})$. Typically, they are only bounded and we need to extend the domain of the operator p_B^t to some class of bounded functionals. But from our point of view it would be very naive to hope that a global solution to the hierarchy (1.16)–(1.18) can be obtained for all initial data. Even in the case of a finite number of particles the singularity of the interaction potential does not allow us to define the evolution of arbitrary initial state. Generally speaking one can expect existence of a solution only if the initial correlation functions are chosen in a proper way. In this article we consider a class of initial functionals which correspond to some perturbations of the equilibrium state $\mu=\mu_\phi$ which is constructed by ϕ. The idea is that, as the equilibrium state is a perturbation of the free state (Poisson ideal gas), the nonequilibrium state should be some perturbation of the equilibrium Gibbs state. Such a choice of the initial state is very natural from a physical point of view and were used by many authors. Our main result (Theorem 4.1) is the following. Consider an initial state μ_0 which corresponds to a superstable potential

$$V=\phi+\psi, \tag{1.20}$$

where ϕ is the potential by which our dynamics (1.1) is governed and ψ is a superstable, lower regular interaction potential (see Sec. III). For the given measure μ_0 we consider a family of finite volume measures μ_0^Λ [for bounded $\Lambda\in\mathfrak{B}(\mathbb{R}^d)$] and the corresponding family of initial correlation functionals $k_0^\Lambda(\eta)$:[15]

$$k_0^\Lambda(\eta)=\int_{\Gamma_0}\lambda_\sigma(d\gamma)\mathcal{D}_0^\Lambda(\eta\cup\gamma) \tag{1.21}$$

with

$$\mathcal{D}_0^\Lambda(\eta)=Z_\Lambda^{-1}\mathbb{1}_{\Gamma_\Lambda}(\eta)e^{-\beta U_V(\eta)},\quad \eta\in\Gamma_0, \tag{1.22}$$

$$Z_\Lambda=\int_{\Gamma_0}\lambda_\sigma(d\eta)\mathbb{1}_{\Gamma_\Lambda}(\eta)e^{-\beta U_V(\eta)}. \tag{1.23}$$

For such initial correlation functionals we construct a solution of (1.16) as

$$k_t^\Lambda(\eta)=(p_B^t k_0^\Lambda)(\eta). \tag{1.24}$$

Our main technical result consists in the proof of a bound, uniform in Λ, for these correlation functionals:

$$k_t^\Lambda(\eta)\leqslant c_1^{|\eta|},\quad \eta\in\Gamma_0\quad c_1=c_1(z,\beta,T),\quad t\in[0,T], \tag{1.25}$$

for any time interval $[0,T]$. We obtain this result using the well-known technique of superstability estimates in classical statistical mechanics[28] and its generalization to the quantum case with Boltzman statistics.[29]

In our case this technique needs some modification. We should also note that as in Ref. 29 we need the restriction $d\leqslant 3$ on the dimension d of the system. It is connected with estimating the contribution of long Wiener trajectories in a functional integral representation for the correlation functions. Using (1.25) and the continuity in time (uniformly in Λ) [see (4.27)] we conclude that there exists a thermodynamic limit for k_t^Λ and these limit functionals k_t satisfy the equation (1.16) in a weak sense.

The structure of this paper is as follows: In Sec. II we construct the operator p_B^t and derive a representation for k_t^Λ. In Sec. III we discuss the class of interactions. In Sec. IV we recall some auxiliary constructions and formulate our main result. The proof of the main theorem is presented in Sec. V. The basic technical lemmas are outlined in the Appendix.

II. CORRELATION FUNCTIONS

In this section we construct the semigroup connected with the diffusion hierarchy (1.16)–(1.18) and derive a representation for the finite volume correlation functions (1.24). Let us define an operator K_0 on quasi-observables as

$$K_0G := (KG)\restriction\Gamma_0. \tag{2.1}$$

Then we can construct the operator

$$H_F := K_0\hat{H}K_0^{-1}. \tag{2.2}$$

On smooth quasi-observables the operator H_F acts by the following formulas

$$H_FG = ((H_FG)^{(n)}(x)_n)_{n=0}^\infty, \quad G = ((G)^{(n)}(x)_n)_{n=0}^\infty, \tag{2.3}$$

where

$$(H_FG)^{(n)}(x)_n = (H_F^{(n)}G^{(n)})(x)_n = \sum_{j=1}^n \left(-\frac{1}{\beta}\Delta_{x_j} + \nabla_{x_j}U_\phi(x)_n\cdot\nabla_{x_j}\right)G^{(n)}(x)_n. \tag{2.4}$$

$H_F^{(n)}$ is the generator of the stochastic dynamics for an n-particle system:

$$dx_i(t) = -\sum_{i\neq j=1}^n \nabla\phi(x_i(t)-x_j(t))dt + \sqrt{\frac{2}{\beta}}\quad dw_i(t), \quad i=1,\dots,n. \tag{2.5}$$

The problem of existence of the stochastic dynamics (2.5) with a singular potential is analyzed in Refs. 30 and 31. The operator $H_F^{(n)}$ is generated by the Dirichlet form

$$(H_F^{(n)}G^{(n)},G^{(n)})_{L^2(\Gamma_0^{(n)},\mu_\phi^{(n)})} = \frac{1}{\beta}\sum_{j=1}^n \int_{\Gamma_0^{(n)}} |\nabla_jG^{(n)}|^2 d\mu_\phi^{(n)}, \tag{2.6}$$

where

$$\mu_\phi^{(n)} := e^{-\beta U_\phi(\cdot)_n}\sigma^{(n)} \tag{2.7}$$

and $\sigma^{(n)}$ is defined in (1.7).

Then using (1.14)–(1.15) and (2.1)–(2.2) one can write for p_B^t the following representation:

$$p_B^t = e^{-tH_B} = K_0^* e^{-tH_F^*}(K_0^{-1})^* = De^{-tH_F^*}D^{-1}. \tag{2.8}$$

Here the operators $D := K_0^*$ and D^{-1} are defined in $L^1(\Gamma_0,\lambda_{\xi\sigma})$, $\xi>2$, by the following formulas (see Ref. 12 for details):

$$(DF)(\eta) = \int_{\Gamma_0}\lambda_\sigma(d\gamma)F(\eta\cup\gamma), \tag{2.9}$$

$$(D^{-1}F)(\eta) = \int_{\Gamma_0}\lambda_\sigma(d\gamma)(-1)^{|\gamma|}F(\eta\cup\gamma). \tag{2.10}$$

Remark 2.1: In our approach the representation (2.8) for p_B^t is a direct consequence of the Kolmogorov equation (1.4) without any reference to the hierarchical structure of (1.17) and (1.18). In the same way from the Liouville equation one can obtain the corresponding representation for the Hamiltonian dynamics.[14] Representations like (2.8) appeared earlier. They were obtained by application of the method of ''creation'' and ''annihilation'' operators for classical statistical mechanics (see Refs. 32–35). For connections with the diffusion hierarchy see Ref. 19.

Remark 2.2: It will be clear from the considerations below that in the case of a stable interaction potential ϕ for which $-\Delta\phi$ is also stable, the operator p_B^t can be defined on a Banach space $L_{\beta,\xi}$ with the norm

$$\|G\|_{\beta,\xi}=\int_{\Gamma_0}\lambda_{\xi\sigma}(d\eta)e^{(1/2)\beta U_\phi(\eta)}|G(\eta)|<\infty,\quad G\in L^1_{\beta,\xi}. \tag{2.11}$$

To obtain a representation for finite volume correlation functions k_t^Λ we take into account the definition of the operator D and rewrite (1.21) in the form

$$k_0^\Lambda(\eta)=(D\mathcal{D}_0^\Lambda)(\eta). \tag{2.12}$$

Then due to (2.8) and (1.20) the following representation is true:

$$k_t^\Lambda(\eta)=\left(D\left[e^{-tH_F^*}\left(\frac{1}{Z_\Lambda}e^{-\beta U_\phi}e^{-\beta U_\psi}\mathbb{1}_{\Gamma_\Lambda}\right)\right]\right)(\eta)=\left(D\left[\frac{1}{Z_\Lambda}e^{-tH_F}(e^{-\beta U_\psi}\mathbb{1}_{\Gamma_\Lambda})e^{-\beta U_\phi}\right]\right)(\eta), \tag{2.13}$$

where we use the fact that the operator H_F [see (2.4)] is a self-adjoint operator in $L^2(\Gamma_0,e^{-\beta U_\phi}\lambda_\sigma)$.

Now, to get an integral representation for k_t^Λ we use a functional integral representation for the operator e^{-tH_F} in (2.13). First of all, note that the operator H_F has the Fock structure (2.3) and (2.4), so we only need a representation for $e^{-tH_F^{(n)}}$ in $L^2(\Gamma_0^{(n)},\mu_\phi^{(n)})$. To get it we use the well-known ground state transformation (see, e.g., Ref. 36, Sec. 2, and Ref. 23, Chap. 7)

$$L^2(\Gamma_0^{(n)},\mu_\phi^{(n)})\ni f\mapsto e^{-(1/2)\beta U_\phi}f\in L^2(\Gamma_0^{(n)},\sigma^{(n)}). \tag{2.14}$$

The corresponding generator $\tilde{H}_F^{(n)}$ in $L^2(\Gamma_0^{(n)},\sigma^{(n)})$ has the following form,

$$\tilde{H}_F^{(n)}=-\frac{1}{\beta}\sum_{j=1}^n\Delta_{x_j}+\tilde{V}(x)_n, \tag{2.15}$$

with the effective potential

$$\tilde{V}(x)_n=\tilde{V}^+(x)_n+\tilde{V}^{(-\Delta\phi)}(x)_n:=\sum_{j=1}^n\left(\frac{\beta}{4}|\nabla_{x_j}U_\phi(x)_n|^2-\frac{1}{2}\Delta_{x_j}U_\phi(x)_n\right). \tag{2.16}$$

For the domain of the operator $\tilde{H}_F^{(n)}$ we have $\mathfrak{D}(\tilde{H}_F^{(n)})\supset C_0^\infty(\Gamma_0^{(n)})$, where $C_0^\infty(\Gamma_0^{(n)})$ denotes C^∞-functions on $\Gamma_0^{(n)}$ with compact supports. It can be shown that for any superstable potential ϕ the effective potential $\tilde{V}(x)_n$ is bounded from below for any fixed n. But for the class of potentials under consideration it is even superstable (see Sec. III). Therefore, we can apply the Feynman–Kac formula for the kernel of the semigroup $e^{-t\tilde{H}_F^{(n)}}$, where $\tilde{H}_F^{(n)}$ is considered in the sense of a form sum (2.15) Ref. 37, Chap. 2. As a result, we get

$$(e^{-tH_F^{(n)}})((x)_n;(y)_n)=e^{(1/2)\beta U_\phi(x)_n-(1/2)\beta U_\phi(y)_n}\int_{(\Omega^{t\beta})^n}\prod_{j=1}^n W^{t\beta}_{x_j;y_j}(d\omega_j)e^{-\beta\int_0^{t\beta}d\tau\tilde{V}(\omega(\tau))_n}, \tag{2.17}$$

where

$$\Omega^{t_\beta} := C([0,t_\beta] \to \mathbb{R}^d), \quad t_\beta = t\beta^{-1}, \tag{2.18}$$

$W^{t_\beta}_{x;y}$ is the conditional Wiener measure on the space Ω^{t_β} with conditions $\omega_j(t_\beta) = x_j$ and $\omega_j(0) = y_j$. It implies the following useful representation:

$$k_t^\Lambda(\eta) = \int_{\mathbb{R}^{dm}} d\xi \int_{(\Omega^{t_\beta})^m} W^{t_\beta}_{\eta;\xi}(d\omega)_m \rho_t^\Lambda(\omega)_m, \tag{2.19}$$

where $\eta = \{x_1, \ldots, x_m\}$, $\xi = \{y_1, \ldots, y_m\}$, $d\xi = dy_1 \cdots dy_m$, and

$$\rho_t^\Lambda(\omega)_m = \sum_{n \geqslant 0} \frac{1}{n!} \int \tilde{\sigma}_\Lambda(\omega_{m+1}) \cdots \int \tilde{\sigma}_\Lambda(\omega_{m+n}) \tilde{D}_0^\Lambda(\omega(0))_{m+n} e^{-\tilde{U}(\omega)_{m+n}}. \tag{2.20}$$

In (2.20) we use the following notations:

$$\tilde{U}(\omega)_{m+n} := \frac{1}{2}\beta U_\phi(x)_{m+n} + \int_0^{t_\beta} d\tau [U_{-\Delta\phi}(\omega(\tau))_{m+n} + U^+_{\nabla\phi}(\omega(\tau))_{m+n}], \tag{2.21}$$

$$U^+_{\nabla\phi}(x)_{m+n} := \sum_{j=1}^{m+n} \left[\frac{1}{4}\beta |\nabla_{x_j} U_\phi(x)_{m+n}|^2 \right] \geqslant 0, \tag{2.22}$$

$$\tilde{D}_0^\Lambda(\omega(0))_{m+n} := e^{(1/2)\,\beta U_\phi(\omega(0))_{m+n}} \mathcal{D}_0^\Lambda(\omega(0))_{m+n}, \tag{2.23}$$

and

$$\int \tilde{\sigma}_\Lambda(d\omega)(\cdots) = z \int dx \int_\Lambda dy \int W^{t_\beta}_{x;y}(d\omega)(\cdots). \tag{2.24}$$

A representation like (2.19) and (2.20) was obtained also in Refs. 17 and 18 as the generalized solution of the finite volume diffusion hierarchy (1.18).

Remark 2.3: It is not hard to show that the sequence $k_t^\Lambda(\eta)$ is positive-definite in the sense of Refs. 12 and 13, which is the following.

Definition 2.1:[13] The sequence $k_t^\Lambda(\eta)$ is positive-definite if

$$\int_{\Gamma_0} (G \star \overline{G})(\eta) k_t^\Lambda(\eta) \lambda_\sigma(d\eta) \geqslant 0 \quad \textit{for all } G \in B_{bs}(\Gamma_0). \tag{2.25}$$

Here $B_{bs}(\Gamma_0)$ is the set of all bounded measurable functions with bounded support, $\overline{G}$ denotes the complex conjugate of G, and $\star$-star is the convolution, which is defined in the following way:

$$K(G_1 \star G_2) = KG_1 \cdot KG_2. \tag{2.26}$$

(See Ref. 13 for details.)

Now, inserting (1.24) into (2.25) and using the representation (2.8), (2.12), (2.17) and the property (2.26) (which is true, also, for K_0 [see (2.1)] we obtain

$$\int_{\Gamma_0}(G\star\overline{G})(\eta)p_t D\mathcal{D}_0^{\Lambda}(\eta)\lambda_\sigma(d\eta)$$

$$=\int_{\Gamma_0}(G\star\overline{G})(\eta)K_0^* e^{-tH_F^*}D^{-1}D\mathcal{D}_0^{\Lambda}(\eta)\lambda_\sigma(d\eta)$$

$$=\int_{\Gamma_0}e^{-tH_F}(K_0G)(\eta)(K_0\overline{G})(\eta)\mathcal{D}_0^{\Lambda}(\eta)\lambda_\sigma(\eta)$$

$$=\int_{\Gamma_0}\lambda_\sigma(d\eta)\int_{(\mathbb{R}^d)^{|\eta|}}d\eta'(e^{-tH_F^{|\eta|}})(\eta|\eta')|(K_0G)(\eta')|^2\mathcal{D}_0^{\Lambda}(\eta)\geqslant 0 \qquad (2.27)$$

Positive definiteness together with the bound (1.25) gives a possibility to reconstruct the corresponding sequence of states (measures) μ_t^{Λ}.

Representation (2.19) and (2.20) is reminiscent to the representation of reduced density matrices by correlation functionals in quantum statistical mechanics with Boltzman statistics (see Refs. 38 and 39). This analogy enables us to apply powerful techniques from quantum statistical mechanics in the considered model. Following Ref. 40, we construct the configuration space $\Gamma_{\Omega^{t_\beta}}$ over the space Ω^{t_β} of Wiener trajectories in $\mathbb{R}^d$. Define configuration $\tilde{\gamma}$ as the infinite set of trajectories $\omega\in\Omega^{t_\beta}$ such that the set of values of these trajectories at time $\tau=0$ is a configuration $\gamma^0\in\Gamma$. Then define the configuration space of trajectories with initial points $\omega(0)$ in $\Lambda\in\mathfrak{B}_c(\mathbb{R}^d)$:

$$\Gamma_{\Omega^{t_\beta}_\Lambda}:=\{\tilde{\gamma}\in\Gamma_{\Omega^{t_\beta}}|\,\gamma^0\in\Gamma_\Lambda\}.$$

In the same way the Lebesgue–Poisson measure $\lambda_{\tilde{\sigma}}^{\Lambda}$ with intensity measure $\tilde{\sigma}_\Lambda$ is defined by (1.7). Then for the "correlation functionals" $\rho_t^{\Lambda}(\tilde{\eta})$, $\tilde{\eta}\in\Gamma_{\Omega^{t_\beta}_\Lambda}$, the following representation is true:

$$\rho_t^{\Lambda}(\tilde{\eta})=\int_{\Gamma_{\Omega^{t_\beta}_\Lambda}}\lambda_{\tilde{\sigma}}^{\Lambda}(d\tilde{\gamma})\tilde{D}_0^{\Lambda}(\eta^0\cup\gamma^0)e^{-\tilde{U}(\tilde{\eta}\cup\tilde{\gamma})}, \qquad (2.28)$$

where $\tilde{U}(\tilde{\eta}\cup\tilde{\gamma})$ is defined by (2.21) with $\tilde{\eta}\cup\tilde{\gamma}=\{\omega_1,\ldots,\omega_{m+n}\}$ and $\tilde{D}_0^{\Lambda}$ as defined in (2.23).

Remark 2.4: In the following we write $\eta,\gamma,\xi,\ldots,\Omega,\Omega_\Lambda$, instead of $\tilde{\eta},\tilde{\gamma},\tilde{\xi},\ldots,\Omega^{t_\beta},\Omega^{t_\beta}_\Lambda$ and $\eta^\tau,\gamma^\tau,\xi^\tau,\ldots,\ldots,\tau\in[0,t_\beta]$ for the sets of values of the corresponding configurations at time τ. Note that these sets for $\tau>0$ are not configurations in Γ_0 because some points of their values can coincide (intersection of trajectories).

III. THE CLASS OF INTERACTION POTENTIALS

In this section we describe a class of interaction potentials which allow us to solve the problem formulated in the Introduction. As it was mentioned in Remark 2.2, even to define the operator p_B^t on $L^1_{\beta,\xi}$ we have to consider a rather narrow class of interaction potentials. The restrictions on the potential imposed below are, however, rather dictated by the technique of the superstability estimates for functional integrals. We hope that the stochastic dynamics, actually, exists for a more wide class of potentials and initial states. This point of view is supported by the fact that the equilibrium stochastic dynamics exists for a wide class of physically reasonable potentials (see, e.g., Ref. 2).

To define the said class of superstable interactions we denote by $\overline{\Delta}$ a partition of $\mathbb{R}^d$ into half open unit cubes Δ centered at the points $r\in\mathbb{Z}^d$ (see Ref. 28 for details):

$$\mathbb{R}^d=\bigcup_{\Delta\subset\overline{\Delta}}\Delta,\quad \forall\Delta,\Delta'\in\overline{\Delta},\quad \Delta\cap\Delta'=\varnothing.$$

We assume the following conditions to hold:
(A1) Smoothness:

$$\phi, \quad \psi \in C^3(\mathbb{R}^d \backslash \{0\}).$$

(A2) Superstability:

$$\forall i = 1,2,3 \quad \exists A_i > 0, \quad B_i \geqslant 0: \quad U_{v_i}(\gamma) \geqslant \sum_{\Delta \in \Delta}{}_{-} (A_i |\gamma_\Delta|^2 - B_i |\gamma_\Delta|),$$

with $v_1 = \phi$, $v_2 = -\Delta\phi$ and $v_3 = \psi$.
(A3) Lower-regularity:
For any $X, Y \subset \mathbb{R}^d$ and configurations $\gamma_X \in \Gamma_X$, $\gamma_Y \in \Gamma_Y$, define

$$W_{v_i}(\gamma_X | \gamma_Y) = \sum_{x \in \gamma_X, y \in \gamma_Y} v_i(x-y). \tag{3.1}$$

Then

$$-W_{v_i}(\gamma_X | \gamma_Y) \leqslant \sum_{\Delta, \Delta' \in \Delta}{}_{-} \Psi_{v_i}(\Delta, \Delta') |\gamma_\Delta| |\gamma_{\Delta'}|, \tag{3.2}$$

where

$$\Psi_v(\Delta, \Delta') = \sup_{x \in \Delta, x' \in \Delta'} v_-(x - x'),$$

and $v_- = -\min(v, 0)$. We also require the existence of positive decreasing functions $\Psi_i(k)$ on positive integers such that

$$\Psi_i(k) \geqslant \sup_{\Delta, \Delta' \in \bar{\Delta}; d(\Delta, \Delta') = k} \Psi_{v_i}(\Delta, \Delta') \tag{3.3}$$

and

$$\sum_{k=0}^{\infty} \Psi_i(k) k^{d + \mu_i - 1} = F_{\mu_i} < +\infty \tag{3.4}$$

with $\mu_1 = \mu_3 > \frac{1}{2}$, $\mu_2 > -\frac{3}{2}$ and

$$d(\Delta, \Delta') = \max_{1 \leqslant \alpha \leqslant d} \inf_{x \in \Delta, x' \in \Delta'} |x^{(\alpha)} - x'^{(\alpha)}|.$$

Now we describe some class Φ of potentials which satisfy (A.1)–(A.3). Let

$$\begin{gathered} \phi(x) = \phi_+(x) + \phi_{st}(x), \\ \phi_+(0) = +\infty, \quad \phi_+(x) > 0, \end{gathered} \tag{3.5}$$

$$\begin{gathered} -\Delta\phi_+(0) = +\infty, \quad -\Delta\phi_+(x) > 0, \\ \phi_{st}(x) = \frac{1}{(2\pi)^d} \int dk e^{ixk} \tilde{\phi}(k), \quad \phi(k) \geqslant 0, \end{gathered} \tag{3.6}$$

$$\int dk\tilde{\phi}(k)<\infty, \quad \int dkk^2\tilde{\phi}(k)<\infty. \tag{3.7}$$

As an example (for $d=3$) of such a potential we can choose some function which has an asymptotic behavior near the origin like

$$\phi_+(x)\sim\frac{C_1}{|x|^\alpha}, \quad 0<\alpha\leqslant 1 \quad for \quad |x|<r_0, \quad r_0>0,$$

and is sufficiently fast decreasing as $|x|\nearrow+\infty$. This is clear from a direct calculation which gives

$$-\Delta\frac{1}{|x|^\alpha}=\frac{\alpha(1-\alpha)}{|x|^{\alpha+2}}, \tag{3.8}$$

which is positive for $\alpha<1$.

IV. RUELLE'S CONSTRUCTIONS. MAIN RESULT

Our main technical tool is the technique of superstability estimates proposed by Ruell[28] for classical statistical mechanics. Later Esposito *et al.*[29] generalized this technique for the case of quantum statistical mechanics and proved the boundedness of the reduced density matrices (RDMs) for the Maxwell–Boltzmann statistics.

In this section we briefly recall some basic constructions which were made in Refs. 28 and 29.

A. Λ_q-cubs

For some $\alpha>0$ (to be fixed later) let

$$l_q=[e^{\alpha q}], \quad q\in\mathbb{N}, \tag{4.1}$$

where $[x]$ is the integer part of $x\in\mathbb{R}^+$ and

$$\Lambda_q=[-l_q-\tfrac{1}{2},l_q+\tfrac{1}{2}]^d, \quad |\Lambda_q|=(2l_q+1)^d. \tag{4.2}$$

We also set the origin in the center of some cube $\Delta_1\in\overline{\Delta}$. So, every cube Λ_q is the union of cubes Δ from $\overline{\Delta}$. And for convenience we suppose that for one of the trajectories $\omega\in\eta$ we have $\omega(0)=0\in\Delta_1\subset\mathbb{R}^d$. Following Ref. 29 we also introduce the sequence

$$\varphi(q)=q|\Lambda_q|. \tag{4.3}$$

We extensively use the following properties (see Ref. 29 for details). For given $\varepsilon>0$, $\alpha>0$ $\exists s_0$ such that for $s\geqslant s_0$

$$1+\alpha<\frac{l_{s+1}}{l_s}<e^{\alpha(1+\varepsilon)},$$

$$\frac{\varphi(s+1)}{\varphi(s)}<e^{\alpha(d+\varepsilon(d+1))}, \tag{4.4}$$

or for $\varepsilon<\varepsilon_0=1-2\alpha e^{2\alpha}$ (α is sufficiently small)

$$\frac{l_{s+1}}{l_s}<1+2\alpha,$$

$$\frac{\varphi(s+1)}{\varphi(s)}<(1+2\alpha)^{d+1}. \tag{4.5}$$

We also need the following lemma:
Lemma 4.1 (see Ref. 29): Let

$$r(k)=\min\{r\in\mathbb{N}|l_{q+r}>l_q+k,\quad \forall q\geqslant 1,\quad k\in\mathbb{N}\}. \tag{4.6}$$

Then

$$r(k)\leqslant 1+\frac{1}{\alpha}\log(k+2). \tag{4.7}$$

B. An extension of the functionals $\rho_t^\Lambda(\eta)$

The functionals ρ_t^Λ are defined on the configuration space Γ_{Ω_Λ}, where Ω_Λ is the space of continuous trajectories $\omega(\tau)$ [see (2.18)] with $\omega(0)\in\Lambda$. But in the construction we are going to apply we need to consider functionals ρ_t^Λ on the trajectories which take values in the bounded cube Λ_q or in its compliment Λ_q^c. In this case some trajectories can be discontinuous because they take their values in Λ_q not for all $\tau\in[0,t_\beta]$ but only in some intervals $[\tau_1,\tau_2]$, $[\tau_3,\tau_4]$, etc. So for $\tau\in(\tau_2,\tau_3),\ldots$ they are not defined. In this case the definition of $\tilde{U}(\eta_{\Lambda_q}\cup\gamma)$ and therefore $\rho_t^\Lambda(\eta_{\Lambda_q})$ becomes ambiguous. To avoid these difficulties we repeat the construction proposed in Ref. 29.

Let $\mathfrak{B}([0,t_\beta])$ be the σ-algebra of Borel sets in $[0,t_\beta]$ with Ω_B the set of all measurable functions:

$$\tilde{\omega}:B\to\mathbb{R}^d,\quad B\in\mathfrak{B}([0,t_\beta]). \tag{4.8}$$

Now we define a new configuration space by

$$\Gamma_{\tilde{\Omega}}=\bigcup_{n\geqslant 0}\Gamma_{\tilde{\Omega}}^{(n)}, \tag{4.9}$$

where for $n=0$ $\Gamma_{\tilde{\Omega}}^{(0)}$ is a nonempty set which, however, consists of the trajectories $\tilde{\omega}$ whose domain B have zero Lebesgue measure and

$$\Gamma_{\tilde{\Omega}}^{(n)}=\tilde{\Omega}_1^{\otimes n-symm},\quad \tilde{\Omega}_1=\bigcup_{B\in\mathfrak{B}([0,t_\beta])}\Omega_B. \tag{4.10}$$

Then, instead of $\tilde{U}(\omega)_{m+n}=\tilde{U}(\eta\cup\gamma)$, $\eta=\{\omega_1,\ldots,\omega_m\}$, $\gamma=\{\omega_{m+1},\ldots,\omega_{m+n}\}$ we define $\tilde{U}(\tilde{\eta}\cup\gamma)$ by the same formula (2.21) and (2.22), but instead of $U_{v_k}(\omega(\tau))_{m+n}$, $k=1,2$ ($v_1=\phi, v_2=-\Delta\phi$) we set for $\tilde{\omega}_j\in\tilde{\Omega}_1$

$$\sum_{1\leqslant i<j\leqslant m+n}\chi_{D(\tilde{\omega}_i)\cap D(\tilde{\omega}_j)}(\tau)v_k(\tilde{\omega}_i(\tau)-\tilde{\omega}_j(\tau)), \tag{4.11}$$

where $D(\tilde{\omega})$ is the domain of $\tilde{\omega}$. For fixed $\tilde{\eta}\in\Gamma_{\tilde{\Omega}}$ the function

$$\tilde{U}(\tilde{\eta}\cup\cdot):\Gamma_\Omega\to\mathbb{R}$$

is measurable on Γ_Ω w.r.t. the σ-algebra of Borel sets corresponding to the topology of point-wise convergence (see Ref. 29 for details). Finally, we define

$$\tilde{\rho}_t^\Lambda(\tilde{\eta})=\int_{\Gamma_{\Omega_\Lambda}}\lambda_{\tilde{\sigma}}^\Lambda(d\tilde{\gamma})\tilde{D}_0^\Lambda(\tilde{\eta}^0\cup\gamma^0)e^{-\tilde{U}(\tilde{\eta}\cup\gamma)}, \tag{4.12}$$

which is an extension of definition (2.28) [here $\tilde{\eta}$ has a different sense than in (2.28) (see Remark 2.4)].

It is clear that for $\eta \in \Gamma_{\Omega_\Lambda}$

$$\rho_t^\Lambda(\eta) = \tilde{\rho}_t^\Lambda(\tilde{\eta}). \tag{4.13}$$

Then for any bounded measurable $X \subset \Lambda$ we define the map $\pi_X : \Gamma_{\Omega_\Lambda} \to \Gamma_{\tilde{\Omega}_\Lambda}$, such that for any $\gamma \in \Gamma_{\Omega_\Lambda}$

$$\pi_X \gamma = (\pi_X \omega_1, \ldots, \pi_X \omega_{|\gamma|}), \tag{4.14}$$

where $\pi_X \omega_j \in \tilde{\Omega}_\Lambda$ and its domain is the measurable set

$$B = \{\tau \in [0, t_\beta] \,|\, \omega(\tau) \in X\}.$$

If B has nonzero Lebesgue measure, then $(\pi_X \omega)(\tau) = \omega(\tau)$, $\tau \in B$, and if B has zero measure, then $\pi_X \omega \in \Gamma_{\tilde{\Omega}}^{(0)}$. We need also the map $s : \Gamma_{\Omega_\Lambda} \to \Gamma_{\tilde{\Omega}_\Lambda}$, which is

$$\gamma \to s(\gamma) = \bigcup_{\Delta \in \overline{\Delta}} \pi_\Delta \gamma. \tag{4.15}$$

The union is taken over all $\Delta \in \overline{\Delta}$, such that $\pi_\Delta \gamma$ has a domain of nonzero Lebesgue measure. It is clear that

$$\tilde{\rho}_t^\Lambda(\tilde{\eta}) = \tilde{\rho}_t^\Lambda(s(\eta)). \tag{4.16}$$

C. Partitions of Γ_{Ω_Λ}

For every $\tau \in [0, t_\beta]$ and a given configuration $\tilde{\eta} \in \Gamma_{\tilde{\Omega}_\Lambda}$ we introduce some characteristics of a given configuration $\gamma \in \Gamma_{\Omega_\Lambda}$:

$$E_q^\tau(\xi) = E_{\Lambda_q}^\tau(\xi) = \sum_{\Delta \subset \Lambda_q} |\xi_\Delta^\tau|^2, \quad \xi = \tilde{\eta} \cup \gamma, \tag{4.17}$$

where $|\xi_\Delta^\tau|$ is the number of all trajectories from ξ which take values in Δ at time τ. We also denote $E^\tau(\xi)$ by the same expression (4.17) with summation over all $\Delta \in \overline{\Delta}$.

Then we define three factors

$$E_q^{(1)}(\xi) = E_q^{t_\beta}(\xi), \tag{4.18}$$

$$E_q^{(2)}(\xi) = \int_0^{t_\beta} d\tau E_q^\tau(\xi), \tag{4.19}$$

$$E_q^{(3)}(\xi) = E_q^0(\xi), \tag{4.20}$$

which correspond to the factors $\exp\{-1/2\beta U_\phi(\tilde{\eta}^{t_\beta} \cup \gamma^{t_\beta}\}$, $\exp\{\beta U_{\Delta\phi}(\tilde{\eta} \cup \gamma)\}$ and $\tilde{D}_0^\Lambda(\tilde{\eta}^0 \cup \gamma^0)$, respectively, to be controlled, and define

$$E_q(\xi) = \sum_{i=1}^{3} E_q^{(i)}(\xi). \tag{4.21}$$

Following Ref. 29 we can now construct a partition of Γ_{Ω_Λ} in the following way. For some large integer q_0 (to be fixed later) we introduce

$$\Gamma_{q_0-1}=\{\gamma\in\Gamma_{\Omega_\Lambda}|E_m(\xi)\leqslant\varphi(m) \quad \text{for all} \quad m\geqslant q_0-1\}, \tag{4.22}$$

and for $q\geqslant q_0$

$$\Gamma_q=\{\gamma\in\Gamma_{\Omega_\Lambda}|E_{q-1}(\xi)>\varphi(q-1), \quad \text{but} \quad E_m(\xi)\leqslant\varphi(m) \quad \text{for} \quad m\geqslant q\}. \tag{4.23}$$

Then for $q\geqslant q_0-1$ let $\chi_q(\gamma)$ be an indicator function of the set Γ_q and for the partition

$$\Gamma_{\Omega_\Lambda}=\bigcup_{q\geqslant q_0-1}\Gamma_q \tag{4.24}$$

we consider the partition of the unity:

$$1=\sum_{q\geqslant q_0-1}\chi_q(\gamma). \tag{4.25}$$

D. Main result

Theorem 4.1: *For the interactions $\phi(x)$ $(x\in\mathbb{R}^d,\ d\leqslant 3)$, which satisfy (A1)–(A3), and for initial distributions (1.21)–(1.23) there exist constants $c_1=c_1(z,\beta,T)$ and $c_2=c_2(z,\beta,T)$ such that*

$$k_t^\Lambda(x)_m\leqslant c_1^m, \quad \eta\equiv\{x_1,\ldots,x_m\}\in\Gamma_\Lambda. \tag{4.26}$$

For any $t_1,t_2\in[0,T]$

$$|\langle k_{t_1}^\Lambda,\varphi\rangle-\langle k_{t_2}^\Lambda,\varphi\rangle|\leqslant c_2^m\|\varphi\|_m|t_1-t_2|, \tag{4.27}$$

uniformly in Λ and $t\in[0,T]$. Here

$$\langle k_t^\Lambda,\varphi\rangle=\int_{\mathbb{R}^{dm}}k_t^\Lambda(x)_m\varphi(x)_m(dx)^m, \tag{4.28}$$

where $(dx)^m=dx_1\cdot\cdots\cdot dx_m$, for $(x)_m=\{x_1,\ldots,x_m\}$, $\varphi\in C_0^\infty(\mathbb{R}^{dm})$,

$$c_2^m=\max\{m\xi_1^m\beta^{-1}, \quad m(m-1)\xi_1^m, \quad m\xi_1^{m+1}\}, \tag{4.29}$$

and

$$\|\varphi\|_m=\max_{1\leqslant j\leqslant m}\|\Delta_j\varphi\|_{L^1(\mathbb{R}^{md})}+\max_{j\neq k}\|\nabla_j\varphi\cdot\nabla_k\phi\|_{L^1(\mathbb{R}^{md})}+\max_j\|\nabla\phi\|_{L^1(\mathbb{R}^d)}\|\nabla_j\varphi\|_{L^1(\mathbb{R}^{md})}. \tag{4.30}$$

Remark 4.1: For potentials $\phi\in\Phi$ it is clear that $\|\nabla\phi\|_{L^1(\mathbb{R}^d)}<\infty$ (see Sec. III).

Remark 4.2: From (4.26), by compactness, we can choose a sequence $(\Lambda_n)_{n=1}^\infty$, $\Lambda_n\subset\Lambda_{n+1}$, $\Lambda_n\nearrow\mathbb{R}^d$, so that we get a limit point (in the weak sense) for $k_t^{\Lambda_n}$. Hence by diagonal argument we obtain the existence of a corresponding limit for any rational $t\in[0,T]$. Then from the continuity property (4.27) the existence of a weak-limit for k_t^Λ follows for all $t\in[0,T]$. And, finally, using positive-definiteness [see Remark 2.3, (2.25)–(2.27)] of k_t^Λ for any $\Lambda\subset\mathbb{R}^d$ we get a limit state μ_t (not unique), such that $K^*\mu_t=\rho_{\mu_t}=k_t\lambda_\sigma$.

V. PROOF OF THE MAIN THEOREM

First we note that neglecting the positive part of the effective potential $\tilde{V}(x)_n$ [see (2.16)] we get

$$\tilde{\rho}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda) \leqslant \tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda), \tag{5.1}$$

where

$$\tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda) = \tilde{\rho}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda)\big|_{\tilde{V}^+ \equiv 0}.$$

Then, the main technical point of the proof is the following proposition.

Proposition 5.1: Under the same hypothesis as in Theorem 4.1 there exist a small $\alpha > 0$, a sufficiently large integer $q_0 = q_0(\alpha)$, constants $h(q_0), K(q_0)$, and a positive decreasing function $\varepsilon(q)$ such that

$$\tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda) \leqslant C_0 e^{-(1/4)\,\beta A E(\eta_{\Lambda_{q_0}})} \tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_{\Lambda^c_{q_0}}) + \sum_{q \geqslant q_0} C_q e^{-(1/4)\,\beta A E(\tilde{\eta}_{\Lambda_q})} \tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_{\Lambda^c_q}), \tag{5.2}$$

with

$$A = \min\{A_1, \quad 2A_2, \quad A_3\},$$

$$C_0 = e^{h(q_0)+K(q_0)}, \quad C_q = e^{-(1/8)\,\beta A \varphi(q-1)+\varepsilon(q)\varphi(q-1)+K(q_0)}, \quad q \geqslant q_0.$$

The proof of Theorem 4.1 follows from the next lemma.

Lemma 5.1: Let

$$S(\tilde{\eta}) = \{\Delta \in \overline{\Delta} \,|\, \exists\, \tau \in [0, t_\beta] \quad \textit{and} \quad \omega \in \tilde{\eta} \quad \textit{such that} \quad \omega(\tau) \in \Delta\}.$$

Then

$$\rho^{\Lambda}_{t_\beta}(\tilde{\eta}) \leqslant e^{-(1/4)\,\beta A E(\tilde{\eta}) + \delta |S(\tilde{\eta})|}, \tag{5.3}$$

with $\delta > \log D$, $D = C_0 + \Sigma_{q \geqslant q_0} C_q$.

Proof: We shall proceed by induction. Let $\tilde{\eta}'$ be a subconfiguration of $\tilde{\eta}$. We assume that (5.2) is true for any such $\tilde{\eta}'$. Then from (5.2)

$$\begin{aligned}\tilde{\tilde{\rho}}^{\Lambda}_{t_\beta}(\tilde{\eta}_\Lambda) &\leqslant C_0 e^{-AE(\tilde{\eta}_{\Lambda_{q_0}}) - AE(\tilde{\eta}_{\Lambda^c_{q_0}}) + \delta |S(\tilde{\eta}_{\Lambda^c_{q_0}})|} + \sum_{q \geqslant q_0} C_q e^{-AE(\tilde{\eta}_{\Lambda_q}) - AE(\tilde{\eta}_{\Lambda^c_q}) + \delta |S(\tilde{\eta}_{\Lambda^c_q})|} \\ &\leqslant e^{-AE(\tilde{\eta}_\Lambda) + \delta |S(\tilde{\eta}_\Lambda)|},\end{aligned}$$

since $|S(\tilde{\eta}_{\Lambda^c_q})| \leqslant |S(\tilde{\eta}_\Lambda)| - 1$. Taking into account (5.1) we get (5.3). □

Proof of Theorem 4.1: Using (5.3) from (2.19) we get

$$k^{\Lambda}_t(x)_m \leqslant z^m \prod_{j=1}^{m} \int dy_j \int W^{t_\beta}_{x_j, y_j}(d\omega_j) e^{-AE(\omega_j) + \delta |S(\omega_j)|}.$$

Using the Schwartz inequality, the estimate [see Ref. 29, (A.21)]

$$\int W^{t_\beta}_{x,y}(d\omega) e^{2\delta |S(\omega)|} \leqslant (2\pi t_\beta)^{-d/2} I(2\delta), \quad I(2\delta) = \int W^{t_\beta}_{0,0}(d\omega) e^{2\delta |S(\omega)|},$$

and the trivial estimate

$$\int dy \left(\int W^{t_\beta}_{x,y}(d\omega) \right)^{1/2} \leqslant 2^{3d/4} \pi^{d/4} t^{d/4}$$

we obtain (4.26) with

$$c_1 = z((4\pi)^d I(2\delta))^{1/2}.$$

In the same way one can prove Eq. (4.27). Indeed, we have by (1.18) that

$$\langle k^\Lambda_{t_1}, \varphi\rangle - \langle k^\Lambda_{t_2}, \varphi\rangle = \int_{t_1}^{t_2} d\tau \left\langle \frac{dk^\Lambda_\tau}{d\tau}, \varphi \right\rangle$$

$$= \int_{t_1}^{t_2} d\tau \sum_{j=1}^{m} [\langle k^\Lambda_\tau, \Delta_j \varphi\rangle - \langle k^\Lambda_\tau, \nabla_j \varphi \cdot \nabla_j U_\phi\rangle - \langle\langle k^\Lambda_\tau, \nabla_j \phi\rangle \nabla_j \varphi\rangle].$$

Using (4.26) we get (4.27) with the constants (4.29) and (4.30). □

Proof of Proposition 5.1: Inserting (4.25) into (4.12) we get

$$\tilde{\tilde{\rho}}^\Lambda_t(\tilde{\eta}_\Lambda) = \sum_{q \geqslant q_0 - 1} I_q(\tilde{\eta}_\Lambda), \tag{5.4}$$

with

$$I_q(\tilde{\eta}_\Lambda) = \int \lambda^\Lambda_{\tilde{\sigma}}(d\gamma) \chi_q(\gamma) \tilde{D}^\Lambda_0(\tilde{\eta}^0_\Lambda \cup \gamma^0) e^{-\tilde{\tilde{U}}(\tilde{\eta}\cup\gamma)}, \tag{5.5}$$

where

$$\tilde{\tilde{U}}(\tilde{\eta}\cup\gamma) = \tilde{U}(\tilde{\eta}\cup\gamma) - \tilde{V}^+(\eta\cup\gamma). \tag{5.6}$$

To estimate (5.5) we construct a further partition of Γ_q:[29]

$$\Gamma_q = \Gamma_{q,\Lambda} = \Gamma_{q,\Lambda_q} \cup \Gamma_{q,\Lambda^c_q} \cup \Gamma^s_{q,\partial\Lambda_q} \cup \Gamma^l_{q,\partial\Lambda_q},$$

where Γ_{q,Λ_q} is the configuration of those trajectories which are completely contained in Λ_q, Γ_{q,Λ^c_q} are trajectories completely outside of Λ_q, i.e., in Λ^c_q, $\Gamma^s_{q,\partial\Lambda_q}$ are short trajectories, which cross the boundary of Λ_q but do not leave Λ_{q+2} and $\Gamma^l_{q,\partial\Lambda_q}$ are long trajectories, which cross $\partial\Lambda_q$ and leave Λ_{q+2}. By the infinite-divisibility of the Poisson–Lebesgue measure $\lambda_{\tilde{\sigma}}$, for any function $F(\gamma) \in L^1(\Gamma_{\Omega_\Lambda}, \lambda^\Lambda_{\tilde{\sigma}})$ which can be represented as

$$F(\gamma) = F_1(\gamma_{\Lambda_q}) F_2(\overline{\gamma}_{\Lambda^c_q}) F_3(\zeta_{\partial\Lambda_q}) F_4(\overline{\zeta}_{\partial\Lambda_q}) \tag{5.7}$$

for

$$\gamma = \gamma_{\Lambda_q} \cup \overline{\gamma}_{\Lambda^c_q} \cup \zeta_{\partial\Lambda_q} \cup \overline{\zeta}_{\partial\Lambda_q}, \quad \gamma_{\Lambda_q} \in \Gamma_{\Lambda_q}, \quad \overline{\gamma}_{\Lambda^c_q} \in \Gamma_{\Lambda^c_q}, \quad \zeta_{\partial\Lambda_q} \in \Gamma^s_{\partial\Lambda_q}, \quad \overline{\zeta}_{\partial\Lambda_q} \in \Gamma^l_{\partial\Lambda_q}$$

the following formula is true:

$$\int \lambda^\Lambda_{\tilde{\sigma}}(d\gamma) F(\gamma) = \int_{\Gamma_{q,\Lambda_q}} \lambda^{\Lambda_q}_{\tilde{\sigma}}(d\gamma) F_1(\gamma) \int_{\Gamma_{q,\Lambda^c_q}} \lambda^{\Lambda^c_q}_{\tilde{\sigma}}(d\overline{\gamma}) F_2(\overline{\gamma})$$

$$\times \int_{\Gamma^s_{q,\partial\Lambda_q}} \lambda^\Lambda_{\tilde{\sigma}}(d\zeta) F_3(\zeta) \int_{\Gamma^l_{q,\partial\Lambda_q}} \lambda^\Lambda_{\tilde{\sigma}}(d\overline{\zeta}) F_4(\overline{\zeta}).$$

But in our case the function

$$F(\gamma)=\chi_q(\gamma)\tilde{D}_0^{\Lambda}(\tilde{\eta}_{\Lambda}^0\cup\gamma_{\Lambda}^0)e^{-\tilde{\tilde{U}}(\tilde{\eta}\cup\gamma)} \tag{5.8}$$

does not satisfy (5.7). So, our next step is to estimate (5.8) as a product of some functions as in (5.7).

Due to (5.6), (2.21) and (2.22) we have

$$\tilde{\tilde{U}}(\tilde{\eta}\cup\gamma)=\frac{1}{2}\beta U_{v_1}(\tilde{\eta}^{t_\beta}\cup\gamma^{t_\beta})+\beta\int_0^{t_\beta}d\tau U_{v_2}(\tilde{\eta}^{\tau}\cup\gamma^{\tau}),$$

with $v_1=\phi$, and $v_2=-\Delta\phi$. Then for any $\tau\in[0,t_\beta]$ we can write for the energy $U_{v_i}(\tilde{\eta}^{\tau}\cup\gamma^{\tau})$ the following decomposition:

$$\begin{aligned}U_{v_i}(\tilde{\eta}^{\tau}\cup\gamma^{\tau})=&U_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q}\cup\gamma^{\tau}_{\Lambda_q}\cup(\pi_{\Lambda_q}\zeta)^{\tau}\cup(\pi_{\Lambda_q}\overline{\zeta})^{\tau})+U_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q^c}\cup\overline{\gamma}^{\tau}_{\Lambda_q^c})+U_{v_i}((\pi_{\Lambda_q^c}\zeta)^{\tau}\cup(\pi_{\Lambda_q^c}\overline{\zeta})^{\tau})\\&+W_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q}\cup\gamma^{\tau}_{\Lambda_q}\cup(\pi_{\Lambda_q}\zeta)^{\tau}\cup(\pi_{\Lambda_q}\overline{\zeta})^{\tau}|\tilde{\eta}^{\tau}_{\Lambda_q^c}\cup\overline{\gamma}^{\tau}_{\Lambda_q^c}\cup(\pi_{\Lambda_q^c}\zeta)^{\tau}\cup(\pi_{\Lambda_q^c}\overline{\zeta})^{\tau})\\&+W_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q^c}\cup\overline{\gamma}^{\tau}_{\Lambda_q^c}|(\pi_{\Lambda_q^c}\zeta)^{\tau})+W_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q^c}\cup\overline{\gamma}^{\tau}_{\Lambda_q^c}|(\pi_{\Lambda_q^c}\overline{\zeta})^{\tau}),\end{aligned} \tag{5.9}$$

where in the same way as for $\tilde{U}$ we use the substitution (4.11) to define the interaction energy W_{v_i} for $\tilde{\omega}\in\tilde{\Omega}_1$. Now to estimate the various terms in (5.9) we prove some lemmas.

Lemma 5.2: For each positive, integer q and $\tau\in[0,t_\beta]$

$$U_{v_i}(\tilde{\eta}^{\tau}_{\Lambda_q}\cup\gamma^{\tau}_{\Lambda_q}\cup(\pi_{\Lambda_q}\zeta)^{\tau}\cup(\pi_{\Lambda_q}\overline{\zeta})^{\tau})\geqslant\frac{1}{4}A_iE_q^{\tau}(\xi)+\frac{1}{2}A_iE_q^{\tau}(\tilde{\eta}_{\Lambda_q})-\frac{B_i^2}{A_i}|\Lambda_q|. \tag{5.10}$$

Proof: The proof follows from Lemma A.1 (see the Appendix) and the definition of $E_q^{\tau}(\xi)$. □

By the stability condition we have

$$U_{v_i}((\pi_{\Lambda_q^c}\zeta)^{\tau}\cup(\pi_{\Lambda_q^c}\overline{\zeta})^{\tau})\geqslant-B_i(|\zeta|+|\overline{\zeta}|). \tag{5.11}$$

Lemma 5.3: Let ξ_a and ξ_a' be subconfigurations of $\xi\in\Gamma_q$ and ξ_a contained in Λ_{q+a} and ξ_a' in Λ_q^c. Then for any $\tau\in[0,t_\beta]$ there exist a small enough α, sufficiently large $q_0^{(1)}$, a constant $h_i^{(a)}(q_0^{(1)})$ and a decreasing function $\varepsilon_i^{(a)}(q)$ on the integers, such that for each $q\geqslant q_0^{(1)}-1$

$$-W_{v_i}(\xi_a^{\tau}|\xi_a'^{\tau})\leqslant\begin{cases}h_i^{(a)}(q_0^{(1)}) & \text{for } q=q_0^{(1)}-1,\\ \varepsilon_i^{(a)}(q)\varphi(q-1) & \text{for } q\geqslant q_0^{(1)}.\end{cases} \tag{5.12}$$

Remark 5.1: We use Lemma 5.3 with $a=0$ for the fourth term in (5.9) ($\xi_0=\tilde{\eta}_{\Lambda_q}\cup\gamma_{\Lambda_q}$, $\xi_0'=\tilde{\eta}_{\Lambda_q^c}\cup\overline{\gamma}_{\Lambda_q^c}\cup\pi_{\Lambda_q^c}\xi\cup\pi_{\Lambda_q^c}\overline{\zeta}$) and with $a=2$ for the fifth term of (5.9) ($\xi_2=\pi_{\Lambda_q^c}\zeta$, $\xi_2'=\tilde{\eta}_{\Lambda_q^c}\cup\overline{\gamma}_{\Lambda_q^c}$).

Proof: Let us prove the lemma for $a=0$, $i=1$ and for $q\geqslant q_0^{(1)}$ which we chose later. Taking $i=1$, $a=0$ and $\tau=t_\beta$ in Lemma A.2 and using the fact that

$$E^{(1)}_{q+1\setminus q-1}(\xi^{t_\beta})\leqslant E_{q+1\setminus q-1}(\xi)=E_{q+1}(\xi)-E_{q-1}(\xi)$$

and because of $\xi\in\Gamma_q$, $E_{q-1}(\xi)>\varphi(q-1)$ and $E_m(\xi)\leqslant\varphi(m)$ for $m\geqslant q$, we have

$$-W_{v_1}(\xi_0^{t_\beta}|\xi_0'^{t_\beta}) \leqslant \frac{1}{2}F_{\mu_1}[\varphi(q+1)-\varphi(q-1)]+\frac{1}{2}\beta\varepsilon_1^{(1)}(q)\varphi(q) + \frac{1}{2}\beta\varepsilon_2^{(2)}(q)\varphi(q)\sum_{k=1}^{\infty}(a_k^{(1)}-a_{k+1}^{(1)})\varphi(q+k+1), \tag{5.13}$$

where $a_k^{(1)}=\Psi_1(l_{q+k}-l_q)$. Then from (4.5) we have

$$\varphi(q+1)-\varphi(q-1)<[(1+2\alpha)^{2d+2}-1]\varphi(q-1), \tag{5.14}$$

$$\varphi(q)<(1+2\alpha)^{d+1}\varphi(q-1). \tag{5.15}$$

From the definitions (4.1)–(4.3), choosing α sufficiently small and

$$q_0^{(1)}>-\frac{2}{\alpha}\log(1-e^{-2\alpha}), \tag{5.16}$$

it is easy to calculate that $q+k+1<(2/\alpha)\log(l_{q+k+1}-l_q+1)$ and

$$\sum_{k=1}^{\infty}(a_k^{(1)}-a_{k+1}^{(1)})\varphi(q+k+1)\leqslant c(\alpha)\sum_{l_{q+1}-l_q}^{\infty}\Psi_1(m)(2m+1)^d\log(m+1)=c(\alpha)\varepsilon_0(q) \tag{5.17}$$

with $c(\alpha)=2\alpha^{-1}(1+\alpha)$. Now from (5.13)–(5.16) we have (5.12) for $q\geqslant q_0^{(1)}$ with

$$\varepsilon_1^{(0)}(q)=\tfrac{1}{2}\beta F_{\mu_1}[(1+2\alpha)^{2d+2}-1]+\tfrac{1}{2}\beta\varepsilon_1^{(1)}(q)(1+2\alpha)^{d+1} + \tfrac{1}{2}\beta\varepsilon_2^{(1)}(q)(1+2\alpha)^{d+1}c(\alpha)\varepsilon_0(q). \tag{5.18}$$

The proofs for the cases $i=2$ and $a=2,i=1,2$ are the same.

Now we consider the case $q=q_0^{(1)}-1$. The only difference in the proof lies in estimating the first term in Eq. (A2). As $\gamma\in\Gamma_{q_0-1}$ this term cannot be very small and we estimate it by

$$E^{t_\beta}_{q_0^{(1)}\setminus q_0^{(1)}-2}(\xi^{t_\beta})\leqslant E_{q_0}(\xi)\leqslant\varphi(q_0^{(1)}).$$

Then inequality (5.12) for $q=q_0^{(1)}-1$ holds with

$$h_i^{(a)}=[\tfrac{1}{2}\beta F_{\mu_i}+\tfrac{1}{2}\beta\varepsilon_1^{(i)}(q_0^{(1)})+\tfrac{1}{2}\beta\varepsilon_2^{(i)}(q_0^{(i)})]\varepsilon(q_0^{(1)}).$$

□

And finally the sixth term of (5.9) can be estimated by

Lemma 5.4: Let $\overline{\zeta}$ be some subconfiguration of $\gamma\in\Gamma_q$, contained in Λ_m, $m>q$. Then there exist a $q_0^{(2)}$ large enough and some constant $b=b(\alpha,d)$, such that for each $q\geqslant q_0^{(2)}$

$$-\tfrac{1}{2}\beta W_{v_1}((\pi_{\Lambda_q^c}\overline{\zeta})^{t_\beta}|\,\widetilde{\eta}^{t_\beta}_{\Lambda_q^c}\cup(\pi_{\Lambda_q^c}\gamma)^{t_\beta})\leqslant\tfrac{1}{2}\beta bF_{\mu_1}|\overline{\zeta}|\varphi(m)^{1/2}, \tag{5.19}$$

$$-\beta W_{v_2}(\pi_{\Lambda_q^c}\overline{\zeta}|\,\widetilde{\eta}_{\Lambda_q^c}\cup\pi_{\Lambda_q^c}\gamma)\leqslant tbF_{\mu_2}|\overline{\zeta}|\varphi(m)^{1/2}. \tag{5.20}$$

Proof: The proofs of (5.19) and (5.20) are almost the same. Let us prove for example (5.19). Using Lemma A.3. with $\tau=t_\beta$, $\xi_1=\pi_{\Lambda_q^c}\overline{\zeta}$, $\xi_2=\widetilde{\eta}_{\Lambda_q^c}\cup\pi_{\Lambda_q^c}\gamma$ and taking into account that for $m>q$

$$E^{t_\beta}_{m+r(k)}(\xi) \leqslant E_{m+r(k)}(\xi) \leqslant \varphi(m+r(k)),$$

as $\xi = \tilde{\eta} \cup \gamma$ and $\gamma \in \Gamma_q$ we get

$$-\frac{1}{2}\beta W_{v_1}(\cdots|\cdots) \leqslant \frac{1}{2}\beta b_1 |\overline{\zeta}| \sum_{k=1}^{\infty} \Psi_1(k)(k+1)^{(d-1)/2} \varphi(m+r(k))^{1/2}.$$

[See for $r(k)$ Eqs. (4.6) and (4.7).] Using (4.4), (4.7) and (3.4) we get (5.19) with $b = b_1 \exp[\alpha/2(d+\varepsilon(d+1))] 2^{d-1+\mu}$, $\varepsilon = \min\{1-2\alpha e^{2\alpha}, (2\mu-1)(\alpha+1)^{-1}\}$ and $q_0^{(2)} = s_0$ (see (4.4), (4.5) for definition of s_0). □

And finally we present some inequalities for the initial density distribution (1.21)–(1.23).

Lemma 5.5: Let the potentials ϕ and ψ satisfy (A.1)–(A.3). *Then*

1^o. *For any $\Lambda_q \subset \Lambda$, $q \geqslant q_0 - 1$, and $\xi^0_\Lambda \in \Gamma_q$ there exist $A_3 > 0$ and $B_3 \geqslant 0$ such that*

$$\tilde{D}^\Lambda_0(\xi^0_\Lambda) \leqslant e^{[-A_3\beta\Sigma_{\Delta\subset\Lambda_q}|\xi^0_\Delta|^2 + B_3\beta\Sigma_{\Delta\subset\Lambda_q}|\xi^0_\Delta|]} \tilde{D}^\Lambda_0(\xi^0_{\Lambda^c_q}) \tag{5.21}$$

2^o. *For any partition*

$$\xi_{\Lambda^c_q} = \overline{\xi}^0_{\Lambda_s \cap \Lambda^c_q} \cup \tilde{\xi}^0_{\Lambda^c_q}, \quad \overline{\xi}^0_{\Lambda_s \cap \Lambda^c_q} \cap \tilde{\xi}^0_{\Lambda^c_q} = \varnothing, \quad s > q, \tag{5.22}$$

there exists $C_3 \geqslant 0$ such that

$$\tilde{D}^\Lambda_0(\xi^0_{\Lambda^c_q}) \leqslant e^{C_3\beta|\overline{\xi}^0_{\Lambda_s\cap\Lambda^c_q}|\varphi(s)^{1/2}} \tilde{D}^\Lambda_0(\tilde{\xi}^0_{\Lambda^c_q}). \tag{5.23}$$

Proof: The proof is a direct consequence of Ruelle's technique.[28]

Now we collect all the estimates (5.10)–(5.12), (5.19), (5.20), (5.21), and (5.23) to obtain for $q \geqslant q_0 = \max\{q_0^{(1)}, q_0^{(2)}\}$ [see (5.16)]:

$$I_q(\tilde{\eta}_\Lambda) \leqslant e^{-(1/4)\,\beta A E_q(\tilde{\eta}_{\Lambda_q}) - (1/8)\,\beta A\varphi(q-1) + \varepsilon_0(q)\varphi(q-1) + \varepsilon_1(q)\varphi(q-1)} \int \lambda^{\Lambda_q}_{\tilde{\sigma}}(d\gamma) \int \lambda^{\Lambda_{q+2}}_{\tilde{\sigma}}(d\zeta) e^{B|\zeta|}$$
$$\times \int \lambda^{\Lambda^c_q}_{\tilde{\sigma}}(d\overline{\gamma}) e^{-\tilde{\tilde{U}}(\tilde{\eta}_{\Lambda^c_q}\cup\overline{\gamma})} \tilde{D}^{\Lambda^c_q}_0(\tilde{\eta}^0_{\Lambda^c_q} \cup \overline{\gamma}^0) \prod_{m \geqslant q+3} \int \lambda^{\Lambda_m}_{\tilde{\sigma}}(d\overline{\zeta}^{(m)}) e^{B|\overline{\zeta}^{(m)}| + C|\overline{\zeta}^{(m)}|\varphi(m)^{1/2}} \tag{5.24}$$

with

$$A = \min\{A_1, \quad 2A_2, \quad 2A_3\},$$

$$B = \max\{\tfrac{1}{2}\beta B_1, \quad TB_2, \quad \beta B_3\},$$

$$C = \max\{\tfrac{1}{2}\beta b F_{\mu_1}, \quad TbF_{\mu_2}, \quad C_3\},$$

and

$$\epsilon_0(q) = \frac{(1+2\alpha)^{d+1}}{q}\left[\frac{\beta B_1^2}{2A_1} + \frac{TB_2^2}{A_2} + \frac{\beta B_3^2}{A_3}\right],$$

$$\varepsilon_1(q) = \sum_{i\in\{1,2\}} \sum_{a\in\{0,2\}} \varepsilon_i^{(a)}(q). \tag{5.25}$$

Now from the definition of the Poisson–Lebesgue measure we get

$$\int \lambda_{\tilde{\sigma}}^{\Lambda_q}(d\gamma) \leqslant e^{\varepsilon_2(q)\varphi(q-1)}, \quad \varepsilon_2(q) = \frac{z(1+2\alpha)^{d+1}}{q}, \tag{5.26}$$

$$\int \lambda_{\tilde{\sigma}}^{\Lambda_{q+2}}(d\zeta) e^{B|\zeta|} \leqslant e^{\varepsilon_3(q)\varphi(q-1)}, \quad \varepsilon_3(q) = \frac{z(1+2\alpha)^{3d+3}}{q} e^B, \tag{5.27}$$

$$\int \lambda_{\tilde{\sigma}}^{\Lambda_q^c}(d\overline{\gamma}) e^{-\tilde{\tilde{U}}(\tilde{\eta}_{\Lambda_q^c} \cup \overline{\gamma})} \tilde{D}_0^{\Lambda_q^c}(\tilde{\eta}^0_{\Lambda_q^c} \cup \overline{\gamma}^0) \leqslant \tilde{\tilde{\rho}}_{t_\beta}^{\Lambda}(\tilde{\eta}_{\Lambda_q^c}). \tag{5.28}$$

Applying the same arguments as in (5.26) and (5.27), making a partition of all long trajectories $\overline{\zeta}$ in (5.24) according to their lengths and using the resummation formula we get

$$I_q^{(4)} \equiv \prod_{m \geqslant q+3} \int \lambda_{\tilde{\sigma}, \partial\Lambda_q}^{\Lambda_m}(d\overline{\zeta}^{(m)}) e^{B|\overline{\zeta}^{(m)}| + C|\overline{\zeta}^{(m)}|\varphi(m)^{1/2}}$$

$$= \sum_{k=0}^{\infty} \frac{e^{Bk}}{k!} \sum_{m_1, \ldots, m_k \geqslant q+3} \int \tilde{\sigma}_{\Lambda_{m_1}}(d\overline{\zeta}^{(m_1)}) \cdots \tilde{\sigma}_{\Lambda_{m_k}}(d\overline{\zeta}^{(m_k)}) e^{C\Sigma_{j=1}^k \varphi(m_j)^{1/2}}.$$

Then we use (see Ref. 29 or 38)

$$\int \tilde{\sigma}_{\Lambda_m}(d\overline{\zeta}^{(m)}) \leqslant z \frac{|\Lambda_m|}{(2\pi t_\beta)^{d/2}} e^{-c\,(l_m^2/2t_\beta)(\alpha^2/(1+2\alpha)^4}$$

with $c = c(d)$ and get

$$I_q^{(4)} \leqslant e^{ze^B f(T_\beta)}, \quad T_\beta = T/\beta, \tag{5.29}$$

where

$$f(T_\beta) = \sum_{m \geqslant q_0+3} (2l_m+1)^d \exp\left\{ -c \frac{l_m^2}{2t_\beta} \frac{\alpha^2}{(1+2\alpha)^4} + Cm^{1/2}(2l_m+1)^{d/2} \right\}.$$

Obviously we have $f(T_\beta) < \infty$ for $d \leqslant 3$.

As a result we get (5.1) for $q \geqslant q_0$ with $\varepsilon(q) = \Sigma_{0 \leqslant j \leqslant 3} \varepsilon_j(q)$ and $K = ze^B f(T_\beta)$.

In the same way we have for $q = q_0 - 1$

$$I_{q_0-1} \leqslant e^{-1/4\,\beta A E_{q_0}(\tilde{\eta}_{\Lambda_{q_0}}) + h(q_0) + K} \tilde{\rho}^{\Lambda}(\tilde{\eta}_{\Lambda_{q_0}^c}),$$

with

$$h(q_0) = \sum_{i \in \{1,2\}} \sum_{a \in \{0,2\}} h_i^{(a)}(q_0).$$

As a result we get (5.1) from (5.24), (5.26)–(5.29) with $\varepsilon(q) = \Sigma_{0 \leqslant j \leqslant 3} \varepsilon_j(q)$ and $K(q_0) = ze^B f(T_\beta)$. □

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APPENDIX: PROOF OF THE BASIC LEMMAS

Lemma A.1: For any $\tau\in[0,t_\beta]$ *and* $q\in\mathbb{N}$ *and* $\tilde{\eta}^\tau,\gamma^\tau\subset\Lambda_q$,

$$U_{v_i}(\tilde{\eta}^\tau_{\Lambda_q}\cup(\pi_{\Lambda_q}\gamma)^\tau)\geqslant\frac{1}{4}A_iE^\tau_q(\xi^\tau)+\frac{1}{2}A_iE^\tau_q(\tilde{\eta}^\tau_{\Lambda_q})-\frac{B_i^2}{A_i}|\Lambda_q|. \tag{A1}$$

Proof: From the superstability condition (A.2) (see Sec. III) we obtain

$$U_{v_i}(\tilde{\eta}^\tau_{\Lambda_q}\cup(\pi_{\Lambda_q}\gamma)^\tau)\geqslant A_i\sum_{\Delta\subset\Lambda_q}|\xi^\tau_\Delta|^2-B_i\sum_{\Delta\subset\Lambda_q}|\xi^\tau_\Delta|.$$

Then (A1) follows from the inequalities $-n\geqslant-A_in^2/4B_i-B_i/A_i$ and $E^\tau_q(\xi)\geqslant E^\tau_q(\tilde{\eta})$. □

Lemma A.2: Let $\tau\in[0,t_\beta]$, $q\in\mathbb{N}$ *and* $\xi_1\in\Gamma_{\tilde{\Omega}_{\Lambda_{q+a}}}$ *with* $a=0$ *or* $a=2$, $\xi\in\Gamma_{\tilde{\Omega}_{\Lambda_q^c}}$, $\xi_1\cup\xi_2\subset\xi\in\Gamma_q$. *Then there exist positive, decreasing functions* $\varepsilon_1^{(i)}(q),\varepsilon_2^{(I)}(q)$ *such that*

$$-W_{v_i}(\xi_1^\tau|\xi_2^\tau)\leqslant F_{\mu_i}E^\tau_{q+a+1\setminus q-1}(\xi)+\varepsilon_1^{(i)}(q)E^\tau_{q+a}(\xi)+\varepsilon_2^{(i)}(q)\varphi(q)\sum_{k=1}^{\infty}(a_k^i-a_{k+1}^i)E^\tau_{q+a+k+1}(\xi), \tag{A2}$$

with $a_k^i=\Psi_i(l_{q+a+k}-l_{q+a})$.

Proof: From the regularity assumption (A3),

$$-W_{v_i}(\xi_1^\tau|\xi_2^\tau)\leqslant\frac{1}{2}\sum_{\Delta\subset\Lambda_{q+a}}\sum_{\Delta'\subset\Lambda_q^c}\Psi_i(\Delta,\Delta')[|\xi^\tau_\Delta|^2+|\xi^\tau_{\Delta'}|^2]. \tag{A3}$$

According to the partitions $\Lambda_{q+a}=\Lambda_{q+a-1}\cup(\Lambda_{q+a}\setminus\Lambda_{q+a-1})$, $\Lambda_q^c=(\Lambda_{q+a+1}\setminus\Lambda_q)\cup\Lambda^c_{q+a+1}$ we write down the r.h.s. of (A3) as

$$\begin{aligned}
-W_{v_i}(\xi_1^\tau|\xi_2^\tau)\leqslant&\frac{1}{2}\sum_{\Delta\subset\Lambda_{q+a}\setminus\Lambda_{q-1}}\sum_{\Delta'\subset\Lambda_{q+a+1}\setminus\Lambda_q}\Psi_i(\Delta,\Delta')|\xi^\tau_\Delta|^2\\
&+\frac{1}{2}\sum_{\Delta\subset\Lambda_{q-1}}\sum_{\Delta'\subset\Lambda_{q+a+1}\setminus\Lambda_q}\Psi_i(\Delta,\Delta')|\xi^\tau_\Delta|^2+\frac{1}{2}\sum_{\Delta\subset\Lambda_{q+a}}\sum_{\Delta'\subset\Lambda^c_{q+a+1}}\Psi_i(\Delta,\Delta')|\xi^\tau_\Delta|^2\\
&+\frac{1}{2}\sum_{\Delta\subset\Lambda_{q+a}}\sum_{\Delta'\subset\Lambda_{q+a+1}\setminus\Lambda_q}\Psi_i(\Delta,\Delta')|\xi^\tau_\Delta|^2\\
&+\frac{1}{2}\sum_{\Delta\subset\Lambda_{q+a}}\sum_{\Delta'\subset\Lambda^c_{q+a+1}}\Psi_i(\Delta,\Delta')|\xi^\tau_{\Delta'}|^2\\
\leqslant&\frac{1}{2}F_{\mu_i}E^\tau_{q+a\setminus q-1}(\xi)+\frac{1}{2}F^{(i)}(l_q-l_{q-1})E^\tau_{q-1}(\xi)+\frac{1}{2}F^{(i)}(l_{q+a+1}-l_{q+a})E^\tau_{q+a}(\xi)\\
&+\frac{1}{2}F_{\mu_i}E^\tau_{q+a+1\setminus q}(\xi)+\frac{1}{2}\sum_{\Delta\in\Lambda_{q+a}}\sum_{k=1}^{\infty}\Psi_i(l_{q+a+k}-l_{q+a})E_{q+a+k+1\setminus q+a+k}(\xi)\\
\leqslant&F_{\mu_i}E^\tau_{q+a+1\setminus q-1}(\xi)+F^{(i)}(l_q-l_{q-1})E^\tau_{q+a}(\xi)\\
&+\frac{1}{2}|\Lambda_{q+a}|\sum_{k=1}^{\infty}(a_k-a_{k+1})E^\tau_{q+a+k+1}(\xi),
\end{aligned}$$

where we have used the summation over layers $\Lambda_{q+a+k+1}\backslash\Lambda_{q+a+k}$, some resummation formula. As a result we obtain (A2) with $\varepsilon_1^{(i)}(q)=F^{(i)}(l_q-l_{q-1})=\sup_{\Delta\in\Lambda_{q-1}}\Sigma_{\Delta'\in\Lambda_q^c}\Psi_i(\Delta,\Delta')$ and $\varepsilon_2^{(i)}=2^{-1}(q+a)^{-1}$. □

Lemma A.3: Let $\tau\in[0,t_\beta]$, $q\in\mathbb{N}$, ξ_1 *contained in* Λ_s, $s>q$, ξ_2, *contained in* Λ_q^c *and* $\xi_1\cup\xi_2\subset\xi\in\Gamma_q$. *Then there exists* $q_0^{(2)}$ *such that for* $q\geqslant q_0^{(2)}$

$$-W_{v_i}(\xi_1^\tau|\xi_2^\tau)\leqslant b_1|\xi_1^\tau|\sum_{k=0}^{\infty}\Psi_i(k)(k+1)^{(d-1)/2}(E^\tau_{s+r(k)}(\xi))^{1/2}, \tag{A4}$$

with $b_1=b_1(d)$ *and* $r(k)$, *which is defined in (4.6).*

Proof: Using the regularity assumption (A.3) and Schwartz inequality we get

$$\begin{aligned}-W_{v_i}(\xi_1^\tau|\xi_2^\tau)&\leqslant\sum_{\Delta\in\Lambda_s}\sum_{\Delta'\in\Lambda_q^c}\Psi(\Delta,\Delta')|\xi^\tau_{1,\Delta}||\xi^\tau_{2,\Delta'}|\\&\leqslant\sum_{k=0}^{\infty}\Psi_i(k)\sum_{\Delta\in\Lambda_s}|\xi^\tau_{1,\Delta}|\left(\sum_{\Delta',d(\Delta,\Delta')=k}1^2\right)^{1/2}\left(\sum_{\Delta',d(\Delta,\Delta')=k}|\xi^\tau_{2,\Delta'}|^2\right)^{1/2}.\end{aligned}$$

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Generating Gowdy cosmological models*

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Using the analogy with stationary axisymmetric solutions, we present a method to generate new analytic cosmological solutions of Einstein's equation belonging to the class of T^3 Gowdy cosmological models. We show that the solutions can be generated from their data at the initial singularity and present the formal general solution for arbitrary initial data. We exemplify the method by constructing the Kantowski–Sachs cosmological model and a generalization of it that corresponds to an unpolarized T^3 Gowdy model. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Gowdy metrics,[1,2] which are exact solutions of Einstein's vacuum field equations, represent cosmological models with various possible topologies ($S^3, S^1\times S^2, T^3$) and are spatially compact inhomogeneous space–times admitting two commuting spacelike Killing vector fields. They are of special importance for the study of formation of singularities in general relativity. Many efforts[3–6] have been made in order to derive and analyze these types of solutions, especially by using numerical methods. The physical structure of these metrics is sufficiently simple to expect that the singularities can be analyzed in detail, but their mathematical structure is sufficiently complicated so that the global dynamical behavior is still far from being completely understood. One of the most intriguing questions concerns the structure of the curvature singularity that is expected to appear at certain spacelike boundary of the associated space–time. Many studies have been devoted to the so-called ''asymptotically velocity term dominated'' (AVTD) behavior which states that near the singularity each point in space is characterized by a different spatially homogeneous cosmology.[8] The idea of AVTD behavior was originally proposed in Ref. 9 more than 30 years ago, but is still being debated. Numerical analysis of the Gowdy models have shown that they do become AVTD near the singularity, except at a set of isolated points, where there are ''spikes'' in the behavior of the metric functions. The origin of these spikes is investigated in Ref. 6. Gowdy metrics have been also analyzed as toy models in quantum midisuperspace gravity.[7]

Numerical methods have been extensively used to investigate Gowdy models, but only recently it has been argued that solutions generating techniques can be applied in this case[10–12] to generate new solutions and that even a ''simple change of coordinates'' can be applied to reinterpret certain stationary axisymmetric solutions as $S^1\times S^2$ Gowdy cosmological models.[13] The reason why these methods can be used also in this case is due to the well-known fact that the solution generating techniques are applicable to any space–time which admits two (commuting) Killing vector fields. In this work, we will concentrate on T^3 Gowdy cosmological models and will see that a complex coordinate transformation, together with a complex change of metric functions, allows us to apply in a straightforward manner the well-known solution generating

*We would like to dedicate this work to the memory of Professor Nail Sibgatullin who unexpectly passed away on March 12, 2004.

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techniques that have been intensively used for stationary axisymmetric solutions.

This paper is organized as follows: In Sec. II we derive the ''transformation'' that relates stationary axisymmetric solutions with Gowdy T^3 models. We will show that due to this analogy, the AVTD behavior in Gowdy T^3 is mathematically equivalent to the behavior of stationary asixymmetric solutions near the axis of symmetry. In Sec. III we show that Sibgatullin's method for constructing solutions can be applied in the case of Gowdy T^3 models and in Sec. IV we present several examples of exact solutions generated by using this method. Finally, Sec. V is devoted to the conclusions and some remarks about different possibilities of generalizing the results derived in this work.

II. STATIONARY AXISYMMETRIC SOLUTIONS AND GOWDY T^3 MODELS

Consider the line element for stationary axisymmetric spacetimes in the Lewis–Papapetrou form[14]

$$ds^2=-e^{2\psi}(dT+\omega d\phi)^2+e^{-2\psi}[e^{2\gamma}(d\rho^2+dz^2)+\rho^2 d\phi^2], \tag{1}$$

where ψ, ω, and γ are functions of the nonignorable coordinates ρ and z. The ignorable coordinates T and ϕ are associated with the two Killing vector fields $\eta_{\mathrm{I}}=\partial/\partial T$ and $\eta_{\mathrm{II}}=\partial/\partial\phi$. The field equations take the form

$$\psi_{\rho\rho}+\frac{1}{\rho}\psi_\rho+\psi_{zz}+\frac{e^{4\psi}}{2\rho^2}(\omega_\rho^2+\omega_z^2)=0, \tag{2}$$

$$\omega_{\rho\rho}-\frac{1}{\rho}\omega_\rho+\omega_{zz}+4(\omega_\rho\psi_\rho+\omega_z\psi_z)=0, \tag{3}$$

$$\gamma_\rho=\rho(\psi_\rho^2-\psi_z^2)-\frac{e^{4\psi}}{4\rho^2}(\omega_\rho^2-\omega_z^2), \tag{4}$$

$$\gamma_z=2\rho\psi_\rho\psi_z-\frac{1}{2\rho}e^{4\psi}\omega_\rho\omega_z, \tag{5}$$

where the lower indices represent partial derivative with respect to the corresponding coordinate.

Consider now the following coordinate transformation $(\rho,t)\rightarrow(\tau,\sigma)$ and the complex change of coordinates $(\phi,z)\rightarrow(\delta,\chi)$ defined by

$$\rho=e^{-\tau},\quad T=\sigma,\quad z=i\chi,\quad \phi=i\delta, \tag{6}$$

and introduce the functions P, Q, and λ by means of the relationships

$$\psi=\frac{1}{2}(P-\tau),\quad Q=i\omega,\quad \gamma=\frac{1}{2}\left(P-\frac{\lambda}{2}-\frac{\tau}{2}\right). \tag{7}$$

Introducing Eqs. (6) and (7) into the line element (1), we obtain

$$-ds^2=e^{-\lambda/2}e^{\tau/2}(-e^{-2\tau}d\tau^2+d\chi^2)+e^{-\tau}[e^P(d\sigma+Qd\delta)^2+e^{-P}d\delta^2]. \tag{8}$$

Let us take $\tau\geqslant 0$ (what seems reasonable in virtue that the radial coordinate $\rho=e^{-\tau}\geqslant 0$) and ''compactify'' the new coordinates as $0\leqslant\chi,\ \sigma,\ \delta\leqslant 2\pi$ (a less reasonable condition since in general $-\infty<z<+\infty$ and $T\geqslant 0$). The line element (8) with the coordinates τ, χ, σ, and δ in the range given above is known as the line element for Gowdy T^3 cosmological models.[6] Furthermore, one can verify by direct calculation that the action of the transformations (6) and (7) on the field

equations (2)–(5) yields exactly the field equations for the Gowdy cosmological models which after some algebraic manipulations can be written as a set of two second order differential equations for P and Q,

$$P_{\tau\tau}-e^{-2\tau}P_{\chi\chi}-e^{2P}(Q_\tau^2-e^{-2\tau}Q_\chi^2)=0, \tag{9}$$

$$Q_{\tau\tau}-e^{-2\tau}Q_{\chi\chi}+2(P_\tau Q_\tau-e^{-2\tau}P_\chi Q_\chi)=0, \tag{10}$$

and two first order differential equations for λ

$$\lambda_\tau=P_\tau^2+e^{-2\tau}P_\chi^2+e^{2P}(Q_\tau^2+e^{-2\tau}Q_\chi^2), \tag{11}$$

$$\lambda_\chi=2(P_\chi P_\tau+e^{2P}Q_\chi Q_\tau). \tag{12}$$

It should be emphasized that this method for ''deriving'' the Gowdy line element from the stationary axisymmetric one involves real as well as complex transformations at the level of coordinates and metric functions. It is, therefore, necessary to demand that the resulting metric functions P, Q, and λ be real. That means that in general it is not possible to take an axisymmetric stationary solution and apply the transformations to obtain a Gowdy cosmological model. If the resulting functions are not real, they cannot be physical reasonable solutions to the real equations (9)–(12). These transformations can be used only as a guide to get some insight into the form of the new solutions. In any case, the corresponding field equations have to be invoked in order to confirm the correctness of the solution.

A very useful form for analyzing the field equations of space–times with two (commuting) Killing vector fields is the Ernst representation. In fact, this convenient form for the field equations was first proposed for axisymmetric stationary solutions,[15] but since then it has been applied in many different configurations.[16–18] Here we will present the Ernst representation of the main field equations (9) and (10) which is especially adapted to the coordinates used here. To this end, let us introduce a new coordinate t and a new function $R=R(t,\chi)$ by means of the equations[10–13]

$$t=e^{-\tau}, \quad R_t=te^{2P}Q_\chi, \quad R_\chi=te^{2P}Q_t. \tag{13}$$

Then, the field equation (9) can be expressed as

$$t^2\left(P_{tt}+\frac{1}{t}P_t-P_{\chi\chi}\right)+e^{-2P}(R_t^2-R_\chi^2)=0, \tag{14}$$

whereas Eq. (10) for the function Q turns out to be equivalent to the integrability condition $R_{t\chi}=R_{\chi t}$. However, an alternative and convenient equation is obtained by introducing Eq. (13) directly into Eq. (10). So we obtain

$$te^P\left(R_{tt}+\frac{1}{t}R_t-R_{\chi\chi}\right)-2[(te^P)_tR_t-(te^P)_\chi R_\chi]=0, \tag{15}$$

an equation which of course becomes an identity if the integrability condition $R_{t\chi}=R_{\chi t}$ is satisfied. We can now introduce the complex Ernst potential E and the complex gradient operator D as

$$E=te^P+iR, \quad \text{and} \quad D=\left(\frac{\partial}{\partial t},i\frac{\partial}{\partial\chi}\right), \tag{16}$$

which allow us to write the main field equations in the *Ernst-type representation*

$$\mathrm{Re}(E)\left(D^2E+\frac{1}{t}Dt\,DE\right)-(DE)^2=0. \tag{17}$$

It is easy to verify that the field equations (14) and (15) can be obtained as the real and imaginary part of the Ernst equation (17), respectively. For the sake of completeness, we rewrite the system of first order, partial, differential equations (11) and (12) in terms of the Ernst potential:

$$\lambda_t = -\frac{t}{2}(C_+ C_+^* + C_- C_-^*), \tag{18}$$

$$\lambda_\chi = -\frac{t}{2}(C_+ C_+^* - C_- C_-^*), \tag{19}$$

where

$$C_\pm = \frac{1}{\mathrm{Re}(E)}(E_t \pm E_\chi) - \frac{1}{t}, \tag{20}$$

and the asterisk denotes complex conjugation.

If the Ernst potential E is known, then it is easy to recover the metric functions P, Q, and λ which enter the line element (8) of Gowdy T^3 cosmological models. In fact, from Eq. (16) one can algebraically construct the functions P and R. Then the function Q can be obtained by solving the system of two first order partial differential equations given in (13). Notice that the integrability condition of this last system is satisfied by virtue of Eq. (17). Finally, the system (18) and (19) for the function λ can be solved by quadratures since its integrability condition coincides with the Ernst equation (17). Consequently, all the information about any Gowdy T^3 cosmological model is contained in the corresponding Ernst potential.

One of the most important properties of the Ernst representation (17) is that it is very appropriate to investigate the symmetries of the field equations. In particular, the symmetries of the Ernst equation for stationary axisymmetric spacetimes have been used to develop the modern solution generating techniques,[19] like the Bäcklund method, Belinsky–Zakharov inverse scattering method, the Hoenselaers–Kinnersley–Xanthopoulos method, and others (for an introductory review and detailed references, see Ref. 20). In all these methods it is necessary to start from a given ''seed'' solution which has to be specified in the whole space–time (except, perhaps, in the regions where the metric possesses true curvature singularities). An alternative approach for exploring the symmetries inherent in the Ernst equation was explicitly developed by Sibgatullin[21] and consists of constructing exact solutions to the Ernst equation from initial data specified only on certain hypersurface (submanifold) of the space–time. For instance, in the case of stationary axisymmetric space–times, Sibgatullin's method allows one to construct exact solutions from their data on the axis of symmetry. In the following sections we will show that Sibgatullin's method can be applied in the case of Gowdy cosmological models and will present several examples of its application.

III. CONSTRUCTING SOLUTIONS FROM AVTD DATA

As we have mentioned above, an important property of Gowdy cosmological models is its AVTD behavior near the initial singularity. In the case of T^3 models it can be shown that the singularity is approached in the limit $\tau \to \infty$. The AVTD behavior implies that at the singularity all spatial derivatives of the field equations can be neglected and only the temporal behavior is relevant. On the other hand, the transformation (6) indicates that the limit $\tau \to \infty$ is equivalent to the limit $\rho \to 0$; however, this is true only at the level of coordinates and a more detailed analysis is necessary to make sure that this analogy is also valid at the level of explicit solutions. To this end, let us consider the system of partial differential equations for ψ and ω given in Eqs. (2) and (3). If we neglect the spatial dependence on z, which accoring to the transformation (6) is equivalent to the spatial dependence on χ in Gowdy models, then we obtain a system of differential equations which can be solved by quadratures and yields

$$\psi=\tfrac{1}{2}\ln[a(\rho^{1+c}+b^2\rho^{1-c})],\quad \omega=\frac{ib}{a(\rho^{1+c}+b^2\rho^{1-c})}+id, \tag{21}$$

where a, b, c, and d are arbitrary real functions of z. Clearly, this solution is meaningless when considered as a stationary axisymmetric spacetime. However, if we now follow the prescription given in Eqs. (6) and (7) for obtaining Gowdy models, we will find that solution (21) ''corresponds'' to the Gowdy model

$$P=\ln[a(e^{-c\tau}+b^2e^{c\tau})],\quad Q=\frac{b}{a(e^{-2c\tau}+b^2)}+d, \tag{22}$$

where now a, b, c, and d are to be considered as arbitrary real functions of the coordinate χ. It is straightforward to verify that the expressions given in Eq. (22) satisfy the Gowdy field equations (9) and (10) in its ''truncated'' form, i.e., when the spatial derivatives are neglected. The solution (22) is known in the literature as the AVTD solution for Gowdy T^3 models[6] and dictates the behavior of these models near the singularity $\tau\to\infty$. Thus, we have ''derived'' the AVTD solution starting from its stationary axisymmetric counterpart. This is a further indication that the behavior of Gowdy models at the initial singularity is mathematically equivalent to the behavior of stationary axisymmetric solutions at the axis. For the sake of completeness we also quote here the value of the function λ corresponding to the AVTD solution (22) that can be obtained by integrating Eq. (11):

$$\lambda=\lambda_0-c^2\ln t, \tag{23}$$

where λ_0 is an additive constant. Furthermore, the corresponding AVTD Ernst potential can be obtained by introducing Eq. (22) into Eqs. (16) and (17). Then,

$$E=a[e^{-(1+c)\tau}+b^2e^{-(1-c)\tau}]+iR^{\mathrm{avtd}}\quad\text{with}\quad R^{\mathrm{avtd}}_{\chi}=-2abc. \tag{24}$$

If we define

$$E(\tau\to\infty,\chi)=e(\chi) \tag{25}$$

as the Ernst potential at the singularity, we see from Eq. (24) that for $c\in(-1,1)$ only the imaginary part remains, $e(\chi)=iR^{\mathrm{avtd}}$. This means that the real part of $e(\chi)$ is arbitrary and since R^{avtd} is given in terms of the real part it is also arbitrary. If $c\notin(-1,1)$, the Ernst potential diverges at the singularity for arbitrary values of the functions a and b. In the limiting case $c=\pm1$, the Ernst potential at the singularity is regular, but again no conditions appear for the behavior of the functions a and b. Consequently, the AVTD behavior does not impose any conditions on the function $e(\chi)$. We will now see that it is possible to use this function to construct the corresponding Ernst potential $E(\tau,\chi)$.

Sibgatullin's method[21] has been developed to construct exact stationary axisymmetric solutions starting from their data on the axis of symmetry. It is based upon the fact that the Ernst equation possesses symmetry properties associated with an infinite-dimensional Lie group which transforms one solution of this equation into another solution of the same equation. This implies remarkable analyticity properties that make it possible to reduce the Ernst equation to a system of linear integral equations which can be integrated explicitly if initial data is known, for instance, on the axis of symmetry. It is clear that the Ernst-type representation (17) possesses similar symmetry properties. On the other hand, we have shown that the behavior of stationary axisymmetric solutions near the axis is mathematically equivalent to the behavior of Gowdy T^3 cosmological models near the singularity. Thus, it should be possible to construct Gowdy cosmological models starting from the value of the corresponding Ernst potential at the singularity. It turns out that Sibgatullin's method can be generalized in a straightforward manner to include the case of Gowdy models. A detailed explanation of the procedure necessary to obtain the system of linear integral equations

associated with the Ernst equation is given in Ref. 21. Here we will only quote the main steps of the construction. Assume that the value of the Ernst potential is known at the initial singularity, i.e., $e(\chi)$ is given. Then, the Ernst potential can be generated by means of the integral equation

$$E(t,\chi)=\frac{1}{\pi}\int_{-1}^{1}\frac{e(\xi)\mu(\xi)}{\sqrt{1-s^2}}ds, \tag{26}$$

where the unknown function $\mu(\xi)$ has to be found from the singular integral equation

$$\int_{-1}^{1}\frac{\mu(\xi)[e^*(\eta)+e(\xi)]}{(s-\kappa)\sqrt{1-s^2}}ds=0, \tag{27}$$

with the normalization condition

$$\int_{-1}^{1}\frac{\mu(\xi)}{\sqrt{1-s^2}}ds=\pi, \tag{28}$$

where $\xi=\chi+ts,\ \eta=\chi+t\kappa,$ with $s,\kappa\in[-1,1]$.

Notice that for this method no condition is imposed on the behavior of $e(\chi)$. This is in accordance with the result obtained above about the AVTD behavior of the Ernst potential near the singularity. Once $e(\chi)$ is given in any desired form, one only has to calculate the integral (26) to find the Ernst potential. However, to calculate this integral one first has to find the function $\mu(\xi)$ by means of the singular equation (27) and the normalization condition (28). In practice, for a given $e(\xi)$ one has to make a reasonable ansatz for $\mu(\xi)$ such that it allows the existence of solutions for the integral singular equation (27).

IV. EXAMPLES OF GOWDY T^3 MODELS

The cases where the Ernst potential at the initial singularity behaves as a rational function are relatively easy to analyze. In this section we will present two such examples. Let us consider the following simple example of an Ernst potential at the singularity

$$e(\chi)=\frac{\chi_0-\chi}{\chi_0+\chi}, \tag{29}$$

where χ_0 is a real constant. The first step of the construction is to find the unknown function μ according to Eqs. (27) and (28). A reasonable ansatz is again a rational function[21]

$$\mu=A_0+\frac{A_1}{\xi-\xi_1}, \tag{30}$$

where ξ_1 is the root of the equation $e(\xi)+\tilde{e}(\xi)=0$ (in this case $\xi_1=\chi_0$) and A_0, A_1, are functions of t and χ. To handle the integrals which follow from the singular integral equation we use the following standard formulas

$$\int_{-1}^{1}\frac{ds}{\sqrt{1-s^2}}=\pi, \tag{31}$$

$$\int_{-1}^{1}\frac{ds}{(a+isb)\sqrt{1-s^2}}=\frac{\pi}{\sqrt{a^2+b^2}}, \tag{32}$$

$$\int_{-1}^{1}\frac{ds}{(s-\kappa)(s-\gamma)\sqrt{1-s^2}}=\frac{\pi}{(\kappa-\gamma)\sqrt{\gamma^2-1}}, \tag{33}$$

where a, b, and γ are arbitrary constants.

Introducing Eq. (30) into the normalization condition (28), we obtain

$$A_0+\frac{A_1}{r_-}=1, \tag{34}$$

where $r_-=\sqrt{(\chi-\chi_0)^2-t^2}$, whereas the integral singular equation (27) leads to

$$A_0-\frac{A_1(r_++r_-)}{2\chi_0 r_-}=0\,. \tag{35}$$

The last two equations can be used to find the explicit values of A_0 and A_1 which then can be replaced in the result of the integration of Eq. (26) and yield

$$E(t,\chi)=-A_0-\frac{A_1-2\chi_0A_0}{r_+}=\frac{2\chi_0-r_+-r_-}{2\chi_0+r_++r_-}, \tag{36}$$

where $r_+=\sqrt{(\chi+\chi_0)^2-t^2}$. It is easy to check that indeed this is a solution to the Ernst equation (17). Since the resulting Ernst potential is real, the solution corresponds to a polarized ($Q=0$) Gowdy model. The expression for the metric function P can easily be obtained from the definition (16) and Eq. (36), and the remaining function λ can be calculated (up to an additive constant) by quadratures from Eqs. (18) and (19):

$$\lambda=\ln\left[\frac{1}{t}\frac{(r_+r_-)^2}{(r_++r_-+2\chi_0)^4}\right]. \tag{37}$$

The physical significance of this solution becomes plausible in a different system of coordinates which we introduce in two steps. Let us first introduce in the (τ,χ)-sector of the line element (8) coordinates x and y by means of the relationships

$$e^{-2\tau}=t^2=\chi_0^2(1-x^2)(1-y^2),\quad \chi=\chi_0xy, \tag{38}$$

or the inverse transformation law

$$x=\frac{r_++r_-}{2\chi_0},\quad y=\frac{r_+-r_-}{2\chi_0}, \tag{39}$$

so that the metric functions become

$$P=\ln\left[\frac{1-x}{\chi_0\sqrt{(1-x^2)(1-y^2)}(1+x)}\right],\quad \lambda=\ln\left[\frac{(x^2-y^2)^2}{\chi_0\sqrt{(1-x^2)(1-y^2)}(1+x)^4}\right]. \tag{40}$$

The second transformation affects now all the sectors of the line element (8) and is defined by

$$x=\frac{T}{\chi_0}-1,\quad y=\cos\theta,\quad \sigma=r,\quad \delta=\phi. \tag{41}$$

Then, after some algebraic manipulations, the metric can be written as

$$-ds^2=-\left(\frac{2\chi_0}{T}-1\right)^{-1}dT^2+\left(\frac{2\chi_0}{T}-1\right)dr^2+T^2(d\theta^2+\sin^2\theta d\phi^2), \tag{42}$$

an expression that can immediately be recognized as the Kantowski–Sachs cosmological model.[23,24] Thus, we have shown that the Kantowski–Sachs metric can be constructed from the value of its Ernst potential at the singularity (29).

Consider now the more general case

$$e(\chi)=\frac{\chi_0-\chi-i\chi_1}{\chi_0+\chi+i\chi_1}, \tag{43}$$

where χ_0 and χ_1 are real constants. The unknown function $\mu(\xi)$ can be sought in the form

$$\mu=A_0+\frac{A_1}{\xi-\xi_1}+\frac{A_2}{\xi-\xi_2}, \tag{44}$$

where $\xi_{1,2}=\pm\alpha=\pm\sqrt{\chi_0^2-\chi_1^2}$ are the roots of the equation $e(\xi)+e^*(\xi)=0$. Substituting Eq. (44) in the integral equation (27) we obtain the system

$$-A_0+\frac{A_1}{\chi_0+i\chi_1+\alpha}+\frac{A_2}{\chi_0+i\chi_1-\alpha}=0\,, \tag{45}$$

$$-\frac{A_1(\alpha+i\chi_1)}{r_-(\chi_0+i\chi_1+\alpha)}+\frac{A_2(\alpha-i\chi_1)}{r_+(\chi_0+i\chi_1-\alpha)}=0\,, \tag{46}$$

where $r_\pm=\sqrt{(\chi\pm\alpha)^2-t^2}$. On the other hand, the normalization condition (28) yields

$$A_0+\frac{A_1}{r_-}+\frac{A_2}{r_+}=1\,, \tag{47}$$

an equation which together with Eqs. (45) and (46) form a closed algebraic system that determines the coefficients of the function μ:

$$\begin{aligned}
A_0&=\frac{\alpha(r_++r_-)+i\chi_1(r_+-r_-)}{\alpha(r_++r_-)+i\chi_1(r_+-r_-)+2\alpha\chi_0},\\
A_1&=\frac{r_-(\alpha-i\chi_1)(\chi_0+i\chi_1+\alpha)}{\alpha(r_++r_-)+i\chi_1(r_+-r_-)+2\alpha\chi_0},\\
A_2&=\frac{r_+(\alpha+i\chi_1)(\chi_0+i\chi_1-\alpha)}{\alpha(r_++r_-)+i\chi_1(r_+-r_-)+2\alpha\chi_0}.
\end{aligned} \tag{48}$$

Finally, we calculate the Ernst potential according to Eq. (26) and obtain

$$E(t,\chi)=-A_0+\frac{A_1(\chi_0-i\chi_1-\alpha)}{r_-(\chi_0+i\chi_1+\alpha)}+\frac{A_2(\chi_0-i\chi_1+\alpha)}{r_+(\chi_0+i\chi_1-\alpha)}=\frac{2\alpha\chi_0-\alpha(r_++r_-)-i\chi_1(r_+-r_-)}{2\alpha\chi_0+\alpha(r_++r_-)+i\chi_1(r_+-r_-)}. \tag{49}$$

The calculation of the corresponding metric functions can be carried out as described in the last section. When integrating the systems of first order differential equations (13) for Q and (18) and (19) for λ, constants of integration appear which we choose such that a simpler representation is obtained in terms of the coordinates used. To write down the final form of the metric functions it is convenient to use the coordinates (x, y) as defined in Eq. (39) with χ_0 replaced by α. Then

$$P=\ln\frac{\chi_0^2-\alpha^2x^2-\chi_1^2y^2}{\alpha\sqrt{(1-x^2)(1-y^2)}[(\chi_0+\alpha x)^2+\chi_1^2y^2]}\,, \tag{50}$$

$$Q=\frac{2\chi_1\chi_0(1-y^2)(\chi_0+\alpha x)}{\chi_0^2-\alpha^2x^2-\chi_1^2y^2}, \tag{51}$$

$$\lambda=\ln\frac{\chi_0^3(x^2-y^2)^2}{\sqrt{(1-x^2)(1-y^2)}[(\chi_0+\alpha x)^2+\chi_1^2y^2]^2}. \tag{52}$$

This metric corresponds to an unpolarized generalization of the Kantowski–Sachs cosmological model which is obtained in the limiting case $\chi_1=0$.

It is easy to see that near the singularity ($\tau\to\infty$) the general Ernst potential (49) approaches the corresponding AVTD potential as given in Eq. (43). This could be interpreted as an indirect proof of the AVTD behavior of the solution obtained here. A more direct proof can be given by analyzing the hyperbolic velocity $v=\sqrt{P_\tau^2+e^{2P}Q_\tau^2}$ (see Ref. 4). In terms of the coordinates x and y, the hyperbolic velocity of the solutions (50) and (51) is given as a rather cumbersome expression. Nevertheless, it is possible to perform an analysis of its behavior by considering the different domains of the coordinates according to the definition equation (39). One can show that in general $0\leqslant v<1$ which according to Ref. 4 implies that the solution is AVTD.

An important property of the method presented here is that it allows us to calculate an arbitrary Gowdy T^3 cosmological solution with any degree of accuracy. To this end, let us expand in Eq. (26) the value of the Ernst potential $e(\xi)$ in Fourier series,

$$e(\xi)=\sum_{k=0}^{\infty} e_k(t,\chi)\cos(k\varphi), \tag{53}$$

where $e_0=e(\chi)$ and we have represented the parameter s as $s=\cos\varphi$. Then the unknown function $\mu(\xi)$ can be expanded in a similar way,

$$\mu(\xi)=\sum_{k=0}^{\infty} \mu_k(t,\chi)\cos(k\varphi). \tag{54}$$

The normalization condition (28) can easily be calculated and implies that $\mu_0=1$. Furthermore, the general solution of the integral equation (26) can be written as[21]

$$E(t,\chi)=e(\chi)+\frac{1}{2}\sum_{k=1}^{\infty} e_k\mu_k. \tag{55}$$

According to Eq. (27), the coefficients μ_k have to satisfy the following system of algebraic equations:

$$\sum_{l=1}^{\infty} \mu_k(e_{k+l}-e^*_{k+l}+e_{|k-l|}-e^*_{|k-l|})=-2e_k. \tag{56}$$

Thus, once the value of the Ernst potential is given at the initial singularity [$e(\chi)=E(\chi,\tau\to\infty)$] the general solution of the Ernst equation reduces to an infinite series with coefficients satisfying a set of pure algebraic equations.

V. CONCLUSIONS

We have shown that it is possible to generate Gowdy T^3 cosmological models starting from their data near the initial singularity. To this end, we first show that the Gowdy T^3 line element can be obtained from the line element of stationary axisymmetric solutions by means of complex transformation that involves the metric functions and the coordinates. The behavior of stationary axisymmetric solutions at the axis of symmetry is shown to be mathematically equivalent to the

behavior of Gowdy T^3 models near the singularity. In particular, we have derived the AVTD solution from its stationary axisymmetric counterpart. We then use the Ernst representation of the field equations and apply Sibgatullin's method to the Ernst potential which can be given at the singularity as any arbitrary function of the angle coordinate χ. In particular, we have shown that the Kantowski–Sachs cosmological model can be derived in this manner by starting from a specific form of the Ernst potential in terms of a rational function. We then have found an unpolarized generalization of the Kantowski–Sachs cosmological model. This generalization has been obtained in the same way as the Kerr metric is obtained from its value at the axis of symmetry by using Sibgatullin's method.[21] It is possible to consider more general examples of Ernst potentials at the axis in terms of rational functions. It turns out that the system of integral equations (27) and (28) forms a closed algebraic system from which the value of the function $\mu(\xi)$ can be found and the expression for the Ernst potential can be calculated.[22] This method could also be applied in the case of Gowdy cosmological models considered here.

By expanding the value of the Ernst potential at the singularity in terms of a Fourier series, it is possible to write explicitly the general solution for this type of models (including the unpolarized case) by using only a recurrence algebraic formula. This is a result that could find some application in numerical investigations since it allows us to ''control'' the accuracy of the analysis by truncating the series at any desired level.

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On the extra phase correction to the semiclassical spin coherent-state propagator

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The problem of an origin of the Solari–Kochetov extra-phase contribution to the naive semiclassical form of a generalized phase-space propagator is addressed with the special reference to the su(2) spin case which is the most important in applications. While the extra-phase correction to a flat phase-space propagator can straightforwardly be shown to appear as a difference between the principal and the Weyl symbols of a Hamiltonian in the next-to-leading order expansion in the semiclassical parameter, the same statement for the semiclassical spin coherent-state propagator holds provided the Holstein–Primakoff representation of the su(2) algebra generators is employed. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The spin coherent-state path integral appears to be very useful in many physical problems that involve quantum su(2) spins. In particular, one of its most significant practical applications is the study of spin tunneling in the semiclassical limit.[1–4] However, as it was remarked in Ref. 5, the straightforward computation of the semiclassical propagator[6] or the tunnel splitting[7] yields results that are incorrect beyond the leading semiclassical order. Examples of other systems where the large spin limit gives a good qualitative picture, while the first quantum correction is either ignored or fixed by heuristic considerations, can be found in Ref. 8.

Recently, Stone *et al.*[5] have restored the reliability of the semiclassical expression for the spin coherent-state propagator, thus effectively rehabilitating the use of the continuous-time spin coherent-state path integral. The crucial point in that approach is the recognition of an importance and the explanation of the origin of a previously discovered quantum correction[9–11] to the naive form of the semiclassical coherent-state propagator. It has been pointed out that the functional determinant arising from the evaluation of the functional integral about the classical path possesses a U(1) gauge anomaly, its proper regularization resulting in the extra-phase contribution. Originally Solari[9] obtained this extra-phase correction through a careful calculation of the path integral in the discrete-time approximation. Kochetov[10] derived it independently considering the continuous-time version of the spin coherent-state path integral in the semiclassical limit. A discrete-time evaluation similar to that of Solari was carried out by Vieira and Sacramento[11] who have also reproduced the same result.

The relevance of the Solari–Kochetov phase has been justified in the application of the spin coherent-state path integral to the calculation of the tunnel splitting of the classically degenerate ground state for a family of models that includes a realistic approximation to the molecular magnet Fe_8.[8] It has been also noticed in Ref. 12 that the modification of the Gutzwiller trace formula[13] for systems with a coupling of the translational and spin degrees of freedom should also contain this extra phase in the combined limit $\hbar \to 0$, $S \to \infty$, $\hbar S = \text{const}$.

In this article we offer a point of view on the origin of the Solari–Kochetov phase, which complements the analysis made in Ref. 5.

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To establish our notations we briefly outline in Sec. II some basic facts concerning quantization on cotangent bundles and coadjoint group orbits, the phase space manifolds that are most frequently encountered in applications. In Sec. III we consider in detail semiclassical propagators on flat phase spaces. We observe that the arising extra phase can be interpreted as a difference between the principal and the Weyl symbols of a Hamiltonian in the next-to-leading order in $\hbar$. On the other hand, various symbols, or various quantization schemes, are closely related to the operator ordering procedures. One can then alternatively state that the extra phase is the difference between the naive classical Hamiltonian and the expectation value of the Weyl-ordered operator.[14] Obviously, both formulations are equivalent, though the former provides a more efficient way to compute the extra phases, since it is based on the Wigner–Weyl calculus and implies an extensive use of the Moyal formula.[15]

In Sec. IV we discuss the semiclassical spin coherent-state propagator and its specific ingredient—the Solari–Kochetov phase. We also briefly outline the relation between the covariant and contravariant quantization schemes which are usually employed for the path integral construction in the spin case.

To obtain the Solari–Kochetov phase using the analogy with the flat case we, in the first place, need a proper definition of a Weyl symbol of the quantum spin Hamiltonian. The point is that a standard Weyl quantization is well-defined on a classical phase space M, provided it appears as a cotangent bundle to a certain configuration space Q, $M=T^*Q$. While Q may in principle be a compact manifold, T^*Q is always noncompact. A classical phase space of a spin is, however, a compact finite volume manifold, the two-sphere S^2, which is not a cotangent bundle. Therefore, there does not seem to exist any natural global definition of appropriate Weyl symbols of the su(2) spin operators.

To partly circumvent this apparent difficulty, we employ in Sec. V a special Holstein–Primakoff representation of the su(2) algebra.[16] It expresses the su(2) generators in terms of $\hat{a}$, $\hat{a}^\dagger$, $\hat{a}^\dagger\hat{a}$—the standard generators of the Heisenberg–Weyl algebra, and allows for a formal application of the standard Wigner–Weyl calculus to spin Hamiltonians. We then are able to define the Weyl symbols of the spin operators, provided the semiclassical representations of su(2) are considered, and to determine their difference from the components of the classical spin. This difference appears to be well-defined in the semiclassical limit $S\to\infty$, exactly reproducing the Solari–Kochetov phase.

II. PHASE-SPACE QUANTIZATION

The classical phase space can be thought of as a pair (M,w) where M is a $2n$-dimensional Riemannian manifold and w stands for a closed nondegenerate symplectic two-form on it. A group of canonical transformations G acting on M transitively leaves w invariant. Quantization on M amounts to constructing a complex line bundle over M with a connection one-form θ such that $d\theta=w$. A quantum Hilbert space is then constructed out of sections of the bundle. When lifted to the bundle, the action of G gives rise to a unitary but reducible representation of G. In order to select an irreducible component, the action of G is restricted to the subspace of those sections which are covariantly constant along n linearly independent vector fields $\chi_1,\ldots,\chi_n$ on M such that $w(\chi_i,\chi_j)=0$. This procedure is usually referred to as fixing of the polarization.[17]

To illustrate these definitions we briefly discuss two examples of phase spaces, which appear to be our main concern here, cotangent bundles and coadjoint group orbits.

Local coordinates on a cotangent bundle $M=T^*Q$ can always be separated into "coordinates," q^j, and "momenta," p_j, which are canonically conjugated to the q^j, with the globally defined canonical symplectic one-form $\theta=(1/\hbar)(p^j dq_j-q^j dp_j)$. Covariantly constant sections $f(q,p)$ along the vector field $\chi=\partial_p$ (we put for simplicity $n=1$) are then defined by

$$\nabla_p f:=(\partial_p+i\theta_p)f=0, \tag{1}$$

where $f(q,p)\sim e^{ipq/\hbar}\psi(q)$. The quantum Hilbert space appears then as the space of square-integrable functions $\psi(q)$. When considering the time evolution, one usually picks up initial and

final states as the eigenstates of the operator $\hat{q}$, $\hat{q}|q_0\rangle = q_0|q_0\rangle$, which corresponds to the choice $\psi(q) \sim \delta(q-q_0)$. Analogously, the choice $\chi = \partial_q$ results in quantization in terms of the p-dependent sections, $f(q,p) \sim e^{-ipq/\hbar}\psi(p)$. In the following we will be considering quantum propagators on T^*Q having the form

$$K(p_f, q_i, T) := \langle p_f | e^{-i\hat{H}T/\hbar} | q_i \rangle, \tag{2}$$

where initial and final quantum states belong to different polarizations.

Formally, the Weyl symbol of the operator $\hat{H}(\hat{q},\hat{p})$ is given by

$$H_W(q,p) = \int_Q dx \sqrt{g} e^{ipx/\hbar} \langle q - x/2 | \hat{H} | q + x/2 \rangle, \tag{3}$$

where g denotes the determinant of a restriction of a full metric tensor onto Q. As already said, the separation of the local coordinates into (q,p) is defined on a cotangent bundle globally (because θ exists globally). Accordingly, the symbol $H_W(q,p)$ is defined on the phase space manifold T^*Q globally as well.

The second important class of classical phase spaces is the so-called coadjoint orbits of Lie groups.[17] These symplectic G-homogeneous manifolds appear as natural classical phase spaces in the instances where quantum Hamiltonians allow for representations in terms of the Lie group generators. For example, the quantum spin dynamics is governed by a Hamiltonian built out of the su(2) generators. Spin classical phase space appears then as an SU(2) orbit—the two-sphere S^2,[18] which is a compact curved manifold. It can be covered by two local charts with complex coordinates $(z,\overline{z})$ and $(w,\overline{w})$ defined by projections from the North and South Poles, respectively.

Since there is no globally defined symplectic one-form on S^2, it does not admit a global separation of coordinates into q's and p's. Instead, the locally defined su(2) symplectic one-forms (in the representation with spin S) $\theta_1 = iS(\overline{z}dz - zd\overline{z})/(1+|z|^2)$ and $\theta_2 = iS(\overline{w}dw - wd\overline{w})/(1+|w|^2)$, where $w = 1/z$, are related in the charts' overlap by a U(1) gauge transformation, $\theta_1 = \theta_2 + iSd\log(z/\overline{z})$.

The covariantly constant section of the monopole $P(S^2, U(1))$ bundle that forms a quantum Hilbert space for spin can be chosen as an su(2) coherent state. In particular,

$$\nabla_{\overline{z}} |z\rangle_1 := (\partial_{\overline{z}} + i\theta_{1\ \overline{z}})|z\rangle_1 = 0, \tag{4}$$

where $|z\rangle_1$ denotes the su(2) coherent state in the local chart $(z,\overline{z})$. The su(2) quantum phase-space propagator can then be written down in the form

$$K(\overline{z_f}, z_i, T) := {}_1\langle z_f | e^{-i\hat{H}T/\hbar} | z_i \rangle_1, \tag{5}$$

where the initial and final states belong to different polarizations.

Given a spin quantum Hamiltonian $\hat{H}$, its classical symbol may be conveniently chosen as an expectation value in the coherent state, the so-called covariant symbol of the spin-dependent operator, $H_1^{cov}(\overline{z},z) = {}_1\langle z|\hat{H}|z\rangle_1$. In spite of its appearance, this symbol is defined globally on S^2: the $P(S^2,U(1))$ local sections are related in the charts' overlap by the U(1) gauge transformation

$${}_2\langle 1/z | z \rangle_1 = (z/\overline{z})^S \in U(1). \tag{6}$$

Therefore, $H_1^{cov}(\overline{z},z) = H_2^{cov}(\overline{w},w)$ for $w = 1/z$.

Concluding the section, we may state: though it might be in principle possible to construct a Weyl symbol for the su(2) spin locally on S^2, there seems to be no way to extend such a definition globally to the whole sphere.

III. FLAT PHASE-SPACE PROPAGATOR

The well-known van Vleck representation for the semiclassical propagator on a flat configuration space[19] has its counterpart in the phase space T^*R^2 which is the semiclassical approximation for the propagator (2)

$$K(p_f,q_i,T)=\frac{1}{\sqrt{2\pi\hbar}}\left(-\frac{\partial^2\mathcal{R}_{cl}}{\partial p_f\partial q_i}\right)^{1/2}e^{i\mathcal{R}_{cl}(p_f,q_i,T)/\hbar}, \tag{7}$$

where

$$\mathcal{R}_{cl}(p_f,q_i,T)=-\frac{1}{2}(p_f q_{cl}(T)+p_{cl}(0)q_i)+\int_0^T dt\left(-\frac{1}{2}(\dot{p}_{cl}q_{cl}-p_{cl}\dot{q}_{cl})-H(q_{cl},p_{cl})\right). \tag{8}$$

The classical dynamics of the system is governed by the principal symbol $H(q,p)$ of the quantum Hamiltonian $\hat{H}$:

$$\dot{q}=\frac{\partial H(q,p)}{\partial p},\quad q(0)=q_i, \tag{9}$$

$$\dot{p}=-\frac{\partial H(q,p)}{\partial q},\quad p(T)=p_f. \tag{10}$$

We would also call $H(q,p)$ the naive classical Hamiltonian since it can be obtained by just "dropping hats" in $\hat{H}$.

Formally, the principal symbol $H(q,p)$ is obtained in the limit $\hbar\to 0$ of the Weyl symbol (3). The Weyl symbol of the product of two operators is given by the Moyal product[15] of two respective symbols. The Moyal formula can be written in the symbolic form

$$(\hat{F}\hat{G})_W=F_W{*}G_W=F_W\,e^{i\hbar\mathcal{L}/2}\,G_W, \tag{11}$$

where the operator

$$\mathcal{L}=\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}-\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} \tag{12}$$

is associated with the Poisson bracket

$$F_W\mathcal{L}G_W=\{F_W,G_W\}_{q,p}=\frac{\partial F_W}{\partial q}\frac{\partial G_W}{\partial p}-\frac{\partial F_W}{\partial p}\frac{\partial G_W}{\partial q}. \tag{13}$$

Expanding (11) into a series of $\hbar$, we obtain the leading and the next-to-leading contributions to the Moyal formula

$$(\hat{F}\hat{G})_W=F_W G_W+\frac{i\hbar}{2}\{F_W,G_W\}_{q,p}+O(\hbar^2). \tag{14}$$

Respectively, the leading contribution to the Weyl symbol of the commutator

$$([\hat{F},\hat{G}])_W=(\hat{F}\hat{G}-\hat{G}\hat{F})_W=F_W{*}G_W-G_W{*}F_W=i\hbar\{F_W,G_W\}_{q,p}+O(\hbar^3) \tag{15}$$

establishes the "correspondence principle" between commutators and Poisson brackets.

However, the expression (7) is, in general, incorrect. Besides the Morse index that accounts for the number of conjugate points,[20] there may appear another discrepancy between the repre-

sentation of (7) and that of a correct asymptotic propagator. It happens when the quantum Hamiltonian contains the terms that mix $\hat{q}$ and $\hat{p}$. Unless $\hat{H}$ is Weyl (symmetrically) ordered, it is not sufficient to take into account just the principal symbol $H(q,p)$ for the calculation of $\mathcal{R}_{cl}$.

Thus, we make here the following proposition: in the semiclassical evaluation of the propagator of type (7) it is necessary to use the Weyl symbol of the quantum Hamiltonian:

$$H_W(q,p)=H(q,p)-\delta H(q,p)+O(\hbar^2), \quad \delta H(q,p)\sim O(\hbar). \tag{16}$$

Though the classical dynamics is governed by the principal symbol, or naive classical Hamiltonian, $H(q,p)$, the next order term $\delta H(q,p)$ divided by $\hbar$, nevertheless, contributes to the phase of the semiclassical propagator. If the quantum Hamiltonian is a polynomial in $\hat{q}$ and $\hat{p}$, it is easy to calculate $\delta H(q,p)$ using the Moyal formula (14) and the obvious fact that $(\hat{q})_W=q$ and $(\hat{p})_W=p$.

Let us introduce the complex variables

$$\alpha=\frac{1}{\sqrt{2}}(q+ip), \quad \overline{\alpha}=\frac{1}{\sqrt{2}}(q-ip). \tag{17}$$

They are normalized to be the Weyl symbols of the operators

$$\hat{A}=\frac{1}{\sqrt{2}}(\hat{q}+i\hat{p}), \quad \hat{A}^{\dagger}=\frac{1}{\sqrt{2}}(\hat{q}-i\hat{p}), \tag{18}$$

which satisfy the commutation relation

$$[\hat{A},\hat{A}^{\dagger}]=\hbar. \tag{19}$$

We can define the Weyl symbols $F_W(\overline{\alpha},\alpha)$ and $G_W(\overline{\alpha},\alpha)$ and the Poisson bracket

$$\{F_W(\overline{\alpha},\alpha),G_W(\overline{\alpha},\alpha)\}_{\overline{\alpha},\alpha}=i\left(\frac{\partial F_W}{\partial\overline{\alpha}}\frac{\partial G_W}{\partial\alpha}-\frac{\partial F_W}{\partial\alpha}\frac{\partial G_W}{\partial\overline{\alpha}}\right) \tag{20}$$

by making a change of variables (17) in $F_W(q,p)$ and $G_W(q,p)$ and in the Poisson bracket (13), respectively. In turn, after the transformation (18) the operator which is Weyl-ordered in $\hat{A},\hat{A}^{\dagger}$ converts into the operator Weyl-ordered in $\hat{q},\hat{p}$. Note also that for the Weyl-ordered operator (either in $\hat{A},\hat{A}^{\dagger}$ or in $\hat{q},\hat{p}$), its Weyl symbol yields the principal symbol, the higher order terms being identically zero. This justifies the above definition of the Weyl symbols $F_W(\overline{\alpha},\alpha)$ and $G_W(\overline{\alpha},\alpha)$.

Taking into account a definite correspondence between the symbols and the ordering procedures, we can therefore interpret the emergence of the extra phase $\delta H/\hbar$ as an artifact of the operator ordering.

For a more detailed explanation, we would like to discuss the results of Ref. 21. In particular, there has been established the relation between semiclassical results for a propagator obtained within different quantization schemes. The ''λ-quantization'' infers the choice of the λ-symbol[22]

$$H^{(\lambda)}(\overline{\alpha},\alpha)=\mathrm{Tr}[\hat{H}\hat{R}_{\lambda}(\overline{\alpha},\alpha)], \quad \lambda\in[0,1], \tag{21}$$

where

$$\hat{R}_{\lambda}(\overline{\alpha},\alpha)=\frac{1}{\pi\hbar}\int d^2\xi e^{-(1-2\lambda)\overline{\xi}\xi/2\hbar}e^{\{\xi(\overline{\alpha}-\hat{A}^{\dagger})-\overline{\xi}(\alpha-\hat{A})\}/\hbar}. \tag{22}$$

The particular cases of $\lambda=0,\frac{1}{2},1$ correspond to the covariant (coherent-state), Weyl and contravariant symbols, respectively. The arbitrary λ-symbol is linked to the covariant symbol through the relation

$$H^{(0)}(\overline{\alpha},\alpha)=(\hat{T}_\lambda(\Delta)H^{(\lambda)})(\overline{\alpha},\alpha),\quad \hat{T}_\lambda(\Delta)=e^{\hbar\lambda\Delta}, \tag{23}$$

where $\Delta=\partial^2/\partial\alpha\partial\overline{\alpha}$ is the Laplace–Beltrami operator on the complex plane.

In the semiclassical limit $\hbar\to 0$ the expression (23) can be expanded as

$$H^{(0)}=H^{(\lambda)}+\hbar\lambda\Delta H^{(\lambda)}+O(\hbar^2). \tag{24}$$

Therefore, for arbitrary $\lambda,\lambda'\in[0,1]$ we have

$$H^{(\lambda')}=H^{(\lambda)}-\hbar(\lambda'-\lambda)\Delta H^{(\lambda)}+O(\hbar^2). \tag{25}$$

The expression for the semiclassical propagator reads[21]

$$K_{scl}^{flat}=\left(i\frac{\partial^2\mathcal{R}_{cl}^{(\lambda)}}{\partial\overline{\alpha}_f\partial\alpha_i}\right)^{1/2}\exp\left\{i\frac{\mathcal{R}_{cl}^{(\lambda)}}{\hbar}+i\left(\frac{1}{2}-\lambda\right)\int_0^T B^{(\lambda)}dt\right\}, \tag{26}$$

where

$$\mathcal{R}^{(\lambda)}(\overline{\alpha}_f,\alpha_i,T)=-\frac{i}{2}(\overline{\alpha}_f\alpha_{cl}(T)+\overline{\alpha}_{cl}(0)\alpha_i-|\alpha_f|^2-|\alpha_i|^2)$$
$$+\int_0^T dt\left(-\frac{i}{2}(\dot{\overline{\alpha}}_{cl}\alpha_{cl}-\overline{\alpha}_{cl}\dot{\alpha}_{cl})-H^{(\lambda)}(\overline{\alpha}_{cl},\alpha_{cl})\right) \tag{27}$$

and

$$B^{(\lambda)}=\Delta H^{(\lambda)}=\Delta H^{(1/2)}+O(\hbar)=\Delta H^{(0)}+O(\hbar). \tag{28}$$

The terms of the order $O(\hbar)$ in $B^{(\lambda)}$ as well as the dependence of the prefactor on λ are inessential due to the very structure of the asymptotic expression (26). $O(\hbar)$-terms are also negligible in the classical equations of motion:

$$\dot{\alpha}=-i\frac{\partial H^{(\lambda)}}{\partial\overline{\alpha}}+O(\hbar),\quad \alpha(0)=\alpha_i, \tag{29}$$

$$\dot{\overline{\alpha}}=i\frac{\partial H^{(\lambda)}}{\partial\alpha}+O(\hbar),\quad \overline{\alpha}(T)=\overline{\alpha}_f. \tag{30}$$

Note that for $\lambda=\frac{1}{2}$ (Weyl quantization) the B-term drops out from (26). Since the semiclassical propagator should not depend on λ, i.e., on the choice of the quantization scheme, the extra-phase correction just compensates for the difference between λ and Weyl symbols in the next-to-leading order in $\hbar$ [see (25) for $\lambda'=\frac{1}{2}$].

Suppose that the quantum Hamiltonian $\hat{H}$ belongs to a family of specifically ordered Hamiltonians,[23] also parametrized by $\lambda\in[0,1]$,

$$\hat{H}_\lambda(\hat{A}^\dagger,\hat{A})=\frac{1}{(\pi\hbar)^2}\int d^2\alpha d^2\beta H(\overline{\alpha},\alpha)e^{(1-2\lambda)\overline{\beta}\beta/2\hbar}e^{\{\beta(\overline{\alpha}-\hat{A}^\dagger)-\overline{\beta}(\alpha-\hat{A})\}/\hbar}, \tag{31}$$

where the particular cases of $\lambda=0,\frac{1}{2},1$ correspond to the normal, Weyl and antinormal orderings, respectively. One can establish the one-to-one correspondence between the operators (31) and the

symbols (21). It follows from the observation that the λ-symbol of the λ-ordered operator yields the principal symbol $H(\overline{\alpha},\alpha)$. Thus, the result (26) of Ref. 21 actually proves our proposition for the Hamiltonians (31).

The problem of the extra-phase contribution was often encountered in the coherent-state semiclassics based on the covariant quantization scheme. We can illustrate it with the following example.

Let us consider the normally ordered operator

$$\hat{H}_{\lambda=0}=\sum_{m,n} h_{mn}\hat{A}^{\dagger m}\hat{A}^{n}. \tag{32}$$

Its covariant (coherent-state) symbol

$$H^{(0)}(\overline{\alpha},\alpha)=\langle\alpha|\hat{H}_0|\alpha\rangle=\sum_{m,n} h_{mn}\overline{\alpha}^{m}\alpha^{n} \tag{33}$$

is found from (21) with $\lambda=0$, or, equivalently, by taking an expectation value in the Heisenberg-Weyl coherent state

$$|\alpha\rangle=e^{-\overline{\alpha}\alpha/2\hbar}e^{\alpha\hat{A}^{\dagger}/\hbar}|0\rangle, \quad \langle\alpha|\alpha\rangle=1. \tag{34}$$

Obviously, the covariant symbol (33) coincides with the principal symbol.

The Weyl symbol of (32) is

$$H^{(1/2)}=\sum_{m,n} h_{mn}\overline{\alpha}^{m}\alpha^{n}+\frac{i\hbar}{2}\sum_{m,n} h_{mn}\{\overline{\alpha}^{m},\alpha^{n}\}_{\overline{\alpha},\alpha}+O(\hbar^2)=H^{(0)}-\frac{\hbar}{2}\Delta H^{(0)}+O(\hbar^2). \tag{35}$$

Thus, we can deduce that

$$\frac{\delta H}{\hbar}=\frac{1}{2}\Delta H^{(0)}. \tag{36}$$

The same expression for the phase correction has been derived in Ref. 24, where the WKB approximation in the Bargmann representation has been considered. In the case $h_{11}=\omega$ and $h_{mn}=0$ for $m,n\neq 1$, we see that $\delta H/\hbar=\omega/2$. When multiplied by T, it exactly coincides with the required phase correction to the semiclassical coherent-state propagator of the harmonic oscillator. Its inclusion is sometimes referred to as a restoration of zero-point energy in the first order of $\hbar$.

IV. SEMICLASSICAL SPIN COHERENT-STATE PROPAGATOR

A quantum spin Hamiltonian $\hat{H}=\hat{H}(\hat{\mathbf{s}})$ is a function of spin algebra generators which satisfy the su(2) commutation relations

$$[\hat{s}_+,\hat{s}_-]=2\hat{s}_3, \quad [\hat{s}_3,\hat{s}_\pm]=\pm\hat{s}_\pm, \tag{37}$$

where $\hat{s}_\pm=\hat{s}_1\pm i\hat{s}_2$.

There actually exist two quantization schemes for spin[25]—covariant and contravariant—that are usually employed for the path-integral construction and its further semiclassical approximations.

The covariant quantization scheme is based on the coherent-state representation of the quantum Hamiltonian: the covariant symbol is defined as an expectation value

$$H^{cov}(\overline{z},z)\equiv H(\overline{z},z)={}_1\langle z|\hat{H}|z\rangle_1 \tag{38}$$

in the spin coherent state

$$|z\rangle_1=(1+\overline{z}z)^{-S}e^{z\hat{s}_+}|S,-S\rangle, \quad {}_1\langle z|z\rangle_1=1, \tag{39}$$

where $|S,-S\rangle$ is the lowest spin state in the $2S+1$-dimensional representation of SU(2). The second family of the spin coherent states is given by

$$|w\rangle_2=(1+\overline{w}w)^{-S}e^{w\hat{s}_-}|S,S\rangle, \quad {}_2\langle w|w\rangle_2=1, \tag{40}$$

$|S,S\rangle$ being the highest spin state.

In the sequel, all spin coherent states will be drawn from the first family, $|z\rangle:=|z\rangle_1$.

The spin coherent-state propagator (5) can be approximated in the semiclassical limit $S\to\infty$ by

$$K_{scl}(\overline{z}_f,z_i,T)=\left(i\frac{(1+\overline{z}_f z_{cl}(T))(1+\overline{z}_{cl}(0)z_i)}{2S}\frac{\partial^2\mathcal{R}_{cl}}{\partial z_i\partial\overline{z}_f}\right)^{1/2}e^{i\mathcal{R}_{cl}(\overline{z}_f,z_i,T)+(i/2)\int_0^T\phi_{SK}(t)dt}. \tag{41}$$

The validity of this formula has been proven in Ref. 5. It has been also shown that the degree of its accuracy, assuming errors of at most $O(1/S)$, is uniform in T.

The leading contribution to the phase of K_{scl} is the classical action

$$\begin{aligned}\mathcal{R}_{cl}(\overline{z}_f,z_i,T)=&-iS\{\ln[(1+\overline{z}_f z_{cl}(T))(1+\overline{z}_{cl}(0)z_i)]-\ln[(1+|z_f|^2)(1+|z_i|^2)]\}\\&+\int_0^T\left\{-iS\frac{\dot{\overline{z}}_{cl}z_{cl}-\overline{z}_{cl}\dot{z}_{cl}}{1+\overline{z}_{cl}z_{cl}}-H(\overline{z}_{cl},z_{cl})\right\}dt.\end{aligned} \tag{42}$$

(Note the distinction up to a factor of i in our notation and that of Ref. 5 as well as the difference in the normalization of the spin coherent states.) Classical trajectories $z_{cl}(t),\overline{z}_{cl}(t)$ are to be found from the classical equations of motion

$$\dot{z}=-i\frac{(1+\overline{z}z)^2}{2S}\frac{\partial H}{\partial\overline{z}}, \quad z(0)=z_i, \tag{43}$$

$$\dot{\overline{z}}=i\frac{(1+\overline{z}z)^2}{2S}\frac{\partial H}{\partial z}, \quad \overline{z}(T)=z_f. \tag{44}$$

The Solari–Kochetov phase, or the first quantum phase correction to K_{scl}, is expressed through

$$\phi_{SK}(t)=\frac{1}{2}\left(\frac{\partial}{\partial\overline{z}}\frac{(1+\overline{z}z)^2}{2S}\frac{\partial H}{\partial z}+\frac{\partial}{\partial z}\frac{(1+\overline{z}z)^2}{2S}\frac{\partial H}{\partial\overline{z}}\right)\Bigg|_{z=z_{cl},\overline{z}=\overline{z}_{cl}} \tag{45}$$

and represents the main subject of our discussion.

In particular, for a Hamiltonian linear in the spin operators

$$\hat{H}=\mathbf{C}\cdot\hat{\mathbf{s}}=\tfrac{1}{2}C_+\hat{s}_-+\tfrac{1}{2}C_-\hat{s}_+ +C_3\hat{s}_3, \tag{46}$$

where $C_\pm=C_1\pm iC_2$, we obtain the spin coherent-state symbol

$$H(\overline{z},z)=S\frac{C_+z+C_-\overline{z}}{1+\overline{z}z}-SC_3\frac{1-\overline{z}z}{1+\overline{z}z}, \tag{47}$$

and the Solari–Kochetov phase correction

$$\tfrac{1}{2}\phi_{SK}=-\tfrac{1}{4}(C_+z_{cl}+C_-\overline{z}_{cl})+\tfrac{1}{2}C_3. \tag{48}$$

Another example is the Hamiltonian of the Lipkin–Meshkov–Glick (LMG) model[26]

$$\hat{H}_{LMG}=\frac{w}{\sqrt{2}(2S-1)}(\hat{s}_+^2+\hat{s}_-^2)+\frac{Sw}{\sqrt{2}}, \tag{49}$$

which is quadratic in the spin operators. In this case we have

$$H_{LMG}(\bar{z},z)=\sqrt{2}Sw\frac{\bar{z}^2+z^2}{(1+\bar{z}z)^2}+\frac{Sw}{\sqrt{2}} \tag{50}$$

and

$$\frac{1}{2}\phi_{SK}^{LMG}=-\frac{w}{\sqrt{2}}\frac{(\bar{z}^2+z^2)(2+\bar{z}z)}{(1+\bar{z}z)^2}. \tag{51}$$

The latter has been calculated in Ref. 8, and its inclusion into the semiclassical propagator has provided the correct result for the tunnel splitting of the ground state in the LMG model.

To complete the presentation of the semiclassical spin propagator, we would also like to mention another quantization scheme which relies on the contravariant symbol $H^{ctr}(\bar{z},z)$ given by

$$\hat{H}=\frac{2S+1}{\pi}\int\frac{d^2z}{(1+\bar{z}z)^2}H^{ctr}(\bar{z},z)|z\rangle\langle z|. \tag{52}$$

As follows from Ref. 25, the relation between the covariant and contravariant symbols in the semiclassical limit $S\to\infty$ reads

$$H^{cov}(\bar{z},z)=[1+\Delta+O(1/S^2)]H^{ctr}(\bar{z},z), \tag{53}$$

where

$$\Delta=\frac{(1+\bar{z}z)^2}{2S}\frac{\partial^2}{\partial z\partial\bar{z}} \tag{54}$$

is the Laplace–Beltrami operator acting on the complex projective plane $CP^1=S^2$ which is a Kähler homogeneous manifold SU(2)/U(1). In view of (53), one may convert formula (41) into a form suitable for the quantization by contravariant symbols.

V. SOLARI–KOCHETOV PHASE FROM HOLSTEIN–PRIMAKOFF REPRESENTATION

Now we would like to derive the Solari–Kochetov phase exploiting the paradigm of the Sec. III. For this purpose we employ the Holstein–Primakoff representation[16] for the spin operators

$$\begin{aligned}\hat{s}_+&=\hat{s}_1+i\hat{s}_2=\hat{a}^\dagger\sqrt{2S-\hat{a}^\dagger\hat{a}},\\ \hat{s}_-&=\hat{s}_1-i\hat{s}_2=\sqrt{2S-\hat{a}^\dagger\hat{a}}\,\hat{a},\\ \hat{s}_3&=\hat{a}^\dagger\hat{a}-S,\end{aligned} \tag{55}$$

in terms of the standard annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ with the commutation relation $[\hat{a},\hat{a}^\dagger]=1$. It is easy to check that the operators (55) satisfy the su(2) algebra (37) as well as

$$\tfrac{1}{2}(\hat{s}_+\hat{s}_-+\hat{s}_-\hat{s}_+)+\hat{s}_3^2=S(S+1). \tag{56}$$

Besides the representation (55), there actually exist other representations of the spin algebra in terms of bosonic operators. For the review of their properties and applications in physics, we refer to Refs. 27 and 28.

It is also worth mentioning that in Ref. 29, where the instanton picture of spin tunneling in the LMG model was also considered, the sort of the Holstein–Primakoff representation was used in order to obtain the correct ground-state energy splitting. The authors established some heuristic rule which, however, required an adequate interpretation (see Discussion in Ref. 29). Our approach will allow us to refine their prescription and to establish the link to the consideration of the LMG model made in Ref. 8.

Let us introduce the semiclassical parameter $h=1/(2S)$ and define $\hat{A}=\hat{a}\sqrt{h}$ and $\hat{A}^\dagger=\hat{a}^\dagger\sqrt{h}$, such that

$$[\hat{A},\hat{A}^\dagger]=h. \tag{57}$$

We also define the operators

$$\begin{aligned}\hat{S}_+&=h\hat{s}_+=\hat{A}^\dagger\sqrt{1-\hat{A}^\dagger\hat{A}},\\ \hat{S}_-&=h\hat{s}_-=\sqrt{1-\hat{A}^\dagger\hat{A}}\,\hat{A},\\ \hat{S}_3&=h\hat{s}_3=\hat{A}^\dagger\hat{A}-\tfrac{1}{2},\end{aligned} \tag{58}$$

which satisfy the commutation relations

$$[\hat{S}_+,\hat{S}_-]=2h\hat{S}_3,\quad [\hat{S}_3,\hat{S}_\pm]=\pm h\hat{S}_\pm. \tag{59}$$

The square root in (58) should be understood as an expansion in a Taylor series

$$\sqrt{1-x}=1+\sum_{l=1}^{\infty} b_l x^l \tag{60}$$

with x replaced by $\hat{A}^\dagger\hat{A}$.

One can immediately notice that the operators (58), when expressed through $\hat{A}$ and $\hat{A}^\dagger$, do not depend explicitly on h, and that (57) is similar to (19). This enables us to apply formally the Moyal formula (14) with the Poisson bracket (20) to the operators (58), replacing everywhere $\hbar$ by h. Considering α and $\overline{\alpha}$ to be the ''Weyl symbols'' of $\hat{A}$ and $\hat{A}^\dagger$, respectively, we can thus define the ''Weyl symbols'' of the operators (58).

First we find

$$(\hat{A}^\dagger\hat{A})_W=\overline{\alpha}\alpha-\frac{h}{2}+O(h^2), \tag{61}$$

$$(\hat{A}\hat{A}^\dagger)_W=\overline{\alpha}\alpha+\frac{h}{2}+O(h^2), \tag{62}$$

$$((\hat{A}^\dagger\hat{A})^l)_W=(\overline{\alpha}\alpha)^l-\frac{hl}{2}(\overline{\alpha}\alpha)^{l-1}+O(h^2). \tag{63}$$

Exploiting the latter relation and the trivial equality

$$\frac{d}{dx}\sqrt{1-x}=-\frac{1}{2\sqrt{1-x}}=\sum_{l=1}^{\infty} l b_l x^{l-1} \tag{64}$$

we establish

$$(\sqrt{1-\hat{A}^\dagger\hat{A}})_W=\sqrt{1-\overline{\alpha}\alpha}+\frac{h}{4}\frac{1}{\sqrt{1-\overline{\alpha}\alpha}}+O(h^2). \tag{65}$$

Further use of the Moyal formula (14) leads to the desired definitions

$$(\hat{S}_+)_W=(\hat{A}^\dagger\sqrt{1-\hat{A}^\dagger\hat{A}})_W=\overline{\alpha}\sqrt{1-\overline{\alpha}\alpha}+\frac{h}{2}\frac{\overline{\alpha}}{\sqrt{1-\overline{\alpha}\alpha}}+O(h^2),$$

$$(\hat{S}_-)_W=(\sqrt{1-\hat{A}^\dagger\hat{A}}\hat{A})_W=\alpha\sqrt{1-\overline{\alpha}\alpha}+\frac{h}{2}\frac{\alpha}{\sqrt{1-\overline{\alpha}\alpha}}+O(h^2), \tag{66}$$

$$(\hat{S}_3)_W=\left(\hat{A}^\dagger\hat{A}-\frac{1}{2}\right)_W=\overline{\alpha}\alpha-\frac{1}{2}-\frac{h}{2}+O(h^2).$$

We can construct the approximate realization of the su(2) algebra with respect to the Poisson bracket (20). Taking into account (15) and the commutation relations (59) we deduce that

$$i\{(\hat{S}_+)_W,(\hat{S}_-)_W\}_{\overline{\alpha},\alpha}=2(\hat{S}_3)_W+O(h^2), \tag{67}$$

$$i\{(\hat{S}_3)_W,(\hat{S}_\pm)_W\}_{\overline{\alpha},\alpha}=\pm(\hat{S}_\pm)_W+O(h^2). \tag{68}$$

These formulas can be checked by straightforward calculation using (66).

There exists, however, a subtlety that should be spelled out here. The spin operators (58) act in the finite Hilbert space in contrast to the operators $\hat{q},\hat{p}$ and $\hat{H}(\hat{q},\hat{p})$ in the flat case which act in a different—infinite—Hilbert space. Nevertheless, the ''Weyl symbols'' (66) of the operators (58) do make sense locally in the semiclassical limit $h\to 0$, and, as we shall see, reproduce the Solari–Kochetov phase. Similarly to the flat case, we are going to recognize it for a Hamiltonian linear in the spin operators

$$\hat{H}=\frac{1}{h}\mathbf{C}\cdot\hat{\mathbf{S}}=\frac{1}{h}\left[\frac{1}{2}C_+\hat{S}_-+\frac{1}{2}C_-\hat{S}_++C_3\hat{S}_3\right] \tag{69}$$

in the difference between its principal and ''Weyl symbols''

$$H(\overline{\alpha},\alpha)-H_W(\overline{\alpha},\alpha)=\delta H(\overline{\alpha},\alpha)+O(h). \tag{70}$$

[There is a small distinction in notations in comparison with the flat case since the classical action and the naive classical Hamiltonian for spin are already divided by the semiclassical parameter h and therefore $H(\overline{\alpha},\alpha)$ and $\delta H(\overline{\alpha},\alpha)$ are of order $O(h^{-1})$ and $O(1)$, respectively.]

According to (66) the principal symbol and the next-order correction of (69) are given, respectively, by

$$H(\overline{\alpha},\alpha)=\frac{1}{h}\left[\frac{1}{2}C_+\alpha\sqrt{1-\overline{\alpha}\alpha}+\frac{1}{2}C_-\overline{\alpha}\sqrt{1-\overline{\alpha}\alpha}+C_3\left(\overline{\alpha}\alpha-\frac{1}{2}\right)\right], \tag{71}$$

$$\delta H(\overline{\alpha},\alpha)=-\frac{C_+\alpha+C_-\overline{\alpha}}{4\sqrt{1-\overline{\alpha}\alpha}}+\frac{1}{2}C_3. \tag{72}$$

To compare these expressions with (47) and (48), respectively, we use the Darboux transformation

$$z=\frac{\alpha}{\sqrt{1-\bar{\alpha}\alpha}},\quad \bar{z}=\frac{\bar{\alpha}}{\sqrt{1-\bar{\alpha}\alpha}}. \tag{73}$$

It makes the Kähler symplectic structure locally flat and converts the classical equations of motion (44) into

$$\dot{\alpha}=-ih\frac{\partial H(\bar{\alpha},\alpha)}{\partial\bar{\alpha}}+O(h),\quad \dot{\bar{\alpha}}=ih\frac{\partial H(\bar{\alpha},\alpha)}{\partial\alpha}+O(h). \tag{74}$$

The terms $O(h)$ appear due to the finiteness of the $(\alpha,\bar{\alpha})$ phase space which is a disc on the complex plane. However, they become negligible as $h\to 0$. All the other terms in (74) have the order $O(1)$.

Thus, after the transformation (73) we observe the coincidence of the principal symbols (47) and (71) and obtain the desired relation

$$\tfrac{1}{2}\phi_{SK}=\delta H. \tag{75}$$

Our consideration is not restricted to the case of Hamiltonians linear in spin operators. The formula (75) can be proved valid when the Hamiltonian is a more general element of the enveloping algebra (i.e., a polynomial in spin operators).

Let us consider, for example, the Hamiltonian

$$\hat{H}=c\cdot\frac{(2S-n)!}{(2S-1)!}(\hat{s}_+^n+\hat{s}_-^n), \tag{76}$$

where n is an arbitrary integer number. For $n=2$ and $c=w/\sqrt{2}$ it coincides (up to the constant factor) with the Hamiltonian of the LMG model (49).

We note that it is important to introduce the S-dependent coefficient in (76) so that to make the respective covariant symbol proportional to S:

$$H^{cov}=c\cdot 2S\frac{\bar{z}^n+z^n}{(1+\bar{z}z)^n}. \tag{77}$$

This allows us to identify (77) with the principal symbol, or classical Hamiltonian, which contains the leading-in-S term only.

First, we calculate the Solari–Kochetov phase according to the original formula (45), and obtain

$$\frac{1}{2}\phi_{SK}=-c\cdot\frac{n}{2}\frac{(\bar{z}^n+z^n)(n+\bar{z}z)}{(1+\bar{z}z)^n}. \tag{78}$$

Now we would like to show that the same expression can be obtained from (75) using the Holstein–Primakoff representation. We rewrite the Hamiltonian (76) in terms of the operators (58),

$$\hat{H}=c\cdot h^{-n}\frac{(h^{-1}-n)!}{(h^{-1}-1)!}(\hat{S}_+^n+\hat{S}_-^n), \tag{79}$$

and find its ''Weyl symbol''

$$(\hat{H})_W = c\cdot\frac{1}{h}\left(1+\frac{hn(n-1)}{2}\right)\left[\frac{\overline{z}^n+z^n}{(1+\overline{z}z)^n}+\frac{hn}{2}\,\frac{\overline{z}^n+z^n}{(1+\overline{z}z)^{n-1}}\right]+O(h)$$
$$=c\cdot\left[\frac{1}{h}\,\frac{\overline{z}^n+z^n}{(1+\overline{z}z)^n}+\frac{n}{2}\,\frac{(\overline{z}^n+z^n)(n+\overline{z}z)}{(1+\overline{z}z)^n}\right]+O(h). \tag{80}$$

This expression is derived due to

$$(\hat{S}_+^n)_W=(\overline{\alpha}\sqrt{1-\overline{\alpha}\alpha})^n+\frac{hn}{2}\,\overline{\alpha}^n(\sqrt{1-\overline{\alpha}\alpha})^{n-2}+O(h^2)=\frac{\overline{z}^n}{(1+\overline{z}z)^n}+\frac{hn}{2}\,\frac{\overline{z}^n}{(1+\overline{z}z)^{n-1}}+O(h^2), \tag{81}$$

$$(\hat{S}_-^n)_W=(\alpha\sqrt{1-\overline{\alpha}\alpha})^n+\frac{hn}{2}\,\alpha^n(\sqrt{1-\overline{\alpha}\alpha})^{n-2}+O(h^2)=\frac{z^n}{(1+\overline{z}z)^n}+\frac{hn}{2}\,\frac{z^n}{(1+\overline{z}z)^{n-1}}+O(h^2), \tag{82}$$

and

$$\frac{(N-n)!}{N!}=N^{-n}\left(1+\frac{1}{N}\,\frac{n(n-1)}{2}+O\left(\frac{1}{N^2}\right)\right), \tag{83}$$

for $N\equiv 2S=h^{-1}$. The relations (73) have been also employed.

Thus, we see that the leading term in (80) coincides with (77), and the next-to-leading term is in agreement with (78). We note that in our derivation of the Solari–Kochetov phase it was important to expand in a series of h the h-dependent coefficient—the ratio of two factorials—which was inherited from the quantum Hamiltonian (79).

VI. DISCUSSION

We put forward a proposition to determine the extra-phase correction in the semiclassical expression for a propagator as the difference between the principal and the Weyl symbol of the quantum Hamiltonian. Based on the Wigner–Weyl calculus, it becomes a well-defined and efficient computational prescription.

We offered to exploit this paradigm for the case of the spin propagator, making use of the Holstein–Primakoff representation of the su(2) algebra. However, there exists a subtle issue concerning the finiteness of the spin Hilbert space. It also shows up on the classical level: the classical phase space in such a representation is a flat disc which has finite volume. Nevertheless, in the semiclassical limit $S\to\infty$ the difference between the principal and the ''Weyl symbols'' appears to be well-defined. This is also confirmed by the possibility to construct the su(2) algebra realization in terms of the Poisson bracket $i\{\cdot,\cdot\}_{\overline{\alpha},\alpha}$ with the required accuracy [modulo terms $O(h^2)$]. Obviously, this amounts to defining the spin Weyl symbols only locally.

We applied the developed prescription for the calculation of the phase correction to the semiclassical spin coherent-state propagator for systems with the Hamiltonian which is either linear or nonlinear in spin operators. The presented consideration can be straightforwardly generalized for any Hamiltonian which is a polynomial in spin operators. Our prescription is rather simple from a computational point of view, and it does not require the use of the polynomial tensor operators (cf. Ref. 14).

In summary, we would like to motivate the usefulness of the ''Weyl symbol'' for spin with the following reference. The idea to introduce such a symbol is employed in order to reveal the similarity between the phase corrections to the semiclassical flat and spin propagators, and it appears quite naturally when one considers the semiclassical limit of the Holstein–Primakoff (HP) representation including the next-to-leading term. In Ref. 29 the Lipkin–Meshkov–Glick (LMG) model (quadratic in spin) has been considered using the sort of the HP representation. The authors recognized the necessity of the phase correction to the semiclassical spin propagator within their

approach and formulated the heuristic rule for its calculation. However, they stated the lack of its adequate interpretation. On the other hand, the consideration of the LMG model made in Ref. 8 uses the original Solari–Kochetov expression for the phase correction. The relation between these two approaches is missing, although both of them have led to the correct result. Thus, introducing the ''Weyl symbol'' for spin helps to bridge the gap between two different interpretations of the same extra-phase correction.

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Green functions of the Dirac equation with magnetic-solenoid field

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Various Green functions of the Dirac equation with a magnetic-solenoid field (the superposition of the Aharonov–Bohm field and a collinear uniform magnetic field) are constructed and studied. The problem is considered in $2+1$ and $3+1$ dimensions for the natural extension of the Dirac operator (the extension obtained from the solenoid regularization). Representations of the Green functions as proper time integrals are derived. The nonrelativistic limit is considered. For the sake of completeness the Green functions of the Klein–Gordon particles are constructed as well. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1699483]

I. INTRODUCTION

In the present paper we continue our previous study[1–3] of the Dirac equation with a magnetic-solenoid field, constructing and studying various Green functions of this equation. We recall that the magnetic-solenoid field is the collinear superposition of the constant uniform magnetic field and the Aharonov–Bohm (AB) field. The AB field is a field of an infinitely long and infinitesimally thin solenoid. Recently the interest in such a field configuration has been renewed in connection with planar physics problems, quantum Hall effect, and the Aharonov–Bohm effect in cyclotron and synchrotron radiations.[4–9]

In principle, the Green functions can be constructed whenever complete sets of solutions of the Dirac equations are available. In this connection, one should recall that solutions of the Dirac equation with the magnetic-solenoid field in $2+1$ and $3+1$ dimensions were obtained in Ref. 1. The singularity of the AB field demands a special attention to the correct definition of the Dirac operator. The need for self-adjoint extensions in the case of the Dirac Hamiltonian with the pure AB field in $2+1$ dimensions was recognized in Refs. 10 and 11 where certain boundary conditions at the origin were established. The regularized case and peculiarities of the behavior of a spinning particle in the presence of the magnetic string were considered in Refs. 12 and 13. The problem of the self-adjoint extension of the Dirac operator with the magnetic-solenoid field was studied in Refs. 2, 3, and 14. In $2+1$ dimensions, a one-parametric family of self-adjoint Dirac Hamiltonians specified by the corresponding boundary conditions at the AB solenoid was constructed, and the spectrum and eigenfunctions for each value of the extension parameter were found. In $3+1$ dimensions, a two-parametric family of the self-adjoint Dirac Hamiltonians was constructed on the condition that the spin polarization is conserved. The corresponding spectrum and eigenfunctions for each value of the extension parameters were found as well. In Refs. 2 and 3 the procedure of solenoid regularization was also considered. The procedure implies considering the finite solenoid and then making its radius go to zero. This procedure specifies some particular boundary conditions. The values of the extension parameters corresponding to the solenoid regularization case were determined in $2+1$ and $3+1$ dimensions. Further, we call the corresponding extension the natural extension. Nonrelativistic propagators for the spinless and spin-1/2 particle

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moving in the pure AB field were considered mainly in the relation to the AB effect. The propagator of the spinless particle was found in Refs. 15, 16, and 17 as a sum of partial propagators corresponding to homotopically different paths in the covering space of the physical background. The nonrelativistic propagator of the spin-1/2 particle in the AB field for a particular value of the self-adjoint extension parameter was discussed in Ref. 18. The relativistic scalar case for the AB field was studied in Ref. 19. The propagators and the AB effect in general gauge theories were considered in Refs. 20 and 21. Recently, vacuum polarization effects in the AB field have aroused great interest, see, for example, Refs. 22 and 23 and references therein.

In the present paper, we construct and study the Green functions of the Dirac particle in the magnetic-solenoid field in $2+1$ and $3+1$ dimensions. The physical importance of the problem is stressed by the fact that the knowledge of the Green functions in such a configuration allows one to study quantum (and quantum field) effects in the magnetic-solenoid field on a regular base. A technical specificity of the problem is related to the necessity to take into account all the peculiarities related to the self-adjoint extension problem of the Dirac operator in the background under consideration. In Sec. II we consider the $(2+1)$-dimensional case in detail. Here, constructing the Green functions, we use the exact solutions of the Dirac equation that are related to the specific values of the extension parameter. These values correspond to the natural extension, see above. The representations of the Green functions as proper time integrals are derived. In addition, we calculate the nonrelativistic Green functions as well. In Sec. III we extend the results to the $(3+1)$-dimensional case. In the Appendix, for the sake of completeness, we present the Green functions of the relativistic scalar particle.

We note that the magnetic-solenoid field belongs to such type of fields that do not violate the vacuum stability. For such fields a unique stable vacuum exists, and quantum field definitions of the Green functions below hold true.[24] In particular, the causal propagator $S^c(x,x')$ and the anticausal propagator $S^{\bar{c}}(x,x')$ are defined by the expressions

$$S^c(x,x')=i\langle 0|T\hat{\psi}(x)\hat{\bar{\psi}}(x')|0\rangle, \tag{1}$$

$$S^{\bar{c}}(x,x')=i\langle 0|\hat{\psi}(x)\hat{\bar{\psi}}(x')T|0\rangle, \tag{2}$$

where $\hat{\psi}(x)$ is the quantum spinor field in the Furry representation, satisfying the Dirac equation with the magnetic-solenoid field, $|0\rangle$ is the vacuum in this representation. The symbol of the T-product acts on both sides: it orders the field operators to its right-hand side and antiorders them to its left-hand side. The functions $S^c(x,x')$, $S^{\bar{c}}(x,x')$ can be expressed via the functions $S^{\mp}(x,x')$,

$$S^c(x,x')=\theta(\Delta x^0)S^-(x,x')-\theta(-\Delta x^0)S^+(x,x'), \quad \Delta x^0=x^0-x^{0\prime}, \tag{3}$$

$$S^{\bar{c}}(x,x')=\theta(-\Delta x^0)S^-(x,x')-\theta(\Delta x^0)S^+(x,x'), \tag{4}$$

and the latter can be calculated via a complete set ${}_{\pm}\psi_a(x)$ of solutions of the Dirac equation with the magnetic-solenoid field as

$$S^{\mp}(x,x')=i\sum_a {}_{\pm}\psi_a(x)\,\overline{{}_{\pm}\psi_a(x')}. \tag{5}$$

The solutions with the subscript $(+)$ belong to the positive energy spectrum, whereas the solutions with the subscript $(-)$ belong to the negative energy spectrum. Via a all possible quantum numbers are denoted.

The Dirac equation with the magnetic-solenoid field has the form

$$(\gamma^\nu P_\nu - M)\psi(x)=0. \tag{6}$$

Here $P_\nu = i\partial_\nu - qA_\nu(x)$, $x=(x^\nu)$, q is an algebraic charge, for electrons $q=-e<0$, M is the electron mass, and $A_\nu(x)$ are potentials of the magnetic-solenoid field. In the $(3+1)$-dimensional case $\nu=0,1,2,3$ and γ^ν are the corresponding gamma-matrices. In the $(2+1)$-dimensional case $\nu=0,1,2$ and in what follows, we employ the letter Γ to denote the gamma-matrices. We use for these matrices the following representation:

$$\Gamma^0=\sigma^3, \quad \Gamma^1=i\sigma^2, \quad \Gamma^2=-i\sigma^1,$$

where σ^i are the Pauli matrices. In cylindric coordinates (φ,r), $x^1=r\cos\varphi$, $x^2=r\sin\varphi$, the potentials of the magnetic-solenoid field have the form

$$A_0=0, \quad eA_1=[l_0+\mu+A(r)]\frac{\sin\varphi}{r}, \quad eA_2=-[l_0+\mu+A(r)]\frac{\cos\varphi}{r},$$

$$(A_3=0 \text{ in } 3+1), \quad A(r)=eBr^2/2. \tag{7}$$

Here B is the magnitude of the uniform magnetic field, and the magnitude B^{AB} of the AB field is given by the expression $B^{\mathrm{AB}}=\Phi\,\delta(x^1)\,\delta(x^2)$, where Φ is the AB-solenoid flux, $(l_0+\mu)=\Phi/\Phi_0$, $\Phi_0=2\pi/e$. It is supposed that l_0 is integer and $0\leqslant\mu<1$.

The functions $S^{\mp}(x,x')$ obey the Dirac equation (6), whereas the causal and anticausal propagators obey the nonhomogeneous Dirac equations:

$$(\gamma^\nu P_\nu - M)S^c(x,x') = -\delta(x-x'), \quad (\gamma^\nu P_\nu - M)S^{\bar{c}}(x,x') = \delta(x-x').$$

We note that the commutation function $S(x,x')$, the advanced $S^{\mathrm{adv}}(x,x')$ and the retarded $S^{\mathrm{ret}}(x,x')$ Green functions can be expressed in terms of $S^c(x,x')$, $S^{\bar{c}}(x,x')$ as follows:

$$S(x,x')=S^-(x,x')+S^+(x,x')=\mathrm{sgn}(\Delta x^0)[S^c(x,x')-S^{\bar{c}}(x,x')], \tag{8}$$

$$S^{\mathrm{adv}}(x,x')=-\theta(-\Delta x^0)S(x,x'), \quad S^{\mathrm{ret}}(x,x')=\theta(\Delta x^0)S(x,x'). \tag{9}$$

II. 2+1 DIMENSIONAL CASE

A. Sets of exact solutions

First we study the $(2+1)$-dimensional case, for which, as known,[2,3] the Dirac operator with the magnetic-solenoid field in $2+1$ dimensions possesses a one-parameter family of self-adjoint extensions. That provides a one-parameter family of boundary conditions at the origin. Following Refs. 2 and 3, we denote the extension parameter as Θ. Generally speaking, the AB symmetry is violated for the spinning particle, which is therefore sensible to the solenoid flux sign. As was demonstrated in Refs. 2 and 3, the values $\Theta=\pm\pi/2$ correspond to the natural extension, $\Theta=-\pi/2$ if the flux is positive and $\Theta=\pi/2$ if the flux is negative. Below we present a set of solutions ${}_\pm\psi_a(x)$ of (6) which we will use for Green function construction according to the formulas (5). We consider the problem separately for two values of the extension parameter.

We start with the case $\Theta=-\pi/2$. The positive energy spectrum is given by ${}_+\varepsilon$ and the negative energy spectrum is given by ${}_-\varepsilon$,

$${}_+\varepsilon=-{}_-\varepsilon=\sqrt{M^2+\omega}. \tag{10}$$

Both branches are determined by the spectrum of the quantity ω which is defined below. The solutions ${}_\pm\psi_a(x)$ can be expressed via the solutions $u(x)$ of the squared Dirac equation. The latter solutions have the form

$$\begin{gathered} {}_\pm u_{m,l,\sigma}(x)=e^{-i\,{}_\pm\varepsilon x^0}u_{m,l,\sigma}(x_\perp), \\ x_\perp=(x^1,x^2), \quad m=0,1,\ldots, \quad l=0,\pm1,\ldots, \quad \sigma=\pm1, \end{gathered} \tag{11}$$

where

$$u_{m,l,\sigma}(x_\perp)=\sqrt{\gamma}g_l(\varphi)\phi_{m,l,\sigma}(r)v_\sigma, \quad l\neq 0,$$

$$u_{m,0,+1}(x_\perp)=\sqrt{\gamma}g_0(\varphi)\phi_{m,0,+1}(r)v_{+1},$$

$$u_{m,0,-1}(x_\perp)=\sqrt{\gamma}g_0(\varphi)\phi^{ir}_{m,-1}(r)v_{-1}, \quad \gamma=e|B|,$$

and

$$g_l(\varphi)=\frac{1}{\sqrt{2\pi}}\exp\left\{i\varphi\left[l-l_0-\frac{1}{2}(1+\sigma^3)\right]\right\},$$

$$v_{+1}=\begin{pmatrix}1\\0\end{pmatrix}, \quad v_{-1}=\begin{pmatrix}0\\1\end{pmatrix}.$$

The functions $\phi_{m,l,\sigma}(r)$, $\phi^{ir}_{m,-1}(r)$ are expressed via the Laguerre functions $I_{m+\alpha,m}(\rho)$ as

$$\begin{gathered}\phi_{m,l,\sigma}(r)=I_{m+|\nu|,m}(\rho), \quad \phi^{ir}_{m,-1}(r)=I_{m-\mu,m}(\rho),\\ \rho=\gamma r^2/2, \quad \nu=\mu+l-(1+\sigma)/2.\end{gathered} \tag{12}$$

We recall that the Laguerre functions $I_{m+\alpha,m}(\rho)$ are related to the Laguerre polynomials $L^\alpha_m(x)$ [8.970, 8.972.1 (Ref. 25)] as

$$I_{m+\alpha,m}(x)=\sqrt{\frac{m!}{\Gamma(m+\alpha+1)}}e^{-x/2}x^{\alpha/2}L^\alpha_m(x).$$

For the magnetic field $B>0$, the spectrum of ω corresponding to the functions $u_{m,l,\sigma}(x_\perp)$ is

$$\omega=\begin{cases}2\gamma(m+l+\mu), & l-(1+\sigma)/2\geqslant 0,\\ 2\gamma(m+(1+\sigma)/2), & l-(1+\sigma)/2<0,\end{cases} \tag{13}$$

except the functions $u_{m,0,-1}(x_\perp)$ for which the spectrum of ω is

$$\omega=2\gamma m. \tag{14}$$

Then the complete set ${}_\pm\psi_a$ with $a=(m,l)$ has the form

$${}_\pm\psi_{m,l}(x)=N(\Gamma P+M)\,{}_\pm u_{m,l,-1}(x). \tag{15}$$

The latter form provides correct expressions both for $\omega\neq 0$ and $\omega=0$, since the states with $\omega=0$ can only be expressed in terms of the spinors with $\sigma=-1$ [we note that ${}_+\psi\equiv 0$ for $\omega=0$, nevertheless it is convenient to remain in (11) u_+ with ${}_+\varepsilon=M$]. The normalization factor with respect to the usual inner product $(\psi,\psi')=\int\psi^\dagger(x)\psi'(x)\mathrm{d}\mathbf{x}$ reads

$$N=\begin{cases}[2|{}_\pm\varepsilon|(|{}_\pm\varepsilon|-M)]^{-1/2}, & \omega\neq 0,\\ [2M]^{-1}, & \omega=0.\end{cases}$$

The quantum number l characterizes the angular momentum of the particle, m is the radial quantum number, see Ref. 1.

For $B<0$ the spectrum of states differs nontrivially from the expressions given by Eqs. (13) and (14). Here ω corresponding to $u_{m,l,\sigma}(r)$ is

$$\omega=\begin{cases} 2\gamma(m-l+1-\mu), & l-(1+\sigma)/2<0, \\ 2\gamma(m+(1-\sigma)/2), & l-(1+\sigma)/2\geqslant 0, \end{cases} \tag{16}$$

except the functions $u_{m,0,-1}(x_\perp)$ for which the spectrum of ω is

$$\omega=2\gamma(m+1-\mu). \tag{17}$$

Now we go to the case with the extension parameter $\Theta=\pi/2$. We recall that one needs for self-adjoint extensions of the radial Dirac Hamiltonian only in the subspace $l=0$ to which we refer to as the critical subspace. Thus, the only solutions in the $l=0$ subspace must be subjected to the one of asymptotic condition from a one-parametric family of boundary conditions as $r\to 0$. By this reason for $\Theta=\pi/2$, the solutions only differ from (11) in the subspace $l=0$,

$$\begin{gathered} u_{m,0,+1}(x_\perp)=\sqrt{\gamma}g_0(\varphi)\phi^{ir}_{m,+1}(r)\upsilon_{+1}, \quad \phi^{ir}_{m,+1}(r)=I_{m+\mu-1,m}(\rho), \\ u_{m,0,-1}(x_\perp)=\sqrt{\gamma}g_0(\varphi)\phi_{m,0,-1}(r)\upsilon_{-1}, \end{gathered} \tag{18}$$

where the spectrum for $u_{m,0,+1}(x_\perp)$ is given as

$$\omega=2\gamma(m+\mu), \quad B>0, \tag{19}$$

$$\omega=2\gamma m, \quad B<0. \tag{20}$$

B. Construction of Green functions

The main point in constructing the Green functions is the summations in the representation (5). In the case under consideration, this summation can be done with the help of special relations which can be established for the solutions of the Dirac equation.

Let us start with the calculation of the Green functions for the extension parameter $\Theta=-\pi/2$ and $B>0$. In this case, taking into account that the eigenfunctions u of the equation $[(\Gamma P_\perp)^2+\omega]u=0$ corresponding to any $\omega\neq 0$ obey the equations

$$\begin{gathered} \Gamma P_\perp\, {}_\pm u_{m_+,l,-\sigma}(x)=-i\sqrt{\omega}\,{}_\pm u_{m_-,l,\sigma}(x), \quad l\leqslant 0, \quad P_\perp=(0,P_1,P_2), \\ \Gamma P_\perp\, {}_\pm u_{m,l,-\sigma}(x)=i\sqrt{\omega}\,{}_\pm u_{m,l,\sigma}(x), \quad l\geqslant 1, \quad m_\pm=m+(1\pm\sigma)/2, \end{gathered} \tag{21}$$

and the explicit form of the solutions ${}_\pm\psi_{m,l}$, one can verify that for $|\varepsilon|\neq M$ the following relations hold true:

$$\begin{gathered} {}_\pm\psi_{m,l}(x)\,{}_\pm\overline{\psi}_{m,l}(x')=(\Gamma P+M)\frac{1}{2\,{}_\pm\varepsilon}e^{-i\,{}_\pm\varepsilon\Delta x^0}\sum_{\sigma=\pm 1}\phi_{m_-,l,\sigma}(x_\perp,x'_\perp)\Xi_\sigma, \quad l\leqslant 0, \\ {}_\pm\psi_{m,l}(x)\,{}_\pm\overline{\psi}_{m,l}(x')=(\Gamma P+M)\frac{1}{2\,{}_\pm\varepsilon}e^{-i\,{}_\pm\varepsilon\Delta x^0}\sum_{\sigma=\pm 1}\phi_{m,l,\sigma}(x_\perp,x'_\perp)\Xi_\sigma, \quad l\geqslant 1, \end{gathered} \tag{22}$$

where

$$\begin{gathered} \phi_{m,l,\sigma}(x_\perp,x'_\perp)=\frac{\gamma}{2\pi}e^{i[l-l_0-(1+\sigma)/2]\Delta\varphi}I_{m+\alpha,m}(\rho)I_{m+\alpha,m}(\rho'), \\ \Delta\varphi=\varphi-\varphi', \quad \alpha=\begin{cases} \mu+l-(1+\sigma)/2, & l\geqslant 1, \\ -[\mu+l-(1+\sigma)/2], & l\leqslant 0, \end{cases} \quad \Xi_{\pm 1}=(1\pm\sigma^3)/2. \end{gathered} \tag{23}$$

The above relations and Eqs. (3) and (5) allow us to represent the causal Green function in the following form:

$$S^c(x,x')=(\Gamma P+M)\Delta^c(x,x'),$$
$$\Delta^c(x,x')=i\sum_{m,l,\sigma}\left[\theta(\Delta x^0)\frac{e^{-i_+\varepsilon\Delta x^0}}{2_+\varepsilon}-\theta(-\Delta x^0)\frac{e^{-i_-\varepsilon\Delta x^0}}{2_-\varepsilon}\right]\phi_{m,l,\sigma}(x_\perp,x'_\perp)\Xi_\sigma. \tag{24}$$

Then we can use the representations

$$\theta(\Delta x^0)\frac{e^{-i_+\varepsilon\Delta x^0}}{2_+\varepsilon}-\theta(-\Delta x^0)\frac{e^{-i_-\varepsilon\Delta x^0}}{2_-\varepsilon}=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{-ip_0\Delta x^0}}{\varepsilon^2-p_0^2-i\epsilon}\mathrm{d}p_0, \tag{25}$$

$$\frac{1}{\varepsilon^2-p_0^2-i\epsilon}=i\int_0^\infty e^{-i(\varepsilon^2-p_0^2)s}\,\mathrm{d}s, \tag{26}$$

in Eq. (24). Integrating over p_0, we obtain finally

$$\Delta^c(x,x')=\int_0^\infty f(x,x',s)\mathrm{d}s,$$
$$f(x,x',s)=\frac{1}{2(\pi s)^{1/2}}e^{(-i\Delta x_0^2/4s)}e^{i\pi/4}e^{-iM^2s}i\sum_{m,l,\sigma}e^{-i\omega s}\phi_{m,l,\sigma}(x_\perp,x'_\perp)\Xi_\sigma. \tag{27}$$

The path of the integration over s is deformed so that it goes slightly below the singular points $s_k=k\pi/\gamma$, $k=1,2,\ldots$.

Using (5), (22), and the representation

$$-\theta(-\Delta x^0)\frac{e^{-i_+\varepsilon\Delta x^0}}{2_+\varepsilon}+\theta(\Delta x^0)\frac{e^{-i_-\varepsilon\Delta x^0}}{2_-\varepsilon}=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{-ip_0\Delta x^0}}{\varepsilon^2-p_0^2+i\epsilon}\mathrm{d}p_0,$$
$$\frac{1}{\varepsilon^2-p_0^2+i\epsilon}=i\int_{-0}^{-\infty}e^{-i(\varepsilon^2-p_0^2)s}\,\mathrm{d}s, \tag{28}$$

instead of (25) and (26) we obtain from (4),

$$S^{\bar c}(x,x')=(\Gamma P+M)\Delta^{\bar c}(x,x'),\quad \Delta^{\bar c}(x,x')=\int_{-0}^{-\infty}f(x,x',s)\mathrm{d}s, \tag{29}$$

where $f(x,x',s)$ is given by Eq. (27). The negative values for s are defined as $s=|s|e^{-i\pi}$, and the path of integration over s is deformed so that it goes slightly below the singular points $-s_k$.

We now consider the summations in (27). Applying the formula [8.976(1) (Ref. 25)] we can sum over m to get

$$\sum_{m=0}^{\infty}e^{-i2m\gamma s}I_{m+\alpha,m}(\rho)I_{m+\alpha,m}(\rho')=\exp\left\{\frac{i}{2}(\rho+\rho')\cot(\gamma s)\right\}\frac{e^{i\alpha\gamma s}e^{i\gamma s}}{2i\sin(\gamma s)}e^{-i\pi\alpha/2}J_\alpha(z),$$
$$z=\sqrt{\rho\rho'}/\sin(\gamma s), \tag{30}$$

where $J_\alpha(z)$ are the Bessel functions [8.402 (Ref. 25)], and for negative s we take $\arg s=-\pi+0$.

Similar results can be obtained for the case $B<0$. Here one should use the solutions corresponding to the spectrum of ω (16) and (17). Then these results can be united to obtain expressions which hold true for any sign of B,

$$f(x,x',s)=\sum_{l=-\infty}^{\infty} f_l(x,x',s), \quad f_l(x,x',s)=A(s)\sum_{\sigma=\pm 1}\Phi_{l,\sigma}(s)e^{-i\sigma eBs}\Xi_\sigma,$$
$$A(s)=\frac{eB}{8\pi^{3/2}s^{1/2}\sin(eBs)}\exp\left\{\frac{i\pi}{4}-iM^2s-il_0\Delta\varphi\right\}$$
$$\times\exp\left\{-\frac{i(\Delta x_0)^2}{4s}+\frac{ieB}{4}(r^2+r'^2)\cot(eBs)\right\}, \tag{31}$$

$$\Phi_{l,\sigma}(s)=e^{il_\sigma\Delta\varphi}e^{-i(l_\sigma+\mu)eBs}e^{-i\pi|l_\sigma+\mu|/2}J_{|l_\sigma+\mu|}(z), \quad l_\sigma=l-(1+\sigma)/2, \quad l\neq 0,$$
$$\Phi_{0,+1}(s)=e^{-i\Delta\varphi}e^{i(1-\mu)eBs}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z), \quad \Phi_{0,-1}(s)=e^{-i\mu eBs}e^{i\pi\mu/2}J_{-\mu}(z). \tag{32}$$

Now we consider the summation over l. One can see that the following relations hold true:

$$\sum_{l=1}^{\infty}\Phi_{l,-1}(s)=\sum_{l=1}^{\infty}\Phi_{l+1,+1}(s)=e^{-i\mu eBs}Y(z,\Delta\varphi-eBs,\mu),$$

$$\sum_{l=-1}^{-\infty}\Phi_{l,-1}(s)=\sum_{l=-1}^{-\infty}\Phi_{l+1,+1}(s)=e^{-i\mu eBs}Y(z,-\Delta\varphi+eBs,-\mu),$$

where

$$Y(z,\eta,\mu)=a_1(z)+\tilde{Y}(z,\eta,\mu), \quad \tilde{Y}(z,\eta,\mu)=\sum_{l=2}^{\infty}a_l(z), \quad a_l(z)=e^{i\eta l}(-i)^{l+\mu}J_{l+\mu}(z). \tag{33}$$

The evaluation of the sum in (33) can be done in a similar way to what was done in Ref. 26. There exist all $\partial_z a_l(z)$ on the half-line, $0<z<\infty$, and the relation [8.471 (2) (Ref. 25)], $\partial_z J_\nu(z)=[J_{\nu-1}(z)-J_{\nu+1}(z)]/2$, can be used. The series $\tilde{Y}(z,\eta,\mu)$ converges and the series of derivatives $\Sigma_{l=2}^{\infty}\partial_z a_l(z)$ converges uniformly in $(0,\infty)$. It is a sufficient condition to write down $\partial_z\tilde{Y}(z,\eta,\mu)=\Sigma_{l=2}^{\infty}\partial_z a_l(z)$. Thus, one arrives to a differential equation with respect to $Y(z,\eta,\mu)$,

$$\frac{d}{dz}Y(z,\eta,\mu)=-Y(z,\eta,\mu)i\cos\eta+\frac{1}{2}(-i)^{\mu}[-ie^{i\eta}J_\mu(z)+J_{1+\mu}(z)]. \tag{34}$$

that is true on the half-line, $0<z<\infty$. The solution of (34) reads

$$Y(z,\eta,\mu)=\frac{1}{2}(-i)^{\mu}\int_0^z e^{i(y-z)\cos\eta}[-ie^{i\eta}J_\mu(y)+J_{1+\mu}(y)]dy. \tag{35}$$

This is also valid for $Y(z,-\eta,-\mu)$.

It is useful to introduce the following function:

$$f_{nc}(x,x',s)=\sum_{l\neq 0}f_l(x,x',s).$$

It defines the part of the Green functions that is the same for all extensions. With the help of the function $Y(z,\eta,\mu)$ (33), (35) one can write

$$f_{nc}(x,x',s)=A(s)e^{-i\mu eBs}e^{-ieBs\sigma^3}\{Y(z,\Delta\varphi-eBs,\mu)+Y(z,-\Delta\varphi+eBs,-\mu)$$
$$+[e^{-i\pi\mu/2}J_{\mu}(z)-e^{-i(\Delta\varphi-eBs)}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z)]\Xi_{+1}\}. \tag{36}$$

The function $f_0(x,x',s)$ is specific for each extension. It is reasonable to mark it with a superscript that assumes the values of the extension parameter. Thus, for $\Theta=-\pi/2$,

$$f_0^{(-\pi/2)}(x,x',s)=A(s)e^{-i\mu eBs}[e^{-i\Delta\varphi}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z)\Xi_{+1}+e^{-ieBs\sigma^3}e^{i\pi\mu/2}J_{-\mu}(z)\Xi_{-1}]. \tag{37}$$

Accordingly, the function $f(x,x',s)$ acquires the same superscript,

$$f^{(-\pi/2)}(x,x',s)=f_{nc}(x,x',s)+f_0^{(-\pi/2)}(x,x',s). \tag{38}$$

For the extension parameter $\Theta=\pi/2$, one obtains

$$f_0^{(\pi/2)}(x,x',s)=A(s)e^{-i\mu eBs}[e^{-i\Delta\varphi}e^{-i\pi(\mu-1)/2}J_{\mu-1}(z)\Xi_{+1}+e^{-ieBs\sigma^3}e^{-i\pi\mu/2}J_{\mu}(z)\Xi_{-1}],$$
$$f^{(\pi/2)}(x,x',s)=f_{nc}(x,x',s)+f_0^{(\pi/2)}(x,x',s). \tag{39}$$

Besides, one can consider particles with "spin-down" polarization in $2+1$ dimensions. The corresponding wave functions $\psi^{(-1)}(x)$ can be presented as

$$\psi^{(-1)}(x)=\sigma^1(\Gamma P-M)u(x)\,,$$

where $u(x)$ are solutions (11) of the squared Dirac equation. The propagator related to such particles can be expressed in terms of the function $\Delta^c(x,x')$ (24),

$$S^c_{(-1)}(x,x')=-\sigma^1(\Gamma P-M)\Delta^c(x,x')\sigma^1\,.$$

At this point we should make some remarks.

One can see that there exists a simple relation between scalar Green functions and Green functions of the squared Dirac equation (for the above considered extensions). Consider this relation in the example of causal Green functions. First of all, we note that the Klein–Gordon equation differs from the squared Dirac equation by the Zeeman interaction term. Then we can see (remembering the origin of the quantum number l for both spinning and spinless particles) that the scalar propagator can be derived from $\Delta^c(x,x')$ by only retaining the terms with $\sigma=-1$ only. The term $eB\sigma^3$, which is responsible for the Zeeman interaction with the uniform magnetic field, has to be removed. The Zeeman interaction with the solenoid flux, influencing the terms with $l=0$, depends on the flux sign and can be repulsive or attractive. The repulsive contact interaction case is physically equivalent to the spinless case, since in both cases the corresponding wave functions vanish at the origin. The necessary boundary condition is realized for the extension parameter $\Theta=\pi/2$. Thus, one can obtain the scalar Green functions using the coefficients of Ξ_{-1} in $f_l(x,x',s)$ (31), (32) and $f_0^{(\pi/2)}(x,x',s)$ (39). By following such prescriptions, one arrives at the expression (A1) obtained by direct calculation.

In the spinless case there is no physically preferred orientation of the plane x^1x^2. Therefore, the solenoid flux direction does not matter, i.e., the AB symmetry, $l_0\to l_0+1$, is conserved. The direction of the uniform magnetic field does not matter as well. This can be observed from the explicit form of the Green functions (A1) where the change $B\to -B$ is equivalent to the choice of the opposite orientation of the plane, $l\to -l$, $\Delta\varphi\to-\Delta\varphi$, $\Phi\to-\Phi$. In the spinning case the given spin direction breaks the symmetry related to the plane orientation. The Zeeman interaction of the spin with the background violates the AB symmetry as well as the symmetry with respect to the change $B\to -B$.

As is known, influence of the solenoid flux on the particle is observed only when the flux is not equal to an integral number of quanta ($\mu\neq 0$). In this connection it is instructive to consider

the Green functions for the particular case $\mu=0$. We note that the part $f_{nc}(x,x',s)$ (36) of the function $f(x,x',s)$ is regular everywhere, while the part $f_0(x,x',s)$ is singular at the origin. Thus, taking the limit $\mu\to 0$ in (36) and using the relation $J_1(y)=-J_0'(y)$ we get

$$f_{nc}(x,x',s)=A(s)e^{-ieBs\sigma^3}\{e^{-iz\cos(\Delta\varphi-eBs)}-J_0(z)+[J_0(z)+ie^{-i(\Delta\varphi-eBs)}J_1(z)]\Xi_{+1}\}.$$

The corresponding expression for $f_0(x,x',s)$ can be obtained in the following way. We restrict the range of z to $0<\delta<z<\infty$, where $\delta\ll 1$. Then we take the limit $\mu\to 0$ and use the continuity of the Bessel functions with respect to its index. At the end we construct the analytic continuation of the obtained expressions over the interval $(0,\delta)$. Thus, starting from either (37) or (39) we get

$$f_0(x,x',s)=A(s)[-ie^{-i\Delta\varphi}J_1(z)\Xi_{+1}+e^{ieBs}J_0(z)\Xi_{-1}],$$

where the superscript is no longer necessary. Thus, the explicit form of $f(x,x',s)$ is

$$f(x,x',s)=\frac{eB}{8\pi^{3/2}s^{1/2}\sin(eBs)}\exp\left\{\frac{i\pi}{4}-\frac{i(\Delta x_0)^2}{4s}-iM^2s-ieBs\sigma^3\right\}$$
$$\times\exp\left\{-il_0\Delta\varphi+\frac{ieB}{4}(r^2+r'^2)\cot(eBs)-\frac{ieBrr'\cos(\Delta\varphi-eBs)}{2\sin(eBs)}\right\}. \quad (40)$$

Making a transformation to Cartesian coordinates in (40) and setting $l_0=0$, one can obtain the known result of the uniform magnetic field, see for example, Ref. 27.

C. Nonrelativistic case

Consideration of the Green functions in the background under question in the nonrelativistic case is important for various physical applications. Below we study this case in detail. The solutions of the Schrödinger equation for "spin-up" particles $(+)$ and antiparticles $(-)$ in the case $\Theta=-\pi/2$ read

$$_+\phi_{m,l}(x)=e^{-iEx^0}\sqrt{\frac{\gamma}{2\pi}}e^{i(l-l_0-1)\varphi}\phi_{m,l,+1}(r),\quad E=\frac{\omega_{m,l,\sigma}}{2M},$$
$$_-\phi_{m,l}(x)=e^{-iEx^0}\sqrt{\frac{\gamma}{2\pi}}e^{-i(l-l_0)\varphi}\phi_{m,l,-1}(r),\quad l\neq 0, \quad (41)$$

$$_-\phi_{m,0}(x)=e^{-iEx^0}\sqrt{\frac{\gamma}{2\pi}}e^{il_0\varphi}\phi^{ir}_{m,-1}(r), \quad (42)$$

where the values $\omega_{m,l,\sigma}$ are defined by m,l,σ with the help of formulas (13), (14) for $B>0$, and (16), (17) for $B<0$. The solutions $_+\phi_{m,l}(x)$ ($_-\phi_{m,l}(x)$) for the "spin-down" case can be obtained from the solutions $_-\phi_{m,l}(x)$ ($_+\phi_{m,l}(x)$) for the "spin-up" case with the change $\varphi\to-\varphi$ in (41), (42).

The retarded Green functions for particles and antiparticles are defined as

$$S^{\mathrm{ret},(\pm)}(x,x')=\theta(\Delta x^0)\sum_l S_l^{(\pm)}(x,x'),\quad S_l^{(\pm)}(x,x')=i\sum_m {}_\pm\phi_{m,l}(x)\,{}_\pm\phi^*_{m,l}(x'),$$
$$S^{(\pm)}_{nc}(x,x')=\sum_{l\neq 0}S_l^{(\pm)}(x,x'), \quad (43)$$

where the part $S^{(\pm)}_{nc}(x,x')$ is the same for all extensions, whereas $S_0^{(\pm)}(x,x')$ is specific for each extension. Carrying out the summations in (43) one obtains

$$S_l^{(\pm)}(x,x')=A_{nr}(x,x')e^{\mp i\gamma\tau}e^{\pm i(l_\pm-l_0)\Delta\varphi}e^{-i|l_\pm+\mu|\gamma\tau}e^{-i\pi|l_\pm+\mu|/2}J_{|l_\pm+\mu|}(z_{nr}),$$

$$A_{nr}(x,x')=\frac{\gamma}{4\pi\sin(\gamma\tau)}\exp\left[\frac{i}{2}(\rho+\rho')\cot(\gamma\tau)\right], \tag{44}$$

$$S_{nc}^{(+)}(x,x')=A_{nr}(x,x')e^{-il_0\Delta\varphi}e^{-i(1+\mu)eB\tau}\{e^{-i\pi\mu/2}J_\mu(z_{nr})-e^{-i\Delta\varphi}e^{ieB\tau}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z_{nr})$$
$$+Y(z_{nr},\Delta\varphi-eB\tau,\mu)+Y(z_{nr},-\Delta\varphi+eB\tau,-\mu)\}, \tag{45}$$

$$S_{nc}^{(-)}(x,x')=A_{nr}(x,x')e^{il_0\Delta\varphi}e^{i(1-\mu)eB\tau}\{Y(z_{nr},-\Delta\varphi-eB\tau,\mu)+Y(z_{nr},\Delta\varphi+eB\tau,-\mu)\}, \tag{46}$$

$$z_{nr}=\sqrt{\rho\rho'}/\sin(\gamma\tau),\quad \tau=\Delta x^0/2M,\quad l_\pm=l-(1\pm1)/2,\quad l\neq0,$$

whereas for $l=0$,

$$S_0^{(+)(\mp\pi/2)}(x,x')=A_{nr}(x,x')e^{-i(l_0+1)\Delta\varphi}e^{-i\mu eB\tau}e^{\mp i\pi(1-\mu)/2}J_{\pm(1-\mu)}(z_{nr}), \tag{47}$$

$$S_0^{(-)(\mp\pi/2)}(x,x')=A_{nr}(x,x')e^{il_0\Delta\varphi}e^{i(1-\mu)eB\tau}e^{\pm i\pi\mu/2}J_{\mp\mu}(z_{nr}). \tag{48}$$

The Green function in the "spin-down" case can be obtained with the change $\Delta\varphi\to-\Delta\varphi$ in (44)–(48) and with the change $S^{(\pm)}$ by $S^{(\mp)}$ in all the functions $S(x,x')$ in (44)–(48). Thus, one can see that the Green functions for the nonrelativistic particle is irregular at $r=0$ when the contact interaction is attractive.

We note that for the limiting case $B=0$ (the uniform magnetic field is absent), $S_l^{(+)(-\pi/2)}(x,x')$ coincide with the known expression for the spinless particle,[15–17] which is natural in the case of a repulsive contact interaction. $S_l^{(+)(\pi/2)}(x,x')$ for $B=0$ coincide with the corresponding expressions obtained in Ref. 18.

III. 3+1 DIMENSIONAL CASE

To obtain the Green functions in $3+1$ dimensions we use the orthonormalized solutions ${}_\pm\Psi_{p_3,m,l,\sigma}(x)$ of the Dirac equation found in Refs. 2 and 3. The quantum numbers m, l have the same meaning as in the $(2+1)$-dimensional case, p_3 is the x^3 component of the momentum, and σ is the spin quantum number. The positive energy spectrum is given by ${}_+\varepsilon$ and the negative energy spectrum is given by ${}_-\varepsilon$. They both are expressed via the quantity ω as

$${}_+\varepsilon=-{}_-\varepsilon=\sqrt{M^2+p_3^2+\omega}. \tag{49}$$

The spectra of ω are given in (13), (14) for $B>0$, and in (16), (17) for $B<0$. For $\omega\neq0$, one can present the solutions ${}_\pm\Psi_{p_3,m,l,\sigma}$ in the following form:

$${}_\pm\Psi_{p_3,m,l,\sigma}(x)=N(\gamma^\nu P_\nu+M)\,{}_\pm U_{p_3,m,l,\sigma}(x),$$

$${}_\pm U_{p_3,m,l,\sigma}(x)=\frac{1}{\sqrt{2\pi}}\,e^{-i\,{}_\pm\varepsilon x^0-ip_3x^3}U_{m,l,\sigma}(x_\perp),$$

$$U_{m,l,\sigma}(x_\perp)=\begin{pmatrix}u_{m,l,\sigma}(x_\perp)\\ \sigma^3u_{m,l,\sigma}(x_\perp)\end{pmatrix},\quad N=[2|{}_\pm\varepsilon|(|{}_\pm\varepsilon|+p_3)]^{-1/2}, \tag{50}$$

whereas for $\omega=0$,

$${}_\pm\Psi_{p_3,0,l,-\xi}(x)=N(\gamma^\nu P_\nu+M)\,{}_\pm U_{p_3,0,l,-\xi}(x),\quad \xi=\mathrm{sgn}(B),$$

where $u_{m,l,\sigma}(x_\perp)$ are the two-spinors defined in (11).

We are going to construct the Green functions using the solutions that correspond to the natural extensions of the Dirac operator, i.e., for the extension parameters chosen as $\Theta_{+1}=\Theta_{-1}=\Theta$, and $\Theta=\pm\pi/2$. First we consider the case $\Theta=-\pi/2$, and $B>0$. We note that for $\omega\neq 0$,

$$\gamma^\nu P_{\perp\nu}U_{m,l,-\sigma}=i\sqrt{\omega}U_{m,l,\sigma}, \quad l\geqslant 1,$$
$$\gamma^\nu P_{\perp\nu}U_{m_+,l,-\sigma}=-i\sqrt{\omega}U_{m_-,l,\sigma}, \quad l\leqslant 0, \tag{51}$$

where $P_\perp=(0,P_1,P_2,0)$. The summations in (5) can be done similarly to the $(2+1)$-dimensional case by the help of some important relations derived by us for the solutions (50). Namely, for the states with a given $\omega\neq 0$, the following relations hold true:

$$\sum_{\sigma=\pm 1} {}_\pm\Psi_{p_3,m,l,\sigma}(x)\,{}_\pm\overline{\Psi}_{p_3,m,l,\sigma}(x')$$
$$=\sum_{\sigma=\pm 1}\frac{1}{2\,{}_\pm\varepsilon}(\gamma^\nu P_\nu+M)\frac{1}{2}(1+\sigma\Sigma^3)\,{}_\pm\phi_{p_3,m,l,\sigma}(x,x'), \quad l\geqslant 1,$$
$$\sum_{\sigma=\pm 1} {}_\pm\Psi_{p_3,m_+,l,-\sigma}(x)\,{}_\pm\overline{\Psi}_{p_3,m_+,l,-\sigma}(x')$$
$$=\sum_{\sigma=\pm 1}\frac{1}{2\,{}_\pm\varepsilon}(\gamma^\nu P_\nu+M)\frac{1}{2}(1+\sigma\Sigma^3)\,{}_\pm\phi_{p_3,m_+,l,-\sigma}(x,x'), \quad l\leqslant 0, \tag{52}$$

and for $\omega=0$, we have

$${}_\pm\Psi_{p_3,0,l,-1}(x)\,{}_\pm\overline{\Psi}_{p_3,0,l,-1}(x')=\frac{1}{2\,{}_\pm\varepsilon}(\gamma^\nu P_\nu+M)\frac{1}{2}(1-\Sigma^3)\,{}_\pm\phi_{p_3,0,l,-1}(x,x'),$$

where

$${}_\pm\phi_{p_3,m,l,\sigma}(x,x')=\frac{1}{2\pi}e^{-i\,{}_\pm\varepsilon\Delta x^0-ip_3\Delta x^3}\phi_{m,l,\sigma}(x_\perp,x'_\perp), \quad \Delta x^3=x^3-x'^3. \tag{53}$$

The functions $\phi_{m,l,\sigma}(x_\perp,x'_\perp)$ are defined in (23). Therefore,

$$S^c(x,x')=(\gamma^\nu P_\nu+M)\Delta^c(x,x'),$$
$$\Delta^c(x,x')=i\sum_{m,l,\sigma}\int_{-\infty}^{\infty}dp_3\frac{1}{2}(1+\sigma\Sigma^3)\Big[\theta(\Delta x^0)\frac{1}{2\,{}_+\varepsilon}\,{}_+\phi_{p_3,m,l,\sigma}(x,x')$$
$$-\theta(-\Delta x^0)\frac{1}{2\,{}_-\varepsilon}\,{}_-\phi_{p_3,m,l,\sigma}(x,x')\Big]. \tag{54}$$

Applying the relations (25),(26), one obtains the proper time integral representation for Δ^c,

$$\Delta^c(x,x')=\int_0^\infty f(x,x',s)ds, \quad f(x,x',s)=\sum_{l=-\infty}^{\infty}f_l(x,x',s),$$
$$f_l(x,x',s)=D(s)\sum_{\sigma=\pm 1}\Phi_{l,\sigma}(s)e^{-i\sigma eBs}\frac{1}{2}(1+\sigma\Sigma^3),$$

$$D(s)=\frac{eB}{16\pi^2 s\sin(eBs)}\exp\left\{\frac{i}{4s}[(\Delta x_3)^2-(\Delta x_0)^2]-iM^2 s\right\}$$
$$\times\exp\left\{-il_0\Delta\varphi+\frac{ieB}{4}(r^2+r'^2)\cot(eBs)\right\}, \tag{55}$$

where $\Phi_{l,\sigma}(s)$ are defined in (32).

Carrying out similar calculations for $B<0$ one can verify that (55) is valid for both signs of B. Therefore, for any sign of B, we get

$$f_{nc}(x,x',s)=\sum_{l\neq 0} f_l(x,x',s)=D(s)e^{-ieBs(\mu+\Sigma^3)}\Big\{Y(z,\Delta\varphi-eBs,\mu)+Y(z,-\Delta\varphi+eBs,-\mu)$$
$$+[e^{-i\pi\mu/2}J_\mu(z)-e^{-i(\Delta\varphi-eBs)}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z)]\frac{1}{2}(1+\Sigma^3)\Big\},$$

$$f_0^{(-\pi/2)}(x,x',s)=\tfrac{1}{2}D(s)e^{-i\mu eBs}[e^{-i\Delta\varphi}e^{-i\pi(1-\mu)/2}J_{1-\mu}(z)(1+\Sigma^3)$$
$$+e^{ieBs}e^{i\pi\mu/2}J_{-\mu}(z)(1-\Sigma^3)],$$

$$f^{(-\pi/2)}(x,x',s)=f_{nc}(x,x',s)+f_0^{(-\pi/2)}(x,x',s), \tag{56}$$

Using the corresponding solutions for the case $\Theta=\pi/2$, we obtain

$$f_0^{(\pi/2)}(x,x',s)=\tfrac{1}{2}D(s)e^{-i\mu eBs}[e^{-i\Delta\varphi}e^{-i\pi(\mu-1)/2}J_{\mu-1}(z)(1+\Sigma^3)+e^{ieBs}e^{-i\pi\mu/2}J_\mu(z)(1-\Sigma^3)],$$

$$f^{(\pi/2)}(x,x',s)=f_{nc}(x,x',s)+f_0^{(\pi/2)}(x,x',s). \tag{57}$$

IV. SUMMARY

Various Green functions of the Dirac equation with the magnetic-solenoid field are constructed as sums over exact solutions of this equation. We stress that doing that we had to take into account all the peculiarities related to the self-adjoint extension problem of the Dirac operator in the background under consideration. Both $2+1$ and $3+1$ dimensional cases are considered. Compact form for the Green functions was obtained thanks to the important relations (22) and (52) derived by us for the exact solutions under consideration. The representations of the Green functions as proper time integrals are constructed. The kernels of the proper time integrals are represented both as infinite sums over the orbital quantum number l and as simple integrals. The Green functions are obtained for two natural self-adjoint extensions, one for the positive solenoid flux and the other one for the negative solenoid flux. The physical motivation for the choice of these extensions is their correspondence to the presence of the point-like magnetic field at the origin and their close relation to the MIT boundary conditions.[23,28,29] Thus, the considered cases are of most interest for applications. Other values of the extension parameter correspond to additional contact interactions,[30] and some of the values are of physical interest as well. To find a closed form of Green functions for the arbitrary value of the extension parameter is a more complicated task. The spectra of the corresponding extensions in the critical subspace are no longer periodic for such a situation that requires to apply more exquisite calculation methods. We suppose to consider this issue in the future.

In addition, the nonrelativistic Green functions are constructed. The latter Green functions are represented for all possible types of $2+1$ dimensional nonrelativistic particles.

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APPENDIX

For the sake of completeness we consider here the Green functions for the scalar particle. They are defined by Eqs. (3), (4), (8), and (9), where $S^{\mp}(x,x')$ read

$$S^{\mp}(x,x') = \pm i \sum {}_{\pm}\phi_n(x)\, {}_{\pm}\phi_n^*(x'),$$

and ${}_{\pm}\phi_n(x)$ form a complete set of orthonormalized solutions of the Klein–Gordon equation. Here we consider the natural extension of the Klein–Gordon operator for which solutions in $2+1$ dimensions and the related spectrum read[3]

$${}_{\pm}\phi_{m,l}(x) = \frac{1}{\sqrt{2\varepsilon}}\, e^{-i\,{}_{\pm}\varepsilon x^0} \sqrt{\frac{\gamma}{2\pi}}\, e^{i(l-l_0)\varphi} I_{m+|l+\mu|,m}(\rho),$$

$${}_{\pm}\varepsilon = \pm\sqrt{M^2+\omega}, \quad \omega = \gamma[1+2m+|l+\mu|+\xi(l+\mu)],$$

$$l = 0,\pm 1,\pm 2,\ldots, \quad m = 0,1,2,\ldots .$$

Using Eqs. (25), (26), (28), and (30), we calculate the causal and anticausal propagators. They have the form

$$S^c(x,x') = \int_0^{\infty} f^{sc}(x,x',s)\mathrm{d}s, \quad S^{\bar{c}}(x,x') = \int_{-0}^{-\infty} f^{sc}(x,x',s)\mathrm{d}s,$$

$$f^{sc}(x,x',s) = \sum_l f_l^{sc}(x,x',s)\,,$$

$$f_l^{sc}(x,x',s) = A(s) e^{il\Delta\varphi} e^{-i(l+\mu)eBs} e^{-i\pi|l+\mu|/2} J_{|l+\mu|}\,, \tag{A1}$$

$$f^{sc}(x,x',s) = A(s) e^{-i\mu eBs}[e^{-i\pi\mu/2} J_{\mu}(z) + Y(z,\Delta\varphi - eBs,\mu) + Y(z,-\Delta\varphi + eBs,-\mu)],$$

where $A(s)$ is given in (31), and $Y(z,\eta,\mu)$ in (33), (35). The expression (A1) can be generalized for the $(D+1)$-dimensional case, where D is the number of spacial dimensions, with the substitution $A(s)$ in (A1) by $A^{(D)}(s)$,

$$A^{(D)}(s) = A(s)\exp\left\{\frac{i}{4s}\sum_{k=3}^{D}(\Delta x_k)^2\right\}\left(\frac{e^{-i\pi/2}}{4\pi s}\right)^{(D-2)/2}, \quad D \geqslant 3.$$

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The role of the irreducible representations of the Poincaré group in solving Maxwell's equations

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Maxwell's equations are universally solved when the charge and current densities are given, without reference to the transformation properties of the fields or charge density–current density four vector. However these transformation properties are generally held to be *essential* physical properties of the fields and the charge density–current density four-vector. They are required if the consequences of relativity are to hold. The way the fields and four-vectors transform constitutes a representation of the Poincaré group which can be reduced to the irreducible representations of that group first given by Wigner. The use of the irreducible representations corresponds to the expansion of the fields and currents into modes which have the simplest possible transformation properties. These modes can be identified as wave functions of particles of spin 1 and mass m $(0 \leqslant m < \infty)$. We compare the solutions of Maxwell's equations utilizing the ''usual'' time-dependent Green's function and the method introduced in this paper. The solutions are identical, if we assume that the fields created by the time-dependent sources have the same initial values for the fields. Among the new results, we demonstrate the mechanism by which one can transform transverse fields for which the charge density is zero to fields that are partially longitudinal and for which the charge density source is not zero under Poincaré transformations of the space–time coordinates. We give a concrete example of a transverse current density source and one for a longitudinal current density source and show that sources lead to a mass spectrum of the photons. Longitudinal current densities always lead to *noncausal* (as noncausal is commonly understood) solutions for the fields. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND SUMMARY

The Poincaré group is the Lorentz group to which is added the translations of space and time. It seems universally accepted that the electromagnetic fields transform under the Poincaré transformations as an antisymmetric tensor and the current–density, charge density transform as a four-vector, These requirements are at the heart of special relativity and its extension to general relativity. Maxwell's equations are invariant under transformations of this group. However, strange as it might seem, Maxwell's equations do not seem to have been solved under the requirement of Poincaré invariance as a constraint. The intent of this paper is to solve Maxwell's equations under this requirement. We proceed by expanding the field tensor and the current-density, charge-density four-vector into the irreducible representations of the Poincaré group first given by Wigner. Such representations are the simplest representations and the expansions *must* exist for invariance. This method of obtaining solutions leads to surprising results. Only the discrete zero mass and nonzero mass representations of spin 1 and positive energy are involved in the expansions. The zero-mass expansions can be used for transverse fields (i.e., photons), *only* if the mass zero components of transverse part of the current density vector vanishes. Second, if there is a transverse, time-dependent current density which does not have a time interval during which the current vanishes,

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only nonzero mass representations may appear in the expansions of the currents and fields. However, once the zero mass components are removed in this latter case, the solution of Maxwell's equations obtained using the method of expansions of the present paper are identical to the ''usual'' solution obtained through the use of time-dependent Green's functions if the initial conditions of both methods of solution are the same.

Another result is that solutions of Maxwell's equations, with *longitudinal* current densities and corresponding charge densities as sources, are not causal even though the *transverse* field solutions originating from transverse current densities are! Possibly this paradox can be resolved by redefining causality.

Only nonzero mass representations can occur in the transverse current densities that are used as sources for transverse fields. Is it possible that when the sources are operative, photons have mass? What is the nature of these masses? Can they be sources of gravity or can they be attracted by other masses? It would seem difficult to answer these questions experimentally, but the use of Poincaré invariance brings the possibility of photons with mass to one's attention.

II. INTEGRATION OF MAXWELL'S EQUATIONS USING TIME-DEPENDENT GREEN'S FUNCTIONS

Maxwell's equations in Gaussian units are

$$\begin{aligned}
\vec{\nabla}\times\vec{E}(\vec{x};t) &= -\frac{1}{c}\frac{\partial\vec{H}(\vec{x};t)}{\partial t},\\
\vec{\nabla}\times\vec{H}(\vec{x};t) &= \frac{1}{c}\frac{\partial\vec{E}(\vec{x};t)}{\partial t}+\frac{4\pi}{c}\vec{j}(\vec{x};t),\\
\vec{\nabla}\cdot\vec{E}(\vec{x};t) &= 4\pi\rho(\vec{x};t),\\
\vec{\nabla}\cdot\vec{H}(\vec{x};t) &= 0\,.
\end{aligned} \tag{1}$$

We shall solve these equations using group theory. However, they can also be solved as an initial value problem using a time-dependent Green's function. Do these two methods give different results? To make the discussion as clear as we can, we shall address the problem of the creation of a transverse electromagnetic field by a pulsed transverse current density. Let the time interval that the pulse is on be given by $t_1<t<t_2$. We shall assume that there is no proper subinterval such that the transverse current density $\vec{j}(\vec{x};t)$ vanishes.[1] The solution of the initial value problem for the case that there is no electromagnetic field before the current density is turned on is[2]

$$\begin{aligned}
\vec{E}(\vec{x};t) &= \frac{4\pi}{c^2}\int_{t_1}^{t}\mathrm{d}t'\int\mathrm{d}\vec{x}'\,\frac{\partial^2}{\partial t^2}D(\vec{x}-\vec{x}';t-t')\vec{j}_T(\vec{x}',t'),\\
\vec{H}(\vec{x};t) &= \frac{4\pi}{c}\vec{\nabla}\times\int_{t_1}^{t}\mathrm{d}t'\int\mathrm{d}\vec{x}'\,\frac{\partial}{\partial t}D(\vec{x}-\vec{x}';t-t')\vec{j}_T(\vec{x}',t')\,.
\end{aligned} \tag{2}$$

In the above equations $t>t_1$. Moreover, the function $D(\vec{x};t)$ is

$$D(\vec{x};t)=\frac{1}{4\pi r}\eta(r-ct)\quad\text{where } r=|\vec{x}| \tag{3}$$

and $\eta(x)$ is the Heaviside function

$$\eta(x)=\begin{cases}0 & \text{if } x<0\\ 1 & \text{if } x\geqslant 0\,.\end{cases} \tag{4}$$

The current density $\vec{j}_T(\vec{x};t)$ is the transverse part of the current density.

We now state an important theorem. Let there be a second way of solving Maxwell's equations with the initial condition that the field be zero for $t<t_1$. The two methods of solution will yield the same result. The proof is simple. Let $\vec{\Delta}_E(\vec{x};t)$ and $\vec{\Delta}_H(\vec{x};t)$ be the difference of the fields of the two solutions. Then $\vec{\Delta}_E$ and and $\vec{\Delta}_H$ satisfy Maxwell's equations without current densities as a source. Then the requirement that the the two original fields be zero when $t<t_1$ leads immediately to $\vec{\Delta}_E=\vec{\Delta}_H\equiv 0$. The solution obtained using group theory and that using Green's functions will look different but will be the same. For the sake of completeness we shall indicate a vector potential $\vec{A}(\vec{x};t)$ in the radiation gauge which can be used to obtain the general transverse electromagnetic field of Eqs. (2) and (3),

$$\vec{A}(\vec{x};t)=-\frac{4\pi}{c}\int_{t_1}^{t}\mathrm{d}t'\int \mathrm{d}\vec{x}'\frac{\partial}{\partial t}D(\vec{x}-\vec{x}';t-t')\vec{j}_T(\vec{x}';t').$$

Then

$$\vec{E}(\vec{x};t)=-\frac{1}{c}\frac{\partial}{\partial t}\vec{A}(\vec{x};t),$$

$$\vec{H}(\vec{x};t)=\vec{\nabla}\times\vec{A}(\vec{x};t)\,. \tag{5}$$

III. EIGENFUNCTIONS OF THE CURL OPERATOR

The irreducible representations of the Poincaré group for zero mass representations are given in Ref. 3, and for nonzero mass representations in the format of Foldy and Shirokov.[4]

For the sake of brevity we shall assume that the reader has available two published papers in which the writer has expanded wave functions in terms of the finite mass and massless representations.[5,6] We shall also use the eigenfunctions of the curl operator discussed in Ref. 7. We shall repeat some of the material in Ref. 7 with slight changes in notation. The eigenfunctions of the curl operator constitute a generalization of the three-dimensional Fourier transformation. They enable us to handle simply problems involving the curl and divergence operators as they act on vector fields. Let us introduce three-component "vectors" [8] $\vec{Q}(\vec{p},\lambda)$ for $\lambda=0,\pm 1$ and a real vector $\vec{p}$ by

$$\vec{Q}(\vec{p},0)=-\frac{\vec{p}}{p},$$

$$\vec{Q}(\vec{p},\lambda)=-\frac{\lambda}{\sqrt{2}}\left(\frac{p_1(p_1+i\lambda p_2)}{p(p+p_3)}-1,\frac{p_2(p_1+i\lambda p_2)}{p(p+p_3)}-i\lambda,\frac{p_1+i\lambda p_2}{p}\right)\quad\text{for }\lambda=\pm 1\,. \tag{6}$$

These vectors satisfy the orthogonality and completeness relations

$$\vec{Q}^*(\vec{p},\lambda)\cdot\vec{Q}(\vec{p},\lambda')=\delta_{\lambda,\lambda'}\,,$$

$$\sum_{\lambda=0,\pm 1}Q_i^*(\vec{p},\lambda)Q_j(\vec{p},\lambda)=\delta_{i,j}\,. \tag{7}$$

In Eq. (7) $Q_i(\vec{p},\lambda)$ is the ith component of $\vec{Q}(\vec{p},\lambda)$.

Further properties of the vectors $\vec{Q}(\vec{p},\lambda)$ are

$$\vec{p}\cdot\vec{Q}(\vec{p},\lambda)=0 \qquad \text{for} \quad \lambda=\pm 1,$$

$$\vec{p}\cdot\vec{Q}(\vec{p},0)=-p \quad \text{where} \quad p=|\vec{p}|,$$

$$\vec{p}\times\vec{Q}(\vec{p},\lambda)=-i\lambda p\vec{Q}(\vec{p},\lambda), \tag{8}$$

$$\vec{Q}^*(\vec{p},\lambda)=-\vec{Q}(\vec{p},-\lambda) \qquad \text{for} \quad \lambda=\pm 1,$$

$$\vec{Q}^*(-\vec{p},\lambda)=-\frac{p_1-\lambda i p_2}{p_1+\lambda i p_2}\vec{Q}(\vec{p},\lambda)\,.$$

The eigenfunctions $\vec{\chi}(\vec{x}|\vec{p},\lambda)$ of the $\vec{\nabla}\times$ operator are

$$\vec{\chi}(\vec{x}|\vec{p},\lambda)=\frac{e^{i\vec{p}\cdot\vec{x}}}{(2\pi)^{3/2}}\vec{Q}(\vec{p},\lambda)\,. \tag{9}$$

From the orthogonality and completeness properties of the vectors $\vec{Q}(\vec{p},\lambda)$ [Eq. (7)] we deduce these properties of the vectors $\vec{\chi}(\vec{x}|\vec{p},\lambda)$,

$$\int d\vec{x}\,\vec{\chi}^*(\vec{x}|\vec{p},\lambda)\cdot\vec{\chi}(\vec{x}|\vec{p}\,',\lambda')=\delta_{\lambda,\lambda'}\delta(\vec{p}-\vec{p}\,'),$$

$$\sum_{\lambda=0,\pm 1}\int d\vec{p}\,\chi_i^*(\vec{x}|\vec{p},\lambda)\vec{\chi}(\vec{x}\,'|\vec{p},\lambda)=\delta_{i,j}\delta(\vec{x}-\vec{x}\,')\,, \tag{10}$$

where $\chi_i(\vec{x}|\vec{p},\lambda)$ is the ith component of $\vec{\chi}(\vec{x}|\vec{p},\lambda)$. These eigenvectors have the properties

$$\vec{\nabla}\times\vec{\chi}(\vec{x}|p,\lambda)=\lambda p\vec{\chi}(\vec{x}|\vec{p},\lambda),$$

$$\vec{\nabla}\cdot\vec{\chi}(\vec{x}|\vec{p},\lambda)=0 \qquad \text{for} \quad \lambda=\pm 1,$$

$$\vec{\nabla}\cdot\vec{\chi}(\vec{x}|\vec{p},0)=\frac{-ip}{(2\pi)^{3/2}}e^{i\vec{p}\cdot\vec{x}}, \tag{11}$$

$$\vec{\chi}^*(\vec{x}|\vec{p},\lambda)=-\frac{p_1-i\lambda p_2}{p_1+i\lambda p_2}\vec{\chi}(\vec{x}|-\vec{p},\lambda),$$

$$\int d\vec{x}\,\vec{\chi}^*(\vec{x}|\vec{p},\lambda)\cdot\vec{\chi}^*(\vec{x}|\vec{p}\,',\lambda')=-\frac{p_1-i\lambda p_2}{p_1+i\lambda p_2}\delta(\vec{p}+\vec{p}\,')\delta_{\lambda,\lambda'}\,.$$

From the properties of the eigenvectors we see that *every* vector $\vec{V}(\vec{x})$ can be decomposed uniquely into a sum of two vectors,

$$\vec{V}(\vec{x})=\vec{V}_L(\vec{x})+\vec{V}_T(\vec{x}), \tag{12}$$

where

$$\vec{V}_L(\vec{x})=\int d\vec{p}\,g(\vec{p},0)\vec{\chi}(\vec{x}|\vec{p},0),$$

$$\vec{V}_T(\vec{x})=\sum_{\lambda=\pm 1}\int d\vec{p}\,g(\vec{p},\lambda)\vec{\chi}(\vec{x}|\vec{p},\lambda) \quad \text{and where}$$

$$g(\vec{p},\lambda)=\int \mathrm{d}\vec{x}\,\vec{\chi}^{\,*}(\vec{x}|\vec{p},\lambda)\cdot\vec{V}(\vec{x})\,. \tag{13}$$

Since

$$\begin{aligned}\vec{\nabla}\times\vec{V}_L(\vec{x})&=0,\\ \vec{\nabla}\cdot\vec{V}_T(\vec{x})&=0,\end{aligned} \tag{14}$$

$\vec{V}_L(\vec{x})$ is the longitudinal part of $\vec{V}(\vec{x})$ and $\vec{V}_T(\vec{x})$ is the transverse part in the Helmholtz decomposition of the vector. It is seen that $\vec{V}_L(\vec{x})$ and $\vec{V}_T(\vec{x})$ are linearly independent. Indeed they are orthogonal in the following sense:

$$\int \mathrm{d}\vec{x}\,\vec{V}_L^{*}(\vec{x})\cdot\vec{V}_T(\vec{x})=0\,. \tag{15}$$

IV. THE SOLUTION OF THE TIME-DEPENDENT MAXWELL'S EQUATIONS USING GROUP THEORY

A. The Bateman–Cunningham form of the equations

We proceed to solve Maxwell's equations using the irreducible representations of the Poincaré group.

A very convenient way of writing Maxwell's equations is the following: Define the vector $\vec{\psi}(\vec{x};t)$ by

$$\vec{\psi}(\vec{x};t)=\vec{E}(\vec{x};t)-i\vec{H}(\vec{x};t)\,. \tag{16}$$

Then Maxwell's equations are

$$\begin{aligned}\vec{\nabla}\times\vec{\psi}(\vec{x};t)&=-i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}(\vec{x};t)-4\pi\frac{\vec{j}(\vec{x};t)}{c},\\ \vec{\nabla}\cdot\vec{\psi}(\vec{x};t)&=4\pi\rho(\vec{x};t)\,.\end{aligned} \tag{17}$$

The vector $\vec{\psi}(\vec{x};t)$ undergoes relatively simple transformations under the coordinate transformations of the Poincaré group (see Refs. 5 and 6). Without going into details at this time, it can be shown that the helicity operator $\vec{P}\cdot\vec{J}/|\vec{P}|$, where $\vec{P}=\{P_1,P_2,P_3\}$ are the infinitesimal generators of the translations and $\vec{J}=\{J_1,J_2,J_3\}$ are the infinitesimal generators of the rotations, has only a finite number of point eigenvalues. Since imaginary mass and continuous zero mass have an *infinite* number of eigenvalues for the helicity operator, such representations are precluded in the expansion of $\vec{\psi}(\vec{x};t)$. Thus we need only consider discrete 0 mass representations and real mass representations for spin 1 in the expansion of $\vec{\psi}(\vec{x};t)$.

B. Mass and Maxwell's equations

One of the labels used in characterizing the irreducible representations is the *mass* m. The range of m is $0\leqslant m<\infty$. Let us denote the four-vector current density by $\iota(\vec{x};t)$:

$$\iota(\vec{x};t)\rightarrow\{c\rho(\vec{x};t),\vec{j}(\vec{x};t)\}. \tag{18}$$

The field $\vec{\psi}(\vec{x};t)$ is a sum of representations corresponding to m. It can be shown that the range and values of m in the decomposition of $\vec{\psi}(\vec{x};t)$ are the same as those for $\iota(\vec{x};t)$. Let us assume that m can take on discrete values $\{m_1,m_2,\ldots\}$ and continuous values in some range $\mathcal{R}$. Then

$\vec{\psi}(\vec{x};t)$ can be written as a sum of representations over the discrete values of m and an integral over the continuous values.[9] Then $\vec{\psi}(\vec{x};t)$ and $\iota(\vec{x};t)$ can be written as a sum of representations over the discrete values of m and an integral over the continuous values,

$$\vec{\psi}(\vec{x};t)=\sum_{m_i}\ \vec{\psi}_{m_i}(\vec{x};t)+\int_{\mathcal{R}}\mathrm{d}m\ \vec{\psi}_m(\vec{x};t),$$
$$\iota(\vec{x};t)=\sum_{m_i}\ \iota_{m_i}(\vec{x};t)+\int_{\mathcal{R}}\mathrm{d}m\ \iota_m(\vec{x};t)\ . \tag{19}$$

For any value of m, $\vec{\psi}_m(\vec{x};t)$ and $\iota_m(\vec{x};t)$ satisfy Maxwell's equations:

$$\vec{\nabla}\times\vec{\psi}_m(\vec{x};t)=-i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_m(\vec{x};t)-4\pi i\frac{\vec{j}_m(\vec{x};t)}{c},$$
$$\vec{\nabla}\cdot\vec{\psi}_m(\vec{x};t)=4\pi\rho_m(\vec{x};t)\ . \tag{20}$$

If we prescribe the irreducible representations in $\iota_m(\vec{x};t)$, we can find the irreducible representations in $\vec{\psi}_m(\vec{x};t)$ through these equations.

In the next sections we shall give the irreducible representations for $\vec{\psi}_m(\vec{x};t)$ and $\iota_m(\vec{x};t)$. Surprisingly, the case for which $m=0$ is quite different than that for which $m\neq 0$.[10]

V. THE REDUCTION OF $\vec{\psi}_m(\vec{x};t)$ AND $\iota_m(\vec{x};t)$ FOR ZERO MASS

The $m=0$ representations are considered first. They correspond to a point eigenvalue of m at $m=0$. We use the results of Ref. 6 with the notation of Ref. 7,

$$\vec{\psi}_0(\vec{x};t)=\vec{\psi}_{0,L}(\vec{x};t)+\vec{\psi}_{0,T}(\vec{x};t)\ , \tag{21}$$

where $\vec{\psi}_{0,L}(\vec{x};t)$ is the longitudinal part of $\vec{\psi}_0(\vec{x};t)$ and $\vec{\psi}_{0,T}(\vec{x};t)$ is the transverse part,

$$\vec{\psi}_{0,L}(\vec{x};t)=-\int\frac{\mathrm{d}\vec{p}}{p}[\vec{\chi}(\vec{x}|\vec{p},0)f_0(\vec{p},0)e^{-ipct}+\vec{\chi}^*(\vec{x}|\vec{p},0)h_0^*(\vec{p},0)e^{ipct}],$$
$$\vec{\psi}_{0,T}(\vec{x};t)=-\sum_{\lambda=\pm 1}\int\frac{\mathrm{d}\vec{p}}{p}[p^{-\lambda}\vec{\chi}(\vec{x}|\vec{p}\lambda)f_0(\vec{p},\lambda)e^{-ipct}+p^{\lambda}\vec{\chi}^*(\vec{x}|\vec{p},\lambda)h_0^*(\vec{p},\lambda)e^{ipct}]\ . \tag{22}$$

The functions $f_0(\vec{p},\lambda)$, $h_0(\vec{p},\lambda)$ transform under the irreducible representations of the Poincaré group for mass zero, positive energy, and helicity λ. We shall show how these functions may be obtained from similar functions in the expansion of $\iota_0(\vec{x};t)$.

The vector part of $\iota_0(\vec{x};t)$, which is the current density $\vec{j}_0(\vec{x};t)$, is expanded as[11]

$$\vec{j}_0(\vec{x};t)=\vec{j}_{0,L}(\vec{x};t)+\vec{j}_{0,T}(\vec{x};t)\ , \tag{23}$$

where $\vec{j}_{0,L}(\vec{x};t)$ is the longitudinal part of the current density and $\vec{j}_{0,T}(\vec{x};t)$ is the transverse part,

$$\frac{\vec{j}_{0,L}(\vec{x};t)}{c}=\int\mathrm{d}\vec{p}\,[\vec{\chi}(\vec{x}|\vec{p},0)k_0(\vec{p},0)e^{-icpt}+\chi^*(\vec{x}|\vec{p},0)k_0^*(\vec{p},0)e^{icpt}],$$
$$\frac{\vec{j}_{0,T}(\vec{x};t)}{c}=\sum_{\lambda=\pm 1}\int\frac{\mathrm{d}\vec{p}}{p}[\vec{\chi}(\vec{x}|\vec{p},\lambda)k_0(\vec{p},\lambda)e^{-icpt}+\vec{\chi}^*(\vec{x}|\vec{p},\lambda)k_0^*(\vec{p},\lambda)e^{icpt}]\ . \tag{24}$$

Finally, the charge density $\rho_0(\vec{x};t)$ is coupled to the longitudinal part of the current density through

$$\rho_0(\vec{x};t)=\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}\vec{p}[k_0(\vec{p},0)e^{i(\vec{p}\cdot\vec{x}-cpt)}+k_0^*(\vec{p},0)e^{-i(\vec{p}\cdot\vec{x}-cpt)}\,. \tag{25}$$

The three amplitudes $k_0(\vec{p},\lambda)$ for $\lambda=0,\pm1$ *are independent of each other*. If $k_0(\vec{p},0)\equiv0$, then the current density is purely transverse and the charge density is zero. More generally, Maxwell's equations can be solved independently for the transverse and longitudinal fields. From the properties of the vectors $\vec{\chi}(\vec{x}|\vec{p},0)$, it is seen that the equation of continuity is satisfied:

$$\frac{\partial\rho_0(\vec{x};t)}{\partial t}+\vec{\nabla}\cdot\vec{j}_{0,L}(\vec{x};t)=0\,. \tag{26}$$

A. The solution of Maxwell's equations for the transverse fields in terms of the transverse current densities

Maxwell's equations for the transverse fields in terms of the transverse currents are

$$\vec{\nabla}\times\vec{\psi}_{0,T}(\vec{x};t)=-i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{0,T}(\vec{x};t)-4\pi i\frac{\vec{j}_{0.T}(\vec{x};t)}{c},$$
$$\vec{\nabla}\cdot\vec{\psi}_{0,T}(\vec{x};t)=0\,. \tag{27}$$

We turn our attention to the first term of Eq. (27). It is not clear at this point whether this set of equations can be integrated. We shall show that *they cannot be integrated unless the transverse current density is identically zero*. The only solution, then, is a solution of Maxwell's equations without sources, i.e., a radiation field. One finds from Eq. (22)

$$\vec{\nabla}\times\vec{\psi}_{0,t}(\vec{x};t)+i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{0.T}(\vec{x};t)=-\sum_{\lambda=\pm1}\int\frac{\mathrm{d}\vec{p}}{p}\{p^{-\lambda}p\times[\lambda+1]\vec{\chi}(\vec{x}|\vec{p},\lambda)f_0(\vec{p},\lambda)e^{-icpt}$$
$$+p^{\lambda}p[\lambda-1]\vec{\chi}^*(\vec{x}|\vec{p},\lambda)h_0^*(\vec{p},\lambda)e^{icpt}\}\,. \tag{28}$$

Summing over λ we have

$$\vec{\nabla}\times\vec{\psi}_{0,T}(\vec{x};t)+i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{0,T}(\vec{x};t)=-2\int\frac{\mathrm{d}\vec{p}}{p}\{\vec{\chi}(\vec{x}|\vec{p},1)f_0(\vec{p},1)e^{-icpt}$$
$$-\vec{\chi}^*(\vec{x}|\vec{p},-1)h_0^*(\vec{p},-1)e^{icpt}\}\,, \tag{29}$$

or

$$\vec{\nabla}\times\vec{\psi}_{0,T}(\vec{x};t)+i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{0,T}(\vec{x};t)=-2\int\frac{\mathrm{d}\vec{p}}{p}\{\vec{\chi}(\vec{x};t)f_0(\vec{p},1)e^{-icpt}+\ \mu(\vec{p},-1)\vec{\chi}(\vec{x}|-\vec{p},-1)$$
$$\times h_0^*(\vec{p},-1)e^{icpt}\}\,. \tag{30}$$

In Eq. (30) and later

$$\mu(\vec{p},\lambda)=\frac{p_1-i\lambda p_2}{p_1+i\lambda p_2}. \tag{31}$$

In Eq. (31) use $-\vec{p}$ as the variable of integration in the term involving $\vec{\chi}(\vec{x}|-\vec{p},-1)$. Then Eq. (30) leads to

$$\vec{\nabla}\times\vec{\psi}_{0,T}(\vec{x};t)+i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{0,T}(\vec{x};t)=-2\int\frac{d\vec{p}}{p}[\vec{\chi}(\vec{x}|\vec{p},1)f_0(\vec{p},1)e^{-icpt}+\mu(\vec{p},-1)\vec{\chi}(\vec{x}|\vec{p},-1)h_0^*(-\vec{p},-1)e^{icpt}]. \tag{32}$$

Similarly,

$$\vec{j}_{0,T}(\vec{x};t)=\sum_{\lambda=\pm1}\int\frac{d\vec{p}}{p}\vec{\chi}(\vec{x}|\vec{p},\lambda)[k_0(\vec{p},1)e^{-icpt}-\mu(\vec{p},\lambda)k_0^*(-\vec{p},\lambda)e^{icpt}]. \tag{33}$$

The vectors $\vec{\chi}(\vec{x}|\vec{p},1)$ and $\vec{\chi}(\vec{x}|\vec{p},-1)$ are linearly independent. We first equate the coefficients on both sides of Eq. (27),

$$f_0(\vec{p},1)e^{-ipct}=2\pi i[k_0(\vec{p},1)e^{-icpt}-\mu(\vec{p},1)k_0^*(-\vec{p},1)e^{icpt}]. \tag{34}$$

On using the fact that e^{icpt} and e^{-icpt} are also linearly independent, we find on equating the coefficients of e^{icpt},

$$k_0(\vec{p},1)\equiv0. \tag{35}$$

Similarly

$$k_0(\vec{p},-1)\equiv0\,. \tag{36}$$

Thus from Eq. (33), we have the result that the *transverse current is zero for zero mass representations as a condition of integrability*.

The functions $f_0(\vec{p},-1)$ and $h_0(\vec{p},1)$ are not obtained by this substitution, since the coefficients in front of these quantities are zero. The amplitudes are arbitrary. The vector $\vec{\psi}_{0,T}(\vec{x};t)$ using these undetermined amplitudes, namely,

$$\vec{\psi}_{0,T}(\vec{x};t)=-\int\frac{d\vec{p}}{p}[\vec{\chi}(\vec{x}|\vec{p},-1)f_0(\vec{p},-1)e^{-icpt}\vec{\chi}^*(\vec{x}|\vec{p},1)h_0^*(\vec{p},1)e^{icpt}], \tag{37}$$

is an arbitrary solution of the *homogeneous* Maxwell's equations. The functions $f_0(\vec{p},-1)$ and $h_0(\vec{p},1)$ can be obtained by imposing initial conditions on the transverse electromagnetic fields $\vec{E}_{0,T}(\vec{x};t)$ and $\vec{H}_{0,T}(\vec{x};t)$ or, equivalently on $\vec{E}_{0,T}(\vec{x};t)$ and $(\partial/\partial t)\vec{E}_{0,T}(\vec{x};t)$.

B. The solution for the longitudinal fields in terms of the longitudinal current densities

The longitudinal field $\vec{\psi}_{0,L}(\vec{x};t)$ has as its expansion the first of Eq. (22). Since the right-hand side of Eq. (20) is real,

$$H_{0,L}\equiv0\,. \tag{38}$$

Thus we need only find $\vec{E}_{0,L}(\vec{x};t)$. The two equations from which $\vec{E}_{0,L}(\vec{x};t)$ can be calculated are

$$\vec{\nabla}\cdot\vec{E}_{0,L}(\vec{x};t)=4\pi\rho_{0,L}(\vec{x};t), \tag{39}$$

$$\frac{\partial}{\partial t}\vec{E}_{0,L}(\vec{x};t)=-4\pi\vec{j}_{0,L}(\vec{x};t). \tag{40}$$

The ''traditional'' way of finding $\vec{E}_{0,L}(\vec{x};t)$ is to use Eq. (39). Since $\vec{E}_{0,L}(\vec{x};t)$ is longitudinal, we may introduce the scalar potential $V_0(\vec{x};t)$:

$$\vec{E}_{0,L}(\vec{x};t)=-\vec{\nabla}V_0(\vec{x};t)\,. \tag{41}$$

Then, on substituting into Eq. (39), one obtains Poisson's equation,

$$\nabla^2 V_0(\vec{x};t) = -4\pi\rho_0(\vec{x};t)\,. \tag{42}$$

On using the well-known solution of Eq. (42), the longitudinal field is

$$\vec{E}_{0,L}(\vec{x};t) = \vec{\nabla}\int \mathrm{d}\vec{x}\frac{\rho_0(\vec{x};t)}{|\vec{x}-\vec{x}\,'|}\,. \tag{43}$$

This result is a generalization of the static situation. It has the consequence, however, that the longitudinal field will not be causal. A change in $\rho_0(\vec{x};t)$, in general, would cause a change in the field which is transmitted instantaneously over entire space. Moreover, from Eq. (43) it is seen that $\vec{E}_{0,L}(\vec{x};t)$ falls off as $1/r^2$, as is the case with most static fields.

To test this situation mathematically, Keller[12] has suggested using Eq. (40) to obtain the longitudinal fields, assuming that the current density, rather than the charge density, is given. The charge density is then obtained from Eq. (39). We shall give a simple example later to show that the use of current densities or charge densities gives the same results.

Using Eqs. (25) and (24) we see that both $\vec{j}_{0,L}(\vec{x};t)$ depend upon the *single* complex function $k_0(\vec{p},0)$. One finds

$$f_0(\vec{p},0) = h_0(\vec{p},0) = 4\pi k_0(\vec{p},0)\,. \tag{44}$$

Thus $\vec{\psi}_{0,L}(\vec{x};t)$ is real as before. *Any* complex function $k_0(\vec{p},0)$ can be used to provide a longitudinal electric field. On the other hand, *longitudinal electric fields cannot exist without a charge density*. Though we have shown this result for $m=0$, an identical proof holds for arbitrary positive values of m.

VI. THE REDUCTION OF $\vec{\psi}_m(\vec{x};t)$ AND $\iota_m(\vec{x};t)$ FOR NONZERO MASS SOLUTIONS OF MAXWELL'S EQUATIONS

We now consider nonzero mass expansions of $\vec{\psi}(\vec{x};t) = \vec{E}(\vec{x};t) - i\vec{H}(\vec{x};t)$ into the irreducible representations of the Poincaré group corresponding to nonzero mass m and spin 1. The subscript m will be used to indicate that we are working in such a representation. The energy $c\,\omega(m,p)$ will appear where

$$\omega(m,p) = \sqrt{m^2c^2+p^2}\,. \tag{45}$$

Equation (4.15) of Ref. 6 gives us the reduction of $\vec{\psi}_m(\vec{x};t)$ to the irreducible representations of mass m and spin 1 in the Foldy–Shirokov form. Using a vector notation the reduction is

$$\begin{aligned}\vec{\psi}_m(\vec{x};t) = mc\Bigg[\int \frac{\mathrm{d}\vec{p}}{\omega(m,p)} e^{i[\vec{p}\cdot\vec{x}-c\,\omega(m,p)t]}\Bigg\{\omega(m,p)\vec{f}_m(\vec{p}) - \frac{\vec{p}}{\omega(m,p)+mc}[\vec{p}\cdot\vec{f}_m(\vec{p})] \\ - i[\vec{p}\vec{f}_m(\vec{p})]\Bigg\} + \int \frac{\mathrm{d}\vec{p}}{\omega(m,p)} e^{-i[\vec{p}\cdot\vec{x}-c\,\omega(m,p)t]}\Bigg\{\omega(m,p)\vec{h}_m^{\,*}(\vec{p}) \\ - \frac{\vec{p}}{\omega(m,p)+mc}[\vec{p}\cdot\vec{h}_m^{\,*}(\vec{p})] - i[\vec{p}\times\vec{h}_m^{\,*}(\vec{p})]\Bigg\}\Bigg]\,.\end{aligned} \tag{46}$$

The vectors $\vec{f}_m(\vec{p})$ and $\vec{h}_m(\vec{p})$ are in the space of vectors on which the operators of the irreducible representations act.

In order to split $\vec{\psi}_m(\vec{x};t)$ into its transverse and longitudinal parts we introduce the helicity representation of Ref. 11. We expand the vectors $\vec{f}_m(\vec{p})$ and $\vec{h}_m(\vec{p})$ as follows:[13]

$$\vec{f}_m(\vec{p}) = \sum_{\lambda=0,\pm1} \vec{Q}(\vec{p},\lambda) i^{\lambda} f_m(\vec{p},\lambda),$$
$$\vec{h}_m(\vec{p}) = \sum_{\lambda=0,\pm1} \vec{Q}(\vec{p},\lambda) i^{\lambda} h_m(\vec{p},\lambda)\,. \tag{47}$$

Using the results of our earlier discussion of the eigenfunctions of the curl operator, we can now expand $\vec{\psi}_m(\vec{x};t)$ in terms of these eigenfunctions. We can thereby express $\vec{\psi}_m(\vec{x};t)$ as the sum of its longitudinal and transverse parts:[14]

$$\vec{\psi}_m(\vec{x};t) = \vec{\psi}_{m,L}(\vec{x};t) + \vec{\psi}_{m,T}(\vec{x};t), \tag{48}$$

where

$$\vec{\psi}_{m,L}(\vec{x};t) = 2\,\mathrm{Re}\, imc \int \frac{d\vec{p}}{\omega(m,p)} [\vec{\chi}(\vec{x}|\vec{p},0) f_m(\vec{p},0) e^{-ic\omega(m,p)t} + \vec{\chi}^*(\vec{x}|\vec{p},0) h_m^*(\vec{p},0) e^{ic\omega(m,p)t}]\,. \tag{49}$$

The transverse part, namely, $\vec{\psi}_{m,T}(\vec{x};t)$ is

$$\vec{\psi}_{m,T}(\vec{x};t) = mci \sum_{\lambda=\pm1} \lambda \int \frac{d\vec{p}}{\omega(m,p)} [(\omega(m,p) - \lambda p)\vec{\chi}(\vec{x}|\vec{p},\lambda) f_m(\vec{p},\lambda) e^{-ic\omega(m,p)t}$$
$$+ (\omega(m,p) + \lambda p)\vec{\chi}^*(\vec{x}|\vec{p},\lambda) h_m^*(\vec{p},\lambda) e^{ic\omega(m,p)t}]. \tag{50}$$

The reduction of the four-vector current density $\iota_m(\vec{x};t)$ into its longitudinal and transverse parts is similar. The longitudinal part $\vec{j}_{m,L}(\vec{x};t)$ is

$$\frac{\vec{j}_{m,L}(\vec{x};t)}{c} = 2\,\mathrm{Re}\, imc \sum_{\lambda=\pm1} \int d\vec{p}\,\vec{\chi}(\vec{x}|\vec{p},0) k_m(\vec{p},0) e^{-ic\omega(m,p)t}. \tag{51}$$

In the above and subsequent equations Re means "real part" of the mathematical expression which follows.

The transverse part of the current density, denoted by $\vec{j}_{m,T}(\vec{x};t)$ is

$$\frac{\vec{j}_{m,T}(\vec{x};t)}{c} = 2\,\mathrm{Re}\, imc \sum_{\lambda=\pm1} \lambda \int \frac{d\vec{p}}{\omega(m,p)} \vec{\chi}(\vec{x}|\vec{p},\lambda) k_m(\vec{p},\lambda) e^{-ic\omega(m,p)t}\,. \tag{52}$$

Finally, the charge density $\rho_m(\vec{x};t)$ is given in terms of the longitudinal component of the current density by

$$\rho(\vec{x};t) = -2\,\mathrm{Re}\frac{mc}{(2\pi)^{3/2}} \int \frac{d\vec{p}}{\omega(m,p)} k_m(\vec{p},0) e^{i[\vec{p}\cdot\vec{x} - c\omega(m,p)t}\,. \tag{53}$$

The transverse current density $j_{m,T}(\vec{x};t)$ satisfies the required divergence condition

$$\vec{\nabla}\vec{j}_{m,T}(\vec{x};t) = 0\,.$$

The longitudinal part of the current density and charge density satisfy the requisite equation of continuity:

$$\vec{\nabla}\cdot\vec{j}_{m,L}(\vec{x};t) + \frac{\partial\rho(\vec{x};t)}{\partial t} = 0\,.$$

There is an essential distinction between the $m=0$ and the $m\neq 0$ cases. In the $m=0$ case. the amplitudes $k_0(\vec{p},\lambda)$ transform into new amplitudes under changes of frame *which do not involve summations over* λ. That is, the variable λ is an *invariant* of all the transformations of the Poincaré group. A consequence is that longitudinal fields and current densities remain longitudinal fields and current densities under all transformations of the group. Similarly, transverse fields and current densities remain transverse fields and current densities under all the transformations. *This result is not true for nonzero mass*.[15]

A. The solution of Maxwell's equations for the transverse fields in terms of the transverse current densities

We want now to find the solution of Maxwell's equations for the transverse fields in terms of the transverse current densities. Thus we wish to solve

$$\vec{\nabla}\times\vec{\psi}_{m,T}(\vec{x};t)=-i\frac{1}{c}\frac{\partial}{\partial t}\vec{\psi}_{m,T}-4\pi i\frac{\vec{j}_{m,T}(\vec{x};t)}{c},$$
$$\vec{\nabla}\cdot\vec{\psi}_{m,T}(\vec{x};t)=0\,, \tag{54}$$

for $m\neq 0$.

As in the massless case, the second of Eq. (54) is trivially satisfied. Our attention is thus directed to the first of the equations. Then

$$f_m(\vec{p},\lambda)=-h_m(\vec{p},\lambda)=-\frac{4\pi i k_m(\vec{p},\lambda)}{m^2c^2}\qquad \text{for}\quad \lambda=\pm 1\,. \tag{55}$$

Hence,

$$\vec{\psi}_{m,T}(\vec{x};t)=\frac{4\pi}{mc}\sum_{\lambda=\pm 1}\lambda\int\frac{d\vec{p}}{\omega(m,p)}\{[(\omega(m,p)-\lambda p)\vec{\chi}(\vec{x}|\vec{p},\lambda)k_m(\vec{p},\lambda)e^{-ic\omega(m,p)t}]$$
$$+[(\omega(m,p)+\lambda p)\vec{\chi}^*(\vec{x}|\vec{p},\lambda)k_m^*(\vec{p},\lambda)e^{ic\omega(m,p)t}]\}. \tag{56}$$

However,

$$\vec{\psi}_{m,T}(\vec{x};t)=\vec{E}_{m,T}(\vec{x};t)-i\vec{H}_{m,T}(\vec{x};t) \tag{57}$$

so that

$$\vec{E}_{m,T}(\vec{x};t)=\frac{4\pi}{mc}\sum_{\lambda=\pm 1}\lambda\int d\vec{p}[\vec{\chi}(\vec{x}|\vec{p},\lambda)k_m(\vec{p},\lambda)e^{-ic\omega(m,p)t}+\vec{\chi}^*(\vec{x}|\vec{p},\lambda)k_m^*(\vec{p},\lambda)e^{ic\omega(m,p)t}], \tag{58}$$

$$\vec{H}_{m,T}(\vec{x};t)=-\frac{4\pi i}{mc}\sum_{\lambda=\pm 1}\int\frac{p\,d\vec{p}}{\omega(m,p)}[\vec{\chi}(\vec{x}|\vec{p},\lambda)k_m(\vec{p},\lambda)e^{-ic\omega(m,p)t}$$
$$-\vec{\chi}^*(\vec{x}|\vec{p},\lambda)k_m^*(\vec{p},\lambda)e^{ic\omega(m,p)t}]\,.$$

It is readily proved that the fields of Eq. (58) satisfy Maxwell's equations with the current given by Eq. (52). *For* $m\neq 0$ *the transverse current density determines the transverse electromagnetic field completely. There is no room for initial conditions*. One must add a solution of the homogeneous Maxwell's equations, which will contain modes of zero mass only, if initial conditions are to be imposed.

B. An example of a simple transverse current density and its transverse field

All transverse current densities and corresponding solutions for the fields are given by function $k_m(\vec{p},\lambda)$ for $\lambda=\pm 1$. We shall take the function $k_m(\vec{p},\lambda)$ to be particularly simple:

$$k_m(\vec{p},\lambda)=J\delta(p_x)\delta(p_y)\delta(p_z-P)\delta_{\lambda,\mu}. \tag{59}$$

In the above equation $\mu=+1$ or $\mu=-1$ and $P>O$. In analogy to the scalar case, the general transverse current and corresponding electromagnetic field are superpositions of such vector waves.[16] The current density $\vec{j}_{m,T}$ has an x and a y component,[17]

$$\begin{aligned} j_x(z;t)&=-\frac{1}{\sqrt{4\pi^3}}\frac{J}{\omega(m,P)}\sin[Pz-c\omega(m,P)t],\\ j_y(z;t)&=-\frac{1}{\sqrt{4\pi^3}}\frac{J\mu}{\omega(m,P)}\cos[Pz-c\omega(m,P)t],\\ j_z(z;t)&\equiv 0\,. \end{aligned} \tag{60}$$

We can now give the physical meaning of μ (or more generally λ). If μ or (λ) equals 1, $\vec{j}$ is *circularly* polarized in a direction *opposite* to the direction of propagation. If μ or λ equals -1, the wave is circularly polarized in the direction of propagation. Circular polarization is a more relativistic notion than linear polarization. Moreover, circular polarization has only *two* values, whereas linear polarization must be described by a continuum of values.

We can also find the electromagnetic fields, also circular polarized, from Eq. (54),

$$\begin{aligned} E_x(z;t)&=\frac{2J\mu}{m\sqrt{\pi}}\cos[Pz-c\omega(m,P)t],\\ E_y(z;t)&=-\frac{2J}{m\sqrt{\pi}}\sin[Pz-c\omega(m,P)t],\\ E_z(z;t)&\equiv 0,\\ H_x(z;t)&=-\frac{2J}{m\sqrt{\pi}}\frac{P}{\omega(m,P)}\sin[Pz-c\omega(m,P)t],\\ H_y(z;t)&=\frac{2J}{m\sqrt{\pi}}\frac{P\mu}{\omega(m,P)}\cos[Pz-c\omega(m,P)t],\\ H_z(z;t)&\equiv 0\,. \end{aligned} \tag{61}$$

It is perhaps useful to note that when $P\to\infty$ so that $\omega(m,P)\to P$, the solution for mass m becomes that for zero mass, i.e., for the source-free circularly polarized electromagnetic wave with amplitude $2J/m$. This result is consistent with the observation that when the momentum of a massive particle is sufficiently high, many results reduce to the case of a zero mass particle, i.e., a photon in the usual sense.

C. The solution for the longitudinal fields in terms of the longitudinal current densities

We now can proceed to find the longitudinal fields in terms of the charge densities and longitudinal current densities. In a development very close to that for the zero mass case we have

$$\vec{H}_{m,L}(\vec{x};t)\equiv 0,$$
$$f_m(\vec{p},0)=h_m(\vec{p},0)=4\pi k_m(\vec{p},0)\,. \tag{62}$$

The longitudinal electric field, longitudinal current density, and charge density are closely related superpositions of waves. Since these waves have a finite velocity for a given value of $\vec{p}$, they are causal in a sense. *Any* choice of $k_m(\vec{p},0)$ (including $m=0$) will lead to a longitudinal wave of mass m. We have thus given longitudinal currents which give rise to electric fields which are longitudinally polarized. In a later section we shall give a simple example of a longitudinal current density, charge density, and time-dependent longitudinal electric field, which gives a competing view about the notion of causality for longitudinal fields.

D. Transverse fields when there are no transverse current densities

It is clear, using the above-mentioned methods, that there can be no time-dependent longitudinal fields for $m\neq 0$ as well as $m=0$ if there are no longitudinal current densities and corresponding charge densities. We can also ask the question what are the *transverse* fields if there are no transverse currents. One can show that the only fields are the zero mass fields which we discussed earlier.

VII. THE INITIAL VALUE PROBLEM FOR ELECTROMAGNETIC FIELDS: GENERAL CONSIDERATIONS

Usually electromagnetic problems are solved in a time-independent setting. We are more interested, however, in cases in which the current density and charge density are pulsed time.[18] For this reason we use the time-dependent approach which uses the full set of the time-dependent Maxwell's equations. Thus let us consider current densities $\vec{j}(\vec{x};t)$ and charge densities $\rho(\vec{x};t)$ which are nonzero only during the time interval $t_1<t<t_2$.[19] Let us consider the case before the pulse is turned on, i.e., for $t<t_1$. The only solution of Maxwell's equations for transverse waves are those corresponding to $m=0$. The solution is found as an initial value problem in which $\vec{E}_{0,T}(\vec{x};t_0)$ and $\vec{H}_{0,T}(\vec{x};t_0)$ are given for $t_0<t_1$. The solution in terms of influence functions is identical to that of the nonrelativistic treatment (Ref. 6)

For $t>t_2$ our solution for the field is again a transverse field without a current source. The initial conditions are those for the homogeneous transverse field as $t\rightarrow t_2$ from below. For $t_1<t<t_2$ we require that the currents that contain nonzero mass modes be present. As we shall see in the following, we shall require that the range of mass is $0_+<m<\infty$. Single mass fields are exceptional if the current density is prescribed. In particular, the value of $m=0$ is *excluded* because there can be no transverse currents in this case. Instead, we can pick m as close to 0 as we like from above.

VIII. A SET OF FOUR-DIMENSIONAL EIGENFUNCTIONS OF THE CURL OPERATOR: EVALUATION OF THE EXPANSION COEFFICIENTS

A. Orthogonality of the eigenfunctions

For the sake of a more nearly ''manifestly covariant'' notation, we shall enlarge our definitions slightly. We define the four-dimensional eigenfunctions of the curl operator $\vec{\vec{\Xi}}(\vec{x};t|\vec{p},\lambda,m)$ by

$$\vec{\vec{\Xi}}(\vec{x};t|\vec{p},\lambda,m)=\frac{1}{(2\pi)^{1/2}}e^{-ic\omega(m,p)t}\vec{\chi}(\vec{x}|\vec{p},\lambda)\,. \tag{63}$$

Theorem: The four-dimensional eigenfunctions $\vec{\vec{\Xi}}(\vec{x};t|\vec{p},\lambda,m)$ satisfy the orthogonality relations

$$\int d\vec{x} \int_{-\infty}^{\infty} dt\, \vec{\Xi}^*(\vec{x};t|\vec{p},\lambda,m)\cdot\vec{\Xi}(\vec{x};t|\vec{p}\,'\lambda',m') = \frac{1}{c^3}\delta(\vec{p}-\vec{p}\,')\delta_{\lambda,\lambda'}\delta(m-m')\frac{\omega(m,p)}{m}. \tag{64}$$

From Eqs. (10) and (63),

$$\int d\vec{x} \int_{-\infty}^{\infty} dt\, \vec{\Xi}^*(\vec{x};t|\vec{p},\lambda,m)\cdot\vec{\Xi}(\vec{x};t|p',\lambda',m') = \frac{1}{2\pi}\delta(\vec{p}-\vec{p}\,')\int_{-\infty}^{\infty} dt \exp\{ict[\omega(m',p)-\omega(m,p)]\}$$

$$= \frac{1}{c}\delta(\vec{p}-\vec{p}\,')\delta_{\lambda,\lambda'}\delta[\omega(m',p)-\omega(m,p)]. \tag{65}$$

But on using δ-function identities and the fact that $m+m'\geqslant 0$,

$$\begin{aligned}\delta[\omega(m',p)-\omega(m,p)] &= \delta[(\omega(m',p)-\omega(m,p))(\omega(m',p)+\omega(m,p))] \\ &\quad\times[(\omega(m',p)+\omega(m,p))] \\ &= \delta[((m'c)^2+p^2)-((mc)^2+p^2)](\omega(m',p)+\omega(m,p)) \\ &= \frac{1}{c^2}\delta[(m'-m)(m'+m)](\omega(m',p)+\omega(m,p)) \\ &= \frac{1}{c^2}\delta(m'-m)\frac{\omega(m,p)}{m}.\end{aligned} \tag{66}$$

On using Eq. (66) in Eq. (65), Eq. (64) follows.

Finally, one can show

$$\int d\vec{x} \int_{-\infty}^{\infty} dt\, \vec{\Xi}^*(\vec{x};t|\vec{p},\lambda,m)\cdot\vec{\Xi}^*(\vec{x};t|\vec{p}\,',\lambda',m') = 0. \tag{67}$$

B. Eigenfunctions and eigenvalues of the mass

The functions $k_m(\vec{p},\lambda)$ are eigenfunctions corresponding to eigenvalues m in the continuous spectrum of the mass $0\leqslant m<\infty$ except in the following cases: If there are values of m in the vicinity of $m_1, m_2, \ldots$ such that

$$k_m(\vec{p},\lambda) = \delta(m-m_i)\hat{k}_{m_i}(\vec{p},\lambda) \tag{68}$$

and such that

$$\sum_{\lambda=\pm 1} m_i \int \frac{d\vec{p}}{\omega(m_i,p)}|\hat{k}_{m_i}(\vec{p},\lambda)|^2 < \infty, \tag{69}$$

then m_i is a *point* eigenvalue of the mass for which the corresponding eigenfunction is $\hat{k}_{m_i}(\vec{p},\lambda)$. Point eigenvalues can be added to the current density by choosing functions $\hat{k}_{m_i}(\vec{p},\lambda)$ which satisfy Eq. (69). Generally we shall be interested in nonzero point eigenvalues, since a zero point eigenvalue in the current density is a situation in which Maxwell's equations cannot be integrated. The case in which $m=0$ in the *continuous* spectrum contributes nothing.[20]

C. The completeness relation for the eigenfunctions

In a rather similar fashion one can obtain the completeness *Theorem* if there are no point eigenvalues m_i,

$$\sum_{\lambda=0,\pm1}\int_0^\infty m\,dm\int\frac{d\vec{x}}{\omega(m,p)}\Xi_i^*(\vec{x};t|\vec{p},\lambda,m)\Xi_j(\vec{x}';t'|\vec{p},\lambda,m)=\frac{1}{c^3}\delta_{i,j}\delta(\vec{x}-\vec{x}')\,\delta(t-t')\,. \tag{64a}$$

In Eq. (64a) $\Xi_i(\vec{x};t|\vec{p},\lambda,m)$ is the ith component of the vector $\vec{\Xi}(\vec{x};t|\vec{p},\lambda,m)$.

We shall now restrict our discussion to the $m>0$ case, since that for $m=0$ has already been discussed. For a general transverse current density $\vec{j}_T(\vec{x};t)$ we have the expansion

$$\frac{\vec{j}_T(\vec{x};t)}{c}=\sqrt{8\pi}\,c\,\mathrm{Re}\,i\sum_{\lambda=\pm1}\int_0^\infty m\,dm\int\frac{d\vec{p}}{\omega(m,p)}\vec{\Xi}(\vec{x};t|\vec{p},\lambda,m)k_m(\vec{p},\lambda)\,. \tag{70}$$

Thus for $\lambda=\pm1$,[21]

$$k_m(\vec{p},\lambda)=\frac{-ic^2}{\sqrt{2\pi}}\int_{-\infty}^\infty dt\int d\vec{x}\,\vec{\Xi}^*(\vec{x},t|\vec{p},\lambda,m)\cdot\vec{j}_T(\vec{x};t). \tag{71}$$

Also

$$\begin{aligned}\vec{E}_T(\vec{x};t)&=\mathrm{Re}\frac{\sqrt{128\pi^3}}{c^3}\sum_{\lambda=\pm1}\lambda\int_0^\infty\frac{dm}{m}\int d\vec{p}\,\vec{\Xi}(\vec{x};t|\vec{p},\lambda,m)k_m(\vec{p},\lambda),\\ \vec{H}_T(\vec{x};t)&=\mathrm{Re}\frac{\sqrt{128\pi^3}}{c^3}i\sum_{\lambda=\pm1}\int_0^\infty\frac{dm}{m}\int\frac{p\,d\vec{p}}{\omega(m,p)}\vec{\Xi}(\vec{x};t|\vec{p},\lambda,m)k_m(\vec{p},\lambda)\,.\end{aligned} \tag{72}$$

The longitudinal part of the current density is

$$\vec{j}_L(\vec{x};t)=2\sqrt{2\pi}\,c\,\mathrm{Re}\int_0^\infty m\,dm\int d\vec{p}\;\vec{\Xi}(\vec{x};t|\vec{p},0,m)k_m(\vec{p},0)\,. \tag{73}$$

The charge density is

$$\rho(\vec{x};t)=-2\,\mathrm{Re}\frac{1}{(2\pi)^{3/2}}\int_0^\infty m\,dm\int\frac{p\,d\vec{p}}{\omega(m,p)}k_m(\vec{p},0)\,e^{i[\vec{p}\cdot\vec{x}-c\omega(m,p)t]}\,. \tag{74}$$

The equation of continuity is again satisfied.

Because of the completeness and orthogonality relations, *any* current density $\vec{j}(\vec{x};t)=\vec{j}_T(\vec{x};t)+\vec{j}_L(\vec{x};t)$ can be expanded as in Eqs. (70) and (73). The charge density *must* be given by Eq. (74).[22] In the expansions we can include point eigenvalues m_i by requiring corresponding $\delta(m-m_i)$ functions in the coefficients $k_m(\vec{p},\lambda)$.

The expansions for the four-current density or for fields do not in themselves assure us that the theory is Poincaré-invariant. One must have the same expansions in *any* frame of reference. This invariance of expansions can be achieved by requiring the amplitudes $k_m(\vec{p},\lambda)$ to transform as mass m, spin 1, and positive energy representations in the helicity description of the irreducible representations of the Poincaré group.

IX. VELOCITY OF CURRENT DENSITY WAVES AND ELECTROMAGNETIC WAVES

Equations (54) and (55) indicate that for waves of a single frequency, current-density and fields, the waves propagate with a velocity $c\omega(m,p)/p$. That is, these waves propagate with a velocity greater than the speed of light. Relativity is generally thought to preclude this result. The usual reconciliation with relativity involves the assumption that we are dealing with a *group* and that it is the group whose velocity we require. The usual expressions for the group velocity follow:

$$v_g = c\left\{\frac{\partial}{\partial p}\omega(m,p)\right\}_{p=p_0} = \frac{cp_0}{\omega(m,p_0)} < c\,. \tag{75}$$

In deriving this result it is assumed that $k_m(\vec{p},\lambda)$ has a sharp peak at $p \equiv |\vec{p}| = p_0$.[23]

One of the difficulties which we have found is that one has approximate periodicity in p-space even when the peak is not extremely sharp.[24]

However, the principal difficulty, as pointed out by Stratton, is that it is hard to define velocity in a dispersive medium. When the mass is zero, velocity is relatively easy to define because the wave moves rigidly with increasing time. One can follow any point as it moves. When there is dispersion, it is not clear how to define velocity because the wave changes form with time.

X. IS A QUANTUM INTERPRETATION FOR MASSIVE PHOTONS POSSIBLE? A BASIS FOR CONJECTURES

We have not needed a quantum interpretation for the complex amplitudes $k_m(\vec{p},\lambda)$ to obtain our results. In the spirit of the application of group theory to quantum mechanics it is tempting to call the complex amplitudes $k_m(\vec{p},\lambda)$ wave functions of a particle of spin 1 and mass m. Perhaps one can be made more comfortable with this idea by reviewing the process by which the dynamical variables of relativistic quantum particles are introduced from classical analogues and how they are related to the infinitesimal generators of the Poincaré group. This relationship is implicit or explicit in most treatments of the application of the theory of Poincaré groups to elementary particle theory.

A. The infinitesimal generators of the Poincaré group

1. Poincaré transformations: Parametrization of the transformations

Let us consider the time–space four-vector x^μ with the components $\{x^0 = -x_0 = ct, x^i = x_i\}$ for $i = 1,2,3$. We define the *translation transformation* $T(a^\mu)$ as mapping x^μ into the four-vector x'^μ where

$$x^{\mu\prime} = T(a^\mu)x^\mu \equiv x^\mu - a^\mu. \tag{76}$$

The inverse transformation $T^{-1}(a^\mu)$ is

$$T^{-1}(a^\mu)x^\mu = x^\mu + a^\mu\,. \tag{77}$$

To define the pure rotation transformation and pure Lorentz transformation it is convenient to regard the four-vector x^μ as being a column vector which we shall denote by x_c. We use $\vec{x}$ to denote the vector which is made up of the space components of x_c. The proper *rotation transformation* is accomplished using a three-by-three matrix acting on $\vec{x}$ to produce a vector $\vec{x}'$. The transformation is such that the length of $\vec{x}'$ is equal to the length of $\vec{x}$ and the determinant of the matrix is unity. The component x^0 of x_c is unaffected by this transformation. The matrix is called the rotation matrix and is uniquely characterized by a vector $\vec{\theta}$. By one of Euler's theorems on rotations, *every proper rotation can be accomplished by a rotation around an axis*. The direction of $\vec{\theta}$ is the direction of the axis of rotation and $\theta = |\vec{\theta}|$, $(0 < \theta < 2\pi)$ is the angle of rotation. We therefore parametrize the rotation by $\vec{\theta}$ and denote both the rotation and the associated matrix by

$R(\vec{\theta})$. As is well known the product of two rotations is also a rotation. That is, if one performs two rotations one after the other, the resulting transformation is also a rotation. One says that the set of rotations form a group.

The *pure Lorentz transformation* maps the set of time–space coordinates from an initial frame to a moving from whose axes are parallel to the axes of the original frame and whose origins coincide at time $t=0$ in both frames. In addition one requires that the sign of time is preserved, or to use an accepted term, the transformation is orthochronous. The transformation and the associated 4×4 transformation matrix will be denoted by $L(\vec{\beta})$, where the direction of $\vec{\beta}$ points in the direction of the line connecting the origin of the moving frame to the origin of the fixed frame. The absolute value $\beta=|\vec{\beta}|$ is found from

$$\cosh\beta=\frac{1}{\sqrt{1-(v/c)^2}}, \tag{78}$$

where v is the velocity of the moving frame with respect to the original frame. The set of pure Lorentz transformations do *not* form a group, since the product of two Lorentz transformations involves the introduction of a rotation matrix.

The Poincaré group can have many parametrizations but the number of independent parameters is ten. We shall parametrize the group using the four parameters, which are the components of the column vector a^μ, the three components of $\vec{\theta}$, and the three components of $\vec{\beta}$. An element of the Poincaré transformation will be written as $G(a^\mu,\vec{\theta},\vec{\beta})$ where

$$G(a^\mu,\vec{\theta},\vec{\beta})=T(a^\mu)R(\vec{\theta}),L(\vec{\beta})\,. \tag{79}$$

The multiplication law

$$G(a^\mu,\vec{\theta},\vec{\beta})G(a^{\mu'},\vec{\theta}',\vec{\beta}')=G(a^{\mu''},\vec{\theta}'',\vec{\beta}'') \tag{80}$$

is obtained by carrying out the transformations of the four-vector x^μ in the order indicated. One will be able to find the set of parameters $a^{\mu''},\vec{\theta}'',\vec{\beta}''$ in terms of the sets $a^\mu,\vec{\theta},\vec{\beta}$ and $a^{\mu'},\vec{\theta}',\vec{\beta}'$. The transformations also include the identity $G(0,0,0)$ and the inverse of $G(a^\mu,\vec{\theta},\vec{\beta})$, namely $L(-\vec{\beta})R(-\vec{\theta})T(-a^\mu)$. The abstract Poincaré consists of elements which we shall also label by $G(a^\mu,\vec{\theta},\vec{\beta})$ which are in a one-to-one correspondence with the set of transformations. To have a representation of the group we must have Hilbert space upon which unitary operators $\mathcal{G}(a^\mu,\vec{\theta},\vec{\beta})$ acting on elements of the Hilbert space have the same multiplication properties as the abstract group elements $G(a^\mu.\vec{\theta},\vec{\beta})$. In general, the Hilbert space of representations can be split up into subspaces on which the operators of the representation can act without taking the vectors in the subspace out of the subspace. One of the objectives of representation theory is to find all of the subspaces which have no other proper subspaces in them that can support a representation. Each such subspace and the operators having the group properties acting on it constitute an *irreducible* representation of the group. What we have done in Refs. 5 and 6 and applied in the present paper is to show how one can obtain the irreducible representation of the electromagnetic fields and currents and find solutions of Maxwell's equations with sources in terms of the irreducible representations. Moreover, the solutions satisfy the relativistic properties required of them. In what follows we shall discuss the relationship between the group operators and the dynamical variables of relativistic particles to indicate where our conjecture comes from. Instead of using $\mathcal{G}$ as above to indicate the unitary operators which represent the group elements, we shall use G to prevent an overload of notation.

2. The infinitesimal generators of the representation

The group member $T(a^\mu)=G(a^\mu,0,0), R(\vec{\theta})=G(0,\vec{\theta},0), L(\vec{\beta})=G(0,0,\vec{\beta})$ can be written in the form

$$T(a^\mu)=\exp\left(i\sum_{\mu=0,1,2,3} a_\mu P^\mu\right),$$

$$R(\vec{\theta})=\exp(i\vec{\theta}\cdot\vec{J}), \tag{81}$$

$$L(\vec{\beta})=\exp(i\vec{\beta}\cdot\vec{K})\,.$$

In Eq. (81) P^μ ($\mu=0,1,2,3$) are Hermitian operators and are the infinitesimal generators of the translation operators. Similarly J^i and K^i are the infinitesimal generators of the rotation and pure Lorentz transformation operators.

One can find the commutation rules for the infinitesimal generators from the multiplication laws of the unitary operators $G(a^\mu,\vec{\theta},\vec{\beta})$. For later use it is convenient to introduce the operator $H=cP^0$, which will be called the energy operator or Hamiltonian. The commutation rules for the infinitesimal generators are

$$\begin{gathered}
[H,P^i]=0,\\
[P^i,P^j]=0,\\
[J^1,J^2]=J^3 \quad \text{(cyc.)},\\
[J^i,P^i]=0,\\
[J^1,P^2]=[P^1,J^2]=iP^3 \quad \text{(cyc.)},\\
[J^i,K^i]=0,\\
[J^1,K^2]=[K^1,K^2]=iK^3 \quad \text{(cyc.)},\\
[K^1,K^2]=-iJ^3 \quad \text{(cyc.)},\\
[K^i,H]=icP^i,\\
[K^i,P^j]=i\delta_{ij}\,.
\end{gathered} \tag{82}$$

We have indicated that the infinitesimal generators can be obtained from the finite unitary operators which represent the group. Remarkably, one can find *all* the irreducible representations of the infinitesimal generators and integrate them to obtain the unitary operators.

If the infinitesimal generators are given in an irreducible representation, then the operator M defined by

$$M=\frac{1}{c}\sqrt{\frac{H^2}{c^2}-\sum_{i=1}^{3}(P^i)^2} \tag{83}$$

is a real positive number called the ''mass.'' Those representations for which $M=0$ and which are of interest to us, are further classified by their helicity λ, again a constant for each representation which takes on one of the values $\lambda=0,\pm1$. These representations for which $\lambda=\pm1$ are identified with a free photon. For $M>0$ the helicity no longer labels the representation but the ''spin,'' which in our case is unity, is a label. The sign of the energy is another marker for the irreducible

representations for both $M=0$ and $M>0$. The negative energy representations are ''converted'' to positive energy representations through the use of anti-unitary operators. The ''wave functions'' which we have introduced in Sec. III are in the Hilbert space of the irreducible representations of the Poincaré group.

B. The dynamical variables of quantized relativistic particles

We shall motivate our conjectures that the irreducible representations of the Poincaré group introduce the notion of photons with mass. We shall show that knowing the irreducible representations of the Poincaré group is equivalent to knowing the quantum dynamical variables of a particle of spin 1.

Quantization of classical particle dynamics is carried out by replacing the classical Poisson bracket of two classical dynamical variables by a commutator of corresponding quantum operators divided by i times Planck's constant, i.e.,

$$\{a,b\}\rightarrow\frac{[A,B]}{i\hbar}.$$

In the above a and b are two classical dynamical variables and A,B are the corresponding quantum dynamical variables.

The dynamical variables of an unquantized relativistic particle are taken to be the three components of the momentum $p^i=p_i$, the energy $H=c\sqrt{m^2c^2+\Sigma_{i=1}^3(p^i)^2}$ and the angular momentum tensor $J^{\mu\nu}=x^\mu p^\nu-x^\nu p^\mu$.[25] The time-like component of the momentum four momentum–energy four-vector p^0 is $p^0=H/c$.

The angular momentum tensor is written in nonrelativistic form as

$$J^1=J^{23}\quad(\text{cyc.}),\tag{84}$$

$$K^i=J^{0i}.\tag{85}$$

The quantities J^i are the components of the angular momentum vector. The dynamical variables K^i are called ''boosts'' and are somewhat analogous to the position variables x^i.

We now denote the quantum dynamical variable analogues by the subscript ''q'' and the operators corresponding to the infinitesimal generators without this subscript. We find that the quantum variables satisfy the *same* commutation rules as the infinitesimal generators up to a scale factor. All the quantum relativistic dynamical variables are given by

$$\begin{aligned}P_q^i&=P^i\hbar,\\ J_q^i&=J^i\hbar,\\ K_q^i&=K^i\hbar,\\ H_q&=H\hbar.\end{aligned}\tag{86}$$

If m is the mass in the Poincaré description (dimension *time/length*^{2}) and m_q in the quantized particle description (dimension *mass*), then

$$m_q=m\hbar\ .\tag{87}$$

The functions which we have called $k_m(\vec{p},\lambda)$ are wave functions upon which the infinitesimal generators of the Poincaré representations *and* the dynamical variables of quantized relativistic particles act. It should also be noted that the quantum particle operators have the correct physical

dimensions. For example, if the Poincaré infinitesimal generators P^i (or rather their eigenvalues) have the dimension 1/*length*, then the eigenvalues of the particle operators P_q^i have the correct dimensions of linear momentum.

We shall give an example of how the commutation relations of the quantum operators are obtained from the Poisson brackets of the classical dynamical variables. Let K^1 and K^2 be the classical boost dynamical variables,

$$\begin{aligned} K^1 &= x^0 p^1 - x^1 p^0, \\ K^2 &= x^0 p^2 - x^2 p^0. \end{aligned} \tag{88}$$

Furthermore,

$$p^0 = \sqrt{m^2 c^2 + \sum_{i=1}^{3} (p^i)^2}. \tag{89}$$

Then the Poisson bracket of K^1, K^2 is

$$\{K^1, K^2\} = \sum_{i=1}^{3} \left[\frac{\partial K^1}{\partial x^i} \frac{\partial K^2}{\partial p^i} - \frac{\partial K^2}{\partial x^i} \frac{\partial K^1}{\partial p^i} \right]. \tag{90}$$

Also

$$\begin{aligned} \frac{\partial K^1}{\partial x^i} &= -\delta_{i1} p^0, \\ \frac{\partial K^2}{\partial p^i} &= -x^2 \frac{\partial p^0}{\partial p^i}. \end{aligned} \tag{91}$$

But

$$\frac{\partial p^0}{\partial p^i} = \frac{p^i}{p^0}. \tag{92}$$

Thus

$$\sum_{i=1}^{3} \left[\frac{\partial K^1}{\partial x^i} \frac{\partial K^2}{\partial p^i} \right] = x^2 p^1. \tag{93}$$

Similarly,

$$\sum_{i=1}^{3} \left[\frac{\partial K^2}{\partial x^i} \frac{\partial K^1}{\partial p^i} \right] = x^1 p^2. \tag{94}$$

Therefore the Poisson bracket is

$$\{K^1, K^2\} = x^2 p^1 - x^1 p^2 = -J^3. \tag{95}$$

To introduce quantization we replace K^1, K^2, J^3 by Hermitian operators and the Poisson bracket by the commutator

$$\{K^1, K^2\} \rightarrow \frac{[K_q^1, K_q^2]}{i\hbar} = -J_q^3, \tag{96}$$

or

$$[K_q^1, K_q^2] = -i\hbar J_q^3$$

as required.

XI. MOVING FRAMES OF REFERENCE AND THE CREATION OF LONGITUDINAL FIELDS FROM TRANSVERSE AND THE CONVERSE

We shall now prove that even if one starts out with a purely transverse current density and a transverse field in an original frame of reference, a longitudinal current density and field appear in a frame of reference moving with respect to the first. Moreover, in the moving frame there will be a charge density, even if there were none in the original frame in which Eq. (53) holds. For a purely transverse field $k_m(\vec{p},0) \equiv = 0$.

Let us consider a frame moving along the z axis such that the space coordinates of the moving frame remain parallel to those of the original frame and that the two frames coincide when the time t equals zero in both frames. Then the coordinates in the new frame are related to those of the old by

$$\begin{aligned} ct' &= \frac{ct}{\sqrt{1-(v/c)^2}}, \\ z' &= \frac{z}{\sqrt{1-(v/c)^2}} - ct\frac{v/c}{\sqrt{1-(v/c)^2}}, \\ x' &= x, \\ y' &= y. \end{aligned} \tag{97}$$

The amplitudes in the original frame will be denoted by $k_m(\vec{p},\lambda)$ and that in the moving frame by $k'_m(\vec{p},\lambda)$. Then the principal result of this section is taken from Ref. 11:

$$k'_m(\vec{p},\lambda) = \exp[i\beta\mathcal{J}_3]k_m(\vec{p},\lambda). \tag{98}$$

In Eq. (98) $\mathcal{J}_3$ is the infinitesimal boost operator which operates on $k_m(\vec{p},\lambda)$ in a manner described in Ref. 11. As before, the scalar β is related to the velocity v of the Lorentz transformation Eq. (97) as follows:

$$\cosh\beta = \frac{1}{\sqrt{1-(v/c)^2}}. \tag{99}$$

The exponent operator in Eq. (98) is a *global* operator which represents the effect of a *finite* Lorentz transformation as in Eq. (97). Let us consider the case in which the velocity of the moving frame v is much less than the velocity of light.[26] Then

$$\begin{aligned} \frac{v}{c} &\ll 1, \\ \beta &\approx \frac{v}{c}. \end{aligned} \tag{100}$$

For such velocities

$$\exp[i\beta\mathcal{J}_3]\approx 1+i\frac{v}{c}\mathcal{J}_3. \tag{101}$$

Thus on using Eq. (2.6) of Ref. 11

$$k'_m(\vec{p},\lambda)\approx\left[1-\frac{v\,\omega(m,p)}{c}\frac{\partial}{\partial p_3}\right]k_m(\vec{p},\lambda)+i\frac{v}{c}\frac{mc}{p^2}(p_1T_1+p_2T_2)k_m(\vec{p},\lambda). \tag{102}$$

The operators T_1 and T_2 act only on the variable $\lambda=0,\pm 1$ in $k_m(\vec{p},\lambda)$. It is these operators which can introduce longitudinal polarization even when the amplitude $k_m(\vec{p},0)\equiv 0$. Conversely, if the field is longitudinally polarized in the original frame, it will generally have a transverse component in the moving frame.[27]

To show how T_1 and T_2 act on $k_m(\vec{p},\lambda)$ we introduce the related operators $T^{\pm}$ through

$$T^{\pm}=T_1\pm T_2. \tag{103}$$

Then

$$\begin{aligned} T^+k_m(\vec{p},\lambda)&=\sqrt{2-\lambda}\,\sqrt{1+\lambda}\,k_m(\vec{p},\lambda-1),\\ T^-k_m(\vec{p},\lambda)&=\sqrt{2+\lambda}\,\sqrt{1-\lambda}\,k_m(\vec{p},\lambda+1)\,. \end{aligned} \tag{104}$$

From the above equation we see that our assertion is proved.

XII. A SIMPLE EXAMPLE: A SPHERE OF CONSTANT CHARGE DENSITY UNDER PULSED ROTATIONS

We shall consider the source of electromagnetic waves to be a sphere of radius a which contains a charge of uniform density ρ. The origin of the sphere is at the origin of coordinates. For time $t<-\tau$ and $t>\tau$, where $\tau>0$, the sphere is stationary. But for $-\tau<t<\tau$ the sphere rotates about the z axis with a constant angular velocity Ω. For $t<-\tau$ and $t>\tau$ there is no current at all, either transverse or longitudinal. Since the charge density is constant in time, the equation of continuity is trivially satisfied. For $-\tau<t<\tau$ the current is purely transverse and again the equation of continuity is satisfied.

A. The longitudinal field

We shall first dispose of the problem of finding the longitudinal current density and the longitudinal electromagnetic field. It is obvious that the longitudinal current density is zero and that the longitudinal field is a purely electrostatic field with only a radial component $E_r(r)$ given by

$$E_r(r)=\frac{Q}{r^2}\qquad \text{for}\quad r>a\,. \tag{105}$$

B. The transverse current density

The transverse current density $\vec{j}_T(\vec{x})$ during the time $-\tau<t<\tau$ is

$$\vec{j}_T(\vec{x})=\rho(r)\vec{v}\,, \tag{106}$$

$$\rho(r)=\begin{cases}\rho & \text{for}\quad r<a\\ 0 & \text{for}\quad r>a.\end{cases} \tag{107}$$

We define the vector angular velocity $\vec{\Omega}=\Omega\vec{k}$ where $\vec{k}$ is the unit vector on the z axis. Then $\vec{v}=\vec{\Omega}\times\vec{x}$.

Polar coordinates in $\vec{x}$ space will be denoted by $\{r,\hat{\theta},\hat{\phi}\}$. In $\vec{p}$ space they will be indicated by $\{p,\theta,\phi\}$. In terms of polar coordinates

$$\vec{j}_T(\vec{x})=\rho(r)\Omega r\sin\hat{\theta}\,\vec{a}_{\hat{\phi}} \tag{108}$$

for $-\tau<t<\tau$. For all other values of t, $\vec{j}_T\equiv 0$. The vector $\vec{a}_{\hat{\phi}}$ is the unit vector in $\vec{x}$ space in the $\hat{\phi}$ direction.

C. Generalized spherical harmonics

It is now convenient to introduce generalized spherical (or surface) harmonics $Y_j^{\mu,\lambda}(\theta,\phi)$. The number j is either 0 or a positive integer or half-odd integer. The numbers λ,μ take on the values $-j,-j+1,\ldots,j-1,j$. The generalized spherical harmonics are useful when describing functions, vectors, and tensors.[28] These functions are generalized spherical harmonics in the sense that a subset of them are ''ordinary'' spherical harmonics,

$$Y_j^{\mu,0}(\theta,\phi)\equiv Y_{j,\mu}(\theta,\phi) \tag{109}$$

when j is an integer.[29] The generalized spherical harmonics satisfy the following orthogonality and completeness relations:

$$\begin{aligned}&\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\sin\theta\,\mathrm{d}\theta\,Y_j^{m,n}{}^*(\theta,\phi)\,Y_{j'}^{m',n}(\theta,\phi)=\delta_{j,j'}\delta_{m,m'},\\&\sum_{j=|n|}^{\infty}\sum_{m=-j}^{j}Y_j^{m,n}(\theta,\phi)\,Y_j^{m,n}{}^*(\theta',\phi')\sin\theta=\delta(\theta-\theta')\,\delta(\phi-\phi').\end{aligned} \tag{110}$$

The spherical harmonics $Y_1^{\mu,\lambda}(\theta,\phi)$ play a central role. Explicitly they are given by[30]

$$\begin{aligned}Y_1^{1,1}(\theta,\phi)&=\frac{1}{4}\sqrt{\frac{3}{\pi}}(1+\cos\theta),\\Y_1^{1,0}(\theta,\phi)&=-\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin\theta,\\Y_1^{1,-1}(\theta,\phi)&=\frac{1}{4}\sqrt{\frac{3}{\pi}}e^{2i\phi}(1-\cos\theta),\\Y_1^{0,1}(\theta,\phi)&=-\sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin\theta,\\Y_1^{0,-1}(\theta,\phi)&=-\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin\theta,\\Y_1^{-1,1}(\theta,\phi)&=\frac{1}{4}\sqrt{\frac{3}{\pi}}e^{-2i\phi}(1-\cos\theta),\\Y_1^{-1,0}(\theta,\phi)&=\sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin\theta,\\Y_1^{-1,-1}(\theta,\phi)&=\frac{1}{4}\sqrt{\frac{3}{\pi}}(1+\cos\theta).\end{aligned} \tag{111}$$

D. Calculation of the wave function $k_m(\vec{p},\lambda)$

In this section we shall compute $k_m(\vec{p},\lambda)$ from the current density Eq. (108) by using Eq. (65). We only need find $k_m(\vec{p},\lambda)$ for $\lambda=\pm 1$, since the current density is transverse so that $k_m(\vec{p},0)\equiv 0$.

Through the use of the formulas for $\vec{\Xi}(\vec{x},t|\vec{p},\lambda,m)$,

$$k_m(\vec{p},\lambda)=\frac{\rho\Omega}{(2\pi)^2}\int_{-\tau}^{\tau}\mathrm{d}t\, e^{ic\omega(m,p)t}\int_0^{\infty}r^3\,\mathrm{d}r\int_0^{2\pi}\mathrm{d}\hat{\phi}\int_0^{\pi}\sin^2\hat{\theta}\,\mathrm{d}\hat{\theta}[\vec{a}_{\hat{\phi}}\cdot\vec{Q}^*(\vec{p},\lambda)]e^{-i\vec{p}\cdot\vec{x}}. \tag{112}$$

But

$$\int_{-\tau}^{\tau}\mathrm{d}t\, e^{ic\omega(m,p)t}=2\,\frac{\sin c\omega(m,p)\tau}{c\omega(m,p)}. \tag{113}$$

Now we shall evaluate the integral

$$\int_0^{2\pi}\mathrm{d}\hat{\phi}\int_0^{\pi}\mathrm{d}\hat{\theta}\sin^2\hat{\theta}[\vec{a}_{\hat{\phi}}\cdot\vec{Q}^*(\vec{p},\lambda)]e^{-i\vec{p}\cdot\vec{x}}.$$

We recollect that $\hat{\phi}$ and $\hat{\theta}$ refer to the polar angles of $\vec{x}$ and ϕ and θ refer to the polar angles of $\vec{p}$. The expression in square brackets in the above double integral involves the two sets of polar angles.

It can be shown that

$$\vec{a}_{\hat{\phi}}\cdot\vec{Q}^*(\vec{p},\lambda)=-i\sqrt{\frac{2\pi}{3}}\sum_{\mu=\pm 1}e^{-i\mu\hat{\phi}}Y_1^{\mu\lambda}(\theta,\phi). \tag{114}$$

Also

$$e^{-i\mu\hat{\phi}}\sin\hat{\theta}=\sqrt{\frac{8\pi}{3}}\,\mu Y_1^{*\mu 0}(\hat{\theta},\hat{\phi}) \tag{115}$$

and

$$e^{-i\vec{p}\cdot\vec{x}}=4\pi\sum_{q=0}^{\infty}\sum_{s=-q}^{q}(-i)^q j_q(pr)Y_q^{*s0}(\theta,\phi)Y_q^{s0}(\hat{\theta},\hat{\phi}). \tag{116}$$

In the above equation $j_n(x)$ is the usual spherical Bessel function. (Of course $p=|\vec{p}|$ and $r=|\vec{x}|$.) On using the orthogonality properties of the generalized spherical harmonics we have

$$k_m(\vec{p},\lambda)=-\frac{8}{3}\rho\Omega\,\frac{\sin\omega(m,p)c\tau}{c\omega(m,p)}\sum_{\mu=\pm 1}\mu Y_1^{\mu\lambda}(\theta,\phi)Y_1^{*\mu 0}(\theta,\phi)\int_0^a\mathrm{d}r\, r^3 j_1(pr). \tag{117}$$

On using the explicit forms for the generalized spherical harmonics

$$\sum_{\mu=\pm 1}\mu\, Y_1^{\mu\lambda}(\theta,\phi)Y_1^{*\mu 0}(\theta,\phi)=-\sqrt{2}\,\frac{3}{8\pi}\lambda e^{-i\lambda\phi}\sin\theta \tag{118}$$

and thus

$$k_m(\vec{p},\lambda)=\frac{\sqrt{2}}{\pi}\rho\Omega\,\frac{\sin[\omega(m,p)c\tau]}{c\omega(m,p)}\lambda e^{-i\lambda\phi}\sin\theta\int_0^a\mathrm{d}r\, r^3 j_1(pr). \tag{119}$$

We need only evaluate the integral. We give this integral below:

$$\int_0^a \mathrm{d}r\, r^3 j_1(pr) = \frac{1}{p^4} G(pa)\,, \tag{120}$$

where $G(x)$ is the function

$$G(x) = 3x\cos x + (-3+x^2)\sin x\,. \tag{121}$$

Thus we have found the transform of the current density explicitly as

$$k_m(\vec{p},\lambda) = \frac{\sqrt{2}}{\pi}\rho\Omega\,\frac{\sin[\omega(m,p)c\tau]}{c\,\omega(\vec{p},\lambda)}\lambda e^{-i\lambda\phi}\sin\theta\frac{1}{p^4}G(pa)\,. \tag{122}$$

One can also write Eq. (122) in terms of dimensionless variables,

$$k_m(\vec{p},\lambda) = \mathcal{C}\hat{k}_m(\vec{\hat{p}},\lambda)\,. \tag{123}$$

In Eq. (123) $\mathcal{C} = (\sqrt{2}/\pi)\rho\Omega a^3\tau$. The function $\hat{k}_m$ is the dimensionless form of k_m and is given in terms of the dimensionless variables $\hat{m}$, $\hat{p}$ and χ defined below:

$$\hat{k}_{\hat{m}}(\vec{\hat{p}},\lambda) = \frac{\sin[\sqrt{\hat{m}^2+\hat{p}^2}\,\chi]}{\sqrt{\hat{m}^2+\hat{p}^2}}\lambda e^{-i\lambda\phi}\sin\theta\frac{G(\hat{p})}{\hat{p}^4},$$

$$\hat{p} = pa,$$

$$\chi = \frac{c\tau}{a},$$

$$\hat{m} = mca\,. \tag{124}$$

When we consider $k_m(\vec{p},\lambda)$ to be a wave function used in fractions to provide probability distributions, we may set $\mathcal{C}$ to be equal to unity, since it cancels out in the numerator and denominator of the ratio. We can then drop the caret over the variables and evaluate probabilities in a dimensionless setting.

1. Use of $k_m(\vec{p},\lambda)$ to find the mass distribution for the rotating sphere of charge

It is not a difficult matter to find the electromagnetic field due to the rotating sphere of charge. The easiest way, perhaps, is to calculate $\vec{E}(\vec{x};t)$ and $\vec{H}(\vec{x};t)$ using Eq. (72). We focus our attention on finding the consequences of considering $k_m(\vec{p},\lambda)$ to be the wave function of a massive photon.

2. Consequences of the notion of a massive photon: Arguments for and against its existence

We shall use Eq. (122) as the wave function. We shall concentrate on obtaining the probability of finding the mass m in an interval when the current is on.

Knowledge of the wave function $k_m(\vec{p},\lambda)$ enables us to obtain the probability distribution $P(m)$ that the mass m lies in the interval Δ as

$$\int_\Delta P(m)\mathrm{d}m\,.$$

From quantum mechanics,

$$P(m)=\frac{m\sum_{\lambda=\pm1}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dp[p^2/\omega(m,p)]|k_m(\vec{p},\lambda)|^2}{\int_0^{\infty}dm\,m\sum_{\lambda=\pm1}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dp[p^2/\omega(m,p)]|k_m(\vec{p},\lambda)|^2}. \tag{125}$$

Then the probability that a measurement of mass m in a small interval Δ about m_0 is

$$P(m_0)\Delta\,. \tag{126}$$

At this point it seems desirable to give arguments for and against the existence of massive photons based on the requirements of relativity as a constraint on the solutions of Maxwell's equations. The principal reason for identifying $k_m(\vec{p},\lambda)$ with the photon wave function is that when this identification is carried out for the case of no current density, this identification leads to the correct results for zero-mass photons, including second quantization. Also one obtains the correct decompositions for both the real and complex vector fields and for solutions of the Dirac equation for both zero- and nonzero masses.[31] Furthermore, as indicated earlier, the function $k_m(\vec{p},\lambda)$ is the *only* wave function[32] for quantized relativistic particles of spin 1. The electromagnetic fields cannot be expressed in terms of any other function if they are to transform under Lorentz transformations in the customary way.

The principal argument against massive photons is that they have not yet been found. (But neither have they been sought for in modern times.) Another argument against their existence is that $P(m)$ which gives the mass distribution is, in our example, independent of the charge density ρ or angular velocity Ω of the rotating sphere of charge, though the strength of the electromagnetic field *does* depend on these quantities. Perhaps the independence of $P(m)$ on $\rho\Omega$ is one of the paradoxes of quantum theory as opposed to classical theory. A somewhat similar situation exists for the electron–positron field for which the ''sea of electrons'' is assumed to fill the negative energy band, even when no electron is lifted out of the sea and the sea cannot be observed.

XIII. EVALUATION OF THE PROBABILITY DISTRIBUTION OF MASS $P(m)$ IN OUR EXAMPLE

We shall now evaluate the probability distribution $P(m)$ of Eq. (125), which will give an indication of which masses to expect in our problem. The masses m are perhaps the most interesting aspect of photons with mass.

A. The evaluation of the denominator

We denote the denominator by D,

$$D=\sum_{\lambda=\pm1}\int_0^{2\pi}d\phi\int_0^{\pi}\sin^3\theta\int_0^{\infty}dm\,m\int_0^{\infty}\frac{dp}{p^6}\frac{\sin^2[\omega(m,p)\chi]}{[\omega(m,p)]^3}[G(p)]^2. \tag{127}$$

Summing over λ and integrating over θ and ϕ allow us to write

$$D=E\int_0^{\infty}dm\,m\int_0^{\infty}\frac{dp}{p^6}\frac{\sin^2[\omega(m,p)\chi]}{[\omega(m,p)]^3}[G(p)]^2\,. \tag{128}$$

In the above equation E is a numerical constant which will cancel out in the ratio of numerator and denominator in the expression for $P(m)$. We may thus set $E=1$. We shall now carry out the integration over m.

We introduce the variable ξ by

$$\xi=\omega(m,p)\chi\,.$$

Then

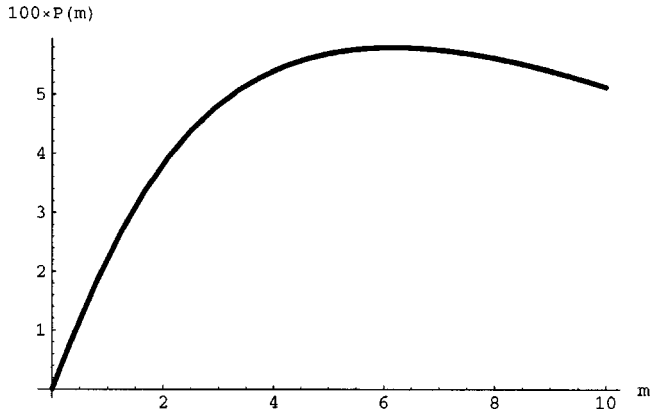

FIG. 1. The probability density $P(m)$ for $\chi=0.1$.

$$\int_0^\infty \mathrm{d}m \frac{m \sin^2[\omega(m,p)\chi]}{[\omega(m,p)]^3} = \chi \int_{\chi p}^\infty \frac{\sin^2 \xi}{\xi^2} = \chi\left[\frac{\pi}{2} - \mathrm{Si}(2\chi p) + \frac{\sin^2 \chi p}{\chi p}\right]. \tag{129}$$

Thus the denominator of the probability ratio is

$$D = \chi \int_0^\infty \frac{dp}{p^6}\left[\frac{\pi}{2} - \mathrm{Si}(2\chi p) + \frac{\sin^2 \chi p}{\chi p}\right]|G(p)|^2 . \tag{130}$$

This integral is a single integral over p which we shall evaluate numerically for several values of the nondimensional time χ.

B. The expression for the probability density

We shall now give the probability density $P(m)$ in terms of the dimensionless variables m,χ.

We shall denote the probability density, at the nondimensional time χ, by $P(m,\chi)$. The probability that a measurement of the mass m will give a value of m within an interval Δ about m at the nondimensional time χ is $P(m,\chi)\Delta$ where

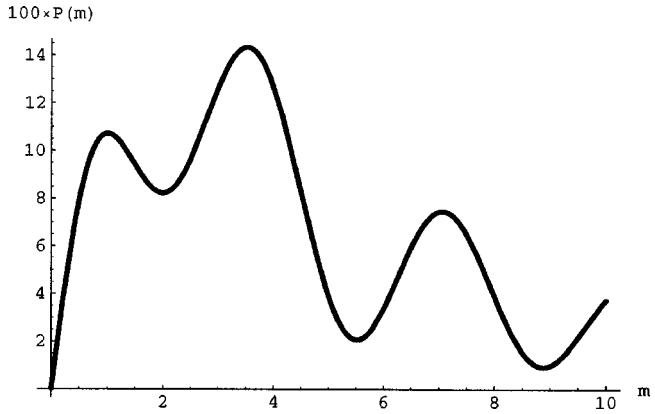

FIG. 2. The probability density $P(m)$ for $\chi=1.0$.

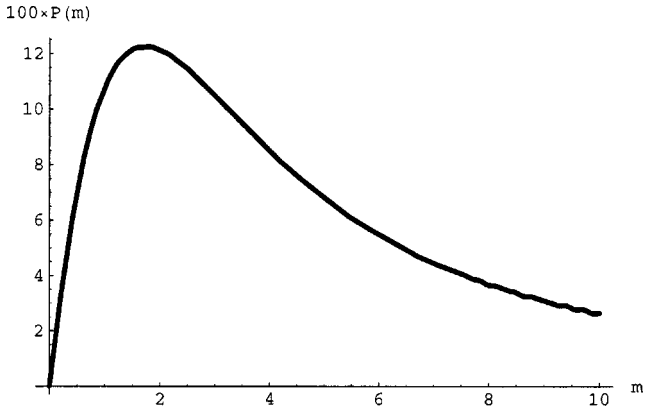

FIG. 3. The probability density $P(m)$ for $\chi=10.0$.

$$P(m,\chi)=\frac{1}{\chi}\frac{m\int_0^\infty \frac{dp}{p^6}\frac{\sin^2[\omega(m,p)\chi]}{[\omega(m,p)]^3}[G(p)]^2}{\int_0^\infty \frac{dp}{p^6}\left[\frac{\pi}{2}-\mathrm{Si}(2\chi p)+\frac{\sin^2\chi p}{\chi p}\right][G(p)]^2}. \tag{131}$$

C. Figures for $P(m)$ for several values of time interval of rotation

We have calculated and graphed $P(m)$ for three values of χ, namely, $\chi=0.1$, 1.0, and 10. These three values of χ are representative of the cases for which $c\tau$ is short, equal to long, respectively, compared to the radius a of the sphere which contains the charge (Figs. 1–3).[33]

It is clear from these graphs that there is a continuous distribution of masses for the problem which we have discussed. The writer hopes to obtain probability distributions for other transverse current distributions.

XIV. A DISCUSSION OF THE LONGITUDINAL FIELD: AN EXAMPLE OF A TIME-DEPENDENT LONGITUDINAL CURRENT DENSITY AND THE ASSOCIATED LONGITUDINAL ELECTRIC FIELD

Most of our discussion has centered on time-dependent transverse current densities and transverse electromagnetic fields because these are of great practical interest. But longitudinal current densities and longitudinal electric fields (there are no magnetic fields) also have properties which are surprising. We shall give an example which can, perhaps, be tested experimentally.

A. General considerations of longitudinal current densities and electric fields

Longitudinal current densities as a source of fields are much more easily treated mathematically than transverse current densities and fields. If we have a longitudinal current density, Maxwell's equations become

$$\frac{\partial}{\partial t}\vec{E}_L(\vec{x};t)=-4\pi\vec{j}_L(\vec{x};t),$$

$$\vec{H}_L(\vec{x};t)\equiv 0, \tag{132}$$

$$\vec{\nabla}\cdot\vec{E}_L(\vec{x};t)=4\pi\rho(\vec{x};t).$$

It would appear that we could use either the longitudinal current density $\vec{j}(\vec{x};t)$ or the charge density $\rho(\vec{x};t)$ and get the same answer. We shall see that this is, in fact, true.

We shall assume that the current density is pulsed and that it is zero for $t<-T<0$ and $t>T$. We can use Professor Keller's suggested method of solving Eq. (132) without reducing the fields and currents to irreducible representations of the Poincaré group. Thus we find the electric field $\vec{E}_L(\vec{x};t)$ from the first of Eq. (132):

$$\vec{E}_L(\vec{x};t)=\begin{cases}\vec{E}_{s0}(\vec{x}) & \text{for} \quad t<-T,\\ E_{s0}(\vec{x})-4\pi\int_{-T}^{t}\vec{j}_L(\vec{x};t')dt' & \text{for} \quad -T<t<T\\ E_{s0}(\vec{x})-4\pi\int_{-T}^{T}\vec{j}_L(\vec{x};t')dt' & \text{for} \quad t>T.\end{cases} \tag{133}$$

In the above equation $\vec{E}_{s0}(\vec{x})$ is the static electric field which may exist before the longitudinal current is pulsed. It could be due to a static charge density. When $t>T$, the electric field is again independent of time and may be regarded as the static field due to a charge distribution arising from the pulsed current. Thus for $t>T$ we write $\vec{E}_L(\vec{x};t)\equiv\vec{E}_{s1}(\vec{x})$. We first solve the problem for which $\vec{E}_{s0}(\vec{x})\equiv 0$. The charge density after the current density pulse has been initiated is then

$$\rho(\vec{x};t)=\begin{cases}\dfrac{1}{4\pi}\vec{\nabla}\cdot\vec{E}_L(\vec{x};t)\\ 0 \quad \text{for} \quad t<-T\\ -\displaystyle\int_{-T}^{t}dt'\,\vec{\nabla}\cdot\vec{j}_L(\vec{x},t') \quad \text{for} \quad t>-T.\end{cases} \tag{134}$$

Clearly the equation of continuity is satisfied.

B. Example: An expanding balloon with surface charge

As an example, we consider an expanding balloon, the surface of which has an index of refraction close to unity. The expansion starts at time $t=-T$, at which time the radius of the balloon is R_0 and continuous to time $t=T$ at which time the radius is R_1. The radius for any time t with $-T<t<T$ is denoted by $R(t)$. The radius is assumed to grow with constant velocity u. Thus

$$\begin{aligned}R(t)&=ut+\frac{R_1+R_0}{2},\\ u&=\frac{R_1-R_0}{2T}.\end{aligned} \tag{135}$$

The total charge in the balloon is Q which is uniformly distributed on the surface of the balloon. The charge distribution $\rho(\vec{x};t)$ is then

$$\rho(\vec{x};t)=\frac{Q}{4\pi}\frac{\delta(r-r(t))}{R^2(t)}. \tag{136}$$

Thus $\rho(\vec{x};t)$ depends only upon r and t. It is readily verified that

$$\int \mathrm{d}\vec{x}\,\rho(\vec{x};t)=Q \tag{137}$$

as required. The current density is

$$\vec{j}(\vec{x};t)=\begin{cases}\rho(\vec{x};t)\vec{u} & \text{for } -T<t<T\\ 0 \text{ for all other values of } t,\end{cases} \tag{138}$$

and $\vec{u}=u\vec{a}_r$ where $\vec{a}_r$ is e unit vector along the radius. We can find the electric field from Eq. (132). Initially we set $\vec{E}_{s0}=0$.

Then

$$\vec{E}_L(\vec{x};t)=\begin{cases}0 & \text{for } t<-T\\ -\dfrac{Q}{r^2} & \text{for } -T<t<T \text{ and } R_0<r<R(t)\\ -\dfrac{Q}{r^2}\vec{a}_r & \text{for } t>T \text{ and } R_0<r<R_1\,.\end{cases} \tag{139}$$

In all domains of space–time other than those appearing in Eq. (139) $\vec{E}_L(\vec{x};t)=0$.

This result for $\vec{E}_l(\vec{x};t)$ would be valid if the charge on the balloon were created instantaneously at time $t=-T$. A more realistic approach would be to put the charge on the balloon *before* the balloon began to expand. In this case

$$\vec{E}_{s0}(\vec{x};t)=\begin{cases}0 & \text{for } r<R_0\\ \dfrac{Q}{r^2}\vec{a}_r & \text{for } r>R_0\,.\end{cases} \tag{140}$$

We now add this field to the field of Eq. (139). We obtain

$$\vec{E}_{L\ total}=\begin{cases}0 & \text{for } r<R(t)\\ \dfrac{Q}{r^2}\vec{a}_r & \text{for } r>R(t).\end{cases} \tag{141}$$

This result is precisely the same as though we used Gauss's theorem as is generally done finding the field due to a spherical distribution of charge in elementary potential theory.

This result is general. One can use electrostatic theory with time-dependent source densities $\rho(\vec{x};t)$ to obtain longitudinal fields. We shall now prove this theorem in general. The proof is a generalization of a similar theorem for zero mass components of the field which we treated earlier.

Since $\vec{E}_L(\vec{x};t)$ is a longitudinal (i.e., irrotational) field, the field can be represented as a gradient of a scalar potential.

$$\vec{E}_L(\vec{x};t)=-\vec{\nabla}V(\vec{x};t). \tag{142}$$

Then the last of Eq. (132) becomes

$$\nabla^2V(\vec{x};t)=-4\pi\rho(\vec{x};t)\,. \tag{143}$$

This equation is, of course, Poisson's equation for potentials with a source distribution $\rho(\vec{x};t)$. Then the longitudinal field is easily solved for

$$\vec{E}_L(\vec{x};t)=\vec{\nabla}\int d\vec{x}\frac{\rho(\vec{x}';t)}{|\vec{x}-\vec{x}'|}. \tag{144}$$

Thus the *time-dependent* longitudinal field is easily obtained from a *time-dependent* source distribution. This result is a simple generalization of the method of obtaining electrostatic fields from source distributions.

There is an astonishing consequence. *Longitudinal fields are not causal! Maxwell's equations have noncausal solutions!* Longitudinal electric fields travel with infinite speed just as Newtonian gravitational fields do.

We are left with a problem, if causality, as usually understood, is to be preserved. It would seem that Maxwell's equations have to be modified. Otherwise, if we want to keep Maxwell's equations as they are, we shall have to alter our notion of the meaning of causality. From an experimental point of view, one should test whether indeed a change in the longitudinal fields travel with a finite speed if the source distribution is changed abruptly.

The problem of causality of all solutions of Maxwell's equations seems not to have been generally understood or discussed, at least in modern times.

To finish the discussion of longitudinal electric fields, the longitudinal current density can be found from the first of Eq. (132) or, equivalently, from the equation of continuity. If one starts with this current density and solves for the longitudinal field, one gets the same field that one started with and the same charge density. The circle is closed.

ACKNOWLEDGMENT

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[1] If there are such subintervals, we may consider the current density to be a series of pulses, the fields of each of which can be added to form the solution because of the linearity of Maxwell's equations.

[2] See, e.g., H. E. Moses, J. Math. Phys. **25**, 1905 (1984). We take this opportunity to correct an error in that paper. Equation (4.42) is incorrect and the current density in Eq. (4.43) is transverse.

[3] J. S. Lomont and H. E. Moses, J. Math. Phys. **3**, 405 (1962).

[4] L. L. Foldy, Phys. Rev. **102**, 568 (1956); Yu. M. Shirokov, Zh. Eksp. Theor. Fiz. **3**, 1196 (1957) [Sov. Phys. JETP **13**, 240 (1961)].

[5] H. E. Moses, J. Math. Phys. **8**, 1134 (1967).

[6] H. E. Moses, J. Math. Phys. **9**, 16 (1968).

[7] H. E. Moses, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. **21**, 114 (1971).

[8] These quantities strictly speaking are not vectors, since their transformation properties under rotations are not quite the proper ones. See Ref. 7 for the rotation properties of the eigenfunctions.

[9] One can introduce a measure function to describe the range of values of m.

[10] The helicity realization for $m \neq 0$ resembles the $m=0$ case more closely than the equivalent Foldy–Shirokov realization. When $m \to 0$, the mass helicity representation approaches the direct sum of *three* zero-mass representations corresponding to the three values of helicity of the nonzero mass representations. H. E. Moses, Ann. Phys. (N.Y.) **60**, 275 (1970).

[11] In Ref. 6 we have given the expansion of the real four-vector which is comprised of the scalar and vector potential satisfying the Lorentz condition. The same expansion applies to $\iota(\vec{x};t)$ when the equation of continuity is satisfied.

[12] J.B. Keller (private communication).

[13] We recollect that for a fixed value of $\vec{p}$ the vectors $\vec{Q}(\vec{p},\lambda)$ constitute a basis in three-dimensional space. We have absorbed some numerical factors in the functions $f_m(\vec{p})$ and $h_m(\vec{p})$.

[14] The functions $f_m(\vec{p},\lambda)$, $h_m(\vec{p},\lambda)$, and $k_m(\vec{p},\lambda)$ transform under the irreducible helicity representations of the Poincaré group (Ref. 11) corresponding to particles of mass m, spin 1, and *positive* energy.

[15] This consequence of the properties of Poincaré transformations will be discussed more fully in a later section.

[16] For simplicity we take J to be real.

[17] We have dispensed with the showing of several nonessential variables and constants.

[18] In practice this is the way to create source-free electromagnetic fields.

[19] The effect of repeated pulses, even those of different shapes in time and space, can be obtained by superposition.

[20] In integrals any point in the continuous spectrum is of zero measure.

[21] We have used Eq. (67). Moreover, we have made the replacement $\lambda k_m(\vec{p},\lambda) \to k_m(\vec{p},\lambda)$.

[22] Choosing the current density and evaluating the charge density later is close to the suggestion made by Professor J. B. Keller.

[23] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941), p. 330ff. A rather complete discussion of group and phase velocity is given for one-dimensional propagation.

[24] H. E. Moses and A. F Quesada, J. Math. Phys. **15**, 748 (1974).

[25] The four-vector x^μ is not quantized because space and time cannot be quantized in the same way.

[26] This is often the case in experimental settings. One could, however, consider any velocity including high velocities encountered in astronomy and particle accelerators using the results of Ref. 10.

[27] This result suggests the possibility of generating transverse waves from longitudinal fields by launching the longitudinal fields in a moving frame of reference. We may study this matter more fully later.

[28] H. E. Moses, Ann. Phys. (Leipzig) **41**, 166 (1967). They are the Jacob–Wick functions in a notation that emphasizes their role as generalizations of the usual spherical harmonics.
[29] We use the notation of A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University, Princeton, 1960) for $Y_{j,\mu}$.
[30] H. E. Moses and A. F. Quesada, Arch. Ration. Mech. Anal. **50**, 194, (1971).
[31] See, e.g., H. E. Moses, Phys. Rev. A **22**, 2069 (1980).
[32] Within unitary transformations.
[33] Of course, the usual *caveats* apply with respect to the accuracy of numerical computations.

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Group averaging in the (p,q) oscillator representation of $SL(2,\mathbb{R})$

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We investigate refined algebraic quantization with group averaging in a finite-dimensional constrained Hamiltonian system that provides a simplified model of general relativity. The classical theory has gauge group $SL(2,\mathbb{R})$ and a distinguished $\mathfrak{o}(p,q)$ observable algebra. The gauge group of the quantum theory is the double cover of $SL(2,\mathbb{R})$, and its representation on the auxiliary Hilbert space is isomorphic to the (p,q) oscillator representation. When $p\geqslant 2$, $q\geqslant 2$ and $p+q\equiv 0 \pmod 2$, we obtain a physical Hilbert space with a nontrivial representation of the $\mathfrak{o}(p,q)$ quantum observable algebra. For $p=q=1$, the system provides the first example known to us where group averaging converges to an indefinite sesquilinear form. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1689001]

I. INTRODUCTION

In quantization of constrained systems, an elegant proposal to obtain a physical inner product is to average unconstrained quantum states in an auxiliary Hilbert space over the gauge group.[1–13] When the averaging is formulated within refined algebraic quantization[4,8,12] and converges in a sufficiently strong sense, it provides either the unique rigging map, and hence the unique inner product on the states that satisfy the constraints, or a proof that the system does not admit a rigging map.[8] Given the equivalence of refined algebraic quantization to a wide class of methods of choosing the physical inner product,[13,14] group averaging thus provides considerable control over the quantization.

When the gauge group is compact, the averaging necessarily converges. For a noncompact gauge group the averaging need not converge on all of the auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ but may still converge on a suitable dense linear subspace Φ, and this is sufficient for recovering the physical Hilbert space $\mathcal{H}_{\text{RAQ}}$. The choice of the test space Φ thus has a mathematical role in ensuring convergence, but it also has a deep physical role in that Φ determines the algebra of operators represented on $\mathcal{H}_{\text{RAQ}}$.[8,14] While quantization with group averaging can be carried out without the explicit construction of any physical observables, in concrete examples one may wish to choose Φ so that certain explicitly known physical observables of interest are contained in the algebra represented on $\mathcal{H}_{\text{RAQ}}$.

In this paper we study a quantum mechanical system whose constraints mimic the Hamiltonian structure of general relativity.[15] The constraint set consists of two ''Hamiltonian''-type constraints, quadratic in the momenta, and one ''momentum''-type constraint, linear in the momenta, and the classical gauge group generated by these constraints is $SL(2,\mathbb{R})$. The unreduced phase space is $T^*\mathbb{R}^{p+q}\simeq\mathbb{R}^{2(p+q)}$, where $p\geqslant 1$ and $q\geqslant 1$. The system was introduced by Montesinos, Rovelli and Thiemann with $p=q=2$,[16] and its quantization with $p=q=2$ was studied in Refs. 10 and 16–18 within Ashtekar's algebraic quantization,[19,20] in Ref. 21 within algebraic constraint quantization,[22,23] in Refs. 10 and 24–26 within group theoretic quantization,[27,28] and in Ref. 10 within refined algebraic quantization with group averaging.[4,8] All these quantizations

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relied in one way or another on a distinguished classical $\mathfrak{o}(2,2)$ observable algebra, constructing a quantum theory in which these observables are promoted into quantum operators. Within group averaging,[10] it was in particular found that a judicious choice for the test space is necessary to achieve both convergence of the averaging and the inclusion of the $\mathfrak{o}(2,2)$ observables in the physical operator algebra.

For $p>2$ and $q=2$, the system has been studied in the context of a ''two-time'' physical interpretation in Refs. 29–32. The case $p=q=2$ is currently being studied[33] within the master constraint program.[34] Related systems with $\mathrm{SL}(2,\mathbb{R})$ gauge invariance have been studied in Refs. 35–37.

We wish to quantize this system with group averaging for general p and q, using test states built from eigenstates of the harmonic oscillator Hamiltonians that arise in the oscillator representation of $\mathrm{SL}(2,\mathbb{R})$.[38] When $p\geqslant 2$, $q\geqslant 2$ and $p+q\equiv 0 \pmod 2$, we obtain a quantum theory in which the classical $\mathfrak{o}(p,q)$ observables are promoted into a nontrivially represented operator algebra. When $(p,q)=(1,3)$ or $(3,1)$, we obtain a quantum theory with a one-dimensional physical Hilbert space that is annihilated by all the $\mathfrak{o}(p,q)$ observables. For other values of p and q we recover no physical Hilbert space. In particular, for $p=q=1$ the group averaging converges to an *indefinite* sesquilinear form, in a sense strong enough for the uniqueness theorem of Ref. 8 to imply that the system admits no rigging maps. This is the first example known to us in which group averaging fails to produce a Hilbert space owing to indefiniteness of the would-be inner product.

We show further that all our group averaging quantum theories can be obtained within Ashtekar's algebraic quantization,[19,20] using the $\mathfrak{o}(p,q)$ observables to determine the physical inner product, and we display explicitly the correspondence between the two schemes. We have not gained sufficient control over the $\mathfrak{o}(p,q)$ algebra to ascertain whether algebraic quantization might for some p and q yield also quantum theories not recovered by the group averaging, but we show that this does not happen for $p+q\equiv 1 \pmod 2$, nor does it happen for $p+q\equiv 0 \pmod 2$ if $p\leqslant 3$ and $q\leqslant 3$.

We also give a detailed description of the classical reduced phase space. The reduced phase space contains a symplectic manifold if and only if $p\geqslant 2$ and $q\geqslant 2$. This manifold is separated by the $\mathfrak{o}(p,q)$ observables, and it is connected if and only if $p\geqslant 3$ and $q\geqslant 3$. This suggests that interesting quantum theories should exist only when $p\geqslant 2$ and $q\geqslant 2$, possibly with some subtleties when $\min(p,q)=2$. As outlined above, this agrees with our findings.

The rest of the article is as follows. Section II introduces and analyzes the classical system. Section III discusses algebraic quantization, laying out the task for general p and q and completing it for $\max(p,q)\leqslant 3$. Refined algebraic quantization with group averaging is carried out in Sec. IV for $\min(p,q)\geqslant 3$ and in Sec. V for other values of p and q.

Section VI presents a summary and concluding remarks. Appendix A collects some basic properties of $\mathrm{SL}(2,\mathbb{R})$, and Appendixes B–E contain the proofs of several technical results stated in the main text.

II. CLASSICAL SYSTEM

In this section we analyze a classical constrained system with the unreduced phase space $T^*\mathbb{R}^{p+q}$, where $p\geqslant 1$ and $q\geqslant 1$. The system was introduced for $p=q=2$ in Ref. 16, and our discussion of the gauge transformations and the distinguished $\mathfrak{o}(p,q)$ observables generalizes the observations of Ref. 16 in a straightforward manner. We shall, however, show that the structure of the reduced phase space depends sensitively on p and q.

A. The system

The system is defined by the action

$$S=\int dt\,(\mathbf{p}\cdot\dot{\mathbf{u}}+\boldsymbol{\pi}\cdot\dot{\mathbf{v}}-NH_1-MH_2-\lambda D), \tag{2.1}$$

where $\mathbf{u}$ and $\mathbf{p}$ are real vectors of dimension $p \geqslant 1$, $\mathbf{v}$ and $\boldsymbol{\pi}$ are real vectors of dimension $q \geqslant 1$, and the overdot denotes differentiation with respect to t. $\mathbf{p}$ and $\boldsymbol{\pi}$ are, respectively, the momenta conjugate to $\mathbf{u}$ and $\mathbf{v}$, the symplectic structure is

$$\Omega = \sum_{i=1}^{p} dp_i \wedge du_i + \sum_{j=1}^{q} d\pi_j \wedge dv_j, \tag{2.2}$$

and the phase space is $\Gamma := T^*\mathbb{R}^{p+q} \simeq \mathbb{R}^{2(p+q)}$. N, M and λ are Lagrange multipliers associated with the constraints

$$\begin{aligned} H_1 &:= \tfrac{1}{2}(\mathbf{p}^2 - \mathbf{v}^2), \\ H_2 &:= \tfrac{1}{2}(\boldsymbol{\pi}^2 - \mathbf{u}^2), \\ D &:= \mathbf{u}\cdot\mathbf{p} - \mathbf{v}\cdot\boldsymbol{\pi}. \end{aligned} \tag{2.3}$$

The Poisson algebra of the constraints is the $\mathfrak{sl}(2,\mathbb{R})$ Lie algebra (see Appendix A),

$$\begin{aligned} \{H_1, H_2\} &= D, \\ \{H_1, D\} &= -2H_1, \\ \{H_2, D\} &= 2H_2, \end{aligned} \tag{2.4}$$

and the system is a first class constrained system.[39,40] The finite gauge transformations on Γ generated by the constraints are

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} \mapsto g \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix}, \quad \begin{pmatrix} \boldsymbol{\pi} \\ \mathbf{v} \end{pmatrix} \mapsto g \begin{pmatrix} \boldsymbol{\pi} \\ \mathbf{v} \end{pmatrix}, \tag{2.5}$$

where g is an $\mathrm{SL}(2,\mathbb{R})$ matrix. The gauge group is thus $\mathrm{SL}(2,\mathbb{R})$. As the Hamiltonian is a sum of the constraints, the constraints entirely determine the dynamics.

B. Classical observables

Recall that an observable is a function on Γ whose Poisson brackets with the first class constraints vanish when the first class constraints hold.[40] Consider on Γ the functions $\mathcal{O}_{kj} := x_k \times x_j$, where $x_k = (u_k, p_k)^T$ for $1 \leqslant k \leqslant p$, $x_{p+k} = (\pi_k, v_k)^T$ for $1 \leqslant k \leqslant q$, and the cross stands for the scalar-valued cross product on $\mathbb{R}^2$. As the $\mathrm{SL}(2,\mathbb{R})$ action on $\mathbb{R}^2$ preserves areas, (2.5) shows that $\mathcal{O}_{kj}$ are invariant under the gauge transformations. Hence $\mathcal{O}_{kj}$ are observables. The Poisson algebra of these observables is the $\mathfrak{o}(p,q)$ Lie algebra,

$$\{\mathcal{O}_{ij}, \mathcal{O}_{kl}\} = g_{ik}\mathcal{O}_{jl} - g_{il}\mathcal{O}_{jk} + g_{jl}\mathcal{O}_{ik} - g_{jk}\mathcal{O}_{il}, \tag{2.6}$$

where

$$g_{ik} = \mathrm{diag}(\underbrace{1,\ldots,1}_{p}, \underbrace{-1,\ldots,-1}_{q})_{ik}.$$

The algebra generated by $\{\mathcal{O}_{ij}\}$ is denoted by $\mathcal{A}_{\mathrm{class}}$. The finite transformations that $\mathcal{A}_{\mathrm{class}}$ generates on Γ are

$$\begin{pmatrix} \mathbf{u} \\ \boldsymbol{\pi} \end{pmatrix} \mapsto R \begin{pmatrix} \mathbf{u} \\ \boldsymbol{\pi} \end{pmatrix}, \quad \begin{pmatrix} \mathbf{p} \\ \mathbf{v} \end{pmatrix} \mapsto R \begin{pmatrix} \mathbf{p} \\ \mathbf{v} \end{pmatrix}, \tag{2.8}$$

where R is an $O(p,q)$ matrix, in the connected component $O_c(p,q)$. Note that as none of the above relies on the constraints being satisfied, the $SL(2,\mathbb{R})$ action (2.5) and the $O_c(p,q)$ action (2.8) commute on all of Γ, not just on the subset where the constraints hold.

It will be useful to decompose the basis $\{\mathcal{O}_{ij}\}$ of $\mathcal{A}_{\text{class}}$ as $\mathfrak{o}(p,q)=\mathfrak{o}(p)\oplus\mathfrak{o}(q)\oplus\mathfrak{p}$, where $\mathfrak{p}$ is spanned by the observables transverse to those in the Lie algebra of the maximal compact subgroup $O_c(p)\times O_c(q)$.[41] Explicitly, we write

$$\begin{aligned} A_{ij} &:= \mathcal{O}_{ij} = u_i p_j - u_j p_i, \quad 1\leqslant i\leqslant p,\ 1\leqslant j\leqslant p, \\ B_{ij} &:= \mathcal{O}_{p+i,p+j} = v_i \pi_j - v_j \pi_i, \quad 1\leqslant i\leqslant q,\ 1\leqslant j\leqslant q, \\ C_{ij} &:= \mathcal{O}_{i,p+j} = u_i v_j - p_i \pi_j, \quad 1\leqslant i\leqslant p,\ 1\leqslant j\leqslant q, \end{aligned} \tag{2.9}$$

where $A_{ij}\in\mathfrak{o}(p)$, $B_{ij}\in\mathfrak{o}(q)$ and $C_{ij}\in\mathfrak{p}$.

Other observables of interest in $\mathcal{A}_{\text{class}}$ are the Casimir elements of the universal enveloping algebra of $\mathfrak{o}(p,q)$.[42] We consider only the quadratic Casimir observable,

$$\mathcal{C} := \frac{1}{2}\sum_{ijkl} g_{ij}g_{kl}\mathcal{O}_{ik}\mathcal{O}_{jl} = \sum_{i<j}(A_{ij})^2 + \sum_{i<j}(B_{ij})^2 - \sum_{i,j}(C_{ij})^2 = -4H_1H_2 - D^2, \tag{2.10}$$

where the last equality follows by direct computation. When the constraints hold, $\mathcal{C}$ thus vanishes.

C. Reduced phase space

Let $\overline{\Gamma}$ be the subset of Γ where the constraints hold. The reduced phase space, denoted by $\mathcal{M}$, is the quotient of $\overline{\Gamma}$ under the gauge action (2.5). As the Hamiltonian is a linear combination of the constraints, there is no dynamics on $\mathcal{M}$, and $\mathcal{M}$ can be identified with the space of classical solutions. As the functions in $\mathcal{A}_{\text{class}}$ are gauge invariant, they project to functions on $\mathcal{M}$: We use for these functions the same symbols.

For $p=q=2$, the generic sectors of $\mathcal{M}$ were found in Refs. 16 and 21 and the global properties of $\mathcal{M}$ were exhibited in Ref. 10. We now analyze $\mathcal{M}$ for general $p\geqslant 1$ and $q\geqslant 1$.

Γ is clearly connected. Hence also $\mathcal{M}$ is connected.

To proceed, we decompose $\overline{\Gamma}$ into three subsets. Let $\overline{\Gamma}_0=\{\mathsf{q}_0\}$, where q_0 is the origin of Γ, $\mathbf{u}=\mathbf{p}=\mathbf{0}=\mathbf{v}=\boldsymbol{\pi}$. Let $\overline{\Gamma}_{\text{ex}}$ contain all other points of $\overline{\Gamma}$ at which at least one of the pairs $(\mathbf{u},\mathbf{p})$ and $(\mathbf{v},\boldsymbol{\pi})$ is linearly dependent. Finally, let $\overline{\Gamma}_{\text{reg}}$ contain the rest of $\overline{\Gamma}$. We refer to $\overline{\Gamma}_{\text{ex}}$ and $\overline{\Gamma}_{\text{reg}}$ as respectively the "exceptional" and "regular" parts of $\overline{\Gamma}$. We show in Appendix B that the gradients of the constraints are all vanishing on $\overline{\Gamma}_0$, linearly dependent but not all vanishing on $\overline{\Gamma}_{\text{ex}}$, and linearly independent on $\overline{\Gamma}_{\text{reg}}$. $\overline{\Gamma}_0$ and $\overline{\Gamma}_{\text{ex}}$ are nonempty for all p and q, while $\overline{\Gamma}_{\text{reg}}$ is nonempty if and only if $p\geqslant 2$ and $q\geqslant 2$.

As $\overline{\Gamma}_0$, $\overline{\Gamma}_{\text{ex}}$ and $\overline{\Gamma}_{\text{reg}}$ are preserved by the gauge transformations, they project onto disjoint subsets of $\mathcal{M}$. We denote these sets respectively by $\mathcal{M}_0$, $\mathcal{M}_{\text{ex}}$ and $\mathcal{M}_{\text{reg}}$ and analyze each in turn.

1. $\mathcal{M}_0$

$\mathcal{M}_0$ contains only one point, the projection of q_0. All observables in $\mathcal{A}_{\text{class}}$ vanish on $\mathcal{M}_0$.

2. $\mathcal{M}_{\text{ex}}$

As $\mathsf{q}_0\notin\overline{\Gamma}_{\text{ex}}$, the constraints $H_1=0=H_2$ show that all points in $\overline{\Gamma}_{\text{ex}}$ have $(\mathbf{u},\mathbf{p})\neq(\mathbf{0},\mathbf{0})$ and $(\mathbf{v},\boldsymbol{\pi})\neq(\mathbf{0},\mathbf{0})$. Given a point at which the pair $(\mathbf{u},\mathbf{p})$ is linearly dependent, there thus exists a gauge-equivalent point with $\mathbf{u}=\mathbf{0}$ and $\mathbf{p}^2=1$, at which the constraints imply $\boldsymbol{\pi}=\mathbf{0}$ and $\mathbf{v}^2=1$. Given a point at which the pair $(\mathbf{v},\boldsymbol{\pi})$ is linearly dependent, a similar argument shows that there exists a gauge-equivalent point at which $\boldsymbol{\pi}=\mathbf{0}$, $\mathbf{v}^2=1$, $\mathbf{u}=\mathbf{0}$ and $\mathbf{p}^2=1$. Thus, each point in $\overline{\Gamma}_{\text{ex}}$ is gauge-equivalent to a point that satisfies

$$\mathbf{v}^2=\mathbf{p}^2=1,\ \mathbf{u}=\mathbf{0}=\boldsymbol{\pi}. \tag{2.11}$$

It follows that both the pair $(\mathbf{u},\ \mathbf{p})$ and the pair $(\mathbf{v},\ \boldsymbol{\pi})$ are linearly dependent on $\overline{\Gamma}$.

The gauge transformations that preserve the set (2.11) act on it either trivially or by

$$(\mathbf{v},\mathbf{p})\mapsto(-\mathbf{v},-\mathbf{p}). \tag{2.12}$$

$\mathcal{M}_{\rm ex}$ can therefore be represented as the quotient of the set (2.11), with topology $S^{p-1}\times S^{q-1}$, under the $\mathbb{Z}_2$ action generated by (2.12). If in particular $p=1$ (respectively $q=1$), $\mathcal{M}_{\rm ex}$ has topology S^{q-1} (S^{p-1}). If $p=q=1$, $\mathcal{M}_{\rm ex}$ contains just two points.

Other representations of $\mathcal{M}_{\rm ex}$ are obtained by replacing in (2.11) the first equations by $\mathbf{v}^2=\mathbf{p}^2=r$, where r is an arbitrary prescribed positive number. This shows that in the topology of $\mathcal{M}$ induced from Γ, every open set that includes $\mathcal{M}_0$ includes also $\mathcal{M}_{\rm ex}$.

Equations (2.9) and (2.11) show that all observables in $\mathcal{A}_{\rm class}$ vanish on $\mathcal{M}_{\rm ex}$. Equations (2.2) and (2.11) show that the projection of the symplectic form Ω vanishes on $\mathcal{M}_{\rm ex}$. We refer to $\mathcal{M}_{\rm ex}$ as the ''exceptional'' part of $\mathcal{M}$.

3. $\mathcal{M}_{\rm reg}$

When $p=1$ or $q=1$ (or both), $\overline{\Gamma}_{\rm reg}$ and hence also $\mathcal{M}_{\rm reg}$ are empty. We now assume $p\geqslant 2$ and $q\geqslant 2$.

We show in Appendix B that the gradients of the constraints are linearly independent on $\overline{\Gamma}_{\rm reg}$. It follows (Ref. 40, Sec. 1.1.2 and Appendix 2A) that $\mathcal{M}_{\rm reg}$ is a manifold of dimension $2p+2q-6$ with a symplectic form induced from Γ. We refer to $\mathcal{M}_{\rm reg}$ as the ''regular'' part of $\mathcal{M}$.

Given a point in $\Gamma_{\rm reg}$, the linear independence of the pair $(\mathbf{u},\ \mathbf{p})$ implies that there exists a gauge-equivalent point at which $\mathbf{u}\cdot\mathbf{p}=0$ and $\mathbf{u}^2=\underline{\mathbf{p}}^2>0$. The constraints imply that at this point $\mathbf{v}\cdot\boldsymbol{\pi}=0$, $\mathbf{v}^2=\mathbf{p}^2$ and $\boldsymbol{\pi}^2=\mathbf{u}^2$. Hence each point in $\Gamma_{\rm reg}$ is gauge-equivalent to a point that satisfies

$$\mathbf{u}^2=\mathbf{p}^2=\mathbf{v}^2=\boldsymbol{\pi}^2>0,\ \mathbf{u}\cdot\mathbf{p}=\mathbf{v}\cdot\boldsymbol{\pi}=0. \tag{2.13}$$

The gauge transformations that preserve the set (2.13) are (2.5) with

$$g=\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}, \tag{2.14}$$

where $0\leqslant\theta<2\pi$. It follows that $\mathcal{M}_{\rm reg}$ can be represented as the quotient of the set (2.13) under the $U(1)$ action given by (2.5) and (2.14).

We show in Appendix C that $\mathcal{A}_{\rm class}$ separates $\mathcal{M}_{\rm reg}$: Given two distinct points in $\mathcal{M}_{\rm reg}$, there exist functions in $\mathcal{A}_{\rm class}$ that take distinct values at the two points.

For $p=q=2$, $\mathcal{M}_{\rm reg}$ consists of four connected components,[10,16,21] which can be pairwise joined into two connected symplectic manifolds by adding certain points from $\mathcal{M}_{\rm ex}$.[10]

Suppose $p=2$ and $q>2$. Within each gauge equivalence class in (2.13), there is a unique representative at which $p_1=0$ and $u_1>0$. It follows that at this point $p_2\neq 0$ and $u_2=0$. A gauge transformation by $g=\mathrm{diag}(|p_2|,|p_2|^{-1})$ brings this point to

$$\mathbf{v}^2=1,\ \mathbf{v}\cdot\boldsymbol{\pi}=0,\ \boldsymbol{\pi}^2>0,\ \mathbf{p}=(0,\epsilon),\ \mathbf{u}=(|\boldsymbol{\pi}|,0), \tag{2.15}$$

where $\epsilon=\pm 1$. For each ϵ, the set (2.15) is recognized as the cotangent bundle over S^{q-1}, with the zero fibers omitted. Hence $\mathcal{M}_{\rm reg}$ consists of two connected components, given by (2.15) with the respective values of ϵ. Equations (2.2) and (2.15) show that the symplectic structure of this cotangent bundle description is precisely the symplectic structure induced from Γ. For each ϵ, it is possible to include the zero fibers by allowing $\boldsymbol{\pi}^2=0$ in (2.15); this means adding from $\mathcal{M}_{\rm ex}$ the subset represented uniquely by (2.11) with $\mathbf{p}=(0,\epsilon)$ and $\boldsymbol{\pi}=\mathbf{0}$. Note that because of the identification (2.12) in (2.11), this subset of $\mathcal{M}_{\rm ex}$ is the same for both signs of ϵ. The mechanism of

pairwise smoothly joining the disconnected sectors for $q=2$ (Ref. 10) is not available now because the fibers without origin are disconnected for $q=2$ but connected for $q>2$.

The case $q=2$ and $p>2$ is isomorphic to $p=2$ and $q>2$.

When $p>2$ and $q>2$, $\mathcal{M}_{\mathrm{reg}}$ is connected. We have not found a simpler description of the global properties in this case. Convenient local gauge fixings are introduced in Appendix C.

III. ALGEBRAIC QUANTIZATION

In this section we apply the algebraic quantization framework of Ref. 19, adopting $\mathcal{A}_{\mathrm{class}}$ as the classical observable algebra whose complex conjugation relations are promoted into adjointness relations. Seeking solutions to the quantum constraints by separation of variables, we show in Sec. III A that necessary conditions for obtaining a quantum theory with a nontrivially represented observable algebra are $p\geqslant 2$, $q\geqslant 2$ and $p+q\equiv 0 \pmod 2$. The case $p=q=2$ was analyzed in Refs. 10 and 16. In Sec. III B we complete the quantization for $p=q=3$.

Detailed expositions of algebraic quantization can be found in Refs. 19 and 20.

A. Setup for $p\geqslant 1$ and $q\geqslant 1$

We take the elementary "position" and "momentum" operators to act on smooth functions $\Psi(\mathbf{u},\mathbf{v})$ as

$$\begin{aligned} &\hat{\mathbf{u}}\Psi(\mathbf{u},\mathbf{v})=\mathbf{u}\Psi(\mathbf{u},\mathbf{v}), \quad \hat{\mathbf{p}}\,\Psi(\mathbf{u},\mathbf{v})=-i\boldsymbol{\nabla}_u\Psi(\mathbf{u},\mathbf{v}),\\ &\hat{\mathbf{v}}\,\Psi(\mathbf{u},\mathbf{v})=\mathbf{v}\Psi(\mathbf{u},\mathbf{v}), \quad \hat{\boldsymbol{\pi}}\Psi(\mathbf{u},\mathbf{v})=-i\boldsymbol{\nabla}_v\Psi(\mathbf{u},\mathbf{v}), \end{aligned} \tag{3.1}$$

so that $[\hat{u}_k,\hat{p}_j]=i\delta_{kj}$ and $[\hat{v}_k,\hat{\pi}_j]=i\delta_{kj}$. Inserting these operators into the classical constraints (2.3) and making a judicious ordering choice, we obtain the quantum constraints

$$\hat{H}_1 := -\tfrac{1}{2}(\Delta_u+\mathbf{v}^2), \tag{3.2a}$$

$$\hat{H}_2 := -\tfrac{1}{2}(\Delta_v+\mathbf{u}^2), \tag{3.2b}$$

$$\hat{D} := -i\left(\mathbf{u}\cdot\boldsymbol{\nabla}_u-\mathbf{v}\cdot\boldsymbol{\nabla}_v+\frac{p-q}{2}\right), \tag{3.2c}$$

where Δ_u (respectively, Δ_v) stands for the Laplacian in $\mathbf{u}$ ($\mathbf{v}$). The nonderivative term in $\hat{D}$ is needed to make the commutators close as the $\mathfrak{sl}(2,\mathbb{R})$ Lie algebra,

$$\begin{aligned} &[\hat{H}_1,\hat{H}_2]=i\hat{D},\\ &[\hat{H}_1,\hat{D}]=-2i\hat{H}_1,\\ &[\hat{H}_2,\hat{D}]=+2i\hat{H}_2. \end{aligned} \tag{3.3}$$

We define the quantum observables $\hat{\mathcal{O}}_{ij}$ by substituting the elementary quantum operators (3.1) in the expressions of the classical observables $\mathcal{O}_{ij}$. These quantum observables commute with the quantum constraints (3.2), and their commutators form the $\mathfrak{o}(p,q)$ Lie algebra, obtained by hatting (2.6) and multiplying the right-hand side by i. As $\mathcal{O}_{ij}$ are real, we introduce on the algebra generated by $\{\hat{\mathcal{O}}_{ij}\}$ an antilinear involution by $\hat{\mathcal{O}}_{ij}^{\star}=\hat{\mathcal{O}}_{ij}$. We denote the resulting star-algebra of quantum observables by $\mathcal{A}_{\mathrm{phys}}^{(\star)}$.

Following (2.9), we decompose the basis of $\mathcal{A}_{\mathrm{phys}}^{(\star)}$ as

$$\hat{A}_{ij} := \hat{\mathcal{O}}_{ij} = -i(u_i \partial_{u_j} - u_j \partial_{u_i}), \quad 1 \leqslant i \leqslant p,\ 1 \leqslant j \leqslant p;$$

$$\hat{B}_{ij} := \hat{\mathcal{O}}_{p+i,p+j} = -i(v_i \partial_{v_j} - v_j \partial_{v_i}), \quad 1 \leqslant i \leqslant q,\ 1 \leqslant j \leqslant q; \tag{3.4}$$

$$\hat{C}_{ij} := \hat{\mathcal{O}}_{i,p+j} = u_i v_j + \partial_{u_i} \partial_{v_j}, \quad 1 \leqslant i \leqslant p,\ 1 \leqslant j \leqslant q.$$

The quantum quadratic Casimir observable is

$$\hat{\mathcal{C}} := \frac{1}{2} \sum_{ijkl} g_{ij} g_{kl} \hat{\mathcal{O}}_{ik} \hat{\mathcal{O}}_{jl} = \sum_{i<j} (\hat{A}_{ij})^2 + \sum_{i<j} (\hat{B}_{ij})^2 - \sum_{i,j} (\hat{C}_{ij})^2$$

$$= -2(\hat{H}_1 \hat{H}_2 + \hat{H}_2 \hat{H}_1) - \hat{D}^2 - \frac{1}{4}(p+q)(p+q-4), \tag{3.5}$$

where the last equality follows by direct computation. In contrast to the classical Casimir (2.10), $\hat{\mathcal{C}}$ vanishes on states annihilated by the constraints only for $p+q=4$.

We seek states annihilated by the constraints,

$$\hat{H}_1 \Psi(\mathbf{u},\mathbf{v}) = 0,\ \hat{H}_2 \Psi(\mathbf{u},\mathbf{v}) = 0,\ \hat{D} \Psi(\mathbf{u},\mathbf{v}) = 0, \tag{3.6}$$

by separation of variables. If $p \geqslant 2$ and $q \geqslant 2$, we make the ansatz

$$\Psi(\mathbf{u},\mathbf{v}) = \psi(u,v) Y_{lk_u}(\theta^{(u)}) Y_{jk_v}(\theta^{(v)}), \tag{3.7}$$

where $u := |\mathbf{u}|$, $v := |\mathbf{v}|$ and $Y_{lk_u}(\theta^{(u)})$ [respectively $Y_{jk_v}(\theta^{(v)})$] are the spherical harmonics on unit S^{p-1} in $\mathbf{u}$ (S^{q-1} in $\mathbf{v}$).[43,44] Here $\theta^{(u)}$ denotes the coordinates on S^{p-1}, the index l ranges over non-negative integers, the eigenvalue of the scalar Laplacian on S^{p-1} is $-l(l+p-2)$, the index k_u labels the degeneracy for each l, and similarly for the quantities appearing in $Y_{jk_v}(\theta^{(v)})$. We extend the ansatz (3.7) to $p=1$, in which case $\theta^{(u)} := u_1/u \in \{1,-1\}$, $l \in \{0,1\}$, the index k_u takes only a single value and can be dropped, and the spherical harmonics are $Y_l(\theta^{(u)}) := (\theta^{(u)})^l/\sqrt{2}$, and similarly for $q=1$. For all $p \geqslant 1$ and $q \geqslant 1$, Eqs. (3.6) then reduce to

$$\left[\frac{1}{u^{p-3}} \frac{\partial}{\partial u} \left(u^{p-1} \frac{\partial}{\partial u} \right) - l(l+p-2) + u^2 v^2 \right] \psi(u,v) = 0, \tag{3.8a}$$

$$\left[\frac{1}{v^{q-3}} \frac{\partial}{\partial v} \left(v^{q-1} \frac{\partial}{\partial v} \right) - j(j+q-2) + u^2 v^2 \right] \psi(u,v) = 0, \tag{3.8b}$$

$$\left(u \frac{\partial}{\partial u} - v \frac{\partial}{\partial v} + \frac{p-q}{2} \right) \psi(u,v) = 0. \tag{3.8c}$$

The general solution to (3.8c) is $\psi(u,v) = u^{(2-p)/2} v^{(2-q)/2} \chi(\zeta)$, where $\zeta := uv$. Substituting this in (3.8a) and (3.8b), we find that the indices satisfy

$$2l + p = 2j + q \tag{3.9}$$

and $\chi(\zeta)$ satisfies the Bessel equation of order $l + (p-2)/2$.[43]

Equation (3.9) shows that solutions exist only when $p+q \equiv 0 \pmod 2$. If $p=1$ or $q=1$, inspection of (3.9) further shows that solutions exist only when $(p,q) = (1,1)$, (1,3) or (3,1). Let us consider these exceptional cases first.

When $p=q=1$, the linearly independent solutions are $\Psi_{\pm}:=\exp(\pm iu_1v_1)$, $\mathcal{A}^{(\star)}_{\text{phys}}$ is generated by the single observable $\hat{C}_{11}$, and $\hat{C}_{11}\Psi_{\pm}=\pm i\Psi_{\pm}$. The representation of $\mathcal{A}^{(\star)}_{\text{phys}}$ on $\mathcal{V}_{\text{phys}}:=\text{span}\{\Psi_{\pm}\}$ is irreducible, but the only sesquilinear forms in which $\hat{C}_{11}$ is symmetric have indefinite signature.

When $p=1$ and $q=3$, the only (smooth) solution is $\Psi_0:=v^{-1}\sin(u_1v)$, which is annihilated by all operators in $\mathcal{A}^{(\star)}_{\text{phys}}$. Promoting $\text{span}\{\Psi_0\}$ into a one-dimensional Hilbert space gives thus a quantum theory in which $\mathcal{A}^{(\star)}_{\text{phys}}$ is represented trivially. The situation for $p=3$ and $q=1$ is similar.

We therefore see that necessary conditions for obtaining a quantum theory with a nontrivial representation of $\mathcal{A}^{(\star)}_{\text{phys}}$ are $p\geqslant 2$, $q\geqslant 2$ and $p+q\equiv 0 \pmod 2$. When these conditions hold, we have found for the quantum constraints the linearly independent solutions

$$\Psi_{ljk_uk_v}:=\delta_{2l+p,2j+q}\,u^{(2-p)/2}v^{(2-q)/2}J_{l+(p-2)/2}(uv)Y_{lk_u}(\theta^{(u)})Y_{jk_v}(\theta^{(v)}), \tag{3.10}$$

where $J_{l+(p-2)/2}$ is the Bessel function of the first kind.[43] The Bessel function of the second kind has been excluded to make $\Psi_{ljk_uk_v}$ smooth at $uv=0$. The motivation for this exclusion may be debatable within algebraic quantization, but we shall see that it is precisely the smooth solutions (3.10) that will emerge from group averaging in Secs. IV and V.

To proceed, we would need to examine the representation of $\mathcal{A}^{(\star)}_{\text{phys}}$ on $\text{span}\{\Psi_{ljk_uk_v}\}$. The representation of the $\mathfrak{o}(p)\oplus\mathfrak{o}(q)$ subalgebra is given directly by its representation on the spherical harmonics,[43,44] but the observables $\hat{C}_{ij}$ mix the states in a more complicated way. The special case $p=q=2$ was analyzed in Refs. 10 and 16. In Sec. III B we address the special case $p=q=3$.

B. Completion for $p=q=3$

When $p=q=3$, the states (3.10) can be written as

$$\Psi_{lmn}=j_l(uv)Y_{lm}(\theta^{(u)})Y_{ln}(\theta^{(v)}), \tag{3.11}$$

where l ranges over non-negative integers, $j_l(uv)$ is the spherical Bessel function of the first kind of order l,[43] m and n are integers satisfying $|m|\leqslant l$ and $|n|\leqslant l$ and the Y's are the usual spherical harmonics on S^2.[43] We write $\mathcal{V}_{\text{phys}}:=\text{span}\{\Psi_{lmn}\}$.

We introduce for $\mathcal{A}^{(\star)}_{\text{phys}}$ the basis

$$\begin{gathered}
\hat{L}_3:=\hat{A}_{12},\\
\hat{L}_{\pm}:=\hat{A}_{23}\pm i\hat{A}_{31},\\
\hat{J}_3:=\hat{B}_{12},\\
\hat{J}_{\pm}:=\hat{B}_{23}\pm i\hat{B}_{31},\\
\hat{C}_0:=\hat{C}_{33},\\
\hat{C}_1^{\pm}:=\hat{C}_{31}\pm i\hat{C}_{32},\\
\hat{C}_2^{\pm}:=\hat{C}_{13}\pm i\hat{C}_{23},\\
\hat{C}_3^{\pm}:=(\hat{C}_{11}+\hat{C}_{22})\pm i(\hat{C}_{21}-\hat{C}_{12}),\\
\hat{C}_4^{\pm}:=(\hat{C}_{11}-\hat{C}_{22})\pm i(\hat{C}_{21}+\hat{C}_{12}).
\end{gathered} \tag{3.12}$$

TABLE I. The action of $\mathcal{A}_{\text{phys}}^{(\star)}$ on $\mathcal{V}_{\text{phys}}$. Whenever the indices of a Ψ on the right-hand side go outside the allowed range, the numerical coefficient vanishes and the term is understood as zero.

$$
\begin{aligned}
\hat{L}_3\Psi_{lmn} &= m\Psi_{lmn}\\
\hat{J}_3\Psi_{lmn} &= n\Psi_{lmn}\\
\hat{L}_\pm\Psi_{lmn} &= \sqrt{(l\pm m+1)(l\mp m)}\,\Psi_{l,m\pm1,n}\\
\hat{J}_\pm\Psi_{lmn} &= \sqrt{(l\pm n+1)(l\mp n)}\,\Psi_{l,m,n\pm1}\\
\hat{C}_0\Psi_{lmn} &= \frac{\sqrt{(l-m+1)(l+m+1)(l-n+1)(l+n+1)}}{2l+3}\Psi_{l+1,m,n}\\
&\quad+\frac{\sqrt{(l-m)(l+m)(l-n)(l+n)}}{2l-1}\Psi_{l-1,m,n}\\
\hat{C}_1^\pm\Psi_{lmn} &= \mp\frac{\sqrt{(l-m+1)(l+m+1)(l\pm n+1)(l\pm n+2)}}{2l+3}\Psi_{l+1,m,n\pm1}\\
&\quad\pm\frac{\sqrt{(l-m)(l+m)(l\mp n)(l\mp n-1)}}{2l-1}\Psi_{l-1,m,n\pm1}\\
\hat{C}_2^\pm\Psi_{lmn} &= \mp\frac{\sqrt{(l\pm m+1)(l\pm m+2)(l-n+1)(l+n+1)}}{2l+3}\Psi_{l+1,m\pm1,n}\\
&\quad\pm\frac{\sqrt{(l\mp m)(l\mp m-1)(l-n)(l+n)}}{2l-1}\Psi_{l-1,m\pm1,n}\\
\hat{C}_3^\pm\Psi_{lmn} &= -\frac{\sqrt{(l\pm m+1)(l\pm m+2)(l\mp n+1)(l\mp n+2)}}{2l+3}\Psi_{l+1,m\pm1,n\mp1}\\
&\quad-\frac{\sqrt{(l\mp m)(l\mp m-1)(l\pm n)(l\pm n-1)}}{2l-1}\Psi_{l-1,m\pm1,n\mp1}\\
\hat{C}_4^\pm\Psi_{lmn} &= +\frac{\sqrt{(l\pm m+1)(l\pm m+2)(l\pm n+1)(l\pm n+2)}}{2l+3}\Psi_{l+1,m\pm1,n\pm1}\\
&\quad+\frac{\sqrt{(l\mp m)(l\mp m-1)(l\mp n)(l\mp n-1)}}{2l-1}\Psi_{l-1,m\pm1,n\pm1}
\end{aligned}
$$

Note that the $\hat{L}$'s (respectively, $\hat{J}$'s) are a standard raising and lowering operator basis for the $\mathfrak{o}(3)$ algebra in $\mathbf{u}$ ($\mathbf{v}$).[43] The action of the basis (3.12) on $\mathcal{V}_{\text{phys}}$ can be computed from standard properties of the spherical harmonics and spherical Bessel functions[43,45] and is displayed in Table I. It follows that $\mathcal{V}_{\text{phys}}$ is invariant under $\mathcal{A}_{\text{phys}}^{(\star)}$. We show in Appendix D that the representation of $\mathcal{A}_{\text{phys}}^{(\star)}$ on $\mathcal{V}_{\text{phys}}$ is irreducible.

The star-relations of the basis (3.12) read

$$
\begin{gathered}
(\hat{L}_3)^\star=\hat{L}_3,\\
(\hat{L}_\pm)^\star=\hat{L}_\mp,\\
(\hat{J}_3)^\star=\hat{J}_3,\\
(\hat{J}_\pm)^\star=\hat{J}_\mp,\\
(\hat{C}_0)^\star=\hat{C}_0,\\
(\hat{C}_k^\pm)^\star=\hat{C}_k^\mp,\ 1\leqslant k\leqslant 4.
\end{gathered}
\tag{3.13}
$$

From Table I it follows by direct computation that these star-relations coincide with the adjoint relations in the inner product

$$(\Psi_{lmn},\Psi_{l'm'n'})_{\mathrm{AQ}} := (2l+1)\,\delta_{ll'}\delta_{mm'}\delta_{nn'}. \tag{3.14}$$

We show in Appendix D that the only inner products on $\mathcal{V}_{\mathrm{phys}}$ with this property are multiples of (3.14).

The physical Hilbert space is the Cauchy completion of $\mathcal{V}_{\mathrm{phys}}$ in the inner product (3.14). It carries by construction a densely defined representation of $\mathcal{A}^{(\star)}_{\mathrm{phys}}$ in which the quadratic $\mathfrak{o}(3,3)$ Casimir (3.5) has the value -3.

IV. REFINED ALGEBRAIC QUANTIZATION FOR $p\geqslant 3$, $q\geqslant 3$

We now turn to refined algebraic quantization. In this section we take $p\geqslant 3$ and $q\geqslant 3$. The remaining values of p and q will be treated in Sec. V.

We employ refined algebraic quantization with group averaging as formulated in Ref. 8. A review can be found in Ref. 12 and an outline adapted to the present situation in Ref. 10.

A. Auxiliary Hilbert space and representation of the gauge group

We introduce the auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}}\simeq L^2(\mathbb{R}^{p+q})$ of square integrable functions $\Psi(\mathbf{u},\mathbf{v})$ in the inner product

$$(\Psi_1,\Psi_2)_{\mathrm{aux}} := \int d^p\mathbf{u}\, d^q\mathbf{v}\, \overline{\Psi_1}\Psi_2, \tag{4.1}$$

where the overline denotes complex conjugation. The quantum constraints (3.2) are essentially self-adjoint on $\mathcal{H}_{\mathrm{aux}}$, and exponentiating $-i$ times their algebra yields a unitary representation of the universal covering group of $\mathrm{SL}(2,\mathbb{R})$. Denoting this representation by U, the group elements in the Iwasawa decomposition (A3) are represented by

$$U(\exp(\mu e^-)) = \exp(-i\mu\hat{H}_2), \tag{4.2a}$$

$$U(\exp(\lambda h)) = \exp(-i\lambda\hat{D}), \tag{4.2b}$$

$$U(\exp[\theta(e^+-e^-)]) = \exp(-i\theta(\hat{H}_1-\hat{H}_2)). \tag{4.2c}$$

The operators in (4.2a) and (4.2b) act as

$$[\exp(-i\mu\hat{H}_2)\Psi](\mathbf{u},\mathbf{v}) = \int \frac{d^q\mathbf{v}'}{(2\pi i\mu)^{q/2}} \exp\left[\frac{i}{2}\left(\frac{(\mathbf{v}-\mathbf{v}')^2}{\mu}+\mu\mathbf{u}^2\right)\right]\Psi(\mathbf{u},\mathbf{v}'), \tag{4.3a}$$

$$[\exp(-i\lambda\hat{D})\Psi](\mathbf{u},\mathbf{v}) = \exp\left[\frac{\lambda}{2}(q-p)\right]\Psi(e^{-\lambda}\mathbf{u},e^{\lambda}\mathbf{v}). \tag{4.3b}$$

In (4.2c) we have $\hat{H}_1-\hat{H}_2=\hat{H}^{\mathrm{sho}}_{\mathbf{u}}-\hat{H}^{\mathrm{sho}}_{\mathbf{v}}$, where $\hat{H}^{\mathrm{sho}}_{\mathbf{u}}$ and $\hat{H}^{\mathrm{sho}}_{\mathbf{v}}$ are the harmonic oscillator Hamiltonians of unit mass and angular frequency in respectively $\mathbf{u}$ and $\mathbf{v}$. It follows that $U(\exp[\theta(e^+-e^-)])$ is periodic in θ with period 2π when $p+q\equiv 0 \pmod 2$ and with period 4π when $p+q\equiv 1 \pmod 2$. This means that the gauge group is $\mathrm{SL}(2,\mathbb{R})$ when $p+q\equiv 0 \pmod 2$ and the double cover of $\mathrm{SL}(2,\mathbb{R})$ when $p+q\equiv 1 \pmod 2$. U is isomorphic to the (p,q) oscillator representation of the double cover of $\mathrm{SL}(2,\mathbb{R})$[38] via the Fourier transform in $\mathbf{v}$.

B. Test space

The next step is to introduce a linear space of test states in $\mathcal{H}_{\mathrm{aux}}$. The harmonic oscillator Hamiltonians in $U(\exp[\theta(e^+-e^-)])$ suggest that we make use of the harmonic oscillator eigenstates in $\mathbf{u}$ and $\mathbf{v}$,

$$\Psi_{ljmnk_uk_v}(\mathbf{u},\mathbf{v}) := u^l v^j e^{-(1/2)(u^2+v^2)} L_m^{\tilde{l}}(u^2) L_n^{\tilde{j}}(v^2) Y_{lk_u}(\theta^{(u)}) Y_{jk_v}(\theta^{(v)}), \tag{4.4}$$

where l, j, m and n are non-negative integers, $\tilde{l}$ and $\tilde{j}$ are defined by

$$\tilde{l} := l + (p-2)/2, \quad \tilde{j} := j + (q-2)/2, \tag{4.5}$$

$u := |\mathbf{u}|$, $v := |\mathbf{v}|$, the L's are the generalized Laguerre polynomials[45,46] and the Y's are the spherical harmonics in the notation of Sec. III. These states satisfy

$$\begin{aligned} \hat{H}^{\text{sho}}_{\mathbf{u}} \Psi_{ljmnk_uk_v} &= E_u \Psi_{ljmnk_uk_v}, \quad E_u := 2m + l + (p/2) = 2m + \tilde{l} + 1, \\ \hat{H}^{\text{sho}}_{\mathbf{v}} \Psi_{ljmnk_uk_v} &= E_v \Psi_{ljmnk_uk_v}, \quad E_v := 2n + j + (q/2) = 2n + \tilde{j} + 1, \end{aligned} \tag{4.6}$$

and they are orthogonal in $\mathcal{H}_{\text{aux}}$,

$$(\Psi_{ljmnk_uk_v}, \Psi_{l'j'm'n'k_u'k_v'})_{\text{aux}} = \frac{\Gamma(l+m+(p/2))\Gamma(j+n+(q/2))}{4\Gamma(m+1)\Gamma(n+1)} \delta_{ll'}\delta_{jj'}\delta_{mm'}\delta_{nn'}\delta_{k_uk_u'}\delta_{k_vk_v'}. \tag{4.7}$$

We set $\Phi_0 := \text{span}\{\Psi_{ljmnk_uk_v}\} = \{P(\mathbf{u},\mathbf{v})\exp[-\frac{1}{2}(u^2+v^2)]\}$, where $P(\mathbf{u},\mathbf{v})$ is an arbitrary polynomial in $\{u_i\}$ and $\{v_i\}$. Φ_0 is clearly dense in $\mathcal{H}_{\text{aux}}$ and mapped to itself by the quantum constraints (3.2).

Let G denote the gauge group, and let dg be the (left and right) invariant Haar measure on G. An L^1 function h on G defines on $\mathcal{H}_{\text{aux}}$ the bounded operator $\hat{h} := \int_G dg\, h(g) U(g)$, and the set of all such operators generates an algebra $\hat{\mathcal{A}}_G$. Starting with Φ_0, we first take the closure under the algebra generated by $\{U(g)|g \in G\}$, then take the closure under $\hat{\mathcal{A}}_G$, and adopt the resulting space Φ as our test space. Φ is a dense linear subspace of $\mathcal{H}_{\text{aux}}$, invariant under both $\hat{\mathcal{A}}_G$ and the algebra generated by $\{U(g)|g \in G\}$, and it hence satisfies the test space postulates of Ref. 8.

C. Physical Hilbert space

We now construct a rigging map by averaging states in Φ over G.

We define on Φ the sesquilinear form

$$(\phi_2, \phi_1)_{\text{ga}} := \int_G dg\, (\phi_2, U(g)\phi_1)_{\text{aux}}. \tag{4.8}$$

We show in Appendix E, Theorem E.3, that the integral in (4.8) is absolutely convergent for all $\phi_1, \phi_2 \in \Phi$, and $(\cdot\,,\cdot)_{\text{ga}}$ is hence well defined. We also show that $(\cdot\,,\cdot)_{\text{ga}}$ vanishes for $p+q \equiv 1 \pmod 2$. For the rest of this subsection we take $p+q \equiv 0 \pmod 2$.

Let Φ^* be the algebraic dual of Φ and let $f[\phi]$ denote the dual action of $f \in \Phi^*$ on $\phi \in \Phi$. We define the antilinear map $\eta: \Phi \to \Phi^*$ by

$$\eta(\phi_1)[\phi_2] := (\phi_1, \phi_2)_{\text{ga}}, \tag{4.9}$$

and we define on the image of η the sesquilinear form $(\cdot\,,\cdot)_{\text{RAQ}}$ by

$$(\eta(\phi_1), \eta(\phi_2))_{\text{RAQ}} := \eta(\phi_2)[\phi_1]. \tag{4.10}$$

We need to investigate whether the image of η is nontrivial and whether $(\cdot\,,\cdot)_{\text{RAQ}}$ is positive definite. If yes, η is a rigging map and the physical Hilbert space is the Cauchy completion of the image of η in $(\cdot\,,\cdot)_{\text{RAQ}}$.

Note first that if $\phi_i \in \Phi$ and $h_i \in L^1(G)$, (4.8) and (4.9) imply[8]

$$\eta(\hat{h}_1\phi_1)[\hat{h}_2\phi_2]=\overline{\left(\int_G dg\, h_1(g)\right)}\left(\int_G dg\, h_2(g)\right)\eta(\phi_1)[\phi_2] \tag{4.11}$$

and $\eta(\phi_1)[U(g)\phi_2]=\eta(U(g)\phi_1)[\phi_2]=\eta(\phi_1)[\phi_2]$ for all g. Hence it suffices to evaluate $\eta(\phi_1)[\phi_2]$ for $\phi_1,\phi_2\in\Phi_0$.

By Proposition E.4 in Appendix E, Fubini's theorem implies that we can represent the image of η as functions on $\mathbb{R}^{p+q}=\{(\mathbf{u},\mathbf{v})\}$, acting on $\phi\in\Phi$ by

$$f[\phi]=\int d^p\mathbf{u}\, d^q\mathbf{v}\, f(\mathbf{u},\mathbf{v})\phi(\mathbf{u},\mathbf{v}), \tag{4.12}$$

and evaluate η by

$$\eta(\phi)=\overline{\int_G dg\, U(g)\phi}, \tag{4.13}$$

where the integral is taken in the sense of pointwise convergence on $\mathbb{R}^{p+q}$. The value of (4.13) can be read off from the results in Appendix D.1 of Ref. 10, by matching our (E6) to Eq. (D3) in Ref. 10. The result is

$$\eta(\Psi_{ljmnk_uk_v})=4\pi^2(-1)^m\,\delta_{mn}\frac{\Gamma(l+m+(p/2))}{(2l+p-2)\Gamma(m+1)}\overline{\Psi_{ljk_uk_v}}, \tag{4.14}$$

where $\Psi_{ljk_uk_v}$ is as in (3.10). The action of $\overline{\Psi_{ljk_uk_v}}$ on Φ_0 reads (Ref. 46, p. 244)

$$\overline{\Psi_{l'j'k'_uk'_v}}[\Psi_{ljmnk_uk_v}]=(-1)^m\delta_{2l+p,2j+q}\delta_{ll'}\delta_{jj'}\delta_{mn}\delta_{k_uk'_u}\delta_{k_vk'_v}\frac{\Gamma(l+m+(p/2))}{2\Gamma(m+1)}. \tag{4.15}$$

Hence the image of η is nontrivial and spanned by $\{\overline{\Psi_{ljk_uk_v}}\}$. From (4.10), (4.14) and (4.15) we find

$$(\overline{\Psi_{l'j'k'_uk'_v}},\overline{\Psi_{ljk_uk_v}})_{\mathrm{RAQ}}=\frac{2l+p-2}{8\pi^2}\,\delta_{2l+p,2j+q}\delta_{ll'}\delta_{jj'}\delta_{k_uk'_u}\delta_{k_vk'_v}. \tag{4.16}$$

Hence $(\cdot\,,\cdot)_{\mathrm{RAQ}}$ is positive definite, η is a rigging map, and we have a physical Hilbert space $\mathcal{H}_{\mathrm{RAQ}}$. The group averaging sesquilinear form on Φ_0 reads

$$\begin{aligned}(\Psi_{l'j'm'n'k'_uk'_v},\Psi_{ljmnk_uk_v})_{\mathrm{ga}}=&\,2\pi^2(-1)^{m+m'}\,\delta_{2l+p,2j+q}\delta_{mn}\delta_{m'n'}\delta_{ll'}\delta_{jj'}\delta_{k_uk'_u}\delta_{k_vk'_v}\\&\times\frac{\Gamma(l+m'+(p/2))\Gamma(l+m+(p/2))}{(2l+p-2)\Gamma(m'+1)\Gamma(m+1)}.\end{aligned} \tag{4.17}$$

The uniqueness theorem of Ref. 8 shows that every rigging map for our triple $(\mathcal{H}_{\mathrm{aux}},U,\Phi)$ is a multiple of the group averaging rigging map η.

The algebra $\mathcal{A}^{(\star)}_{\mathrm{phys}}$ is represented on $\mathcal{H}_{\mathrm{aux}}$ by (3.4). This representation leaves Φ invariant and commutes with $U(g)$, and the star-relation in this representation coincides with the adjoint map on $\mathcal{H}_{\mathrm{aux}}$. It follows that $\mathcal{H}_{\mathrm{RAQ}}$ carries an antilinear representation ρ of $\mathcal{A}^{(\star)}_{\mathrm{phys}}$, such that the star-relation coincides with the adjoint map on $\mathcal{H}_{\mathrm{RAQ}}$. In the notation of (3.4),

$$\rho(\hat{O}_{ij}):f\mapsto\overline{\hat{O}_{ij}\bar{f}}. \tag{4.18}$$

This shows that the algebraic quantization set up in Sec. III yields a quantum theory anti-isomorphically embedded in our group averaging quantum theory whenever $p\geqslant 3$, $q\geqslant 3$ and p

$+q\equiv 0 \pmod 2$, even though we were able to complete the algebraic quantization explicitly only for $p=q=3$. Apart from $p=q=3$, we do, however, not know whether this quantum theory is the *only* one arising from the algebraic quantization for $p\geqslant 3$, $q\geqslant 3$ and $p+q\equiv 0 \pmod 2$.

V. REFINED ALGEBRAIC QUANTIZATION FOR $p<3$ OR $q<3$

In Sec. IV we assumed $p\geqslant 3$ and $q\geqslant 3$. We now discuss refined algebraic quantization for lower p or q. By interchange of $\mathbf{u}$ and $\mathbf{v}$, it suffices to consider $p\leqslant q$.

A. $p=1$, $q>3$

When $p=1$ and $q>3$, we define $\mathcal{H}_{\text{aux}}$ and Φ as in Sec. IV. The u_1 dependence of the test states (4.4) can be written in terms of Hermite polynomials as $H_{l+2m}(u_1)\exp(-\frac{1}{2}u_1^2)$ (Ref. 46, p. 240), but the notation in (4.4) covers also $p=1$, the spherical harmonics on S^0 being as described in Sec. III A. We drop the redundant index k_u and write

$$\phi_{ljmnk}(u_1,\mathbf{v}) := \Psi_{ljmn0k} = u^l v^j e^{-(1/2)(u^2+v^2)} L_m^{\tilde{l}}(u^2) L_n^{\tilde{j}}(v^2) Y_l(\theta^{(u)}) Y_{jk}(\theta^{(v)}), \tag{5.1}$$

where $l\in\{0,1\}$ and $\tilde{l}=l-\frac{1}{2}$.

As a preliminary, let $Y_{j0}(\theta^{(v)})$ denote the zonal spherical harmonics, which depend only on v_q/v and are given by Gegenbauer polynomials.[43] The recursion relations for the Gegenbauer polynomials and the generalized Laguerre polynomials[46] allow an explicit computation of the action of $\hat{C}_{1q}$ on ϕ_{ljmn0}. We find

$$\begin{aligned}\hat{C}_{1q}\phi_{0jmn0} = &-W_{qj}[(n+\tilde{j})\phi_{1,j-1,m-1,n,0}+(n+1)\phi_{1,j-1,m,n+1,0}]\\ &+W_{q,j+1}(\phi_{1,j+1,m-1,n-1,0}+\phi_{1,j+1,mn0}),\end{aligned} \tag{5.2a}$$

$$\begin{aligned}\hat{C}_{1q}\phi_{1jmn0} = &\,W_{qj}[(m+\tfrac{1}{2})(n+\tilde{j})\phi_{0,j-1,mn0}+(m+1)(n+1)\phi_{0,j-1,m+1,n+1,0}]\\ &-W_{q,j+1}[(m+\tfrac{1}{2})\phi_{0,j+1,m,n-1,0}+(m+1)\phi_{0,j+1,m+1,n0}],\end{aligned} \tag{5.2b}$$

where

$$\begin{aligned}W_{qj} &:= 2\left[\frac{j(j+q-3)}{(2j+q-2)(2j+q-4)}\right]^{1/2} \text{ for } j>0,\\ W_{q0} &:= 0,\end{aligned} \tag{5.3}$$

and any ϕ_{ljmn0} on the right-hand side with $m<0$ or $n<0$ is understood as zero.

Now, by Theorem E.3, the group averaging converges in absolute value. When q is even, the θ dependence in (E7) shows that the image of η is trivial. In the rest of this subsection we take q odd and show that the image of η is trivial also in this case.

It suffices to show that $(\phi_{l'j'm'n'k'},\phi_{ljmnk})_{\text{ga}}$ vanishes. When $l=l'=1$, we can proceed as in Sec. IV C and the result follows from (4.17). When $l=0$ or $l'=0$, (E7) shows that it suffices to consider $(\phi_{0jm'n'0},\phi_{0jmn0})_{\text{ga}}$. The θ-dependence in (E7) shows that the integral over θ gives zero unless $2m=2n+j+(q-1)/2$, and a similar observation with $U(g)$ conjugated to act on the first argument shows that the integral over θ gives zero unless $2m'=2n'+j+(q-1)/2$. When $q=5+4a$, $a=0,1,\ldots$, it therefore suffices to consider $(\phi_{0,2s,n'+s+a+1,n'},\phi_{0,2s,n+s+a+1,n})_{\text{ga}}$, where s, n and n' are non-negative integers and we have suppressed the last index of the ϕ's, understood to take the value zero. When $q=3+4b$, $b=1,2,\ldots$, it similarly suffices to consider $(\phi_{0,2s+1,n'+s+b+1,n'},\phi_{0,2s+1,n+s+b+1,n})_{\text{ga}}$, where s, n and n' are non-negative integers.

Let $q=3+4b$, $b=1,2,\ldots$. Recall that $\hat{C}_{1q}$ is self-adjoint in $\mathcal{H}_{\text{aux}}$ and commutes with $U(g)$. We compute

$$W_{q,2s+1}[(n+s+b+\tfrac{1}{2})(\phi_{0,2s+1,n'+s+b+1,n'},\phi_{0,2s+1,n+s+b,n-1})_{\mathrm{ga}}+(n+s+b+1)$$
$$\times(\phi_{0,2s+1,n'+s+b+1,n'},\phi_{0,2s+1,n+s+b+1,n})_{\mathrm{ga}}]$$
$$=-(\phi_{0,2s+1,n'+s+b+1,n'},\hat{C}_{1q}\phi_{1,2s,n+s+b,n})_{\mathrm{ga}}$$
$$=-(\hat{C}_{1q}\phi_{0,2s+1,n'+s+b+1,n'},\phi_{1,2s,n+s+b,n})_{\mathrm{ga}}=0, \tag{5.4}$$

where the first equality follows from (5.2b) and the last from (5.2a) and (4.17). By induction in n, (5.4) implies $(\phi_{0,2s+1,n'+s+b+1,n'},\phi_{0,2s+1,n+s+b+1,n})_{\mathrm{ga}}=0$.

Let then $q=5+4a$, $a=0,1,\ldots$. An argument similar to (5.4) shows that $(\phi_{0,2s,n'+s+a+1,n'},\phi_{0,2s,n+s+a+1,n})_{\mathrm{ga}}$ vanishes for $s>0$. When $s=0$, we compute

$$W_{q1}[(n+a+\tfrac{3}{2})(n+2a+\tfrac{5}{2})(\phi_{0,0,n'+a+1,n'},\phi_{0,0,n+a+1,n})_{\mathrm{ga}}+(n+a+2)(n+1)$$
$$\times(\phi_{0,0,n'+a+1,n'},\phi_{0,0,n+a+2,n+1})_{\mathrm{ga}}]$$
$$=(\phi_{0,0,n'+a+1,n'},\hat{C}_{1q}\phi_{1,1,n+a+1,n})_{\mathrm{ga}}=(\hat{C}_{1q}\phi_{0,0,n'+a+1,n'},\phi_{1,1,n+a+1,n})_{\mathrm{ga}}=\ 0, \tag{5.5}$$

where the last equality follows from (5.2a) and (4.17). By induction in n, it therefore suffices to consider $(\phi_{0,0,n'+a+1,n'},\phi_{0,0,a+1,0})_{\mathrm{ga}}$. A similar argument in n' shows that it suffices to consider $(\phi_{0,0,a+1,0},\phi_{0,0,a+1,0})_{\mathrm{ga}}$.

In $(\phi_{0,0,a+1,0},U(g)\phi_{0,0,a+1,0})_{\mathrm{aux}}$, we use (E7) and perform the elementary integration over $\mathbf{v}$. We then integrate over G in the Haar measure $dg=\frac{1}{2}dz\,d\mu\,d\theta$. The integration over θ is elementary. Changing the variables in the inner integral from u to $y:=u^2/z$ and in the outer integral from μ to $t:=\mu z/(z+1)$, we find that $(\phi_{0,0,a+1,0},\phi_{0,0,a+1,0})_{\mathrm{ga}}$ equals a numerical constant times

$$\int_0^\infty dz\,\frac{z^{a+1/2}}{(z+1)^{2a+3/2}}\int_{-\infty}^{\infty}\frac{dt}{(1+it)^{2a+5/2}}\int_0^\infty dy\,y^{-1/2}L_{a+1}^{-1/2}(zy)\,L_{a+1}^{-1/2}(y)$$
$$\times\exp\left[-\frac{1}{2}(z+1)(1-it)y\right]. \tag{5.6}$$

We interchange the order of the dt and dy integrals in (5.6), justified by the absolute convergence of the double integral, and perform the dt integral as a contour integral, finding that (5.6) equals a numerical constant times

$$\int_0^\infty dz\,z^{a+1/2}\int_0^\infty dy\,y^{2a+1}L_{a+1}^{-1/2}(zy)\,L_{a+1}^{-1/2}(y)\exp[-(z+1)y]. \tag{5.7}$$

In (5.7) we interchange the order of the dz and dy integrals, justified by the absolute convergence of the double integral. Changing the variable in the new inner integral from z to $x:=zy$, we obtain

$$\int_0^\infty dy\,y^{a-1/2}L_{a+1}^{-1/2}(y)\,e^{-y}\int_0^\infty dx\,x^{a+1/2}L_{a+1}^{-1/2}(x)\,e^{-x}. \tag{5.8}$$

The integrals in (5.8) have factorized, and the integral over y vanishes by the orthogonality of the generalized Laguerre polynomials.[46]

B. $p=1$, $q=3$

When $p=1$ and $q=3$, we define $\mathcal{H}_{\mathrm{aux}}$ as in Sec. IV. With Φ defined as in Sec. IV, the integral in (4.8) is not absolutely convergent for $l=j=0$, and we have not found a weaker unambiguous

sense of convergence. The θ-dependence in (E7) however suggests that if group averaging can be made well-defined, it should annihilate states with $l=j=0$. We shall achieve this by suitably modifying the test space.

Dropping the redundant index k_u, we introduce the states ϕ_{ljmnk} by (5.1) with $q=3$. We define $\Phi_0^{\mathrm{mod}} := \mathrm{span}(\{\phi_{ljmnk} | l+j>0\} \cup \{\psi_{mn}\})$, where

$$\psi_{mn} := \frac{2}{\sqrt{3}}\left[\left(m+\frac{1}{2}\right)\left(n+\frac{3}{2}\right)\phi_{00mn0} + (m+1)(n+1)\,\phi_{00,m+1,n+1,0}\right]. \tag{5.9}$$

Using the basis (3.4) of $\mathcal{A}_{\mathrm{phys}}^{(\star)}$, properties of the spherical harmonics on S^2 (Refs. 43 and 45) and properties of the generalized Laguerre polynomials,[46] it can be verified that Φ_0^{mod} is invariant under $\mathcal{A}_{\mathrm{phys}}^{(\star)}$. In particular, formulas (5.2) and (5.3) hold with $q=3$, implying

$$\hat{C}_{13}\phi_{11mn0} = \psi_{mn} - \frac{4}{\sqrt{15}}\left[\left(m+\frac{1}{2}\right)\phi_{0,2,m,n-1,0} + (m+1)\,\phi_{0,2,m+1,n,0}\right], \tag{5.10a}$$

$$\begin{aligned}\hat{C}_{13}\psi_{mn} = {} & \tfrac{4}{3}\left(m+\tfrac{1}{2}\right)\left(n+\tfrac{3}{2}\right)\left(\phi_{11,m-1,n-1,0} + \phi_{11mn0}\right) + \tfrac{4}{3}(m+1)(n+1) \\ & \times\left(\phi_{11mn0} + \phi_{11,m+1,n+1,0}\right).\end{aligned} \tag{5.10b}$$

We claim that Φ_0^{mod} is dense in $\mathcal{H}_{\mathrm{aux}}$. If this were not the case, there would exist a nonzero vector $y=\Sigma_{ljmnk} a_{ljmnk}\phi_{ljmnk} \in \mathcal{H}_{\mathrm{aux}}$ that is orthogonal to all vectors in Φ_0^{mod}. By (4.7), orthogonality with each ϕ_{ljmnk} with $l+j>0$ implies $a_{ljmnk}=0$ for $l+j>0$. By (4.7) and (5.9), orthogonality with each ψ_{mn} implies $a_{00mn0}+a_{00,m+1,n+1,0}=0$, from which (4.7) further shows that y has finite norm only if y is the zero vector. Hence Φ_0^{mod} is dense in $\mathcal{H}_{\mathrm{aux}}$.

Following Sec. IV with Φ_0 replaced by Φ_0^{mod}, we first take the closure of Φ_0^{mod} under the algebra generated by $\{U(g)|g\in G\}$, then take the closure under $\hat{\mathcal{A}}_G$, and adopt the resulting space Φ^{mod} as our test space. Φ^{mod} is a dense linear subspace of $\mathcal{H}_{\mathrm{aux}}$, invariant under $\mathcal{A}_{\mathrm{phys}}^{(\star)}$, $\hat{\mathcal{A}}_G$ and the algebra generated by $\{U(g)|g\in G\}$, and satisfies hence the test space postulates of Ref. 8. We show in Appendix E, Theorem E.5, that the integral in (4.8) converges in absolute value for all $\phi_1, \phi_2 \in \Phi^{\mathrm{mod}}$.

To evaluate $(\phi_2,\phi_1)_{\mathrm{ga}}$ on Φ^{mod}, it suffices to consider $\phi_1, \phi_2 \in \Phi_0^{\mathrm{mod}}$. When both ϕ_1 and ϕ_2 have $l=1$, we can proceed as in Sec. IV C, arriving at (4.12)–(4.17). When ϕ_1 and ϕ_2 have differing values of l, j or k, (E7) shows that $(\phi_2,\phi_1)_{\mathrm{ga}}$ vanishes. What remains is $(\phi_{0jm'n'k}, \phi_{0jmnk})_{\mathrm{ga}}$ with $j>0$ and $(\psi_{m'n'}, \psi_{mn})_{\mathrm{ga}}$. The vanishing of the former follows as in Sec. V A, noting that (5.4) holds also for $b=0$. For the latter, we use (5.10a), the self-adjointness of $\hat{C}_{13}$ on $\mathcal{H}_{\mathrm{aux}}$ and the vanishing of $(\psi_{m'n'}, \phi_{0jmn0})_{\mathrm{ga}}$ for $j>0$ and compute

$$(\psi_{m'n'}, \psi_{mn})_{\mathrm{ga}} = (\psi_{m'n'}, \hat{C}_{13}\phi_{11mn0})_{\mathrm{ga}} = (\hat{C}_{13}\psi_{m'n'}, \phi_{11mn0})_{\mathrm{ga}} = 0, \tag{5.11}$$

where the last equality follows from (5.10b) and (4.17).

The evaluation of $(\phi_2,\phi_1)_{\mathrm{ga}}$ is now complete. The only nonzero contribution comes from states with $l=1$, in which case formulas (4.12)–(4.17) hold. The image of η is one-dimensional, spanned by $\{\overline{\Psi_0}\}$, where Ψ_0 is the state (3.10) with $l=1$ and $j=0$ and reads explicitly (Ref. 43, Sec. 7.11) $\Psi_0 = v^{-1}\sin(u_1 v)$. The inner product (4.16) is positive definite, and we obtain a one-dimensional physical Hilbert space $\mathcal{H}_{\mathrm{RAQ}}$.

As Φ_0^{mod} is invariant under $\mathcal{A}_{\mathrm{phys}}^{(\star)}$, $\mathcal{H}_{\mathrm{RAQ}}$ carries an antilinear representation of $\mathcal{A}_{\mathrm{phys}}^{(\star)}$. A direct calculation shows that all operators in this representation annihilate $\overline{\Psi_0}$, and the representation is trivial. The quantum theory found in algebraic quantization in Sec. (III A) is thus anti-isomorphically embedded in the group averaging quantum theory.

C. $p=1$, $q=2$

When $p=1$ and $q=2$, and $\mathcal{H}_{\rm aux}$ and Φ are as in Sec. IV, the integral in (4.8) is not absolutely convergent for $l=j=0$. It may be possible to modify the $l=j=0$ sector of Φ as in Sec. V B above, but as now $p+q\equiv 1 \pmod 2$, any test space built from linear combinations of the harmonic oscillator eigenfunctions will give an η with trivial image.

D. $p=q=1$

When $p=q=1$, and $\mathcal{H}_{\rm aux}$ and Φ are as in Sec. IV, the integral in (4.8) is not absolutely convergent for $l=0$ or $j=0$ and is unambiguously divergent for example for $\phi_1=\phi_2=\Psi_{0000}$.

We attempt to cure the divergence by modifying the zero angular momentum sector. For technical simplicity, we choose at the outset to work with states that are symmetric under $(u_1,v_1)\mapsto(-u_1,-v_1)$.

Let $\mathcal{H}^{\rm s}_{\rm aux}\subset\mathcal{H}_{\rm aux}$ be the Hilbert subspace of vectors symmetric under $(u_1,v_1)\mapsto(-u_1,-v_1)$. Dropping the redundant indices k_u and k_v, we write

$$\phi_{lmn}(u_1,v_1) := \Psi_{llmn00} = u^l v^l e^{-(1/2)(u^2+v^2)} L^{\tilde{l}}_m(u^2) L^{\tilde{l}}_n(v^2) Y_l(\theta^{(u)}) Y_l(\theta^{(v)}), \tag{5.12}$$

where $l\in\{0,1\}$ and $\tilde{l}=l-\frac{1}{2}$. $\{\phi_{lmn}\}$ is clearly an orthogonal basis for $\mathcal{H}^{\rm s}_{\rm aux}$.

Let $\Phi^{\rm s}_0 := {\rm span}\{\psi_{mn},\phi_{1mn}\}$, where

$$\psi_{mn} := 2[(m+\tfrac{1}{2})(n+\tfrac{1}{2})\phi_{0mn} + (m+1)(n+1)\phi_{0,m+1,n+1}]. \tag{5.13}$$

We then find (Ref. 46, p. 241)

$$\hat{C}_{11}\psi_{mn} = 4[(m+\tfrac{1}{2})(n+\tfrac{1}{2})(\phi_{1mn}+\phi_{1,m-1,n-1}) + (m+1)(n+1)(\phi_{1mn}+\phi_{1,m+1,n+1})], \tag{5.14a}$$

$$\hat{C}_{11}\phi_{1mn} = \psi_{mn}, \tag{5.14b}$$

where $\hat{C}_{11}$ (3.4) is the single generator of $\mathcal{A}^{(\star)}_{\rm phys}$. Hence $\Phi^{\rm s}_0$ is invariant under $\mathcal{A}^{(\star)}_{\rm phys}$, and it can be shown as in Sec. V B that $\Phi^{\rm s}_0$ is dense in $\mathcal{H}^{\rm s}_{\rm aux}$. We build from $\Phi^{\rm s}_0$ a test space $\Phi^{\rm s}$ satisfying the postulates of Ref. 8 as in Sec. V B. The integral in (4.8) then converges in absolute value for all $\phi_1,\phi_2\in\Phi^{\rm s}$: The proof is a verbatim adaptation of that of Theorem E.5.

We need to evaluate $(\phi_2,\phi_1)_{\rm ga}$ on $\Phi^{\rm s}$. It suffices to consider $\phi_1,\phi_2\in\Phi^{\rm s}_0$. Clearly $(\psi_{m'n'},\phi_{1mn})_{\rm ga}=0$. For $(\phi_{1m'n'},\phi_{1mn})_{\rm ga}$ we proceed as in Sec. IV C and arrive at (4.12)–(4.17), the last of which reads

$$(\phi_{1m'n'},\phi_{1mn})_{\rm ga} = 2\pi^2(-1)^{m+m'}\delta_{mn}\delta_{m'n'}\frac{\Gamma(m+\frac{3}{2})\Gamma(m'+\frac{3}{2})}{\Gamma(m+1)\Gamma(m'+1)}. \tag{5.15}$$

To find $(\psi_{m'n'},\psi_{mn})_{\rm ga}$, we use the self-adjointness of $\hat{C}_{11}$ on $\mathcal{H}^{\rm s}_{\rm aux}$ and compute

$$\begin{aligned}(\psi_{m'n'},\psi_{mn})_{\rm ga} &= (\psi_{m'n'},\hat{C}_{11}\phi_{1mn})_{\rm ga}\\ &= (\hat{C}_{11}\psi_{m'n'},\phi_{1mn})_{\rm ga}\\ &= -2\pi^2(-1)^{m+m'}\delta_{mn}\delta_{m'n'}\frac{\Gamma(m+\frac{3}{2})\Gamma(m'+\frac{3}{2})}{\Gamma(m+1)\Gamma(m'+1)},\end{aligned} \tag{5.16}$$

where the first equality follows from (5.14b) and the last one from (5.14a) and (5.15).

We see that $(\cdot\,,\cdot)_{\rm ga}$ is an *indefinite* sesquilinear form. Hence the map η defined by (4.9) is not a rigging map and we do not recover a Hilbert space. The indefiniteness of $(\cdot\,,\cdot)_{\rm ga}$ further implies, by the uniqueness theorem of Ref. 8, that the triple $(\mathcal{H}^{\rm s}_{\rm aux}, \underline{U}, \underline{\Phi}^{\rm s})$ admits no rigging maps.

The image of η is two-dimensional, spanned by $\{\overline{\Psi_{00}}, \overline{\Psi_{11}}\}$, where Ψ_{00} and Ψ_{11} are given by (3.10) and read explicitly (Ref. 43, Sec. 7.11)

$$\Psi_{00} = \frac{1}{\sqrt{2\pi}} \cos(u_1 v_1), \tag{5.17a}$$

$$\Psi_{11} = \frac{1}{\sqrt{2\pi}} \sin(u_1 v_1). \tag{5.17b}$$

The manifestly indefinite sesquilinear form (4.10) on the image of η is given by (4.16). The representation of $\mathcal{A}^{(\star)}_{\rm phys}$ induced on the image of η by (4.12) is anti-isomorphic to the representation obtained in Sec. III A on the solution space to the algebraic quantization constraints.

E. $p=2$, $q>2$

When $p=2$ and $q>2$, we define $\mathcal{H}_{\rm aux}$ and Φ as in Sec. IV. Theorem E.3 in Appendix E shows that the group averaging converges in absolute value.

When q is odd, the θ dependence in (E7) shows that the image of η is trivial.

Suppose then that q is even. When $l>0$ and $l'>0$, we arrive at Eqs. (4.12)–(4.17) as in Sec. IV C. When $l=0$ or $l'=0$, it can be shown that $(\Psi_{l'j'm'n'k'_u k'_v}, \Psi_{ljmnk_u k_v})_{\rm ga}$ vanishes: The arguments follow those in Sec. V A so closely that we will not spell them out here. This means that Eqs. (4.12)–(4.17) hold for all values of the indices in the sense that terms involving $\delta_{2l+1,2j+q}$ for $l=0$ are understood to vanish. Hence the situation is similar to that for $p\geqslant 3$, $q\geqslant 3$ and $p+q \equiv 0 \pmod 2$ in Sec. IV. The image of η is nontrivial, $(\cdot\,,\cdot)_{\rm RAQ}$ is positive definite, η is a rigging map, and the representation of $\mathcal{A}^{(\star)}_{\rm phys}$ on the physical Hilbert space is as described at the end of Sec. IV C.

F. $p=q=2$

The case $p=q=2$ was analyzed in Ref. 10. Group averaging does not converge on the test space of Sec. IV, but the $l=j=0$ sector of the test space can be modified so that group averaging converges and the physical observable algebra includes $\mathcal{A}^{(\star)}_{\rm phys}$. The physical Hilbert space decomposes into a direct sum of four Hilbert subspaces, each of them carrying a distinct representation of $\mathcal{A}^{(\star)}_{\rm phys}$.

VI. DISCUSSION

We have discussed the quantization of a constrained system with unreduced phase space $\mathbb{R}^{2(p+q)}$, classical gauge group $\mathrm{SL}(2,\mathbb{R})$ and a distinguished $\mathfrak{o}(p,q)$ algebra of classical observables. We employed refined algebraic quantization, using group averaging on an auxiliary Hilbert space to find the inner product on the physical Hilbert space. We took care to select the quantization input so that when a quantum theory is recovered, the classical $\mathfrak{o}(p,q)$ algebra gets promoted into an operator algebra represented on the physical Hilbert space.

When $p\geqslant 2$, $q\geqslant 2$, $p+q>4$ and $p+q\equiv 0 \pmod 2$, we found a quantum theory with a nontrivial representation of the $\mathfrak{o}(p,q)$ observables. For $p=q=2$, a similar result was obtained in Ref. 10. For $(p,q)=(1,3)$ or $(3,1)$, we found a quantum theory with a one-dimensional Hilbert space and a trivial representation of the $\mathfrak{o}(p,q)$ observables. For other values of p and q we found no quantum theory.

We also discussed Ashtekar's algebraic quantization, solving first the quantum constraints without an inner product and then promoting the classical $\mathfrak{o}(p,q)$ algebra into operators whose star-relations determine the physical inner product. For all values of p and q for which

group averaging gave a quantum theory, algebraic quantization gave a quantum theory that is (anti-)isomorphically embedded in the group averaging theory. For $p=q=3$, we showed that this algebraic quantization theory is unique.

With both algebraic quantization and group averaging, qualitative changes emerged depending on whether p and q are less than, equal to, or greater than 2. This could be expected from the properties of the classical reduced phase space: The reduced phase space contains a symplectic manifold when and only when $\min(p,q)\geqslant 2$, and this symplectic manifold is connected when and only when $\min(p,q)\geqslant 3$. However, a phenomenon not expected on classical grounds was that neither algebraic quantization nor group averaging gave a quantum theory for $p+q\equiv 1 \pmod 2$. The technical reason was that both quantization schemes represented the $\mathfrak{o}(p)\oplus\mathfrak{o}(q)$ subalgebra of $\mathfrak{o}(p,q)$ by integer-valued rather than half-integer-valued angular momenta. Obtaining quantum theories for $p+q\equiv 1 \pmod 2$ by some ''fermionic'' modification might be an interesting challenge.

For $p=q=1$, both algebraic quantization and group averaging failed to give a quantum theory, for closely related reasons. Algebraic quantization led to a two-dimensional vector space of solutions to the constraints, but requiring the $\mathfrak{o}(1,1)$ generator to be symmetric forced the sesquilinear form on this vector space to be indefinite. In group averaging, a judicious choice of the test space ensured convergence of the averaging and the inclusion of the $\mathfrak{o}(1,1)$ generator in the would-be physical observable algebra, but the outcome was the same indefinite sesquilinear form on the same two-dimensional vector space as in algebraic quantization. It is not clear whether the case $p=q=1$ has physical interest, especially as the reduced phase space consists of just three points, non-Hausdorff close to each other, but from the mathematical point of view this provides the first example known to us where group averaging fails to produce a Hilbert space owing to indefiniteness of the would-be inner product. As the uniqueness theorem of Ref. 8 does not assume positive definiteness, the theorem is applicable here and implies that our test space admits no rigging maps.

We assumed throughout $p\geqslant 1$ and $q\geqslant 1$. If either p or q vanishes, the action (2.1) still defines a classical theory, but the reduced phase space then consists of a single point. Algebraic quantization in the representation of Sec. III gives no solutions to the constraints, and when group averaging based on the harmonic oscillator eigenstates converges, it gives an identically vanishing sesquilinear form owing to the θ dependence in $U(g)\Psi$ (E7).

Finally, one would like to characterize the representations of $\mathfrak{o}(p,q)$ on our physical Hilbert spaces in terms of invariants,[42] as done in Refs. 10, 16, and 21 for $p=q=2$. The value of the quadratic Casimir operator can be read off from (3.5). As our representation of the gauge group on the auxiliary Hilbert space is isomorphic to the oscillator representation of $\mathrm{SL}(2,\mathbb{R})$,[38] the joint representation theory of the dual pair $(\mathrm{O}(p,q),\mathrm{SL}(2,\mathbb{R}))$[47,48] may be useful with this question.

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APPENDIX A: SL(2,$\mathbb{R}$)

In this appendix we collect some relevant properties of $\mathrm{SL}(2,\mathbb{R})$. The notation follows Ref. 38.

$\mathrm{SL}(2,\mathbb{R})$ consists of real 2×2 matrices with unit determinant. The Lie algebra $\mathfrak{sl}(2,\mathbb{R})$ is spanned by the matrices

$$h:=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad e^{+}:=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad e^{-}:=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, \tag{A1}$$

whose commutators are

$$[h, e^+] = 2e^+,$$
$$[h, e^-] = -2e^-, \tag{A2}$$
$$[e^+, e^-] = h.$$

Elements of $SL(2,\mathbb{R})$ have the unique Iwasawa decomposition

$$g = \exp(\mu e^-)\exp(\lambda h)\exp[\theta(e^+ - e^-)], \tag{A3}$$

or explictly

$$g = \begin{pmatrix} 1 & 0 \\ \mu & 1 \end{pmatrix}\begin{pmatrix} e^\lambda & 0 \\ 0 & e^{-\lambda} \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{A4}$$

where $\mu \in \mathbb{R}$, $\lambda \in \mathbb{R}$ and $0 \leqslant \theta < 2\pi$. The unique Iwasawa decomposition of the universal covering group of $SL(2,\mathbb{R})$ is given by (A3) with $-\infty < \theta < \infty$, and that of the double cover by $0 \leqslant \theta < 4\pi$. The left and right invariant Haar measure reads $dg = e^{2\lambda}\, d\lambda\, d\mu\, d\theta$.

APPENDIX B: LINEAR INDEPENDENCE OF THE CONSTRAINTS

In this appendix we show that the gradients of the constraints are all vanishing on $\overline{\Gamma}_0$, linearly dependent but not all vanishing on $\overline{\Gamma}_{\text{ex}}$, and linearly independent on $\overline{\Gamma}_{\text{reg}}$.

From (2.3), the gradients of the constraints read

$$dH_1 = \sum_i (p_i dp_i - v_i dv_i),$$
$$dH_2 = \sum_i (\pi_i d\pi_i - u_i du_i), \tag{B1}$$
$$dD = \sum_i (u_i dp_i + p_i du_i - \pi_i dv_i - v_i d\pi_i).$$

For $\alpha, \beta, \gamma \in \mathbb{R}$, the equation $\alpha dH_1 + \beta dH_2 + \gamma dD = 0$ is equivalent to

$$\gamma\mathbf{u} + \alpha\mathbf{p} = \mathbf{0} = -\beta\mathbf{u} + \gamma\mathbf{p},$$
$$\gamma\boldsymbol{\pi} + \alpha\mathbf{v} = \mathbf{0} = -\beta\boldsymbol{\pi} + \gamma\mathbf{v}. \tag{B2}$$

$\overline{\Gamma}_0$ is clearly the set where the gradients of all the constraints vanish.

On $\overline{\Gamma}_{\text{ex}}$, we saw in Sec. II that each point can be brought to the form (2.11) by a gauge transformation (2.5) with some $g \in SL(2,\mathbb{R})$. Given such a g, (B2) is satisfied by $\alpha = (g_{12})^2$, $\beta = -(g_{11})^2$ and $\gamma = g_{11}g_{12}$, where at least one of α and β must be nonvanishing since $\det(g) \neq 0$. Hence the gradients of the constraints are linearly dependent on $\overline{\Gamma}_{\text{ex}}$.

On $\overline{\Gamma}_{\text{reg}}$, the pair $(\mathbf{u}, \mathbf{p})$ [as well as the pair $(\mathbf{v}, \boldsymbol{\pi})$] is linearly independent, and (B2) implies $\alpha = \beta = \gamma = 0$. Hence the gradients of the constraints are linearly independent on $\overline{\Gamma}_{\text{reg}}$.

APPENDIX C: SEPARATION OF $\mathcal{M}_{\text{reg}}$ BY $\mathcal{A}_{\text{class}}$

In this appendix we show that the classical observable algebra $\mathcal{A}_{\text{class}}$ separates $\mathcal{M}_{\text{reg}}$. We assume $p \geqslant 2$ and $q \geqslant 2$, which is necessary and sufficient for $\mathcal{M}_{\text{reg}}$ to be nonempty. The case $p = q = 2$ was treated in Refs. 10, 16, and 21.

Let $\mathcal{M}_i$, $1\leqslant i\leqslant p$, be the subset of $\mathcal{M}_{\rm reg}$ whose points have a representative in $\overline{\Gamma}_{\rm reg}$ satisfying the gauge conditions (2.13) with $u_i^2+p_i^2>0$. It follows that $\mathcal{M}_i\cap\mathcal{M}_j\neq\varnothing$ for all i and j and

$$\mathcal{M}_{\rm reg}=\bigcup_{i=1}^{p}\mathcal{M}_i. \tag{C1}$$

Lemma C.1: Let $\tilde{a}\in\mathcal{M}_{\rm reg}$ and $\tilde{b}\in\mathcal{M}_{\rm reg}$ such that there is no $\mathcal{M}_i$ containing both $\tilde{a}$ and $\tilde{b}$. Then $\mathcal{A}_{\rm class}$ separates $\tilde{a}$ and $\tilde{b}$.

Proof: Let $a=(\mathbf{u},\mathbf{p},\mathbf{v},\boldsymbol{\pi})\in\overline{\Gamma}_{\rm reg}$ and $b=(\mathbf{u}',\mathbf{p}',\mathbf{v}',\boldsymbol{\pi}')\in\overline{\Gamma}_{\rm reg}$ be representatives of, respectively, $\tilde{a}$ and $\tilde{b}$, each satisfying (2.13). As the pair $(\mathbf{u},\mathbf{p})$ is linearly independent, there exist $i\neq j$ such that $u_ip_j-u_jp_i\neq0$. It follows that $\tilde{a}\in\mathcal{M}_i\cap\mathcal{M}_j$. By assumption then $\tilde{b}\notin\mathcal{M}_i\cup\mathcal{M}_j$, which implies $u_i'=p_i'=u_j'=p_j'=0$. Hence $A_{ij}(\tilde{a})=u_ip_j-u_jp_i\neq0$ but $A_{ij}(\tilde{b})=u_i'p_j'-u_j'p_i'=0$, which shows that the observable A_{ij} in (2.9) separates $\tilde{a}$ and $\tilde{b}$. ■

Remark: Repeating the proof with $\tilde{a}$ and $\tilde{b}$ interchanged shows that points satisfying the conditions of Lemma C.1 exist only for $p\geqslant4$.

Theorem C.1: $\mathcal{A}_{\rm class}$ separates $\mathcal{M}_{\rm reg}$.

Proof: By Lemma C.1, it suffices to consider individually each $\mathcal{M}_k$.

From now on let $\mathcal{M}_k$ be fixed. We saw in Sec. II C 3 that $\mathcal{M}_{\rm reg}$ can be represented as the quotient of the set (2.13) under the $U(1)$ action given by (2.5) with (2.14). Within $\mathcal{M}_k$, each $U(1)$ equivalence class in (2.13) has a unique representative that satisfies $p_k=0$ and $u_k>0$. Performing on this representative a gauge transformation (2.5) with $g=\mathrm{diag}(u_k^{-1},u_k)$, we obtain a point in Γ satisfying

$$\begin{gathered}\mathbf{u}^2=\boldsymbol{\pi}^2>0,\quad \mathbf{p}^2=\mathbf{v}^2>0,\\ \mathbf{u}\cdot\mathbf{p}=\mathbf{v}\cdot\boldsymbol{\pi}=0,\\ p_k=0,\quad u_k=1.\end{gathered} \tag{C2}$$

It follows that $\mathcal{M}_k$ can be represented as the subset of Γ satisfying (C2).

Let now $\tilde{a},\tilde{b}\in\mathcal{M}_k$ such that $A(\tilde{a})=A(\tilde{b})$ for all $A\in\mathcal{A}_{\rm class}$. Let $a=(\mathbf{u},\mathbf{p},\mathbf{v},\boldsymbol{\pi})$ and $b=(\mathbf{u}',\mathbf{p}',\mathbf{v}',\boldsymbol{\pi}')$ be the respective representatives of $\tilde{a}$ and $\tilde{b}$ in the gauge (C2). We shall show that $a=b$. We use the basis (2.9) of $\mathcal{A}_{\rm class}$.

Consider the observables A_{ij}. From $A_{ij}(\tilde{a})=A_{ij}(\tilde{b})$ we obtain

$$u_ip_j-u_jp_i=u_i'p_j'-u_j'p_i', \tag{C3}$$

where $1\leqslant i\leqslant p$ and $1\leqslant j\leqslant p$. With $i=k$ and $j\neq k$, the gauge conditions (C2) show that (C3) reduces to $p_j=p_j'$. The gauge conditions (C2) imply directly that $p_k=p_k'$. Hence $\mathbf{p}=\mathbf{p}'$.

Multiplying (C3) by p_j and summing over j gives

$$\mathbf{p}^2u_i-(\mathbf{u}\cdot\mathbf{p})p_i=(\mathbf{p}\cdot\mathbf{p}')u_i'-(\mathbf{u}'\cdot\mathbf{p})p_i'. \tag{C4}$$

Using $\mathbf{p}=\mathbf{p}'$ and (C2), (C4) reduces to $u_i=u_i'$. Hence $\mathbf{u}=\mathbf{u}'$.

Consider then the observables C_{ij}. From $C_{ij}(\tilde{a})=C_{ij}(\tilde{b})$ we obtain

$$u_iv_j-p_i\pi_j=u_i'v_j'-p_i'\pi_j', \tag{C5}$$

where $1\leqslant i\leqslant p$ and $1\leqslant j\leqslant q$. With $i=k$, (C2) shows that (C5) reduces to $v_j=v_j'$. Hence $\mathbf{v}=\mathbf{v}'$.

Substituting $\mathbf{u}=\mathbf{u}'$, $\mathbf{p}=\mathbf{p}'$ and $\mathbf{v}=\mathbf{v}'$ in (C5) gives $p_i(\pi_j-\pi_j')=0$. As $\mathbf{p}^2>0$, this implies $\pi_j=\pi_j'$. Hence $\boldsymbol{\pi}=\boldsymbol{\pi}'$. ■

APPENDIX D: $\mathcal{A}^{(\star)}_{\text{phys}}$ ON $\mathcal{V}_{\text{phys}}$ FOR $p=q=3$

In this appendix we analyze the representation of $\mathcal{A}^{(\star)}_{\text{phys}}$ on $\mathcal{V}_{\text{phys}}$ for $p=q=3$, displayed in Table I. We show first that this representation is irreducible. We then show that the only inner products in which the star-relations (3.13) become adjoint relations are multiples of (3.14).

Proposition D.1: Let $U\subset\mathcal{V}_{\text{phys}}$ be a linear subspace invariant under $\mathcal{A}^{(\star)}_{\text{phys}}$, $U\neq\{0\}$. Then $U=\mathcal{V}_{\text{phys}}$.

Proof: Recall that the operator $\widehat{L^2}:=\hat{L}_0^2+\frac{1}{2}(\hat{L}_+\hat{L}_-+\hat{L}_-\hat{L}_+)$ satisfies $\widehat{L^2}\Psi_{lmn}=l(l+1)\Psi_{lmn}$. Let $u\in U$, $u\neq 0$. Then $u=\Sigma a_{lmn}\Psi_{lmn}$, where only finitely many a_{lmn} are nonzero. Let l_0 be the largest l for which some a_{lmn} is nonzero. Then $u^{(1)}:=\Pi_{l<l_0}[\widehat{L^2}-l(l+1)]u=k\Sigma_{mn}a_{l_0mn}\Psi_{l_0mn}$, where $k\neq 0$. Acting on $u^{(1)}$ finitely many times with $\hat{L}_+$ and $\hat{J}_+$ gives the vector $u^{(2)}=a^{(2)}\Psi_{l_0l_0l_0}\neq 0$, and $u^{(3)}:=(\hat{L}_-)^{l_0}(\hat{J}_-)^{l_0}u^{(2)}=a^{(3)}\Psi_{l_000}\neq 0$. Hence $\Psi_{l_000}\in U$.

A direct computation from Table I shows that $\hat{J}_-\hat{C}_1^+\Psi_{l00}-(l-1)\hat{C}_0\Psi_{l00}$ is a nonzero multiple of $\Psi_{l+1,00}$ for all l and $\hat{J}_-\hat{C}_1^+\Psi_{l00}+(l+1)\hat{C}_0\Psi_{l00}$ is a nonzero multiple of $\Psi_{l-1,00}$ for $l>0$. It follows by induction that $\Psi_{l00}\in U$ for all l. Acting on Ψ_{l00} with $\hat{L}_\pm$ and $\hat{J}_\pm$ shows that $\Psi_{lmn}\in U$ for all values of the indices. ■

Proposition D.2: Let $(\cdot,\cdot)$ *be an inner product in which the star-relations* (3.13) *become adjoint relations. Then* $(\Psi_{lmn},\Psi_{l'm'n'})=r(2l+1)\delta_{ll'}\delta_{mm'}\delta_{nn'}$, *where* r *is a positive constant.*

Proof: The adjointness relations imply that the operator $\widehat{L^2}$ introduced in the proof of Proposition D.1 is self-adjoint. Hence $l'(l'+1)(\Psi_{lmn},\Psi_{l'm'n'})=(\Psi_{lmn},\widehat{L^2}\Psi_{l'm'n'})=(\widehat{L^2}\Psi_{lmn},\Psi_{l'm'n'})=l(l+1)(\Psi_{lmn},\Psi_{l'm'n'})$, which shows that $(\Psi_{lmn},\Psi_{l'm'n'})$ vanishes for $l\neq l'$. By standard angular momentum techniques in the $\mathfrak{o}(3)$ subalgebras generated, respectively, by the $\hat{L}$'s and the $\hat{J}$'s (see, for example, Ref. 49), we then find

$$(\Psi_{lmn},\Psi_{l'm'n'})=A_l\delta_{ll'}\delta_{mm'}\delta_{nn'}, \tag{D1}$$

where A_l depends only on l.

To determine A_l, we use the self-adjointness of $\hat{C}_0$. Writing $\Psi_l:=\Psi_{l00}$ and using the action of $\hat{C}_0$ from Table I and (D1), we compute

$$\begin{aligned}\frac{(l+1)^2}{2l+1}A_l&=\frac{(l+1)^2}{2l+1}(\Psi_l,\Psi_l)\\&=(\Psi_l,\hat{C}_0\Psi_{l+1})\\&=(\hat{C}_0\Psi_l,\Psi_{l+1})\\&=\frac{(l+1)^2}{2l+3}(\Psi_{l+1},\Psi_{l+1})\\&=\frac{(l+1)^2}{2l+3}A_{l+1},\end{aligned} \tag{D2}$$

from which by induction $A_l=(2l+1)A_0$. ■

APPENDIX E: CONVERGENCE OF THE GROUP AVERAGING

In this appendix we provide the group averaging convergence results needed in the main text. When not mentioned otherwise, p and q are arbitrary positive integers.

To begin, consider $U(g)\Psi_{ljmnk_uk_v}$. Writing g in the Iwasawa decomposition (A3), (4.2) gives

$$U(g)=\exp(-i\mu\hat{H}_2)\exp(-i\lambda\hat{D})\exp(-i\theta(\hat{H}_1-\hat{H}_2)). \tag{E1}$$

As $\Psi_{ljmnk_uk_v}$ is an eigenstate of $\hat{H}_1-\hat{H}_2$ with eigenvalue E_u-E_v, (4.3) yields

$$U(g)\Psi_{ljmnk_uk_v}=\frac{z^{(\tilde{j}-\tilde{l})/2}e^{-i\theta(E_u-E_v)}}{(2\pi i\mu)^{q/2}}Y_{lk_u}(\theta^{(u)})\int_0^\infty dv'\,u^l(v')^{j+q-1}L_m^{\tilde{l}}(u^2/z)L_n^{\tilde{j}}(z(v')^2)$$
$$\times\exp\left[-\frac{1}{2}\left(\frac{u^2}{z}+z(v')^2\right)+\frac{i}{2}\left(\mu u^2+\frac{v^2+(v')^2}{\mu}\right)\right]$$
$$\times\int d\Omega_{v'}\exp\left(-\frac{i}{\mu}(\mathbf{v}\cdot\mathbf{v}')\right)Y_{jk_v}(\theta^{(v')}), \tag{E2}$$

where $z:=e^{2\lambda}$ and we are assuming $\mu\neq 0$, $\mathbf{v}\neq\mathbf{0}$ and $\mathbf{u}\neq\mathbf{0}$.

We need to evaluate the angular integral in (E2). Suppose $q>2$. We write $\mathbf{v}\cdot\mathbf{v}'=vv'\cos\gamma$ and expand the exponential under the angular integral by (Ref. 44, p. 98)

$$e^{it\cos\gamma}=\frac{1}{2}\Gamma\left(\frac{q-2}{2}\right)\sum_{a=0}^{\infty}i^a(2a+q-2)\frac{J_{(q-2+2a)/2}(t)}{(t/2)^{(q-2)/2}}C_a^{(q-2)/2}(\cos\gamma). \tag{E3}$$

We then expand the Gegenbauer polynomial $C_a^{(q-2)/2}(\cos\gamma)$ as

$$C_a^{(q-2)/2}(\cos\gamma)=\frac{4\pi^{q/2}}{\Gamma((q-2)/2)(2a+q-2)}\sum_k Y_{ak}(\theta^{(v)})\overline{Y_{ak}(\theta^{(v')})}, \tag{E4}$$

which follows from formula 11.4(2) in Ref. 43 (correcting a typographical error in the normalization factor, as seen from the final step of the proof on p. 247). Using the orthonormality of the spherical harmonics, we obtain

$$\int d\Omega_{v'}\exp\left(-\frac{i}{\mu}(\mathbf{v}\cdot\mathbf{v}')\right)Y_{jk_v}(\theta^{(v')})=(2\pi)^{q/2}i^{-j}\left(\frac{vv'}{\mu}\right)^{(2-q)/2}J_{(q-2+2j)/2}(vv'/\mu)Y_{jk_v}(\theta^{(v)}). \tag{E5}$$

For $q=2$, (E5) follows by recognizing the angular integral as a representation of J_j, and for $q=1$ it follows from the relation of $J_{\pm 1/2}$ to trigonometric functions (Ref. 43, Secs. 7.3.1 and 7.11). Hence, for all $p\geqslant 1$ and $q\geqslant 1$, we have

$$U(g)\Psi_{ljmnk_uk_v}=\frac{i^{-\tilde{j}-1}z^{(\tilde{j}-\tilde{l})/2}e^{-i\theta(E_u-E_v)}}{\mu}Y_{lk_u}(\theta^{(u)})Y_{jk_v}(\theta^{(v)})\,u^{(2-p)/2}v^{(2-q)/2}$$
$$\times\int_0^\infty dv'\,u^{\tilde{l}}(v')^{\tilde{j}+1}J_{\tilde{j}}(vv'/\mu)L_m^{\tilde{l}}(u^2/z)L_n^{\tilde{j}}(z(v')^2)$$
$$\times\exp\left[-\frac{1}{2}\left(\frac{u^2}{z}+z(v')^2\right)+\frac{i}{2}\left(\mu u^2+\frac{v^2+(v')^2}{\mu}\right)\right]. \tag{E6}$$

Performing the integral in (E6) gives (Ref. 50, formula 7.421.4)

$$U(g)\Psi_{ljmnk_uk_v}=e^{-i\theta(E_u-E_v)}z^{(\tilde{j}-\tilde{l})/2}(1+i\mu z)^{-\tilde{j}-1}\left(\frac{1-i\mu z}{1+i\mu z}\right)^n Y_{lk_u}(\theta^{(u)})Y_{jk_v}(\theta^{(v)})$$
$$\times u^l v^j L_m^{\tilde{l}}(u^2/z)\,L_n^{\tilde{j}}\left(\frac{zv^2}{1+\mu^2z^2}\right)\times\exp\left[-\frac{1}{2}\left(\frac{1}{z}-i\mu\right)u^2-\frac{1}{2}\left(\frac{z}{1+i\mu z}\right)v^2\right]. \tag{E7}$$

We can now use (E7) to prove the convergence results.

Proposition E.1: Let $\tilde{l}+\tilde{j}>0$. *Then* $(\Psi_{l'j'm'n'k_u'k_v'}, U(g)\Psi_{ljmnk_uk_v})_{\text{aux}}$ *is integrable in absolute value over* G.

Proof: It suffices to consider $l'=l$, $j'=j$, $k_u'=k_u$ and $k_v'=k_v$, for otherwise the integrand vanishes.

In $\overline{\Psi_{ljm'n'k_uk_v}}U(g)\Psi_{ljmnk_uk_v}$, we use (4.4) and (E7) and expand the product of the generalized Laguerre polynomials as a sum of numerical constants times terms of the form

$$(u^2)^{r'}(v^2)^{s'}\left(\frac{u^2}{z}\right)^{r}\left(\frac{zv^2}{1+\mu^2z^2}\right)^{s}, \tag{E8}$$

where r, s, r' and s' are non-negative integers. Integrating over **u** and **v** term by term, we find that $(\Psi_{ljm'n'k_uk_v}, U(g)\Psi_{ljmnk_uk_v})_{\text{aux}}$ is a sum of terms whose respective absolute values are numerical constants times

$$\frac{z^{(\tilde{l}+\tilde{j})/2+1+s+r'}(1+\mu^2z^2)^{(s'-s)/2}}{[(z+1)^2+\mu^2z^2]^{1+(\tilde{l}+\tilde{j}+r+r'+s+s')/2}}. \tag{E9}$$

An elementary analysis shows that sufficient conditions for (E9) to be integrable over G in the Haar measure $e^{2\lambda}\,d\lambda\,d\mu\,d\theta=\frac{1}{2}dz\,d\mu\,d\theta$ are

$$\begin{aligned}\tilde{l}+\tilde{j}+2r+2s&>0,\\ \tilde{l}+\tilde{j}+1+r+2s&>0,\end{aligned} \tag{E10}$$

which hold since $\tilde{l}+\tilde{j}>0$ by assumption. ■

Proposition E.2: Let $\tilde{l}+\tilde{j}>0$ *and* $p+q\equiv 1 \pmod 2$. *Then the value of the integral in Proposition E.1 is zero.*

Proof: As $p+q\equiv 1 \pmod 2$, G is the double cover of $\mathrm{SL}(2,\mathbb{R})$ and the range of θ in (E1) is θ is $0\leqslant\theta<4\pi$. By Proposition E.1, we may perform the integral over θ first, and the θ-dependence in (E7) shows that this integral evaluates to zero. ■

Theorem E.3: *Let* $p\geqslant 2$, $q\geqslant 2$ *and* $p+q>4$. *Then the integral in (4.8) converges in absolute value for all* $\phi_1,\phi_2\in\Phi$. *If* $p+q\equiv 1 \pmod 2$, *the value of the integral is zero.*

Proof: It suffices to consider $\phi_1,\phi_2\in\{\Psi_{ljmnk_uk_v}\}$. The inequalities on p and q imply that the conditions of Propositions E.1 and E.2 are satisfied. ■

Proposition E.4: Let $\tilde{l}>0$ *and* $\tilde{j}>0$. *Then* $\overline{\Psi_{ljm'n'k_uk_v}}U(g)\Psi_{ljmnk_uk_v}$ *is integrable in absolute value over* $G\times\mathbb{R}^{p+q}$.

Proof: In $\overline{\Psi_{ljm'n'k_uk_v}}U(g)\Psi_{ljmnk_uk_v}$, we use (4.4) and (E7), expand the product of the generalized Laguerre polynomials as in the proof of Proposition E.1 and consider the individual terms in this expansion. We now *first* take the absolute value and then integrate. The integrals over θ, $\theta^{(u)}$ and $\theta^{(v)}$ are bounded by constants, the integrals over u and v are convergent and easily performed, and an elementary analysis shows that the remaining $\int dz\,d\mu$ integral is convergent provided $\tilde{l}>0$ and $\tilde{j}>0$. ■

Theorem E.5: *Let* $p=1$, $q=3$ *and let* Φ^{mod} *be as in Sec. V B. Then the integral in (4.8) converges in absolute value for all* $\phi_1,\phi_2\in\Phi^{\text{mod}}$.

Proof: The only case not covered by Proposition E.1 is $\phi_1=\psi_{mn}$, $\phi_2=\psi_{m'n'}$.

In $\overline{\psi_{m'n'}}U(g)\psi_{mn}$, we use (5.12), (5.13) and (E7) and expand the generalized Laguerre polynomials of argument u^2/z and $zv^2/(1+\mu^2z^2)$ as polynomials in their respective arguments. Inequalities (E10) in the proof of Proposition E.1 show that it suffices to keep only the constant

terms of these polynomials. Doing this, and integrating over u_1 and $\mathbf{v}$ by 7.414.8 in Ref. 50, we obtain two terms whose absolute values are numerical constants times

$$\frac{z^2}{[(z+1)^2+\mu^2 z^2]^2}\times\left[\frac{(z-1)^2+\mu^2 z^2}{(z+1)^2+\mu^2 z^2}\right]^{(m'+n')/2}, \tag{E11}$$

which is integrable in the measure $dz\,d\mu$. ■

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On the generalized function calculus for infrared and ultraviolet singular quantum fields

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New theorems on properties of the generalized functions defined on Gelfand–Shilov's spaces S^0_α are established. These functional classes are universal for the operator realization of quantum field theories whose infrared or/and ultraviolet behavior is more singular than that of the standard Wightman quantum field theories (QFT's). The leading role in these applications is played by the notion of a carrier cone of analytic functional which generalizes and replaces the notion of support of distribution. An explicit representation for the generalized functions with a given carrier cone is obtained. It is proved that the restrictions of functionals defined on S^0_α to the spaces with smaller subscripts have the same carrier cones. The precise characterization of the relation between the carrier cones of multilinear forms with respect to their arguments and the carrier cones of their associated generalized functions is given. Applications of the obtained results to indefinite metric QFT and to nonlocal models are discussed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1695094]

I. INTRODUCTION

In this paper, we present some results concerning the generalized function classes required for the operator realization and nonperturbative investigation of quantum field theory (QFT) models with singular infrared or/and ultraviolet behavior. These classes are considerably wider than that of tempered distributions used originally for formulating the general principles of QFT,[1,2] and than those of ultradistributions corresponding to the strictly localizable Jaffe fields.[3] Moreover, they provide a means for the efficient treatment of singularities much more severe than those of hyperfunctions proposed for further elaborating the axiomatic approach and, particularly, establishing a more symmetrical relation between QFT in Minkowski space–time and Euclidean field theory.[4] The suitable test function spaces are S^β_α introduced by Gelfand and Shilov,[5] with the superscript satisfying $\beta<1$. The spaces S^0_α are minimal among them, and their dual spaces S'^0_α consisting of continuous linear functionals defined on S^0_α provide us with the most general framework for constructing the mentioned QFT models. The properties of functionals of this class are just the subject of our investigation. The theorems established below have obvious analogues for $0<\beta<1$ and the proofs are even simpler in that case. The space S'^0_α is exactly the Fourier-transformed space of Roumieu's ultradistributions[6] of class $\{k^{\alpha k}\}$ and the study of its properties is also interesting from this viewpoint.

The highly singular generalized functions have long been used in the theory of nonlocal interactions for generalizing the Wightman axiomatic approach (see, e.g., Ref. 7 for a review) as well as for constructing phenomenological models.[8] At present this is perhaps the best developed branch of nonlocal QFT which is interesting in view of a possible interplay with string theory and even proposed as an alternative to string theory.[9] There are also attempts to connect it with noncommutative field theory.[10,11] The main motivation for the study of generalized function classes S'^0_α is the desire to obtain a generalization of the distributional and hyperfunctional cal-

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culus required for the consistent quantization of gauge theories in a generic covariant gauge. The relevance of Gelfand–Shilov's spaces to this problem was first pointed out by Moschella and Strocchi.[12,13] In particular, the use of them enables one to obtain the complete operator realization[14,15] of the Wick-ordered entire functions of indefinite metric free fields that enter as building blocks in the exact solutions of some simple gauge models.

In nonlocal field theory, the singularities are ultraviolet by their nature and fields are well defined on averaging with configuration-space test functions belonging to S_α^β with a suitable $\beta<1$. On the contrary, when dealing with gauge theories and indefinite metric infrared singularities, we have to use such test functions in momentum space. In both cases, the main difficulty is that these functions are analytic and cannot vanish in any nontrivial domain. Because of this, the possibility of the proper generalization of the microcausality axiom in the former case and of the spectral condition in the latter is not immediately evident. It has been shown,[16,17] however, that an angular localizability property is preserved even for $\beta=0$ and every functional $v\in S_\alpha'^0$ has a unique minimal carrier cone which can be called the "quasisupport" of v. It is natural to use this notion for the mentioned generalizations. As shown in Ref. 18, there is an interrelation between this notion and the concept of analytic wave front set of ultradistribution. By taking this fact into account, it has been possible to construct a new derivation[18,19] of the CPT and spin-statistics theorems which covers nonlocal quantum fields with arbitrary high energy behavior. This approach was also applied[20] to Euclidean formulation of QFT without positivity[21] and an appropriate generalization of the reconstruction theorem was suggested.

However, there are several questions concerning properties of the generalized functions of the class $S_\alpha'^0$, which have not been given due attention although they are important for further developments. The aim of this paper is to give the complete and clear answers to three of them.

In Sec. II, on doing some preliminaries, we derive a structure theorem for elements of $S_\alpha'^0$ with a given carrier cone. It is well known that the structure of usual Schwartz's distributions supported by a closed set M is described by the representation

$$(v,f)=\sum_{|q|\leqslant N}\int D^q f\,\mathrm{d}\mu_q,$$

where μ_q are measures of tempered growth, whose supports can be chosen contained in M if this set satisfies some regularity conditions. This representation is widely used in applications and was generalized to ultradistributions.[6,22] An analogous representation for elements of $S'^0=S_\infty'^0$ was assumed in some works[23] on nonlocal QFT. However, as explained in Ref. 18, its rigorous derivation from the basic definitions, e.g., from those of Refs. 16 and 17 is a nontrivial task. The main difficulty in deriving such representations, which has been pointed by Komatsu[22] and is often overlooked by other authors, lies in the need of proving the equivalence of two natural but a priori different topologies on a subspace of an inductive limit, see below. To our knowledge, there is no consideration of this issue for $S_\alpha'^0$ in the existing literature. It should be emphasized that the structure theorem of Sec. II is helpful in actual applications, for instance, it is required for extending the theory of Lorentz invariant distributions to the functional classes under study, see Ref. 24.

In Sec. III we consider the relation between the carrier properties of a multilinear form w defined on $S_\alpha^0(\mathbb{R}^{d_1})\times\cdots\times S_\alpha^0(\mathbb{R}^{d_n})$ and those of the generalized function v determined by w on $S_\alpha^0(\mathbb{R}^{d_1+\cdots+d_n})$ by the nuclear theorem. In the QFT context, w is a vacuum expectation value and v is the corresponding Wightman function. If w regarded as a functional of $f_j\in S_\alpha^0(\mathbb{R}^{d_j})$, with other variables held fixed, is carried by K_j, then the product $K_1\times\cdots\times K_n$ is a carrier of v, but these two properties proved to be nonequivalent. So, the situation is distinct from the case of the usual distributions and this raises the question of what really is the relevant property of v. This point is important for the extension[20] of the Osterwalder–Schrader theory to infrared singular fields. Moreover, a similar subtlety should be taken into account in deriving the reconstruction theorem for QFT in terms of Fourier hyperfunctions. Since translating the carrier properties of w

into those of v presents difficulties and this procedure was not described anywhere, we will perform it in a simple manner, by using the uniform boundedness principle.

In Sec. IV, we show that the notion of carrier cone is independent of the index α specifying the test function space. More precisely, we prove that the restriction of $v \in S'^0_\alpha$ to any nontrivial smaller space $S^0_{\alpha'}$, $\alpha' < \alpha$, has the same carrier cones as v. Such a proof is also lacking in the literature, although this question is not only of theoretical significance but raises in concrete applications. For instance, it faces us in proving[19] that the vacuum expectation value $\langle \Phi_0, [\phi(x), \phi(x')]_{\overset{-}{(+)}} \Psi_0 \rangle$, where ϕ is a nonlocal field of the class S'^0_α with an integer (half-integer) spin, is carried by the closed cone $\{(x,x') \in \mathbb{R}^8 : (x-x')^2 \geqslant 0\}$.

We will attempt to elucidate the above questions with a minimal amount of technical work. In particular, where possible, we use the language of Hilbert space theory familiar to theoretical physicists and apply theorem quoting proofs. Some technical details are moved to the Appendix. The final section contains conclusions and outlook.

II. STRUCTURE THEOREM

We start by recalling the original definition[5] of the space $S^0_\alpha(\mathbb{R}^d)$. It consists of all smooth functions on $\mathbb{R}^d$ such that

$$|D^q f(x)| \leqslant C b^{|q|} e^{-|x/a|^{1/\alpha}}, \tag{1}$$

where C, a, b are positive constants depending on f. The choice of norm in $\mathbb{R}^d$ is inessential here because all these norms are equivalent, and it can be adapted to each specific application. The space is nontrivial for $\alpha > 1$ only, and this condition is supposed to be met throughout what follows. The definition of $S^0_\alpha(\mathbb{R}^d)$ can be reformulated in terms of complex variables since every element of this space allows an analytic continuation to the whole of $\mathbb{C}^d$ and the resulting entire functions satisfy the estimate $|f(x+iy)| \leqslant C \exp\{-|x/a|^{1/\alpha} + b|y|\}$. Analogous spaces can be associated[16,17] with cones in $\mathbb{R}^d$. Namely, if $U \subset \mathbb{R}^d$ is an open cone, then $S^0_\alpha(U)$ is defined to be the space of all smooth functions on $\mathbb{R}^d$ satisfying (1) for $x \in U$. It is natural to regard this space as the inductive limit of the Banach spaces $S^{0,b}_{\alpha,a}(U)$ whose norms are defined by

$$\|f\|_{U,a,b} = \sup_{x \in U} \sup_{q \in \mathbb{Z}^d_+} |b^{-|q|} \partial^q f(x)| \, e^{|x/a|^{1/\alpha}}, \tag{2}$$

where $\mathbb{Z}_+$ is the set of non-negative integers. This limit coincides with that of the Banach spaces $E^{0,b}_{\alpha,a}(U)$ of entire functions endowed with the norms

$$\|f\|'_{U,a,b} = \sup_{z \in \mathbb{C}^d} |f(z)| \exp\{|x/a|^{1/\alpha} - b\,\delta_U(x) - b|y|\} \quad (z = x+iy), \tag{3}$$

where $\delta_U(x)$ is the distance of x from U.

A closed cone $K \subset \mathbb{R}^d$ is said to be a carrier of $v \in S'^0_\alpha$ if v can be continuously extended to each of $S^0_\alpha(U)$, where $U \supset K \setminus \{0\}$. (If this inclusion holds, we say that K is compact in U and use also the notation $U \ni K$.[25]) Taking into account that S^0_α is dense in every space $S^0_\alpha(U)$,[17] this means that v belongs to the dual space of the inductive limit $S^0_\alpha(K) = \varinjlim_{U \ni K} S^0_\alpha(U)$, which is identified with a vector subspace of S'^0_α. In order to gain a better insight into the construction of Sec. III, we remark that $\{U : U \ni K\}$ is a directed set and $S^0_\alpha(U)$ is an increasing family of spaces only if the closed cone K is nondegenerate. For the degenerate cone consisting of the origin, its associated space $S^0_\alpha(\{0\})$ is the space of all entire analytic functions of order 1 and finite type, i.e., satisfying the estimate $|f(z)| \leqslant C e^{b|z|}$, $z \in \mathbb{C}^d$. By Theorem 6 of Ref. 16 every element $f \in S^0_\alpha(\{0\})$ allows the decomposition $f = f_+ + f_-$, where $f_\pm \in S^0_\alpha(U_\pm)$ and $U_\pm$ are arbitrary open

cones such that $\overline{U}_+ \cap \overline{U}_- = \{0\}$. Because of this, the inductive topology on $S^0_\alpha(\{0\})$ determined by the canonical injections $S^0_\alpha(U) \to S^0_\alpha(\{0\})$, where U runs through all open cones, coincides with that determined by the two injections $S^0_\alpha(U_\pm) \to S^0_\alpha(\{0\})$.

The space $S^0_\alpha(U)$ can also be represented[16] as the inductive limit of the Hilbert spaces $H^{0,b}_{\alpha,a}(U)$ of entire functions with the scalar products

$$\langle f, g\rangle_{U,a,b} = \int \overline{f(z)}\, g(z)\, e^{2(|x/a|^{1/\alpha} - b\,\delta_U(x) - b|y|)}\, \mathrm{d}x\, \mathrm{d}y. \tag{4}$$

As a consequence, it is a nuclear DFS space, i.e., strong dual of a nuclear Fréchet–Schwartz space. Spaces of this type, for which the abbreviation DFN is also used, have nice topological properties convenient in applications and exploited below. In particular, we will use Pták's version[26] of the open mapping theorem, which shows that every continuous linear mapping of a DFS space onto a barrelled space is open. Clearly, an analogous representation is possible in terms of real variables and that is just what we need now. Let $L^{0,b}_{\alpha,a}(U)$ be the space of all infinitely differentiable functions on $\mathbb{R}^d$ for which the norm corresponding to the scalar product

$$(f, g)_{U,a,b} = \sum_q\ b^{-2|q|} \int_U \overline{\partial^q f(x)}\, \partial^q g(x)\, e^{2|x/a|^{1/\alpha}}\, \mathrm{d}x \tag{5}$$

is finite.

Lemma 1: For any open cone U, the space $S^0_\alpha(U)$ coincides with the inductive limit $\lim_{\to} L^{0,b}_{\alpha,a}(U)$ $(a,b \to \infty)$.

For the proof we refer to Appendix A.

Theorem 1: *Let U be an open cone in $\mathbb{R}^d$. Every $v \in S'^0_\alpha(U)$ can be written as*

$$v(f) = \sum_q\ \int_U v_q(x)\, \partial^q f(x)\, \mathrm{d}x, \tag{6}$$

where v_q are locally integrable functions satisfying the condition

$$\sum_q\ b^{|q|} \int_U |v_q(x)|\, e^{-|x/a|^{1/\alpha}}\, \mathrm{d}x < \infty \quad \textit{for all} \quad a,b>0. \tag{7}$$

In particular, such a representation is valid for any functional of class S'^0_α whose quasisupport is contained in $U \cup \{0\}$.

Proof: Lemma 1 enables us to reduce the derivation of this representation to Riesz's theorem characterizing the dual of a Hilbert space. At first we replace the exponential that occurs in definition (5) by the function $(1+|x|)^{-2d} \Sigma_{k \in \mathbb{Z}^d_+} x^{2k} a^{-2|k|} k^{-2\alpha k}$. This leaves the limit space $\lim_{\to} L^{0,b}_{\alpha,a}(U)$ unaltered because

$$c \exp\left(\frac{2\alpha}{e} \sum_{j=1}^d |x_j|^{1/\alpha}\right) \leqslant \sum_k \frac{x^{2k}}{k^{2\alpha k}} \leqslant C_\epsilon \exp\left(\frac{2\alpha}{e} \sum_{j=1}^d |(1+\epsilon)x_j|^{1/\alpha}\right),$$

where $\epsilon > 0$ can be taken arbitrarily small. For the spaces modified in such a way, we keep the same notation $L^{0,b}_{\alpha,a}(U)$ and introduce another family of Hilbert spaces. Namely, let $\mathcal{L}^{0,b}_{\alpha,a}(U)$ be the space consisting of twice multi-indexed sequences $F = \{f_{kq}\}$ of square-integrable functions on U and endowed with the scalar product

$$(G, F)_{U,a,b} = \sum_{k,q}\ a^{-2|k|} b^{-2|q|} k^{-2\alpha k} \int_U \overline{g_{kq}(x)}\, f_{kq}(x)\, \mathrm{d}x. \tag{8}$$

Then $L^{0,b}_{\alpha,a}(U)$ is identified with a subspace of $\mathcal{L}^{0,b}_{\alpha,a}(U)$ by means of the mapping

$$i: f \to f_{kq} = (1+|x|)^{-d} x^k \partial^q f. \tag{9}$$

This subspace, being complete, is evidently closed. Let us provide the image of $\varinjlim L^{0,b}_{\alpha,a}(U)$ in $\varinjlim \mathcal{L}^{0,b}_{\alpha,a}(U)$ with the topology induced by that of the latter space.

Lemma 2: The space $\varinjlim L^{0,b}_{\alpha,a}(U)$ *has the same continuous dual space as the subspace* $i(\varinjlim L^{0,b}_{\alpha,a}(U))$ *of* $\varinjlim \mathcal{L}^{0,b}_{\alpha,a}(U)$.

Proof: For brevity we introduce the designations,

$$L_\nu = L^{0,\nu}_{\alpha,\nu}(U), \quad \mathcal{L}_\nu = \mathcal{L}^{0,\nu}_{\alpha,\nu}(U) \quad (\nu = 1,2,\dots), \quad L = \varinjlim L_\nu, \quad \mathcal{L} = \varinjlim \mathcal{L}_\nu.$$

Since the unit closed ball in a Hilbert space is weakly compact, the continuous injections $\mathcal{L}_\nu \to \mathcal{L}_{\nu+1}$ are evidently weakly compact. Therefore the statement of interest follows from Theorem 7 of Ref. 27. To apply it, we only need to verify that L is closed in $\mathcal{L}$. Let $F \in \mathcal{L}_\mu \backslash L$. Since L_μ is closed in $\mathcal{L}_\mu$, there exists a ball $\mathcal{B}_\mu = \{G \in \mathcal{L}_\mu : \|G\|_\mu \leqslant \epsilon\}$ such that $(F+\mathcal{B}_\mu) \cap L_\mu = \varnothing$. The mapping $\mathcal{L}_\mu \to \mathcal{L}_{\mu+1}$ is continuous under the weak topologies, therefore $\mathcal{B}_\mu$ is weakly compact not only in $\mathcal{L}_\mu$ but also in $\mathcal{L}_{\mu+1}$. The subspace $L_{\mu+1}$ does not meet $F+\mathcal{B}_\mu$, because $L_{\mu+1} \cap \mathcal{L}_\mu = L_\mu$, and so $0 \notin F+\mathcal{B}_\mu+L_{\mu+1}$. Furthermore $L_{\mu+1}$ is weakly closed in $\mathcal{L}_{\mu+1}$ since subspaces have the same closure under any topology consistent with duality. By Theorem I.1.1 of Ref. 26, the set $F+\mathcal{B}_\mu+L_{\mu+1}$ is also weakly closed. Hence, there is a ball $\mathcal{B}_{\mu+1} = \{G \in \mathcal{L}_{\mu+1} : \|G\|_{\mu+1} \leqslant \epsilon_1\}$ such that $\mathcal{B}_{\mu+1} \cap (F+\mathcal{B}_\mu+L_{\mu+1}) = \varnothing$ or, equivalently, $(F+\mathcal{B}_\mu+\mathcal{B}_{\mu+1}) \cap L_{\mu+1} = \varnothing$. The set $\mathcal{B}_\mu+\mathcal{B}_{\mu+1}$ is absolutely convex and weakly compact in $\mathcal{L}_{\mu+1}$ as well as in $\mathcal{L}_{\mu+2}$. We proceed along the same lines and obtain an increasing sequence of absolutely convex neighborhoods $\mathcal{U}_\nu$ of F in the spaces $\mathcal{L}_\nu$, $\nu \geqslant \mu$, such that $\mathcal{U}_\nu$ are disjoint with L_ν. The subspace L does not meet their union which is a neighborhood of F in $\mathcal{L}$ by the definition of inductive topology. Therefore, L is indeed closed in $\mathcal{L}$ and Lemma 2 is proved.

Thus, every $v \in S'^0_\alpha(U)$ may be regarded as a continuous linear form on a subspace of $\varinjlim \mathcal{L}^{0,b}_{\alpha,a}(U)$ and, by the Hahn–Banach theorem, it has a continuous extension $\hat{v}$ to the whole space. Now the Riesz theorem shows that, for every a and b, there is a unique $G \in \mathcal{L}^{0,b}_{\alpha,a}(U)$ such that $\hat{v}(F) = (G,F)_{U,a,b}$ for all $F \in \mathcal{L}^{0,b}_{\alpha,a}(U)$. Using the designation $h_{kq} = a^{-2|k|} b^{-2|q|} k^{-2\alpha k} g_{kq}$, this may be rewritten as

$$\hat{v}(F) = \sum_{k,q} \int_U \overline{h_{kq}(x)} f_{kq}(x)\, \mathrm{d}x\,. \tag{10}$$

The functions h_{kq} belong to $L^2(U)$ and do not depend on a and b. In fact, each of h_{kq} is entirely determined by the values of $\hat{v}$ on those F all of whose components are zero except f_{kq} which is an arbitrary element of $L^2(U)$, and all such F's are contained in every space $\mathcal{L}^{0,b}_{\alpha,a}(U)$. Substituting the specified F's in (10), setting $f_{kq} = h_{kq}$ and using the continuity of $\hat{v}$ on $\mathcal{L}^{0,b}_{\alpha,a}(U)$, we obtain

$$|\hat{v}(h_{kq})| = \|h_{kq}\|^2_{L^2(U)} \leqslant C\|h_{kq}\|_{U,a,b} = Ca^{-|k|} b^{-|q|} k^{-\alpha k} \|h_{kq}\|_{L^2(U)}\,. \tag{11}$$

Taking into account that (11) holds for any positive a and b (although with different constants C), we can change a for $2a$ and b for $2b$ and obtain

$$\sum_{k,q} a^{|k|} b^{|q|} k^{\alpha k} \|h_{kq}\|_{L^2(U)} < \infty, \tag{12}$$

which again is valid for all a, b. When being applied to elements of the initial space by the embedding rule (9), Eq. (10) takes the form

$$v(f)=\sum_{k,q}\int x^k v_{kq}(x)\,\partial^q f(x)\,\mathrm{d}x, \tag{13}$$

where $v_{kq}(x)\overset{\text{def}}{=}(1+|x|)^{-d}\overline{h_{kq}(x)}$. These functions are integrable on U and, applying Schwarz's inequality, we see that (12) holds true after replacing $\|h_{kq}\|_{L^2(U)}$ by $\|v_{kq}\|_{L^1(U)}$. Then making use of the inequality $k^{\alpha k}/|x^k|\geqslant\exp\{-(\alpha d/e)|x|^{1/\alpha}\}$, we conclude that

$$\sum_{k,q} b^{|q|}\int |x^k v_{kq}(x)|\,e^{-|x/a|^{1/\alpha}}\,\mathrm{d}x<\infty,$$

where a and b are arbitrary positive numbers as before. By Levi's theorem, the convergence of the number series $\Sigma_k\int|x^k v_{kq}|\exp\{-|x/a|^{1/\alpha}\}\,\mathrm{d}x$ implies that the series $\Sigma_k|x^k v_{kq}|$ converges almost everywhere to a function integrable with the weight $\exp\{-|x/a|^{1/\alpha}\}$. Calling this function v_q and performing the k summation in (13), which is possible by the same argument, we arrive at (7) and finish the proof.

The above derivation is vastly simplified in the case of functionals carried by the origin. By means of the mapping $f\to f_q=\partial^q f(0)$, the space $S^0_\alpha(\{0\})$ is identified with the inductive limit of the Hilbert spaces whose elements are sequences of complex numbers satisfying $\Sigma b^{-|q|}|f_q|^2<\infty$. Therefore, every $v\in S'^0_\alpha(\{0\})$ can be written as $\Sigma v_q\partial^q\delta(x)$. Clearly, the analogue of (7) is of the form $\lim_{|q|\to\infty}|v_q|^{1/|q|}=0$. This simple fact is helpful, for instance, in proving[24] that every Lorentz invariant functional $v\in S'^0_\alpha(\mathbb{R}^4)$ carried by the closed light cone $\overline{\mathbb{V}}$ admits a Lorentz invariant splitting into two functionals of the same class with carriers $\overline{\mathbb{V}}_+$ and $\overline{\mathbb{V}}_-$.

Remark 1: Komatsu's theorem[27] is called for the derivation of representation (6) because in general the topology induced on a subspace by an inductive limit topology is different from the inductive limit of induced topologies. That theorem shows that the discrepancy between these topologies is unessential in the case of injective limits of weakly compact sequences of locally convex spaces. The replacement of the Banach spaces with the original norms (2) by an equivalent sequence of Hilbert spaces makes it possible to exploit this property. We could show that $S^0_\alpha(U)$ is topologically isomorphic to its image in $\varinjlim\mathcal{L}^{0,b}_{\alpha,a}(U)$, but there is no need to appeal to this more subtle fact here.

Remark 2: The case $\beta>0$ differs only by the additional factor $q^{\beta q}$ on the right-hand sides of the analogues of (6) and (7). When $\beta>1$, the use of measures instead of integrable functions is preferable, because their supports can be chosen contained in $\operatorname{supp} v$. However, this gives no advantage in the nonlocalizable case $\beta<1$. The results of the next section show that not every $v\in S'^0_\alpha(K)$ admits a representation like (6) with measures supported by K.

When applied to the vacuum expectation values in QFT's with singular infrared or ultraviolet behavior, Theorem 1 exhibits their structure and distinguishing features as opposed to those of the usual Wightman functions.[1,2] In extending the axiomatic approach to fields whose infrared singularities violate positivity, it is natural to assume that the Wightman functions $w_n(x_1,\ldots,x_n)$ are well defined as ultradistributions of class $\{k^{\alpha k}\}$ with a suitable α. Then the most general formulation of spectral condition is the requirement that the Fourier transforms of the functionals W_n related to the translation invariant w_n's by $W_{n-1}(x_1-x_2,\ldots,x_{n-1}-x_n)=w_n(x_1,\ldots,x_n)$ be carried by the closed cone $\overline{\mathbb{V}}_+^{(n-1)}$, where $\overline{\mathbb{V}}_+=\{p\in\mathbb{R}^4: p^2\geqslant 0, p_0\geqslant 0\}$. A Paley–Wiener–Schwartz-type theorem[17] shows that this condition makes possible the analytic continuation of the Wightman functions into the usual domains containing Euclidean points and moreover, it is the weakest one ensuring such an analyticity. On the other hand, dealing with nonlocal ultraviolet singular fields $\{\phi_\iota\}$ defined on $S^0_\alpha(\mathbb{R}^4)$ in configuration representation, we say that ϕ_ι and $\phi_{\iota'}$ commute (anticommute) asymptotically for large spacelike separations of their arguments if the functional $\langle\Phi,[\phi_\iota(x),\phi_{\iota'}(x')]_{-\atop(+)}\Psi\rangle$ is carried by the closed cone

$$\{(x,x') \in \mathbb{R}^8 : (x-x')^2 \geqslant 0\} \tag{14}$$

for any Φ, Ψ belonging to the cyclic space D_0 generated from the vacuum by polynomials in the fields $\{\phi_\iota\}$. Theorem 1 clarifies, in particular, the relation between the asymptotic commutativity and some other generalizations of local commutativity which were proposed for extending the PCT and spin-statistics theorems to nonlocal fields. In particular, a representation similar to (6) was assumed and exploited[23] for functionals defined on $S^0 = S^0_\infty$. However this space is not a DFS space and has more complicated topological structure, which leaves open the question of rigorous derivation of that representation. From a technical point of view, the employment of S^0_α is more convenient and in this respect it is desirable to be sure that the restriction of $v \in S'^0$ to S^0_α has the same carrier cones as v. Below we argue that this is the case.

III. CARRIERS OF FUNCTIONALS DEFINED BY MULTILINEAR FORMS

The theory of multilinear forms on products of test function spaces is important for the applications of interest because the vacuum expectation values of quantum fields are just such forms. As known, in the standard axiomatics[1,2] these are uniquely extendable to tempered distributions by Schwartz's nuclear theorem and the content of theory can be reformulated in terms of these Wightman distributions. We want to show that such a possibility is preserved in the more general framework of spaces S^0_α and then we face the problem of continuous extension of multilinear forms to the completions of their domains in a weaker topology. This matter is much more complicated than continuous extension of linear forms (see, e.g., Ref. 26) but we will show that in our case it suffices to use the barrelledness of S^0_α. This property is practically equivalent to the applicability of the uniform boundedness principle which is well known in the theory of Hilbert spaces. It is inherited by inductive topologies and because of this the spaces S^0_α, being the inductive limits of Hilbert spaces, possess this property. A subtlety is that S^0_α are nonmetrizable and we cannot identify topological properties with their sequential form. When A and B are sets in a nonmetrizable topological space, we say that A is sequentially dense in B if every point of B is the limit of a sequence lying in A and convergent in the topology of this space.

Lemma 3: If L is a sequentially dense subspace of a locally convex space E_1 and E_2 is a barrelled space, then every bilinear separately continuous form w defined on $L \times E_2$ has a unique extension to $E_1 \times E_2$ which is bilinear and separately continuous.

Proof: For each fixed $g \in E_2$, the form $w(f,g)$ can be uniquely extended to E_1 by continuity. Letting $\hat{w}$ denote this extension, we have to show that it is linear and continuous in g for each fixed $f \in E_1$. That is just what is ensured by the barrelledness of E_2, because if $f_\nu \in L$, $f_\nu \to f$, then regarding f_ν as elements of E_2' [whose values on g are $w(f_\nu,g)$] and applying Theorem 4.6 of Ref. 26, we see that their pointwise convergence to $f(g) = w(f,g)$ implies that $f(g)$ is also an element of E_2'.

We now note that every multilinear separately continuous form w on $S^0_\alpha(U_1) \times \cdots \times S^0_\alpha(U_n)$ defines a unique linear functional $v \in S'^0_\alpha(U_1 \times \cdots \times U_n)$ such that

$$w(f_1, \ldots, f_n) = v(f_1 \otimes \cdots \otimes f_n), \quad f_j \in S^0_\alpha(U_j)\,. \tag{15}$$

In the case of bilinear forms, this is an immediate consequence of the relation[17]

$$S^0_\alpha(U_1) \hat{\otimes}_\iota S^0_\alpha(U_2) = S^0_\alpha(U_1 \times U_2), \tag{16}$$

where the index ι indicates that the tensor product space is equipped with the inductive topology and the hat means the corresponding completion. Under this topologization, the dual space of the tensor product is canonically identified with the space of bilinear separately continuous forms.[26] In the general case of multilinear forms, we may use the corresponding generalization of formula (16), derivable analogously. It perhaps should be noted that for DFN spaces the binary operation $\hat{\otimes}_\iota$ is associative and this gives another way for drawing the same conclusion.

Theorem 2: *Let K_j be closed cones in $\mathbb{R}^{d_j}$, $j=1,\dots n$, and let w be a multilinear separately continuous form on $S^0_\alpha(\mathbb{R}^{d_1})\times\cdots\times S^0_\alpha(\mathbb{R}^{d_n})$ with the following property:*

(∗) *For every j, the cone K_j is a carrier of all the linear functionals on $S^0_\alpha(\mathbb{R}^{d_j})$ that are determined by $w(f_1,\dots,f_n)$ with the arguments $f_i, i\neq j$, held fixed.*

Then the functional v defined by w in $S'^0_\alpha(\mathbb{R}^{d_1+\cdots+d_n})$ is carried by the cone $K_1\times\cdots\times K_n$.

Proof: For the sake of simplicity, we set $d_j=d$ for all j. It suffices to show that every cone $\mathbb{R}^{d(j-1)}\times K_j\times\mathbb{R}^{d(n-j)}$ is a carrier of v, because then their intersection is also a carrier by Theorem 2 of Ref. 16. We put $j=1$ without loss of generality. Let $n=2$ and let U_1 be an open cone in $\mathbb{R}^d$ such that $K_1\Subset U_1$. According to Theorem 5 of Ref. 17, every element of $S^0_\alpha(U_1)$ can be approximated by elements of some $H^{0,b}_{\alpha,a}(\mathbb{R}^d)$ in the norm of $H^{0,b}_{\alpha,a}(U_1)$. So, by Lemma 3, w can be extended to a bilinear separately continuous form on $S^0_\alpha(U_1)\times S^0_\alpha(\mathbb{R}^d)$. This form in turn determines a continuous linear functional on $S^0_\alpha(U_1\times\mathbb{R}^d)$, which is an extension of v because $S^0_\alpha(\mathbb{R}^d)\otimes S^0_\alpha(\mathbb{R}^d)$ is dense in in $S^0_\alpha(\mathbb{R}^{2d})$. Thus, v allows a continuous extension even to a space larger than $S^0_\alpha(K_1\times\mathbb{R}^d)$ since, for every open cone U in which $K_1\times\mathbb{R}^d$ is compact, there is a U_1 such that $U_1\times\mathbb{R}^d\subset U$, but the converse is not in general true. Next we use the induction on n. Consider an n-linear form w $(n>2)$ as bilinear on $L\times E_2$, where $L=\overset{n-1}{\otimes} S^0_\alpha(\mathbb{R}^d)$ and $E_2=S^0_\alpha(\mathbb{R}^d)$. By the induction hypothesis, it is separately continuous under the topology induced on L by that of $S^0_\alpha(U_1\times\mathbb{R}^{d(n-2)})$. Every element of the latter space can be approximated by elements of L in the norm of $H^{0,b}_{\alpha,a}(U_1\times\mathbb{R}^{d(n-1)})$ with a and b large enough. This follows from the same approximation theorem combined with Lemma 1 of Ref. 17 which shows that, for any pair of open cones, $H^{0,b}_{\alpha,a}(U_1\times U_2)=H^{0,b}_{\alpha,a}(U_1)\otimes H^{0,b}_{\alpha,a}(U_2)$ with the Hilbert tensor product on the right. Applying Lemma 3 again, we conclude that v has a continuous extension to $S^0_\alpha(U_1\times\mathbb{R}^{d(n-1)})$ and so the cone $K_1\times\mathbb{R}^{d(n-1)}$ is a carrier of v as was to be proved.

In order to characterize precisely those elements of $S'^0_\alpha(\mathbb{R}^{d_1+\cdots+d_n})$ that are generated by the multilinear forms with property (∗), we use the following definition.

Definition: Let K_j be closed cones in $\mathbb{R}^{d_j}$, $j=1,\dots,n$. We denote by $S^0_\alpha(K_1,\dots,K_n)$ the linear span of the images of the canonical mappings $S^0_\alpha(U_1\times\cdots\times U_n)\to S^0_\alpha(\{0\})$, where U_j runs through the open cones in $\mathbb{R}^{d_j}$ such that $K_j\Subset U_j$, and endow it with the inductive topology by these mappings. If $v\in S'^0_\alpha(\mathbb{R}^{d_1+\cdots+d_n})$ has a continuous extension to $S^0_\alpha(K_1,\dots,K_n)$, then we say that v is multiplicatively carried by the cone $K_1\times\cdots\times K_n$.

It can be shown that this definition is equivalent to Definition 2 of Ref. 20, where the term ''strong'' was used instead of ''multiplicative'' and auxiliary spaces associated with arbitrary cones were exploited. Because of the obvious inclusion $S^0_\alpha(K_1\times\cdots\times K_n)\subset S^0_\alpha(K_1,\dots,K_n)$, any multiplicative carrier cone of a functional is its carrier cone.

Lemma 4: For any system of closed cones, $S^0_\alpha(K_1,\dots,K_n)$ is a DFN space.

Proof: It suffices to take well-known inheritance properties of DFN spaces into account. In particular, finite direct sums, quotient spaces (modulo closed subspaces) and injective limits of sequences of DFN spaces are DFN. So, the conclusion of Lemma 4 is evident if all K_j are nondegenerate, because then $S^0_\alpha(U_1\times\cdots\times U_n)$ is an increasing family equivalent to an increasing sequence. Now, let some of K_j be degenerate. We form new systems $(K'_1,\dots,K'_n)$ and $(K''_1,\dots,K''_n)$, replacing the degenerate cones by the positive orthants in the first case and by negative ones in the second case and leaving the other cones unchanged. From the decomposition theorem of Ref. 16, it follows that every element of $S^0_\alpha(K_1,\dots,K_n)$ can be decomposed into a sum of functions belonging to $S^0_\alpha(K'_1,\dots,K'_n)$ and $S^0_\alpha(K''_1,\dots,K''_n)$. When being endowed with the inductive topology with respect to the latter spaces, $S^0_\alpha(K_1,\dots,K_n)$ becomes a DFN space, because then it is identified with a quotient space of direct sum of two DFN spaces, and this topology coincides with the original one by the open mapping theorem.

It is not difficult to show that $S^0_\alpha(K_1\times\cdots\times K_n)=S^0_\alpha(K_1,\dots,K_n)$ only in the two trivial cases when all K_j are degenerate or when $K_j=\mathbb{R}^{d_j}$ for all j, and only then their duals coincide because DFN spaces are reflexive. The proof of this assertion is beyond the scope of the present paper, but we give a simple explaining example. Namely, let $K_1=\mathbb{R}$ and let K_2 be the nonpositive semiaxis $\overline{\mathbb{R}}_-$. Clearly $e^z\in S^0_\alpha(\mathbb{R}_-)$ for any $\alpha>1$ and $f_1(z_1)\,e^{z_2}\in S^0_\alpha(\mathbb{R},\overline{\mathbb{R}}_-)=S^0_\alpha(\mathbb{R}\times\mathbb{R}_-)$ for every f_1

$\in S^0_\alpha(\mathbb{R})$. According to Ref. 5, the space $S^0_\alpha(\mathbb{R})$ contains a non-negative function f_0 such that $f_0(0)>0$ and $|f_0(x+iy)|\leqslant e^{-2|x|^{1/\alpha}+|y|}$. The convolution $f_1(x)=\int e^{-|\xi|^{1/\alpha}} f_0(x-\xi)\,\mathrm{d}\xi$ also belongs to $S^0_\alpha(\mathbb{R})$ and satisfies the lower bound

$$f_1(x)\geqslant \int_{-1}^{+1} e^{-|x-\xi|^{1/\alpha}} g_\alpha(\xi)\,\mathrm{d}\xi \geqslant e^{-(|x|+1)^{1/\alpha}} \int_{-1}^{+1} g_\alpha(\xi)\,\mathrm{d}\xi \geqslant c\, e^{-|x|^{1/\alpha}}. \tag{17}$$

The estimate (17) shows that the function $f_1(z_1)\,e^{z_2}$ increases indefinitely along each of the real rays lying in the half-plane $x_2>0$ and hence does not belong to any space $S^0_\alpha(U)$, where $U\ni\mathbb{R}\times\overline{\mathbb{R}}_-$. It follows that $S'^0_\alpha(\mathbb{R},\overline{\mathbb{R}}_-)\neq S'^0_\alpha(\mathbb{R}\times\overline{\mathbb{R}}_-)$.

Theorem 3: *A functional $v\in S'^0_\alpha(\mathbb{R}^{d_1+\cdots+d_n})$ is generated by a multilinear form on $S^0_\alpha(\mathbb{R}^{d_1})\times\cdots\times S^0_\alpha(\mathbb{R}^{d_n})$ with property $(*)$ if and only if it has a continuous extension to $S^0_\alpha(K_1,\ldots,K_n)$.*

Proof: We may use the l-norm $|x|=\Sigma|x_j|$ in $\mathbb{R}^{d_1+\cdots+d_n}$ and substitute $\Sigma|x_j|^{1/\alpha}$ for $|x|^{1/\alpha}$ in definition (3). Then $\delta_{U_1\times\cdots\times U_n}(x)=\Sigma\,\delta_{U_j}(x)$ and the indicator function defined by the exponential in (3) is multiplicative. It follows that the mapping $f_j\to f_1\otimes\cdots\otimes f_j\otimes\cdots\otimes f_n$ from $S^0_\alpha(U_j)$ to $S^0_\alpha(U_1\times\cdots\times U_n)$ is continuous and hence the multilinear forms that correspond to functionals in $S'^0_\alpha(K_1,\ldots,K_n)$ possess property $(*)$. To derive the converse implication $(*)\Rightarrow v\in S'^0_\alpha(K_1,\ldots,K_n)$, which is the main point of the theorem under discussion, we need two lemmas.

Lemma 5: Let U_1, U_2, and U be open cones in $\mathbb{R}^{d_1}$, $\mathbb{R}^{d_2}$, and $\mathbb{R}^d$, respectively, and let $V_1\Subset U_1$, $V_2\Subset U_2$. Then every function $f\in S^0_\alpha(U_1\times U_2\times U)$ allows a decomposition of the form $f=f_1+f_2$, where $f_1\in S^0_\alpha(V_1\times\mathbb{R}^{d_2}\times U)$ and $f_2\in S^0_\alpha(\mathbb{R}^{d_1}\times V_2\times U)$.

This is a simplified version of Lemma 2 in Ref. 20.

Lemma 6: Let E be a vector space and let L_0, L_1, L_2 be its subspaces endowed with locally convex topologies and such that $L_0\subset L_1\cap L_2$. Assume that L_1+L_2 and $L_1\cap L_2$ are equipped with the inductive and projective topologies, respectively. If L_0 is dense in each of L_1, L_2, $L_1\cap L_2$ and the injections $L_0\to L_1$, $L_0\to L_2$ are continuous, then

$$(L_1+L_2)'=L_1'\cap L_2',$$

where the dual spaces are regarded as vector subspaces of L_0'.

Proof: Note that L_0 is dense in L_1+L_2 if it is dense in L_1 and L_2 and so the natural mapping $(L_1+L_2)'\to L_0'$ is injective along with $L_1'\to L_0'$ and $L_2'\to L_0'$. Clearly, $(L_1+L_2)'\subset L_1'\cap L_2'$ and we only need to show the converse inclusion. Let $v\in L_1'\cap L_2'$ and let v_1, v_2 be its continuous extensions to L_1, L_2. Since the projective topology on $L_1\cap L_2$ is the upper bound of the topologies induced by those of L_1 and L_2, the functionals v_1 and v_2 are continuous on $L_1\cap L_2$ and hence coincide on this subspace by the denseness condition. Therefore, the formula $\hat{v}(f_1+f_2)=v_1(f_1)+v_2(f_2)$ defines a linear extension of v to L_1+L_2 which is continuous by the definition of inductive topology.

End of the proof of Theorem 3: We again set $d_j=d$ for simplicity. Let w be a multilinear form with property $(*)$. In deriving Theorem 2, we have shown that its associated functional v belongs to $S'^0_\alpha(\mathbb{R}^{d(j-1)},K_j,\mathbb{R}^{d(n-j)})$ for every $j=1,\ldots,n$. At first assume that $K_j\neq\{0\}$ for all j. Denote by E the space $S^0_\alpha(K_1,K_2,\mathbb{R}^{d(n-2)})$ and by L_1 and L_2 the images of $S^0_\alpha(K_1,\mathbb{R}^{d(n-1)})$ and $S^0_\alpha(\mathbb{R}^d,K_2,\mathbb{R}^{d(n-2)})$ in this space. By Lemma 5, we have $E=L_1+L_2$. If the sum is endowed with the inductive topology, then this equality holds not only algebraically but also topologically by the open mapping theorem. The intersection $L_1\cap L_2$ is identified, as a set, with the inductive limit of directed family of spaces $S^0_\alpha(U)$, where U is the union of open cones $U_1\times\mathbb{R}^{d(n-1)}$ and $\mathbb{R}^d\times U_2\times\mathbb{R}^{d(n-2)}$, with U_1, U_2 running through the conic neighborhoods of K_1, K_2. By the approximation theorem,[17] S^0_α is dense in each of them and so in $L_1\cap L_2$ endowed with the inductive limit topology which is obviously stronger than the projective topology determined by the injections $L_1\cap L_2\to L_1$, $L_1\cap L_2\to L_2$. Applying Lemma 6, we conclude that $v\in S'^0_\alpha(K_1,K_2,\mathbb{R}^{d(n-2)})$. Repeating the same line of argument, we obtain v

$\in S'^{0}_{\alpha}(K_1,K_2,K_3,\mathbb{R}^{d(n-3)})$ and so on. Now, let some of K_j be degenerate. Then we set $E=S^0_\alpha(K_1,\ldots,K_n)$, $L_1=S^0_\alpha(K'_1,\ldots,K'_n)$, and $L_2=S^0_\alpha(K''_1,\ldots,K''_n)$, where the systems of cones are defined in Lemma 4. From what has been said, it follows that $v\in L'_1\cap L'_2$ and applying Lemma 6 completes the proof.

It should be noted that in the usual case of tempered distributions on $\mathbb{R}^{d_1}\times\cdots\times\mathbb{R}^{d_n}$, the situation is quite different because the projections of their supports onto $\mathbb{R}^{d_j}$ certainly contain supports of those distributions that are obtained by fixing the other arguments. Clearly, this difference has its origin in using the conic neighborhoods (in other words, the radial compactification of $\mathbb{R}^d$) in the definition of carrier cones of the functionals belonging to $S'^{0}_{\alpha}(\mathbb{R}^d)$.

When applied to nonlocal fields defined on the test function space $S^0_\alpha(\mathbb{R}^4)$, Theorems 2 and 3 enable one to express the asymptotic commutativity condition stated in Sec. II in terms of the corresponding generalized Wightman functions on $S^0_\alpha(\mathbb{R}^{4n})$. Namely, the functional defined by

$$\langle\Psi_0,\phi_{\iota_1}(x_1)\cdots\phi_{\iota_{k-1}}(x_{k-1})[\phi_{\iota_k}(x_k),\phi_{\iota_{k+1}}(x_{k+1})]_{\substack{-\\(+)}}\phi_{\iota_{k+2}}(x_{k+2})\cdots\phi_{\iota_n}(x_n)\Psi_0\rangle,$$

where the sign $-$ or $+$ corresponds to the type of commutation relation between ϕ_{ι_k} and $\phi_{\iota_{k+1}}$, is carried and even multiplicatively carried by the cone $\mathbb{R}^{4(k-1)}\times\mathbb{V}^8\times\mathbb{R}^{4(n-k-1)}$, with $\mathbb{V}^8$ defined by (14). As a consequence, that condition is actually fulfilled on a larger domain D_1 spanned by the vacuum Ψ_0 and all vectors of the form

$$\int \phi_{\iota_1}(x_1)\ldots\phi_{\iota_n}(x_n)\,f(x_1,\ldots,x_n)\;\mathrm{d}x_1\cdots\mathrm{d}x_n\,\Psi_0\quad(n=1,2,\ldots),$$

where $f\in S^0_\alpha(\mathbb{R}^{4n})$. The notion of multiplicative carrier cone is particularly essential for formulating the spectral condition for the quantum fields whose infrared singularities violate positivity and, specifically, for generalizing the Osterwalder–Schrader theorem to such QFT's.[20] The employment of this notion results in effective estimates for the Schwinger functions and enables one to develop Euclidean formulation in complete analogy to the usual case of tempered distribution fields. It is significant that the spectral condition stated in such a way is fulfilled for the Wick ordered entire functions of indefinite metric free fields.

IV. INDEPENDENCE OF THE QUASISUPPORT FROM THE INDEX α

Theorem 4: *Let $v\in S'^{0}_{\alpha}$ and let $1<\alpha'<\alpha$. If the restriction $v|S^0_{\alpha'}$ is carried by a closed cone K, then so is v.*

Proof: This statement, combined with the obvious converse implication, can be expressed by the relation

$$S'^{0}_{\alpha}\cap S'^{0}_{\alpha'}(K)=S'^{0}_{\alpha}(K),\tag{18}$$

where all the spaces are regarded as vector subspaces of $S'^{0}_{\alpha'}$, which is permissible by the approximation theorem.[17] For $K=\{0\}$, equality (18) is valid by definition and the cone K will henceforth be assumed nontrivial. We begin by deriving the dual formula

$$S^0_\alpha(K)=S^0_\alpha+S^0_{\alpha'}(K)\tag{19}$$

and then apply Lemma 6. Let $f\in E^{0,b}_{\alpha,1}(U)$, $U\ni K$. [Taking advantage of the dilation invariance of the spaces involved, we set $a=1$ without loss of generality. From now on, we shall also use the Euclidean norm in $\mathbb{R}^d$ and the system of norms (3) dropping the prime.] Choose a non-negative function $\chi_0\in C^\infty_0$ with support in the ball $B_\epsilon=\{x:|x|<\epsilon\}$ and such that $\int\chi_0(x)\,\mathrm{d}x=1$ and set

$$\chi(x)=\int_U\chi_0(x-\xi)\,\mathrm{d}\xi.$$

Let us consider the decomposition

$$f=f_1+f_2,\quad f_1(z)=f(z)\chi(x),\quad f_2(z)=f(z)(1-\chi(x)).$$

The functions f_1 and f_2 are not analytic but behave properly at infinity of $\mathbb{C}^d$. Indeed, we have

$$|f_1(z)|\leqslant\|f\|_{U,1,b}\exp\{-|x|^{1/\alpha}+b|y|+b\epsilon\} \tag{20}$$

since $\delta_U(x)\leqslant\epsilon$ for $x\in\operatorname{supp}\chi$. Further, let V be an open cone such that $K\Subset V\Subset U$. Then there is a constant $\gamma>0$ such that $\delta_V(x)\geqslant\gamma|x|$ for all points of $\operatorname{supp}(1-\chi)$ except for a compact subset. At these points, we have $b\,\delta_U(x)\leqslant b\,\delta_V(x)\leqslant\overline{b}\,\delta_V(x)-\overline{\gamma}|x|$, where $\overline{b}>b$ and $\overline{\gamma}=\overline{b}-b$. Therefore,

$$|f_2(z)|\leqslant C\,\|f\|_{U,1,b}\exp\{-\overline{\gamma}|x|+b|y|+\overline{b}\,\delta_V(x)\}. \tag{21}$$

To obtain an analytic decomposition, we write

$$f=f_1'+f_2',\quad f_1'=f_1-\psi,\quad f_2'=f_2+\psi$$

and subject ψ to the equations

$$\frac{\partial\psi}{\partial\overline{z}_j}=\eta_j,\quad \text{where}\quad \eta_j\overset{\text{def}}{=}f\frac{\partial\chi}{\partial\overline{z}_j}=\frac{1}{2}f\frac{\partial\chi}{\partial x_j}\quad (j=1,\ldots,d). \tag{22}$$

The functions $\eta_j(z)$ are nonzero only for $x\in\partial U+B_\epsilon$, where ∂U is the boundary of U, and satisfy the estimate

$$|\eta_j(z)|\leqslant C_j\|f\|_{U,1,b}\exp\{-|x|^{1/\alpha}+b|y|\}. \tag{23}$$

It remains to verify that there exists a solution of Eqs. (22) with the required behavior at infinity. First we shall show that this behavior can be characterized by a plurisubharmonic function, which enables us to apply an existence theorem due to Hörmander.[28]

Lemma 7: For every pair U', U of open cones in $\mathbb{R}^d$ such that $U'\Subset U$ and for each system of numbers $\alpha,\alpha',b,b',\epsilon$ satisfying $\alpha>\alpha'>1$, $b'>\sqrt{d}\,b>0$, $0<\epsilon<1/b$, there is a plurisubharmonic function $\rho(z)$ with the following properties:

$$\rho(z)\geqslant-|x|^{1/\alpha}+b|y|\quad \textit{for}\ \ x\in\partial U+B_\epsilon, \tag{24}$$

$$\rho(z)\leqslant-|x|^{1/\alpha}+b'|y|+C\quad \textit{everywhere}, \tag{25}$$

$$\rho(z)\leqslant-|x|^{1/\alpha'}+b'|y|+C\quad \textit{for}\ \ x\in U', \tag{26}$$

where C is a sufficiently large constant.

The proof of this lemma is given in Appendix B.

Let us go on with our proof of Theorem 4. We choose a cone U' so that $V\Subset U'\Subset U$, take a function ρ defined by Lemma 7, and denote by ϱ the strictly plurisubharmonic function $2\rho+(d+3)\ln(1+|z|^2)$. Using (23) and (24), we see that $\eta_j\in L^2(\mathbb{C}^d,e^{-\varrho}\varkappa^{-1}\,d\lambda)$, where $d\lambda$ stands for the Lebesgue measure on $\mathbb{C}^d$ and

$$\varkappa\overset{\text{def}}{=}\inf_{\zeta}\sum_{j,k}\frac{\partial^2\varrho(z)}{\partial z_j\partial\overline{z}_k}\frac{\zeta_j\overline{\zeta}_k}{|\zeta|^2}\geqslant(d+3)\inf_{\zeta}\sum_{j,k}\frac{\partial^2\ln(1+|z|^2)}{\partial z_j\partial\overline{z}_k}\frac{\zeta_j\overline{\zeta}_k}{|\zeta|^2}\geqslant\frac{d+3}{(1+|z|^2)^2},$$

with the last lower bound taken from Ref. 28, Sec. 15.1. The functions η_j satisfy the consistency conditions $\partial\eta_j/\partial\overline{z}_k=\partial\eta_k/\partial\overline{z}_j$ by definition, and Theorem 15.1.1 of Ref. 28 shows that the system of Eqs. (22) has a solution ψ such that

$$\int |\psi|^2 e^{-\varrho}\,\mathrm{d}\lambda \leqslant \int |\eta|^2 e^{-\varrho}\varkappa^{-1}\,\mathrm{d}\lambda \leqslant \frac{1}{d+3}\int \frac{|\eta|^2 e^{-2\rho}}{(1+|z|^2)^{d+1}}\,\mathrm{d}\lambda \leqslant C'\|f\|^2_{U,1,b}, \tag{27}$$

where we made use of (23) and (24) in the last step. This implies that

$$\psi \in L^2(\mathbb{C}^d, e^{2(|x/a|^{1/\alpha}-b''|y|)}\,\mathrm{d}\lambda) \quad \text{and} \quad \psi \in L^2(\mathbb{C}^d, e^{2(|x/a|^{1/\alpha'}-b''|y|-b'\,\delta_V(x))}\,\mathrm{d}\lambda)$$

for each $a>1$ and for each $b''>\sqrt{d}\,b$. The former membership relation is ensured by (25) and the latter follows from (26) since for $x \notin U'$, we have $\delta_V(x) \geqslant \gamma'|x|$ with some $\gamma'>0$ and the exponent in question evidently does not exceed $-\varrho+C''$ by (25) again. Referring back to (4), (20), and (21), we conclude that the analytic functions f_1' and f_2' belong, respectively, to the spaces $H^{0,b''}_{\alpha,a}$ and $H^{0,b''}_{\alpha',a}(V)$ and so relation (19) is proved. To complete the proof, it remains to verify that $S^0_{\alpha'}$ is dense in the intersection $S^0_\alpha \cap S^0_{\alpha'}(K)$ endowed by its natural (i.e., projective) topology. This is considerably simpler than proving the denseness of $S^0_{\alpha'}$ in $S^0_{\alpha'}(K)$ since the elements of intersection decrease like $\exp(-|x|^{1/\alpha})$ outside the cone K, in contrast to an arbitrary function in $S^0_{\alpha'}(K)$ which has an exponential growth. Namely, an approximating sequence φ_ν can be constructed by setting $\varphi_\nu=\sigma_\nu\varphi$, where $\sigma_\nu(z)$ is a sequence of Riemann sums for the integral $\int\sigma_0(z-\xi)\,\mathrm{d}\xi$, with σ_0 a function in $S^0_{\alpha'}$ whose integral is unity. The sequence $\varphi_\nu \in S^0_{\alpha'}$ is obviously bounded in both the spaces S^0_α and $S^0_{\alpha'}(K)$ and converges to φ uniformly on compact subsets of $\mathbb{C}^d$ by the Vitali–Montel theorem. Thus, by the standard argument,[5] $\varphi_\nu \to \varphi$ in the topology of either of these spaces. Applying Lemma 6 concludes the proof.

Corollary: Let V be an open connected cone in $\mathbb{R}^d$ and let $\alpha'>1$. Suppose that $g(\zeta)$ is an analytic function on the tubular domain $\mathbb{R}^d+iV$ with the property that, for any $\varepsilon,R>0$ and every cone $V' \Subset V$,

$$|g(\zeta)| \leqslant C_{\varepsilon,R}(V')\exp\{\varepsilon\,|\mathrm{Im}\,\zeta|^{-1/(\alpha'-1)}\} \quad (\mathrm{Im}\,\zeta \in V',\ |\zeta| \leqslant R). \tag{28}$$

If the boundary value of g is an ultradistribution of class $\{k^{\alpha k}\}$, where $\alpha>\alpha'$, then this function satisfies a stronger bound of the same type, with α substituted for α'.

This is a direct consequence of Theorem 4 combined with Theorem 4 of Ref. 17 which shows that the Laplace transformation is an isomorphism of the algebra of analytic functions with growth property (28) onto the space $S'^0_\alpha(V^*)$, where V^* is the dual cone of V.

Remark 3: An analogue of Theorem 4 for S'^β_α, where $0<\beta<1$, can be derived more easily. Namely, it suffices to apply Theorem 5.18 of Ref. 24 which shows that, for v in S'^β_α, the condition of belonging to $S'^\beta_\alpha(K)$ amounts to a falloff property of the convolution $v*f$, $f \in S^\beta_{1-\beta}$, in the complementary cone $\complement K$. Any similar proof is impossible for $\beta=0$ because of the absence of a smallest space among the family S^0_α.

Theorem 4 has been stated in Ref. 19 without a proof and used there in deriving some auxiliary theorems, which generalize the well-known fact that the odd Lorentz invariant distributions have support in the closed light cone and which play a significant part in proving the CPT invariance of nonlocal QFT's satisfying the asymptotic commutativity condition as well as in extending the spin-statistics relation to nonlocal fields. The role of Theorem 4 in these applications can be illustrated, in particular, by the following example.

Theorem 5: *Let ϕ be a field defined on the space S^0_α, $\alpha>2$, and satisfying all the standard axioms except temperedness and locality. Assume it transforms according to an irreducible representation of the group* $\mathrm{SL}(2,\mathbb{C})$ *and let $W(x_1-x_2)$ be the Wightman generalized function determined by the vacuum expectation value $\langle\Psi_0, \phi(x_1)\phi^*(x_2)\Psi_0\rangle$. Then the closed light cone $\overline{\mathbb{V}}=\{\xi:\xi^2\geqslant 0\}$ is a carrier of the functional*

$$W(\xi) \mp W(-\xi), \tag{29}$$

where the upper and lower signs correspond to the cases of integer and half-integer spin, respectively.

In deriving Theorem 5 we are to regularize the ultraviolet behavior of W through the multiplication of the Fourier transform $\tilde{W}$ by the Lorentz invariant function $\omega(p/\mu)$, where $\omega(p)=\omega_0(p^2)$, $\omega_0 \in S_0^{\alpha'}(\mathbb{R})$, $1<\alpha'<\alpha$, $\operatorname{supp}\omega_0 \subset (-1,1)$, and $\omega_0(t)=1$ for $|t|\leqslant 1/2$. Theorem 7 of Ref. 19 shows that the regularized functional $\tilde{W}_\mu$ allows a continuous extension to the space $S^{\alpha'}_{\alpha-\alpha'}$. In particular, if $\alpha>2$ and $\alpha'<\alpha-1$, then $\tilde{W}_\mu$ has no worse than exponential growth of the order $1/(\alpha-\alpha')<1$ and hence its Laplace transform $\mathbf{W}_\mu$ is well defined and holomorphic in the usual tubular domain $\mathbb{R}^4-i\mathbb{V}_+$. This enables us to apply the Bargmann–Hall–Wightman theorem[1,2] and to assert that the support of the functional $F_\mu \overset{\text{def}}{=} W_\mu(\xi) \mp W_\mu(-\xi)$, which is defined on the space $S^{\alpha-\alpha'}_{\alpha'}$ containing functions of compact support providing $\alpha'<\alpha-1$, lies in $\overline{\mathbb{V}}$ and therefore F_μ has a continuous extension to $S^0_{\alpha'}(\mathbb{V})$. The extension $\hat{F}_\mu$ can be defined by $(\hat{F}_\mu, f)=(F_\mu, \chi f)$, where χ is a multiplier for $S^{\alpha-\alpha'}_{\alpha'}$ which is equal to 1 in an ϵ-neighborhood of $\overline{\mathbb{V}}$, vanishes outside the 2ϵ-neighborhood and satisfies the estimate $|\partial^q \chi(x)| \leqslant C h^{|q|} q^{(\alpha-\alpha')q}$. It is readily verified that the multiplication by χ is a continuous map from $S^0_{\alpha'}(\mathbb{V})$ into $S^{\alpha-\alpha'}_{\alpha'}$. Taking into account that the Fourier transforms of functions belonging to $E^{0,b}_{\alpha',a}$ have support in the ball of radius $\sim b$, where $\omega(p/\mu)=1$ for μ large enough, and using the denseness of $S^0_{\alpha'}$ in $S^0_{\alpha'}(\mathbb{V})$, we conclude that the nonregularized functional (29) also has a continuous extension to $S^0_{\alpha'}(\mathbb{V})$. Finally, Theorem 4 makes possible a further extension to $S^0_\alpha(\overline{\mathbb{V}})$, which completes the proof. In the same manner it is used in deriving an analogue[19] of Theorem 5 for the n-point vacuum expectation values.

V. CONCLUDING REMARKS

A number of works (see, e.g., Ref. 23 and references therein) on nonlocal QFT exploit another Gelfand–Shilov's class of test-function spaces S^β, $\beta<1$. The generalized functions belonging to S'^β have the same type of singularity as elements of S'^β_α but grow at infinity no faster than a polynomial. Their carrier cones can be defined[24] in a manner analogous to that used in Sec. II. As pointed in Sec. II, the spaces S^β_α are more convenient in operation because their topological structure is simpler, and in this respect it is worth noting that the restriction of $v \in S'^\beta$ to S^β_α has the same carrier cones as v. The proof of this fact for $\beta=0$ is more complicated than the derivation of Theorem 4, but the above construction can be adapted to this case by using Lemma 5.11 of Ref. 24. Theorem 4 can also be extended to the multiplicative carriers. As already remarked, the notion of multiplicative carrier cone is best suited for generalization of the spectral condition to gain the Euclidean formulation of local QFT's without positivity. Perhaps it is reasonable to impose an analogous condition on the generalized functions that serve as kernels of the positive semidefinite scalar product defining an auxiliary Hilbert structure[29] which is associated with the set of Wightman functions to identify the physical states. It is hardly surprising that highly singular generalized functions should be incorporated into the mathematical tools of quantum field theory with indefinite metric. This simply brings the distributional framework of QFT into coordination with the presence of nonphysical degrees of freedom and appears to be essential for the complete implementation of the gauge symmetry. What is more, the employment of such a formalism might contribute to a better insight into the Higgs effect and the confinement mechanism, as discussed in Refs. 13 and 14. The theorems established in Refs. 16–18 and complemented by the results presented here enable one to work with the analytic functionals in S'^0_α almost as easily as with the usual tempered distributions and may be of use in the further rigorous investigation of the singular QFT models.

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APPENDIX A: PROOF OF LEMMA 1

We denote the norm of $L^{0,b}_{\alpha,a}(U)$ by $\|\cdot\|''_{U,a,b}$. Let $\xi\in U$, and suppose that the neighborhood $B(\xi,\epsilon)=\{x:|x-\xi|<\epsilon\}$ of this point is contained in U. Then $\|\partial^q f\|_{L^2(B)} \leqslant C_\epsilon \|f\|''_{U,a,b}\, b^{|q|}\, e^{-|\xi/a|^{1/\alpha}}$. By Sobolev's lemma we have

$$|\partial^q f(\xi)|\leqslant C'_\epsilon \sum_{|k|\leqslant[d/2]+1} \|\partial^{q+k} f\|_{L^2(B)} \leqslant C''_\epsilon \|f\|''_{U,a,b}\, b^{|q|}\, e^{-|\xi/a|^{1/\alpha}}. \tag{A1}$$

Therefore, every element of $L^{0,b}_{\alpha,a}(U)$ allows an analytic continuation to the whole of $\mathbb{C}^d$. If f_ν is a Cauchy sequence in this space, than it converges uniformly on compact sets of $\mathbb{C}^d$ and hence its limit f is an entire function. All derivatives $\partial^q f$ are obviously square integrable on U with the weight $\exp\{2|x/a|^{1/\alpha}\}$ and the positive series determining $\|f\|''^{\,2}_{U,a,b}$ is convergent since its partial sums are bounded by the number $\sup_\nu \|f_\nu\|''^{\,2}_{U,a,b}$. Thus, $L^{0,b}_{\alpha,a}(U)$ is a Hilbert space. For each $a>a'$ and $b>b'$, we have $\|f\|''_{U,a,b}\leqslant C\|f\|_{U,a',b'}$ and hence the Banach space $S^{0,b'}_{\alpha,a'}(U)$ with norm (A1) is continuously embedded into $L^{0,b}_{\alpha,a}(U)$. Conversely, using inequality (A1) at the points of U whose distance to the boundary is greater than ϵ and applying the Taylor expansion to estimate $\partial^q f$ elsewhere, we see that the norm $\|f\|''_{U,a,b}$ is not weaker than $\|f\|_{U,a,b}$. Thus the limit spaces in question are indeed the same.

APPENDIX B: PROOF OF LEMMA 7

Let u be a unit vector in $\mathbb{R}^d$ and $\theta>0$. We denote by R_u the ray $\{\lambda u:\lambda\geqslant 0\}$ and by $K_{u,\theta}$ the circular cone $\{\lambda x:|x-u|\leqslant\theta,\ \lambda\geqslant 0\}$. Assume that θ is less than the angular separation between the cones U, U'. It suffices to prove that, for every $u\in\partial U$, there exists a plurisubharmonic function $\rho_u(z)$ bounded by (25) and satisfying estimates of the form (24) and (26) but for $x\in R_u+B_\epsilon$ and for $x\notin K_{u,\theta}$, respectively. Then the upper envelope

$$\rho(z)=\overline{\lim_{z'\to z}}\ \sup\{\rho_u(z'):u\in\partial U,\ |u|=1\} \tag{B1}$$

satisfies all the required conditions because $U'\subset\subset K_{u,\theta}$ for every $u\in\partial U$. The function (B1) is plurisubharmonic since the family $\{\rho_u\}$ is locally uniformly bounded above. The space $S^{\alpha'}_0(\mathbb{R})$, which is the Fourier transform of $S^0_{\alpha'}(\mathbb{R})$, contains a non-negative even function ω such that $\operatorname{supp}\omega\subset[-\delta,\delta]$, $\int\omega(t)\,dt=1$, and $|\omega^{(k)}(t)|\leqslant A_0 a_0^k k^{\alpha' k}$, where a_0 and δ can be taken arbitrarily small, see Ref. 5, Sec. IV.8.3. Let Ω be the convolution of ω by the characteristic function of the segment $|t|\leqslant b+\delta$ and let $1+2\delta/b<\pi/3$. Then $\cos\xi t>1/2$ for $|\xi|<1/b$ and $t\in\operatorname{supp}\Omega$. Let us estimate the Laplace transform $\tilde\Omega(\zeta)$ of Ω in the strip $|\operatorname{Re}\zeta|<1/b$. Taking into account that $\int\Omega(t)\ dt=2(b+\delta)$, we get

$$|\tilde\Omega(\zeta)|\geqslant\operatorname{Re}\int e^{it\zeta}\Omega(t)\,dt\geqslant\frac{1}{2}\int_{|t|>b} e^{-t\operatorname{Im}\zeta}\,\Omega(t)\,dt\geqslant\frac{1}{2}e^{b|\operatorname{Im}\zeta|}\int_{t>b}\Omega(t)dt=\frac{\delta}{2}e^{b|\operatorname{Im}\zeta|}. \tag{B2}$$

Therefore, the subharmonic function $\rho_0(z)=\ln(2|\tilde\Omega(z)|/\delta)$ is bounded from below by $b|\operatorname{Im}\zeta|$ in that strip. According to Ref. 5, we have $\tilde\Omega\in E^{0,b+2\delta}_{\alpha',1}$ if a_0 is small enough, and so

$$\rho_0(\zeta)\leqslant-|\operatorname{Re}\zeta|^{1/\alpha'}+(b+2\delta)|\operatorname{Im}\zeta|+A. \tag{B3}$$

We may assume without loss of generality that u is the first basis vector and then define ρ_u to be the upper envelope of the family

$$\rho_0(z_1-\xi)+\sum_{j>1}\rho_0(z_j)-|\xi|^{1/\alpha},\quad \xi>-\epsilon.$$

If $x\in R_u+B_\epsilon$, then $x_1>-\epsilon$ and $|x_j|<\epsilon<1/b$ for all $j>1$. Setting $\xi=x_1$, we see that (B2) ensures the required lower bound on ρ_u. Further, using (B3) and the elementary inequalities $\Sigma_{j>1}|x_j|^{1/\alpha'}\geqslant\Sigma_{j>1}|x_j|^{1/\alpha}-C'$, $|x_1-\xi|^{1/\alpha}+|\xi|^{1/\alpha}\geqslant|x_1|^{1/\alpha}$, and $\Sigma|y_j|\leqslant\sqrt{d}|y|$, we conclude that ρ_u satisfies (25) provided δ is small enough. Finally, if $x\notin\pm K_{u,\theta}$, then $\Sigma_{j>1}|x_j|^{1/\alpha'}\geqslant|\theta' x|^{1/\alpha'}$ with some $\theta'>0$, and if $x\in -K_{u,\theta}$, we have $|x_1-\xi|\geqslant|x_1|$ for $\xi\geqslant 0$ and $|x_1-\xi|^{1/\alpha'}\geqslant|x_1|^{1/\alpha'}-\epsilon^{1/\alpha'}$ for the rest of ξ. Therefore, the last desired bound on ρ_u is also satisfied and so Lemma 7 is proved.

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Integrable and superintegrable quantum systems in a magnetic field

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Integrable quantum mechanical systems with magnetic fields are constructed in two-dimensional Euclidean space. The integral of motion is assumed to be a first or second order Hermitian operator. Contrary to the case of purely scalar potentials, quadratic integrability does not imply the separation of variables in the Schrödinger equation. Moreover, quantum and classical integrable systems do not necessarily coincide: the Hamiltonian can depend on the Planck constant $\hbar$ in a nontrivial manner. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1695447]

I. INTRODUCTION

The purpose of this article is to study the integrability properties of a quantum particle moving in an external magnetic field. More specifically, we will consider the Schrödinger equation in a two-dimensional Euclidean space with the Hamiltonian

$$H=-\frac{\hbar^2}{2}(\partial_x^2+\partial_y^2)-\frac{i\hbar}{2}[A(x,y)\partial_x+\partial_x A(x,y)+B(x,y)\partial_y+\partial_y B(x,y)]+V(x,y). \tag{1.1}$$

The vector and scalar potentials (A,B) and V are to be determined from the requirement that the system should be integrable, i.e., a well-defined quantum mechanical operator X should exist, that commutes with the Hamiltonian, i.e.,

$$[H,X]=0. \tag{1.2}$$

In this particular study, we shall restrict to the case when X is a first or second order polynomial in the momenta. We shall be particularly interested in the case of superintegrable systems, when two independent operators, X_1 and X_2, commuting with the Hamiltonian exist. In general, X_1 and X_2 do not commute with each other, but together generate an algebra of operators, commuting with H.

In classical mechanics, integrable systems are of interest, because they have regular trajectories. Indeed, their motion is restricted to a torus in phase space. Superintegrable systems are even more regular. Trajectories are completely determinded by the values of the $2n-1$ integrals of motion. In particular, all bounded trajectories are periodic, as in the case of the harmonic oscillator, or Kepler problem.

In quantum mechanics, integrability, i.e., the existence of n integrals of motion, provides a complete set of quantum numbers, characterizing the system. Moreover, it simplifies the calcula-

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tion of energy levels and wave functions. Superintegrability, in all cases studied so for, entails exact solvability. This means that energy levels in superintegrable systems can be calculated algebraicly, i.e., they satisfy algebraic rather than transcendental equations.

Previous searches for integrable and superintegrable systems in quantum mechanics concentrated on scalar potentials only.[1–10] It was established that for scalar potentials the existence of first and second order integrals of motion implies the separation variables in the Schrödinger equation, and also in the Hamilton–Jacobi equation in classical mechanics. Moreover, for scalar potentials and second order integrals of motion, classical and quantum integrable systems coincide (i.e., classical and quantum potentials are the same).

Surprisingly, when third order integrals are considered, a new phenomenon occurs: integrable and superintegrable quantum systems that have no classical counterpart.[11–14] Indeed, in the classical limit $\hbar \to 0$ the potential vanishes, $V(x,y) \to 0$ and we obtain free motion.

Previous studies of integrability in magnetic fields were conducted in the framework of classical mechanics.[15,16] It was established that the existence of second order integrals of motion in the presence of magnetic fields no longer implies the separation of variables. However, the integrals of motion were still classified into equivalence classes under the action of the Euclidean group and the highest order terms have the same form as in the case of a purely scalar potential.

In this paper we restrict ourselves to the two-dimensional Euclidean space $E(2)$, the Hamiltonian (1.1) and to first, or second order integrals. In Sec. II we formulate the problem of finding the integrals of motion, first in the classical, then in the quantum case. We show that the determining equations in the two cases are the same for first order integrals of motion, not however for second order ones. Section III is devoted to first order integrals of motion. They are shown to exist if and only if the magnetic field and an effective scalar potential are invariant under either translations, or rotations. We also show that superintegrability with two (or more) first order integrals occurs only for a constant magnetic field and effective potential. In Sec. IV we consider a specific class of second order operators which we call ''Cartesian integrals.'' In the absence of a magnetic field they lead to separation of variables in Cartesian coordinates. We also show that superintegrability with one Cartesian integral and a second integral of any (quadratic) type occurs only for a constant magnetic field. In the Cartesian case there is no difference between classical and quantum integrability. Polar integrability and superintegrability are investigated in Sec. V. All cases of integrability with one ''polar'' integral of motion are identified. The quantum case differs from the classical one and the magnetic field can depend on the Planck constant $\hbar$ in a nontrivial manner. In Sec. VI we show that a polar integral can exist simultaneously with any other independent second order integral only if the magnetic field is constant. The final Sec. VII is devoted to conclusions and open problems.

II. FORMULATION OF THE PROBLEM

A. Classical mechanics

Since we will be comparing results in quantum and classical mechanis, let us briefly recapitulate some results obtained earlier.[15,16] The classical counterpart of the Hamiltonian (1.1) is

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + A(x,y)p_x + B(x,y)p_y + V(x,y), \tag{2.1}$$

where p_x and p_y are the momenta conjugate to x and y, respectively. The classical equations of motion in the Hamiltonian form are

$$\dot{x} = \frac{\partial H}{\partial p_x} = p_x + A, \quad \dot{y} = \frac{\partial H}{\partial p_y} = p_y + B,$$

$$\dot{p}_x = -\frac{\partial H}{\partial x} = -V_x - A_x p_x - B_x p_y, \quad \dot{p}_y = -\frac{\partial H}{\partial y} = -V_y - A_y p_x - B_y p_y. \tag{2.2}$$

The equation of motion (2.2) can be rewritten in the Newton form as

$$\ddot{x} = -W_x + \Omega \dot{y},$$

$$\ddot{y} = -W_y - \Omega \dot{x}, \tag{2.3}$$

$$W = V - \tfrac{1}{2}(A^2 + B^2),$$

$$\Omega = A_y - B_x. \tag{2.4}$$

The equations of motion (2.3) are invariant under a gauge transformation of the potentials

$$V(x,y) \to \tilde{V}(x,y) = V + (\mathbf{A}, \nabla\phi) + \tfrac{1}{2}(\nabla\phi)^2,$$

$$\mathbf{A}(x,y) \to \tilde{\mathbf{A}}(x,y) = \mathbf{A} + \nabla\phi, \tag{2.5}$$

where we have put $\mathbf{A} = (A,B)$ and $\phi = \phi(x,y)$ is an arbitrary smooth function. Thus, the quantities that are of actual physical importance are the magnetic field Ω and the effective potential W.

A classical first integral of motion is postulated to have the form

$$C = f_1(x,y)\dot{x} + f_2(x,y)\dot{y} + m(x,y). \tag{2.6}$$

The determining equations for the funtions f_1, f_2, and m are obtained from the requirement

$$\{H,C\} = \frac{dC}{dt} = 0, \tag{2.7}$$

when Eq. (2.2) are satisfied, i.e., C is a constant on the solutions of the equations of motion and Poisson commutes with the Hamiltonian.

Similarly, a classical second order integral of motion has the form

$$C = g_1(x,y)\dot{x}^2 + g_2(x,y)\dot{y}^2 + g_3(x,y)\dot{x}\dot{y} + k_1(x,y)\dot{x} + k_2(x,y)\dot{y} + m(x,y). \tag{2.8}$$

The determining equations for the functions g_i, k_i, and m are again obtained from the condition (2.7).

The equations for the coefficients of the first and second order classical integrals of motion were derived and partially solved elsewhere.[15,16] We shall give them again below as classical limits of the corresponding equations in the quantum case. To facilitate a comparison, we must rewrite the classical integrals in terms of momenta, rather than velocities, i.e., substitute $\dot{x} = p_x + A$, $\dot{y} = p_y + B$.

B. Quantum mechanics

In quantum mechanics an integral of motion will be a Hermitian operator X that commutes with the Hamiltonian H.

Let us first consider a first order integral in the momenta:

$$X = -\frac{i\hbar}{2}(f_1\partial_x + \partial_x f_1 + f_2\partial_y + \partial_y f_2) + f_1 A + f_2 B + m. \tag{2.9}$$

The classical limit of the operator (2.9) is the integral (2.6); f_1, f_2, and m are functions of x and y.

The commutator $[X,H]$ with H as in Eq. (1.1) will contain second, first, and zero order terms in the derivatives. Setting the coefficients of all of them equal to zero, we obtain the following set of determining equations:

$$f_{1,x}=0,\ \ f_{2,y}=0,\ \ f_{1,y}+f_{2,x}=0, \tag{2.10}$$

$$-f_2\Omega+m_x=0,\ \ f_1\Omega+m_y=0,\ \ f_1W_x+f_2W_y=0. \tag{2.11}$$

We see that the Planck constant $\hbar$ does not figure in Eqs. (2.10) and (2.11). Hence these equations must coincide with their classical limit, and indeed, they do.[15] In particular, Eq. (2.10) implies

$$f_1=\alpha y+\beta,\ \ f_2=-\alpha x+\gamma, \tag{2.12}$$

where α, β, and γ are real constants. Hence the leading terms (independent of A, B, and m) of the operator X of Eq. (2.9) lie in the Lie algebra $e(2)$ of the Euclidean group $E(2)$, generated by

$$P_1=-i\hbar\partial_x,\ P_2=-i\hbar\partial_y,\ L_3=-i\hbar(y\partial_x-x\partial_y). \tag{2.13}$$

Thus, we have

$$X=\alpha L_3+\beta P_1+\gamma P_2+\alpha(yA-xB)+\beta A+\gamma B+m. \tag{2.14}$$

We shall write the second order operator corresponding to the integral (2.8), after symmetrization, as

$$\begin{aligned}X=&-\tfrac{1}{2}\hbar^2\{2g_1\partial_x^2+2g_2\partial_y^2+2g_3\partial_x\partial_y+(2g_{1,x}+g_{3,y})\partial_x+(2g_{2,y}+g_{3,x})\partial_y+g_{1,xx}+g_{2,yy}+g_{3,xy}\}\\&-\frac{i\hbar}{2}\{(4g_1A+2g_3B+2k_1)\partial_x+(4g_2B+2g_3A+2k_2)\partial_y+2g_1A_x+2g_{1,x}A+2g_2B_y+2g_{2,y}B\\&+g_3A_y+g_3B_x+Ag_{3,y}+Bg_{3,x}+k_{1,x}+k_{2,y}\}+g_1A^2+g_2B^2+g_3AB+k_1A+k_2B+m.\end{aligned} \tag{2.15}$$

The commutativity condition $[H,X]=0$ implies the following set of determining relations:

$$g_{1,x}=0,\ \ g_{2,y}=0,\ \ g_{1,y}+g_{3,x}=0,\ \ g_{2,x}+g_{3,y}=0, \tag{2.16}$$

$$\begin{gathered}k_{1x}-g_3\Omega=0,\ \ k_{2y}+g_3\Omega=0,\\2\Omega(g_1-g_2)+k_{1y}+k_{2x}=0,\\2g_1W_x+g_3W_y+k_2\Omega-m_x=0,\\2g_2W_y+g_3W_x-k_1\Omega-m_y=0,\end{gathered} \tag{2.17}$$

$$k_1W_x+k_2W_y+\frac{\hbar^2}{4}(g_{2x}\Omega_y-g_{1y}\Omega_x)=0. \tag{2.18}$$

Equations (2.16) and (2.17) are the same as the classical ones.[15] Equation (2.18) is however different. It involves the Planck constant and reduces to the classical case only in the limit $\hbar\to 0$. Thus, in the presence of a nonconstant magnetic field $\Omega(x,y)$, classical and quantum integrability differ!

Equation (2.16) can be solved as in the classical case[15] and they imply

$$\begin{gathered}g_1=\alpha y^2-\beta y+\delta,\\g_2=\alpha x^2+\gamma x+\zeta,\\g_3=-2\alpha xy+\beta x-\gamma y+\xi,\end{gathered} \tag{2.19}$$

where the greek letters represent real constants. Substituting (2.19) into (2.15) we obtain the operator X in the form

$$X=\alpha[(L_3+yA-xB)^2+\hbar^2]-\tfrac{1}{2}\beta[(L_3+yA-xB)(P_1+A)+(P_1+A)(L_3+yA-xB)]$$
$$-\tfrac{1}{2}\gamma[(L_3+yA-xB)(P_2+B)+(P_2+B)(L_3+yA-xB)]+\delta(P_1+A)^2+\zeta(P_2+B)^2$$
$$+\xi(P_1+A)(P_2+B)-\frac{i\hbar}{2}(2k_1\partial_x+k_{1,x}+2k_2\partial_y+k_{2,y})+k_1A+k_2B+m. \tag{2.20}$$

Thus, the leading part of Eq. (2.20) lies in the enveloping algebra of $e(2)$. For $A=B=0$ this coincides with the case of a scalar potential.[1,2,17] As in the scalar case we can simplify Eq. (2.20) by Euclidean transformations and linear combinations with the Hamiltonian. The operator X is transformed into a similar operator, with new values of the constants $\alpha,\ldots,\xi$. Four classes of such operators exist, represented by

$$X_C=(P_1+A)^2-\frac{i\hbar}{2}(2k_1\partial_x+k_{1,x}+2k_2\partial_y+k_{2,y})+k_1A+k_2B+m, \tag{2.21}$$

$$X_R=(L_3+yA-xB)^2+\hbar^2-\frac{i\hbar}{2}(2k_1\partial_x+k_{1,x}+2k_2\partial_y+k_{2,y})+k_1A+k_2B+m, \tag{2.22}$$

$$X_P=-\frac{1}{2}\{(L_3+yA-xB)(P_1+A)+(P_1+A)(L_3+yA-xB)\}$$
$$-\frac{i\hbar}{2}(2k_1\partial_x+k_{1,x}+2k_2\partial_y+k_{2,y})+k_1A+k_2B+m, \tag{2.23}$$

$$X_E=(L_3+yA-xB)^2+\hbar^2+\sigma[(P_1+A)^2-(P_2+B)^2]$$
$$-\frac{i\hbar}{2}(2k_1\partial_x+k_{1,x}+2k_2\partial_y+k_{2,y})+k_1A+k_2B+m,\quad \sigma>0. \tag{2.24}$$

In the case of a purely scalar potential the existence of a commuting operator of the type X_C, X_R, X_P, or X_E implies that the Schrödinger equation will allow separation of variables in Cartesian, polar, parabolic, or elliptic coordinates, respectively. In the last case σ is related to the interfocal distance for the elliptic coordinates.

Substituting Eq. (2.19) into Eq. (2.18) we obtain

$$k_1W_x+k_2W_y+\frac{\hbar^2}{4}[(2\alpha x+\gamma)\Omega_y-(2\alpha y-\beta)\Omega_x]=0. \tag{2.25}$$

Thus, for the special case $\alpha=\beta=\gamma=0$ classical and quantum integrability will coincide.

III. FIRST ORDER INTEGRABILITY AND SUPERINTEGRABILITY

A first order integral (2.9) in quantum mechanics will exist if the overdetermined system (2.10) and (2.11) has a solution. The general solution of Eq. (2.10) is given by Eq. (2.12). Substituting into (2.11) we obtain

$$(\alpha x-\gamma)\Omega+m_x=0,\ (\alpha y+\beta)\Omega+m_y=0,\ (\alpha y+\beta)W_x+(-\alpha x+\gamma)W_y=0. \tag{3.1}$$

We are only interested in cases with a magnetic field present, i.e., $\Omega \neq 0$. With no loss of generality, we need only distinguish two cases:

1. $\alpha=1$, $\beta=\gamma=0$.

We obtain

$$W=W(\rho),\ \Omega=\Omega(\rho),\ \rho=\sqrt{x^2+y^2}. \tag{3.2}$$

We see that in this case the magnetic field Ω and the effective scalar potential must be spherically symmetric. The potentials in the Hamiltonian (1.1) can by a gauge transformation be taken into

$$A=\int \frac{\Omega(\rho)\rho d\rho}{\sqrt{\rho^2-x^2}},\ B=0,\ V=W(\rho)+\tfrac{1}{2}A^2. \tag{3.3}$$

The integral of motion is

$$X=L_3+y\int \frac{\Omega(\rho)\rho d\rho}{\sqrt{\rho^2-x^2}}-\int \rho\Omega(\rho)d\rho. \tag{3.4}$$

2. $\alpha=\beta=0$, $\gamma=1$.

The magnetic field and effective potential are translationally invariant

$$\Omega=\Omega(x),\ W=W(x), \tag{3.5}$$

and we can take

$$A=\Omega y,\ B=0,\ V=W+\tfrac{1}{2}y^2\Omega^2,$$

$$X=P_2+\int \Omega(x)dx. \tag{3.6}$$

The system (1.1) will be first order superintegrable if at least two first order integrals (2.14) exist. This is only possible if the magnetic field and effective potential are constant:

$$\Omega=\Omega_0,\ W=W_0. \tag{3.7}$$

In this case actually three operators commuting with the Hamiltonian exist and we have

$$H=\frac{1}{2}(i\hbar\partial_x-\Omega y)^2-\frac{\hbar^2}{2}\partial_y^2, \tag{3.8}$$

$$X_1=P_1,\ X_2=P_2+x\Omega_0,\ X_3=L_3-\tfrac{1}{2}(x^2-y^2)\Omega_0, \tag{3.9}$$

where we have chosen the gauge to be such that

$$A=\Omega_0 y,\ B=0,\ V=\tfrac{1}{2}\Omega^2y^2. \tag{3.10}$$

The classical equations of motion (2.2) are easily solved. The trajectories are circles (and are hence all closed). The Schrödinger equation allows the separation of variables in Cartesian coordinates. The solution is

$$\Psi(x,y)=e^{i(\lambda/\hbar)x}f(y), \tag{3.11}$$

where $f(y)$ satisfies the harmonic oscillator equation

$$f''-\left\{\left(\frac{\Omega y+\lambda}{\hbar}\right)^2-\frac{2E}{\hbar^2}\right\}f=0. \tag{3.12}$$

The integrals of motion (3.9), together with the constant Ω, satisfy the commutation relations of a central extension of the Euclidean Lie algebra:

$$[X_1,X_2]=-i\hbar\Omega_0,\ [X_3,X_1]=-i\hbar X_2,\ [X_3,X_2]=i\hbar X_1. \tag{3.13}$$

Only three of the integrals X_1, X_2, X_3, and H can be independent and indeed they satisfy

$$X_1^2+X_2^2+2\Omega_0X_3-2H=0. \tag{3.14}$$

In polar coordinates the Schrödinger equation

$$\left\{\frac{1}{2}\left(i\hbar\cos(\phi)\partial_r-\frac{\sin(\phi)}{r}\partial_\phi-\Omega r\sin(\phi)\right)^2-\frac{1}{2}\left(\sin(\phi)\partial_r+\frac{\cos(\phi)}{r}\partial_\phi\right)^2\right\}\Psi=E\Psi \tag{3.15}$$

R-separates,[16,18] rather than separates, and we have

$$\Psi(r,\phi)=e^{-(i/4)\,\Omega r^2\sin 2\phi}J_m(kr)e^{im\phi},\ \ k^2=2E+m\Omega, \tag{3.16}$$

where $J_m(kr)$ is a Bessel function.

IV. CARTESIAN INTEGRABILITY AND SUPERINTEGRABILITY

A. Integrability

In order to find integrable systems with a second order operator commuting with the Hamiltonian, we must solve the system (2.16)–(2.18). To do this, we first transform X to its canonical form, i.e., one of (2.21)–(2.24). We start with the simplest case, namely X_C of (2.21). We call this the ''Cartesian'' case, because for a purely scalar potential it corresponds to separation of variables in Cartesian coordinates. It corresponds to $\alpha=\beta=\gamma=\zeta=\xi=0$ and $\delta=1$ in Eq. (2.20). Equation (2.25) implies that the determining equations (2.16), (2.17), and (2.18) are the same in the classical and quantum cases [the $\hbar^2$ term in Eq. (2.18) vanishes]. For purely scalar potentials $\Omega=k_1=k_2=0$ we reobtain the known result $W=W_0(y)+m(x)$.[1] From now on we assume $\Omega\neq0$. For completeness, we reproduce the result obtained earlier[15] in the classical case, since it is valid in the quantum case as well:

$$\Omega=f_{xx}+g_{yy},$$

$$W=\frac{a}{3}(g-f)^3-\frac{b+d}{2}(g-f)^2+(c+k-e)(g-f),$$

$$k_1=-g_y,\ k_2=-f_x,$$

$$m=-\frac{a}{3}(g^3+2f^3-3gf^2)+b(fg-f^2)+\frac{d}{2}(g^2-f^2)+c(g-2f)+eg-kf. \tag{4.1}$$

Here a, b, c, d, e, and k are constants and the functions $f=f(x)$ and $g=g(y)$ satisfy

$$f_{xx}=af^2+bf+c,\ \ g_{yy}=-ag^2+dg+e,$$

$$f_x\neq0,\ \ g_y\neq0. \tag{4.2}$$

Two exceptional cases occur when we have $f_x=0$ or $g_y=0$. These however imply $\Omega=\Omega(x)$, $W=W(x)$ or $\Omega=\Omega(y)$, $W=W(y)$, respectively. Then a first order invariant exists and the second order one is simply its square. The general solution of Eq. (4.2) are elliptic functions.

B. Cartesian superintegrability

We shall now assume that Ω and W are such that one Cartesian integral X_1 exists, i.e., they satisfy Eq. (4.1). We require that a second integral X_2 of the type (2.20) should exist, in addition to the considered Cartesian one. We can simplify the integral X_2 by translation and by linear combinations with X_1 and H. Rotations cannot be used, since they would change the form of the operator X_1 and of the Hamiltonian. Two cases must be considered, $\alpha\neq 0$ and $\alpha=0$.

Case 1: $\alpha\neq 0$

We set $\alpha=1$, by a translation we transform $(\beta,\gamma)\rightarrow(0,0)$, by linear combinations we set $(\delta,\zeta)\rightarrow(0,0)$. We are left with an operator X_2 in the form (2.20) with $\alpha=1$, $\beta=\gamma=\delta=\zeta=0$. The constant ξ and functions k_1, k_2 and m must be determined from the system (2.17) and (2.18). Let us consider the case when Ω and W are as in Eq. (4.1). The first two equations imply

$$k_1=-2y(xf_x-f)-x^2yg_{yy}+\xi f_x+\xi xg_{yy}+C_1(y),$$

$$k_2=xy^2f_{xx}+2x(yg_y-g)-\xi yf_{xx}-\xi g_y+C_2(x). \tag{4.3}$$

We substitute k_1, k_2, Ω, and W into the remaining four equations and investigate their compatibility. After somewhat lengthy calculations we obtain a simple result: the equations are compatible for $\Omega\neq 0$ if and only if Ω and W are constant. We arrive at the case (3.7), already investigated in Sec. III.

Case 2: $\alpha=0$

In order to obtain an independent second order integral we must have $\beta^2+\gamma^2\neq 0$ and we can normalize $\beta^2+\gamma^2=1$ and put $\delta=\zeta=\xi=0$ (by linear combinations with H and X_1). The set of Eqs. (2.16)–(2.18) is then again compatible only for Ω and W constant.

The conclusion of this section is that for $\Omega\neq 0$ Cartesian superintegrability with two second order integrals exists only in a trivial sense. Thus $\Omega=\Omega_0$, $W=W_0$ and all second order integrals are reducible: they are polynomials in the three first order ones.

V. POLAR INTEGRABILITY

We now request that one second order integral should exist and that it be of the form (2.22). We shall call this operator X_R a polar type integral. Let us transform the determining equations (2.17) and (2.18) to polar coordinates $x=r\cos(\phi)$, $y=r\sin(\phi)$. The resulting equations are

$$P_r=0,\ P+Q_\phi=0, \tag{5.1}$$

$$2r^3\Omega-P_\phi-rQ_r+Q=0, \tag{5.2}$$

$$m_\phi-2r^2W_\phi+rP\Omega=0,\ \ m_r-Q\Omega=0, \tag{5.3}$$

$$\frac{\hbar^2}{2}\Omega_\phi+PW_r+\frac{1}{r}QW_\phi=0, \tag{5.4}$$

where we have put $P=k_1\cos(\phi)+k_2\sin(\phi)$ and $Q=-k_1\sin(\phi)+k_2\cos(\phi)$.

We see that Eq. (5.4) contains a term proportional to $\hbar^2$. It follows that in this case quantum integrable systems will differ from classical ones, at least if we have $\Omega_\phi\neq 0$. In the classical limit $\hbar\rightarrow 0$ the quantum systems will reduce to classical ones, or to free motion. This is a new phenomenon. In the absence of magnetic fields, classical and quantum systems with second order integrals of motion coincide.

Equations (5.1) imply

$$P=-f'(\phi),\quad Q=f(\phi)+R(r), \tag{5.5}$$

with $f(\phi)$ and $R(r)$ to be determined. We shall use primes and dots to denote derivatives with respect to ϕ and r, respectively. We again assume $\Omega\neq 0$. Indeed, for $\Omega=0$ we obtain the known case of a scalar potential, separable in polar coordinates: $W=W_0(r)+W_1(\phi)/r^2$.

We solve Eq. (5.2) for the magnetic field

$$\Omega=-\frac{1}{2r^3}(f''+f+R-r\dot{R}). \tag{5.6}$$

From Eq. (5.3) we obtain a compatibility condition ($m_{r\phi}=m_{\phi r}$), namely,

$$2r^2W_{r\phi}+4rW_{\phi}+\frac{3f'}{2r^3}(f''+f+R-r\dot{R})+\frac{f'\ddot{R}}{2r}+\frac{1}{2r^3}(f+R)(f'''+f')=0. \tag{5.7}$$

Using Eq. (5.4) to eliminate W_ϕ from Eq. (5.7), we obtain, for

$$f+R\neq 0,\quad f'\neq 0 \tag{5.8}$$

an equation for $W(r,\phi)$ that we can solve

$$W_{rr}+\frac{(3(f+R)-r\dot{R})}{r(f+R)}W_r-\frac{\hbar^2\dot{R}(f'''+f')}{4r^3f'(f+R)}+\frac{3(f+R)}{4r^6}(f''+f+R-r\dot{R})$$
$$+\frac{(f+R)\ddot{R}}{4r^4}+\frac{(f+R)^2}{4r^6f'}(f'''+f')=0. \tag{5.9}$$

We obtain

$$W=\frac{\hbar^2(f'''+f')}{8r^2f'}-\frac{3f(f''+f)}{32r^4}-\frac{f'''}{8f'}r^6\dot{u}^2-\frac{r^2}{8}(r^3\ddot{u}+3r^2\dot{u})^2-\frac{f^2(f'''+f')}{32f'r^4}-\frac{Ff}{2r^2}$$
$$+\left(\frac{3f''}{8}+\frac{ff'''}{8f'}\right)r\dot{u}+\frac{3f''}{4}u-\frac{f}{4r}(r^3\ddot{u}+3r^2\dot{u})+Fr^3\dot{u}+W_0, \tag{5.10}$$

where $F=F(\phi)$ and $W_0(\phi)$ are two new functions, introduced as integration "constants." We have also introduced the functions $u(r)$ and $S(r)$, satisfying

$$\dot{S}(r)=\frac{1}{r^3}R(r),\ \dot{u}(r)=\frac{1}{r^3}S(r). \tag{5.11}$$

Let us first consider the two special cases in Eq. (5.8).

For $f(\phi)+R(r)=0$, Eq. (5.6) implies $\Omega=0$ and we are not interested in this case.

In the case $f'(\phi)=0$ we have

$$P=0,\quad Q=Q(r),\quad W=W(r),\quad m=\frac{Q^2}{4r^2},$$

$$k_1=-Q(r)\sin(\phi),\quad k_2=Q(r)\cos(\phi), \tag{5.12}$$

and the classical and quantum cases coincide. Moreover, a first order integral exists and the second order one is its square.

Let us return to the generic case (5.10) with conditions (5.8) satisfied. We substitute W of Eq. (5.10) into Eqs. (5.3) and (5.4) to obtain

$$m=\frac{ff''}{4r^2}+\frac{f^2}{4r^2}+\frac{fR}{2r^2}-\frac{f''S}{2}+\frac{R^2}{4r^2}+m_0(\phi), \tag{5.13}$$

$$m_0'=2\,f'F, \tag{5.14}$$

$$\dddot{u}+\frac{6}{r}\ddot{u}-\frac{r^3\dot{u}^2}{2}\left(\frac{f'''}{f'}\right)'\frac{1}{f'}+\left(\frac{6}{r^2}+\frac{C}{2r^2f'}+\frac{4F'}{f'}\right)\dot{u}+\frac{3f'''}{r^3f'}u+\frac{4A}{r^7f'}+\frac{4B}{r^5f'}+\frac{4W_0'}{r^3f'}=0, \tag{5.15}$$

where

$$A=-\frac{9ff'''}{32}-\frac{f^2}{32}\left(\frac{f'''}{f'}\right)'-\frac{15f'f''}{32}-\frac{3ff'}{4},$$

$$B=\frac{\hbar^2}{8}\left(\frac{f'''}{f'}\right)'-\frac{fF'}{2}-\frac{3f'F}{2},$$

$$C=6f'''+f\left(\frac{f'''}{f'}\right)'. \tag{5.16}$$

The next task is to solve Eq. (5.15). Notice that this is not a partial differential equation. It involves four unknown functions $u(r)$, $f(\phi)$, $F(\phi)$, and $W_0(\phi)$, each depending on one variable only. Hence, we can consider this equation to be an ordinary differential equation for $u(r)$, and then establish the compatibility conditions on the other unknowns for which the ϕ dependence will cancel. The complete analysis is rather lengthy and involves the consideration of many special cases. We shall only present the main arguments and final results.

Case 1:

$$\left(\left(\frac{f'''}{f'}\right)'\left(\frac{1}{f'}\right)\right)'=0. \tag{5.17}$$

All subcases lead to the following solution (or special cases thereof):

$$f=C_0+C_1\cos(\phi)+C_2\sin(\phi),$$

$$F=K_1,\quad W_0=K_2f+K_3. \tag{5.18}$$

Equation (5.15) then reduces to

$$\dddot{u}+\frac{6}{r}\ddot{u}+\frac{3}{r^2}\dot{u}-\frac{3}{r^3}u-\frac{15C_0}{8r^7}-\frac{6K_1}{r^5}+\frac{4K_2}{r^3}=0. \tag{5.19}$$

The general solution of Eq. (5.19) is

$$u=-\frac{C_0}{8r^4}+\frac{2K_1}{r^2}+\frac{4K_2}{3}+ar+\frac{b}{r}+\frac{c}{r^3}, \tag{5.20}$$

and hence we have

$$S=\frac{C_0}{2r^2}-4K_1+ar^3-br-\frac{3c}{r},$$

$$R=-C_0+3ar^5-br^3+3cr. \tag{5.21}$$

Finally, the magnetic field and effective potential in this case are

$$\Omega = 6ar^2 - b, \tag{5.22}$$

$$W = -2ar(C_1\cos(\phi) + C_2\sin(\phi)) + \frac{ab}{2}r^4 - 3acr^2 - a^2r^6. \tag{5.23}$$

Since Ω does not depend on ϕ the classical and quantum cases are the same. The corresponding classical integral of motion is

$$\begin{aligned} C_R = {} & (x\dot{y} - y\dot{x})^2 + (-C_2 - (3ar^5 - br^3 + 3cr)\sin(\phi))\dot{x} + (C_1 + (3ar^5 - br^3 + 3cr)\cos(\phi))\dot{y} \\ & - \frac{3bcr^2}{2} + \frac{9acr^4}{2} - \frac{3abr^6}{2} + 2C_1ar^3\cos(\phi) - C_1br\cos(\phi) + 2C_2ar^3\sin(\phi) \\ & - C_2br\sin(\phi) + \frac{9a^2r^8}{4} + \frac{b^2r^4}{4} + \frac{9c^2}{4}. \end{aligned} \tag{5.24}$$

Case 2:

$$\left(\left(\frac{f'''}{f'}\right)'\left(\frac{1}{f'}\right)\right)' \neq 0. \tag{5.25}$$

A complete analysis[19] shows that Eq. (5.15) in this case is consistent only if we have

$$u = \frac{a}{8r^4} + \frac{b}{2r^2} + c \tag{5.26}$$

and hence

$$S = -\frac{a}{2r^2} - b, \quad R = a. \tag{5.27}$$

Moreover, the function $f(\phi)$ must satisfy

$$(f+a)^2\left(\frac{f'''}{f'}\right)' + 24f'(f+a) + 9f'''(f+a) + 15f'f'' = 0. \tag{5.28}$$

The functions $F(\phi)$ and $W_0(\phi)$ are given explicitly in terms of $f(\phi)$ as

$$F = -\frac{bf'''}{4f'} + \frac{\hbar^2}{4(f+a)^3}\left((f+a)^2\frac{f'''}{f'} - 2(f+a)f'' + (f')^2\right) + \frac{C_1}{(f+a)^3},$$

$$W_0 = \frac{b^2f'''}{8f'} + bF - \frac{3cf''}{4} + C_2. \tag{5.29}$$

We integrate Eq. (5.28) twice and put $y = f + a$ to obtain the second order equation

$$y'' = -\frac{2}{y}(y')^2 - 3y + \frac{4A}{y} + \frac{B^2 - A^2}{y^3}, \tag{5.30}$$

where A and B are constants.

This equation has a first integral K, in terms of which we have

$$y^4(y')^2 = -y^6 + 2Ay^4 + (B^2 - A^2)y^2 + K. \tag{5.31}$$

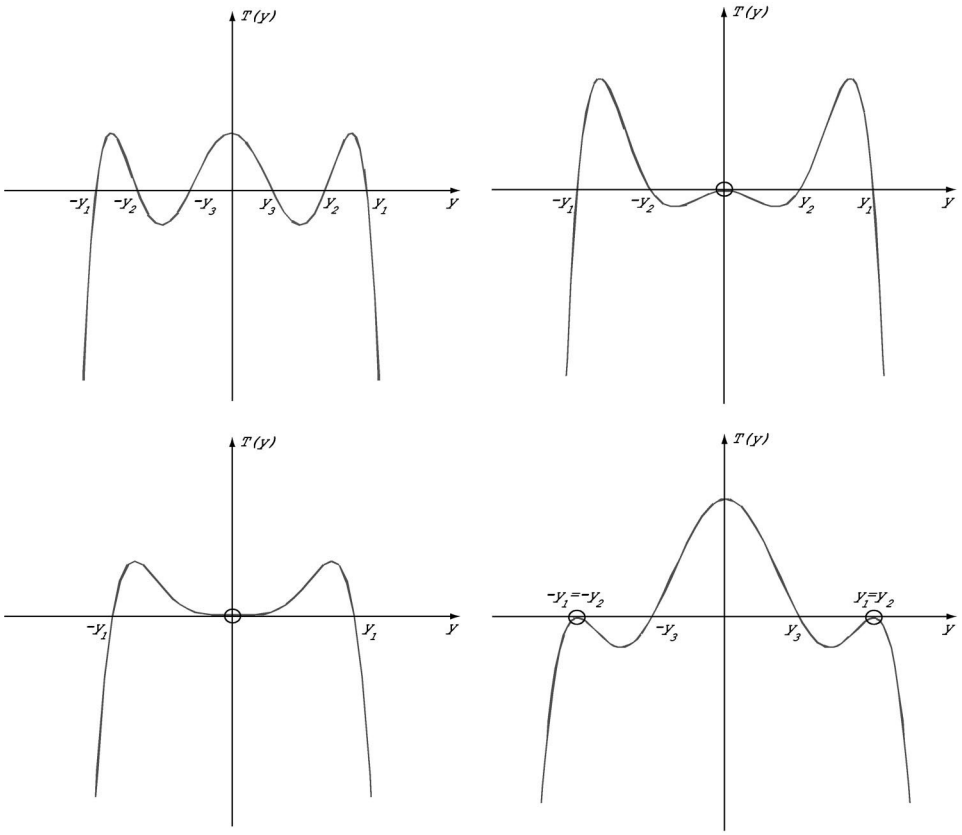

FIG. 1. Roots of the polynomial $T(y)$ in Eq. (5.32). (a) Three pairs of simple roots; (b) one quadruple root, a pair of single ones; (c) one double root, two pairs of single ones; (d) one pair of double roots and one of simple ones.

This equation can be written as a quadrature that will express the independent variable ϕ as a function of y in terms of elliptic integrals. The results are not very illuminating, so instead of presenting them, we restrict ourselves to some special cases. Let us first rewrite Eq. (5.31) as

$$y^4(y')^2 = -(y^2-y_1^2)(y^2-y_2^2)(y^2-y_3^2) \equiv T(y), \tag{5.32}$$

where the roots y_1, y_2, and y_3 are related to the constants A, B, and K by the formulas

$$K = y_1^2 y_2^2 y_3^2, \quad B^2 - A^2 = -(y_1^2 y_2^2 + y_2^2 y_3^2 + y_3^2 y_1^2), \quad 2A = y_1^2 + y_2^2 + y_3^2. \tag{5.33}$$

If all the roots y_i are real and distinct, the behavior of the polynomial $T(y)$ as a function of y is shown in Fig. 1(a).

If all roots are distinct ($0 < y_3 < y_2 < y_1 < \infty$), real periodic solutions are obtained for $-y_3 \leqslant y \leqslant y_3$, $y_2 \leqslant y \leqslant y_1$, and $-y_1 \leqslant y \leqslant y_2$. However, these are expressed in terms of elliptic functions and the period is not a multiple of π. Constant solutions of Eq. (5.32) are obviously $y = \pm y_k$, $k = 1,\ 2$ or 3.

Elementary ϕ dependent real finite periodic solutions are obtained whenever the polynomial $T(y)$ has multiple roots. The corresponding solutions are

(1) $y_3 = y_2 = 0$, $y_1 > 0$ [see Fig. 1(b)]

$$y = y_1 \sin(\phi - \phi_0); \tag{5.34}$$

(2) $0 = y_3 < y_2 < y_1$ [see Fig. 1(c)]

$$y=\pm\frac{1}{\sqrt{2}}\sqrt{y_1^2+y_2^2+(y_1^2-y_2^2)\sin 2(\phi-\phi_0)} \tag{5.35}$$

or in terms of A and B:

$$y=\pm\sqrt{A+B\sin 2(\phi-\phi_0)}; \tag{5.36}$$

(3) $0<y_3<y_2=y_1$ [see Fig. 1(d)].

In this case we give the solution y implicitly as

$$-2\sqrt{y_1^2-y_3^2}\arcsin\left(\frac{y}{y_3}\right)+y_1\left(\arcsin\left(\frac{y_3^2+yy_1}{y_3(y+y_1)}\right)\right)-\arcsin\left(\frac{y_3^2-yy_1}{y_3(y-y_1)}\right)=\pm 2\sqrt{y_1^2-y_3^2}(\phi-\phi_0). \tag{5.37}$$

The solution is real, finite, and periodic for $-y_3\leqslant y\leqslant y_3$.

For any solution $y(\phi)$ of Eq. (5.31) we obtain a magnetic field and effective potential in the form

$$\Omega=-\frac{f''+f+a}{2r^3}, \tag{5.38}$$

$$W=\frac{\hbar^2}{8r^2}\left(1+\frac{2f''}{f+a}-\frac{(f')^2}{(f+a)^2}\right)-\frac{(f+a)^2}{32r^4}\left(\frac{f'''}{f'}+4\right)-\frac{3f''(f+a)}{32r^4}-\frac{C_1}{2r^2(f+a)^2}+C_2. \tag{5.39}$$

The functions P, Q, and m figuring in the polar integral are

$$P=-f'(\phi),\quad Q=f(\phi)+a,$$

$$m=\frac{ff''+(f+a)^2+af''}{4r^2}-\frac{bf''}{2}-\frac{C_1}{(f+a)^2}+\frac{\hbar^2}{4(f+a)^2}(2(f+a)f''-(f')^2). \tag{5.40}$$

Let us sum up the results of this section. Three different cases of polar integrability exist. They are given by Eqs. (5.12), (5.22)–(5.24) and (5.38)–(5.40), respectively. The last case provides an example where the quantum system and the classical one differ. Indeed, the Planck constant figures explicitly in the effective potential W and in the integral of motion.

VI. POLAR SUPERINTEGRABILITY

Let us assume that we have a Hamiltonian (1.1) that is "polar integrable," i.e., allows an integral of motion of the form X_R as in Eq. (2.22). The magnetic field Ω and effective potential W must hence have one of the three forms established in Sec. V. For the system to be superintegrable, it must allow at least one further integral, by assumption of the form (2.20). We can simplify this second integral by linear combinations with X_R and with H and also by rotations, since they will not destroy the form of X_R (nor H). Thus, in Eq. (2.20) we take $\alpha=0$, $\zeta=-\delta$. Furthermore, we can assume $\beta^2+\gamma^2\neq 0$, since otherwise we would be in the case of Cartesian superintegrability, already treated in Sec. IV. By a rotation and normalization, we can set $\beta=1$, $\gamma=0$. It follows that the second integral X_2 is of the parabolic type, conjugate to X_P of Eq. (2.23).

The determining equations for X_2, obtained from (2.17) and (2.18) are

$$k_{1,x}-(x+\xi)\Omega=0,\ k_{2,y}+(x+\xi)\Omega=0, \tag{6.1}$$

$$-2\beta\Omega y+k_{1,y}+k_{2,x}=0, \tag{6.2}$$

$$-2yW_x+(x+\xi)W_y+k_2\Omega-m_x=0,$$

$$(x+\xi)W_x-k_1\Omega-m_y=0, \tag{6.3}$$

$$k_1W_x+k_2W_y+\frac{\hbar^2}{4}\beta\Omega_x=0. \tag{6.4}$$

For each of the three polar integrable systems we obtain the same result, namely, Eqs. (6.1)–(6.4) are compatible only if $\Omega=\Omega_0$ and $W=W_0$ are constant. Then we have three first order integrals and the corresponding second order integrals are polynomial in the first order ones.

VII. CONCLUSIONS

We have constructed all integrable quantum systems with a vector and scalar potential [as in Eq. (1.1)] that possess either a first order integral, or a second order one of the Cartesian, or polar type.

It is interesting to compare such systems with a nonzero magnetic field Ω with systems allowing a scalar potential only.

(1) The first difference is that for $\Omega\neq0$ quantum and classical integrable systems with second order integrals do not necessarily coincide. The Planck constant $\hbar$ can figure in a nontrivial way in the potentials and integrals of motion.
(2) The existence of a first order integral of motion implies a geometrical symmetry, both for $\Omega\neq0$ and $\Omega=0$. Indeed, a first order integral exists if and only if we have either $\Omega=\Omega(r)$, $W=W(r)$, or $\Omega=\Omega(y)$, $W=W(y)$ (up to Euclidean transformations). The functions Ω and W are arbitrary in both cases.
(3) The existence of a second order integral for $\Omega=0$ implies that the Schrödinger equation will allow separation of variables in Cartesian, polar, parabolic, or elliptic coordinates. In each case the potential $V(x,y)$ depends on two arbitrary functions of one variable. For $\Omega\neq0$ the coordinates no longer separate. The requirement that an irreducible second order integral should exist for $\Omega\neq0$ is much more restrictive than for $\Omega=0$. The quanttities $\Omega(x,y)$ and $W(x,y)$ again depend on two functions of one variable, however these functions obey certain ordinary differential equations. They are hence determined completely, up to some arbitrary constants. For instance, in the Cartesian case, they are elliptic functions, or degenerate cases of elliptic functions.
(4) For $\Omega=0$ four families of superintegrable systems in $E(2)$ exist,[1] each depending on three parameters. For $\Omega\neq0$ we have shown that superintegrability with first order integrals of the Cartesian, or polar type, exists only for Ω and W constant.

Several related problems are presently under consideration. To complete the study of quadratic integrability in $E(2)$ for $\Omega\neq0$ we must still consider parabolic and elliptic integrability. For $\Omega=0$ their is a close relation between superintegrability and exact solvability.[20] For $\Omega\neq0$ the requirement of superintegrability seems to be too restrictive. An important question is whether some of the integrable systems found in this article are actually exactly solvable.

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A statistical complexity measure with nonextensive entropy and quasi-multiplicativity

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The properties of a statistical complexity measure that are characterized by nonextensivity in entropy have been investigated, which is of so-called disequilibrium type. Considering the composition law for two systems with different nonextensivities (quasi-multiplicativity), a nontrivial relation between the nonextensive parameters and the fluctuating bit number in information theory has been mentioned. To see the time evolution of the nonextensive complexity measure, we examine systems having a lognormal distribution, the underlying dynamics for which is known to obey a random multiplicative process in the presence of a boundary constraint. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1695600]

I. INTRODUCTION

In recent times, quantifying the complexity of a system has been the chief focus of study across various branches of science and has been drawing renewed attention.[1–3] Up to the present date, different definitions of the complexity have been proposed. Among these, a few notable definitions include algorithmic complexities (Kolmogorov–Chaitin complexity[4] and Lempel-Ziv complexity[5]), effective measure of complexity by Grassberger,[6] logical depth by Bennett,[7] and thermodynamical depth by Lloyd and Pagels.[8] These definitions of complexities have been useful in describing the symbolic dynamics of maps; however, they have the disadvantage of complicated calculations. Especially in physics, a measure of statistical complexity is considerably essential. In most of the proposals for complexity measures, utilizing the concept of entropy or relevant information can be regarded as a basic ingredient for quantifying the phenomenon. In the last few years, keen interest in developing new definitions for statistical measure of complexity based on probabilistic descriptions of physical systems has emerged. One of these is the disequilibrium-based complexity, i.e., LMC(López-Ruiz–Mancini–Calbet)[9] complexity measure C (defined as $C=H\cdot D$ where H is the Shannon entropy and D disequilibrium) that has adopted quadratic distances of each state for assessing the equiprobability. The other one is the simple measure for complexity proposed by SDL (Shiner, Davison, and Landsberg).[10] It is defined as the product of a measure of *order* and a measure of *disorder* in a system.

Another current proposal in the applications is to determine the innovative uses of conventional entropy, which are known as the multiscale entropy[11] and the diffusion entropy analysis[12] (these studies use the Shannon entropy without resorting to the introduction of a new complexity measure). In these past studies, considerable attention has been paid to extract the useful information in order to discriminate, for example, health and disease from a physiologic time series and we require a quantification of their complexities. Their leitmotif was to overcome the fact that an increase in conventional entropy does not always accommodate a growth of dynamical complexity.

In the present study, we intend to use nonextensive entropy instead of extensive (additive) Shannon entropy for defining the statistical measure of complexity from its starting point. The

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rationale for adopting nonextensive entropy is as follows: It is difficult to imagine that the complexity of a system becomes twice its original when the system size is doubled. However, when two or more systems are merged, it seems rather natural to assume that complexity of a system increases or decreases on the basis of symmetry, hierarchy, and acclimation. Although the nonextensivity property of the LMC measure has already been described in Ref. 13, we shall clamp its nonadditive feature on entropy in order to incorporate this assumption into the measure.

We seek a possibility for defining a statistical measure of complexity based on the Tsallis entropy[14] instead of the Shannon entropy for C (another notation will be used subsequently) and take a stance that the statistical complexity measure should vanish or be negligible for both highly ordered and highly disordered systems. As explained in an earlier paper,[9] these extreme situations with zero complexity correspond with the perfect crystal in the former case and the ideal gas in the latter case. In order to describe the perfect crystals, only a minimal amount of information is needed because the constituent atoms are symmetrically arrayed completely. A sufficient amount of information on the crystals is available from the lattice constant and symmetry (fcc, bcc, etc.) only. On the other hand, the state of a system can be found in the phase space with an equal probability in the case of ideal gases. In such a case, we have to specify a large number of variables for defining the system; therefore, it requires maximum information. These two states are extrema in terms of the order and information, and we assume that the system has a finite complexity at an intermediate state.[3]

In effect, we do not regard nonextensivity as an impediment to the legitimate definition of the statistical measure of complexity, because various kinds of physical systems exist for which the traditional extensive statistical mechanics appears to be inadequate.[15,16] Therefore, a nonextensive thermostatistics can be a possible basis for providing a descriptive framework for dealing with the above mentioned complexity measure. In this sense, the complexity measure as well as entropy need not be extensive. Therefore, examining the consequences of using a nonextensive entropy for the complexity measure might provide a hint posed by some applications. For this purpose, we have presented some properties of the complexity measure and have also shown that it retains some properties of the LMC.

The paper has been organized as follows: In Sec. II, the statistical measure of complexity is introduced with the nonextensive entropy of Tsallis and the basic properties are investigated along the lines of Ref. 17. The nonadditivity in the complexity measure is associated with the fluctuating bit number of systems on the basis of the concept of quasi-additivity in Sec. III. In Sec. IV, the time evolution of the present complexity measure is demonstrated by applying the constrained random multiplicative process. Finally, the results of the present study are summarized in the last section. The exact expressions of the complexity measure are given in the Appendix for a few probability distributions, which are often encountered in natural sciences.

II. A NONEXTENSIVE STATISTICAL MEASURE OF COMPLEXITY AND ITS PROPERTIES

In the present study, a continuous expression instead of the discrete one is considered. In general, translation of any entropy from its discrete form to the continuous form requires mathematical precision. However, in this case, we simply assume that the continuous entropy of Tsallis takes the form[18]

$$H_q(p(x)) = \frac{1}{1-q}\left[\int p^q(x)dx - 1\right]. \tag{1}$$

López-Ruiz *et al.*[9] proposed a quantity called the disequilibrium, whose measure is a distance from the equiprobable state. In the discrete case, it is expressed as

$$D(\{p_i\}) = \sum_{i=1}^{n} (p_i - 1/n)^2, \tag{2}$$

where D attains the maximum value for a fully ordered state and vanishes in the case of completely disordered states or equiprobable states. It is interesting to note that the disequilibrium is the same form as the alternative entropy, proposed by Bruckner and Zeilinger[19] in quantum measure of information. In order to make the present paper self-contained, the properties of D are briefly restated. The equiprobable states can be expressed as the rectangular function,

$$p(x)=\begin{cases}\dfrac{1}{2l} & (-l\leqslant x\leqslant l)\\ 0 & (\text{otherwise}),\end{cases} \tag{3}$$

which results in a well-defined disequilibrium for the continuous case. Then, from the definition, we have

$$\int_{-l}^{l}\left(p(x)-\frac{1}{2l}\right)^2 dx=\int_{-l}^{l}p^2(x)dx-\frac{1}{2l}. \tag{4}$$

Moreover, we may redefine the disequilibrium as $D(p(x))=\int_{-l}^{l}p^2(x)dx$, which ensures positivity in any distribution. Accordingly, distributions are measured from equiprobabilities in the course of our consideration. When a system is in the equiprobable state with large l, the value of D is minimum, and when l become small (peaked shape at zero point), then D tends toward infinity. From the view point of the information theory, D is found to be nonextensive[13] since l consecutive sequences of binary variables, $X_i, X_{i+1}, \ldots, X_{i+l-1}\equiv X^{(l)}$, whose values X_i are generated from a discrete finite alphabet of size 2, have the disequilibrium $D(X^{(l)})=\Sigma p^2(x^l)-1/2^l\leqslant 1-2^{-l}$, where $p(x^l)$ is the joint probability over the length sequence l. If the chain of variables is generated by i.i.d. (independent and identically distributed), we can factorize the joint probability into each probability occurring at X_i. However, the above expression is also valid for all Markov chains. Therefore the disequilibrium does not grow linearly with the length of the word l, thereby concluding that the disequilibrium of this sequence becomes nonextensive in the long sequence limit $l\to\infty$. This property is clearly incompatible with the conventional extensive statistical mechanics. Nevertheless, in the subsequent sections, we have concluded that there is no clear reason for measure of complexity to be extensive. Therefore, the disequilibrium without modifying nonextensivity shall be used and the form of multiplying the two nonextensive quantities to obtain a complexity measure would be adopted for the present consideration. The discussion of Catalán *et al.*[17] also holds for the use of the Tsallis entropy in defining the statistical measure of complexity.

The complexity $C_q(p(x))$ for a continuum number of states x with support on the segment $[-l,l]$ with $\int_{-l}^{l}p(x)dx=1$ is defined as follows:

$$C_q(p(x)):=H_q(p(x))D(p(x))=\left(\frac{\int_{-l}^{l}p^q(x)dx-1}{1-q}\right)\left(\int_{-l}^{l}p^2(x)dx\right). \tag{5}$$

To guarantee the positivity of C_q for each continuous distribution, we take the q-exponential[20] of H_q. The new expression $\hat{C}_q$ is regarded as the statistical measure of complexity for the system,

$$\hat{C}_q(p(x)):=\hat{H}_q(p(x))D(p(x))=e_q^{H_q(p(x))}D(p(x)). \tag{6}$$

As for the probability distributions that maximize this type of complexity measure, using ''the maximum complexity approach'' by the Lagrange multipliers method does not help in obtaining the analytical form of the probability distributions p_i's. Therefore, the complexity measure has been regarded as a function of entropy in previous studies.[9,21,22]

A. Properties of $\hat{C}_q$

We investigate the invariance under the β translation and α rescaling transformation on the normalized density function $p(x)$ defined on $\mathbf{R}$, where $\alpha(>0)$ and β are real numbers. The new probability distribution is $p_{\alpha,\beta}(x)=\alpha p[\alpha(x-\beta)]$, which also satisfies the normalization,

$$\int_{\mathbf{R}} p_{\alpha,\beta}(x)dx=1. \tag{7}$$

The effect of the transformation is that β shifts the peak position of the density function while the α determines its broadness. When $\alpha>1$, $p_{\alpha,\beta}(x)$ has a narrow peak, whereas if $\alpha<1$, it becomes broader. After the transformation, we calculate $H_q(p_{\alpha,\beta})$ with the help of the change of variables $y=\alpha(x-\beta)$,

$$\begin{aligned} H_q(p_{\alpha,\beta}(x)) &= \frac{\int_{\mathbf{R}} p^q_{\alpha,\beta}(x)dx-1}{1-q} \\ &= \frac{1}{1-q}\left[\alpha^{q-1}\left(\int_{\mathbf{R}} p^q(y)dy-1\right)+\alpha^{q-1}-1\right] \\ &= \alpha^{q-1}H_q(p)+\ln_q\alpha. \end{aligned} \tag{8}$$

Therefore we have

$$\hat{H}_q(p_{\alpha,\beta}(x))\equiv e_q^{H_q(p_{\alpha,\beta}(x))}=\{1+(1-q)H_q(p_{\alpha,\beta}(x))\}^{1/(1-q)}=\frac{e_q^{H_q(p(x))}}{\alpha}. \tag{9}$$

Since $D(p_{\alpha,\beta}(x))=\alpha D(p(x))$, the new complexity measure is *invariant* under the present transformation:

$$\hat{C}_q(p_{\alpha,\beta}(x))=\hat{H}_q(p_{\alpha,\beta}(x))D(p_{\alpha,\beta}(x))=\frac{e_q^{H_q(p(x))}}{\alpha}\alpha D(p(x))=\hat{C}_q(p). \tag{10}$$

López-Ruiz *et al.*[9] named $\hat{C}_1$ as "the shape complexity" because the translation and rescaling transformation used in the present study do not alter the original shape of distribution curve. It must be noted that this invariance cannot be established when we use the Rényi entropy because of the expression $H_q^{(R)}(p_{\alpha,\beta}(x))=H_q^{(R)}(p)+(q-1)/(1-\alpha)\ln\alpha$. It might be thought that the probability distributions can be analytically determined, which maximizes $\hat{C}_q$, by adopting the maximum complexity approach with a suitable constraint (normalization of probability); however, this approach is not feasible. Hence, it was unavoidable to regard the complexity measure as a function of entropy in Refs. 21 and 22 for further considerations.

B. Invariance under replication

There have been discussions regarding the properties that the complexity measure should possess. Of all these, Lloyd and Pagels[8] insisted on the invariance under replication of distributions. Catalán *et al.*[17] showed $\hat{C}_1$ to be a definite replica invariant; as a result the $\hat{C}_1$ of m replicas for a given distribution are equal to that of the original one. Below, we show, along the lines of Ref. 17, that the use of the Shannon entropy in the complexity measure $\hat{C}$ is not unique choice for this purpose.

Using n copies of the original distribution $p(x)$, which is a compactly supported density function, with $\int_{-\infty}^{\infty}p(x)dx=1$, the mth replica is denoted as

$$p_m(x)=\frac{1}{\sqrt{n}}p[\sqrt{n}(x-\lambda_m)] \quad (1\leqslant m\leqslant n), \tag{11}$$

where λ_m is the center of the mth distribution, $m=1,\ldots,n$, and the support of each $p_m(x)$ is all disjoint. It can be easily observed that the union of all the replicas $s(x)=\Sigma_{i=1}^{n}p_m(x)$ is normalized because $\int_{-\infty}^{\infty}p_m(x)dx=1/n$. Each replica satisfies

$$H_q(p_m(x))=\left(\frac{1}{\sqrt{n}}\right)^{1+q}H_q(p(x))+\frac{(\sqrt{n})^{-1-q}-1}{1-q}, \quad D(p_m)=\frac{D(p)}{n\sqrt{n}}. \tag{12}$$

Since the supports of m replicas on intervals on $\mathbf{R}$ are disjoint, we have the following equations:

$$\begin{aligned}H_q(s(x))&=\frac{\int_{\mathbf{R}}\left(\sum_{i=1}^{n}p_m(x)\right)^q dx-1}{1-q}\\&=\frac{n\int_{\mathbf{R}}p^q(x)dx-1}{1-q}\\&=nH_q(p_m(x))+\frac{n-1}{1-q}\\&=n(\sqrt{n})^{-1-q}H_q(p(x))+\frac{n(\sqrt{n})^{-1-q}-1}{1-q},\end{aligned} \tag{13}$$

$$D(s(x))=\frac{D(p(x))}{\sqrt{n}}. \tag{14}$$

This leads to $\hat{H}_q(s(x))=e_q^{H_q(s(x))}=\sqrt{n}e_q^{H_q(p(x))}$, which makes the complexity measure invariable, i.e., $\hat{C}_q(s(x))=\hat{H}_q(s(x))D(s(x))=\hat{C}_q(p(x))$. Thus, the complexity measure property shown in the LMC case could also be observed when $q\neq 1$.

Continuity is not an evident property in the present definition. To verify the continuity of the complexity measure, let us use a useful concept which was introduced by Catalán *et al.*,[17] i.e., the concept of near-continuity. If similar density functions are given on a common support in similar systems, the associated complexity measures must have values that are close to each other. We discuss this aspect by considering the two rectangular density functions used in the study by Catalán *et al.*[17] One of the density functions is defined on the interval $[-1,0]$ as follows:

$$\xi_{[-1,0]}(x)=\begin{cases}1 & (-1\leqslant x\leqslant 0)\\ 0 & (\text{otherwise}).\end{cases} \tag{15}$$

The other density function is defined on the interval $[-1,L]$ as

$$g_{\delta,L}(x)=\begin{cases}1-\delta & (-1\leqslant x\leqslant 0)\\ \dfrac{\delta}{L} & (0\leqslant x\leqslant L)\\ 0 & (\text{otherwise}),\end{cases} \tag{16}$$

where $0<\delta<1$ and $L>1$. It must be noted that $\lim_{\delta\to 0}g_{\delta,L}(x)=\xi_{[-1,0]}(x)$, thus resulting in the problem of whether or not the $\hat{C}_q$ for each density function converges to the same value in the limiting case. Straightforward calculations indicate $H_q(\xi_{[-1,0]})=0$ and $D(\xi_{[-1,0]})=1$, leading to $\hat{C}_q(\xi_{[-1,0]})=1$ and we obtain the expression

$$H_q(g_{\delta,L}) = \frac{(1-\delta)^q + \delta^q L^{1-q} - 1}{1-q}, \quad D(g_{\delta,L}) = (1-\delta)^2 + \frac{\delta^2}{L}. \tag{17}$$

Therefore, the corresponding complexity measure is expressed as

$$\hat{C}_q(g_{\delta,L}) = [(1-\delta)^q + \delta^q L^{1-q}]^{1/(1-q)} \left[(1-\delta)^2 + \frac{\delta^2}{L} \right]. \tag{18}$$

From the above equation, we can conclude that the support is maintained and the near-continuity condition is satisfied in this limited process irrespective of the value of the nonadditive parameter q:

$$\lim_{\delta \to 0} \hat{C}_q(g_{\delta,L}) = \hat{C}_q(\xi_{[-1,0]}) = 1. \tag{19}$$

Since $[\lim_{L\to\infty} \hat{C}_q(g_{\delta,L}) \to (1-\delta)^{(2-q)/(1-q)}] \neq 1 = \hat{C}_q(\xi_{[-1,0]})$ for $1 < q$ when the support becomes large, the compactness condition is not satisfied despite the fact that they are the δ-neighboring distributions.[23] In such a case, the near-continuity declines in the limit $L \to \infty$.

C. $\hat{C}_q$ in terms of Rényi entropy

The present statistical complexity measure can be expressed with Rényi entropy,[24]

$$H_q^{(R)}(p_i) = \frac{\ln \sum_i p_i^q}{1-q}, \tag{20}$$

which recovers the Shannon entropy as a special case $\lim_{q\to 1} H_q^{(R)} = -\Sigma_i p_i \ln p_i = H^{(S)}$. Since the probability distribution of a system can convey all information that we possess, we often use the entropy as an indication of the degree of randomness. However, the localized or delocalized nature of the system cannot be quantified only by the standard entropy. Therefore, our area of interest is to identify the extent of complexity for a system. For quantification of the characteristics of complexity for a system, the Rényi entropy appears in quantum systems as a measure of localization and ergodicity in phase space,[25] which informs about the shape of distributions. In Ref. 25, it was shown that the differences of Rényi entropies $H_1^{(R)} - H_2^{(R)}$, which are referred to as the structural entropy, can be a candidate for the spatial characterization of one-particle eigenstates (e.g., spatial localization of the charge distributions).

In the previous section, we redefined the disequilibrium D as a squared sum for each distribution measured from a uniform distribution. Since D can be expressed as $D = e^{\ln \Sigma_i p_i^2} = e^{-H_2^{(R)}(p_i)}$, we find that $\hat{C}_1$ can be expressed as follows:

$$\hat{C}_1 = e^{H^{(S)}} D = e^{H_1^{(R)} - H_2^{(R)}}. \tag{21}$$

Similarly, since the Tsallis entropy can be expressed as $H_q(p_i) = (e^{(1-q)H_q^{(R)}} - 1)/(1-q)$, we obtain

$$\hat{C}_q = e_q^{H_q} \cdot D = e^{H_q^{(R)} - H_2^{(R)}}. \tag{22}$$

Accordingly, the present statistical measure of complexity with Tsallis type nonextensive entropy can be expressed by exponential of the difference between qth order Rényi entropy and the second order one. The exact form of $\hat{C}_q$ for the various distributions calculated have been provided in the Appendix. If $q \leqslant 2$ $(q > 2)$, then $\hat{C}_q \geqslant 1$ $(\hat{C}_q < 1)$ holds due to the fact that if $\alpha \leqslant \beta$, then $H_\alpha^{(R)} \geqslant H_\beta^{(R)}$. It is noteworthy that the uniform distribution, which can be viewed as a dispersed or highly delocalized system, has the same complexity value (unity) as that for an extremely local-

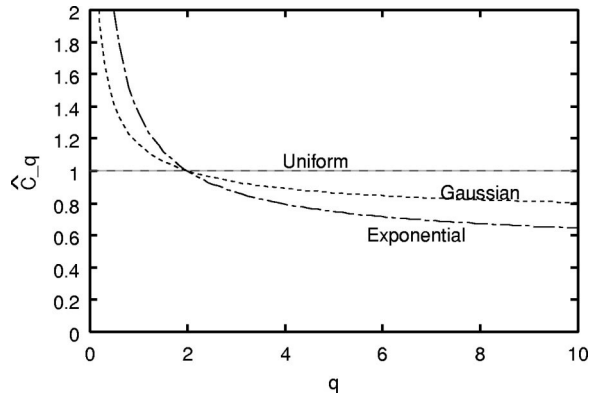

FIG. 1. The behavior of the statistical measure of complexity with respect to q for exponential, Gaussian, and uniform distributions.

ized system. This fact can be easily confirmed by considering a distribution, which assumes the value of $1/\epsilon$ for $-\epsilon/2 \leqslant x \leqslant \epsilon/2$ and 0 for other cases, where ϵ determines the localized region. In this case, therefore, we have $H_q^{(R)} = H_2^{(R)} = \ln \epsilon$. The focus of our attention lies in determining the manner in which a systems's measure of complexity changes when the value of nonextensive parameter is varied. For this purpose, we show the behavior of $\hat{C}_q$ with respect to q in Fig. 1 for three distributions (uniform, Gaussian, and exponential) and in Figs. 2 and 3 for the Weibull distribution and the gamma distribution, respectively.

Although, by definition, $\hat{C}_q$ is made of the two nonextensive quantities, that is, the q-exponentiated Tsallis entropy and the disequilibrium, an assertion regarding its expressivity with an extensive quantity can be made (note that the Rényi entropy is an extensive quantity).

III. THE QUASI-MULTIPLICATIVITY OF $\hat{C}_q$ AND FLUCTUATION OF BIT NUMBER

The quantity $\Sigma_i p_i^q$, which plays a central role in the generalized entropy, can be related to the bit number.[26] The bit number is defined as $B_i = \log p_i$, which has an opposite sign to the information content in Shannon information theory. Assuming that q is close to unity, the Taylor expansion in $q-1$ enables the expression $\Sigma_i p_i^q$ to be written as

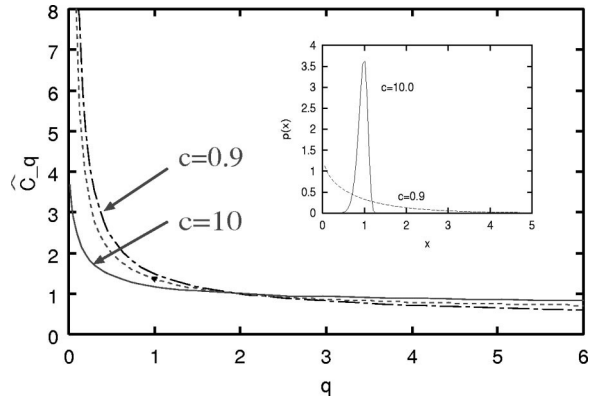

FIG. 2. The behavior of the statistical measure of complexity with respect to q for the Weibull distribution (for $c=0.9$ and $c=10.0$). The dotted curve represents $\hat{C}_q$ for the exponential distribution, which corresponds to the case $c=1$ and the black circle denotes the value $e/2$ when $q=1$. Note that the curves pass through the value 1 when $q=2$ for all the distributions. The inset shows the original distributions when $\alpha=1.0$.

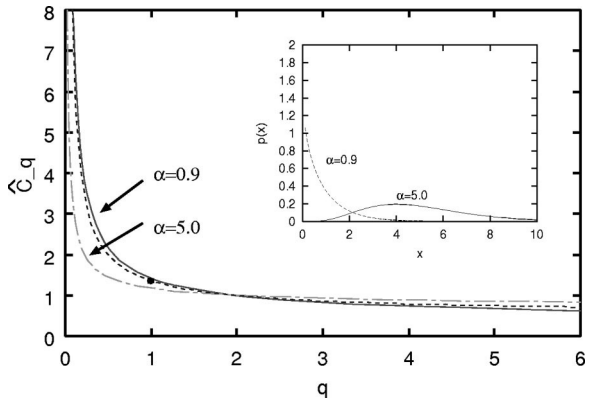

FIG. 3. The behavior of the statistical measure of complexity with respect to q for the gamma distribution (for $\alpha=0.9$ and $\alpha=5.0$). The dotted curve represents $\hat{C}_q$ for the exponential distribution, which corresponds to the case $\alpha=1$ and the black circle denotes the value $e/2$ when $q=1$. Note that the curves pass through the value 1 when $q=2$ for all the distributions. The inset shows the original distributions when $\beta=1.0$.

$$\sum_i p_i^q=\sum_i p_i e^{(q-1)\log p_i}=\sum_{k=0}^{\infty}\frac{\langle B_i^k\rangle(q-1)^k}{k!}, \tag{23}$$

where $\langle B_i^k\rangle=\Sigma_i p_i B_i^k$. Thus, the expectation value of the negative bit number comprises the Shannon entropy. When a joint probability of N systems is factorized into each component and the number of events is the same for all components, Eq. (24) is obtained using the formula shown in Eq. (25):

$$\begin{aligned}\sum_{i_1,\ldots,i_N} p_{i_1,\ldots,i_N}^q&=\left(\sum_i p_i^q\right)^N\\&=\left(\sum_{k=0}^{\infty}\frac{(q-1)^k\langle B_i^k\rangle}{k!}\right)^N\\&=\sum_{\Sigma_s n_s=N}\frac{N!}{n_1!n_2!\cdots}(1)^{n_1}((q-1)\langle B_i\rangle)^{n_2}\cdots\left(\frac{(q-1)^s\langle B_i^s\rangle}{s!}\right)^{n_s}\cdots,\end{aligned} \tag{24}$$

$$(A_1+A_2+\cdots)^N=\sum_{\Sigma_s n_s=N}\frac{N!}{n_1!n_2!\cdots}(A_1)^{n_1}(A_2)^{n_2}\cdots(A_s)^{n_s}\cdots. \tag{25}$$

In what follows, we consider the case $N=2$ and assume that two independent systems X and Y, each of which has a different nonadditive index (q_X and q_Y, respectively) and both these systems are unified to form one system $X+Y$ with a new nonadditive index q_{new} such that the composition of the statistical measure of complexity is as follows:

$$\hat{C}_{q_X}^X(p_i)\times\hat{C}_{q_Y}^Y(p_j)=\hat{C}_{q_{new}}^{X+Y}(p_{ij}). \tag{26}$$

This may be referred to as ''the composition law by multiplication.'' ''The composition law by sum'' inevitably involves the issue of additivity or nonadditivity in entropy, whereas the multiplication conflation does not incur this problem. Subsequently, we assume that the two systems are identical in the level of their probability distributions, which ensures that the fluctuation of the bit number is the same during the composition process as shall be seen in the following sections.

To begin with, the quantity $\ln(\Sigma_i p_i^q)$ can be expanded as $(q-1)\langle B_i\rangle-(q-1)^2(\langle B_i^2\rangle-\langle B_i\rangle^2)/2+O((q-1)^3)$. If the first two terms in Eq. (23) are regarded as infinitesimal quantities compared to unity, then the single Rényi entropy can be expressed as

$$H_q^{(R)}=-\langle B_i\rangle-\tfrac{1}{2}(q-1)(\langle B_i^2\rangle-\langle B_i\rangle^2)+\cdots. \tag{27}$$

When a higher order moment of the bit number in the expression of entropy is required, higher order terms need to be incorporated in $q-1$ for $\ln(1+x)$ type expansion. For our present focus, it is sufficient to expand it up to the second order in $q-1$ because the fluctuation of the bit number appears as the coefficient of $q-1$. Therefore, $\hat{C}_{q_X}^X$ is approximately expressed as

$$\hat{C}_{q_X}^X=e^{H_{q_X}^{(R)}-H_2^{(R)}}\sim e^{(1-q_X/2)(\langle B_i^2\rangle-\langle B_i\rangle^2)} \quad (q_X\sim 1). \tag{28}$$

Accordingly, the product of the statistical measure of complexity for independent systems is reduced to (up to the first order in $q-1$),

$$\hat{C}_{q_X}^X\times\hat{C}_{q_Y}^Y=e^{(1-q_X/2)(\langle B_i^2\rangle-\langle B_i\rangle^2)}e^{(1-q_Y/2)(\langle B_i^2\rangle-\langle B_i\rangle^2)}. \tag{29}$$

On the other hand, by using Eq. (24),

$$\sum_{ij} p_{ij}^{q_{new}}=2\ln\left(\sum_i p_i^{q_{new}}\right)\sim 2(q_{new}-1)\langle B_i\rangle+(q_{new}-1)^2(\langle B_i^2\rangle-\langle B_i\rangle^2)+\cdots, \tag{30}$$

the composed complexity measure $\hat{C}_{q_{new}}^{X+Y}$ satisfies

$$\hat{C}_{q_{new}}^{X+Y}=e^{H_{q_{new}}^{(R)}(p_{ij})-H_2^{(R)}(p_{ij})}\sim e^{-(q_{new}-2)(\langle B_i^2\rangle-\langle B_i\rangle^2)}. \tag{31}$$

Therefore, the present composition law implies a relation among q_X, q_Y, and q_{new}, namely,

$$\left(1-\frac{q_X}{2}\right)+\left(1-\frac{q_Y}{2}\right)=-(q_{new}-2). \tag{32}$$

Based on this, we have $q_{new}=(q_X+q_Y)/2$. If $q_X=q_Y=1$, then q_{new} also becomes unity. For this case, the LMC complexity measure with the exponentiated Shannon entropy was used.

This relation suggests that the composition of two independent systems necessarily involves the average and the variance of bit number when q is close to unity. In other words, the change in the nonadditivity indices relates to the fluctuation of the Shannon entropy. This fact had been indicated when the interpretation of the nonextensive parameter q from the system's fluctuating temperature were analyzed in Ref. 26. If the fluctuation is sufficiently small, i.e., $\langle B_i^2\rangle-\langle B_i\rangle^2 \ll 1$, then Eqs. (28) and (31) are approximately expressed as $(1-q_X/2)b$ and $1-(q_{new}-2)b$, respectively, where we put $b=\langle B_i^2\rangle-\langle B_i\rangle^2$. Therefore, we have the following relation:

$$b=\frac{\frac{1}{2}(q_X+q_Y)-q_{new}}{(1-q_X/2)(1-q_Y/2)}. \tag{33}$$

Note that the above expression is symmetric in q_X and q_Y. When $q_X=q_Y=q_{new}=1$, there is no fluctuation in systems. As special cases, we have two types of *quasi-multiplicativities*.

(i) The case $q_X=q_Y=q$ (type I quasi-multiplicativity): This case corresponds to the situation where two identical systems form a single new system with a new entropic index that is different from its original. This is the case where Beck introduced the concept of quasi-additivity in Ref. 26 in the context of addition of two entropies. In this case, the above relation reduces to

$$b=\frac{q-q_{new}}{(1-q/2)^2}. \tag{34}$$

(ii) The case $q_{new}=q_X$ or $q_{new}=q_Y$ (type II quasi-multiplicativity): This case describes the circumstances where the new entropic index is absorbed either into the index of X or that of Y. Substituting $q_{new}=q_X$ in Eq. (33) and then arranging it, the relation appears as

$$\frac{\langle B_i^2\rangle-\langle B_i\rangle^2}{2}=\frac{1}{q_{new}-2}-\frac{1}{q_Y-2}. \tag{35}$$

In this case, the difference between the reciprocal of the displacements from two in the nonextensive index is equivalent to half of the fluctuation.

IV. TEMPORAL BEHAVIOR OF $\hat{C}_q$ FOR THE RANDOM MULTIPLICATIVE PROCESS

It is noteworthy that both the LMC measure and $\hat{C}_q$ provide time-independent values for the standard diffusion (i.e., Wiener process), indicating that these quantities can measure the shapes of distributions. This time independency comes from the fact that in the standard diffusion process, the dispersion changes with the passage of time; however, the Gaussian forms are maintained during the process (see the Appendix). In this sense, the present disequilibrium based complexity measure captures only the information on shapes of distributions except for the similarity.

It is interesting to observe how the complexity measure evolves with time, or the transient behavior of it. To achieve this end, we examine a lognormal distribution whose form is a result of the Levy and Solomon's random multiplicative processes with a boundary constraint of large time.[27] The random multiplicative process that Levy and Solomon considered is expressed as $x(t+1)=\lambda_t x(t)$ with a stochastic random positive variable λ_t, where $x(t)$ is the position of a particle at time t. The probability distribution for this process at asymptotic time is found to be of the following form:[28]

$$p(x,t)=\frac{1}{\sqrt{2\pi\mathcal{D}t}}\frac{1}{x}\exp\left[-\frac{1}{2\mathcal{D}t}(\ln x-vt)^2\right], \tag{36}$$

where v is the drift velocity, defined as an average of logarithm of λ_t with respect to the probability distribution of λ_t, and $\mathcal{D}$ is its dispersion. Our key interest is in the time regime such that $x\gg e^{(vt+2\mathcal{D}t)}$, whose distributions are clearly distinguished from the power law form $p(x,t)\sim 1/x$. For this distribution, the disequilibrium can be expressed as

$$D(p(x,t))=\int_\epsilon^\infty p^2(x,t)dx=\frac{e^{-(v-\mathcal{D}/4)t}}{2\pi\mathcal{D}t}\int_{\ln\epsilon}^\infty dy e^{-(y-[(2v-\mathcal{D})/2]t)^2/\mathcal{D}t} \tag{37}$$

where $y=\ln x$ is a quantity that arises due to the change of variables. Since the distribution becomes singular at $x=0$, we always set $\epsilon\leqslant x$. This leads the following interpretation: the lower bound ϵ is the boundary that keeps the position of particle away from it at time t (repulsive effect introduced in Ref. 27). The physical description for this process and a derivation based on the random walk analogy are provided in detail in Ref. 28. Furthermore, with the definition of error function $\int_\xi^\infty e^{-z^2}dz=\sqrt{\pi}(1-\mathrm{erf}[\xi])/2$, the following expression is obtained:

$$D(p(x,t))=\frac{e^{-(v-\mathcal{D}/4)}}{4\sqrt{\pi\mathcal{D}t}}(1-\mathrm{erf}[\xi]), \tag{38}$$

where ξ is

$$\xi=\frac{1}{\sqrt{\mathcal{D}t}}\left\{\ln\epsilon-\left(v-\frac{\mathcal{D}}{2}\right)t\right\}. \tag{39}$$

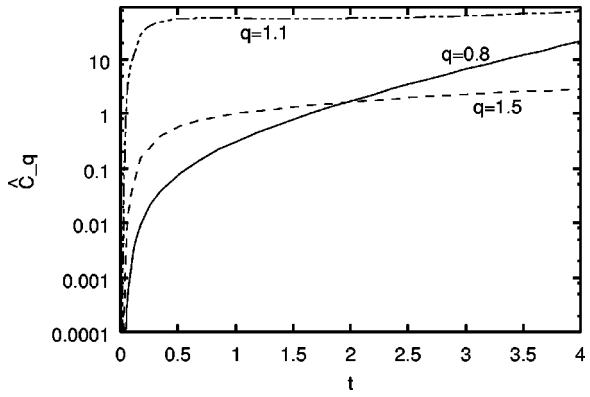

FIG. 4. The change in the complexity measure with time for the random multiplicative process with a boundary constraint for different values of q. The parameters are set as $v=1.5$, $\mathcal{D}=2.5$, and $\epsilon=2.1$.

Since $\xi>0$, the above expression is valid only for $t<\ln\epsilon/(v-\mathcal{D}/2)$. Similarly, the entropy is calculated as

$$H_q(p(x,t))=\frac{\int_\epsilon^\infty p^q(x,t)dx-1}{1-q}. \tag{40}$$

The integral of the numerator for the above equation can be calculated as

$$\int_\epsilon^\infty p^q(x,t)dx=\int_{\ln\epsilon}^\infty dy e^{-(q/2\mathcal{D}t)(y-vt)^2}e^{(1-q)y}=\sqrt{\frac{2\mathcal{D}t}{q}}\frac{\sqrt{\pi}}{2}(1-\mathrm{erf}[\tau])e^{(1-q)(v+[(1-q)/2q]\mathcal{D}t)}, \tag{41}$$

where τ is the lower bound of integration that appears due to the change of variables and attains a positive value,

$$\tau=\sqrt{\frac{q}{2\mathcal{D}t}}\left(\ln\epsilon-\left(v+\frac{1-q}{q}\mathcal{D}\right)t\right)>0. \tag{42}$$

Accordingly, when $q>0(<0)$, the above expression describes the time range $\ln\epsilon/(v+(1-q)\mathcal{D}/q)<t(>t)$. Therefore, the following expression is obtained:

$$\begin{aligned}e_q^{H_q(p(x,t))}&=[1+(1-q)H_q(p(x,t))]^{1/(1-q)}\\&=\sqrt{2\pi\mathcal{D}t}(2\sqrt{q})^{1/(q-1)}(1-\mathrm{erf}[\tau])^{1/(1-q)}e^{(v+[(1-q)/2q]\mathcal{D}t)}.\end{aligned} \tag{43}$$

Combining this with Eqs. (38) and (39), we have the expression

$$\hat{C}_q(p(x,t))=\frac{\sqrt{2}}{4}(2\sqrt{q})^{1/(q-1)}(1-\mathrm{erf}[\xi])(1-\mathrm{erf}[\tau])^{1/(1-q)}e^{[(2-q)/4q]\mathcal{D}t}. \tag{44}$$

In general, $\hat{C}_q$ exhibits varied behavior depending on the value of diffusion constant and that of the boundary constraint. The temporal evolution for some parameter values has been shown in Figs. 4 and 5.

V. SUMMARY

In this work, a statistical complexity measure has been examined with a nonextensive entropy based on the LMC type (disequilibrium-based) measure. The LMC measure can be regarded as

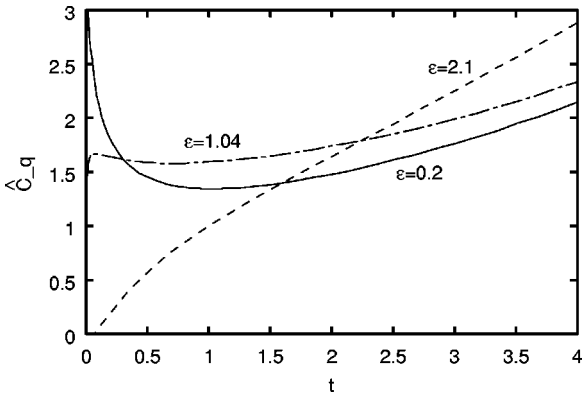

FIG. 5. The change in the complexity measure with time for the random multiplicative process with a boundary constraint for different values of ϵ, with nonextensivity fixed at $q=1.5$. The values of parameters for v and $\mathcal{D}$ are identical to those used in Fig. 4.

one class of measures that satisfies the so-called one-hump criterion—possessing concavity with respect to the order parameter such as entropy.[2,3,29] The more general types of complexity measure are categorized according to their behavior as a function of disorder (or order) using SDL classification[10] with two parameters, and this is referred to as the simple measure for complexity (see also consequent discussions for its validity[13,30–32]). Although it is difficult to choose a specific measure among these, we think that the LMC type complexity measure deserves to be investigated as a prototype. In the LMC measure, the one-hump criterion is realized by using a quantity of disequilibrium. Hence, this criterion has been retained in this study.

In general, analyzing the compositions of two systems that are characterized by different nonextensive parameters is essential because the probability of two complex systems having the same nonextensive value may be rare. In the case of a physical system, a series of analyses has led to the conclusion that the entropy composition with the same nonextensive parameter results in the equibration (the zeroth law of thermodynamics) that occurs when normalized temperature is used over the system's temperature itself.[33] The concept of the quasi-multiplicativity was introduced for the composed system, thereby the idea of defining the statistical complexity measure in terms of a system's bit number leads to the formulation of two kinds of quasi-multiplicativity under the condition where the nonextensivity is small ($q\sim 1$).

Although static distributions yield single values corresponding to their shapes, it is interesting to note how the present measure of complexity changes with time under a specific (often nonlinear) dynamics. In ordinary diffusion process (i.e., Wiener process), the shape of distribution maintains the Gaussian form during its evolution, resulting in that the present measure of complexity yields a constant value. As a specific illustration, a random multiplicative process was considered, in which probability distribution of the position of a particle at asymptotic time obeys a lognormal distribution. Observations revealed that the measure increased with time for different values of q; however, the relation depends on the value of the lower bound (boundary condition).

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APPENDIX: $\hat{C}_q$ AND $\hat{C}$ FOR DIFFERENT KINDS OF DISTRIBUTIONS

Given below are the explicit forms of the present complexity measure defined by Eq. (6) [equivalently by Eq. (22)] for some distribution functions, which are often encountered in the various branches of science.

1. Uniform distribution

$$p(x)=\frac{1}{\beta-\alpha} \quad (\alpha\leqslant x\leqslant\beta). \tag{A1}$$

We have $H^{(S)}(p(x))=-\int_{\alpha}^{\beta}p(x)\ln p(x)dx=\ln(\beta-\alpha)$. Furthermore, $H_q^{(R)}(p(x))=\ln(\beta-\alpha)$, $\forall q$ whence $\hat{C}_q=\hat{C}=1$.

2. Gaussian distribution

$$p(x)=\frac{1}{\sqrt{2\pi\sigma^2}}e^{-x^2/2\sigma^2} \quad (0<\sigma). \tag{A2}$$

We have $H^{(S)}(p(x))=-\int_{-\infty}^{\infty}p(x)\ln p(x)dx=\ln(\sqrt{2\pi}\sigma)+\frac{1}{2}$. Furthermore, $H_q^{(R)}(p(x))=(\ln\sqrt{q})/(q-1)+\ln(\sqrt{2\pi}\sigma)$ and $H_2^{(R)}(p(x))=\ln(\sqrt{2\pi}\sigma)+(\ln 2)/2$. Hence $\hat{C}_q=\sqrt{q^{1/(q-1)}/2}$ and $\hat{C}=\sqrt{e/2}$.

3. Exponential distribution

$$p(x)=\frac{1}{\lambda}e^{-x/\lambda} \quad (x,\lambda>0). \tag{A3}$$

We have $H^{(S)}(p(x))=-\int_{0}^{\infty}p(x)\ln p(x)dx=\ln\lambda+1$. Furthermore, $H_q^{(R)}(p(x))=\ln\lambda-(\ln q)/(1-q)$ and $H_2^{(R)}(p(x))=\ln(2\lambda)$. Hence $\hat{C}_q=q^{1/(q-1)}/2$ and $\hat{C}=e/2$. Note that $\lim_{q\to 1}\hat{C}_q=e/2=\hat{C}$.

4. Pareto distribution

$$p(x)=\frac{ak^a}{x^{a+1}} \quad (0<a, \quad 0<k\leqslant x). \tag{A4}$$

We have $H^{(S)}(p(x))=-\int_{k}^{\infty}p(x)\ln p(x)dx=\ln(k/a)+1+1/a$. Furthermore, $H_q^{(R)}(p(x))=\ln[[k/(q(a+1)-1)](a/k)^q]/(1-q)$ and $H_2^{(R)}(p(x))=\ln[k(2a+1)/a^2]$. Hence $\hat{C}_q=(k/a)\,e^{1+1/a}[[k/(q(a+1)-1)](a/k)^q]^{1/(1-q)}$ and $\hat{C}=ae^{(1+1/a)}/(2a+1)$.

5. Weibull distribution

$$p(x)=\frac{c}{\alpha}x^{c-1}e^{-x^2/\alpha} \quad (x,c,\alpha>0). \tag{A5}$$

$H^{(S)}(p(x))=-\int_{0}^{\infty}p(x)\ln p(x)dx=[(c-1)/c]\,\gamma+\ln(\alpha^{1/c}/c)+1$, where $\gamma=0.577\,215\,66\ldots$ is Euler's constant. Furthermore, $H_q^{(R)}(p(x))=[1/(1-q)]\ln[c^{q-1}\alpha^{(1-q)/c}q^{q(1/c-1)-1/c}\Gamma(q(1-1/c)+1/c))]$ and $H_2^{(R)}(p(x))=\ln[c\alpha^{-1/c}2^{1/c-2}\Gamma(2-1/c)]^{-1}$. Hence $\hat{C}_q=2^{1/c-2}q^{q/(q-1)-1/c}\Gamma(2-1/c)[\Gamma(q(1-1/c)+1/c)]^{1/(1-q)}$. The value of $\hat{C}$ is calculated to be $2^{1/c-2}e^{1+(1-1/c)\gamma}\Gamma(2-1/c)$.

Remark: When $c=1$, $\hat{C}$ and $\hat{C}_q$ are reduced to $e/2$ and $q^{1/(q-1)}/2$, respectively, because the Weibull distribution recovers the exponential distribution. The form $\hat{C}_q$ is independent of the scale parameter α; however, it is affected by the value of the shape parameter c.

6. Gamma distribution

$$p(x)=\frac{x^{\alpha-1}e^{-x/\beta}}{\beta^{\alpha}\Gamma(\alpha)} \quad (x,\alpha,\beta>0). \tag{A6}$$

We have $H^{(S)}(p(x))=-\int_0^{\infty}p(x)\ln p(x)dx=\ln(\beta\Gamma(\alpha))+(1-\alpha)\psi(\alpha)+\alpha$, where $\psi(\alpha)=d\Gamma(\alpha)/d\alpha$ is the digamma function. Then $\hat{C}=e^{(1-\alpha)\psi(\alpha)+\alpha}2^{1-2\alpha}\Gamma(2\alpha-1)/\Gamma(\alpha)$. On the other hand, we have $H_q^{(R)}(p(x))=[\,1/(1-q)\,]\ln[\beta^{1-q}q^{-q(\alpha-1)-1}\Gamma(q(\alpha-1)+1)/[\Gamma(\alpha)]^q]$ and $H_2^{(R)}(p(x))=-\ln[2^{1-2\alpha}\Gamma(2\alpha-1)/\beta[\Gamma(\alpha)]^2]$. Hence $\hat{C}_q=2^{1-2\alpha}q^{[q/(q-1)\,]\alpha-1}\Gamma(2\alpha-1)[\Gamma(\alpha)]^{q/(q-1)-2}\times[\Gamma(q(\alpha-1)+1)]^{1/(1-q)}$.

Remark: When $\alpha=1$, $\hat{C}$ and $\hat{C}_q$ are reduced to $e/2$ and $q^{1/(q-1)}/2$, respectively, because the gamma distribution recovers the exponential distribution. The scale parameter β does not get modified to the form $\hat{C}_q$; however, it is influenced by the value of the shape parameter α.

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Associated Bessel functions and the discrete approximation of the free-particle time evolution operator in cylindrical coordinates

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A central finite difference approximation for the radial contribution Δ_r to the Laplacian $\nabla^2=\Delta_r+\Delta_{r_\perp}(r)$ is considered in a three-dimensional cylindrical coordinate system (r,θ,z). A free-particle Schrödinger time evolution operator is constructed by exponentiation, $e^{(i/2)\,\xi\nabla^2}=\cdots e^{-(1/2)\xi^2[\Delta_r,\Delta_{r_\perp}(r)]}\ e^{(i/2)\,\xi\Delta_{r_\perp}(r)}\ e^{(i/2)\,\xi\Delta_r}\to\cdots e^{(i/2)\,\xi\Delta_r}$. Denoting the central finite difference approximation of Δ_r by $(1/\Delta r^2)\,\mathbb{T}$, the matrix $\mathbb{S}\equiv e^{(i/2)\,\lambda\mathbb{T}}$, with $\lambda=\xi/\Delta r^2$, is shown to be similar to a particular unitary representation U_{VK} of the group of motions on Euclidean three-space that has been described by Vilenkin and Klimyk. The matrix elements of U_{VK} generalize the Bessel function and provide an approximation of the leading term in the radial contribution to the evolution operator. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1695601]

I. INTRODUCTION

We work in standard cylindrical coordinates (r,θ,z) and denote the Laplacian as $\nabla^2=\partial^2/\partial r^2+(1/r)(\partial/\partial r)+(1/r^2)(\partial^2/\partial\theta^2)+\partial^2/\partial z^2\equiv\Delta_r+\Delta_{\theta z}(r)$, where $\Delta_r=\partial^2/\partial r^2+(1/r)(\partial/\partial r)$. Let $\mathcal{H}=-(\hbar^2/2m)\,\nabla^2$ denote the Hamiltonian of a free spinless particle of mass m, and $\Psi(r,\theta,z,t)$ denote its Schrödinger wavefunction. Integration of the Schrödinger equation gives

$$\Psi(r,\theta,z,t+\delta t)=e^{\delta t\partial_t}\Psi(r,\theta,z,t)=e^{(i\hbar\,\delta t/2m)\ \nabla^2}\Psi(r,\theta,z,t). \tag{1}$$

The evolution operator may be expanded using the Zassenhaus formula as

$$e^{(i\hbar\,\delta t/2m)\,\nabla^2}=\cdots e^{A_3\delta t^3}e^{A_2\delta t^2}e^{(i\hbar\,\delta t/2m)\,\Delta_{\theta z}(r)}\,e^{(i\hbar\,\delta t/2m)\,\Delta_r}, \tag{2}$$

where the $A_2,A_3,\ldots$ are anti-Hermitian operators. To each order in δt the decomposition of the evolution operator is in terms of unitary operators, so that the norm of Ψ is preserved as the "dynamics" unfolds. A numerical algorithm based on this expansion will be unconditionally stable. In this note we develop a unitary approximation for the radial contribution to $e^{(i\hbar\,\delta t/2m)\,\nabla^2}$ in terms of a set of special functions, the *associated Bessel functions*, that have been defined by Vilenkin and Klimyk.

We employ a uniform discrete lattice approximation with lattice spacing Δr for the radial coordinate $r\to r_n=(n+\frac{1}{2})\Delta r, n\in\mathbb{N}\quad(n=0,1,2,\ldots)$. The action of Δ_r on Ψ is approximated by $\{\Delta_r\,\Psi\}_n\approx(1/\Delta r^2)\,(\mathbb{T}\Psi)_n$ where $(\mathbb{T}\Psi)_n=\Psi_{n+1}-2\,\Psi_n+\Psi_{n-1}+[1/2\,(n+\frac{1}{2})]\,(\Psi_{n+1}-\Psi_{n-1})$. The matrix elements of $\mathbb{T}$ are

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$$\mathbb{T}_{nn'} = \delta_{n\,n'-1}\left(1+\frac{1}{2\,(n+\frac{1}{2})}\right)) + \delta_{n\,n'}(-2) + \delta_{n\,n'+1}\left(1-\frac{1}{2\,(n+\frac{1}{2})}\right), \tag{3}$$

where $n,n' \in \mathbb{N}$. Let $\lambda = \hbar\ \delta t/m\ \Delta r^2$. We show below that a unitary approximation to $e^{(i\hbar\,\delta t/2m)\,\Delta_r}$ is given by

$$\mathbb{S} = e^{(i/2)\,\lambda \mathbb{T}}, \tag{4}$$

up to a similarity transformation. It will be seen that the matrix elements of $\mathbb{S}$ have a simple, remarkable realization in terms of Vilenkin and Klimyk's associated Bessel functions.

II. ELEMENTARY PROPERTIES OF $\mathbb{S}$

Let us define matrices $\hat{\mathbb{T}}$ and $\hat{\mathbb{S}}$ by

$$\hat{\mathbb{T}}_{nn'} = \delta_{n\,n'-1}\left(1+\frac{1}{2\,n+1}\right) + \delta_{n\,n'+1}\left(1-\frac{1}{2\,n+1}\right), \tag{5}$$

where $n,n' \in \mathbb{N}$, and

$$\hat{\mathbb{S}} = e^{(i/2)\,\lambda \hat{\mathbb{T}}}, \tag{6}$$

so that $\mathbb{S} = e^{-i\lambda}\, e^{(i/2)\,\lambda \hat{\mathbb{T}}} = e^{-i\lambda}\,\hat{\mathbb{S}}$. This is a change of variable that deletes the diagonal matrix elements from $\hat{\mathbb{T}}$ and removes the simple exponential λ-dependence from $\hat{\mathbb{S}}$.

We also define a "weight" matrix $\mathbb{W}$ by

$$\mathbb{W}_{n\,n'} = \delta_{n\,n'}\sqrt{2n+1}, \tag{7}$$

$n,n' \in \mathbb{N}$. $\mathbb{W}$ corresponds to the radial weight function r in this cylindrical coordinate system. It is not too difficult to show that the similarity transform of $\hat{\mathbb{S}}$ by $\mathbb{W}$, $\mathbb{U} = \mathbb{W}\hat{\mathbb{S}}\mathbb{W}^{-1} = \mathbb{W}e^{(i/2)\,\lambda \hat{\mathbb{T}}}\mathbb{W}^{-1} = e^{(i/2)\,\lambda \mathbb{W}\hat{\mathbb{T}}\mathbb{W}^{-1}}$ is a unitary matrix. For brevity we put $\mathbb{Q} \equiv \mathbb{W}\hat{\mathbb{T}}\mathbb{W}^{-1}$ so that $\mathbb{U} = e^{(i/2)\,\lambda \mathbb{Q}}$.

Lemma 1: $\mathbb{Q}$ *is symmetric and* $\mathbb{U} = e^{(i/2)\,\lambda \mathbb{Q}}$ *is unitary.*

Proof: To show that $\mathbb{Q}$ is symmetric consider

$$\begin{aligned}
\mathbb{Q}_{n\,n'} &= (\mathbb{W}\hat{\mathbb{T}}\mathbb{W}^{-1})_{n\,n'} \\
&= \sqrt{\frac{2n+1}{2n'+1}}(\hat{\mathbb{T}})_{n\,n'} \\
&= \sqrt{\frac{2n+1}{2n'+1}}\left[\delta_{n\,n'-1}\left(1+\frac{1}{2\,n+1}\right) + \delta_{n\,n'+1}\left(1-\frac{1}{2\,n+1}\right)\right] \\
&= \sqrt{\frac{2n+1}{2n'+1}}[\delta_{n\,n'-1} + \delta_{n\,n'+1}] + \sqrt{\frac{1}{(2n+1)(2n'+1)}}[\delta_{n\,n'-1} - \delta_{n\,n'+1}] \\
&\equiv \sqrt{\frac{2n+1}{2n'+1}}\,\sigma_{n\,n'} + \sqrt{\frac{1}{(2n+1)(2n'+1)}}\,\Delta_{n\,n'},
\end{aligned}$$

where σ is symmetric and Δ is antisymmetric. We see that $\mathbb{Q}_{n\,n'} - \mathbb{Q}_{n'\,n} = 2\sqrt{1/(2n+1)(2n'+1)}[(n-n')\,\sigma_{n\,n'} + \Delta_{n\,n'}]$. Clearly $(n-n')\,\sigma_{n\,n'} + \Delta_{n\,n'}$ is (possibly) nonvanishing only when $n' = n \pm 1$. However, in both cases $(n-n')\,\sigma_{n\,n'} + \Delta_{n\,n'} = 0$. Hence $\mathbb{Q}$ is symmetric (thus $\mathbb{U}$ is also symmetric). The fact that $\mathbb{Q}$ is a real symmetric matrix implies that $\mathbb{U} = e^{(i/2)\,\lambda \mathbb{Q}}$ is unitary. □

Since $\mathbb{U}$ is unitary and symmetric and $\mathbb{U}_{n\,n'} = \sqrt{(2n+1)/(2n'+1)}\,\hat{\mathbb{S}}_{n\,n'}$ we immediately have

$$\hat{\mathbb{S}}_{n'\,n} = \hat{\mathbb{S}}^T_{n\,n'} = \frac{2n+1}{2n'+1}\ \hat{\mathbb{S}}_{n\,n'}, \tag{8}$$

where ^{T} denotes the transpose. This is equivalent to

$$\hat{\mathbb{S}}^T = \mathbb{W}^2 \ \hat{\mathbb{S}} \ \mathbb{W}^{-2}. \tag{9}$$

III. GENERATING FUNCTION FOR THE $\hat{\mathbb{S}}_{n\,n'}(\lambda)$

We now turn to the problem of expressing the matrix elements $\hat{\mathbb{S}}_{n\,n'}(\lambda)$ in terms of known special functions. We note that, for each $n \in \mathbb{N}$, $\Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda)\hat{\mathbb{S}}^*_{n'\,n}(\lambda) = 1$, so that each row of $\hat{\mathbb{S}}(\lambda)$, $\{\hat{\mathbb{S}}_{n\,n'}(\lambda)\}_{n' \in \mathbb{N}}$ defines a square summable sequence.

We shall construct a vector generating function with components $h_n(\lambda, \xi)$, where $n \in \mathbb{N}$, $-1 \leqslant \xi \leqslant 1$ and $\lambda \in \mathbb{R}$, that will yield the matrix elements $\hat{\mathbb{S}}_{n\,n'}(\lambda)$ upon "projection" onto suitable basis functions. Let $P_n(\xi)$ denote the Legendre polynomial of order n satisfying $[(n+1)/(2n+1)]P_{n+1}(\xi) + [n/(2n+1)]P_{n-1}(\xi) = \xi P_n(\xi)$. For each row of $\hat{\mathbb{S}}(\lambda)$, a generating function is defined as a simple discrete Fourier–Legendre transform of the columns of this row of $\hat{\mathbb{S}}(\lambda)$ with weights $P_{n'}(\xi)$,

$$h_n(\lambda, \xi) \equiv \sum_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) P_{n'}(\xi) = \sum_{n'=0}^{\infty} \frac{2n'+1}{2n+1} \hat{\mathbb{S}}_{n'\,n}(\lambda) P_{n'}(\xi). \tag{10}$$

Since $|P_{n'}(\xi)| \leqslant 1$ and $\{\hat{\mathbb{S}}_{n\,n'}(\lambda)\}_{n' \in \mathbb{N}} \in \ell^2_\lambda$, this series is convergent for $-1 \leqslant \xi \leqslant 1$ and $\lambda \in \mathbb{R}$.

The generating function may be associated with a partial differential equation whose solution depends on initial values provided by the following.

Lemma 2:

$$\sum_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) = \sum_{n'=0}^{\infty} \frac{2n'+1}{2n+1} \hat{\mathbb{S}}_{n'\,n}(\lambda) = e^{i\lambda}. \tag{11}$$

Proof: Note that $\mathbb{T}$ (*not* $\hat{\mathbb{T}}$) annihilates constant vectors. Let Φ denote the constant column vector with a one in each row, $\Phi_n = 1$, $n = 0,1,2,\ldots$. Then $\mathbb{T}\Phi = 0$ and $\mathbb{S}\Phi = \Phi = e^{-i\lambda}\hat{\mathbb{S}}\Phi$. The action of $\hat{\mathbb{S}}$ on Φ is $(\hat{\mathbb{S}}\Phi)_n = \Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda)\Phi_{n'} = \Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda)$, which must yield $(\hat{\mathbb{S}}\Phi)_n = e^{i\lambda}\Phi_n = e^{i\lambda}$. Hence $\Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) = \Sigma_{n'=0}^{\infty} [(2n'+1)/(2n+1)] \ \hat{\mathbb{S}}_{n'\,n}(\lambda) = e^{i\lambda}$.

With this initial value in hand, it is not difficult to calculate the following.

Lemma 3:

$$e^{i\lambda\,\xi} P_n(\xi) = \sum_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) P_{n'}(\xi), \tag{12}$$

where $P_{n'}(\xi)$ is a Legendre polynomial satisfying $[(n'+1)/(2n'+1)]P_{n'+1}(\xi) + [n'/(2n'+1)]P_{n'-1}(\xi) = \xi P_{n'}(\xi)$.

Proof: Let $h_n(\lambda, \xi) \equiv \Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) P_{n'}(\xi) = \Sigma_{n'=0}^{\infty} [(2n'+1)/(2n+1)] \ \hat{\mathbb{S}}_{n'\,n}(\lambda) P_{n'}(\xi)$. $h_n(\lambda, \xi)$ is subject to the "initial" conditions $h_n(0, \xi) = \Sigma_{n'=0}^{\infty} \delta_{n\,n'} P_{n'}(\xi) = P_n(\xi)$ and $h_n(\lambda, 1) = \Sigma_{n'=0}^{\infty} \hat{\mathbb{S}}_{n\,n'}(\lambda) = e^{i\lambda}$ by Lemma 2.

To generate a partial differential equation for $h_n(\lambda, \xi)$, consider the one-parameter subgroup $\hat{\mathbb{S}}_{n\,n'}(\lambda + \lambda') = \Sigma_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,k}(\lambda)\hat{\mathbb{S}}_{k\,n'}(\lambda')$. The Fourier–Legendre transformation yields $h_n(\lambda + \lambda', \xi) = \Sigma_{n'=0}^{\infty} \Sigma_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,k}(\lambda) \hat{\mathbb{S}}_{k\,n'}(\lambda') P_{n'}(\xi)$. Differentiating this result with respect to λ', then putting $\lambda' = 0$ yields $(\partial/\partial\lambda) h_n(\lambda, \xi) = [(\partial/\partial\lambda') h_n(\lambda + \lambda', \xi)]_{\lambda'=0} = \Sigma_{n'=0}^{\infty} \Sigma_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,k}(\lambda)[(\partial/\partial\lambda')\hat{\mathbb{S}}_{k\,n'} \times (\lambda')]_{\lambda'=0} P_{n'}(\xi) = (i/2) \Sigma_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,k}(\lambda) \Sigma_{n'=0}^{\infty} \mathbb{T}_{k\,n'} P_{n'}(\xi) = i \Sigma_{k=0}^{\infty} \hat{\mathbb{S}}_{n\,k}(\lambda) [[(k+1)/(2k+1)] \times P_{k+1}(\xi) + [k/(2k+1)] P_{k-1}(\xi)] = i \Sigma_{k=0}^{\infty} \xi P_k(\xi) \hat{\mathbb{S}}_{n\,k}(\lambda) = i\,\xi\, h_n(\lambda, \xi)$. Integration and application of the initial conditions gives $h_n(\lambda, \xi) = P_n(\xi)\, e^{i\,\lambda\,\xi}$. □

IV. MATRIX ELEMENTS $\mathbb{U}_{n\,n'}$ AS KNOWN SPECIAL FUNCTIONS

An integral representation of $\mathbb{U}_{n\,n'}=\sqrt{(2n+1)/(2n'+1)}\,\hat{\mathbb{S}}_{n\,n'}$ and an expansion in terms of spherical Bessel functions may obtained by multiplying Eq. (12) by $P_h(\xi)\,d\,\xi$ and integrating over $-1\leqslant\xi\leqslant+1$. This gives the following theorem.

Theorem 1 ($\hat{\mathbb{U}}_{n\,n'}(\lambda)$):

$$\begin{aligned}\mathbb{U}_{n\,n'}(\lambda)&=\frac{\sqrt{(2n+1)(2n'+1)}}{2}\int_{-1}^{+1}e^{i\lambda\,\xi}P_n(\xi)P_{n'}(\xi)d\,\xi\\&=\frac{\sqrt{(2n+1)(2n'+1)}}{2\pi}\sum_{k=0}^{\min(n\,n')}i^{n+n'-2k}[2(n+n'-2k)+1]\\&\quad\times\frac{(n+n'-k)!}{(n-k)!(n'-k)!k!}\,\frac{\Gamma(n-k+\frac{1}{2})\Gamma(n'-k+\frac{1}{2})\Gamma(k+\frac{1}{2})}{\Gamma(n+n'-k+\frac{3}{2})!}\,j_{n+n'-2k}(\lambda)\\&=J^{4}_{n\,n'\,0}(-i\lambda).\end{aligned}\tag{13}$$

Here j_n denotes a spherical Bessel function of the first kind. For reference, we recall that the recursion relations for the spherical Bessel functions are $(2n+1)\,j_n'(\lambda)=n\,j_{n-1}(\lambda)-(n+1)\,j_{n+1}(\lambda)$ and $(2n+1)\,j_n(\lambda)=\lambda\,[j_{n-1}(\lambda)+j_{n+1}(\lambda)]$ (Ref. 2), and that $j_n(0)=\delta_{n\,0}$.

In the next to last equation of Eq. (13) we have used Bauer's addition theorem (Ref. 4, p. 368) $e^{i\lambda\xi}=\Sigma_{h=0}^{\infty}(2h+1)i^h j_h(\lambda)\,P_h(\xi)$ and Adams'[1] product decomposition

$$\begin{aligned}P_n(\xi)P_{n'}(\xi)=\frac{1}{2\pi}\sum_{k=0}^{\min(n\,n')}&[2(n+n'-2k)+1]\frac{(n+n'-k)!}{(n-k)!(n'-k)!k!}\\&\times\frac{\Gamma(n-k+\frac{1}{2}\Gamma(n'-k+\frac{1}{2})\Gamma(k+\frac{1}{2})}{\Gamma(n+n'-k+\frac{3}{2})!}P_{n+n'-2k}(\xi)\,.\end{aligned}\tag{14}$$

In the last equation of Eq. (13), $J^{4}_{n\,n'\,0}(-i\lambda)$ denotes the matrix elements of Vilenkin and Klimyk's unitary irreducible representation of the group of motions on Euclidean three-space that generalizes the Bessel function [Ref. 3, p. 101, Eq. (5)]. They have named these functions *associated Bessel functions*. This correspondence is discussed in more detail in the Conclusion.

V. USEFUL RECURRENCE RELATIONS

Recurrence relations can reduce the amount of computation required to calculate a number of the $\hat{\mathbb{S}}_{n\,n'}$ when using a set of these functions in a zeroth-order approximation to the solution of a scattering problem.

A simple recurrence relation may be obtained from

$$-2\,i\,\frac{\partial}{\partial\lambda}\mathbb{S}_{n\,n'}(\lambda)=[\hat{\mathbb{T}}\hat{\mathbb{S}}]_{n\,n'}=[\hat{\mathbb{S}}\hat{\mathbb{T}}]_{n\,n'}\,.\tag{15}$$

The result is consistent with the recurrence relation obtained by differentiating Eq. (13) with respect to λ and using $(2n'+1)\xi\,P_{n'}(\xi)=(n'+1)P_{n'+1}(\xi)+n'\,P_{n'-1}(\xi)$. More generally, a generator of parity recurrence relations for the $\hat{\mathbb{S}}_{n\,n'}(\lambda)$ may be obtained by differentiating Eq.

(12) with respect to ξ, then multiplying by $(1-\xi^2)$ and recalling the Legendre polynomial recurrence relation $(1-\xi^2)(\partial/\partial\xi)\,P_n(\xi)=n\,[P_{n-1}(\xi)-\xi\,P_n(\xi)]$. This yields

$$\begin{aligned}
&(1-\xi^2)(\partial/\partial\xi)\{e^{i\lambda\,\xi}P_n(\xi)\}\\
&\quad=e^{i\lambda\,\xi}\{i\lambda\,(1-\xi^2)P_n(\xi)+n\,[P_{n-1}(\xi)-\xi\,P_n(\xi)]\}\\
&\quad=[i\lambda\,(1-\xi^2)-n\,\xi\,]\{e^{i\lambda\,\xi}P_n(\xi)\}+n\,\{e^{i\lambda\,\xi}P_{n-1}(\xi)\}\\
&\quad=[i\lambda\,(1-\xi^2)-n\,\xi\,]\left\{\sum_{k=0}^{\infty}\hat{\mathbb{S}}_{n\,k}(\lambda)\,P_k(\xi)\right\}+n\left\{\sum_{k=0}^{\infty}\hat{\mathbb{S}}_{n-1\,k}(\lambda)\,P_k(\xi)\right\}\\
&\quad=\sum_{k=0}^{\infty}\hat{\mathbb{S}}_{n\,k}(\lambda)\,(1-\xi^2)\,\frac{\partial}{\partial\xi}P_k(\xi)=\sum_{k=0}^{\infty}\hat{\mathbb{S}}_{n\,k}(\lambda)\;k\,[P_{k-1}(\xi)-\xi\,P_k(\xi)].
\end{aligned}$$

Hence

$$\sum_{k=0}^{\infty}\,[\hat{\mathbb{S}}_{n\,k}(\lambda)\,\{[i\lambda\,(1-\xi^2)+(k-n)\,\xi\,]P_k(\xi)-k\,P_{k-1}(\xi)\}+n\,\hat{\mathbb{S}}_{n-1\,k}(\lambda)\,P_k(\xi)]=0. \quad (16)$$

Multiplying Eq. (16) by $d\,\xi$ and integrating over $-1\leqslant\xi\leqslant+1$ yields, for $n>0$,

$$i\,\lambda\,(\;\hat{\mathbb{S}}_{0\,n}(\lambda)-\;\hat{\mathbb{S}}_{2\,n}(\lambda)\,)-\frac{3}{2}(2+n)\hat{\mathbb{S}}_{1\,n}(\lambda)+n\,\frac{3}{2}\,\frac{(2n+1)}{(2n-1)}\hat{\mathbb{S}}_{0\,n-1}(\lambda)=0. \quad (17)$$

Here we have used $1=P_0(\xi), \xi=P_1(\xi), \xi^2=\frac{1}{3}(P_0(\xi)+2P_2(\xi))$.

The general relation is obtained by multiplying Eq. (16) by $P_h(\xi)\,d\,\xi$ and integrating over $-1\leqslant\xi\leqslant+1$. We may assume that $h>0$ since the case $h=0$ has just been evaluated. We obtain the following.

Proposition 1 (General parity recurrence relation): The parity recursion relations for the $\hat{\mathbb{S}}_{h\,n}(\lambda)$, $h=0,1,2,\ldots$, *are given by Eq. (17) for* $h=0$ *and*

$$\begin{aligned}
&i\lambda\,\frac{2(h^2+h-1)(2h+1)}{(2h+3)(2h-1)}\hat{\mathbb{S}}_{h\,n}(\lambda)\;-i\lambda\,\frac{(h+1)(h+2)}{(2h+3)}\hat{\mathbb{S}}_{h+2\;n}(\lambda)-i\lambda\,\frac{h(h-1)}{(2h-1)}\hat{\mathbb{S}}_{h-2\;n}(\lambda)\\
&\quad-(h+2+n)(h+1)\,\hat{\mathbb{S}}_{h+1\;n}(\lambda)+h(h-1-n)\,\hat{\mathbb{S}}_{h-1\;n}(\lambda)\\
&\quad+\frac{n(2n+1)}{(2n-1)(2h+1)}\hat{\mathbb{S}}_{h\;n-1}(\lambda)\;=0
\end{aligned} \quad (18)$$

for $h>0$.

VI. CONCLUSION

In this section we adopt the notation of Vilenkin and Klimyk.[3] Let $ISO(n-1)$ denote the group of motions of $n-1$-dimensional Euclidean space $\mathbb{E}_{n-1}$. Let $\mathbf{x}\in\mathbb{E}_{n-1}$; every $g\in ISO(n-1)$ has the action $g\mathbf{x}=k\mathbf{x}+\mathbf{a}$, where $k\in SO(n-1)$ is a rotation of $\mathbb{E}_{n-1}$ about the origin and $\mathbf{a}\in\mathbb{R}^{n-1}$. The group $ISO(n-1)$ is isomorphic to the group of $n\times n$ real matrices of the form

$$g(k,\mathbf{a})=\begin{pmatrix} k & \mathbf{a}\\ \mathbf{0}^T & 1\end{pmatrix},$$

where $\mathbf{0}^T=(0,\ldots,0)$ has $n-1$ components.

Let

$$D^{n}_{k\,m\,j}=\frac{2^{2j+n-5}}{\pi}\Gamma^{2}\left(j+\frac{n-3}{2}\right)\left[\frac{(k-j)!(m-j)!(2k+n-3)(2m+n-3)}{(k+j+n-4)!(m+j+n-4)!}\right]^{1/2}, \tag{19}$$

$\mathbf{a}_r^T=(0,\ldots,0,r)$ and $g_r=g(\text{identity},\mathbf{a}_r)$; Vilenkin and Klimyk[3] show that the matrix elements $t^{n\,R}_{k\,m\,j}(g_r)$ of the representation $T^{n\,R}(g_r)$ of $ISO(n-1)$ possess the integral representation

$$t^{n\,R}_{k\,m\,j}(g_r)=D^{n}_{k\,m\,j}\int_0^{\pi} e^{R\,r\,\cos(\phi)}C^{j+(n-3)/2}_{k-j}(\cos(\phi))C^{j+(n-3)/2}_{m-j}(\cos(\phi))\sin^{2j+n-3}(\phi)\,d\phi\,, \tag{20}$$

where C^j_k is the Gegenbauer polynomial. The representation is unitary when $R=i\,\rho,\rho\in\mathbb{R}$. In our case we see that $\mathbb{U}_{n\,n'}(\lambda)=J^{4}_{n\,n'\,0}(-i\lambda)$. Vilenkin and Klimyk show that $J^{n}_{k\,m\,j}(-i\,R\,r)=t^{n\,R}_{k\,m\,j}(g_r)$ defines a generalization of the Bessel function that they call the associated Bessel functions. Hence the associated Bessel functions $J^{4}_{n\,n'\,0}(-i\lambda)$ provide an approximation for the leading term in the radial contribution of the evolution operator.

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Curvature singularity of the distributional Bañados, Teitelboim, and Zanelli black hole geometry

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For the nonrotating Bañados, Teitelboim, and Zanelli black hole, the distributional curvature tensor field is found. It is shown to have singular parts proportional to a δ-distribution with support at the origin. This singularity is related, through Einstein field equations, to a point source. Coordinate invariance and independence on the choice of differentiable structure of the results are addressed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1699482]

I. INTRODUCTION

The $(2+1)$-dimensional black hole of Bañados, Teitelboim, and Zanelli (BTZ)[1,2] provides us with a useful model to study various classical and quantum aspects of black hole physics.[3] The BTZ black hole shares many of the properties of the more complicated $(3+1)$-dimensional Kerr black hole. However, it differs from the Kerr solution in which it is asymptotically anti–de Sitter rather than asymptotically flat. Furthermore, by admitting closed time-like curves, the rotating BTZ black hole has no curvature singularities. Nevertheless, when there is no angular momentum the space–time fails to be Hausdorff at the origin and turns out to be singular.[2]

The purpose of this work is to analyze the distributional BTZ black hole geometry for the nonrotating case. There are several reasons to carry out such analysis. The nonrotating BTZ black hole provides an example of a singular space–time whose singularities cannot be identified with the unboundedness of some scalar constructed from the curvature tensor. In this sense, it resembles the well-known conical singularities[4] whose meaning has attracted wide interest for many years.[5] On the other hand, besides the fact that the distributional analysis has not been considered hitherto, regularization procedures required to multiply distributions need not be invoked in the calculation of the distributional nonrotating BTZ black hole curvature tensor. Most of the distributional treatments of the $(3+1)$-dimensional Schwarzschild[6–8] and Kerr black holes[7] rely on suitable regularization procedures; while general regularization procedures using Colombeau's generalized functions[9] to obtain the distributional curvature associated to the Schwarzschild[10] and Kerr geometries[11] and to a conical singularity[12–14] have been put forward (see also Refs. 6 and 15 for other approaches to conical singularities). We show that the nonrotating BTZ black hole metric belongs to the class of semiregular metrics, as defined in Ref. 16, for which a direct distributional meaning may be assigned to the curvature tensor field. Notice that not many semiregular metrics are known. It has been shown that the $(3+1)$-dimensional Minkowski metric with an angular deficit, and a certain kind of traveling wave metric are semiregular.[16] Recently, the metric associated to the $(2+1)$-dimensional space–time around a point source[4] was demonstrated to be a third example.[8]

In order to consider the coordinate dependence of the results, the distributional description of the BTZ black hole space–time is carried out in Schwarzschild coordinates and in Kerr–Schild coordinates. We find the distributional Ricci and Einstein tensor fields for the nonrotating BTZ

black hole, which turn out to be equivalent in both coordinate systems. This indicates that, although the intermediate calculations depend upon the choice of coordinates, the final result does not. Remarkably, a complete agreement with what is physically expected is found. The distributional curvature tensor becomes, besides the constant curvature part, a δ-distribution supported at the origin. Furthermore, this singularity is related through Einstein field equations to a point source.

The paper is organized as follows. In the next section, following the procedure of Ref. 16, the distributional curvature and Einstein tensor fields are found for the nonrotating BTZ solution in Schwarzschild coordinates. In Sec. III, we carry out the distributional analysis using the Kerr–Schild form of the BTZ solution, and the question of whether one can also obtain these results as the distributional limit of a suitable regularized metric is addressed. The last section is devoted to summarize and discuss the coordinate invariance (and differentiable structure dependence) of our results.

II. BTZ BLACK HOLE IN SCHWARZSCHILD COORDINATES

The nonrotating BTZ black hole solution[1,2] written in Schwarzschild coordinates is given by

$$g_{ab}=-\left(-m+\frac{r^2}{l^2}\right)\mathrm{d}t_a\,\mathrm{d}t_b+\left(-m+\frac{r^2}{l^2}\right)^{-1}\mathrm{d}r_a\,\mathrm{d}r_b+r^2\,\mathrm{d}\varphi_a\,\mathrm{d}\varphi_b\,, \tag{1}$$

where $-\infty<t<\infty$, $0<r<\infty$, and $0\leqslant\varphi<2\pi$, with the surfaces $\varphi=0,2\pi$ identified. The dimensionless quantity m is the mass parameter. In $(2+1)$-dimensions we have

$$R_{abc}{}^{d}=g_{ac}R_b{}^{d}-g_{bc}R_a{}^{d}+\delta_b{}^{d}R_{ac}-\delta_a{}^{d}R_{bc}-\tfrac{1}{2}(g_{ac}\delta_b{}^{d}-g_{bc}\delta_a{}^{d})R \tag{2}$$

and from (1) we obtain

$$R_{ab}=-\frac{2}{l^2}g_{ab}\,. \tag{3}$$

Hence, (1) has constant negative curvature.

The BTZ metric (1) is a solution of the vacuum Einstein field equations with cosmological constant $\Lambda=-1/l^2$,

$$R_{ab}-\tfrac{1}{2}g_{ab}R+\Lambda g_{ab}=0, \tag{4}$$

and may be obtained by identifying certain points of (the covering manifold of) the anti–de Sitter space.[1,2] For $m>0$, (1) describes a black hole of mass m with horizon at $r_+=\sqrt{m}l$. For $m\leqslant 0$ the horizon disappears and there is no black hole. The solution with $-1<m<0$ may be associated to the metric generated by a point source at the origin.[17] The solution with $m=-1$ is anti–de Sitter space. The massless black hole, $m=0$, is commonly considered as the vacuum state. For a review of the properties of BTZ black holes see Ref. 3.

In (1), $\sqrt{g_{\varphi\varphi}}=r$ represents the radius associated with the proper circumference. Therefore with $x=r\cos\varphi$ and $y=r\sin\varphi$ we have

$$g_{ab}=\eta_{ab}+\left(1+m-\frac{r^2}{l^2}\right)\mathrm{d}t_a\,\mathrm{d}t_b-\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right)\frac{1}{r^2}(x\,\mathrm{d}x_a+y\,\mathrm{d}y_a)(x\,\mathrm{d}x_b+y\,\mathrm{d}y_b), \tag{5}$$

where $r=\sqrt{x^2+y^2}$ and η_{ab} is the ordinary Minkowski metric on $\mathcal{R}^3$. The metric (5) is singular when $r=0$, except for $m=-1$. This singularity is not a coordinate singularity. The spinless BTZ black hole is geodesically incomplete[18] and the singularity at $r=0$ corresponds to fixed points of

the identifications from which the BTZ solution is obtained.[19] Assuming that (5) can be extended to $r=0$, we look for the distributional curvature tensor and its relation with a possible distributional source.

Suppose $(\mathcal{M},g_{ab})$ are given such that

(1) g_{ab} and $(g^{-1})^{ab}$ exist almost everywhere and are locally integrable,
(2) the weak first derivative $\nabla_c g_{ab}$ of g_{ab} in a smooth derivative operator ∇_c exists and the tensors

$$C^c_{ab}\equiv \tfrac{1}{2}(g^{-1})^{cd}(\nabla_a g_{bd}+\nabla_b g_{ad}-\nabla_d g_{ab}), \tag{6}$$

and $C^d_{m[b}C^m_{a]c}$ are locally integrable.

Following Ref. 16, these are sufficient conditions for $R_{abc}{}^d$ to be definable as a distribution by the usual coordinate formula,

$$R_{abc}{}^d=\tilde{R}_{abc}{}^d+2\nabla_{[b}C^d_{a]c}+2C^d_{m[b}C^m_{a]c}, \tag{7}$$

where $\tilde{R}_{abc}{}^d$ is the curvature tensor associated to the smooth derivative operator ∇_c and we shall say that g_{ab} is a semiregular metric.

A semiregular metric may have no distributional Einstein tensor due to the fact that contractions of the metric with the curvature tensor may have no sense as distributions. Stronger conditions can be imposed to isolate the class of metrics for which the distributional meaning of the Einstein tensor is ensured, but then the distributional curvature tensor must have its support on a submanifold of codimension of at most one.[20] Metrics for surface layers[21] lie in this class, but neither strings nor point particles can be described by metrics in this class. Alternatively, by considering Colombeau's generalized functions,[9] distributional curvatures can be defined for those cases where a direct calculation would not work, but we will not consider it here.

We shall prove that (5) is a semiregular metric. We take for the differentiable structure that in which $t,x,$ and y form a smooth chart. For a test tensor field U^{ab} on $\mathcal{R}^3$ we have

$$\begin{aligned} g_{ab}[U^{ab}]\equiv\int_{\mathcal{R}^3} g_{ab}U^{ab}\omega_\eta=\int_{\mathcal{R}^3}\eta_{ab}U^{ab}\omega_\eta+\int_{\mathcal{R}^3}\left(1+m-\frac{r^2}{l^2}\right)U^{tt}\omega_\eta \\ -\int_{\mathcal{R}^3}\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right)\mathrm{d}r_a\,\mathrm{d}r_b U^{ab}\omega_\eta, \end{aligned} \tag{8}$$

where ω_η is the volume element associated to η_{ab} and it is understood that all tensor components are Cartesian components as functions of Cartesian coordinates. For $m>0$ we require that U^{ab} be a test tensor with support on $r<\sqrt{m}l$, while for $m<0$ we simply require that U^{ab} be a test tensor of compact support. The black vacuum can not be handled in the Schwarzschild-type coordinates because the last term in the right-hand side of (8) is not locally integrable for $m=0$. Note that, with this choice, the natural volume element ω_g associated to g_{ab} agrees with the volume element ω_η of η_{ab}.

It follows that

$$\begin{aligned} g_{ab}[U^{ab}]=\int_{\mathcal{R}^3}\eta_{ab}U^{ab}\omega_\eta+\int_{\mathcal{R}^3}\left(1+m-\frac{r^2}{l^2}\right)U^{tt}\omega_\eta-\int_{\mathcal{R}^3}\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right) \\ \times(\cos^2\varphi U^{xx}+\cos\varphi\sin\varphi(U^{xy}+U^{yx})+\sin^2\varphi U^{yy})\omega_\eta. \end{aligned} \tag{9}$$

Therefore, g_{ab} is locally integrable for $m\neq 0$.

Next, let U_{ab} be a test tensor field on $\mathcal{R}^3$. For

$$(g^{-1})^{ab}\equiv\eta^{ab}+\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right)\partial_t^a\partial_t^b-\left(1+m-\frac{r^2}{l^2}\right)\partial_r^a\partial_r^b, \tag{10}$$

we have

$$(g^{-1})^{ab}[U_{ab}]=\int_{\mathcal{R}^3}\eta^{ab}U_{ab}\omega_\eta+\int_{\mathcal{R}^3}\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right)\ U_{tt}\omega_\eta-\int_{\mathcal{R}^3}\left(1+m-\frac{r^2}{l^2}\right)$$
$$\times(\cos^2\varphi U_{xx}+\cos\varphi\sin\varphi(U_{xy}+U_{yx})+\sin^2\varphi U_{yy})\omega_\eta. \tag{11}$$

Therefore, $(g^{-1})^{ab}$ is locally integrable for $m\neq 0$.

We now calculate the weak derivative in η_{ab} of g_{ab}. Let U^{abc} be a test tensor field. We find

$$\nabla_c g_{ab}[U^{cab}]\equiv-\int_{\mathcal{R}^3}g_{ab}\nabla_c U^{cab}\omega_\eta=\int_{\mathcal{R}^3}W_{cab}U^{cab}\omega_\eta, \tag{12}$$

where W_{cab} is the locally integrable but not locally square integrable tensor given by

$$W_{cab}=-\frac{2r}{l^2}\mathrm{d}r_c\left(\mathrm{d}t_a\,\mathrm{d}t_b+\left(m-\frac{r^2}{l^2}\right)^{-2}\mathrm{d}r_a\,\mathrm{d}r_b\right)-\frac{1}{r}\left(\frac{l^2+ml^2-r^2}{ml^2-r^2}\right)r\,\mathrm{d}\varphi_c(r\,\mathrm{d}\varphi_a\,\mathrm{d}r_b+r\,\mathrm{d}r_a\,\mathrm{d}\varphi_b). \tag{13}$$

From (6), we find

$$C^c_{ab}=\frac{-r(ml^2-r^2)}{l^4}\mathrm{d}t_a\,\mathrm{d}t_b\,\partial^c_r-\frac{r}{ml^2-r^2}(\mathrm{d}r_a\,\mathrm{d}t_b+\mathrm{d}t_a\,\mathrm{d}r_b)\partial^c_t$$
$$+\frac{r}{ml^2-r^2}\mathrm{d}r_a\,\mathrm{d}r_b\,\partial^c_r+\frac{1}{r}\,\frac{ml^2+l^2-r^2}{l^2}r^2\,\mathrm{d}\varphi_a\,\mathrm{d}\varphi_b\,\partial^c_r, \tag{14}$$

which is locally integrable. On the other hand,

$$2C^d_{m[b}C^m_{a]c}=\frac{4r}{ml^2-r^2}\mathrm{d}t_{[a}\mathrm{d}r_{b]}\left(\frac{r}{ml^2-r^2}\mathrm{d}r_c\,\partial^d_t-\frac{r(ml^2-r^2)}{l^4}\mathrm{d}t_c\,\partial^d_r\right)$$
$$-2\,\frac{ml^2+l^2-r^2}{(ml^2-r^2)l^2}(r^2\,\mathrm{d}\phi_{[a}\mathrm{d}t_{b]}\,\mathrm{d}\phi_c\partial^d_t-r^2\,\mathrm{d}\phi_{[a}\mathrm{d}r_{b]}\,\mathrm{d}\phi_c\,\partial^d_r), \tag{15}$$

which is locally integrable. Hence, g_{ab} is a semiregular metric in the differentiable structure chosen.

Now, contracting (7) and using (14) and (15) we find for the Ricci tensor of g_{ab},

$$R_{ac}[U^{ac}]\equiv-\int_{\mathcal{R}^3-B_\varepsilon}C^b_{ac}\nabla_b U^{ac}\omega_\eta-\int_{\mathcal{R}^3-B_\varepsilon}C^b_{ma}C^m_{bc}U^{ac}\omega_\eta, \tag{16}$$

where

$$-\int_{\mathcal{R}^3-B_\varepsilon}C^b_{ac}\nabla_b U^{ac}\omega_\eta=\int_{r=\varepsilon}\mathrm{d}r_b\,C^b_{ac}U^{ac}\sigma+\int_{r>\varepsilon}\nabla_b C^b_{ac}U^{ac}\omega_\eta, \tag{17}$$

with σ the volume element induced on the surface $r=$constant by the metric η_{ab}, B_ε is the ε-ball around the origin with $\varepsilon\to 0$ and

$$\nabla_b C^b_{ac}=-\frac{2(ml^2-2r^2)}{l^4}\mathrm{d}t_a\,\mathrm{d}t_c+2\,\frac{ml^2}{(ml^2-r^2)^2}\mathrm{d}r_a\,\mathrm{d}r_c-2\,\frac{r^2}{l^2}\mathrm{d}\varphi_a\,\mathrm{d}\varphi_c, \tag{18}$$

which is a locally integrable tensor.

From (16) and (15), (17), and (18) we find

$$R_{ac}[U^{ac}]=\pi(1+m)\int \mathrm{d}t(U^{xx}(t,\vec{0})+U^{yy}(t,\vec{0}))-\frac{2}{l^2}\int_{\mathcal{R}^3} g_{ac}U^{ac}\omega_\eta, \tag{19}$$

where g_{ac} is the locally integrable tensor defined by (9). Thus we obtain

$$R_{ac}=\pi(1+m)\,\delta^{(2)}_{(0)}(\mathrm{d}x_a\,\mathrm{d}x_c+\mathrm{d}y_a\,\mathrm{d}y_c)-\frac{2}{l^2}g_{ac}\,. \tag{20}$$

Note that $\forall m>-1$, the Ricci tensor has a singular part proportional to a δ distribution. As expected, for $m=-1$ the singular part of the curvature is absent, as follows from the fact that in this case we have AdS_3 space–time. Since for $-1<m<0$, there is no horizon, we have a naked singularity at $r=0$. For $m>0$ we have a singularity at $r=0$ hidden by a horizon at $r_+=\sqrt{m}l$. As stated before, for $m=0$ the metric (8) is not a semiregular metric and the massless BTZ black hole cannot be properly discussed from the above derivation.

We now calculate the Einstein tensor of g_{ab}. Following Ref. 8 we will concentrate on the mixed-index Einstein tensor field $G^a{}_b$. Define

$$\begin{aligned}G^a{}_b=R^a{}_b-\tfrac{1}{2}(g^{-1})^{cd}\tilde{R}_{cd}\delta^a{}_b+(g^{-1})^{cd}C^e_{m[c}C^m_{e]d}\delta^a{}_b\\ +\nabla_{[c}(C^e_{e]d}(g^{-1})^{cd})\,\delta^a{}_b+C^e_{d[c}\nabla_{e]}(g^{-1})^{cd}\delta^a{}_b\,,\end{aligned} \tag{21}$$

where

$$R^a{}_b=(g^{-1})^{ac}\tilde{R}_{cb}+2\nabla_{[c}(C^c_{d]b}(g^{-1})^{ad})+2C^c_{b[c}\nabla_{d]}(g^{-1})^{ad}+2(g^{-1})^{ad}C^c_{m[c}C^m_{d]b}\,. \tag{22}$$

We shall say that (21) is the Einstein tensor distribution of (5), whenever each term in the right-hand sides of (21) and (22) may be interpreted as a distribution.

From (14), (15), and (22) we find

$$\begin{aligned}R^d{}_c=\nabla_b((g^{-1})^{ad}C^b{}_{ac})=\nabla_b\Big(-\frac{r}{l^2}\partial^d_t\,\mathrm{d}t_c\,\partial^b_r-\frac{rl^2}{(ml^2-r^2)^2}\partial_t\,\mathrm{d}r_c\,\partial^b_t+\frac{r}{l^2}\partial^d_r\,\mathrm{d}t_c\,\partial^b_t\\ --\frac{r}{l^2}\partial^d_r\,\mathrm{d}r_c\,\partial^b_r+\frac{ml^2+l^2-r^2}{rl^2}\partial^d_\varphi\,\mathrm{d}\varphi_c\,\partial^b_r\Big).\end{aligned} \tag{23}$$

Note that the right-hand side of (23) is the derivative of a locally integrable tensor. Therefore a distributional meaning can be given to (23).

An analogous calculation to that of (20) leads to

$$R^a{}_b=\pi(1+m)\,\delta^{(2)}_{(0)}(\partial^a_x\,\mathrm{d}x_b+\partial^a_y\,\mathrm{d}y_b)-\frac{2}{l^2}(\partial^a_t t_b+\partial^a_x\,\mathrm{d}x_a+\partial^a_y\,\mathrm{d}y_b). \tag{24}$$

Finally, from (14) and (15) and (21) and (24) we obtain

$$G^a{}_b-\frac{1}{l^2}(\partial^a_t t_b+\partial^a_x\,\mathrm{d}x_a+\partial^a_y\,\mathrm{d}y_b)=-\pi(1+m)\,\delta^{(2)}_{(0)}\partial^a_t\,\mathrm{d}t_b\,. \tag{25}$$

Remarkably enough, the right-hand side of (25) resembles the physically expected result for the distributional energy momentum tensor $T^a{}_b=-m\,\delta^{(3)}_{(0)}\partial^a_t\,\mathrm{d}t_b$ of the Schwarzschild four-dimensional black hole.[22,6–8,10] (The Schwarzschild metric is not a semiregular metric and cannot be handled with the methods used here to obtain its distributional curvature.[8])

Now, let us consider the dependence of these results on the coordinate system. Note that whether or not a metric is semiregular depends in general on the differentiable structure imposed on the manifold. In this section, the choice of the manifold differentiable structure was made on

the basis of an interpretation of the coordinate system in which the metric is given: we use Cartesian coordinates associated with the Schwarzschild coordinates. In the next section the distributional curvature and Einstein tensor fields are evaluated using the Kerr–Schild form of the BTZ metric. This amounts to change both the coordinates and the differentiable structure.

III. BTZ BLACK HOLE IN KERR–SCHILD COORDINATES

In previous works the Kerr–Schild form of the Schwarzschild metric has been proved to be useful, from both conceptual and technical points of view, for the analysis of the distributional Schwarzschild geometry from quite different approaches.[22,7,11,10] In the following we shall prove that the nonrotating BTZ solution in Kerr–Schild coordinates is a semiregular metric.

The AdS_3 black hole solution of BTZ is given in the Kerr–Schild form by[23]

$$g_{ab}=\eta_{ab}+f\,k_a k_b\,, \tag{26}$$

where $r=\sqrt{x^2+y^2}$ and

$$f=\left(1+m-\frac{r^2}{l^2}\right),\quad k_a=\mathrm{d}t_a+\frac{1}{r}(x\,\mathrm{d}x_a+y\,\mathrm{d}y_a), \tag{27}$$

with $k^a=\eta^{ab}k_b$ a null vector field with respect to η_{ab} and g_{ab}. It follows that there are two metrical structures, η_{ab} and g_{ab}, associated to the manifold. Furthermore,

$$k^a\nabla_a k^b=k^a\nabla_a^g k^b=0, \tag{28}$$

where ∇_a and ∇_a^g are the derivatives in η_{ab} and g_{ab}, respectively, i.e., k^a is geodetic with respect to η_{ab} and g_{ab}. Hence, the conditions of the Kerr–Schild class are met by the decomposition (26) and (27), a fact that will be used later. We choose as the underlying manifold structure that of $\mathcal{R}^3$ with the smooth metric η_{ab} in Cartesian coordinates $\{t,x,y\}$. Note that in Kerr–Schild coordinates r is a spacelike coordinate $\forall r>0$, which is not the case in Schwarzschild-type coordinates. Note also that the natural volume element ω_g associated to g_{ab} agrees with the volume element ω_η of η_{ab}.

Now,

$$(g^{-1})^{ab}=\eta^{ab}-\left(1+m-\frac{r^2}{l^2}\right)\left(\partial_t^a-\frac{1}{r}(x\partial_x^a+y\partial_y^a)\right)\left(\partial_t^b-\frac{1}{r}(x\partial_x^b+y\partial_y^b)\right). \tag{29}$$

Clearly, g_{ab} and $(g^{-1})^{ab}$ are locally bounded and locally integrable $\forall m$.

The weak derivative in η_{ab} of g_{ab} exists almost everywhere and is given by

$$\nabla_c g_{ab}[U^{cab}]=\int_{\mathcal{R}^3}W_{cab}U^{cab}\omega_\eta, \tag{30}$$

where

$$W_{cab}=-\frac{r}{l^2}\mathrm{d}r_c(\mathrm{d}t_a+\mathrm{d}r_a)(\mathrm{d}t_b+\mathrm{d}r_b)+\frac{1}{r}\left(1+m-\frac{r^2}{l^2}\right)r\,\mathrm{d}\varphi_c(r\,\mathrm{d}\varphi_a(\mathrm{d}t_b+\mathrm{d}r_b)$$
$$+(\mathrm{d}t_a+\mathrm{d}r_a)r\,\mathrm{d}\varphi_b), \tag{31}$$

which is locally integrable $\forall m$.

From (6), it follows

$$C^c{}_{ab}=\frac{2r}{l^2}(\mathrm{d}r_a(\mathrm{d}t_b+\mathrm{d}r_b)+\mathrm{d}r_b(\mathrm{d}t_a+\mathrm{d}r_a))(\partial_t^c-\partial_r^c)+\frac{2r}{l^2}\left(1+m-\frac{r^2}{l^2}\right)(\mathrm{d}t_a+\mathrm{d}r_a)(\mathrm{d}t_b+\mathrm{d}r_b)$$
$$\times(\partial_t^c-\partial_r^c)+\frac{2r}{l^2}(\mathrm{d}t_a+\mathrm{d}r_a)(\mathrm{d}t_b+\mathrm{d}r_b)\partial_r^c-\frac{2}{r}\left(1+m-\frac{r^2}{l^2}\right)r^2\,\mathrm{d}\varphi_a\,\mathrm{d}\varphi_b(\partial_t^c-\partial_r^c), \tag{32}$$

which is locally integrable $\forall m$. Note that $C^b{}_{ab}=0$.

Finally, from (32) we find

$$2C^d_{m[b}C^m_{a]c}=2\frac{r^2}{l^4}(\mathrm{d}t_a\,\mathrm{d}r_b-\mathrm{d}r_a\,\mathrm{d}t_b)(\mathrm{d}t_c+\mathrm{d}r_c)(\partial_t^d-\partial_r^d)-\frac{1}{l^2}\left(1+m-\frac{r^2}{l^2}\right)$$
$$\times((\mathrm{d}t_a+\mathrm{d}r_a)r\,\mathrm{d}\varphi_b-r\,\mathrm{d}\varphi_a(\mathrm{d}t_b+\mathrm{d}r_b))r\,\mathrm{d}\varphi_c(\partial_t^d-\partial_r^d), \tag{33}$$

which is locally integrable $\forall m$. Therefore the metric (26) is semiregular. Furthermore, since (26) is a semiregular metric $\forall m$, we can now consider the distributional geometry of the BTZ black hole including the $m=0$ black vacuum.

We now calculate the Ricci tensor of (26). We have

$$R_{ac}[U^{ac}]=-\int_{\mathcal{R}^3-B_\varepsilon}C^b{}_{ac}\nabla_b U^{ac}\omega_\eta-\int_{\mathcal{R}^3-B_\varepsilon}\frac{2r}{l^2}k_ak_c\,U^{ac}\omega_\eta. \tag{34}$$

An analogous calculation to that of (20) leads to

$$R_{ac}=\pi(1+m)\,\delta^{(2)}_{(0)}(\mathrm{d}x_a\,\mathrm{d}x_c+\mathrm{d}y_a\,\mathrm{d}y_c)-\frac{2}{l^2}g_{ac}, \tag{35}$$

where g_{ac} is the locally integrable tensor (26). Note that (35) is equivalent to (20) which was obtained using Schwarzschild-type coordinates.

Calculations analogous to the ones done previously show that

$$R^a{}_b=\pi(1+m)\,\delta^{(2)}_{(0)}(\partial_x^a\,\mathrm{d}x_b+\partial_y^a\,\mathrm{d}y_b)-\frac{2}{l^2}(\partial_t^a t_b+\partial_x^a\,\mathrm{d}x_b+\partial_y^a\,\mathrm{d}y_b), \tag{36}$$

which is equivalent to (24) and

$$G^a{}_b-\frac{1}{l^2}(\partial_t^a t_b+\partial_x^a\,\mathrm{d}x_a+\partial_y^a\,\mathrm{d}y_b)=-\pi(1+m)\,\delta^{(2)}_{(0)}\partial_t^a\,\mathrm{d}t_b \tag{37}$$

which is equivalent to (25).

Now, it would be interesting to see if the distributional curvatures obtained above can also be obtained employing regularization methods. This is far from being obvious, since for conical singularities the results of the regularization approaches taken so far[6,12–14,8] are in disagreement with the ones obtained following the procedure of Ref. 16 which is the one that we have employed. A property of the Kerr–Schild class of metrics is that the mixed Ricci curvature tensor takes the form

$$R^a{}_b=\tfrac{1}{2}(\nabla^a\nabla_c(fk^ck_b)+\nabla^b\nabla_c(fk_ck^a)+\nabla^c\nabla_c(fk^ak_b)) \tag{38}$$

(recall that ∇_a is the derivative in η_{ab}) which allows a distributional evaluation whenever fk^ak_b is a well-defined distribution.[7] However, it should be kept in mind that due to the nonlinear character of the curvatures, we must first regularize, then carry out the nonlinear operations and finally compute the distributional limits.

For the metric tensor (26) and (27), f is indeed a smooth function and although k_a is a nonsmooth vector field, fk^ak_b is a locally integrable tensor field,

$$fk^a k_b[U^b{}_a]=\int_{\mathcal{R}^3} fk^a k_b\, U^b{}_a \omega_\eta=\int_{\mathcal{R}^3}\left(1+m-\frac{r^2}{l^2}\right)(U^t{}_t+\cos\varphi(U^x{}_t+U^t{}_x)+\sin\varphi(U^y{}_t+U^t{}_y)$$
$$+\cos^2\varphi\, U^x{}_x+\cos\varphi\sin\varphi(U^x{}_y+U^y{}_x)+\sin^2\varphi\, U^y{}_y)\omega_\eta. \quad (39)$$

Hence, due to the fact that (38) turns out to be second derivatives of a distribution it is then possible to carry out the calculation, without specifying the regularization procedure, requiring only that the regularization chosen retains the Kerr–Schild form of the metric (for a discussion on this point see Refs. 7, 11, and 10).

Now, let us exemplify the calculation of the distributional Ricci tensor field by the evaluation of the first term of (38) explicitly. We have

$$\nabla^a\nabla_c(fk^c k_b)[U^b{}_a]\equiv\int_{\mathcal{R}^3-B_\varepsilon} fk^c k_b\nabla^a\nabla_c U^b{}_a\omega_\eta$$
$$=-\int_{r=\varepsilon} \mathrm{d}r_c\, fk^c k_b\nabla^a U^b{}_a\sigma+\int_{r=\varepsilon}\partial_r^a\nabla_c(fk^c k_b)U^b{}_a\sigma$$
$$+\int_{r>\varepsilon}\nabla^a\nabla_c(fk^c k_b)U^b{}_a\omega_\eta. \quad (40)$$

The first term on the right-hand side of (40) is of order ε and vanishes in the limit $\varepsilon\to 0$, the third term contributes to the Ricci curvature in the region $\mathcal{R}^3-B_\varepsilon$. For the second term we have

$$\int_{r=\varepsilon}\partial_r^a\nabla_c(fk^c k_b)U^b{}_a\sigma=\int_{r=\varepsilon}\left(-\frac{2r}{l^2}+\left(1+m-\frac{r^2}{l^2}\right)\frac{1}{r}\right)(\mathrm{d}t_b+\mathrm{d}r_b)\,\partial_r^a U^b{}_a\,\sigma$$
$$=\pi(1+m)\int \mathrm{d}t(U^x{}_x(t,\vec{0})+U^y{}_y(t,\vec{0}))$$
$$=\pi(1+m)\,\delta^{(2)}_{(0)}(\partial_x^a\,\mathrm{d}x_b+\partial_y^a\,\mathrm{d}y_b)[U^b{}_a]. \quad (41)$$

Analogous calculations for the remaining terms of (38) lead to

$$R^a{}_b=\pi(1+m)\,\delta^{(2)}_{(0)}(\partial_x^a\,\mathrm{d}x_b+\partial_y^a\,\mathrm{d}y_b)-\frac{2}{l^2}(\partial_t^a t_b+\partial_x^a\,\mathrm{d}x_b+\partial_y^a\,\mathrm{d}y_b), \quad (42)$$

and we obtain for the Einstein tensor

$$G^a{}_b=-\pi(1+m)\,\delta^{(2)}_{(0)}\partial_t^a\,\mathrm{d}t_b+\frac{1}{l^2}(\partial_t^a t_b+\partial_x^a\,\mathrm{d}x_a+\partial_y^a\,\mathrm{d}y_b), \quad (43)$$

which are the same results obtained in (36) and (37).

IV. DISCUSSIONS

As noted above, the distributional Ricci tensor fields (20) and (35) are equivalent, as is the case with the mixed index versions (24) and (36). We take (35) and (36), which are valid $\forall m$, as the distributional R_{ab} and $R^a{}_b$ Ricci tensor fields. The nonrotating BTZ black hole geometry is singular and this singularity is a curvature singularity proportional to a δ-distribution supported at the origin. As follows from (35) and (36), even for the $m=0$ black vacuum this singularity is present. As expected, for $m=-1$ (anti–de Sitter space–time) a nonsingular space–time is recovered.

On the other hand, (25) and (37) are equivalent. Hence, we take (37) as the distributional Einstein tensor field $G^a{}_b$ of the nonrotating BTZ black hole. As expected on physical grounds, the distributional energy momentum tensor $T^a{}_b$ of the BTZ black hole geometry is then given by

$$T^a{}_b = -(1+m)\,\delta^{(2)}_{(0)}\partial^a_t\,\mathrm{d}t_b\,, \tag{44}$$

where we have set the gravitational constant G equal to $\frac{1}{8}$. Note that (44) is a nonzero distribution for $m=0$. The constant shift in the mass is due to the fact that in (1) the zero point of energy has been set so that the mass vanishes when the horizon size, the length of the minimal geodesic of the horizon, goes to zero.[2] As follows from the fact that the singular parts of the distributional curvature and Einstein tensor fields are equal to zero only for $m=-1$, if the zero of energy is adjusted so that anti–de Sitter space has zero mass then $1+m\to m$.

Finally, let us briefly discuss the coordinate independence of these results. As already mentioned in Sec. II, whether or not a given metric is semiregular depends in general on the differentiable structure imposed on the underlying manifold. In Secs. II and III, the choice of the differentiable structure was made on the basis of an interpretation of the coordinate system in which the metric is given. In this sense, the choice of coordinates determines the differentiable structure of the underlying manifold. Here we find that the distributional curvature and Einstein tensor fields are well defined and that they are equivalent in both descriptions. Furthermore, we have shown that the same distributional mixed index Ricci and Einstein tensor fields can be obtained by standard regularization approaches. Thus, in a restricted sense, the present distributional treatment in Schwarzschild and Kerr–Schild coordinates provides invariant results for the distributional curvature and Einstein tensor fields of the BTZ black hole geometry.

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Applications and generalizations of Fisher–Hartwig asymptotics

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Fisher–Hartwig asymptotics refers to the large n form of a class of Toeplitz determinants with singular generating functions. This class of Toeplitz determinants occurs in the study of the spin–spin correlations for the two-dimensional Ising model, and the ground state density matrix of the impenetrable Bose gas, amongst other problems in mathematical physics. We give a new application of the original Fisher–Hartwig formula to the asymptotic decay of the Ising correlations above T_c, while the study of the Bose gas density matrix leads us to generalize the Fisher–Hartwig formula to the asymptotic form of random matrix averages over the classical groups and the Gaussian and Laguerre unitary matrix ensembles. Another viewpoint of our generalizations is that they extend to Hankel determinants the Fisher–Hartwig asymptotic form known for Toeplitz determinants. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1699484]

ENCOMIUM

In celebration of Freeman Dyson on his

$$\left(32\left(\frac{40960001}{25600}\right)^3-6\left(\frac{40960001}{25600}\right)+\sqrt{\left[32\left(\frac{40960001}{25600}\right)^3-6\left(\frac{40960001}{25600}\right)\right]^2-1}\right)^{1/6}\ \text{th}$$

birthday. (This radical appears in the works on Ramanujan,[1] who is very dear to Dyson.)

Dyson's legendary works[2] on random matrices are now standards in physics, mathematics and fields far(ther) afield. These works and, in particular his powerful log-Coulomb gas model, developed to liberate the mathematics where none yet exists, are the very essential tools in our ongoing pursuits.[3]

I. INTRODUCTION

Fisher–Hartwig asymptotics refers to the large n form of a class of Toeplitz determinants $D_n[g]$. By definition, the entries of the latter depend only on the difference of the row and column indices, and thus

$$D_n[g]=\det[g_{j-k}]_{j,k=1,\ldots,n} \tag{1.1}$$

for some $\{g_k\}_{k=0,\pm1,\pm2,\ldots}$. Crucial to the structure of the asymptotic form of (1.1) are analytic properties of the so-called symbol

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$$g(\theta) := \sum_{n=-\infty}^{\infty} g_n e^{in\theta}, \tag{1.2}$$

or more particularly the decay of the Fourier coefficients of $\log g(\theta)$. Explicitly, let

$$\log g(\theta) = \sum_{p=-\infty}^{\infty} c_p e^{ip\theta}. \tag{1.3}$$

Then if

$$\sum_{p=-\infty}^{\infty} |p| c_p c_{-p} < \infty \tag{1.4}$$

a strong form of the Szegö limit theorem (see, e.g., Refs. 4 and 5) asserts that for $n \to \infty$,

$$D_n[g] = \exp\left(n c_0 + \sum_{k=1}^{\infty} k c_k c_{-k} + o(1) \right). \tag{1.5}$$

Two cases for which (1.4) will not hold are when $g(\theta)$ has a jump discontinuity or a zero for some $-\pi < \theta \leqslant \pi$. It is for such singular symbols (in the case of a zero it is the logarithm of the symbol which is singular) that Fisher and Hartwig[6] sought the asymptotic form of (1.1). Symbols with singularities of this type have the functional form

$$\begin{aligned} \log g(\theta) &= \log a(\theta) - i \sum_{r=1}^{R} b_r \arg e^{i(\theta_r + \pi - \theta)} + \sum_{r=1}^{R} a_r \log |2 - 2\cos(\theta - \theta_r)| \\ &= \log a(\theta) + \sum_{r=1}^{R} ((a_r + b_r)\log(1 + e^{i(\theta - (\theta_r + \pi))}) + (a_r - b_r)\log(1 + e^{i(\theta_r + \pi - \theta)})). \end{aligned} \tag{1.6}$$

Here $-\pi < \arg z \leqslant \pi$ and $a(\theta)$ is assumed to be sufficiently smooth that if we write

$$\log a(\theta) = \sum_{p=-\infty}^{\infty} c_p e^{ip\theta} \tag{1.7}$$

[cf. (1.3)] then the condition (1.4) holds. By using data following from the fact that special cases of (1.6) correspond to Toeplitz determinant expressions for the spin–spin correlation in the two-dimensional Ising model at criticality (see Sec. II below), the asymptotic form of which had previously been calculated,[7] Fisher and Hartwig[6] conjectured that for some range of parameter values $\{a_r\}_{r=1,\ldots,R}$, $\{b_r\}_{r=1,\ldots,R}$,

$$D_n[g] \underset{n \to \infty}{\sim} e^{c_0 n} e^{\sum_{r=1}^{R} (a_r^2 - b_r^2)\log n} E, \tag{1.8}$$

where E is independent of n. Subsequently this was proved for various ranges of parameter values (see e.g., Ref. 8) and furthermore the constant was determined to be given by

$$\begin{aligned} E = e^{\sum_{k=1}^{\infty} k c_k c_{-k}} \prod_{r=1}^{R} e^{-(a_r + b_r)\log a_-(\theta_r)} e^{-(a_r - b_r)\log a_+(\theta_r)} \prod_{1 \leqslant r \neq s \leqslant R} (1 - e^{i(\theta_s - \theta_r)})^{-(a_r + b_r)(a_s - b_s)} \\ \times \prod_{r=1}^{R} \frac{G(1 + a_r + b_r) G(1 + a_r - b_r)}{G(1 + 2a_r)}, \end{aligned} \tag{1.9}$$

where G is the Barnes G-function and

$$\log a_+(\theta) := \sum_{p=1}^{\infty} c_p e^{ip\theta}, \quad \log a_-(\theta) := \sum_{p=-\infty}^{-1} c_p e^{ip\theta}. \tag{1.10}$$

Our interest is in applications and generalizations of the Fisher–Hartwig asymptotic formula (1.8). We begin in Sec. II with an application of (1.8) to the calculation of the asymptotic form of the spin–spin correlation for the two-dimensional Ising model above criticality. In Sec. III the well-known equivalence of the Toeplitz determinant (1.1) to a random matrix average over the unitary group $\mathrm{U}(n)$ is revised. This average is in turn equivalent to the partition function of the one-component log-gas on a circle, subject to a one-body potential with Boltzmann factor $g(\theta)$ at the special coupling $\beta=2$. As such there is a natural generalization for couplings $\beta>0$, and in the case $b_r=0$, $r=1,\ldots,R$ this can be used to predict the corresponding generalization of (1.8). Moreover, in the special case $a(\theta)=1$, $R=1$ the sought asymptotic form can be deduced from an exact formula valid for general a_r, b_r. This can be used to extend the conjectured generalization of (1.8) to nonzero b_r.

In Sec. IV we recall the problem of computing the asymptotic form of the density matrix for impenetrable bosons in Dirichlet and Neumann boundary conditions. This is immediately identifiable as an average over the classical groups $\mathrm{Sp}(N)$ and $\mathrm{O}^+(2N)$, respectively, with the function being averaged over having two zeros, and thus analogous to the random matrix formulation of the Toeplitz determinant (1.1) with symbol (1.6) in the case $R=2$, $b_r=0$. We point out that the same class of averages over the groups $\mathrm{O}^+(2N+1)$ or $\mathrm{O}^-(2N+1)$ result from considering the density matrix for the impenetrable Bose gas in the case of mixed Dirichlet and Neumann boundary conditions. In Ref. 9 the sought asymptotics were calculated on the basis of a combination of analytic and log-gas arguments, and a Fisher–Hartwig-type generalization (with $b_r=0$) conjectured. The conjecture of Ref. 9 can used to predict the asymptotic form in the case of mixed Dirichlet and Neumann boundary conditions. Moreover we show that this asymptotic form can be proved by making use of asymptotic formulas recently obtained[10] for Toeplitz plus Hankel determinants

$$\det[a_{j-k}+a_{j+k+1}]_{j,k=0,\ldots,n-1} \tag{1.11}$$

in the case of singular generating functions (1.6).

In addition to averages over the classical groups, the study of the density matrix for impenetrable bosons naturally leads to the question of obtaining the asymptotic form of averages over the eigenvalue probability density function for the GUE and LUE, in the case that the function being averaged over has zeros. Here the GUE denotes the Gaussian unitary ensemble of random Hermitian matrices, and the LUE denotes the Laguerre unitary ensemble of positive definite matrices with complex entries. These random matrix averages are equivalent to pure Hankel determinants,

$$\det[a_{j+k}]_{j,k=0,\ldots,n-1}, \quad a_n = \int_{-\infty}^{\infty} a(x) x^n \, d\mu(x), \tag{1.12}$$

where $d\mu(x)=e^{-x^2}\,dx$ for the GUE and $d\mu(x)=x^a e^{-x}\,dx$, $x>0$ for the LUE. Conjectures for such asymptotic forms are given in Sec. V. The paper ends with some concluding remarks on the universal form for Hankel asymptotics in Sec. VI, and attention is also drawn to the fluctuation formula perspective of our asymptotic results.

II. SPIN–SPIN CORRELATIONS FOR THE TWO-DIMENSIONAL ISING MODEL

In the two-dimensional Ising model on a square lattice each site (i,j) of the lattice exists in one of two possible states $\sigma_{ij}=\pm 1$ with coupling between nearest neighbors in the horizontal and vertical directions. Explicitly, the joint probability density function for a particular configuration $\{\sigma_{ij}\}$ of the states on a $(2N+1)\times(2N+1)$ lattice is given by

$$P_{2N+1}(\{\sigma_{ij}\})=\frac{1}{Z_{2N+1}}\exp\left(K_1\sum_{j=-N}^{N}\sum_{i=-N}^{N-1}\sigma_{ij}\sigma_{i+1\,j}+K_2\sum_{i=-N}^{N}\sum_{j=-N}^{N-1}\sigma_{ij}\sigma_{i\,j+1}\right), \tag{2.1}$$

where Z_{2N+1} is the normalization. The spin–spin correlation function between the spin σ_{00} at the center of the lattice, and the spin $\sigma_{i^*j^*}$ at site (i^*,j^*) is, in the infinite lattice limit, defined as

$$\langle\sigma_{00}\sigma_{i^*j^*}\rangle=\lim_{N\to\infty}\sum_{\{\sigma_{ij}\}}\sigma_{00}\sigma_{i^*j^*}P_{2N+1}(\{\sigma_{ij}\}). \tag{2.2}$$

Onsager knew of, but never published (see instead, e.g., Ref. 11) a Toeplitz determinant form for the case of (2.2) for which $(i^*,j^*)=(n,n)$ and thus lies on the diagonal. Explicitly

$$\langle\sigma_{00}\sigma_{nn}\rangle=\det[a_{i-j}]_{i,j=1,\ldots,n},\quad a_p=\frac{1}{2\pi}\int_{-\pi}^{\pi}h(\theta)e^{-ip\theta}\,\mathrm{d}\theta, \tag{2.3}$$

where

$$h(\theta):=\left(\frac{1+(1/k)e^{-i\theta}}{1+(1/k)e^{i\theta}}\right)^{1/2},\quad k=\sinh 2K_1\sinh 2K_2. \tag{2.4}$$

Also, in the case of (2.2) with $(i^*,j^*)=(0,n)$ so that the two spins lie in the same row, Onsager and Kaufmann[12] expressed (2.2) as the sum of two Toeplitz determinants. A different approach to this problem was undertaken by Potts and Ward,[13] who obtained instead the single Toeplitz determinant form

$$\langle\sigma_{00}\sigma_{0n}\rangle=\det[\tilde{a}_{i-j}]_{i,j=1,\ldots,n},\quad \tilde{a}_p=\frac{1}{2\pi}\int_{-\pi}^{\pi}\tilde{h}(\theta)e^{-ip\theta}\,\mathrm{d}\theta, \tag{2.5}$$

where

$$\tilde{h}(\theta):=\left(\frac{(1+\alpha_1e^{i\theta})(1+\alpha_2e^{-i\theta})}{(1+\alpha_1e^{-i\theta})(1+\alpha_2e^{i\theta})}\right)^{1/2} \tag{2.6}$$

with

$$\alpha_1:=e^{-2K_2}\tanh K_1,\quad \alpha_2:=\frac{e^{-2K_2}}{\tanh K_1}.$$

The formula obtained in Ref. 12 was shown to be identical to (2.3), (2.4) by Montroll, Potts, and Ward.[14] We remark that if α_1,α_2 in (2.6) and k in (2.4) are regarded as parameters not specified by K_1,K_2, then setting $\alpha_1=0,\alpha_2=1/k$ in the former gives (2.4).

A detailed study of the asymptotic form of (2.6) was undertaken by Wu.[7] Indeed, it was the asymptotic form of (2.5) at the critical coupling

$$\alpha_1<\alpha_2=1 \tag{2.7}$$

obtained in Ref. 7 which, partially at least, inspired the formulation of the Fisher–Hartwig asymptotic formula (1.8).[6] To see how (1.8) relates to (2.5) with parameters (2.7), note

$$\log \tilde{h}(\theta)|_{\alpha_2=1} = \log\left(\frac{1+\alpha_1 e^{i\theta}}{1+\alpha_1 e^{-i\theta}}\right)^{1/2} + i \arg e^{-i\theta/2}. \tag{2.8}$$

For $|\alpha_1|<1$ this has the structure of (1.6) with

$$a(\theta) = \left(\frac{1+\alpha_1 e^{i\theta}}{1+\alpha_1 e^{-i\theta}}\right)^{1/2}, \quad R=1, \quad b_r = -\frac{1}{2}, \quad a_r = 0, \quad \theta_r = -\pi.$$

Recalling the definitions (1.3) [with $g(\theta)$ replaced by $a(\theta)$] and (1.10), application of (1.8) implies

$$\langle \sigma_{00}\sigma_{0n}\rangle|_{\substack{\alpha_2=1 \\ \alpha_1<1}} \underset{n\to\infty}{\sim} \left(\frac{1+\alpha_1}{1-\alpha_1}\right)^{1/4} \frac{\sqrt{\pi}G^2(1/2)}{n^{1/4}}, \tag{2.9}$$

where use has been made of the functional equation

$$G(z+1) = \Gamma(z)G(z),$$

in agreement with the result of Wu.

The high temperature phase corresponds to couplings

$$\alpha_1 < 1 < \alpha_2, \quad \alpha_1\alpha_2 < 1. \tag{2.10}$$

In this case $\log \tilde{h}(\theta)$ is of the form (1.6) with

$$a(\theta) = \left(\frac{(1+\alpha_1 e^{i\theta})(1+e^{i\theta}/\alpha_2)}{(1+\alpha_1 e^{-i\theta})(1+e^{-i\theta}/\alpha_2)}\right)^{1/2}, \quad R=1, \quad b_r=-1, \quad a_r=0, \quad \theta_r=-\pi. \tag{2.11}$$

With $R=1, b_r=-1, a_r=0$ we see that the Fisher–Hartwig asymptotic formula (1.8) breaks down because according to (1.9) the constant E contains the factor $G(0)=0$ and thus vanishes. To obtain the asymptotics in this case the approach taken in Ref. 7 was to relate it back to the original strong Szegö theorem, multiplied by an auxiliary factor. Here we will show that by transforming (2.6), a form of $\log \tilde{h}(\theta)$ can be obtained which has the general structure (1.6) but is distinct from the specification (2.11). We will see that applying the Fisher–Hartwig formula then correctly reproduces the result of Wu for the leading asymptotic decay in the high temperature phase.

For this purpose, let us introduce the notation $f(\theta) \equiv g(\theta)$ to mean that

$$\int_{-\pi}^{\pi} f(\theta) e^{-ip\theta}\, d\theta = c^{-p} \int_{-\pi}^{\pi} g(\theta) e^{-ip\theta}\, d\theta$$

for some c independent of p. According to the definitions (2.6) and (2.11) we have $\tilde{h}(\theta) = e^{-i\theta} a(\theta)$. Now, since with $z=e^{i\theta}$, $\tilde{h}(\theta)$ is an analytic function of z in the annulus $1/\alpha_2 < |z| < \alpha_2$, by Cauchy's theorem

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{h}(\theta) e^{-ip\theta}\, d\theta = \int_{\mathcal{C}} \tilde{h}(\theta) z^{-p} \frac{dz}{2\pi i z}$$

for any simple closed contour encircling the origin in this annulus. Choosing $\mathcal{C}$ to be the circle with radius α_2 (the outer boundary of the annulus) shows

$$\tilde{h}(\theta) \equiv \frac{e^{-i\theta}}{\alpha_2}\left(\frac{1+\alpha_1\alpha_2 e^{i\theta}}{1+(\alpha_1/\alpha_2)e^{-i\theta}}\right)^{1/2}\frac{(1+e^{i\theta})^{1/2}}{(1+e^{-i\theta}/\alpha_2^2)^{1/2}}$$
$$= \frac{1}{\alpha_2}\frac{1}{(1+e^{-i\theta}/\alpha_2^2)^{1/2}}\left(\frac{1+\alpha_1\alpha_2 e^{i\theta}}{1+(\alpha_1/\alpha_2)e^{-i\theta}}\right)^{1/2} e^{-3i\theta/4}|1+e^{i\theta}|^{1/2}.$$

This is of the form (1.6) with

$$a(\theta) = \frac{1}{\alpha_2}\frac{1}{(1+e^{-i\theta}/\alpha_2^2)^{1/2}}\left(\frac{1+\alpha_1\alpha_2 e^{i\theta}}{1+(\alpha_1/\alpha_2)e^{-i\theta}}\right)^{1/2}, \quad R=1, \quad b_r=-\frac{3}{4}, \quad a_r=\frac{1}{4}, \quad \theta_r=-\pi. \tag{2.12}$$

Application of (1.8) implies

$$\langle \sigma_{00}\sigma_{0n}\rangle|_{\substack{\alpha_1<1<\alpha_2 \\ \alpha_1\alpha_2<1}} \underset{n\to\infty}{\sim} \frac{\alpha_2^{-n}}{(\pi n)^{1/2}}(1-\alpha_1^2)^{1/4}(1-\alpha_2^{-2})^{-1/4}(1-\alpha_1\alpha_2)^{-1/2} \tag{2.13}$$

in agreement with the result of Wu.[7] Moreover the Fisher–Hartwig formula (1.8) with $R=1$ has been proved[15] for parameter values satisfying all three of the inequalities,

$$\mathrm{Re}\, a_1 \geqslant 0, \quad \mathrm{Re}\, a_1 + \mathrm{Re}\, b_1 > -1, \quad \mathrm{Re}\, a_1 - \mathrm{Re}\, b_1 > -1.$$

These inequalities are satisfied by the parameters in (2.12) and so the Fisher–Hartwig formula provides a proof of (2.13).

III. β-GENERALIZATION OF THE FISHER–HARTWIG FORMULA

It is well known, and easy to verify, that the Toeplitz determinant (1.2) can be written as a random matrix average according to

$$D_n[g] = \left\langle \prod_{l=1}^{n} g(\theta_l) \right\rangle_{\mathrm{U}(n)}. \tag{3.1}$$

Here $\mathrm{U}(n)$ refers to the eigenvalue probability density function for the unitary group

$$\frac{1}{(2\pi)^n n!}\prod_{1\leqslant j<k\leqslant n}|e^{i\theta_k}-e^{i\theta_j}|^2, \quad -\pi<\theta_l\leqslant\pi. \tag{3.2}$$

As first noted by Dyson,[2] (3.2) is proportional to the Boltzmann factor for the one-component log-potential Coulomb gas on a circle, at the special coupling $\beta=2$. From the log-gas viewpoint a natural generalization of (3.2) is the probability density function $C\beta E_n$ proportional to the Boltzmann factor for the same statistical mechanical system but with general coupling $\beta>0$,

$$\frac{1}{(2\pi)^n C_{n,\beta}}\prod_{1\leqslant j<k\leqslant n}|e^{i\theta_k}-e^{i\theta_j}|^\beta, \quad C_{n,\beta}=\frac{\Gamma(n\beta/2+1)}{(\Gamma(\beta/2+1))^n}. \tag{3.3}$$

The identity (3.1) then allows us to formulate a β-generalization of the Toeplitz determinant (1.2) as the average

$$D_n^{(\beta)}[g] := \left\langle \prod_{l=1}^{n} g(\theta_l) \right\rangle_{C\beta E_n}. \tag{3.4}$$

Choosing $g(\theta)$ according to (1.6) in this we obtain a natural β-generalization of the Toeplitz determinant with a Fisher–Hartwig symbol. In the case $b_r=0$, $r=1,\dots,R$, the log-gas viewpoint can be used to conjecture the corresponding analogue of the asymptotic formula (1.8).

Let

$$Z_n^{(\beta)}[g(\theta)] := \frac{1}{(2\pi)^n}\int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_n \prod_{l=1}^{n} g(\theta_l) \prod_{1\leqslant j<k\leqslant n} |e^{i\theta_k}-e^{i\theta_j}|^{\beta}. \tag{3.5}$$

As the first step, guided by both the log-gas viewpoint and the structure of (1.8), we conjecture the factorization

$$\frac{Z_n^{(\beta)}\left[a(\theta)\prod_{j=1}^{R}|e^{i\theta}-e^{i\phi_j}|^{q_j\beta}\right]}{Z^{(\beta)}_{n+\Sigma_{j=1}^{R}q_j}[1]} \sim e^{-\Sigma_{j=1}^{R}q_j \log a(\theta_j)} \frac{Z_n^{(\beta)}[a(\theta)]}{Z^{(\beta)}_{n+\Sigma_{j=1}^{R}q_j}[1]} \frac{Z_n^{(\beta)}\left[\prod_{j=1}^{R}|e^{i\theta}-e^{i\phi_j}|^{q_j\beta}\right]}{Z^{(\beta)}_{n+\Sigma_{j=1}^{R}q_j}[1]}. \tag{3.6}$$

From the work of Johansson,[5,16] with the Fourier expansion of $\log a(\theta)$ specified by (1.7) and assuming the coefficients satisfy (1.4), it has been proved for general $\beta>0$ that

$$\frac{Z^{(\beta)}_{n+Q}[a(\theta)]}{Z^{(\beta)}_{n+Q}[1]} \sim e^{c_0(n+Q)} e^{(2/\beta)\Sigma_{k=1}^{\infty} k c_k c_{-k}}. \tag{3.7}$$

Regarding the second ratio on the right-hand side of (3.6), as first noted in Refs. 17 and 18 and revised in Ref. 20, the log-gas viewpoint suggests that for $n\to\infty$ we have the factorization

$$\prod_{1\leqslant j<k\leqslant R}|e^{i\theta_k}-e^{i\theta_j}|^{\beta q_j q_k} \frac{Z_n^{(\beta)}\left[\prod_{j=1}^{R}|e^{i\theta}-e^{i\phi_j}|^{q_j\beta}\right]}{Z^{(\beta)}_{n+\Sigma_{j=1}^{R}q_j}[1]} \sim \prod_{j=1}^{R} \frac{Z_n^{(\beta)}\left[\prod_{j=1}^{R}|e^{i\theta}-e^{i\phi_j}|^{q_j\beta}\right]}{Z^{(\beta)}_{n+q_j}[1]}. \tag{3.8}$$

The large-n expansion of a ratio closely related to the product on the right-hand side of (3.8) is known for β rational, in particular

$$\beta/2 = s/r, \quad s \text{ and } r \text{ relatively prime}. \tag{3.9}$$

Thus we have[18]

$$\prod_{j=1}^{R} \frac{Z_n^{(\beta)}\left[\prod_{j=1}^{R}|e^{i\theta}-e^{i\phi_j}|^{q_j\beta}\right]}{Z_n^{(\beta)}[1]} \sim n^{q^2\beta/2} A_q, \tag{3.10}$$

where

$$A_q := r^{-q^2\beta/2} \prod_{\nu=0}^{r-1}\prod_{p=0}^{s-1} \frac{G^2(q/r+\nu/r-p/s+1)}{G(2q/r+\nu/r-p/s+1)G(\nu/r-p/s+1)}. \tag{3.11}$$

Finally, the formula for $C_{n,\beta}$ in (3.3) together with Stirling's formula shows

$$\frac{Z_n^{(\beta)}[1]}{Z^{(\beta)}_{n+q}[1]} \sim (\Gamma(\beta/2+1))^q (n\beta/2)^{-q\beta/2}. \tag{3.12}$$

Combining the above results gives the sought β-generalization of the Fisher–Hartwig formula in the case $b_r=0$.

Conjecture 1: Let β be rational and of the form (3.9), and let $a(\theta)$ be as assumed for the validity of (3.7). For $q_j\beta>-1$ we expect

$$\left\langle \prod_{l=1}^{N} \left(a(\theta_l) \prod_{j=1}^{R} |e^{i\theta_l} - e^{i\phi_j}|^{q_j \beta} \right) \right\rangle_{C\beta E_n} \underset{n\to\infty}{\sim} e^{c_0(n+\sum_{j=1}^{R} q_j)} n^{(\beta/2)\sum_{j=1}^{R} q_j^2} E^{(\beta)}, \tag{3.13}$$

where, with A_q specified by (3.11),

$$E^{(\beta)} = e^{-\sum_{j=1}^{R} q_j \log a(\theta_j)} e^{(2/\beta)\sum_{k=1}^{\infty} k c_k c_{-k}} \prod_{1\le j<k\le R} |e^{i\theta_k} - e^{i\theta_j}|^{-\beta q_j q_k} \prod_{j=1}^{R} A_{q_j}. \tag{3.14}$$

It is of interest to extend Conjecture 1 to include a factor

$$\prod_{j=1}^{R} e^{-i(\beta/2) b_r \arg e^{i(\phi_j + \pi - \theta)}} \tag{3.15}$$

in the average, and so obtain a β-generalization of the Fisher–Hartwig formula for general parameters. Although we do not have a log-gas interpretation of the factor (3.15), the case $R=1$ substituted in (3.13) with $a(\theta)=1$ gives an average which can be evaluated in closed form, and the corresponding asymptotics computed for rational β. This together with the structure of the original Fisher–Hartwig formula (1.8), (1.9) allows us to formulate the sought β-generalization.

Now, by rotational invariance, independent of the value of ϕ

$$\begin{aligned} \left\langle \prod_{l=1}^{n} e^{-i(\beta/2) b \arg e^{i(\phi+\pi-\theta_l)}} |e^{i\theta_l} - e^{i\phi}|^{\beta q} \right\rangle_{C\beta E_n} &= \left\langle \prod_{l=1}^{n} e^{i\beta b \theta_l/2} |1 + e^{i\theta_l}|^{\beta q} \right\rangle_{C\beta E_n} \\ &= \frac{Z_n^{(\beta)}[e^{i\beta b\theta/2}|1+e^{i\theta}|^{\beta q}]}{Z_n^{(\beta)}[1]}. \end{aligned} \tag{3.16}$$

But, from the theory of the Selberg integral (see, e.g., Ref. 3), we know the right-hand side of (3.16) has the explicit gamma function evaluation

$$\frac{f_n(2cq,c)}{f_n(c(q+b),c) f_n(c(q-b),c)}, \quad \text{where } f_n(\alpha,c) := \prod_{j=0}^{n-1} \frac{(\alpha+jc)!}{(jc)!}, \quad c := \beta/2. \tag{3.17}$$

For $c \in \mathbb{Z}^+$ it was shown in Ref. 18 that

$$f_n(\alpha,c) \underset{n\to\infty}{\sim} \exp(\alpha n \log n) c^{\alpha n} e^{-\alpha n} n^{-(c-1)\alpha/2 + \alpha^2/2c} \prod_{p=0}^{c-1} \frac{G(-p/c+1)}{G((\alpha-p)/c+1)}, \tag{3.18}$$

while for r and s relatively prime

$$f_{rn}(\alpha, s/r) = \prod_{\nu=0}^{r-1} \frac{f_n(\alpha + s\nu/r, s)}{f_n(s\nu/r, s)}. \tag{3.19}$$

Using (3.19) and (3.18) in (3.17) it follows that for β rational of the form (3.9),

$$\left\langle \prod_{l=1}^{n} e^{i\beta b\theta_l/2} |1 + e^{i\theta_l}|^{\beta q} \right\rangle_{C\beta E_{rn}} \underset{n\to\infty}{\sim} (rn)^{(\beta/2)(q^2-b^2)} A_{q,b}, \tag{3.20}$$

where

$$A_{q,b} := r^{-(q^2-b^2)\beta/2} \prod_{\nu=0}^{r-1} \prod_{p=0}^{s-1} \frac{G((q+b)/r+\nu/r-p/s+1)G^2((q-b)/r+\nu/r-p/s+1)}{G(2q/r+\nu/r-p/s+1)G(\nu/r-p/s+1)}. \tag{3.21}$$

Note that in the case $b=0$ this reduces to (3.11), (3.10) as it must.

Knowing how, from the Fisher–Hartwig formula (1.8), (1.9), to generalize from the case $R=1$, general parameters, and the case general R but $b_r=0$ $(r=1,\dots,R)$, to the case of general parameters and general R lets us use (3.13) and (3.20) to formulate a β-generalization of the Fisher–Hartwig formula for general parameters.

Conjecture 2: Let β be rational and of the form (3.9), and let $a(\theta)$ be as assumed for the validity of (3.7). We expect, for some range of parameters $\{b_j\}$ and $\{q_j\}$,

$$\left\langle \prod_{l=1}^{n} a(\theta_l) \prod_{j=1}^{R} e^{-i(\beta/2)b_j \arg e^{i(\phi_j+\pi-\theta_l)}} |e^{i\theta_l}-e^{i\phi_j}|^{q_j\beta} \right\rangle_{C\beta E_n} \underset{n\to\infty}{\sim} e^{c_0 n} n^{(\beta/2)\Sigma_{j=1}^{R}(q_j^2-b_j^2)} \tilde{E}(\beta), \tag{3.22}$$

where, with $A_{q,b}$ specified by (3.21),

$$\tilde{E}(\beta) = e^{(2/\beta)\Sigma_{k=1}^{\infty} k c_k c_{-k}} \prod_{r=1}^{R} e^{-(q_r+b_r)\log a_-(\theta_r)} e^{-(q_r-b_r)\log a_+(\theta_r)}$$

$$\times \prod_{1\le r\ne s\le R} (1-e^{i(\theta_s-\theta_r)})^{-\beta(q_r+b_r)(q_s-b_s)/2} \prod_{j=1}^{R} A_{q_j,b_j}. \tag{3.23}$$

IV. FISHER–HARTWIG ASYMPTOTICS FOR AVERAGES OVER THE ORTHOGONAL AND SYMPLECTIC GROUPS

A problem in mathematical physics which, along with the Ising correlations, motivated the Fisher–Hartwig formula (1.8) is the impenetrable Bose gas on a circle. If the circle has circumference length L, it was shown by Lenard[19] that the ground state density matrix $\rho_{N+1}^{C}(x)$ has the Toeplitz determinant form

$$\rho_{N+1}^{C}(x;0) = \frac{1}{L} \det[a_{j-k}^{C}(x)]_{j,k=1,\dots,N},$$
$$a_l^{C}(x) := \frac{1}{2\pi} \int_{-\pi}^{\pi} |e^{2\pi i x/L} + e^{i\theta}||1+e^{i\theta}| e^{-il\theta}\, d\theta. \tag{4.1}$$

The symbol in (4.1) is of the form (1.6) with

$$a(\theta)=1, \quad R=2, \quad a_1=a_2=\tfrac{1}{2}, \quad b_1=b_2=0, \quad \theta_1=0, \quad \theta_2=2\pi x/L. \tag{4.2}$$

Now a fundamental issue relating to the Bose gas is the occupation λ_0 of the zero momentum state, which quantifies the phenomenon of Bose–Einstein condensation (see, e.g., Ref. 20). In the present system, which is translationally invariant, λ_0 is related to the density matrix by the simple formula

$$\lambda_0 = \int_0^L \rho_{N+1}^{C}(x;0)\, dx = L \int_0^1 \rho_{N+1}^{C}(LX;0)\, dX. \tag{4.3}$$

For fixed $0<X<1$ one thus seeks the $L\to\infty$ asymptotic form of $\rho_{N+1}^{C}(LX;0)$. In an unpublished work as of 1968, made available to the authors of Ref. 6 and subsequently published in 1972,[21] Lenard obtained for the sought expansion

$$\rho_{N+1}^{C}(LX;0)\sim\rho_0\frac{G^4(3/2)}{\sqrt{2\pi}}\left(\frac{\pi}{N\sin(\pi X)}\right)^{1/2}, \tag{4.4}$$

where ρ_0 denotes the bulk density. Lenard obtained (4.4) as an upper bound, which soon after was shown to be attained by Widom.[22] Applying the Fisher–Hartwig formula (1.8) with variables (4.2) reproduces (4.4).

According to (3.1) the Toeplitz formula (4.1) can equivalently be written as the U(N) average

$$\rho_{N+1}^{C}(x;0)=\frac{1}{L}\left\langle\prod_{l=1}^{N}\left|2\sin\left(\frac{\pi x}{L}-\frac{\theta_l}{2}\right)\right|\left|2\sin\frac{\theta_l}{2}\right|\right\rangle_{\mathrm{U}(N)}. \tag{4.5}$$

The study of the ground state density matrices for the impenetrable Bose gas on a line of length L with Dirichlet or Neumann boundary conditions leads to formulas analogous to (4.5), only now the averages are with respect to the eigenvalue probability density functions for the classical groups Sp(N) and $\mathrm{O}^+(2N)$, respectively (see, e.g., Ref. 3 for the specification of these PDFs). Thus one has[20]

$$\begin{aligned}\rho_{N+1}^{D}(x;y)&=\frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}\left\langle\prod_{l=1}^{N}\left|2\left(\cos\frac{\pi x}{L}-\cos\theta_l\right)\right|\left|2\left(\cos\frac{\pi y}{L}-\cos\theta_l\right)\right|\right\rangle_{\mathrm{Sp}(N)},\\ \rho_{N+1}^{N}(x;y)&=\frac{1}{2L}\left\langle\prod_{l=1}^{N}\left|2\left(\cos\frac{\pi x}{L}-\cos\theta_l\right)\right|\left|2\left(\cos\frac{\pi y}{L}-\cos\theta_l\right)\right|\right\rangle_{\mathrm{O}^+(2N)}.\end{aligned} \tag{4.6}$$

Impenetrable bosons on the interval $[0,L]$ with Dirichlet boundary conditions at $x=0$ and Neumann boundary conditions at $x=L$ also relate to a classical group. Thus from the fact that the single particle wave functions are given by

$$\phi_k^M(x)=\sqrt{\frac{2}{L}}\sin\frac{\pi(k-1/2)x}{L}\quad(k=1,2,\dots)$$

(the superscript M stands for "mixed") we see that the ground state wave function

$$\psi_0^M(x_1,\dots,x_N)=\frac{1}{\sqrt{N!}}|\det[\,\phi_k^M(x_j)\,]_{j,k=1,\dots,N}|$$

has the product form

$$\psi_0^M(x_1,\dots,x_N)=\frac{1}{\sqrt{N!}}\left(\frac{1}{2\sqrt{L}}\right)^N\prod_{l=1}^{N}2\sin(\pi x_l/2L)\prod_{1\le j<k\le N}2|\cos\pi x_k/L-\cos\pi x_j/L|.$$

The square of this quantity coincides with the eigenvalue PDF of the classical group $\mathrm{O}^+(2N+1)$ with $\theta=\pi x/L$ (for this we ignore the fixed eigenvalue at $\theta=0$). From this fact, as in the derivation of (4.6) detailed in Ref. 20, it follows that

$$\rho_{N+1}^{M}(x;y)=\frac{2}{L}\sin\frac{\pi x}{2L}\sin\frac{\pi y}{2L}\left\langle\prod_{l=1}^{N}\left|2\left(\cos\frac{\pi x}{L}-\cos\theta_l\right)\right|\left|2\left(\cos\frac{\pi y}{L}-\cos\theta_l\right)\right|\right\rangle_{\mathrm{O}^+(2N+1)}. \tag{4.7}$$

Using a combination of analytic calculations based on the Selberg correlation integral,[23] and physical arguments based on log-gas analogies, the large N, fixed $x/L, y/L, N/L$ limit of the density matrices (4.6) was computed in Ref. 9 to be equal to

$$\rho^D_{N+1}(x;y)\sim\rho^N_{N+1}(x;y)\sim\rho\frac{G^4(3/2)}{\sqrt{2N}}\frac{(X(1-X))^{1/8}(Y(1-Y))^{1/8}}{|X-Y|^{1/2}}\Bigg|_{\substack{X=(1+\cos\,\pi x/L)/2\\ Y=(1+\cos\,\pi y/L)/2}}. \tag{4.8}$$

Here we will show how recent rigorous asymptotic analysis[10] of Toeplitz and Hankel determinants (1.11) with Fisher–Hartwig-type symbols can be used to prove that $\rho^M_{N+1}(x;y)$ exhibits the same asymptotic form (4.8). We will also show how a result of Ref. 10 can be used to confirm the asymptotic form of a more general class of averages over $\mathrm{O}^+(2N+1)$ which can be deduced from a conjecture in Ref. 9, and how this conjecture in turn can be used to predict analogous asymptotics in the case of averages over $\mathrm{Sp}(N)$ and $\mathrm{O}^+(2N)$.

To begin we require a simple to verify identity noted in Ref. 24.

Lemma 1: Suppose $g(\theta)=g(-\theta)$ *and set* $g_j=(1/2\pi)\int_{-\pi}^{\pi}g(\theta)e^{-ij\theta}\,\mathrm{d}\theta$. *We have*

$$\det[g_{j-k}+g_{j+k+1}]_{j,k=0,\dots,N-1}=\left\langle\prod_{j=1}^{N}g(\theta_j)\right\rangle_{\mathrm{O}^-(2N+1)}=\left\langle\prod_{j=1}^{N}g(\pi-\theta_j)\right\rangle_{\mathrm{O}^+(2N+1)}. \tag{4.9}$$

Note that by the assumption on $g(\theta)$ the matrix in (4.9) is symmetric. Also, the average in (4.7) is an even function of θ_l and corresponds to the special case

$$\begin{aligned}g(\theta)&=2\left|\cos\frac{\pi x}{L}-\cos\theta\right|\,2\left|\cos\frac{\pi y}{L}-\cos\theta\right|\\&=\left(\left|2-2\cos\left(\theta-\frac{\pi x}{L}\right)\right|\left|2-2\cos\left(\theta+\frac{\pi x}{L}\right)\right|\left|2-2\cos\left(\theta-\frac{\pi y}{L}\right)\right|\left|2-2\cos\left(\theta+\frac{\pi y}{L}\right)\right|\right)^{1/2}\end{aligned} \tag{4.10}$$

of (4.9). We observe that (4.10) is an example of a symbol of the form (1.6). Fortunately, recent rigorous works[25,10] have determined the asymptotic form of the Hankel plus Toeplitz determinant in (4.9) for all symbols (1.6), with the restriction that for $g(\theta)$ even [the case of interest in relation to (4.9)], $\theta_r\neq 0,\pm\pi$. Let us recall the result of Ref. 10, Theorem 6.1, simplified so that it relates to the even case of (1.6) with each $b_r=0$.

Theorem 1: *Let*

$$\log g(\theta)=\log a(\theta)+\sum_{r=1}^{R}a_r(\log(2|\cos\theta-\cos\theta_r|)), \tag{4.11}$$

where $a(\theta)$ *is an even periodic function with the property that the Fourier expansion of its logarithm (1.7) satisfies (1.4), together with some technical assumptions (for the latter, which may not be necessary, see Ref. 10). We have*

$$\det[g_{j-k}+g_{j+k+1}]_{j,k=0,\dots,N-1}\sim e^{(N+\Sigma_{j=1}^{R}a_j)c_0}(2N)^{\Sigma_{r=1}^{R}a_r^2}E, \tag{4.12}$$

where

$$\begin{aligned}E=&\prod_{r=1}^{R}\frac{G^2(1+a_r)}{G(1+2a_r)}e^{1/2\,\Sigma_{k=1}^{\infty}kc_k^2+\Sigma_{k=1}^{\infty}c_{2k-1}}e^{-\Sigma_{j=1}^{N}a_j\log a(\theta_j)}\\&\times\prod_{r=1}^{R}\frac{|1-e^{i\theta_r}|^{a_r}}{|1+e^{i\theta_r}|^{a_r}|1-e^{2i\theta_r}|^{a_r^2}}\prod_{1\leqslant r<s\leqslant R}(|1-e^{i(\theta_r-\theta_s)}||1-e^{i(\theta_r+\theta_s)}|)^{-2a_ra_s}.\end{aligned} \tag{4.13}$$

Recalling (4.9) it follows from Theorem 1 that

$$\left\langle \prod_{j=1}^{N} \left| 2\left(\cos\frac{\pi x}{L} - \cos\theta_j \right) \right| \left| 2\left(\cos\frac{\pi y}{L} - \cos\theta_j \right) \right| \right\rangle_{\mathrm{O}^-(2N+1)}$$
$$\sim (2N)^{1/2} G^4(3/2) \frac{|1+e^{\pi i x/L}|^{1/4}}{|1-e^{\pi i x/L}|^{3/4}} \frac{|1+e^{\pi i y/L}|^{1/4}}{|1-e^{\pi i y/L}|^{3/4}} \frac{1}{|1-e^{\pi i (x-y)/L}|^{1/2} |1-e^{\pi i (x+y)/L}|^{1/2}}. \tag{4.14}$$

Substituting this in (4.7) shows

$$\rho_{N+1}^{M}(x,y) \sim \frac{(2N)^{1/2}}{2L} G^4(3/2) \frac{|1-e^{2\pi i x/L}|^{1/4} |1-e^{2\pi i y/L}|^{1/4}}{|1-e^{\pi i (x-y)/L}|^{1/2} |1-e^{\pi i (x+y)/L}|^{1/2}}$$
$$= \rho \frac{G^4(3/2)}{\sqrt{2N}} \frac{(X(1-X))^{1/8} (Y(1-Y))^{1/8}}{|X-Y|^{1/2}} \Big|_{\substack{X=(1+\cos \pi x/L)/2 \\ Y=(1+\cos \pi y/L)/2}}, \tag{4.15}$$

thus rigorously establishing the asymptotic form (4.8) derived, but not rigorously proved, in Ref. 9 for the cases of Dirichlet and Neumann boundary conditions.

The eigenvalue distributions for $\mathrm{Sp}(N)$, $\mathrm{O}^+(2N)$, $\mathrm{O}^-(2N+1)$, and $\mathrm{O}^+(2N+1)$ are proportional to

$$\prod_{l=1}^{N} (1+\cos\theta_l)^{\lambda_1} (1-\cos\theta_l)^{\lambda_2} \prod_{1 \leqslant j < k \leqslant N} (\cos\theta_k - \cos\theta_j)^2, \quad 0 \leqslant \theta_l \leqslant \pi \tag{4.16}$$

for $(\lambda_1,\lambda_2)=(1,1)$, $(0,0)$, $(1,0)$, and $(0,1)$, respectively (our convention is not to include the delta function corresponding to a fixed eigenvalue, nor the delta functions corresponding to the conjugate eigenvalues). Thus to obtain the asymptotics of the averages in (4.6) it is sufficient to obtain the asymptotics of

$$\left\langle \prod_{l=1}^{N} \prod_{r=1}^{R} (2|\cos\theta_l - \cos\phi_r|)^{2a_r} \right\rangle_{C_N(\lambda_1,\lambda_2)}, \tag{4.17}$$

where $C_N(\lambda_1,\lambda_2)$ refers to the normalized form of (4.16). In the cases $(\lambda_1,\lambda_2)=(1,0)$ or $(0,1)$, due to the identity (4.9), we can read off the asymptotic form from (4.12). But for general (λ_1,λ_2) the asymptotic form of (4.17) is not included in Theorem 1. Instead, we will use a conjecture from Ref. 9 to formulate the result.

Let us first recall the conjectured asymptotic form from Ref. 9. Define

$$H_{n,\lambda_1,\lambda_2}[f(x)] := \int_0^1 dx_1 \cdots \int_0^1 dx_n \prod_{l=1}^{n} f(x_l) x_l^{\lambda_1} (1-x_l)^{\lambda_2} \prod_{1 \leqslant j < k \leqslant n} |x_k - x_j|^2. \tag{4.18}$$

Then the argument given in Ref. 9 predicts

$$\frac{H_{n,\lambda_1,\lambda_2}\left[e^{h(x)} \prod_{r=1}^{R} |y_r - x|^{2q_r} \right]}{H_{n+\Sigma_{j=1}^{R} q_j,\lambda_1,\lambda_2}[1]} \sim \exp\left[\frac{n + \sum_{r=1}^{R} q_r + (\lambda_1+\lambda_2)/2}{\pi} \int_0^1 \frac{h(x)}{[x(1-x)]^{1/2}} dx \right]$$
$$\times \exp\left[\sum_{r=1}^{R} (-q_r + q_r^2) \log 2n \right] K, \tag{4.19}$$

where

$$K=\prod_{j=1}^{R} y_j^{-\lambda_1 q_j}(1-y_j)^{-\lambda_2 q_j}\prod_{1\leqslant j<k\leqslant R}|y_k-y_j|^{-2q_jq_k}e^{-(\lambda_1 h(0)+\lambda_2 h(1))/2}e^{-\Sigma_{r=1}^{R}q_r h(y_r)}$$
$$\times\exp\left[\frac{1}{4\pi^2}\int_0^1 dx\,\frac{h(x)}{(x(1-x))^{1/2}}\int_0^1 dy\,\frac{h'(y)(y(1-y))^{1/2}}{x-y}\right]$$
$$\times\prod_{r=1}^{R}(y_r(1-y_r))^{-q_r^2/2}\prod_{r=1}^{R}\frac{1}{\pi^{q_r}}\frac{G^2(q_r+1)}{G(2q_r+1)}. \tag{4.20}$$

[Unfortunately there are a number of inaccuracies in the reporting of the conjecture in Ref. 9. The term $H_{n+\Sigma_{j=1}^{R}q_j,\lambda_1,\lambda_2}[1]$ in the denominator on the left-hand side of (4.19) has mistakenly been written as $H_{n,\lambda_1,\lambda_2}[1]$ in Eqs. (90), (94), (96), and (97); the factors $\Pi_{j=1}^{R}y_j^{-\lambda_1 q_j}(1-y_j)^{-\lambda_2 q_j}$ are missing and should be paired with $\Pi_{1\leqslant j<k\leqslant R}|y_k-y_j|^{-2q_jq_k}$ throughout; and the term $e^{-(\lambda_1+\lambda_2)[h(0)+h(1)]/4}$ in (96) and (97) should read $e^{-(\lambda_1 h(0)+\lambda_2 h(1))/2}$.]

In preparation for relating this to the average (4.17) let

$$h\left(\frac{1}{2}(1+\cos\theta)\right)=c_0+2\sum_{n=1}^{\infty}c_n\cos n\theta. \tag{4.21}$$

We then have that

$$\frac{1}{\pi}\int_0^1\frac{h(x)}{(x(1-x))^{1/2}}dx=\frac{1}{\pi}\int_0^{\pi}h\left(\frac{1}{2}(1+\cos\theta)\right)d\theta=c_0, \tag{4.22}$$

$$\frac{1}{2}(\lambda_1 h(0)+\lambda_2 h(1))=\frac{1}{2}(\lambda_1+\lambda_2)c_0+\sum_{n=1}^{\infty}c_n(\lambda_1+(-1)^n\lambda_2), \tag{4.23}$$

while (4.21) together with the cosine expansion

$$\log(2|\cos\theta-\cos\phi|)=-\sum_{n=1}^{\infty}\frac{2}{n}\cos n\theta\cos n\phi$$

shows

$$\frac{1}{4\pi^2}\int_0^1 dx\,\frac{h(x)}{(x(1-x))^{1/2}}\int_0^1 dy\,\frac{h'(y)(y(1-y))^{1/2}}{x-y}=\frac{1}{2}\sum_{n=1}^{\infty}nc_n^2. \tag{4.24}$$

Also, as noted in Ref. 9,

$$H_{n,a,b}[1]=\frac{G(n+1+a)G(n+1+b)G(n+1+a+b)}{G(1+a)G(1+b)G(2n+1+a+b)}G(n+2). \tag{4.25}$$

Since[26]

$$\log\frac{G(n+1+a)}{G(n+1+b)}\underset{n\to\infty}{\sim}(b-a)n+\frac{a-b}{2}\log(2\pi)+\left((a-b)n+\frac{a^2-b^2}{2}\right)\log n+o(1) \tag{4.26}$$

we deduce

$$\frac{H_{n,a,b}[1]}{H_{n+Q,a,b}[1]}\sim\frac{2^{4nQ+2Q^2+2Q(a+b)}}{(2\pi n)^Q}. \tag{4.27}$$

Finally we note that under the change of variables

$$x_l = \tfrac{1}{2}(1+\cos\theta_l)$$

the integrand in (4.18) contains as a factor the (un-normalized) eigenvalue probability density function (4.16). Explicitly, with $\tilde{h}(\theta) := h(1/2\,(1+\cos\theta))$ we have

$$\left.\frac{H_{n,\lambda_1,\lambda_2}\left[e^{h(x)}\prod_{r=1}^{R}|y_r-x|^{2q_r}\right]}{H_{n,\lambda_1,\lambda_2}[1]}\right|_{y_r=1/2(1+\cos\phi_r)} = \left\langle \prod_{l=1}^{n} e^{\tilde{h}(\theta_l)}\prod_{r=1}^{R}\left|\frac{1}{2}(\cos\phi_r-\cos\theta_l)\right|^{2q_r}\right\rangle_{C_N(\lambda_1,\lambda_2)}. \tag{4.28}$$

Making use of (4.22)–(4.28) shows that the asymptotic formula (4.19) for the integral (4.18) is equivalent to an asymptotic formula generalizing Theorem 1.

Conjecture 3: Let $\log a(\theta)$ *have the Fourier expansion (1.7), with coefficients satisfying (1.4). We expect that for* $N\to\infty$,

$$\left\langle \prod_{l=1}^{N} a(\theta_l)\prod_{r=1}^{R}|2(\cos\phi_r-\cos\theta_l)|^{2a_r}\right\rangle_{C_N(\lambda_1+1/2,\lambda_2+1/2)} \sim e^{(N+\sum_{r=1}^{R}a_r)c_0}(2N)^{\sum_{r=1}^{R}a_r^2}\tilde{K}, \tag{4.29}$$

where, with E specified by (4.13),

$$\tilde{K}=\prod_{r=1}^{R}\frac{1}{|1+e^{i\phi_r}|^{2(\lambda_1-1)a_r}|1+e^{i\phi_r}|^{2\lambda_2 a_r}}e^{-\sum_{n=1}^{\infty}c_n(\lambda_1-1+(-1)^n\lambda_2)}E. \tag{4.30}$$

We can apply some checks to (4.19). As already remarked, with $(\lambda_1,\lambda_2)=(1,0)$ the probability density function $C_N(\lambda_1,\lambda_2)$ coincides with the eigenvalue probability density function for $\mathrm{O}^-(2N+1)$, and (4.29) must coincide with (4.12), as indeed it does. Also, changing variables $\theta_l\mapsto\pi-\theta_l$ and interchanging λ_1 and λ_2 leaves (4.16) invariant, and thus the average (4.17) invariant if we also set $\phi_r\mapsto\pi-\phi_r$, $a(\theta)\mapsto a(\pi-\theta)$ [and thus $c_n\mapsto(-1)^n c_n$]. Recalling the definition (4.13) of E we see that (4.30) exhibits this symmetry. Another check follows from a factorization identity, relating an average over the unitary group to a product of averages over the orthogonal and symplectic groups.[27,24,28]

Proposition 1: With $g(\theta)=g(-\theta)$ *we have*

$$\left\langle \prod_{l=1}^{2N+1} g(\theta_l)\right\rangle_{\mathrm{U}(2N+1)} = \left\langle \prod_{l=1}^{N+1} g(\theta_l)\right\rangle_{\mathrm{O}^+(2N+2)}\left\langle \prod_{l=1}^{N} g(\theta_l)\right\rangle_{\mathrm{Sp}(N)}. \tag{4.31}$$

With

$$g(\theta)=a(\theta)\prod_{r=1}^{R}(2|\cos\theta-\cos\phi_r|)^{2a_r}$$

in (4.31) we see that the conjectured asymptotic form (4.29) for the right-hand side is consistent with the Fisher–Hartwig formula (1.8).

The identity (4.31) is also of interest for providing an exact formula for the product of the density matrix in Dirichlet boundary conditions and in Neumann boundary conditions. Thus recalling (4.6) we see from (4.31) that

$$\frac{1}{L^2}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}\left\langle \prod_{l=1}^{2N+1}\left|2\left(\cos\frac{\pi x}{L}-\cos\theta_l\right)\right|\left|2\left(\cos\frac{\pi x}{L}-\cos\theta_l\right)\right|\right\rangle_{\mathrm{U}(2N+1)}$$
$$=\rho^N_{N+2}(x,y)\rho^D_{N+1}(x,y).$$

V. IMPENETRABLE BOSONS IN A HARMONIC TRAP AND RANDOM MATRIX AVERAGES OVER THE GUE AND LUE

From a physical viewpoint the most relevant setting for the impenetrable Bose gas is confinement by a harmonic potential (see Refs. 20 and 29 and references therein). Then the ground state wave function ψ_0^H is proportional to

$$\prod_{l=1}^{N} e^{-x_l^2/2}\prod_{1\leqslant j<k\leqslant N}|x_k-x_j|,$$

and $|\psi_0^H|^2$ is identical to the eigenvalue probability density function for the Gaussian unitary ensemble of complex Hermitian matrices. The combination of log-gas arguments and analytic calculation based on the Selberg correlation integral used to analyze (4.18) was used in Ref. 29 to analyze the asymptotic form of

$$e^{-\Sigma_{j=1}^R 2Nq_r y_r^2}\frac{G_{N,\sqrt{2N}}\left[\prod_{r=1}^{R}|x-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}, \tag{5.1}$$

where

$$G_{N,a}[f(x)]:=\int_{-\infty}^{\infty}\mathrm{d}x_1\cdots\int_{-\infty}^{\infty}\mathrm{d}x_N\prod_{l=1}^{N}f(x_l)e^{-a^2x_l^2}\prod_{1\leqslant j<k\leqslant N}|x_k-x_j|^2, \tag{5.2}$$

in the special case $R=2$, $q_1=q_2=1/2$ which specifies the ground state density matrix. As our first point of interest we will generalize this calculation to general R and q_r $(q_r>-1/2)$.

The log-gas perspective[18] suggests the factorization

$$\prod_{1\leqslant j<k\leqslant R}|y_j-y_k|^{2q_jq_k}e^{-\Sigma_{r=1}^R 2Nq_ry_r^2}\frac{G_{N,\sqrt{2N}}\left[\prod_{r=1}^{R}|x-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}$$
$$\underset{N\to\infty}{\sim}\prod_{r=1}^{R}e^{-2Nq_ry_r^2}\frac{G_{N,\sqrt{2N}}[|x-y_r|^{2q_r}]}{G_{N+q_r,\sqrt{2N}}[1]}. \tag{5.3}$$

Next, from the theory of Selberg correlation integrals,[23] for $q_r\in\mathbb{Z}_{\geqslant 0}$ we have the duality formula[30]

$$\frac{G_{N,a}[(x-y_r)^{2q_r}]}{G_{N,a}[1]}=\frac{G_{2q_r,a}[(y_r+ix)^N]}{G_{2q_r,a}[1]}. \tag{5.4}$$

It is a fairly straightforward exercise, detailed in Ref. 30, Sec. 5.3 for a related problem, to use the saddle point method to compute the large N expansion of the integral on the right-hand side of (5.4). One finds

$$e^{-2Nq_rx_r^2}G_{2q_r,\sqrt{2N}}[(y_r+ix)^N]\underset{N\to\infty}{\sim}\binom{2q_r}{q_r}(G_{q_r,1}[1])^2e^{-q_rN}2^{-2q_rN}(4N)^{-q_r^2}(1-y_r^2)^{q_r^2/2}. \tag{5.5}$$

Also, we know (see, e.g., Ref. 3) the exact evaluation

$$G_{n,1}[1]=2^{-n(n-1)/2}\pi^{n/2}G(n+2), \tag{5.6}$$

which together with the asymptotic expansion (4.26) implies

$$\frac{G_{N,\sqrt{2N}}[1]}{G_{N+q,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}\frac{2^{2Nq+q^2-q}}{\pi^q}e^{qN}N^{-q}. \tag{5.7}$$

Combining (5.4)–(5.7) gives the asymptotic formula

$$e^{-2Nq_ry_r^2}\frac{G_{N,\sqrt{2N}}[|x-y_r|^{2q_r}]}{G_{N+q_r,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}\frac{G^2(q_r+1)}{G(2q_r+1)}\frac{2^{2q_r^2-q_r}}{\pi^{q_r}}N^{q_r^2-q_r}(1-y_r^2)^{q_r^2/2} \tag{5.8}$$

which we have proved for $q_r\in\mathbb{Z}_{\geqslant 0}$, and conjecture as being valid for all $q_r>-1/2$. This same result can also be deduced from results in Ref. 31. Substituting this in (5.3) gives the sought asymptotic form of (5.1).

Conjecture 4: Let $q_r>-1/2$, and let $G_{N,a}[f]$ be given by (5.2). We expect

$$e^{-\Sigma_{r=1}^R 2Nq_ry_r^2}\frac{G_{N,\sqrt{2N}}\left[\prod_{r=1}^R|x-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}\prod_{1\leqslant j<k\leqslant R}|y_j-y_k|^{-2q_jq_k}\times\prod_{r=1}^R\frac{G^2(q_r+1)}{G(2q_r+1)}\frac{2^{2q_r^2-q_r}}{\pi^{q_r}}N^{q_r^2-q_r}(1-y_r^2)^{q_r^2/2}. \tag{5.9}$$

An extension of (5.9) can also be formulated. Let $a(x)$ be analytic on $[-1,1]$. Then it has rigorously been proved that[16]

$$\frac{G_{N,\sqrt{2N}}[e^{a(x)}]}{G_{N,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}\exp\left(\frac{2N}{\pi}\int_{-1}^1 a(x)\sqrt{1-x^2}\,dx\right)\times\exp\left(\frac{1}{4\pi^2}\int_{-1}^1 dx\,\frac{a(x)}{(1-x^2)^{1/2}}\int_{-1}^1 dy\,\frac{a'(y)(1-y^2)^{1/2}}{x-y}\right). \tag{5.10}$$

The structure of (4.19) in the case $\lambda_1=\lambda_2=0$ suggests how (5.10) can be combined with (5.9) to generalize the latter.

Conjecture 5: Let $a(x)$ be analytic on $[-1,1]$. It is expected that

$$e^{-\Sigma_{r=1}^R 2Nq_ry_r^2}\frac{G_{N,\sqrt{2N}}\left[e^{a(x)}\prod_{r=1}^R|x-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}(\text{RHS}\,(5.10))|_{N\mapsto N+\Sigma_{r=1}^R q_r}(\text{RHS}\,(5.9))e^{-\Sigma_{r=1}^R q_r a(y_r)}. \tag{5.11}$$

We remark that in the special case $a(x)=kx$, Conjecture 5 can be reduced to Conjecture 4. To see this, use completion of squares to note

$$G_{N,\sqrt{2N}}\left[e^{kx}\prod_{r=1}^R|x-y_r|^{2q_r}\right]=e^{k^2/8}G_{N,\sqrt{2N}}\left[\prod_{r=1}^R\left|x+\frac{k}{2N}-y_r\right|^{2q_r}\right].$$

According to Conjecture 4 we have

$$e^{-\Sigma_{r=1}^R 2Nq_r(y_r-k/4N)^2}\frac{G_{N,\sqrt{2N}}\left[e^{kx}\prod_{r=1}^R|x+\frac{k}{2N}-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}\underset{N\to\infty}{\sim}\text{RHS}\,(5.10)$$

and thus

$$e^{-\Sigma_{r=1}^R 2Nq_r y_r^2}\frac{G_{N,\sqrt{2N}}\left[e^{kx}\prod_{r=1}^R|x-y_r|^{2q_r}\right]}{G_{N+\Sigma_{r=1}^R q_r,\sqrt{2N}}[1]}\sim e^{k^2/8}\,\text{RHS}\,(5.10)\,e^{-\Sigma_{r=1}^R q_r y_r}.$$

Since (4.24) gives

$$\frac{1}{4\pi^2}\int_{-1}^1 dx\,\frac{a(x)}{(1-x^2)^{1/2}}\int_{-1}^1 dy\,\frac{a'(y)(1-y^2)^{1/2}}{x-y}\bigg|_{a(x)=kx}=\frac{k^2}{8}$$

this is in agreement with (5.11).

Let us now turn our attention to a variation of the impenetrable Bose gas in a harmonic well, which also has the features of being related to a random matrix ensemble. In reduced units, the Hamiltonian for the system is

$$H=-\sum_{j=1}^N\frac{\partial^2}{\partial x_j^2}+\sum_{j=1}^N\left(a'(a'-1)\frac{1}{x_j^2}+x_j^2\right),\quad x_j>0. \tag{5.12}$$

Thus in addition to the harmonic well, the particles are restricted to the half line by a repulsive potential (requiring $a'>1$) at the origin proportional to $1/r^2$. This is the noninteracting case of the so-called type B Calogero–Sutherland Hamiltonian,[32] for which the interacting case has $1/r^2$ pair repulsion. The ground state wave function for (5.12) is proportional to

$$\prod_{l=1}^N e^{-x_l^2/2}(x_l^2)^{a'/2}\prod_{1\le j<k\le N}|x_k^2-x_j^2|. \tag{5.13}$$

We recognize the square of the ground state wave function as being identical to the probability density function for the singular values of $n\times N$ complex Gaussian matrices with $a'=n-N+1/2$ (see, e.g., Ref. 3, Chap. 2). Changing variables $x_l^2\mapsto x_l$ this is refered to as the Laguerre unitary ensemble. The problem of computing the asymptotic form of the density matrix for this system suggests analyzing the asymptotic form of the more general quantity

$$\prod_{r=1}^R y_r^{2a'q_r}e^{-4Nq_ry_r^2}\frac{L_N\left[\prod_{r=1}^R|x^2-y_r^2|^{2q_r}\right]}{L_{N+\Sigma_{r=1}^R q_r}[1]}, \tag{5.14}$$

where

$$L_N[f]:=\int_0^\infty dx_1\cdots\int_0^\infty dx_N\prod_{l=1}^N f(x_l)x_l^{2a'}e^{-4Nx_l^2}\prod_{1\le j<k\le N}|x_k^2-x_j^2|^2, \tag{5.15}$$

in analogy with (5.1).

From a log-gas perspective, the integrand in (5.15) corresponds to a one-component system interacting on the half-line $x>0$, subject to a one-body confining potential $2Nx^2-(a'-1/2)\log x$. In addition to the electrostatic energy $-\log|x-x'|$ at the point x due to the interaction with a charge at x', there is also a term $-\log|x+x'|$ due to the interaction with an image charge at $-x'$ (outside the system, since $x'>0$). In keeping with the image charge interpretation, for each charge at x one requires a term $-\frac{1}{2}\log|2x|$ to account for the interaction between a charge and its own image (the factor of 1/2 is because this energy is shared between the charge and its image, the latter being outside the system). From this viewpoint we can interpret

$$\prod_{1\leqslant j<k\leqslant R}|y_k^2-y_j^2|^{2q_jq_k}\prod_{r=1}^{R}(2y_r)^{q_r^2}e^{-q_r4Ny_r^2}|y_r|^{(2a'-1)q_r}\frac{L_N\Big[\prod_{r=1}^{R}|x^2-y_r^2|^{2q_r}\Big]}{2^{\sum_{r=1}^{R}q_r}L_{N+\sum_{r=1}^{R}q_r}[1]}$$

as a ratio of partition functions for log-gas systems, and analogous to (5.3) we expect the factorization into

$$\prod_{r=1}^{R}(2y_j)^{q_j^2}e^{-q_r4Ny_r^2}|y_r|^{(2a'-1)q_r}\frac{L_N[|x^2-y_r^2|^{2q_r}]}{2^{q_r}L_{N+q_r}[1]} \tag{5.16}$$

for $N\to\infty$.

To analyze (5.16) in the limit $N\to\infty$ we make the change of variables $x_l^2\mapsto x_l$ and introduce

$$\widetilde{L}_{N,c}[f]:=\int_0^\infty dx_1\cdots\int_0^\infty dx_N\prod_{l=1}^{N}f(x_l)x_l^{a'-1/2}e^{-cx_l}\prod_{1\leqslant j<k\leqslant N}(x_k-x_j)^2 \tag{5.17}$$

so that it reads

$$\prod_{r=1}^{R}(2y_r)^{q_r^2}e^{-q_r4Ny_r^2}y_r^{(2a'-1)q_r}\frac{\widetilde{L}_{N,4N}[|x-y_r^2|^{2q_r}]}{\widetilde{L}_{N+q_r,4N}[1]}. \tag{5.18}$$

To proceed further, we use the fact that for $q\in\mathbb{Z}_{\geqslant 0}$ we have the duality formula[33]

$$\frac{\widetilde{L}_{N,c}[|x-t|^{2q}]}{\widetilde{L}_{N,c}[1]|_{a\mapsto a+2q}}=\frac{1}{M_{2q}(a,N)}\int_{-1/2}^{1/2}dx_1\cdots\int_{-1/2}^{1/2}dx_{2q}\prod_{l=1}^{2q}e^{\pi ix_l(a-N)}$$

$$\times|1+e^{2\pi ix_l}|^{a+N}e^{-cte^{2\pi ix_l}}\prod_{1\leqslant j<k\leqslant 2q}|e^{2\pi ix_k}-e^{2\pi ix_j}|^2, \tag{5.19}$$

where on the right-hand side $a=a'-1/2$ and

$$M_n(a,b):=\int_{-1/2}^{1/2}dx_1\cdots\int_{-1/2}^{1/2}dx_n\prod_{l=1}^{n}e^{\pi ix_l(a-b)}|1+e^{2\pi ix_l}|^{a+b}\prod_{1\leqslant j<k\leqslant n}|e^{2\pi ix_k}-e^{2\pi ix_j}|^2$$

$$=\frac{G(n+1+a+b)}{G(1+a+b)}\frac{G(1+a)}{G(n+1+a)}\frac{G(1+b)}{G(n+1+b)}G(n+2) \tag{5.20}$$

(for the last equality see, e.g., Ref. 3). If we suppose temporarily that $a\in Z_{\geqslant 0}$, the right-hand side of (5.19) with $c=4N$ can be written as the contour integral

$$\frac{1}{M_{2q}(a,-N)}\int_{\mathcal{C}}\frac{dz_1}{2\pi iz_1}\cdots\int_{\mathcal{C}}\frac{dz_{2q}}{2\pi iz_{2q}}\prod_{l=1}^{2q}(1+z_l)^a(1+1/z_l)^Ne^{-4Ntz_l}\prod_{1\leqslant j<k\leqslant 2q}(z_k-z_j)(1/z_k-1/z_j), \tag{5.21}$$

where $\mathcal{C}$ is any simple closed contour which encircles the origin. To analyze this for $N\to\infty$, following Ref. 33 where the case $q=1$ was considered, we note the N-dependent terms in the integrand have a stationary point when

$$z=z_\pm:=-\tfrac{1}{2}\pm i\tfrac{1}{2}(1/t-1)^{1/2}. \tag{5.22}$$

By deforming the contour $\mathcal{C}$ to pass through z_+ for q of the integrations, and to pass through z_- for the remaining q integrations, we readily deduce from the representation (5.21) of (5.19) that

$$
\begin{aligned}
&e^{-q_r 4Ny_r^2} y_r^{(2a'-1)q_r} (2y_r)^{q_r^2} \widetilde{L}_{N,4N}[|x-y_r^2|^{2q_r}] \\
&\quad = \frac{\widetilde{L}_{N,4N}[1]|_{a'\mapsto a'+2q_r}}{M_{2q_r}(a'-1/2,N)} e^{-q_r 4Ny_r^2} y_r^{(2a'-1)q_r} (2y_r)^{q_r^2} \binom{2q_r}{q_r} e^{-4Ny_r^2 q_r(z_+ + z_-) + Nq_r \log|1+1/z_+|^2} \\
&\qquad \times \frac{1}{|z_+|^{4q_r^2}} |z_+ - z_-|^{2q_r^2} |1+z_+|^{q_r(2a'-1)} \left(\frac{1}{2\pi}\right)^{2q_r} \\
&\qquad \times \left| \frac{N}{2} \left(\frac{1}{z_+^2} - \frac{1}{(1+z_+)^2} \right) \right|^{-q_r^2} (G_{q_r}[1])^2.
\end{aligned} \tag{5.23}
$$

Now, with $t = y_r^2$ in (5.22)

$$
\begin{gathered}
z_+ + z_- = -1, \quad \left| 1 + \frac{1}{z_+} \right|^2 = 1, \quad |z_+ - z_-|^2 = \left(\frac{1}{y_r^2} - 1 \right), \\
|1+z_+|^2 = |z_+|^2 = \frac{1}{4y_r^2}, \quad \left| \frac{1}{z_+^2} - \frac{1}{(1+z_+)^2} \right| = 16 y_r^4 \left(\frac{1}{y_r^2} - 1 \right)^{1/2},
\end{gathered} \tag{5.24}
$$

so the right-hand side of (5.23) simplifies to

$$
\frac{\widetilde{L}_{N,4N}[1]|_{a'\mapsto a'+2q_r}}{M_{2q_r}(a'-1/2,N)} N^{-q_r^2} \left(\frac{1}{2\pi} \right)^{2q_r} \binom{2q_r}{q_r} 2^{2q_r^2} 2^{-q_r(2a'-1)} (G_{q_r}[1])^2 (1-y_r^2)^{q_r^2/2}. \tag{5.25}
$$

Furthermore we know (see, e.g., Ref. 3)

$$
\widetilde{L}_{N,c}[1] = c^{-N^2 - N(a'-1/2)} \frac{G(N+2)G(a'+N+1/2)}{G(a'+1/2)}, \tag{5.26}
$$

and making use of (5.22) it follows from the asymptotic expansion (4.26) that

$$
\frac{\widetilde{L}_{N,4N}[1]|_{a'\mapsto a'+2q_r}}{\widetilde{L}_{N+q_r,4N}[1] M_{2q_r}(a'-1/2,N)} N^{-q_r^2} \sim 2^{2(q_r^2 + q_r(a'-1/2))} N^{q_r^2 - q_r}. \tag{5.27}
$$

Substituting (5.27) in (5.25), evaluating $G_{q_r}[1]$ therein according to (5.6) and simplifying we obtain the $N \to \infty$ expansion

$$
e^{-q_r 4Ny_r^2} y_r^{(2a'-1)q_r} (2y_r)^{q_r^2} \frac{L_N[|x^2-y_r^2|^{2q_r}]}{2^{q_r} L_{N+q_r}[1]} \sim \frac{G^2(q_r+1)}{G(2q_r+1)} \frac{2^{3q_r^2 - q_r}}{\pi^{q_r}} N^{q_r^2 - q_r} (1-y_r^2)^{q_r^2/2}, \tag{5.28}
$$

proved for $q_r \in \mathbb{Z}_{\geqslant 0}$ and expected to be true for all $q_r > -1/2$. Substituting this in (5.16) gives, as a conjecture, the sought asymptotic form of (5.14).

Conjecture 6: For $N \to \infty$, and assuming $q_r > -1/2$ for each $r = 1, \ldots, R$,

$$\prod_{r=1}^{R} y_r^{2a'q_r} e^{-4Nq_r y_r^2} \frac{L_N\left[\prod_{r=1}^{R} |x^2-y_r^2|^{2q_r}\right]}{L_{N+\Sigma_{r=1}^{R} q_r}[1]} \sim \prod_{1\leqslant j<k\leqslant R} |y_k^2-y_j^2|^{-2q_jq_k} \times \prod_{r=1}^{R} \frac{G^2(q_r+1)}{G(2q_r+1)} \frac{2^{2q_r^2}}{\pi^{q_r}} N^{q_r^2-q_r} y_r^{-q_r^2+q_r} (1-y_r^2)^{q_r^2/2}. \tag{5.29}$$

It is of interest to extend (5.29) in an analogous way to how (5.11) extends (5.9). First we use (4.19) with $q_r=0$, and (5.10) to conjecture that for $a(x)$ analytic on [0,1],

$$\frac{L_N[e^{a(x)}]}{L_N[1]} \sim \exp\left(\frac{4(N+(2a'-1)/4)}{\pi} \int_0^1 a(x)\sqrt{1-x^2}\,dx\right) \times \exp\left(\frac{1}{\pi^2}\int_0^1 dx \frac{a(x)}{(1-x^2)^{1/2}} \int_0^1 dy \frac{ya'(y)(1-y^2)^{1/2}}{x^2-y^2}\right) e^{-a'a(0)/2}. \tag{5.30}$$

Combining this with (5.29) as in (5.11) gives us the LUE analogue of Conjecture 5.

Conjecture 7: Let $a(x)$ be analytic on [0,1]. *It is expected that*

$$\prod_{r=1}^{R} y_r^{2a'q_r} e^{-4Nq_r y_r^2} \frac{L_N\left[e^{a(x)}\prod_{r=1}^{R} |x^2-y_r^2|^{2q_r}\right]}{L_{N+\Sigma_{r=1}^{R} q_r}[1]} \underset{N\to\infty}{\sim} (\text{RHS}\,(5.30))\big|_{N\to N+\Sigma_{r=1}^{R} q_r} \times (\text{RHS}\,(5.29)) e^{-\Sigma_{r=1}^{R} q_r a(y_r)}. \tag{5.31}$$

We can check the consistency of (5.11) and (5.31). For this we make use of a factorization identity analogous to Proposition 1.[28]

Proposition 2: Let $g(\theta)=g(-\theta)$. We have

$$\frac{G_{2N,a}[g(x)]}{G_{2N,a}[1]} = \frac{L_{N,a}^{(0)}[g(x)]}{L_{N,a}^{(0)}[1]} \frac{L_{N,a}^{(2)}[g(x)]}{L_{N,a}^{(2)}[1]}, \tag{5.32}$$

where

$$L_{N,a}^{(p)}[g(x)] := \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \prod_{l=1}^{N} g(x_l)|x_l|^p e^{-a^2x_l^2} \prod_{1\leqslant j<k\leqslant N} (x_k^2-x_j^2)^2.$$

Let $a(x)$ be even and choose

$$a=\sqrt{4N}, \quad g(x)=e^{a(x)}\prod_{r=1}^{R} |x^2-y_r^2|^{2q_r}.$$

According to Conjecture 5,

$$e^{-2a^2\Sigma_{r=1}^{R} q_r y_r^2} \frac{G_{2N,a}[g(x)]}{G_{2(N+\Sigma_{r=1}^{R} q_r),a}[1]} \underset{N\to\infty}{\sim} \exp\left(\frac{4}{\pi}\left(2N+2\sum_{r=1}^{R} q_r\right)\int_0^1 a(x)\sqrt{1-x^2}\,dx\right) \times \exp\left(\frac{1}{\pi^2}\int_0^1 dx \frac{a(x)}{(1-x^2)^{1/2}} \int_0^1 dy \frac{ya'(y)(1-y^2)^{1/2}}{x^2-y^2}\right) \times \prod_{1\leqslant j<k\leqslant R} |y_j^2-y_k^2|^{-4q_jq_k} \prod_{r=1}^{R} (1-y_r^2)^{q_r^2} |2y_r|^{-2q_r^2} \times \left(\prod_{r=1}^{R} \frac{G^2(q_r+1)}{G(2q_r+1)} \frac{2^{2q_r^2-q_r}}{\pi^{q_r}} (2N)^{q_r^2-q_r}\right)^2 e^{-2\Sigma_{r=1}^{R} q_r a(y_r)}. \tag{5.33}$$

For the right-hand side of (5.32) as implied by Conjecture 7 to be consistent with this we require

$$2^{4\Sigma_{r=1}^{R}q_r}\frac{G_{2N,\sqrt{4N}}[1]}{L_N[1]|_{a'=0}L_N[1]|_{a'=1}}\sim\frac{G_{2(N+\Sigma_{r=1}^{R}q_r),\sqrt{4N}}[1]}{L_{N+\Sigma_{r=1}^{R}q_r}[1]|_{a'=0}L_{N+\Sigma_{r=1}^{R}q_r}[1]|_{a'=1}}. \tag{5.34}$$

But the method of derivation of (5.32) given in Ref. 28 shows that for general n,

$$\frac{G_{2n,\sqrt{4n}}[1]}{L_n|_{a'=0}L_n|_{a'=1}}=2^{2n}\frac{(2n)!}{(n!)^2}\sim\frac{2^{4n}}{(\pi n)^{1/2}},$$

verifying (5.34).

Let us now apply Conjecture 7 to the calculation of the density matrix $\rho_{N+1}^{L}(x,y)$ for the state (5.13) with $N+1$ particles,

$$\rho_{N+1}^{L}(x,y):=\frac{N+1}{C_{N+1}}e^{-x^2/2-y^2/2}(xy)^{a'}\int_0^\infty dx_1\cdots\int_0^\infty dx_N\prod_{l=1}^{N}x_l^{2a'}e^{-x_l^2}|x^2-x_l^2||y^2-y_l^2|$$

$$\times\prod_{1\leqslant j<k\leqslant N}(x_k^2-x_j^2)^2, \tag{5.35}$$

where

$$C_{N+1}:=\int_0^\infty dx_1\cdots\int_0^\infty dx_{N+1}\prod_{l=1}^{N+1}x_l^{2a'}e^{-x_l^2}\prod_{1\leqslant j<k\leqslant N+1}(x_k^2-x_j^2)^2.$$

In terms of the average (5.15) we thus have

$$2\sqrt{N}\rho_{N+1}^{L}(2\sqrt{N}X,2\sqrt{N}Y)=(N+1)e^{-2NX^2-2NY^2}(XY)^{a'}\frac{L_N\left[\prod_{l=1}^{N}|x^2-X^2||x^2-Y^2|\right]}{L_{N+1}[1]}.$$

On the right-hand side we can apply Conjecture 7 with $R=2$, $q_1=q_2=1/2$ and so obtain the asymptotic form

$$2\sqrt{N}\rho_{N+1}^{L}(2\sqrt{N}X,2\sqrt{N}Y)\sim 2\sqrt{N}\,\frac{G^4(3/2)}{\pi}\,\frac{(XY)^{1/4}}{|X^2-Y^2|^{1/2}}(1-X^2)^{1/8}(1-Y^2)^{1/8}. \tag{5.36}$$

The asymptotic form (5.36) can in turn be used to specify the occupations λ_j of the low-lying effective single particle states ϕ_j, which by definition satisfy the eigenvalue equation

$$\int\rho_N(x,y)\,\phi_j(y)\,dy=\lambda_j\phi_j(x). \tag{5.37}$$

Thus, with $x=2\sqrt{N}X$, $y=2\sqrt{N}Y$ and j fixed, introducing the scaled effective single particle states[34,20]

$$(4N)^{1/2}\phi_j(x)\mapsto\varphi_j(X),$$

substituting (5.38) and using the fact that $\rho_N^L(x,y)$ is supported on $x,y\in[0,2\sqrt{N}]$ we obtain the explicit integral equation

$$2\int_0^1\frac{X^{1/4}(1-X^2)^{1/8}\varphi_j(X)}{|X^2-Y^2|^{1/2}}\,dX=\overline{\lambda}_j\frac{\varphi_j(Y)}{Y^{1/4}(1-Y^2)^{1/8}}, \tag{5.38}$$

where

$$\lambda_j = \sqrt{N}\frac{G^4(3/2)}{\pi}\overline{\lambda}_j . \tag{5.39}$$

We see immediately that the occupations of the low-lying effective single particle states are proportional to $\sqrt{N}$, as has been found for the impenetrable Bose gas in periodic boundary conditions,[19,20] in a harmonic trap[34,29] and in Dirichlet and Neumann boundary conditions.[9] An appropriate analysis similar to that undertaken in Ref. 29, Appendix B gives the same upper bound on $\overline{\lambda}_0$ as found for the same quantity in the case of the harmonic trap,[29] but a detailed analysis of (5.38) remains.

VI. CONCLUDING REMARKS

A. Universal form for Hankel asymptotics

Analogous to (3.1), Hankel determinants are related to log-gas partition functions according to the formula

$$\begin{aligned}\det[a_{j+k}]_{j,k=0,\dots,n-1} &= \frac{1}{n!}\int_{-\infty}^{\infty} dx_1\, e^{-nV(x_1)}\cdots\int_{-\infty}^{\infty} dx_n\, e^{-nV(x_n)}\prod_{l=1}^{n} a(x_l)\prod_{1\le j<k\le n}(x_k-x_j)^2 \\ &=: A_n(e^{-nV(x)})[a(x)],\end{aligned} \tag{6.1}$$

where

$$a_p = \int_{-\infty}^{\infty} a(x)x^p e^{-nV(x)}\,dx.$$

For $V(x)$ an even degree polynomial independent of n with positive leading coefficient and no real zeros, it was proved by Johansson[16] that

$$\begin{aligned}\frac{A_n(e^{-nV(x)})[e^{a(x)}]}{A_n(e^{-nV(x)})[1]} &\underset{n\to\infty}{\sim} \exp\left(n\int_{c_1}^{c_2} a(x)\rho(x)\,dx\right) \\ &\quad\times\exp\left(\frac{1}{4\pi^2}\int_{c_1}^{c_2} dx\,\frac{a(x)}{\sqrt{(x-c_1)(c_2-x)}}\int_{c_1}^{c_2} dy\,\frac{a'(y)\sqrt{(y-c_1)(c_2-y)}}{x-y}\right).\end{aligned} \tag{6.2}$$

Here $\rho(x)$ is the scaled density in the log-gas system corresponding to $A_n(e^{-nV(x)})[1]$, supported on $[c_1,c_2]$ and normalized so that

$$\int_{c_1}^{c_2}\rho(x)\,dx = 1.$$

The asymptotic formula (5.10) corresponds to the special case $V(x)=\frac{1}{2}x^2$, $\rho(x)=(2/\pi)\sqrt{1-x^2}$ of (6.2). To extend Conjecture 5 to more general V this suggests we simply write the latter in terms of $\rho(x)$.

Conjecture 8: Under the conditions of the validity of (6.2) we expect

$$e^{-n\Sigma_{r=1}^{R} q_r V(y_r)} \frac{A_n(e^{-nV(x)})\left[e^{a(x)} \prod_{j=1}^{r} |x-y_j|^{q_j} \right]}{A_{n+\Sigma_{j=1}^{R} q_j}(e^{-nV(x)})[e^{a(x)}]}$$

$$\underset{n\to\infty}{\sim} e^{-\Sigma_{r=1}^{R} q_r a(y_r)} \prod_{1\leqslant j<k\leqslant R} |y_k-y_j|^{-2q_jq_k} \times \prod_{r=1}^{R} \frac{G^2(q_r+1)}{G(2q_r+1)} (2\pi n)^{q_r^2-q_r} (\rho(y_r))^{q_r^2}. \tag{6.3}$$

We remark that in the case $R=1$, $e^{a(x)}=1$, this conjecture (together with some corroborative analysis) was formulated earlier by Brézin and Hikami[31] (see also Ref. 35).

Conjecture 7 can similarly be extended, although we work with the quantity (5.17) in favor of (5.15) so as to have a Hankel determinant interpretation according to (6.1). In the log-gas system corresponding to (5.17) one has $\rho(x)=(2/\pi x^{1/2})(1-x)^{1/2}$. Recalling the equality between (5.16) and (5.18), and writing $y_r^2 \mapsto y_r$, $a(x^{1/2}) \mapsto a(x)$ we see that Conjecture 7 can be rewritten to imply

$$\prod_{r=1}^{R} y_r^{(a'-1/2)q_r} e^{-4Nq_ry_r} \frac{\widetilde{L}_{N,4N}\left[e^{a(x)} \prod_{r=1}^{R} |x-y_r|^{2q_r} \right]}{\widetilde{L}_{N+\Sigma_{r=1}^{R} q_r,4N}[e^{a(x)}]}$$

$$\underset{N\to\infty}{\sim} e^{-\Sigma_{r=1}^{R} q_r a(y_r)} \prod_{1\leqslant j<k\leqslant R} |y_k-y_j|^{-2q_jq_k} \times \prod_{r=1}^{R} \frac{G^2(q_r+1)}{G(2q_r+1)} (2\pi N)^{q_r^2-q_r} (\rho(y_r))^{q_r^2}, \tag{6.4}$$

thus assuming the universal form (6.3) and suggesting the following analogue of (6.2) and Conjecture 8.

Conjecture 9: Let $V(x)$ be a polynomial independent of n, with positive leading coefficient and no real zeros on $[0,\infty)$. Let

$$\widetilde{A}_n(x^\alpha e^{-nV(x)})[a(x)] := \frac{1}{n!} \int_0^\infty dx_1\, x_1^\alpha e^{-nV(x_1)} \cdots \int_0^\infty dx_n\, x_n^\alpha e^{-nV(x_n)} \prod_{l=1}^{n} a(x_l) \prod_{1\leqslant j<k\leqslant n} (x_k-x_j)^2. \tag{6.5}$$

Analogous to (6.2) we expect that

$$\frac{\widetilde{A}_n(x^\alpha e^{-nV(x)})[e^{a(x)}]}{\widetilde{A}_n(x^\alpha e^{-nV(x)})[1]} \underset{n\to\infty}{\sim} \exp\left(n \int_0^{c_2} a(x)\rho(x)\, dx \right) \times \exp\left(\frac{1}{4\pi^2} \int_0^{c_2} dx \frac{a(x)}{\sqrt{x(c_2-x)}} \int_{c_1}^{c_2} dy \frac{a'(y)\sqrt{y(c_2-y)}}{x-y} \right), \tag{6.6}$$

where $\rho(x)$ is the scaled density in the log-gas corresponding to $\widetilde{A}_n(x^\alpha e^{-nV(x)})[1]$, with support on $[0,c_2]$. Furthermore, with the same meaning of $\rho(x)$, we expect

$$\prod_{r=1}^{R} y_r^\alpha e^{-nq_rV(y_r)} \frac{\widetilde{A}_n(x^\alpha e^{-nV(x)})\left[e^{a(x)} \prod_{j=1}^{r} |x-y_j|^{q_j} \right]}{\widetilde{A}_{n+\Sigma_{j=1}^{R} q_j}(x^\alpha e^{-nV(x)})[e^{a(x)}]} \underset{n\to\infty}{\sim} \text{RHS}\,(6.3). \tag{6.7}$$

As a final comment on this point, we note that the universal form given by the right-hand side of (6.3) is also exhibited by the Fisher–Hartwig formula (1.8). Thus, with $z_r := e^{i\theta_r}$ we see that

$$\frac{D_n\left[e^{a(\theta)}\prod_{r=1}^{R}|e^{i\theta}-z_r|\right]}{D_{n+\Sigma_{j=1}^{R}}[e^{a(\theta)}]} \underset{n\to\infty}{\sim} \mathrm{RHS}\,(6.3)\big|_{\substack{y_r=z_r\\ \rho(y)=N/2\pi}}.$$

B. Further Toeplitz and Hankel structures

The identity (4.9) of Lemma 1 has counterparts for averages over $\mathrm{Sp}(N)$ and $\mathrm{O}^+(2N)$.[24]

Lemma 2: Suppose $g(\theta)=g(-\theta)$, set $g_j=(1/2\pi)\int_{-\pi}^{\pi} g(\theta)e^{-ij\theta}\,d\theta$, and let $C_N(\lambda_1,\lambda_2)$ refer to the normalized form of (4.16). We have

$$\begin{aligned}\det[a_{j-k}+a_{j+k}]_{j,k=0,\dots,N-1} &= \left\langle \prod_{j=1}^{N} g(\theta_j)\right\rangle_{\mathrm{O}^+(2N)} = \left\langle \prod_{j=1}^{N} g(\theta_j)\right\rangle_{C_N(0,0)},\\ \det[a_{j-k}-a_{j+k+2}]_{j,k=0,\dots,N-1} &= \left\langle \prod_{j=1}^{N} g(\theta_j)\right\rangle_{\mathrm{Sp}(N)} = \left\langle \prod_{j=1}^{N} g(\theta_j)\right\rangle_{C_N(1,1)}.\end{aligned} \tag{6.8}$$

Choosing $g(\theta)$ as in (4.11), Conjecture 3 gives the asymptotic behavior of the right-hand sides in (6.8), and thus the conjectured form of these Toeplitz and Hankel structures.

C. Fluctuation formula perspective and future directions

Let $p := p(x_1,\dots,x_N)$ be an N-dimensional probability density function. The stochastic quantity $A=\Sigma_{j=1}^{N} a(x_j)$, with the $\{x_j\}$ sampled from p, is referred to as a linear statistic. Its distribution $P_A(t)$ is defined by

$$P_A(t)=\left\langle \delta\left(t-\sum_{j=1}^{N} a(x_j)\right)\right\rangle_p, \tag{6.9}$$

and taking the Fourier transform of this gives

$$\tilde{P}_A(k)=\left\langle \prod_{j=1}^{N} e^{ika(x_j)}\right\rangle_p. \tag{6.10}$$

The structure of the average (6.10) is common to the averages studied in this paper. As an illustration of the content of the asymptotic formulas from this viewpoint, consider Johansson's result (3.7). Written in terms of the average (3.1) with $g(\theta)=e^{ika(\theta)}$, it reads

$$D_n^{(\beta)}[e^{ika(\theta)}] \underset{n\to\infty}{\sim} e^{ikc_0 n}e^{-(2/\beta)k^2\Sigma_{n=1}^{\infty} nc_n c_{-n}}, \tag{6.11}$$

where $\{c_n\}_{n=0,\pm1,\dots}$ are the Fourier coefficients in the expansion of $a(\theta)$,

$$a(\theta)=\sum_{n=-\infty}^{\infty} c_n e^{in\theta}. \tag{6.12}$$

A key feature of the exponents in the exponentials on the right-hand side of (6.11) is that they form a quadratic polynomial in k. Thus substituting this in (6.9) and taking the inverse transform gives the Gaussian distribution

$$P_A(t) \underset{n\to\infty}{\sim} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-(t-\mu)^2/2\sigma^2} \tag{6.13}$$

with

$$\mu = nc_0, \quad \sigma^2 = \frac{4}{\beta} \sum_{p=1}^{\infty} p c_p c_{-p}. \tag{6.14}$$

As noted by Johansson,[5] in the case $\beta = 2$ this gives a Gaussian fluctuation formula interpetation of Szegö's theorem. A peculiar feature is that although the mean is proportional to n, the variance is O(1), so fluctuations are strongly suppressed. It is formulas of the type (6.13), (6.14) which led to the successful theoretical explanation of the phenomenon of universal conductance fluctuations in mesoscopic wires (see, e.g., Ref. 36), in which the conductance—an order N quantity—is written as a linear statistic of certain eigenvalues and is shown to have O(1) fluctuations with variance given by an analytic formula of the type (6.14).

All our generalizations of the Fisher–Hartwig formula involve a term of the form $e^{Q^2 \log n}$ as the first correction to the leading order behavior $e^{c_0 n}$. However again when written as an average of the type (6.10) the exponential of a quadratic in k again results. Consider for example (3.13). With $\{c_n\}$ specified by (6.12) we have

$$\langle e^{ika(\theta) + ik\beta \Sigma_{j=1}^R q_j \log|e^{i\theta} - e^{i\phi_j}|} \rangle_{C\beta E_n} \underset{n\to\infty}{\sim} e^{ikc_0 n} e^{-k^2(\beta/2)(\Sigma_{j=1}^R q_j^2)\log n}$$

and thus, as first noted in Ref. 37, with

$$A = \sum_{l=1}^{N} \left(a(\theta_l) + \beta \sum_{j=1}^{R} q_j \log|e^{i\theta_l} - e^{i\phi_j}| \right)$$

the asymptotic form of the corresponding distribution is given by the Gaussian (6.13) with

$$\mu = nc_0, \quad \sigma^2 = \beta \left(\sum_{j=1}^{R} q_j^2 \right) \log n.$$

Thus the variance diverges logarithmically. This class of Gaussian fluctuation theorem has found use in the application of random matrix theory to the study of the statistical properties of the zeros of the Riemann zeta function.[38,39] The study of the statistical properties of the zeros of families of L-functions requires averages over the different classical groups.[40–43] We might anticipate that our new results of Sec. IV will find application in this topic.

Of course it remains to prove the conjectures of this paper. Of these, Conjecture 2 is the most general, as it involves Fisher–Hartwig-type parameters $\{q_j\}$, $\{b_j\}$ as well as the log-gas type parameter β. It is also of interest to extend Conjectures 3, 8, and 9 to this level of generality. Another direction of generality is to extend the domain of integration from a circle or line to a two-dimensional region.[44,45]

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Adiabatic approximation of the Schrödinger–Poisson system with a partial confinement: The stationary case

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Asymptotic quantum transport models of a two-dimensional gas are presented. The models are the stationary versions of those introduced in a previous paper by Ben Abdallah, Méhats, Pinaud. The starting point is a singular perturbation of the three-dimensional stationary Schrödinger–Poisson system posed on bounded domain. The electron injection in the device is modeled thanks to open boundary conditions. Under a small density assumption, the asymptotics lead to a full two-dimensional first-order approximation of the initial model. An intermediate model, called the ''2.5D adiabatic model'' in Ben Abdallah, Méhats, Pinaud is then introduced. It shares the same structure as the limit but is shown to be a second-order approximation of the three-dimensional model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1688432]

I. INTRODUCTION

The paper presents the stationary versions of the models previously analyzed in Ref. 11. These models, first introduced in Refs. 32 and 33 in a formal approach, were originally implemented in a stationary framework and with open boundary conditions. The objective of the paper is, as for Ref. 11, to prove rigorously the asymptotics derived in Refs. 32 and 33. Before going into the details, we recall the motivations of the introduction of open boundary conditions and confined systems.

In nanoscale semiconductor, the electronic transport can be described in various ways. Very often, like in resonant tunneling diodes,[15,22,29,31] the electrons are injected, through a wave guide or quantum wire, into an active device where all the important physical effects take place. Consequently, due to the ultrashort scale, a quantum description is needed into the device while in the leads, two situations are possible: the transport can be considered either as classical or as quantum. Then, the different descriptions have to be connected at the interface lead-active region. A quantum–quantum case was first treated in Ref. 26 thanks to the introduction of suitable boundary conditions and was analyzed in Ref. 6 while a classical–quantum one was studied in Ref. 5. Some other examples of such coupling can be found in Refs. 7, 8, 12, and 18.

Besides, the operation of many quantum devices relies on the formation of a bidimensional electron gas. Such a system is obtained by confining the electrons in one direction and allowing for transport in the two other directions, the confining appearing at some junctions between different layers. The reduced extension of the electron gas results, at low temperature, in an increase of the mobility and therefore to a ballistic transport.[2,25,30] Again, at this level, several strategies can be used: the transport along the nonconfined directions can be considered either as classical or as quantum. The classical–quantum description give rises to the theory of sub-bands which is widely used in the semiconductor physics literature.[2,3,17,38] Such a model has been rigourously derived in Ref. 9 and analyzed in Ref. 10.

The situation described in the paper is a fully quantum model: a heterostructure coupled to electrons reservoirs through wave guides is considered. The electrons behavior is assumed to be

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quantum both in the device and in the leads and the electrons gas is assumed to be confined in a particular direction. The initial model is a three-dimensional Schrödinger–Poisson system, where the electrons are described by a mixed state,

$$-\Delta \Psi_\lambda^\varepsilon + \frac{1}{\varepsilon^2} V_c\left(\frac{z}{\varepsilon}\right)\Psi_\lambda^\varepsilon + V^\varepsilon \Psi_\lambda^\varepsilon = E^\varepsilon \Psi_\lambda^\varepsilon, \tag{1.1}$$

$$-\Delta V^\varepsilon = n^\varepsilon, \tag{1.2}$$

$$n^\varepsilon = \int_\Lambda |\Psi_\lambda^\varepsilon|^2 \, \mathrm{d}\mu(\lambda) + \text{boundary conditions}, \tag{1.3}$$

where μ represents the statistics of the injected electrons and λ is a set of quantum numbers with values in Λ, and ε can be seen as the ratio between the kinetic and the confining energies of the electrons, see Ref. 11 for more details on the scaling. The external potential $(1/\varepsilon^2)\, V_c(z/\varepsilon)$ is a confining potential and the potential V^ε is the self-consistent potential due to space charge effects and is expected to be slowly varying in the z direction. Due to the strong confinement, the wave functions concentrate around the plane $\{z=0\}$ and the transport effects are almost two dimensional. In Ref. 11, in a time-dependent and whole space picture, the limit $\varepsilon \to 0$ was performed. The electronic density $n^\varepsilon(t,x,z)$ concentrates into a surface density $n_s(t,x)\,\delta(z)$ and the limit model was called *2D surface density model*. This model involves bidimensional Schrödinger equations, coupled to a bidimensional equation for the potential. An intermediate model, called the *2.5D adiabatic model*, first introduced in Refs. 32 and 33, was also derived and was shown to be a second order approximation of the initial model. This model couples 2D Schrödinger equations and a 3D equation for the potential. It has been shown numerically in Refs. 32 and 33, that the 2.5D model gives results in a very good agreement with those of the 3D model with a much lower computational cost. In this paper, we will develop a similar strategy to justify the asymptotics in the stationary framework. The differences in the analysis come from the boundedness of the transport domain and the stationary character of the problem. This requires to derive new estimates for the Poisson equation and to take particular care of the existence and uniqueness theory of the nonlinear stationary problem. More precisely, the results are proven under three main hypothesis: the first one states that the electrons are injected into the device on the ground state and is necessary in order to obtain ε-independent estimates. The two others hypothesis are directly related to uniqueness result concerning the solutions of the open Schrödinger–Poisson system stated in Ref. 6. In order to have uniqueness, one requires a weak coupling between the Schrödinger and the Poisson equations and also requires a statistics of injection avoiding the bound states of the device.

Within the time-dependent picture, quantum confining on very general surfaces have been previously investigated in Refs. 16, 23, and 28 for the linear Schrödinger equation. As pointed out in Ref. 37, the quantum constrained system can be related to the Born–Oppenheimer theory for molecular dynamics.[24,35] Even if these theories are mainly developed in a time-dependent and linear framework, they share similar properties with the problem presented in this paper. In the different cases, the electron dynamics is located on the eigenspaces of the confining (or transverse) Hamiltonian and is governed by an effective potential. In the present work, the main difficulty stems from the nonlinearity due to the Coulombian interaction.

The paper is organized as follows: in Sec. II we introduce the spectral elements of the confining operator, which enable to define the 2.5D adiabatic model; then we present in details the different models where special care is given to boundary conditions; the main results of the paper are presented in Sec. III; in Sec. IV we obtain some ε-independent estimates for (1.1)–(1.3) and we give existence and uniqueness results for the approximate models; in Sec. V, we prove that the 2.5D model is a second order approximation while in Sec. VI, the 2D model is proven to be only

a first order approximation; Sec. VII is devoted to some extensions and comments; finally, an appendix contains some basic results on the Schrödinger equation and some regularity estimates for the Poisson equation which are used all along the paper.

II. NOTATIONS AND PRESENTATION OF THE MODELS

In the paper, Ω_0 denotes a regular domain of dimension 2. First, we define the following functional space.

Definition 2.1: Let $1 \leqslant p,\ q \leqslant +\infty$. *Then*

$$L_x^q L_z^p = \left\{ u \in L^1(\Omega_0 \times \mathbb{R}), \quad \|u\|_{L^{q,p}} = \left(\int_{\Omega_0} \|u(x,\cdot)\|_{L^p(\mathbb{R})}^q \, \mathrm{d}x \right)^{1/q} < +\infty \right\}$$

(*with an obvious generalization of this definition for* $q = +\infty$). In the sequel, $L^p(\Omega_0 \times \mathbb{R})$ will be more simply denoted L^p.

For a function $f = f(z)$ belonging to $L^1(\mathbb{R})$ we denote $\langle f \rangle = \int_{\mathbb{R}} f(z)\mathrm{d}z$. In particular, if $n(x,z)$ is the particle density, the surface density is defined by $n_s(x) = \langle n(x,\cdot) \rangle$.

A. Spectrum of the confinement operator

We introduce the properties of the confining potential V_c. We assume that it satisfies the

Assumption 2.2: The rescaled confining potential $V_c = V_c(z)$ *is a non-negative real-valued function in* $L^2_{loc}(\mathbb{R})$ *such that*

$$\lim_{|z| \to +\infty} V_c(z) = +\infty.$$

Under this assumption, the operator $A = -\frac{1}{2}(d^2/dz^2) + V_c$ defined on $X = L^2(\mathbb{R})$ with the domain

$$\mathcal{D}(A) = \{ u \in H^2(\mathbb{R}) \ \text{ such that } \ V_c\, u \in L^2(\mathbb{R}) \}$$

is self-adjoint, non-negative, and has a compact resolvent (see, e.g., Ref. 34). Hence, its spectrum is purely discrete and consists in a strictly increasing sequence of non-negative real numbers tending to infinity $(E_p)_{p \in \mathbb{N}^*}$. Moreover, the associated eigenfunctions $(\chi_p)_{p \in \mathbb{N}^*}$, chosen real-valued, form an orthonormal basis of $L^2(\mathbb{R})$ and verify

$$\forall a > 0, \quad \forall p \in \mathbb{N}^*, \quad \exists C_{a,p} > 0, \quad \text{such that,} \quad \forall z \in \mathbb{R}, \quad |\chi_p(z)| \leqslant C_{a,p}\, e^{-a|z|}. \tag{2.1}$$

The partial Hamiltonian involved in (1.1) is obtained by rescaling A:

$$A^\varepsilon = -\frac{1}{2}\frac{d^2}{dz^2} + V_c^\varepsilon = -\frac{1}{2}\frac{d^2}{dz^2} + \frac{1}{\varepsilon^2} V_c\left(\frac{z}{\varepsilon}\right).$$

This operator A^ε on $X = L^2(\mathbb{R})$ has the domain

$$\mathcal{D}(A^\varepsilon) = \{ u \in H^2(\mathbb{R}) \ \text{ such that } \ V_c^\varepsilon\, u \in L^2(\mathbb{R}) \}.$$

Its eigenfunctions $(\chi_p^\varepsilon)_{p \in \mathbb{N}^*}$ and eigenvalues $(E_p^\varepsilon)_{p \in \mathbb{N}^*}$ can be deduced by a simple rescaling from those of A:

$$\chi_p^\varepsilon(z) = \frac{1}{\sqrt{\varepsilon}} \chi_p\left(\frac{z}{\varepsilon}\right), \quad E_p^\varepsilon = \frac{E_p}{\varepsilon^2}.$$

We shall denote by Π_p^ε the orthogonal projector on $span(\chi_p^\varepsilon)$. The space $L^2(\mathbb{R}^2, span(\chi_p^\varepsilon))$ will be called the pth subband. With an abuse of notation, we shall also denote by Π_p^ε the orthogonal projector $\mathbb{I} \otimes \Pi_p^\varepsilon$ of $L^2(\mathbb{R}^3)$ on $L^2(\mathbb{R}^2, span(\chi_p^\varepsilon))$.

The following technical lemma, proved in Ref. 11, will be used several times in this paper.

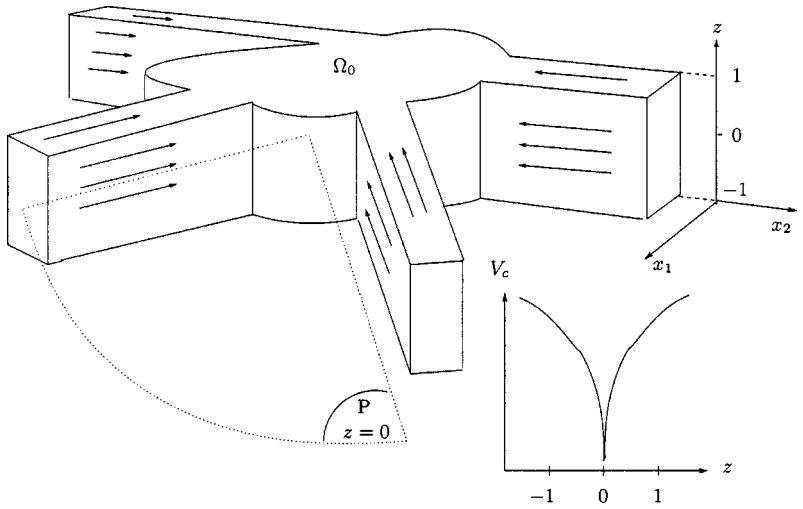

FIG. 1. The device projected in $\{z\in[-1,1]\}$.

Lemma 2.3: Let $V^\varepsilon \in W^{1,\alpha}(\mathbb{R})$ *with* $\alpha\in[1,+\infty]$. *Then for any* $p\in\mathbb{N}^*$ *we have*

$$\|[\Pi_p^\varepsilon, V^\varepsilon]\|_{\mathcal{L}(L^2(\mathbb{R}))} \leqslant C_p\, \varepsilon^{1-1/\alpha}\, \|\partial_z V^\varepsilon\|_{L^\alpha(\mathbb{R})},$$

where $[\cdot,\cdot]$ *denotes the commutator of operators and* C_p *only depends on* p.

Notice that this type of commutator estimates was already used in the semiclassical analysis of electrons motion in periodic crystals. In that case, the projector is the projector on the energy bands related to the Bloch decomposition, see Refs. 27 and 4.

B. Definition of the models

For the sake of completeness, the open boundary conditions introduced in Ref. 26 are derived step by step in Appendix A. We set now the geometry of the device.

The device domain consists in an active region, denoted by $\Omega_0\times\mathbb{R}$ connected to semi-infinite electrons reservoirs by n leads $\Omega_j\times\mathbb{R}$, $j=1,...,n$, see Fig. 1 for a schematic drawing of the device in $\Omega_0\times[-1,1]$ and Fig. 2. The full domain of the device is $\Omega\times\mathbb{R}$, where $\Omega=\cup_{j=0}^n\Omega_j$. The boundary of Ω_0 is split into a part Γ_0 and n parts Γ_j, $j=1,...,n$. We denote by ω_0 the boundary $(\Gamma_0\times\mathbb{R})\cup(\Omega_0\times\{z=\pm\infty\})$. The transport directions are denoted by $x:=(x_1,x_2)$ and the confined direction by z. The local coordinates of the lead j, $j\neq 0$ are denoted by η_j and ξ_j, see Fig. 2. The confining potential insures that the electrons stay around the plane $P=\{x\in\Omega, z=0\}$, see Figs. 1 and 2.

1. The 3D model

The 3D model is obtained by coupling the Poisson equation to a set of Schrödinger equations to be solved on the domain $\Omega_0\times\mathbb{R}$ with open boundary conditions. A single electron injected with an energy E^ε is represented by a wave function Ψ^ε solution of the Schrödinger equation

$$-\Delta\Psi^\varepsilon(x,z)+(V_c^\varepsilon(z)+V^\varepsilon(x,z))\Psi^\varepsilon(x,z)=E^\varepsilon\,\Psi^\varepsilon(x,z) \quad \text{in } \Omega_0\times\mathbb{R}, \tag{2.2}$$

where V_c^ε is a confining potential and V^ε is, up to now, a given potential supported only in $\Omega_0\times\mathbb{R}$. Ψ^ε satisfies the nonhomogeneous open boundary conditions derived in Appendix A:

$$\left.\frac{\partial\Psi^\varepsilon}{\partial\eta_j}\right|_{\Gamma_j}=\mathbb{Z}_j^{3D}[E^\varepsilon](\Psi^\varepsilon)+\mathbb{S}_j^{3D}[E^\varepsilon], \tag{2.3}$$

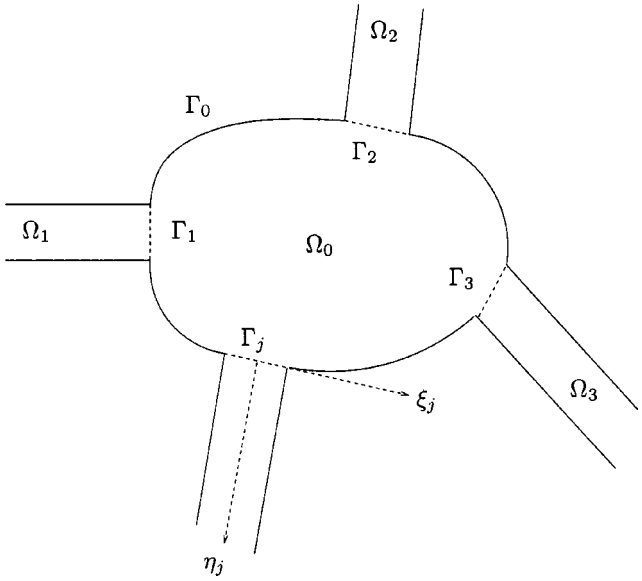

FIG. 2. The plane P.

$$\Psi^\varepsilon = 0 \quad \text{on} \quad \omega_0 . \tag{2.4}$$

The electrons populate the different sub-bands starting from the first sub-band. In Ref. 11, a model close to the one presented is analyzed in the time-dependent picture. Therein, the ε-independent estimates are obtained using crucially the Stricharz estimates introduced by Castella in Ref. 14 in order to solve the Schrödinger–Poisson system in L^2. This theory does not use H^1 energy estimates. Obviously, within the stationary framework, the Stricharz estimates are not available and one needs H^1 theory to obtain energy estimates. In the time-dependent picture, when the initial condition has a nonzero component on a sub-band with index $p \geqslant 2$, ε-independent *a priori* bounds in H^1 are only derived on a small time interval while the time interval can be made arbitrarily large for wave functions supported only on the first sub-band. Therefore, there is a little hope to obtain estimates for the stationary problem if the electrons populate the upper sub-bands. Consequently, we will only focus on the electrons injected on this first sub-band by assuming the following hypothesis.

*Assumption 2.4: Let Θ_m^j and $\mathcal{E}_m^j$ be the eigenfunctions and eigenvalues of the j*th *transversal Schrödinger operator $-\partial_{\xi_j}^2$ with Dirichlet boundary conditions. Then, we suppose that the electrons are injected in the lead j_0, on the first sub-band, on the transversal mode m_0 and with a longitudinal kinetic energy k^2. This implies that $\mathbb{S}_j^{3\mathrm{D}} = -2\,\delta_j^{j_0}\, ik\, \Theta_{m_0}^j\, \chi_1^\varepsilon$ and $E^\varepsilon = E_1^\varepsilon + \mathcal{E}_{m_0}^{j_0} + k^2$.*

The wave functions Ψ^ε are thus parametrized by $\lambda = (m_0, j_0, k)$, $\Psi^\varepsilon := \Psi_\lambda^\varepsilon$ (the dependence on the parameter 1 of first sub-band is omitted). Notice that the assumption is compatible with some physical situations called electrical quantum limit, see for instance the numerical simulations in Refs. 32 and 33, where only the first sub-band is populated. This hypothesis is often verified in structures like T-stubs, quantum couplers, or various types of transistors. Indeed, in two-dimensional electron gases, the electron occupancy in the second sub-band is usually a small fraction (typically less than 10%) of the total electron density, see Refs. 36 and 20. Nervertheless, in parabolic quantum well structures, the electrons population in the sub-bands can be carefully controlled and the densities in two lowest sub-band can be similar to within 30%, see Refs. 19 and 21.

Assumption 2.4 thus implies that the boundary condition (2.3) reads

$$\left.\frac{\partial \Psi_\lambda^\varepsilon}{\partial \eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{3D}[E_1^\varepsilon + E_\lambda](\Psi_\lambda^\varepsilon) - 2\,\delta_j^{j_0}\, ik\, \Theta_{m_0}^j\, \chi_1^\varepsilon. \tag{2.5}$$

In order to take into account self-consistent effects, the electrons are supposed to be injected in the state λ by a source in the leads and the electronic density is assumed to be in a mixed state. It reads

$$n^\varepsilon(x,z) = \int_\Lambda |\Psi_\lambda^\varepsilon(x,z)|^2 \, d\mu(\lambda) = \sum_{j_0=1}^{n} \sum_{m_0=1}^{\infty} \int_{\mathbb{R}_+^\star} \Phi(j_0,m_0,k) |\Psi_{j_0,m_0,k}^\varepsilon(x,z)|^2 \, dk, \tag{2.6}$$

where $\Phi(j_0,m_0,k)$ is the statistics of injection and Λ is the set

$$\Lambda = [0,\ldots,n] \times \mathbb{N}^\star \times \mathbb{R}_+^\star .$$

The electrons being charged particles, they generate a self-consistent potential V^ε through the Poisson equation. It is assumed that the nonlinear interaction takes place only in the active region, the domain $\Omega_0 \times \mathbb{R}$. Hence, V^ε solves

$$-\Delta V^\varepsilon = n^\varepsilon \quad \text{on } \Omega_0 \times \mathbb{R}, \tag{2.7}$$

$$V^\varepsilon = 0 \quad \text{on } \partial\Omega_0 \times \mathbb{R}, \tag{2.8}$$

$$V^\varepsilon \to 0 \quad \text{as } |z| \to \infty. \tag{2.9}$$

The fact that the electrons are injected on the first sub-band does not imply that the wave function Ψ_λ^ε has only a contribution on this sub-band. Indeed, the different sub-bands are coupled through the z-dependence of V^ε. Nevertheless, it will be shown that the upper sub-bands are weakly populated since the potential V^ε is slowly varying with respect to the variable z. The 3D model finally read as follows.

The 3D model:

$$\begin{gathered}
-\Delta \Psi_\lambda^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi_\lambda^\varepsilon(x,z) = (E_1^\varepsilon + E_\lambda)\, \Psi_\lambda^\varepsilon(x,z) \quad \text{in } \Omega_0 \times \mathbb{R}, \\
\Psi_\lambda^\varepsilon = 0 \quad \text{on } \omega_0; \ \Psi_\lambda^\varepsilon \text{ satisfies } (2.5) \quad \text{on } \Gamma_j \times \mathbb{R}, \quad j \neq 0, \\
-\Delta V^\varepsilon = n^\varepsilon \quad \text{on } \Omega_0 \times \mathbb{R}, \quad n^\varepsilon(x,z) = \int_\Lambda |\Psi_\lambda^\varepsilon(x,z)|^2 \, d\mu(\lambda), \\
V^\varepsilon = 0 \quad \text{on } \partial\Omega_0 \times \mathbb{R}; \ V^\varepsilon \to 0 \quad \text{as } |z| \to \infty.
\end{gathered} \tag{2.10}$$

Existence and uniqueness: The model presented in Ref. 6 is slighty different from the 3D model but the results can be easily adapted. It is proven in Ref. 6 that, for a general μ satisfying an assumption of boundedness of the support, the 3D model admits a weak solution Ψ_λ^ε in $H^1(\Omega_0 \times \mathbb{R})$. More precisely, the obtained density reads

$$n^\varepsilon = \int_\Lambda |\Psi_\lambda^\varepsilon|^2 \, d\mu(\lambda) + \quad \text{sum of bound states.}$$

This last statement means that the electrons having adequate energies are trapped into the active region. In other words, the bound states of the device can be excited by the injected beam of electrons (see Ref. 6 for more details). This implies, conjugated with the nonlinear character of the problem, the nonuniqueness of the solutions. Morever, the wave function satisfies estimates of the type

$$\|\Psi_\lambda^\varepsilon\|_{L^2} \leqslant \frac{C}{|\mathcal{E}^\varepsilon - E_\lambda|}, \tag{2.11}$$

where $\mathcal{E}^\varepsilon$ denotes an energy of the bound states. This leads to a nonintegrable singularity in the computation of the density. To derive the asymptotic models, the nonuniqueness property is not fundamental but in order to obtain error estimates, we need to recover uniqueness. This can be done thanks to the uniqueness result of Ref. 6: if the bound states are avoided by the statistics μ and if the nonlinearity is supposed to be weak enough the solutions are unique. Moreover, the fact that the bound states are avoided implies also, thanks to (2.11), some uniform bounds with respect to λ. This leads to the following definition.

Definition 2.5: Assume that V^ε is a given regular potential. Consider the operator $-\Delta + V_c^\varepsilon + V^\varepsilon - E_1^\varepsilon$ equipped with Dirichlet boundary conditions on ω_0 and with the homogeneous transparent boundary conditions (2.3) on $\Gamma_j \times \mathbb{R}$, $j=1,..,n$ with $\mathbb{S}_j^{3D}[E_1^\varepsilon + E_\lambda] := 0$. According to Ref. 6, this operator has a purely discrete spectrum and we will call "energies of the bound states" its eigenvalues $(\mathcal{E}_i^\varepsilon(V^\varepsilon))_{i \geqslant 1}$.

In order to simplify the analysis and to avoid additional technicalities, we set in the simplest way to make the electrons avoid the bound states, see Ref. 6. The requirement is given by the following

Assumption 2.6: The measure μ has a bounded support such that, for $\lambda \in supp\ \mu$, there exists $C>0$, ε-independent such that

$$C \leqslant \mathcal{E}_1^\varepsilon(0) - E_\lambda .$$

This implies that the electrons avoid all the bound states. Indeed, by the maximum principle, V^ε is positive and then $\mathcal{E}_1^\varepsilon(0) \leqslant \mathcal{E}_1^\varepsilon(V^\varepsilon)$. Notice that above, this choice of μ is ε-independent since $\mathcal{E}_1^\varepsilon(0)$ is also ε-independent. This assumption is rather stringent in the general case and some ways to waive this restriction are proposed in Sec. VII. Nevertheless, in the case of confined devices at low temperatures, this hypothesis may nearly be verified. Indeed, in these structures, the typical statistics of injection is a Fermi–Dirac statistics. It reads

$$\Phi(E^\varepsilon) = \frac{1}{1 + \exp\left(\dfrac{E_F^\varepsilon - E^\varepsilon}{k_B T}\right)},$$

where k_B is the Boltzmann constant, T the temperature, and E_F^ε the rescaled Fermi level. In practical,

$$E_F^\varepsilon = E_1^\varepsilon + \mathcal{O}(1),$$

and the Fermi–Dirac reads

$$\Phi(E^\varepsilon) = \frac{1}{1 + \exp\left(\dfrac{E_\lambda + \mathcal{O}(1)}{k_B T}\right)},$$

which exhibits an exponential decay at low temperatures and also at high energies.

The theorem of Ref. 6 reads, for given ε, after a slight adaptation.

Theorem 2.7: *(Ref. 6) There exists $\delta(\varepsilon)$ positive, such that for every μ satisfying assumption 2.6 and*

$$\mu(\Lambda) < \delta(\varepsilon)$$

the 3D model admits a unique solution.

We shall see in the sequel that $\delta(\varepsilon)$ can be chosen ε-independent.

2. The 2D surface density model

The 2D surfacic density model is the coupling between many 2D Schrödinger equations and a 2D potential. When ε goes to zero, $|\chi_p^\varepsilon|^2$ concentrates around 0 and becomes then a Dirac measure. This leads to the definition of the limit model by replacing the self-consistent potential by its trace on the plane $\{x\in\Omega_0, z=0\}$ and by replacing the 3D density by a 2D density multiplied by a Delta measure. The boundary condition (2.5) becomes

$$\left.\frac{\partial\psi_\lambda}{\partial\eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{2D}[E_\lambda](\psi_\lambda) - 2\,\delta_j^{j_0}\, ik\,\Theta_{m_0}^j, \tag{2.12}$$

where

$$\mathbb{Z}_j^{2D}[E_\lambda](\psi_\lambda) = \sum_{m=1}^{N^j(E_\lambda)} ik_m^j(E_\lambda)\psi_{m,j}(0)\Theta_m^j(\xi_j) - \sum_{m=N^j(E_\lambda)+1}^{\infty} k_m^j(E_\lambda)\,\psi_{m,j}(0)\,\Theta_m^j(\xi_j).$$

The 2D surface density model then reads

$$\begin{gathered}
-\Delta_x\psi_\lambda(x) + V(x,0)\psi_\lambda(x) = E_\lambda\,\psi_\lambda \quad \text{in } \Omega_0,\\
\psi_\lambda = 0 \quad \text{on } \Gamma_0;\ \psi_\lambda \text{ satisfies (2.12) on } \Gamma_j,\quad j\neq 0,\\
-\Delta V(x,z) = n_s(x)\delta(z) \quad \text{on } \Omega_0\times\mathbb{R},\quad n_s = \int_\Lambda |\psi_\lambda|^2\,d\mu(\lambda),\\
V = 0 \quad \text{on } \partial\Omega_0\times\mathbb{R};\ \lim_{|z|\to\infty} V = 0 \quad \text{a.e. on } \Omega_0.
\end{gathered} \tag{2.13}$$

Definition 2.8: Assume that V is a given regular potential. Consider the operator $-\Delta_x + V(\cdot,0)$ equipped with Dirichlet boundary conditions on Γ_0 and with the homogeneous transparent boundary conditions (2.12) on Γ_j, $j=1,..,n$ without source term. According to Ref. 6, this operator has a purely discrete spectrum and we will call "energies of the 2D bound states" its eigenvalues $(\mathcal{E}_i(V(\cdot,0))_{i\geqslant 1}$.

3. The 2.5D model

The 2.5D adiabatic model is an intermediate model between the fully 3D model and the 2D surfacic density one. It takes into account the small thickness of the electron gas and consists in coupling a set of two-dimensional Schrödinger equations and the three-dimensional Poisson equation:

$$\begin{gathered}
-\Delta_x\psi_\lambda^\varepsilon + \langle V^\varepsilon|\chi_1^\varepsilon|^2\rangle\,\psi_\lambda^\varepsilon(x) = E_\lambda\,\psi_\lambda^\varepsilon \quad \text{in } \Omega_0,\\
\psi_\lambda^\varepsilon = 0 \quad \text{on } \Gamma_0;\ \psi_\lambda^\varepsilon \text{ satisfies (2.12)} \quad \text{on } \Gamma_j,\quad j\neq 0,\\
-\Delta V^\varepsilon = n^\varepsilon|\chi_1^\varepsilon|^2 \quad \text{on } \Omega_0\times\mathbb{R},\ n^\varepsilon = \int_\Lambda |\psi_\lambda^\varepsilon|^2\,d\mu(\lambda),\\
V^\varepsilon = 0 \quad \text{on } \partial\Omega_0\times\mathbb{R};\ \lim_{|z|\to\infty} V^\varepsilon = 0 \quad \text{a.e. on } \Omega_0.
\end{gathered} \tag{2.14}$$

Remark 2.9: According to Definition 2.8, the energies of the bound states of the 2.5D model are naturaly denoted by $(\mathcal{E}_i(\langle V^\varepsilon|\chi_1^\varepsilon|^2\rangle))_{i\in\mathbb{N}^\star}$. Morever, if V is a potential independent of the variable z, it comes easily that $\mathcal{E}_i(V) = \mathcal{E}_i^\varepsilon(V)$.

III. MAIN RESULTS

In this paper, we will prove the following theorems.

Theorem 3.1: *Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, there exists η positive ε-independent such that, for every μ satisfying Assumption 2.6 and*

$$\mu(\Lambda) < \eta,$$

the 3D model (2.10) and the 2.5D adiabatic model (2.14) admit unique weak solutions, respectively, denoted by $(\Psi_\lambda^{3D}, V^{3D})$ and by $(\psi_\lambda^{2.5D}, V^{2.5D})$. Moreover, η can be chosen such that we have the following error estimates, uniformly in λ, for $\alpha>0$, for $p\in[1,2)$,

$$\|\Psi_\lambda^{3D} - \psi_\lambda^{2.5D}\chi_1^\varepsilon\|_{W^{1,p}(\Omega_0, L^2(\mathbb{R}))} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.1}$$

$$\|V^{3D} - V^{2.5D}\|_{W^{1,p}(\Omega_0, L^\infty(\mathbb{R}))} = \mathcal{O}(\varepsilon^{2-\alpha}). \tag{3.2}$$

Furthermore the surfacic densities defined by $n_s^{3D} = \int_\Lambda \langle |\Psi_\lambda^{3D}|^2\rangle \, d\mu(\lambda)$ and $n_s^{2.5D} = \int_\Lambda |\psi_\lambda^{2.5D}|^2 \, d\mu(\lambda)$ satisfy

$$\|n_s^{3D} - n_s^{2.5D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{2-\alpha}) \quad \forall \alpha>0, \quad \forall p\in[1,2). \tag{3.3}$$

Theorem 3.2: *Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, there exists η positive ε-independent such that, for every μ satisfying Assumption 2.6 and*

$$\mu(\Lambda) < \eta,$$

as $\varepsilon\to 0$, the unique solution $(\psi_\lambda^{2.5D}, n^{2.5D}, V^{2.5D})$ of the 2.5D adiabatic model converges to the unique solution $(\phi^{2D}, n_s^{2D}, V^{2D})$ of the 2D surfacic density model (2.13) in the following sense: for $\alpha>0$, for $p\in[1,2)$,

$$\|\psi_\lambda^{2.5D} - \phi^{2D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.4}$$

$$\|V^{2.5D} - V^{2D}\|_{W^{1,p}(\Omega_0, L^\infty(\mathbb{R}))} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.5}$$

$$\|n_s^{2.5D} - n_s^{2D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.6}$$

where $n_s^{2D} = \int_\Lambda |\phi_\lambda^{2D}|^2 \, d\mu(\lambda)$ and $n_s^{2.5D} = \int_\Lambda |\psi_\lambda^{2.5D}|^2 \, d\mu(\lambda)$. Furthermore, we have the following bound from below:

$$\|V^{2D} - V^{2.5D}\|_{L^2} + \|n_s^{2D} - n_s^{2.5D}\|_{L^2} \geq C\,\varepsilon, \tag{3.7}$$

where C does not depend on ε.

A straightforward consequence of these theorems is the following.

Corollary 3.3: Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, under the notations of Theorems 3.1 and 3.2, there exists η positive ε-independent such that, for every μ satisfying Assumption 2.6 and

$$\mu(\Lambda) < \eta,$$

the 3D model converges as $\varepsilon\to 0$ to the 2D model. Furthermore, we have the estimate

$$C_1\,\varepsilon \leq \|V^{2D} - V^{3D}\|_{L^2} + \|n_s^{2D} - n_s^{3D}\|_{L^2} \leq C_2\,\varepsilon^{1-\alpha}.$$

IV. ε-INDEPENDENT ESTIMATES AND WELL-POSEDNESS

In this section, we shall obtain some ε-independent estimates for the 3D and the 2.5D models. To this aim, we will use Proposition A.1 for both models. Besides, the well-posedness of the 2D and 2.5D models will also be studied.

Proposition 4.1: Let V^ε and Ψ^ε_λ be the solutions of the 3D model. Then, under assumption 2.2, 2.4, and 2.6 we have the following estimates, uniformly in λ,

$$\|\Psi^\varepsilon_\lambda\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leqslant C, \tag{4.1}$$

$$\|(\mathbb{I}-\Pi^\varepsilon_1)\Psi^\varepsilon_\lambda\|_{L^2}\leqslant C\,\varepsilon, \tag{4.2}$$

$$\|V^\varepsilon\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leqslant C \quad for \;\; p\in(1,\infty),\;\; s<\tfrac{3}{2},\quad p(1+2s)<8, \tag{4.3}$$

$$\|(\mathbb{I}-\Pi^\varepsilon_1)\Psi^\varepsilon_\lambda\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leqslant C\,\varepsilon^{1-\alpha},\quad \alpha>0, \tag{4.4}$$

where C is ε-independent.

Proof: The proof of (4.1) and (4.2) is a direct application of Proposition A.1 Indeed, according to the maximum principle V^ε is positive and according to hypothesis 2.4, Ψ^ε_λ satisfies the boundary condition (A10) with $a=1$. It suffices to apply (A12) and (A13) with $f=0$ to conclude.

The estimate (4.3) will be obtained by using the regularity properties of the Poisson equation given in Appendix B. To this aim, we first remark that $\int_\Lambda|\nabla_x\Psi^\varepsilon_\lambda|^2 d\mu(\lambda)\;\in L^1$ and $\int_\Lambda|\Psi^\varepsilon_\lambda|^2 d\mu(\lambda)\in L^p_x L^1_z$, for all $p\in[1,\infty)$, thanks to (4.1) and the embedding $H^1(\Omega_0)\hookrightarrow L^p(\Omega_0)$, $p<\infty$. This implies by interpolation, that for $r<2$,

$$\nabla_x n^\varepsilon = 2\,\mathrm{Re}\int_\Lambda \overline{\Psi^\varepsilon_\lambda}\,\nabla_x\Psi^\varepsilon_\lambda\, d\mu(\lambda)\in L^{r,1}.$$

It suffices then to apply (B3) to conclude.

To prove (4.4), we form the quantity $w^\varepsilon_\lambda:=(\mathbb{I}-\Pi^\varepsilon_1)\Psi^\varepsilon_\lambda$. It can be easily seen that w^ε_λ solves

$$-\Delta w^\varepsilon_\lambda+(V^\varepsilon_c(z)+V^\varepsilon(x,z))w^\varepsilon_\lambda=(E^\varepsilon_1+E_\lambda)\,w^\varepsilon_\lambda+[\Pi^\varepsilon_1,V^\varepsilon]\Psi^\varepsilon_\lambda \tag{4.5}$$

with boundary conditions (A10) with $a=0$ and (A11). Hence, the estimate (A12) of Appendix A with $f=[\Pi^\varepsilon_1,V^\varepsilon]\Psi^\varepsilon_\lambda$ implies

$$\|w^\varepsilon_\lambda\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leqslant C\|[\Pi^\varepsilon_1,V^\varepsilon]\Psi^\varepsilon_\lambda\|_{L^2}\leqslant C\,\varepsilon^{1-1/p}\|\partial_z V^\varepsilon\|_{L^4_x L^p_z}\|\Psi^\varepsilon_\lambda\|_{L^4_x L^2_z}$$

thanks to Lemma 2.3. We conclude the proof by using (4.1) and by noticing that (4.3) implies that $\partial_z V^\varepsilon$ is bounded in $L^4_x L^p_z$ for any $p<\infty$, thanks to the embedding $H^{1/2-(1/p)}(\mathbb{R})\hookrightarrow L^p(\mathbb{R})$, for $p\in[2,\infty)$, see Ref. 1. □

Proposition 4.2: Let V^ε and ψ^ε_λ be the solutions of the 2.5D model. Then, under Assumptions 2.2, 2.4, and 2.6, we have the following estimates, uniformly in λ,

$$\|\psi^\varepsilon_\lambda\|_{H^1(\Omega_0)}\leqslant C, \tag{4.6}$$

$$\|V^\varepsilon\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leqslant C \quad for \;\; p\in(1,\infty),\quad s<\tfrac{3}{2},\quad p(1+2s)<8, \tag{4.7}$$

where C is ε-independent.

Proof: To prove (4.6) and in order to apply Proposition A.1, we form artificially the function $\Phi^\varepsilon_\lambda(x,z):=\psi^\varepsilon_\lambda(x)\,\chi^\varepsilon_1(z)$ which solves

$$-\Delta\Phi^\varepsilon_\lambda+(V^\varepsilon_c+\langle V^\varepsilon\,|\chi^\varepsilon_1|^2\rangle)\Phi^\varepsilon_\lambda=(E^\varepsilon_1+E_\lambda)\,\Phi^\varepsilon_\lambda \quad \text{in}\;\; \Omega_0\times\mathbb{R}$$

equipped with boundary conditions (A10) with $a=1$ and (A11). (A12) concludes then the proof since V^ε is positive by the maximum principle.

The estimate (4.7) is proven analogously to (4.3) by using (4.6). □

The existence and uniqueness of solution for the 2.5D and the 2D models are direct applications of Theorem 7.2 of Ref. 6. The result is the following.

Theorem 4.3: *Let Assumptions 2.2, 2.4, and 2.6 be verified. Let* $\Psi_\lambda^{3D}\in H^1(\Omega_0\times\mathbb{R})$ *be a solution of the 3D model. Then, there exists an* η *positive such that, for every* μ *satisfying Assumption 2.6 and*

$$\mu(\Lambda)<\eta,$$

the 3D, the 2.5D, and the 2D models admit unique weak solutions. The solutions in $H^1(\Omega_0)$ *of the 2.5D and the 2D models are, respectively, denoted by* $\psi_\lambda^{2.5D}$ *and* ϕ_λ^{2D}. *Moreover, we have the estimates, uniformly in* λ,

$$\|\phi_\lambda^{2D}\|_{H^1(\Omega_0)}\leqslant C, \tag{4.8}$$

$$\|V^{2D}\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leqslant C \quad for \;\; p\in(1,\infty), \quad s<\tfrac{3}{2}, \quad p(1+2s)<8. \tag{4.9}$$

Sketch of the proof: The basic tools are the Leray–Schauder fixed point theorem and the regularity properties of the Poisson equation. The positivity of the potentials V^{2D} and $V^{2.5D}$ coupled to Assumption 2.6 imply direct bounds on the densities thanks to (A12) with $f=0$ and $a=1$. It follows, thanks to the Poisson equation, Lemmas B.1 and B.2, some compactness properties of the mapping and then to the existence result. The uniqueness is given by the fact that the fixed point procedures become contractions if the densities are small enough in L^1 norm. To this aim, we notice that, thanks to (4.1), (4.6) for n^{3D} and $n^{2.5D}$, and thanks to (A12) for n^{2D},

$$\|n^{3D}\|_{L^1}\leqslant C\mu(\Lambda),\;\; \|n^{2.5D}\|_{L^1}\leqslant C\mu(\Lambda), \quad \|n^{2D}\|_{L^1}\leqslant C\mu(\Lambda),$$

and then it suffices to choose η small enough such that each of the Leray–Schauder mappings are contractions. Equations (4.8) and (4.9) are direct applications of (A12) and Lemma B.2.

V. THE 2.5D MODEL IS A SECOND ORDER APPROXIMATION

In this section, we end the proof of Theorem 3.1 initiated in the preceding section. The used strategies are the same as Ref. 11. We assume that we are under the hypothesis of Theorem 4.3 which insure that the 3D and 2.5D models admit unique solutions. We denote respectively, by $(\Psi_\lambda^{3D},V^{3D})$ and $(\psi_\lambda^{2D},V^{2D})$, these solutions. We start by proving (3.2) by setting $V^{3D}-V^{2.5D}=V+R_1^\varepsilon+R_2^\varepsilon$ with

$$-\Delta V=|\chi_1^\varepsilon|^2(n_s^{3D}-n^{2.5D}), \quad -\Delta R_1^\varepsilon=r_1^\varepsilon, \quad -\Delta R_2^\varepsilon=r_2^\varepsilon$$

equipped with boundary conditions (B2) and where

$$n_s^{3D}=\int_\Lambda\int_{\mathbb{R}}|\Pi_1^\varepsilon\Psi_\lambda^{3D}|^2\,\mathrm{d}z\,\mathrm{d}\mu(\lambda), \quad r_1^\varepsilon=2\,\mathrm{Re}\int_\Lambda\overline{\Pi_1^\varepsilon\Psi_\lambda^{3D}}\;\;(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D}\,\mathrm{d}\mu(\lambda),$$

$$r_2^\varepsilon=\int_\Lambda|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D}|^2\,\mathrm{d}\mu(\lambda).$$

Estimating the remainder terms R_1^ε *and* R_2^ε*:* Thanks to (4.1) and (4.4), we have directly, for $r<2$ and $\delta>0$,

$$\|r_1^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant C\,\varepsilon^{1-\delta},$$

$$\|r_2^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta},$$

$$\|z\,r_1^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant\|z\chi_1^\varepsilon\|_{L^2(\mathbb{R})}\,\varepsilon^{1-\alpha}\leqslant C\,\varepsilon^{2-\alpha}.$$

This implies that R_2^ε is almost of order two while R_1^ε is, up to now, almost of order one. To get one order more for R_1^ε, we will use (B5) of Appendix B. To this aim, we remark by orthogonality of $\Pi_1^\varepsilon\Psi_\lambda^{3\mathrm{D}}$ and $(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3\mathrm{D}}$ that

$$\int_{\mathbb{R}} r_1^\varepsilon(x,z)\,\mathrm{d}z=0.$$

Thereby, (B5) applies. Choosing $s=\frac{1}{2}+\alpha$, $\beta=1-2\alpha$ with α positive and close to 0, we obtain, for all δ positive and $p<2$,

$$\|R_1^\varepsilon\|_{W^{1,p}(\Omega_0,H^{1/2+\alpha}(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta},$$

$$\|R_2^\varepsilon\|_{W^{1,p}(\Omega_0,H^{1/2+\alpha}(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta}$$

which leads to bounds in $W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))$ thanks to the embedding $H^{1/2+\alpha}(\mathbb{R})\hookrightarrow L^\infty(\mathbb{R})$ for all α positive.

It remains now to treat V. In order to estimate $|\chi_1^\varepsilon|^2(n_s^{3\mathrm{D}}-n^{2.5\mathrm{D}})$, we use the Schrödinger equation solved by $w_\lambda^\varepsilon:=\Pi_1^\varepsilon\Psi_\lambda^{3\mathrm{D}}-\chi_1^\varepsilon\,\psi_\lambda^{2.5\mathrm{D}}$:

$$-\Delta w_\lambda^\varepsilon+V_c^\varepsilon w_\lambda^\varepsilon+\langle V^{3\mathrm{D}}\,|\chi_1^\varepsilon|^2\rangle\,w_\lambda^\varepsilon=(E_1^\varepsilon+E_\lambda)w_\lambda^\varepsilon+f^\varepsilon+g^\varepsilon$$

equipped with the transparent homogeneous boundary conditions (A10) with $a=0$ and where

$$f^\varepsilon=-\Pi_1^\varepsilon\,V^{3\mathrm{D}}\,(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3\mathrm{D}},\quad g^\varepsilon=\langle(V^{2.5\mathrm{D}}-V^{3\mathrm{D}})\,|\chi_1^\varepsilon|^2\rangle\chi_1^\varepsilon\psi_\lambda^{2.5\mathrm{D}}.$$

Remarking that

$$\Pi_1^\varepsilon\,V^{3\mathrm{D}}\,(\mathbb{I}-\Pi_1^\varepsilon)=\Pi_1^\varepsilon[\Pi_1^\varepsilon,V^{3\mathrm{D}}],$$

we deduce from Lemma 2.3, (4.3) and (4.4) that, for δ strictly positive,

$$\|f^\varepsilon\|_{L^2}\leqslant C\,\varepsilon^{1-1/p}\|\partial_z V^{3\mathrm{D}}\|_{L_x^4L_z^p}\|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}=\mathcal{O}(\varepsilon^{2-\delta})$$

thanks to the embedding $H^{\frac{1}{2}-(1/p)}(\mathbb{R})\hookrightarrow L^p(\mathbb{R})$, for $p\in[2,\infty)$. Besides, according to (4.6), for $r>2$

$$\|g^\varepsilon\|_{L^2}\leqslant C\|V^{3\mathrm{D}}-V^{2\mathrm{D}}\|_{L_x^rL_z^\infty}$$

and we obtain finally, thanks to (A12), (4.22), and (4.6), that

$$\|w_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leqslant C\|f^\varepsilon\|_{L^2}+C\|g^\varepsilon\|_{L^2}\leqslant\mathcal{O}(\varepsilon^{2-\delta})+C\|V^{3\mathrm{D}}-V^{2\mathrm{D}}\|_{L_x^rL_z^\infty},$$

$$\|n_s^{3\mathrm{D}}-n^{2.5\mathrm{D}}\|_{W^{1,p}(\Omega_0)}\leqslant C\mu(\Lambda)^{1/2}\left(\int_\Lambda\|w_\lambda^\varepsilon\|^2_{H^1(\Omega_0,L^2(\mathbb{R}))}\,\mathrm{d}\mu(\lambda)\right)^{1/2}$$

$$\leqslant\mathcal{O}(\varepsilon^{2-\delta})+C\,\mu(\Lambda)\,\|V^{3\mathrm{D}}-V^{2\mathrm{D}}\|_{L_x^rL_z^\infty},$$

for $\delta>0$, $r>2$, and $p<2$. Applying (B3) in order to bound V, we find, according to the above estimate,

$$\|V\|_{W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))} \leqslant C\,\varepsilon^{2-\delta} + C\,\mu(\Lambda)\,\|V^{3D}-V^{2D}\|_{L^r_x L^\infty_z}.$$

Gathering now the different estimates on R_1^ε, R_2^ε, and V leads to

$$\|V^{3D}-V^{2D}\|_{W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))} \leqslant C\,\varepsilon^{2-\delta} + C\,\mu(\Lambda)\,\|V^{3D}-V^{2D}\|_{L^r_x L^\infty_z}.$$

Choosing $r \leqslant [2p/(2-p)]$ and $\mu(\Lambda)$ small enough end the proof thanks to the embedding $W^{1,p}(\Omega_0) \hookrightarrow L^r(\Omega_0)$.

VI. THE 2D MODEL IS A FIRST ORDER APPROXIMATION

In this section, we end the proof of Theorem 3.2. We first assume that we are under the hypothesis of Theorem 4.3 which insure that the 2D and 2.5D models admit unique solutions. We denote, respectively, by $(\psi_\lambda^{2.5D}, V^{2.5D})$ and $(\phi_\lambda^{2D}, V^{2D})$, these solutions. We start by proving (3.5) by writing

$$-\Delta(V^{2.5D}-V^{2D}) = |\chi_1^\varepsilon|^2(n_s^{2.5D}-n_s^{2D}) + n_s^{2D}(|\chi_1^\varepsilon|^2-\delta(z)) \tag{6.1}$$

equipped with the boundary conditions (B2). In order to apply (B3) to (6.1), we first estimate the quantity $n_s^{2.5D}-n_s^{2D}$ by using the Schrödinger equation solved by $w_\lambda^\varepsilon := \chi_1^\varepsilon(\psi_\lambda^{2.5D}-\phi_\lambda^{2D})$:

$$-\Delta w_\lambda^\varepsilon + V_c^\varepsilon w_\lambda^\varepsilon + \langle V^{2.5D}\,|\chi_1^\varepsilon|^2\rangle\, w_\lambda^\varepsilon = (E_1^\varepsilon + E_\lambda) w_\lambda^\varepsilon + f^\varepsilon$$

equipped with the transparent homogeneous boundary conditions (A10) with $a=0$ and where

$$f^\varepsilon = (V^{2D}(\cdot,0) - \langle V^{2.5D}\,|\chi_1^\varepsilon|^2\rangle)\chi_1^\varepsilon\phi_\lambda^{2D}.$$

Estimating the source term f^ε: We have

$$\begin{aligned}\|f^\varepsilon\|_{L^2} &\leqslant (\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z} + \|\langle (V^{2D}(\cdot,0)-V^{2D})\,|\chi_1^\varepsilon|^2\rangle\|_{L^p(\Omega_0)})\|\phi_\lambda^{2D}\|_{H^1(\Omega_0)} \\ &\leqslant C\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z} + C\|\partial_z V^{2D}\|_{L^p_x L^\alpha_z}\langle z^{1-1/\alpha}|\chi_1^\varepsilon|^2\rangle, \\ p>2 &\leqslant C\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z} + \mathcal{O}(\varepsilon^{1-\delta}), \quad \delta>0,\end{aligned}$$

where we used the estimates (4.8), (4.9) and the embeddings $H^1(\Omega_0) \hookrightarrow L^q(\Omega_0)$, $q<\infty$ and $H^{1/2-(1/\alpha)}(\mathbb{R}) \hookrightarrow L^\alpha(\mathbb{R})$, $\alpha \in [2,\infty)$. Applying now (A12) in order to estimate w_λ^ε, we obtain uniformly in λ, thanks to the above estimate of the source term f^ε, for $p>2$, $\delta>0$, and $r<2$,

$$\|w_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))} \leqslant C\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z} + \mathcal{O}(\varepsilon^{1-\delta}), \tag{6.2}$$

$$\|n_s^{2.5D}-n_s^{2D}\|_{W^{1,r}(\Omega_0)} \leqslant C\mu(\Lambda)\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z} + \mathcal{O}(\varepsilon^{1-\delta}). \tag{6.3}$$

It remains now to estimate the second part on the right-hand side of (B2). To this aim, we find, according to (B6), for $r<2$, $p(1+2(s+\beta)) \leqslant 4r$, $s+\beta<\frac{3}{2}$,

$$\|(-\Delta)^{-1}(n_s^{2D}(|\chi_1^\varepsilon|^2-\delta(z)))\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))} \leqslant C\langle z|\chi_1^\varepsilon|^2\rangle^\beta \|n_s^{2D}\|_{W^{1,r}(\Omega_0)}.$$

Since $\|n_s^{2D}\|_{W^{1,r}(\Omega_0)}$ is bounded for $r \leqslant 2$ thanks to (4.8) and since $\langle z|\chi_1^\varepsilon|^2\rangle = \mathcal{O}(\varepsilon)$ thanks to 2.1, we have finally, by choosing $\beta = 1-\delta$, $s = \frac{1}{2} + (\delta/2)$,

$$\|(-\Delta)^{-1}(n_s^{2D}(|\chi_1^\varepsilon|^2-\delta(z)))\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))} \leqslant \mathcal{O}(\varepsilon^{1-\delta}). \tag{6.4}$$

We are able now to estimate the difference $V^{2D}-V^{2.5D}$ by applying (B3). Gathering the bounds (6.1), (6.3), and (6.4) and thanks to the embedding $H^{1/2+\alpha}(\mathbb{R})\hookrightarrow L^\infty(\mathbb{R})$, $\alpha>0$, we find, for $\delta>0$, $q<2$, and $p>2$,

$$\|V^{2D}-V^{2.5D}\|_{W^{1,q}(\Omega_0,L^\infty(\mathbb{R}))}\leqslant C\mu(\Lambda)\|V^{2D}-V^{2.5D}\|_{L^p_x L^\infty_z}+\mathcal{O}(\varepsilon^{1-\delta}).$$

Choosing $p\leqslant 2q/(2-q)$ and $\mu(\Lambda)$ small enough end the proof of (3.5).

In order to prove (3.4) and (3.6), it suffices to apply (3.5), (6.2), and (6.3).

The estimate from below: For the proof of (3.7), we introduce $(e_i,\lambda_i)_{i\in\mathbb{N}^*}$, the Hilbertian decomposition of the x-Laplacian equipped with Dirichlet boundary condition on $\partial\Omega_0$. Let $g\in L^2(\Omega_0\times\mathbb{R})$ and let u be the solution of $-\Delta u=g$ on the domain $\Omega_0\times\mathbb{R}$ with Dirichlet boundary conditions on $\partial(\Omega_0\times\mathbb{R})$. It can be easily seen that the Fourier transform $\hat{u}$ of u reads

$$\hat{u}(x,\xi)=\sum_{i\geqslant 1}\frac{(\hat{g}(\cdot,\xi),e_i(\cdot))_{L^2_x}}{\lambda_i+\xi^2}e_i(x)$$

and thus, thanks to the Fourier–Plancherel equality

$$\|u\|^2_{L^2}=\|(-\Delta)^{-1}g\|^2_{L^2}=\sum_{i\geqslant 1}\int_{\mathbb{R}}d\xi\left|\frac{(\hat{g},e_i)_{L^2_x}}{\lambda_i+\xi^2}\right|^2.$$

Hence, using the above equality, we find

$$\begin{aligned}\|(-\Delta)^{-1}(n_s^{2D}(|\chi_1^\varepsilon|^2-\delta(z)))\|^2_{L^2}&=\sum_{i\geqslant 1}\int_{\mathbb{R}}d\xi\left|\frac{(n_s^{2D},e_i)_{L^2_x}}{\lambda_i+\xi^2}\right|^2\left|\int_{\mathbb{R}}|\chi_1^\varepsilon|^2(e^{-i\xi z}-1)\,dz\right|^2\\&\geqslant\sum_{i\geqslant 1}\left|\frac{(n_s^{2D},e_i)_{L^2_x}}{\lambda_i+1}\right|^2\int_0^1 d\xi\left|\int_{\mathbb{R}}|\chi_1^\varepsilon|^2(e^{-i\xi z}-1)\,dz\right|^2\\&\geqslant C\,\|n_s^{2D}\|^2_{H^{-1}(\Omega_0)}\int_0^1 d\xi\left|\int_{\mathbb{R}}|\chi_1|^2(e^{-i\varepsilon\xi z}-1)\,dz\right|^2.\end{aligned}\tag{6.5}$$

Moreover, pointwise in ξz, as $\varepsilon\to 0$, we have

$$\frac{e^{-i\,\varepsilon\,\xi\,z}-1}{-i\,\varepsilon\,\xi\,z}\to 1.$$

Consequently, defining h by

$$\frac{h(\varepsilon)}{\varepsilon^2}=\frac{1}{\varepsilon^2}\int_0^1 d\xi\left|\int_{\mathbb{R}}|\chi_1|^2(e^{-i\varepsilon\xi z}-1)\,dz\right|^2,$$

the Lebesgue dominated convergence theorem implies that

$$\frac{h(\varepsilon)}{\varepsilon^2}\to\frac{1}{3}\left|\int_{\mathbb{R}}z\,|\chi_1|^2\,dz\right|^2=C.$$

To conclude, we come back to (6.1) and (6.5). By noticing that $\|n_s^{2D}\|_{H^{-1}(\Omega_0)}=C$, there exists finally C_0 ε-independent such that

$$\|V^{2D}-V^{2.5D}\|^2_{L^2}+\|n_s^{2D}-n_s^{2.5D}\|^2_{L^2}\geqslant\|(-\Delta)^{-1}(n_s^{2D}(|\chi_1^\varepsilon|^2-\delta(z)))\|^2_{L^2}\geqslant C_0\,\varepsilon^2.$$

This ends the proof.

VII. REMARKS

We considered here a model without exterior potential. The analysis still holds if a regular enough potential is added, for instance, a potential in $L^p(\Omega_0, W^{1,\infty}(\mathbb{R}))$, with $p>2$.

We also assumed that the open set Ω_0 is regular. This hypothesis can be weakened if the boundary conditions prescribed for the Poisson equation are modified: for instance, considering a square, we put Dirichlet boundary conditions in two parallel interfaces and Neumann conditions in the orthogonal ones.

All the analysis presented in the paper strongly relies on the Assumption 2.6 which is essential in order to obtain existence and uniqueness results. We conjecture that all the results still hold if this assumption is replaced by the

Assumption 7.1: The measure μ has a bounded support and there exists δ positive, ε-independent, such that, $\forall i \geqslant 1$,

$$\inf_{\lambda \in supp\ \mu} |E_\lambda - \mathcal{E}_i(0)| > \delta,$$

where the $\mathcal{E}_i$ are the energies of the bound states introduced in Definition 2.8.

This assumption means that the statistics avoids the bound states of the linear open Schrödinger equation, see Ref. 6 for more details. To prove the theorems under this framework, one has to show that the statistics still avoids the bound states when considering a nonzero self-consistent potential. This can be done by a careful analysis of the open Schrödinger equation and by setting a statistics whose total mass is weak enough such that there exists $\eta(\delta)$ such that, $\forall i \geqslant 1$,

$$\inf_{\lambda \in \mathrm{supp}\ \mu} |E_\lambda - \mathcal{E}_i(V^\varepsilon)| > \eta(\delta).$$

On the other hand, following again,[6] a limit absorption procedure can be performed as well. One may add to the energy E^ε, a complex term $i\nu$ with $\nu>0$. Then all the results applies without Assumption 2.6. Then, the limit ν goes to zero has to be investigated and the difficulty in this step is to obtain ν-independent estimates. This will require a precise statement of the rate of convergence in ν in order to preserve the different errors estimates. To conclude, the Assumption 2.6 can be actually weakened but this improvment involves more technicalities than in the present analysis and not directly related to the purpose of this work.

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APPENDIX A: THE LINEAR SCHRÖDINGER EQUATION ON OPEN DOMAINS

In this section, we derive the open boundary conditions introduced in Ref. 6 and we give some estimates for the solution of the Schrödinger equation equipped with such conditions. More precisely, we seek a generalized eigenfunction Ψ^ε solution of the Schrödinger equation associated with the energy E^ε, this means

$$-\Delta\Psi^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi^\varepsilon(x,z) = E^\varepsilon\,\Psi^\varepsilon(x,z) \quad \text{in } \Omega\times\mathbb{R}, \tag{A1}$$

$$\Psi^\varepsilon \text{ is bounded}, \tag{A2}$$

$$\Psi^\varepsilon = 0 \quad \text{on } \partial(\Omega\times\mathbb{R}), \tag{A3}$$

where V_c^ε is a confining potential and was defined in Introduction and V^ε is a given regular potential, supported only in $\Omega_0\times\mathbb{R}$. The equation (A1) is, in the lead j,

$$(-\partial_z^2-\Delta_{\xi_j,\eta_j})\Psi^\varepsilon(\xi_j,\eta_j,z)+V_c^\varepsilon(z)\Psi^\varepsilon(\xi_j,\eta_j,z)=E^\varepsilon\,\Psi^\varepsilon(\xi_j,\eta_j,z),\quad j\neq 0, \tag{A4}$$

where ξ_j and η_j are the local coordinates of the lead j, see Fig. 2. The boundary conditions are obtained by explictly solving the Schrödinger equation in each lead. For this purpose, let Θ_m^j and $\mathcal{E}_m^j$, be the eigenfunctions and eigenvalues of the jth transversal Schrödinger operator $-\partial_{\xi_j}^2$ with Dirichlet boundary conditions. Ψ^ε can be written under the form, in the lead j,

$$\Psi^\varepsilon(\eta_j,\xi_j,z)=\sum_p\ \Pi_p^\varepsilon\Psi^\varepsilon=\sum_{p,m}\ \Psi_{p,m,j}^\varepsilon(\eta_j)\Theta_m^j(\xi_j)\chi_p^\varepsilon(z),$$

where $\Psi_{p,m,j}^\varepsilon$ is the component of Ψ^ε on the basis $(\Theta_m^j\otimes\chi_p^\varepsilon)_{p,m}$ and solves

$$-\frac{\partial^2\Psi_{m,p,j}^\varepsilon}{\partial\eta_j^2}=(E^\varepsilon-E_p^\varepsilon-\mathcal{E}_m^j)\Psi_{m,p,j}^\varepsilon. \tag{A5}$$

Hence, setting

$$k_m^j(E^\varepsilon-E_p^\varepsilon)=\sqrt{|E^\varepsilon-E_p^\varepsilon-\mathcal{E}_m^j|},$$

$$N^j(E^\varepsilon-E_p^\varepsilon)=\sup\{m\geqslant 1,\ E^\varepsilon-E_p^\varepsilon>\mathcal{E}_m^j\},$$

we obtain

$$\Psi_{m,p,j}^\varepsilon(\eta_j)=a_{m,p}^j e^{-ik_m^j\eta_j}+b_{m,p}^j e^{ik_m^j\eta_j}\quad\text{if } m\leqslant N^j(E^\varepsilon-E_p^\varepsilon), \tag{A6}$$

$$\Psi_{m,p,j}^\varepsilon(\eta_j)=b_{m,p}^j e^{-k_m^j\eta_j}\quad\text{if } m>N^j(E^\varepsilon-E_p^\varepsilon). \tag{A7}$$

The modes associated with $m\leqslant N^j(E^\varepsilon-E_p^\varepsilon)$ are the propagating modes and the modes associated with $m>N^j(E^\varepsilon-E_p^\varepsilon)$ are the evanescent modes. The coefficients $a_{m,p}^j$ are known whereas the $b_{m,p}^j$ are the reflection–transmission coefficients and deduced from the solution. The boundary conditions on Γ_j are obtained by eliminating the $b_{m,p}^j$ coefficients and the result is,[6,26]

$$\left.\frac{\partial\Psi^\varepsilon}{\partial\eta_j}\right|_{\Gamma_j}=\mathbb{Z}_j^{3\mathrm{D}}[E^\varepsilon](\Psi^\varepsilon)+\mathbb{S}_j^{3\mathrm{D}}[E^\varepsilon], \tag{A8}$$

where

$$\mathbb{Z}_j^{3\mathrm{D}}[E^\varepsilon](\Psi^\varepsilon)=\sum_{p=1}^{\infty}\left(\sum_{m=1}^{N^j(E^\varepsilon-E_p^\varepsilon)} ik_m^j(E^\varepsilon-E_p^\varepsilon)\Psi_{p,m,j}^\varepsilon(0)\,\Theta_m^j(\xi_j)\right.$$

$$\left.-\sum_{m=N^j(E^\varepsilon-E_p^\varepsilon)+1}^{\infty} k_m^j(E^\varepsilon-E_p^\varepsilon)\,\Psi_{p,m,j}^\varepsilon(0)\,\Theta_m^j(\xi_j)\right)\chi_p^\varepsilon,$$

$$\mathbb{S}_j^{3\mathrm{D}}[E^\varepsilon]=-2\sum_{p=1}^{\infty}\sum_{m=1}^{N^j(E^\varepsilon-E_p^\varepsilon)} ik_m^j(E^\varepsilon-E_p^\varepsilon)\,a_{m,p}^j\,\Theta_m^j(\xi_j)\,\chi_p^\varepsilon(z).$$

To summarize, the problem is solved only on the bounded domain $\Omega_0\times\mathbb{R}$ with the boundary conditions (A8) and $\Psi=0$ on ω_0.

We rewrite now these boundary conditions in the case of the nonlinear transport model of Sec. II B 1. According to Assumption 2.4, the energy E^ε is equal to $E_1^\varepsilon + E_\lambda$, where $E_\lambda = E_{m_0}^{j_0} + k^2$ and $a_{m,p}^j = \delta_p^1\, \delta_m^{m_0}\, \delta_j^{j_0}$. This implies that $\mathbb{S}_j^{3D}$ takes the simpler form

$$\mathbb{S}_j^{3D}[E_1^\varepsilon + E_\lambda] = -2\, \delta_j^{j_0}\, ik\, \Theta_{m_0}^j(\xi_j)\, \chi_1^\varepsilon(z).$$

Finally, in order to derive estimates for more general problems, we consider the following system:

$$-\Delta \Psi^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi^\varepsilon(x,z) = (E_1^\varepsilon + E_\lambda)\, \Psi^\varepsilon(x,z) + f(x,z) \quad \text{in } \Omega_0 \times \mathbb{R}, \tag{A9}$$

$$\left.\frac{\partial \Psi^\varepsilon}{\partial \eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{3D}[E_1^\varepsilon + E_\lambda](\Psi^\varepsilon) - 2a\, \delta_j^{j_0}\, ik\, \Theta_{m_0}^j(\xi_j)\, \chi_1^\varepsilon(z), \tag{A10}$$

$$\Psi^\varepsilon = 0 \quad \text{on } \omega_0, \tag{A11}$$

where a is a positive parameter and f a given source term. The well-poseness of this system has been studied in Ref. 6.

Proposition A.1: Let Ψ^ε be the solution of (A9)–(A11). Let $f \in L^2(\Omega_0 \times \mathbb{R})$, $V^\varepsilon \in L^\infty(\Omega_0 \times \mathbb{R})$ and V^ε non-negative a.e. Then, under Assumption 2.2, 2.4, and 2.6, we have, uniformly in λ,

$$\|\Psi^\varepsilon\|_{H^1(\Omega_0, L^2(\mathbb{R}))} \leqslant C\,(2a + \|f\|_{L^2}), \tag{A12}$$

$$\|(\mathbb{I} - \Pi_1^\varepsilon)\Psi^\varepsilon\|_{L^2} \leqslant C\,\varepsilon\,(2a + \|f\|_{L^2}), \tag{A13}$$

where C is a generic constant ε-independent.

Proof: Consider the kinetic energy along x and the kinetic energy along z defined by

$$\mathcal{E}_{\text{kin},x}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} |\nabla_x \Psi^\varepsilon|^2\, dx\, dz, \quad \mathcal{E}_{\text{kin},z}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} |\partial_z \Psi^\varepsilon|^2\, dx\, dz.$$

The potential energy and the external potential energy are, respectively, defined by

$$\mathcal{E}_{\text{pot}}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} V^\varepsilon |\Psi^\varepsilon|^2\, dx\, dz, \quad \mathcal{E}_{\text{ext}}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} V_c^\varepsilon\, |\Psi^\varepsilon|^2 dx\, dz.$$

We introduce also the energy coming from the boundary terms

$$\mathcal{E}_{BC}^\varepsilon = -\sum_{j=1}^n \int_{\Gamma_j \times \mathbb{R}} \left.\frac{\partial \Psi^\varepsilon}{\partial \eta_j}\right|_{\Gamma_j} \overline{\Psi^\varepsilon}\, d\xi_j\, dz.$$

A standard energy estimate for the Schrödinger equation, obtained after multiplication of (A9) by $\overline{\Psi_\lambda^\varepsilon}$ and some integration by parts, yields

$$\mathcal{E}_{\text{kin},x}^\varepsilon + \mathcal{E}_{\text{kin},z}^\varepsilon + \mathcal{E}_{\text{pot}}^\varepsilon + \mathcal{E}_{\text{ext}}^\varepsilon + \text{Re}\, \mathcal{E}_{BC}^\varepsilon = (E_1^\varepsilon + E_\lambda)\|\Psi^\varepsilon\|_{L^2}^2 + \int_{\Omega_0 \times \mathbb{R}} f\, \overline{\Psi^\varepsilon} dx\, dz, \tag{A14}$$

$$\text{Im}\, \mathcal{E}_{BC}^\varepsilon = 0. \tag{A15}$$

Besides, the boundary condition (A10) implies that

$$\mathrm{Re}\,\mathcal{E}^{\varepsilon}_{BC}=\sum_{j=1}^{n}\sum_{p=1}^{\infty}\sum_{m=N^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)+1}^{\infty}k_m^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)|\Psi^{\varepsilon}_{p,m,j}|^2-2a\,k\,\mathrm{Im}\,\Psi^{\varepsilon}_{1,m_0,j_0}, \tag{A16}$$

$$\mathrm{Im}\,\mathcal{E}^{\varepsilon}_{BC}=\sum_{j=1}^{n}\sum_{p=1}^{\infty}\sum_{m=1}^{N^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)}k_m^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)|\Psi^{\varepsilon}_{p,m,j}|^2+2a\,k\,\mathrm{Re}\,\Psi^{\varepsilon}_{1,m_0,j_0}=0, \tag{A17}$$

and we first deduce from (A16) and (A17) that

$$|\Psi^{\varepsilon}_{1,m_0,j_0}|\leqslant 2a \tag{A18}$$

$$0\leqslant \mathrm{Re}\,\mathcal{E}^{\varepsilon}_{BC}+2a\,k\,\mathrm{Im}\,\Psi^{\varepsilon}_{1,m_0,j_0}. \tag{A19}$$

Moreover, according to Ref. 6, the operator $-\Delta+V_c^\varepsilon+V^\varepsilon-E_1^\varepsilon$ equipped with (A10) and (A11) with $a=0$, has a compact resolvent and denote $(\mathcal{E}_i^\varepsilon(V^\varepsilon))_{i\in\mathbb{N}^*}$ its spectrum and $(\Phi_i^\varepsilon)_{i\in\mathbb{N}^*}$ its associated eigenvectors. Since $V^\varepsilon\geqslant 0$, then $\mathcal{E}_1^\varepsilon(V^\varepsilon)\geqslant\mathcal{E}_1^\varepsilon(0)$ and it can be easily seen that $\mathcal{E}_1^\varepsilon(0)$ is ε-independent. It follows, after a projection of Ψ^ε on the basis $(\Phi_i^\varepsilon)_{i\in\mathbb{N}^*}$ that

$$\mathcal{E}^{\varepsilon}_{\mathrm{kin},x}+\mathcal{E}^{\varepsilon}_{\mathrm{kin},z}+\mathcal{E}^{\varepsilon}_{\mathrm{pot}}+\mathcal{E}^{\varepsilon}_{\mathrm{ext}}+\mathrm{Re}\,\mathcal{E}^{\varepsilon}_{BC}+2a\,k\,\mathrm{Im}\,\Psi^{\varepsilon}_{1,m_0,j_0}-E_1^\varepsilon\|\Psi^\varepsilon\|_{L^2}^2=\sum_{i\geqslant 1}\mathcal{E}_i^\varepsilon(V^\varepsilon)|(\Psi^\varepsilon,\Phi_i^\varepsilon)|^2.$$

Injecting this relation in (A14) leads to

$$(\mathcal{E}_1^\varepsilon(0)-E_\lambda)\|\Psi^\varepsilon\|_{L^2}^2\leqslant\sum_{i\geqslant 1}(\mathcal{E}_i^\varepsilon(V^\varepsilon)-E_\lambda)|(\Psi^\varepsilon,\Phi_i^\varepsilon)|^2\leqslant 4a^2k+\|f\|_{L^2}\|\Psi^\varepsilon\|_{L^2},$$

where we used (A18) for the second inequality while the first inequality follows from the fact that $\mathcal{E}_i^\varepsilon(0)\leqslant\mathcal{E}_i^\varepsilon(V^\varepsilon)$ since V^ε is positive. We use now crucially Assumption 2.6 which implies that $\mathcal{E}_1^\varepsilon(0)-E_\lambda>C$, where C is ε-independent and this gives the L^2 estimate, uniform in λ,

$$\|\Psi^\varepsilon\|_{L^2}\leqslant C(2a\sqrt{k}+\|f\|_{L^2}). \tag{A20}$$

To conclude the proof, we come back to (A14) and by using (A19) and (A20), we obtain

$$\mathcal{E}^{\varepsilon}_{\mathrm{kin},x}+\mathcal{E}^{\varepsilon}_{\mathrm{kin},z}+\mathcal{E}^{\varepsilon}_{\mathrm{pot}}+\mathcal{E}^{\varepsilon}_{\mathrm{ext}}\leqslant E_1^\varepsilon\|\Psi^\varepsilon\|_{L^2}^2+C(4a^2+\|f\|_{L^2}^2),$$

where C depends on $\sup_{\lambda\in\mathrm{supp}\,\mu}E_\lambda$. Since

$$\mathcal{E}^{\varepsilon}_{\mathrm{kin},z}+\mathcal{E}^{\varepsilon}_{\mathrm{ext}}=\sum_{p=1}^{\infty}E_p^\varepsilon\|\Pi_p^\varepsilon\Psi^\varepsilon\|_{L^2}^2$$

and since V^ε is non-negative, we have $\mathcal{E}^{\varepsilon}_{\mathrm{pot}}\geqslant 0$ and finally

$$\mathcal{E}^{\varepsilon}_{\mathrm{kin},x}+\frac{1}{\varepsilon^2}(E_2-E_1)\|(\mathbb{I}-\Pi_1^\varepsilon)\Psi^\varepsilon\|_{L^2}^2\leqslant C(4a^2+\|f\|_{L^2}^2)$$

which ends the proof. □

APPENDIX B: THE POISSON EQUATION WITH $L^r_xL^1_z$ DENSITIES

This section deals with the regularity of the solution of the Poisson equation

$$-\Delta V=n \quad \text{on} \quad \Omega_0\times\mathbb{R}, \tag{B1}$$

$$V(\cdot,z)=0 \quad \text{on } \partial\Omega_0, \qquad \lim_{|z|\to\infty} V(x,z)=0. \tag{B2}$$

In the whole section, $L^p_x L^q_z$ denotes the spaces introduced in Definition 2.1.

Lemma B.1: (i) Let V be the solution of (B1) and (B2), let $n\in L^r_x L^1_z$ *with* $r\in(1,\infty)$. *Then for* $s<\frac{3}{2}$ *and* $p(1+2s)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L^r_x L^1_z}. \tag{B3}$$

(ii) Besides, for $s<\frac{1}{2}$ *and* $p(3+2s)\leqslant 4r$, *we have also*

$$\|\nabla_x V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L^r_x L^1_z}. \tag{B4}$$

(iii) Let $n\in L^r_x L^1_z$ *such that* $z\,n\in L^r_x L^1_z$, *with* $r\in(1,+\infty)$ *and* $\int_{\mathbb{R}} n(\cdot,z)\mathrm{d}z=0$. *Then, for* $0\leqslant\beta\leqslant 1$, $p\in[2,+\infty)$, $s+\beta<\frac{3}{2}$ *and* $p(1+2(s+\beta)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|z\,n\|^{\beta}_{L^r_x L^1_z}\|n\|^{1-\beta}_{L^r_x L^1_z}. \tag{B5}$$

(iv) Assume that $n(x,z)=n_s(x)\,(\rho(z)-\delta(z))$ *where* $n_s\in L^r(\Omega_0)$ *with* $r\in(1,+\infty)$, *where* $\rho\in L^1(\mathbb{R})$, *non-negative such that* $z\,\rho\in L^1(\mathbb{R})$ *and* $\|\rho\|_{L^1(\mathbb{R})}=1$. *Then, for* $0\leqslant\beta\leqslant 1$, $p\in[2,+\infty)$, $s+\beta<\frac{3}{2}$ *and* $p(1+2(s+\beta)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|z\,\rho\|^{\beta}_{L^1}\|n_s\|_{L^r(\Omega_0)}. \tag{B6}$$

Proof: Taking the Fourier transform of (B1) with respect to z leads to

$$-\Delta_x\hat{V}(x,\xi)+\xi^2\,\hat{V}(x,\xi)=\hat{n}(x,\xi),$$

where

$$\hat{V}(x,\xi)=\int_{\mathbb{R}} V(x,z)\,e^{-i\,z\,\xi}\,\mathrm{d}z, \quad \hat{n}(x,\xi)=\int_{\mathbb{R}} n(x,z)\,e^{-i\,z\,\xi}\,\mathrm{d}z. \tag{B7}$$

Since $-\Delta_x$, equipped with Dirichlet boundary conditions on Ω_0, is a sectorial operator on $L^p(\Omega_0)$, for $p\in(1,+\infty)$, we have

$$\|\hat{V}(\cdot,\xi)\|_{L^p(\Omega_0)}\leqslant\frac{1}{\xi^2}\|-\Delta_x\hat{V}(\cdot,\xi)+\xi^2\hat{V}(\cdot,\xi)\|_{L^p(\Omega_0)}\leqslant\frac{1}{\xi^2}\|\hat{n}(\cdot,\xi)\|_{L^p(\Omega_0)}. \tag{B8}$$

Moreover, (B8), (B7), and standard elliptic estimates imply

$$\|\hat{V}(\cdot,\xi)\|_{W^{2,p}(\Omega_0)}\leqslant C\|\hat{n}(\cdot,\xi)\|_{L^p(\Omega_0)}, \tag{B9}$$

where C does not depend on ξ. Besides, for $p\geqslant 2$, we have thanks to the Hölder inequality,

$$\begin{aligned}\|V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))}&=\int_{\Omega_0}\left(\int_{\mathbb{R}}(1+\xi^{2s})\,|\hat{V}(x,\xi)|^2\,\mathrm{d}\xi\right)^{p/2}\mathrm{d}x\\&\leqslant\left\|\frac{1}{1+\xi^{\alpha}}\right\|_{L^{p/(p-2)}(\mathbb{R})}\int_{\Omega_0}\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,|\hat{V}(x,\xi)|^p\,\mathrm{d}\xi\,\mathrm{d}x\\&\leqslant C\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,\|\hat{V}(\cdot,\xi)\|^r_{L^r(\Omega_0)}\|\hat{V}(\cdot,\xi)\|^{p-r}_{L^\infty(\Omega_0)}\,\mathrm{d}\xi,\end{aligned} \tag{B10}$$

as soon as

$$0 \leqslant 1-\frac{2}{p} < \alpha, \quad 1 \leqslant r \leqslant p \leqslant \infty.$$

Coupling now (B8) and (B9) and using the embedding $W^{2,r}(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, for $r>1$, leads to

$$\begin{aligned}\|V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))} &\leqslant C\int_{\mathbb{R}} (1+\xi^{(2s+\alpha)p/2})\,\|\hat{V}(\cdot,\xi)\|^r_{L^r(\Omega_0)}\,\|\hat{V}(\cdot,\xi)\|^{p-r}_{W^{2,r}(\Omega_0)}\,\mathrm{d}\xi \\ &\leqslant C\int_{\mathbb{R}} (1+\xi^{2r-(2s+\alpha)p/2})^{-1}\,\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)}\,\mathrm{d}\xi \\ &\leqslant C\|n\|^p_{L^r_x L^1_z} \quad \text{if } \frac{1}{\xi^{2r-(2s+\alpha)p/2}} \in L^1([1,+\infty)),\end{aligned} \tag{B11}$$

where we used the fact that $|\hat{n}(x,\xi)| \leqslant \|n(x,\cdot)\|_{L^1(\mathbb{R})}$. After some easy algebra, this gives the final conditions for (B3),

$$2 \leqslant p < \infty, \quad s \leqslant \tfrac{3}{2}, \quad p(1+2s) < 4r.$$

For (B4), we use a classical interpolation equality in Ref. 13 which insures that

$$\|\nabla_x \hat{V}\|_{L^p(\Omega_0)} \leqslant C\|\Delta_x \hat{V}\|^{1/2}_{L^r(\Omega_0)}\ \ \|\hat{V}\|^{1/2}_{L^t(\Omega_0)} \leqslant C\|\Delta_x \hat{V}\|^{1/2}_{L^r(\Omega_0)}\ \ \|\hat{V}\|^{r/2r}_{L^r(\Omega_0)}\ \ \|\hat{V}\|^{1/2[1-(r/t)]}_{L^\infty(\Omega_0)} \tag{B12}$$

with $1/p = \frac{1}{2}[(1/t) + (1/r).]$ This inequality implies, together with (B8), (B9), for $t \geqslant r > 1$,

$$\|\nabla_x \hat{V}\|_{L^p(\Omega_0)} \leqslant \frac{C}{\xi^{r/t}} \|\hat{n}\|_{L^r(\Omega_0)}. \tag{B13}$$

Replacing V by $\nabla_x V$ in (B11), using estimates (B9) and (B13), we obtain by proceeding as for (B11),

$$\begin{aligned}\|\nabla_x V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))} &\leqslant \left\| \frac{1}{1+\xi^\alpha} \right\|_{L^{p/(p-2)}(\mathbb{R})}\ \int_{\Omega_0}\int_{\mathbb{R}} (1+\xi^{(2s+\alpha)p/2})\,|\nabla_x \hat{V}(x,\xi)|^p\,\mathrm{d}\xi\,\mathrm{d}x \\ &\leqslant C\int_{\mathbb{R}} (1+\xi^{rp/t-(2s+\alpha)p/2})^{-1}\,\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)}\,\mathrm{d}\xi \leqslant C\|n\|^p_{L^r_x L^1_z}\end{aligned}$$

as soon as

$$0 \leqslant 1-\frac{2}{p} < \alpha, \quad \frac{1}{p} = \frac{1}{2}\left(\frac{1}{t}+\frac{1}{r}\right), \quad r \leqslant t, \quad \frac{rp}{t} - \frac{1}{2}(2s+\alpha)p > 1.$$

This concludes the proof of (B4) after some easy manipulations.

We end now the proof of Lemma B.1 by proving (B5). If $\int_{\mathbb{R}} n\,\mathrm{d}z = 0$, it can easily remarked that

$$\left|\frac{\hat{n}(x,\xi)}{\xi}\right| = \left|\frac{1}{\xi}\int_{\mathbb{R}} (e^{-i\,z\,\xi}-1)n(x,z)\,\mathrm{d}z\right| \leqslant \|z n(x,.)\|_{L^1(\mathbb{R})},$$

since $|e^{-i\,z\,\xi}-1| \leqslant |z\,\xi|$, $\forall (k,\xi) \in \mathbb{R}^2$. This leads to, thanks to (B11),

$$\|V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))} \leqslant C\int_{\mathbb{R}} (1+\xi^{2r-(2s+\alpha)p/2-\beta p})^{-1}\left(\frac{\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)}}{\xi^p}\right)^{\beta}(\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)})^{1-\beta}\,\mathrm{d}\xi$$

$$\leqslant C\|z\,n\|^{\beta p}_{L^r_x L^1_z}\|n\|^{(1-\beta)p}_{L^r_x L^1_z} \quad \text{if} \quad \frac{1}{\xi^{2r-(2(s+\beta)+\alpha)p/2}} \in L^1([1,+\infty)),$$

which gives the result.

For (B6), we just remark that

$$\hat{n}(x,\xi) = n_s(x)\int_{\mathbb{R}} (e^{-i\,z\,\xi}-1)\rho(z)\,\mathrm{d}z$$

which is exactly the same form as above. □

In the same way, if n is given by $n(x,z) := n_s(x)\,\delta(z)$, we have the following.

Lemma B.2: (i) Let V be the solution of (B1) and (B2) with $n(x,z) := n_s(x)\delta(z)$, *where* $n_s \in L^r(\Omega_0)$ *with* $r \in (1,\infty)$. *Then, for* $s < \frac{3}{2}$ *and* $p(1+2s) \leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))} \leqslant C\|n\|_{L^r(\Omega_0)}. \tag{B14}$$

Besides, for $s < \frac{1}{2}$ *and* $p(3+2s) \leqslant 4r$, *we have also*

$$\|\nabla_x V\|_{L^p(\Omega_0,H^s(\mathbb{R}))} \leqslant C\|n\|_{L^r(\Omega_0)}. \tag{B15}$$

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Group-cohomology refinement to classify *G*-symplectic manifolds

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''Pseudo-cohomology,'' as a refinement of Lie group cohomology, is soundly studied aiming at classifying the symplectic manifolds associated with Lie groups. In this study, the framework of symplectic cohomology provides fundamental new insight, which enriches the analysis previously developed in the setting of Cartan–Eilenberg $H^2(G,\mathrm{U}(1))$ cohomology. © *2004 American Institute of Physics.*
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I. INTRODUCTION

From the strict mathematical point of view, the orbits of the coadjoint representation of Lie groups provide a source for symplectic manifolds on which a given Lie group acts as a group of symplectomorphisms, i.e., G-symplectic manifolds. Even, for finite-dimensional semisimple groups, this mechanism essentially exhausts all models of they. These G-symplectic manifolds could then be considered as phase spaces of physical systems for which G can be called the ''basic symmetry.'' From the physical point of view, however, the simplest physical systems (the free nonrelativistic particle, for instance) possess a phase space endowed with a symplectic form whose associated Poisson bracket realizes the Lie algebra of a central extension of the basic ''classical'' symmetry. Central extensions of Lie groups by U(1), associated with projective unitary representations, were classified long ago by Bargmann[1] by means of the cohomology group $H^2(G,\mathrm{U}(1))$.[2] Later, the momentum map from the phase space to the coalgebra $\mathcal{G}^*$ of the basic ''classical'' symmetry group, constructed with the set of Noether invariants of the physical system, was used by Souriau[3] to define the symplectic cohomology group $H^1_S(G,\mathcal{G}^*)$ characterizing equivalently the central extensions of a simply connected group G.

In this paper we revisit the notion of Lie group ''pseudo-cohomology'' in an attempt to classify all possible (quantizable) G-symplectic manifolds for an arbitrary Lie group G, in such a way that both coadjoint orbits and phase spaces realizing central extensions can be put together into (''pseudo''-)cohomology classes. By the way, the prefix ''pseudo'' had its origin[4] in the fact that the corresponding central extensions are trivial from the mathematical point of view, the associated cocycle being a coboundary, although they behave as if they were non-trivial in some aspects, as we shall show.

Our study here is made in the language of symplectic cohomology of Lie groups. The insight provided by the natural and explicit role of phase spaces in symplectic cohomology offers a more intuitive understanding of the significance of pseudo-cohomology in classifying dynamics, as well as an easier mathematical handling which allows a generalization of the mathematical results obtained in its original presentation.[5,6]

Roughly speaking, pseudo-cohomology emerges as a refinement of the equivalence classes of 2-cocycles in the cohomology group $H^2(G,\mathrm{U}(1))$. The first clues for the need of such a refinement occurred when studying the problem of the Inönü-Wigner contraction of centrally extended

Lie groups (see Saletan[7]). An example of this need appears in the contraction Poincaré $\rightarrow$Galileo where a special kind of trivial 2-cocycles in the Poincaré group, become true (nontrivial) 2-cocycles for the Galileo group in the $c\rightarrow\infty$ limit. The underlying reason is that, while the 2-cocycle is well-behaved in the limit, its generating function is not, thus occurring a generation of cohomology.[4] The second indication for the need of pseudo-cohomology appeared in the context of generalized Hopf fibrations of semi-simple Lie groups related to Čech (true, i.e., noncoboundary) cocycles of coadjoint orbits. Such pseudo-cocycles play in fact a fundamental role in the explicit construction of the local exponent associated with Lie-algebra cocycles of the corresponding Kac–Moody groups.[8]

In spite of these antecedents, the importance of pseudo-cohomology is more evident in the framework of Group Approach to Quantization (GAQ), a group theoretical quantization scheme designed for obtaining the dynamics of a physical system out of a Lie group.[9] In particular, GAQ starts from a central extension $\tilde{G}$ of a Lie group G by U(1) in such a way that the symplectic form of the classical phase space is derived from the 2-cocycle which defines the central extension. Nevertheless, the correspondence between central extensions and symplectic forms is not one-to-one. The most obvious illustration of this is the case of groups with trivial cohomology group $H^2(G,\mathrm{U}(1))$ (such as the Poincaré group in $3+1$ dimensions or finite-dimensional semisimple groups). In fact, even though these groups do not admit nontrivial central extensions, genuine symplectic structures and dynamics can be derived out of them.[4,8] The rationale for this is the existence of 2-cocycles which are coboundaries, and therefore trivial from the cohomological point of view, but which do define authentic symplectic structures. Coboundaries with this property are called *pseudo-cocycles*, giving rise to trivial central extension referred to as *pseudo-extensions*.

The study of this mechanism and the characterization of the classes of pseudo-extensions associated with nonequivalent symplectic structures, led in an explicit way to the notion of pseudo-cohomology, constituting the more systematic and clarifying approach to the problem.[5,6] This *standard* view of pseudo-cohomology is described in the next section.

II. PSEUDO-COHOMOLOGY IN GAQ

As commented in the introduction, GAQ is a formalism devised for obtaining the (quantum or classical) dynamics of a physical system out of a Lie group (of its symmetries). The starting point is a central extension $\tilde{G}$ of the symmetry group G by U(1) (or $\mathbb{R}$ to recover the classical dynamics), determined by a 2-cocycle (local exponent) $\xi: G\times G\rightarrow\mathbb{R}$. The group law then reads

$$g''=g'*g, \quad \zeta''=\zeta'\zeta e^{i\xi(g',g)}, \tag{1}$$

where $g'',g',g\in G$ and $\zeta'',\zeta',\zeta\in\mathrm{U}(1)$. On the Lie group $\tilde{G}$ we have at our disposal left- and right-invariant vector fields. If we choose a coordinate system $(\{g^i\}_{i=1}^{\dim G},\zeta)$ in $\tilde{G}$, a basis for the vector fields is given by $\tilde{X}_i^L$ and $\tilde{X}_i^R$, respectively, and their dual sets of left- and right-invariant 1-forms are denoted by $\theta^{L(i)}$ and $\theta^{R(i)}$, respectively. One of the left-invariant 1-forms, $\Theta\equiv\theta^{L(\zeta)}$, the U(1)-component of the left-invariant canonical 1-form on the Lie group $\tilde{G}$, is chosen as the connection 1-form of the principal bundle $\mathrm{U}(1)\rightarrow\tilde{G}\rightarrow G$, thus defining a notion of *horizontality*.

This connection 1-form, named the quantization 1-form, depends directly on the 2-cocycle ξ and can be used to define a symplectic structure in a unique manner. In fact, if $\mathcal{G}_\Theta$ is the characteristic distribution of Θ, i.e., the intersection of the kernel of Θ and $\mathrm{d}\Theta$, then $\tilde{G}/\mathcal{G}_\Theta$ is a quantum manifold P.[9,10] This means that $\tilde{G}/\mathcal{G}_\Theta$ is a contact manifold with contact 1-form $\Theta|_P$. The quantum manifold P is in turn a U(1) Principal bundle $\mathrm{U}(1)\rightarrow P\xrightarrow{\pi}S$ with base a symplectic manifold, $S=P/\mathrm{U}(1)$ endowed with a symplectic form ω such that $\pi^*\omega=\mathrm{d}\Theta$.

The symplectic structure (S,ω) is not completely determined by the cohomology class to which the 2-cocycle ξ belongs. In fact, different yet cohomologous 2-cocycles can lead to completely different symplectic structures (S,ω) (think, for instance, of a semisimple Lie group, with trivial cohomology but with many different kinds of symplectic structures determined by its coadjoit orbits). This phenomenon suggests, again, a refinement in the classification of 2-cocycles in such a way that a one-to-one correspondence between the refined classes and the symplectic structures could be established. This refinement will define pseudo-cohomology. Therefore, the latter is intrinsically tied to the classification of possible symplectic structures constructed out of a Lie group.

The main idea for the definition of these subclasses in $H^2(G,\mathrm{U}(1))$ can be intuited from the expression of Θ in terms of the 2-cocycle ξ:

$$\Theta = \frac{\mathrm{d}\zeta}{i\zeta} + \left.\frac{\partial \xi(g',g)}{\partial g^i}\right|_{g'=g^{-1}} \mathrm{d}g^i. \tag{2}$$

If, now, a 2-coboundary $\xi_\lambda(g',g)=\lambda(g'*g)-\lambda(g')-\lambda(g)$ generated by the function $\lambda: G \to \mathbb{R}$, is added to ξ, the expression for the new quantization 1-form Θ' [as the U(1)-component of the canonical 1-form for the centrally extended Lie group defined by $\xi+\xi_\lambda$] is given by

$$\Theta' = \Theta + \Theta_\lambda = \Theta + \lambda_i^0 \theta^{L(i)} - \mathrm{d}\lambda, \tag{3}$$

where $\lambda_i^0 \equiv [\partial\lambda(g)/\partial g^i]|_{g=e}$. Thus, the new term Θ_λ added to the connection 1-form Θ by the inclusion of a 2-coboundary depends only, up to a total differential, on the gradient at the identity λ^0 of the generating function $\lambda(g)$. In fact, if we denote $\Theta_{\lambda^0}=\lambda_i^0\theta^{L(i)}$, then the total differential disappears when the presymplectic 2-form $\mathrm{d}\Theta$ is considered, in such a way that $\mathrm{d}\Theta' = \mathrm{d}\Theta + \mathrm{d}\Theta_{\lambda^0}$.

From these considerations two conclusions can be drawn:

(i) A 2-coboundary contributes nontrivially to the connection 1-form Θ and to the symplectic structure determined by $\mathrm{d}\Theta$, if and only if $\lambda^0 \neq 0$.

(ii) This contribution depends only (up to a total differential, which does not affect the symplectic structure) on the local properties of the generating function $\lambda(g)$ at the identity of the group, through its gradient at the identity λ^0.

A 2-coboundary ξ_λ such that $\lambda^0 \neq 0$ is named a *pseudo-cocycle*. The name reflects the fact that they are trivial 2-cocycles but, from the dynamical point of view, behave as if they were nontrivial. If we consider the group G centrally extended by this pseudo-cocycle ξ_λ, the extended group $\tilde{G}$ is isomorphic to $G\times\mathrm{U}(1)$. However, we will refer to this extension as a *pseudo-extension*, to underline the fact that, although trivial as a central extension, it can lead to a nontrivial symplectic structure and nontrivial dynamics.

The next point to explore is the conditions under which two different 2-coboundaries, ξ_λ and $\xi_{\lambda'}$, generated by functions λ and λ' with different gradients at the identity λ^0 and λ'^0, determine the same symplectic structure (S,ω), up to symplectomorphisms. This condition will define a refined equivalence relation inside each cohomology class. For the sake of simplicity, we shall restrict ourselves to simply connected Lie groups.

The clue in the definition of the new equivalence relation is given by the fact that λ^0 defines an element of $\mathcal{G}^*$, the dual of the Lie algebra $\mathcal{G}$ of G, usually named the *coalgebra*. This can be seen by noting that $\Theta_{\lambda^0}=\lambda_i^0\theta^{L(i)}$ defines, at the identity of G, an element of $\mathcal{G}^*$ given by $\Theta_{\lambda^0}|_{g=e}=\lambda^0$. It is also important to note that $\Theta_\lambda|_{g=e}=0\in\mathcal{G}^*$ (due to the presence of $\mathrm{d}\lambda$), in such a way that the quantization 1-form Θ verifies $\Theta|_{g=e}=(0,\ldots,0,1)\in\tilde{\mathcal{G}}^*$, whatever the 2-cocycle ξ we are considering (here $\tilde{\mathcal{G}}^*$ is the dual of the extended algebra $\tilde{\mathcal{G}}$ associated with the extended group $\tilde{G}$). This fact will be of relevance in the relationship between pseudo-cohomology and symplectic cohomology.

Once we have established that $\lambda^0 \in \mathcal{G}^*$, it is natural to propose their classification in accordance with the coadjoint orbits. This will prove to be the correct ansatz, provided we use the correct coadjoint action.

A bit of notation is in order. Let us denote the equivalence class of the cocycle ξ, defining a certain central extension $\tilde{G}$ of G by U(1), by $[[\xi]] \in H^2(G,\mathrm{U}(1))$. We are going to introduce a further partition in each class $[[\xi]]$ into equivalence subclasses $[\xi]$.

For the sake of clarity, we shall firstly define this partition for the trivial cohomology class $[[\xi]]_0$, made out of trivial cocycles, i.e., 2-coboundaries ξ_λ. This would be enough for groups with trivial cohomology $H^2(G,\mathrm{U}(1))=0$ (that is, with only the trivial class), such as finite-dimensional semisimple groups or the Poincaré group (in $3+1$ dimensions). It is also valid for fully centrally extended groups $\tilde{G}$, for which $H^2(\tilde{G},\mathrm{U}(1))=0$. The case of groups with nontrivial cohomology or nonfully central-extended groups $\tilde{G}$, with $H^2(\tilde{G},\mathrm{U}(1))\neq 0$, will be considered in Sec. II B.

A. The trivial class

Given a Lie group G, a natural action of G on $\mathcal{G}^*$ is provided by the coadjoint action *Coad*, defined as the dual of the adjoint action of G on $\mathcal{G}$. More explicitly, with the adjoint action of G on $\mathcal{G}$ given by $Adg(X)=(R^T_{g^{-1}}L^T_g)(e)\cdot X$, where $g\in G$, $X\in\mathcal{G}$ and L^T_g, R^T_g stand for the tangent application to the left and right translations, respectively, the coadjoint action $Coad{:}G \rightarrow Aut(\mathcal{G}^*)$ has the form $Coad(g)\mu(X)=\mu(Adg^{-1}(X))$, where $\mu\in\mathcal{G}^*$. It is also convenient to make explicit the infinitesimal version of this action. Linearizing on the g variable we obtain the coadjoint action of the Lie algebra on the coalgebra: $(Coad)^T(e)\equiv coad{:}\mathcal{G}\rightarrow End(\mathcal{G}^*)$. Its explicit expression is given by $coadX(\mu)(Y)=\mu(ad\ \ X(Y))=\mu([X,Y])$, with $X,Y\in\mathcal{G}$ and $\mu \in \mathcal{G}^*$.

The orbits of this action are specially relevant in our study. Given a point $\mu\in\mathcal{G}^*$, the orbit through this point by the action of the whole group G is $Orb(\mu)=\{Coad(g)\mu \ / \ g\in G\}$, diffeomorphic to G/G_μ where G_μ is the isotropy group of μ. The coadjoint action determines a foliation of $\mathcal{G}^*$ in orbits, in such a way that any point belongs to one (and just one) orbit [by definition, the point μ belongs to $Orb(\mu)$], and two points in the same orbit are always connected by the coadjoint action.

Coadjoint orbits of Lie groups are interesting from the physical point of view since they possess a natural symplectic structure $[Orb(\mu),\omega]$ with the symplectic form given by

$$\omega_\nu(X_\nu,Y_\nu)=\nu([X,Y]),X_\nu,Y_\nu\in T_\nu(Orb(\mu)), \tag{4}$$

where $\nu\in Orb(\mu)\subset\mathcal{G}^*$, $X_\nu,Y_\nu\in T_\nu(Orb(\mu))$ and $X\in\mathcal{G}$ is related to $X_\nu\in T_\nu(Orb(\mu))$ by $X_\nu = coad(X)\nu$, and analogously for Y_ν and Y (note we are using the fact that $\mathcal{G}^*$ is a linear space in order to identify its points with tangent vectors).

There is a close relationship between pseudo-extensions and coadjoint orbits, that can be stated as follows. A pseudo-extension characterized by the generating function $\lambda(g)$ with gradient at the identity $\lambda^0\neq 0$ defines a presymplectic form $\mathrm{d}\Theta_\lambda=\mathrm{d}\Theta_{\lambda^0}$ depending only on λ^0. In the trivial case we are discussing in this section, the quotient of $\tilde{G}$ by the characteristic subalgebra $\mathcal{G}_{\Theta_{\lambda^0}}\equiv\ker\Theta_\lambda\cap\ker\mathrm{d}\Theta_{\lambda^0}$, defines a quantum manifold P, and the quotient $S=\tilde{G}/(G_{\Theta_{\lambda^0}}\times\mathrm{U}(1)) \sim G/G_{\Theta_{\lambda^0}}$ is a symplectic manifold with symplectic form ω_{λ^0} given by $\pi^*\omega_{\lambda^0}=\mathrm{d}\Theta_{\lambda^0}$, where $\pi{:}\ P\rightarrow S$ is the canonical projection and $G_{\Theta_{\lambda^0}}$ is the (connected) subgroup associated with $\mathcal{G}_{\Theta_{\lambda^0}}$. $G/G_{\Theta_{\lambda^0}}$ is in fact locally diffeomorphic to a coadjoint orbit (the one passing through λ^0). This can be seen by noting the following:

(a) The presymplectic form adopts the expression

$$\mathrm{d}\Theta_{\lambda^0}=\tfrac{1}{2}\lambda^0_k C^k_{ij}\theta^{L(i)}\wedge\theta^{L(j)}, \tag{5}$$

when using the Maurer–Cartan equations, and therefore,

$$d\Theta_{\lambda^0}(X_i^L, X_j^L) = \lambda_k^0 C_{ij}^k = \lambda^0([X_i^L, X_j^L]) \tag{6}$$

where $\{X_i^L\}$ is a basis for $\mathcal{G}$ and $\lambda^0 \in \mathcal{G}^*$, thus reproducing (4) (before falling down to the quotient).

(b) The characteristic group $G_{\Theta_{\lambda^0}}$ coincides with (the connected component of) the isotropy group of λ^0, G_{λ^0} under the coadjoint action, thus defining (locally) the same quotient space. At the infinitesimal level, a vector $Y = Y^i X_i^L$ belongs to $\mathcal{G}_{\Theta_{\lambda^0}}$ if $Y^i \lambda_k^0 C_{ij}^k = 0, \forall j$, which is the same condition for Y to belong to $\mathcal{G}_{\lambda^0}$.

Using the transformation properties of left-invariant 1-forms under translation by the group, it is easy to check that

$$Ad(g)^*(\Theta_{\lambda^0}) = \Theta_{Coad(g)\lambda^0}, \tag{7}$$

where $Ad(g)^*$ denotes the pull-back of the adjoint action of the group on itself (conjugation), acting on $\theta^{L(i)}$, and on the right-hand side $Coad(g)$ acts on λ^0.

Although the connection 1-form is given by Θ_λ rather than Θ_{λ^0}, the symplectic form is determined by just λ^0, and it transforms in a similar way,

$$Ad(g)^*(d\Theta_{\lambda^0}) = d\Theta_{Coad(g)\lambda^0}. \tag{8}$$

These results can be summarized in the following proposition.

Proposition 1: Let G be a Lie group and consider two coboundaries ξ_{λ_1} and ξ_{λ_2} with generating functions $\lambda_1(g)$ and $\lambda_2(g)$, defining the (trivial) central extensions $\tilde{G}_1$ and $\tilde{G}_2$, respectively. If Θ_{λ_1} and Θ_{λ_2} are the quantization one-forms associated with each group, and $G_{\Theta_{\lambda_1^0}}$ and $G_{\Theta_{\lambda_2^0}}$ their respective characteristic subgroups, the two symplectic spaces $\tilde{G}_1/(G_{\Theta_{\lambda_1^0}} \times \mathrm{U}(1))$ and $\tilde{G}_2/(G_{\Theta_{\lambda_2^0}} \times \mathrm{U}(1))$, with symplectic forms given by $\omega_{\lambda_1^0}$ and $\omega_{\lambda_2^0}$ such that $d\Theta_{\lambda_1^0} = \pi^* \omega_{\lambda_1^0}$ and $d\Theta_{\lambda_2^0} = \pi^* \omega_{\lambda_2^0}$, respectively, are symplectomorphic if there exists $h \in G$ such that

$$\lambda_1^0 = Coad(h)\lambda_2^0, \tag{9}$$

the symplectomorphism being given by $Ad(h)$:

$$d\Theta_{\lambda_1^0} = Ad(h)^* \, d\Theta_{\lambda_2^0}. \tag{10}$$

Proof: It simply remains to prove that the two spaces $\tilde{G}_1/(G_{\Theta_{\lambda_1^0}} \times \mathrm{U}(1))$ and $\tilde{G}_2/(G_{\Theta_{\lambda_2^0}} \times \mathrm{U}(1))$ are diffeomorphic. Since the extensions are trivial, $\tilde{G}_i$, $i = 1,2$ are isomorphic to $G \times \mathrm{U}(1)$, therefore $\tilde{G}_i/(G_{\Theta_{\lambda_i^0}} \times \mathrm{U}(1)) \approx G/G_{\Theta_{\lambda_i^0}}$, $i = 1,2$. If $\lambda_1^0 = Coad(h)\lambda_2^0$, then $G_{\Theta_{\lambda_1^0}}$ and $G_{\Theta_{\lambda_2^0}}$ are conjugated subgroups by the adjoint action and this implies that the two spaces $G/G_{\Theta_{\lambda_i^0}}$, $i = 1,2$ are diffeomorphic.

This suggests us to define the equivalence relation in $[[\xi]]_0$ in the following way.

Definition 1: Two coboundaries ξ_λ and $\xi_{\lambda'}$ with generating functions λ and λ', respectively, belong to the same equivalence subclass $[\xi]$ of $[[\xi]]_0$ if and only if the gradients at the identity of the generating functions are related by

$$\lambda^{0\prime} = Coad(g)\lambda^0, \tag{11}$$

for some $g \in G$.

We shall denote by $[\xi]_{\lambda^0}$ the equivalence class of coboundaries "passing through" λ^0. The equivalence relation introduced in this way will be named pseudo-cohomology, even though this

equivalence relation does not define a cohomology in the usual sense, and the subclass of (trivial) central extensions defined by all $\xi_\lambda \in [\xi]_{\lambda^0}$ will be called the central pseudo-extension associated with $[\xi]_{\lambda^0}$.

The condition $\lambda^{0\prime} = Coad(g)\lambda^0$ means that λ^0 and $\lambda^{0\prime}$ are related by the coadjoint action of the group G. Therefore, λ^0 and $\lambda^{0\prime}$ lie in the same coadjoint orbit of G in $\mathcal{G}^*$. A pseudo-cohomology class is therefore directly associated with a coadjoint orbit in $\mathcal{G}^*$.

If $\lambda^{0\prime} = \lambda^0$, then ξ_λ, $\xi_{\lambda'} \in [\xi]_{\lambda^0}$. Thus, we can always choose a representative element in each subclass "linear" in the local coordinate system, $\xi_{\lambda^0}(g) = \lambda^0_i g^i$. If the local coordinates $\{g^i\}$ are canonical, and if we restrict ourselves to canonical 2-cocycles (see Ref. 1), then two cohomologous 2-cocycles differ in a 2-coboundary ξ_λ with $\lambda(g)$ linear in the canonical coordinates. Then pseudo-cohomology is a further partition of "linear" coboundaries into equivalence classes through the coadjoint action of the group G on $\mathcal{G}^*$ (for the trivial class, at the moment).

However, the correspondence between pseudo-cohomology classes and coadjoint orbits for a Lie group G is not onto. The relation is established in the following theorem.

Proposition 2: Pseudo-cohomology classes are associated with coadjoint orbits which satisfy an integrality condition: the symplectic 2-form ω naturally defined on the coadjoint orbit by (4) has to be of integer class.

In fact, this integrality condition is required for ξ_{λ^0} to define a global coboundary on G; nonintegral coadjoint orbits of G cannot be related to central pseudo-extensions of G, since they do not define a proper (global) Lie group.

Proof: A (pseudo-)centrally extended Lie group gives rise to a quantum manifold in the sense of geometric quantization (see Sec. II) when taking quotient by the characteristic subalgebra.[9] Therefore, as a consequence of the necessary and sufficient condition for the existence of a quantization of a given symplectic manifold (see Refs. 10 and 9), the closed 2-form on the coadjoint orbit is of integer class.

Let us see another way of looking at the integrality condition. The vector λ^0 is an element of $\mathcal{G}^*$ and, therefore, it is a linear mapping from $\mathcal{G}$ to $\mathbb{R}$. It is easy to check that when restricted to $\mathcal{G}_{\lambda^0}$ (the Lie algebra of the isotropy group G_{λ^0} of the coadjoint orbit passing through λ^0), λ^0 defines a one-dimensional representation of the latter. Then, the integrality condition on the coadjoint orbit parallels the requirement for λ^0 of being exponentiable (integrable) to a unitary character of the group G_{λ^0} (note however that this remark resorts to the level of representation theory of the group, whereas the above-stated theorem involves only the Lie group structure).

This relationship between integrality condition of the coadjoint orbit and "integrality" of the character defined by λ^0 reveals, in passing, that the coadjoint orbit method of Kostant–Kirillov,[11,12] intended to obtain unitary irreducible representations of Lie groups using (what in Physics is now known as) geometric quantization[10] on coadjoint orbits of Lie groups, is a particular case of the induced representation technique of Mackey.[13]

Let us denote by $\check{G}$ the central pseudo-extension of G, characterized by ξ_{λ^0}. It defines a central pseudo-extension of $\mathcal{G}$:

$$[\check{X}^L_i, \check{X}^L_j] = C^k_{ij}(\check{X}^L_k + \lambda^0_k X_0), \tag{12}$$

where X_0 is the (central) generator associated with U(1) (our convention is to take $X_0 = iI$ in any faithful unirrep of $\check{G}$). The left-invariant vector fields of $\check{G}$ (denoted with check) are related to those of G by

$$\check{X}^L_i = X^L_i + (X^L_i \lambda - \lambda^0_i) X_0, \tag{13}$$

with a similar relation for the right-invariant vector fields.

From this point of view, central pseudo-extensions are on the same footing as true (nontrivial) central extensions, and we can employ with them the same techniques for obtaining (projective) unirreps of G (especially for semisimple Lie groups). Once a projective representation of G

(which is a true representation of $\check{G}$, the pseudo-extended group) has been obtained in this way, in order to obtain the true (nonprojective) representations of G associated with it we simply redefine the generators in the following way:

$$\check{X}_i^L \to \check{X}_i^L + \lambda_i^0 X_0 = X_i^L + (X_i^L \lambda) X_0 , \tag{14}$$

or, equivalently, redefine the functions of the Hilbert space carring the representation by multiplying them by an appropriate factor.

B. Nontrivial classes

Let us consider now nontrivial cohomology classes $[[\xi]] \neq [[\xi]]_0$, in the case of groups G with nontrivial cohomology, or extended groups $\tilde{G}$ which still admit further central extensions, that is, with $H^2(\tilde{G}, \mathrm{U}(1)) \neq 0$.

In order to proceed, a representative element $\xi \in [[\xi]]$ must be chosen. We can add to ξ a coboundary ξ_λ generated by a function λ, with nontrivial gradient at the identity of G. The resulting cocycle $\xi' = \xi + \xi_\lambda$ defines a new central extension $\tilde{G}'$ of G isomorphic, from the group-theoretical point of view, to $\tilde{G}$. The question is whether these pseudo-extensions can be classified into equivalence classes leading to the same symplectic structures, as in the case of the trivial class of Sec. II A. The naive classification in coadjoint orbits of the group G does not work in this case (since there is a mixture of true cohomology and pseudo-cohomology), and there is no clue, at this level, of how the classification should be done.

The direct relation between pseudo-cohomology and coadjoint orbits obtained for the trivial class, allows us to resort to symplectic cohomology, as a tool for classifying symplectic structures (see Sec. III), to come in our help. In this framework, it will be shown that a classification of pseudo-cocyles in the nontrivial classes is possible and entails a slight generalization with respect to that of the trivial class, in the sense that the classification should be done using the deformed coadjoint action (associated with the central extension determined by the nontrivial class we are considering).

III. SYMPLECTIC COHOMOLOGY

In the preceding section we have seen how GAQ can be used to define symplectic structures out of a Lie group, naturally leading to the notion of pseudo-cohomology. In this section we review a different approach to the discussion of the symplectic structures defined in terms of a Lie group G. First, we briefly recall the fundamentals of the so-called symplectic cohomology of G. The rationale for this structure can be found in the context of momentum mapping (Ref. 3 and below). Second, we use this mathematical structure to classify a family of symplectic spaces which generalize the ones obtained by the coadjoint action of a group G.

A. Lie group cohomology. Symplectic cohomology

Given a Lie group G, an Abelian Lie group A and a (left) action L of G on A, we define the n-cochains γ_n as mappings

$$\gamma_n : G \times \overset{n)}{\cdots} \times G \to A, \tag{15}$$

in such a way that the standard sum of mappings

$$(\gamma_n + \gamma_n')(g_1, \ldots, g_n) = \gamma_n(g_1, \ldots, g_n) + \gamma_n'(g_1, \ldots, g_n) \tag{16}$$

endows the space of n-cochains, denoted as $C_L^n(G,A)$, with the structure of an Abelian group. The coboundary operators $\delta: C_L^n(G,A) \to C_L^{n+1}(G,A)$ are defined by

$$(\delta\gamma_n)(g_1,\ldots,g_n,g_{n+1}) \equiv L(g_1)(\gamma_n)(g_2,\ldots,g_n,g_{n+1}) + \sum_{i=1}^{n} (-1)^i \gamma_n(g_1,\ldots,g_i g_{i+1},g_{i+2},\ldots,g_{n+1}) + (-1)^{n+1}\gamma_n(g_1,\ldots,g_n), \tag{17}$$

satisfying the nilpotency condition $\delta\circ\delta=0$. We can define the subspaces of n-cochains $Z^n \equiv Ker(\delta)\subset C_L^n(G,A)$, whose elements are *closed n-cochains* and $B^n\equiv \mathrm{Im}(\delta)\subset C_L^n(G,A)$, whose elements are n-coboundaries. Two exact n-cochains are equivalent if their difference is a coboundary. Cohomology groups are defined by this equivalence

$$H_L^n(G,A)=\frac{Z^n}{B^n} \tag{18}$$

and their elements are called *n-cocycles*. For the first cohomology groups the expression of (17) takes the form

$$(\delta\gamma_0)(g)=L(g)\gamma_0-\gamma_0,$$

$$(\delta\gamma_1)(g_1,g_2)=L(g_1)\gamma_1(g_2)-\gamma_1(g_1g_2)+\gamma_1(g_1),$$

$$(\delta\gamma_2)(g_1,g_2,g_3)=L(g_1)\gamma_2(g_2,g_3)+\gamma_2(g_1,g_2g_3)-\gamma_2(g_1g_2,g_3)-\gamma_2(g_1,g_2). \tag{19}$$

As we will see below, the generalization of the coadjoint action and its associated orbits naturally involves a cohomological structure. In order to address this point, we consider the general elements above and choose $A=\mathcal{G}^*$ and $L=Coad$, i.e., the coadjoint action of G on $\mathcal{G}^*$. This choice leads in particular to the cohomology group $H^1_{Coad}(G,\mathcal{G}^*)$, where a 1-cocycle $\gamma: G\rightarrow\mathcal{G}^*$ is characterized by $(\delta\gamma\equiv 0)$

$$\gamma(g'g)=Coad(g')\gamma(g)+\gamma(g'), \tag{20}$$

meanwhile a 1-coboundary has the form $(\Delta_\mu\equiv\delta\mu)$

$$\Delta_\mu=Coad(g)\mu-\mu, \quad g\in G,\mu\in\mathcal{G}^* \quad . \tag{21}$$

Symplectic cohomology $H_S(G,\mathcal{G}^*)$ is defined out of this cohomology group by restricting the 1-cocycles to functions γ which satisfy the following antisymmetry condition on its differential γ^T:

$$\gamma^T(e)(X,Y)\equiv\gamma^T(e)\cdot X(Y), \qquad \gamma^T(e)(X,Y)=-\gamma^T(e)(Y,X) \quad \forall X,Y\in\mathcal{G}. \tag{22}$$

The reason for this condition will be apparent in the next section.

For the sake of completeness, we mention that the cohomology group $H^2(G,\mathrm{U}(1))$ we found in the preceding section and which classifies the central extensions of the Lie group G, is obtained by setting $A=\mathrm{U}(1)$ and L as the trivial representation in the general construction above of Lie group cohomology. Second and third lines in (19) then define the expression of a coboundary and the cocycle condition.

B. Deformed coadjoint orbits

As we have seen in Sec. II A, orbits of the coadjoint action of a group G on its coalgebra $\mathcal{G}^*$ constitute a class of symplectic manifolds characterized in terms of group-theoretical structures.

Symplectic cohomology provides a way of introducing a notion of *affine-deformations* of coadjoints actions which allow us to generalize the notion of coadjoint orbit. Defining the mapping $g \mapsto Coad_\gamma(g)$

$$Coad_\gamma(g)\mu_0 \equiv Coad(g)\mu_0 + \gamma(g), \quad \mu_0 \in \mathcal{G}^*, \tag{23}$$

the condition for this expression to actually define a (left) action of G on $\mathcal{G}^*$, i.e., $Coad_\gamma(g'g)\mu = Coad_\gamma(g')(Coad_\gamma(g)\mu)$, reduces to expression (20), which is simply the cocycle condition in $H_S(G,\mathcal{G}^*)$.

On the other hand, and denoting the orbit of $Coad_\gamma$ through the point $\mu_0 \in \mathcal{G}^*$ by $Orb_\gamma(\mu_0)$, we note that γ functions which differ by a coboundary, (21), define the same set of orbits. In fact, since

$$Coad_{\gamma+\Delta_\mu}(g)\mu_0 = Coad_\gamma(g)\mu_0 + Coad(g)\mu - \mu = Coad_\gamma(g)(\mu+\mu_0) - \mu, \forall g \in G, \forall \mu_0 \in \mathcal{G}^*, \tag{24}$$

we realize that $Orb_{\gamma+\Delta_\mu}(\mu_0)$ and $Orb_\gamma(\mu_0+\mu)$ coincide modulo a translation by μ. Therefore, if we allow μ to vary on $\mathcal{G}^*$, each element in $H^1_{Coad}(G,\mathcal{G}^*)$ characterizes a family of orbits (modulo translations) obtained from the deformed coadjoint action on $\mathcal{G}^*$.

Finally, the antisymmetry condition on $\gamma^T(e)$ is necessary in order to define a symplectic structure on $Orb_\gamma(\mu)$. If we define

$$\Gamma(X,Y) \equiv \gamma^T(e)\cdot X(Y) \tag{25}$$

the following theorem follows (Ref. 3).

Theorem: The orbit $Orb_\gamma(\mu) \subset \mathcal{G}^*$ admits a symplectic form ω which is pointwise given by

$$\omega_\nu(X_\nu, Y_\nu) = \nu([X,Y]) + \Gamma(X,Y), \quad \nu \in Orb_\gamma(\mu), X_\nu, Y_\nu \in T_\nu(Orb_\gamma(\mu)), \tag{26}$$

where $X \in \mathcal{G}$ is related to $X_\nu \in T_\nu(Orb_\gamma(\mu))$ by $X_\nu = coad_\gamma(X)\nu$ and analogously for Y_ν and Y [where $coad_\gamma \equiv (Coad_\gamma)^T(e)$].

C. Convergence with the problem of central extensions

In Sec. II the techniques of GAQ were used in order to define a specific symplectic structure that could be used as the support for the Hamiltonian description of a classical system. The algorithm started from a U(1)-centrally extended Lie group $\tilde{G}$, where the 2-cocycle which defines the central extension permits the identification of the set of variables building the sought phase space (for concreteness, those coordinates associated with nonvertical vector fields which are absent from the characteristic module of $\Theta \equiv \theta^{L(\zeta)}$). However, the object classifying the nonisomorphic U(1)-central extensions of G, $H^2(G,\mathrm{U}(1))$, is not fine enough in order to classify the specific symplectic spaces, since some ambiguity still remains linked to the choice of the particular coboundary for the 2-cocycle.

In an analogous manner, the approach followed in this section, based on deformed coadjoint actions, permits the classification of the different classes of deformed coadjoint orbits by the elements of $H_S(G,\mathcal{G}^*)$, but not the characterization of individual symplectic spaces.

Therefore, the crucial mathematical structures of both approaches, the groups $H^2(G,\mathrm{U}(1))$ and $H_S(G,\mathcal{G}^*)$, respectively, need to be refined in order to account for such specific symplectic manifolds.

Even at this intermediate step, a nontrivial convergence occurs between the conceptually different problems of classifying the central extensions of a given Lie group G by U(1), on the one hand, and the affine deformations of the coadjoint actions on $\mathcal{G}^*$, on the other hand. In fact, the same object classifies the solutions to both problems, since $H^2(G,\mathrm{U}(1)) \approx H_S(G,\mathcal{G}^*)$.

Although we shall dwell on this point in Sec. III C 2, we can outline this equivalence by noting that, for simply connected groups, the isomorphism $H^2(\mathcal{G},\mathrm{U}(1)) \approx H^2(G,\mathrm{U}(1))$ is satisfied

and therefore it is enough to discuss the equivalence at the infinitesimal level. (On behalf of concision, we avoid a presentation of Lie algebra cohomology and refer the reader to standard references like Ref. 14. We just note that for simply connected groups, Lie algebra cohomology emerges as an infinitesimal version of Lie group cohomology.) In fact, the cocycle condition (20) implies the following condition on its differential $\Gamma(X,Y)$:

$$\Gamma([X,Y],Z)+\Gamma([Y,Z],X)+\Gamma([Z,X],Y)=0, \tag{27}$$

which, together with the antisymmetry condition (22), $\Gamma(X,Y)=-\Gamma(Y,X)$ defines a 2-cocycle in $H^2(\mathcal{G},\mathrm{U}(1))$ [from the point of view of the central extensions of the Lie algebra $\mathcal{G}$ (27) is simply the Jacobi identity for the central generator in the Lie algebra; see Ref. 14]. Likewise the infinitesimal expression of the coboundary condition (21) implies

$$\Gamma_{cob}(X,Y)=\mu([X,Y]) \quad \text{for some} \quad \mu\in\mathcal{G}^*, \tag{28}$$

which is the coboundary condition in $H^2(\mathcal{G},\mathrm{U}(1))$.

In Sec. II, pseudo-extensions have been introduced as the element necessary to account for the specific symplectic manifolds, that we can construct out of a Lie group G via a central extension of it. However the discussion was carried out only for the trivial class of $H^2(G,\mathrm{U}(1))$. For the nontrivial cohomology classes the analysis was not so straightforward. However the convergence with the approach based on symplectic cohomology, and which aims directly at the problem of defining symplectic structures completely in terms of a Lie group, sheds a new light on the problem. From this perspective, the characterization of a specific symplectic structure for a (in general nontrivial) cohomology class γ of $H^2(\mathcal{G},\mathrm{U}(1))\approx H^2(G,\mathrm{U}(1))$, simply parallels the characterization of a particular orbit in the family of orbits defined by $Coad_\gamma$.

1. Singularization of coadjoint orbits in symplectic cohomology

In order to singularize a specific symplectic manifold out of the family defined by a cocycle in $H_S(G,\mathcal{G}^*)$, i.e., in order to characterize a particular deformed coadjoint orbit, we have two options.

(i) We can fix a pair (γ,μ_0), where γ specifies the cocycle which defines the deformation of the action and μ_0 precises a point in the orbit. In this case, varying the second entry we scan all the possible orbits.

(ii) Alternatively, we can fix the point μ_0 in the coalgebra and vary instead the representative of the cocycle γ by modifying the coboundary, Δ_μ. Since the coalgebra is a linear space, there is a canonical choice for the fixed point μ_0: the zero vector. We can see from expression (24) that the set of spaces constructed this way is the same that the one derived with option (i), although translated with respect to them in such a way that all these spaces share the zero vector in $\mathcal{G}^*$.

However both characterizations are redundant since different pairs (γ,μ_0), or alternatively different specific representatives $\gamma+\Delta_\mu$, give rise essentially to the same orbits. Therefore it is necessary to establish an equivalence relationship in order to eliminate this ambiguity. The analysis of Sec. II A. establishing the relationship between specific symplectic structures and pseudo-cohomology understood as a refinement of a true cohomology, suggests us to choose the characterization (ii) for the deformed orbits. In fact, it directly leads to a refinement of symplectic cohomology, intrinsically tied to group cohomology.

In this sense we have to determine under which conditions two coboundaries Δ_μ and $\Delta_{\mu'}$ generate the same orbit. A direct computation shows that if there exists an element $h\in G$ such that $\mu=Coad_\gamma(h)\mu'$ (that is, if μ and $\mu'\in\mathcal{G}^*$ belong to the same γ-orbit) then

$$Coad_{\gamma+\Delta_\mu}(g)\,0=Coad_{\gamma+\Delta_{\mu'}}(gh)\,0+\mu'-\mu \quad \forall g\in G. \tag{29}$$

Since $\mu'-\mu$ is independent of g, spaces spanned by the action of $Coad_{\gamma+\Delta_\mu}$ and $Coad_{\gamma+\Delta'_\mu}$ through the zero in $\mathcal{G}^*$ coincide, modulo a rigid translation. These orbits are trivially symplectomorphic, the symplectomorphism being this translation in $\mathcal{G}^*$.

Summarizing with the language of symplectic cohomology, individual symplectic spaces associated with deformed coadjoints actions are classified by refinement of symplectic cohomology in such a way that two coboundaries Δ_μ and $\Delta_{\mu'}$ are equivalent if μ and μ' belong to the same γ-orbit. In other words, these individual symplectic spaces are classified by elements $\mu\in\mathcal{G}^*$ modulo the corresponding γ-deformed coadjoint action. Note the similarity with Definition 1, to which it directly generalizes in the context of deformed coadjoint orbits.

2. Pseudo-cohomology from symplectic cohomology

In this section we see in a more systematic way the close relation between pseudo-cohomology and symplectic cohomology for the nontrivial classes $(H^2(G,\mathrm{U}(1))\neq 0)$. The idea is to investigate how the coadjoint action *Coad* of G on $\mathcal{G}^*$ is modified by a central extension. The result is that when G is centrally extended by a 2-cocycle ξ, the coadjoint action of the extended group $\tilde{G}$, denoted by $\widetilde{Coad}$, acting on $\tilde{\mathcal{G}}^*=\mathcal{G}^*\times\mathbb{R}$, turns out to be

$$\widetilde{Coad}(\tilde{g})\tilde{\mu}=(Coad(g)\mu+\mu_\zeta F(g),\mu_\zeta), \tag{30}$$

where $\tilde{g}=(g,\zeta)\in\tilde{G}$, $\zeta\in\mathrm{U}(1)$ and $\tilde{\mu}=(\mu,\mu_\zeta)\in\tilde{\mathcal{G}}^*$. Here $F(g)\in\mathcal{G}^*$, and it is related to the 2-cocyle ξ through the quantization 1-form θ, by $F_i(g)=i_{\tilde{X}_i^R}\Theta$. These functions are nothing other than the Noether invariants of the classical theory.[9] Observe that $\widetilde{Coad}(\tilde{g})$ does not depend on ζ, and that μ_ζ does not change by this extended action [these two facts are related to the central character of U(1)]. Since the case $\mu_\zeta=0$ reproduces the original coadjoint action *Coad* of G, let us suppose $\mu_\zeta\neq 0$.

From (30) it can be derived that $\widetilde{Coad}(g)$ can be restricted to the foliations of $\tilde{\mathcal{G}}^*$ of constant μ_ζ, which can be identified with $\mathcal{G}^*$. Since $\widetilde{Coad}$ is an action, so it is its restriction, and this implies that $F(g)$ must verify the condition (this relation can also be checked by direct computation):

$$F(g'g)=Coad(g')F(g)+F(g'). \tag{31}$$

Therefore Noether invariants are nothing other than 1-cocycles for the coadjoint action *Coad* of G. Even more, they are symplectic, since its differential at the identity is precisely the Lie algebra 2-cocycle. Therefore, $\widetilde{Coad}$ can be identified with a deformed coadjoint action $Coad_\gamma$, with $\gamma(g)=\mu_\zeta F(g)$.

Without losing generality, we can take $\mu_\zeta=1$. Let us see what happens to $Coad_\gamma$ when we add to ξ a coboundary ξ_λ generated by $\lambda(g)$. A simple calculation shows that γ changes to $\gamma'=\gamma+\gamma_\lambda$, where γ_λ is given by

$$\gamma_\lambda(g)=Coad(g)\lambda^0-\lambda^0. \tag{32}$$

Surprisingly, γ_λ is a symplectic coboundary, associated with $\lambda^0\in\mathcal{G}^*$, and, what is more important, it depends just on λ^0, not on the particular choice of λ. This simple relation has deep consequences since it provides the close relation between pseudo-cocycles and symplectic cohomology. It also guides us in the correct definition of subclasses of pseudo-cocycles for the nontrivial case, using the characterization of single coadjoint orbits found in the symplectic cohomology setting (see Sec. III C 1).

According to this, and since the quantization 1-form Θ for any central extension $\tilde{G}$ characterized by the 2-cocycle ξ always verifies $\Theta|_e=(0,0,\ldots,1)$ (that is, $\mu=0$ and $\mu_\zeta=1$), we can singularize a deformed orbit in $\mathcal{G}^*$ by considering

$$\widetilde{Coad}(\tilde{g})\,\Theta|_e=(Coad_\gamma(g)\,0,1)=(Coad(g)\,0+F(g),1)=(F(g),1). \tag{33}$$

That is, this orbit is the image of the Noether invariants. This fact simply affirms that Noether invariants parametrize classical phase spaces.

The question now is that if we add to the 2-cocycle ξ a pseudo-cocycle ξ_λ generated by $\lambda(g)$ with gradient at the identity λ^0, does it define a new deformed coadjoint orbit? Can we define an equivalence relation among pseudo-cocycles as for the case of the trivial class?

Again, from the symplectic cohomology framework (see Sec. III C 1), we have the answer. First we define the following.

Definition 2: Two coboundaries ξ_λ and $\xi_{\lambda'}$ with generating functions λ and λ', respectively, define two cocycles $\xi+\xi_\lambda$, $\xi+\xi_{\lambda'}$ belonging to the same equivalence subclass $[\xi]$ of $[[\xi]]$ if and only if the gradients at the identity of the generating functions are related by

$$\lambda^{0\prime} = Coad_\gamma(g)\lambda^0, \tag{34}$$

for some $g \in G$, where $Coad_\gamma$ stands for the deformed coadjoint action, which is equivalent to the coadjoint action $\widetilde{Coad}$ of $\tilde{G}$ on $\tilde{\mathcal{G}}^* = \mathcal{G}^* \times \mathbb{R}$, where $\tilde{G}$ is the central extension associated with the two-cocycle ξ.

According to this definition, equivalent pseudo-extensions (for the nontrivial class $[[\xi]]$) are determined by generating functions whose gradient at the identity lie in the same coadjoint orbit of $\tilde{G}$.

The ultimate justification of this definition is the following proposition.

Proposition 3: Given a Lie group G and a 2-cocycle ξ on G, consider the two coboundaries ξ_{λ_1} and ξ_{λ_2} with generating functions $\lambda_1(g)$ and $\lambda_2(g)$. Define the central extensions $\tilde{G}_1$ and $\tilde{G}_2$ characterized by the two-cocycles $\xi+\xi_{\lambda_1}$ and $\xi+\xi_{\lambda_2}$, respectively, and construct the quantization 1-forms $\Theta_1 = \Theta + \Theta_{\lambda_1}$ and $\Theta_2 = \Theta + \Theta_{\lambda_2}$, following expressions (2) *and* (3). *The two symplectic spaces $\tilde{G}_1/(G_{\Theta_1} \times U(1))$ and $\tilde{G}_2/(G_{\Theta_2} \times U(1))$, with symplectic forms ω_1 and ω_2, such that $d\Theta_1 = \pi^*\omega_1$ and $d\Theta_2 = \pi^*\omega_2$, respectively, are symplectomorphic if there exists $h \in G$ such that*

$$\lambda_1^0 = Coad_\gamma(h)\lambda_2^0, \tag{35}$$

the symplectomorphism being given by $\widetilde{Ad}(\tilde{h})$,

$$d\Theta_1 = (\widetilde{Ad}(\tilde{h}))^*\, d\Theta_2, \tag{36}$$

where $\tilde{h}$ is such that $p(\tilde{h}) = h$, with $p: \tilde{G} \to G$ the canonical projection.

Proof: Even though the result can be shown by direct calculation, the most straightforward derivation comes from splitting the central extension into two steps. First, the central extension by ξ alone is constructed, and this group $\tilde{G}$ is taken as the departing point for a second trivial extension by ξ_{λ_1} and ξ_{λ_2}. The study of the trivial class in $\tilde{G}$ amounts for the study of that nontrivial class in G characterized by the cocycle ξ. At this point we can apply Proposition 1 to the trivial extension of $\tilde{G}$ and then take advantage of the identification between the nontrivial part ($\mathcal{G}^*$-component in $\tilde{\mathcal{G}}^*$) of $\widetilde{Coad}$ in $\tilde{G}$ and $Coad_\gamma$ in G, which follows from expression (30) and its subsequent discussion. This leads directly to the claimed result.

As in the case of the trivial class, the correspondence between pseudo-cohomology classes in $[[\xi]]$ and ''deformed'' coadjoint orbits in $\mathcal{G}^*$ is not onto. Only when we demand these coadjoint orbits to satisfy the integrality condition (that is, to be quantizable), the correspondence with pseudo-cohomology classes is one-to-one. The proof of this statement is the same as in the trivial case, see Ref. 9.

IV. SIMPLE PHYSICAL EXAMPLES

For the sake of completeness we shall include some simple examples of relevant elementary physical phase spaces which can be obtained along the general lines here drawn.

A. The Poincaré group in 1+1 dimensions

The simplest physical example of a phase space associated with a pseudo-cocycle corresponds to the $1+1$ dimensional relativistic particle. The ordinary Poincaré group in $3+1$ dimensions is the semidirect product of the Lorentz group (SO(3,1)) by the four-dimensional space–time translations. In $1+1$ dimensions, any element g can be parametrized by two space–time translations x^0, x, and the boost velocity $v \equiv c\,\mathrm{th}\,\chi$ in SO(1,1), or $u=\gamma v$, where $\gamma = 1/\sqrt{1-v^2/c^2}$.

We should comment that although the standard $3+1$ Poincaré group has trivial cohomology, the $1+1$-Poincaré group admits a nontrivial cocycle associated with the space–time translation subgroup. However, we shall disregard this cocycle, which has no $3+1$ dimensional analogue (that is, we shall restrict ourselves to the trivial cohomology class). We dwell, therefore, on the setting of Sec. II A.

The composition law, in terms of the parametrization $(x^0 \equiv ct, x, u)$, is

$$x^{0\prime\prime} = x^{0\prime} + \gamma' x^0 + \frac{u'}{c} x,$$

$$x'' = x' + \gamma' x + \frac{u'}{c} x^0,$$

$$u'' = \gamma u' + \gamma' u. \tag{37}$$

Right- and left-invariant vector fields are easily obtained by deriving the group law,

$$X^L_{x^0} = \gamma \frac{\partial}{\partial x^0} + \frac{u}{c}\frac{\partial}{\partial x}, \quad X^R_{x^0} = \frac{\partial}{\partial x^0},$$

$$X^L_{x} = \gamma \frac{\partial}{\partial x} + \frac{u}{c}\frac{\partial}{\partial x^0}, \quad X^R_{x} = \frac{\partial}{\partial x},$$

$$X^L_{u} = \gamma \frac{\partial}{\partial u}, \quad X^R_{u} = \gamma \frac{\partial}{\partial u} + \frac{x^0}{c}\frac{\partial}{\partial x} + \frac{x}{c}\frac{\partial}{\partial x^0}\ . \tag{38}$$

The Lie algebra $\mathcal{G}$ of the $1+1$ Poincaré group is the one satisfied by, say, left-invariant vector fields,

$$[X^L_{x^0}, X^L_x] = 0,$$

$$[X^L_{x^0}, X^L_u] = -\frac{1}{c} X^L_x, \tag{39}$$

$$[X^L_x, X^L_u] = -\frac{1}{c} X^L_{x^0},$$

and the Casimir for this algebra is $\hat{C} = (X^L_{x^0})^2 - (X^L_x)^2$.

The left-invariant 1-forms (dual to the set of left-invariant vector fields) are given by

$$\theta^{L(x^0)} = \gamma\, \mathrm{d}x^0 - \frac{u}{c}\mathrm{d}x,$$

$$\theta^{L(x)} = -\frac{u}{c}\mathrm{d}x^0 + \gamma\, \mathrm{d}x,$$

$$\theta^{L(u)} = \frac{1}{\gamma}\mathrm{d}u\ . \tag{40}$$

We can parametrize a vector λ^0 in $\mathcal{G}^*$ by its expansion coefficients in the basis associated with, say, the left-invariant forms on the group, $\theta^{L(i)}$, at the identity e of the group. That is, $\lambda^0 = -P_0\theta^{L(x^0)}|_e + P\theta^{L(x)}|_e - K\theta^{L(u)}|_e$ (the minus signs are chosen for convenience, to reproduce standards results).

We shall construct all possible pseudo-extensions of the $1+1$ Poincaré group by means of an arbitrary pseudo-cocycle generated by a function with nontrivial gradient $\lambda^0 \in \mathcal{G}^*$ at the identity. Let us define the generating function $\lambda(g) = -P_0x^0 + Px - Ku$, whose gradient at the identity is λ^0 (note that we have chosen a linear function in the coordinates).

The question is how many different (nonequivalent) pseudo-extensions can we construct for the $1+1$ Poincaré group. The answer, as we already know, is given by the different coadjoint orbits in $\mathcal{G}^*$.

The generating function $\lambda(g)$ previously introduced defines a pseudo-cocycle $\xi_\lambda = \lambda(g'*g) - \lambda(g') - \lambda(g)$,

$$\xi_\lambda(g',g) = -P_0\left((\gamma'-1)x^0 + \frac{u'}{c}x\right) + P\left((\gamma'-1)x + \frac{u'}{c}x^0\right) - K((\gamma-1)u' + (\gamma'-1)u). \tag{41}$$

This defines a central pseudo-extension $\tilde{G}$ of G by U(1), with group law given by (37) together with

$$\zeta'' = \zeta'\zeta e^{i\xi_\lambda(g',g)}. \tag{42}$$

Left- and right-invariant vector fields for the pseudo-extended group are ($X_0 = \partial/\partial\phi$, $\phi = -i\ln\zeta$)

$$\begin{aligned}
\tilde{X}^L_{x^0} &= \gamma\frac{\partial}{\partial x^0} + \frac{u}{c}\frac{\partial}{\partial x} + \left(-P_0(\gamma-1) + P\frac{u}{c}\right)X_0,\\
\tilde{X}^L_{x} &= \gamma\frac{\partial}{\partial x} + \frac{u}{c}\frac{\partial}{\partial x^0} + \left(-P_0\frac{u}{c} + P(\gamma-1)\right)X_0,\\
\tilde{X}^L_{u} &= \gamma\frac{\partial}{\partial u} + K(\gamma-1)X_0,\\
\tilde{X}^R_{x^0} &= \frac{\partial}{\partial x^0},\\
\tilde{X}^R_{x} &= \frac{\partial}{\partial x},\\
X^R_{u} &= \gamma\frac{\partial}{\partial u} + \frac{x^0}{c}\frac{\partial}{\partial x} + \frac{x}{c}\frac{\partial}{\partial x^0} + \left(-P_0\frac{x}{c} + P\frac{x^0}{c} - K(\gamma-1)\right)X_0.
\end{aligned} \tag{43}$$

The Lie algebra $\tilde{\mathcal{G}}$ of the pseudo-extended group is

$$\begin{aligned}
[\tilde{X}^L_{x^0}, \tilde{X}^L_{x}] &= 0,\\
[\tilde{X}^L_{x^0}, \tilde{X}^L_{u}] &= -\frac{1}{c}(\tilde{X}^L_{x} + PX_0),\\
[\tilde{X}^L_{x}, \tilde{X}^L_{u}] &= -\frac{1}{c}(\tilde{X}^L_{x^0} - P_0X_0).
\end{aligned} \tag{44}$$

The quantization 1-form is given by

$$\Theta = \frac{d\zeta}{i\zeta} - P_0\theta^{L(x^0)} + P\theta^{L(x)} - K\theta^{L(u)} - d\lambda$$

$$= \frac{d\zeta}{i\zeta} - P_0(\theta^{L(x^0)} - dx^0) + P(\theta^{L(x)} - dx) - K(\theta^{L(u)} - du), \tag{45}$$

where $\theta^{L(i)}$ are given by Eq. (40). The characteristic subalgebra is generated by $\mathcal{G}_\Theta = \langle P_0\tilde{X}^L_{x^0} + P\tilde{X}^L_x\rangle$.

The Noether invariants are defined as $F_i = i_{\tilde{X}^R_i}\Theta$, which can be rewritten as $F_i = i_{X^R_i}\theta^{L(j)}\lambda^0_j - \lambda^0_i$, where $i_{X^R_i}\theta^{L(j)}$ turn out to be the matrix elements associated with the coadjoint action. That is, for the case of trivial cohomology (or the trivial cohomology class), Noether invariants coincide with symplectic coboundaries γ_λ [see Eq. (32)]. In this case, the coadjoint action is given by the matrix

$$Coad(x^0,x,u) = \begin{pmatrix} \gamma & -\frac{u}{c} & 0 \\ -\frac{u}{c} & \gamma & 0 \\ \frac{\gamma x}{c} - \frac{ux^0}{c^2} & \frac{\gamma x^0}{c} - \frac{ux}{c^2} & 1 \end{pmatrix}. \tag{46}$$

The Noether invariants prove to be, then

$$F_{x^0} = -(\gamma - 1)P_0 - \frac{u}{c}P,$$

$$F_x = \frac{u}{c}P_0 + (\gamma - 1)P,$$

$$F_u = -\left(\frac{\gamma x}{c} - \frac{ux^0}{c^2}\right)P_0 + \left(\frac{\gamma x^0}{c} - \frac{ux}{c^2}\right)P. \tag{47}$$

The Noether invariants are not independent but, rather, they satisfy the relation

$$(F_{x^0} - P_0)^2 - (F_x + P)^2 = P_0^2 - P^2 \equiv C. \tag{48}$$

The function $C:\mathcal{G}^* \to \mathbb{R}$ is named a Casimir function, and it is invariant under the coadjoint action. Casimir functions are closely related to Casimir operators, in fact they can be considered the classical (commutative) version of the Casimir operators. Since they are invariant under the coadjoint action, coadjoint orbits are included in the level sets of the Casimir functions.

With the help of the Casimir functions we can obtain the coadjoint orbits in $\mathcal{G}^*$ avoiding their direct computation, which can be rather involved. For the case of the $1+1$ Poincaré group there is a single Casimir function, the one already found $C = P_0^2 - P^2$, whose level sets are conics since it is a quadratic function. We should only care about the fact that level sets can be disconnected (coadjoint orbits of connected Lie groups are connected) or, even nondifferentiable manifolds. In these cases, the level set is the disjoint union of two or more (even infinite) coadjoint orbits.

Three cases should be distinguished: $C>0, C<0$, or $C=0$.

(1) In the case $C>0$ we have $P_0 = \pm\sqrt{C+P^2}$ and $K \in \mathbb{R}$. This is the translation in the K axis of the upper and lower hyperbolas, with vertices $(\pm\sqrt{C},0,K)$, respectively.

(2) In the case $C<0$ we have $P=\pm\sqrt{C+P_0^2}$ and $K\in\mathbb{R}$. This is the translation in the K axis of the left and right hyperbolas, with vertices $(0,\pm\sqrt{-C},K)$, respectively.
(3) In the case $C=0$ we have $P_0=\pm P$ and $K\in\mathbb{R}$. This is the union of four half-planes, $(\pm P,P,K)$ with either $P>0$ or $P<0$, and $K\in\mathbb{R}$, and the union of zero-dimensional coadjoint orbits $(0,0,K)$, $K\in\mathbb{R}$.

Physically, the case $C>0$ corresponds to the mass shell condition $P_0^2-P^2=C=m^2c^2$, representing relativistic particles with rest mass $m=\pm\sqrt{C}/c$, or particles with positive and negative energies $P_0=\pm\sqrt{m^2c^2+P^2}$ (they can be also interpreted as particles moving forward and backward in time). The case $C<0$ corresponds to tachyons with "imaginary mass" $m=\sqrt{C}/c$ moving in the right and left directions (with $P>0$ or $P<0$, respectively). And the case $C=0$ corresponds to photons moving forward and backward in time and in the right and left direction.

When passing to $3+1$ dimensions, and discarding the spin, the case $C>0$ remains essentially the same, the two sheets (for each value of C) of the mass shell condition. The case $C<0$, due to rotations, become a single connected orbit for each value of C (a particle moving to the right can be converted to a particle moving to the left by a rotation). In the case $C=0$, the four half-planes become two coadjoint orbits, associated with the future and past light cones. The zero-dimensional orbits $(0,0,K)$ with $K\neq 0$ do not have a counterpart in $3+1$ dimensions [the origin $(0,0,0)$ is always a zero dimensional orbit for any Lie group].

Now we select a particular point λ^0 in each coadjoint orbit, which will be used to define a pseudo-extension of the $1+1$ Poincaré group (different choices of λ^0 in the same coadjoint orbit will lead to equivalent pseudo-extensions). For the case $C=m^2c^2>0$, the easiest choice is $\lambda^0=(\pm mc,0,0)$ [note that, by our sign convention, particles with positive energy are associated with $(-mc,0,0)$]. For the case $C<0$, we can use $\lambda^0=(0,\pm\sqrt{-C},0)$, and for the case $C=0$ we use $\lambda^0=(\pm\nu,\pm\nu,0)$ with $\nu>0$.

Finally, all coadjoint orbits satisfy the integrality condition, therefore there is a one-to-one correspondence between coadjoint orbits and pseudo-cohomology classes for this group.

Group contraction Poincaré→Galileo

Coming back to the original motivation for pseudo-cohomology in terms of Inönü–Wigner contractions, we shall present an example of generation of cohomology from pseudo-cohomology by means of group contraction.

In general, given a pseudo-cohomology class and the corresponding quantization group $\tilde{G}$, with quantization 1-form Θ, an Inönü–Wigner contraction with respect to the characteristic subgroup G_Θ of Θ automatically leads to a contracted group $\tilde{G}_c$ which proves to be a nontrivial extension by U(1) of the contraction G_c of G by the same subgroup G_Θ.

Let us consider the pseudo-cohomology class of the $1+1$ Poincaré group associated with the upper sheet of the mass-shell $P_0^2-P^2=m^2c^2$. We can choose as representative point $\lambda^0=(-mc,0,0)$, and consider the pseudo-extension associated with the pseudo-cocycle ξ_λ with generating function,

$$\lambda(g)=-mcx^0, \tag{49}$$

so that

$$\xi_\lambda(g',g)=-mc(x^{0\prime\prime}-x^{0\prime}-x^0)=-mc\left((\gamma'-1)x^0+\frac{u'}{c}x\right)=-(p^{0\prime}-mc)x^0-p'x, \tag{50}$$

where $p\equiv mu$ and $p^0\equiv\sqrt{m^2c^2+p^2}=mc\,\gamma$.

We should realize that in the nonrelativistic limit, $c\to\infty$, ξ_λ is well-behaved, in fact

$$\xi_\lambda\to\xi_m\equiv-mv'x-\tfrac{1}{2}mv'^2t, \tag{51}$$

which coincides with the true cocycle of the $1+1$ version of the Galilei group (64) (see the next section), whereas λ, itself, proves to be ill-defined.

Particularizing (43) for this case we have the left-invariant vector fields,

$$\tilde{X}^L_{x^0}=\gamma\frac{\partial}{\partial x^0}+\frac{u}{c}\frac{\partial}{\partial x}-mc(\gamma-1)X_0,$$

$$\tilde{X}^L_{x}=\gamma\frac{\partial}{\partial x}+\frac{u}{c}\frac{\partial}{\partial x^0}-muX_0,$$

$$\tilde{X}^L_{u}=\gamma\frac{\partial}{\partial u} \tag{52}$$

with commutation relations

$$[\tilde{X}^L_{x^0},\tilde{X}^L_{x}]=0,$$

$$[\tilde{X}^L_{x^0},\tilde{X}^L_{u}]=-\frac{1}{c}\tilde{X}^L_{x},$$

$$[\tilde{X}^L_{x},\tilde{X}^L_{u}]=-\frac{1}{c}(\tilde{X}^L_{x^0}-mcX_0), \tag{53}$$

and it should be again remarked that, under the nonrelativistic limit, (53) goes to the $1+1$ version of the Galilean algebra (68).

The left-invariant 1-form Θ is

$$\Theta=p\,\mathrm{d}x-(p^0-mc)\mathrm{d}x^0+\frac{\mathrm{d}\zeta}{i\zeta}, \tag{54}$$

and its differential

$$\mathrm{d}\Theta=\mathrm{d}p\wedge\mathrm{d}x-\frac{p}{p^0}\mathrm{d}p\wedge\mathrm{d}x^0 \tag{55}$$

is a presymplectic form that, taking quotient by the characteristic subalgebra, becomes the symplectic form on the upper sheet of the mass-shell $P_0^2-P^2=m^2c^2$, i.e., the co-adjoint orbit of mass m in the co-algebra of the Poincaré group. The symplectic structure also goes, in the limit $c\to\infty$, to the symplectic structure of the $1+1$ version of the Galilei group (69) and (70).

B. Phase space of the nonrelativistic spinning particle

The next example corresponds to a family of phase spaces associated with a refinement of a nontrivial cohomology class in the $3+1$ Galilei group. In order to illustrate the ideas in Sec. III, we first discuss the classification of these spaces as orbits of deformed coadjoint actions [in the spirit of option (ii) in Sec. III C 1], and then we present the results in the framework of central extensions (Sec. III C 2).

1. Deformed coadjoint orbits

Let us explicitly write the composition law of the $3+1$ Galilei group,

$$\begin{aligned}
t''&=t'+t,\\
\vec{x}\,''&=\vec{x}\,'+R(\vec{\epsilon}\,')\vec{x}+\vec{v}\,'t,\\
\vec{v}\,''&=\vec{v}\,'+R(\vec{\epsilon}\,')\vec{v},\\
\vec{\epsilon}\,''&=\sqrt{1-\frac{\epsilon'^2}{4}}\,\vec{\epsilon}+\sqrt{1-\frac{\epsilon^2}{4}}\,\vec{\epsilon}\,'-\frac{1}{2}\vec{\epsilon}\,'\times\vec{\epsilon},
\end{aligned} \tag{56}$$

where the rotation matrix $R(\vec{\epsilon})$ has the explicit form

$$R(\vec{\epsilon})=(1-\epsilon^2/2)I-\sqrt{1-\frac{\epsilon^2}{4}}\,\vec{\epsilon}\times\,\cdot+\frac{1}{2}(\vec{\epsilon}\cdot\ \ )\vec{\epsilon}\,. \tag{57}$$

We can parametrize a vector μ in the coalgebra by its expansion coefficients in the basis associated with the left-invariant forms, $\theta^{L(i)}$, at the identity element e of the group. That is, $\mu=-E\,\theta^{L(t)}|_e+P_i\theta^{L(x^i)}|_e-Q_i\theta^{L(v^i)}|_e+J_i\theta^{L(\epsilon^i)}|_e$. The coadjoint action, $Coad(t,\vec{x},\vec{v},\vec{\epsilon})$, has then the expression

$$\begin{gathered}(-E',\vec{P}',-\vec{Q}',\vec{J}')=Coad(t,\vec{x},\vec{v},\vec{\epsilon})(-E,\vec{P},-\vec{Q},\vec{J})\\ E'=E+\vec{v}\cdot R(\vec{\epsilon})\vec{P},\\ \vec{P}'=R(\vec{\epsilon})\vec{P},\\ \vec{Q}'=R(\vec{\epsilon})\vec{Q}-tR(\vec{\epsilon})\vec{P},\\ \vec{J}'=R(\vec{\epsilon})\vec{J}+\vec{x}\times R(\vec{\epsilon})\vec{P}-\vec{v}\times R(\vec{\epsilon})\vec{Q}.\end{gathered} \tag{58}$$

As discussed previously, the study of the symplectic manifolds obtained by deforming this coadjoint action demands the introduction of a symplectic cocycle γ. In the case of the $3+1$ Galilei group, there exists a one-dimensional family (vector space) of nontrivial cohomology classes. A representative (a basis) for this family can be chosen as[3]

$$\gamma_m(t,\vec{x},\vec{v},\vec{\epsilon})=m(-\tfrac{1}{2}\vec{v}\cdot\vec{v},\vec{v},-\vec{x}+\vec{v}t,\vec{x}\wedge\vec{v}), \tag{59}$$

where the parameter m will be related to the mass of the free particle. In order to classify the symplectic manifolds, we construct different representatives of the symplectic cocycle by first correcting γ_m with a symplectic coboundary Δ_μ and, then, applying $Coad_{\gamma_m+\Delta_\mu}$ to the 0 vector. Choosing as the generator of the coboundary the vector $\mu=(-E_0,0,0,j\vec{n})$, where $\vec{n}$ is an arbitrary unit vector and E_0 is considered the ''internal energy,'' we find

$$\Delta_\mu=Coad(t,\vec{x},\vec{v},\vec{\epsilon})(-E_0,0,0,j\vec{n})-(-E_0,0,0,j\vec{n})=(0,0,0,jR(\vec{\epsilon})\vec{n}-j\vec{n}). \tag{60}$$

The orbits are then generated by the action

$$\begin{gathered}Coad_{\gamma_m+\Delta_\mu}(t,\vec{x},\vec{v},\vec{\epsilon})0=\left(-\frac{m}{2}\vec{v}\cdot\vec{v},m\vec{v},-m(\vec{x}-\vec{v}t),m\vec{x}\wedge\vec{v}+jR(\vec{\epsilon})\vec{n}-j\vec{n}\right),\\ \forall t,\vec{x},\vec{v},\vec{\epsilon}.\end{gathered} \tag{61}$$

From this expression, one can characterize the orbits as subspaces in $\mathbb{R}^{1+3+3+3}$ defined by the constraints

$$E=\frac{1}{2m}\vec{P}^2,\quad (\vec{J}-(m\vec{x}\wedge\vec{v}-j\vec{n}))^2=j^2. \tag{62}$$

In the case $j\neq 0$, this is an eight-dimensional space, which can be seen as the topological product of $\mathbb{R}^{3+3}$ parametrized by the position and momentum of the particle, $(\vec{Q},\vec{P})$, times a sphere of radius j related to a *spinning* angular momentum. These orbits could be regarded as the classical

phase space for the quantization of the free particle with mass m and spin j. In the case $j=0$, the second constraint expands into three, $\vec{J}=\vec{x}\wedge m\vec{v}$, giving rise to the six-dimensional phase space of a particle without spin.

Finally, we note that these spaces in fact exhaust all possible orbits. This can be seen by using the result that orbits are classified by elements $\mu\in\mathcal{G}^*$ modulo γ-orbits: Δ_μ and $\Delta_{\mu'}$ give rise (modulo a rigid translation) to the same orbit if and only if the relation $\mu'=Coad_\gamma(h)\mu$ holds for some h. In our case, $\mu=(-E_0,0,0,j\vec{n})$, and denoting $h=(t,\vec{x},\vec{v},\vec{\epsilon})$, we find

$$\mu'=\left(-E_0-\frac{m}{2}\vec{v}\cdot\vec{v},m\vec{v},-m(\vec{x}-\vec{v}t),jR(\vec{\epsilon})\vec{n}+m\vec{x}\wedge\vec{v}\right). \tag{63}$$

Under free variation of the parameters in this expression, $\mathbb{R}^{10}$ is fully spanned. In addition, noting that the parameter E_0 simply induces a rigid translation of the orbits, we conclude that $\mu=(0,0,0,j\vec{n})$ covers all possible different cases up to symplectomorphism (in fact, it suffices with varying j, the direction of $\vec{n}$ being irrelevant).

2. Quotient spaces in the extended Galilei group

We now study the way in which this family of symplectic spaces parametrized by j, emerges from pseudo-cohomology classes. First, the Galilei group must be extended by introducing a new group variable ζ. The composition law (56) is completed with

$$\zeta''=\zeta'\zeta e^{i\xi_m(g',g)}e^{i\xi_j(g',g)},$$

where $\xi_m(g',g)$ is the "standard" cocycle given by

$$\xi_m(g',g)=-m\vec{v}'\cdot R(\vec{\epsilon}')\vec{x}-\tfrac{1}{2}m\vec{v}'^2t, \tag{64}$$

and $\xi_j(g',g)$ is the pseudo-cocycle generated by the function of the rotation parameters (with nontrivial gradient at the identity)

$$\lambda_j(g)\equiv j\vec{n}\cdot\vec{\epsilon}. \tag{65}$$

Again, $\vec{n}$ is an arbitrary unit vector in the "spin-quantization direction." In this way, the explicit law for the parameter $\phi\equiv -i\,\mathrm{Log}\,\zeta$ is

$$\begin{aligned}\phi''=\phi'+\phi-m\left(\vec{v}'\cdot R(\vec{\epsilon}')\vec{x}+\frac{1}{2}\vec{v}'^2t\right)\\ +j\vec{n}\cdot\left(\sqrt{1-\frac{\epsilon'^2}{4}}\vec{\epsilon}+\sqrt{1-\frac{\epsilon^2}{4}}\vec{\epsilon}\,'-\frac{1}{2}\vec{\epsilon}\,'\times\vec{\epsilon}-\vec{\epsilon}\,'-\vec{\epsilon}\right).\end{aligned} \tag{66}$$

The left-invariant vector fields are straightforwardly computed,

$$\tilde{X}_t^L = \frac{\partial}{\partial t} + \vec{v}\cdot\frac{\partial}{\partial \vec{x}} - \frac{1}{2}mv^2 X_0,$$

$$\tilde{X}_{\vec{x}}^L = \left(\frac{\partial}{\partial \vec{x}} - m\vec{v}X_0\right)\cdot R(\vec{\epsilon}),$$

$$\tilde{X}_{\vec{v}}^L = \frac{\partial}{\partial \vec{v}}\cdot R(\vec{\epsilon}),$$

$$\tilde{X}_{\vec{\epsilon}}^L = \sqrt{1-\frac{\epsilon^2}{4}}\frac{\partial}{\partial \vec{\epsilon}} - \frac{1}{2}\vec{\epsilon}\times\frac{\partial}{\partial \vec{\epsilon}} + j\left(\left(\sqrt{1-\frac{\epsilon^2}{4}}-1\right)\vec{n} - \frac{1}{2}\vec{\epsilon}\times\vec{n}\right)X_0,$$

$$\tilde{X}_\phi^L = \frac{\partial}{\partial \phi} \equiv X_0, \tag{67}$$

providing the following nontrivial commutators:

$$\begin{aligned}
&[\tilde{X}_{\epsilon^i}^L, \tilde{X}_{\epsilon j}^L] = \eta_{ij.}^{\ k}(\tilde{X}_{\epsilon^k}^L + jn_k X_0),\\
&[\tilde{X}_t^L, \tilde{X}_{v^i}^L] = -\tilde{X}_{x^i}^L, \qquad [\tilde{X}_{\epsilon^i}^L, \tilde{X}_{xj}^L] = \eta_{ij.}^{\ k}\tilde{X}_{x^k}^L,\\
&[\tilde{X}_{x^i}^L, \tilde{X}_{vj}^L] = m\delta_{ij}X_0, \qquad [\tilde{X}_{\epsilon^i}^L, \tilde{X}_{vj}^L] = \eta_{ij.}^{\ k}\tilde{X}_{vk}^L.
\end{aligned} \tag{68}$$

Again, from (67), the precontact 1-form Θ and the presymplectic 2-form $d\Theta$ can be derived, with the result

$$\Theta = m\vec{v}\cdot d\vec{x} - \frac{1}{2}mv^2\,dt + \frac{(\vec{n}\times\vec{S})\cdot d\vec{S}}{j+\vec{S}\cdot\vec{n}} + \frac{d\zeta}{i\zeta}, \tag{69}$$

$$d\Theta = m\,d\vec{v}\wedge d\vec{x} - m\vec{v}\cdot d\vec{v}\wedge dt + \frac{\vec{n}\cdot(d\vec{S}\overset{\times}{\wedge}d\vec{S})}{2\vec{n}\cdot\vec{S}}, \tag{70}$$

where we have introduced the "spin" parameter $\vec{S}\equiv jR(\vec{\epsilon})\vec{n}$ (which is related to Noether invariants for the rotations group).

Finally, the quotient of the Galilei group by the kernel of $d\Theta$ leads to the $4+4$ dimensional symplectic manifolds with the topology $\mathbb{R}^3\times\mathbb{R}^3\times S^2$, for $j\neq 0$, and to $\mathbb{R}^3\times\mathbb{R}^3$, for $j=0$. It must be stressed that the half-integral value of the spin, j, is associated with the winding number of the application $e^{i\lambda_j}: \mathrm{SU}(2)\to\mathrm{U}(1)$, which generate the cocycle $e^{i\xi_j}$, where SU(2) is the universal covering of the rotation subgroup, SO(3).

We can make explicit contact with the deformed coadjoint orbit approach, by illustrating the formula (33), where $F(g)=(F_1(g),\ldots,F_{10}(g))=(i_{\tilde{X}_1^R}\Theta,\ldots,i_{\tilde{X}_{10}^R}\Theta)$. Calculating the right-invariant vector fields,

$$\tilde{X}_t^R = \frac{\partial}{\partial t},$$

$$\tilde{X}_{\vec{x}}^R = \frac{\partial}{\partial \vec{x}},$$

$$\tilde{X}^R_{\vec{v}} = t\frac{\partial}{\partial \vec{x}} + \frac{\partial}{\partial \vec{v}} - m\vec{x}X_0,$$

$$\tilde{X}^R_{\vec{\epsilon}} = \vec{x}\times\frac{\partial}{\partial \vec{x}} + \vec{v}\times\frac{\partial}{\partial \vec{v}} + \sqrt{1-\frac{\epsilon^2}{4}}\frac{\partial}{\partial \vec{\epsilon}} + \frac{1}{2}\vec{\epsilon}\times\frac{\partial}{\partial \vec{\epsilon}} + j\left(\left(\sqrt{1-\frac{\epsilon^2}{4}}-1\right)\vec{n} + \frac{1}{2}\vec{\epsilon}\times\vec{n}\right)X_0,$$

$$\tilde{X}^R_{\phi} = \frac{\partial}{\partial \phi} \equiv X_0, \tag{71}$$

we obtain

$$F(t,\vec{x},\vec{v},\vec{\epsilon}) = (i_{\tilde{X}^R_1}\Theta, \ldots, i_{\tilde{X}^R_{10}}\Theta) = (-\tfrac{1}{2}m\vec{v}^2, m\vec{v}, -m(\vec{x}-t\vec{v}), \vec{x}\wedge m\vec{v} + jR(\epsilon)\vec{n} - j\vec{n}),$$

which is exactly the set of representatives for the symplectic cocycle, $\gamma_m(t,\vec{x},\vec{v},\vec{\epsilon}) + \Delta_\mu$, that we have employed in the discussion of the symplectic orbits for the Galilei group.

V. FINAL REMARKS

In this paper we have established a neat characterization of the concept of pseudo-cohomology as the mathematical object classifying the single G-symplectic spaces that can be constructed out of a Lie group G. The role of symplectic cohomology has been crucial in this analysis: (a) on the one hand, it provides a clearer setting for the problem than the one based on central extensions; (b) on the other hand, it offers a straightforward bridge for the translation of the results into the language of central extensions.

This characterization is something more than an academic problem, since these symplectic spaces constitute the classical phase spaces of the quantum theories associated with a fundamental symmetry. The *a priori* knowledge of the available classical structures provides a most valuable information in the study of the quantum theory. In this sense, and although this paper focuses on the discussion of classical structures, a remark on their quantum counterparts is in order. In fact, once the classification of symplectic spaces (deformed coadjoint orbits) associated with a symmetry group has been done by means of pseudo-cohomology, the question on the existence of nonequivalent quantizations corresponding to a given coadjoint orbit S naturally arises. As is well-known from geometric quantization[3] (see also Ref. 10) such a variety of nonisomorphic quantum manifolds is classified by $\pi_1^*(S)$, i.e., the dual group of the first homotopy group of the classical phase space. Although this problem goes beyond the scope of the present work, where we are interested in the classification of symplectic spaces, not in their quantization, let us remark that when considering multiply connected coadjoint orbits there exists the possibility of finding pseudo-cocycles associated with the same coadjoint orbit and which leads to nonequivalent representations (see the end of Sec. II A for the relation between pseudo-extensions and quantization), hence to nonequivalent quantizations. These pseudo-cocycles are generated by nonhomotopic functions having the same gradient at the identity. An example of this situation can be found in the case of the SL(2,$\mathbb{R}$) group which admits two nonequivalent classes of unirreps associated with the multiply connected coadjoint orbits.[15,16] A precise analysis of this example can be seen in Ref. 17. As a consequence, the classification of nonequivalent representations associated with the same coadjoint orbit would require a further refinement in the characterization of pseudo-cohomology classes.

It should be stressed that although pseudo-cohomology with values on U(1) classifies quantizable G-symplectic manifolds through the integrality condition, general classical G-symplectic manifolds can be regained by considering pseudo-cohomology with values on the additive group R, rather than U(1). In fact, the Group Approach to Quantization recovers Classical Mechanics, in the Hamilton–Jacobi version, by just considering the additive group $\mathbb{R}$ instead of the multiplicative one U(1), the former being a local approximation to the latter.

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Integrable mixing of A_{n-1} type vertex models

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Given a family of monodromy matrices $\mathsf{T}_0,\mathsf{T}_1,\ldots,\mathsf{T}_{K-1}$ corresponding to integrable anisotropic vertex models of $A_{n_\mu-1}$ type, $\mu=0,1,\ldots,K-1$, we built up a related mixed vertex model by means of gluing the lattices on which they are defined, in such a way that integrability property is preserved. The gluing process is implemented through one-dimensional representations of rectangular quantum matrix algebras $\mathrm{A}(R_{n_{\mu-1}}:R_{n_\mu})$, namely, the *gluing matrices* ζ_μ. Algebraic Bethe ansatz is applied on a pseudovacuum space with a selected basis and, for each element of this basis, it yields a set of nested Bethe ansatz equations matching up to the ones corresponding to an A_{m-1} quasiperiodic model, with m equal to $\min_{\mu\in\mathbb{Z}_K}\{\mathrm{rank}\,\zeta_\mu\}$. © *2004 American Institute of Physics.*
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I. INTRODUCTION

There exists a deep link between solvable two-dimensional vertex models in statistical mechanics and the quantum Yang–Baxter (YB) equation, where it appears as a condition for integrability related to some basic quantities of the model.[1,2] This linking relies on the existence of an underlying symmetry, the quantum group,[3,4] which comes to provide a nice algebraic framework to study these systems. There, solutions of the YB equation are representations of some quadratic relations defining the quantum group structure and, through a process called baxterization,[5] they connect with the monodromy matrices of the model. From an algebraic point of view, baxterization makes an ordinary quantum group into a YB algebra. In this way, different representations of a YB algebra lead to different integrable lattice models.

The main aim of this work is to present a gluing process of models associated to several YB algebras preserving the integrability of the total system. We restrict ourselves to those YB algebras YB_n, $n\in\mathbb{N}$, coming from baxterization of the quantum groups $\mathrm{A}(R_n)$,[4] i.e., the duals of $U_q(\mathrm{su}_n)$.[3] Beside algebras YB_n, the gluing process also involves their rectangular generalizations $\mathrm{YB}_{n,m}$, defined as the spectral parameter dependent versions of the rectangular quantum matrix algebras $\mathrm{A}(R_n:R_m)$.[6] Here $\mathrm{A}(R_n:R_n)=\mathrm{A}(R_n)$ and, accordingly, $\mathrm{YB}_{n,n}=\mathrm{YB}_n$. The process is based on the existence of algebra homomorphisms $\mathrm{YB}_{n,m}\to\mathrm{YB}_{n,p}\otimes\mathrm{YB}_{p,m}$, the cocomposition maps, that generalize the concept of coproduct in a bialgebra. Such maps can be used to build up representations of a given YB algebra YB_n as a product of representations of another algebras YB_m, $m\neq n$, in an analogous way as the standard coproduct is used for building up usual tensor representations. More precisely, given families T_μ and ζ_μ, $\mu=0,1,\ldots,K-1$, of representations of YB_{n_μ} and $\mathrm{YB}_{n_{\mu-1},n_\mu}$, respectively, cocomposition maps ensure operator $\mathsf{T}^{\mathrm{mix}}=\zeta_0\dot{\otimes}\mathsf{T}_0\dot{\otimes}\cdots\dot{\otimes}\zeta_{K-1}\dot{\otimes}\mathsf{T}_{K-1}$ is a representation of $\mathrm{YB}_{n_{K-1}}$ (symbol $\dot{\otimes}$ will be defined in the next section). If each T_μ defines the monodromy matrix of a given vertex model, we say $\mathsf{T}^{\mathrm{mix}}$ is that of the mixed model with gluing matrices ζ_μ.

We shall see that this procedure is compatible with the algebraic Bethe ansatz method for solving these models, in the sense there exists a set of pseudovacuum vectors with respect to which these techniques can be applied. Moreover, we show a set of nested Bethe ansatz equations identical to the ones corresponding to an A_{m-1} quasiperiodic model, with m equal to $\min_{\mu\in\mathbb{Z}_K}\{\mathrm{rank}\,\zeta_\mu\}$, is related to each one of these vectors.

This work is organized as follows: in Sec. II, we review some well known facts on the connection between YB algebras and integrable lattice models; in Sec. III, we describe the gluing process and the gluing matrices as one-dimensional representations of the rectangular YB algebras; finally in Sec. IV, we prove integrability of mixed vertex models, showing that diagonalization of mixed transfer matrices reduces to solve nested Bethe equations of a family of A-type vertex models.

II. YANG–BAXTER ALGEBRAS AND INTEGRABLE VERTEX MODELS

To start with, we describe briefly the connection between two-dimensional vertex models and A_{n-1} type solutions of the YB equation.

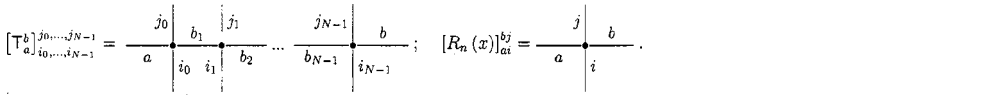
Let us consider the class of YB operators or constant R-matrices,

$$[R_n]^{kl}_{ab}=\begin{cases} q\,\delta^k_a\,\delta^{kl}, & a=b;\\ \delta^k_a\,\delta^l_b+(q-1/q)\,\delta^l_a\;\delta^k_b, & a<b;\\ \delta^k_a\,\delta^l_b, & a>b; \end{cases}\qquad 1\leqslant a,b,k,l\leqslant n; \tag{1}$$

$q\in\mathbb{C}\backslash\{0,1\}$, related to the standard Hopf algebra deformations of the simple Lie algebras A_{n-1}, i.e., the quantum groups $U_q(\mathrm{su}_n)$ and $\mathrm{A}(R_n)$, $n\in\mathbb{N}$. Baxterization process yields the spectral parameter dependent versions $R_n(x)=xR_n-PR_n^{-1}P/x$ of each R_n, with $P^{kl}_{ij}=\delta^l_i\delta^k_j$ the permutation matrix and $x\in\mathbb{C}$. Then, for every $N\in\mathbb{N}$ a related integrable (inhomogeneous) lattice model[7] is defined by a monodromy matrix $\mathsf{T}\doteq\mathsf{T}^{(n,N)}(x;\alpha)$ with entries (sum over repeated indices convention is assumed)

$$\mathsf{T}^b_a=\mathsf{R}^{b_1}_a(x/\alpha_0)\otimes\mathsf{R}^{b_2}_{b_1}(x/\alpha_1)\otimes\cdots\otimes\mathsf{R}^{b}_{b_{N-1}}(x/\alpha_{N-1}),\qquad 1\leqslant a,b\leqslant n, \tag{2}$$

being $\alpha=(\alpha_0,\ldots,\alpha_{N-1})$ a vector of $\mathbb{C}^N$. Operators $\mathsf{R}^b_a(x):\mathbb{C}^n\to\mathbb{C}^n$ are entries of a matrix $\mathsf{R}=\mathsf{R}(x)$ such that $[\mathsf{R}^b_a(x)]^j_i=[R_n(x)]^{bj}_{ai}$ in the canonical basis of $\mathbb{C}^n$. Compact notation $\mathsf{T}=\mathsf{R}\,\dot\otimes\cdots\dot\otimes\,\mathsf{R}$, where $\dot\otimes$ denotes matrix multiplication between consecutive factors, will be used. Note that $\mathsf{T}^{(n,1)}=\mathsf{R}^n=\mathsf{R}$. These models are the anisotropic analogs of the A_{n-1} invariant vertex models with periodic boundary conditions. Quasiperiodic versions[7] are given by elements Υ in the symmetry group of $R_n(x)$, i.e., $\Upsilon\in\mathrm{GL}(n)$ and $[R_n(x),\Upsilon\otimes\Upsilon]=0$. Related monodromy matrices read $\mathsf{T}^\Upsilon=\mathsf{T}\cdot\Upsilon$. Equation (2) defines operators $\mathsf{T}^b_a:(\mathbb{C}^n)^{\otimes N}\to(\mathbb{C}^n)^{\otimes N}$ that describe the statistical weights assigned to each vertex configuration in a given row of the lattice, graphically,



If the lattice has N' rows, the partition function is $\mathsf{Z}=\mathrm{trace}(\mathsf{t}^{N'})$, being $\mathsf{t}=\Sigma_a\mathsf{T}^a_a$ the transfer matrix. On the other hand, the operators $\mathsf{T}^b_a(x;\alpha)$, as it is well known, give a representation of the YB algebra related to $R_n(x)$. This algebra, which we shall indicate YB_n, is generated by indeterminates $\mathsf{T}^j_i(x)$, $1\leqslant i,j\leqslant n$; $x\in\mathbb{C}$, subject to relations

$$[R_n(x/y)]^{kl}_{ij}\,\mathsf{T}^r_k(x)\,\mathsf{T}^s_l(y)=\mathsf{T}^l_j(y)\,\mathsf{T}^k_i(x)\,[R_n(x/y)]^{rs}_{kl};\qquad 1\leqslant i,j,r,s\leqslant n. \tag{3}$$

These relations entail the formal integrability of the system. In fact, by taking the trace, one gets $[\mathsf{t}(x),\mathsf{t}(y)]=0$ for all $x,y\in\mathbb{C}$, i.e., the transfer matrix is a generating function of *conserved quantities*. Beside this, the model is effectively solved by means of algebraic Bethe ansatz,[8,9,10] where the central ingredient is the existence of an eigenstate $\omega\in(\mathbb{C}^n)^{\otimes N}$ of each entry T^a_a (and consequently of the transfer matrix t), such that $\mathsf{T}^b_a\,\omega=0$ for all $a\neq b$ and $a\geqslant 2$, and $\mathsf{T}^b_1\,\omega\neq c\,\omega$, $\forall c\in\mathbb{C}$, for all $b\geqslant 2$. For latter convenience, let us express T in the block form

$$\mathsf{T}=\begin{bmatrix}\mathsf{A} & \mathsf{B}_j\\ \mathsf{C}_i & \mathsf{D}_{ij}\end{bmatrix};\qquad 1\leqslant i,j\leqslant n-1,$$

i.e., define $\mathsf{A}\doteq\mathsf{T}_1^1$, $\mathsf{B}_j\doteq\mathsf{T}_1^{j+1}$, $\mathsf{C}_i\doteq\mathsf{T}_{i+1}^1$ and $\mathsf{D}_{ij}\doteq\mathsf{T}_{i+1}^{j+1}$. Then, ω is an eigenstate of A and of each diagonal entry D_{ii}, fulfilling $\mathsf{C}_i\,\omega=0$ and $\mathsf{D}_{ij}\,\omega=0$ for $i\neq j$. A vector satisfying these conditions is called *pseudovacuum vector*. On the other hand, since $\mathsf{B}_j\,\omega=\mathsf{T}_1^{j+1}\,\omega\neq c\,\omega$ for all j, each $\mathsf{B}_j(x)$ plays the role of a creation operator. Applying them repeatedly on ω (varying j from 1 to $n-1$ and x satisfying the so-called Bethe equations) we generate new eigenstates for the transfer matrix, namely the *Bethe vectors*, giving *a priori* a complete set of eigenstates for t. In such a case we say the system is exactly solvable or completely integrable.[11] Nevertheless, sometimes not only a vector but a *pseudovacuum subspace*[12,13] is needed in order to insure complete integrability. This will be our case.

Since each YB_n is a bialgebra, with coalgebra structure

$$\Delta:\mathsf{T}_i^j(x)\mapsto\mathsf{T}_i^k(x)\otimes\mathsf{T}_k^j(x),\quad \varepsilon:\mathsf{T}_i^j(x)\mapsto\delta_i^j, \tag{4}$$

for every couple of monodromy matrices $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(n,P)}$ as above we have another one,

$$\mathsf{T}^{(n,N+P)}=\mathsf{T}^{(n,N)}\dot{\otimes}\,\mathsf{T}^{(n,P)},\quad \text{with entries}\quad \mathsf{T}_a^{b(n,N+P)}=\mathsf{T}_a^{c(n,N)}\otimes\mathsf{T}_c^{b(n,P)},$$

giving again a representation of YB_n. Furthermore, if ω and ϕ are the pseudovacuums of $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(n,P)}$, then $\omega\otimes\phi$ defines a pseudovacuum for $\mathsf{T}^{(n,N+P)}$. Consequently the enlarged model, or the *gluing* of $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(n,P)}$, is also integrable. In particular, thermodynamic limit $N\to\infty$ preserves integrability. But, can we glue models which give representations of different YB algebras, e.g., YB_n and YB_m with $n\neq m$, and such that a pseudovacuum exists for the resulting model? The aim of this paper is to answer last question. More precisely, we build up from a family $\{\mathsf{T}_\mu:\mu\in\mathbb{Z}_K\}$ of *pure* models, i.e., $\mathsf{T}_\mu=\mathsf{T}^{(n_\mu,N_\mu)}$, $n_\mu,N_\mu\in\mathbb{N}$, a *mixing* of them by means of gluing the lattices on which they are defined, in such a way that resulting mixed model can be solved by means of algebraic Bethe ansatz techniques.

III. THE GLUING PROCESS

For any pair (R_n,R_m) of matrices (1), there exist an associated quadratic algebra $\mathrm{A}(R_n:R_m)$. They are called rectangular quantum matrix algebras.[6] There are also parameter dependent versions, the algebras $\mathrm{YB}_{n,m}$, generated by indeterminates $\mathsf{T}_i^j(x)$, $1\leqslant i\leqslant n$, $1\leqslant j\leqslant m$ and $x\in\mathbb{C}$, and defined by the quadratic relations

$$[R_n(x/y)]_{ij}^{kl}\,\mathsf{T}_k^r(x)\,\mathsf{T}_l^s(y)=\mathsf{T}_j^l(y)\,\mathsf{T}_i^k(x)\,[R_m(x/y)]_{kl}^{rs}, \tag{5}$$

$1\leqslant i,j\leqslant n$, $1\leqslant r,s\leqslant m$. Obviously, $\mathrm{YB}_{n,n}=\mathrm{YB}_n$. In the same way as for the constant case,[6,14] there exist homomorphisms

$$\Delta_p:\mathrm{YB}_{n,m}\to\mathrm{YB}_{n,p}\otimes\mathrm{YB}_{p,m};\quad n,m,p\in\mathbb{N}; \tag{6}$$

inherited from the cocomposition notion of the internal $coHom$ objects, enjoying the coassociativity property $(\Delta_p\otimes id)\Delta_r=(id\otimes\Delta_r)\Delta_p$.[15] In the $n=m=p$ cases, these reduce to the usual comultiplication maps [see Eq. (4)]. In particular, we have morphisms

$$\mathrm{YB}_m\to\mathrm{YB}_{m,n}\otimes\mathrm{YB}_n\otimes\mathrm{YB}_{n,m}\otimes\mathrm{YB}_m$$

for all n,m. Now, consider pure monodromy matrices $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(m,P)}$ related to YB_n and YB_m, and representations λ and β of $\mathrm{YB}_{m,n}$ and $\mathrm{YB}_{n,m}$, respectively, where λ and β denote rectangular matrices whose coefficients are representative of the corresponding generator algebra elements. Mentioned morphism implies $\lambda\dot{\otimes}\mathsf{T}^{(n,N)}\dot{\otimes}\beta\dot{\otimes}\mathsf{T}^{(m,P)}$ gives a representation of YB_m. As we do not want to add new degrees of freedom others than the related to the original models $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(m,P)}$, we ask λ and β to be constant (i.e., spectral parameter independent) one-dimensional representations. In this case $\lambda\dot{\otimes}\mathsf{T}^{(n,N)}\dot{\otimes}\beta\dot{\otimes}\mathsf{T}^{(m,P)}$ gives an operator on $(\mathbb{C}^n)^{\otimes N}\otimes(\mathbb{C}^m)^{\otimes P}$, which

we shall call the *gluing* of $\mathsf{T}^{(n,N)}$ and $\mathsf{T}^{(m,P)}$ through matrices λ and β. It is worth remarking that this is not the gluing operation defined by Majid and Markl.[6] Physically, λ and β define vertices with statistical weights

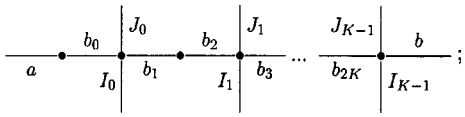
$$\lambda_a^b \quad \text{and} \quad \beta_c^d, \quad 1 \leqslant a,d \leqslant m \quad \text{and} \quad 1 \leqslant b,c \leqslant n.$$

In general, for a family of pure monodromy matrices as described above, we can define a *mixing* of them, namely,

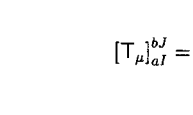
$$\mathsf{T}^{\mathrm{mix}} = \lambda_0 \dot{\otimes} \mathsf{T}_0 \dot{\otimes} \lambda_1 \dot{\otimes} \mathsf{T}_1 \dot{\otimes} \cdots \dot{\otimes} \lambda_{K-1} \dot{\otimes} \mathsf{T}_{K-1}, \tag{7}$$

where each λ_μ is a constant one-dimensional representation of the rectangular YB algebra $\mathrm{YB}_{n_{\mu-1},n_\mu}$ $(\mathrm{mod}\, K)$. Graphically,

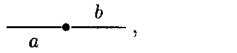
$$[\mathsf{T}_a^{b\ mix}]_{I_0,\ldots,I_{K-1}}^{J_0,\ldots,J_{K-1}} =$$



$$[\mathsf{T}_\mu]_{aI}^{bJ} =$$



$$; \quad [\lambda_\mu]_a^b =$$



being I_μ and J_μ multi-indices for spaces $(\mathbb{C}^{n_\mu})^{\otimes N_\mu}$ on which each T_μ acts. Since the quadratic relations (5) and the cocomposition maps (6), one may see that $\mathsf{T}^{\mathrm{mix}}$ provides a representation of $\mathrm{YB}_{n_{K-1}}$. This is a direct consequence of the algebra map

$$\mathrm{YB}_{n_{K-1}} \to \mathrm{YB}_{n_{K-1},n_0} \otimes \mathrm{YB}_{n_0} \otimes \mathrm{YB}_{n_0,n_1} \otimes \cdots \otimes \mathrm{YB}_{n_{K-2},n_{K-1}} \otimes \mathrm{YB}_{n_{K-1}}. \tag{8}$$

Of course, these representations are highly reducible in general, as we shall see later.

A. Constant one-dimensional representations of $\mathrm{YB}_{n,m}$

Representations λ_μ appearing in (7) match exactly with one-dimensional representations of $\mathrm{A}(R_n:R_m)$, i.e., rectangular matrices $\lambda \in \mathrm{Mat}[n \times m]$ in $\mathbb{C}$ such that

$$[R_n]_{ij}^{kl}\, \lambda_k^r \lambda_l^s = \lambda_j^l\, \lambda_i^k [R_m]_{kl}^{rs}; \quad 1 \leqslant i,j \leqslant n, \ \ 1 \leqslant r,s \leqslant m. \tag{9}$$

We are considering the same parameter $q \neq 0,1$ for all involved R-matrices. Otherwise, the only solution to (9) is the trivial one. Using an explicit form of R_n given in (1), the last equation is equivalent to

$$\lambda_i^r \lambda_j^r = 0, \quad 1 \leqslant r \leqslant m, \ \ 1 \leqslant i \leqslant j \leqslant n,$$

$$\lambda_i^r \lambda_i^s = 0, \quad 1 \leqslant r < s \leqslant m, \ \ 1 \leqslant i \leqslant n,$$

$$\lambda_i^r \lambda_j^s = 0, \quad 1 \leqslant r < s \leqslant m, \ \ 1 \leqslant j < i \leqslant n.$$

First and second lines imply coefficients of λ in a given column and row, respectively, are null except for almost one of them. The last line says, if $\lambda_i^j \neq 0$, then all coefficients λ_a^b with $i < a$, $b < j$, and with $a < i$, $j < b$, are null. Thus, each solution λ of (9) is a diagonal matrix to which columns and rows of zeros were added. From that it follows immediately the set of solutions for

all m,n form a semigroupoid, or a category, generated by the Abelian groups $\mathcal{D}_n$ of invertible $n\times n$ diagonal matrices, and also by matrices $\sigma_i^n \in \mathrm{Mat}[n\times(n+1)]$ and $\partial_i^n \in \mathrm{Mat}[(n+1)\times n]$, $i=1,\ldots,n+1$, $n\in\mathbb{N}$, given by

$$\sigma_i^n = \begin{bmatrix} Id_{(i-1)\times(i-1)} & O_{(i-1)\times(n-i+2)} \\ O_{1\times(i-1)} & O_{1\times(n-i+2)} \\ O_{(n-i)\times(i-1)} & Id_{(n-i)\times(n-i+2)} \end{bmatrix},$$

$$\partial_i^n = \begin{bmatrix} Id_{(i-1)\times(i-1)} & O_{(i-1)\times 1} & O_{(i-1)\times(n-i)} \\ O_{(n-i+2)\times(i-1)} & O_{(n-i+2)\times 1} & Id_{(n-i+2)\times(n-i)} \end{bmatrix},$$

being $O_{n,m}$ the $n\times m$ null matrix. In fact, a general solution of Eq. (9) has the form

$$\lambda = \partial_{j_b}^{n-1}\cdots\ \partial_{j_1}^{k}\, D\, \sigma_{i_1}^{k}\cdots\ \sigma_{i_a}^{m-1} \in \mathrm{Mat}[n\times m];$$

$$a,b\geqslant 0, \quad m-a=n-b=k\geqslant 0, \tag{10}$$

with $i_1\leqslant\cdots\leqslant i_a\leqslant m$, $j_1\leqslant\cdots\leqslant j_b\leqslant n$, and $D\in\mathcal{D}_k$. If a (resp. b) is equal to zero, then factors of type σ (resp. ∂) do not appear. Such a solution has k nonnull entries equal to the diagonal elements of D, a number a of null columns in positions $i_1,\ldots,i_a$, and b null rows in positions $j_1,\ldots,j_b$. Note that rank $\lambda=k$.

Matrices σ_i^n and ∂_i^m, which give solutions to (9) for $m=n+1$ and $n=m+1$, respectively, are related each other by matrix transposition, i.e., $\partial_i^n=(\sigma_i^n)^t$, and enjoy relations

$$\sigma_j^{n-1}\,\sigma_i^n=\sigma_i^{n-1}\sigma_{j+1}^n, \qquad i\leqslant j;$$

$$\partial_i^{n+1}\,\partial_j^n=\partial_{j+1}^{n+1}\,\partial_i^n, \qquad i\leqslant j;$$

$$\sigma_j^{n+1}\,\partial_i^{n+1}=\partial_i^n\,\sigma_{j-1}^n, \qquad i<j;$$

$$\sigma_j^n\,\partial_i^n=Id, \qquad i=j;$$

$$\sigma_j^{n+1}\,\partial_i^{n+1}=\partial_{i-1}^n\,\sigma_j^n, \qquad i\geqslant j+1.$$

In spite of these relations, they do **not** define the simplicial category. Note that, for instance, $\sigma_j^n\,\partial_{j+1}^n\neq Id$. Nevertheless we name $\Delta=\vee_{n,m\in\mathbb{N}}\Delta_{n,m}$ the category formed out by them.

On the other hand, as it is well known, the group of diagonal matrices $\mathcal{D}_n$ defines precisely the symmetry group of R_n, given by matrices $D\in\mathrm{GL}(n)$ such that $[R_n,D\otimes D]=0$. Moreover, they are also the symmetry group of $R_n(x)$ or $R_n(x,y)=R_n(x/y)$. Let us mention that, when $R_n(x,y)$ is changed by a similarity transformation $Q(x)\otimes Q(y)$ such that $Q_k^l(x)=\delta_k^l\,x^{2l/n}$, the group enlarges to $\mathcal{D}_n\times\mathbb{Z}_n$.[7] This is why systems related to such R-matrices were called $\mathbb{Z}_n$-symmetric vertex models.[16]

Elements $D\in\mathcal{D}_n$ give rise to multiparametric solutions $(id\otimes D)^{-1}R_n(D\otimes id)$ of the YB equation,[17] and related twist transformations of original quantum groups.[14,18] Associated integrable models differ from the original ones by a twisting of the boundary conditions.[19] We shall see later that also in mixed models the role of matrices D is to make a twist on the boundary conditions.

The commutation relations between elements of $\mathcal{D}=\vee_{n\in\mathbb{N}}\mathcal{D}_n$ and Δ can be written

$$D\,\sigma_i^n=\sigma_i^n\,D_i^+, \qquad \partial_i^n\,D=D_i^+\,\partial_i^n,$$

$$\sigma_i^{n-1}\,D=D_i^-\,\sigma_i^{n-1}, \qquad D\,\partial_i^{n-1}=\partial_i^{n-1}\,D_i^-, \tag{11}$$

being $D_i^+ = \mathrm{diag}(d_1,\ldots,d_{i-1},1,d_i,\ldots,d_n)$ and $D_i^- = \mathrm{diag}(d_1,\ldots,d_{i-1},d_{i+1},\ldots,d_n)$ whenever $D = \mathrm{diag}(d_1,\ldots,d_n) \in \mathcal{D}_n$. It is worth mentioning that λ can also be expressed as a product $\lambda = \zeta D'$, where $\zeta \in \Delta$ is obtained from λ by taking $D = Id$, and $D' \in \mathcal{D}_n$ is the result of passing D to the right, through matrices σ's, using commutation rules (11).

B. Equivalent forms for a mixed monodromy matrix

From results of last section, it is clear that any mixed model has a monodromy matrix

$$\lambda_0 \cdot \mathsf{R}_0 \dot{\otimes} \lambda_1 \cdot \mathsf{R}_1 \dot{\otimes} \cdots \dot{\otimes} \lambda_{N-1} \cdot \mathsf{R}_{N-1}, \tag{12}$$

with $\mathsf{R}_\nu = \mathsf{R}^{n_\nu}$ for some related dimension n_ν, and $\lambda_\nu = \zeta_\nu D_\nu$, where ζ_ν is in $\Delta_{n_{\nu-1},n_\nu}$ and D_ν in $\mathcal{D}_{n_\nu}$. Here $\nu \in \mathbb{Z}_N$. Equation (7) corresponds to the case in which there exist K numbers N_μ, $\mu \in \mathbb{Z}_K$, giving a partition of N and such that

$$\mathsf{R}_{M_\mu} = \cdots = \mathsf{R}_{M_\mu + N_\mu - 1} = \mathsf{R}^{n_{M_\mu}} \quad \text{and} \quad \lambda_\nu = Id_{n_\nu} \ \text{ for } \ \nu \neq M_0,\ldots,M_{K-1}, \tag{13}$$

being $M_0 = 0$ and $M_\mu = \Sigma_{\sigma=0}^{\mu-1} N_\sigma$ for $1 \leqslant \mu \leqslant K-1$. Furthermore, Eq. (12) can be brought to an equivalent form

$$\mathsf{T}^{\mathrm{mix}} = \zeta_0 \cdot \mathsf{R}_0 \dot{\otimes} \zeta_1 \cdot \mathsf{R}_1 \dot{\otimes} \cdots \dot{\otimes} \zeta_{N-1} \cdot \mathsf{R}_{N-1}\, \Upsilon, \tag{14}$$

where Υ is an element of $\mathcal{D}_{n_{N-1}}$. To see that, let us define matrices $D_\nu^{(k)} \in \mathcal{D}_{n_k}$, $k \in \mathbb{Z}_N$, by

$$D_\nu^{(k)} = \begin{cases} Id_{n_k}, & 0 \leqslant k < \nu, \\ D_\nu, & k = \nu, \end{cases}$$

and for each $k > \nu$ by the solution of $D_\nu \zeta_{\nu+1} \zeta_{\nu+2} \cdots \zeta_k = \zeta_{\nu+1} \zeta_{\nu+2} \cdots \zeta_k D_\nu^{(k)}$. We mean by "the solution" of the last equation the inversible diagonal matrix $D_\nu^{(k)}$ that arises when passing, in the first member, the matrix D_ν to the right using (11). Then (12) and (14) are similar through $\Pi_{\nu \in \mathbb{Z}_N} \otimes_{k \in \mathbb{Z}_N} D_\nu^{(k)}$, and $\Upsilon = \Pi_{\nu \in \mathbb{Z}_N} D_\nu^{(N-1)}$.

In other words, every mixed model is physically equivalent to a twisted version of another one whose corresponding matrices λ_ν are in the category Δ. The role of matrices D's is to implement a twisting of the boundary conditions. Accordingly, we can describe each mixing $\mathsf{T}^{\mathrm{mix}}$ in terms of a family of elements $\zeta_\nu \in \Delta_{n_{\nu-1},n_\nu}$, the *gluing matrices*, and a diagonal matrix $\Upsilon = \mathrm{diag}(\tau_1,\ldots,\tau_{n_{N-1}})$ of $\mathcal{D}_{n_{N-1}}$, the *boundary matrix*.

Another useful expression for the monodromy matrices of these models can be given from the following observation. Any matrix $\lambda \in \Delta_{n,m}$ of rank k (note that $k \leqslant m,n$) may be written $\lambda = P\,\hat{\lambda}\,P'$, where $\hat{\lambda} = \partial_n^{n-1} \cdots \partial_{k+1}^k \sigma_{k+1}^k \cdots \sigma_m^{m-1} \in \mathrm{Mat}[n \times m]$, that is,

$$\hat{\lambda} = \begin{pmatrix} Id_k & O_{k\times(m-k)} \\ O_{(n-k)\times k} & O_{(n-k)\times(m-k)} \end{pmatrix}, \tag{15}$$

and P, P' are appropriate permutations. More precisely, if

$$\lambda = \partial_{j_b}^{n-1} \cdots \partial_{j_1}^k \sigma_{i_1}^k \cdots \sigma_{i_a}^{m-1}, \quad i_1 \leqslant \cdots \leqslant i_a \leqslant m, \quad j_1 \leqslant \cdots \leqslant j_b \leqslant n$$

[see Eq. (10)], then we can choose, for instance, $P \in \mathrm{Mat}[n]$ and $P' \in \mathrm{Mat}[m]$ to be

$$P = C_{j_b,n}\, C_{j_{b-1},n} \cdots C_{j_1,n} \qquad \text{and} \qquad P' = C_{i_1,m} \cdots C_{i_{a-1},m}\, C_{i_a,m},$$

respectively, being $C_{r,s}$, $r \leqslant s$, the matrix that acting on the right (resp. left) makes a cyclic permutation sending the sth column (resp. row) to the rth one, and acts as an identity for the rest

of columns (resp. rows). Hence, for a given family of gluing matrices we have $\zeta_\nu = P_\nu \hat{\zeta}_\nu P'_\nu$. Introducing last expression for ζ_ν into Eq. (14), and making a similarity transformation $\otimes_{\nu\in\mathbb{Z}_N} P'_\nu$, an equivalent system

$$\tilde{\mathsf{T}}^{\mathrm{mix}} = P_0\ \hat{\zeta}_0 \cdot \tilde{\mathsf{R}}_0 \cdot Q_0 \dot{\otimes} \hat{\zeta}_1 \cdot \tilde{\mathsf{R}}_1 \cdot Q_1 \dot{\otimes} \cdots \dot{\otimes} \hat{\zeta}_{N-2} \cdot \tilde{\mathsf{R}}_{N-2} \cdot Q_{N-2} \dot{\otimes} \hat{\zeta}_{N-1} \cdot \tilde{\mathsf{R}}_{N-1}\, P'_{N-1}\, \Upsilon, \quad (16)$$

where $Q_\nu = P'_\nu P_{\nu+1}$ and $\tilde{\mathsf{R}}_\nu = (P'_\nu \otimes P'_\nu)\, \mathsf{R}_\nu\, (P'_\nu \otimes P'_\nu)^{-1}$, follows. That is,

$$\tilde{\mathsf{T}}^{\mathrm{mix}} = (\otimes_{\nu\in\mathbb{Z}_N} P'_\nu)\, \mathsf{T}^{\mathrm{mix}}\, (\otimes_{\nu\in\mathbb{Z}_N} P'_\nu)^{-1}. \quad (17)$$

It can be seen for an arbitrary permutation that

$$\tilde{\mathsf{R}}^a_a(x) = \mathsf{R}^a_a(x), \quad \text{and} \quad \tilde{\mathsf{R}}^b_a(x) = x^{2\varepsilon_{ab}}\, \mathsf{R}^b_a(x) \quad \text{for} \quad a \neq b, \quad (18)$$

where coefficients ε_{ab} takes values $-1,0,1$ depending on the considered permutation. We shall show in the next section that mixed models with

$$P_0 = P'_{N-1} = Id_{n_{N-1}}, \quad \text{and} \quad Q_\nu = Id_{n_\nu}, \ \forall \nu \in \mathbb{Z}_{N-1}, \quad (19)$$

are solvable by means of algebraic Bethe ansatz techniques [actually, (19) can be slightly relaxed and ask $Q_\nu = Id_{n_\nu}, \forall \nu \in \mathbb{Z}_N$, instead]. Furthermore, we shall see complete integrability implies transfer matrix obtained from (16) is similar to the trace of

$$\mathsf{T}^{\mathrm{mix}} = \hat{\zeta}_0 \cdot \mathsf{R}_0 \dot{\otimes} \hat{\zeta}_1 \cdot \mathsf{R}_1 \dot{\otimes} \cdots \dot{\otimes} \hat{\zeta}_{N-1} \cdot \mathsf{R}_{N-1}\, \Upsilon. \quad (20)$$

Thus, we can solve all vertex models with gluing matrices $\zeta_\nu = P_\nu \hat{\zeta}_\nu P'_\nu$ satisfying (19) by solving those with $\mathsf{T}^{\mathrm{mix}}$ given in Eq. (20). In addition, all $\hat{\zeta}_\nu$ can be supposed to have the same rank.

IV. INTEGRABILITY OF MIXED VERTEX MODELS

In order to show exact solvability of these models (or unless of a subclass of them), since needed commutation rules follow from map (8), we must prove there exists a suitable set of pseudovacuum vectors for $\mathsf{T}^{\mathrm{mix}}$ from which all its eigenstates and corresponding eigenvalues can be constructed. In other terms, using block form

$$\mathsf{T}^{\mathrm{mix}} = \begin{bmatrix} \mathsf{A}^{\mathrm{mix}} & \mathsf{B}^{\mathrm{mix}}_j \\ \mathsf{C}^{\mathrm{mix}}_i & \mathsf{D}^{\mathrm{mix}}_{ij} \end{bmatrix}; \quad 1 \leqslant i,j \leqslant n_{N-1} - 1,$$

we look for elements $\Phi \in \mathcal{H}^{\mathrm{mix}} = \otimes_{\nu\in\mathbb{Z}_N} \mathbb{C}^{n_\nu}$ which are eigenvectors of $\mathsf{A}^{\mathrm{mix}}$ and of each diagonal entry $\mathsf{D}^{\mathrm{mix}}_{ii}$, such that $\mathsf{C}^{\mathrm{mix}}_i \Phi = 0$, and $\mathsf{D}^{\mathrm{mix}}_{ij} \Phi = 0$ for $i \neq j$. In this way, we build up recursively all eigenvalues and eigenstates by applying repeatedly operators $\mathsf{B}^{\mathrm{mix}}_j$ to the mentioned vectors. Completeness problem will be studied separately. Of course, the smaller the rank of involved gluing matrices, the smaller the set of monomials in $\mathsf{B}^{\mathrm{mix}}_j$ and the bigger the number of pseudovacuum vectors we need to construct the complete set of eigenstates. In the singular case for which $\mathrm{rank}\zeta_\nu = 0$ for some ν, we have $\mathsf{T}^{\mathrm{mix}} = 0$ and accordingly every vector of $\mathcal{H}^{\mathrm{mix}}$ is trivially a pseudovacuum vector, and no creation operator is needed in order to diagonalize the transfer matrix $\mathsf{t}^{\mathrm{mix}}$. Note in this case, operators $\mathsf{B}^{\mathrm{mix}}_j$ are null. Thus we can have pseudovacuum vectors which are annihilated by operators $\mathsf{B}^{\mathrm{mix}}_j$ and still be able to build up an eigenstate basis for $\mathsf{t}^{\mathrm{mix}}$.

We actually show exact solvability for a particular class of mixed models. Concretely, we concentrate ourself in monodromy matrices whose related gluings ζ_ν satisfy Eq. (19).

A. The pseudovacuum subspace

Let us first consider the mixed models with monodromy matrices $\mathsf{T}^{\mathrm{mix}}$ defined by Eq. (20), that is, each $\zeta_\nu = \hat{\zeta}_\nu$ is of the form (15). They are a particular case of those with gluing matrices satisfying (19). At the end of this section the general case will be addressed. In order to simplify our calculations, we shall suppose

$$m \doteq \operatorname{rank} \zeta_0 \leqslant \operatorname{rank} \zeta_\nu \qquad \text{for all} \qquad \nu \in \mathbb{Z}_N . \tag{21}$$

This can be reached by a similarity transformation cyclically permuting tensor factors of the linear space $\mathcal{H}^{\mathrm{mix}}$. Of course, $m \leqslant \operatorname{rank} \zeta_\nu \leqslant \min\{n_{\nu-1}, n_\nu\} \pmod N$. Also, we suppose $m > 0$, since for $m = 0$ diagonalization of $\mathsf{T}^{\mathrm{mix}}$ is immediate. Note that (21) implies

$$\mathsf{T}_a^{b\ \mathrm{mix}} = 0 \qquad \text{for} \qquad a > m, \tag{22}$$

and in particular

$$\mathsf{t}^{\mathrm{mix}} = \sum_{a=1}^{n_{N-1}} \mathsf{T}_a^{a\ \mathrm{mix}} = \sum_{a=1}^{m} \mathsf{T}_a^{a\ \mathrm{mix}} = \mathsf{A}^{\mathrm{mix}} + \sum_{i=1}^{m-1} \mathsf{D}_{ii}^{\mathrm{mix}} . \tag{23}$$

For $a \leqslant m$ we have (nonsum over b)

$$\mathsf{T}_a^{b\ \mathrm{mix}} = \tau_b [\mathsf{R}^{n_0}]_a^{c_1} \otimes [\mathsf{R}^{n_1}]_{c_1}^{c_2} \cdots [\mathsf{R}^{n_{N-2}}]_{c_{N-2}}^{c_{N-1}} \otimes [\mathsf{R}^{n_{N-1}}]_{c_{N-1}}^{b} , \tag{24}$$

where sum over each c_ν is in the interval $1 \leqslant c_\nu \leqslant \operatorname{rank} \zeta_\nu$.

Let us indicate by $e_1, \ldots, e_n$ the elements of the canonical basis of $\mathbb{C}^n$. Then $\mathcal{H}^{\mathrm{mix}}$ is spanned by vectors of the form $e_{f_0} \otimes \cdots \otimes e_{f_{N-1}}$, which can be identified with an obvious subset F of functions $f : \mathbb{Z}_N \to \mathbb{N} : \nu \mapsto f_\nu$. In particular, given $f \in \mathsf{F}$, we denote Ω^f the corresponding vector of $\mathcal{H}^{\mathrm{mix}}$. We shall show there exists a set of pseudovacuum vectors, on which algebraic Bethe ansatz will be applied, labeled by the subset F_0 of functions

$$f \in \mathsf{F} / \operatorname{Image} f \subset \{1\} \cup \{n \in \mathbb{N} : n > m\}. \tag{25}$$

More precisely, there exist vectors $\Phi^f \in \mathcal{H}^{\mathrm{mix}}$, $f \in \mathsf{F}_0$, expanding a space

$$\mathcal{H}_0 \doteq \operatorname{span}\{\Omega^f \in \mathcal{H}^{\mathrm{mix}} : f \in \mathsf{F}_0\} \subset \mathcal{H}^{\mathrm{mix}}, \tag{26}$$

namely, the pseudovacuum subspace, and fulfilling

$$\mathsf{A}^{\mathrm{mix}} \Phi^f = \tau_1 \, d \prod_{\nu \in f^{-1}(1)} G(x/\alpha_\nu) \, \Phi^f ,$$

$$\mathsf{D}_{ii}^{\mathrm{mix}} \Phi^f = \tau_{i+1} \, d \, \Phi^f (i < m), \qquad \mathsf{D}_{i \neq j}^{\mathrm{mix}} \Phi^f = \mathsf{C}_i^{\mathrm{mix}} \Phi^f = 0, \tag{27}$$

being $d = \Pi_{\nu \in \mathbb{Z}_N} 1/G(x/\alpha_\nu)$ and $G(x) = (xq - 1/qx)/(x - 1/x)$. In particular for the *equal rank case*, i.e., if $\operatorname{rank} \zeta_\nu = m$ for all ν, then $\Phi^f = \Omega^f$. Note that $\mathcal{H}_0 \subset \ker \mathsf{C}_i^{\mathrm{mix}}\ \forall i$.

We also show

$$\mathsf{B}_j^{\mathrm{mix}} \Phi^f \neq c \, \Phi^f \qquad \text{if} \quad 1 \in \operatorname{Image} f ; \quad \text{otherwise,} \quad \mathsf{B}_j^{\mathrm{mix}} \Phi^f = 0 ; \tag{28}$$

i.e., each $\mathsf{B}_j^{\mathrm{mix}}$ creates new states when $f^{-1}(1) \neq \varnothing$. Using that we construct a set of Bethe vectors from each Φ^f, with j from 1 to m and $f^{-1}(1) \neq \varnothing$, and generate in this way all eigenstates of the transfer matrix.

To find the vectors Φ^f we need some previous results.

1. The action of $\mathsf{T}^{\mathrm{mix}}$ on vectors Ω^f

Let us evaluate the entries $\mathsf{T}_a^{b\ \mathrm{mix}}$ on each vector Ω^f. From Eq. (22) it follows that $\mathsf{T}_a^{b\ \mathrm{mix}}\Omega^f=0$ for all $a>m$. So we only consider $a\leqslant m$. As usual,[7] we normalize operators $\mathsf{R}_a^b=\mathsf{R}^{n_\nu\, b}_{\ \ a}(x/\alpha_\nu):\mathbb{C}^{n_\nu}\to\mathbb{C}^{n_\nu}$ in such a way that on the canonical basis of $\mathbb{C}^{n_\nu}$,

$$\mathsf{R}_a^b\, e_k=\begin{cases}\delta_a^b/G(x/\alpha_\nu)\, e_k, & k\neq a,\\ (\delta_a^b+(1-\delta_a^b)\, c_{\mathrm{sg}(b-a)}(x/\alpha_\nu))\, e_b, & k=a,\end{cases} \tag{29}$$

being $c_\pm(x)=(q-1/q)\ x^{\pm 1}/(xq-1/qx)$. Then, from (24) and the first part of (29), it follows that

$$\mathsf{T}_a^{b\ \mathrm{mix}}\Omega^f=\tau_b\,\delta_a^b\prod_{\nu\in\mathbb{Z}_N}1/G(x/\alpha_\nu)\,\Omega^f=\tau_a\,\delta_a^b\,d\,\Omega^f \tag{30}$$

if $a\notin\mathrm{Image}\, f$, i.e., if $f(\nu)\neq a$ for all $\nu\in\mathbb{Z}_N$. In particular

$$\mathsf{T}_a^{b\ \mathrm{mix}}\Omega^f=0\qquad\text{if}\qquad a\notin\mathrm{Image}\, f\cup\{b\}. \tag{31}$$

Also, if $f\in\mathsf{F}_0$ and $1<a\leqslant m$, since in this case $a\notin\mathrm{Image}\, f$ [see (25)], we have that

$$\begin{gathered}\mathsf{D}_{ii}^{\mathrm{mix}}\Omega^f=\mathsf{T}_{i+1}^{i+1\ \mathrm{mix}}\Omega^f=\tau_{i+1}\,d\,\Omega^f,\quad\text{for}\quad 1\leqslant i<m,\\ \mathsf{D}_{ij}^{\mathrm{mix}}\Omega^f=\mathsf{T}_{i+1}^{j+1\ \mathrm{mix}}\Omega^f=0,\quad\text{for}\quad 1\leqslant i,j<m,\quad i\neq j,\\ \mathsf{C}_i^{\mathrm{mix}}\Omega^f=\mathsf{T}_{i+1}^{1\ \mathrm{mix}}\Omega^f=0,\quad\text{for}\quad 1\leqslant i<m,\end{gathered} \tag{32}$$

putting $i=a-1$ in (30). Otherwise, let σ_a be the first integer such that $f(\sigma_a)=a$, that is, $f(\nu)\neq a$ for all $\nu<\sigma_a$ and $f(\sigma_a)=a$. Let us write

$$\Omega^f=\Omega^{g^a}\otimes e_a\otimes\Omega^{f^a},\qquad\text{with}\qquad g^a,f^a:\mathbb{Z}_{\sigma_a},\mathbb{Z}_{N-\sigma_a-1}\to\mathbb{N}. \tag{33}$$

If $\sigma_a=N-1$, we take Ω^{f^a} equal to 1. Then, using (24) and (29) again (note that a does not belong to Image g^a) we have

$$\mathsf{T}_a^{b\ \mathrm{mix}}\Omega^f=\sum_{i=1}^{\mathrm{rank}\,\zeta_{\sigma_a}}C_{a,i}\,\Omega^{g^a}\otimes e_i\otimes\hat{\mathsf{T}}_i^{b\ \mathrm{mix}}\Omega^{f^a},$$

$$C_{a,i}=D_{a,i}\prod_{\nu<\sigma_a}1/G(x/\alpha_\nu);\quad D_{a,i}=\delta_a^i+(1-\delta_a^i)\,c_{\mathrm{sg}(i-a)}(x/\alpha_{\sigma_a}). \tag{34}$$

Here, operators $\hat{\mathsf{T}}_i^{b\ \mathrm{mix}}$ are given by the last $N-\sigma_a-1$ factors of $\mathsf{T}^{\mathrm{mix}}$. From Eq. (31) applied to $\hat{\mathsf{T}}_i^{b\ \mathrm{mix}}\Omega^{f^a}$, since $C_{a,i}\neq 0$ for all $1\leqslant i\leqslant\mathrm{rank}\,\zeta_{\sigma_a}$, the nonzero terms of (34) are those with i inside $I_a=\{i\in\mathrm{Image}\, f^a\cup\{b\}:i\leqslant\mathrm{rank}\,\zeta_{\sigma_a}\}$. If b is the unique element of I_a and $b\notin\mathrm{Image}\, f^a$, then

$$\mathsf{T}_a^{b\ \mathrm{mix}}\Omega^f=\tau_b\,C_{a,b}\left(\prod_{\nu\neq\sigma_a}1/G(x/\alpha_\nu)\right)\Omega^{g^a}\otimes e_b\otimes\Omega^{f^a}=\tau_b\,C_{a,b}\,d\,G(x/\alpha_{\sigma_a})\,\Omega^{g^a}\otimes e_b\otimes\Omega^{f^a}. \tag{35}$$

Otherwise, suppose there exists $c_1\in I_a\cap\mathrm{Image}\, f^a$, and let σ_{ac_1} be the first integer such that $f^a(\sigma_{ac_1}-\sigma_a)=c_1$. Then $\hat{\mathsf{T}}_{c_1}^{b\ \mathrm{mix}}\Omega^{f^a}=\Sigma_{i\in I_{ac_1}}C_{ac_1,i}\,\Omega^{g^{ac_1}}\otimes e_i\otimes\hat{\mathsf{T}}_i^{b\ \mathrm{mix}}\Omega^{f^{ac_1}}$ with

$$C_{ac_1,i}=D_{c_1,i}\prod_{\sigma_a<\nu<\sigma_{ac_1}}1/G(x/\alpha_\nu),\qquad \Omega^{f^a}=\Omega^{g^{ac_1}}\otimes e_{c_1}\otimes\Omega^{f^{ac_1}},$$

$$I_{ac_1}=\{i\in\text{Image}\,f^{ac_1}\cup\{b\}:i\leqslant\text{rank}\,\zeta_{\sigma_{ac_1}}\}.$$

A recursive process easily follows and the generic term reads

$$\hat{\mathsf{T}}^{b\ \text{mix}}_{c_k}\Omega^{f^{ac_1\cdots c_{k-1}}}=\sum_{i\in I_{ac_1\cdots c_k}}C_{ac_1\cdots c_k,i}\,\Omega^{g^{ac_1\cdots c_k}}\otimes e_i\otimes\hat{\mathsf{T}}^{b\ \text{mix}}_{i}\Omega^{f^{ac_1\cdots c_k}},$$

with $C_{ac_1\cdots c_k,i}=D_{c_k,i}\,\Pi_{\sigma_{ac_1\cdots c_{k-1}}<\nu<\sigma_{ac_1\cdots c_k}}1/G(x/\alpha_\nu)$. Of course, $c_1\in I_a\cap\text{Image}\,f^a$,

$$I_{ac_1c_2\cdots c_{j-1}}=\{i\in\text{Image}\,f^{ac_1c_2\cdots c_{j-1}}\cup\{b\}:i\leqslant\text{rank}\,\zeta_{\sigma_{ac_1\cdots c_{j-1}}}\}\tag{36}$$

and $c_j\in I_{ac_1c_2\cdots c_{j-1}}\cap\text{Image}\,f^{ac_1c_2\cdots c_{j-1}}$ for $2\leqslant j\leqslant k$. The process ends when $b\in I_{ac_1\cdots c_k}$, $b\notin\text{Image}\,f^{ac_1\cdots c_k}$, and we choose $c_{k+1}=b$. In this case

$$\hat{\mathsf{T}}^{b\ \text{mix}}_{c_k}\Omega^{f^{ac_1\cdots c_{k-1}}}=\tau_b\,C_{ac_1\cdots c_k,b}\prod_{\nu>\sigma_{ac_1\cdots c_k}}1/G(x/\alpha_\nu)\,\Omega^{g^{ac_1\cdots c_k}}\otimes e_b\otimes\Omega^{f^{ac_1\cdots c_k}}.$$

In particular, writing $\mathsf{T}^{b\ \text{mix}}_{a}\Omega^{f}=\Sigma_{g\in\mathsf{F}}\,t^{fg}_{ab}\,\Omega^{g}$ we have the given sequence of numbers $c_1,\ldots,c_k\in\text{Image}\,f$ defined by a function g such that $t^{fg}_{ab}\neq0$, being

$$\Omega^{g}=\Omega^{g^a}\otimes e_{c_1}\otimes\Omega^{g^{ac_1}}\otimes e_{c_2}\otimes\Omega^{g^{ac_1c_2}}\otimes\cdots\otimes\Omega^{g^{ac_1c_2\cdots c_{k-1}}}\otimes e_{c_k}\otimes\Omega^{g^{ac_1\cdots c_k}}\otimes e_b\otimes\Omega^{f^{ac_1c_2\cdots c_k}}.\tag{37}$$

Note that Ω^f can be written

$$\Omega^{f}=\Omega^{g^a}\otimes e_a\otimes\Omega^{g^{ac_1}}\otimes e_{c_1}\otimes\Omega^{g^{ac_1c_2}}\otimes\cdots\otimes\Omega^{g^{ac_1c_2\cdots c_{k-1}}}\otimes e_{c_{k-1}}\otimes\Omega^{g^{ac_1c_2\cdots c_k}}\otimes e_{c_k}\otimes\Omega^{f^{ac_1c_2\cdots c_k}}.\tag{38}$$

Furthermore, defining $J_{fg}=\{\sigma_a,\sigma_{ac_1},\ldots,\sigma_{ac_1\cdots c_k}\}$ and $c_0=a$, and recalling $c_{k+1}=b$, we have [compare with Eq. (35)]

$$t^{fg}_{ab}=\tau_b\,d\prod_{j=1}^{k+1}D_{c_{j-1},c_j}\prod_{\nu\in J_{fg}}G(x/\alpha_\nu).\tag{39}$$

If $\#[f^{-1}(a)]=k+1$ and $a=b$, the sequence of numbers $c_i=a$, $i=1,\ldots,k$, corresponds to the vector $\Omega^g=\Omega^f$. Also, $J_{ff}=f^{-1}(a)$ and accordingly, since $D_{a,a}=1$,

$$t^{ff}_{aa}=\tau_a\,d\prod_{\nu\in f^{-1}(a)}G(x/\alpha_\nu).\tag{40}$$

Comparing (37) and (38), we see that functions g such that $t^{fg}_{ab}\neq0$ necessarily satisfy

$$\text{Image}\,g\cup\{a\}=\text{Image}\,f\cup\{b\}.\tag{41}$$

In addition, for each element $\mu\in\text{Image}\,f$, $\mu\neq a,b$, function g must hold

$$\#[g^{-1}(\mu)]=\#[f^{-1}(\mu)],\tag{42}$$

and

$$\#[g^{-1}(a)]=\#[f^{-1}(a)]-(1-\delta_{ab}),$$
$$\#[g^{-1}(b)]=\#[f^{-1}(b)]+(1-\delta_{ab}). \tag{43}$$

Now, defining the classes of functions $C\subset\mathsf{F}$, in such a way that $f,g\in C$ iff

$$\text{Image}\, f=\text{Image}\, g \qquad \text{and} \qquad \#[f^{-1}(\mu)]=\#[g^{-1}(\mu)]$$

for all μ contained in their respective images, we can write

$$\mathsf{T}_a^{b\ \text{mix}}\,\Omega^f=\sum_{g\in C_{-a}^{+b}} t_{ab}^{fg}\,\Omega^g, \qquad \text{if} \quad f\in C, \tag{44}$$

where C_{-a}^{+b} is the class given by functions g satisfying (41), (42), and (43). Let us note that $C=C_{-a}^{+b}$ iff $a=b$. Then, denoting

$$\mathcal{H}_X\doteq\text{span}\{\Omega^f\in\mathcal{H}^{\text{mix}}: f\in X\} \quad \text{for each} \quad X\subset\mathsf{F}, \tag{45}$$

spaces $\mathcal{H}_C$ are $\mathsf{T}_a^{a\ \text{mix}}$-invariant for all a. On the other hand, when $a\neq b$ (since $C\neq C_{-a}^{+b}$), vector Ω^f cannot be written as a linear combination of vectors Ω^g's appearing in (44) (they form a linearly independent set of vectors). That is, $\mathsf{T}_a^{b\ \text{mix}}\,\Omega^f$ is not proportional to Ω^f. Also, if $a\notin\text{Image}\, f$, then $C_{-a}^{+b}=\varnothing$ and consequently $\mathsf{T}_a^{b\ \text{mix}}\,\Omega^f=0$, such as follows from Eq. (30) for $a\neq b$. Last observations translate for operators $\mathsf{B}_j^{\text{mix}}$ into equations

$$\mathsf{B}_j^{\text{mix}}\,\Omega^f\neq c\,\Omega^f, \quad \text{if} \quad f^{-1}(1)\neq\varnothing; \quad \mathsf{B}_j^{\text{mix}}\,\Omega^f=0 \quad \text{otherwise.} \tag{46}$$

Let us briefly study the reducibility of the action on $\mathcal{H}^{\text{mix}}$ of the algebra generated by operators T^{mix}. It follows from Eq. (36) that, if $M=\max_\nu\{\text{rank}\,\zeta_\nu\}$, numbers $c_1,\ldots,c_k$ and $c_{k+1}=b$ must be smaller than or equal to M. This implies $\mathsf{T}_a^{b\ \text{mix}}=0$ for $b>M$, and we can restrict ourselves to the $a,b\leqslant M$ case. Also, comparing (37) and (38), if $f(\nu)>M$ then $g(\nu)=f(\nu)$. As a consequence, besides (41), (42), and (43), condition

$$g(\nu)=f(\nu) \quad \forall\,\nu\in\mathbb{Z}_N \quad \text{such that} \quad g(\nu),f(\nu)>M \tag{47}$$

is necessary in order to have $t_{ab}^{fg}\neq 0$. Thus, defining the classes $E\subset\mathsf{F}$ as those whose functions satisfy (47), it is clear that spaces $\mathcal{H}_E$ are invariant under the action of T^{mix}. It actually can be found smaller invariant spaces inside $\mathcal{H}_E$, depending *locally* on the ranks of gluing matrices, but we will not discuss it here.

For the equal rank case we have $m=M$, and accordingly the classes E are in bijection with elements of F_0. Thus, we can decompose $\mathcal{H}^{\text{mix}}$ into T^{mix}-invariant subspaces $\mathcal{H}_{E(f)}$ labeled by elements of F_0. In addition, by a simple inspection of coefficients (39), it can be shown the actions on $\mathcal{H}_{E(f)}$ and $\mathcal{H}_{E(g)}$ are equivalent provided $f^{-1}(1)=g^{-1}(1)$. Moreover, in the homogeneous case, namely, $\alpha_\nu=1$ for all ν, above equivalence still holds when $\#[f^{-1}(1)]=\#[g^{-1}(1)]$.

In the following subsection we diagonalize (when possible) the operator A^{mix} restricted to each $\mathcal{H}_C$, and show its eigenvectors, when $C\subset\mathsf{F}_0$, are precisely the pseudovacuum vectors we are looking for.

2. Diagonalization of A^{mix} and vectors Φ^f

Let us consider a class of functions C. Using Eqs. (40) and (44) for $a=b=1$, and defining $a_{fg}\doteq t_{11}^{fg}$ for $f\neq g$, we have that

$$\mathsf{A}^{\text{mix}}\,\Omega^f=a_f\,\Omega^f+\sum_{g\in C, g\neq f} a_{fg}\,\Omega^g, \qquad a_f=\tau_1\,d\prod_{\nu\in f^{-1}(1)} G(x/\alpha_\nu). \tag{48}$$

Now, we are going to show there exists a total order relation between the functions of C, such that w.r.t. this order we can write

$$\mathsf{A}^{\mathrm{mix}}\,\Omega^f = a_f\,\Omega^f + \sum_{g<f} a_{fg}\,\Omega^g. \tag{49}$$

In other words, operator $\mathsf{A}^{\mathrm{mix}}$ restricted $\mathcal{H}_C$ is represented by a triangular matrix w.r.t. the resulting ordered basis [recall Eq. (45) for $X=C$].

To see that, let us consider a function $f\in C$. Assign to f_ν the number 1 if $f_\nu=1$ or 0 if $f_\nu \neq 1$. Denote b^f the binary expression related to the sequence $f_0,\ldots,f_{N-1}$. From Eqs. (37) and (38) for $a=b=1$, we see that $b^f>b^g$ (as real numbers) for $f\neq g$, since unless one $f_\nu=1$ were moved to the right. This implies $a_{fg}=0$ if $b^f\leqslant b^g$, that is,

$$\mathsf{A}^{\mathrm{mix}}\,\Omega^f = a_f\,\Omega^f + \sum_{b^g<b^f} a_{fg}\,\Omega^g. \tag{50}$$

So let us define an order $<$ between the elements of C by saying $g<f$ if $b^g<b^f$, and when $b^g=b^f$ we choose an arbitrary order. Using that and equation above, Eq. (49) follows immediately.

Since eigenvalues of $\mathsf{A}^{\mathrm{mix}}$ are given by the numbers a_f, in order to insure its diagonalizability we can ask the considered model to be completely inhomogeneous, i.e., $\alpha_\nu\neq\alpha_\mu$ for all $\nu,\mu\in\mathbb{Z}_N$. Then $a_f\neq a_g$ provided $f^{-1}(1)\neq g^{-1}(1)$. Thus, eigenvalues are distinct, unless those related to the fth and gth rows for which $f^{-1}(1)=g^{-1}(1)$. But $f^{-1}(1)\neq g^{-1}(1)$ if $b^f>b^g$. Therefore [see Eq. (50)], $\mathsf{A}^{\mathrm{mix}}$ does not mix vectors related to rows with the same diagonal entries, and accordingly $\mathsf{A}^{\mathrm{mix}}$ is diagonalizable. Actually, we just can insure $\mathsf{A}^{\mathrm{mix}}=\mathsf{A}^{\mathrm{mix}}(x)$ is diagonalizable for almost all values x of the spectral parameter. Note that for some isolated points $x_o\in\mathbb{C}$, we can have $a_f(x_o)=a_g(x_o)$, in spite of condition $f^{-1}(1)\neq g^{-1}(1)$ holds.

Using usual recursion formulas for diagonalizing triangular matrices, we can define for each subspace $\mathcal{H}_C$ the basis Φ^f, $f\in C$, given by

$$\Phi^f = \begin{cases} \Omega^{\min_C}, & f=\min_C, \\ \Omega^f + \sum_{g<f} \chi_{fg}\,\Phi^g, & f>\min_C, \end{cases} \tag{51}$$

with

$$\chi_{fg} = \begin{cases} a_{g^+g}/(a_{g^+}-a_g), & f=g^+, \\ \left(a_{fg} - \sum_{g<h<f} a_{fh}\,\chi_{hg}\right)/(a_f-a_g), & f>g^+. \end{cases} \tag{52}$$

Here $\min_C$ is the minimal $f\in C$ w.r.t. the defined order, and g^+ is the first element in C bigger than g. Equation (52) must be understood as a recursive formula on f for each g. Because $[\mathsf{A}^{\mathrm{mix}}(x),\mathsf{A}^{\mathrm{mix}}(x')]=0$ for all $x,x'\in\mathbb{C}$ [that follows from commutation relations given in (3)], operators $\mathsf{A}^{\mathrm{mix}}(x)$ can be diagonalized simultaneously. Thus numbers χ_{fg} and vectors Φ^f do not depend on the spectral parameter.

Let us note diagonal entries $\mathsf{D}^{\mathrm{mix}}_{ii}$ can be diagonalized as above. But this is not enough to diagonalize $\mathsf{t}^{\mathrm{mix}}$, since operators $\mathsf{A}^{\mathrm{mix}}$ and $\mathsf{D}^{\mathrm{mix}}_{ii}$ do not commute among themselves. Nevertheless, last operators restricted to $\mathcal{H}_0$ do commute, and accordingly can be simultaneously diagonalized. This follows from the facts that $\mathcal{H}_0\subset\ker\mathsf{C}^{\mathrm{mix}}_i$ and that Eq. (3) implies

$$[\,\mathsf{D}^{\mathrm{mix}}_{ii}(x),\mathsf{A}^{\mathrm{mix}}(y)] = -\mathsf{B}^{\mathrm{mix}}_i(x)\,\mathsf{C}^{\mathrm{mix}}_i(y)\,c_-(x/y) + \mathsf{B}^{\mathrm{mix}}_i(y)\,\mathsf{C}^{\mathrm{mix}}_i(x)\,c_+(x/y).$$

Now, let us see that vectors Φ^f for $f\in\mathsf{F}_0$, given by (51) and (52), satisfy Eqs. (27) and (28). Since they are eigenvectors of $\mathsf{A}^{\mathrm{mix}}$ with eigenvalues a_f, the first part of (27) follows immediately.

For the second part, note Φ^f is a linear combination of vectors Ω^g with g inside C. Also note, if $f\in \mathsf{F}_0$, then the class defined by f is inside F_0 too. Hence, using Eq. (32) we arrive at the wanted result. The same happens for (28) using Eq. (46).

For the equal rank case, it can be shown that $a_{fg}=0$ for all $f\in \mathsf{F}_0$. In fact, sets $I_{1c_1\cdots c_j}$ defined by (36) (putting $a=b=1$) has 1 as the unique element, and consequently the only possible sequence is $c_i=1$ for $i=1,\ldots,\#[f^{-1}(1)]-1$. Such sequence corresponds to the vector Ω^f. Then, the latter is an eigenvector of $\mathsf{A}^{\mathrm{mix}}$ (without any inhomogeneity condition). In other words, $\mathsf{A}^{\mathrm{mix}}$ restricted to $\mathcal{H}_0$ is represented by a diagonal matrix for the basis Ω^f, $f\in \mathsf{F}_0$, and accordingly $\Phi^f=\Omega^f$.

To end this subsection let us say last results, valid for monodromy matrices $\mathsf{T}^{\mathrm{mix}}$ of the form (20), also holds for those given by Eq. (16) and satisfying condition (19). In fact, on the canonical basis $e_1,\ldots,e_{n_\nu}$ of $\mathbb{C}^{n_\nu}$, using Eqs. (18) and (29), we have that

$$\tilde{\mathsf{R}}_{a}^{b\ \ n_\nu} e_k=\begin{cases} \delta_a^b/G(x/\alpha_\nu)\, e_k, & k\neq a,\\ (\,\delta_a^b+(1-\delta_a^b)\,(x/\alpha_\nu)^{2\varepsilon^\nu_{ab}}\, c_{\mathrm{sg}(b-a)}(x/\alpha_\nu))\, e_b, & k=a. \end{cases}$$

Then, applying $\tilde{\mathsf{T}}_a^{b\ \ \mathrm{mix}}$ to a vector Ω^f we arrive at Eqs. (30) or (34), depending on Image f, where the second term of coefficients C_i [see Eq. (34)] must be just changed by a factor $(x/\alpha_\sigma)^{2\varepsilon^\sigma_{ai}}$. Therefore, all above results follow. In particular, all we have said for $\mathsf{A}^{\mathrm{mix}}$ is also true for $\tilde{\mathsf{A}}^{\mathrm{mix}}$, and the former is diagonalizable iff so is the latter. There is a minor change in coefficients a_{fg}, and consequently in the linear combinations (51) that define eigenvectors of $\tilde{\mathsf{A}}^{\mathrm{mix}}$. Denoting the latter by $\tilde{\Phi}^f$, and recalling Eq. (17), we conclude

Theorem 1: *Given a mixed vertex model* $\mathsf{T}^{\mathrm{mix}}=\zeta_0\cdot\mathsf{R}_0\dot{\otimes}\zeta_1\cdot\mathsf{R}_1\dot{\otimes}\cdots\dot{\otimes}\zeta_{N-1}\cdot\mathsf{R}_{N-1}\,\Upsilon$, *with gluing matrices* $\zeta_\nu=P_\nu\hat{\zeta}_\nu P'_\nu$ *satisfying Eqs. (19) and (21), and assuming* $\mathsf{A}^{\mathrm{mix}}$ *is diagonalizable (e.g.,* $\mathsf{T}^{\mathrm{mix}}$ *is completely inhomogeneous), it follows that vectors*

$$\Phi^f\doteq(\otimes_{\nu\in\mathbb{Z}_N}P'_\nu)^{-1}\,\tilde{\Phi}^f,\qquad f\in \mathsf{F}_0,$$

are pseudovacuum states for $\mathsf{T}^{\mathrm{mix}}$ *satisfying Eqs. (27) and (28). When* $\mathrm{rank}\zeta_\nu=m\ \forall\nu$, $\mathsf{A}^{\mathrm{mix}}$ *is diagonalizable and* $\Phi^f\doteq(\otimes_{\nu\in\mathbb{Z}_N}P'_\nu)^{-1}\,\Omega^f$. □

All that can be rephrased in terms of our original mixed monodromy matrices, i.e., in the form (7). We just must regard them as particular cases of (12) subject to (13).

B. Nested Bethe equations

Let $\mathsf{T}^{\mathrm{mix}}$ be a monodromy matrix as that given in theorem above. Thanks to the algebra embeddings $\mathrm{YB}_{n-1}\hookrightarrow\mathrm{YB}_n$, $n>1$, which are a direct consequence of equations

$$[R_{n-1}]^{kl}_{ab}=[R_n]^{kl}_{ab},\qquad \text{for } 1\leqslant a,b,k,l\leqslant n-1,$$

it follows that $\mathsf{T}_a^{b\ \ \mathrm{mix}}$ for $a,b\leqslant m$ satisfy relations corresponding to the YB algebra YB_m. Then, following standard techniques for each $\Phi^f\in\mathcal{H}_0$,[7,20] that is, proposing as eigenstates for $\mathsf{t}^{\mathrm{mix}}$ [see (23)] the Bethe vectors

$$\Psi^f=\Psi^{j_1\cdots j_{r_1}}\mathsf{B}^{\mathrm{mix}}_{j_1}(x_1;\alpha)\,\cdots\,\mathsf{B}^{\mathrm{mix}}_{j_r}(x_r;\alpha)\,\Phi^f,\qquad j_1,\ldots,j_r<m,$$

and separating in the so-called *wanted* and *unwanted* terms, we arrive at a set of nested Bethe ansatz equations which in its recursive form are given by

$$\frac{\prod_{p=1}^{r_1}G(x_k^{(1)}/x_p^{(1)})}{\prod_{\nu\in f^{-1}(1)}G(x_k^{(1)}/\alpha_\nu)}\Lambda_1(x_k^{(1)})+\tau_1\prod_{p=1}^{r_1}G(x_p^{(1)}/x_k^{(1)})=0,$$

$$\frac{\prod_{p=1}^{r_l} G(x_k^{(l)}/x_p^{(l)})}{\prod_{v=1}^{r_{l-1}} G(x_k^{(l)}/x_v^{(l-1)})}\Lambda_l(x_k^{(l)})+\tau_l\prod_{p=1}^{r_l} G(x_p^{(l)}/x_k^{(l)})=0 \quad (l>1), \tag{53}$$

and

$$\Lambda_{m-1}(x)=\tau_m,$$

$$\Lambda_l(x)=\frac{\prod_{p=1}^{r_{l+1}} G(x/x_p^{(l+1)})}{\prod_{u=1}^{r_l} G(x/x_u^{(l)})}\Lambda_{l+1}(x)+\tau_{l+1}\prod_{p=1}^{r_{l+1}} G(x_p^{(l+1)}/x) \quad (l<m-2), \tag{54}$$

where $l=1,\ldots,m-1$, $k=1,\ldots,r_l$, and $0\leqslant r_l\leqslant r_{l-1}\leqslant\#[f^{-1}(1)]$. Thus, Bethe equations related to a given $\Phi^f\in\mathcal{H}_0$, are the ones corresponding to an A_{m-1} type quasiperiodic vertex model with $n_f\doteq\#[f^{-1}(1)]$ sites per row and inhomogeneity vector $\alpha_f=(\alpha_{\nu_0},\alpha_{\nu_1},\ldots,\alpha_{\nu_{n_f-1}})$, such that $\nu_i\in f^{-1}(1)$ and $\nu_i<\nu_{i+1}$ for all $i\in\mathbb{Z}_{n_f}$.

When $\#[f^{-1}(1)]=0$ we have no Bethe equations. Note in this case $\mathsf{B}_j^{\mathrm{mix}}\Phi^f=0$ for all $j<m$ [see Eq. (28)].

For each solution

$$\mathbf{x}=\{\mathbf{x}^{(l)}=(x_1^{(l)},\ldots,x_{r_l}^{(l)}):l=1,\ldots,m-1\}$$

of Eqs. (53) and (54),

$$\Lambda^f(x;\mathbf{x})=d\prod_{k=1}^{r_1} G(x/x_k^{(1)})\,\Lambda_1(x)+\tau_1\,d\prod_{\nu\in f^{-1}(1)} G(x/\alpha_\nu)\prod_{k=1}^{r_1} G(x_k^{(1)}/x) \tag{55}$$

gives an eigenvalue of $\mathsf{t}^{\mathrm{mix}}$. Note that $\Lambda^f(x;\mathbf{x})=\Lambda^g(x;\mathbf{x})$ if $f^{-1}(1)=g^{-1}(1)$. This is the main source of degeneracy for the transfer matrix. It can be seen each $\Lambda^f(x;\mathbf{x})$ differs by a factor $\Pi_{\nu\notin f^{-1}(1)}1/G(x/\alpha_\nu)$ from the corresponding eigenvalue related to the mentioned A_{m-1} model. Eigenvectors $\Psi^f(\mathbf{x})$, i.e., the Bethe vectors, can also be given recursively, but now through vectors $\Psi_l\in(\mathbb{C}^{m-l})^{\otimes r_l}$ with coordinates $(\Psi_l)^{j_1\cdots j_{r_l}}$ (w.r.t. the canonical basis of $\mathbb{C}^{m-l}$) such that

$$\Psi^f(\mathbf{x})=(\Psi_1)^{j_1\cdots j_{r_1}}\mathsf{B}_{j_1}^{\mathrm{mix}}(x_1^{(1)};\alpha)\cdots\mathsf{B}_{j_{r_1}}^{\mathrm{mix}}(x_{r_1}^{(1)};\alpha)\,\Phi^f, \tag{56}$$

for $1\leqslant l\leqslant m-2$

$$\Psi_l=(\Psi_{l+1})^{j_1\cdots j_{r_{l+1}}}\mathsf{B}_{j_1}^{(m-l,r_l)}(x_1^{(l+1)};\mathbf{x}^{(l)})\cdots\mathsf{B}_{j_{r_{l+1}}}^{(m-l,r_l)}(x_{r_{l+1}}^{(l+1)};\mathbf{x}^{(l)})\,\omega_l,$$

and $\Psi_{m-1}=1$. Here $j_1,\ldots,j_{r_{l+1}}<m$. We are denoting by ω_l the pseudovacuum for the pure monodromy matrix $\mathsf{T}^{(m-l,r_l)}$. Let us mention, in the lth level of the nesting process the involved monodromy matrix actually is the twisting

$$\mathsf{T}^{(m-l,r_l)}\cdot\Upsilon_l, \qquad \text{being} \qquad \Upsilon_l=\mathrm{diag}(\tau_1,\ldots,\tau_{m-l}),$$

which also has ω_l as pseudovacuum vector.

Summing up, we have constructed a set of eigenvectors for $\mathsf{t}^{\mathrm{mix}}$ by applying creation operators $\mathsf{B}_j^{\mathrm{mix}}$'s over all Φ^f, $f\in\mathsf{F}_0$. In the following section we address the combinatorial completeness of that set of states.

By last, let us say that Eqs. (53) and (54) do not depend either on permutations P_ν,P'_ν defining the gluing matrices of $\mathsf{T}^{\mathrm{mix}}$ (recall conditions of theorem above), or on the set of ranks of the latter. They only depend on the minimum $m=\min_\nu\{\mathrm{rank}\,\zeta_\nu\}$ of that set, on the boundary matrix

Υ, and on the inhomogeneity vector α. Hence, assuming complete integrability, the spectrum of the related transfer matrix $\mathrm{t}^{\mathrm{mix}}$, which would be given by the numbers $\Lambda^f(x;\mathbf{x})$ defined in (55), only depends on m, Υ, and α. Accordingly,

Theorem 2: *Assuming complete integrability, every mixed model with gluing matrices satisfying Eq. (19) is physically equivalent to one with monodromy matrix of the form (20) and satisfying the equal rank condition:* $\operatorname{rank}\zeta_\nu = m$ *for all* ν. □

C. Combinatorial completeness

In this section we are going to show that Eq. (56) (varying indices j from 1 to m, functions f in F_0, and $\mathbf{x}$ along solutions of (53) and (54)) defines unless $\dim \mathcal{H}^{\mathrm{mix}} = \Pi_{\nu\in\mathbb{Z}_N} n_\nu$ different vectors. That is to say, we have a set of Bethe vectors from which, *a priori*, a basis of eigenstates for the related transfer matrix can be extracted. To see that, we shall assume combinatorial completeness of Bethe ansatz equations related to the A_{n-1} vertex models, i.e., for a model with N sites in a row we suppose there is unless $(n-1)^r\binom{N}{r}$ different solutions for the Bethe equations corresponding to r creation operators. This has been shown[21] for $n=2$, but we do not know about any similar result for bigger n. In our case, we would be saying for each vector Φ^f with $f \in \mathsf{F}_0$, there exists unless a number $(m-1)^r\binom{n_f}{r}$ of different solutions of (53) and (54) corresponding to $r_1 = r$ creation operators. Recall that $n_f = \#[f^{-1}(1)]$. Let us first see why this assumption is useful for our purposes.

It is enough to analyze the case of monodromy matrices given by (20). The other cases, i.e., those given by (14) and satisfying (19), follow analogously. So let us come back to Sec. IV A 1 and consider the action of operators $\mathsf{B}_j^{\mathrm{mix}}$ with $j<m$, on vectors Ω^f with $f\in\mathsf{F}_0$. Suppose first that $\operatorname{rank}\zeta_\nu = m$ for all ν. For $a=1$ and $b=j+1$, sequences $c_i=1$, $i=1,\ldots,k$, with $1\leqslant k<n_f$ define terms proportional to vectors $\Omega^g=\Omega^{f_{\mu,j}}$, with $\mu\in f^{-1}(1)$, $f_{\mu,j}(\nu)=f(\nu)$ for all $\nu\neq\mu$ and $f_{\mu,j}(\mu)=j+1$. That is, we change a vector e_1 by a vector e_{j+1} in position $\mu\in f^{-1}(1)$. They are the only possible sequences. Thus, the action of each $\mathsf{B}_j^{\mathrm{mix}}$, $j=1,\ldots,m-1$, on a vector Ω^f gives rise to a linear combination of n_f linearly independent vectors. Existence of n_f different solutions to Eqs. (53) and (54) for $r_1=1$ and for each j, is a necessary condition to obtain n_f l.i. eigenstates from the set of Bethe vectors. Then, varying j from 1 to $m-1$, we shall have, *a priori*, $(m-1)\,n_f$ l.i. eigenstates. Applying $\mathsf{B}_i^{\mathrm{mix}}$ and $\mathsf{B}_j^{\mathrm{mix}}$ we have $(m-1)^2$ vectors, each one of them having $n_f(n_f-1)/2$ l.i. terms. In general, if we apply r creation operators to Ω^f, we have $(m-1)^r$ vectors with related $\binom{n_f}{r}$ terms. Now it becomes clear why our assumption is needed. The same argument can be given for the general rank case. There, when an operator $\mathsf{B}_j^{\mathrm{mix}}$ acts on Ω^f we have as above the terms proportional to $\Omega^{f_{\mu,j}}$, $\mu\in f^{-1}(1)$, together with additional terms given by vectors $\Omega^{h_{\sigma,j}}$ with h belonging to the same class of f. Thus, the latter appears as terms when $\mathsf{B}_j^{\mathrm{mix}}$ is applied to Ω^h. Accordingly, in order to avoid overcounting, we do not have to take them into account.

Let us come back to our original problem. If combinatorial completeness holds there exists unless a number $\Sigma_{r=0}^{n_f}(m-1)^r\binom{n_f}{r} = ((m-1)+1)^{n_f} = m^{n_f}$ of Bethe vectors for each function $f\in\mathsf{F}_0$. Thus, since $0\leqslant n_f\leqslant N$ for every $f\in\mathsf{F}$, the total number of Bethe vectors is $\Sigma_{f\in\mathsf{F}_0} m^{n_f} = \Sigma_{k=0}^{N} m^k p_k$, being p_k the number of functions $f\in\mathsf{F}_0$ such that $n_f=k$. Let us calculate p_k. It is clear that the number of functions f in F_0 with the same preimage $f^{-1}(1)$ is

$$\prod_{\nu\in\mathbb{Z}_N}(n_\nu - m)^{\varepsilon_\nu}, \quad \varepsilon_\nu = \begin{cases} 0, & \nu\in f^{-1}(1), \\ 1, & \text{otherwise.} \end{cases} \tag{57}$$

In terms of numbers $\varepsilon_0,\ldots,\varepsilon_{N-1}$, the condition $n_f=\#[f^{-1}(1)]=k$ can be characterized by an equality $\varepsilon_0+\cdots+\varepsilon_{N-1}=N-k$. Then, in order to obtain p_k we must sum over all configurations of $\varepsilon_0,\ldots,\varepsilon_{N-1}$ (ε_ν equal to 0 or 1), such that last condition holds, i.e.,

$$p_k=\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}(n_\nu-m)^{\varepsilon_\nu}\,\delta_{\varepsilon_0+\cdots+\varepsilon_{N-1},N-k}. \tag{58}$$

Accordingly,

$$\begin{aligned}\sum_{k=0}^{N}m^k p_k&=\sum_{k=0}^{N}m^k\left(\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}(n_\nu-m)^{\varepsilon_\nu}\,\delta_{\varepsilon_0+\cdots+\varepsilon_{N-1},N-k}\right)\\&=\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}(n_\nu-m)^{\varepsilon_\nu}\sum_{k=0}^{N}m^k\,\delta_{\varepsilon_0+\cdots+\varepsilon_{N-1},N-k}\\&=\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}(n_\nu-m)^{\varepsilon_\nu}\,m^{N-(\varepsilon_0+\cdots+\varepsilon_{N-1})}\\&=m^N\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}\left(\frac{n_\nu}{m}-1\right)^{\varepsilon_\nu}.\end{aligned}$$

But

$$\begin{aligned}\sum_{\varepsilon_0,\ldots,\varepsilon_{N-1}}\prod_{\nu\in\mathbb{Z}_N}\left(\frac{n_\nu}{m}-1\right)^{\varepsilon_\nu}&=\prod_{\nu\in\mathbb{Z}_N}\left(\sum_{\varepsilon_\nu}\left(\frac{n_\nu}{m}-1\right)^{\varepsilon_\nu}\right)\\&=\prod_{\nu\in\mathbb{Z}_N}\left(\left(\frac{n_\nu}{m}-1\right)^0+\left(\frac{n_\nu}{m}-1\right)\right)\\&=\prod_{\nu\in\mathbb{Z}_N}\frac{n_\nu}{m}\\&=m^{-N}\prod_{\nu\in\mathbb{Z}_N}n_\nu,\end{aligned}$$

and consequently $\Sigma_{f\in\mathsf{F}_0}m^{n_f}=\Pi_{\nu\in\mathbb{Z}_N}n_\nu$, as we wanted to see.

V. CONCLUSIONS

From the last equation we see that, under conditions of Theorem 1 and assuming complete integrability, $\mathcal{H}^{\mathrm{mix}}$ can be decomposed into a direct sum of m^{n_f}-dimensional spaces $\mathcal{H}_f$, each one of them generated by the Bethe vectors related with some f inside F_0. Note this sum, in general, is not orthogonal w.r.t. the usual scalar product in $\otimes_{\nu\in\mathbb{Z}_N}\mathbb{C}^{n_\nu}$. Thinking of the quantum spin ring related to our vertex model, whose Hamiltonian H is constructed from the logarithmic derivative (if there exists) of the transfer matrix, states of $\mathcal{H}_f$ can be interpreted as those of an anisotropic A_{m-1} type spin chain with n_f sites, which are *localized* on the subring $\mathbb{Z}_{n_f}\sim f^{-1}(1)\subset\mathbb{Z}_N$. In other words, we have decomposed a mixed spin model as a direct sum of A_{m-1} type ones with different numbers of sites and generically different inhomogeneities. Multiplicity of these models is given by (57) [recall eigenvalues (55) only depend on f through $f^{-1}(1)$]. In connection with Theorem 2 let us say that for the equal rank case, since we have $\mathcal{H}_f=\mathcal{H}_{E(f)}$ (see at the end of Sec. IV A 1), described decomposition (which results orthogonal) and mentioned multiplicity are direct consequences of the facts that last spaces are $\mathsf{T}^{\mathrm{mix}}$-invariant, and that corresponding actions on spaces $\mathcal{H}_f$ and $\mathcal{H}_g$ are equivalent when $f^{-1}(1)=g^{-1}(1)$.

In the homogeneous case we have in addition actions on $\mathcal{H}_f$ and $\mathcal{H}_g$ are equivalent still when $n_f=n_g$. In other terms, for the homogeneous equal rank case we can write $\mathcal{H}^{\mathrm{mix}}$ as the orthogonal direct sum $\mathcal{H}^{\mathrm{mix}}=\oplus_{k=0}^{N}\mathbb{C}^{p_k}\otimes\mathcal{H}_{f_k}$ [see (58) for numbers p_k], being f_k some function with $n_{f_k}=k$.

Concluding, we have presented a procedure for gluing different integrable vertex models in such a way that the integrability of the whole system is preserved. This procedure relies on some generalization of the coalgebra structure to the case of rectangular quantum matrices and their representations, enhancing the deep linking between these algebraic structures and integrability.

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Double product integrals and Enriquez quantization of Lie bialgebras I: The quasitriangular identities

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Let $\mathcal{T}(\mathcal{L})$ be the space of all tensors over a Lie algebra $\mathcal{L}$ in which the Lie bracket is obtained by taking commutators in an associative algebra. We show that $\mathcal{T}(\mathcal{L})$ becomes a Hopf algebra when equipped with a noncommutative modification of the shuffle product together with the standard coproduct. A definition is given of directed double product integrals as iterated single product integrals driven by formal power series with coefficients in the tensor product of $\mathcal{L}$ with an appropriate associative algebra. For the Hopf algebra $\mathcal{T}(\mathcal{L})[[h]]$ of formal power series we show that elements $R[h]$ of $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$ satisfying $(\Delta\otimes\mathrm{id})R[h]=R[h]^{13}R[h]^{23}$, $(\mathrm{id}\otimes\Delta)R[h]=R[h]^{13}R[h]^{12}$, and which are unitalized by the counit in either copy of $\mathcal{T}(\mathcal{L})$, can be characterized as such directed double product integrals $\Pi\Pi(1+\vec{d}\otimes\vec{d}r[h])$ where $r[h]$ is a formal power series with coefficients in $\mathcal{L}\otimes\mathcal{L}$ and vanishing constant term. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Enriquez[1] has introduced a new method of functorial quantization of Lie bialgebras based on deformation of the Hopf algebra got by equipping the vector space of tensors $\mathcal{T}(\mathcal{L})$ over a Lie bialgebra $\mathcal{L}$ with the shuffle multiplication, defined by

$$(L_1\otimes L_2\otimes\cdots\otimes L_m)(L_{m+1}\otimes L_{m+2}\otimes\cdots\otimes L_{m+n})=\sum_{\pi\in S_{m,n}} L_{\pi(1)}\otimes L_{\pi(2)}\otimes\cdots\otimes L_{\pi(m+n)}, \quad (1)$$

where $S_{m,n}$ is the set of permutations of $(1,2,\ldots,m+n)$ which conserve the order of $(1,2,\ldots,m)$ and of $(m+1,m+2,\ldots,m+n)$, and the coproduct defined by

$$\Delta(L_1\otimes L_2\otimes\cdots\otimes L_m)=\sum_{k=0}^{m}(L_1\otimes L_2\otimes\cdots\otimes L_k)\otimes(L_{k+1}\otimes L_{k+2}\otimes\cdots\otimes L_m). \quad (2)$$

Enriquez' method suggests an alternative more algebraic approach to the quantization problem to that of Etingof and Kazhdan.[2]

In Ref. 4 it was shown that in the case of a Lie algebra $\mathcal{L}$ whose Lie bracket is formed by taking commutators in a not necessarily unital associative algebra, $\mathcal{T}(\mathcal{L})$ can be equipped with a noncommutative associative unital multiplication in which the homogeneous components of the product $\gamma=\alpha\beta$ of two tensors are given in terms of those of α and β by

$$\gamma_n=\sum_{A\cup B=\{1,2,\ldots,n\}}\alpha^A_{|A|}\beta^B_{|B|}. \quad (3)$$

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Here the sum is over all 3^n ordered pairs (A,B) of not necessarily disjoint subsets whose union is $\{1,2,\ldots,n\}$, and we use the place notation that $\alpha^A_{|A|}$ indicates that the homogeneous component $\alpha_{|A|}$ is placed in the tensor product of the $|A|$ copies of $\mathcal{L}$ within $\otimes^n\mathcal{L}$ labeled by the elements of A, $\beta^B_{|B|}$ is defined analogously, so that since $A\cup B=\{1,2,\ldots,n\}$ all copies of $\mathcal{L}$ within $\otimes^n\mathcal{L}$ are occupied by $\alpha^A_{|A|}\beta^B_{|B|}$, and double occupancies are reduced using the multiplication in $\mathcal{L}$. The shuffle product (1) corresponds to restricting the sum in (3) to disjoint pairs (A,B). Alternatively we may define the multiplication (3) by bilinear extension of its action on homogeneous product tensors, which is:

$$(L_1\otimes L_2\otimes\cdots\otimes L_m)(L_{m+1}\otimes L_{m+2}\otimes\cdots\otimes L_{m+n})=\sum_{j=m\vee n}^{m+n}\sum_{(P_1,P_2,\ldots,P_j)\in\mathcal{P}_j} L_{P_1}\otimes L_{P_2}\otimes\cdots\otimes L_{P_j}, \tag{4}$$

where $\mathcal{P}_j$ is the set of ordered partitions $(P_1,P_2,\ldots,P_j)$ of $\{1,2,\ldots,m+n\}$ into j subsets such that:

(i) Each subset P is either a singleton $\{i\}$, in which case $L_P=L_i$, or a pair $\{k,l\}$ with $k\in\{1,2,\ldots,m\}$ and $l\in\{m+1,m+2,\ldots,m+n\}$, in which case $L_P=L_kL_l$;
(ii) the permutation $(P_1,P_2,\ldots,P_j)$ of $(1,2,\ldots,m+n)$, in which each pair is in increasing order, is an element of $S_{m,n}$.

Remark: We are grateful to the referee for the interesting observation that the multiplication (4) is similar to the general product formula for multizeta functions

$$\zeta(s_1,s_2,\ldots,s_m)=\sum_{1\leqslant j_1<j_2<\cdots<j_m<\infty} j_1^{s_1}j_2^{s_2}\cdots j_m^{s_m},$$

of interest in number theory, namely,

$$\zeta(s_1,s_2,\ldots,s_m)\zeta(s_{m+1},s_{m+2},\ldots,s_{m+n})=\sum_{j=m\vee n}^{m+n}\sum_{(P_1,P_2,\ldots,P_j)\in\mathcal{P}_j}\zeta(s_{P_1},s_{P_2},\ldots,s_{P_k}),$$

where $s_P=s_j$ if P is a singleton $\{j\}$ and $s_P=s_j+s_k$ if P is a pair $\{j,k\}$.

Motivated by quantum stochastic calculus, we refer to (3) or (4) as the *Itô shuffle product* and the corresponding algebra as the *Itô shuffle algebra*. We shall show below that this algebra is also a Hopf algebra under the co-product (2). The subspace $\mathcal{S}(\mathcal{L})$ of $\mathcal{T}(\mathcal{L})$ comprising symmetric tensors is a sub-Hopf algebra isomorphic to the universal enveloping $\mathcal{U}$ algebra of $\mathcal{L}$.

By replacing (3) by

$$\gamma_n=\sum_{A\cup B=\{1,2,\ldots,n\}} h^{|A\cap B|}\alpha^A_{|A|}\beta^B_{|B|},$$

we can make $\mathcal{T}(\mathcal{L})[[h]]$ into a formal deformation of the Enriquez-type.[9]

Enriquez' method depends firstly on finding an element $R[h]$ of the deformed Hopf algebra which satisfies the quasitriangular identities

$$(\Delta\otimes\mathrm{id})R[h]=R[h]^{13}R[h]^{23},\quad(\mathrm{id}\otimes\Delta)R[h]=R[h]^{13}R[h]^{12}. \tag{5}$$

In the present work we shall find a characterization of such elements of the Hopf algebra $\mathcal{T}(\mathcal{L})\times[[h]]$ as directed double product integrals, whose definition will now be explained.

We introduce *right* and *left differential maps* $\vec{d}$ and $\overleftarrow{d}$ from $\mathcal{T}(\mathcal{L})$ to $\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ and to $\mathcal{L}\otimes\mathcal{T}(\mathcal{L})$ by linear extension of their actions on homogeneous product tensors

$$\vec{d}(L_1\otimes L_2\otimes\cdots\otimes L_m)=(L_1\otimes L_2\otimes\cdots\otimes L_{m-1})\otimes L_m,$$

$$\overleftarrow{d}(L_1\otimes L_2\otimes\cdots\otimes L_m)=L_1\otimes(L_2\otimes L_3\cdots\otimes L_m).$$

When $\mathcal{T}(\mathcal{L})$ is equipped with the shuffle product (1) these satisfy the Leibniz formulas

$$\overleftarrow{d}(\alpha\beta)=\overleftarrow{d}(\alpha)\beta+\alpha\overleftarrow{d}(\beta), \tag{6}$$

in which $\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ and $\mathcal{L}\otimes\mathcal{T}(\mathcal{L})$ are regarded as $\mathcal{T}(\mathcal{L})$-bimodules using the natural tensorial actions got by linear extension of

$$\alpha(\beta\otimes L)=(\alpha\otimes L)\beta=(\alpha\beta)\otimes L,\quad \alpha(L\otimes\beta)=(L\otimes\alpha)\beta=L\otimes(\alpha\beta). \tag{7}$$

To see that (6) holds for $\vec{d}$, for example, we may decompose into two parts the sum on the right-hand side of (1) according to whether or not $\pi(m+n)$ belongs to $\{1,2,\ldots,m\}$ or to $\{m+1,m+2,\ldots,m+n\}$, and then apply $\vec{d}$ to both sides. It is evident from actions on homogeneous product tensors that the iterates

$$\overleftrightarrow{d}^{(n)}=(\overleftarrow{d}\otimes\mathrm{id}_{\otimes^{n-1}\mathcal{L}})\circ(\overleftarrow{d}\otimes\mathrm{id}_{\otimes^{n-2}\mathcal{L}})\circ\cdots\circ\overleftarrow{d},\quad n=1,2,\ldots,$$

of both the left and right differential maps satisfy

$$\textcircled{+}_{n=0}^{\infty}\overleftrightarrow{d}^{(n)}=\Delta,$$

where we make the identifications

$$\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})=\bigoplus_{n=0}^{\infty}(\mathcal{T}(\mathcal{L})\otimes(\otimes^n\mathcal{L}))=\bigoplus_{n=0}^{\infty}((\otimes^n\mathcal{L})\otimes\mathcal{T}(\mathcal{L})). \tag{8}$$

If we replace the shuffle product (1) by the Itô shuffle product (4) we find, instead of the Leibniz formula (6), the *Leibniz–Itô formula*

$$\overleftarrow{d}(\alpha\beta)=\overleftarrow{d}(\alpha)\beta+\alpha\overleftarrow{d}(\beta)+\overleftarrow{d}(\alpha)\overleftarrow{d}(\beta), \tag{9}$$

where now the first two terms on the right-hand side refer to the tensorial actions defined by (7), but in which the multiplications are now given by (3), and the third term refers to the tensor product multiplication of the Itô shuffle product in $\mathcal{T}(\mathcal{L})$ with the given multiplication in $\mathcal{L}$. (9) may be seen to hold for $\vec{d}$, for example, by decomposing the inner sum on the right-hand side of (4) into three parts, according to whether the final element L_{S_j} is such that S_j is a singleton $\{i\}\subset\{1,2,\ldots,m\}$, a singleton $\{k\}\subset\{m+1,m+2,\ldots,m+n\}$ or a pair $\{i,k\}$.

The Leibniz formula (6) shows that the right or left differential map defines a differential calculus in the sense of Woronowicz[10] when $\mathcal{T}(\mathcal{L})$ is equipped with the shuffle product and $\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ or $\mathcal{L}\otimes\mathcal{T}(\mathcal{L})$ is equipped with the tensorial biaction defined by (7). In the case of the Itô shuffle product the Leibniz–Ito formula (9) can be reduced to the Leibniz formula (6) by modifying either the right or left actions. For example, if we define $\vec{\bullet}$: $(\mathcal{T}(\mathcal{L})\otimes\mathcal{L})\times\mathcal{T}(\mathcal{L})\to\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ by

$$M\vec{\bullet}\alpha=M\alpha+M\vec{d}\alpha,$$

where the first term is the tensorial action (7) with Itô shuffle product and the second is the tensor product multiplication in $\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ then, using the formula (9), it may be verified that $\vec{\bullet}$ defines a right action, compatible with the corresponding left tensorial action, in terms of which (9) assumes the Leibniz form

$$\vec{d}(\alpha\beta)=\vec{d}(\alpha)\vec{\bullet}\beta+\alpha\vec{d}(\beta).$$

Alternatively a similar modification may be made to the left action to achieve the Leibniz formula. But the asymmetry of the two corresponding Woronowicz calculus (which are not bicovariant in the sense of Ref. 10) make them impractical to use in what follows. Henceforth we always assume that $\mathcal{T}(\mathcal{L})$ is equipped with the Itô shuffle product and that $\mathcal{T}(\mathcal{L})$ acts correspondingly on $\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ or $\mathcal{L}\otimes\mathcal{T}(\mathcal{L})$ according to (7), so that (9) holds. Correspondingly, we regard the space $\mathcal{T}(\mathcal{L})\times[[h]]$ of formal power series as a Hopf algebra under the convolution multiplication formed from the Itô shuffle multiplication and action of Δ on coefficients.

In Ref. 7 we formulated an algebraic theory of product integrals of the form $\Pi(1+dL[h])$ where $L[h]$ is an element of the space $h\mathcal{L}[[h]]$ of formal power series with coefficents in $\mathcal{L}$ and with vanishing zero order coefficient. While this theory is originally formulated in terms of a quantum stochastic calculus of which the associative algebra $\mathcal{L}$ is the algebra of Itô differentials, its algebraic character ensures a reformulation independent of the quantum stochastic context, and that each product integral of the theory has an indefinite version living in $\mathcal{S}(\mathcal{L})[[h]]$, or equivalently in $\mathcal{U}[[h]]$. In this form, in view of Ref. 4, the theory can be set up for an arbitrary commutator Lie algebra $\mathcal{L}$. Product integrals of this type are characterized among all elements $X[h]$ of $\mathcal{S}(\mathcal{L})[[h]]$ by the grouplikeness conditions

$$\varepsilon(X[h])=1,\ \ \Delta(X[h])=X[h]\otimes X[h], \tag{10}$$

where ε denotes the co-unit. Note that the simple product integral $X[h]=\Pi(1+dL[h]$ can be defined as the solution of the differential equation

$$dX[h]=X[h]\otimes dL[h],\ \ \varepsilon(X[h])=1, \tag{11}$$

whose unique solution is well defined algebraically.[3]

In Ref. 8 we developed a corresponding theory of double product integrals of the form $\Pi\Pi(1+dr[h])$ where $r[h]$ is an element of $h(\mathcal{L}\otimes\mathcal{L})[[h]]$, again in the quantum stochastic context. In order to obtain a theory whose indefinite version would live in $(\mathcal{U}\otimes\mathcal{U})[[h]]$ or equivalently in $(\mathcal{S}(\mathcal{L})\otimes\mathcal{S}(\mathcal{L}))[[h]]$ the double products were symmetrized in a way which prevents them from enjoying some cogent mathematical properties.

In the present work we shall develop a theory of double product integrals without the symmetry assumption, which thus live not in $(\mathcal{S}(\mathcal{L})\otimes\mathcal{S}(\mathcal{L}))[[h]]$, but in $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$. We must now distinguish between forward, mixed, and backward double products $\Pi\Pi(1+\vec{d}\otimes\vec{d}r[h])$, $\Pi\Pi(1+\vec{d}\otimes\overleftarrow{d}r[h])$, $\Pi\Pi(1+\overleftarrow{d}\otimes\vec{d}r[h])$ and $\Pi\Pi(1+\overleftarrow{d}\otimes\overleftarrow{d}r[h])$, for which we also use the abbreviated notations $\overrightarrow{\Pi\Pi}(1+dr[h])$, $\overrightarrow{\Pi\Pi}(1+dr[h])$, $\overleftarrow{\Pi\Pi}(1+dr[h])$, and $\overleftarrow{\Pi\Pi}(1+dr[h])$, respectively. We shall show that each such double product integral can be defined, in two different ways, as a simple product integral, which is the solution of an algebraic differential equation, generalizing (11), but in which the driving term which generalizes $L[h]$ has coefficients living in the tensor product of $\mathcal{L}$ with another associative algebra called the system algebra, and is itself also essentially a simple product integral of the same type driven by $r[h]\in h(\mathcal{L}\otimes\mathcal{L})[[h]]$ where one of the two copies of $\mathcal{L}$ plays the role of the system algebra. That the two definitions agree may be regarded as loosely analogous to Fubini's theorem.[5] More precisely the agreement may be regarded as a continuous algebraic version of the identity

$$\prod_j^{\rightarrow}\left(\prod_k^{\rightarrow}(1+x_{j,k})\right)=\prod_k^{\rightarrow}\left(\prod_j^{\rightarrow}(1+x_{j,k})\right), \tag{12}$$

which holds[8] whenever the elements $x_{j,k}$ of a unital associative algebra are weakly commuting in the sense that $x_{j,k}$ commutes with $x_{j',k'}$ whenever $j\neq j'$ and $k\neq k'$ (but not necessarily when $j=j'$ but $k\neq k'$, for example).

We shall show that these double product integrals can then be characterized analogously to (10), for example, an element $R[h]$ of $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$ is of form $\overrightarrow{\prod}(1+dr[h])$ if and only if it satisfies (5) as well as

$$(\varepsilon\otimes\mathrm{id})R[h]=(\mathrm{id}\otimes\varepsilon)R[h]=1.$$

The next stage in Enriquez' quantization procedure is to require that $R[h]$ satisfy, in addition to (5), the quantum Yang–Baxter equation

$$R[h]^{12}R[h]^{13}R[h]^{23}=R[h]^{23}R[h]^{13}R[h]^{12}, \tag{13}$$

in $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$. In a subsequent paper we shall establish a condition on $r[h]$ necessary and sufficient for the mixed double integral $\overrightarrow{\prod}(1+dr[h])$ to satisfy (13).

We use the following notational conventions. If $\mathcal{A}$ is a vector space we denote by $\mathcal{A}[[h]]$ the space of formal power series with coefficients in $\mathcal{A}$ and by $h\mathcal{A}[[h]]$ the subspace of $\mathcal{A}[[h]]$ of elements for which the coefficient of h^0 is zero. When $\mathcal{A}$ is a not necessarily unital associative algebra we equip $\mathcal{A}[[h]]$ with the convolution product

$$\sum_{N=0}^{\infty}h^N A_N\sum_{N=0}^{\infty}h^N B_N=\sum_{N=0}^{\infty}h^N\sum_{j=0}^{N}A_{N-j}B_j\,.$$

Linear maps from $\mathcal{A}$ are extended to $\mathcal{A}[[h]]$ by action on the coefficients. If $\mathcal{V}_1,\mathcal{V}_2,\ldots,\mathcal{V}_n$ are vector spaces and π is a permutation of $(1,2,\ldots,n)$, we denote by τ_π the linear map from $\mathcal{V}_1\otimes\mathcal{V}_2\otimes\cdots\otimes\mathcal{V}_n$ to $\mathcal{V}_{\pi(1)}\otimes\mathcal{V}_{\pi(2)}\otimes\cdots\otimes\mathcal{V}_{\pi(n)}$ which appropriately permutes the components of product tensors.

II. $\mathcal{T}(\mathcal{L})$ AS A HOPF ALGEBRA WITH THE ITÔ SHUFFLE PRODUCT

Let $\mathcal{L}$ be a finite dimensional associative algebra, not necessarily unital, over a field $\mathbb{F}$ of characteristic zero fixed once and for all. We are interested in $\mathcal{L}$ as a Lie algebra under the commutator Lie bracket $[L,K]=LK-KL$ and in the universal enveloping algebra $\mathcal{U}$ of this Lie algebra. Let

$$\mathcal{T}(\mathcal{L})=\bigoplus_{n=0}^{\infty}(\otimes^n\mathcal{L}),$$

denote the vector space of all tensors over $\mathcal{L}$. It is well known that $\mathcal{T}(\mathcal{L})$ becomes a Hopf algebra under the coproduct Δ defined by linear extension of its action on homogeneous product tensors (2) when the multiplication is the shuffle product (1); we call this the *shuffle* Hopf algebra. The antipode is defined by linear extension of the map

$$L_1\otimes L_2\otimes\cdots\otimes L_m\mapsto(-1)^m L_m\otimes L_{m-1}\otimes\cdots\otimes L_1\,. \tag{14}$$

Our first task is to show that $\mathcal{T}(\mathcal{L})$ remains a Hopf algebra under the coproduct Δ when the shuffle multiplication is replaced by (3).

Theorem 1: Δ *is multiplicative for the Itô shuffle product* (3).

Proof: Let $\alpha,\beta\in\mathcal{T}(\mathcal{L})$. To lighten notation we temporarily denote the right differential map $\vec{d}$ by d. We show that, for $n=0,1,2,\ldots$, the nth rank component of $\Delta(\alpha\beta)$ under the identification (8), which is

$$((d\otimes\mathrm{id}_{\otimes^{n-1}\mathcal{L}})\circ(d\otimes\mathrm{id}_{\otimes^{n-2}\mathcal{L}})\circ\cdots\circ d)(\alpha\beta),$$

is equal to the nth rank component of $\Delta(\alpha)\Delta(\beta)$, which by (3) is

$$\sum_{A\cup B=\{1,2,\ldots,n\}} (((d\otimes \mathrm{id}_{\otimes^{|A|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|A|-2}\mathcal{L}})\circ\cdots\circ d)(\alpha))^A,$$

$$(((d\otimes \mathrm{id}_{\otimes^{|B|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|B|-2}\mathcal{L}})\circ\cdots\circ d)(\beta))^B.$$

Here we use the place notation that, for example, the superscript A indicates that the term to which it is attached occupies the tensor product of $\mathcal{T}(\mathcal{L})$ and those copies of $\mathcal{L}$ within $\otimes^n\mathcal{L}$ labeled by elements of A and the two terms are multiplied using the multiplication (3) in $\mathcal{T}(\mathcal{L})$ together with that in $\mathcal{L}$ in case of double occupancy. The proof is by induction on n beginning with the observation that when $n=0$ both expressions are equal to $\alpha\beta$. For general nonzero n we divide the sum in the second expression into three parts depending on whether n belongs to $A\cap B^c$, to $A^c\cap B$, or to $A\cap B$, and write it as

$$\sum_{C\cup D=\{1,2,\ldots,n-1\}} \{(((d\otimes \mathrm{id}_{\otimes^{|C|}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|C|-1}\mathcal{L}})\circ\cdots\circ d)(\alpha))^{C\cup\{n\}}(((d\otimes \mathrm{id}_{\otimes^{|D|-1}\mathcal{L}})$$
$$\circ(d\otimes \mathrm{id}_{\otimes^{|D|-2}\mathcal{L}})\circ\cdots\circ d)(\beta))^D+(((d\otimes \mathrm{id}_{\otimes^{|C|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|C|-2}\mathcal{L}})\circ\cdots\circ d)(\alpha))^C$$
$$\times(((d\otimes \mathrm{id}_{\otimes^{|D|}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|D|-1}\mathcal{L}})\circ\cdots\circ d)(\beta))^{D\cup\{n\}}$$
$$+(((d\otimes \mathrm{id}_{\otimes^{|C|}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|C|-1}\mathcal{L}})\circ\cdots\circ d)(\alpha))^{C\cup\{n\}}$$
$$\times(((d\otimes \mathrm{id}_{\otimes^{|D|}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|D|-1}\mathcal{L}})\circ\cdots\circ d)(\beta))^{D\cup\{n\}}\}.$$

This may be expressed as

$$(d\otimes \mathrm{id}_{\otimes^n\mathcal{L}})\Bigg(\sum_{C\cup D=\{1,2,\ldots,n-1\}} (((d\otimes \mathrm{id}_{\otimes^{|C|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|C|-2}\mathcal{L}})\circ\cdots\circ d)(\alpha))^C$$
$$\times(((d\otimes \mathrm{id}_{\otimes^{|D|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|D|-2}\mathcal{L}})\circ\cdots\circ d)(\beta))^D\Bigg),$$

as is seen by applying the Leibniz–Itô formula (9) to each product occuring in the latter sum. Making the inductive assumption that

$$\sum_{C\cup D=\{1,2,\ldots,n-1\}} (((d\otimes \mathrm{id}_{\otimes^{|C|-1}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{|C|-2}\mathcal{L}})\circ\cdots\circ d)(\alpha))^C(((d\otimes \mathrm{id}_{\otimes^{|D|-1}\mathcal{L}})$$
$$\circ(d\otimes \mathrm{id}_{\otimes^{|D|-2}\mathcal{L}})\circ\cdots\circ d)(\beta))^D$$
$$=((d\otimes \mathrm{id}_{\otimes^{n-2}\mathcal{L}})\circ(d\otimes \mathrm{id}_{\otimes^{n-3}\mathcal{L}})\circ\cdots\circ d)(\alpha\beta)$$

completes the proof. □

Equipped with the Itô product and the co-product Δ, $\mathcal{T}(\mathcal{L})$ becomes a bialgebra equipped with the same unit $1_{\mathcal{T}(\mathcal{L})}=(1_{\mathbb{F}},0,0,\ldots)$ and co-unit

$$\varepsilon:\mathcal{T}(\mathcal{L})=\bigoplus_{n=0}^{\infty}\otimes^n\mathcal{L}\ni(\alpha_0,\alpha_1,\alpha_2,\ldots)\mapsto\alpha_0,$$

as the shuffle Hopf algebra. Since the Itô multiplication acts on homogeneous tensors by adding terms of lower rank to the shuffle product the argument that a deformation bialgebra of a Hopf algebra is itself a Hopf algebra[3] may be adapted to conclude that the new bialgebra is equipped with a antipode whose action on homogeneous tensors is got by adding lower rank terms to (14). We call the resulting Hopf algebra the *Itô–Hopf algebra*.

III. SIMPLE PRODUCT INTEGRALS WITH A SYSTEM ALGEBRA

Let $\mathcal{A}$ be a possibly nonunital associative algebra which we call the *system algebra*. Let $l[h]$ be an element of $h(\mathcal{A}\otimes\mathcal{L})[[h]]$ and write $l[h]=\Sigma_{j=1}^{d} l_j[h]\otimes L^j$ where $l_j[h]\in\mathcal{A}_0[h]$ and $(L^1,L^2,\ldots,L^d)$ is a basis for $\mathcal{L}$. We consider the infinite sum

$$\sum_{n=1}^{\prime\prime\prime} l[h]\boxtimes l[h]\boxtimes\cdots\boxtimes\overset{(n)}{l}[h]=\sum_{n=1}^{\infty}\boxtimes^n l[h]. \tag{15}$$

Here the notation is as follows. The composition $\boxtimes$ denotes multiplication in $h\mathcal{A}[[h]]$ and tensoring in $\mathcal{L}$, thus

$$\boxtimes^n l[h]=\sum_{j_1,\ldots,j_n=1}^{d}\prod_{r=1}^{n} l_{j_r}[h]\otimes(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N}).$$

The sum (15) can be rearranged as a well defined element $\Sigma_{N=1}^{\infty}h^N X_N$ of $h(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$.[7] If $\mathcal{A}$ is unital then the element $X[h]=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+\Sigma_{N=1}^{\infty}h^N X_N$ of $(\mathcal{A}\otimes T(L))[[h]]$ is the unique solution of the algebraic differential equation

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X[h]=X[h]\boxtimes dl[h],\quad (\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}}.$$

We denote it by ${}_{\mathcal{A}}\Pi(1+\vec{d}l[h])$. In the nonunital case we define the original rearranged sum (15) in $h(\mathcal{A}\otimes T(L))[[h]]$ to be the *decapitated* product integral ${}_{\mathcal{A}}\hat{\Pi}(1+\vec{d}l[h])$. In a similar way, starting from an element $m[h]=\Sigma_{j=1}^{d}L^j\otimes m_j[h]$ of $h(\mathcal{L}\otimes A)[[h]]$ we define the product integrals

$$\begin{aligned}\prod{}_{\mathcal{A}}(1+\vec{d}m[h])&=1_{\mathcal{T}(\mathcal{L})\otimes\mathcal{A}}+\sum_{n=1}^{\infty}\boxtimes^n m[h]\\&=1_{\mathcal{T}(\mathcal{L})\otimes\mathcal{A}}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N})\otimes\prod_{r=1}^{N}m_{j_r}[h],\end{aligned}$$

in $(\mathcal{T}(\mathcal{L})\otimes\mathcal{A})[[h]]$ in the unital case, and

$$\widehat{\prod}{}_{\mathcal{A}}(1+\vec{d}m[h])=\sum_{n=1}^{\infty}\boxtimes^n m[h]=\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N})\otimes\prod_{r=1}^{N}m_{j_r}[h],$$

in $h(\mathcal{T}(\mathcal{L})\otimes\mathcal{A})[[h]]$ when $\mathcal{A}$ is nonunital. Thus the position of the subscript $\mathcal{A}$ indicates whether the system algebra is tensored to the right or the left of $\mathcal{T}(\mathcal{L})$. We distinguish these *forward* product integrals from the corresponding *backward* product integrals

$${}_{\mathcal{A}}\prod(1+\overleftarrow{d}l[h]),\quad {}_{\mathcal{A}}\widehat{\prod}(1+\overleftarrow{d}l[h]),\quad \prod{}_{\mathcal{A}}(1+\overleftarrow{d}m[h]),\quad \widehat{\prod}{}_{\mathcal{A}}(1+\overleftarrow{d}m[h]),$$

which are solutions of left differential equations. For example,

$$\begin{aligned}{}_{\mathcal{A}}\prod(1+\overleftarrow{d}l[h])&=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+\tilde{\boxtimes}^n l[h]\\&=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes(L^{j_N}\otimes L^{j_{N-1}}\otimes\cdots\otimes L^{j_1}),\end{aligned}$$

where the symbol $\tilde{\boxtimes}$ denotes multiplication in $\mathcal{A}[[h]]$ combined with tensoring in the opposite direction in $\mathcal{L}$, so that for example $(a\otimes L)\ \tilde{\boxtimes}(b\otimes K)=ab\otimes(K\otimes L)$. ${}_{\mathcal{A}}\Pi(1+\overleftarrow{d}l[h])$ solves the differential equation

$$(\mathrm{id}_{\mathcal{A}}\otimes\tilde{d})X[h]=dl[h]\boxtimes X[h],\quad (\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}}.$$

The theorem which follows generalizes to the case where there is a nontrivial system algebra the characterization[7] of grouplike elements of $\mathcal{S}(\mathcal{L})[[h]]$ as simple product integrals. In preparation for the proof, note that

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\varepsilon\otimes\mathrm{id}_{\mathcal{L}})\circ(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\vec{d})\circ\Delta=\vec{d},$$

as follows from comparison of actions of the two sides on product tensors, and hence

$$(\mathrm{id}_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}\otimes\varepsilon\otimes\mathrm{id}_{\mathcal{L}})\circ(\mathrm{id}_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}\otimes\vec{d})\circ(\mathrm{id}_{\mathcal{A}}\otimes\Delta)=\mathrm{id}_{\mathcal{A}}\otimes\vec{d}. \tag{16}$$

The symbol $\boxtimes$ is used now to denote the operation from $(\mathcal{A}\otimes T(L))[[h]]\times(\mathcal{A}\otimes T(L))[[h]]$ to $(\mathcal{A}\otimes T(L)\otimes T(L))[[h]]$ got by tensoring multiplication from $\mathcal{A}\times\mathcal{A}$ to $\mathcal{A}$ with the tensor product composition from $\mathcal{T}(\mathcal{L})\times\mathcal{T}(\mathcal{L})$ to $\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})$. We regard Δ as a map from $\mathcal{T}(\mathcal{L})[[h]]$ to $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$ by action on coefficients.

Theorem 2: *Let $l[h]\in h(\mathcal{A}\otimes L)[[h]]$ where $\mathcal{A}$ is assumed unital. Then*

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)\prod_{\mathcal{A}}(1+\vec{d}l[h])=\prod_{\mathcal{A}}(1+\vec{d}l[h])\boxtimes\prod_{\mathcal{A}}(1+\vec{d}l[h])$$

and

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)\prod_{\mathcal{A}}(1+\vec{d}l[h])=1_{\mathcal{A}}.$$

Conversely, let $X[h]$ be an element of $(\mathcal{A}\otimes T(L))[[h]]$ satisfying

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)X[h]=X[h]\boxtimes X[h],\quad (\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}}. \tag{17}$$

Then there exists an element $l[h]\in h(\mathcal{A}\otimes L)[[h]]$ such that $X[h]=\prod_{\mathcal{A}}(1+\vec{d}l[h])$.

Proof: Applying the map $\mathrm{id}_{\mathcal{A}}\otimes\Delta$ to

$$\prod_{\mathcal{A}}(1+\vec{d}l[h])=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N}),$$

using (2) we obtain

$$\begin{aligned}
&1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes\sum_{s=0}^{N}(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_s})\otimes(L^{j_{s+1}}\otimes L^{j_{s+2}}\otimes\cdots\\
&\quad\otimes L^{j_N})=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})}+\sum_{N=1}^{\infty}\left(\sum_{j_1,j_2,\ldots j_s=1}^{d}\sum_{s=0}^{N}\prod_{r=1}^{s}l_{j_r}[h]\otimes(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_s})\right)\\
&\quad\boxtimes\left(\sum_{j_{s+1},j_{s+2},\ldots,j_N=1}^{d}\prod_{r=s+1}^{N}l_{j_r}[h]\otimes(L^{j_{s+1}}\otimes L^{j_{s+2}}\otimes\cdots\otimes L^{j_N})\right)\\
&=\Bigg(1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}\\
&\quad+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N})\Bigg)\\
&\quad\boxtimes\left(1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N})\right)\\
&=\left(\prod_{\mathcal{A}}(1+\vec{d}l[h])\right)\boxtimes\left(\prod_{\mathcal{A}}(1+\vec{d}l[h])\right),
\end{aligned}$$

also

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)\,{}_{\mathcal{A}}\prod\,(1+\vec{d}l[h])=1_{\mathcal{A}}+\sum_{N=1}^{\infty}\sum_{j_1,j_2,\ldots,j_N=1}^{d}\prod_{r=1}^{N}l_{j_r}[h]\otimes\varepsilon(L^{j_1}\otimes L^{j_2}\otimes\cdots\otimes L^{j_N})=1_{\mathcal{A}},$$

as required.

To prove the converse we adapt the corresponding proof for the case $\mathcal{A}=\mathbb{F}$.[4] Thus let $X[h]$ satisfy (17) and be of form $1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+Y[h]$, where $Y[h]\in h(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$. Applying $(\mathrm{id}_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}\otimes\varepsilon\otimes\mathrm{id}_{\mathcal{L}})\circ(\mathrm{id}_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}\otimes\vec{d})$ to $(\mathrm{id}_{\mathcal{A}}\otimes\Delta)X[h]=X[h]\boxtimes X[h]$ and using (16) we obtain that $X[h]$ satisfies the differential equation

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X[h]=X[h]\boxtimes dl[h],\quad(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}},$$

where $l[h]=(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon\otimes\mathrm{id}_{\mathcal{L}})X[h]\in\mathcal{A}\otimes\mathcal{T}(\mathcal{L})[[h]]$. Comparing coefficients of h^0 we see that

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X_0=X_0\boxtimes dl_0,\quad(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X_0=1_{\mathcal{A}}.$$

Since $\vec{d}$ is degree reducing on the graded algebra $\mathcal{T}(\mathcal{L})$ this can hold only if $l_0=0$. Hence $l[h]\in h(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$ and the proof is complete. □

Corollary 3: Let $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ where $\mathcal{A}$ is possibly nonunital. Then the element $Y[h]={}_{\mathcal{A}}\hat{\Pi}(1+\vec{d}l[h])$ of $(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$ satisfies

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)Y[h]=Y[h]\otimes1_{\mathcal{T}(\mathcal{L})}+\tau_{(1,3,2)}(Y[h]\otimes1_{\mathcal{T}(\mathcal{L})})+Y[h]\boxtimes Y[h]$$

and

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)Y[h]=0_{\mathcal{A}}.$$

Conversely, let $Y[h]$ be an element of $(\mathcal{A}\otimes T(\mathcal{L}))[[h]]$ satisfying these conditions. Then there exists an element $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ such that $Y[h]={}_{\mathcal{A}}\hat{\Pi}(1+\vec{d}l[h])$.

Proof: We adjoin a unit to $\mathcal{A}$ if it lacks one. Then the Corollary follows from the Theorem by writing ${}_{\mathcal{A}}\Pi(1+\vec{d}l[h])=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\hat{\Pi}(1+\vec{d}l[h])$ and $X[h]=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+Y[h]$. □

Analogous characterisations hold to those of Theorem 2 and its corollary for product integrals of form $\Pi\,{}_{\mathcal{A}}(1+\vec{d}m[h])$ and $\hat{\Pi}\,{}_{\mathcal{A}}(1+\vec{d}m[h])$. To formulate the analogues for backward directed products we need the composition $\tilde{\boxtimes}$ in which elements of $\mathcal{A}$ are multiplied and elements of $\mathcal{T}(\mathcal{L})$ are tensored, but in the reverse direction.

Theorem 4: *Let $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ where $\mathcal{A}$ is assumed unital. Then*

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)\,{}_{\mathcal{A}}\prod\,(1+\tilde{d}l[h])={}_{\mathcal{A}}\prod\,(1+\tilde{d}l[h])\,\tilde{\boxtimes}\,{}_{\mathcal{A}}\prod\,(1+\tilde{d}l[h])$$

and

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)\,{}_{\mathcal{A}}\prod\,(1+\tilde{d}l[h])=1_{\mathcal{A}}.$$

Conversely, let $X[h]$ be an element of $(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$ satisfying

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)X[h]=X[h]\tilde{\boxtimes}X[h],\quad(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}}.\tag{18}$$

Then there exists an element $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ such that $X[h]={}_{\mathcal{A}}\Pi(1+\tilde{d}l[h])$.

This Theorem and its Corollary which follows are proved analogously to Theorem 2 and its Corollary.

Corollary 5: Let $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ *where* $\mathcal{A}$ *is possibly nonunital. Then the element* $Y[h]={}_{\mathcal{A}}\hat{\Pi}(1+\tilde{d}l[h])$ *of* $(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$ *satisfies*

$$(\mathrm{id}_{\mathcal{A}}\otimes\Delta)Y[h]=Y[h]\otimes 1_{\mathcal{T}(\mathcal{L})}+\tau_{(1,3,2)}(Y[h]\otimes 1_{\mathcal{T}(\mathcal{L})})+Y[h]\tilde{\boxtimes}Y[h]$$

and

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)Y[h]=0_{\mathcal{A}}.$$

Conversely, let $Y[h]$ *be an element of* $(\mathcal{A}\otimes\mathcal{T}(\mathcal{L}))[[h]]$ *satisfying these conditions. Then there exists an element* $l[h]\in h(\mathcal{A}\otimes\mathcal{L})[[h]]$ *such that* $Y[h]={}_{\mathcal{A}}\hat{\Pi}(1+\tilde{d}l[h])$.

Now let $l[h]=\Sigma_{j=1}^{d}l_j[h]\otimes L^j$ and $m[h]=\Sigma_{k=1}^{d}m_k[h]\otimes L^k$ be elements of $h(\mathcal{A}\otimes\mathcal{L})[[h]]$. We say that they are $\mathcal{A}$-commuting if each $l_j[h]$ commutes with each $m_k[h]$ as elements of $\mathcal{A}[[h]]$. $\mathcal{A}$-commuting elements $h(\mathcal{L}\otimes\mathcal{A})[[h]]$ are defined analogously.

Theorem 6: *Let* $l[h]$ *and* $m[h]$ *be* $\mathcal{A}$*-commuting elements of* $h(\mathcal{A}\otimes\mathcal{L})[[h]]$ *and let*

$$n[h]=l[h]+m[h]+l[h]m[h],$$

where $l[h]m[h]$ *is formed using the tensor product associative multiplication in* $\mathcal{A}\otimes\mathcal{L}$*. Then if* $\mathcal{A}$ *is unital*

$${}_{\mathcal{A}}\prod(1+\vec{d}l[h])\,{}_{\mathcal{A}}\prod(1+\vec{d}m[h])={}_{\mathcal{A}}\prod(1+\vec{d}n[h]),$$

and in the nonunital case

$${}_{\mathcal{A}}\widehat{\prod}(1+\vec{d}l[h])+{}_{\mathcal{A}}\widehat{\prod}(1+\vec{d}m[h])+{}_{\mathcal{A}}\widehat{\prod}(1+\vec{d}l[h])\,{}_{\mathcal{A}}\widehat{\prod}(1+\vec{d}k[h])={}_{\mathcal{A}}\widehat{\prod}(1+\vec{d}n[h]).$$

Proof: In the unital case $X[h]={}_{\mathcal{A}}\Pi(1+\vec{d}l[h])$ and $Y[h]\,{}_{\mathcal{A}}\Pi(1+\vec{d}m[h])$ are, respectively, the unique solutions of the differential equations

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X[h]=X[h]\boxtimes dl[h],\quad(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h]=1_{\mathcal{A}}$$

and

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})Y[h]=Y[h]\boxtimes dm[h],\quad(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)Y[h]=1_{\mathcal{A}}.$$

By the Leibniz–Itô formula, their product satisfies

$$\begin{aligned}(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})(X[h]Y[h])&=((\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X[h])Y[h]+X[h](\mathrm{id}_{\mathcal{A}}\otimes\vec{d})Y[h]\\&\quad+((\mathrm{id}_{\mathcal{A}}\otimes\vec{d})X[h])(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})Y[h]\\&=(X[h]\boxtimes dl[h])Y[h]+X[h](Y[h]\boxtimes dm[h])\\&\quad+(X[h]\boxtimes dl[h])(Y[h]\boxtimes dm[h])\\&=X[h]Y[h]\boxtimes dl[h]+X[h]Y[h]\boxtimes dm[h]+X[h]Y[h]\boxtimes dl[h]dm[h]\\&=X[h]Y[h]\boxtimes dn[h],\end{aligned}$$

where in the penultimate line we used the $\mathcal{A}$-commutativity of $l[h]$ and $m[h]$. Also, since ε is multiplicative,

$$(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)(X[h]Y[h])=(\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)X[h](\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)Y[h]=1_{\mathcal{A}}.$$

Thus $Z[h]=X[h]Y[h]$ is the unique solution of the differential equation

$$(\mathrm{id}_{\mathcal{A}}\otimes\vec{d})Z[h]=Z[h]\boxtimes dn[h],\quad (\mathrm{id}_{\mathcal{A}}\otimes\varepsilon)Z[h]=1_{\mathcal{A}},$$

which is ${}_{\mathcal{A}}\Pi(1+\vec{d}l[h])$. If $\mathcal{A}$ is nonunital we adjoin a unit. Then, by the unital case,

$$\left(1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}l[h])\right)\left(1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}k[h])\right)=\left(1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}n[h])\right),$$

that is

$$1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}l[h])+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}k[h])+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}l[h])_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}k[h])$$

$$=1_{\mathcal{A}\otimes\mathcal{T}(\mathcal{L})}+{}_{\mathcal{A}}\widehat{\prod}\,(1+\vec{d}n[h])$$

Cancelling the unit on both sides completes the proof. □

Analogous results hold for backward product integrals and for right system algebras.

IV. DEFINITION OF DOUBLE PRODUCT INTEGRALS

Now let $r[h]$ be an element of $h(\mathcal{L}\otimes\mathcal{L})[[h]]$. Regarding the left copy of $\mathcal{L}$ in $\mathcal{L}\otimes\mathcal{L}$ as the system algebra we may form the decapitated product integral ${}_{\mathcal{L}}\hat{\Pi}(1+\vec{d}r[h])$. This is an element of $h(\mathcal{L}\otimes\mathcal{T}(\mathcal{L}))[[h]]$, so, regarding $\mathcal{T}(\mathcal{L})$ as a unital right system algebra, we may form the product integral $\Pi_{\mathcal{T}(\mathcal{L})}(1+\vec{d}({}_{\mathcal{L}}\hat{\Pi}(1+\vec{d}r[h])))$. In the same way, regarding the right copy of $\mathcal{L}$ in $\mathcal{L}\otimes\mathcal{L}$ as the system algebra, we may form, first the decapitated product integral $\hat{\Pi}_{\mathcal{L}}(1+\vec{d}r[h])$ in $(\mathcal{T}(\mathcal{L})\otimes\mathcal{L})[[h]]$, and then the product integral ${}_{\mathcal{T}(\mathcal{L})}\Pi(1+\vec{d}(\hat{\Pi}_{\mathcal{L}}(1+\vec{d}r[h])))$. We shall prove the "Fubini theorem," that ${}_{\mathcal{T}(\mathcal{L})}\Pi(1+\vec{d}(\hat{\Pi}_{\mathcal{L}}(1+\vec{d}r[h])))$ and $\Pi_{\mathcal{T}(\mathcal{L})}(1+\vec{d}({}_{\mathcal{L}}\hat{\Pi}(1+\vec{d}r[h])))$ are equal, so that we may define their common value to be the double product integral $\Pi\Pi(1+\vec{d}\otimes\vec{d}r[h])$ $=\overrightarrow{\Pi}^{\rightarrow}(1+dr[h])$. By changing directions of the single products we define $\overrightarrow{\Pi}^{\leftarrow}(1+dr[h])$, $\overleftarrow{\Pi}^{\rightarrow}(1+dr[h])$, and $\overleftarrow{\Pi}^{\leftarrow}(1+dr[h])$ similarly. For example,

$$\overrightarrow{\prod}^{\leftarrow}(1+dr[h])=\prod_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left({}_{\mathcal{L}}\widehat{\prod}\,(1+\vec{d}r[h])\right)\right)=\prod_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left(\widehat{\prod}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right).$$

We shall prove the Fubini theorem by showing that both definitions are equivalent to a third more explicit but less intuitive form, in fact essentially the unsymmetrized version of the definition used in Ref. 8. To describe this third form we need some combinatorial preliminaries.

For each natural number N let $\mathcal{M}(N)$ denote the set of rectangular matrices M all of whose entries M_{jk} are either 0 or 1 with the properties that each row and each column contains at least one entry 1, that is $\Sigma_k M_{jk}>0$ for each fixed j and $\Sigma_j M_{jk}>0$ for each fixed k, and the total number of entries 1 is N, $\Sigma_{j,k}M_{jk}=N$. For example $\mathcal{M}(1)=\{[1]\}$ and

$$\mathcal{M}(2)=\left\{\begin{bmatrix}1&0\\0&1\end{bmatrix},\begin{bmatrix}0&1\\1&0\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix},[1\ \ 1]\right\}.$$

Each $\mathcal{M}(N)$ is finite since an element can have at most N rows and columns and each entry must be 0 or 1. Let $M\in\mathcal{M}(N)$ have m rows and n columns. We are going to define a corresponding element $\Pi_M r[h]$ of $((\otimes^m\mathcal{L})\otimes(\otimes^n\mathcal{L}))[[h]]$.

We say that an ordering $\omega=((j_1,k_1),(j_2,k_2),\ldots,(j_{mn},j_{mn}))$ of the elements of the Cartesian product $\{1,2,\ldots,m\}\times\{1,2,\ldots,n\}$ is *allowed* if (j,k) precedes (j',k') whenever both $j<j'$ and $k<k'$. For example, the *row* and *column* orderings

$$\omega_{\rightarrow}=((1,1),(1,2),\ldots,(1,n),(2,1),(2,2),\ldots,(2,n),\ldots,(m,1),(m,2),\ldots,(m,n)),$$

$$\omega_{\downarrow}=((1,1),(2,1),\ldots,(m,1),(1,2),(2,2),\ldots,(m,2),\ldots,(1,n),(2,n),\ldots,(m,n)),$$

are allowed orderings, but there are many others.

Given an allowed ordering $\omega=(P_1,P_2,\ldots,P_{mn})$ we construct the corresponding *reduced ordering* $\omega_M=(Q_1,Q_2,\ldots,Q_N)=((j_1,k_1),(j_2,k_2),\ldots,(j_N,k_N))$ by deleting from ω those $P=(j,k)$ for which the matrix element $M_{j,k}=0$. Finally we define the element $\Pi_M^{(\omega)}r[h]$ of $((\otimes^m\mathcal{L})\otimes(\otimes^n\mathcal{L}))[[h]]$ using place notation as

$$\prod_M^{(\omega)} r[h]=r[h]^{(j_1,k_1)}r[h]^{(j_2,k_2)}\ldots r[h]^{(j_N,k_N)}.$$

Here the coefficients of the formal power series $r[h]^{(j,k)}$ occupies the jth copy of $\mathcal{L}$ in $\otimes^m\mathcal{L}$ and the kth copy of $\mathcal{L}$ in $\otimes^n\mathcal{L}$. The defining properties of $\mathcal{M}(N)$ ensure that every copy of $\mathcal{L}$ in $\otimes^m\mathcal{L}$ and in $\otimes^n\mathcal{L}$ is occupied; multiple occupancies are reduced using the multiplication in $\mathcal{L}$.

Lemma 7: $\Pi_M^{(\omega)}r[h]$ *is independent of the choice of allowed ordering* ω.

Proof: By adjoining a unit and setting all terms with $M_{j,k}=0$ equal to this, we may assume that all $M_{j,k}=1$. The second term of the allowed ordering ω must be either (1,2) or (2,1) since any other choice would make it impossible to subsequently place at least one of these terms. Let us show that if the second term is (1,2) then $\Pi_M^{(\omega)}r[h]=\Pi_M^{(\omega_{\rightarrow})}r[h]$. A similar argument shows that if the second term is (2,1) then $\Pi_M^{(\omega)}r[h]=\Pi_M^{(\omega_{\downarrow})}r[h]$. Since it follows from (12) that $\Pi_M^{(\omega_{\rightarrow})}r[h]=\Pi_M^{(\omega_{\downarrow})}r[h]$, this proves the Lemma. Suppose that the second, third,..., kth terms of ω are $(1,2),(1,3),\ldots,(1,k)$ but the $(k+1)$th is not $(1,k+1)$. [Then it must be (2,1).] If $k=n$ we may detach the first row to the left of the ordering and argue by induction that the ordering of the remaining $(m-1)n$ terms is equivalent to the corresponding row ordering and hence, reattaching the first row, that $\Pi_M^{(\omega)}r[h]=\Pi_M^{(\omega_{\rightarrow})}r[h]$. If $k<n$ then $r[h]^{1,k+1}$ commutes with all preceding terms except $r[h]^{1,1},r[h]^{1,2},\ldots,r[h]^{1,k}$ since these are of the form $r[h]^{j,k'}$ with $j>1$ and $k'<k$. Hence we may move $r[h]^{1,k+1}$ to immediately follow $r[h]^{1,1}r[h]^{1,2}\cdots r[h]^{1,k}$, effectively increasing k by 1. Iterating, we arrive at the case $k=n$ already proved. □

We denote by $\Pi_M r[h]$ the common value of the products $\Pi_M^{(\omega)}r[h]$. It is evidently a formal power series of which the coefficents of $h^0,h^1,h^2,\ldots,h^{N-1}$ vanish. Thus $\Sigma_{N=1}^{\infty}\Sigma_{M\in\mathcal{M}(N)}\,\Pi_M r[h]$ is a well defined element of $h(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$. We can also rearrange it as

$$\sum_{N=1}^{\infty}\sum_{M\in\mathcal{M}(N)}\prod_M r[h]=\sum_{m,n=1}^{\infty}\sum_{M\in\mathcal{M}_{m,n}}\prod_M r[h],$$

where $\mathcal{M}_{m,n}$ denotes the finite subset of $\cup_{N=1}^{\infty}\mathcal{M}(N)$ consisting of $m\times n$ matrices.

For natural numbers m,n, we introduce the sets $\mathcal{A}_{m,n}$ of ordered m-tuples $A=(A_1,A_2,\ldots,A_m)$ of nonempty subsets whose union is $\{1,2,\ldots,n\}$, and $\mathcal{B}_{m,n}$ of ordered n-tuples $(B_1,B_2,\ldots,B_n)$ of nonempty subsets whose union is $\{1,2,\ldots,m\}$. There is a one–one correspondence between elements of $\mathcal{M}_{m,n}$, $\mathcal{A}_{m,n}$, and $\mathcal{B}_{m,n}$ given by

$$M_{j,k}=1\Leftrightarrow k\in A_j\Leftrightarrow j\in B_k,\quad j=1,2,\ldots,m,\ k=1,2,\ldots,n.$$

For each $M\in\mathcal{M}_{m,n}$, evaluating $\Pi_M r[h]$ using the row allowed ordering we get

$$\prod_M r[h] = (r[h]^{1,a_{1,1}} \boxtimes r[h]^{1,a_{1,2}} \boxtimes \cdots \boxtimes r[h]^{1,a_{1,|A_1|}}) \\ \boxtimes \quad (r[h]^{2,a_{2,1}} \boxtimes r[h]^{2,a_{2,2}} \boxtimes \cdots \boxtimes r[h]^{2,a_{2,|A_2|}}) \\ \boxtimes \quad \cdots \\ \boxtimes \quad (r[h]^{m,a_{m,1}} \boxtimes r[h]^{m,a_{m,2}} \boxtimes \cdots \boxtimes r[h]^{m,a_{m,|A_m|}}),$$

where the corresponding elements of $\mathcal{A}_{m,n}$ are given by $A_j = \{a_{j,1} < a_{j,2} < \cdots < a_{j,|A_j|}\}$, $j = 1,2,\ldots,m$. Here the inner compositions $\boxtimes$ denote multiplication in $\mathcal{L}$ on the left and tensoring on the right, while the outer compositions $\boxtimes$ denote tensoring on the left and tensoring disjoint indices and multiplying coincident indices on the right. Thus in particular

$$\sum_{N=1}^{\infty} \sum_{M \in \mathcal{M}(N)} \prod_M r[h] = \sum_{m,n=1}^{\infty} \sum_{A \in \mathcal{A}_{m,n}} (r[h]^{1,a_{1,1}} \boxtimes r[h]^{1,a_{1,2}} \boxtimes \cdots \boxtimes r[h]^{1,a_{1,|A_1|}}) \\ \boxtimes \quad (r[h]^{2,a_{2,1}} \boxtimes r[h]^{2,a_{2,2}} \boxtimes \cdots \boxtimes r[h]^{2,a_{2,|A_2|}}) \\ \boxtimes \quad \cdots \\ \boxtimes \quad (r[h]^{m,a_{m,1}} \boxtimes r[h]^{m,a_{m,2}} \boxtimes \cdots \boxtimes r[h]^{m,a_{m,|A_m|}}). \tag{19}$$

Similarly, using the column allowed ordering, we get

$$\sum_{N=1}^{\infty} \sum_{M \in \mathcal{M}(N)} \prod_M r[h] = \sum_{m,n=1}^{\infty} \sum_{B \in \mathcal{B}_{m,n}} (r[h]^{b_{1,1},1} \boxtimes r[h]^{b_{2,1},2} \boxtimes \cdots \boxtimes r[h]^{b_{|B_1|},1}) \\ \boxtimes \quad (r[h]^{b_{1,2},2} \boxtimes r[h]^{b_{2,2},2} \boxtimes \cdots \boxtimes r[h]^{b_{|B_2|},2}) \\ \boxtimes \quad \cdots \\ \boxtimes \quad (r[h]^{b_{1,n},n} \boxtimes r[h]^{b_{2,n},n} \boxtimes \cdots \boxtimes r[h]^{b_{|B_n|},n}), \tag{20}$$

where the elements of $B \in \mathcal{B}_{m,n}$ are given by $B_k = \{b_{1,k} < b_{2,k} < \cdots < b_{|B_k|,k}\}$, $k = 1,2,\ldots,n$.

We are now ready to prove the multiplicative Fubini theorem.

Theorem 8:

$$\prod_{\mathcal{T}(\mathcal{L})} \left(1 + \vec{d}\left(\widehat{\prod_{\mathcal{L}}} (1 + \vec{d}r[h])\right)\right) = 1_{\mathcal{T}(\mathcal{L}) \otimes \mathcal{T}(\mathcal{L})} + \sum_{N=1}^{\infty} \sum_{M \in \mathcal{M}(N)} \prod_M r[h] \\ = {}_{\mathcal{T}(\mathcal{L})}\prod \left(1 + \vec{d}\left(\widehat{\prod_{\mathcal{L}}} (1 + \vec{d}r[h])\right)\right).$$

Proof: To prove the first equality let us denote the element $\hat{\Pi}_{\mathcal{L}}(1 + \vec{d}r[h]))$ of $\mathcal{L} \otimes \mathcal{T}(\mathcal{L})$ by $R[h]$ and use place notation to write it in the form

$$R[h] = \sum_{N=1}^{\infty} r[h]^{1,N+1} \boxtimes r[h]^{1,N+2} \boxtimes \cdots \boxtimes r[h]^{1,2N},$$

where $\boxtimes$ denotes multiplication in the left hand copy of $\mathcal{L}$ and tensoring in $\mathcal{L}$ on the right. Thus

$$\prod_{\mathcal{T}(\mathcal{L})} \left(1 + \vec{d}\left(\widehat{\prod_{\mathcal{L}}} (1 + \vec{d}r[h])\right)\right) = 1_{\mathcal{T}(\mathcal{L}) \otimes \mathcal{T}(\mathcal{L})} + \sum_{N=1}^{\infty} R[h]^1 \boxtimes R[h]^2 \boxtimes \cdots \boxtimes R[h]^N,$$

where now the superscripts denote places in $\otimes^N \mathcal{L}$ and $\boxtimes$ now denotes tensoring in $\mathcal{L}$ on the left and multiplication in $\mathcal{T}(\mathcal{L})$ on the right. Carrying out these multiplications using (3) we obtain

$$\prod_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left(\widehat{\prod_{\mathcal{L}}}(1+\vec{d}r[h])\right)\right)$$

$$\begin{aligned}
&= 1_{\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})}+\sum_{m,n=1}^{\infty}\sum_{A\in\mathcal{A}_{m,n}}(r[h]^{1,a_{1,1}}\boxtimes r[h]^{1,a_{1,2}}\boxtimes\cdots\boxtimes r[h]^{1,a_{1,|A_1|}})\\
&\quad\boxtimes\ (r[h]^{2,a_{2,1}}\boxtimes r[h]^{2,a_{2,2}}\boxtimes\cdots\boxtimes r[h]^{2,a_{2,|A_{2v}|}})\\
&\quad\boxtimes\ \cdots\\
&\quad\boxtimes\ (r[h]^{m,a_{m,1}}\\
&\quad\boxtimes\ r[h]^{m,a_{m,2}}\boxtimes\cdots\boxtimes r[h]^{m,a_{m,|A_m|}}),
\end{aligned}$$

which is precisely $1_{\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})}+\Sigma_{N=1}^{\infty}\Sigma_{M\in\mathcal{M}(N)}\Pi_M r[h]$ by (19). The second equality is proved similarly using (20). □

V. CHARACTERIZATION THEOREM

Theorem 9: *Double product integrals satisfy the pairs of relations*

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\overrightarrow{\prod}(1+dr[h])=\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,2}\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,3},$$

$$(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overrightarrow{\prod}(1+dr[h])=\left(\overrightarrow{\prod}(1+dr[h])^{1,3}\left(\overrightarrow{\prod}(1+dr[h])\right)^{2,3},\right.$$

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\overrightarrow{\prod}(1+dr[h])=\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,3}\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,2},$$

$$(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overrightarrow{\prod}(1+dr[h])=\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,3}\left(\overrightarrow{\prod}(1+dr[h])\right)^{2,3},$$

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\overleftarrow{\prod}(1+dr[h])=\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,2}\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,3},$$

$$(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overleftarrow{\prod}(1+dr[h])=\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,3}\left(\overleftarrow{\prod}(1+dr[h])\right)^{2,3},$$

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\overleftarrow{\prod}(1+dr[h])=\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,3}\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,2},$$

$$(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overleftarrow{\prod}(1+dr[h])=\left(\overleftarrow{\prod}(1+dr[h])\right)^{2,3}\left(\overleftarrow{\prod}(1+dr[h])\right)^{1,3},$$

in $(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$, *together with*

$$(\varepsilon\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overset{**}{\prod}(1+dr[h])=(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\varepsilon)\overset{**}{\prod}(1+dr[h])=1_{\mathcal{T}(\mathcal{L})},\tag{21}$$

in each case. Conversely if $R[h]\in(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$ *satisfies any one of these pairs of relations together with (21) then there exists an element* $r[h]\in h(\mathcal{L}\otimes L)[[h]]$ *such that* $R[h]=\overset{**}{\Pi}(1+dr[h])$.

Proof: We shall prove the characterziation theorem for forward double product integrals $\overrightarrow{\Pi}\overrightarrow{\Pi}(1+dr[h])$; the others are proved similarly using appropriate variants of Theorems 2 and 4 and their corollaries.

Writing $\overrightarrow{\Pi}\overrightarrow{\Pi}(1+dr[h])=\Pi_{\mathcal{T}(\mathcal{L})}(1+\vec{d}({}_{\mathcal{L}}\hat{\Pi}(1+\vec{d}r[h])))$ and using Theorem 2 we get

$$\begin{aligned}(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\overrightarrow{\prod}(1+dr[h]) &= (\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)\left({}_{\mathcal{T}(\mathcal{L})}\prod\left(1+\vec{d}\left(\widehat{\prod}{}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right)\right)\\ &= \left({}_{\mathcal{T}(\mathcal{L})}\prod\left(1+\vec{d}\left(\widehat{\prod}{}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right)\right)\\ &\boxtimes \left({}_{\mathcal{T}(\mathcal{L})}\prod\left(1+\vec{d}\left(\widehat{\prod}{}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right)\right)\\ &= \left(\overrightarrow{\prod}(1+dr[h])\right)^{1,2}\left(\overrightarrow{\prod}(1+dr[h])\right)^{1,3}.\end{aligned}$$

Also

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\varepsilon)\overrightarrow{\prod}(1+dr[h])=(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\varepsilon)\left({}_{\mathcal{T}(\mathcal{L})}\prod\left(1+\vec{d}\left(\widehat{\prod}{}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right)\right)=1_{\mathcal{T}(\mathcal{L})}.$$

Similarly, writing $\overrightarrow{\Pi}\overrightarrow{\Pi}(1+dr[h])=\Pi_{\mathcal{T}(\mathcal{L})}(1+\vec{d}({}_{\mathcal{L}}\hat{\Pi}(1+\vec{d}r[h])))$ and using the analogue of Theorem 2 for right system algebras we have

$$\begin{aligned}(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overleftarrow{\prod}(1+dr[h]) &= (\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\left(\prod{}_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left({}_{\mathcal{L}}\widehat{\prod}(1+\vec{d}r[h])\right)\right)\right)\\ &= \left(\prod{}_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left({}_{\mathcal{L}}\widehat{\prod}(1+\vec{d}r[h])\right)\right)\right)\\ &\boxtimes \left(\prod{}_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left({}_{\mathcal{L}}\widehat{\prod}(1+\vec{d}r[h])\right)\right)\right)\\ &= \left(\overrightarrow{\prod}(1+dr[h])\right)^{1,3}\left(\overrightarrow{\prod}(1+dr[h])\right)^{2,3}\end{aligned}$$

and

$$(\varepsilon\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\overleftarrow{\prod}(1+dr[h])=(\varepsilon\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})\left(\prod{}_{\mathcal{T}(\mathcal{L})}\left(1+\vec{d}\left({}_{\mathcal{L}}\widehat{\prod}(1+\vec{d}r[h])\right)\right)\right)=1_{\mathcal{T}(\mathcal{L})},$$

as required.

Conversely let $R[h]\in(\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L}))[[h]]$ satisfy

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\Delta)R[h]=(R[h])^{1,2}(R[h])^{1,3}, \tag{22}$$

$$(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})R[h]=(R[h])^{1,3}(R[h])^{2,3}, \tag{23}$$

$$(\mathrm{id}_{\mathcal{T}(\mathcal{L})}\otimes\varepsilon)R[h]=(\varepsilon\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})R[h]=1_{\mathcal{T}(\mathcal{L})}. \tag{24}$$

Using the converse of Theorem 2 we deduce from (22) and the left hand equation of (24) that $R[h]=_{\mathcal{T}(\mathcal{L})}\Pi(1+\vec{d}l[h])$ for some element $l[h]\in h(\mathcal{T}(\mathcal{L})\otimes\mathcal{L})[[h]]$. We express $R[h]=_{\mathcal{T}(\mathcal{L})}\Pi(1+\vec{d}l[h])$ as

$$R[h]=(1_{\mathcal{T}(\mathcal{L})},l[h],l[h]\boxtimes l[h],\ldots,\boxtimes^n l[h],\ldots), \tag{25}$$

as an element of $\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})=\oplus_{n=0}^{\infty}(\mathcal{T}(\mathcal{L})\otimes(\otimes^n\mathcal{L}))$, where $\boxtimes$ denotes multiplication in $\mathcal{T}(\mathcal{L})$ on the left and tensoring in $\mathcal{L}$ on the right. Using the right hand equation of (24) and the multiplicativity of ε, we find that

$$1_{\mathcal{T}(\mathcal{L})}=(\varepsilon\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})R[h]=(1_{\mathbb{F}},(\varepsilon\otimes\mathrm{id}_{\mathcal{L}})l[h],\otimes^2((\varepsilon\otimes\mathrm{id}_{\mathcal{L}})l[h]),\ldots,\otimes^n((\varepsilon\otimes\mathrm{id}_{\mathcal{L}})l[h]),\ldots),$$

from which, since $1_{\mathcal{T}(\mathcal{L})}=(1_{\mathbb{F}},0,0,\ldots)$, it follows that

$$(\varepsilon\otimes\mathrm{id}_{\mathcal{L}})l[h]=0_{\mathcal{L}}. \tag{26}$$

Similarly, applying $\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})}$ to both sides of (25) and using (23) we get

$$\begin{aligned}&(1_{\mathcal{T}(\mathcal{L})},l[h],l[h]\boxtimes l[h],\ldots,\boxtimes^n l[h],\ldots)\boxtimes(1_{\mathcal{T}(\mathcal{L})},l[h],l[h]\boxtimes l[h],\ldots,\boxtimes^n l[h],\ldots)\\&\quad=(R[h])^{1,3}(R[h])^{2,3}\\&\quad=(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})R[h]\\&\quad=(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})(1_{\mathcal{T}(\mathcal{L})},l[h],l[h]\boxtimes l[h],\ldots,\boxtimes^n l[h],\ldots),\end{aligned}$$

where the outer $\boxtimes$ on the left denotes tensoring in $\mathcal{T}(\mathcal{L})$ on the left and multiplication in $\mathcal{T}(\mathcal{L})=\oplus_{n=0}^{\infty}(\otimes^n\mathcal{L})$ on the right. We compare the entries in $\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})\otimes\mathcal{L}$ within $\oplus_{n=0}^{\infty}[\mathcal{T}(\mathcal{L})\otimes\mathcal{T}(\mathcal{L})\otimes(\otimes^n\mathcal{L})]$ in this identity. From (3) contributions to the entry on the left can come only from composing terms of rank not exceeding 1. Thus we find that

$$\tau_{(1,3,2)}(l[h]\otimes 1_{\mathcal{T}(\mathcal{L})})+1_{\mathcal{T}(\mathcal{L})}\otimes l[h]+l[h]\boxtimes l[h]=(\Delta\otimes\mathrm{id}_{\mathcal{T}(\mathcal{L})})l[h]. \tag{27}$$

Using the analogue of Corollary 3 for right system algebras it follows from (26) and (27) that $l[h]=\hat{\Pi}_{\mathcal{L}}(1+\vec{d}r[h])$ for some $r[h]\in h(\mathcal{L}\otimes\mathcal{L})[[h]]$. Hence

$$R[h]=_{\mathcal{T}(\mathcal{L})}\prod\left(1+\vec{d}\left(\widehat{\prod}_{\mathcal{L}}(1+\vec{d}r[h])\right)\right)=\overrightarrow{\prod}^{\rightarrow}(1+dr[h]).$$

□

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 45, NUMBER 5 MAY 2004

Comment on "Double product integrals and Enriquez quantization of Lie bialgebras I: The quasitriangular identities" [Hudson and Pulmannová, J. Math. Phys. 45, 2090 (2004)]

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The purpose of this article is to derive both the ''Fubini theorem'' and the ''quasitriangular relations'' shown by the authors of the preceding paper[1] at the same time, not using the results of their Sec. IV. We first recall these results, using the notation of the paper.

Let $r[h] \in h\mathcal{L} \otimes \mathcal{L}[[h]]$. Set

$$X = \sum_{n>0} r^{0,1} \cdots r^{0,n} \in h\mathcal{L} \otimes \mathcal{T}(\mathcal{L})[[h]]$$

[the product of $\mathcal{L}$ is used in the factor $\mathcal{L}$, concatenation is used in $\mathcal{T}(\mathcal{L})$],

$$Z = \sum_{n \geqslant 0} X^{1,\infty} \cdots X^{n,\infty} \in \mathcal{T}(\mathcal{L}) \otimes \mathcal{T}(\mathcal{L})[[h]]$$

[concatenation in the first $\mathcal{T}(\mathcal{L})$, product in the second $\mathcal{T}(\mathcal{L})$],

$$Y = \sum_{n>0} r^{1,\infty} \cdots r^{n,\infty} \in h\mathcal{T}(\mathcal{L}) \otimes \mathcal{L}[[h]]$$

(concatenation then product),

$$Z' = \sum_{n \geqslant 0} Y^{0,1} \cdots Y^{0,n} \in \mathcal{T}(\mathcal{L}) \otimes \mathcal{T}(\mathcal{L})[[h]]$$

(product then concatenation).

Theorem 1: *(1) ("Fubini theorem") $Z = Z'$. (2) ("Quasitriangular relations")*

$$(\Delta \otimes \mathrm{id})(Z) = Z^{1,3} Z^{2,3}, \quad (\mathrm{id} \otimes \Delta)(Z) = Z^{1,3} Z^{1,2}.$$

Proof: Let $\mathcal{T}(\mathcal{L})_0 = \oplus_{i>0} \mathcal{L}^{\otimes i}$, $\tilde{\mathcal{L}} = \mathcal{L} \oplus \mathbb{F}1$ ($\tilde{\mathcal{L}}$ is $\mathcal{L}$ with a unit adjoined).

Lemma 2: The map $\alpha: \mathcal{T}(\tilde{\mathcal{L}}) \to \mathcal{L}$, $1 \mapsto 1$, and taking $x \in \mathcal{T}(\mathcal{L})_0$ to its homogeneous component x_1 of rank 1 is an algebra homomorphism.

Proof of Lemma: Clear.

Proof of Theorem: We have obviously $(\Delta \otimes \mathrm{id})(Z) = Z^{1,3} Z^{2,3}$. Let us prove $(\mathrm{id} \otimes \Delta)(Z) = Z^{1,3} Z^{1,2}$. Set $u = (\mathrm{id} \otimes \Delta)(Z)$ and $v = Z^{1,3} Z^{1,2}$. Then $u, v \in \mathcal{T}(\mathcal{L})^{\otimes 3}[[h]]$. Moreover both u and v satisfy $(\Delta \otimes \mathrm{id}^{\otimes 2})(x) = x^{1,3,4} x^{2,3,4}$. To apply Theorem 4 of Hudson and Pulmannova it remains to check that

$$(\alpha \otimes \mathrm{id}^{\otimes 2})(u) = (\alpha \otimes \mathrm{id}^{\otimes 2})(v).$$

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Now $(\alpha\otimes \mathrm{id}^{\otimes 2})(u)=(\mathrm{id}\otimes\Delta)(X)$ and $(\alpha\otimes \mathrm{id}^{\otimes 2})(v)=X^{1,3}X^{1,2}$ using the Lemma and the fact that $(\alpha\otimes \mathrm{id})(Z)=X$. Since $(\mathrm{id}\otimes\Delta)(X)=X^{1,3}X^{1,2}$ we are done. Therefore, Z satisfies both quasitriangularity identities.

Z' obviously satisfies $(\mathrm{id}\otimes\Delta)(Z')=(Z')^{1,3}(Z')^{1,2}$. Since Z also satisfies this relation we will apply Theorem 4 of Hudson and Pulmannova to prove $Z'=Z$. For this we need to prove that $(\mathrm{id}\otimes\alpha)(Z)=(\mathrm{id}\otimes\alpha)(Z')$. Now the Lemma implies that

$$(\mathrm{id}\otimes\alpha)(Z)=\sum_{n\geqslant 0}(\mathrm{id}\otimes\alpha)(X)^{1,\infty}\cdots(\mathrm{id}\otimes\alpha)(X)^{n,\infty},$$

and since $(\mathrm{id}\otimes\alpha)(X)=1$ we get $(\mathrm{id}\otimes\alpha)(Z)=Y$. We also have $(\mathrm{id}\otimes\alpha)(Z')=Y$, so by Theorem 4 of Hudson and Pulmannova, $Z=Z'$. This proves "Fubini's theorem." Since $Z=Z'$, Z' also satisfies both quasitriangularity identities. □

[1] R. L. Hudson and S. Pulmannova, "Double product integrals and Enriquez quantization of Lie bialgebras I: The quasitriangular identities," J. Math. Phys. **45**, 2090–2105 (2004).

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Erratum: "Properties of the symplectic structure of general relativity for spatially bounded space–time regions" [J. Math. Phys. 43, 3984 (2002)]

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The left side of Eqs. (3.15) and (3.24) should contain a projection operator "$\mathcal{P}_S$" with respect to the 2-surface S: i.e.,

$$\mathcal{P}_S(\mathcal{L}_v \epsilon_{ab}) = \kappa(v)\epsilon_{ab}$$

and

$$\mathcal{P}_S(\mathcal{L}_{\theta^\pm} \epsilon_{ab}) = \kappa^\pm \epsilon_{ab}\,.$$

The sentences before and after Eqs. (4.53)–(4.55), (4.62)–(4.65), (4.79)–(4.81), and (4.89)–(4.91) all refer to 2-spheres S that lie outside any horizon.

The sentence after Eq. (4.91) should refer to the *normal part of* P^a.

In Eq. (4.37), the log expressions are missing a term R^2: i.e.,

$$\ln(R^2 + \kappa(u)/\kappa(v)).$$

Likewise, the formula in the sentence after Eq. (4.37) should be changed to

$$(P^{\mathrm{D}}_{\|})_a = \tfrac{1}{2}\nabla^S_a \ln(R^2 + \kappa(u)/\kappa(v)).$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 45, NUMBER 5 MAY 2004

Erratum: "Covariant Hamiltonian boundary conditions in General Relativity for spatially bounded space–time regions" [J. Math. Phys. 43, 5531 (2002)]

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The right-side of Eq. (3.55) should contain the final equality "$=8\epsilon_{ebcd}\theta_e^\alpha\theta_\beta^a\delta\Gamma_a{}^{\alpha\beta}(\theta)$": i.e.,

$$\Theta_{bcd}(\theta,\delta\theta)=12\theta_{[c}^\mu\theta_d^\nu\delta\tilde{\Gamma}_{b]\mu\nu}(\theta)=8\epsilon_{ebcd}\theta_e^\alpha\theta_\beta^a\delta\Gamma_a{}^{\alpha\beta}(\theta).$$

In Eq. (3.69), a "δ" is missing on $J_{abc}(\xi;\theta)$: i.e.,

$$\Omega_\Sigma(\theta,\delta\theta,\mathcal{L}_\xi\theta)=\int_\Sigma \delta J_{abc}(\xi;\theta)-4\xi^d\mathcal{E}^\mu_{[abc}(\theta)\,\delta\theta_{d]\mu}-\int_{\partial\Sigma}\xi^c\Theta_{abc}(\theta,\delta\theta).$$

The sentence before Eq. (3.74) should have at the end: ", using identity (3.4),"

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Nonsingular G_2 stiff fluid cosmologies

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In this paper we analyze Abelian diagonal orthogonally transitive space–times with spacelike orbits for which the matter content is a stiff perfect fluid. The Einstein equations are cast in a suitable form for determining their geodesic completeness. A sufficient condition on the metric of these space–times is obtained, that is fairly easy to check and to implement in exact solutions. These results confirm that nonsingular space–times are abundant among stiff fluid cosmologies. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1705715]

I. INTRODUCTION

After the discovery of the first nonsingular perfect fluid cosmological model by Senovilla,[1] the possibility of constructing regular cosmologies was renewed. The interest for regular cosmologies had stifled for nearly 30 years due to the powerful singularity theorems (cf., for instance, Refs. 2 and 3), which seemed to preclude such space–times under very general requirements, such as chronology protecting, energy and generic conditions. The open way to regular cosmologies was found in the violation of some technical premises of the theorems. For instance, in Ref. 4 it was shown that the Senovilla space–time did not possess a compact achronal set without edge and could not have closed trapped surfaces.

However, the first results were not encouraging. The extension of the Senovilla solution to a family of space–times left the set of regular models limited to a zero-measure subset surrounded by space–times with Ricci and Weyl curvature singularities.[5] During the following decade only a few new nonsingular cosmologies were added to the list.[6]

Another estrategy to approach singularities arose with the publication of regularity theorems.[7–9] Whereas singularity theorems stated general sufficient conditions for the appearance of singularities, these theorems aimed the contrary, namely particular conditions to achieve regular space–times.

The application of the conclusions of Ref. 8 to a restricted family of stiff fluids provided an unexpected result. The set of known nonsingular perfect fluid cosmologies was enlarged with a huge family depending on two nearly arbitrary functions.[10]

The purpose of this paper is the extension of those results to determine which space–times among Abelian diagonal orthogonally transitive space–times with spacelike orbits and with a stiff fluid as matter content are nonsingular. Instead of restricting to an integrable family of solutions of the Einstein equations, we analyze the whole set of diagonal cylindrical stiff fluid space–times with a spacelike transitivity surface element.

With this aim in mind we write in Sec. II the Einstein equations for such space–times and we cast them in a form suitable for the application of the theorems. The analysis of the restrictions imposed by regularity conditions is done in Sec. III. Finally in Sec. IV we check the possibility of constructing regular space–times with nonvaninishing matter scalar space averages on Cauchy hypersurfaces in order to support the validity of a regularity conjecture by Senovilla.[11]

II. EQUATIONS FOR G_2 STIFF FLUID SPACE–TIMES

As it has been stated in the introduction, we shall focus on space–times endowed with an Abelian orthogonally transitive group of isometries G_2 acting on spacelike surfaces, since this is the framework where most nonsingular space–times have been found so far. We further impose that generators for the group can be found that are mutually orthogonal. We follow Ref. 8 for writing the Einstein equations for such space–times using a formalism based on differential forms.

If the generators of the isometry group are chosen to be $\{\xi,\eta\}$, we may write an orthonormal tetrad, $\{\theta^0,\theta^1,\theta^2,\theta^3\}$, where just θ^2 and θ^3 lie in $\mathrm{lin}\{\xi,\eta\}$. We may impose that these 1-forms be Lie-invariant under the isometry group.[12] The metric is written as

$$ds^2=-\theta^0\otimes\theta^0+\theta^1\otimes\theta^1+\theta^2\otimes\theta^2+\theta^3\otimes\theta^3. \tag{1}$$

Making use of the spacelike congruence for θ^2 and its kinematical quantities, we may define the tetrad basis according to the vanishing torsion equations,

$$d\theta^0=\nu\wedge\theta^1, \tag{2a}$$

$$d\theta^1=\nu\wedge\theta^0, \tag{2b}$$

$$d\theta^2=\alpha\wedge\theta^2, \tag{2c}$$

$$d\theta^3=(\beta-\alpha)\wedge\theta^3, \tag{2d}$$

where ν is just a connection in the $\theta^0-\theta^1$ subspace, α is an ''acceleration'' for θ^2 and β is related to the expansion of the surface element in the $\theta^2-\theta^3$ subspace, since $d(\theta^2\wedge\theta^3)=\beta\wedge\theta^2\wedge\theta^3$.

The integrability conditions for these equations are easily obtained by exterior differentiation of the system,

$$d\beta=0, \tag{3a}$$

$$d\alpha=0. \tag{3b}$$

Finally, Einstein field equations are written in terms of these differential forms as an exterior system,

$$d*\alpha+\beta\wedge*\alpha=(\tfrac{1}{2}T-T_{22})\,\theta^0\wedge\theta^1, \tag{4a}$$

$$d*\beta+\beta\wedge*\beta=(T_{11}-T_{00})\,\theta^0\wedge\theta^1, \tag{4b}$$

$$d\nu+\alpha\wedge*\alpha-\beta\wedge*\alpha=\tfrac{1}{2}(T_{00}-T_{11}+T_{22}+T_{33})\,\theta^0\wedge\theta^1, \tag{4c}$$

$$d*\tilde{\beta}+\beta\wedge*\tilde{\beta}+2(\alpha-\beta)\wedge*\tilde{\alpha}+2\,\nu\wedge\tilde{\beta}=(T_{00}+T_{11})\,\theta^0\wedge\theta^1, \tag{4d}$$

$$d\tilde{\beta}+\beta\wedge\tilde{\beta}+2(\alpha-\beta)\wedge\tilde{\alpha}+2\,\nu\wedge*\tilde{\beta}=2T_{01}\theta^0\wedge\theta^1, \tag{4e}$$

for a matter content defined by the energy-momentum tensor $T=T_{ab}\theta^a\otimes\theta^b$.

The tilde denotes a reflection in the $\theta^0-\theta^1$ subspace, that is, if $\alpha=a\,\theta^0+b\,\theta^1$, then $\tilde{\alpha}=a\,\theta^0-b\,\theta^1$. The $*$ denotes the Hodge duality operator in the same subspace, $*\alpha=-a\,\theta^1-b\,\theta^0$.

Integration of the first Bianchi equations (3a) and (3b),

$$\alpha=-dU, \tag{5a}$$

$$\beta = \frac{d\ln\rho}{\rho}, \tag{5b}$$

allows integration of Cartan equations in terms of two functions, z, ϕ,

$$\theta^2 = e^{-U}\,dz, \quad \theta^3 = \rho e^{U}\,d\phi, \tag{6}$$

that we take as coordinates in order to write the metric in a conventional form,

$$g = e^{2K}(-dt^2 + dr^2) + e^{-2U}\,dz^2 + \rho^2 e^{2U}\,d\phi^2. \tag{7}$$

The coordinates are adapted to the Killing fields, so that $\xi = \partial_z$, $\eta = \partial_\phi$. The nonignorable coordinates t, r are chosen so that the metric is isotropic in the subspace spanned by θ^0 and θ^1,

$$\theta^0 = e^{K}\,dt, \quad \theta^1 = e^{K}\,dr. \tag{8}$$

The range for these coordinates is the usual one,

$$-\infty < t, \quad z < \infty, \quad 0 < r < \infty, \quad 0 < \phi < 2\pi, \tag{9}$$

if we require the space–time to be cylindrically symmetric. The remaining metric functions, K, U, and ρ, depend just on t and r.

The connection in this case is $\nu = *dK$.

This is the general framework for an orthogonally transitive diagonal space–time with spacelike orbits. If the matter content is a perfect fluid with 4-velocity u, pressure p, and density μ, the Bianchi equations for such energy-momentum tensor,

$$T = \mu u \otimes u + p\,(g + u \otimes u), \tag{10}$$

may be written in compact expressions involving the kynematical 1-forms,

$$du + \frac{1}{\mu + p}\,dp \wedge u = 0, \tag{11a}$$

$$d*u + \left(\beta + \frac{d\mu}{\mu + p}\right) \wedge *u = 0, \tag{11b}$$

which state that the fluid is irrotational.

We might choose $\theta^0 = u$ for writing the Einstein equations, as it was done in Ref. 10, but since we aim full generality, we shall not follow that way and explore arbitrary possibilities of alignment for this 1-form. Preserving the unitarity of u, we may parametrize it in terms of a function ξ,

$$u = -\theta^0 \cosh\xi - \theta^1 \sinh\xi, \tag{12}$$

so that the Einstein equations for a perfect fluid take the following form:

$$U_{tt} - U_{rr} + \frac{1}{\rho}(U_t\rho_t - U_r\rho_r) = \frac{p-\mu}{2}e^{2K}, \tag{13a}$$

$$\rho_{tt} - \rho_{rr} = (\mu - p)\rho e^{2K}, \tag{13b}$$

$$K_t\rho_r + K_r\rho_t = \rho_{tr} + U_t\rho_r + U_r\rho_t + 2\rho U_t U_r + e^{2K}\rho\frac{\mu + p}{2}\sinh 2\xi, \tag{13c}$$

$$K_t\rho_t+K_r\rho_r=\frac{\rho_{tt}+\rho_{rr}}{2}+U_t\rho_t+U_r\rho_r+\rho\left(U_t^2+U_r^2+e^{2K}\frac{\mu+p}{2}\cosh 2\xi\right), \tag{13d}$$

$$K_{rr}-K_{tt}+\frac{U_r\rho_r-U_t\rho_t}{\rho}+U_r^2-U_t^2=\frac{\mu+p}{2}e^{2K}, \tag{13e}$$

and the energy-momentum conservation laws yield

$$K_r-\xi_t+\frac{p_r\cosh^2\xi+(\mu_t-p_t)\sinh\xi\cosh\xi-\mu_r\sinh^2\xi}{\mu+p}+\frac{\rho_t\cosh\xi-\rho_r\sinh\xi}{\rho}\sinh\xi=0, \tag{14a}$$

$$K_t-\xi_r+\frac{\mu_t\cosh^2\xi+(p_r-\mu_r)\sinh\xi\cosh\xi-p_t\sinh^2\xi}{\mu+p}+\frac{\rho_t\cosh\xi-\rho_r\sinh\xi}{\rho}\cosh\xi=0. \tag{14b}$$

The system of equations becomes much simpler if we restrict to stiff fluids, $\mu=p$,

$$U_{tt}-U_{rr}+\frac{1}{\rho}(U_t\rho_t-U_r\rho_r)=0, \tag{15a}$$

$$\rho_{tt}-\rho_{rr}=0, \tag{15b}$$

$$\frac{K_t\rho_r+K_r\rho_t}{\rho}=\frac{\rho_{tr}+U_t\rho_r+U_r\rho_t}{\rho}+2U_tU_r+e^{2K}p\sinh 2\xi, \tag{15c}$$

$$\frac{K_t\rho_t+K_r\rho_r}{\rho}=\frac{\rho_{tt}+\rho_{rr}}{2\rho}+\frac{U_t\rho_t+U_r\rho_r}{\rho}+U_t^2+U_r^2+e^{2K}p\cosh 2\xi, \tag{15d}$$

$$K_{rr}-K_{tt}+\frac{U_r\rho_r-U_t\rho_t}{\rho}+U_r^2-U_t^2=p\,e^{2K}, \tag{15e}$$

$$K_r-\xi_t+\frac{p_r}{2p}+\frac{\rho_t\cosh\xi-\rho_r\sinh\xi}{\rho}\sinh\xi=0, \tag{15f}$$

$$K_t-\xi_r+\frac{p_t}{2p}+\frac{\rho_t\cosh\xi-\rho_r\sinh\xi}{\rho}\cosh\xi=0. \tag{15g}$$

The reason why the stiff fluid equations are easy to integrate is that the metric functions U, ρ decouple from the pressure, which only appears in the equations for the conformal factor K. Therefore the stiff fluid case is fairly similar to vaccuum and can be generated from this one.

A further simplification can be obtained if we take ρ as coordinate. This is fully compatible with an isotropic parametrization, since equation (15b),

$$0=d*\beta+\beta\wedge*\beta=d\left(\frac{*d\rho}{\rho}\right)+\frac{d\rho\wedge*d\rho}{\rho^2}=\frac{d*\mathrm{d}\rho}{\rho},$$

states that $*d\rho$ is also an exact differential form.

We take $\rho=r$ as a spatial coordinate, since every known nonsingular solution has a surface element with spacelike gradient. With this choice of coordinates the differential system becomes even simpler,

$$U_{tt}-U_{rr}-\frac{U_r}{r}=0, \tag{16a}$$

$$K_t=U_t+2rU_tU_r+e^{2K}pr\sinh 2\xi, \tag{16b}$$

$$K_r=U_r+r(U_t^2+U_r^2)+e^{2K}pr\cosh 2\xi, \tag{16c}$$

$$K_{rr}-K_{tt}+\frac{U_r}{r}+U_r^2-U_t^2=pe^{2K}, \tag{16d}$$

$$K_r-\xi_t+\frac{p_r}{2p}-\frac{\sinh^2\xi}{r}=0, \tag{16e}$$

$$K_t-\xi_r+\frac{p_t}{2p}-\frac{\sinh\xi\cosh\xi}{r}=0. \tag{16f}$$

The integrability condition, $K_{rt}=K_{tr}$, for (16b) and (16c) requires that a combination of functions be an exact differential form,

$$dH=e^{2K}rp(\sinh 2\xi\,dt+\cosh 2\xi\,dr), \tag{17}$$

from which we can read ξ and the pressure, if K is known,

$$\tanh 2\xi=\frac{H_t}{H_r},\quad |p|=\frac{e^{-2K}}{r}\sqrt{H_r^2-H_t^2}. \tag{18}$$

The integrability of dH is also a consequence of the energy-momentum conservation equations (16e) and (16f).

For consistency these expressions imply that the gradient of H be spacelike and that H_r be positive in order to have positive pressure.

The simple case, $\xi=0$, for which u is parallel to the time direction corresponds to $H=\gamma r^2/2$, where γ is a positive constant.

The remaining system of differential equations,

$$U_{tt}-U_{rr}-\frac{U_r}{r}=0, \tag{19a}$$

$$H_{rr}-H_{tt}=\frac{\sqrt{H_r^2-H_t^2}}{r}, \tag{19b}$$

$$K_t=U_t+2rU_tU_r+H_t, \tag{19c}$$

$$K_r=U_r+r(U_t^2+U_r^2)+H_r, \tag{19d}$$

is formed by a reduced wave equation in polar coordinates for U on the plane and a nonlinear wave equation for H. Once these equations are solved, we are left with a quadrature for K. The integrability of this quadrature is guaranteed by the other equations.

As it has already been stated, these equations are pretty similar to those of vaccuum. The only diference is the additional conformal factor defined by H.

Regularity of the metric at the axis $r=0$ is already implicit in the equations, provided that metric functions are regular. Following Ref. 13, we have a regular axis whenever

$$\lim_{r\to 0}\frac{\langle \mathrm{grad}\,\Delta,\mathrm{grad}\,\Delta\rangle}{4\Delta}=e^{2(U-K)}|_{r=0}=1,\quad \Delta=\langle\partial_\phi,\partial_\phi\rangle=r^2e^{2U}. \tag{20}$$

But according to Eqs. (17), (19c), and (19d), K and U are equal at the axis, except for a constant, since

$$K_r(t,0)=U_r(t,0),\quad K_t(t,0)=U_t(t,0), \tag{21}$$

if pressure and K are regular functions, so that $H_t(t,0)=0=H_r(t,0)$, and therefore condition (20) is fulfilled either by taking the constant equal to zero or conveniently rescaling the angular coordinate.

The problem of obtaining solutions for H is solved by the Wainright–Ince–Marshman formalism.[14] Solutions to (19b) may be generated from solutions of the reduced wave equation on the plane with timelike gradient,

$$\sigma_{tt}-\sigma_{rr}-\frac{\sigma_r}{r}=0,\quad \sigma_t^2-\sigma_r^2>0, \tag{22}$$

by a quadrature identical to the one which defines $K-U$ in the vacuum case,

$$H_t=2r\sigma_t\sigma_r, \tag{23a}$$

$$H_r=r(\sigma_t^2+\sigma_r^2). \tag{23b}$$

The functions H generated by this mechanism have trivially a spacelike gradient and positive radial derivative. The fluid properties may be read directly from the generating function,

$$\tanh 2\xi=\frac{2\sigma_t\sigma_r}{\sigma_t^2+\sigma_r^2},\quad p=e^{-2K}(\sigma_t^2-\sigma_r^2). \tag{24}$$

The function that generates the $\xi=0$ case is $\sigma=\sqrt{\gamma}t$.

Using this formalism, the remaining system of equations is formed by a quadrature and two reduced wave equations,

$$U_{tt}-U_{rr}-\frac{U_r}{r}=0, \tag{25a}$$

$$\sigma_{tt}-\sigma_{rr}-\frac{\sigma_r}{r}=0, \tag{25b}$$

$$K_t=U_t+2rU_tU_r+2r\sigma_t\sigma_r, \tag{25c}$$

$$K_r=U_r+r(U_t^2+U_r^2)+r(\sigma_t^2+\sigma_r^2). \tag{25d}$$

III. NONSINGULAR MODELS

We have obtained a fairly simple system of equations (25a)–(25c) that will be useful for analyzing the regularity of the solutions. Following Ref. 2 we take causal geodesic completeness as our definition for regularity.

Even if we have regular metric components, geodesic completeness of the space–time is not guaranteed and we have to check explicitly that every timelike and lightlike geodesic in the space–time can be extended to all values of the affine parameter, that is, in the parametrization for which the geodesic equations take the form

$$\ddot{x}^i+\Gamma^i_{jk}\dot{x}^j\dot{x}^k=0, \tag{26}$$

in terms of the Christoffel symbols.

Fortunately, results concerning causal geodesic completeness of diagonal Abelian orthogonally transitive space–times have already been obtained in Ref. 8. The conclusions of that paper may be condensed in two theorems. We follow the simplified version of Ref. 10.

Theorem 1: A diagonal Abelian orthogonally transitive space–time with spacelike orbits endowed with a metric in the form (7) with C^2 metric functions K,U,ρ, where ρ has a spacelike gradient, is future causally geodesically complete provided that along causal geodesics.

(1) For large values of t and increasing r,
   (a) $(K-U-\ln\rho)_r+(K-U-\ln\rho)_t\geqslant 0$, and either $(K-U-\ln\rho)_r\geqslant 0$ or $|(K-U-\ln\rho)_r|\leqslant(K-U-\ln\rho)_r+(K-U-\ln\rho)_t$,
   (b) $K_r+K_t\geqslant 0$, and either $K_r\geqslant 0$ or $|K_r|\leqslant K_r+K_t$,
   (c) $(K+U)_r+(K+U)_t\geqslant 0$, and either $(K+U)_r\geqslant 0$ or $|(K+U)_r|\leqslant(K+U)_r+(K+U)_t$.
(2) For large values of t, a constant b exists such that

$$\left.\begin{matrix} K(t,r)-U(t,r) \\ 2K(t,r) \\ K(t,r)+U(t,r)+\ln\rho(t,r)\end{matrix}\right\}\geqslant -\ln|t|+b.$$

Theorem 2: A diagonal Abelian orthogonally transitive space–time with spacelike orbits endowed with a metric in the form (7) with C^2 metric functions K,U,ρ, where ρ has a spacelike gradient, is past causally geodesically complete provided that along causal geodesics.

(1) For small values of t and increasing r,
   (a) $(K-U-\ln\rho)_r-(K-U-\ln\rho)_t\geqslant 0$, and either $(K-U-\ln\rho)_r\geqslant 0$ or $|(K-U-\ln\rho)_r|\leqslant(K-U-\ln\rho)_r-(K-U-\ln\rho)_t$.
   (b) $K_r-K_t\geqslant 0$, and either $K_r\geqslant 0$ or $|K_r|\leqslant K_r-K_t$.
   (c) $(K+U)_r-(K+U)_t\geqslant 0$, and either $(K+U)_r\geqslant 0$ or $|(K+U)_r|\leqslant(K+U)_r-(K+U)_t$.
(2) For small values of t, a constant b exists such that

$$\left.\begin{matrix} K(t,r)-U(t,r) \\ 2K(t,r) \\ K(t,r)+U(t,r)+\ln\rho(t,r)\end{matrix}\right\}\geqslant -\ln|t|+b.$$

Therefore now we just have to verify under which conditions these theorems can be applied to stiff fluid space–times. Since the theorems do not make use of Einstein equations, it is expected that when we take them into account the conditions will not be so restrictive as they seem.

We begin with future-pointing geodesics. The first part of the theorem is a set of conditions on the derivatives of the metric functions.

(1)

(a) From (19c) and (19d) we obtain

$$(K-U-\ln\rho)_t+(K-U-\ln\rho)_r=r(U_t+U_r)^2+H_t+H_r-\frac{1}{r}.$$

The sum of the derivatives of H is always positive, since $H_r>|H_t|$ in order to have positive pressure. In fact, this is the $r(\sigma_t+\sigma_r)^2$ term in the Wainright–Ince–Marshman formalism. This expression is positive if either $|U_t+U_r|$ or H_t+H_r ($|\sigma_t+\sigma_r|$ in the Wainright–Ince–Marshman formalism) does not decrease as $1/r$ or faster for large values of t and r. That is, we need either U or H to overcome the negative term. Under such conditions, the second part of the premise,

$$(K-U-\ln\rho)_r=r(U_t^2+U_r^2)+H_r-\frac{1}{r}\geqslant 0,$$

is also satisfied.

(b) Once (1) (a) is fulfilled, this condition,

$$K_t+K_r=U_t+U_r+r(U_t+U_r)^2+H_t+H_r>0,$$

is trivial, since the only possible negative contribution would be that of U_t+U_r and this is counteracted by H_t+H_r if it decreases as $1/r$ or faster, or by $r(U_t+U_r)^2$ if it does not. Following a similar line of thought we also conclude that

$$K_r=U_r+r(U_t^2+U_r^2)+H_r$$

is positive for large values of t and r.

(c) The last set of conditions on the derivatives,

$$(K+U)_t+(K+U)_r=2(U_t+U_r)+r(U_t+U_r)^2+H_t+H_r\geqslant 0,$$
$$K_r+U_r=2U_r+rU_r^2+H_r\geqslant 0,$$

is also a consequence of (1) (a). Therefore the first part of the theorem is satisfied if

$$\left.\begin{array}{c} r^{1-\varepsilon}|U_r+U_t| \\ \text{or} \\ r^{1-\varepsilon}(H_r+H_t) \end{array}\right\} \not\to 0 \tag{27}$$

for large values of t and r. The conclusion for past-pointing geodesics is quite similar. We just have to change the sign of the time derivatives,

$$\left.\begin{array}{c} r^{1-\varepsilon}|U_r-U_t| \\ \text{or} \\ r^{1-\varepsilon}(H_r-H_t) \end{array}\right\} \not\to 0 \tag{28}$$

for large values of r and small values of t. For instance, these restrictions are trivial for the $\xi=0$ case, since $H=\gamma r^2/2$ does not decrease.

(2) The dependence on the matter content of the space–time may be removed from these conditions, since we may write

$$K(t,r)=U(t,r)+\int_0^r dr'(r'U_r^2(t,r')+r'U_t^2(t,r')+H_r(t,r'))=U(t,0)+\int_0^r dr'\,K_r(t,r'), \tag{29}$$

and according to (19d) or (25d) K_r is a positive term if the first part of the theorem is satisfied.

(a) The first condition is tautological since

$$K(t,r)-U(t,r)=\int_0^r dr'\,(r'U_r^2(t,r')+r'U_t^2(t,r')+H_r(t,r'))>0.$$

(b) For geodesics along the axis, this condition requires for large values of the time coordinate that

$$K(t,0)=U(t,0)\geqslant -\tfrac{1}{2}\ln|t|+b, \tag{30}$$

and for general geodesics the only difference is the positive term in (29). Therefore (30) is the only restriction for all geodesics.

(c) The same restriction is achieved likewise when applied to the expression $K+U+\ln\rho$.

Therefore we are left with just three regularity conditions on the metric of an Abelian diagonal orthogonally transitive space–time with spacelike orbits and with a stiff perfect fluid as matter content. We may summarize these results in two theorems:

Theorem 3: A cylindrical space–time with a stiff perfect fluid as matter content, endowed with a metric in the form (7) with C^2 metric functions K,U,ρ is future geodesically complete if the gradient of the surface element is spacelike and

(1) For large values of t, $U(t,0) \geqslant -\frac{1}{2}\ln|t|+b$.
(2) Either $r^{1-\varepsilon}|U_r+U_t|$ or $r^{1-\varepsilon}(H_r+H_t)$ does not tend to zero for large values of t and r.

Theorem 4: A cylindrical space–time with a stiff perfect fluid as matter content, endowed with a metric in the form (7) with C^2 metric functions K,U,ρ is past geodesically complete if the gradient of the surface element is spacelike and

(1) For small values of t, $U(t,0) \geqslant -\frac{1}{2}\ln|t|+b$.
(2) Either $r^{1-\varepsilon}|U_r-U_t|$ or $r^{1-\varepsilon}(H_r-H_t)$ does not tend to zero for small values of t and large values of r.

For vaccuum space–times both theorems hold just dropping the conditions on the derivatives of H.

The restrictions imposed by both theorems in order to have a nonsingular space–time are rather simple to implement, since U is just a solution of the wave equation and H is related to another one. We may state that regularity conditions are quite weak for stiff fluids, since it is very easy to provide solutions that fulfill such requirements. For instance,

Corollary: A metric with arbitrary H and a function U which grows for large $|t|$ and for large r makes the spacetime geodesically complete.

It is not difficult to derive such functions. The solutions to the reduced wave equation in the plane can be written as solutions of the initial value problem,

$$U_{tt}-U_{rr}-\frac{U_r}{r}=0,$$
$$U(0,r)=f(r), \quad U_t(0,r)=g(r). \tag{31}$$

The solution to this problem can be written in closed form,[15]

$$U(x,y,t)=\frac{1}{2\pi}\int_0^{2\pi}d\phi\int_0^t dR\,R\frac{g(x+R\cos\phi,y+R\sin\phi)}{\sqrt{t^2-R^2}}$$
$$+\frac{1}{2\pi}\frac{\partial}{\partial t}\int_0^{2\pi}d\phi\int_0^t dR\,R\frac{f(x+R\cos\phi,y+R\sin\phi)}{\sqrt{t^2-R^2}}, \tag{32}$$

for initial data $U(x,y,0)=f(x,y)$, $U_t(x,y,0)=g(x,y)$, taking into account that f and g are to have circular symmetry.

If we split U in U_f and U_g, the terms depending, respectively, on the initial data for U and its derivative, we notice that U_f is even in the time coordinate whereas U_g is odd. This implies that if U_f satisfies the first condition in theorem 3 for future-pointing geodesics, it will fulfill it for past-pointing geodesics too. On the contrary, if U_g satisfies it for future-pointing geodesics, it may not fulfill it for past-pointing ones, unless it behaves for large values of $|t|$ slower than a logarithm. Therefore one is to require either that U_f dominates over U_g for large $|t|$ or that both terms behave slower than a logarithm in order to have nonsingular behavior.

IV. DISCUSSION

In this paper we have derived sufficient conditions for an Abelian diagonal orthogonally transitive space–time with spacelike orbits and with a stiff perfect fluid as matter content to be geodesically complete. One of the metric functions appears to be determinant for the regularity of the space–time. These conditions are easy to check and do not mean much restriction on these space–times.

This means that nonsingular space–times are not as scarce as it was thought, considering the reduced list of geodesically complete perfect fluid cosmologies in the literature. Further work is

needed with more generic symmetries and matter contents in order to clarify the issue, since stiff perfect fluids are rather peculiar. They may be interpreted as a massless scalar field and they are the limiting case for which a barotropic perfect fluid with linear equation of state satisfies every energy condition. These space–times also fulfill the generic condition and are causally stable.

The latter assert is true since they possess a cosmic time, which is the coordinate t. This coordinate has a timelike gradient everywhere. Therefore,[2] these space–times satisfy weaker causality conditions. For instance, the chronology condition is true for them and no closed causal curves are possible.

As it was stated in the introduction, the existence of these nonsingular space–times is possible because they do not possess causally trapped sets. They obviously do not contradict then the singularity theorems. They just fall out of their scope.

Another interesting point that is worthwhile mentioning is that the regularity theorems appear to encourage a growing K for large values of $|t|$. This seems to support a conjecture that states that the spatial average value of the pressure in nonsingular space–times is zero,[11] since p decreases with large K according to (24),

$$p=e^{-2K}(\sigma_t^2-\sigma_r^2). \tag{33}$$

In our regular space–times, constant t sheets are Cauchy hypersurfaces and we may write the whole system of equations as an initial value problem for U, K, and H for any constant t. Without breaking the generality of the result, we may focus on $t=0$. The initial value problem can be stated as

$$U_{tt}-U_{rr}-\frac{U_r}{r}=0, \tag{34a}$$

$$\sigma_{tt}-\sigma_{rr}-\frac{\sigma_r}{r}=0, \tag{34b}$$

$$K_t=U_t+2r(U_tU_r+\sigma_t\sigma_r), \tag{34c}$$

$$U(0,r)=f(r), \quad U_t(0,r)=g(r), \tag{34d}$$

$$\sigma(0,r)=f_\sigma(r), \quad \sigma_t(0,r)=g_\sigma(r), \tag{34e}$$

$$K(0,r)=h(r), \tag{34f}$$

and the remaining equation in the system,

$$K_r=U_r+r(U_t^2+U_r^2+\sigma_t^2+\sigma_r^2), \tag{35}$$

is used to complete the initial data,

$$h(r)=U(0,0)+\int_0^r dr'\,K_r(0,r')=f(r)+\int_0^r dr'\,r'\{g(r)^2+f'(r)^2+g_\sigma(r')^2+f'_\sigma(r')^2\}. \tag{36}$$

In order to know the pressure on the hypersurface $t=0$ we just have to prescribe the initial data,

$$p(0,r)=e^{-2h(r)}\{g_\sigma(r)^2-f'_\sigma(r)^2\}. \tag{37}$$

We show that it must necessarily vanish at infinity if the space–time is causally geodesically complete.

If the term $g_\sigma^2 - f_\sigma'^2$ in the pressure does not tend to zero at infinity, the σ terms would contribute to h as r^2 (if $g_\sigma^2 + f_\sigma'^2$ tends to a constant) or greater. Unless a negative f overcomes this quadratic term, we would have a pressure decreasing as a Gaussian exponential and the average on $t=0$ would be zero.

But f cannot beat a quadratic term, because the f' term in the integral would mean a positive r^4 contribution to h, and we would have again a negative exponential. That is, if $g_\sigma^2 - f_\sigma'^2$ does not vanish at infinity, it grows much slower than the exponential term decreases and the pressure tends to zero.

The only possibility we have left then is a positive exponential. This means a negative h. If we want f to overcome just the f' term in h, we require $|f(r)| \leqslant \ln r$ for large values of r, a very narrow strip.

But we also need to keep under control the σ terms in h. They remain bounded for large values of r if $r^2(g_\sigma^2 + f_\sigma'^2)$ tends to zero. This means that the σ term in the pressure decreases faster than r^{-2}. Admitting that $h(r)$ might behave as $-\ln r$ for large r, the exponential in the pressure would be a r^2 term, that cannot compensate the σ term.

Therefore, pressure tends to zero for large r on constant time hypersurfaces, thereby supporting Senovilla's conjecture in Ref. 11.

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The appearance of the resolved singular hypersurface in the classical phase space of the Lie group SU(n)

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A classical phase space with a suitable symplectic structure is constructed together with functions which have Poisson brackets algebraically identical to the Lie algebra structure of the Lie group SU(n). In this phase space we show that the orbit of the generators corresponding to the simple roots of the Lie algebra give rise to fibers that are complex lines containing spheres. There are $n-1$ spheres on a fiber and they intersect in exactly the same way as the Cartan matrix of the Lie algebra. This classical phase space bundle, being compact, has a description as a variety. Our construction shows that the variety containing the intersecting spheres is exactly the one obtained by resolving the singularities of the variety $x_0x_1-x_2^n=0$ in $\mathcal{C}^3$. A direct connection between this singular variety and the classical phase space corresponding to the Lie group SU(n) is thus established. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1723700]

I. INTRODUCTION

It has long been known that there is an intriguing algebraic correspondence between the Cartan matrix of simply laced Lie groups and the intersection matrix of spheres that appear when certain simple singularities are resolved.[1] The reason for such a correspondence has also been long known within the framework of algebraic groups.[2] That this correspondence might be more than a mathematical curiosity was established when it was shown that duality in string theory made effective use of such a link.[3] A type 2A string compactified on a $K3$ surface (a four-dimensional surface) was conjectured to be dual to a heterotic string compactified on T^4 (the four torus). A test of this conjecture required the zero mass excitations in the two theories to match. The zero mass excitations at the type 2A end came from certain singular points that appear on the $K3$ surface in a certain limit while those at the heterotic string end came from gauge excitations associated with an SU(n) Lie group. The excitations at the type 2A end were ''classical'' solitonic-type excitations while those at the heterotic end were ''quantum'' gauge excitations. This result suggests that a link between minimally resolved singularities and the ''classical limit'' of simply laced Lie groups might exist.

In this paper we establish such a link. We demonstrate this link explicitly for the Lie groups SU(2), SU(3), and SU(4). Generalization to SU(n) is then straightforward. We find, using a Gauss decomposition Z_+HZ_-, where Z_+ is an upper triangular matrix with unit diagonal elements, H is a diagonal matrix, Z_- is a lower triangular matrix with unit diagonal elements that the classical phase space, in which Poisson brackets mirror the Lie algebra structure, can be constructed using a standard coherent state approach.[4] We use the Gauss decomposition in order to use the Borel–Weil Theorem. This theorem shows how irreducible representations of a compact Lie group G can

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be constructed as holomorphic sections over G/T, where T is the maximal torus of G. The approach thus describes the group in terms of complex variables and is thus a natural setting for making contact between the group and complex algebraic varieties. We have

Borel–Weil Theorem 1 (Ref. 5): *The space of holomorphic sections of the line bundle L_λ over G/T is nontrivial if λ is the highest weight of an irreducible representation of G. When λ is the highest weight then this space of holomorphic sections is a realization of the representation space V_λ of G.*

The coherent state approach is an explicit way of implementing the Borel–Weil Theorem. Use is made, in this approach, of the fact that $G/T=G_c/B$, where G_c is the complexification of G and B is the Borel subgroup. In terms of the Gauss decomposition B is generated by H and Z_-. It is in this framework that we search for and identify classical phase space. For SU(n) the phase space is CP^{n-1}. This is a Kähler symplectic manifold. It is identified cleanly in G_c/B as follows. We first introduce some definitions. Triangular matrices with unit diagonal elements are called unipotent. Z_+,Z_- are unipotent. We claim that by using unipotent group elements of a special kind we can construct the required Kähler symplectic manifold. To do this the unipotent elements used must have two special features. First they must mutually commute. Second the number of elements that commute with the these unipotent elements must equal the rank r of the group. Such elements are called regular. In this coherent state approach the symplectic structure is derived from a Kähler potential which we construct from a scalar product using the group elements described acting on the highest weight vector for the fundamental representation. It is then shown that the expectation value of the generators of the Lie algebra have Poisson brackets, defined in terms of this symplectic structure, isomorphic to the Lie algebra of the group. On this Kähler phase space a fiber bundle structure can be constructed whose fibers are complex curves, containing intersecting spheres. The fiber bundle considered is constructed from the orbit of group elements arising from the simple roots of the corresponding Lie algebra. In our construction we classify the unipotent elements of Z_+ in the following way:

One class has a centralizer (elements of the group commuting among themselves) of dimension equal to the rank r of the group. These are the regular elements. The other class comes from the generators of the Lie algebra for simple roots. These are unipotent elements that commute with $r+2$ group elements. Such elements are called subregular. These unipotent subregular elements play a crucial role in our construction. The special unipotent regular elements are used to construct classical phase space. This is done by acting on the highest weight vector with the the elements described. Choosing to work with the highest weight vector is the way the quotienting of G_c by B is implemented in this framework. The unipotent subregular elements acting on a point of this phase space give rise to a fiber containing intersecting spheres. The way these spheres intersect can be summarized in the form of an intersection matrix. This intersection matrix is found to be identical to the negative of the Cartan matrix of the Lie algebra. We show this explicitly for SU(3) where there are two intersecting spheres, for SU(4) where there are three spheres and for SU(n) where there are $n-1$ spheres. Precisely such intersecting spheres also appear when certain singular points are resolved on the hypersurface $x_0x_1-x_2^n=0$, where $(x_0,x_1,x_2)\in\mathcal{C}^3$, the space of three complex variables. In Sec. II we summarize the basic facts we need from the theory of resolution of singularities. In Sec. III the classical phase space for the Lie groups SU(2), SU(3), and SU(4) is constructed and the link with the resolved singularities established. Finally in Sec. IV we summarize our conclusions.

II. RESOLVING SINGULARITIES

Consider the hypersurface V_n in $\mathcal{C}^3$ defined by the algebraic equation:

$$V_n(x_0,x_1,x_2)=x_0x_1-x_2^n=0, \tag{1}$$

where n is an integer $\geqslant 2$ and $(x_0,x_1,x_2)\in\mathcal{C}^3$. We have the following definition:[1,6]

Definition: A point $(x_0,x_1,x_2)\in V_n=0$ is a singular point of the hypersurface if $\partial_{x_i}V_n=0$ at that point.

It follows from the definition that the point (0,0,0) i.e., the origin is a singular point of the hypersurface $V_n \equiv x_0 x_1 - x_2^n = 0$, for $n \geqslant 2$. Indeed a simple definition of this hypersurface as an orbifold is possible. To see this set $x_0 = \xi^n$, $x_1 = \eta^n$, $x_2 = \xi\eta$, where $(\xi, \eta) \in \mathcal{C}^2$. We note that in terms of these variables ξ, η the equation $x_0 x_1 - x_2^n = 0$ is identically satisfied, i.e., ξ, η parametrize the hypersurface $V_n = 0$. There is however one restriction on the variables ξ, η when they are on the hypersurface $V_n = 0$ namely the point (ξ, η) must be identified with $(\omega^{1/n}\xi, \omega^{-1/n}\eta)$, where ω is an nth root of identity $(\omega^n = 1)$. Thus the hypersurface $V_n = 0$ can be identified with the orbifold $\mathcal{C}^2/\mathcal{Z}_n$ with $\mathcal{Z}_n$ action defined by $(\xi, \eta) \to (\omega^{1/n}\xi, \omega^{-1/n}\eta)$, $\omega^n = 1$.

There is a standard method of minimally resolving this singularity,[1,6] i.e., of constructing a globally well defined hypersurface which is in 1–1 correspondence with the original hypersurface $V_n = 0$ except at the point (0,0,0). The singular point is "blown up." We describe this procedure first for the case $n = 2$ and $n = 3$ and then for the general case where $n > 3$.

Let us introduce the space $\mathcal{C}^3 \times \mathcal{P}^2$, where $\mathcal{P}^2$ is the complex projective two space (henceforth we denote $\mathcal{CP}^n$ by $\mathcal{P}^n$). Points in $\mathcal{C}^3 \times \mathcal{P}^2$ can be written as the pair $((x_0, x_1, x_2), [s_0, s_1, s_2])$ where $(x_0, x_1, x_2) \in \mathcal{C}^3$ and $[s_0, s_1, s_2]$ is an element of $\mathcal{P}^2$, i.e., it represents the equivalence class of points (s_0, s_1, s_2) under the equivalence relation $(s_0, s_1, s_2) \sim \lambda(s_0, s_1, s_2)$, where λ is a complex number $\neq 0$. Next we introduce the space $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$. This is defined as the set:

$$\mathcal{C}^3(\mathcal{P}^2, \mathcal{R}) = \{(x_0, x_1, x_2), [s_0, s_1, s_2] | x_i s_j = x_j s_i, \forall i, j\}. \tag{2}$$

Geometrically the restriction $x_i s_j = x_j s_i$ means that s_i is proportional to x_i. This gives a space consisting of points (x_0, x_1, x_2) in $\mathcal{C}^3$ and lines through the origin and these points. These lines are elements of $\mathcal{P}^2$. Thus for all points in $\mathcal{C}^3$, other than the origin, the element of $\mathcal{P}^2$ is uniquely fixed by (x_0, x_1, x_2). There is thus a 1–1 correspondence between points in $\mathcal{C}^3$ and the pair of points in $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$ defined by Eq. (2). For the origin however the situation is different. When $x_0 = x_1 = x_2 = 0$, there is no restriction on $[s_0, s_1, s_2]$. Thus the origin of $\mathcal{C}^3$ is replaced by the entire $\mathcal{P}^2$ in $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$; it is "blown up." Let us now study the way the hypersurface $x_0 x_1 - x_2^2 = 0$ behaves in $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$. To see the way the singular point in $V_2 = 0$ in $\mathcal{C}^3$ gets mapped in $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$ we approach the origin in $\mathcal{C}^3$. This is done by scaling the points (x_0, x_1, x_2) in $\mathcal{C}^3$ by t and letting $t \to 0$. Note that the constraints $x_i s_j = x_j s_i \forall i, j$ imply that $x_i = k s_i$ (where k = constant). Thus $(t x_0, t x_1, t x_2) = t k (s_0, s_1, s_2)$, i.e., we get from Eqs. (1) and (2) in the $t \to 0$ limit, points on $V_2 = 0$ satisfy $s_0 s_1 - s_2^2 = 0$ in $\mathcal{P}^2$. We now have the following theorem.

Theorem 2 (Ref. 7): *A polynomial equation of degree n in $\mathcal{P}^2$ describes a compact Riemann surface of genus g with $g = \frac{1}{2}(n-1)(n-2)$.*

In our case the polynomial equation $s_0 s_1 - s_2^2 = 0$ in $\mathcal{P}^2$ is of degree 2. Hence the surface in $\mathcal{P}^2$ is a genus zero surface, i.e., topologically it is a sphere. Thus the singular point of the hypersurface $x_0 x_1 - x_2^2 = 0$ in $\mathcal{C}^3$ is replaced by a sphere in $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$. The singularity has been resolved by a process of "blowing up" tuning the singular point into a sphere. We next consider the case $n = 3$. Repeating the procedure for the $n = 2$ case we find, the points $[s_0, s_1, s_2]$ satisfying Eq. (1) for $n = 3$, i.e., $V_3 = 0$ and Eq. (2) in the vicinity of the origin now have to satisfy the polynomial equation $t^2(s_0 s_1 - k t s_2^3) = 0$, i.e., the equation $s_0 s_1 = 0$ in the $t \to 0$ limit. This gives a pair of spheres $\mathcal{P}^1$'s in $\mathcal{P}^2$ (theorem 2) corresponding to setting $s_0 = 0$, $s_1 = 0$. These two spheres intersect once at the point (0,0,1) in $\mathcal{P}^2$. For $n \geqslant 4$, we again get the equation $s_0 s_1 = 0$ in the limit $t \to 0$ and a pair of spheres. However the intersection of these spheres is still a singular point. To see this we choose to describe $\mathcal{C}^3(\mathcal{P}^2, \mathcal{R})$ by first selecting a point in $\mathcal{P}^2$, say, (s_0, s_1, s_2) with $s_2 \neq 0$. Choosing this point does not uniquely fix a point in $\mathcal{C}^3$ but gives a line through the point (s_0, s_1, s_2) and the origin in $\mathcal{C}^3$. Let us set $s_2 = y_2$ $s_0 = y_0 y_2$, $s_1 = y_1 y_2$, where $(y_0, y_1, y_2) \in \mathcal{C}^3$. Finally set $y_2 = x_2$. Then $x_0 = y_0 y_2$, $x_1 = y_1 y_2$, and $0 = x_0 x_1 - x_2^n = y_2^2(y_0 y_1 - y_2^{n-2}) = 0$. By construction $y_2 \neq 0$. So $y_0 y_1 - y_2^{n-2} = 0$. For $n \geqslant 4$ this hyperplane has a singularity at the origin $y_0 = y_1 = y_2 = 0$, where $s_0 = 0$, $s_1 = 0$. The process of blowing up has to be repeated. The spheres produced by this process of blowing up self-intersect in an invariant way. Following a standard procedure[1] it can be shown that the self-intersection of the spheres can be taken to be -2. We

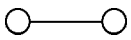

FIG. 1. Dynkin diagram 1.

summarize the results presented regarding the way the spheres in the ''resolved singularity'' intersect in the form of a matrix. For $n=3$, we have the intersection matrix $\left(\begin{smallmatrix}-2 & 1\\ 1 & -2\end{smallmatrix}\right)$. For $n=4$ we have

$$\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}.$$

This intersection information can be encoded in the form of a Dynkin diagram shown in Fig. 1 where each dot denotes a sphere with self intersection -2 and a line joining two dots denote intersection between two spheres with intersection number one. The construction described here extends to the case of arbitrary n where the diagram is shown in Fig. 2.

III. THE CLASSICAL PHASE SPACE FOR THE LIE GROUPS SU(2), SU(3), AND SU(4)

We now look at the classical origins of the Lie groups SU(2), SU(3), and SU(4) in the following sense. The groups have a local structure encoded by their Lie algebras. We will call the associated phase space, defined with a suitable symplectic structure, the classical counterpart of the Lie group if functions on the phase space can be constructed which have Poisson brackets algebraically identical to the Lie algebra structure of the Lie group. The construction we will describe involves coherent states associated with the Lie group of interest.[4] We start by quickly summarising the results for SU(2). This simple example contains a crucial ingredient needed for our subsequent analysis. Let us introduce the highest weight representation for SU(2), which we write as the vector $\left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)$. The coherent state $|\lambda\rangle$ is then defined as

$$|\lambda\rangle = e^{\lambda J_+}\begin{pmatrix}0\\1\end{pmatrix},\quad J_+ = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \equiv e_{12},\quad \langle\lambda|\lambda\rangle = (1+\lambda\bar{\lambda}), \tag{3}$$

λ being a complex variable. We then construct the Kähler potential $V(\lambda,\bar{\lambda}) = k\cdot\log(1+\lambda\bar{\lambda})$. This gives rise to a symplectic form on the coordinate chart $\lambda_0 \neq 0$ in $\mathcal{P}^1$ as well as the Fubini–Study metric,[6,8] where $\lambda = \lambda_1/\lambda_0$. The symplectic structure is given by

$$\omega_{\lambda\bar{\lambda}} = \partial_\lambda \partial_{\bar{\lambda}} V(\lambda\bar{\lambda}), \omega = \omega_{\lambda\bar{\lambda}} d\lambda \wedge d\bar{\lambda} + \omega_{\bar{\lambda}\lambda} d\bar{\lambda}\wedge d\lambda, \tag{4}$$

where the symplectic matrix is given by

$$[\omega] = k\cdot\begin{pmatrix} 0 & \dfrac{1}{(1+\lambda\bar{\lambda})^2} \\ -\dfrac{1}{(1+\lambda\bar{\lambda})^2} & 0 \end{pmatrix}, \tag{5}$$

k is a constant. We next note that

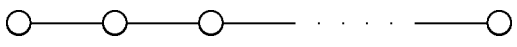

FIG. 2. Dynkin diagram 2.

$$X_+ = \frac{\langle \lambda | J_+ | \lambda \rangle}{\langle \lambda | \lambda \rangle} = \frac{2\lambda}{1+\lambda\bar{\lambda}},$$

$$X_- = \frac{\langle \lambda | J_- | \lambda \rangle}{\langle \lambda | \lambda \rangle} = \frac{2\bar{\lambda}}{1+\lambda\bar{\lambda}},$$

$$X_0 = \frac{\langle \lambda | J_0 | \lambda \rangle}{\langle \lambda | \lambda \rangle} = \frac{1-\lambda\bar{\lambda}}{1+\lambda\bar{\lambda}}, \tag{6}$$

with $J_- = e_{21}$, $J_+ = e_{12}$, $J_0 = e_{11} - e_{22}$, where e_{ij} stands for the 3×3 matrix with one in the ijth position and zero elsewhere, and X_+, X_-, X_0 are functions on the phase space $\mathcal{P}^1$ described by the complex variable λ and the symplectic form ω given by Eq. (4).

Furthermore $X_+X_- + X_0^2 = 1$, i.e., these functions represent points on S^2. Also

$$\{X_+, X_-\} = (\omega^{-1})_{\lambda\bar{\lambda}}\partial_\lambda X_+ \partial_{\bar{\lambda}} X_- + (\omega^{-1})_{\bar{\lambda}\lambda}\partial_{\bar{\lambda}} X_+ \partial_\lambda X_- = 2iX_0,$$

$$\{X_0, X_\pm\} = \pm X_\pm, \tag{7}$$

for suitable choice of k. Thus the expectation values of the generators $J_\pm$, J_0 in the normalized state vector $|\lambda\rangle$ represent the classical functions whose quantization, achieved by replacing Poisson brackets by commutators leads to the Lie algebra structure. The classical phase space of SU(2) is thus S^2 or $\mathcal{P}^1$. Note that the presence of S^2 could be spotted simply by evaluating $\int \omega d\lambda \wedge d\bar{\lambda} = 4\pi$, where ω is given by Eq. (4) and noting that the curvature of the phase space manifold is constant and positive. Also the metric on the phase space derived from the Kähler potential can be seen to be precisely the metric on S^2. The emergence of S^2 for the Lie group SU(2) is the key observation we want to record. For the groups SU(3), SU(4) we will construct appropriate Kähler forms which describe the classical phase space associated with these groups. It will then be demonstrated that the fiber obtained from the orbit of the generators corresponding to simple roots of the Lie algebra acting on this phase space contain intersecting spheres. The spheres can easily be identified by the presence of nontrivial cycles with $\int \omega = 4\pi$ on the fiber and a sphere metric in an appropriate subspace. The intersection properties of these spheres can be determined by using the methods of differential topology.[6] We demonstrate that the spheres described intersect in a manner precisely mirroring the Dynkin diagram of the group. Such a result was established by Tits and Steinberg in a different setting (see the theorem by Tits and Steinberg in the article by Brieskorn in Ref. 2). We saw in Sec. II that the spheres present when the singular hypersurface considered there was resolved also contain intersecting spheres of exactly the same kind. We now make use of the following theorems:

Chow's Theorem 3 (Refs. 6, 7): *A compact hypersurface can always be represented by an algebraic variety in a higher dimensional projective space.*

Theorem 4 (Ref. 7): *A complex curve in $\mathcal{C}^n$ can always be embedded in $\mathcal{C}^3$.*

The space constructed here is compact and hence the system can be represented as an algebraic variety and the intersecting spheres, present in $\mathcal{C}^{n-1}$, can be embedded in $\mathcal{C}^3$.

With the help of these theorems we see that the fibers containing the intersecting spheres can be embedded in $\mathcal{C}^3$. Thus the two different mathematical objects: the resolved singular curve and the algebraic curve present in the phase space bundle of SU(n) both live in $\mathcal{C}^3$ and both contain the same number of spheres that intersect in the same way.

Now for the details. For SU(3) we again work with the fundamental representation and introduce the coherent state

$$|\nu_1,\nu_2\rangle = e^{\nu_1 e_{13}} e^{\nu_2 e_{23}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \nu_1 \\ \nu_2 \\ 1 \end{pmatrix}. \tag{8}$$

Note that

$$g = e^{\nu_1 e_{13} + \nu_2 e_{23}} = \begin{pmatrix} 1 & 0 & \nu_1 \\ 0 & 1 & \nu_2 \\ 0 & 0 & 1 \end{pmatrix}$$

has generators e_{13}, e_{23} that commute. Furthermore g commutes with e_{13} and e_{23} so that dimension of the center of g is 2 = rank of SU(3). It is thus a regular element in SU(3,c). The element is also unipotent as it is an upper triangular matrix with unit diagonal elements.

The Kähler potential is given by

$$V(\nu_1,\nu_2,\overline{\nu_1},\overline{\nu_2}) = k\cdot \log\langle \nu_1,\nu_2|\overline{\nu_1},\overline{\nu_2}\rangle = k\cdot \log(1+\nu_1\overline{\nu_1}+\nu_2\overline{\nu_2}) = k\cdot \log\langle \nu|\nu\rangle \tag{9}$$

and the symplectic structure determined by

$$\omega_{i\bar{j}} = k\cdot \partial_{\nu_i}\partial_{\overline{\nu_j}} V, \omega = \omega_{i\bar{j}} d\nu_i \wedge d\overline{\nu_j} \tag{10}$$

is precisely that on $\mathcal{P}^2$ (Refs. 6 and 8) in the coordinate chart $\nu_0' \neq 0$, (ν_0',ν_1',ν_2') being the homogeneous coordinates and ν_1,ν_2 stand for ν_1'/ν_0' and ν_2'/ν_0'. Also the symplectic structure (10) can be proved to be global.[6] It is then easy to verify that the commutation relations of SU(3) are reflected in the Poisson brackets between the functions $\langle e_{ij}\rangle$ and $\langle e_{kl}\rangle$, where

$$\langle e_{ij}\rangle = \frac{\langle \nu_1\nu_2|e_{ij}|\nu_1\nu_2\rangle}{\langle \nu_1\nu_2|\nu_1\nu_2\rangle}.$$

Note that

$$[\omega] = \begin{pmatrix} 0 & a & 0 & b \\ -a & 0 & -b' & 0 \\ 0 & b' & 0 & c \\ -b & 0 & -c & 0 \end{pmatrix}, \tag{11}$$

$$[\omega^{-1}] = \frac{1}{ac-bb'} \begin{pmatrix} 0 & -c & 0 & b' \\ c & 0 & -b & 0 \\ 0 & b & 0 & -a \\ -b' & 0 & a & 0 \end{pmatrix}, \tag{12}$$

where

$$a = \partial_{\nu_1}\partial_{\overline{\nu_1}} \log\langle \nu|\nu\rangle, b = \partial_{\nu_1}\partial_{\overline{\nu_2}} \log\langle \nu|\nu\rangle, c = \partial_{\nu_2}\partial_{\overline{\nu_2}} \log\langle \nu|\nu\rangle \tag{13}$$

and prime stands for complex conjugate.

We now proceed to construct fibers on this phase space:

The generators corresponding to the simple roots of SU(3) are e_{12}, e_{23} and the group elements $\in Z_+$ are $e^{\mu e_{12}}$, $e^{\lambda e_{23}}$. They are unipotent subregular elements $\in Z_+$. To see this set $x = e^{\mu e_{12}}$. Then $y = e^{\alpha e_{13} + \beta(h_1+2h_2) + \gamma e_{32} + \delta e_{12}} \in \mathrm{SU}(3,c)$, where α, β, γ, δ are complex parameters, commutes with x. So dimension of the center of x in SU(3,c) is $4 = 2+2 =$ rank of SU(3) + 2. Thus x is subregular in SU(3,c). Similarly the element $e^{\lambda e_{23}}$ is subregular. We now consider the orbits

of $e^{\mu e_{12}}$ and $e^{\lambda e_{23}}$ at the base point on the phase space

$$\begin{pmatrix} \nu_1 \\ \nu_2 \\ 1 \end{pmatrix}.$$

We have then μ-orbit and λ-orbit as the fiber elements as

$$\begin{pmatrix} \nu_1 \\ \nu_2 \\ 1 \end{pmatrix}$$

and

$$\begin{pmatrix} \nu_1 \\ \nu_2+\lambda \\ 1 \end{pmatrix}.$$

Relabeling the first orbit as

$$\begin{pmatrix} z_1 \\ \nu_2 \\ 1 \end{pmatrix}$$

we can associate with it a Kähler potential $\log(1+z_1\overline{z_1})$. This is a sphere $\mathcal{P}^1$. Similarly the λ orbit is also a sphere. To demonstrate that these two spheres intersect with intersection number 1 we consider

$$e^{\mu e_{12}} e^{\lambda e_{23}} \begin{pmatrix} \nu_1 \\ \nu_2 \\ 1 \end{pmatrix}.$$

The common z_1-z_2 (the first two coordinates) plane has an associated Kähler potential $\log(1+z_1\overline{z_1}+z_2\overline{z_2})$. The symplectic structure is then given by Eq. (10) with $i,j=1,2$. We now note the following theorems:

Theorem 5 (Ref. 6): *The de Rham cohomology and Dolbeault cohomology groups for $\mathcal{P}^n$ are related*:

$$H_{\partial}^{p,p}(\mathcal{P}^n) \cong H_{DR}^{2p} \cong C.$$

Theorem 6 (Ref. 6): *The intersection of the two surfaces $\mathcal{C}_i$ and $\mathcal{C}_j$ are given by $\mathcal{C}_i \cdot \mathcal{C}_j = 1/(4\pi)^2 \int \omega_i \wedge \omega_j$, where the integration is in the space containing the surface $\mathcal{C}_i$ and $\mathcal{C}_j$ and is a space of dimension four and ω_i, ω_j are (de Rham cohomology) elements of $H_{DR}^2(M,R)$.*

The cohomology groups associated with the symplectic form constructed are Dolbeault cohomology groups while the intersection formula is valid for de Rham cohomology groups. However for $\mathcal{P}^n$ they are equivalent (Theorem 5). We can thus determine intersection of spheres by simply evaluating $(1/(4\pi)^2)\int \omega \wedge \omega$, where the relevant four-dimensional manifold (complex dimension 2) is the common z_1-z_2 plane. This is precisely seen to be one. Thus the two spheres on the fiber intersect once with intersection number one.

The procedure outlined can be repeated for SU(4). This time

$$|\nu\rangle = |\nu_1, \nu_2, \nu_3\rangle = e^{\nu_1 e_{14}} e^{\nu_2 e_{24}} e^{\nu_3 e_{34}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \\ 1 \end{pmatrix} \tag{14}$$

and the Kähler potential is

$$V(\nu_1, \nu_2, \nu_3, \overline{\nu_1}, \overline{\nu_2}, \overline{\nu_3}) = k \cdot \log\langle \nu|\nu\rangle = k \cdot \log(1 + \nu_1\overline{\nu_1} + \nu_2\overline{\nu_2} + \nu_3\overline{\nu_3}). \tag{15}$$

Here again

$$\omega_{i,\bar{j}} = \partial_{\nu_i}\partial_{\overline{\nu_j}} \log\langle \nu|\nu\rangle, \omega = \omega_{i,\bar{j}} d\nu_i \wedge d\overline{\nu_j} \tag{16}$$

is a symplectic structure on $\mathcal{P}^3$. The corresponding $[\omega]$ and $[\omega^{-1}]$ matrices are given by

$$[\omega] = \begin{pmatrix} 0 & a & 0 & b & 0 & c \\ -a & 0 & -b' & 0 & -c' & 0 \\ 0 & b' & 0 & d & 0 & f \\ -b' & 0 & -d & 0 & -f' & 0 \\ 0 & c' & 0 & f' & 0 & g \\ -c & 0 & -f & 0 & -g & 0 \end{pmatrix}, \tag{17}$$

where the primed entries stand for complex conjugates and

$$[\omega^{-1}] = \frac{1}{N} \begin{pmatrix} 0 & dg - ff' & 0 & fc' - gb' & 0 & b'f' - dc' \\ ff' - dg & 0 & bg - cf' & 0 & cd - bf & 0 \\ 0 & cf' - bg & 0 & ag - cc' & 0 & bc' - af' \\ gb' - fc' & 0 & cc' - ag & 0 & af - b'c & 0 \\ 0 & bf - cd & 0 & b'c - af & 0 & ad - bb' \\ dc' - b'f' & 0 & af' - bc' & 0 & bb' - ad & 0 \end{pmatrix}, \tag{18}$$

where

$$N^2 = \det[\omega], \quad a = \partial_{\nu_1}\partial_{\overline{\nu_1}} \log\langle \nu|\nu\rangle, \quad b = \partial_{\nu_1}\partial_{\overline{\nu_2}} \log\langle \nu|\nu\rangle, \quad c = \partial_{\nu_1}\partial_{\overline{\nu_3}} \log\langle \nu|\nu\rangle,$$

$$d = \partial_{\nu_2}\partial_{\overline{\nu_2}} \log\langle \nu|\nu\rangle, \quad f = \partial_{\nu_2}\partial_{\overline{\nu_3}} \log\langle \nu|\nu\rangle, \quad g = \partial_{\nu_3}\partial_{\overline{\nu_3}} \log\langle \nu|\nu\rangle, \tag{19}$$

and the prime denotes complex conjugate. Using $[\omega^{-1}]$ from Eq. (18) it is again straightforward to verify that the commutation relations of SU(4) are reflected in the Poisson bracket between the functions $\langle e_{ij}\rangle$ and $\langle e_{kl}\rangle$ where again $\langle e_{ij}\rangle \equiv \langle \nu|e_{ij}|\nu\rangle / \langle \nu|\nu\rangle$.

Finally we look at the fiber. The unipotent subregular elements corresponding to the simple roots are $e^{\mu e_{12}}$, $e^{\lambda e_{23}}$, and $e^{\rho e_{34}}$. So we have μ, λ, and ρ orbits on the fiber at the base point

$$\begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \\ 1 \end{pmatrix}.$$

Each element acts on a 2-complex dimensional subspace. It is easy to determine, as we have shown for the SU(3) case that an individual orbit is $\mathcal{P}^1$ on the fiber. Two generators intersect if

they act on a common subspace i.e., group elements corresponding to e_{12} and e_{23} both act on the space labeled by 2, while e_{34} and e_{12} have no common subspace. A differential topology way of spotting this is to construct the vector obtained by acting $e^{\mu e_{12}}\, e^{\lambda e_{23}}$, say, on the base point. The variables μ, λ appear in the 1,2 position. Setting the variables corresponding to 1,2 as z_1, z_2 the symplectic structure can be constructed from the corresponding Kähler potential and

$$\frac{1}{(4\pi)^2}\int \omega\wedge\omega=\frac{1}{(4\pi)^2}\int 2(\omega_{z_1\bar{z}_1}\omega_{z_2\bar{z}_2}-\omega_{z_1\bar{z}_2}\omega_{z_2\bar{z}_1})dz_1\wedge d\bar{z}_1\wedge dz_2\wedge d\bar{z}_2$$

gives the intersection. Similarly e_{23}, e_{34} will give rise to intersection in the subspace z_2-z_3. The intersection corresponding to e_{12}, e_{34} will be zero since they have no subspace in common. Here we have to evaluate $\int\omega\wedge\omega$ in the subspace 1,2 or 3,4 in each of which $\omega\wedge\omega$ vanishes. Hence there is no intersection. The intersection properties of the orbits described easily generalizes to the case of SU(n). For SU(n) the symplectic structure will come from the group elements constructed from the generators e_{12}, $e_{13},\ldots,e_{1n}$ while the simple roots are $e_{12},e_{23},\ldots,e_{n,n-1}$. It is the orbit of the group elements generated by these simple roots acting at any point on phase space that give fibers containing $n-1$ intersecting spheres.

IV. CONCLUSIONS

We have shown in two examples, i.e., for SU(3) and SU(4) how a classical phase space can be associated with these groups. In this phase space the orbit of the generators corresponding to the simple roots of the Lie algebra gives rise to intersecting spheres as fibers. For SU(n) the fiber of the bundle consists of $n-1$ (equal to the rank of SU(n)) intersecting spheres. These spheres intersect precisely as the negative of the Cartan matrix of SU(n). A simple understanding of how this happens is provided in our work. The structure of SU(n), contained in the commutation properties of the simple roots of its Lie algebra, is exactly the structure used to construct the orbit of these generators in phase space. This structure in phase space gives rise to the resolved variety associated with a singular variety. An algebraic group demonstration of the relationship between simple singularities of the ADE type and simply laced Lie groups of ADE type was proved by Brieskorn,[2] where the role of the unipotent subregular elements of the groups was stressed and the earlier result regarding intersecting spheres of Tits and and Steinberg (theorem by Tits and Steinberg discussed in the article by Brieskorn in Ref. 2) stated. Our explicit construction uses unipotent regular elements of a special kind (viz., ones involving mutually commuting generators) to construct classical phase space and confirms the role played by subregular unipotent elements for making contact with resolved singularity. In our physically motivated approach it is geometrically very clear why unipotent subregular elements are crucial: they are the group elements that come from the simple roots of the Lie algebra. The classical phase space for SU(n) is shown explicitly to be contained in G_c/B as CP^{n-1}. The orbit of the generators of the simple roots of the corresponding Lie algebra then provide a local trivialization of a bundle contained in G_c/B with the classical phase space as the base. It is in the fiber of this space that the variety corresponding to the resolved singularity is contained. Our construction extends easily to SU(n). Extention of the construction described here to the D,E groups should be straightforward. It is pleasing that classical phase space is where the resolved singular variety corresponding to $x_0x_1-x_2^n=0$ makes its appearance. Our work thus provides confirmation of the classical/quantum correspondence discovered in string theory between groups and singularities.

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Perturbations of ground states in weakly interacting quantum spin systems

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We consider a general weak bounded finite range perturbation of a general free quantum spin Hamiltonian on a lattice. We prove that if the free Hamiltonian has a nondegenerate ground state and a spectral gap, then the perturbation also has a ground state, and estimate the localization of the spectrum in the corresponding ground state representation. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND RESULTS

We consider a weak finite range perturbation of a free quantum lattice Hamiltonian with a nondegenerate ground state and a spectral gap. It is natural to expect that in this situation there must exist some sort of a general perturbation theory for the ground and low-lying excited states, and in this report we establish certain results supporting this point of view.

This problem has been studied earlier for a variety of models. A possible approach here is to obtain the ground state as a zero temperature limit of temperature Gibbs states, which can be analyzed using Trotter-type (in particular, Feynman–Kac) formulas and cluster expansions; low-lying excitations can also be analyzed in this way.[1,3,6,17,18,20] In Refs. 7, 8 Kennedy and Tasaki used this method to develop a general perturbation theory for weak quantum perturbations of classical systems with a finite spin space.

There is, however, a more direct way to the ground states, suggested by Kirkwood and Thomas in Ref. 9. The key idea is to write a special ansatz for it and substitute into the Schrödinger equation. The resulting (Kirkwood–Thomas) equation can then be solved in a sense uniformly in the volume. These authors applied this technique to obtain infinite volume ground states and to establish short- or long-range order in certain spin-1/2 models.

The method was subsequently generalized to higher spins and used to prove the uniqueness of a translationally invariant ground state by Matsui in Refs. 13, 14. In Ref. 4, Datta and Kennedy simplified it and employed to find quasi-particle states. In particular, they showed that the Kirkwood–Thomas equation can be conveniently viewed as a fixed point equation for certain contraction mapping. Also see Ref. 5 for an application to interface states.

In this paper we give a further generalization of the method. While in the previous applications it was assumed that the Hilbert space of the model is realized as a functional space and the ground state as a Gibbs measure, we show that this is not necessary and the method works in the general C^*-algebraic framework (though a significant role in the proofs is played by a commutative subalgebra).

We give now the precise statements.

We consider a quantum spin system on the lattice $\mathbb{Z}^\nu$. Suppose that for each $x \in \mathbb{Z}^\nu$ there is a Hilbert space $\mathcal{H}_x$ (generally infinite-dimensional) assigned to this site. The Hilbert space of the model confined to a finite volume $\Lambda \subset \mathbb{Z}^\nu$ is then

$$\mathcal{H}_\Lambda := \otimes_{x \in \Lambda} \mathcal{H}_x .$$

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In $\mathcal{H}_\Lambda$ we consider a Hamiltonian H_Λ, having the form

$$H_\Lambda = H_{\Lambda,0} + \Phi_\Lambda .$$

Here $H_{\Lambda,0}$ is a free Hamiltonian:

$$H_{\Lambda,0} = \sum_{x \in \Lambda} h_x .$$

We assume that each h_x is a non-negative self-adjoint, generally unbounded operator on $\mathcal{H}_x$ with a nondegenerate ground state $\Omega_x \in \mathcal{H}_x$:

$$h_x \Omega_x = 0,$$

and a uniform in an x spectral gap:

$$h_x|_{\mathcal{H}_x \ominus \Omega_x} \geqslant \mathbf{1}. \tag{1}$$

In order to introduce the perturbation Φ_Λ we fix a finite subset $\Lambda_0 \subset \mathbb{Z}^\nu$ and set

$$\Phi_\Lambda = \sum_{x \in \mathbb{Z}^\nu : \Lambda_0 + x \subset \Lambda} \phi_x . \tag{2}$$

Here $\Lambda_0 + x$ is a shift of Λ_0 and ϕ_x a self-adjoint bounded operator on $\mathcal{H}_{\Lambda_0 + x}$. Since Φ_Λ is bounded, H_Λ is self-adjoint and $\mathrm{Dom}\,(H_\Lambda) = \mathrm{Dom}\,(H_{\Lambda,0})$. We will assume that $\sup_{x \in \mathbb{Z}^\nu} \|\phi_x\|$ is finite and small enough.

The first theorem shows the existence of the finite volume ground states and gives a spectral localization estimate.

Theorem 1: *There exists a constant $c_1 = c_1(\Lambda_0) > 0$ such that if $\sup_x \|\phi_x\| < c_1$ then for any finite Λ the Hamiltonian H_Λ has a nondegenerate ground state Ω_Λ:*

$$H_\Lambda \Omega_\Lambda = E_\Lambda \Omega_\Lambda , \quad H_\Lambda|_{\mathcal{H}_\Lambda \ominus \Omega_\Lambda} > E_\Lambda \mathbf{1}.$$

Moreover, denote

$$\tilde{H}_\Lambda := H_\Lambda - E_\Lambda \mathbf{1}.$$

There exists a constant $c_2 = c_2(\Lambda_0)$ such that

$$\mathrm{Sp}(\tilde{H}_\Lambda) \subset \bigcup_{a \in \mathrm{Sp}(H_{\Lambda,0})} \{z : |z - a| \leqslant c_2 \sup_x \|\phi_x\| a\}. \tag{3}$$

In particular, this gives a lower bound on the spectral gap:

$$\tilde{H}_\Lambda|_{\mathcal{H}_\Lambda \ominus \Omega_\Lambda} \geqslant (1 - c_2 \sup_x \|\phi_x\|)\mathbf{1}. \tag{4}$$

The second result concerns the thermodynamic limit of the ground states. Let $\mathcal{B}(\mathcal{H}_\Lambda)$ be the algebra of bounded operators in $\mathcal{H}_\Lambda$ for any finite Λ, and

$$\mathcal{A}_\infty := \bigcup_{\Lambda \subset \mathbb{Z}^\nu, |\Lambda| < \infty} \mathcal{B}(\mathcal{H}_\Lambda)$$

the full local algebra. Define the ground states found above as states on $\mathcal{B}(\mathcal{H}_\Lambda)$ (i.e., normalized positive linear functionals):

$$\omega_\Lambda(A) := (A\Omega_\Lambda, \Omega_\Lambda), \quad A \in \mathcal{B}(\mathcal{H}_\Lambda),$$

where Ω_Λ is assumed normalized. Let $\Lambda \nearrow \mathbb{Z}^\nu$ mean that Λ converges to $\mathbb{Z}^\nu$ in the sense that it eventually contains any finite subset.

Theorem 2: *There exists the thermodynamic limit of the finite volume ground states as a state ω_∞ on the quasi-local algebra $\overline{\mathcal{A}_\infty}$, in the sense that for any $A \in \mathcal{A}_\infty$ one has*

$$\omega_\Lambda(A) \overset{\Lambda \nearrow \mathbb{Z}^\nu}{\to} \omega_\infty(A).$$

Finally we consider the thermodynamic limit of the Hamiltonian. Let $(\mathcal{H}_\infty, \pi_\infty, \Omega_\infty)$ be the cyclic representation of $\overline{\mathcal{A}_\infty}$, associated with the state ω_∞:

$$(\pi_\infty(A)\Omega_\infty, \Omega_\infty)_{\mathcal{H}_\infty} = \omega_\infty(A).$$

Theorem 3: *There exists a self-adjoint operator H_∞ on $\mathcal{H}_\infty$, which is the weak resolvent limit of $\tilde{H}_\Lambda$ in the following sense: for any $A, B \in \mathcal{A}_\infty$ and $z \in \mathbb{C}\backslash\mathbb{R}$,*

$$((\tilde{H}_\Lambda - z)^{-1} A\Omega_\Lambda, B\Omega_\Lambda) \overset{\Lambda \nearrow \mathbb{Z}^\nu}{\to} ((H_\infty - z)^{-1}\pi_\infty(A)\Omega_\infty, \pi_\infty(B)\Omega_\infty).$$

Moreover, $H_\infty\Omega_\infty = 0$ and estimates (3),(4) hold with $\tilde{H}_\Lambda, \mathcal{H}_\Lambda, \Omega_\Lambda$ replaced by $H_\infty, \mathcal{H}_\infty, \Omega_\infty$, and $\mathrm{Sp}(H_{\Lambda,0})$ replaced by

$$\mathrm{Sp}(H_{\infty,0}) := \left\{ \sum_{x \in \mathbb{Z}^\nu} a_x \,\middle|\, a_x \in \mathrm{Sp}(h_x), a_x \neq 0 \ \textit{only for finitely many } x \right\}.$$

We prove our main result, Theorem 1, in two steps: first we find the ground state (in some implicit form), and then prove the spectral estimate (3). In the first step we follow the procedure developed by Datta and Kennedy in Ref. 4. We rewrite the Kirkwood–Thomas equation as a fixed point equation for a certain mapping, which is proved to be a contraction on a properly defined set. We introduce, however, a different, more general ansatz for the ground state, which allows us to treat abstract Hamiltonians without referring to special functional realizations.

Our derivation of the spectral estimate (3) partly relies on ideas from the Malyshev–Minlos method of isolating invariant many-particle subspaces of cluster operators.[12] [We remark that if the model is translationally invariant and $\mathrm{Sp}(h_x)$ discrete, then $\mathrm{Sp}(H_{\infty,0})$ is also discrete and H_∞ is expected to have a particle structure. Some of the one-particle subspaces can then be obtained as the invariant subspaces corresponding to certain isolated components of the spectrum induced by the relation (3).[2,3,10,15,16,19,20]] But technically our treatment is different and more simple than in the original Malyshev–Minlos approach. Namely, we explicitly represent the renormalized Hamiltonian as a sum of an operator similar to the free Hamiltonian and a relatively bounded, in some special sense, perturbation. The conclusion about the spectrum then follows directly from resolvent expansions relevant for relatively bounded perturbations, like in the well-known Kato–Rellich and KLMN theorems.

A natural conjecture for the model considered in our report is the uniqueness of the infinite volume ground state. We plan to give a proof of this in a subsequent publication.

II. PROOF OF THEOREM 1

In this section we fix a finite volume Λ (throughout the paper all the proper subsets of $\mathbb{Z}^\nu$ will be finite); the dependence on Λ will be occasionally suppressed in the notation.

By the standard perturbation theory, H_Λ has a nondegenerate ground state if $\sup_x \|\phi_x\| < c$ with some constant c, depending on Λ. We will show that the constant can in fact be chosen independent of Λ, and the ground state can be found in the form of some multiplicative expression. First we introduce some notation. Let

$$\mathcal{H}'_x := \mathcal{H}_x \ominus \Omega_x$$

and

$$\mathcal{H}'_I := \otimes_{x\in I}\mathcal{H}'_x, \quad \Omega_{I,0} := \otimes_{x\in I}\Omega_x,$$

for any $\varnothing \neq I \subset \Lambda$. Throughout the paper by u_I, v_I, etc. we will always denote vectors from $\mathcal{H}'_I$.

It follows that

$$\mathcal{H}_\Lambda \ominus \Omega_{\Lambda,0} = \bigoplus_{\varnothing\neq I\subset\Lambda} \mathcal{H}'_I \otimes \Omega_{\Lambda\setminus I,0} \tag{5}$$

(with $\mathcal{H}'_\Lambda \otimes \Omega_{\varnothing,0} \equiv \mathcal{H}'_\Lambda$). Now let $\tilde{\Omega}_\Lambda$ be the ground state vector of H_Λ, normalized by the condition

$$(\tilde{\Omega}_\Lambda, \Omega_{\Lambda,0}) = 1.$$

Then there exists a unique collection of vectors $\{u_I \in \mathcal{H}'_I\}_{\varnothing\neq I\subset\Lambda}$ such that

$$\tilde{\Omega}_\Lambda = \Omega_{\Lambda,0} + \sum_{\varnothing\neq I\subset\Lambda} u_I \otimes \Omega_{\Lambda\setminus I,0}, \tag{6}$$

and finding $\tilde{\Omega}_\Lambda$ is reduced to finding this collection. It is more natural, however, to search for the corresponding truncated objects, rather than u_I themselves. Namely, for any collection $\{u_I \in \mathcal{H}'_I\}_{\varnothing\neq I\subset\Lambda}$ we can define another collection $\{v_I \in \mathcal{H}'_I\}_{\varnothing\neq I\subset\Lambda}$ by

$$u_I = \sum_{\{I_1,\ldots,I_k\}\in\mathcal{P}(I)} \otimes_{l=1}^{k} v_{I_l}, \quad \forall I \subset \Lambda, I \neq \varnothing, \tag{7}$$

where $\mathcal{P}(I)$ is the set of all partitions of I into disjoint nonempty subsets. Such a collection exists and is uniquely determined by the inverse relation

$$v_I = \sum_{\{I_1,\ldots,I_k\}\in\mathcal{P}(I)} (-1)^{k-1}(k-1)! \otimes_{l=1}^{k} u_{I_l}. \tag{8}$$

The perturbed ground state $\tilde{\Omega}_\Lambda$ can be obtained from $\Omega_{\Lambda,0}$ by a "dressing transformation," connected with the above decompositions. For any $v_I \in \mathcal{H}'_I$, define the one-dimensional "creation operator" $\hat{v}_I \in \mathcal{B}(\mathcal{H}_I)$ by

$$\hat{v}_I \Omega_{I,0} = v_I, \quad \hat{v}_I|_{\mathcal{H}_I \ominus \Omega_{I,0}} = 0. \tag{9}$$

These operators have some useful properties. First of all, they commute: for any u_I, v_J one has

$$[\hat{u}_I, \hat{v}_J] = 0. \tag{10}$$

Moreover,

$$\hat{u}_I \hat{v}_J = 0, \quad \text{if } I \cap J \neq \varnothing. \tag{11}$$

Finally,

$$\|\hat{v}_I\| = \|v_I\|. \tag{12}$$

Now it easily follows from (10), (11) that for any collection $\{v_I\}_{\varnothing\neq I\subset\Lambda}$,

$$\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}=\Omega_{\Lambda,0}+\sum_{\varnothing\neq I\subset\Lambda}\sum_{\{I_1,\dots,I_k\}\in\mathcal{P}(I)}(\otimes_{l=1}^{k}v_{I_l})\otimes\Omega_{\Lambda\setminus I,0}.$$

So we see that a collection $\{v_I\}_{\varnothing\neq I\subset\Lambda}$ is related to $\tilde{\Omega}_\Lambda$ by Eqs. (6), (7) if and only if

$$\tilde{\Omega}_\Lambda=\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}. \tag{13}$$

Since the decomposition (5) is invariant with respect to $H_{\Lambda,0}$, relations (7), (8) imply that the rhs of (13) lies in $\mathrm{Dom}(H_\Lambda)(=\mathrm{Dom}(H_{\Lambda,0}))$ if and only if $v_I\in\mathrm{Dom}(H_{I,0})$ for all I (where $H_{I,0}=\Sigma_{x\in I}h_x$).

We will find $\tilde{\Omega}_\Lambda$ in the form (13). Precisely, let us fix any $\lambda>1$. We will show that there exists a constant $c_1=c_1(\lambda,\Lambda_0)>0$ such that if $\sup_x\|\phi_x\|<c_1$ then $\tilde{\Omega}_\Lambda$ has the form (13) with

$$\max_{x\in\Lambda}\sum_{I\subset\Lambda:x\in I}\|H_{I,0}v_I\|\lambda^{d_I+1}\leqslant 1, \tag{14}$$

where d_I is the minimal length of a connected graph containing I.

To this end we substitute the ansatz (13) into the Schrödinger equation,

$$H_\Lambda\tilde{\Omega}_\Lambda=E_\Lambda\tilde{\Omega}_\Lambda, \tag{15}$$

and find

$$\exp\left(-\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)H_\Lambda\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}=E_\Lambda\Omega_{\Lambda,0}. \tag{16}$$

Recall that $H_\Lambda=H_{\Lambda,0}+\Phi_\Lambda$. A simple computation shows that for any $x\in\Lambda$,

$$\begin{aligned}h_x\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}&=\sum_{I\subset\Lambda:x\in I}\sum_{J\subset\Lambda\setminus I}\sum_{\{I_1,\dots,I_k\}\in\mathcal{P}(J)}(h_xv_I)\otimes(\otimes_l v_{I_l})\otimes\Omega_{\Lambda\setminus(I\sqcup J)}\\&=\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\sum_{\varnothing\neq I\subset\Lambda}h_x\hat{v}_I\Omega_{\Lambda,0}\end{aligned}$$

(by $\sqcup$ we denote a disjoint union). Therefore

$$\exp\left(-\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)H_{\Lambda,0}\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}=H_{\Lambda,0}\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\Omega_{\Lambda,0}=\sum_{\varnothing\neq I\subset\Lambda}\widehat{H_{I,0}v_I}\Omega_{\Lambda,0},$$

and Eq. (16) becomes

$$\sum_{\varnothing\neq I\subset\Lambda}\widehat{H_{I,0}v_I}\Omega_{\Lambda,0}+\exp\left(-\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Phi_\Lambda\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat{v}_I\right)\Omega_{\Lambda,0}=E_\Lambda\Omega_{\Lambda,0}. \tag{17}$$

Now, let $P_I:\mathcal{H}_\Lambda\to\mathcal{H}'_I$ be the operator, defined for each $I\subset\Lambda$ by

$$u=\sum_{I\subset\Lambda}(P_Iu)\otimes\Omega_{\Lambda\setminus I,0},\quad\forall u\in\mathcal{H}_\Lambda$$

(where $\mathcal{H}'_\varnothing\equiv\mathbb{C}$). Let T be the map on the linear space of collections $\{v_I\}_{\varnothing\neq I\subset\Lambda}$, defined by

$$T(\{v_I\}_{\varnothing\neq I\subset\Lambda}):=\{u_I\}_{\varnothing\neq I\subset\Lambda}, \tag{18}$$

where

$$u_I := -(H_{I,0}|_{\mathcal{H}_I'})^{-1} P_I \exp\Big(-\sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big) \Phi_\Lambda \exp\Big(\sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big) \Omega_{\Lambda,0}. \tag{19}$$

The inverse $(H_{I,0}|_{\mathcal{H}_I'})^{-1}$ is well-defined, since the spectral gap condition (1) implies

$$H_{I,0}|_{\mathcal{H}_I'} \geqslant |I| \mathbf{1}. \tag{20}$$

We see now that Eq. (17) is equivalent to the fixed point (Kirkwood–Thomas) equation,

$$T(\{v_I\}_{\varnothing \neq I \subset \Lambda}) = \{v_I\}_{\varnothing \neq I \subset \Lambda}, \tag{21}$$

on the space of collections [the eigenvalue E_Λ has been eliminated; it can be found by substituting the solution of (21) onto the lhs of (17) and taking the scalar product with $\Omega_{\Lambda,0}$]. Consider the Banach space $\mathcal{K}_\lambda$ of collections $\{v_I \in \mathcal{H}_I' \cap \mathrm{Dom}\,(H_{I,0})\}_{\varnothing \neq I \subset \Lambda}$, equipped with the norm

$$\|\{v_I\}_{\varnothing \neq I \subset \Lambda}\|_\lambda := \max_{x \in \Lambda} \sum_{I \subset \Lambda : x \in I} \|H_{I,0} v_I\| \lambda^{d_I + 1}. \tag{22}$$

We will show that T is a contraction in the unit ball in this space and hence has there a unique fixed point.

Let us first estimate $\|T(\{u_I\}) - T(\{v_I\})\|_\lambda$ for any two collections $\{u_I\}, \{v_I\} \in \mathcal{K}_\lambda$. We begin by expanding (19) using the identity

$$\exp\Big(-\sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big) \Phi_\Lambda \exp\Big(\sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big) = \sum_{k=0}^{\infty} \frac{1}{k!} \underbrace{\Big[\ldots\Big[}_{k} \Phi_\Lambda, \sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big], \ldots, \sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big] \tag{23}$$

(with the $k=0$ term equal to Φ_Λ). Let

$$T = \sum_{k=0}^{\infty} \frac{1}{k!} T^{(k)},$$

where $T^{(k)}$ is the contribution to T coming from the k-th term in (23). It follows that

$$\|T(\{u_I\}) - T(\{v_I\})\|_\lambda \leqslant \sum_{k=1}^{\infty} \frac{1}{k!} \|T^{(k)}(\{u_I\}) - T^{(k)}(\{v_I\})\|_\lambda \tag{24}$$

(because $T^{(0)}$ is a constant map). To estimate the k-th term in this sum we use (2) and write

$$\underbrace{\Big[\ldots\Big[}_{k} \Phi_\Lambda, \sum_{\varnothing \neq I \subset \Lambda} \hat{u}_I\Big], \ldots, \sum_{\varnothing \neq I \subset \Lambda} \hat{u}_I\Big] - \underbrace{\Big[\ldots\Big[}_{k} \Phi_\Lambda, \sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big], \ldots, \sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I\Big]$$

$$= \sum_{l=1}^{k} \sum_{y : \Lambda_0^+ y \in \Lambda} \sum_{\varnothing \neq I_1, \ldots, I_k \subset \Lambda} [\ldots[[[\ldots[\phi_y, \hat{u}_{I_1}], \ldots, \hat{u}_{I_{l-1}}], \hat{u}_{I_l} - \hat{v}_{I_l}], \hat{v}_{I_{l+1}}], \ldots, \hat{v}_{I_k}]. \tag{25}$$

So we see that

$$T^{(k)}(\{u_I\}) - T^{(k)}(\{v_I\}) = \sum_{l=1}^{k} T_l^{(k)}(\{u_I\}, \{v_I\}), \tag{26}$$

where $T_l^{(k)}$ is the contribution to $T^{(k)}(\{u_I\})-T^{(k)}(\{v_I\})$ from the lth term in (25), i.e., for $l=1$,

$$T_1^{(k)}(\{u_I\}_{\varnothing\neq I\subset\Lambda},\{v_I\}_{\varnothing\neq I\subset\Lambda})=\{w_I\}_{\varnothing\neq I\subset\Lambda},$$

where

$$w_I=-(H_{I,0}|_{\mathcal{H}_I'})^{-1}P_I\sum_{y:\Lambda_0+y\in\Lambda}\ \sum_{\varnothing\neq I_1,\ldots,I_k\subset\Lambda}[\ldots[[\phi_y,\hat{u}_{I_1}-\hat{v}_{I_1}],\hat{v}_{I_2}],\ldots,\hat{v}_{I_k}]\Omega_{\Lambda,0},$$

etc. We will consider the $l=1$ term first. By (22),

$$\|T_1^{(k)}(\{u_I\},\{v_I\})\|_\lambda=\max_{x\in\Lambda}\sum_{I\subset\Lambda:x\in I}\left\|\sum_{y:\Lambda_0+y\in\Lambda}\ \sum_{\varnothing\neq I_1,\ldots,I_k\subset\Lambda}P_I[\ldots[[\phi_y,\hat{u}_{I_1}-\hat{v}_{I_1}],\hat{v}_{I_2}],\ldots,\hat{v}_{I_k}]\Omega_{\Lambda,0}\right\|\lambda^{d_I+1}. \tag{27}$$

Now we make some observations concerning

$$P_I[\ldots[[\phi_y,\hat{u}_{I_1}-\hat{v}_{I_1}],\hat{v}_{I_2}],\ldots,\hat{v}_{I_k}]\Omega_{\Lambda,0}. \tag{28}$$

Expanding the commutators, we see that the norm of this expression does not exceed

$$2^k\sup_z\|\phi_z\|\|u_{I_1}-v_{I_1}\|\prod_{s=2}^{k}\|v_{I_s}\|, \tag{29}$$

because of (12). Next, note that (28) can be nonzero only if

$$I_s\cap(\Lambda_0+y)\neq\varnothing,\quad \forall s=1,\ldots,k \tag{30}$$

and

$$I=\bigsqcup_{s=1}^{k}(I_s\backslash(\Lambda_0+y))\sqcup J,\ \text{with some}\ J\subset\Lambda_0+y. \tag{31}$$

Indeed, since $\hat{u}_{I_1}-\hat{v}_{I_1},\hat{v}_{I_2},\ldots,\hat{v}_{I_k}$ commute with each other, (28) can be nonzero only if $[\phi_y,\hat{u}_{I_1}-\hat{v}_{I_1}]\neq 0$ and $[\phi_y,\hat{v}_{I_s}]\neq 0$ for all $s=2,\ldots,k$, which implies (30). To see (31), note that after expanding the commutators in (28) we get 2^k terms of the form

$$P_I\hat{w}_{I_{\sigma(1)}}\cdots\hat{w}_{I_{\sigma(t)}}\phi_y\hat{w}_{I_{\sigma(t+1)}}\ldots\hat{w}_{I_{\sigma(k)}}\Omega_{\Lambda,0}, \tag{32}$$

where

$$w_{I_s}:=\begin{cases}u_{I_1}-v_{I_1}, & \text{for } s=1,\\ v_{I_s}, & \text{else,}\end{cases}$$

and σ is a permutation. If (28) is nonzero, then at least one of the terms (32) is nonzero. For this term, by (11) $I_{\sigma(1)},\ldots,I_{\sigma(t)}$ do not overlap and also $I_{\sigma(t+1)},\ldots,I_{\sigma(k)}$ do not overlap, so that it has the form

$$P_I\hat{w}^{(1)}_{I^{(1)}}\phi_y\hat{w}^{(2)}_{I^{(2)}}\Omega_{\Lambda,0}, \tag{33}$$

where $I^{(1)}=\sqcup_{s=1}^{t} I_{\sigma(s)}, I^{(2)}=\sqcup_{s=t+1}^{k} I_{\sigma(s)}$ and $w^{(1)}_{I^{(1)}}=\otimes_{s=1}^{t} w_{I_{\sigma(s)}}, w^{(2)}_{I^{(2)}}=\otimes_{s=t+1}^{k} w_{I_{\sigma(s)}}$. As $\phi_y \in \mathcal{B}(\mathcal{H}_{\Lambda_0+y})$,

$$\phi_y \hat{w}^{(2)}_{I^{(2)}} \Omega_{\Lambda,0} = \sum_{K \subset \Lambda_0+y} \hat{w}^{(3)}_{K \sqcup (I^{(2)} \setminus (\Lambda_0+y))} \Omega_{\Lambda,0},$$

with some vectors $w^{(3)}_{K\sqcup(I^{(2)}\setminus(\Lambda_0+y))} \in \mathcal{H}'_{K\sqcup(I^{(2)}\setminus(\Lambda_0+y))}$. It follows that (33) can be nonzero only if $I^{(1)} \cap (I^{(2)} \setminus (\Lambda_0+y))=\varnothing$ and $I=I^{(1)} \sqcup (I^{(2)} \setminus (\Lambda_0+y)) \sqcup K$ with some $K \subset \Lambda_0+y, K \cap I^{(1)}=\varnothing$, in which case (33) equals

$$w^{(1)}_{I^{(1)}} \otimes w^{(3)}_{K\sqcup(I^{(2)}\setminus(\Lambda_0+y))}.$$

In particular, this implies (31).

Now, for any given $y, I_1, \ldots, I_k$ there exist at most $2^{|\Lambda_0|}$ sets I obeying (31). Further, (30) implies the inequality

$$d_I \leqslant d_{(\cup_{s=1}^{k} I_s) \cup (\Lambda_0+y)} \leqslant \sum_{s=1}^{k} d_{I_s} + d_{\Lambda_0}, \tag{34}$$

which in turn implies

$$\lambda^{d_I+1} \leqslant \lambda^{d_{\Lambda_0}-k+1} \prod_{s=1}^{k} \lambda^{d_{I_s}+1} \leqslant \lambda^{d_{\Lambda_0}} \prod_{s=1}^{k} \lambda^{d_{I_s}+1}.$$

It follows from these observations and the bound (29) that (27) does not exceed

$$\max_{x \in \Lambda} \sum^{(x)} \|u_{I_1} - v_{I_1}\| \lambda^{d_{I_1}+1} \left(\prod_{s=2}^{k} \|v_{I_s}\| \lambda^{d_{I_s}+1} \right) \lambda^{d_{\Lambda_0}} 2^k 2^{|\Lambda_0|} \sup_z \|\phi_z\|, \tag{35}$$

where $\Sigma^{(x)}$ is the sum over all those $y, I_1, \ldots, I_k$, for which $I_s \cap (\Lambda_0+y) \neq \varnothing, s=1,\ldots,k$, and $x \in (\cup_{s=1}^{k} I_s) \cup (\Lambda_0+y)$. We will estimate (35) by rearranging summation in it. Since $x \in (\cup_{s=1}^{k} I_s) \cup (\Lambda_0+y)$, and because $I_2, \ldots, I_k$ enter into (35) symmetrically, we have

$$\sum^{(x)} \leqslant \sum_1^{(x)} + \sum_2^{(x)} + (k-1) \sum_3^{(x)},$$

where

$$\sum_1^{(x)} := \sum_{y:\Lambda_0+y \ni x} \sum_{z_1,\ldots,z_k \in \Lambda_0+y} \sum_{I_s \ni z_s, s=1,\ldots,k},$$

$$\sum_2^{(x)} := \sum_{I_1 \ni x} \sum_{y:(\Lambda_0+y)\cap I_1 \neq \varnothing} \sum_{z_2,\ldots,z_k \in \Lambda_0+y} \sum_{I_s \ni z_s, s=2,\ldots,k},$$

$$\sum_3^{(x)} := \sum_{I_2 \ni x} \sum_{y:(\Lambda_0+y)\cap I_2 \neq \varnothing} \sum_{z_1,z_3,\ldots,z_k \in \Lambda_0+y} \sum_{I_s \ni z_s, s=1,3,\ldots,k}.$$

First we estimate the $\Sigma_1^{(x)}$ term. Since y and each of z_s can be chosen in at most $|\Lambda_0|$ ways, this term does not exceed

$$|\Lambda_0|^{k+1}\left(\max_{z_1}\sum_{I_1\ni z_1}\|u_{I_1}-v_{I_1}\|\lambda^{d_{I_1}+1}\right)\left(\prod_{s=2}^{k}\max_{z_s}\sum_{I_1\ni z_s}\|v_{I_s}\|\lambda^{d_{I_s}+1}\right)\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_z\|\phi_z\|. \quad (36)$$

Recall that for any I and w_I,

$$\|H_{I,0}w_I\|\geqslant|I|\|w_I\|, \quad (37)$$

by (20). It follows then by the definition of the norm (22) that

$$(36)\leqslant|\Lambda_0|^{k+1}\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_z\|\phi_z\|\|\{u_I-v_I\}\|_\lambda\|\{v_I\}\|_\lambda^{k-1}.$$

The $\Sigma_2^{(x)}$ term does not exceed

$$|I_1||\Lambda_0|^k\left(\max_{x}\sum_{I_1\ni x}\|u_{I_1}-v_{I_1}\|\lambda^{d_{I_1}+1}\right)\left(\prod_{s=2}^{k}\max_{z_s}\sum_{I_1\ni z_s}\|v_{I_s}\|\lambda^{d_{I_s}+1}\right)\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_z\|\phi_z\|, \quad (38)$$

because y can be chosen in at most $|I_1||\Lambda_0|$ ways, while each of z_s can be chosen then in at most $|\Lambda_0|$ ways. Again, by (37) and the definition of the norm, (38) is not greater than

$$|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_z\|\phi_z\|\|\{u_I-v_I\}\|_\lambda\|\{v_I\}\|_\lambda^{k-1}. \quad (39)$$

Similarly, the $\Sigma_3^{(x)}$ term can be bounded by (39) too. We conclude that

$$\|T_1^{(k)}(\{u_I\},\{v_I\})\|_\lambda\leqslant(k+|\Lambda_0|)|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_x\|\phi_x\|\|\{u_I-v_I\}\|_\lambda\|\{v_I\}\|_\lambda^{k-1}. \quad (40)$$

If $l=2,\ldots,k$, we have a similar bound for $T_l^{(k)}$ with $\|\{v_I\}\|_\lambda^{k-1}$ replaced by $\|\{u_I\}\|_\lambda^{l-1}\|\{v_I\}\|_\lambda^{k-l}$ in (40). Finally, if $\|\{v_I\}\|_\lambda\leqslant1$ and $\|\{u_I\}\|_\lambda\leqslant1$, then by (24),(26),

$$\|T(\{u_I\})-T(\{v_I\})\|_\lambda\leqslant\sum_{k=1}^{\infty}\frac{1}{k!}k(k+|\Lambda_0|)|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_x\|\phi_x\|\|\{u_I-v_I\}\|_\lambda. \quad (41)$$

So we see that if $\sup_x\|\phi_x\|\leqslant c_1'$, where

$$c_1'=\frac{1}{2}\left(\sum_{k=1}^{\infty}\frac{1}{(k-1)!}(k+|\Lambda_0|)|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\right)^{-1}, \quad (42)$$

then

$$\|T(\{u_I\})-T(\{v_I\})\|_\lambda\leqslant\tfrac{1}{2}\|\{u_I-v_I\}\|_\lambda,$$

for any two collections $\{u_I\},\{v_I\}$ from the unit ball.

Now we estimate $\|T(\{v_I\})\|_\lambda$. Consider the zero collection $\{0\}$ and note that $T^{(k)}(\{0\})=0$ for $k\geqslant1$; hence

$$\|T(\{0\})\|_\lambda=\|T^{(0)}(\{0\})\|_\lambda=\max_x\sum_{I\ni x}\left\|\sum_{y:\Lambda_0+y\ni x}P_I\phi_y\Omega_{\Lambda,0}\right\|\lambda^{d_I+1}\leqslant|\Lambda_0|2^{|\Lambda_0|}\lambda^{d_{\Lambda_0}+1}\sup_x\|\phi_x\|.$$

In particular, if $\sup_x\|\phi_x\|\leqslant c_1''\coloneqq(|\Lambda_0|2^{|\Lambda_0|}\lambda^{d_{\Lambda_0}+1})^{-1}/2$, then $\|T(\{0\})\|_\lambda\leqslant1/2$. It follows that if $\sup_x\|\phi_x\|\leqslant c_1\coloneqq\min(c_1',c_1'')$; then for any $\{v_I\}$ from the unit ball we have

$$\|T(\{v_I\})\|_\lambda\leqslant\|T(\{v_I\})-T(\{0\})\|_\lambda+\|T(\{0\})\|_\lambda\leqslant1/2+1/2=1.$$

So we see that if $\sup_x \|\phi_x\| \leqslant c_1$, then T is a contraction in the unit ball in $\mathcal{K}_\lambda$, and hence the Kirkwood–Thomas equation (21) there has a unique solution, which we will denote by $\{v_I^{(gs)}\}_{\varnothing \neq I \subset \Lambda}$. It obeys condition (14) and the vector

$$\tilde{\Omega}_\Lambda = \exp\left(\sum_{\varnothing \neq I \subset \Lambda} \hat{v}_I^{(gs)} \right) \Omega_{\Lambda,0}$$

is a solution of the Schrödinger equation (15) with some E_Λ. However, we have not proved yet that this $\tilde{\Omega}_\Lambda$ is the ground state and that it is non-degenerate. This will be seen from the spectral analysis of H_Λ given below.

Note first that any $u \in \mathcal{H}_\Lambda$ can be uniquely expanded as

$$u = \sum_{I \subset \Lambda} \hat{u}_I \tilde{\Omega}_\Lambda ,$$

with some $u_I \in \mathcal{H}_I'$ (where $\hat{u}_\varnothing$ is a multiple of **1**). Indeed, by the commutativity of the creation operators this relation is equivalent to

$$\exp\left(- \sum_{\varnothing \neq K \subset \Lambda} \hat{v}_K^{(gs)} \right) u = \sum_{I \subset \Lambda} \hat{u}_I \Omega_{\Lambda,0} ,$$

i.e.,

$$u_I = P_I \exp\left(- \sum_{\varnothing \neq K \subset \Lambda} \hat{v}_K^{(gs)} \right) u . \tag{43}$$

It is easy to check that $u \in \mathrm{Dom}\,(H_\Lambda)$ iff $u_I \in \mathrm{Dom}\,(H_{I,0})$ for all I.

Now recall that we defined $\tilde{H}_\Lambda = H_\Lambda - E_\Lambda \mathbf{1}$, so that $\tilde{H}_\Lambda \tilde{\Omega}_\Lambda = 0$. Below we will decompose $\tilde{H}_\Lambda$ into the sum

$$\tilde{H}_\Lambda = \tilde{H}_{\Lambda,0} + \tilde{\Phi}_\Lambda ; \tag{44}$$

$\tilde{H}_{\Lambda,0}$ will be a ''simple'' operator and $\tilde{\Phi}_\Lambda$ will be ''small'' with respect to $\tilde{H}_{\Lambda,0}$; both will have $\tilde{\Omega}_\Lambda$ as a zero eigenvector.

To this end take some $I \subset \Lambda$ and $u_I \in \mathcal{H}_I' \cap \mathrm{Dom}\,(H_{I,0})$. First we note that

$$H_{\Lambda,0} \hat{u}_I \tilde{\Omega}_\Lambda = \hat{u}_I H_{\Lambda,0} \tilde{\Omega}_\Lambda + \widehat{H_{I,0} u_I} \tilde{\Omega}_\Lambda .$$

Indeed, if $H_{\Lambda,0}$ is bounded, this formula follows because

$$\widehat{H_{I,0} u_I} = [H_{\Lambda,0}, \hat{u}_I];$$

for an unbounded $H_{\Lambda,0}$ one can justify it by a direct calculation. Then

$$\tilde{H}_\Lambda \hat{u}_I \tilde{\Omega}_\Lambda = \hat{u}_I \tilde{H}_\Lambda \tilde{\Omega}_\Lambda + \widehat{H_{I,0} u_I} \tilde{\Omega}_\Lambda + [\Phi_\Lambda, \hat{u}_I] \tilde{\Omega}_\Lambda = \widehat{H_{I,0} u_I} \tilde{\Omega}_\Lambda + [\Phi_\Lambda, \hat{u}_I] \tilde{\Omega}_\Lambda .$$

So we can define the operators $\tilde{H}_{\Lambda,0}, \tilde{\Phi}_\Lambda$ on $\mathrm{Dom}\,(\tilde{H}_{\Lambda,0}) := \mathrm{Dom}\,(H_{\Lambda,0})$ and $\mathrm{Dom}\,(\tilde{\Phi}_\Lambda) := \mathcal{H}_\Lambda$ by

$$\tilde{H}_{\Lambda,0} \hat{u}_I \tilde{\Omega}_\Lambda := \widehat{H_{I,0} u_I} \tilde{\Omega}_\Lambda , \quad \tilde{\Phi}_\Lambda \hat{u}_I \tilde{\Omega}_\Lambda := [\Phi_\Lambda, \hat{u}_I] \tilde{\Omega}_\Lambda , \tag{45}$$

and by linearity. We will rewrite $\tilde{\Phi}_\Lambda$ in a more convenient form using creation operators. Namely, for all $I, J \subset \Lambda$ and $u_I \in \mathcal{H}_I'$, define $(F_\Lambda u_I)_J \in \mathcal{H}_J'$ by

$$\tilde{\Phi}_\Lambda \hat{u}_I \tilde{\Omega}_\Lambda = \sum_{J\subset\Lambda} \widehat{(F_\Lambda u_I)_J} \tilde{\Omega}_\Lambda . \tag{46}$$

Applying (43), we find

$$\begin{aligned}(F_\Lambda u_I)_J &= P_J \exp\left(-\sum_{\varnothing\neq K\subset\Lambda} \hat{v}_K^{(gs)}\right)[\Phi_\Lambda,\hat{u}_I]\exp\left(\sum_{\varnothing\neq K\subset\Lambda} \hat{v}_K^{(gs)}\right)\Omega_{\Lambda,0}\\ &= P_J \sum_{s=0}^{\infty} \frac{1}{s!}\Bigg[\underbrace{\dots\Bigg[}_{s}[\Phi_\Lambda,\hat{u}_I],\sum_{\varnothing\neq K\subset\Lambda}\hat{v}_K^{(gs)}\Bigg],\dots,\sum_{\varnothing\neq K\subset\Lambda}\hat{v}_K^{(gs)}\Bigg]\Omega_{\Lambda,0}. \end{aligned}\tag{47}$$

Let us estimate $\Sigma_J\|(F_\Lambda u_I)_J\|$. Recall that

$$P_J[\dots[[\phi_y,\hat{u}_I],\hat{v}_{K_1}^{(gs)}],\dots,\hat{v}_{K_s}^{(gs)}]\Omega_{\Lambda,0}, \tag{48}$$

can be nonzero only if $(\Lambda_0+y)\cap I\neq\varnothing$ and $(\Lambda_0+y)\cap K_t\neq\varnothing$ for all $t=1,\dots,s$. Moreover, for $y,K_1,\dots,K_s$ fixed there are at most $2^{|\Lambda_0|}$ different sets J, for which (48) can be nonzero. Using also the fact that the norm of (48) is not greater than $2^{s+1}\|\phi_y\|\|u_I\|\Pi_{t=1}^s\|v_{K_t}^{(gs)}\|$, we find that

$$\begin{aligned}\sum_{J\subset\Lambda}\|(F_\Lambda u_I)_J\| &\leqslant \|u_I\|\sup_x\|\phi_x\|\\ &\times\sum_{s=0}^{\infty}\frac{2^{s+1+|\Lambda_0|}}{s!}\sum_{y:(\Lambda_0+y)\cap I\neq\varnothing}\ \sum_{y_1,\dots,y_s\in\Lambda_0+y}\ \sum_{K_t\ni y_t,t=1,\dots,s}\ \prod_{t=1}^{s}\|v_{K_t}^{(gs)}\|.\end{aligned}$$

Recall that $\|\{v_I^{(gs)}\}\|_\lambda\leqslant 1$ and hence $\max_x\Sigma_{K\ni x}\|v_K^{(gs)}\|\leqslant 1$. It follows that

$$\sum_{J\subset\Lambda}\|(F_\Lambda u_I)_J\|\leqslant\|u_I\|\sup_x\|\phi_x\||I|\sum_{s=0}^{\infty}\frac{2^{s+1+|\Lambda_0|}}{s!}|\Lambda_0|^{s+1}.$$

So if we set

$$c_2=\sum_{s=0}^{\infty}\frac{2^{s+1+|\Lambda_0|}}{s!}|\Lambda_0|^{s+1},$$

then

$$\sum_{J\subset\Lambda}\|(F_\Lambda u_I)_J\|\leqslant c_2\sup_x\|\phi_x\|\|H_{I,0}u_I\|. \tag{49}$$

By assumption and (42), $\sup_x\|\phi_x\|<c_1'<1/c_2$, so the inequality (49) indicates a sort of ''relative boundedness'' of $\tilde{\Phi}_\Lambda$ wrt $\tilde{H}_{\Lambda,0}$. Our spectral estimate (3) will follow from this inequality. Let us introduce a new norm $\|\cdot\|_1$ (equivalent to the usual norm) in $\mathcal{H}_\Lambda$ by

$$\left\|\sum_{I\subset\Lambda}\hat{u}_I\tilde{\Omega}_\Lambda\right\|_1 := \sum_{I\subset\Lambda}\|u_I\|.$$

Then for any $z\notin \mathrm{Sp}\,(H_{\Lambda,0})$,

$$\|\tilde{\Phi}_\Lambda(\tilde{H}_{\Lambda,0}-z)^{-1}\|_1=\max_{I\subset\Lambda}\sup_{\|u_I\|=1}\sum_{J\subset\Lambda}\|(F_\Lambda(H_{I,0}-z)^{-1}u_I)_J\|$$

$$\leqslant\max_{I\subset\Lambda}\sup_{\|u_I\|=1}c_2\sup_x\|\phi_x\|\|H_{I,0}(H_{I,0}-z)^{-1}u_I\|=\sup_{a\in\,\mathrm{Sp}\,(H_{\Lambda,0})}\frac{c_2\sup_x\|\phi_x\|a}{|z-a|}.$$

Let

$$f(a):=\frac{c_2\sup_x\|\phi_x\|a}{|z-a|},$$

and suppose now that

$$z\in\mathcal{O}_\Lambda:=\bigcap_{a\in\,\mathrm{Sp}\,(H_{\Lambda,0})}\{z\in\mathbb{C}:|z-a|>c_2\sup_x\|\phi_x\|a\}. \tag{50}$$

Then $f(a)<1$ for all $a\in\mathrm{Sp}\,(H_{\Lambda,0})$. Clearly f is continuous on the closed set $\mathrm{Sp}\,(H_{\Lambda,0})$, and $\lim_{a\to+\infty}f(a)=c_2\sup_x\|\phi_x\|<1$. It follows that $\sup_{a\in\,\mathrm{Sp}\,(H_{\Lambda,0})}f(a)<1$ and therefore

$$\|\tilde{\Phi}_\Lambda(\tilde{H}_{\Lambda,0}-z)^{-1}\|_1<1. \tag{51}$$

Let

$$S_{\Lambda,N}(z):=(\tilde{H}_{\Lambda,0}-z)^{-1}\sum_{k=0}^{N}(-\tilde{\Phi}_\Lambda(\tilde{H}_{\Lambda,0}-z)^{-1})^k.$$

Then by (51),

$$S_{\Lambda,N}(z)\overset{N\to\infty}{\to}S_\Lambda(z):=(\tilde{H}_{\Lambda,0}-z)^{-1}\sum_{k=0}^{\infty}(-\tilde{\Phi}_\Lambda(\tilde{H}_{\Lambda,0}-z)^{-1})^k,$$

with a bounded $S_\Lambda(z)$. Moreover,

$$(\tilde{H}_\Lambda-z)S_{\Lambda,N}(z)=(\tilde{H}_{\Lambda,0}-z+\tilde{\Phi}_\Lambda)S_{\Lambda,N}(z)=\mathbf{1}+(-1)^N(\tilde{\Phi}_\Lambda(\tilde{H}_{\Lambda,0}-z)^{-1})^{N+1}\overset{N\to\infty}{\to}\mathbf{1}.$$

The closedness of $\tilde{H}_\Lambda$ thus implies $(\tilde{H}_\Lambda-z)S_\Lambda(z)=\mathbf{1}$. Since $\tilde{H}_\Lambda$ is self-adjoint, this means that $\tilde{H}_\Lambda-z$ is invertible for $z\in\mathcal{O}_\Lambda$, which proves the spectral estimate (3).

Now to finish the proof of Theorem 1 it remains to show that $\tilde{\Omega}_\Lambda$ is a nondegenerate ground state of $\tilde{H}_\Lambda$. It follows from (3) that $\tilde{H}_\Lambda\geqslant 0$, so $\tilde{\Omega}_\Lambda$ is a ground state. The nondegeneracy can be deduced by a continuity argument. Consider the family of operators $H_\Lambda^{(\delta)}=H_{\Lambda,0}+\delta\Phi_\Lambda$ parametrized by $\delta\in[0,1]$. If $\tilde{H}_\Lambda^{(\delta)}=H_\Lambda^{(\delta)}-E_\Lambda^{(\delta)}$ are the corresponding renormalized operators, they all obey the common spectral estimate (3) and hence 0 is an isolated eigenvalue for all of them. By the continuity of the resolvents $(H_\Lambda^{(\delta)}-z)^{-1}$ in δ it follows then that the multiplicity of 0 is constant in δ, i.e., identically equals 1.

III. PROOF OF THEOREM 2

In the previous section we showed that if $\sup_x\|\phi_x\|<c_1$, then for any finite Λ the ground state of H_Λ can be found by solving the Kirkwood–Thomas equation $T_\Lambda(\{v_I\}_{\varnothing\neq I\subset\Lambda})=\{v_I\}_{\varnothing\neq I\subset\Lambda}$, where T_Λ is the map (18)–(19) on the Banach space $\mathcal{K}_{\lambda,\Lambda}$ of collections $\{v_I\in\mathcal{H}_I'\cap\mathrm{Dom}\,(H_{I,0})\}_{\varnothing\neq I\subset\Lambda}$, equipped with the norm (22). This map is a contraction in the unit ball in $\mathcal{K}_{\lambda,\Lambda}$ and has a unique fixed point $\{v_I^{(\Lambda,gs)}\}_{\varnothing\neq I\subset\Lambda}$ there.

In fact, one can consider the Kirkwood–Thomas equation for an arbitrary, not necessarily finite, subset of $\mathbb{Z}^\nu$, and in particular for $\mathbb{Z}^\nu$ itself. Namely, let $\mathcal{K}_{\lambda,\infty}$ be the Banach space of collections $\{v_I \in \mathcal{H}_I' \cap \mathrm{Dom}\,(H_{I,0})\}_{\varnothing \neq I \subset \mathbb{Z}^\nu}$ with I running over the finite subsets of $\mathbb{Z}^\nu$. The norm is defined as in (22), but with $\sup_{x\in\mathbb{Z}^\nu}$ instead of $\max_{x\in\Lambda}$ and with summation extended to all finite $I \ni x$. The map T_∞ can be defined by

$$T_\infty(\{v_I\}_{\varnothing\neq I\subset\mathbb{Z}^\nu}) := \left\{ \lim_{\Lambda \nearrow \mathbb{Z}^\nu} u_I^{(\Lambda)} \right\}_{\varnothing\neq I\subset\mathbb{Z}^\nu},$$

where

$$\{u_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda} := T_\Lambda(\{v_I\}_{\varnothing\neq I\subset\Lambda}).$$

Alternatively, one can define T_∞ directly, using the commutator expansion (23) with the summation extended to all finite subsets. Conditions (30), (31) and uniform bounds derived in the previous section ensure that T_∞ is well-defined and is a contraction in the unit ball of $\mathcal{K}_{\lambda,\infty}$. The corresponding Kirkwood–Thomas equation $T_\infty(\{v_I\}_{\varnothing\neq I\subset\mathbb{Z}^\nu}) = \{v_I\}_{\varnothing\neq I\subset\mathbb{Z}^\nu}$ then has there a unique solution, which we will denote by $\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\mathbb{Z}^\nu}$. We begin by proving that the finite volume solutions converge to this infinite volume solution.

Lemma 1: Let $\tilde{d}_{I;\Lambda^c}$ be the minimal length of a connected graph containing I and at least one point of $\Lambda^c := \mathbb{Z}^\nu \setminus \Lambda$. There exists $\tilde{c} = \tilde{c}(\lambda, \Lambda_0) > 0$ such that if $\sup_x \|\phi_x\| < \tilde{c}$ then for any finite Λ,

$$\max_{x\in\Lambda} \sum_{I\subset\Lambda : I\ni x} \|H_{I,0}(v_I^{(\Lambda,gs)} - v_I^{(\infty,gs)})\| \lambda^{\tilde{d}_{I;\Lambda^c}+1} \leqslant 1.$$

In particular, for any I,

$$v_I^{(\Lambda,gs)} \overset{\Lambda\nearrow\mathbb{Z}^\nu}{\longrightarrow} v_I^{(\infty,gs)}.$$

Proof: Let $\Delta v_I^{(\Lambda)} := v_I^{(\Lambda,gs)} - v_I^{(\infty,gs)}$ for $\varnothing \neq I \subset \Lambda$. Then the collection $\{\Delta v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda}$ satisfies the fixed point equation,

$$\{\Delta v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda} = T_{\Lambda;\Lambda^c}(\{\Delta v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda}), \tag{52}$$

where the map $T_{\Lambda;\Lambda^c}$ on $\mathcal{K}_{\lambda,\Lambda}$ is defined by

$$T_{\Lambda;\Lambda^c}(\{v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda}) := T_\Lambda(\{v_I^{(\infty,gs)} + v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda}) - \{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\Lambda}. \tag{53}$$

Let us introduce a new norm $\|\cdot\|_{\lambda,\Lambda;\Lambda^c}$ in $\mathcal{K}_{\lambda,\Lambda}$ by

$$\|\{v_I\}_{\varnothing\neq I\subset\Lambda}\|_{\lambda,\Lambda;\Lambda^c} := \max_{x\in\Lambda} \sum_{I\subset\Lambda : I\ni x} \|H_{I,0} v_I\| \lambda^{\tilde{d}_{I;\Lambda^c}+1}.$$

This new norm is clearly equivalent to the old norm $\|\cdot\|_{\lambda,\Lambda}$, defined by (22). We will prove that $T_{\Lambda;\Lambda^c}$ is a contraction in the unit ball in $\mathcal{K}_{\lambda,\Lambda}$ wrt this new norm, if $\sup_x \|\phi_x\| < \tilde{c}$ with some $\tilde{c} = \tilde{c}(\lambda, \Lambda_0)$ (there is no loss of generality in this assumption, since c_1 in the hypothesis of Theorem 1 can be taken smaller).

Indeed, for any two collections $\{u_I\}, \{v_I\} \in \mathcal{K}_{\lambda,\Lambda}$ by (53) we have

$$\|T_{\Lambda;\Lambda^c}(\{u_I\}) - T_{\Lambda;\Lambda^c}(\{v_I\})\|_{\lambda,\Lambda;\Lambda^c} = \|T_\Lambda(\{v_I^{(\infty,gs)} + u_I\}_{\varnothing\neq I\subset\Lambda}) - T_\Lambda(\{v_I^{(\infty,gs)} + v_I\}_{\varnothing\neq I\subset\Lambda})\|_{\lambda,\Lambda;\Lambda^c}.$$

We can estimate this norm in the same way as we estimated $\|T_\Lambda(\{u_I\})-T_\Lambda(\{v_I\})\|_{\lambda,\Lambda}$ in the previous section; the only difference is the factor $\lambda^{\tilde{d}_{I;\Lambda^c}+1}$ instead of λ^{d_I+1} in the definition of the norm. So instead of (34) we use the inequality

$$\tilde{d}_{I;\Lambda^c}\leqslant\tilde{d}_{(\cup_{s=1}^k I_s)\cup(\Lambda_0+y);\Lambda^c}\leqslant\tilde{d}_{I_l;\Lambda^c}+\sum_{s\neq l} d_{I_s}+d_{\Lambda_0}.$$

As a result we arrive at the following analog of (41):

$$\|T_{\Lambda;\Lambda^c}(\{u_I\})-T_{\Lambda;\Lambda^c}(\{v_I\})\|_{\lambda,\Lambda;\Lambda^c}\leqslant\sum_{k=1}^{\infty}\frac{k+|\Lambda_0|}{(k-1)!}|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_x\|\phi_x\|\|\{u_I-v_I\}\|_{\lambda,\Lambda;\Lambda^c}$$
$$\times(\max(\|\{v_I^{(\infty,gs)}+u_I\}\|_{\lambda,\Lambda},\|\{v_I^{(\infty,gs)}+v_I\}\|_{\lambda,\Lambda}))^{k-1}. \quad (54)$$

Suppose that $\|\{u_I\}\|_{\lambda,\Lambda;\Lambda^c}\leqslant 1$ and $\|\{v_I\}\|_{\lambda,\Lambda;\Lambda^c}\leqslant 1$. From the inequalities $\|\cdot\|_{\lambda,\Lambda}\leqslant\|\cdot\|_{\lambda,\Lambda;\Lambda^c}$ and $\|\{v_I^{(\infty,gs)}\}\|_{\lambda,\Lambda}\leqslant 1$ we see that $\max(\cdots)\leqslant 2$ in (54). It follows that if $\sup_x\|\phi_x\|<\tilde{c}$, where

$$\tilde{c}=\frac{1}{2}\left(\sum_{k=1}^{\infty}\frac{k+|\Lambda_0|}{(k-1)!}|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{2k-1+|\Lambda_0|}\right)^{-1},$$

then

$$\|T_{\Lambda;\Lambda^c}(\{u_I\})-T_{\Lambda;\Lambda^c}(\{v_I\})\|_{\lambda,\Lambda;\Lambda^c}\leqslant\tfrac{1}{2}\|\{u_I-v_I\}\|_{\lambda,\Lambda;\Lambda^c}.$$

Now let us estimate $\|T_{\Lambda;\Lambda^c}(\{0\})\|_{\lambda,\Lambda;\Lambda^c}$, which equals

$$\|T_\Lambda(\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\Lambda})-\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\Lambda}\|_{\lambda,\Lambda;\Lambda^c}. \quad (55)$$

Recall that $\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\mathbb{Z}^\nu}=T_\infty(\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\mathbb{Z}^\nu})$; so the norm (55) can be estimated by expanding $T_\infty(\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\mathbb{Z}^\nu})$ and $T_\Lambda(\{v_I^{(\infty,gs)}\}_{\varnothing\neq I\subset\Lambda})$ into commutator series in $P_I[\cdots[\phi_x,\hat{v}_{I_1}^{(\infty,gs)}],\ldots,\hat{v}_{I_k}^{(\infty,gs)}]\Omega_{\Lambda,0}$ and comparing the resulting terms. Clearly, the expansion for T_∞ contains that for T_Λ; the extra terms are those for which $I_t\not\subset\Lambda$ for some t. For such I_t we have $\tilde{d}_{I_t;\Lambda^c}=d_{I_t}$ and hence we can write

$$\tilde{d}_{I;\Lambda^c}\leqslant\sum_{s=1}^{k} d_{I_s}+d_{\Lambda_0},$$

instead of (34). Repeating again the estimates of the previous section, we find

$$\|T_{\Lambda;\Lambda^c}(\{0\})\|_{\lambda,\Lambda;\Lambda^c}\leqslant\sum_{k=1}^{\infty}\frac{k+|\Lambda_0|}{(k-1)!}|\Lambda_0|^k\lambda^{d_{\Lambda_0}}2^{k+|\Lambda_0|}\sup_x\|\phi_x\|,$$

which is less than 1/2 if $\sup_x\|\phi_x\|<\tilde{c}$.

Hence $T_{\Lambda;\Lambda^c}$ is a contraction in the $\|\cdot\|_{\lambda,\Lambda;\Lambda^c}$-unit ball and Eq. (52) has a unique solution there. It only remains to check that this solution is the same as $\{\Delta v_I^{(\Lambda)}\}_{\varnothing\neq I\subset\Lambda}$. This again follows by a continuity argument. Consider, as before, the family $H_\Lambda^{(\delta)}=H_{\Lambda,0}+\delta\Phi_\Lambda$, $\delta\in[0,1]$. As is easy to see, both $\{\Delta v_I^{(\delta,\Lambda)}\}_{\varnothing\neq I\subset\Lambda}$ and the above-mentioned solution continuously depend on δ; since they are equal for $\delta=0$, they are equal for all δ. □

The remaining part of the proof is quite analogous to the standard cluster expansion for Gibbs fields and our exposition will be sketchy.

Let A act on $\mathcal{H}_\Lambda$; then, by definition,

$$\omega_\Lambda(A)=\frac{(A\tilde\Omega_\Lambda,\tilde\Omega_\Lambda)}{\|\tilde\Omega_\Lambda\|^2}.$$

First consider the "partition function" $Z_\Lambda:=\|\tilde\Omega_\Lambda\|^2$. We have

$$Z_\Lambda=\left\|\exp\left(\sum_{\varnothing\neq I\subset\Lambda}\hat v_I^{(\Lambda,gs)}\right)\Omega_{\Lambda,0}\right\|^2=1+\sum_{\varnothing\neq I\subset\Lambda}\left\|\sum_{\{I_1,\dots,I_k\}\in\mathcal{P}(I)}\otimes_{s=1}^k v_{I_s}^{(\Lambda,gs)}\right\|^2.$$

For any $\Lambda_1\subset\Lambda$, set

$$Z_{\Lambda_1}^{(\Lambda)}:=1+\sum_{\varnothing\neq I\subset\Lambda_1}\left\|\sum_{\{I_1,\dots,I_k\}\in\mathcal{P}(I)}\otimes_{s=1}^k v_{I_s}^{(\Lambda,gs)}\right\|^2.$$

In particular $Z_\Lambda^{(\Lambda)}=Z_\Lambda, Z_\varnothing^{(\Lambda)}=1$. Then for any nonempty $\Lambda_1\subset\Lambda$ and any $x\in\Lambda_1$,

$$Z_{\Lambda_1}^{(\Lambda)}=Z_{\Lambda_1\setminus\{x\}}^{(\Lambda)}+\sum_{\Lambda_2\subset\Lambda_1:\Lambda_2\ni x}K_{\Lambda_2}^{(\Lambda)}Z_{\Lambda_1\setminus\Lambda_2}^{(\Lambda)},\tag{56}$$

where

$$K_{\Lambda_2}^{(\Lambda)}:=\sum_{\substack{\{I_1,\dots,I_k\},\{J_1,\dots,J_l\}\in\mathcal{P}(\Lambda_2):\\ \{I_1,\dots,I_k,J_1,\dots,J_l\}\text{conn.}}}(\otimes_{s=1}^k v_{I_s}^{(\Lambda,gs)},\otimes_{t=1}^l v_{J_t}^{(\Lambda,gs)}),\tag{57}$$

and summation in the last formula is over *connected* double partitions of Λ_2, i.e., such that the collection $\{I_1,\dots,I_k,J_1,\dots,J_l\}$ cannot be decomposed into two non-empty subcollections, whose unions do not overlap. Now suppose that A acts on $\mathcal{H}_{\Lambda_1}$ and $\varnothing\neq\Lambda_1\subset\Lambda$. Then

$$\omega_\Lambda(A)=\sum_{\Lambda_2\subset\Lambda\setminus\Lambda_1}M_{A,\Lambda_1,\Lambda_2}^{(\Lambda)}\frac{Z_{\Lambda\setminus(\Lambda_1\sqcup\Lambda_2)}^{(\Lambda)}}{Z_\Lambda},\tag{58}$$

where

$$M_{A,\Lambda_1,\Lambda_2}^{(\Lambda)}:=\sum_{\Lambda_3,\Lambda_4\subset\Lambda_1}\sum_{\substack{\{I_1,\dots,I_k\}\in\mathcal{P}(\Lambda_2\sqcup\Lambda_3),\\ \{J_1,\dots,J_l\}\in\mathcal{P}(\Lambda_2\sqcup\Lambda_4):\\ \{I_1,\dots,I_k,J_1,\dots,J_l,\Lambda_1\}\text{conn.}}}(A\otimes_{s=1}^k v_{I_s}^{(\Lambda,gs)},\otimes_{t=1}^l v_{J_t}^{(\Lambda,gs)}).$$

Lemma 2 (cluster estimates): If $\lambda\geqslant 2$ *and* $\sup_x\|\phi_x\|<c_1(\lambda,\Lambda_0)$, *then for any* $x\in\Lambda$,

$$\sum_{\Lambda_1\ni x}|K_{\Lambda_1}^{(\Lambda)}|\lambda^{d_{\Lambda_1}+1}\leqslant 1,\tag{59}$$

and for any $\varnothing\neq\Lambda_1\subset\Lambda$ *and* $A\in\mathcal{B}(\mathcal{H}_{\Lambda_1})$,

$$\sum_{\Lambda_2\subset\Lambda\setminus\Lambda_1}|M_{A,\Lambda_1,\Lambda_2}^{(\Lambda)}|\lambda^{d_{\Lambda_1\sqcup\Lambda_2}}\leqslant c_{\Lambda_1}\|A\|,\tag{60}$$

with some constant c_{Λ_1}.

Proof: We will prove (59); (60) is analogous. All the connected double partitions of finite sets containing x can be uniquely generated by a successive choice of I's and J's as follows. For any

nonempty $I\subset\mathbb{Z}^\nu$ fix some $x(I)\in I$. Choose $I_1\ni x$. Then proceed by induction. Suppose we have already chosen a connected family $\{I_1,\ldots,I_k,J_1,\ldots,J_l\}$ such that the I's are mutually disjoint, and the J's are mutually disjoint. Set

$$\Lambda^{(k+l)}:=[(\sqcup_{n=1}^k I_n)\setminus(\sqcup_{n=1}^l J_n)]\sqcup[(\sqcup_{n=1}^l J_n)\setminus(\sqcup_{n=1}^k I_n)]$$

and consider two possibilities.

(1) $\Lambda^{(k+l)}=\varnothing$. Then the family $\{I_1,\ldots,I_k,J_1,\ldots,J_l\}$ forms a connected double partition of some set containing x.

(2) $\Lambda^{(k+l)}\neq\varnothing$. Then consider $x(\Lambda^{(k+l)})$. If $x(\Lambda^{(k+l)})\in(\sqcup_{n=1}^k I_n)\setminus(\sqcup_{n=1}^l J_n)$; then choose J_{l+1} such that $J_{l+1}\ni x(\Lambda^{(k+l)})$ and $J_{l+1}\cap(\sqcup_{n=1}^l J_n)=\varnothing$. Otherwise, if $x(\Lambda^{(k+l)})\in(\sqcup_{n=1}^l J_n)\setminus(\sqcup_{n=1}^k I_n)$, choose I_{k+1} such that $I_{k+1}\ni x(\Lambda^{(k+l)})$ and $I_{k+1}\cap(\sqcup_{n=1}^k I_n)=\varnothing$. Then repeat the inductive step.

Clearly, all the connected double partitions of finite sets containing x can be obtained in this way. Now we bound the scalar product in (57) by $\Pi_{s=1}^k\|v_{I_s}^{(\Lambda,gs)}\|\Pi_{t=1}^l\|v_{J_t}^{(\Lambda,gs)}\|$. If $\{I_1,\ldots,I_k,J_1,\ldots,J_l\}$ is a connected double partition of Λ_1, then $d_{\Lambda_1}\leqslant\Sigma_{s=1}^k d_{I_s}+\Sigma_{t=1}^l d_{J_t}$. It follows that

$$\sum_{\Lambda_1\ni x}|K_{\Lambda_1}^{(\Lambda)}|\lambda^{d_{\Lambda_1}+1}\leqslant\lambda\sum_{n=2}^{\infty}\left(\max_y\sum_{I\ni y}\|v_I^{(\Lambda,gs)}\|\lambda^{d_I}\right)^n$$

(n is the number of elements in a double partition). Using the bound (14) and the inequality $\lambda\geqslant 2$, we find

$$\sum_{\Lambda_1\ni x}|K_{\Lambda_1}^{(\Lambda)}|\lambda^{d_{\Lambda_1}+1}\leqslant\lambda\sum_{n=2}^{\infty}\lambda^{-n}=\frac{1}{\lambda-1}\leqslant 1.$$

□

The desired convergence of $\omega_\Lambda(A)$ follows now for sufficiently large λ from the expansions (56), (58), cluster estimates and Lemma 1 by standard arguments.[11]

IV. PROOF OF THEOREM 3

We introduce the commutative subalgebras $\mathcal{U}_\Lambda,\mathcal{U}_\infty$, generated by the creation operators:

$$\mathcal{U}_\Lambda:=\left\{\sum_{I\subset\Lambda}\hat{u}_I\,\middle|\,u_I\in\mathcal{H}_I'\right\},\quad|\Lambda|<\infty,$$

$$\mathcal{U}_\infty:=\bigcup_{|\Lambda|<\infty}\mathcal{U}_\Lambda.$$

Note that if $A\in\mathcal{U}_\Lambda$, then $\|A\|=\|A\Omega_{\Lambda,0}\|$.

Lemma 3: (a) If $A\in\mathcal{U}_\infty$ and $A\neq 0$, then $\pi_\infty(A)\Omega_\infty\neq 0$.

(b) The set $\pi_\infty(\mathcal{U}_\infty)\Omega_\infty$ is dense in $\mathcal{H}_\infty$.

Proof: (a) Let $A\in\mathcal{U}_\Lambda$; then for any $\Lambda_1\supset\Lambda$ by the commutativity

$$\|A\Omega_{\Lambda_1}\|=\frac{\|A\tilde{\Omega}_{\Lambda_1}\|}{\|\tilde{\Omega}_{\Lambda_1}\|}=\frac{\left\|\exp\left(\sum_{\substack{I\subset\Lambda_1:\\ I\cap\Lambda\neq\varnothing}}\hat{v}_I^{(\Lambda_1,gs)}\right)A\exp\left(\sum_{\substack{I\subset\Lambda_1\setminus\Lambda:\\ I\neq\varnothing}}\hat{v}_I^{(\Lambda_1,gs)}\right)\Omega_{\Lambda_1,0}\right\|}{\left\|\exp\left(\sum_{\substack{I\subset\Lambda_1:\\ I\cap\Lambda\neq\varnothing}}\hat{v}_I^{(\Lambda_1,gs)}\right)\exp\left(\sum_{\substack{I\subset\Lambda_1\setminus\Lambda:\\ I\neq\varnothing}}\hat{v}_I^{(\Lambda_1,gs)}\right)\Omega_{\Lambda_1,0}\right\|}.\tag{61}$$

It follows from the bound (14) that

$$\left\| \exp\left(\pm \sum_{\substack{I\subset\Lambda_1:\\ I\cap\Lambda\neq\varnothing}} \hat{v}_I^{(\Lambda_1,gs)} \right) \right\| \leqslant \exp\left(|\Lambda| \sup_x \sum_{I\ni x} \|v_I^{(\Lambda_1,gs)}\| \right) \leqslant e^{|\Lambda|},$$

and hence

$$(61) \geqslant e^{-2|\Lambda|} \frac{\left\| A \exp\left(\sum_{\substack{I\subset\Lambda_1\setminus\Lambda:\\ I\neq\varnothing}} \hat{v}_I^{(\Lambda_1,gs)} \right) \Omega_{\Lambda_1,0} \right\|}{\left\| \exp\left(\sum_{\substack{I\subset\Lambda_1\setminus\Lambda:\\ I\neq\varnothing}} \hat{v}_I^{(\Lambda_1,gs)} \right) \Omega_{\Lambda_1,0} \right\|} = e^{-2|\Lambda|} \|A\Omega_{\Lambda,0}\| = e^{-2|\Lambda|} \|A\|.$$

Taking the limit $\Lambda_1 \nearrow \mathbb{Z}^\nu$, we find

$$\|\pi_\infty(A)\Omega_\infty\|^2 = \omega_\infty(A^*A) = \lim_{\Lambda_1\nearrow\mathbb{Z}^\nu} \omega_{\Lambda_1}(A^*A) = \lim_{\Lambda_1\nearrow\mathbb{Z}^\nu} \|A\Omega_{\Lambda_1}\|^2 \geqslant e^{-4|\Lambda|}\|A\|^2.$$

(b) Let $A \in \mathcal{A}_\Lambda$, then $A\Omega_\Lambda = \Sigma_{I\subset\Lambda} \hat{u}_I^{(\Lambda)} \Omega_\Lambda$, where

$$u_I^{(\Lambda)} = P_I^{(\Lambda)} \exp\left(- \sum_{\varnothing\neq I\subset\Lambda} \hat{v}_I^{(\Lambda,gs)} \right) A \exp\left(\sum_{\varnothing\neq I\subset\Lambda} \hat{v}_I^{(\Lambda,gs)} \right) \Omega_{\Lambda,0}$$

[see (43)]. Fix A and let $\Lambda \nearrow \mathbb{Z}^\nu$; expanding the rhs and using Lemma 1, one finds that there exist limits,

$$u_I^{(\infty)} := \lim_{\Lambda\nearrow\mathbb{Z}^\nu} u_I^{(\Lambda)},$$

and then, using Theorem 2,

$$A\Omega_\infty = \sum_{I\subset\mathbb{Z}^\nu} \hat{u}_I^{(\infty)} \Omega_\infty,$$

with an absolutely convergent series on the rhs. In particular, it follows that $\pi_\infty(\mathcal{U}_\infty)\Omega_\infty$ is dense in $\mathcal{A}_\infty\Omega_\infty$ and hence in $\mathcal{H}_\infty$. □

Recall that for the renormalized Hamiltonian $\tilde{H}_\Lambda$ in a finite volume Λ we had the decomposition $\tilde{H}_\Lambda = \tilde{H}_{\Lambda,0} + \tilde{\Phi}_\Lambda$, where $\mathrm{Dom}(\tilde{H}_\Lambda) = \{\Sigma_{I\subset\Lambda} \hat{u}_I \Omega_\Lambda | u_I \in \mathcal{H}_I' \cap \mathrm{Dom}(H_{I,0})\}$, and on this domain,

$$\tilde{H}_{\Lambda,0}\left(\sum_{I\subset\Lambda} \hat{u}_I\Omega_\Lambda \right) = \sum_{I\subset\Lambda} \widehat{H_{I,0}u_I}\Omega_\Lambda,$$

$$\tilde{\Phi}_\Lambda\left(\sum_{I\subset\Lambda} \hat{u}_I\Omega_\Lambda \right) = \sum_{I\subset\Lambda} \sum_{J\subset\Lambda} \widehat{(F_\Lambda u_I)_J}\Omega_\Lambda$$

[see (44)–(47)]. Using the expansion (47) and Lemma 1, we find that there exist the limits

$$(F_\infty u_I)_J := \lim_{\Lambda\nearrow\mathbb{Z}^\nu} (F_\Lambda u_I)_J,$$

and, moreover,

$$\sum_{J\subset\mathbb{Z}^\nu} \|(F_\infty u_I)_J\| \leqslant c_2 \sup_x \|\phi_x\| \|H_{I,0}u_I\|, \tag{62}$$

as in (49).

Now we can define the limiting Hamiltonian H_∞. First we define it on the subspace $\mathcal{D}\subset\mathcal{H}_\infty$, consisting of vectors of the form $\pi_\infty(\Sigma_I \hat{u}_I)\Omega_\infty$, where the sum is finite and $u_I \in \mathcal{H}_I' \cap \mathrm{Dom}\,(H_{I,0})$ for all I; then we will take the closure. On the domain $\mathcal{D}$ we set

$$H_\infty|_{\mathcal{D}} := H_{\infty,0} + \Phi_\infty,$$

where

$$H_{\infty,0}\pi_\infty\left(\sum_I \hat{u}_I\right)\Omega_\infty := \pi_\infty\left(\sum_I \widehat{H_{I,0}u_I}\right)\Omega_\infty,$$

$$\Phi_\infty\pi_\infty\left(\sum_I \hat{u}_I\right)\Omega_\infty := \pi_\infty\left(\sum_I \sum_{J\subset\mathbb{Z}^\nu} (\widehat{F_\infty u_I})_J\right)\Omega_\infty.$$

Operator $H_\infty|_{\mathcal{D}}$ is well-defined by Lemma 3(a) and inequality (62). Using Theorem 2 and the symmetricity of the finite-volume Hamiltonians $\tilde{H}_\Lambda$, one deduces that $H_\infty|_{\mathcal{D}}$ is symmetric. Now let H_∞ be the closure of $H_\infty|_{\mathcal{D}}$. First we prove that it is self-adjoint. Let $z\in\mathcal{O}_\infty := \cap_\Lambda \mathcal{O}_\Lambda$, where $\mathcal{O}_\Lambda$ is defined in (50). Then for any $u\in\pi_\infty(\mathcal{U}_\infty)\Omega_\infty$, using inequality (62) and arguing as in the proof of Theorem 1, we see that one can form the series

$$S_{\mathbb{Z}^\nu}(z)u = (H_{\infty,0}-z)^{-1}\sum_{k=0}^{\infty}(-\Phi_\infty(H_{\infty,0}-z)^{-1})^k u, \tag{63}$$

defining an element of $\mathcal{H}_\infty$. The closedness of H_∞ then implies that $S_{\mathbb{Z}^\nu}(z)u\in\mathrm{Dom}\,(H_\infty)$ and $(H_\infty - z)S_{\mathbb{Z}^\nu}(z)u = u$. Since $\pi_\infty(\mathcal{U}_\infty)\Omega_\infty$ is dense in $\mathcal{H}_\infty$ by Lemma 3(b), it follows that $\mathrm{Ran}\,(H_\infty - z) = \mathcal{H}_\infty$ and hence H_∞ is self-adjoint with the series (63) being its resolvent for $u \in \pi_\infty(\mathcal{U}_\infty)\Omega_\infty$ and $z\in\mathcal{O}_\infty\cap(\mathbb{C}\backslash\mathbb{R})$. But the expression (63) is analytic in z in $\mathcal{O}_\infty$ and hence the spectral measure for such u is supported on $\mathbb{R}\backslash\mathcal{O}_\infty$ (this follows, e.g., from Stone's resolvent formula for spectral projectors). By the density of such u's, we conclude that $\mathrm{Sp}\,(H_\infty)\subset\mathbb{R}\backslash\mathcal{O}_\infty$, which is the desired spectral localization estimate.

Now suppose that $A\in\mathcal{U}_\infty$ and $z\in\mathcal{O}_\infty$. Then for any Λ large enough, expressing the resolvent via $S_\Lambda(z)$ and using the expansions for $S_\Lambda, \tilde{\Phi}_\Lambda$, we can find $A_\Lambda\in\mathcal{U}_\Lambda$ such that $(\tilde{H}_\Lambda - z)^{-1}A\Omega_\Lambda = A_\Lambda\Omega_\Lambda$. Since the expansion for $\tilde{\Phi}_\Lambda$ converges to that for Φ_∞, there exists $A_\infty = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} A_\Lambda$, and $(H_\infty - z)^{-1}\pi_\infty(A)\Omega_\infty = \pi_\infty(A_\infty)\Omega_\infty$. It follows then by Theorem 2 that for any $B\in\mathcal{A}_\infty$,

$$((\tilde{H}_\Lambda - z)^{-1}A\Omega_\Lambda, B\Omega_\Lambda) = \omega_\Lambda(B^*A_\Lambda) \overset{\Lambda\nearrow\mathbb{Z}^\nu}{\longrightarrow} \omega_\infty(B^*A_\infty) = ((H_\infty - z)^{-1}\pi_\infty(A)\Omega_\infty, \pi_\infty(B)\Omega_\infty). \tag{64}$$

Since $\pi_\infty(\mathcal{U}_\infty)\Omega_\infty$ is dense in H_∞, this convergence extends to all $A\in\mathcal{A}_\infty$. Finally, the extension to $z\in\mathbb{C}\backslash\mathbb{R}$ follows by Vitali's theorem.

It only remains to show that 0 as an eigenvalue of H_∞ is nondegenerate. Since it is a nondegenerate eigenvalue of $\tilde{H}_\Lambda$ in any finite volume Λ, for any $A\in\mathcal{B}(\mathcal{H}_\Lambda)$ we have

$$(Q_\Lambda A\Omega_\Lambda, A\Omega_\Lambda) = |(A\Omega_\Lambda, \Omega_\Lambda)|^2, \tag{65}$$

where Q_Λ is the projector onto $\mathrm{Ker}\,(\tilde{H}_\Lambda)$ in $\mathcal{H}_\Lambda$. Let γ be a contour in $\mathcal{O}_\infty$, surrounding 0; then by the Cauchy formula $Q_\Lambda = -(2\pi i)^{-1}\int_\gamma(\tilde{H}_\Lambda - z)^{-1}\,dz$ we can use (64) to take the limit $\Lambda\nearrow\mathbb{Z}^\nu$ in (65) and write

$$(Q_\infty\pi_\infty(A)\Omega_\infty, \pi_\infty(A)\Omega_\infty) = |(\pi_\infty(A)\Omega_\infty, \Omega_\infty)|^2,$$

where Q_∞ is the projector onto Ker (H_∞) in $\mathcal{H}_\infty$. Hence, Ker (H_∞) contains only multiples of Ω_∞.

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Histories electromagnetism

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Working within the HPO (History Projection Operator) Consistent Histories formalism, we follow the work of Savvidou on (scalar) field theory [J. Math. Phys. **43**, 3053 (2002)] and that of Savvidou and Anastopoulos on (first-class) constrained systems [Class. Quantum Gravt. **17**, 2463 (2000)] to write a histories theory (both classical and quantum) of Electromagnetism. We focus particularly on the foliation-dependence of the histories phase space/Hilbert space and the action thereon of the two Poincaré groups that arise in histories field theory. We quantize in the spirit of the Dirac scheme for constrained systems. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1723702]

I. INTRODUCTION

Our aim in this paper is to demonstrate the application of certain ideas and techniques that have been developed within the HPO (History Projection Operator) histories formalism over recent years to the theory of Electromagnetism. Specifically, we follow up on two pieces of work which are naturally combined therein:

Field theory. In Ref. 1, Savvidou describes the histories theory of the (classical and quantum) scalar field. This has the important feature that there exist two distinct Poincaré groups. The ''internal'' group is simply the histories analog of that of the standard theory, but there also exists an ''external'' group that explicitly performs changes of the foliation. This is important as it provides a way of relating quantities that are defined with respect to different foliations. These groups arise as a consequence of one of the most powerful and interesting features of histories theories, namely that there exist two distinct types of time transformation each of which represents a distinct *quality* of time: (a) the internal time (''time of becoming''), which is related to the dynamics of the particular system in question, and (b) the external time (''time of being''), which is related to the causal ordering of events, i.e., the kinematics. (For a detailed exposition of the HPO continuous time histories program, the reader is referred to Ref. 2.)

Constrained systems. In Ref. 3, Savvidou and Anastopoulos describe an algorithm for working with systems with first-class constraints within the HPO formalism. They focused specifically on parametrized systems, i.e., those systems whose Hamiltonian is itself a first-class constraint, as a natural precursor to understanding ''histories'' general relativity, and demonstrated that the histories on the reduced phase space *retained* their intrinsic temporal ordering. The quantization algorithm is in the spirit of the Dirac scheme for constrained systems. (For progress with this enterprise, see Refs. 4–6.)

The theory of Electromagnetism, as a field theory with first-class constraints, thus perfectly combines the above pieces of work, but also brings something new to each when studied within the histories framework. In the first instance we shall see explicitly how the histories phase space and reduced phase space depend on the foliation and discuss the importance of the external boost in this respect. Second, we will have to deal with the fact (not tackled in detail in Ref. 3) that our constraints have continuous spectra, and thus the physical Hilbert space cannot be a true linear subspace of the full (unconstrained) Hilbert space.

The outline of the paper is as follows: in Sec. II we give a brief account of those aspects of the

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Histories program most relevant to our needs, and then we present the histories theory of Electromagnetism, starting with the classical theory in Sec. III, and then its quantization in Sec. IV. We conclude in Sec. V.

Finally we note that the classical history theory of vector fields has been studied by Noltingk[7] as well as their BRST quantization,[8] though he follows a fundamentally different approach which centers on defining five component vector fields to incorporate the two times.

II. THE HISTORIES PROGRAM

The consistent histories version of quantum mechanics was originally developed in the 1980s by Griffiths[9] and then built on (each with different emphases) by Omnès[10] and then Gell-Mann and Hartle[11] and Hartle.[12] The main aim (particularly of the latter) was to develop a quantum mechanics of closed systems.

As formulated by Gell-Mann and Hartle, a history, α, is represented by a class operator, C_α, that is a product of Heisenberg picture projection operators. Dynamic information is contained in the decoherence functional, defined on a pair of histories as

$$d(\alpha,\beta)=\mathrm{tr}(C_\alpha^\dagger \rho_0 C_\beta), \tag{2.1}$$

where ρ_0 is the density matrix describing the initial state of the system. If a history is part of a ''consistent'' set, then probabilities (in the usual Kolmogorov sense) may be assigned to the individual histories according to $p(\alpha)=d(\alpha,\alpha)$.

The HPO formalism was developed initially by Isham[13] and Isham and Linden[14] who sought a histories version of single-time quantum logic. To this end they re-defined the class operator as a *tensor* product of *Schrödinger* picture operators, so it would be a genuine projection operator on some suitable ''history'' Hilbert space. This formalism was extended to the case of continuous time histories by Isham and co-workers,[15,16] in which the ''history group''—analogous to the usual Heisenberg–Weyl group—was introduced. However, this structure lacked any clear notion of time evolution. It was only with Savvidou's introduction of the action operator—the quantum analog of the classical Hamilton–Jacobi action functional—that the temporal structure of histories theory was established in the form as it is used now (see Ref. 17). It is these two—the history group and action operator—that are the key elements of any history theory.

A. The history group

By introducing the history group, a HPO theory may be seen as seeking a suitable representation of a certain algebra, e.g., for a (nonrelativistic) particle moving on the real line (see Ref. 2) and a continuous time label, $t\in\mathbb{R}$, the (nonzero) commutation relation is ($\hbar=1$)

$$[x_t,p_{t'}]=i\delta(t-t'). \tag{2.2}$$

This algebra is isomorphic to that of a field theory in one spatial dimension, and field-theoretic techniques are usefully employed to find a suitable representation. Following Araki,[18] the proper representation of this algebra is selected by requiring that the Hamiltonian exist as a self-adjoint operator, and it will come as no surprise that a Fock representation provides the necessary ''history'' Hilbert space.

In histories quantum scalar field theory (see Ref. 1), after foliating Minkowski space with a unit timelike vector, n_μ, we have

$$[\phi(X),\pi(X')]=i\delta^4(X-X'), \tag{2.3}$$

where we are using a ''pseudo-covariant'' notation $X=n\cdot t+x_n$ (x_n is a four vector such that $n\cdot x_n=0$). [We use the metric signature $(+,-,-,-)$.] A representation of this algebra is found in terms of creation and annihilation, $b^\dagger(X)$ and $b(X)$, on the (history) Fock space, $\mathcal{V}_{\mathrm{scalar}}=\exp(L^2(\mathbb{R}^4,d^4X))$. Indeed, it is found that all foliation dependent representations exist *on the same* Fock space.

B. The action operator

The other key element of a histories theory is the action operator, $S(\gamma)$ (see Ref. 17). It is this that is the generator of time transformations of a HPO theory, combining the Liouville operator, $V(\gamma)$, which generates time translations in the external (kinematical) time label, and the Hamiltonian, $H(\gamma)$, which generates time translations in the internal (dynamical) time label. For our nonrelativistic particle, the action would be written as

$$S(\gamma)=V(\gamma)-H(\gamma)=\int dt[p_t\dot{x}_t-H_t(p_t,x_t)](\gamma), \tag{2.4}$$

where H_t is a one parameter family of Hamiltonians.

In the field theory case, we have two Poincaré groups, with the Hamiltonian being the time translations generator of the internal group, and the Liouville being the time translations generator of the external group. The generators of the internal group are time-averaged versions of the generators of the standard group, but it is the external group that is the novel object, as the boost of this group generates *changes of the foliation* as well. Its action on the foliation-dependent scalar field is given by

$$^{\text{ext}}U(\Lambda)^n\phi(X)^{\text{ext}}U(\Lambda)^{-1}=^{\Lambda n}\phi(\Lambda^{-1}X) \tag{2.5}$$

[where $U(\Lambda)$ is the unitary operator that generates the Lorentz transformation] and thus we have a way of relating quantities defined with respect to different foliations.

Finally, we note, without going into great detail, that there is an analogous formalism for classical histories which we will use to write the classical history theory of EM below (see Chap. 5 of Ref. 2 for further details). This involves thinking of a history as a map from the real line into the classical phase space, Γ. A natural symplectic structure can be defined on Π (the history phase space), giving rise to the Poisson algebra. The equations of motion can be expressed by saying that, for any function F on Π, their solutions, γ_{cl}, will satisfy

$$\{F,S\}(\gamma_{\text{cl}}) = 0. \tag{2.6}$$

C. The constrained systems algorithm

The theory of constrained systems was extensively studied by Dirac,[19] though we primarily use Refs. 20 and 21. In essence, a first-class constraint, $\phi(x,p)=0$, is to be seen as a generator of gauge transformations which partitions the phase space, Γ (and, thus, the constraint surface) into orbits. The reduced phase space, Γ_{red}, is then isomorphic to the space of orbits. There exists a unique "reduction" of a function F on Γ to a function $\tilde{F}$ on Γ_{red} if F has a weakly vanishing Poisson bracket with the constraint. Dirac quantization proceeds by constructing the unconstrained Hilbert space, $\mathcal{H}$, writing the constraint as an operator, and then defining the physical Hilbert space as that linear subspace (modulo considerations of the constraint spectrum) of $\mathcal{H}$ which is spanned by those eigenvectors of the constraint whose corresponding eigenvalue is zero.

In histories theory[3] we write the (time-averaged) constraint as $\Phi_\lambda(\gamma)=\int dt\,\lambda(t)\phi(x_t,p_t)\times(\gamma)$. As above, the action of the constraint will partition Π (the history phase space) into orbits, and we can define Π_{red} (the reduced phase space) as the space of equivalence classes of histories on the constraint surface, C_h. (Histories will be equivalent if they lie on the same orbit.) Again, there will be a unique "reduction" of any function, F, on Π to a function, $\tilde{F}$, on Π_{red} if $\{F,\Phi_\lambda\}\approx 0$.

The quantization algorithm for a histories theory follows the spirit of the Dirac scheme, briefly described above. It is implemented, once the constraint is suitably defined as an operator, by first observing that we require

$$d(e^{i\Phi_\lambda}\alpha e^{-i\Phi_\lambda},e^{i\Phi_\lambda}\beta e^{-i\Phi_\lambda})=d(\alpha,\beta). \tag{2.7}$$

To meet this requirement (modulo, as above, issues concerning the nature of the constraint spectrum) we define a projector, E, onto the closed linear subspace of the (unconstrained) history space, $\mathcal{V}$, corresponding to the zero eigenvalue of Φ_λ and then substitute α for $E\alpha E$ in the expression for the decoherence functional (evidently $e^{i\Phi_\lambda}E=E$).

We are now in a position to put these ideas into practice, writing the classical histories theory of Electromagnetism in the next section, and its quantization in the subsequent one.

III. ELECTROMAGNETISM—CLASSICAL

We begin with a brief review of the standard theory.

A. Basics

The EM Action is

$$S=-\frac{1}{4}\int d^4x \;\; F_{\mu\nu}F^{\mu\nu}, \tag{3.1}$$

where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$. The equations of motion are computed from setting $\delta S=0$, and we get

$$\partial^\mu F_{\mu\nu}=0. \tag{3.2}$$

To write this in Hamiltonian form we first define the momentum conjugate to the vector potential:

$$\pi^\mu=\frac{\delta L}{\delta \dot{A}_\mu}=F^{\mu 0}. \tag{3.3}$$

So $\pi^i=\partial^i A^0-\partial^0 A^i=-[(\nabla A^0)^i+\dot{A}^i]=(\underline{E})_i$, and we have the following constraints:

$$\pi^0=0 \tag{3.4}$$

(this is a primary, first-class constraint), and the Gauss Law constraint (this is a secondary, first-class constraint),

$$\partial_i\pi^i=0, \tag{3.5}$$

derived from the consistency condition that the primary constraint be conserved in time, i.e., $\{H,\pi^0\}=0$ (where H is the canonical Hamiltonian given below). In terms of the observable fields, $\underline{E}$ and $\underline{B}=\nabla\times\underline{A}$ the canonical Hamiltonian is written as

$$H=\int d^3x \;\; \left(\frac{1}{2}\underline{E}^2+\frac{1}{2}\underline{B}^2-A^0\nabla\cdot\underline{E}\right). \tag{3.6}$$

1. Poincaré invariance in the standard theory

The generators of the Poincaré group of the standard theory are ''taken over'' (in time-averaged form) to the histories theory as the ''internal'' group. Following Ref. 22, these are derived from the energy–momentum tensor (to which a total divergence has to be added):

$$\tilde{\Theta}^{\mu\nu}=-F^{\mu\rho}\partial^\nu A_\rho+\tfrac{1}{4}\eta^{\mu\nu}F^2+\partial_\rho(F^{\mu\rho}A^\nu). \tag{3.7}$$

The ten generators of the Poincaré group are then written as

$$P^\alpha=\int d^3x \;\; \tilde{\Theta}^{0\alpha}, \tag{3.8}$$

$$M^{\alpha\beta}=\int d^3x\ \ (x^{\alpha}\tilde{\Theta}^{0\beta}-x^{\beta}\tilde{\Theta}^{0\alpha}). \tag{3.9}$$

From these, we deduce the explicit, canonical form of the Hamiltonian, linear momentum, angular momentum and boost generators to be, respectively,

$$H=\int d^3x\left(-\frac{1}{2}\pi_i\pi^i+\frac{1}{2}(\nabla\times\underline{A})^2-A^0\partial_i\pi^i\right), \tag{3.10}$$

$$P_i=\int d^3x\,\pi^j\,\partial_iA_j\,, \tag{3.11}$$

$$J^i=\epsilon^{ijk}\int d^3x(\pi^lx_j\,\partial_kA_l+\pi_jA_k), \tag{3.12}$$

$$K_i=\int d^3x-x_i\left(-\frac{1}{2}\pi_j\pi^j+\frac{1}{2}(\nabla\times\underline{A})^2-A^0\,\partial_j\pi^j\right) \tag{3.13}$$

(where we have chosen $x^0=0$ in the expression for the boost). This algebra closes only weakly, i.e., subject to the Gauss Law constraint, a fact that will be of significance when we come to the quantization.

We now turn to the histories formulation of classical electromagnetism.

B. The histories phase space, Π

The phase space of canonical EM is $\Gamma=(A_i(\underline{x}),\pi_j(\underline{x}))$, and a history is defined to be a path:

$$\gamma:\mathbb{R}\rightarrow\Gamma, \tag{3.14}$$

$$t\mapsto(A_i(t,\underline{x}),\pi_j(t,\underline{x})). \tag{3.15}$$

The space of histories, Π, is defined to be the space of all such smooth paths γ. As explained before we can use a ''covariant-like'' notation, writing $X=n\cdot t+x_n$ where n_μ is a unit time-like vector, so $t=n\cdot X$ and x_n is ''n-spatial,'' i.e., $n\cdot x_n=0$.

However, we wish to find a representation of the time-averaged canonical expressions on the phase space coordinated by $(A_\mu(X),\pi^\nu(X))$. This is so we can write a representation of both the internal *and* external groups on the same space. This is achieved using the n-spatial projector, $P_{\mu\nu}$, introduced earlier, along with the foliating timelike vector, n_μ. In this notation, we write the foliation dependent (canonical) fields ${}^nA_\mu:=P^\nu_\mu A_\nu$ (and likewise for the conjugate momenta). The Hamiltonian is written as

$$H_n=\int d^4X\ \ \left(\frac{1}{2}[P^{\mu\nu}\pi_\mu\pi_\nu+(\nabla^\mu_\sigma A^\sigma)(\nabla_{\mu\delta}A^\delta)]+n^\rho A_\rho P^{\mu\nu}\,\partial_\mu\pi_\nu\right)\chi(n\cdot X) \tag{3.16}$$

(where the subscript ''n'' refers to the particular foliation, and we have introduced the notation $\nabla_{\mu\sigma}A^\sigma\equiv\epsilon_{\mu\nu\rho\sigma}n^\nu\,\partial^\rho A^\sigma$). This is the generator of time translations of the internal group. We then define the Liouville operator (the generator of time translations in the external group):

$$V_n=\int d^4X\ \ \pi^\mu n^\rho\,\partial_\rho A_\mu\,, \tag{3.17}$$

and thus can write the action functional:

$$S_n=V_n-H_n\,. \tag{3.18}$$

It is the action functional that is to be understood as the ''true'' generator of time translations of the theory, naturally intertwining the two modes of time represented by the Hamiltonian and Liouville operators. The fundamental Poisson brackets are now

$$\{A_\mu(X),A_\nu(Y)\}=0=\{\pi^\mu(X),\pi^\nu(Y)\} \tag{3.19}$$

and

$$\{A_\mu(X),\pi^\nu(Y)\}=\delta^\nu_\mu\delta^4(X-Y). \tag{3.20}$$

We now turn to the central issue of Poincaré invariance.

C. The Poincaré groups

As was the case for the scalar field, we seek representations for two Poincaré groups on the history space: one associated with the internal time label, and one associated with the external time label. The generators for spatial translations and spatial rotations will be the same for each group, so we focus our attentions on the time translation and boost generators in each case.

1. The internal Poincaré group

The generators of the internal Poincaré group will be time-averaged versions of the generators of the standard theory [Eqs. (3.10)–(3.13)]. The time translation generator is, of course, just the Hamiltonian of Eq. (3.16) and we define the boost at $s=0$ as

$$^{\text{int}}K(m)=-m_\mu\int d^4X\ \ X^\mu\left(\frac{1}{2}[P^{\mu\nu}\pi_\mu\pi_\nu+(\nabla^\mu_\sigma A^\sigma)(\nabla_{\mu\delta}A^\delta)]+n^\rho A_\rho P^{\mu\nu}\partial_\mu\pi_\nu\right), \tag{3.21}$$

where m_μ is a space-like vector, i.e., $n\cdot m=0$, parametrizing the boost. Given a function A on Π, we can denote the one parameter group of transformations it generates as $s\mapsto T_A(s)$ and its action on the algebra of functions, B, as

$$T_A(s)[B]=\sum_n\frac{s^n}{n!}\underbrace{\{A,\{A,\ldots\{A}_{n\text{-times}},B\ldots.\}\} \tag{3.22}$$

So, we first define the classical analog of the Heisenberg picture fields by

$$T_{\text{H}}(s)[^nA_\mu(X)]=^nA_\mu(X,s), \tag{3.23}$$

$$T_{\text{H}}(s)[^n\pi^\mu(X)]=^n\pi^\mu(X,s), \tag{3.24}$$

and can now see explicitly the sense in which the Hamiltonian generates time translations in the internal time label by looking at its action on the ''Heisenberg'' picture fields:

$$T_{\text{H}}(\tau)[^nA_\mu(X,s)]=^nA_\mu(X,s+\tau), \tag{3.25}$$

$$T_{\text{H}}(\tau)[^n\pi^\mu(X,s)]=^n\pi^\mu(X,s+\tau). \tag{3.26}$$

The internal boost generator will mix the internal time parameter, ''s,'' with the spatial coordinates

$$T_{\text{int}_{K(m)}}[^nA_\mu(X,s)]=^nA_\mu(\Lambda^{-1}(X,s)), \tag{3.27}$$

$$T_{\text{int}_{K(m)}}[^n\pi^\mu(X,s)]=^n\pi^\mu(\Lambda^{-1}(X,s)), \tag{3.28}$$

where $\Lambda^{-1}(X,s)$ is related to (X,s) (the time label "t" is, of course, constant) by the Lorentz boost parametrized by m^μ, i.e., the velocity of the moving frame is given by

$$v^i = c\frac{\tanh|m|m^i}{|m|}. \tag{3.29}$$

2. The external Poincaré group

In contrast to the definition of the generators of the internal group, we use the covariant fields, $(A_\mu(X),\pi^\mu(X))$ in the definition of the generators for the external Poincaré group. These are

$$P^\mu = \int d^4X \;\; \pi^\nu \partial^\mu A_\nu \tag{3.30}$$

and

$$M^{\mu\nu} = \int d^4X[\,\pi^\rho(X^\mu\partial^\nu - X^\nu\partial^\mu)A_\rho] + \sigma^{\mu\nu}, \tag{3.31}$$

where $\sigma^{\mu\nu}$ is the spin term, given by

$$\sigma^{\mu\nu} = \int d^4X(\pi^\mu A^\nu - \pi^\nu A^\mu). \tag{3.32}$$

As before, we are particularly interested in the actions of the time translation generator $V = P^0$ and the boosts generator $K(m) = n_\mu m_\nu M^{\mu\nu}$. These are therefore written as

$$V = \int d^4X \;\; \pi^\mu n^\nu \partial_\nu A_\mu \tag{3.33}$$

and

$${}^{\text{ext}}K(m) = m_\mu \int d^4X[(n\cdot X)\pi^\nu \partial^\mu A_\nu - X^\mu \pi^\rho n^\nu \partial_\nu A_\rho] + n_\mu m_\nu \sigma^{\mu\nu}. \tag{3.34}$$

The effect of the Liouville functional is to generate the following algebra automorphisms, in which we can clearly see that it generates time translation in the external time label:

$$T_V(\tau)[A_\mu(X,s)] = e^{-\tau n_\sigma \partial^\sigma} A_\mu(X,s) = A_\mu(X',s), \tag{3.35}$$

$$T_V(\tau)[\,\pi^\mu(X,s)] = e^{-\tau n_\sigma \partial^\sigma} \pi^\mu(X,s) = \pi^\mu(X',s), \tag{3.36}$$

where X' is the point in $\mathcal{M}$ associated with the pair $(\underline{x}, t+\tau)$.

Let us now turn to the transformations generated by the external boosts. These will mix the external time parameter, "t," with the spatial coordinates. The finite transformations can be written as

$$T_{\text{ext}_{K(m)}}[A_\mu(X,s)] = \Lambda_\mu^\nu A_\nu(\Lambda^{-1}(X),s), \tag{3.37}$$

$$T_{\text{ext}_{K(m)}}[\,\pi^\mu(X,s)] = \Lambda_\nu^\mu \pi^\nu(\Lambda^{-1}(X),s). \tag{3.38}$$

As previously stated, the role of the external group is an interesting one, and it is this that is one of the novel features of histories field theory. The effect of the external boosts is to mix the

spatial coordinate with the external time label "t" and, as the phase space has an implicit foliation dependence, it will also boost the foliation vector itself, thus generating transformations between different foliation-dependent representations.

D. The reduced phase space, Π_{red}

Our next task is to follow the algorithm of Ref. 3 to ascertain a suitable description of the reduced phase space, Π_{red}, on which the true degrees of freedom of the theory are defined. To this end, we are interested in the actions of the constraints on the phase space (and in particular the history constraint surface, C_h) because, by examining their action, we can define suitable coordinates (i.e., ones constant along the orbits) for the reduced phase space Π_{red}.

We write the time-averaged analogs of the constraints of the standard theory as follows:

$$\Psi_\lambda = \int d^4X \;\; \lambda(X) n_\mu \pi^\mu \approx 0, \tag{3.39}$$

$$\Phi_\lambda = \int d^4X \;\; \lambda(X) P^{\mu\nu} \partial_\mu \pi_\nu \approx 0, \tag{3.40}$$

and consider their action on the coordinates of Π. Under Ψ_λ we have

$$(A_\mu(X), \pi^\mu(X)) \rightarrow (A_\mu(X) - \lambda(X) n_\mu, \pi^\mu(X)). \tag{3.41}$$

Under Φ_λ we have

$$(A_\mu(X), \pi^\mu(X)) \rightarrow (A_\mu(X) + P^\rho_\mu \partial_\rho \lambda(X), \pi^\mu(X)). \tag{3.42}$$

Evidently $\pi^\mu(X)$ is constant along the orbits, so we just seek a quantity associated with the vector potential that is gauge invariant.

Equations (3.41) and (3.42) tell us that the transverse components of the vector potential remain constant along the orbits of the constraints and are thus good coordinates for Π_{red}, whereas the scalar and longitudinal components correspond to the degenerate directions of Ψ_λ and Φ_λ, respectively. (This state of affairs is more clearly seen if we use a Fourier transform and work in momentum space.) If we combine this knowledge with a look at the constraints themselves, which (if we were to Fourier transform them) readily show us that the constraint surface, C_h, is defined by $\pi^0 = \pi^L = 0$, where these are, respectively, the scalar and longitudinal components of the conjugate momentum, we can deduce that Π_{red} is suitably coordinated by $(A^\perp_\mu(X), \pi^\perp_\mu(X))$, where the superscript "$\perp$" indicates the transverse components, and these are defined by

$$A^\perp_\mu(X) = \left(\frac{{}^n\partial_\mu \, {}^n\partial^\nu}{{}^n\Delta} - P^\nu_\mu \right) A_\nu(X) \tag{3.43}$$

(and likewise for $\pi^\perp$) and where ${}^n\partial_\mu$ is shorthand for $P^\alpha_\mu \partial_\alpha$ and the (invertible) partial differential operator ${}^n\Delta$ is defined as

$$({}^n\Delta f_\rho)(X) = (P^{\mu\nu} \partial_\mu \partial_\nu) f_\rho(X). \tag{3.44}$$

The (nonzero) Poisson bracket relation on the reduced phase space is given by

$$\{A^\perp_\mu(X), \pi^{\perp\,\nu}(X')\} = T^\nu_\mu \delta^4(X - X'), \tag{3.45}$$

where

$$(T^\nu_\mu f_\nu)(X) \equiv \left(\frac{{}^n\partial_\mu \, {}^n\partial^\nu}{{}^n\Delta} - P^\nu_\mu \right) f_\mu(X). \tag{3.46}$$

We are now in a position to examine whether or not we can write a representation of the two Poincaré groups on Π_{red}.

E. The reduced Poincaré algebras

As explained in Sec. II C, for a function on the whole phase space to reduce to a corresponding function on the reduced phase space, it is necessary that its Poisson bracket with the constraints is weakly zero. We expect to find that the generators of the *internal* Poincaré group reduce to Π_{red}. However, we do not expect to find a full representation of the *external* Poincaré group on the reduced phase space. In Ref. 1 the foliation dependence of the phase space was emphasized but not explicit. In the case of EM we shall see this dependence explicitly as the action of the external boost will affect the definition of Π_{red} and so we do not expect to find a reduced version of this generator. We now turn to the explicit results.

As before, we are only interested in the time translation and boost generators of each Poincaré group and thus we need only compute the Poisson brackets of S, ${}^{\text{int}}K(m)$ and ${}^{\text{ext}}K(m)$ with the constraints. We find the following results (recall that Ψ_λ is the "π^0" constraint and Φ_λ the Gauss Law constraint):

$$\{S,\Psi_\lambda\}=\Psi_{\dot{\lambda}}-\Phi_\lambda\approx 0 \tag{3.47}$$

and

$$\{S,\Phi_\lambda\}=\Phi_{\dot{\lambda}}\approx 0. \tag{3.48}$$

So the action functional weakly commutes with both constraints and so can be reduced to a functional $\tilde{S}$ acting on Π_{red}.

The internal boost generator has the following Poisson brackets with the constraints:

$$\{{}^{\text{int}}K(m),\Psi_\lambda\}=\Phi_{-m_\alpha X^\alpha\lambda}\approx 0 \tag{3.49}$$

and

$$\{{}^{\text{int}}K(m),\Phi_\lambda\}=0. \tag{3.50}$$

This in line with what we expected, i.e., that the generators of the internal Poincaré group commute with the constraints and thus we have a representation of the internal group on Π_{red}. (Of course, something would be quite amiss if we did not have this as the internal group is the histories analog of the Poincaré group of standard Maxwell theory.)

The external boost generator forms the following Poisson brackets with the constraints:

$$\{{}^{\text{ext}}K(m),\Psi_\lambda\}=\Psi_{(n_\beta X^\beta m_\alpha\partial^\alpha-m_\beta X^\beta n_\alpha\partial^\alpha)\lambda}-\int d^4X\ \ \lambda(X)m_\alpha\pi^\alpha \tag{3.51}$$

and

$$\{{}^{\text{ext}}K(m),\Phi_\lambda\}=\Psi_{m_\alpha\partial^\alpha\lambda}+\int d^4X(n_\alpha\partial^\alpha\lambda(X))m_\beta\pi^\beta. \tag{3.52}$$

Neither of these are weakly zero, and so the external boost generator cannot be reduced to Π_{red}.

For those functions that *can* be reduced, we use the coordinates for the reduced phase space that we worked out in the previous section. The Hamiltonian and Liouville functionals on the reduced phase space are written as follows:

$$\tilde{H}=\int d^4X\frac{1}{2}(\pi^{\perp\mu}\pi^{\perp}_{\mu}+A^{\perp n}_{\mu}\,\Delta A^{\perp\mu}), \tag{3.53}$$

$$\tilde{V}=\int d^4X \;\; \pi^{\perp\mu} n_\nu \partial^\nu A^\perp_\mu, \tag{3.54}$$

where we have used, in the expression for the Hamiltonian,

$$A_\mu \, {}^n\Gamma^{\mu\nu} A_\nu = A^\perp_\mu \, {}^n\Delta A^{\perp\mu}, \tag{3.55}$$

with ${}^n\Delta$ defined in Eq. (3.44). Thus the action functional on Π_{red} is written as

$$\tilde{S}=\tilde{V}-\tilde{H}, \tag{3.56}$$

and the classical paths which are solutions to the equations of motion are those which satisfy

$$\{\tilde{S},\tilde{F}\}(\gamma_{\text{cl}})=0, \tag{3.57}$$

for all functions $\tilde{F}$ defined on Π_{red}.

IV. ELECTROMAGNETISM—QUANTIZATION

For the quantization of the theory we continue to follow the algorithm laid down by Savvidou and Anastopolous, which, as outlined in Sec. II C, essentially follows the Dirac scheme. We define the history space, $\mathcal{V}$, by consideration of the history group, and define the constraints thereon. However, as we mentioned, the constraints have continuous spectra, and thus the physical Hilbert space, $\mathcal{V}_{\text{phys}}$, will not be a genuine subspace of the history Hilbert space. This will be explicitly demonstrated. And so we are led to a creative implementation of the algorithm (the central idea here is due to Savvidou[25]), in which the physical Hilbert space is defined separately, based on an analysis, in terms of coherent states, of how the constraints act on $\mathcal{V}$. Appropriate mappings are then defined between $\mathcal{V}$ and $\mathcal{V}_{\text{phys}}$ such that objects on one can be related to objects on the other.

A. The History Hilbert space $\mathcal{V}$

So the first stage is to define the History Hilbert space. Following the methods of Refs. 15 and 1, we start by defining the History Algebra:

$$[A_\mu(X),A_\nu(X')]=0, \tag{4.1}$$

$$[\pi_\mu(X),\pi_\nu(X')]=0, \tag{4.2}$$

$$[A_\mu(X),\pi^\nu(X')]=i\,\delta^\nu_\mu\delta^4(X-X'), \tag{4.3}$$

or, in its more rigorous, smeared form:

$$[A_\mu(f^\mu),A_\nu(f'^\nu)]=0, \tag{4.4}$$

$$[\pi_\mu(h^\mu),\pi_\nu(h'^\nu)]=0, \tag{4.5}$$

$$[A_\mu(f^\mu),\pi^\nu(h_\nu)]=i\int \; d^4X\; \delta^\nu_\mu f^\mu(X) h_\nu(X), \tag{4.6}$$

where $f^\mu(X)$, $h_\mu(X)$ are elements of a suitable space of smearing functions which we will leave unspecified beyond saying that it must at least be a subspace of $\oplus_{i=1\cdots4} L^2_{\mathbb{R}}(\mathbb{R}^4,d^4X)_i$. Let us denote this space $\mathcal{T}_{\mathbb{R}}$. It is natural to seek a Fock representation of this algebra, and this is achieved by first taking the complexification of the space of smearing functions, i.e., $\mathcal{T}_{\mathbb{C}}=\mathcal{T}_{\mathbb{R}}\oplus\mathcal{T}_{\mathbb{R}}$ and then exponentiating the resulting space to give $\mathcal{V}=e^{\mathcal{T}_{\mathbb{C}}}$. The Fock space thus defined will carry a natural representation of the above History Algebra, which we seek explicitly below, in terms of creation and annihilation operators:

$$[b_\mu(X), b^{\dagger\nu}(X)] = \delta_\mu^\nu \delta^4(X - X'). \tag{4.7}$$

1. The representation of (A, π) in terms of $(b^\dagger, b)$

We can easily write a representation of the fully covariant fields $(A_\mu(X), \pi^\mu(X))$:

$$A_\mu(X) = \frac{1}{\sqrt{2}}(b_\mu(X) + b_\mu^\dagger(X)), \tag{4.8}$$

$$\pi_\mu(X) = -\frac{i}{\sqrt{2}}(b_\mu(X) - b_\mu^\dagger(X)). \tag{4.9}$$

However, what we require in order to define the Hamiltonian is foliation-dependent fields. So we start from a normal-ordered analog of the classical unconstrained Hamiltonian:

$${}^nH =: \frac{1}{2}\int d^4X (P^{\mu\nu\,n}\pi_\mu\,{}^n\pi_\nu + {}^nA_\mu\,{}^n\Gamma^{\mu\nu\,n}A_\nu): \tag{4.10}$$

and may think, at first, to define

$${}^nA_\mu(X) = \frac{1}{\sqrt{2}}({}^n\Gamma^\nu_\mu)^{-1/4}(b_\nu(X) + b_\nu^\dagger(X)), \tag{4.11}$$

$${}^n\pi_\mu(X) = -\frac{i}{\sqrt{2}}({}^n\Gamma^\nu_\mu)^{1/4}(b_\nu(X) - b_\nu^\dagger(X)). \tag{4.12}$$

However, there is a problem here, as the operator $\Gamma^{\mu\nu}$ has zero eigenvalues, and is, therefore, not invertible. To see this, it is easier to use ''canonical notation,'' i.e., $\Gamma^{ij} = \partial^i\partial^j - \delta^{ij}\partial_k\partial^k$. We then examine the action of this operator on an element, $f_i(x)$, of the smearing function space—which we split into its transverse and longitudinal components, $f_i = f_i^\perp + f_i^\parallel$—and find

$$\Gamma^{ij}f_i(x) = \Gamma ij(f_i^\perp(x) + f_i^\parallel(x)) = \Gamma^{ij}f_i^\perp(x). \tag{4.13}$$

So the longitudinal components of the smearing functions are the zero eigenvectors of Γ^{ij}. If we now split the Hamiltonian into its transverse and longitudinal parts, we find (reverting to the full ''histories'' notation, and dropping the n superscript for ease),

$$H = \frac{1}{2}\int d^4X (\pi_\mu^\perp\pi^{\perp\mu} + A_\mu^\perp\,{}^n\Delta A^{\perp\mu} + \pi_\mu^\parallel\pi^{\parallel\mu}), \tag{4.14}$$

where the operator ${}^n\Delta$ was defined in Eq. (3.44). And now we see that the transverse part of the Hamiltonian is, in essence, that of the usual ''harmonic oscillators,'' whereas the longitudinal part is that of a ''free particle.'' This form now prompts us towards the correct definition of the fields in terms of the creation and annihilation operators:

$${}^nA_\mu(X) = \frac{1}{\sqrt{2}}\,{}^n\Delta^{-1/4}(b_\mu(X) + b_\mu^\dagger(X)), \tag{4.15}$$

$${}^n\pi_\mu(X) = -\frac{i}{\sqrt{2}}\,{}^n\Delta^{1/4}(b_\mu(X) - b_\mu^\dagger(X)). \tag{4.16}$$

Now, on the one hand, we can consider the Fock space in terms of the orthonormal basis obtained by a continual application of the creation operator on a translationally invariant vacuum state (defined by $b_\mu|0\rangle=0$). However, it has also proved very useful to consider the Fock space in terms of coherent states—indeed, in Ref. 15, these were vital to the demonstration that there exists a natural isomorphism between an exponential Hilbert space and the ''continuous tensor product'' of Hilbert spaces so vital to the Histories program. In the next section, we make use of the technology of coherent states (an excellent reference is Ref. 23) as we seek to define the Physical Hilbert space.

B. The Physical Hilbert space $\mathcal{V}_{\text{phys}}$

Recall that the constraints are written as

$$\Psi_\lambda=\int d^4X\ \ \lambda(X)n_\mu\pi^\mu, \tag{4.17}$$

$$\Phi_\lambda=\int d^4X\ \ \lambda(X)P^{\mu\nu}\partial_\mu\pi_\nu. \tag{4.18}$$

Substituting for the fields in terms of the creation and annihilation operators, these become

$$\Psi_\lambda=\frac{-i}{2}\int d^4X\ \ \lambda(X)n_\mu{}^n\Delta^{1/4}(b^\mu-b^{\dagger\mu}), \tag{4.19}$$

$$\Phi_\lambda=\frac{-i}{2}\int d^4X\ \ \lambda(X)P^{\mu\nu}\partial_\mu{}^n\Delta^{1/4}(b_\nu-b^\dagger_\nu). \tag{4.20}$$

It is clear that these constraints are self-adjoint operators on $\mathcal{V}$, and also that they have continuous spectra, so the physical Hilbert space will not be a genuine subspace. However, by consideration of the Fock space, $\mathcal{V}$, in terms of coherent states we are led naturally to the correct definition of $\mathcal{V}_{\text{phys}}$, and explicitly show in what sense the latter is not a true subspace of the former.

The Weyl operator which generates the (overcomplete) set of coherent states is written as

$$U[f,h]=\exp[i({}^nA_\mu(f^\mu)-{}^n\pi_\nu(h^\nu))]|0\rangle, \tag{4.21}$$

$$=\exp[b^\dagger_\mu(z^\mu)-b_\mu(z^{*\mu})]|0\rangle, \tag{4.22}$$

with $z_\mu(X)=(1/\sqrt{2})\,({}^n\Delta^{1/4}h_\mu(X)+i\,{}^n\Delta^{-1/4}f_\mu(X))$. The un-normalized coherent states on $\mathcal{V}$ are defined for each $z^\mu(X)\in\mathcal{T}_{\mathbb{C}}$ as

$$|\exp z\rangle=e^{b^\dagger_\mu(z^\mu)}|0\rangle. \tag{4.23}$$

Their overlap is given by

$$\langle\exp z|\exp z'\rangle=e^{\langle z,z'\rangle} \tag{4.24}$$

[where the inner product is $\langle z,z'\rangle=\int d^4Xz^*_\mu(X)z'^\mu(X)$] and there exists a measure, $d\sigma[z]$, such that

$$1=\int|\exp z\rangle\langle\exp z|d\sigma[z]. \tag{4.25}$$

(That this measure exists was demonstrated in Ref. 15.) With the aid of this resolution of unity, we can thus define an integral representation of $\mathcal{V}$ in terms of wave functionals, $\psi[z]$:

$$|\psi\rangle = \int |\exp z\rangle\langle \exp z|\psi\rangle d\sigma[z] = \int \psi[z]|\exp z\rangle d\sigma[z]. \tag{4.26}$$

Furthermore, we can write a differential representation of a general operator, O on $\mathcal{V}$:

$$\langle \exp z|:O(b_\mu^\dagger, b_\mu):|\psi\rangle = O\left(z_\mu^*, \frac{\delta}{\delta z_\mu^*}\right)\psi[z]. \tag{4.27}$$

Given this last construction, we can now rewrite the constraint operators as follows:

$$\langle \exp z|\Psi_\lambda|\psi\rangle = \int d^4X g_\mu\left(\frac{\delta}{\delta z^{*\mu}} - z^{*\mu}\right)\psi[z] \tag{4.28}$$

[where $g_\mu(X) = (-i/2)\lambda(X)\,{}^n\Delta^{1/4} n_\mu$] and, similarly,

$$\langle \exp z|\Phi_\lambda|\psi\rangle = \int d^4X w_\mu\left(\frac{\delta}{\delta z^{*\mu}} - z^{*\mu}\right)\psi[z] \tag{4.29}$$

[where $w_\mu(X) = (i/2)P_\mu^\nu \partial_\nu \lambda(X)\,{}^n\Delta^{1/4}$].

So now we can consider the action of the constraints on a general wave functional $\psi[z]$, finding

$$e^{i\Psi_\lambda}\psi[z] = e^{-(1/2)\langle g,g\rangle - i\langle z,g\rangle}\psi[z+ig], \tag{4.30}$$

and, similarly,

$$e^{i\Phi_\lambda}\psi[z] = e^{-(1/2)\langle w,w\rangle - i\langle z,w\rangle}\psi[z+iw]. \tag{4.31}$$

We can now explicitly see that $\mathcal{V}_{\text{phys}}$ will not be a subspace of $\mathcal{V}$ as we require the subspace to be invariant under the action of the constraints, and are thus essentially looking for solutions to the pair of equations

$$\psi[z] = \psi[z+ig], \tag{4.32}$$

$$\psi[z] = \psi[z+iw]. \tag{4.33}$$

The solutions to these will be $\psi[z^\perp]$, where $z_\mu^\perp(X)$ are only the transverse components of $z_\mu(x)$ defined as

$$z_\mu^\perp(X) = \left(\frac{{}^n\partial_\mu\,{}^n\partial^\nu}{{}^n\Delta} - P_\mu^\nu\right) z_\nu(X) \tag{4.34}$$

(where ${}^n\partial_\mu$ is just shorthand for $P_\mu^\rho\partial_\rho$). However, it is clear that the corresponding wave-functionals, $\psi[z^\perp]$, will not be square integrable. To see this, we need only consider $\int\int\int |\psi[z^\perp]|^2 d\sigma[z^\perp]d\sigma[z^0]d\sigma[z^\parallel]$ which will be infinite on account of the contributions from the integrations over the scalar and longitudinal parts. This leads us to the conclusion that what we need to do is to construct the physical Hilbert space *separately* so that the wave-functionals, $\psi[z^\perp]$, *are* square-integrable, and then define a suitable mapping from $\mathcal{V}$ to $\mathcal{V}_{\text{phys}}$.

Equipped with what we know from the classical theory, and what we have ascertained from the analysis above, we construct $\mathcal{V}_{\text{phys}}$ in the usual way—first by positing the algebra

$$[A_\mu(f^{\perp\mu}), A_\nu(f'^{\perp\nu})] = 0, \tag{4.35}$$

$$[\pi_\mu(h^{\perp\mu}), \pi_\nu(h'^{\perp\nu})] = 0, \tag{4.36}$$

$$[A_\mu(f^{\perp\mu}),\pi^\nu(h^\perp_\nu)]=i\int d^4X\ \delta^\nu_\mu f^{\perp\mu}(X)h^\perp_\nu(X), \tag{4.37}$$

where the smearing functions belong to $\mathcal{T}^\perp_{\mathbb{R}}=L^2_{\mathbb{R}}(\mathbb{R}^4,d^4X)\oplus L^2_{\mathbb{R}}(\mathbb{R}^4,d^4X)$. We then take the complexification of this space $\mathcal{T}^\perp_{\mathbb{C}}=\mathcal{T}^\perp_{\mathbb{R}}\oplus\mathcal{T}^\perp_{\mathbb{R}}$ and exponentiate the resulting space to give $\mathcal{V}_{\text{phys}}=e^{\mathcal{T}^\perp_{\mathbb{C}}}$. We can then write a representation of the transverse fields in terms of the creation and annihilation operators of this Fock space:

$${}^nA^\perp_\mu(X)=\frac{1}{\sqrt{2}}{}^n\Delta^{-1/4}(b^\perp_\mu(X)+b^{\perp\dagger}_\mu(X)), \tag{4.38}$$

$${}^n\pi^\perp_\mu(X)=-\frac{i}{\sqrt{2}}{}^n\Delta^{1/4}(b^\perp_\mu(X)-b^{\perp\dagger}_\mu(X)), \tag{4.39}$$

where

$$[b_\mu(z^{\perp\mu}),b^{\dagger\nu}(z'^\perp_\nu)]=\langle z^\perp,z'^\perp\rangle, \tag{4.40}$$

and $z^\perp_\mu(X)=(1/\sqrt{2})\,({}^n\Delta^{1/4}h^\perp_\mu(X)+i\,{}^n\Delta^{-1/4}f^\perp_\mu(X))$.

In direct analogy to $\mathcal{V}$, we can consider $\mathcal{V}_{\text{phys}}$ in terms of the un-normalized coherent states defined by

$$|\exp z^\perp\rangle_{\mathcal{V}_{\text{phys}}}=e^{b^\mu(z^\perp_\mu)}|0\rangle, \tag{4.41}$$

and these will admit a resolution of unity:

$$1=\int|\exp z^\perp\rangle\langle\exp z^\perp|d\sigma[z^\perp], \tag{4.42}$$

and thus an integral representation for $|\psi\rangle\in\mathcal{V}_{\text{phys}}$:

$$|\psi\rangle=\int\psi[z^\perp]|\exp z^\perp\rangle_{\mathcal{V}_{\text{phys}}}d\sigma[z^\perp]. \tag{4.43}$$

We now define a mapping between $\mathcal{V}$ and $\mathcal{V}_{\text{phys}}$:

$$L:\mathcal{V}\to\mathcal{V}_{\text{phys}},$$

$$|\exp z\rangle_{\mathcal{V}}\mapsto L(|\exp z\rangle_{\mathcal{V}})\equiv|\exp z^\perp\rangle_{\mathcal{V}_{\text{phys}}}, \tag{4.44}$$

where $|\exp z^\perp\rangle_{\mathcal{V}_{\text{phys}}}$ is defined as in Eq. (4.41). We define the (continuous) dual mapping:

$$L^\dagger:\mathcal{V}^*_{\text{phys}}\to\mathcal{V}^* \tag{4.45}$$

by

$${}_{\mathcal{V}_{\text{phys}}}\langle\exp z^\perp|L^\dagger|\exp w\rangle_{\mathcal{V}}={}_{\mathcal{V}_{\text{phys}}}\langle\exp z^\perp|L|\exp w\rangle_{\mathcal{V}}. \tag{4.46}$$

We can now use these maps (and the fact that, due to the Riesz Lemma (see, e.g., Ref. 24), there is an isomorphism between a Hilbert space, $\mathcal{H}$, and the space of continuous linear functionals, $\mathcal{H}^*$, from $\mathcal{H}$ to $\mathbb{C}$) to relate objects on $\mathcal{V}_{\text{phys}}$ to objects on $\mathcal{V}$:

$$b_{\mathcal{V}_{\text{phys}}}=Lb_{\mathcal{V}}L^\dagger. \tag{4.47}$$

Having now established the relationship between the ''full'' Hilbert space, $\mathcal{V}$, and the ''physical'' Hilbert space, $\mathcal{V}_{\rm phys}$, we can now turn to the issue of Poincaré invariance and use Eq. (4.47) to define the action operator on $\mathcal{V}_{\rm phys}$.

C. The Poincaré groups

In the case of classical histories electromagnetism, we proved the existence of the two Poincaré groups on the histories phase space, Π, and analyzed their ''reduction'' to the reduced phase space, $\Pi_{\rm red}$, by considering their compatibility with the constraints. We demonstrated the existence of the internal group on Π, finding that the algebra closed only weakly, i.e., was only satisfied on the constraint surface. We then proved the existence of a ''reduced'' internal Poincaré group on $\Pi_{\rm red}$, with the generators written in terms of the transverse components of the fields. We also demonstrated the existence of the external Poincaré on Π, but found that the external boost generator did not commute with the constraints, and thus could not be represented on $\Pi_{\rm red}$. This, as we shall see in greater detail in the quantum case below, results from the fact that Π and $\Pi_{\rm red}$ are foliation dependent, and that the external boost boosts the foliation vector as well. So let us now discuss the issue of Poincaré invariance in the quantum theory.

1. The internal Poincaré group

Our starting point for the internal Poincaré group is (a normal ordered version of) the unconstrained Hamiltonian given in Sec. IV A 1 and repeated here:

$$H=\frac{1}{2}:\int d^4X(\pi_\mu^\perp\pi^{\perp\mu}+A_\mu^{\perp\ n}\Delta A^{\perp\mu}+\pi_\mu^\parallel\pi^{L\mu}):. \tag{4.48}$$

In terms of the creation and annihilation operators [Eqs. (4.38)–(4.39)], this reads as

$$H=\int d^4X\left[b_\mu^{\perp\dagger\ n}\Delta^{1/2}b^{\perp\mu}-\frac{1}{4}((b_\mu^\parallel-b_\mu^{\parallel\dagger})^n\Delta^{1/2}(b^{\parallel\mu}-b^{\parallel\dagger\mu}))\right]. \tag{4.49}$$

However, while the transverse part can easily be shown to exist in the usual way, the longitudinal part does not generate automorphisms which are unitarily implementable on account of the presence of terms quadratic in b_μ and $b_\mu^\dagger$. And so the Hamiltonian does not exist on $\mathcal{V}$ as a self-adjoint operator. Of course, this is no tragedy and we half-expected it anyway as we had already seen in the classical case that the algebra of the internal group closed only weakly.

What is important is that a representation of the internal group can be found on $\mathcal{V}_{\rm phys}$. This is straightforward. The generators are taken straight from the classical case, suitably ordered and then written in terms of $b_\mu^\perp$ and $b_\mu^{\perp\dagger}$ using Eqs. (4.38)–(4.39). They are

$$\tilde{H}=\int d^4Xb_\mu^{\perp\dagger\ n}\Delta^{1/2}b^{\perp\mu}, \tag{4.50}$$

$$\tilde{P}(m)=im_\nu\int d^4Xb_\mu^{\perp\dagger}\,\partial^\nu b^{\perp\mu}, \tag{4.51}$$

$$\tilde{J}(m)=i\epsilon_{\mu\nu\rho\sigma}n^\mu m^\nu\int d^4X(b_\alpha^{\perp\dagger}X^\rho\,\partial^\sigma b^{\perp\alpha}+b^{\perp\dagger\rho}b^{\perp\sigma}), \tag{4.52}$$

$$\tilde{K}(m)=m_\nu\int d^4Xb_\mu^{\perp\dagger\ n}\Delta^{1/4}X^{\nu\ n}\Delta^{1/4}b^{\perp\mu}, \tag{4.53}$$

where we have used an obvious shorthand for operators on $\mathcal{V}_{\rm phys}$ [see Eq. (4.47)], i.e.,

$$b^{\perp\mu}\equiv b^\mu_{\mathcal{V}_{\rm phys}}=Lb^\mu_{\mathcal{V}}L^\dagger. \tag{4.54}$$

The analysis of this group is essentially the same as the classical case. We define the Heisenberg picture fields:

$$b_\mu^\perp(X,s)=e^{is\tilde{H}}b_\mu^\perp(X)e^{-is\tilde{H}}, \tag{4.55}$$

$$b_\mu^{\perp\dagger}(X,s)=e^{is\tilde{H}}b_\mu^{\perp\dagger}(X)e^{-is\tilde{H}}. \tag{4.56}$$

The Hamiltonian generates transformations in the internal time label "s," and the internal boost mixes the internal time parameter with the spatial coordinates. These transformations all happen at constant "t" (where "t" is the external time parameter).

2. The external Poincaré group

As in the case of the scalar field, one of the novel features of histories theories is the existence of a second Poincaré group—the external group—that is associated with the external time label, "t." Again we start from the classical expressions, suitably ordered:

$$P^\mu=:\int d^4X \;\; \pi^\nu\,\partial^\mu A_\nu: \tag{4.57}$$

$$M^{\mu\nu}=:\int d^4X[\,\pi^\rho(X^\mu\partial^\nu-X^\nu\partial^\mu)A_\rho+(\,\pi^\mu A^\nu-\pi^\nu A^\mu)]: \tag{4.58}$$

Note that these expressions use the covariant fields defined in Eqs. (4.8)–(4.9), and thus we write

$$P^\mu=i\int d^4X b^{\dagger\nu}\,\partial^\mu b_\nu, \tag{4.59}$$

$$M^{\mu\nu}=i\int d^4X[\,b^{\dagger\rho}(X^\mu\partial^\nu-X^\nu\partial^\mu)b_\rho+(\,b^{\dagger\mu}b^\nu-b^{\dagger\nu}b^\mu)]. \tag{4.60}$$

As in the classical case, the Liouville operator, $V=n_\mu P^\mu$, generates translations in the external time parameter. And it is the external boost generator, ${}^{\text{ext}}K(m)=n_\mu m_\nu M^{\mu\nu}$ that is of the most importance as we can see in its action on foliation dependent objects:

$$U(\Lambda)^n A_\mu(X)U(\Lambda)^{-1}=\Lambda_\mu^{\ \nu}\,{}^{\Lambda n}A_\nu(\Lambda^{-1}X), \tag{4.61}$$

where $U(\Lambda)=e^{iK(m)}$. The crucial point here is that it generates Lorentz transformations on the foliation vector as well. Let us now analyze this issue in a bit more detail.

Though the set of all coherent states is independent of the foliation vector, n_μ (they are eigenstates of the annihilation operator), the definition of them in terms of the Weyl generator, Eqs. (4.21)–(4.22) is clearly not. It is thus that the Fock space, $\mathcal{V}$, depends upon the choice of foliation. Now, as in the case of the scalar field, all the foliation-dependent representations of the history algebra exist on the same Fock space, $\mathcal{V}$, and ${}^{\text{ext}}K(m)$ relates the objects defined with respect to a foliation "n," with those same objects defined with respect to the foliation "Λn." For example, under ${}^{\text{ext}}K(m)$, the constraint operators will transform

$${}^n\Psi_\kappa \overset{{}^{\text{ext}}K(m)}{\rightarrow} {}^{\Lambda n}\Psi_\kappa, \tag{4.62}$$

$${}^n\Phi_\kappa \overset{{}^{\text{ext}}K(m)}{\rightarrow} {}^{\Lambda n}\Phi_\kappa. \tag{4.63}$$

Now the map L from $\mathcal{V}$ to $\mathcal{V}_{\text{phys}}$ is also evidently n-dependent and thus $\mathcal{V}_{\text{phys}}$ also depends on the choice of foliation used to define $\mathcal{V}$. However, whereas all foliation-dependent representations can

exist on $\mathcal{V}$ (and we can thus talk about transformations between them), the physical Hilbert spaces, ${}^{n}\mathcal{V}_{\text{phys}}$ and ${}^{\Lambda n}\mathcal{V}_{\text{phys}}$ (where, we trust, the point of the added superscript is self-evident), are clearly different. This is why there will be no representation of ${}^{\text{ext}}K(m)$ on $\mathcal{V}_{\text{phys}}$. Mathematically (and analogously to the classical case) this situation is represented by the fact that the external boost does not (weakly) commute with either of the constraints.

Of course, we can still relate the important quantities on ${}^{n}\mathcal{V}_{\text{phys}}$ such as the action, ${}^{n}S$, to those same quantities on ${}^{\Lambda n}\mathcal{V}_{\text{phys}}$ via the prescription given at the end of Sec. IV B, i.e., by mapping back to $\mathcal{V}$, boosting there, and then mapping to ${}^{\Lambda n}\mathcal{V}_{\text{phys}}$.

The other generators will be represented on $\mathcal{V}_{\text{phys}}$, we just make use of Eq. (4.47) to define them. The most important of these is the Liouville operator, and this will be defined on the physical Hilbert space as

$$\tilde{V}=i\int d^4X b_{\nu}^{\perp\dagger} n_{\mu}\partial^{\mu}b^{\perp\nu}. \tag{4.64}$$

This will generate time transformations in the external time label, "t," on the physical Hilbert space. We thus arrive, using Eqs. (4.50) and (4.64), at the definition of the action operator on the physical Hilbert space:

$$\tilde{S}=\tilde{V}-\tilde{H}. \tag{4.65}$$

V. CONCLUSION

Our aim in this paper has been to construct a histories theory of Electromagnetism working in the HPO consistent histories framework. As a vector field theory with two first class constraints, we have built on the work of Savvidou[1] on scalar field theory, as well as demonstrating an application of the constrained systems algorithm developed by Savvidou and Anastopoulos.[3]

Classically, we defined the histories phase space and the two Poincaré groups that are a feature of histories field theories. The constraints partition the constraint surface (and indeed the whole phase space) into orbits, and by defining coordinates that are constant on each orbit, we defined the reduced phase space that carries the physical degrees of freedom of the theory. We stressed the importance of the foliation dependence of the phase space (and thus the reduced phase space) focusing particularly on the action of the external boost generator which transforms between different foliations.

Quantizing within the Dirac scheme, we first constructed the Hilbert space of the unconstrained theory ($\mathcal{V}$), motivated by finding a suitable representation of the History algebra. We then defined the constraints as operators, and, making use of the technology of coherent states, sought to define the physical Hilbert space ($\mathcal{V}_{\text{phys}}$). As the constraints have continuous spectra, this was not going to be a true linear subspace of the full Hilbert space. We got around this issue by analyzing $\mathcal{V}$ in terms of coherent states, which led to a definition of $\mathcal{V}_{\text{phys}}$ in terms of just the transverse components of the vector field and their conjugate momenta (or, more strictly, the space of test functions). We then defined a suitable mapping from $\mathcal{V}$ to $\mathcal{V}_{\text{phys}}$ and used this to define the action operator on $\mathcal{V}_{\text{phys}}$.

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Symmetric informationally complete quantum measurements

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We consider the existence in arbitrary finite dimensions d of a positive operator valued measure (POVM) comprised of d^2 rank-one operators all of whose operator inner products are equal. Such a set is called a ''symmetric, informationally complete'' POVM (SIC–POVM) and is equivalent to a set of d^2 equiangular lines in $\mathbb{C}^d$. SIC–POVMs are relevant for quantum state tomography, quantum cryptography, and foundational issues in quantum mechanics. We construct SIC–POVMs in dimensions two, three, and four. We further conjecture that a particular kind of group-covariant SIC–POVM exists in arbitrary dimensions, providing numerical results up to dimension 45 to bolster this claim. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1737053]

I. INTRODUCTION

In quantum theory, measurements are represented by *positive operator valued measures* (POVMs). A POVM is termed *informationally complete* if its statistics determine completely the quantum state on which the measurement is carried out.[2,4,20,21] In order to be maximally efficient at determining the state, such a measurement should also be *rank-one*; i.e., the measurement operators or *POVM elements* should be positive multiples of projectors onto pure states, in which case each POVM element corresponds uniquely (up to a phase) to a subnormalized vector in $\mathbb{C}^d$. A particularly appealing and potentially useful measurement is one which is *symmetric*, meaning all pairwise inner products between the POVM elements are equal. Such a POVM is a ''symmetric, informationally complete positive operator-valued measure,'' or SIC–POVM for short. The set of vectors comprising a SIC–POVM has also been studied in a very different context, where it has a different name: it is a set of d^2 equiangular lines in $\mathbb{C}^d$, first studied by Lemmens and Seidel[19] and subsequently by many others.[5–7,11,16–18,22,24] In quantum information theory such measurements are relevant to quantum state tomography,[3] quantum cryptography,[9] and to foundational studies[8] where they would make for a particularly interesting ''standard quantum measurement.'' The outstanding question we address in this paper is whether SIC–POVMs exist in any finite dimension.

We conjecture that SIC–POVMs exist in all finite dimensions and, moreover, that there exists in all finite dimensions a SIC–POVM that is covariant under a standard representation of $\mathbb{Z}_d \times \mathbb{Z}_d$. To state the conjecture, let us formalize the definition of a SIC–POVM. The simplest definition is that a SIC–POVM P is a set of d^2 normalized vectors $|\phi_k\rangle$ in $\mathbb{C}^d$ satisfying

$$|\langle \phi_j|\phi_k\rangle|^2 = \frac{1}{d+1}, \quad j \neq k. \tag{1}$$

More precisely, the POVM elements of P are the subnormalized projectors $|\phi_k\rangle\langle\phi_k|/d=\Pi_k/d$, which have pairwise Hilbert–Schmidt inner product $(\Pi_j,\Pi_k)/d^2=\mathrm{Tr}[\Pi_j^\dagger\Pi_k]/d^2=1/d^2(d+1)$ for $j\neq k$. It turns out that the other properties of a SIC–POVM, i.e., completeness and informational completeness, follow from Eq. (1), as we show in Sec. II.

We can now state our conjecture.

Conjecture 1: For any dimension $d\in\mathbb{N}$, let $\{|k\rangle\}_{k=0}^{d-1}$ be an orthonormal basis for $\mathbb{C}^d$, and define

$$\omega=\exp(2\pi i/d),\quad D_{jk}=\omega^{jk/2}\sum_{m=0}^{d-1}\omega^{jm}|k\oplus m\rangle\langle m|\,, \tag{2}$$

where $\oplus$ denotes addition modulo d. Then there exists a normalized $|\phi\rangle\in\mathbb{C}^d$ such that the set $\{D_{jk}|\phi\rangle\}_{j,k=1}^{d}$ is a SIC–POVM P.

Analytic solutions are known for $d=2,3,8$,[16] and to this list we add $d=4$. Additionally, computer calculations reveal numerical solutions (with an accuracy better than 1 part in 10^8) in dimensions up to 45, some derived using the aforementioned group, but others using other suitable groups. These results are detailed herein according to the following plan. Section II states the problem in the language of frame theory and derives a connection to the problem of finding spherical t-designs. Section III specializes to the group-covariant case and explains why our conjecture might be generally true. Section IV presents our analytic solutions for $d=2,3,4$, and Sec. V the method of obtaining the numerical results. Finally, in Sec. VI we discuss possible approaches to a general proof, as well as related open questions.

II. FRAMES AND SPHERICAL *t*-DESIGNS

The concepts of frame theory provide a simple and elegant means of putting our problem in a general setting, for a SIC–POVM is a particular kind of frame. Frames are a generalization of basis sets, with the requirements of orthogonality and normalization relaxed. For a finite-dimensional vector space $\mathcal{H}$, a collection of vectors $|\psi_k\rangle\in\mathcal{H}$ is a frame if there exist constants $0<a\leqslant b<\infty$ such that

$$a\langle\xi|\xi\rangle\leqslant\sum_k|\langle\xi|\psi_k\rangle|^2\leqslant b\langle\xi|\xi\rangle \tag{3}$$

for all $|\xi\rangle\in\mathcal{H}$. Any collection of vectors is a frame in the subspace spanned by the vectors. The constants a and b are called the *frame bounds*, and if $a=b$, the frame is said to be *tight*. The *frame operator* is the positive operator

$$S=\sum_k|\psi_k\rangle\langle\psi_k|. \tag{4}$$

It should be immediately clear that for a tight frame $S=aI$. This tight-frame condition is equivalent to the completeness condition for the corresponding POVM elements $|\psi_k\rangle\langle\psi_k|/a$, and thus rank-one POVMs and tight frames are the same mathematical object.

Now let $\mathbb{S}^d\subset\mathbb{C}^d$ be the subset consisting of vectors that have unit norm. Any frame can be rewritten in terms of the corresponding normalized vectors, but tightness is not preserved under this transformation. For a frame $\{|\psi_k\rangle\in\mathbb{S}^d\}_{k=1}^n$ made up of normalized vectors, the quantity

$$\mathrm{Tr}[S^2]=\sum_{j,k}|\langle\psi_j|\psi_k\rangle|^2 \tag{5}$$

is called the *frame potential*. We consider only frames made up of normalized vectors throughout the following.

A useful theorem due to Benedetto and Fickus[1] states the following.

Theorem 1 (Benedetto–Fickus): *Given any d and n, let $\{|\psi_k\rangle \in \mathbb{S}^d\}_{k=1}^n$ be a set of normalized vectors with frame operator S. Then*

$$\mathrm{Tr}[S^2] \geqslant \max(n, n^2/d). \tag{6}$$

Furthermore, the bound is achieved if and only if $\{|\psi_k\rangle\}$ consists of orthonormal vectors, when $n \leqslant d$, or is a tight frame, when $n \geqslant d$.

Proof: The proof is so simple that we can include it here for completeness. Denoting the ordered eigenvalues of S by $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_d$, we first note that the number of nonzero eigenvalues is at most $q = \min(n,d)$. Thus we have

$$\mathrm{Tr}[S] = n = \sum_{k=1}^{q} \lambda_k \quad \text{and} \quad \mathrm{Tr}[S^2] = \sum_{k=1}^{q} \lambda_k^2. \tag{7}$$

Minimizing $\mathrm{Tr}[S^2]$ subject to the constraint $\mathrm{Tr}[S] = n$ gives the inequality. Equality holds if and only if $\lambda_k = n/q$, $k = 1,\ldots,q$. Thus for $n \leqslant d$, S is a projector onto an n-dimensional subspace, implying that the vectors $|\psi_k\rangle$ are orthogonal, and if $n \geqslant d$, $S = (n/d)I$, implying that the set $\{|\psi_k\rangle\}$ is a tight frame. □

Since the frame potential of P is $\mathrm{Tr}[S^2] = d^3 = n^2/d$, the theorem establishes immediately that P is a tight frame, hence P is also a POVM.

For P to be informationally complete, the d^2 operators $\Pi_k = |\phi_k\rangle\langle\phi_k|$ must be linearly independent so that they span the space of operators. The linear independence follows from considering the rank of their Gram matrix $(\Pi_j, \Pi_k) = \mathrm{Tr}[\Pi_j^\dagger \Pi_k] = (d\delta_{jk} + 1)/(d+1)$, which being circulant (each row is a cyclic shift of the previous row), has eigenvalues given by the Fourier transform of one of the rows. A simple calculation reveals that due to the combination of constant term and Kronecker delta, the eigenvalues are exactly the same as the values in any row. Since no eigenvalues are zero, the Gram matrix has full rank, the projection operators Π_k are linearly independent, and P is informationally complete.

Since every rank-one POVM is a tight frame, a SIC–POVM P is clearly something more. To fully elucidate the properties and applications of P, we need to introduce *spherical t-designs*. Building on the result of Benedetto and Fickus, we can establish a connection between frames and spherical t-designs applicable to the SIC–POVM problem.

A *spherical t-design* is a set of n normalized vectors $\{|\phi_k\rangle \in \mathbb{S}^d\}$ such that the average value of any tth order polynomial $f_t(\psi)$ over the set $\{|\phi_k\rangle\}$ is equal to the average of $f_t(\psi)$ over *all* normalized vectors $|\psi\rangle$. Note that if a set is a t-design, it is also an s-design for all $s \leqslant t$, since an sth order polynomial is also a tth order polynomial. Spherical t-designs were originally developed as subsets of the real sphere S^d; here we apply the concept to the set $\mathbb{S}^d$.

Let $\mathcal{H} = \mathbb{C}^d$, $\mathcal{H}_t$ be the t-fold tensor product of such spaces, and $\mathcal{S}_t$ be the symmetric subspace of $\mathcal{H}_t$, and consider a function $f_t : \mathcal{H} \to \mathbb{C}$ defined as

$$f_t(\psi) = \langle \Psi^t | F_t | \Psi^t \rangle, \quad |\Psi^t\rangle = |\psi\rangle^{\otimes t}, \quad |\psi\rangle \in \mathcal{H}, \tag{8}$$

where the choice of f_t is equivalent to a choice of a symmetric operator $F_t \in \mathcal{B}(\mathcal{S}_t)$. Such a function is a tth order polynomial function on $\mathcal{H}$. We can decompose F_t into a sum of product operators, i.e., $F_t = \Sigma_k \otimes_{j=1}^t A_{j;k}$; thus any such function can be decomposed into monomial terms like

$$\langle \Psi^t | \bigotimes_{j=1}^{t} A_j | \Psi^t \rangle = \prod_{j=1}^{t} \langle \psi | A_j | \psi \rangle. \tag{9}$$

Without loss of generality, we can restrict our attention to such monomial functions and rewrite them as

$$f_t(\psi)=\prod_{j=1}^{t}\mathrm{Tr}[A_j|\psi\rangle\langle\psi|]=\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{t}A_j\right)\Pi_\psi^{\otimes t}\right],\quad \Pi_\psi=|\psi\rangle\langle\psi|. \tag{10}$$

Since the set $\{|\phi_k\rangle\}$ is a t-design if and only if the average of any f_t over $\{|\phi_k\rangle\}$ is equal to its average over all $|\psi\rangle\in\mathbb{S}^d$, we are led to compute the average of an arbitrary monomial term:

$$\langle f_t\rangle=\int \mathrm{d}\psi\,\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{t}A_j\right)\Pi_\psi^{\otimes t}\right]=\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{t}A_j\right)\int \mathrm{d}\psi\,\Pi_\psi^{\otimes t}\right]=\mathrm{Tr}\left[\left(\bigotimes_{j=1}^{t}A_j\right)K_t\right]. \tag{11}$$

Hence we focus on finding K_t, since it effectively takes the average of f_t. A spherical t-design is then a set of vectors for which

$$S_t=\sum_{k=1}^{n}|\Phi_k^t\rangle\langle\Phi_k^t|=nK_t,\quad |\Phi_k^t\rangle=|\phi_k\rangle^{\otimes t}. \tag{12}$$

Note that S_t is the t-fold tensor-product analog of the frame operator S.

To find the operator K_t, note that K_t has support only on the symmetric subspace $\mathcal{S}_t$. Further, because K_t is invariant under any $U^{\otimes t}$ for $U\in\mathrm{SU}(d)$, we conclude that $K_t\propto\Pi_{\mathrm{sym}}$, the projector onto $\mathcal{S}_t$. (Recall that $\mathcal{S}_t$ is an irreducible invariant subspace of the group consisting of the operators $U^{\otimes t}$.) Finally, to determine the constant of proportionality, we consider the average of the trivial function $f_t(\psi)=1$. Equation (11) then becomes $\mathrm{Tr}[K_t]=1$, and since $\mathcal{S}_t$ has dimension $\binom{t+d-1}{d-1}$, we have

$$K_t=\frac{t!(d-1)!}{(t+d-1)!}\Pi_{\mathrm{sym}}. \tag{13}$$

For $t=1$, we see that a 1-design is a tight frame made up of normalized vectors and, hence, also a POVM made up of equally weighted rank-one projectors.

Equation (12) now says that the set $\{|\phi_k\rangle\}$ is a t-design if and only if the set $\{|\Phi_k^t\rangle\}$ is a tight frame on $\mathcal{S}_t$, whence we can apply Theorem 1 to obtain the following result.

Theorem 2: *A set of normalized vectors* $\{|\phi_k\rangle\in\mathbb{S}^d\}_{k=1}^n$ *with* $n\geqslant\binom{t+d-1}{d-1}$ *forms a spherical* t*-design if and only if*

$$\mathrm{Tr}[S_t^2]=\sum_{j,k}|\langle\phi_j|\phi_k\rangle|^{2t}=\frac{n^2t!\,(d-1)!}{(t+d-1)!}. \tag{14}$$

Furthermore, this value is the global minimum of $\mathrm{Tr}[S_t^2]$.

This theorem links the spherical t-design property with the minimization of the tth frame potential, $\mathrm{Tr}[S_t^2]$. Immediately we can infer that every SIC–POVM is a 2-design since $\mathrm{Tr}[S_2^2]=\Sigma_{j,k}|\langle\phi_j|\phi_k\rangle|^4=2d^3/(d+1)$, the required value for a 2-design. The converse is also true, namely, every 2-design with $n=d^2$ elements is a SIC–POVM. To show this, let $\lambda_{jk}=|\langle\phi_j|\phi_k\rangle|^2$, $j\neq k$, and interpret these λ_{jk} as coordinates in $\mathbb{R}^{d^2(d^2-1)}$. Using the values of the frame potentials for a 2-design with $n=d^2$ elements, we can write

$$\sum_{j\neq k}\lambda_{jk}=\mathrm{Tr}(S^2)-d^2=\frac{d^2(d^2-1)}{d+1}\quad\text{and}\quad\sum_{j\neq k}\lambda_{jk}^2=\mathrm{Tr}(S_2^2)-d^2=\frac{d^2(d^2-1)}{(d+1)^2}. \tag{15}$$

The first equation describes a plane and the second a sphere. They intersect at the single tangent point $\lambda_{jk}=1/(d+1)$, thus showing that all 2-designs with d^2 elements are SIC–POVMs. These considerations make clear that the crucial distinguishing property of a SIC–POVM is that it is also a 2-design. Moreover, this ensures that minimizing the second frame potential, as we do in the numerical work reported in Sec. IV, yields vectors that do indeed form a SIC–POVM.

Furthermore, d^2 is the smallest number of elements a 2-design can have, so a SIC–POVM is a *minimal* 2-design (see also Ref. 16). Theorem 2 does not provide the minimum number of states, $n_{\min}$, for a t-design in d dimensions, but we can establish lower bounds. For the $t=2$ case, consider again the steps leading to the definition of the operator K_t. In carrying out the average of the function f_2, we could have written

$$\langle f_2\rangle = \mathrm{Tr}\left[A_2 \int \mathrm{d}\psi\, |\psi\rangle\langle\psi|A_1|\psi\rangle\langle\psi|\right] = \mathrm{Tr}[A_2\mathcal{G}(A_1)] \tag{16}$$

and thus considered the superoperator $\mathcal{G}:\mathcal{B}(\mathbb{C}^d)\to\mathcal{B}(\mathbb{C}^d)$. Here $\mathcal{G}(UAU^\dagger)=U\mathcal{G}(A)U^\dagger$ for any $U\in \mathrm{SU}(d)$, so by Schur's lemma, $\mathcal{G}$ is some linear combination of projectors onto the invariant subspaces of U acting on $\mathcal{B}(\mathbb{C}^d)$. These invariant subspaces are (i) the (d^2-1)-dimensional subspace of traceless operators and (ii) the one-dimensional subspace spanned by the identity operator I. Thus we can write $\mathcal{G}=a\mathcal{I}+b\mathbf{I}$ where $\mathcal{I}(A)=A$ and $\mathbf{I}(A)=\mathrm{Tr}[A]I$ (i.e., $\mathcal{I}$ is the identity superoperator, and $\mathbf{I}$ projects onto the identity operator). To find a and b, we first let $A_1=A_2=I$, which gives the function $f_2(\psi)=1$, so that Eq. (16) yields $d(a+bd)=1$. Next we consider $A_1=A_2=|\phi\rangle\langle\phi|$, for which $\langle f_2\rangle=\int \mathrm{d}\psi\,|\langle\phi|\psi\rangle|^4=a+b$. We can use Eqs. (11) and (13) to show that $\langle f_2\rangle=2/d(d+1)$; combined with the previous result, this implies $a=b=1/d(d+1)$. Therefore, $\mathcal{G}$ has no null subspace, must be rank-d^2, and cannot be constructed from less than d^2 linearly independent rank-one superoperators. Similar arguments can be applied to all spherical t-designs. By similar rearrangements, we can make several different types of operators K_t', and the rank of each serves as a lower bound on the number of vectors required to comprise a t-design.

III. GROUP COVARIANCE

Our results are obtained by considering group-covariant sets, so it is appropriate to specialize to this case. The SIC–POVM P is group covariant if there exists a group G with a d-dimensional projective unitary representation $\{U_g\}$ such that (i) P is invariant under any U_g, i.e., for any $|\phi_j\rangle\in P$ and any U_g, $U_g|\phi_j\rangle\in P$ (up to a phase), and (ii) $\{U_g\}$ acts transitively on P, i.e., for any $|\phi_j\rangle,|\phi_k\rangle\in P$, there exists U_g such that $U_g|\phi_j\rangle=|\phi_k\rangle$ (also up to a phase). Assuming group covariance simplifies the search for SIC–POVMs. We simply search for a fiducial vector such that $P=\{U_g|\phi\rangle\}$ is a SIC–POVM (note that the transitivity property implies that the order of G must be at least d^2). To do this, we use groups such that $\{U_g|\phi\rangle\}$ is a 1-design, i.e., a POVM, for any normalized vector $|\phi\rangle$, and then we search for a particular vector $|\phi\rangle$ such that $|\langle\phi|U_g|\phi\rangle|^2=1/(d+1)$ for all $g\neq e$. All other inner products are then guaranteed to have this value due to the group action.

We suspect the case of group covariance to be general for the following reason. Consider the map $\alpha:\mathbb{S}^d\to\mathcal{B}(\mathbb{C}^d)$ that takes a normalized vector to the corresponding projector, i.e., $\alpha(|\phi_j\rangle)=|\phi_j\rangle\langle\phi_j|$. Now consider the operators

$$\sigma_j=\sqrt{\frac{d}{d-1}}\left(|\phi_j\rangle\langle\phi_j|-\frac{I}{d}\right) \quad . \tag{17}$$

Being both traceless and Hermitian, these operators lie in a subspace of $\mathcal{B}(\mathbb{C}^d)$ that is isomorphic to $\mathbb{R}^{d^2-1}$; indeed, since $(\sigma_j,\sigma_j)=1$, they all lie on the unit sphere in $\mathbb{R}^{d^2-1}$. This sphere is a generalization of the Bloch sphere for two-dimensional systems, the difference being that for $d>2$, not all operators on the sphere are images of vectors in $\mathbb{S}^d$ under the map α. From the SIC–POVM condition (1), one finds immediately that

$$(\sigma_j,\sigma_k)=-\frac{1}{d^2-1} \quad \forall\, j\neq k. \tag{18}$$

This is the condition for the d^2 operators $\{\sigma_j\}$ to form a regular simplex in $\mathbb{R}^{d^2-1}$, whose automorphism group is the permutation group S_{d^2}. Given this result, some group covariance

seems natural. One is tempted to think that from here it is a simple matter to establish the existence of the set P. This is not the case, however, as working in the operator space obscures the very difficult task of determining when a given operator is the image of some element of $\mathbb{S}^d$ under the map α. In the same vein, most of the elements of the permutation group cannot be represented in this framework as unitary transformations of $\mathbb{C}^d$; thus, while we know that any G satisfying the conditions above must be a subgroup of S_{d^2}, it is not obvious which subgroups are candidates.

The outstanding choice for G is the group $\mathbb{Z}_d \times \mathbb{Z}_d$, as described in the conjecture. We note in passing that using this group to find a SIC–POVM makes P a Gabor or Weyl–Heisenberg frame, this being the definition of such a frame;[10] such a SIC–POVM P is useful in defining finite-dimensional analogs of the familiar P and Q quasidistributions of infinite dimensions. The group's usefulness here stems from the fact that, for any normalized $|\psi\rangle \in \mathbb{S}^d$,

$$S_\psi = \sum_{jk} D_{jk} |\psi\rangle\langle\psi| D_{jk}^\dagger = dI, \tag{19}$$

a fact readily checked by direct calculation.

The property in Eq. (19) of producing a 1-design for any input state is quite general. The following argument is adapted from Proposition 3 of Ref. 23. Any set of d^2 orthogonal unitary operators T_j, thus satisfying $\mathrm{Tr}[T_j^\dagger T_k] = d\delta_{jk}$, is a complete set for expanding operators in $\mathcal{B}(\mathbb{C}^d)$; the unitary operators $\{D_{jk}\}$ are one example of operators that satisfy this orthogonality condition. It is a simple matter to turn the completeness relation into $\Sigma_k T_k C T_k^\dagger = d\,\mathrm{Tr}[C] I$ for any operator C. Simply consider the inner product of two arbitrary operators A and B. The completeness relation means that

$$(A,B) = \frac{1}{d} \sum_k (A,T_k)(T_k,B). \tag{20}$$

Setting $A = |\phi_1\rangle\langle\phi_2|$ and $B = |\psi_1\rangle\langle\psi_2|$ [which we can do without loss of generality because such outer products span $\mathcal{B}(\mathbb{C}^d)$], we find

$$\langle\phi_1|\psi_1\rangle\langle\psi_2|\phi_2\rangle = \frac{1}{d} \sum_k \langle\phi_1|T_k|\phi_2\rangle\langle\psi_2|T_k^\dagger|\psi_1\rangle, \tag{21}$$

from which it follows that $\Sigma_k T_k |\phi_2\rangle\langle\psi_2| T_k^\dagger = d\,\langle\psi_2|\phi_2\rangle$, whence the result follows.

Thus the property of producing a 1-design regardless of the fiducial $|\phi_0\rangle$ is common to all groups of size d^2 whose representation operators are a complete, orthogonal set. Such groups were introduced by Knill in connection with quantum error-correcting codes and are called ''nice error bases'' or unitary error bases.[14,15] Klappenecker and Rötteler have kindly detailed all such nice error bases up to dimension 10, so we can apply them to the problem at hand.[12,13,25] Only the nice error bases associated with the group $\mathbb{Z}_d \times \mathbb{Z}_d$ exist in every dimension, thus accounting for our focus on this group.

IV. ANALYTIC SIC–POVMS

Here we concentrate specifically on using the group $\mathbb{Z}_d \times \mathbb{Z}_d$. Fixing the representation operators D_{jk} of this group we can determine the set of fiducial vectors that under the group action make a SIC–POVM. From this we can determine also the number of distinct SIC–POVMs generated by our fixed representation. In three dimensions there are an uncountably infinite number of such covariant SIC–POVMs, but in two dimensions there are just two, and in four, 16. We write the fiducial state as

$$|\phi\rangle = \sum_k r_k e^{i\theta_k} |k\rangle, \tag{22}$$

where we can, of course, immediately choose $\theta_0 = 0$.

A. $d=2$

The two solutions, represented as column vectors in the standard basis, are

$$\left\{ \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3+\sqrt{3}} \\ e^{i\pi/4}\sqrt{3-\sqrt{3}} \end{pmatrix}, \quad \frac{1}{\sqrt{6}} \begin{pmatrix} -\sqrt{3-\sqrt{3}} \\ e^{i\pi/4}\sqrt{3+\sqrt{3}} \end{pmatrix} \right\}. \tag{23}$$

These have a simple interpretation on the Bloch sphere, where the nontrivial group operators are simply rotations by π about the x, y, and z axes, respectively. Then the Bloch vectors of the two fiducial states are $\pm(1,1,1)/\sqrt{3}$, and the two SIC–POVM states thus formed are regular tetrahedra, each one related to the other by inversion of the Bloch vectors.

B. $d=3$

For r_0 satisfying $1/\sqrt{2} < r_0 < \sqrt{2/3}$, define

$$r_\pm(r_0) = \tfrac{1}{2} r_0 \pm \tfrac{1}{2}\sqrt{2 - 3r_0^2}. \tag{24}$$

Hence $0 < r_- \leqslant 1/\sqrt{6} \leqslant r_+ < 1/\sqrt{2} < r_0 \leqslant \sqrt{2/3}$. The complete set of fiducial states, represented as column vectors in the standard basis, is then

$$\left\{ \begin{pmatrix} r_0 \\ r_+ e^{i\theta_1} \\ r_- e^{i\theta_2} \end{pmatrix}, \begin{pmatrix} \text{plus all vectors formed} \\ \text{by permuting of elements} \end{pmatrix} \middle| \ \theta_1, \theta_2 \in \left\{ \frac{\pi}{3}, \pi, \frac{5\pi}{3} \right\}, \frac{1}{\sqrt{2}} < r_0 \leqslant \sqrt{\frac{2}{3}} \right\}$$
$$\cup \left\{ \begin{pmatrix} 1/\sqrt{2} \\ e^{i\theta_1}/\sqrt{2} \\ 0 \end{pmatrix}, \begin{pmatrix} \text{plus all vectors formed} \\ \text{by permuting of elements} \end{pmatrix} \middle| \ 0 \leqslant \theta_1 < 2\pi \right\}. \tag{25}$$

C. $d=4$

Now let

$$r_0 = \frac{1 - 1/\sqrt{5}}{2\sqrt{2-\sqrt{2}}} \quad , \quad r_1 = (\sqrt{2}-1) r_0 \quad , \quad r_\pm = \tfrac{1}{2}\sqrt{1 + 1/\sqrt{5} \pm \sqrt{1/5 + 1/\sqrt{5}}}, \tag{26}$$

along with

$$a = \arccos \frac{2}{\sqrt{5+\sqrt{5}}}, \quad b = \arcsin \frac{2}{\sqrt{5}}, \tag{27}$$

and define the set

$$\Omega \equiv \{((-1)^m(a/2+b/4) + \pi(m+2n+7j+1)/4,\ \pi(2k+1)/2, \quad (-1)^m(-a/2+b/4)$$
$$+ \pi(m+2n+3j+4k+1)/4) \mid j,k,m = 0,1 \ \text{ and } \ n = 0,\ldots,3\}. \tag{28}$$

The complete set of fiducial states, represented as column vectors in the standard basis, is now

TABLE I. Number of SIC–POVM sets generated by a fixed representation of the group $\mathbb{Z}_d \times \mathbb{Z}_d$ in dimensions 2 through 7. The infinity in dimension 3 is uncountable.

d	#(SIC–POVMs)
2	2
3	∞
4	16
5	80
6	96
7	336

$$\left\{ \begin{pmatrix} r_0 \\ r_+ e^{i\theta_+} \\ r_1 e^{i\theta_1} \\ r_- e^{i\theta_-} \end{pmatrix}, \begin{pmatrix} r_0 \\ r_- e^{i\theta_-} \\ r_1 e^{i\theta_1} \\ r_+ e^{i\theta_+} \end{pmatrix}, \begin{pmatrix} \text{plus all vectors formed} \\ \text{by cycling of elements} \end{pmatrix} \middle| \ (\theta_+, \theta_1, \theta_-) \in \Omega \right\}. \tag{29}$$

V. NUMERICAL SIC–POVMS

Because analytic solutions to the SIC–POVM condition (1) are so few, our conjectures are based almost entirely on numerical evidence (even the $d=4$ solution was originally inspired by close examination of numerical solutions). To find numerical instances of P, we simply minimize the second frame potential $\mathrm{Tr}[S_2^2]$ over sets of d^2 normalized vectors generated by a representation of $\mathbb{Z}_d \times \mathbb{Z}_d$ from a vector $|\phi\rangle$. It is also possible to vary independently the d^2 elements of P, but this is much less efficient; taking advantage of the group-covariance conjecture permits us to search a space of $O(d)$ complex parameters instead of $O(d^3)$ complex parameters.

The quantity that we minimize, $\Sigma_{j,k}|\langle\phi|D_{jk}|\phi\rangle|^4$, is proportional to the frame potential because of the group covariance. Since it is a quartic function of $|\phi\rangle$, we have to use numerical methods to minimize it, using either Mathematica (simpler) or C++ (much faster). The method used is an adaptive conjugate gradient method; this has the advantage of converging with exponential rapidity to a local minimum, but the disadvantage of being insensitive to global conditions. As a result, the most time-intensive portion of the computation by far is identifying one of the global minima among the many local minima.

Once the correct minimum is located, we quickly obtain P such that Eq. (1) is satisfied to an accuracy of 10^{-8}. The sole exception to this rule is $d=3$ (where an exact analytic solution is known): in $d=3$ there exists a continuously infinite family of solutions, and this degeneracy makes numerical solution difficult. For every dimension between $d=5$ and $d=45$, however, we have found $\mathbb{Z}_d \times \mathbb{Z}_d$-covariant solutions to within machine precision.[26]

Additionally, in small dimensions, one can attempt an exhaustive search for *all* possible $\mathbb{Z}_d \times \mathbb{Z}_d$-covariant SIC–POVMs, by simply running the minimization many times with differing presumptive fiducial states, tabulating all the while the distinct SIC–POVM fiducial states found. Table I lists the results for the number of distinct SIC–POVMs.

Finally, we have tested some of the other nice error bases tabulated by Klappenecker and Rötteler. These are also easy handled, and although not all groups were tested, at least four groups were found to generate SIC–POVM sets. In the notation of the library of small groups used by GAP3, GAP4, and MAGMA, these groups are G(36,11), G(36,14), G(64,8), and G(81,9). Each of these solutions has an accuracy of 10^{-15} in the individual vector inner products. Perhaps surprisingly, many of the tabulated groups do not seem to yield group-covariant SIC–POVMs.

VI. ODDS AND ENDS

A rigorous proof of existence of SIC–POVMs in all finite dimensions seems tantalizingly close, yet remains somehow distant. Although the numerical evidence makes very clear the relevance of the group $\mathbb{Z}_d \times \mathbb{Z}_d$, this is not definitively established. Given the apparent importance of

$\mathbb{Z}_d \times \mathbb{Z}_d$, it would seem to be just a short step to some general form for an operator whose eigenvectors could be a fiducial state, but a proof by this method has not been forthcoming. For instance, in three dimensions the Fourier transform operator has an eigenvector that is a fiducial state (the one associated with the eigenvalue i), but this does not hold in general. In five dimensions a fiducial vector can be found among the degenerate eigenvectors of a particular $\mathbb{Z}_3$ subgroup of the normalizer of $\mathbb{Z}_d \times \mathbb{Z}_d$ in $\mathrm{SU}(d)$, but there is no such subgroup at all in the normalizer for dimension seven. The group-theoretic structure of SIC–POVMs is exceedingly rich, however, and ongoing efforts to understand the full automorphism group of a SIC–POVM might yield insights into operators that yield fiducial states. We hope that by establishing the framework and providing motivating numerical results in this paper, a proof might be completed.

Finally, regardless of whether their existence can be proved rigorously, SIC–POVMs appear to exist in many dimensions. They might be of use in many areas of quantum information theory—signal ensembles, quasidistributions on discrete phase space, error-correcting codes, and quantum measurement, just to name a few. In addition, they appear to be connected to a number of interesting mathematical problems, including spherical codes and the putative existence of mutually unbiased bases.

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Traveling wave solutions of a generalized modified Kadomtsev–Petviashvili equation

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A method to generate traveling wave solutions of the generalized modified Kadomtsev–Petviashvili equation is reported and several physical solutions, including conditions of their existence, are presented. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1737813]

I. INTRODUCTION

As is well known, the Kadomtsev–Petviashvili equations (KPI, KPII) are universal models for the propagation of weakly nonlinear dispersive long waves which are essentially one directional, with weak transverse effects.[1] Both KPI and KPII have been solved by the inverse scattering technique.[2] Certain physical problems[3,4] motivated the investigation of generalizations of the KP equations.[5] Recently, the $(2+1)$-dimensional modified KP equation[6]

$$\psi_t - \tfrac{1}{8}(\psi_{xxx} - 6\psi^2\psi_x + 6\psi_x\partial_x^{-1}\psi_y + 3\partial_x^{-1}\psi_{yy}) = 0 \tag{1}$$

was solved by a decomposition procedure.[7] The generalized KPI equation

$$(\psi_t + (\psi^{q+1})_x + \psi_{xxx})_x - \psi_{yy} = 0, \quad q \in \mathbb{R} \ , \tag{2}$$

used as a model to describe the evolution of sound waves in antiferromagnetics,[3] was treated by a virial method.[8]

In this article we consider the generalized modified Kadomtsev–Petviashvili equation (gmKPE)

$$\psi_{xt} + ((a + b\psi^q)\psi^q\psi_x)_x + c\psi_{xxxx} - \sigma^2\psi_{yy} = 0, \tag{3}$$

where a,b,c,q are real constants and $\sigma^2 = \pm 1$.

II. TRAVELING WAVE SOLUTIONS

We look for real traveling wave solutions

$$\psi(x,y,t) = g(z), \tag{4}$$

with $z = x + ky + vt$. The ansatz (4) implies $\partial_x^{-1} = k\partial_y^{-1}$ and hence Eqs. (1) and (2) are particular cases of Eq. (3), subject to ansatz (4). Our main purpose is to prove the following theorem.

Theorem: Suppose that q is real, $q \neq 0, \pm 1/2, \pm 1, \pm 2$ and the parameters a,b,c,k,σ,v satisfy the condition

$$\frac{a^2}{(q+1)(q+2)^2} \geqslant \frac{b(v - k^2\sigma^2)}{2q+1}. \tag{5}$$

Then there exists a real and bounded solution of Eq. (3) of the form (4). Moreover, for

$$\frac{k^2\sigma^2-v}{c}<0 \tag{6}$$

this solution is periodic and for

$$\frac{k^2\sigma^2-v}{c}\geqslant 0 \tag{7}$$

this solution is solitary wavelike.

Remark 1: The exact solutions from this Theorem can be found in Eqs. (22) and (23).

Proof of Theorem: Substitution of Eq. (4) into Eq. (3) leads to the ODE

$$(v-k^2\sigma^2+ag^q+bg^{2q})g_{zz}+cg_{zzzz}+(ag^{q-1}+2bg^{2q-1})q(g_z)^2=0 \tag{8}$$

that can be integrated once to yield

$$(v-k^2\sigma^2+ag^q+bg^{2q})g_z+cg_{zzz}=C_1, \tag{9}$$

where C_1 is an arbitrary constant. For simplicity we continue with $C_1=0$. Applying the transformation

$$g(z)=f(z)^{1/q}, \quad q\neq 0 \tag{10}$$

and multiplying by $f^{3-(1/q)}$, Eq. (9) reads

$$\frac{1}{q^3}\{c(q-1)(2q-1)(f_z)^3-3c(q-1)qff_zf_{zz} + q^2f^2((v-k^2\sigma^2+(a+bf)f)f_z+cf_{zzz})\}=0. \tag{11}$$

We look for particular real solutions $f(z)$ of Eq. (11) that satisfy

$$R(f)\equiv(f_z)^2=\alpha f^4+4\beta f^3+6\gamma f^2+4\delta f+\epsilon. \tag{12}$$

As is well known[9,10] these solutions $f(z)$ can be expressed in terms of Weierstrass' elliptic function $\wp$. The coefficients α, β, γ, δ, ϵ in Eq. (12) have to be determined by the parameters of the gmKPE.

Equation (12) implies

$$f_{zz}=2\alpha f^3+6\beta f^2+6\gamma f+2\delta,$$
$$f_{zzz}=6(\gamma+2\beta f+\alpha f^2)f_z. \tag{13}$$

Inserting Eqs. (12) and (13) into Eq. (11) and dividing by f_z one obtains

$$\frac{1}{q^3}\{(bq^2+c\alpha(q+1)(2q+1))f^4+(aq^2+2c\beta(q+1)(q+2))f^3 + (6c\gamma+vq^2-k^2\sigma^2q^2)f^2+2c\delta(q-1)(q-2)f+c\epsilon(q-1)(2q-1)\}=0. \tag{14}$$

The sought for coefficients α, β, γ, δ, ϵ and the parameter q can be determined from Eq. (14). Disregarding the case $q=0$ (the gmKPE is linear in this case) and excluding first the cases

$$q=\pm\tfrac{1}{2},\pm 1,\pm 2, \tag{15}$$

and setting equal to zero the coefficients of f^ν in Eq. (14) one obtains

$$\alpha=-\frac{b\cdot q^2}{c(q+1)(2q+1)},\quad \beta=-\frac{aq^2}{2c(q+1)(q+2)},$$

$$\gamma=\frac{q^2(k^2\sigma^2-v)}{6c},\quad \delta=\epsilon=0,\quad c\neq 0. \tag{16a}$$

If q is equal to one of the values in (15), Eq. (14) yields for $q=-\frac{1}{2}$

$$\beta=-\frac{a}{6c},\quad \gamma=\frac{k^2\sigma^2-v}{24c},\quad \delta=\epsilon=0,\quad b=0,\quad c\neq 0, \tag{16b}$$

and arbitrary α;
for $q=-1$

$$\gamma=\frac{k^2\sigma^2-v}{6c},\quad \delta=\epsilon=0,\quad a=b=0,\quad c\neq 0, \tag{16c}$$

and arbitrary α, β;
for $q=-2$

$$\alpha=-\frac{4b}{3c},\quad \gamma=\frac{2(k^2\sigma^2-v)}{3c},\quad \delta=\epsilon=0,\quad a=0,\quad c\neq 0, \tag{16d}$$

and arbitrary β;
for $q=\frac{1}{2}$

$$\alpha=-\frac{b}{12c},\quad \beta=-\frac{a}{30c},\quad \gamma=\frac{k^2\sigma^2-v}{24c},\quad \delta=0,\quad c\neq 0, \tag{16e}$$

and arbitrary ϵ;
for $q=1$

$$\alpha=-\frac{b}{6c},\quad \beta=-\frac{a}{12c},\quad \gamma=\frac{k^2\sigma^2-v}{6c},\quad c\neq 0, \tag{16f}$$

and arbitrary δ, ϵ;
for $q=2$

$$\alpha=-\frac{4b}{15c},\quad \beta=-\frac{a}{6c},\quad \gamma=\frac{2(k^2\sigma^2-v)}{3c},\quad \epsilon=0,\quad c\neq 0, \tag{16g}$$

and arbitrary δ.

Summing up, a subset of traveling wave solutions to Eq. (3) is determined by the ODE (12) where $f(z)=g(z)^q$. The coefficients α, β, γ, δ, ϵ are given by Eqs. (16) relating the coefficients to the parameters of Eq. (3) (a,b,c,q) and of the ansatz (k,v).

It is known since 1865 (Ref. 11) that solutions to Eq. (12) are given by

$$f(z)=f_0+\frac{\sqrt{R(f_0)}\dfrac{d\wp(z;g_2,g_3)}{dz}+\frac{1}{2}R'(f_0)[\wp(z;g_2,g_3)-\frac{1}{24}R''(f_0)]+\frac{1}{24}R(f_0)R'''(f_0)}{2[\wp(z;g_2,g_3)-\frac{1}{24}R''(f_0)]^2-\frac{1}{48}R(f_0)R'''{}'(f_0)}, \tag{17}$$

where the prime denotes differentiation with respect to f and f_0 is any constant, not necessarily a zero of $R(f)$. The invariants g_2, g_3 of Weierstrass' elliptic function $\wp(z;g_2,g_3)$ are related to the coefficients of $R(f)$ according to[12]

$$g_2 = \alpha\epsilon - 4\beta\delta + 3\gamma^2, \tag{18}$$

$$g_3 = \alpha\gamma\epsilon + 2\beta\gamma\delta - \alpha\delta^2 - \gamma^3 - \epsilon\beta^2. \tag{19}$$

The discriminant [of $\wp$ and R (Ref. 13)]

$$\Delta = g_2^3 - 27g_3^2 \tag{20}$$

is suitable to classify the behavior of $f(z)$. In general, $f(z)$ is periodic.[14] If $\Delta = 0$, $g_2 \geqslant 0$, $g_3 \leqslant 0$, $f(z)$ is solitary wavelike and given by[15]

$$f(z) = f_0 + \frac{R'(f_0)}{4\left[e_1 - \frac{R''(f_0)}{24} + 3e_1 \operatorname{csch}^2(\sqrt{3e_1}z)\right]}, \tag{21}$$

where $e_1 = \sqrt[3]{-g_3}$ and f_0 now is a simple root of $R(f)$. In general, $f(z)$ (according to Eqs. (17) and (21)) is not real and bounded. Conditions for real and bounded solutions $f(z)$ can be obtained by considering the phase diagrams of $R(f)$.[16]

Inspection of Eqs. (16) shows that in most cases $\delta = \epsilon = 0$ holds or either δ or ϵ is zero and ϵ or δ is arbitrary. Thus a large set of solutions of Eq. (12) can be found by choosing $\delta = \epsilon = 0$ in Eqs. (16) simplifying the evaluation of the phase diagrams considerably. Following the lines of Ref. 10 real and bounded solutions $f(z)$ are associated to phase diagrams shown in Fig. 1. The periodic bounded solutions to Eq. (12) are associated to diagrams (a), (e). Choosing f_0 in Eq. (17) as the simple root

$$f_0 = -\frac{4\beta + \sqrt{(4\beta)^2 - 24\alpha\gamma}}{2\alpha}$$

evaluation of Eq. (17) yields

$$f(z) = \frac{-(4\beta + \sqrt{(4\beta)^2 - 24\alpha\gamma})(\gamma - 2\wp(z;3\gamma^2, -\gamma^3))}{2(4\beta^2 - 5\alpha\gamma + \beta\sqrt{(4\beta)^2 - 24\alpha\gamma} - 2\alpha\wp(z;3\gamma^2, -\gamma^3))}, \tag{22}$$

subject to $2\beta^2 - 3\alpha\gamma \geqslant 0$, $\gamma < 0$. These two inequalities are equivalent to the conditions (5) and (6). Thus, a subset of periodic solutions $f(z)$ of Eq. (12) compactly is represented by Eq. (22), where the coefficients α, β, γ are related to the parameters a, b, c, σ^2, k, v according to Eqs. (16a)–(16g).

Solitary wavelike solutions are represented by phase diagrams (b), (c), (d), (f), (g), (h) in Fig. 1.

Evaluation of Eq. (21) yields

$$f_{\pm}(z) = \frac{\gamma(\pm 4\beta + \sqrt{(4\beta)^2 - 24\alpha\gamma})\left(\gamma^2 - 1 + 3\gamma^2 \operatorname{csch}^2\left(\sqrt{\frac{3\gamma^3}{2}}z\right)\right)}{2\left(\pm 4\beta^2 + \beta\sqrt{(4\beta)^2 - 24\alpha\gamma} \mp \alpha\gamma(5+\gamma)^2 \mp 3\alpha\gamma^3 \operatorname{csch}^2\left(\sqrt{\frac{3\gamma^3}{2}}z\right)\right)} \tag{23}$$

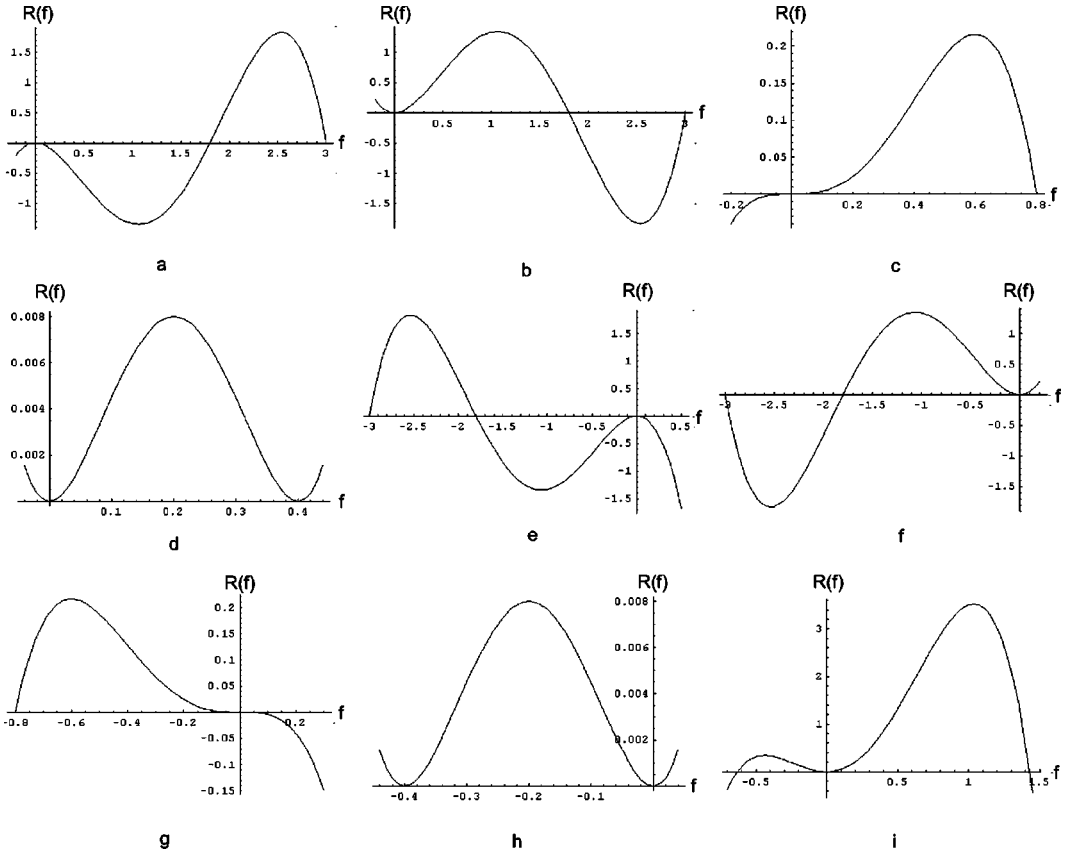

FIG. 1. Phase diagrams associated to real and bounded solutions if $\delta=\epsilon=0$.

for diagrams (b) and (f), where the upper and lower sign corresponds to (b) and (f), respectively, and subject to $\alpha\geqslant 0$, $\gamma>0$ and $2\beta^2-3\alpha\gamma\geqslant 0$. If $\alpha<0$, $\gamma>0$, $2\beta^2-3\alpha\gamma\geqslant 0$ (diagram (i)) two solitary wavelike solutions $f_+(z)$ and $f_-(z)$ exist, represented by Eq. (23). The conditions for these two cases are equivalent to the conditions (5) and (7).

By taking the limiting case ($\gamma\to 0$) of Weierstrass' elliptic function in Eq. (22), diagrams (c), (g) are associated with

$$f(z)=\frac{4\beta}{-\alpha+4\beta^2 z^2}, \tag{24}$$

representing algebraic solitary wavelike solutions.

To find the solutions corresponding to diagrams (d), (h) of Fig. 1 ($\alpha>0,\beta\lesseqgtr 0,\gamma=2\beta^2/3\alpha$) we choose $f_0=-(\beta/\alpha)$ in Eq. (17) and substitute $\wp(z;g_2,g_3)$ for the limiting case $\Delta=0$, $g_3=-(8\beta^6/27\alpha^3)<0$ according to[17]

$$\wp(z;g_2,g_3)=\sqrt[3]{-g_3}\left(1+\frac{3}{\sinh^2(3\sqrt[6]{-g_3}z)}\right)$$

to obtain the kink solitary wavelike solutions

$$f(z)=-\frac{\alpha}{\gamma}\left[1+\tanh\left(\frac{\beta z}{\sqrt{\alpha}}\right)\right],\quad \alpha>0,\quad \beta\lesseqgtr 0. \tag{25}$$

Thus we may conclude that this theorem is proved.

Remark 2: The modified Korteweg–de Vries equation (mKdVE)

$$\psi_t+6\psi^2\psi_x+\psi_{xxx}=0$$

is a particular case of Eq. (3) ($q=1,a=0,b=6,c=1,k=0$). Thus the parameters in (16f) are given by $\alpha=-1,\beta=0,\gamma=-(v/6)$ and δ, ϵ arbitrary. Since we assumed (for simplicity) $\delta=\epsilon=0$ in deriving Eqs. (22)–(25) these solutions belong to the subset of solutions restricted by $\delta=\epsilon=0$ (e.g., if $\gamma=1$ we obtain $f_{\pm}=\pm\sqrt{6}\,\mathrm{sech}(\sqrt{6}z)$ according to Eq. (23)). In this case all solutions (with $\gamma>0$ arbitrary) of the mKdVE exhibit a sech-shape behavior. If $\delta\neq 0,\epsilon\neq 0$ the analysis of the gmKPE and its relation to the mKdVE seems rather involved.

Remark 3: To evaluate the traveling wave (Weierstrass) solutions $\psi=f(x+ky+vt)^{1/q}$ of Eq. (3) we have to discriminate between positive and negative q and between positive and negative f (cf. Fig. 1).[18] If q is positive and f is positive, real and bounded, $\psi(x+ky+vt)$ is real and given by Eqs. (22)–(25) subject to the corresponding constraints (cf. Figs. 1(a)–1(d), partly (i)) for the various triples $\{\alpha,\beta,\gamma\}$ according to Eqs. (16). In this case q is restricted either by (16e)–(16g) or by (16a) with $q>0$, subject to restrictions for α, β, γ so that f is positive (cf. Figs. 1(a)–1(d), partly (i)).

If f is negative, real and bounded, the restrictions for positive q are different. In this case the parameter q must satisfy

$$q=\frac{1}{2m},\quad m\in\mathbb{N}. \tag{26}$$

Thus, the cases (16f), (16g) have to be excluded, the cases (16b), (16e) are consistent with (26) if α, β, γ fullfill the constraints for f to be negative (cf. Figs. 1(e)–1(h), partly (i)). These constraints also must be satisfied in case (16a). Hence one obtains for this case

$$\alpha<0,\ \beta<0,\ \gamma\leqslant 0\quad\text{or}\quad \alpha>0,\ \beta>0,\ \gamma>0\left(\text{or}\ \gamma=\frac{2\beta^2}{3\alpha}\right)\quad\text{or}\quad \alpha<0,\ \gamma>0, \tag{27}$$

with

$$\alpha=\frac{-b}{2c(1+m)(1+2m)},\quad \beta=\frac{-a}{2c(1+2m)(1+4m)},\quad \gamma=\frac{k^2\sigma^2-v}{24cm^2},\quad m\in\mathbb{N} \tag{28}$$

as constraints for $q=1/2m$, if f, represented by Eqs. (22)–(25), is negative, real and bounded. If q is negative, $f(z)$ may be unbounded but $f=0$ must be excluded for $g(z)$ to be real and bounded. The condition $f\neq 0$ is satisfied for a certain interval in (a), (e) of Fig. 1. Phase diagram (a) is associated to $f>0$ so that $g(z)$ is real and bounded for negative q with no further restriction. Diagram (e) is related to $f<0$ leading to $q=-(1/2m),m\in\mathbb{N}$.

It follows from these remarks and the proof of the Theorem that we proved the following corollaries.

Corollary 1: Let $q=-1/2$ or $q=-2$. Assume that in Eq. (3) $b=0$ if $q=-\frac{1}{2}$ and $a=0$ if $q=-2$, respectively. Assume also that the following condition:

$$2\beta^2-3\alpha\gamma\geqslant 0 \tag{29}$$

holds, where α, β, γ satisfy (16b) and (16d), respectively. Then there exists a real and bounded solution of Eq. (3) of the form (4) and this solution is periodic if condition (6) holds and solitary wavelike if condition (7) is valid.

Corollary 2: Let $q=1/2, q=1$ or $q=2$. Assume that inequality (29) is satisfied and the conditions

$$\Delta=0, \quad g_2\geqslant 0, \quad g_3\leqslant 0 \tag{30}$$

hold, where α, β, γ, δ, ϵ are given by (16e), (16f), and (16g), respectively. Then there exists a solitary wavelike solution of Eq. (3) of the form (4) which is real and bounded. If the conditions (30) are not satisfied, then Eq. (3) has a periodic solution of the form (4) which is also real and bounded.

Remark 4: If $q=-1$, we have to assume, in order to use the method, that $a=0$ and $b=0$ (cf. (16c)). In this case Eq. (8) will be linear with constant coefficients (corresponding to $q=0$ in Eq. (3)) and can be solved by standard methods.

III. SUMMARY

We have shown that via an ansatz $\psi(x,y,t)=g(z)=(f(z))^{1/q}$, $z=x+ky+vt$, and subject to the nonlinear ordinary differential equation (12) a rather large set of solutions to the gmKPE can be obtained. Periodic and solitary wave solutions can be presented in compact form in terms of Weierstrass' elliptic functions and its limiting cases ($\Delta=0$, $g_3\leqslant 0$), respectively. A phase diagram analysis (cf. Fig. 1) yields conditions for the existence of real bounded solutions and conditions for the parameters $\{a,b,c,\sigma^2,k,v,q\}$ of the gmKPE.

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[17] In Ref. 14, Eq. (18.12.3), p. 651.
[18] For $q<0$ we disregard unbounded solutions $f(z)$ that satisfy $R(f)\geqslant 0$, $f\neq 0$ (cf. Fig. 1, $3\leqslant f<\infty$ in (b), $-\infty<f\leqslant -3$ in (f)). They may lead to real and bounded $g(z)$ but the physical significance seems doubtful.

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Fine gradings of $o(4,\mathbb{C})$

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A grading of a Lie algebra is called fine if it cannot be further refined. Fine gradings provide basic information about the structure of the algebra. There are six fine gradings of the semisimple Lie algebra of type $A_1 \times A_1$ over the complex number field. An explicit description of all the fine gradings of $A_1 \times A_1$ is given in terms of the four-dimensional representation $o(4,\mathbb{C})$ of the algebra. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1737054]

I. INTRODUCTION

This paper is the fourth one in a series,[1–3] containing description of maximal gradings, i.e., gradings not refinable any further, for simple/semisimple Lie algebras of particular types.

The algebra $D_2 = o(4,\mathbb{C})$ is exceptional among the classical Lie algebras by the fact that it is not simple. It is semisimple and consists of two ideals A_1. This widens its group of automorphisms, and thus the number of its fine gradings is bigger than one would expect for an algebra of dimension 6. Compare that, e.g., $B_2 = C_2$ of dimension 10 has three fine gradings, A_2 of dimension 8 has four fine gradings, $A_3 = D_3$ of dimension 15 has eight fine gradings. All the fine gradings of the three cases mentioned—A_2, $B_2 = C_2$, and $A_3 = D_3$—are found in Refs. 1–3. The fine gradings of $sl(3,\mathbb{C})$ (i.e., A_2) and of its real forms are found in Ref. 1, in Ref. 2 there are the fine gradings of $sp(4,\mathbb{C})$, $o(5,\mathbb{C})$, and of their real forms (i.e., $C_2 = B_2$). Finally, in Ref. 3 the fine gradings of $sl(4,\mathbb{C})$ and $o(6,\mathbb{C})$ (i.e., $A_3 = D_3$) are given.

The nonsimplicity of $o(4,\mathbb{C})$ also implies the rich structures of fine gradings of real forms. Existence of an automorphism that permutes the two ideals $sl(2,\mathbb{C})$ determines which of the fine gradings of $o(4,\mathbb{C})$ appear in the real forms of $o(4,\mathbb{C})$. In principle, one could study the fine gradings of real forms independently of the complex algebra. However, the gradings of real forms are naturally related to the gradings of the complex algebra. For simplicity of the presentation we have chosen to describe the fine gradings of the real forms separately in the forthcoming paper. Let us point out that the number of fine gradings of the real forms varies between two on the real form $o(4)$ and six on the real form $o(2,2)$.

The algebra D_2 has two nonequivalent representations of dimension 4. One of them is of the type $o(4,\mathbb{C}) = \{X \in \mathbb{C}^{4\times 4} \mid XK + KX^T = 0\}$, where $K = K^T$, $\det K \neq 0$. Often one puts $K = I_4$, and then the algebra is represented by matrices that are skew symmetric with respect to transposition.

The second representation of dimension 4 is reducible. It decomposes into two irreducible ones of dimension 2 each. In each of them one of the ideals is represented trivially. In terms of the highest weights of the representations one has the representation $(1)(0)+(0)(1)$, while the first case is irreducible with the highest weight $(1)(1)$. The reducible representation can be written as

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$$\left\{ \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \middle| A,B \in \mathbb{C}^{2\times 2}, \operatorname{tr} A = \operatorname{tr} B = 0 \right\}.$$

Isomorphic gradings in these different representations look different. Moreover, the reducible representation admits a symplectic invariant form so that it can be viewed as representing the subalgebra of type $sl(2,\mathbb{C})+sl(2,\mathbb{C})$ of $sp(4,\mathbb{C})$.

II. PRELIMINARIES

A. Basic terminology

For motivation and for general comments concerning our undertaking, we refer the reader to Refs. 2 and 3. Here we confine ourselves to our immediate task, namely the fine gradings of $o(4,\mathbb{C})$. A *fine grading* Γ of a Lie algebra L is a decomposition of L into a direct sum of subspaces $0 \neq L_j \subset L$, $j \in \mathcal{J}$,

$$\Gamma: L = \bigoplus_{j \in \mathcal{J}} L_j, \tag{1}$$

such that for each pair j,k of indices from the index set $\mathcal{J}$ the commutator fulfills

$$[L_j, L_k] \subset L_l \tag{2}$$

for some $l \in \mathcal{J}$. With suitable choice of the index set $\mathcal{J}$, we are able to ensure that the index l from (2) turns into $[L_j, L_k] \subset L_{j+k}$ for $[L_j, L_k] \neq 0$. In order to do so we embed the index set $\mathcal{J}$ into an additive commutative group. The indices $j \in \mathcal{J}$ can be multicomponent ones. We use here from one up to four components.

A fine grading cannot be further refined while remaining a grading: it decomposes the Lie algebra into a maximal number of subspaces. Particularly interesting are the gradings which decompose the algebra into the sum of one-dimensional subspaces. Indeed, they provide a basis which is convenient to work with. A graded basis reflects structural properties of the Lie algebra such as the simplicity of commutation relations of the generators.

Fine gradings have a special position among all the gradings. That is because out of the fine gradings one can derive all gradings of the algebra, namely by "coarsening" the fine gradings, i.e., merging some of the grading subspaces. However, it is a rather complicated process and currently the result is only known for Lie algebras of rank 2.

Gradings $\Gamma_1: L = \oplus_{j \in \mathcal{I}} L_j$ and $\Gamma_2: L = \oplus_{m \in \mathcal{J}} K_m$ of the Lie algebra L are equivalent when

(i) $|\mathcal{I}| = |\mathcal{J}|$ and

(ii) there exist an automorphism h on L and a bijection $\pi: \mathcal{I} \to \mathcal{J}$ fulfilling the property $h(L_j) = K_{\pi(j)}$ for all $j \in \mathcal{I}$. Equivalence of the gradings Γ_1 and Γ_2 is denoted by $\Gamma_1 \cong \Gamma_2$.

The Lie algebra $o(4,\mathbb{C})$ is a direct sum of two $sl(2,\mathbb{C})$ algebras. Thus some of the fine gradings of $o(4,\mathbb{C})$ arise from fine gradings of $sl(2,\mathbb{C})$. Therefore it is logical to begin by description of fine gradings of the Lie algebra $sl(2,\mathbb{C})$.

B. Fine gradings of the Lie algebra $sl(2,\mathbb{C})$

The Lie algebra $sl(2,\mathbb{C})$ consists of 2×2 matrices with zero trace, i.e.,

$$sl(2,\mathbb{C}) = \left\{ \begin{pmatrix} a & b \\ c & -a \end{pmatrix} \middle| a,b,c \in \mathbb{C} \right\}. \tag{3}$$

Its two fine gradings are notorious. They are also the two types of fine gradings that occur in all the Lie algebras of the type $sl(n,\mathbb{C})$: one is the Cartan (root) grading, the other one is the Pauli grading (studied in Ref. 4). (See Table I.)

TABLE I. The two nonequivalent fine gradings of the Lie algebra $sl(2,\mathbb{C})$; the index sets $\mathcal{J}$ are embedded into additive groups $\mathbb{Z}_3, \mathbb{Z}_2\times\mathbb{Z}_2$, respectively, so that they reflect the commutation relations between the grading subspaces.

Cartan grading	Pauli grading
$\Upsilon_1: sl(2,\mathbb{C}) = L_0 \oplus L_1 \oplus L_2$	$\Upsilon_2: sl(2,\mathbb{C}) = L_{01} \oplus L_{10} \oplus L_{11}$
$L_0 = \mathbb{C}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$L_{01} = \mathbb{C}\cdot\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$L_1 = \mathbb{C}\cdot\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$	$L_{10} = \mathbb{C}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$L_2 = \mathbb{C}\cdot\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$	$L_{11} = \mathbb{C}\cdot\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
$\mathcal{J}\subset\mathbb{Z}_3$	$\mathcal{J}\subset\mathbb{Z}_2\times\mathbb{Z}_2$
$[L_j, L_k] = L_{j+k \bmod 3}$	$[L_{jk}, L_{lm}] = L_{(j+l)(k+m)\bmod 2,2}$
for all $j,k\in\mathcal{J}, j\neq k$	for all $(j,k),(l,m)\in\mathcal{J}, (j,k)\neq(l,m)$

It is convenient to present here also the graphs depicting the commutation relations within the gradings. The vertices of the graph stand for the grading subspaces, each of them denoted by the label of the subspace. It is convenient to visualize a grading as follows. Two vertices are connected by an edge when the two corresponding subspaces do not commute, i.e., their commutator does not equal zero. In that case, necessarily, their commutator must fall into one of the grading subspaces; its label is given by the grading property (2). Note that the labels are always chosen in such a way that the label of the commutator of two subspaces is the sum of labels of the two commuted subspaces (using a suitable modulo). (See Fig. 1.)

An important use of these graphs is the following: **Two fine gradings are equivalent if and only if their graphs of commutators are equivalent.**

Later on, when a fine grading of the Lie algebra $o(4,\mathbb{C})$ is in the form of a direct sum of two fine gradings of $sl(2,\mathbb{C})$, the graph related to that grading is purely composed of two appropriate graphs.

C. MAD-groups on $o(4,\mathbb{C})$

When describing fine gradings of a complex simple Lie algebra L we can follow the result published in Ref. 5 (using subgroups of the group $\mathrm{Aut}\,L$ of all automorphisms on L).

Theorem 2.1: *A decomposition $\Gamma: L = \oplus_j L_j$ is a fine grading of a simple Lie algebra L over an algebraically closed field of characteristic zero if and only if there exists a maximal Abelian subgroup $\mathcal{G}\subset \mathrm{Aut}\,L$ of diagonalizable automorphisms on L (MAD-group) such that Γ is a decomposition of L into simultaneous eigensubspaces L_j of all elements from $\mathcal{G}$.*

But $o(4,\mathbb{C}) = sl(2,\mathbb{C})\times sl(2,\mathbb{C})$ is not simple, so only one implication in the aforesaid theorem holds, thus that each fine grading of $o(4,\mathbb{C})$ is a decomposition of L into simultaneous eigenspaces

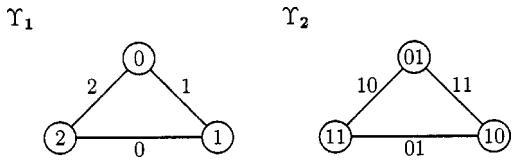

FIG. 1. These graphs depict commutation relations in the two fine gradings of the Lie algebra $sl(2,\mathbb{C})$: Υ_1 represents the Cartan grading and Υ_2 the Pauli grading. When summing the labels in order to obtain the label of the commutator we use mod 3, mod 2,2, respectively, for Υ_1, Υ_2.

of all automorphisms from some MAD-group. But there exists a MAD-group in $\mathrm{Aut}\, o(4,\mathbb{C})$ which generates a grading that is not fine.

However, we use this method with the six nonconjugate MAD-groups on $o(4,\mathbb{C})$. Five of them generate a fine grading of $o(4,\mathbb{C})$, one of them does not; namely the maximal torus. The torus generates a grading with one two-dimensional and four one-dimensional subspaces. Nevertheless, the two-dimensional subspace can be split into two one-dimensional subspaces so that we obtain a decomposition of $o(4,\mathbb{C})$ which remains a grading. All the six (nonequivalent) fine gradings of $o(4,\mathbb{C})$ consist of six one-dimensional subspaces. With each of the fine gradings we provide a graph depicting the commutation relations in the grading. It is obvious from these graphs that the six fine gradings are nonequivalent.

In terms of 4×4 matrices the Lie algebra $o(4,\mathbb{C})$ is expressed as

$$o_K(4,\mathbb{C})=\{X\in\mathbb{C}^{4\times 4}\,|\,XK+KX^T=0\} \tag{4}$$

with $K\in\mathbb{C}^{4\times 4}$ symmetric ($K^T=K$) and nonsingular. All the representations $o_K(4,\mathbb{C})$ are equivalent, and, having a grading on one of them, we can transfer it onto another representation of $o(4,\mathbb{C})$ by $\widetilde{L}_j=\mathrm{Ad}_M L_j$ with a suitable matrix M. We provide our results on the representation $o_K(4,\mathbb{C})$ with

$$K=\begin{pmatrix}0&1\\-1&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix}=\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix},$$

which reflects how $o(4,\mathbb{C})$ arises as a product of two Lie algebras $sl(2,\mathbb{C})$:

$$o(4,\mathbb{C})=\left\{X\in\mathbb{C}^{4\times 4}\,\middle|\,X\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix}+\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix}X^T=0\right\}$$

$$=\left\{\begin{pmatrix}a&b&c&0\\d&e&0&c\\f&0&-e&b\\0&f&d&-a\end{pmatrix}\,\middle|\,a,\ldots,f\in\mathbb{C}\right\}, \tag{5}$$

$$(sl(2,\mathbb{C})\otimes I)+(I\otimes sl(2,\mathbb{C}))=\left\{\begin{pmatrix}A&B\\C&-A\end{pmatrix}\otimes I\right\}+\left\{I\otimes\begin{pmatrix}D&E\\F&-D\end{pmatrix}\right\}$$

$$=\left\{\begin{pmatrix}A+D&E&B&0\\F&A-D&0&B\\C&0&-A+D&E\\0&C&F&-A-D\end{pmatrix}\,\middle|\,A,\ldots,F\in\mathbb{C}\right\}. \tag{6}$$

As well as for each Lie algebra of the type $o(n,\mathbb{C})$ (with the exception of $n=8$), the group $\mathrm{Aut}\, o(4,\mathbb{C})$ contains only inner automorphisms Ad_A with $A\in O(4,\mathbb{C})$,

$$O(4,\mathbb{C})=\{A\in\mathbb{C}^{4\times 4}|AKA^T=K\}.$$

The inner automorphism Ad_A acts on elements $X\in o(4,\mathbb{C})$ by $\mathrm{Ad}_A(X)=A^{-1}XA$.

TABLE II. The full list of nonconjugate maximal Abelian subgroups of diagonalizable automorphisms (MAD-groups) on $o(4,\mathbb{C})$: MAD-group $\mathcal{H}=\{\mathrm{Ad}_A|A\in H_{\mathrm{Ad}}\}$.

	H_{Ad}
$\mathcal{H}_1$	$\{A=\mathrm{diag}(\alpha,\alpha^{-1})\otimes\mathrm{diag}(\beta,\beta^{-1}),\alpha,\beta\in\mathbb{C}\setminus\{0\}\}$
$\mathcal{H}_2$	$\{A=\sigma_j\otimes\sigma_k,\ j,k=0,1,2,3\}$
$\mathcal{H}_3$	$\{A=\sigma_j\otimes\mathrm{diag}(\alpha,\alpha^{-1}),\alpha\in\mathbb{C}\setminus\{0\}\}$
$\mathcal{H}_4$	$\left\{A\in\left\{\pm\begin{pmatrix}\alpha&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&\alpha^{-1}\end{pmatrix},\pm\begin{pmatrix}\alpha&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&\alpha^{-1}\end{pmatrix}\right\},\alpha\in\mathbb{C}\setminus\{0\}\right\}$
$\mathcal{H}_5$	$\left\{A\in\left\{\begin{pmatrix}\varepsilon_1&0&0&0\\0&\varepsilon_2&0&0\\0&0&\varepsilon_2&0\\0&0&0&\varepsilon_1\end{pmatrix},\begin{pmatrix}\varepsilon_1&0&0&0\\0&0&\varepsilon_2&0\\0&\varepsilon_2&0&0\\0&0&0&\varepsilon_1\end{pmatrix},\begin{pmatrix}0&0&0&\varepsilon_1\\0&\varepsilon_2&0&0\\0&0&\varepsilon_2&0\\\varepsilon_1&0&0&0\end{pmatrix},\begin{pmatrix}0&0&0&\varepsilon_1\\0&0&\varepsilon_2&0\\0&\varepsilon_2&0&0\\\varepsilon_1&0&0&0\end{pmatrix}\right\},\varepsilon_j=\pm1\right\}$
$\mathcal{H}_6$	$\left\{A\in\left\{\pm\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\pm\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},\pm\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&-1&0&0\\0&0&0&-1\end{pmatrix},\pm\begin{pmatrix}1&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&-1\end{pmatrix},\right.\right.$ $\left.\left.\pm\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},\pm\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix},\pm\begin{pmatrix}0&0&0&-1\\0&-1&0&0\\0&0&1&0\\1&0&0&0\end{pmatrix},\pm\begin{pmatrix}0&0&0&-1\\0&1&0&0\\0&0&-1&0\\1&0&0&0\end{pmatrix}\right\}\right\}$

As already mentioned, there are six (nonequivalent) fine gradings of $o(4,\mathbb{C})$ corresponding to six (nonconjugate) MAD-groups $\mathcal{H}_1,\ldots,\mathcal{H}_6$ listed in Table II (derived from Ref. 6). The symbols σ_k, $k=0,1,2,3$, stand for 2×2 Pauli matrices,

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&1\\-1&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{7}$$

We describe each MAD-group $\mathcal{H}$ by listing out a group of matrices H_{Ad} such that $\mathcal{H}=\{\mathrm{Ad}_A|A\in H_{\mathrm{Ad}}\}$.

The three MAD-groups $\mathcal{H}_1,\mathcal{H}_2$, and $\mathcal{H}_3$ contain only such automorphisms Ad_A, where A is a direct sum of two parts, $A_1\otimes I$ and $I\otimes A_2$ (with $I,A_1,A_2\in\mathbb{C}^{2\times2}$). It follows that the three fine gradings Γ_1,Γ_2, and Γ_3 generated by $\mathcal{H}_1,\mathcal{H}_2$, and $\mathcal{H}_3$, respectively, have basis elements either in the form $X=Y\otimes I$ or $X=I\otimes Y$, $Y\in sl(2,\mathbb{C})$. They arise as $\Gamma=(\Upsilon_j\otimes I)\oplus(I\otimes\Upsilon_k)$, Υ_j,Υ_k being one of the two fine gradings of $sl(2,\mathbb{C})$ described in Table I.

The remaining three fine gradings $\mathcal{H}_4,\mathcal{H}_5$, and $\mathcal{H}_6$ do not conserve such a nice structure.

III. THE SIX FINE GRADINGS OF THE LIE ALGEBRA $O(4,\mathbb{C})$

As explained in Sec. II C, we find the fine gradings as simultaneous eigensubspaces of all elements (automorphisms) of a MAD-group $\mathcal{H}_k$. But we never need to use all elements from $\mathcal{H}_k$ when searching for the fine grading, but just a few of them, sometimes even one is enough. In this section we provide a list of all the six nonequivalent fine gradings of $o(4,\mathbb{C})$; not only in terms of basis elements of the grading subspaces L_j, but also in terms of so-called grading labels, i.e., indices $j\in\mathcal{J}$ such that $[L_j,L_k]\subset L_{j+k}$ for all $j,k\in\mathcal{J}$, $[L_j,L_k]\neq0$ [as described in (2)]; the index set $\mathcal{J}$ being a subset of a finite additive group. This embedding of $\mathcal{J}$ into an additive group is very

TABLE III. The three fine gradings of $o(4,\mathbb{C})$ which are purely a composition of fine gradings Υ_j of $sl(2,\mathbb{C})$. Υ_1 is the Cartan (root) grading of $sl(2,\mathbb{C})$ with indices from the additive group $\mathbb{Z}_3$, Υ_2 is the Pauli grading of $sl(2,\mathbb{C})$ with indices from the additive group $\mathbb{Z}_2\times\mathbb{Z}_2$.

$\Gamma_1=(\Upsilon_1\otimes I)\oplus(I\otimes\Upsilon_1)$	Cartan/root grading
$\Gamma_2=(\Upsilon_2\otimes I)\oplus(I\otimes\Upsilon_2)$	
$\Gamma_3=(\Upsilon_2\otimes I)\oplus(I\otimes\Upsilon_1)$	

useful because the indices $j\in\mathcal{J}$ provide the vital information on the structure of the fine grading, namely the commutation relations. (It can of course occur that $j+k\notin\mathcal{J}$ for some $j,k\in\mathcal{J}$. In this case, necessarily, $[L_j,L_k]=0$.)

The additive group into which $\mathcal{J}$ is embedded is not uniquely defined. However, we use the smallest possible (regarding its order).

A. Fine gradings of $o(4,\mathbb{C})$ corresponding to the MAD-groups $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$

These fine gradings are composed of gradings Υ_1 and Υ_2 of the algebra $sl(2,\mathbb{C})$ as depicted in Table III. The graded subspaces of Υ_1 are labeled by the group $\mathbb{Z}_3$ and the graded subspaces of Υ_2 are labeled by the group $\mathbb{Z}_2\times\mathbb{Z}_2$. Therefore, the fine grading Γ_1 is labeled by $\mathbb{Z}_3\times\mathbb{Z}_3$, the fine grading Γ_2 is labeled by $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$, and the fine grading Γ_3 is labeled by $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_3$.

The graphs corresponding to the gradings Γ_1, Γ_2, and Γ_3 are formed by two independent components, each of them representing one of the grading Υ_i of $sl(2,\mathbb{C})$.

B. Γ_4, fine grading of $o(4,\mathbb{C})$ corresponding to the MAD-group $\mathcal{H}_4$

Now we are coming to the three fine gradings that cannot be expressed as $(\Upsilon_j\otimes I)\oplus(I\otimes\Upsilon_k)$, Υ_j,Υ_k being fine gradings of $sl(2,\mathbb{C})$. Instead there are only three pairs of commuting grading subspaces (i.e., only three zeroes in all the commutations). (See Fig. 2.)

The fine grading Γ_4 is obtained with the use of just one element

$$\mathrm{Ad}_A\in\mathcal{H}_4,\quad A=\begin{pmatrix}\alpha & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & \dfrac{1}{\alpha}\end{pmatrix};$$

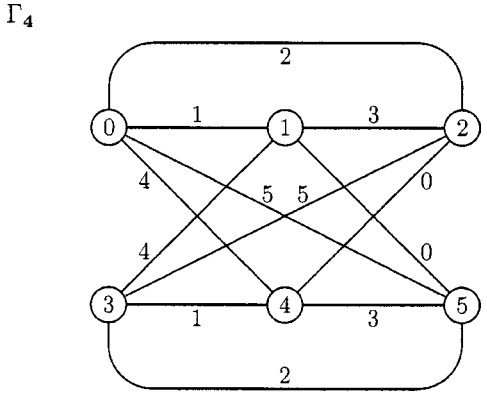

FIG. 2. This graph depicts the commutation relations in the fine grading Γ_4 of $o(4,\mathbb{C})$. The graph is connected and thus the grading is not a direct sum of gradings of $sl(2,\mathbb{C})$ as were the cases of Γ_1, Γ_2, and Γ_3. Commuting two subspaces shows in the graph as summing the respective labels mod 6.

TABLE IV. Eigenvalues of Ad_A corresponding to eigensubspaces L_j, grading subspaces of $o(4,\mathbb{C})$ in the fine grading Γ_4.

Eigensubspace	L_0	L_1	L_2	L_3	L_4	L_5
Eigenvalue	1	α	$-\alpha^{-1}$	-1	$-\alpha$	α^{-1}

the eigenvalues corresponding to the eigensubspaces of Ad_A are listed in Table IV.

The index set $\mathcal{J}$ of indices denoting subspaces L_j equals the additive group $\mathbb{Z}_6$,

$$[L_j,L_k]\subset L_{j+k \bmod 6},$$

$$L_0:X_1=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-1\end{pmatrix},\quad L_3:X_4=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix},$$

$$L_1:X_2=\begin{pmatrix}0&0&0&0\\1&0&0&0\\1&0&0&0\\0&1&1&0\end{pmatrix},\quad L_4:X_5=\begin{pmatrix}0&0&0&0\\1&0&0&0\\-1&0&0&0\\0&-1&1&0\end{pmatrix}, \tag{8}$$

$$L_2:X_3=\begin{pmatrix}0&1&-1&0\\0&0&0&-1\\0&0&0&1\\0&0&0&0\end{pmatrix},\quad L_5:X_6=\begin{pmatrix}0&1&1&0\\0&0&0&1\\0&0&0&1\\0&0&0&0\end{pmatrix}.$$

C. Γ_5, fine grading of $o(4,\mathbb{C})$ corresponding to the MAD-group $\mathcal{H}_5$

All automorphisms from the MAD-group $\mathcal{H}_5$ have just two possible eigenvalues, namely ± 1. Thus at least three automorphisms $\mathrm{Ad}_A\in\mathcal{H}_5$ are needed to split $o(4,\mathbb{C})$ into six one-dimensional eigensubspaces. We use the following triplet $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2},\mathrm{Ad}_{A_3}$:

$$A_1=\begin{pmatrix}0&0&0&1\\0&-1&0&0\\0&0&-1&0\\1&0&0&0\end{pmatrix},\quad A_2=\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix},\quad A_3=\begin{pmatrix}0&0&0&1\\0&1&0&0\\0&0&1&0\\1&0&0&0\end{pmatrix}.$$

The relationship between the grading subspaces L_j of $o(4,\mathbb{C})$ and these automorphisms can be described as follows:

$$L_{jkl}=\{X\in o(4,\mathbb{C})\mid \mathrm{Ad}_{A_1}X=(-1)^jX,\ \ \mathrm{Ad}_{A_2}X=(-1)^kX,\ \ \mathrm{Ad}_{A_3}X=(-1)^lX\},$$

and, clearly, the index set $\mathcal{J}$ is embedded into the additive group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$. (See Fig. 3.)

Let us continue by providing the list of basis elements of the grading subspaces:

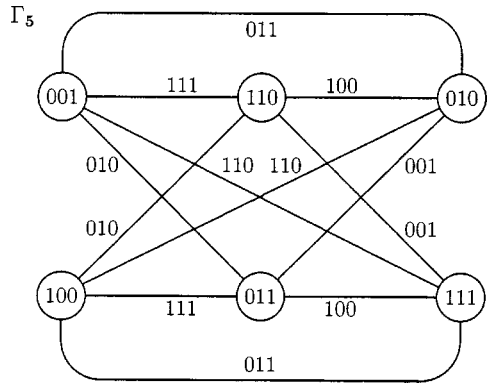

FIG. 3. This graph depicts the commutation relations in the fine grading Γ_5 of $o(4,\mathbb{C})$. Commuting two subspaces shows in the graph as summing the respective labels mod 2,2,2.

$$L_{001}:X_1=\begin{pmatrix} 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 0 \end{pmatrix}, \quad L_{010}:X_4=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$L_{100}:X_2=\begin{pmatrix} 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}, \quad L_{110}:X_5=\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \tag{9}$$

$$L_{111}:X_3=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad L_{011}:X_6=\begin{pmatrix} 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{pmatrix}.$$

The commutation relations are expressed with help of the indices $j \in \mathcal{J}$ by

$$[L_{jkl},L_{mno}] \subset L_{(j+m)(k+n)(l+o)\,\mathrm{mod}\,2,2,2} \quad \text{for } [L_{jkl},L_{mno}] \neq 0.$$

D. Γ_6, fine grading of $o(4,\mathbb{C})$ corresponding to the MAD-group $\mathcal{H}_6$

Finally we have come to the last case, the fine grading generated by the MAD-group $\mathcal{H}_6$. (See Fig. 4.) This MAD-group contains not only automorphisms with eigenvalues ± 1, but also with complex eigenvalues $\pm i$, so we are able to reach a splitting into six one-dimensional subspaces/eigenspaces with the use of two elements $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2} \in \mathcal{H}_6$ only,

$$A_1=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad A_2=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ & 0 & 0 & -1 \end{pmatrix},$$

the latter one with complex eigenvalues. The indices $j \in \mathcal{J} \subset \mathbb{Z}_2 \times \mathbb{Z}_4$ of subspaces L_j are set down in accordance with the eigenvalues by

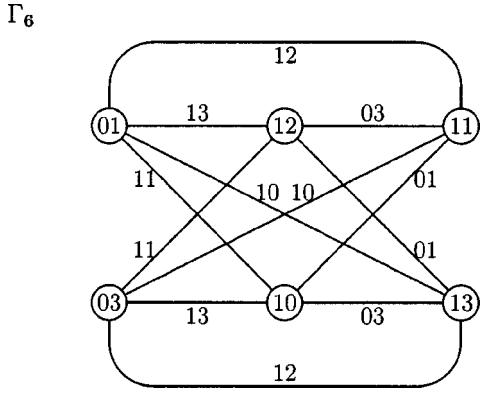

FIG. 4. This graph depicts the commutation relations in the fine grading Γ_6 of $o(4,\mathbb{C})$. Commuting two subspaces shows in the graph as summing the respective labels mod 2,4.

$$L_{jk}=\{X\in o(4,\mathbb{C})\,|\,\mathrm{Ad}_{A_1}X=(-1)^jX,\mathrm{Ad}_{A_2}X=i^kX\}.$$

The list of basis elements of L_j follows:

$$L_{10}:X_1=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-1\end{pmatrix},\quad L_{03}:X_4=\begin{pmatrix}0&1&i&0\\1&0&0&i\\i&0&0&1\\0&i&1&0\end{pmatrix},$$

$$L_{12}:X_2=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix},\quad L_{11}:X_5=\begin{pmatrix}0&1&-i&0\\-1&0&0&-i\\i&0&0&1\\0&i&-1&0\end{pmatrix},\tag{10}$$

$$L_{01}:X_3=\begin{pmatrix}0&1&-i&0\\1&0&0&-i\\-i&0&0&1\\0&-i&1&0\end{pmatrix},\quad L_{13}:X_6=\begin{pmatrix}0&1&i&0\\-1&0&0&i\\-i&0&0&1\\0&-i&-1&0\end{pmatrix}.$$

Commutation relations within this grading are summoned by

$$[L_{jk},L_{lm}]\subset L_{(j+l)(k+m)\bmod 2,4}\quad\text{for }[L_{jk},L_{lm}]\neq 0.$$

E. Nonequivalence of the six fine gradings $\Gamma_1,\ldots,\Gamma_6$

Having two fine gradings $\Gamma_1:L=\oplus_{j\in\mathcal{I}}L_j$ and $\Gamma_2:L=\oplus_{m\in\mathcal{J}}K_m$ of a Lie algebra L, we call Γ_1 and Γ_2 equivalent when both $|\mathcal{I}|=|\mathcal{J}|$ and there exist an automorphism h on L and a bijection $\pi:\mathcal{I}\to\mathcal{J}$ fulfilling the property $h(L_j)=K_{\pi(j)}$ for all $j\in\mathcal{I}$. From the structural point of view equivalent gradings are the same because the commutation relations are the same. Thus we are only interested in nonequivalent fine gradings of $o(4,\mathbb{C})$.

It is a general rule that if $\mathcal{H}_1,\mathcal{H}_2\subset\mathrm{Aut}\,L$ are Abelian subgroups of diagonalizable automorphisms on the Lie algebra L and Γ_1,Γ_2 gradings of L generated by subgroups $\mathcal{H}_1,\mathcal{H}_2$, respectively, then the gradings Γ_1 and Γ_2 are equivalent if and only if the subgroups $\mathcal{H}_1$ and $\mathcal{H}_2$ are

conjugate, i.e., $\mathcal{H}_2 = h^{-1}\mathcal{H}_1 h$ for some $h \in \mathrm{Aut}\, L$. We have six nonconjugate MAD-groups $\mathcal{H}_1,\ldots,\mathcal{H}_6$ in $\mathrm{Aut}\, o(4,\mathbb{C})$ (according to Ref. 6), and thus our six fine gradings $\Gamma_1,\ldots,\Gamma_6$ are nonequivalent, since they are generated by $\mathcal{H}_1,\ldots,\mathcal{H}_6$.

But their nonequivalence can also be easily seen from the graphs provided with each of the fine gradings, since these graphs reflect directly the commutation relations among the grading subspaces.

Clearly none of the gradings $\Gamma_1,\Gamma_2,\Gamma_3$ is equivalent to any of the gradings $\Gamma_4,\Gamma_5,\Gamma_6$, just because of the number of commuting subspaces (one pair of noncommuting subspaces corresponds to one edge in the graph). Nonequivalence of the gradings $\Gamma_1,\Gamma_2,\Gamma_3$ follows from the fact that they arise as compositions of the fine gradings Υ_1,Υ_2 of $sl(2,\mathbb{C})$ as described in Table III, and Υ_1 is not equivalent to Υ_2.

Now it remains to show the nonequivalence of gradings $\Gamma_4,\Gamma_5,\Gamma_6$:

(i) Γ_4 contains a subspace $M = L_0$ such that $[M,L_j] \subset L_j$ for all the grading subspaces L_j; Γ_5,Γ_6 do not contain such a subspace M.

(ii) In Γ_5 there exists a triplet of grading subspaces such that they make up a three-dimensional subalgebra of $o(4,\mathbb{C})$. In the graph they are represented by vertices 1,3,5. Again, this is not the case of Γ_6.

So we have two independent proofs of nonequivalence of our six fine gradings $\Gamma_1,\ldots,\Gamma_6$.

IV. CONCLUSION

There is indeed a number of applications of the fine gradings described above as well as further questions one may ask related to the gradings of both $o(4,\mathbb{C})$ and its real forms:

(i) One of the motivations for studying the gradings in general is given by the graded contractions of a concrete algebra, in particular the contraction of $o(4,\mathbb{C})$ which preserves the chosen grading. Due to the large number of possible gradings such contraction will yield many Lie algebras.

(ii) The inhomogeneous $o(4,\mathbb{C})$, which is a semidirect product of $o(4,\mathbb{C}) \ltimes T_4$, where T_4 is Abelian subalgebra of four translations in $\mathbb{C}^4$, is complex form of the Poincare Lie algebra. This is one of the most exploited algebras of physics. Knowledge of the fine gradings of $o(4,\mathbb{C})$ enables one to describe all fine gradings of complex Poincare Lie algebra and of its representations. Even more interesting would be the contractions of infinite dimensional representations of the Poincare Lie algebra.[7,8]

(iii) Let us notice that $o(4,\mathbb{C})$ is a maximal semisimple subalgebra of the exceptional simple algebra G_2 and thus the six fine gradings found for $o(4,\mathbb{C})$ can be extended to fine gradings of G_2.

(iv) It would be interesting to describe also the gradings in terms of representations and find the eigenspaces of MAD-groups for all the representation spaces.

(v) This work is a basis for study of gradings of the real forms.

(vi) As among the real forms of $o(4,\mathbb{C})$ is the Lorenz algebra $o(3,1)$, one feels motivated to study the gradings of the infinite dimensional representation of $o(3,1)$. Indeed, those are the representations of $o(3,1)$ of particular interest in physics applications.

(vii) It would be useful to know all the gradings of $o(4,\mathbb{C})$ (not only the fine ones) and their hierarchy. There are tens of these gradings because we are dealing with a semisimple algebra.

(viii) Another interesting point to study would be the normalizer of each grading in the group of automorphisms $\mathrm{Aut}\, o(4,\mathbb{C})$. They describe, in particular, the symmetries of the contraction equations, hence they simplify the process of solving the contraction equations.[9]

(ix) Unexplored application of the normalizers is their action on the universal enveloping algebra of $o(4,\mathbb{C})$.

(x) It is useful to notice that, because of the embedding $o(4,\mathbb{C}) \subset sl(4,\mathbb{C})$, we obtain from the eight fine gradings of $sl(4,\mathbb{C})$ the six fine gradings of $o(4,\mathbb{C})$.

(xi) The graphical presentation of the gradings introduced in this paper offers the possibility to study gradings of more complicated Lie algebras in terms of the corresponding graphs.

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Relativistic quantum field theory with a fundamental length

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Since there are indications (from string theory and concrete models) that one must consider relativistic quantum field theories with a fundamental length the question of a suitable framework for such theories arises. It is immediately evident that quantum field theory in terms of tempered distributions and even in terms of Fourier hyperfunctions cannot meet the (physical) requirements. We argue that quantum field theory in terms of *ultra-hyperfunctions* is a suitable framework. For this we propose a set of axioms for the fields and for the sequence of vacuum expectation values of the fields, prove their equivalence, and we give a class of models (analytic, but not entire functions of free fields). © *2004 American Institute of Physics.* [DOI: 10.1063/1.1737055]

I. INTRODUCTION

Relativistic quantum field theory is defined in terms of a set of conditions for which there is strong physical motivation. These conditions are (1) relativistic covariance, (2) energy momentum spectrum compatible with the principles of special relativity, (3) existence of a vacuum state, and (4) completeness of the field. Then there two conditions in which several technical assumptions enter: (5) fields as operator-valued generalized functions (what class of generalized functions?), (6) uniqueness of the vacuum state. Last, but not least, there is the condition of (7) local commutativity of field operators at spacelike separations.

The first mathematically rigorous realization of all these conditions in one theory is that of Wightman and Gårding[1] where fields are defined as operator valued tempered distributions, and a powerful characterization of such a theory in terms of the sequence of vacuum expectation values of the fields has been derived. Soon a number of physically important general results (existence of a PCT operator, connection between spin and statistics, scattering theory, dispersion relations, etc.) were derived. Furthermore one soon learned that theories with nonunique vacuum state can be decomposed into theories with a unique vacuum and one learned that the apparently weaker condition of local commutativity of field operators at sufficiently large spacelike separations implies local commutativity at all spacelike separations. (More details are given in the textbook.[2])

According to string theory there is a length $\ell > 0$ such that one cannot distinguish events which occur in a distance smaller than ℓ. For example, the T-duality of string theory implies the equivalence of two string theories with toroidal compactification whose radii are R and α'/R. Therefore, in string theory, the existence of a fundamental length is suggested. In a distance smaller than the fundamental length, the space–time is melted down (see Refs. 3, 4). Moreover in string theory there is some discussion about space–time uncertainty $\Delta T \Delta X \geqslant \ell_s^2$, which also suggests the existence of a fundamental length (see Refs. 5, 6).

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How can we take the existence of a fundamental length into account in a relativistic quantum field theory?

In Wightman's framework, in terms of the field operators $A(x)$, locality is expressed as the condition that the commutator of the field operators vanishes for spacelike separated points, i.e., by $A(x)A(y)-A(y)A(x)=0$ for all $x,y\in\mathbb{R}^4$ with $(x-y)^2<0$. Even if one replaces this condition by the apparently weaker condition that this commutator vanishes for all points $x,y\in\mathbb{R}^4$ which are spacelike separated and are in a certain distance of at least $\ell>0$ from each other, i.e., $(x-y)^2<-\ell^2<0$, one can prove that this commutator vanishes for all spacelike separated points by using the other axioms of the theory (see, for instance, Theorem 19.3 of Ref. 7).

The situation is the same in hyperfunction quantum field theory (see Ref. 8). The reason is that the n-point functionals in both theories are boundary values of holomorphic functions in $\mathrm{Im}(z_{i+1}-z_i)\in V_+$ and as such, distributions and hyperfunctions have the same type of localization property, expressed by the fact that both form a sheaf over space–time (see, for instance, Ref. 9). Thus, in order to formulate a quantum field theory with a fundamental length, a space of generalized functions different from both Schwartz distributions and Fourier hyperfunctions has to be used.

By a variety of reasons, the problem to formulate relativistic quantum field theory in terms of generalized functions which are different from Schwartz distributions and/or Fourier hyperfunctions, has been addressed in the past. One of the main physical motivations was to be able to describe relativistic quantum field theories not only with polynomial but with exponential high energy behavior. Some prominent articles about this and related problems are Refs. 10–19. In these articles, roughly, it is argued that the resulting theory is nonlocalizable if it is formulated in terms of generalized functions for which the underlying test-function space does not contain test functions of compact support.

In Refs. 19, 20, QFT is formulated in terms of generalized functions over the Gelfand–Shilov space S^0. Such a theory is so singular that the condition of locality cannot be defined in any generalized sense. But instead of it, a condition which is called asymptotic commutativity can be defined. By replacing local commutativity by asymptotic commutativity, PTC theorem, spin-statistics relation and the existence of S-matrix are shown. We do not consider these highly singular cases, but we consider the quasilocal case, i.e., the theory with a fundamental length ℓ indicated from string theory. For this theory, PTC theorem, spin-statistics relation and the existence of S-matrix are valid because the axioms of QFT with a fundamental length is stronger than those of QFT with test-function space S^0.

In Ref. 21 a different position is proposed by arguing that generalized functions are localizable in a natural way as soon as they form a sheaf over space–time (this then allows localizable relativistic quantum fields which do not admit any test function of compact support, Ref. 21).

Clearly, in order to formulate a relativistic quantum field theory with a fundamental length, a different type of generalized functions has to be used. The following simple example will provide some insight into the properties of the class of generalized functions which could be used in theories with fundamental length.

Let $\{a_n\}$ be a sequence of real numbers. The support of the distribution $\Sigma_{i=0}^{N}a_n\delta^{(n)}(x)$ is $\{0\}$, but $\Sigma_{n=0}^{\infty}a_n\delta^{(n)}(x)$ does not define a distribution unless all except finitely many of the coefficients a_n vanish. If $\lim_{n\to\infty}[n!a_n]^{1/n}=0$, then $\Sigma_{n=0}^{\infty}a_n\delta^{(n)}(x)$ converges to a hyperfunction. The support of this limit is the same as the supports of the approximating sums, i.e., the hyperfunction has the support $\{0\}$.

Now consider the case $a_n=a^n/n!$ and take the underlying space of test functions into account. If $f(z)$ is a holomorphic function in $|\mathrm{Im}\,z|<\ell$, then, for $|a|<\ell$, we have

$$\left\langle \sum_{n=0}^{\infty}\frac{a^n}{n!}\delta^{(n)}(x),f(x)\right\rangle=\sum_{n=0}^{\infty}\frac{(-a)^n}{n!}f^{(n)}(0)=f(0-a)=\langle\delta(x+a),f(x)\rangle,$$

that is, as an equation for functionals defined on the function space $\mathcal{T}(T(-\ell,\ell))$ whose elements are holomorphic functions in $T(-\ell,\ell)=\mathbb{R}+i(-\ell,\ell)\subset\mathbb{C}$, the identity

$$\sum_{n=0}^{\infty} \frac{a^n}{n!} \delta^{(n)}(x) = \delta(x+a)$$

holds, i.e., the sequence of generalized functions $S_N = \Sigma_{n=0}^{N} (a^n/n!)\, \delta^{(n)}(x)$ with support $\{0\}$ converges [weakly, in the dual space of $\mathcal{T}(T(-\ell,\ell))$] to the generalized function $\delta(x+a)$ with support $\{-a\}$, as $N \to \infty$. However, if $|a| > \ell$, then this sequence does not converge in $\mathcal{T}(T(-\ell,\ell))'$.

This phenomenon can be understood as follows. If $|a| < \ell$, then elements in $\mathcal{T}(T(-\ell,\ell))'$ do not distinguish between the points $\{0\}$ and $\{-a\}$, but if $|a| > \ell$ then elements in $\mathcal{T}(T(-\ell,\ell))'$ can distinguish between the points $\{0\}$ and $\{-a\}$. Since $|a| < \ell$ is arbitrary, one can say that elements in $\mathcal{T}(T(-\ell,\ell))'$ do not distinguish between points which are separated by less than ℓ. Spaces of functionals with this property have been studied under the name of ultra-hyperfunctions in Refs. 22, 23.

In this paper we propose to formulate relativistic quantum field theory with a fundamental length ℓ in terms of tempered ultra-hyperfunctions, i.e., those ultra-hyperfunctions which admit the Fourier transform as an isomorphism of topological vector spaces. To this end we introduce, in analogy to the test function space $\mathcal{T}(T(-\ell,\ell))$ of the above example, the test-function space $\mathcal{T}(T(\mathbb{R}^4))$ of tempered ultra-hyperfunctions according to Refs. 22, 23. Section II studies the basic properties of this space. Furthermore, the range of the Fourier transform on $\mathcal{T}(T(\mathbb{R}^4))$ is determined. It is a space which we call $H(\mathbb{R}^n;\mathbb{R}^n)$ and which is characterized explicitly as a projective limit of Fréchet spaces. This space too is studied in Sec. II.

The following sections contain our proposal of a relativistic quantum field theory with fundamental length $\ell > 0$ in terms of tempered ultra-hyperfunctions. At first it seems impossible to reconcile the requirements of relativistic covariance with the existence of a fundamental length. Note however that the Poincaré group acts (smoothly) on the test-function space $\mathcal{T}(T(\mathbb{R}^4))$ and thus by duality on the fields. The fundamental length is introduced into the theory by the distinguished localization property of ultra-hyperfunctions.

Naturally, the condition of locality (local commutativity) differs considerably from that of standard quantum field theory. We explain our proposal of *extended local commutativity* which is considered to be the counterpart of local commutativity in standard quantum field theory in two steps.

In a first step we have to ensure that, in a quantum field theory with fundamental length ℓ, field operators $A(x_1)$ and $A(x_2)$ at two distinct points x_1 and x_2 can only be distinguished if the distance between the two points x_1 and x_2 is greater than ℓ. In the light of our discussion of the elementary example given above, we propose to express this condition as follows: The functional

$$\mathcal{T}(T(\mathbb{R}^4)) \otimes \mathcal{T}(T(\mathbb{R}^4)) \ni f_1 \otimes f_2 \to (\Phi, A(f_1)A(f_2)\Psi) \tag{1.1}$$

can be extended continuously to $\mathcal{T}(T(L^\ell))$ in some Lorentz frame, for arbitrary elements Φ, Ψ in the domain of the field operators $A(f)$, where

$$T(L^\ell) = \{(z_1, z_2) \in \mathbb{C}^{4\cdot 2}; |\operatorname{Im} z_1 - \operatorname{Im} z_2|_1 < \ell\}$$

and

$$|x|_1 = |x^0| + |\mathbf{x}|, \quad |\mathbf{x}| = \sqrt{\sum_{i=1}^{3} (x^i)^2}. \tag{1.2}$$

In a second step we introduce our concept of *extended local commutativity* which is defined by the condition that the carrier of the functional on $\mathcal{T}(T(\mathbb{R}^4)) \otimes \mathcal{T}(T(\mathbb{R}^4))$

$$f_1 \otimes f_2 \to (\Phi, A(f_1)A(f_2)\Psi) - (\Phi, A(f_2)A(f_1)\Psi) \tag{1.3}$$

is contained in the set

$$W^{\ell}=\{(z_1,z_2)\in\mathbb{C}^{4\cdot 2};z_1-z_2\in V^{\ell}\},$$

that is, the functional can be extended continuously to $\mathcal{T}(W^{\ell})$, where V^{ℓ} is a complex neighborhood of the light cone V as defined in Sec. III.

The localization properties of tempered ultra-hyperfunction are very different from those of Fourier hyperfunctions and Schwartz distributions, but the spectral condition is not so much different from that of Schwartz distributions because the Fourier transformation of tempered ultra-hyperfunctions are distributions (see Proposition 2.5). From this condition it follows that $W_{n-1}(\zeta)$ is holomorphic in a domain

$$\mathcal{V}_{R,\epsilon}=\bigcup_{i=1}^{n-1}\mathcal{V}_{R,\epsilon,i}, \tag{1.4}$$

where for some $\epsilon,R>0$,

$$\begin{aligned}\mathcal{V}_{R,\epsilon,i}=\{\zeta\in\mathbb{C}^{4(n-1)};&\operatorname{Im}\zeta_i\in V_+ +(\ell-\epsilon,\mathbf{0}),\\ &\operatorname{Im}\zeta_j\in V_+ +(R,\mathbf{0}),\quad j\neq i\}.\end{aligned} \tag{1.5}$$

In Sec. IV we study the basic properties of the sequence of n-point functionals $\mathcal{W}_n$ in a relativistic quantum field theory with fundamental length. As a consequence of the defining conditions we get that the function $W_n(\zeta)$ is analytically continued to (1.4) (Proposition 4.7). $W_n(\zeta)$ is analytically continued to the extended domain which contains real points. This enables us to prove, using extended local commutativity, that $\mathcal{W}_n(z)$ is a symmetric function on its domain of holomorphy (Theorem 4.11).

Having collected all basic properties of the sequence of n-point functionals we can prove in Sec. V, that the fields can be reconstructed from the sequence of its n-point functionals (reconstruction theorem).

Obviously one would like to have examples of ultra-hyperfunction quantum fields. In Sec. VI, we use the reconstruction theorem to show that the field $A(x)=:e^{\phi(x)^2}:$, defined by the free neutral scalar field $\phi(x)$, satisfies all our axioms of a relativistic quantum field theory with a fundamental length.

Finally, in an Appendix, we prove Theorem 2.13 which guarantees the uniqueness of the extensions (1.1) and (1.3).

In order to put our results in a proper perspective we conclude the Introduction with a couple of remarks on related research.

Remark 1.1: The type of generalized functions to be used in a relativistic quantum field theory is not given *a priori*, one must make a choice, in accordance with the physical constraints one would like to incorporate.

In Ref. 14, the test-function space $S^{1,\lambda}(\mathbb{R}^4)$ is used. By this choice, $W_{n-1}(\zeta)$ is analytic in

$$\{\zeta\in\mathbb{C}^{4(n-1)};\operatorname{Im}\zeta_i\in V_+ +\sqrt{2}(\ell,\mathbf{0})\}, \tag{1.6}$$

where $\ell=1/e\lambda$ and the theory of $A(x)=:e^{\phi(x)^2}:$ defined by the free field $\phi(x)$ is excluded because the Wightman function $W_{n-1}(\zeta)$ of $A(x)$ is analytic only in (1.4). However with the choice of the projective limit of these spaces, i.e.,

$$\mathcal{T}(T(\mathbb{R}^4))=\lim_{0\leftarrow\lambda}S^{1,\lambda}(\mathbb{R}^4),$$

a theory of $A(x)=:e^{\phi(x)^2}:$ can be formulated as we are going to show. The absence of the factor $\sqrt{2}$ in (1.5) is due to the choice of the norm (1.2) instead of Euclidean norm.

Remark 1.2: In 1969 Iofa and Fainberg[11] formulated a nonlocalizable quantum field theory. They used the test-function space $\mathcal{M}(\mathbb{R}^{4n})$ with the seminorms

$$\|\tilde{\phi}\|_k = \sup_{p;m\leqslant k} g(k\|p\|^2)|D^m\tilde{\phi}(p)|,$$

where $g(t^2)$ is an entire function of first order growth and type ρ with respect to t, i.e.,

$$\lim_{\|p\|\to\infty} \frac{\ln g(\|p\|^2)}{\|p\|} = \rho.$$

One can show that $\mathcal{M}(\mathbb{R}^{4n})$ is just the space $H(\mathbb{R}^{4n};\mathbb{R}^{4n})$, the space of Fourier transforms of the test-function space $\mathcal{T}(T(\mathbb{R}^{4n}))$ of tempered ultra-hyperfunctions (see Remark 2.3).

The Fourier transform $\tilde{W}_{n-1}(q_1,\ldots,q_{n-1})$ of the n-point functionals $W_{n-1}(\xi_1,\ldots,\xi_{n-1})$ of their theory in the relative coordinates belongs to $\mathcal{M}(\mathbb{R}^{4(n-1)})$, and the growth of $\tilde{W}_{n-1}(q)$ is $\rho_n\sqrt{k_n}$ which depends on n. In Ref. 11, Iofa and Fainberg assume that

$$\overline{\lim_n}\,\rho_n\sqrt{k_n} = \tilde{\ell} > 0. \tag{1.7}$$

Then $W_{n-1}(\zeta)$ is again analytic in (1.6) and excludes the theory of $A(x)=:e^{\phi(x)^2}:$. We do not require condition (1.7) or something equivalent. We think it is too restrictive.

Remark 1.3: As we discussed above, a relativistic quantum field theory with a fundamental length cannot be formulated in terms of generalized functions with standard localization properties. Accordingly one faces the problem of how to include the physical condition of quasilocality or ℓ-locality of the fields. Above we had indicated that we propose to use a condition of extended local commutativity.

In Ref. 11, a condition of quasilocality is defined by symmetry of the (analytically continued) Wightman functions in their domain of holomorphy. In Ref. 14, quasilocality is defined essentially in the same way as our condition of extended local commutativity, i.e., it is defined as a continuity condition of the expectation values of the field commutators in a topology associated to a ℓ-neighborhood of the light cone.

Though the formulation of quasilocality seems to be the same, the properties of Wightman functionals in both theories are different because different types of generalized functions are used.

Remark 1.4: The important result Theorem 4.11, i.e., the result that extended local commutativity implies the symmetry of the analytically continued Wightman functions on their domain of holomorphy or, in the above terminology, quasilocality follows from the standard strategy (see Refs. 2, 14, 24, 25) by using extended tubes $\mathcal{T}^{n-1}_{\text{ext}}(\ell)$ and by proving this symmetry first in real points in these extended tubes $\mathcal{T}^{n-1}_{\text{ext}}(\ell)$.

As in Ref. 14 the symmetry of the Wightman functions at these real points of analyticity (Jost points) is shown first by suitable approximations for sufficiently distant Jost points. For our case of a different type of generalized functions these approximations are done in suitable open neighborhoods of explicitly chosen distant Jost points and all necessary estimates are done explicitly.

II. TEMPERED ULTRA-HYPERFUNCTIONS

For any subset A of $\mathbb{R}^n$, denote by $T(A)=\mathbb{R}^n+iA\subset\mathbb{C}^n$ the tubular set with base A. For a convex compact set K of $\mathbb{R}^n$, $\mathcal{T}_b(T(K))$ is, by definition, the space of all continuous functions f on $T(K)$ which are holomorphic in the interior of $T(K)$ and which satisfy

$$\|f\|^{T(K),j} = \sup\{|z^p f(z)|; z\in T(K), |p|\leqslant j\} < \infty, \quad j=0,1,\ldots, \tag{2.1}$$

where $p=(p_1,\ldots,p_n)$ and $z^p=z_1^{p_1}\cdots z_n^{p_n}$. $\mathcal{T}_b(T(K))$ is a Fréchet space with the seminorms $\|f\|^{T(K),j}$. If $K_1\subset K_2$ are two compact convex sets, we have the canonical injection,

$$\mathcal{T}_b(T(K_2))\to\mathcal{T}_b(T(K_1)). \tag{2.2}$$

For a convex open set O in $\mathbb{R}^n$ we define

$$\mathcal{T}(T(O)) = \lim_{\leftarrow} \mathcal{T}_b(T(K)), \tag{2.3}$$

where K runs through the convex compact sets contained in O and the projective limit is taken following the restriction mappings (2.2).

Definition 2.1: A tempered ultra-hyperfunction *is by definition a continuous linear functional on* $\mathcal{T}(T(\mathbb{R}^n))$.

The Fourier transformation $\mathcal{F}$ is well defined on $\mathcal{T}(T(\mathbb{R}^n))$ by the standard formula (2.8). In order to determine the range of $\mathcal{F}$ on $\mathcal{T}(T(\mathbb{R}^n))$ we introduce another function space.

The gauge functional h_K of a compact convex set $K \subset \mathbb{R}^n$ is defined by

$$h_K(x) = \sup\{\langle x, \xi\rangle; \xi \in K\}. \tag{2.4}$$

For a convex compact set K of $\mathbb{R}^n$, denote by $H_b(\mathbb{R}^n;K)$ the space of all C^∞ functions f on $\mathbb{R}^n$ which satisfy, for $j = 0,1,\ldots,$

$$\|f\|_{K,j} = \sup\{\exp(h_K(x))|D^p f(x)|; x \in \mathbb{R}^n, \ |p| \leqslant j\} < \infty. \tag{2.5}$$

Equipped with the system of seminorms $\|f\|_{K,j}$, $H_b(\mathbb{R}^n;K)$ is a Fréchet space. If $K_1 \subset K_2$ are two compact convex sets, then $h_{K_1} \leqslant h_{K_2}$ and thus one has the canonical injections:

$$H_b(\mathbb{R}^n;K_2) \to H_b(\mathbb{R}^n;K_1). \tag{2.6}$$

For a convex open set $O \subset \mathbb{R}^n$ the space $H(\mathbb{R}^n;O)$ is the projective limit of the spaces $H_b(\mathbb{R}^n;K)$ along the restriction mappings (2.6), i.e.,

$$H(\mathbb{R}^n;O) = \lim_{\leftarrow} H_b(\mathbb{R}^n;K), \tag{2.7}$$

where K runs through the convex compact sets contained in O.

In order to relate the space $H(\mathbb{R}^n;\mathbb{R}^n)$ to the Schwartz space $\mathcal{S}(\mathbb{R}^n)$ we derive a more direct characterization of $H(\mathbb{R}^n;\mathbb{R}^n)$. Observe that for any convex compact set $K \subset \mathbb{R}^n$ there is a number $k > 0$ such that $K \subseteq [-k,k]^n$. For the sets $K = [-k,k]^n$ the gauge function h_K is easily determined:

$$h_K(x) = \sup\{\langle x, \xi\rangle; \xi \in K\} = k\sum_{i=1}^{n} |x_i|,$$

and the system of continuous norms takes the form, using the notation $|x| = \Sigma_{i=1}^n |x_i|$,

$$\|f\|_{K,j} = \sup\{\exp(h_K(x))|D^p f(x)|; \ |p| \leqslant j, x \in \mathbb{R}^n\} = \sup\{e^{k|x|}|D^p f(x)|; \ |p| \leqslant j, x \in \mathbb{R}^n\}.$$

Thus, the space $H(\mathbb{R}^n;\mathbb{R}^n)$ can be defined as the projective limit of the spaces $H_b(\mathbb{R}^n;K)$ along the restriction mappings (2.6), where $K = [-k,k]^n$, $0 < k < \infty$. Accordingly, the space $H(\mathbb{R}^n;\mathbb{R}^n)$ is the space of all $\mathcal{C}^\infty$ functions on $\mathbb{R}^n$ which, together with all derivatives, decrease faster than any (linear) exponential. An easy consequence is the following.

Corollary 2.2:

(1) The space $H(\mathbb{R}^n;\mathbb{R}^n)$ is continuously embedded into the Schwartz space $\mathcal{S}(\mathbb{R}^n)$.
(2) The elements of $\mathcal{S}(\mathbb{R}^n)$ are multipliers for the space $H(\mathbb{R}^n;\mathbb{R}^n)$, and for each $g \in \mathcal{S}(\mathbb{R}^n)$ the map $f \mapsto gf$ is a continuous linear map of $H(\mathbb{R}^n;\mathbb{R}^n)$ into itself.

Proof: See Refs. 22, 23. □

Remark 2.3: Since

$$\lim_{\|p\| \to \infty} \frac{\ln g(\|p\|^2)}{\|p\|} = \rho,$$

it follows that $g(t^2)\sim e^{\rho t}$ as $|t|\to\infty$. Therefore the system of norms

$$\|\tilde{\phi}\|_k=\sup\{g(k\|x\|^2)|D^p\tilde{\phi}(x)|;\quad x\in\mathbb{R}^n,\ |p|\leqslant k\}$$

and

$$\|\tilde{\phi}\|_{K,j}=\sup\{\exp(h_K(x))|D^p\tilde{\phi}(x)|;\quad x\in\mathbb{R}^n,\ |p|\leqslant j\}$$

are equivalent. It follows that the space $\mathcal{M}(\mathbb{R}^n)$ of Iofa and Fainberg[11] and the space $H(\mathbb{R}^n;\mathbb{R}^n)$ are the same.

The following theorem collects the basic facts about the spaces introduced above.

Theorem 2.4: *For the spaces introduced above the following statements hold, for any convex open set O.*

(1) The space $\mathcal{D}(\mathbb{R}^n)$ of all C^∞ functions with compact support is dense in $H(\mathbb{R}^n;O)$.
(2) The space $H(\mathbb{R}^n;\mathbb{R}^n)$ is dense in $H(\mathbb{R}^n;O)$.
(3) $H(\mathbb{R}^m;\mathbb{R}^m)\otimes H(\mathbb{R}^n;\mathbb{R}^n)$ is dense in $H(\mathbb{R}^{m+n};\mathbb{R}^{m+n})$.

Proof: For the proof of the first two items we refer to Refs. 22, 23. To prove the last item let $\alpha(x)\in H(\mathbb{R}^m;\mathbb{R}^m)$ [respectively, $\beta(x)\in H(\mathbb{R}^n;\mathbb{R}^n)$] such that $\alpha(x)=1$ [respectively, $\beta(x)=1$] for $|x|<1$ and $\alpha(x)=0$ [respectively, $\beta(x)=0$] for $|x|\geqslant 2$. If $f\in H(\mathbb{R}^{m+n};\mathbb{R}^{m+n})$ then $f_m(x,y)=\alpha(x/m)\beta(y/m)f(x,y)$ converges to f in $H(\mathbb{R}^{m+n};\mathbb{R}^{m+n})$ and f_m is the limit of a sequence $\{\alpha(x/m)\beta(y/m)P_k(x,y)\}\subset H(\mathbb{R}^m;\mathbb{R}^m)\otimes H(\mathbb{R}^n;\mathbb{R}^n)$ in $H(\mathbb{R}^{m+n};\mathbb{R}^{m+n})$. □

Proposition 2.5: The Fourier transformation $f\mapsto\tilde{f}\equiv\mathcal{F}f$,

$$\tilde{f}(p)=(2\pi)^{-n/2}\int_{\mathbb{R}^n}f(z)e^{i\langle p,z\rangle}\,dz, \tag{2.8}$$

is a topological isomorphism between the spaces $\mathcal{T}(T(O))$ and $H(\mathbb{R}^n;O)$, for any open convex nonempty set $O\subset\mathbb{R}^n$. The inverse transformation is

$$f(z)=\overline{\mathcal{F}}\tilde{f}=(2\pi)^{-n/2}\int_{\mathbb{R}^n}\tilde{f}(p)e^{-i\langle p,z\rangle}\,dp. \tag{2.9}$$

Proof: See Refs. 22, 23. □

Proposition 2.6: Let $O\subset\mathbb{R}^n$ be a nonempty convex open subset. Then the spaces $H(\mathbb{R}^n;O)$ and $\mathcal{T}(T(O))$ are nuclear Fréchet spaces and thus, in particular, reflexive.

Proof: In the case of $O=\mathbb{R}^n$, Hasumi[22] proved this result, and his proof is valid in the general case. We sketch it for $H(\mathbb{R}^n;O)$. Let K be a convex compact subset of O. Then the mapping Φ_K defined by $\phi(f)=\exp(h_K(x))f(x)$ is a continuous linear mapping of $H(\mathbb{R}^n;O)$ into the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. Moreover, if f is C^∞ and $\phi_K(f)\in\mathcal{S}(\mathbb{R}^n)$ for any convex compact subset K of O then $f\in H(\mathbb{R}^n;O)$. Hence $H(\mathbb{R}^n;O)$ is the projective limit of $\mathcal{S}(\mathbb{R}^n)$ with respect to the mappings ϕ_K. Since $\mathcal{S}(\mathbb{R}^n)$ is nuclear, $H(\mathbb{R}^n;O)$ is also nuclear by Proposition 50.1 of Ref. 26. □

Theorem 2.7 (Corollary of Theorem 34.1 of Ref. 26): *Let E be a Fréchet space, E_1 a metrizable space, G a locally convex space. Then a separately continuous bilinear map of $E\times E_1$ into G is continuous.*

Theorem 2.8 (Kernel theorem for ultra-hyperfunctions): *Let M be a separately continuous multilinear map of $[\mathcal{T}(T(\mathbb{R}^4))]^n$ into a Banach space G. Then there is a unique continuous linear map F of $\mathcal{T}(T(\mathbb{R}^{4n}))$ into G such that, for all $f_i\in\mathcal{T}(T(\mathbb{R}^4))$, $i=1,\ldots,n$,*

$$M(f_1,\ldots,f_n)=F(f_1\otimes\cdots\otimes f_n).$$

Proof: It follows from Theorem 2.7 that M is continuous, that is, there exist a constant C and seminorms $\|f\|^{T(K_i),j_i}$ of the form (2.1) such that

$$\|M(f_1,\ldots,f_n)\| \leqslant C\prod_{i=1}^{n} \|f_i\|^{T(K_i),j_i}. \tag{2.10}$$

This shows that M is continuously extended to $\Pi_{i=1}^{n}\mathcal{T}_b(T(K_i))$. For any finite family $K_1,\ldots,K_n$ of compact sets K_i there is $k>0$ such that $K_i\subseteq K=[-k,k]^4$ for $i=1,\ldots,n$. Since $\|f_i\|^{T(K_i),j_i} \leqslant \|f_i\|^{T(K),j_i}$ for all i, we can assume in (2.10): $K_i=K$ for $i=1,\ldots,n$.

Introduce modified Cauchy kernels as follows. Denote

$$h(t)=\prod_{\alpha=0}^{3} \frac{e^{-(t^\alpha)^2}}{2\pi i t^\alpha} \quad \text{and} \quad h_z(t)=h(t-z). \tag{2.11}$$

If $|\mathrm{Im}\, z^\alpha| \geqslant l>k$, then $h_z(t)$ is a continuous function of t in $T(K)$ which is holomorphic in the interior of $T(K)$ and $h_z\in\mathcal{T}_b(T(K))$. Moreover, h_z is a $\mathcal{T}_b(T(K))$-valued continuous function for $|\mathrm{Im}\, z^\alpha| \geqslant l>k$ as follows. Choose $\delta>0$ such that $|\mathrm{Im}\,(z-\zeta)^\alpha| \geqslant l>k$ for $|\zeta|\leqslant\delta$ and fixed z. For any $\epsilon>0$ there exists $R>0$ such that

$$\sup\{|t^p h_{z+\zeta}(t)|; t\in T(K), |t|\geqslant R, |\zeta|\leqslant\delta, |p|\leqslant j\}<\epsilon.$$

Since $h_z(t)$ is uniformly continuous on a compact set $T(K)_R=\{t\in T(K); |t|\leqslant R\}$, for any $\epsilon'>0$ there exists $0<\delta'\leqslant\delta$ such that

$$|h_{z+\zeta}(t)-h_z(t)|=|h_z(t-\zeta))-h_z(t)|<\epsilon',$$

for any $t\in T(K)_R$ and $|\zeta|\leqslant\delta'$. Hence

$$F(z)=M(h_{z_1},\ldots,h_{z_n}) \tag{2.12}$$

is a well-defined vector-valued continuous function for $|\mathrm{Im}\, z_i^\alpha|>l$, $\alpha=0,\ldots,3$, $i=1,\ldots,n$. For any $r>l>0$ and $l<|\mathrm{Im}\, z^\alpha|\leqslant r$, a straightforward estimate shows

$$\begin{aligned}\|h_z\|^{T(K),j} &= \sup\{|t^p h(t-z)|; t\in T(K), |p|\leqslant j\} \\ &= \sup\{|(t+z)^p h(t)|; t+z\in T(K), |p|\leqslant j\} \leqslant C(1+|z|)^j.\end{aligned} \tag{2.13}$$

The inequality

$$\|F(z)\| \leqslant C\prod_{i=1}^{n} (1+|z_i|)^j \tag{2.14}$$

follows from the estimate (2.10) for $l<|\mathrm{Im}\, z_i^\alpha|\leqslant r$.

Next we consider the integration of the vector valued function $F(z)$. For the reader's convenience we recall some useful propositions about Pettis integration of functions whose values are in a Suslin space E. For our purpose, we only have to know that a separable Fréchet space is a Suslin space. In the following propositions, T denotes a set, $\mathcal{A}$ a σ-algebra of subsets of T, and m a σ-finite positive measure defined on $\mathcal{A}$.

Definition 2.9 (Definition 1 of Ref. 27): Let E be a quasicomplete locally convex Hausdorff space. A function $f:T\to E$ is weakly m-summable if $\langle f(\cdot),x'\rangle$ is m-integrable for each $x'\in E'$. The function f is said to be m-summable (or Pettis integrable) if f is weakly m-summable and if for each set $A\in\mathcal{A}$ there exists an element $\int_A f\,dm\in E$ such that $\langle\int_A f\,dm,x'\rangle=\int_A\langle f,x'\rangle dm$ for all $x'\in E'$.

Proposition 2.10 (Theorem 1 of Ref. 27): Given a function $f:T\to E$ with values in a locally convex Suslin space, the following conditions are equivalent:

(a) $f^{-1}(B)\in\mathcal{A}$ for every Borel subsets $B\subset E$,
(b) for every $x'\in E'$ the scalar function $\langle f(\cdot),x'\rangle$ is measurable.

Proposition 2.11 (Theorem 3 of Ref. 27): Let $f:T\to E$ be a measurable function such that $\int|f|_p\,dm<\infty$ for every continuous seminorm p of a quasicomplete locally convex Suslin space E. Then f is m-summable.

Proposition 2.12 (Secs. I, IX of Ref. 27): (a) If $u:E_1\to E_2$ is a continuous linear map, and if $f:T\to E_1$ is summable, then $u\circ f$ is summable and $\int u\circ f\,dm=u\int f\,dm$.

(b) Let $x\to|x|_\beta$ be a lower semicontinuous generalized seminorm on E and $f:T\to E$ measurable. Then $|f(\cdot)|_\beta$ is measurable and $|\int f\,dm|_\beta\leqq\int|f|_\beta\,dm$.

After these preparations, let $\Gamma=\Gamma^+-\Gamma^-$ be the path in $\mathbb{C}$ defined by

$$\Gamma^\pm=\{z\in\mathbb{C};z=\pm x\pm ir,\ \ -\infty<x<\infty\},$$

and $f_j\in\mathcal{T}(T(\mathbb{R}^4))$.

Since $z\to h_z f_j(z)\in\mathcal{T}_b(T(K))$ is continuous and therefore measurable by Proposition 2.10. It follows from the inequality 2.13 and Proposition 2.11 that $h_z f_j(z)$ is summable.

Applying Proposition 2.12 and the Cauchy integral formula

$$\int_{\Gamma^4}h_z f(z)\mathrm{d}z=f(t),$$

we have

$$M(h_{z_1},\ldots,h_{z_{j-1}},f_j,f_{j+1},\ldots,f_n)=M\left(h_{z_1},\ldots,h_{z_{j-1}},\int_{\Gamma^4}h_{z_j}f_j(z_j)\mathrm{d}z_j,f_{j+1},\ldots,f_n\right)$$
$$=\int_{\Gamma^4}M(h_{z_1},\ldots,h_{z_{j-1}},h_{z_j},f_{j+1},\ldots,f_n)f_j(z_j)\mathrm{d}z_j.$$

This gives

$$M(f_1,\ldots,f_n)=\int_{\Gamma^4}\int_{\Gamma^4}\cdots\int_{\Gamma^4}F(z_1,z_2,\ldots,z_n)f_1(z_1)f_2(z_2)\cdots f_n(z_n)\mathrm{d}z_n\cdots\mathrm{d}z_2\,\mathrm{d}z_1$$
$$=F(f_1\otimes\cdots\otimes f_n).$$

Moreover, the integral

$$F(f)=\int_{\Gamma^4}\int_{\Gamma^4}\cdots\int_{\Gamma^4}F(z_1,z_2,\ldots,z_n)f(z_1,z_2,\ldots,z_n)\mathrm{d}z_n\cdots\mathrm{d}z_2\,\mathrm{d}z_1$$

for $f\in\mathcal{T}(T(\mathbb{R}^{4n}))$ defines a continuous mapping,

$$F:\mathcal{T}(T(\mathbb{R}^{4n}))\ni f\to F(f)\in G.$$

In fact, $F(z)f(z)$ is continuous and therefore measurable by Proposition 2.10, and it follows from (2.14) that

$$\|F(z)\|\ \ |f(z)|\leqq C\|f\|^{T(K),j+2}\prod_{i=1}^{n}\ (1+|z_i|)^{-2}$$

for $z\in\Gamma^4$, where $K=[-r,r]^{4n}$. Thus, using Proposition 2.12, we have

$$\|F(f)\|\leqq C'\|f\|^{T(K),j+2}.$$

This completes the proof. □

For an open set V in $\mathbb{R}^n$ and a positive number ϵ introduce the set V^ϵ defined by

$$V^{\epsilon}=\{z\in\mathbb{C}^n;\exists\, x\in V,|\mathrm{Re}\, z-x|+|\mathrm{Im}\, z|_{\beta}<\epsilon\},$$

where $|y|_{\beta}$ is a norm of $\mathbb{R}^n$ satisfying $|y|_{\beta}\geqslant|y|$ for the Euclidean norm $|y|$. Let K_p be the closure of $V^{\epsilon/(1+1/p)}$ in $\mathbb{C}^n$ and $L_p=\{w\in\mathbb{C}^m;|\mathrm{Im}\, w|\leqslant p\}$. Let $U=V^{\epsilon}\times\mathbb{C}^m$ and $M_p=K_p\times L_p$. $\mathcal{T}_b(M_p)$ is, by definition, the space of all continuous functions f on M_p which are holomorphic in the interior of M_p and satisfy, for $k=1,2,\ldots$,

$$\|f\|^{M_p,k}=\sup\{|z^s w^t f(z,w)|;(z,w)\in M_p,|s|+|t|\leqslant k\}<\infty;$$

$\mathcal{T}_b(M_p)$ is a Fréchet space with the seminorms $\|f\|^{M_p,k}$.

If $k<m$, then we have the canonical injections

$$\mathcal{T}_b(M_m)\to\mathcal{T}_b(M_k). \tag{2.15}$$

We define

$$\mathcal{T}(U)=\lim_{\leftarrow}\mathcal{T}_b(M_m), \tag{2.16}$$

where the projective limit is taken following the restriction mappings (2.15).

Theorem 2.13: *$\mathcal{T}(T(\mathbb{R}^{n+m}))$ is dense in $\mathcal{T}(U)$.*

Proof: The proof is similar to the proofs of Proposition 2.4 of Ref. 28 and Proposition 9.1.2 of Ref. 29. For more details we refer to the Appendix. □

Let V be a closed convex cone in $\mathbb{R}^n$ and define the ϵ-neighborhood of V by

$$V_{\epsilon}=\{y;\exists\, x\in V,\ \ |x-y|\leqslant\epsilon\}.$$

Lemma 2.14: There exists a C^{∞}-function ϕ_{ϵ} with support contained in $V_{3\epsilon}$ such that $\phi_{\epsilon}=1$ in V_{ϵ} and

$$|\partial^{\alpha}\phi_{\epsilon}|\leqslant C_{\alpha}\epsilon^{-|\alpha|},$$

where C_{α} depends only on α and n.

Proof: Let χ be a positive C^{∞} function which has support in the unit ball $\{x;|x|<1\}$, such that $\int\chi\,\mathrm{d}x=1$. Then $\chi_{\epsilon}(x)=\epsilon^{-n}\chi(x/\epsilon)$ has the support in the ball $\{x;|x|<\epsilon\}$ and $\int\chi_{\epsilon}\,\mathrm{d}x=1$. Let v be the characteristic function of $V_{2\epsilon}$ and $\phi_{\epsilon}=v*\chi_{\epsilon}$. Then $\phi\in C^{\infty}(\mathbb{R}^n)$ has support in $V_{3\epsilon}$, and $1-\phi_{\epsilon}=(1-v)*\chi_{\epsilon}$ vanishes in V_{ϵ}. Moreover, we have

$$|\partial^{\alpha}\phi_{\epsilon}|\leqslant\int|\partial^{\alpha}\chi_{\epsilon}|\mathrm{d}x=\epsilon^{-|\alpha|}\int|\partial^{\alpha}\chi|\mathrm{d}x,$$

and

$$|\partial^{\alpha}\phi_{\epsilon}|\leqslant C_{\alpha}\epsilon^{-|\alpha|}$$

for $C_{\alpha}>0$. It is clear that C_{α} depends only on α and n. □

Remark 2.15: Note that Lemma 2.14 is just a concise summary of Sec. 1.4 of Ref. 29.

Theorem 2.15: *Let V be a closed convex cone and K a convex compact set in $\mathbb{R}^n$. Define a function $h_{K,V}(\xi)$, $\xi\in\mathbb{R}^n$, and a set V_K^0 as follows [see Eq. (2.4) for the definition of h_K]:*

$$h_{K,V}(\xi)=\sup_{x\in V}h_K(x)-\langle x,\xi\rangle,\quad\text{and}\quad V_K^0=\{\xi\in\mathbb{R}^n;h_{K,V}(\xi)<\infty\}.$$

Then for every $\mu\in H(\mathbb{R}^n;O)'$ with support in the cone V there is a function

$$\hat{\mu}(\zeta)=\langle\mu,e^{i\langle\cdot,\zeta\rangle}\rangle \tag{2.17}$$

with the following properties: $\hat{\mu}$ *is well defined and holomorphic in the interior of* $\mathbb{R}^n \times iV_K^0$ *and satisfies there the following estimate, for a suitable* $K \subset O$,

$$|\hat{\mu}(\zeta)| \leq C(1+|\zeta|)^j \exp(h_{K,V}(\operatorname{Im}\zeta)). \tag{2.18}$$

$\hat{\mu}$ *is called the Fourier–Laplace transform of* μ.

Proof: We choose a C^∞ function ϕ_ϵ with support contained in $V_{3\epsilon}$ such that $\phi_\epsilon = 1$ in V_ϵ and

$$|\partial^\alpha \phi_\epsilon| \leq C_\alpha \epsilon^{-|\alpha|}.$$

Then we have for $\zeta \in \mathbb{R}^n \times iV_K^0$

$$\begin{aligned}|\langle \mu, e^{i\langle \cdot, \zeta\rangle}\rangle| = |\langle \mu, \phi_\epsilon e^{i\langle \cdot, \zeta\rangle}\rangle| &\leq C\|\phi_\epsilon e^{i\langle \cdot, \zeta\rangle}\|_{K,j} \\ &\leq C \sup\{\exp(h_K(x))|D^\alpha(\phi_\epsilon(x)e^{i\langle x,\zeta\rangle})|; |\alpha| \leq j, x \in \mathbb{R}^n\} \\ &\leq C' \exp(h_{K,V}(\operatorname{Im}\zeta) + 3\epsilon|\operatorname{Im}\zeta|) \sum_{|\alpha|\leq j} \epsilon^{-|\alpha|}(1+|\zeta|)^{j-|\alpha|}.\end{aligned}$$

The estimate (2.18) follows if we take $\epsilon = 1/(1+|\zeta|)$. The standard argument shows that $\zeta \to \phi_\epsilon e^{i\langle \cdot, \zeta\rangle} \in H(\mathbb{R}^n; O)$ is complex differentiable in the interior of $\mathbb{R}^n \times iV_K^0$. □

Remark 2.17: Theorem 7.4.2 of Ref. 29 proves this theorem for Schwartz distributions together with its converse.

Remark 2.18: Let $|x|_\infty = \max\{|x^0|, |\mathbf{x}|\}$ be a norm in $\mathbb{R}^4$ and $\overline{V}_+$ the closed forward light cone in $\mathbb{R}^4$. Abbreviate $V = \overline{V}_+^n$ and for $\ell_i > 0$ introduce $h_K(x) = \Sigma_{i=1}^n \ell_i |x_i|_\infty$. Then we estimate

$$h_{K,V}(\xi) = \sup_{x_i \in \overline{V}_+} \sum_{i=1}^n (\ell_i |x_i|_\infty - \langle x_i, \xi_i\rangle) \leq \sum_{i=1}^n \sup_{x_i \in \overline{V}_+} (\ell_i |x_i|_\infty - \langle x_i, \xi_i\rangle).$$

Let V_+ be the open forward light cone. It follows

$$\sup_{x \in \overline{V}_+} -\langle x, \eta\rangle < \infty$$

for $\eta \in V_+$. Let $\xi_i = \eta_i + (\ell_i, \mathbf{0}) \in V_+ + (\ell_i, \mathbf{0})$. Since $|x|_\infty = x^0$ in $\overline{V}_+$, we find

$$\sup_{x_i \in \overline{V}_+} (\ell_i |x_i|_\infty - \langle x_i, \xi_i\rangle) = \sup_{x_i \in \overline{V}_+} (\ell_i x_i^0 - \langle x_i, \eta_i\rangle - x_i^0 \ell_i) = \sup_{x_i \in \overline{V}_+} -\langle x_i, \eta_i\rangle < \infty.$$

Thus the set

$$V_+(\ell_1, \ldots, \ell_n) = \{(\xi_1, \ldots, \xi_n) \in \mathbb{R}^{4n}; \xi_i \in V_+ + (\ell_i, \mathbf{0})\} \tag{2.19}$$

is contained in V_K^0.

III. AXIOMS FOR QUANTUM FIELD THEORIES WITH FUNDAMENTAL LENGTH

The discussion in the Introduction had shown that the framework of standard quantum fields and the framework of hyperfunction quantum fields do not allow a fundamental length in the formulation of the condition of local commutativity. Thus, for such a theory, a new framework has to be used. We argue that quantum fields in terms of ultra-hyperfunctions is a suitable framework. Accordingly we start by listing the defining conditions of an ultra-hyperfunction quantum field theory (UHFQFT) (here we restrict ourselves to the case of a neutral scalar field). We begin in the spirit of our paper[8] by defining such a field as a relativistic quantum field over the test-function

space $E=\mathcal{T}(T(\mathbb{R}^4))$ for ultra-hyperfunctions. While most conditions only need minor modifications, the condition of local commutativity has to be formulated in such a way as to take the existence of a fundamental length into account.

As usual, the defining conditions of an UHFQFT allow one to deduce a set of properties for the sequences of vacuum expectation values or Wightman functions. In the following section a list of conditions for the sequence of all vacuum expectation values is isolated which allow one to reconstruct the ultra-hyperfunction quantum field.

We begin by collecting some properties of the test-function space, in the sense of Ref. 8.

Lemma 3.1: The test-function space $E=\mathcal{T}(T(\mathbb{R}^4))$ has the following properties:

(1) E admits the Fourier transform $\mathcal{F}$ as an isomorphism of topological vector spaces.
(2) On E and $\tilde{E}=\mathcal{F}E$ there are continuous involutions $f\mapsto f^*$ which satisfy $(\mathcal{F}f)^*=\overline{\mathcal{F}f^*}$ for all $f\in E$.
(3) The restricted Poincaré group G acts on E by continuous linear mappings $\alpha_g: E\to E$, $g\in G$ such that for all $f\in E$ and all $g\in G$ one has $\alpha_g(f)^*=\alpha_g(f^*)$, and $g\mapsto\alpha_g(f)$ is a continuous map $G\to E$. G acts on the test-function space $E=\mathcal{T}(T(\mathbb{R}^4))$ as follows:

$$G\ni g=(a,\Lambda)\to\alpha_g(f)(z)=f(\Lambda^{-1}(z-a)).$$

Proof: For the first item see Proposition 2.5. The proof of the second point is a straightforward calculation. For the proof of (3) see the Appendix. □

Definition 3.2: A quadruple $(\mathcal{H},U,\Phi_0,A)$ satisfying conditions (H_i), $i=1,2,3,4,5$ is called a relativistic quantum field theory with fundamental length ℓ *or an* ultra-hyperfunction quantum field theory.

(H_1) *Fields over $E=\mathcal{T}(T(\mathbb{R}^4))$*: A field A over E with state space $\mathcal{H}$, domain $\mathcal{D}$ and cyclic unit vector Φ_0 is specified in the following way.

(a) The state space $\mathcal{H}$ is a separable complex Hilbert space.
(b) The domain $\mathcal{D}$ is a dense subspace of $\mathcal{H}$ containing the cyclic unit vector Φ_0.
(c) The field A is a linear map from E into the algebra $L(\mathcal{D},\mathcal{D})$ of linear operators $\mathcal{D}\to\mathcal{D}$ such that the following conditions hold.

(i) For all $\Phi,\Psi\in\mathcal{D}$, $f\to(\Phi,A(f)\Psi)$ is a continuous linear map $E\to\mathbb{C}$.
(ii) For each $f\in E$, the adjoint operator $A(f)^*$ of the densely defined operator $A(f)$ in $\mathcal{H}$ is an extension of $A(f^*)$.

(H_2) *Poincaré covariance:* A field $(A,\mathcal{H},\mathcal{D},\Phi_0)$ over E is said to be Poincaré covariant if, and only if, there is a unitary continuous representation U of the restricted Poincaré group G on the Hilbert space $\mathcal{H}$ such that, for all $g\in G$ and all $f\in E$,

$$U(g)\mathcal{D}=\mathcal{D},\ U(g)A(f)U(g)^*=A(\alpha_g(f)).$$

(H_3) *Energy-momentum spectrum Σ:* The energy-momentum spectrum Σ of the theory equals the spectrum $\sigma(P)$ of the infinitesimal generator $P=(P^0,P^1,P^2,P^3)$ of the time–space translations in the representation U, i.e.,

$$U(a)=U(a,\mathbf{1})=e^{ia\cdot P},\quad a\in\mathbb{R}^4.$$

$\{p=0\}$ is an isolated eigenvalue of P. The rest of the spectrum of P is contained in the ''forward light cone''

$$V_+=\{(q^0,\mathbf{q})\in\mathbb{R}^4;q^0>|\mathbf{q}|,\mathbf{q}\in\mathbb{R}^3\}.$$

(H_4) *Uniqueness of the vacuum state:* The subspace $\mathcal{H}_0$ of translation invariant vectors in $\mathcal{H}$ is one-dimensional and is generated by the cyclic vector $\Phi_0\in\mathcal{D}$. Accordingly, this cyclic vector Φ_0 is called the vacuum vector of the theory and it follows that

$$\mathcal{D}_0 = \mathrm{lin}\{\Phi_0, A(f_1)\cdots A(f_n)\Phi_0 : f_k \in E, \quad n = 1,2,\ldots\}$$

is dense in $\mathcal{H}$.

Before we can formulate the last condition of local commutativity, respectively, causality in a theory with finite fundamental length ℓ, we need to introduce some notation and formulate some related results. We define the norm $|x|_1$ for $x = (x^0, \mathbf{x}) \in \mathbb{R}^4$ by

$$|x|_1 = |x^0| + |\mathbf{x}|, \quad |\mathbf{x}| = \sqrt{\sum_{i=1}^{3} (x^i)^2},$$

and denote

$$L^\ell = \{x = (x_1, x_2) \in \mathbb{R}^{4\cdot 2}; |x_1 - x_2|_1 < \ell\}.$$

Next define the open set V of all strictly timelike points in $\mathbb{R}^4$ by

$$V = \{\xi \in \mathbb{R}^4; (\xi^0)^2 - \boldsymbol{\xi}^2 > 0\},$$

and the ℓ-neighborhood V^ℓ of V in $\mathbb{C}^4$,

$$V^\ell = \{z \in \mathbb{C}^4; \exists\, x \in V, |\mathrm{Re}\, z - x| + |\mathrm{Im}\, z|_1 < \ell\}.$$

Finally we introduce the set of all pairs of points in $\mathbb{C}^4$ whose difference belongs to this ℓ-neighborhood,

$$W^\ell = \{(z_1, z_2) \in \mathbb{C}^{4\cdot 2}; z_1 - z_2 \in V^\ell\}.$$

Then we can formulate the last defining condition (H_5).

(H_5) *Extended causality or extended local commutativity:* In some Lorentz frame, for any given $\Psi, \Phi \in \mathcal{D}$ and any $\ell' > \ell$, the functional

$$E \otimes E \ni f_1 \otimes f_2 \to (\Phi, A(f_1)A(f_2)\Psi) \in \mathbb{C}$$

can be extended to a continuous linear functional on $\mathcal{T}(T(L^{\ell'}))$ and moreover,

$$E \otimes E \ni f_1 \otimes f_2 \to (\Phi, A(f_1)A(f_2)\Psi) - (\Phi, A(f_2)A(f_1)\Psi) \in \mathbb{C}$$

can be extended to a continuous linear functional on $\mathcal{T}(W^{\ell'})$.

IV. PROPERTIES OF VACUUM EXPECTATION VALUES FOR UHF QUANTUM FIELDS

A. Preliminaries

Given a UHFQFT $(\mathcal{H}, U, \Phi_0, A)$, we want to analyze the properties of its *vacuum expectation values* defined by

$$\mathcal{W}_n(f_1 \otimes \cdots \otimes f_n) = (\Phi_0, A(f_1)\cdots A(f_n)\Phi_0) \quad \forall\, f_i \in E(1), \quad i = 1,\ldots,n, \tag{4.1}$$

for all $n \in \mathbb{N}$.

Proposition 4.1: For any given $\Psi \in \mathcal{D}$ and every $n = 1,2,\ldots$ there is a continuous linear mapping

$$\Psi_n : E(n) \equiv \mathcal{T}(T(\mathbb{R}^{4n})) \to \mathcal{H}$$

satisfying, for all $f_j \in E = E(1)$, $j = 1,\ldots,n$,

$$\Psi_n(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = A(f_1)A(f_2)\cdots A(f_n)\Psi. \tag{4.2}$$

Proof: Let $\Phi,\Psi\in\mathcal{D}$ and $n\in\mathbb{N}$ be given. Then, by the first axiom,

$$\mathcal{T}(T(\mathbb{R}^4))^n\ni(f_1,\ldots,f_n)\to(\Phi,A(f_1)\cdots A(f_n)\Psi)$$

is a separately continuous n-linear form. Therefore Theorem 2.8 implies that there exists $F\in\mathcal{T}(T(\mathbb{R}^{4n}))'$ such that

$$F(f_1\otimes\cdots\otimes f_n)=(\Phi,A(f_1)\cdots A(f_n)\Psi).$$

Next for $g=f_1\otimes\cdots\otimes f_n\in\otimes^n\mathcal{T}(T(\mathbb{R}^4))$, we define $\Psi_n(g)=A(f_1)\cdots A(f_n)\Psi$ and extend it to $\otimes^n\mathcal{T}(T(\mathbb{R}^4))$ by linearity. By Theorem 2.4, for any $f\in\mathcal{T}(T(\mathbb{R}^{4n}))$ there exists a sequence $\{g_\nu\in\otimes^n\mathcal{T}(T(\mathbb{R}^4))\}$ such that $g_\nu\to f$ as $\nu\to\infty$. Therefore $\|\Psi_n(g_\nu)-\Psi_n(g_\mu)\|^2\to0$ as $\nu,\mu\to\infty$. Thus $\Psi_n(g_\nu)$ converges to a vector $\Psi_n(f)$ and evidently $\Psi_n(f)$ is continuous linear mapping from $\mathcal{T}(T(\mathbb{R}^{4n}))$ to $\mathcal{H}$. □

Apply Proposition 4.1 to the special case where $\Psi\in\mathcal{D}$ is the vacuum vector Φ_0 of the theory. Then we have continuous linear mappings

$$\Phi_n:E(n)=\mathcal{T}(T(\mathbb{R}^{4n}))\to\mathcal{H},\quad n=1,2,\ldots$$

which extend the mappings

$$\otimes^nE(1)\ni f_1\otimes\ \cdots\otimes f_n\mapsto A(f_1)A(f_2)\cdots A(f_n)\Phi_0.$$

As an immediate consequence we get the following proposition.

Proposition 4.2: For every $n=1,2,3,\ldots$, the vacuum expectation value (4.1) has a continuous linear extension to an element $\mathcal{W}_n\in\mathcal{T}(T(\mathbb{R}^{4n}))'$.

B. Implications of extended local commutativity I

Proposition 4.3: For any given $n\geqslant2$ and $i\in\{1,\ldots,n-1\}$ introduce the set

$$L_i^\ell=\{x=(x_1,\ldots,x_n)\in\mathbb{R}^{4n};|x_i-x_{i+1}|_1<\ell\}.$$

Then, for any $\ell'>\ell$ and any $1\leqslant i\leqslant n-1$, $\mathcal{W}_n\in\mathcal{T}(T(\mathbb{R}^{4n}))'$ actually belongs to $\mathcal{T}(T(L_i^{\ell'}))'\subset\mathcal{T}(T(\mathbb{R}^{4n}))'$.

Proof: Let $h\in\mathcal{T}(T(\mathbb{R}^{4j}))$ and $g\in\mathcal{T}(T(\mathbb{R}^{4k}))$. It follows from axiom (H_5) that

$$E\otimes E\ni f_1\otimes f_2\to(\Phi_j(h^*),A(f_1)A(f_2)\Phi_k(g))=\mathcal{W}_n(h\otimes f_1\otimes f_2\otimes g)$$

is extended continuously to $\mathcal{T}(T(L^{\ell'}))$, and we have the following separately continuous multilinear form:

$$\mathcal{T}(T(\mathbb{R}^{4j}))\times\mathcal{T}(T(L^{\ell'}))\times\mathcal{T}(T(\mathbb{R}^{4k}))\ni(h,f,g)\to\mathcal{W}_n(h\otimes f\otimes g).$$

According to Theorem 2.7, a separately continuous multilinear form on Fréchet spaces is jointly continuous. Therefore we have

$$|\mathcal{W}_n(h\otimes f\otimes g)|\leqslant C\|h\|^{T(K_1),j_1}\|f\|^{T(K_2),j_2}\|h\|^{T(K_3),j_3},$$

where $\|h\|^{T(K_1),j_1}$, $\|f\|^{T(K_2),j_2}$, $\|h\|^{T(K_3),j_3}$ are some of the defining seminorms of $\mathcal{T}(T(\mathbb{R}^{4j}))$, $\mathcal{T}(T(L^{\ell'}))$, $\mathcal{T}(T(\mathbb{R}^{4k}))$, respectively. The estimate

$$\begin{aligned}&\|h\|^{T(K_1),j_1}\|f\|^{T(K_2),j_2}\|h\|^{T(K_3),j_3}\\&\quad=\sup\{|z_1^{p_1}h(z_1)z_2^{p_2}f(z_2)z_3^{p_3}g(z_3)|;(z_1,z_2,z_3)\in T(K_1\times K_2\times K_3),|p_i|\leqslant j_i\}\\&\quad\leqslant\|h\otimes f\otimes g\|^{T(K_1\times K_2\times K_3),j_1+j_2+j_3}\end{aligned}$$

shows that $\mathcal{W}_n(h\otimes f\otimes g)$ can be extended continuously to $\mathcal{T}(T(L_i^{\ell'}))$ because $\|h\otimes f\otimes g\|^{T(K_1\times K_2\times K_3),j_1+j_2+j_3}$ is one of the defining seminorms. □

In the same way one proves the following proposition.

Proposition 4.4: For $n\geqslant 2$ and $i\in\{1,\ldots,n-1\}$ denote

$$W_i^{\ell}=\{(z_1,\ldots,z_n)\in\mathbb{C}^{4n};z_i-z_{i+1}\in V^{\ell}\}$$

and define

$$c_i^n(f)(z_1,\ldots,z_n)=f(z_1,\ldots,z_i,z_{i+1},\ldots,z_n)-f(z_1,\ldots,z_{i+1},z_i,\ldots,z_n).$$

Then $\mathcal{W}_n\circ c_i^n$ belongs to $\mathcal{T}(W_i^{\ell'})'$ for any $\ell'>\ell$.

C. Analysis of the spectral condition

Let $\tilde{\Phi}_n$ be the Fourier transform of Φ_n defined by

$$\tilde{\Phi}_n(\tilde{f})=\Phi_n(f).$$

For the vector-valued tempered ultra-hyperfunction Φ_n, $\tilde{\Phi}_n$ is a continuous linear mapping,

$$\tilde{\Phi}_n:H(\mathbb{R}^{4n};\mathbb{R}^{4n})\to\mathcal{H},$$

according to Proposition 2.5. In order to analyze the support properties of $\tilde{\Phi}_n$ we proceed as in Refs. 25, 30 and introduce the following change of variables:

$$(q_0,\ldots,q_{n-1})=\chi_n^{-1}(p_1,\ldots,p_n),\quad q_k=\sum_{j=k+1}^{n}p_j,\quad \zeta_0=z_1,\quad \zeta_j=z_{j+1}-z_j,\quad j=1,\ldots,n-1.$$

Then we have

$$p_n=q_{n-1},\quad p_k=q_{k-1}-q_k,\quad k=1,...,n-1,\quad z_k=\sum_{j=0}^{k-1}\zeta_j,\quad k=1,2,\ldots,n,$$

and thus

$$\sum_{j=1}^{n}z_j\cdot p_j=\langle z,p\rangle=\langle z,\chi_n(q)\rangle=\langle\zeta,q\rangle=\sum_{j=0}^{n-1}\zeta_j\cdot q_j.$$

The translation of a function $f\in E(n)$ by $a\in\mathbb{R}^4$ is defined in the natural way as $f_a(x_1,\ldots,x_n)=f(x_1-a,\ldots,x_n-a)$ and thus the Fourier transform of the translated function is $\tilde{f}_a(p_1,\ldots,p_n)=e^{ia\cdot\Sigma_{k=1}^{n}p_k}\tilde{f}(p_1,\ldots,p_n)$. As a function of the variables $(q_0,\ldots,q_{n-1})$ the Fourier transform $\tilde{\Phi}_n$ is denoted by $\tilde{Z}_n$, i.e.,

$$\tilde{Z}_n(\tilde{f}\circ\chi_n)=\tilde{\Phi}_n(\tilde{f}).$$

The unitary group of translations has a spectral representation $U(a)=\int_{\Sigma}e^{ip\cdot a}E(\mathrm{d}p)$ where the spectral measure $E(\mathrm{d}p)$ has its support in Σ. Thus, by spectral calculus, for any integrable continuous function h on $\mathbb{R}^4$,

$$(2\pi)^{-2}\int_{\mathbb{R}^4}h(a)U(a)\mathrm{d}a=\tilde{h}(P)$$

is a bounded function of the generator $P=(P_0,P_1,P_2,P_3)$ of the translation group. For $h \in \mathcal{S}(\mathbb{R}^4)$ we have

$$\begin{aligned}\tilde{h}(P)\Phi_n(f) &= (2\pi)^{-2}\int_{\mathbb{R}^4} h(a)U(a)\Phi_n(f)\mathrm{d}a = (2\pi)^{-2}\int_{\mathbb{R}^4} h(a)\Phi_n(f_a)\mathrm{d}a \\ &= (2\pi)^{-2}\int_{\mathbb{R}^4} h(a)\tilde{\Phi}_n(\tilde{f}_a)\mathrm{d}a = (2\pi)^{-2}\int_{\mathbb{R}^4} \tilde{Z}_n(h(a)\tilde{f}_a\circ\chi_n)\mathrm{d}a \\ &= \tilde{Z}_n\left((2\pi)^{-2}\int_{\mathbb{R}^4} h(a)\tilde{f}_a\circ\chi_n\,\mathrm{d}a\right) = \tilde{Z}_n(\tilde{h}(q_0)\cdot\tilde{f}\circ\chi_n),\end{aligned}$$

where we used Propositions 2.10, 2.11, 2.12 and the relation

$$\int_{\mathbb{R}^4} h(a)\tilde{f}_a(p)\mathrm{d}a = \tilde{h}(q_0)\cdot\tilde{f}(p).$$

The assumptions of Propositions 2.10 and 2.11 are satisfied because of the continuity of $a \to \tilde{f}_a$ which follows from Lemma 3.1 and the fact that $\|\tilde{f}_a\|_{K,j}$ is a polynomially increasing function of a.

If $\tilde{f}\circ\chi_n = \tilde{g}_1\otimes\tilde{g}_2$ with $\tilde{g}_1 \in H(\mathbb{R}^4;\mathbb{R}^4)$ and $\tilde{g}_2 \in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})$ then, for any $h \in \mathcal{S}(\mathbb{R}^4)$, the relation

$$\tilde{h}(P)\tilde{Z}_n(\tilde{g}_1\otimes\tilde{g}_2) = \tilde{Z}_n((\tilde{h}\cdot\tilde{g}_1)\otimes\tilde{g}_2) \tag{4.3}$$

results.

Proposition 4.5: For any $\tilde{g}_2 \in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})$, the vector-valued generalized function

$$H(\mathbb{R}^4;\mathbb{R}^4) \ni \tilde{g}_1 \to \tilde{Z}_n(\tilde{g}_1\otimes\tilde{g}_2)$$

has its support in Σ.

Proof: Take any $\tilde{g}_1 \in \mathcal{D}(\mathbb{R}^4)$ with support in $R^4\backslash\Sigma$. Then there is $\tilde{h} \in \mathcal{D}(\mathbb{R}^4\backslash\Sigma)$ which is equal to 1 on $\operatorname{supp}\tilde{g}_1$. It follows $\tilde{h}\tilde{g}_1 = \tilde{g}_1$ and $\tilde{h}(P) = 0$. We conclude

$$\tilde{Z}_n(\tilde{g}_1\otimes\tilde{g}_2) = \tilde{Z}_n((\tilde{h}\cdot\tilde{g}_1)\otimes\tilde{g}_2) = \tilde{h}(P)\tilde{Z}_n(\tilde{g}_1\otimes\tilde{g}_2) = 0.$$

Hence the support property follows. □

Recall that the vacuum expectation values $\mathcal{W}_n$ have the following representation

$$\mathcal{W}_n(f_n) = \langle\Phi_0,\Phi_n(f_n)\rangle = \langle\Phi_0,\tilde{\Phi}_n(\tilde{f}_n)\rangle = \langle\Phi_0,\tilde{Z}_n(\tilde{f}_n\circ\chi_n)\rangle \tag{4.4}$$

for all $f_n \in \mathcal{T}(T(\mathbb{R}^{4n}))$ and thus $\tilde{f}_n \in H(\mathbb{R}^{4n};\mathbb{R}^{4n})$. Pick a test function $\tilde{h} \in H(\mathbb{R}^4;\mathbb{R}^4)$. Then, because of the spectral properties of the operator P, we know

$$\tilde{h}^*(0)\Phi_0 = \tilde{h}(P)^*\Phi_0, \tag{4.5}$$

and thus if $\tilde{h}(0) = 1$, because of Eq. (4.3),

$$\mathcal{W}_n(f_n) = \langle\Phi_0,\tilde{Z}_n(\tilde{h}(q_0)\cdot\tilde{f}_n\circ\chi_n)\rangle,$$

or, if $\tilde{f}_n = (\tilde{g}_1\otimes\tilde{g}_{n-1})\circ\chi_n^{-1}$ with $\tilde{g}_k \in H(\mathbb{R}^{4k};\mathbb{R}^{4k})$, then

$$\tilde{\mathcal{W}}_n((\tilde{g}_1\otimes\tilde{g}_{n-1})\circ\chi_n^{-1}) = \tilde{\mathcal{W}}_n(((\tilde{h}\cdot\tilde{g}_1)\otimes\tilde{g}_{n-1})\circ\chi_n^{-1}). \tag{4.6}$$

This prepares for the following proposition.

Proposition 4.6: For $n=2,3,\ldots$ *there is* $\tilde{W}_{n-1}\in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})'$ *such that*

(a)

$$\tilde{\mathcal{W}}_n((\tilde{g}_1\otimes\tilde{g}_{n-1})\circ\chi_n^{-1})=\tilde{g}_1(0)\tilde{W}_{n-1}(\tilde{g}_{n-1}) \tag{4.7}$$

for all $\tilde{g}_{n-1}\in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})$ *and all* $\tilde{g}_1\in H(\mathbb{R}^4;\mathbb{R}^4)$, *i.e.*,

$$\tilde{\mathcal{W}}_n\circ\chi_n(q_0,\ldots,q_{n-1})=(2\pi)^2\delta(q_0)\tilde{W}_{n-1}(q_1,\ldots,q_{n-1});$$

(b) $\operatorname{supp}\tilde{W}_{n-1}\subseteq\Sigma^{n-1}$.

Proof: Take any test function $\tilde{h}\in H(\mathbb{R}^4;\mathbb{R}^4)$ with $\tilde{h}(0)=1$. Then, by Eqs. (4.3), (4.1), and (4.5),

$$\begin{aligned}\tilde{\mathcal{W}}_n((\tilde{g}_1\otimes\tilde{g}_{n-1})\circ\chi_n^{-1})&=\langle\Phi_0,\tilde{Z}_n((\tilde{h}\cdot\tilde{g}_1)\otimes\tilde{g}_{n-1})\rangle\\&=\langle\Phi_0,\tilde{g}_1(P)\tilde{Z}_n(\tilde{h}\otimes\tilde{g}_{n-1})\rangle\\&=\langle\tilde{g}_1(P)^*\Phi_0,\tilde{Z}_n(\tilde{h}\otimes\tilde{g}_{n-1})\rangle=\tilde{g}_1(0)\langle\Phi_0,\tilde{Z}_n(\tilde{h}\otimes\tilde{g}_{n-1})\rangle.\end{aligned}$$

Now define a functional $\tilde{W}_{n-1}$ by

$$\tilde{W}_{n-1}(\tilde{g}_{n-1})=\langle\Phi_0,\tilde{Z}_n(\tilde{h}\otimes\tilde{g}_{n-1})\rangle\quad\forall\,\tilde{g}_{n-1}\in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)}). \tag{4.8}$$

The properties of $\tilde{Z}_n$ imply that this functional belongs to $H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})'$. If $\tilde{h}_j\in H(\mathbb{R}^4;\mathbb{R}^4)$ are two test functions with $\tilde{h}_j(0)=1$ for $j=1,2$, then $\tilde{h}=\tilde{h}_1-\tilde{h}_2$ is a test function with $\tilde{h}(0)=0$. Now pick any test function $\tilde{g}$ with $\tilde{g}(0)=1$. Then, as above, we get

$$\langle\Phi_0,\tilde{Z}_n(\tilde{h}\otimes\tilde{g}_{n-1})\rangle=\langle\Phi_0,\tilde{Z}_n((\tilde{g}\cdot\tilde{h})\otimes\tilde{g}_{n-1})\rangle=\tilde{h}(0)\langle\Phi_0,\tilde{Z}_n(\tilde{g}\otimes\tilde{g}_{n-1})\rangle=0.$$

It follows $\langle\Phi_0,\tilde{Z}_n(\tilde{h}_1\otimes\tilde{g}_{n-1})\rangle=\langle\Phi_0,\tilde{Z}_n(\tilde{h}_2\otimes\tilde{g}_{n-1})\rangle$, and this shows that $\tilde{W}_{n-1}$ is well defined by Eq. (4.8) and part (a) follows.

In order to prove the support property (b) take any $\tilde{g}_1\in H(\mathbb{R}^{4j};\mathbb{R}^{4j})$ and $\tilde{g}_2\in H(\mathbb{R}^{4(n-j)};\mathbb{R}^{4(n-j)})$ and denote $\tilde{f}_1=\tilde{g}_1\circ\chi_j^{-1}$, respectively, $\tilde{f}_2=\tilde{g}_2\circ\chi_{n-j}^{-1}$. Explicitly this means

$$\widetilde{(f_1^*)}(p_1,\ldots,p_j)=\bar{\tilde{g}}_1(-p_1-\cdots-p_j,-p_1-\cdots-p_{j-1},\ldots,-p_1),$$

respectively,

$$\tilde{f}_2(p_{j+1},\ldots,p_n)=\tilde{g}_2(p_{j+1}+\cdots+p_n,p_{j+2}+\cdots+p_n,\ldots,p_n).$$

Note that

$$\begin{aligned}\delta(p_1+\cdots+p_n)\widetilde{(f_1^*)}(p_1,\ldots,p_j)&=\delta(p_1+\cdots+p_n)\bar{\tilde{g}}_1(-p_1-\cdots-p_j,-p_1-\cdots-p_{j-1},\ldots,-p_1)\\&=\delta(q_0)\bar{\tilde{g}}_1(q_j,q_{j-1},\ldots,q_1)=\delta(q_0)(\tilde{g}_1)^*(q_1,\ldots,q_j).\end{aligned}$$

Now use part (a) to evaluate

$$\begin{aligned}(\tilde{Z}_j(\tilde{g}_1),\tilde{Z}_{n-j}(\tilde{g}_2))&=(\tilde{\Phi}_j(\tilde{f}_1),\tilde{\Phi}_{n-j}(\tilde{f}_2))=(\Phi_j(f_1),\Phi_{n-j}(f_2))=\mathcal{W}_n(f_1^*\otimes f_2)=\tilde{\mathcal{W}}_n(\widetilde{(f_1^*)}\otimes\tilde{f}_2)\\&=(2\pi)^2\langle\tilde{W}_{n-1}(q_1,\ldots,q_{n-1}),(\tilde{g}_1)^*(q_1,\ldots,q_j)\tilde{g}_2(q_j,\ldots,q_{n-1})\rangle.\end{aligned}$$

Finally choose $\tilde{g}_1=\tilde{g}_{11}\otimes\tilde{g}_{12}$ with $\tilde{g}_{11}\in H(\mathbb{R}^4;\mathbb{R}^4),\tilde{g}_{12}\in H(\mathbb{R}^{4(j-1)};\mathbb{R}^{4(j-1)})$ and $\tilde{g}_2=\tilde{g}_{21}\otimes\tilde{g}_{22}$ with $\tilde{g}_{21}\in H(\mathbb{R}^4;\mathbb{R}^4),\tilde{g}_{22}\in H(\mathbb{R}^{4(n-j-1)};\mathbb{R}^{4(n-j-1)})$. Then the above identity shows that

$$(\tilde{Z}_j(\tilde{g}_1),\tilde{Z}_{n-j}(\tilde{g}_2))=(2\pi)^2\tilde{W}_{n-1}((\tilde{g}_{12})^*\otimes(\bar{\tilde{g}}_{11}\cdot\tilde{g}_{21})\otimes\tilde{g}_{22}),$$

and by Proposition 4.5 and choosing $j=1,\ldots,n-1$, we conclude that the support of $\tilde{W}_{n-1}$ is contained in Σ^{n-1}. □

D. Basic analyticity

According to Proposition 4.6 the distributions $\tilde{W}_{n-1}$ have their supports in $\Sigma^{n-1}\subseteq\overline{V}_+$. Hence we can apply Theorem 2.16 to them and conclude that their Fourier–Laplace transforms $\hat{W}_{n-1}(\zeta_1,\ldots,\zeta_{n-1})$ are analytic in a set which contains $\mathbb{R}^{4(n-1)}+V_+(\ell_1,\ldots,\ell_{n-1})$ for suitable $\ell_i>0$ [see Eq. (2.19)]. Next we take extended local commutativity into account and show that these Fourier–Laplace transforms can be analytically continued to a much larger domain of analyticity described in the following proposition. These analytic continuations of the $\hat{W}_{n-1}$ are denoted by W_{n-1}.

Proposition 4.7: There exist decreasing functions $R_{ij}(r)$ defined for $\ell<r$ such that $W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})$ is holomorphic in

$$\bigcup_{i=1}^{n-1}\{\zeta\in\mathbb{C}^{4(n-1)};\mathrm{Im}\,\zeta_i\in V_+ +(\ell',\mathbf{0}),\quad \mathrm{Im}\,\zeta_j\in V_+ +(R_{ij}(\ell'),\mathbf{0}),\ \ \ell<\ell',j\neq i\},\tag{4.9}$$

and polynomially increasing there.

Proof: Observe the fact that an element in $H(\mathbb{R}^{4(n-1)};O)'$ is an element in $H_b(\mathbb{R}^{4(n-1)};K)'$ for some compact set $K\subset O$. For any compact set K in

$$L_i^{\ell'}=\{y\in\mathbb{R}^{4n};|y_{i+1}-y_i|_1<\ell'\},$$

we can choose $\epsilon,R_{ij}>0$ so that the set

$$K_i^{\epsilon,R}=\{(\eta_0,\ldots,\eta_{n-1})\in\mathbb{R}^{4n};|\eta_i|_1\leqslant\ell'-\epsilon_i,\ \ |\eta_j|_1\leqslant R_{ij},\ \ j\neq i\}$$

contains K, where $\eta_0=y_1$, $\eta_j=y_{j+1}-y_j$ $(j=1,\ldots,n-1)$. It follows from Proposition 4.3 that $\tilde{\mathcal{W}}_n$ is extended to $H(\mathbb{R}^{4n};L_i^{\ell'})$ for any $\ell'>\ell$. This implies that there exist k, $\epsilon_i=\epsilon_i(\ell')$ and $R_{ij}=R_{ij}(\ell')$ such that

$$|\tilde{\mathcal{W}}_n(\tilde{f})|\leqslant C\|\tilde{f}\|_{K_i^{\epsilon,R},k}$$

for $\tilde{f}\in H(\mathbb{R}^{4n};L_i^{\ell'})$. The function $R_{ij}(r)$ can be chosen such that $R_{ij}(\ell')\geqslant R_{ij}(\ell'')$ when $\ell'<\ell''$. Let $|q|_\infty=\max\{|q^0|,|\mathbf{q}|\}$. Then we have

$$h_{K_i^{\epsilon,R}}(q)=(\ell'-\epsilon_i)|q_i|_\infty+\sum_{j\neq i}R_{ij}|q_j|_\infty.$$

Since the support of $\tilde{W}_{n-1}$ is contained in $\overline{V}_+^{n-1}$, it follows from Theorem 2.16 and Remark 2.18 that $W_{n-1}(\zeta)$ is holomorphic in

$$\{\zeta\in\mathbb{C}^{4(n-1)};\mathrm{Im}\,\zeta_i\in V_+ +(\ell',\mathbf{0}),\mathrm{Im}\,\zeta_j\in V_+ +(R_{ij}(\ell'),\mathbf{0}),\ \ \ell<\ell',j\neq i\}$$

and polynomially increasing there for $i=1,\ldots,n-1$. This completes the proof. □

Now choose $R\in\mathbb{R}$ such that $W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})$ is holomorphic on Γ_R^{n-1}, where $\Gamma_R=\mathbb{R}^4\times(iR,0,0,0)\subset\mathbb{C}^4$. This holomorphic function defines a functional on $\mathcal{T}(T(\mathbb{R}^{4(n-1)}))$ (denoted in the same way) according to the following formula:

$$W_{n-1}(g)=\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})g(\zeta_1,\ldots,\zeta_{n-1})\mathrm{d}\zeta_1\cdots\mathrm{d}\zeta_{n-1} \tag{4.10}$$

for all $g\in\mathcal{T}(T(\mathbb{R}^{4(n-1)}))$. One expects that $W_{n-1}(g)=\tilde{W}_{n-1}(\tilde{g})$ holds. We prepare the proof of this basic relation by the following proposition.

Proposition 4.8: Let $k'>k>0$, $K'=\{q\in\mathbb{R}^4;|q|_1\leqslant k'\}$, $K=\{q\in\mathbb{R}^4;|q|_1\leqslant k\}$, $g\in H_b(\mathbb{R}^4;K')$ *and* $g_x(p)=e^{ixp}g(p)$. *Then the mapping*

$$\mathbb{R}^4\ni x\to g_x\in H_b(\mathbb{R}^4;K) \tag{4.11}$$

is continuous at $x=0$.

Proof: The fundamental theorem of calculus gives $e^{izp}-1=izp\int_0^1 e^{itzp}\,\mathrm{d}t$ and thus, using the well-known estimate $(a>0)$ $xe^{-ax}\leqslant 1/ae$, $\forall\, x\geqslant 0$, for $z\neq 0$, $|z|<\delta/2$,

$$\sup_{p\in\mathbb{R}}|e^{izp}-1|e^{-\delta|p|}\leqslant\frac{2}{e\delta}|z|.$$

Observe the decomposition

$$(e^{ixp}-1)=\sum_{k=0}^{3}(e^{ix^kp^k}-1)\prod_{j=k+1}^{3}e^{ix^jp^j}$$

and the obvious bound $|p^j|\leqslant|p|_\infty$. Then the above estimate implies

$$e^{-\delta|p|_\infty}|e^{ix^kp^k}-1|\prod_{j=k+1}^{3}|e^{ix^jp^j}|\to 0$$

as $x\to 0$ uniformly in p. This estimate can easily be extended to include derivatives,

$$|D^\alpha(e^{ixp}-1)|e^{-\delta|p|}=|(ix)^\alpha e^{ixp}|e^{-\delta|p|_\infty}\to 0,$$

as $x\to 0$ uniformly in p. Since $g\in H_b(\mathbb{R}^4;K')$ satisfies

$$|D^qg(p)|e^{k'|p|_\infty}\leqslant M_{q,k'}<\infty,$$

we conclude

$$|D^q(e^{ixp}-1)D^rg(p)|e^{k|p|_\infty}\leqslant M_{r,k'}|D^q(e^{ixp}-1)|e^{-\delta|p|_\infty}\to 0,$$

as $x\to 0$ uniformly in p, where $\delta=k'-k$. By using Leibniz' formula, we finally get

$$|D^q\{(e^{ixp}-1)g(p)\}|e^{k|p|_\infty}\to 0$$

as $x\to 0$, uniformly in p. This shows that the mapping (4.11) is continuous at $x=0$. □

Now consider a C^∞ function f on $\mathbb{R}^4$ with all derivatives bounded such that $f(q)=1$ in the neighborhood Σ_ϵ and $f(q)=0$ outside of $V_{+2\epsilon}\supset\Sigma_{2\epsilon}$. Then for $R>k$, $e^{i\zeta q}f(q)\in H_b(\mathbb{R}^4;K)$ for $\zeta\in\Gamma_R$, and it follows from Proposition 4.8 that the mapping

$$\Gamma_R\ni\zeta\to e^{i\zeta q}f(q)\in H_b(\mathbb{R}^4;K)$$

is continuous, and

$$\|e^{i\zeta q}f(q)\|_{K,j}\leqslant C\prod_{j=1}^{4}(1+|\zeta_j|)^j$$

for some $C>0$. Let $f_{n-1}(q_1,\ldots,q_{n-1})=\Pi_{j=1}^{n-1}f(q_j)$. Then Propositions 2.10 and 2.11 imply that

$$\begin{aligned}\tilde{W}_{n-1}(\tilde{g})=\tilde{W}_{n-1}(f_{n-1}\cdot\tilde{g})&=\tilde{W}_{n-1}\left((2\pi)^{-2(n-1)}\int_{\Gamma_R^{n-1}}f_{n-1}(q)e^{i\langle\zeta,q\rangle}g(\zeta)\mathrm{d}\zeta\right)\\&=(2\pi)^{-2(n-1)}\int_{\Gamma_R^{n-1}}\tilde{W}_{n-1}(f_{n-1}(q)e^{i\langle\zeta,q\rangle})g(\zeta)\mathrm{d}\zeta\\&=(2\pi)^{-2(n-1)}\int_{\Gamma_R^{n-1}}\tilde{W}_{n-1}(e^{i\langle\zeta,q\rangle})g(\zeta)\mathrm{d}\zeta\\&=\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})g(\zeta_1,\ldots,\zeta_{n-1})\mathrm{d}\zeta_1\ldots\mathrm{d}\zeta_{n-1}=W_{n-1}(g).\end{aligned}$$

E. Implications of Poincaré covariance and quasilocality

For $\ell>0$ introduce

$$\mathcal{I}_i^{n-1}(\ell)=\bigcup_{u\in V_+,u^2=1,\ell<\ell'}\mathcal{I}_i^{n-1}(\ell',u),$$

where

$$\mathcal{I}_i^{n-1}(\ell',u)=\{\zeta\in\mathbb{C}^{4(n-1)};\mathrm{Im}\,\zeta_i\in V_+ +\ell' u,\ \ \mathrm{Im}\,\zeta_j\in V_+ +R_{ij}(\ell')u,\ \ j\neq i\}$$

and then

$$\mathcal{I}_{\mathrm{ext},i}^{n-1}(\ell)=\{\zeta\in\mathbb{C}^{4(n-1)};\exists\Lambda\in L_+(\mathbb{C}),\ \ \Lambda\zeta=(\Lambda\zeta_1,\ldots,\Lambda\zeta_{n-1})\in\mathcal{I}_i^{n-1}(\ell)\}.$$

Let $\mathcal{I}^{n-1}=\mathcal{I}^{n-1}(\ell)$ be the convex envelope of $\cup_{i=1}^{n-1}\mathcal{I}_i^{n-1}(\ell)$. Then it follows from Bochner's theorem on tubular domains (see Sec. 17.5 of Ref. 31) that $W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})$ is analytic in $\mathcal{I}^{n-1}$. Moreover, it can be analytically continued to

$$\mathcal{I}_{\mathrm{ext}}^{n-1}=\{\zeta\in\mathbb{C}^{4(n-1)};\exists\Lambda\in L_+(\mathbb{C}),\ \Lambda\zeta=(\Lambda\zeta_1,\ldots,\Lambda\zeta_{n-1})\in\mathcal{I}^{n-1}\},$$

which is equal to the convex envelope of $\cup_{i=1}^{n-1}\mathcal{I}_{\mathrm{ext},i}^{n-1}(\ell)$, since the Bargman–Hall–Wightman theorem holds also in this case. The proof of the ordinary local case (see Ref. 7) is also applicable to our case. $\mathcal{W}_n(z_1,\ldots,z_n)$ is holomorphic in the domain

$$G_n=\{(z_1,\ldots,z_n);(z_2-z_1,\ldots,z_n-z_{n-1})\in\mathcal{I}_{\mathrm{ext}}^{n-1}\}.$$

Denote

$$L_+(\mathbb{C})\ni\Lambda(t)=\begin{pmatrix}\cos t & i\sin t & & & \\ i\sin t & \cos t & & & \\ & & 1 & 0 & \\ & 0 & & & \\ & & 0 & 1 & \end{pmatrix},$$

$$L_+^{\uparrow} \ni R(\theta)=\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ & \sin\theta & \cos\theta & \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Let $j>0$ and introduce the functions

$$E_j(\zeta)=(j/\pi)^{2(n-1)}\exp\left\{-j\sum_{k=1}^{n-1}\sum_{\alpha=0}^{3}(\zeta_k^{\alpha})^2\right\}.$$

Lemma 4.9: Let $R>0$ be a sufficiently large number as specified for (4.10) and $\rho=(\rho_1,\ldots,\rho_{n-1})$ be a real element of $\mathcal{T}_{\text{ext}}^{n-1}$ satisfying $\xi+ia\in G_n$ for $|\xi-\rho|\leqslant\delta$ for some $\delta\geqslant\sqrt{n}R$ and for any real a such that $a_k=(a_k^0,0,0,0)$. Then we have

$$\int_{\Gamma_R^{n-1}} W_{n-1}(\zeta)E_j(\zeta-\rho)\mathrm{d}\zeta\to W_{n-1}(\rho)$$

as $j\to\infty$.

Proof: Since

$$|\exp\{-j(\zeta-\rho)^2\}|\leqslant\exp\{-j[(\xi-\rho)^2-(n-1)R^2]\}$$

and $W_{n-1}(\zeta)$ is polynomially bounded, we have

$$\left|\int_{\Gamma_R^{n-1},|\xi-\rho|\geqslant\delta} W_{n-1}(\zeta)E_j(\zeta-\rho)\mathrm{d}\zeta\right|\leqslant C_{\delta,R}j^{2(n-1)}\exp\{-j(\delta^2-(n-1)R^2)\}$$

for some constant $C_{\delta,R}>0$. Thus, if $\delta^2\geqslant nR^2$ this contribution tends to zero as $j\to\infty$. Changing the path (surface) of integration, we have

$$\int_{\Gamma_R^{n-1},|\xi-\rho|\leqslant\delta} W_{n-1}(\zeta)E_j(\zeta-\rho)\mathrm{d}\zeta=\int_S W_{n-1}(\zeta)E_j(\zeta-\rho)\mathrm{d}\zeta+\int_{|\xi-\rho|\leqslant\delta} W_{n-1}(\xi)E_j(\xi-\rho)\mathrm{d}\xi \tag{4.12}$$

by Cauchy–Poincaré theorem, where

$$S=\{\zeta\in\mathbb{C}^{n-1};|\xi-\rho|=\delta,y_j^0=tR,\leqslant t\leqslant 1,j=1,\ldots,n-1\}.$$

Since $E_j(\zeta-\rho)\to 0$ for $\zeta\in S$ as $j\to\infty$ and S is compact, the first term of (4.12) vanishes while the second term tends to $W_{n-1}(\rho)$ because $E_j(\xi-\rho)$ tends to $\delta(\xi-\rho)$. □

There exist real points ρ satisfying the condition of Lemma 4.9. In fact, it follows from Proposition 4.7 that for any $\ell'>\ell$ there exists $S>0$ such that $\zeta=(\zeta_1,\ldots,\zeta_{n-1})\in\mathcal{I}_k^{n-1}$ for $\zeta_k\in\Gamma_{R'},\zeta_j\in\Gamma_R$ $(j\neq k)$ for all $R\geqslant S$ and $R'\geqslant\ell'$. We suppose $\ell'\leqslant S$.

Let $\rho_j=(ia_j+\alpha_j,3U+\beta_j,b_j,c_j)$ where $U\geqslant S,|\alpha_j|,|\beta_j|\leqslant U$, and a_j,b_j,c_j are arbitrary real numbers. Then $\Lambda(\pi/2)\rho_j=(i(3U+\beta_j),-a_j+i\alpha_j,b_j,c_j)$ and $\rho=(\rho_1,\ldots,\rho_{n-1})\in\mathcal{I}_{\text{ext}}^{n-1}$.

Let $\rho_j=(ia_j+\alpha_j,b_j,3U+\beta_j,c_j)$. Then $R(-\pi/2)\rho_j=(ia_j+\alpha_j,3U+\beta_j,-b_j,c_j)$ and $\rho\in\mathcal{I}_{\text{ext}}^{n-1}$.

Let σ be the permutation of k and $k+1$, that is, $\sigma(k)=k+1,\sigma(k+1)=k$ and $\sigma(j)=j$ for $j\neq k,k+1$, and $r_j=(0,3\sqrt{n}jR,3\sqrt{n}\sigma(j)R,0)$. Then $\rho_j=r_{j+1}-r_j=(0,3\sqrt{n}R,3\sqrt{n}(\sigma(j+1)-\sigma(j))R,0)$ and therefore $\rho\in\mathcal{I}_{\text{ext}}^{n-1}$. Moreover if $|\xi_j-\rho_j|\leqslant\sqrt{n}R$, $\xi+ia\in\mathcal{I}_{\text{ext}}^{n-1}$. Thus ρ satisfies the condition of Lemma 4.9.

Let $\sigma\rho=\rho'=(\rho_1',\ldots,\rho_{n-1}')$, where $\rho_j'=r_{\sigma(j+1)}-r_{\sigma(j)}$. Then $\sigma\rho$ also satisfies the condition of Lemma 4.9 since $\rho_j'=(0,3\sqrt{n}(\sigma(j+1)-\sigma(j))R,3\sqrt{n}jR,0)$.

The transposition σ of z_k and z_{k+1}, $1\leqslant k\leqslant n-1$, is expressed in terms of the difference variables ζ_j in the following way (compare Sec. IV C):

$$\zeta_k\rightarrow\zeta_k'=-\zeta_k,$$

$$\zeta_{k-1}\rightarrow\zeta_{k-1}'=\zeta_{k-1}+\zeta_k,$$

$$\zeta_{k+1}\rightarrow\zeta_{k+1}'=\zeta_{k+1}+\zeta_k,$$

$$\zeta_j'=\zeta_j \text{ for the remaining indices } j.$$

The following proposition follows from Lemma 4.9.

Proposition 4.10: For the points ρ, $\rho'\in\mathcal{I}_{\mathrm{ext}}^{n-1}$ as above one has, as $j\rightarrow\infty$,

$$\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta)(E_j(\zeta-\rho)-E_j(\zeta'-\rho))\mathrm{d}\zeta\rightarrow W_{n-1}(\rho)-W_{n-1}(\rho').$$

The transformation $(z_1,\ldots,z_n)\rightarrow(\zeta_0,\ldots,\zeta_{n-1})=\lambda_n(z_1,\ldots,z_n)$ introduced in Sec. IV C, maps the set $W_k^{\ell'}$ to the set

$$V_k^{\ell'}=\{(\zeta_0,\ldots,\zeta_{n-1})\in\mathbb{C}^{4n};\zeta_k\in V^{\ell'}\}.$$

For $g_1\in\mathcal{T}(T(\mathbb{R}^4))$ and $g_2\in\mathcal{T}(T(\mathbb{R}^{4(n-1)}))$ define

$$f(z_1,\ldots,z_n)=(g_1g_2)(\lambda_n(z_1,\ldots,z_n))\in\mathcal{T}(T(\mathbb{R}^{4n})).$$

As earlier one gets

$$\mathcal{W}_n(f)=\int_{\mathbb{R}^4}g_1(x)\mathrm{d}x\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta_1,\ldots,\zeta_{n-1})g_2(\zeta_1,\ldots,\zeta_{n-1})\mathrm{d}\zeta_1\cdots\mathrm{d}\zeta_{n-1},$$

which corresponds to Eq. (4.7). Therefore we deduce

$$(\mathcal{W}_n\circ c_k^n)(f)=\int_{\mathbb{R}^4}g_1(x)\mathrm{d}x\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta)(g_2(\zeta)-g_2(\zeta'))\mathrm{d}\zeta$$

and the functional

$$\mathcal{T}(T(\mathbb{R}^{4(n-1)}))\ni f\rightarrow\int_{\Gamma_R^{n-1}}W_{n-1}(\zeta)(f(\zeta)-f(\zeta'))\mathrm{d}\zeta$$

belongs to $\mathcal{T}(V_k^{\ell'})'$.

Since $\rho_k=(0,3\sqrt{n}R,-3\sqrt{n}R,0)$,

$$\mathrm{Re}(\zeta_k-\rho_k)^2=(\mathrm{Re}\,\zeta_k-\rho_k)^2-(\mathrm{Im}\,\zeta_k)^2\geqslant(3/\sqrt{n}R-\ell')^2-\ell'^2$$

if $\zeta_k\in V^{\ell'}$, and

$$\sum_{j=1}^{n-1}\mathrm{Re}(\zeta_j-\rho_j)^2\geqslant(3/\sqrt{n}R-\ell')^2-\ell'^2-(n-2)R^2$$

if $\zeta_k\in V_k^{\ell'}$. If we take $R\geqslant\ell'$, this estimate implies

$$\sup_{\zeta \in V_k^{\ell'}, |\mathrm{Im}\,\zeta_j| \leqslant R} |E_j(\zeta-\rho)| \leqslant (j/\pi)^{(n-1)/2} \exp\{-j5nR^2\} \to 0$$

as $j \to \infty$. Similarly we get that for any multi-index p, as $j \to \infty$,

$$\sup_{\zeta \in V_k^{\ell'}, |\mathrm{Im}\,\zeta_j| \leqslant R} |\zeta^p E_j(\zeta-\rho)| \to 0$$

and this in turn gives

$$\int_{\Gamma_R^{n-1}} (W_{n-1}(\zeta) - W_{n-1}(\zeta')) E_j(\zeta-\rho) \mathrm{d}\zeta \to 0$$

for $j \to \infty$. This and Proposition 4.10 show that $W_{n-1}(\rho) = W_{n-1}(\rho')$ and thus

$$\mathcal{W}_n(r_1,\ldots,r_k,r_{k+1},\ldots,r_n) = \mathcal{W}_n(r_1,\ldots,r_{k+1},r_k,\ldots,r_n).$$

Therefore we can formulate the main result of this section as follows:

Theorem 4.11: *On their respective domains of holomorphy the n-point or Wightman functions $\mathcal{W}_n$ are symmetric.*

V. FUNCTIONAL CHARACTERIZATION OF UHQFT

The analysis of the preceding sections has shown that the sequence of vacuum expectation values of an ultra-hyperfunction quantum field theory has a number of specific properties. In analogy to standard quantum field theory we single out a set of properties of these vacuum expectation values which actually characterizes an ultra-hyperfunction quantum field theory up to isomorphisms.

Properties of UHQFT functionals:

(R0) $\mathcal{W}_0 = 1$, $\mathcal{W}_n \in \mathcal{T}(T(\mathbb{R}^{4n}))'$ for $n \geqslant 1$, and $\mathcal{W}_n(f^*) = \overline{\mathcal{W}_n(f)}$, for all $f \in \mathcal{T}(T(\mathbb{R}^{4n})) \equiv E(n)$, where $f^*(z_1,\ldots,z_n) = \overline{f(\overline{z_n},\ldots,\overline{z_1})}$.

(R1) $\mathcal{W}_n(f) = \mathcal{W}_n(f_{(a,\Lambda)})$ for all $(a,\Lambda) \in \mathcal{P}_+^{\uparrow}$, all $f \in \mathcal{T}(T(\mathbb{R}^{4n}))$, and all $n = 1,2,\ldots$.

(R2) For any finite set f_0, $f_1,\ldots,f_N$ of test functions such that $f_0 \in \mathbb{C}$, $f_n \in \mathcal{T}(T(\mathbb{R}^{4n}))$ for $1 \leqslant n \leqslant N$, one has

$$\sum_{m,n=0}^{N} \mathcal{W}_{m+n}(f_m^* \otimes f_n) \geqslant 0.$$

(R3) For all $n = 2,3,\ldots$ and all $i = 1,\ldots,n-1$ denote

$$L_i^{\ell} = \{x = (x_1,\ldots,x_n) \in \mathbb{R}^{4n}; |x_i - x_{i+1}|_1 < \ell\},$$
$$W_i^{\ell} = \{(z_1,\ldots,z_n) \in \mathbb{C}^{4n}; z_i - z_{i+1} \in V^{\ell}\}.$$

Then, for any $\ell' > \ell$,

(i) $\mathcal{W}_n \in \mathcal{T}(T(\mathbb{R}^{4n}))'$ belongs to $\mathcal{T}(T(L_i^{\ell'}))'$ and

(ii) $\mathcal{W}_n \circ c_i^n$ belongs to $\mathcal{T}(W_i^{\ell'})'$,

where

$$(\mathcal{W}_n \circ c_i^n)(f) = \mathcal{W}_n(c_i^n(f)),$$
$$c_i^n(f)(x_1,\ldots,x_n) = f(x_1,\ldots,x_i,x_{i+1},\ldots,x_n) - f(x_1,\ldots,x_{i+1},x_i,\ldots,x_n).$$

(R4) For the Fourier transform $\tilde{\mathcal{W}}_n \in H(\mathbb{R}^{4n};\mathbb{R}^{4n})'$ of $\mathcal{W}_n$, there exists $\tilde{W}_{n-1} \in H(\mathbb{R}^{4(n-1)};\mathbb{R}^{4(n-1)})'$ such that

$$\tilde{\mathcal{W}}_n \circ \chi_n(q_0,\ldots,q_{n-1}) = (2\pi)^2 \delta(q_0) \tilde{W}_{n-1}(q_1,\ldots,q_{n-1})$$

and supp $\widetilde{W}_{n-1} \subset \Sigma^{n-1}$.

(R5) For a spacelike vector $\mathbf{a} \in \mathbb{R}^4$ and $g_n \in E(n)$ introduce, for all $\lambda > 0$,

$$g_{n,\lambda}(x_1,\ldots,x_n) = g_n(x_1 - \lambda \mathbf{a},\ldots,x_n - \lambda \mathbf{a}).$$

Then, for every $f_m \in E(m)$ and $g_n \in E(n)$ as $\lambda \to \infty$,

$$\mathcal{W}_{m+n}(f_m \otimes g_{n,\lambda}) \to \mathcal{W}_m(f_m)\mathcal{W}_n(g_n).$$

The properties (R0)–(R2) are obvious from the definitions. (R3) and (R4) are shown in the preceding section. (R5) is shown without using locality condition as in the book of Jost.[25]

Theorem 5.1 (Reconstruction theorem): *To a given sequence* $(\mathcal{W}_n)_{n \in \mathbb{N}}$ *of tempered ultra-hyperfunctions satisfying the conditions (R0)–(R5), there corresponds a neutral scalar field* $A(f)$ *which obeys all the axioms* (H_1)–(H_5) *and has the given tempered ultra-hyperfunctions as vacuum expectation values. The field A is unique up to isomorphisms.*

Sketch of the proof: The proof of the theorem differs from the standard one (see for instance Refs. 1, 25) only with regard to those points related to local commutativity. Accordingly we comment only on these aspects.

(R3) implies that, for arbitrary $\Phi = \Phi_m(f_m)$ and $\Psi = \Phi_n(g_n)$, the functional

$$E \otimes E \ni h \otimes k \to (\Phi, A(h)A(k)\Psi) = \mathcal{W}_{m+n+2}(f_m^* \otimes h \otimes k \otimes g_n)$$

can be extended continuously to a functional on $\mathcal{T}(T(L^\ell))$ and moreover

$$E \otimes E \ni h \otimes k \to (\Phi, A(h)A(k)\Psi) - (\Phi, A(k)A(h)\Psi)$$

can be extended continuously to a functional on $\mathcal{T}(W^\ell)$. It follows from the Theorems 2.4 and 2.13 that the above extension is unique. This implies H_5. □

VI. MODELS

We are going to construct models of relativistic quantum fields with a fundamental length by constructing a sequence of n-point functionals which satisfies conditions (R0)–(R5) and then applying the reconstruction theorem 5.1. Our starting points are the well-known results of Jaffe[32] on formal Wick power series of free fields. If we consider the power series of a free field ϕ,

$$\rho^{(i)}(x) = \sum_{n=0}^{\infty} a_n^{(i)} \frac{:\phi(x)^n:}{n!}, \tag{6.1}$$

then we have the following theorem.

Theorem 6.1 (Theorem A.1 of Ref. 32): *As a formal power series*

$$(\Omega, \rho^{(1)}(x_1)\cdots\rho^{(n)}(x_n)\Omega) = \sum_{r_{ij}=0;\ 1 \le i<j \le n}^{\infty} \frac{A(R)T^R}{R!}, \tag{6.2}$$

$$r_{ij} = r_{ji}, \quad r_{ii} = 0, \quad R_i = \sum_{j=1}^{n} r_{ij}, \quad A(R) = \prod_{j=1}^{n} a_{R_j}^{(j)},$$

$$R! = \prod_{1 \le i<j \le n} (r_{ij})!, \quad T^R = \prod_{1 \le i<j \le n} (t_{ij})^{r_{ij}}, \tag{6.3}$$

$$t_{ij} = (\Omega, \phi(x_i)\phi(x_j)\Omega) = D_m^{(-)}(x_i - x_j).$$

Therefore

$$(\Omega,\rho^{(i)}(x)\rho^{(i)}(y)\Omega)=\sum_{n=0}^{\infty}\frac{a_n^{(i)2}}{n!}D_m^{(-)}(x-y)^n,$$

$$D_m^{(-)}(x)=(2\pi)^{-3}\int_{\mathbf{R}^3}[2\omega(\mathbf{k})]^{-1}e^{-i\omega(\mathbf{k})x^0}e^{i\mathbf{k}\cdot\mathbf{x}}\,d\mathbf{k}$$

$$[k\cdot x=k^0x^0-\mathbf{k}\cdot\mathbf{x},\quad \omega(\mathbf{k})=\sqrt{\mathbf{k}^2+m^2}].$$

If the coefficients $\{a_n^{(i)}\}$ satisfy $\lim_{n\to\infty}[|a_n^{(i)}|^2/n!]^{1/n}=0$ then the series (6.1) defines a hyperfunction quantum field (see Ref. 33).

Now we assume that for some $\sigma>0$

$$\limsup_{n\to\infty}[|a_n^{(i)}|^2/n!]^{1/n}=\sigma. \tag{6.4}$$

For example, consider

$$\rho(x)=:e^{g\phi(x)^2}:=\sum_{n=0}^{\infty}g^n\frac{:\phi(x)^{2n}:}{n!}=\sum_{n=0}^{\infty}g^n\frac{(2n)!}{n!}\frac{:\phi(x)^{2n}:}{(2n)!}. \tag{6.5}$$

Then

$$\sigma=\lim_{n\to\infty}\left[g^{2n}\frac{(2n)!}{(n!)^2}\right]^{1/2n}=2g$$

and

$$(\Omega,\rho(x)\rho(y)\Omega)=\sum_{n=0}^{\infty}\left(g^n\frac{(2n)!}{n!}\right)^2\frac{1}{(2n)!}D_m^{(-)}(x-y)^{2n}.$$

Since

$$(1-x)^{-\alpha}=1+\alpha x+\frac{\alpha(\alpha+1)}{2!}x^2+\cdots+\frac{\alpha(\alpha+1)\cdots(\alpha+n-1)}{n!}x^n+\cdots,$$

and for $\alpha=1/2$

$$\frac{\alpha(\alpha+1)\cdots(\alpha+n-1)}{n!}=\frac{(2n)!}{4^n n!}\frac{1}{n!},$$

we get, in the sense of formal power series,

$$(\Omega,\rho(x)\rho(y)\Omega)=[1-4g^2D_m^{(-)}(x-y)^2]^{-1/2}. \tag{6.6}$$

Now we investigate the convergence of this power series, in the sense of tempered ultrahyperfunctions. To this end consider the power series

$$\sum_{r_{ij}=0;\ 1\leqslant i<j\leqslant n}^{\infty}\frac{A(R)Z^R}{R!} \tag{6.7}$$

in the variables z_{ij} $(1\leqslant i<j\leqslant n)$, where $Z^R=\Pi_{1\leqslant i<j\leqslant n}(z_{ij})^{r_{ij}}$. Let

$$\|R\| = \sum_{1 \leqslant i < j \leqslant n} r_{ij} \tag{6.8}$$

and $t_{ij} (1 \leqslant i < j \leqslant n)$ be positive constants. Suppose

$$\limsup_{\|R\| \to \infty} \left[\frac{|A(R)| T^R}{R!} \right]^{1/\|R\|} \leqslant 1.$$

Then the fact that the series (6.7) converges if $|z_{ij}| < t_{ij} (1 \leqslant i < j \leqslant n)$ follows from the following theorem of Lemire.

Theorem 6.2: *The associated convergence radii* $(r_1, \ldots, r_n)$ *of a series* $\Sigma a_{\nu_1, \ldots, \nu_n} z_1^{\nu_1} \cdots z_n^{\nu_n}$ *satisfy*

$$\limsup_{\nu_1 + \cdots + \nu_n \to \infty} [|a_{\nu_1, \ldots, \nu_n}| r_1^{\nu_1} \cdots r_n^{\nu_n}]^{1/(\nu_1 + \cdots + \nu_n)} = 1.$$

The multinomial theorem implies

$$R_i! \prod_{j=1, j \neq i}^{n} \frac{t_{ij}^{r_{ij}}}{(r_{ij})!} \leqslant \left(\sum_{j=1, j \neq i}^{n} t_{ij} \right)^{R_i}$$

and according to Eqs. (6.3) and (6.8) we know

$$\sum_{i=1}^{n} R_i = 2\|R\|, \quad \prod_{i=1}^{n} \prod_{j=1, j \neq i}^{n} (r_{ij})! = (R!)^2, \quad \prod_{i=1}^{n} \prod_{j=1, j \neq i}^{n} t_{ij}^{r_{ij}} = (T^R)^2;$$

hence

$$\left[\frac{|A(R)| T^R}{R!} \right]^2 = \frac{\prod_{i=1}^{n} |a_{R_i}^{(i)}|^2 (T^R)^2}{(R!)^2} = \prod_{i=1}^{n} \left(|a_{R_i}^{(i)}|^2 \prod_{j=1, j \neq i}^{n} \frac{t_{ij}^{r_{ij}}}{(r_{ij})!} \right)$$

and

$$\left[\frac{|A(R)| T^R}{R!} \right]^{1/\|R\|} = \prod_{i=1}^{n} \left[|a_{R_i}^{(i)}|^2 \prod_{j=1, j \neq i}^{n} \frac{t_{ij}^{r_{ij}}}{(r_{ij})!} \right]^{1/2\|R\|} = \prod_{i=1}^{n} \left[\frac{|a_{R_i}^{(i)}|^2}{R_i!} R_i! \prod_{j=1, j \neq i}^{n} \frac{t_{ij}^{r_{ij}}}{(r_{ij})!} \right]^{1/2\|R\|}$$

$$\leqslant \prod_{i=1}^{n} \left[\frac{|a_{R_i}^{(i)}|^2}{R_i!} \left(\sum_{j=1, j \neq i}^{n} t_{ij} \right)^{R_i} \right]^{1/2\|R\|} = \prod_{i=1}^{n} \left[\left(\frac{|a_{R_i}^{(i)}|^2}{R_i!} \right)^{1/R_i} \left(\sum_{j=1, j \neq i}^{n} t_{ij} \right) \right]^{R_i/2\|R\|}.$$

Suppose that $t_{kk+1} < 1/\sigma$, and the other t_{ij}'s are so small that

$$\sum_{1 \leqslant i < j \leqslant n} t_{ij} < \frac{1}{\sigma}.$$

This then implies

$$\limsup_{\|R\| \to \infty} \prod_{i=1}^{n} \left[\left(\frac{|a_{R_i}^{(i)}|^2}{R_i!} \right)^{1/R_i} \left(\sum_{j=1, j \neq i}^{n} t_{ij} \right) \right]^{R_i/2\|R\|} \leqslant 1$$

and the power series (6.7) is convergent for $|z_{ij}| < t_{ij} (1 \leqslant i < j \leqslant n)$. Now we consider the case of $m = 0$ for simplicity. In this case the growth of the two-point function of the free field is easier to estimate. Recall

$$D_0^{(-)}(x)=\lim_{\epsilon\to+0}(2\pi)^{-2}[(x^0-i\epsilon)^2-\mathbf{x}^2]^{-1},$$

$$|(x^0-i\epsilon)^2-\mathbf{x}^2|=|x^2-\epsilon^2-2i\epsilon x^0|.$$

We claim that we can find $\epsilon\geqslant 0$ such that

$$|(2\pi)^{-2}[(x^0-i\epsilon)^2-\mathbf{x}^2]^{-1}|<1/\sigma.$$

For $x^2\leqslant 0$, $|x^2-\epsilon^2-2i\epsilon x^0|\geqslant|x^2-\epsilon^2|\geqslant|x^2|+\epsilon^2$, and for $x^2\geqslant 0$, $|x^2-\epsilon^2-2ix^0|\geqslant|x^2-\epsilon^2-2i\epsilon\sqrt{x^2}|=x^2+\epsilon^2$, and $(|x^2|+\epsilon^2)^{-1}<(2\pi)^2/\sigma$ is equivalent to $\epsilon^2>\sigma/(2\pi)^2-|x^2|$. Choose a number $r'>\sqrt{\sigma}/(2\pi)$ and define

$$\epsilon(x)=\sqrt{\max\{r'^2-|x^2|,0\}}. \tag{6.9}$$

For such a choice one has

$$|(2\pi)^{-2}[(x^0-i\epsilon(x))^2-\mathbf{x}^2]^{-1}|<1/\sigma.$$

Finally we fix the fundamental length for these models,

$$\ell=\sqrt{\sigma}/(2\pi). \tag{6.10}$$

It is easily seen that for any $\ell'>\ell$ there exist $\epsilon(x)$ such that

$$\{(x^0+i\epsilon(x),x^1,x^2,x^3);x\in\mathbb{R}^4\}\subset V^{\ell'}.$$

Therefore, for any $\ell'>\ell$ there exists $R>0$ such that (in formal but suggestive notation)

$$W_{n-1}(\zeta)=\mathcal{W}_n(z)=(\Phi_0,\rho(z_1)\cdots\rho(z_k)\rho(z_{k+1})\cdots\rho(z_n)\Phi_0)$$

is a well-defined holomorphic function for

$$\mathrm{Im}\,\zeta_k=\mathrm{Im}(z_{k+1}-z_j)\in V_+ +(\ell',0,0,0)$$

and

$$\mathrm{Im}\,\zeta_j=\mathrm{Im}(z_{j+1}-z_j)\in V_+ +(R,0,0,0)\quad (j\neq k). \tag{6.11}$$

This implies that $\mathcal{W}_n$ satisfies the condition (i) of the axiom (R3). That is, the mapping

$$\mathcal{T}(T(\mathbb{R}^{4n}))\ni f\to\mathcal{W}(f)=\int_{\Pi_{i=0}^{n-1}\Gamma_i}W_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1}$$

is continuous and can be extended continuously to

$$\mathcal{T}(T(L_k^{\ell'}))\ni f\to\mathcal{W}(f)=\int_{\Pi_{i=0}^{n-1}\Gamma_i}W_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1},$$

where, with $\epsilon(x)$ according to (6.9) and R sufficiently large,

$$\Gamma_k=\{(x^0+i\epsilon(x),x^1,x^2,x^3);x\in\mathbb{R}^4\},\quad \Gamma_j=\{(x^0+iR,x^1,x^2,x^3);x\in\mathbb{R}^4\}$$

and $g(\zeta)=f(\zeta_0,\zeta_0+\zeta_1,\ldots,\zeta_0+\cdots+\zeta_{n-1})$. Now consider the formula

$$\prod_{1\leqslant i<j\leqslant n}(t_{i,j})^{r_{i,j}}=(t_{k,k+1})^{r_{k,k+1}}\prod_{1\leqslant i<j\leqslant n,\ i\neq k,\ j\neq k+1}(t_{i,j})^{r_{i,j}}$$
$$\times\prod_{1\leqslant i<k}(t_{i,k})^{r_{i,k}}\prod_{k+1<j\leqslant n}(t_{k,j})^{r_{k,j}}$$
$$\times\prod_{1\leqslant i<k}(t_{i,k+1})^{r_{i,k+1}}\prod_{k+1<j\leqslant n}(t_{k+1,j})^{r_{k+1,j}}.$$

The transposition of x_k and x_{k+1} causes the transposition of $(t_{k,k+1})^{r_{k,k+1}}$ and $(t_{k+1,k})^{r_{k+1,k}}$ in the first line, and the transposition of the second line and the third line. If x_k and x_{k+1} are spacelike separated, then $t_{k,k+1}=t_{k+1,k}$. The function

$$W^k_{n-1}(\zeta)=(\Phi_0,\rho(z_1)\cdots\rho(z_{k+1})\rho(z_k)\cdots\rho(z_n)\Phi_0)$$

is also holomorphic in a domain defined by (6.11) and

$$-\operatorname{Im}\zeta_k\in V_+ +(\ell',0,0,0).$$

Moreover, if ζ_k lies in $\mathbb{R}^4\backslash V^{\ell'}$, the functions $W_{n-1}(\zeta)$ and $W^k_{n-1}(\zeta)$ are well defined and coincide. Thus we have

$$(\mathcal{W}_n\circ c^n_k)(f)=\int_{\Pi_{i=0}^{n-1}\Gamma_i}W_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1}-\int_{-\Gamma_k\Pi_{i\neq k}\Gamma_i}W^k_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1}$$
$$=\int_{\Gamma^{\ell'}_k\Pi_{i\neq k}\Gamma_i}W_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1}-\int_{-\Gamma^{\ell'}_k\Pi_{i\neq k}\Gamma_i}W^k_{n-1}(\zeta)g(\zeta)\mathrm{d}\zeta_0\cdots\mathrm{d}\zeta_{n-1},$$

where

$$\Gamma^\ell_k=\{(x^0+i\epsilon(x),x^1,x^2,x^3);x\in\mathbb{R}^4\cap V^\ell\}$$

and we used the fact that $W_{n-1}(\zeta)$ and $W^k_{n-1}(\zeta)$ coincides for $\zeta_k\in\mathbb{R}^4\backslash V^{\ell'}$. The above formula shows that the functional $\mathcal{W}_n\circ c^n_k$ belongs to $\mathcal{T}(T(W^{\ell'}_k))'$ for any $\ell'>\ell$ which shows condition (ii) of axiom (R3). We can show that $\mathcal{W}_n$'s satisfy the axioms (R0), (R1), (R2), and (R5) in a similar way as Ref. 34 where it is shown that if the coefficients $\{a^{(i)}_n\}$ satisfy $\lim_{n\to\infty}[|a^{(i)}_n|^2/n!]^{1/n}=0$ then the series (6.1) define hyperfunction quantum fields. There, a Wick polynomial $\rho_N(x)$ is introduced as a truncation of $\rho(x)$,

$$\rho_N(x)=\sum_{n=0}^{N}g^n\frac{:\phi(x)^{2n}:}{n!}.$$

Then the Wightman functions $\mathcal{W}^N_n(x)=(\Phi_0,\rho_N(x_1)\cdots\rho_N(x_n)\Phi_0)$ for $\rho_N(x)$ satisfy all the standard Wightman axioms, and they converge weakly to $\mathcal{W}_n(x)=(\Phi_0,\rho(x_1)\cdots\rho(x_n)\Phi_0)$ as $N\to\infty$ in the sense of tempered ultra-hyperfunctions. Thus they satisfy the above axioms. The proof of spectral condition (R4) is easier than the case of hyperfunction quantum field theory because $\widetilde{W}^N_{n-1}(q)$ and $\widetilde{W}_{n-1}(q)$ are distributions, and $\widetilde{W}^N_{n-1}(q)$ converge weakly to $\widetilde{W}_{n-1}(q)$ as $N\to\infty$ in the sense of distributions. Since the limit in the sense of distributions preserves the support, (R4) is valid for $\rho(x)$. Accordingly we formulate the main result of the section.

Theorem 6.3 (Existence of fields with fundamental length): *For a free field ϕ of mass $m=0$ the Wick power series (6.1) (or more specifically (6.5) define ultra-hyperfunction quantum fields with a fundamental length ℓ given by Eqs. (6.4) and (6.10).*

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APPENDIX A: PROOF OF LEMMA 3.1 (3)

Here we show $g\mapsto\alpha_g(f)$ is a continuous map $G\to E=\mathcal{T}(T(\mathbb{R}^4))$. Since Fourier transformation is a homeomorphism between E and $\tilde{E}=\mathcal{F}E=H(\mathbb{R}^4,\mathbb{R}^4)$, it suffices to show the action $G\to\tilde{E}$ is continuous. The following two propositions show this.

Proposition A.1: Let $f\in H(\mathbb{R}^4,\mathbb{R}^4)$. Then, as $h\to 0$,

$$\|(e^{i\langle h,x\rangle}-1)f(x)\|_{K,j}\to 0.$$

Proof: Note that for any $\epsilon>0$, there exists $R>0$ such that

$$\sup_{|x|\geqslant R,|p|\leqslant j}\exp(h_K(x))|D^p(e^{i\langle h,x\rangle}-1)f(x)|<\epsilon$$

uniformly for $|h|\leqslant\delta>0$. The proposition follows from the following identity:

$$\lim_{h\to 0}\sup_{|x|\leqslant R,|p|\leqslant j}\exp(h_K(x))|D^p(e^{i\langle h,x\rangle}-1)f(x)|\to 0.$$

□

Proposition A.2: Let $\Lambda(t)$ be a one-parameter subgroup of the Lorentz group such that $\Lambda(0)=I$, and $f\in H(\mathbb{R}^4,\mathbb{R}^4)$. Then, as $t\to 0$,

$$\|f(\Lambda(t)x)-f(x)\|_{K,j}\to 0.$$

Proof: The proof goes parallel to the preceding proposition. For any $\epsilon>0$, there exists $R>0$ such that uniformly in t, $|t|\leqslant\delta>0$,

$$\sup_{|x|\geqslant R,|p|\leqslant j}\exp(h_K(x))|D^p(f(\Lambda(t)x)-f(x))|<\epsilon.$$

Again the proposition follows from the following identity:

$$\lim_{t\to 0}\sup_{|x|\leqslant R,|p|\leqslant j}\exp(h_K(x))|D^p(f(\Lambda(t)x)-f(x))|\to 0.$$

□

APPENDIX B: PROOF OF THEOREM 2.13

First we recall that V^ϵ is an open set defined by

$$V^\epsilon=\{z\in\mathbb{C}^n;\exists\, x\in V,|\mathrm{Re}\, z-x|+|\mathrm{Im}\, z|_\beta<\epsilon\}$$

for $\epsilon>0$ and an open set V in $\mathbb{R}^n$. K_p is the closure of $V^{\epsilon/(1+1/p)}$ in $\mathbb{C}^n$, $L_p=\{w\in\mathbb{C}^m;|\mathrm{Im}\, w|\leqslant p\}$, and $U=V^\epsilon\times\mathbb{C}^m$, $M_p=K_p\times L_p$.

Lemma B.1: Let f_j be a sequence in $\mathcal{T}(U)$ and $f\in\mathcal{T}(U)$. If the sequence $\|f_j\|^{M_p,k}$ $(j=1,2,\ldots)$ is bounded, and if f_j converges to f uniformly on $M_{p'}\cap\mathbb{C}^{n+m}$ then f_j converges to f in the norms $\|f_j\|^{M_{p'},k'}$ with $p'\leqslant p$ and $k'<k$.

Proof: We may assume $f=0$. Let $C_{p,k}=\sup\{\|f_j\|^{M_p,k},j=1,2,\ldots\}$. For arbitrary $\epsilon>0$ we can choose $R>0$ such that $C_{p,k}R^{k'-k}<\epsilon$. Then

$$|z^s f_j(z)| < C_{p,k} R^{k'-k} < \epsilon \tag{B1}$$

for $z \in M_{p'}$ with $|z| \geqslant R$ and $|s| \leqslant k'$. On the other hand, there exists $N \in \mathbb{N}$ such that $|f_j(z)| < \epsilon R^{-k'}$ for $j > N$ and $z \in M_{p'}$ with $|z| \leqslant R$. This together with (B1) means $\|f_j\|^{M_{p'},k'} < \epsilon$ for $j > N$. □

Lemma B.2: Let $\epsilon > 0$ *and* $C_\epsilon = \exp \sup_{j \in \mathbb{N}} [(n/2)\log(j/\pi) - j\epsilon^2/(1+\delta)]$. *Then* $0 < C_\epsilon < \infty$ *and the function*

$$E_j(z) = (j/\pi)^{n/2} \exp\left\{ -j \sum_{k=1}^{n} z_k^2 \right\}$$

satisfies

$$|E_j(z)| \leqslant C_\epsilon \exp\{-j\Delta |x|^2\}$$

on the set $\{z = x + iy \in \mathbb{C}^n; |x| \geqslant \epsilon$ and $|y| \leqslant \epsilon/(1+\delta)\}$, *where* $\Delta = (\delta^2 + 2\delta)/(1+\delta)^2$.

Proof: See Lemma 2.3 of Ref. 28. □

Now we define for $\epsilon, \delta > 0$,

$$V_\delta^\epsilon = \{z \in \mathbb{C}^n; \exists x \in V, |\mathrm{Re}\, z - x|/(1+\delta) + |\mathrm{Im}\, z|_\beta < \epsilon\}$$

and let $K_{p,\delta}$ denote the closure of

$$V_\delta^{\epsilon/(1+1/p)} = \{z \in \mathbb{C}^n; \exists x \in V, |\mathrm{Re}\, z - x| + (1+\delta)|\mathrm{Im}\, z|_\beta < \epsilon(1+\delta)/(1+1/p)\}$$

in $\mathbb{C}^n$. Observe that $K_{p,\delta} \subset V^\epsilon$ if $\delta < 1/p$.

Proposition B.3: Let $f(z,w) \in \mathcal{T}(U)$ *and define* $f_j^p(z,w)$ *for* $j = 1,2,\ldots,$ *and* $\delta < 1/p$ *by*

$$f_j^p(z,w) = \int_{K_{p,\delta} \cap \mathbb{R}^n} E_j(z-\xi) f(\xi,w) \mathrm{d}\xi,$$

then $f_j^p \in \mathcal{T}(T(\mathbb{R}^{n+m}))$ *and for any* $k > 0$ *and* $0 < p' < p$, *as* $j \to \infty$,

$$\|f_j^p - f\|^{M_{p'},k} \to 0.$$

Proof: Since $E_j(z)$ is entire analytic, $f_j^p(z,w)$ is also entire analytic. $f \in \mathcal{T}(U)$ implies that for any $p > 0, M > 0, N > 0$, there exists a constant C such that

$$|f(z,w)| \leqslant C \frac{1}{(1+|z|^2)^M (1+|w|)^N} \tag{B2}$$

holds for $(z,w) \in M_p$. Let $r > 0$ and estimate the integral accordingly,

$$\begin{aligned}
\sup_{|\mathrm{Im}\, z| \leqslant r, |\mathrm{Im}\, w| \leqslant r} |z^s w^t f_j^p(z,w)| &\leqslant \sup_{|\mathrm{Im}\, z| \leqslant r, |\mathrm{Im}\, w| \leqslant r} \int_{K_{p,\delta} \cap \mathbb{R}^n} |z^s w^t E_j(z-\xi) f(\xi,w)| \mathrm{d}\xi \\
&\leqslant C \sup_{|\mathrm{Im}\, z| \leqslant r} \int_{K_{p,\delta} \cap \mathbb{R}^n} |z^s E_j(z-\xi)| \frac{1}{(1+|\xi|^2)^M} \mathrm{d}\xi \\
&\leqslant C (j/\pi)^{n/2} e^{jr^2} \sup_{x \in \mathbb{R}^n} \int_{K_{p,\delta} \cap \mathbb{R}^n} (r+|x|)^{|s|} e^{-j(x-\xi)^2} \frac{1}{(1+|\xi|^2)^M} \mathrm{d}\xi.
\end{aligned}$$

Since

$$(r+|x|)^{|s|}e^{-j(x-\xi)^2/2}\frac{1}{(1+|\xi|^2)^M}$$

is a bounded function of x and ξ for $M>|s|$, this estimate can be continued by

$$\sup_{|\mathrm{Im}\, z|\leqslant r,|\mathrm{Im}\, w|\leqslant r}|z^s w^t f_j^p(z,w)|\leqslant C'(j/\pi)^{n/2}e^{jr^2}\int_{\mathbb{R}^n}e^{-j(x-\xi)^2/2}\mathrm{d}\xi<\infty.$$

This shows $f_j^p\in\mathcal{T}(T(\mathbb{R}^{n+m}))$. Next we show that the bounds $\|f_j^p\|^{M_p,k}\leqslant C$ for some $C>0$ hold uniformly with respect to j. To show this, we define a surface $\Gamma(z)$ for $z=x+iy\in K_{p,\delta}$ as follows:

$$\Gamma(z):\{\xi\in\mathbb{R}^n;|\xi-x|<(1+\delta)|y|_\beta<\epsilon(1+\delta)/(1+1/p)\}\to K_{p,\delta}\subset V^\epsilon\subset\mathbb{C}^n,$$

$$\xi\to\zeta=\xi+iy\left(1-\frac{|\xi-x|}{(1+\delta)|y|_\beta}\right).$$

Then $f_j^p(z,w)$ is written as

$$f_j^p(z,w)=\int_{K_{p,\delta}\cap\mathbb{R}^n,|\xi-x|\geqslant(1+\delta)|y|_\beta}E_j(z-\xi)f(\xi,w)\mathrm{d}\xi+\int_{\Gamma(z)}E_j(z-\zeta)f(\zeta,w)\mathrm{d}\zeta_1\wedge\cdots\wedge\mathrm{d}\zeta_n. \tag{B3}$$

Let $\epsilon'=\epsilon(1+\delta)/(1+1/p)$ and

$$g_j^p(z,w)=\int_{K_{p,\delta}\cap\mathbb{R}^n,\epsilon'\geqslant|\xi-x|\geqslant(1+\delta)|y|_\beta}E_j(z-\xi)f(\xi,w)\mathrm{d}\xi+\int_{\Gamma(z)}E_j(z-\zeta)f(\zeta,w)\mathrm{d}\zeta_1\wedge\cdots\wedge\mathrm{d}\zeta_n,$$

and

$$h_j^p(z,w)=\int_{K_{p,\delta}\cap\mathbb{R}^n,|\xi-x|\geqslant\epsilon'}E_j(z-\xi)f(\xi,w)\mathrm{d}\xi.$$

The relevant bound for the function h_j is

$$\sup_{(z,w)\in M_p}|z^s w^t h_j^p(z,w)|=\sup_{(z,w)\in M_p}\int_{K_{p,\delta}\cap\mathbb{R}^n,|\xi-x|\geqslant\epsilon'}|z^s w^t E_j(z-\xi)f(\xi,w)|\mathrm{d}\xi$$

$$\leqslant C\sup_{z\in K_{p,\delta}}\int_{K_{p,\delta}\cap\mathbb{R}^n,|\xi-x|\geqslant\epsilon'}|z^s E_j(z-\xi)|\frac{1}{(1+|\xi|^2)^M}\mathrm{d}\xi.$$

For $z=x+iy\in K_{p,\delta}\subset V_\epsilon$ we have $|y|\leqslant|y|_\beta\leqslant\epsilon'/(1+\delta)$ and so, for ξ with $|\xi-x|\geqslant\epsilon'$, by Lemma B.2, we have $|E_j(z-\xi)|\leqslant C_\epsilon\exp(-j\Delta|\xi-x|^2)$ $(j=1,2,\ldots)$. Accordingly we continue this estimate by

$$\leqslant CC_\epsilon\sup_{z\in K_{p,\delta}\cap\mathbb{R}^n}\int_{K_{p,\delta}\cap\mathbb{R}^n,|\xi-x|\geqslant\epsilon'}(|x|+\epsilon/2)^{|s|}\exp(-j\Delta|x-\xi|^2)|\frac{1}{(1+|\xi|^2)^M}\mathrm{d}\xi$$

$$\leqslant C'\int_{\mathbb{R}^n}|\exp(-j\Delta|x-\xi|^2/2)|\mathrm{d}\xi<C'',$$

where C'' does not depend on j.

In order to estimate $g_j^p(z,w)$, take into account that

$$-\mathrm{Re}\langle z-\xi,z-\xi\rangle=-|x-\xi|^2+|y|\leqslant-|x-\xi|^2+|y|_\beta^2\leqslant-|x-\xi|^2(\delta^2+2\delta)/(1+\delta)^2$$
$$=-\Delta|x-\xi|^2$$

if $|x-\xi|>(1+\delta)|y|_\beta$, and

$$-\mathrm{Re}\langle z-\zeta,z-\zeta\rangle=-|x-\xi|^2+|x-\xi|^2/(1+\delta)^2\leqslant-\Delta|x-\xi|^2$$

if $\zeta\in\Gamma(z)$ and $\mathrm{Re}\,\zeta=\xi$. This gives

$$|g_j^p(z,w)|\leqslant C\int_{|\xi-x|\leqslant\epsilon'}(j/\pi)^{n/2}\exp(-j\Delta|x-\xi|^2)\frac{1}{(1+|\xi|^2)^M}\frac{1}{(1+|w|^2)^N}\mathrm{d}\xi$$
$$\leqslant C'\frac{1}{(1+|x|^2)^M}\frac{1}{(1+|w|^2)^N}\int_{|\xi-x|\leqslant\epsilon}(j/\pi)^{n/2}\exp(-j\Delta|x-\xi|^2)\mathrm{d}\xi$$
$$\leqslant C''\frac{1}{(1+|x|^2)^M}\frac{1}{(1+|w|^2)^N}\int_{\mathbb{R}^n}\exp(-j\Delta|\xi|^2)|\mathrm{d}\xi\leqslant C'''\frac{1}{(1+|z|^2)^M}\frac{1}{(1+|w|^2)^N}.$$

Thus we conclude that $\|f_j^p\|^{M_p,k}\leqslant C$ for some positive constant C uniformly in j, i.e., the sequence $\|f_j^p\|^{M_p,k}$ $(j=1,2,\ldots)$ is bounded.

Next we show that the sequence f_j^p converges to f uniformly on $M_{p'}\cap\mathbb{C}^{n+m}$ with $0<p'<p$. Let $(z,w)\in M_{p'}$. It follows from (B2) that $|f(\zeta,w)-f(z,w)|\leqslant C|\mathrm{Re}\,\zeta-\mathrm{Re}\,z|$ for ζ and z in the integral (B3), and therefore we have

$$\left|f_j^p(z,w)-f(z,w)\int_{K_{p,\delta}\cap\mathbb{R}^n}E_j(z-\xi)\mathrm{d}\xi\right|\leqslant C\int(j/\pi)^{n/2}e^{-j\Delta|x-\xi|}|x-\xi|\mathrm{d}\xi\leqslant C'j^{-1/2}.$$

Since $\mathrm{Re}\,\langle z-\xi,z-\xi\rangle$ has a positive lower bound when $z\in K_{p'}$ and $\xi\in\mathbb{R}^n\backslash K_{p,\delta}$,

$$1-\int_{K_{p,\delta}\cap\mathbb{R}^n}E_j(z-\xi)\mathrm{d}\xi=\int_{\mathbb{R}^n\backslash K_{p,\delta}}E_j(z-\xi)\mathrm{d}\xi$$

is exponentially decreasing as $j\to\infty$. It follows from Lemma 1 that $\|f_j^p-f\|^{K_{p'},k}\to0$ as $j\to\infty$. □

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Phase-space Green's functions for modeling time-harmonic scattering from smooth inhomogeneous objects

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The paper deals with inhomogeneous medium Green's functions in the phase-space domain by which the phase-space (local) spectral distributions of the field, scattered by a high contrast object due a genetic time-harmonic incidence, are evaluated. Two forms of phase-space Green's functions are considered: one that links induced sources in the configuration-space to phase-space distributions of the scattered field, while the other one directly links the phase-space distribution of the incident field to phase-space distributions of the scattered field. The scattering mechanism is described in terms of local samplings of the object function which are localized in the object domain according to the scattered- and incidence-processing parameters. Applications in the field of inverse scattering may be expected to yield fast and efficient algorithms, due to the capability of analytically evaluating (forward) scattering Green's functions. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The conventional spectral elements for wave synthesis are Green's functions or plane waves.[1] However, tracking these *global* basis functions in inhomogeneous environments or through interactions with objects is complicated, and the resulting representation integrals are spectrally distributed. Invoking constructive interference yields local observables in the form of ray fields, but in many situations a wider spectral range of basis functions is required.[2] Instead of using global basis functions that lead to distributed integrals, the representation may be localized *a priori* by using phase-space (PS) spectral representations in which the *local* basis wave-functions are beams. Each beam basis function then accounts for the radiation from a finite region in the source domain, thereby leading to compact spectral representations.

Several PS expansion schemes for wave propagation have been introduced. For *point source* configurations the source field can be expanded into an angular spectrum of beams that emanate from the source in all directions[3] (see also extension to the time-domain in Ref. 4). A different class of expansions applies for *extended source* configurations, utilizing a spectrum of shifted and tilted beams which emanate in all directions from all points in the source domain. Several alternative formulations for time-harmonic fields have been introduced:[5–11] In Refs. 8, 10, and 11, they have been placed within a unified PS format in which a PS distribution of beam propagators is *locally* matched to the source distribution. Recently, discrete PS spectral representations have been introduced, based on the discrete Wilson basis[12] and on frame theory.[13]

Inhomogeneous medium Green's functions are of fundamental significance for modeling wave propagation, inverse scattering, numerical methods, etc. Green's functions are wave objects that link sources in the configuration space, $\mathbf{r}'$, to the configuration observation domain, $\mathbf{r}$, by a convolution integral. These wave objects are global in nature in the sense that each point in the $\mathbf{r}'$ source domain contributes to *all* points in the $\mathbf{r}$-observation domain, hence, the difficulty in evaluating of these wave objects, both analytically and numerically. Since modeling wave propagation directly in the configuration-space implies global Green's functions, transferring the fields via phase-space (windowed-) Fourier transform facilitates the search after *localized Green's function*, which can be easily evaluated both asymptotically and numerically (see Ref. 3 and also

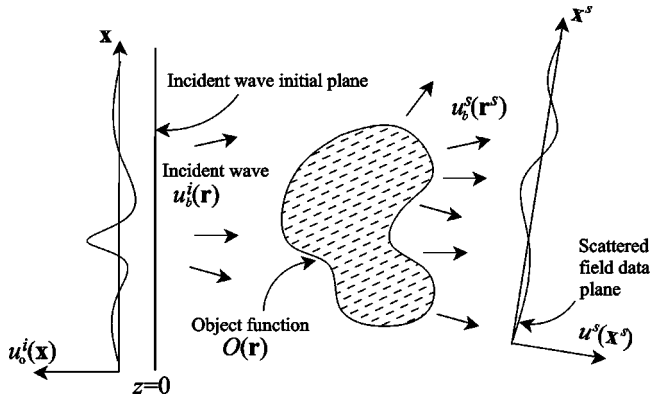

FIG. 1. Physical configuration; the object function $O(\mathbf{r})$ is illuminated by an incident wave $u_b^i(\mathbf{r})$ defined by its initial field distribution over the $z=0$ plane, whereas, the scattered field $u_b^s(\mathbf{r})$ is measured on a data plane $z^s=0$ between which the object is situated.

extension to the time-domain in Ref. 14). Furthermore, since wave interactions with scattering medium have been found to be local in nature, it is suggested that the evaluation of Green's functions should not be carried out in the configuration-space but rather in a *phase-space* (PS) transform domain, which extracts local radiation properties of the data and by that synthesizes local wave-medium interactions.[15,16] The above considerations have been applied in previous publications to the simple case of scattered field due to plane-wave incidence within the Born approximation.[15,16] The present contribution constitutes a general framework for the synthesis and analysis of *inhomogeneous* background scattering due to a *generic* incident wave with applications to inverse scattering, integral equation representation for propagation and scattering, and more.

Following this strategy, we are concerned with the field scattered by an object which is characterized by a wave velocity of $v(\mathbf{r})$, where $\mathbf{r}=(x_1,x_2,z)$ is the conventional Cartesian coordinate system, embedded in a homogeneous medium of save speed v_o (see Fig. 1). The total field $u(\mathbf{r})$, with a $e^{-i\omega t}$ time-dependence assumed and suppressed, satisfies the scalar Helmholtz equation

$$[\nabla^2+k^2(\mathbf{r})]\ \ u(\mathbf{r})=0,\ \ k(\mathbf{r})=\omega/v(\mathbf{r}), \tag{1}$$

subject to Sommerfeld radiation condition $\hat{\mathbf{r}}\cdot\nabla u(\mathbf{r})-iku(\mathbf{r})=o(r^{-1})$, for $r\to\infty$.

In the present investigation, the propagation of the field $u(\mathbf{r})$ in the inhomogeneous medium is formulated by the use of an inhomogeneous background $v_b(\mathbf{r})$ wave speed profile, and the deviation of the scattering medium $v(\mathbf{r})$ from the background $v_b(\mathbf{r})$ is described by the so-called *object function*

$$O(\mathbf{r})=v_o^2[v^{-2}(\mathbf{r})-v_b^{-2}(\mathbf{r})]. \tag{2}$$

The scattering object is illuminated by an incident field, $u_b^i(\mathbf{r})$, defined by the initial field distribution on $z=0$ plane $u_o^i(\mathbf{x})$. Note that $u_o^i(\mathbf{x})$ consists of incident (i.e., having sources in $z<0$ half space) field constituents only, and is therefore, independent of the background medium.

We are concerned with applying PS (local) spectrum techniques to the scattered field, therefore, the scattered field constituents shall be evaluated over planar apertures (observation planes), characterized by $z^s=0$, where $\mathbf{r}^s=(\mathbf{x}^s,z^s)$ with $\mathbf{x}^s=(x_1^s,x_2^s)$ are the Cartesian coordinate system associated with the observation plane (see Fig. 1). The scattered field over the observation plane, $u_b^s(\mathbf{x}^s)\equiv[u(\mathbf{r})-u_b^i(\mathbf{r})]|_{z^s=0}$, satisfies the Lipman–Schwinger integral equation

$$u_b^s(\mathbf{x}^s)=k_o^2\int d^3r'O(\mathbf{r}')u(\mathbf{r}')G_b(\mathbf{r}^s,\mathbf{r}')|_{z^s=0},\ k_o=\omega/v_o, \tag{3}$$

where $u=u_b^i+u_b^s$ is the total field propagating in v_b background medium, and G_b is the inhomogeneous *background* medium Green's function

$$[\nabla^2+k_b^2(\mathbf{r})]\,G_b(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}'),\quad k_b(\mathbf{r})=\omega/v_b(\mathbf{r}). \tag{4}$$

Here and henceforth, subscript b denotes background dependent constituents. Equation (3) describes the scattered field in terms of induced sources, $O(\mathbf{r}')u(\mathbf{r}')$, which are radiating in the perturbed medium $v_b(\mathbf{r})$. The background v_b-medium Green's function, $G_b(\mathbf{r},\mathbf{r}')$, propagates these induced sources to the aperture $z^s=0$ via the spatial convolution integral in (3). Relation (3) has been used for the so-called ''Distorted Wave Born Approximation,'' in which the total field $u(\mathbf{r}')$ on the right-hand side of (3), is replaced by the incident field $u_b^i(\mathbf{r}')$ propagating in the background medium (see also discussion following (15)). This approximation is used for iteratively solving (forward) propagation and scattering problems, and for inverse scattering. In the following sections we will aim at obtaining *PS Green's functions* that link sources to scattered fields in a PS transform domain, rather than in the configuration-space.

II. CONFIGURATION-SPACE TO PHASE-SPACE GREEN'S FUNCTIONS

In order to obtain *PS Green's functions* that link sources to scattered PS field distributions, we shall project the scattered field distribution onto the PS (local) domain. In the next subsections, we shall define the (global) plane-wave spectrum and PS transform of the scattered field which are required for the formulation of the PS Green's function representation.

A. Space-wave-number (global) transforms

The wave number (plane-wave) spectrum, $\tilde{u}_o(\boldsymbol{\xi})$, of an initial field distribution, $u_o(\mathbf{x})$, on a planar surface is defined by the spatial Fourier transform

$$\tilde{u}_o(\boldsymbol{\xi})=\int_{-\infty}^{\infty} d^2x\;\; u_o(\mathbf{x})\exp(-ik_o\,\boldsymbol{\xi}\cdot\mathbf{x}), \tag{5a}$$

where, here and henceforth, plane-wave spectral distribution is denoted by superscript . In (5a), $\boldsymbol{\xi}=(\xi_1,\xi_2)$ is the normalized spatial wave number vector (with respect to $k_o=\omega/v_o$), and $\mathbf{x}=(x_1,x_2)$. Accordingly, the reconstruction of the initial field distribution is

$$u_o(\mathbf{x})=\left(\frac{k_o}{2\pi}\right)^2\int d^2\xi\;\; \tilde{u}_o(\boldsymbol{\xi})\;\; \exp(ik_o\,\boldsymbol{\xi}\cdot\mathbf{x}). \tag{5b}$$

The normalization with respect to the wave number k_o anticipates extension to the time-domain, rendering $\boldsymbol{\xi}$ frequency-independent, with direct geometrical interpretation in terms of the spectral plane-wave propagation angles. For the sake of simplicity, integration limits are omitted on all integrals extending from $-\infty$ to $+\infty$.

B. Phase-space processing of the scattered field

In this section, we summarize the PS analysis and synthesis formalisms that parameterize the scattered field on the initial plane $z^s=0$ (for further details refer to Ref. 11). For the desired *local* spectral analysis of the field distribution, we generate the *PS spectral distribution*, $U_b^s(\overline{\mathbf{X}}^s)$, via a windowed Fourier transform of the distribution in the configuration-space,

$$U_b^s(\overline{\mathbf{X}}^s)=\int d^2x^s\;\; u_b^s(\mathbf{x}^s)\;\; W^{s*}(\mathbf{x}^s;\overline{\mathbf{X}}^s),\quad W^s(\mathbf{x}^s;\overline{\mathbf{X}}^s)=w^s(\mathbf{x}^s-\overline{\mathbf{x}}^s)\exp[ik_o\overline{\boldsymbol{\xi}}^s\cdot(\mathbf{x}^s-\overline{\mathbf{x}}^s)], \tag{6}$$

where, here and henceforth, superscript s denotes scattered field constituents, the asterisk denotes the complex conjugate and $\overline{\mathbf{X}}^s=(\overline{\mathbf{x}}^s,\overline{\boldsymbol{\xi}}^s)$. Here, $w^s(\mathbf{x}^s)$ is a spatial window function, centered at $\mathbf{x}^s=(0,0)$. The vector $\overline{\mathbf{X}}^s$ incorporates the configuration-spectrum *PS coordinates* $(\overline{\mathbf{x}}^s,\overline{\boldsymbol{\xi}}^s)$, whence

$U_b^s(\overline{\mathbf{X}}^s)$ is referred to as a *PS distribution* of the initial field distribution $u_b^s(\mathbf{x}^s)$ over the $z^s=0$ plane. The transform in (6) extracts from $u_b^s(\mathbf{x}^s)$ the local spectrum around the $\overline{\boldsymbol{\xi}}^s$-directed propagation at the window center $\overline{\mathbf{x}}^s$. In typical propagation/scattering problems, the spectrum at a given $\overline{\mathbf{x}}^s$ is localized about a preferred spectral direction $\overline{\boldsymbol{\xi}}^s(\overline{\mathbf{x}}^s)$ that describes the (stationary) direction of propagation of the field at $\overline{\mathbf{x}}^s$ point (the so-called Lagrange manifold). Consequently, the PS spectrum $U^s(\overline{\mathbf{X}}^s)$ is localized *a priori* about the subdomain $(\overline{\mathbf{x}}^s,\overline{\boldsymbol{\xi}}^s)=(\overline{\mathbf{x}}^s,\overline{\boldsymbol{\xi}}^s(\overline{\mathbf{x}}^s))$ in the $\overline{\mathbf{X}}^s$-domain (see synthetic examples in Refs. 8, 11). Note that the PS spectrum of the scattered field depends on the specific background medium profile, $v_b(\mathbf{r})$, since according to (3), both the inhomogeneous medium Green's function, the medium object function, and the incident field propagating in the $v_b(\mathbf{r})$ medium, affect the scattered field.

The degree of spatial and spectral localization achieved by the PS transform can be quantified in terms of the spatial and spectral RMS widths of the window, defined, respectively, by

$$\Delta_{x^s}=\frac{1}{N^s}\left[\int d^2x^s|\mathbf{x}^s|^2\ \ |w^s(\mathbf{x}^s)|^2\right]^{1/2}, \tag{7a}$$

$$\Delta_{\xi^s}=\frac{k_o}{2\pi N^s}\left[\int d^2\xi^s|\boldsymbol{\xi}^s|^2\ \ |\tilde{w}^s(\boldsymbol{\xi}^s)|^2\right]^{1/2}, \tag{7b}$$

where $\tilde{w}^s(\boldsymbol{\xi}^s)$ is the plane-wave distribution (5a) of the window $w^s(\mathbf{x}^s)$, and

$$N^s=\left[\int d^2x^s|w^s(\mathbf{x}^s)|^2\right]^{1/2}=\frac{k_o}{2\pi}\left[\int d^2\xi^s|\tilde{w}^s(\boldsymbol{\xi}^s)|^2\right]^{1/2} \tag{8}$$

is the $\mathcal{L}^2_{\mathbf{x}^s}$ norm of w^s. Note that $\Delta_{x^s}\Delta_{\xi^s}\geqslant 1/k_o$ according to the uncertainty principle. The inverse PS transform is given by[11]

$$u_b^s(\mathbf{x}^s)=\left(\frac{k_o}{2\pi N^s}\right)^2\int d^4\overline{X}^s\ \ U_b^s(\overline{\mathbf{X}}^s)\ \ W^s(\mathbf{x}^s;\overline{\mathbf{X}}^s), \tag{9}$$

where W^s is given in (6). This representation has been used to obtain a PS field representation for homogeneous medium in the 2D (Refs. 8, 17) and 3D (Ref. 11) frequency- and time-domains.

C. PS Green's functions

In order to establish the locally-transformed Data–Object relation, we insert (3) into (6), obtaining

$$U_b^s(\overline{\mathbf{X}}^s)=k_o^2\int d^3r'O(\mathbf{r}')u(\mathbf{r}')B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s), \tag{10}$$

with the scattering propagators

$$B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)=\int d^2x^s\ \ W^{s*}(\mathbf{x}^s;\overline{\mathbf{X}}^s)G_b(\mathbf{r}^s;\mathbf{r}')\big|_{z^s=0}, \tag{11}$$

where $G_b(\mathbf{r},\mathbf{r}')$ is the background medium Green's function in (4) and $W^s(\mathbf{x}^s;\overline{\mathbf{X}}^s)$ is given in (6). Equation (10) describes the local spectrum of the data in terms of a spatial convolution integral of the induced sources $O(\mathbf{r}')u(\mathbf{r}')$ in the configuration-space, with $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$. Comparing relation (10) with the Lipman–Schwinger equation in (3), one finds that the two have essentially the same form. Therefore, $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$ may be regarded as *configuration-space to phase-space* (CS2PS) *Green's function* (see Appendix A for operator representation of the CS2PS Green's function). The CS2PS Green's function propagates the contribution of the configuration-space induced sources to

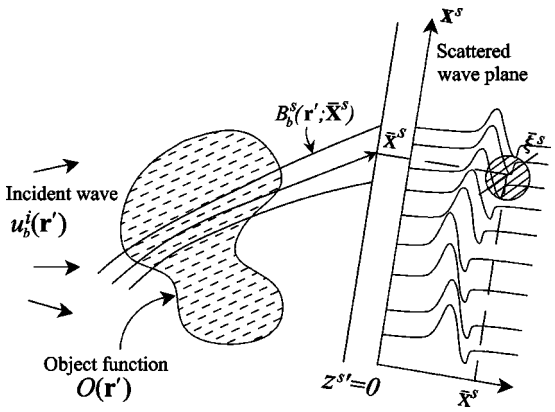

FIG. 2. Configuration-space to phase-space Green's function; the CS2PS Green's function is obtained by a spatial integration of the induced sources $u(\mathbf{r}')O(\mathbf{r}')$ multiplied by the scattering propagator, $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$. This results in a link between the total field propagating in the background medium, and a single phase-space constituent of the scattered field, $U_b^s(\overline{\mathbf{X}}^s)$. The integration domain is limited to points near the B_b^s beam-axis; thus, unlike the Lipman–Schwinger integral (3), the PS spectral distribution of the scattered field synthesizes wave interaction only near the beam-axis.

the PS transform of the data over the observation plane. Also, from (11), we note that the scattering propagators satisfy the wave equation in the v_b background medium, and therefore, for a proper choice of window function w^s, may be evaluated asymptotically using the method described in Sec. IV C (see also Fig. 2). Finally, using $u(\mathbf{r})=u_b^i(\mathbf{r})+u_b^s(\mathbf{r})$, we rewrite (10) in the form

$$U_b^s(\overline{\mathbf{X}}^s)=U_i^s(\overline{\mathbf{X}}^s)+U_s^s(\overline{\mathbf{X}}^s), \tag{12}$$

where

$$U_i^s(\overline{\mathbf{X}}^s)=k_o^2\int d^3r'\,O(\mathbf{r}')u_b^i(\mathbf{r}')B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s), \tag{13}$$

and

$$U_s^s(\overline{\mathbf{X}}^s)=k_o^2\int d^3r'\,O(\mathbf{r}')u_b^s(\mathbf{r}')B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s), \tag{14}$$

in which U_s^i and U_s^s are the contributions of the sources induced by either the incident or scattered fiels, respectively. The above exact formalism may be used for the Distorted Wave Born Approximation (DWBA) in which the total field $u(\mathbf{r}')$ in the exact formulation (3) is replaced by the incident field $u_b^i(\mathbf{r}')$ propagating in the background medium. The DWBA is often used for solving high contrast scattering iteratively, especially in inverse scattering scenarios. In the framework of the DWBA, we may use

$$U_b^s(\overline{\mathbf{X}}^s)\approx U_i^s(\overline{\mathbf{X}}^s). \tag{15}$$

The scattering propagators, $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$, result in a beam wave objects which, for the case of the Gaussian window in (23), are Gaussian beams localized about ray trajectories (i.e., beam-axes). Therefore, the CS2PS mapping in (10) (or (13)), is obtained by integrating over induced sources *locally about beam-axes*. The ray trajectories that describe the beam-axes depend on the background medium v_b and on the processing parameters: $\overline{\mathbf{x}}^s$ determines the emanating point of the ray from the data plane while $\overline{\boldsymbol{\xi}}^s$ sets its direction in the $\mathbf{r}'$ (source) domain (see Fig. 2).

The CS2PS representation in (10) or (12), has several advantages over the Lipman–Schwinger representation: (a) the inhomogeneous Green's function, $G_b(\mathbf{r},\mathbf{r}')$ is difficult to evaluate both analytically and numerically, while the scattering propagators may be evaluated asymptotically (see Sec. IV C); (b) the integration domain in (3) includes the entire object domain, since the induced sources, $O(\mathbf{r}')u(\mathbf{r}')$ exist in the entire object domain and contribute to each point $\mathbf{x}^s$ on the observation plane. Using the CS2PS relation, the integration domain is limited to points near the local Green's function (beam-) axis, since the beam exhibits Gaussian decay away from its axis (see (49) and Fig. 2). Though the induced sources exist in the entire object domain, the PS transform for a given set of PS variables, $\overline{\mathbf{X}}^s$, extracts from the scattered field only those constituents that are scattered in the direction $\overline{\boldsymbol{\xi}}^s$ and are aimed at the point $\overline{\mathbf{x}}^s$; and finally, (c) there exist applications in which the PS spectrum, rather than the scattered field, needs to be evaluated.[15,16] In such cases, direct evaluation using PS Green's function in (10) is more efficient than the conventional route of possibly solving (3), followed by PS processing via (6).

The CS2PS mapping in (10) exhibits *a priori* localization in the source domain only about the coordinates *transverse* to the beam-axis. Furthermore, the incident field $u_b^i(\mathbf{r})$, propagating in the inhomogeneous background medium, $v_b(\mathbf{r})$, has no closed form analytic expression. In the next section, we shall apply local processing to both *scattered* and *incident* fields, resulting in *a priori* localization in all three coordinates, as well as analytical (asymptotic) expressions for the local incident propagators and Green's functions.

III. PHASE-SPACE TO PHASE-SPACE GREEN'S FUNCTIONS

Following the strategy outlined in the previous section, we shall now consider applying PS processing to both *scattered* and *incident* fields. The PS transform operations over the scattered field have been introduced in Sec. II B. Next we define, in a similar way, the operations related to local processing of the incident field.

A. Local processing of the incident field

We generate the *incident field* PS spectral distribution in a way similar to (6), i.e.,

$$U^i(\overline{\mathbf{X}}^i)=\int d^2x \quad u_o^i(\mathbf{x}) \quad W^{i*}(\mathbf{x};\overline{\mathbf{X}}^i), \qquad W^i(\mathbf{x};\overline{\mathbf{X}}^i)=w^i(\mathbf{x}-\overline{\mathbf{x}}^i)\exp[ik_o\overline{\boldsymbol{\xi}}^i\cdot(\mathbf{x}-\overline{\mathbf{x}}^i)], \tag{16}$$

where, as in (6), $w^i(\mathbf{x})$ is a spatial window function. Here and henceforth, superscript i denotes *incident* field constituents and $\overline{\mathbf{X}}^i=(\overline{\mathbf{x}}^i,\overline{\boldsymbol{\xi}}^i)$ are the incidence *PS coordinates*. A key feature in (16) is that, unlike the scattered local spectrum, the incident one is *independent* of the propagation medium, $v_b(\mathbf{r})$. The window's properties (RMS widths, etc.) have been presented in Sec. II B (relations (7), (8)).

Using the inverse transform (as in (9) with $s\rightarrow i$), the PS superposition (16) of the initial field can be propagated into the region $z>0$, giving

$$u_b^i(\mathbf{r})=\left(\frac{k_o}{2\pi N^i}\right)^2\int d^4\overline{X}^i \quad U^i(\overline{\mathbf{X}}^i)B_b^i(\mathbf{r};\overline{\mathbf{X}}^i), \tag{17}$$

where N^i is the $\mathcal{L}_{\mathbf{x}}^2$ norm of w^i (similar to (8)), and the *PS incident propagator* B_b^i is the field radiated by each PS window element $W^i(\mathbf{x};\overline{\mathbf{X}}^i)$ in (9), and can therefore be expressed by Kirchhoff-type integration of the form

$$B_b^i(\mathbf{r};\overline{\mathbf{X}}^i)=\int 2W^i(\mathbf{x};\overline{\mathbf{X}}^i)\partial_{z'}G_b(\mathbf{r};\mathbf{r}')|_{z'=0}, \tag{18}$$

where $G_b(\mathbf{r};\mathbf{r}')$ is the v_b medium Green's function, and W^i is given in (16).

The representation in (17) describes the radiated field as a continuous superposition of shifted and tilted beams, centered at and directed along $\overline{\mathbf{x}}$ and $\overline{\boldsymbol{\xi}}$, respectively. The PS distribution $U^i(\overline{\mathbf{X}}^i)$ defines the excitation strengths of these beams via local matching to the aperture field $u_o^i(\mathbf{x})$.

B. PS Green's functions

By inserting the incident field PS representation in (17) into (13), and inverting the order of integration, one obtains

$$U_i^s(\overline{\mathbf{X}}^s)=\left(\frac{k_o^2}{2\pi N^i}\right)^2\int d^4\overline{X}^i \quad U^i(\overline{\mathbf{X}}^i)\int d^3r' O(\mathbf{r}')B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s). \tag{19}$$

Equation (19) links contributions of PS initial field distribution to the PS scattered field distribution over the $z^s=0$ observation plane in the following manner: the windowed incident (initial-) field distribution is propagated into the $\mathbf{r}'$ configuration-space via the local domain PS incident propagators $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$, which are beam-type wave objects. For a given $\overline{\mathbf{X}}^i$, the beam emanates from the processing-dependent point, $\overline{\mathbf{x}}^i$, in a processing-dependent direction, $\overline{\boldsymbol{\xi}}^i$, into $\mathbf{r}'$ space. The PS scattering propagators, $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$, accumulate, via d^3r' integration, contributions of the incident beams to the local scattered field PS distribution at point $\overline{\mathbf{x}}^s$ on the observation plane, arriving from direction $\overline{\boldsymbol{\xi}}^s$. The PS spectral distribution of the scattered field is obtained by collecting these contributions from all beams emanating from the incidence plane points, in all directions via the $d^4\overline{X}^i$ integration. The contribution of each incident-window element to the scattered PS spectrum is weighted by the PS distribution of the initial incident field.

In order to gain insight into the scattering mechanism, we rewrite (19) in the form

$$U_i^s(\overline{\mathbf{X}}^s)=k_o^2\int d^4\overline{X}^i \quad U^i(\overline{\mathbf{X}}^i)\Psi_b(\overline{\mathbf{X}}^s,\overline{\mathbf{X}}^i), \tag{20}$$

where

$$\Psi_b(\overline{\mathbf{X}}^s,\overline{\mathbf{X}}^i)=\int d^3r' O(\mathbf{r}')\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s), \tag{21}$$

is hereby termed the *phase-space to phase-space* (PS2PS) *Green's function*, and $\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s)$ is a sampling window in the $\mathbf{r}'$-object domain

$$\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s)=\left(\frac{k_o}{2\pi N^i}\right)^2 B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s). \tag{22}$$

Relation (20) presents the PS spectrum of the time-harmonic scattered field distribution in terms of local spatial samples of $O(\mathbf{r})$ (Fig. 3). Since both $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$ and $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$ are beam-like wave objects, the multiplication in (22) results in a *local scattering cell* which exhibits a spatial Gaussian decay away from its center over the intersection of the incident and scattered beam-axes. Here, Λ_b provides windowing along the beam-axis as determined by the PS parameters $\overline{\mathbf{X}}^i$ and $\overline{\mathbf{X}}^s$. The above results imply that the interaction of the incident spectral beam with the object domain, when parameterized in terms of scattered Gaussian beam propagators (i.e., the scattered PS spectrum), occurs as if each scattered beam were *specularly reflected* from the local medium inhomogeneities (see Fig. 3 and further discussion following (56)).

IV. GAUSSIAN WINDOWS

In this section, we examine the special case of Gaussian windows, which have been used extensively for modeling beam propagation since they maximize the PS localization as implied by the uncertainty principle, and yield analytically trackable beam-type propagators.[3,8,14,11]

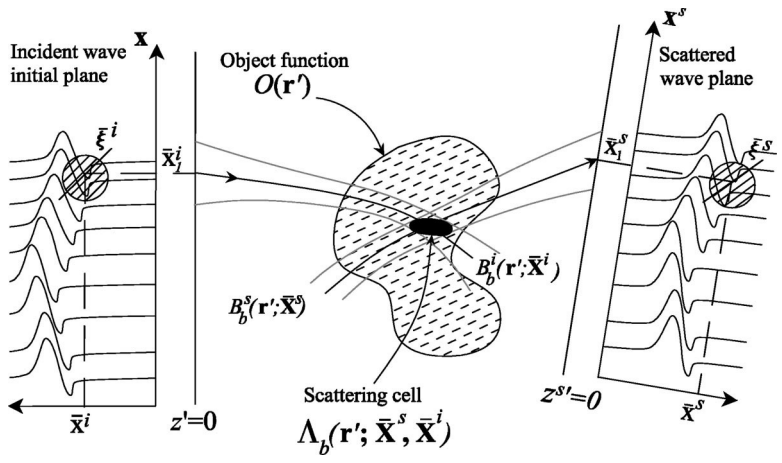

FIG. 3. Phase-space to phase-space mapping phenomenology; the phase-space transform, applied to both incident and scattered field distributions, synthesizes local reflections between isolated local cells, Λ_n, dynamically oriented and located according to the phase-space processing parameters $\bar{\mathbf{X}}^i$ and $\bar{\mathbf{X}}^s$. The PS2PS Green's function in (21) is obtained by a spatial windowing of the object function with the scattering cells.

A. Definitions

For locally (PS-)processing the scattered field distribution, we use a Gaussian window whose spatial and spectral distributions are

$$w^s(\mathbf{x}^s)=\exp\left[\frac{i}{2}k_o\mathbf{x}^s\ \ \mathbf{\Gamma}^s\cdot\mathbf{x}^s\right],\quad \tilde{w}^s(\boldsymbol{\xi}^s)=\frac{2\pi i}{k_o\Gamma^s}\exp\left[-\frac{i}{2}k_o\boldsymbol{\xi}^s\ \ (\mathbf{\Gamma}^s)^{-1}\cdot\boldsymbol{\xi}^s\right], \tag{23}$$

where $\mathbf{\Gamma}^s=\Gamma^s\mathbf{I}$, with $\mathbf{I}$ being the unity matrix and $\Gamma^s=\Gamma^s_r+i\Gamma^s_i$ is the window complex parameter with $\Gamma^s_i>0$. Anticipating extension to the time-domain, definition (23) has been constructed so that the frequency $k_o=\omega/v_o$ appears explicitly in the exponent, while Γ^s is *frequency-independent*. These features may be used to construct collimated time-domain wave objects. $\mathbf{\Gamma}^s$ is a complex symmetric matrix with $\mathrm{Im}\,\mathbf{\Gamma}^s$ positive definite, so that the quadratic phase in the exponent in (23), $\mathbf{x}^s\ \ \mathbf{\Gamma}^s\cdot\mathbf{x}^s=[(x_1^{s2}+x_2^{s2})]\Gamma^s$, has a positive imaginary part that is generating a smooth Gaussian window which is strongest for $|\mathbf{x}^s|=0$ and weakens as $|\mathbf{x}^s|$ increases. The spatial and spectral localization can be quantified in terms of the spatial and spectral RMS widths of the windows given in (7), (8)

$$(N^s)^2=\pi/(k_o\Gamma^s_i),\quad \Delta_{x^s}=1/\sqrt{\Gamma^s_i k_o}=\Delta_{\xi^s}/|\Gamma^s|. \tag{24}$$

Note the uncertainty principle $\Delta_{x^s}\Delta_{\xi^s}=|\Gamma^s|/\Gamma^s_i k_o\geqslant 1/k_o$ with an equality for $\Gamma^s_r=0$.

Following the definition in (23), we shall define the *incident* field distribution processing window, $w^i(\mathbf{x})$, having the same structure as in (23), with the processing parameter Γ^i, i.e.,

$$w^i(\mathbf{x})=\exp\left[\frac{i}{2}k_o\mathbf{x}\ \ \mathbf{\Gamma}^i\cdot\mathbf{x}\right],\quad \mathbf{\Gamma}^i=\Gamma^i\mathbf{I}, \tag{25}$$

etc. All the parametrization and analysis following (23) apply to w^i by replacing $\Gamma^s\to\Gamma^i$ and $\mathbf{x}^s\to\mathbf{x}$ in (23)–(24).

B. Special case: The Born approximation

In order to gain insight into the PS2PS mapping process, we first consider the Born approximation in which the background medium is the *homogeneous* medium v_o. In this case, the background Green's function is free-space Green's function, $G(\mathbf{r},\mathbf{r}')=\exp(ik_o|\mathbf{r}-\mathbf{r}'|)/(4\pi|\mathbf{r}$

$-\mathbf{r}'|$) and the PS propagators and scattering cells yield clear and simple asymptotic expressions. The general scattering over an inhomogeneous background is discussed in Sec. IV C.

1. Asymptotic evaluation of the scattering propagators

The formal integral representation of the scattering propagators using Gaussian windows may be obtained by inserting (23) into (11), with $G_b = G$ being free-space Green's function. Alternatively, a plane-wave spectral representation may be more useful for asymptotic evaluation. In order to obtain such a representation, we insert free-space Green's function plane-wave spectral representation[1]

$$G(\mathbf{r},\mathbf{r}') = \left(\frac{k_o}{2\pi}\right)^2 \int d^2\xi \frac{1}{-2ik_o\zeta} \exp[ik_o(\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{x}') + \zeta|z-z'|)] \tag{26}$$

into (11) and invert the order of integration, yielding

$$B_b^s(\mathbf{r}^s;\overline{\mathbf{X}}^s) = \left(\frac{k_o}{2\pi}\right)^2 \int d^2\xi \frac{i}{2k_o\zeta} \tilde{w}^{s*}(\boldsymbol{\xi}-\overline{\boldsymbol{\xi}}^s) \exp[ik_o(-\boldsymbol{\xi}\cdot(\mathbf{x}^s-\overline{\mathbf{x}}^s) - \zeta z^s)], \tag{27}$$

where $\tilde{w}^s(\boldsymbol{\xi})$ is given in (23). For the Gaussian (scattering) window in (23), the scattering propagator has been evaluated asymptotically in Ref. 15 with connection to the PS processing of pulsed plane-wave excited scattering. It was found there that if the window is "large" on a wavelength scale, $B_b^s(\mathbf{r}^s;\overline{\mathbf{X}}^s)$ in (27) yields collimated beam fields in the $\mathbf{r}'$-domain. Via asymptotic evaluation and paraxial approximation, one obtains

$$B_b^s(\mathbf{r};\overline{\mathbf{X}}^s) = \frac{i}{2k_o\overline{\zeta}^s} \sqrt{\frac{\det\boldsymbol{\Gamma}^i(z_b^s)}{\det\boldsymbol{\Gamma}^s(0)}} \exp\left[ik_o\left(-z_b^s + \frac{1}{2}\mathbf{x}_b^s\boldsymbol{\Gamma}^s(z_b^s)\cdot\mathbf{x}_b^s\right)\right], \tag{28}$$

where

$$\boldsymbol{\Gamma}^s(z_b^s) = \begin{bmatrix} (-z_b^s - \overline{\zeta}^{s2}/\Gamma^{s*})^{-1} & 0 \\ 0 & (-z_b^s - 1/\Gamma^{s*})^{-1} \end{bmatrix}, \tag{29}$$

with $\overline{\zeta}^s = \sqrt{1-\overline{\boldsymbol{\xi}}^s\cdot\overline{\boldsymbol{\xi}}^s}$. In (28), we utilize the *beam-coordinates* $(x_{b_1}^s, x_{b_2}^s, z_b^s)$, defined, for a given PS point $\overline{\mathbf{X}}^s$, by the rotation transformation

$$\begin{bmatrix} x_{b_1}^s \\ x_{b_2}^s \\ z_b^s \end{bmatrix} = \begin{bmatrix} \cos\overline{\vartheta}^s\cos\overline{\varphi}^s & \cos\overline{\vartheta}^s\sin\overline{\varphi}^s & -\sin\overline{\vartheta}^s \\ -\sin\overline{\varphi}^s & \cos\overline{\varphi}^s & 0 \\ \sin\overline{\vartheta}^s\cos\overline{\varphi}^s, & \sin\overline{\vartheta}^s\sin\overline{\varphi}^s & \cos\overline{\vartheta}^s \end{bmatrix} \begin{bmatrix} x_1^s - \overline{x}_1^s \\ x_2^s - \overline{x}_2^s \\ z^s \end{bmatrix}, \tag{30}$$

where $(\overline{\vartheta}^s, \overline{\varphi}^s)$ are the spherical angles associated with the unit-vector (see Fig. 4)

$$\hat{\overline{\boldsymbol{\kappa}}}^s = (\overline{\boldsymbol{\xi}}^s, \overline{\zeta}^s) = (\sin\overline{\vartheta}^s\cos\overline{\varphi}^s, \sin\overline{\vartheta}^s\sin\overline{\varphi}^s, \cos\overline{\vartheta}^s). \tag{31}$$

Thus, the z_b^s axis coincides with the beam-axis in the positive (outward) $\hat{\overline{\boldsymbol{\kappa}}}^s$ direction; the transverse coordinates $\mathbf{x}_b^s = (x_{b_1}^s, x_{b_2}^s)$ are rotated such that $x_{b_2}^s$ is parallel to the z^s plane while $x_{b_1}^s$ lies in the plane $(\overline{\boldsymbol{\xi}}^s, \hat{\overline{\boldsymbol{\kappa}}}^s)$ with its positive direction defined so that $\overline{\boldsymbol{\xi}}^s\cdot\hat{\mathbf{x}}_{b_1}^s > 0$ (see Fig. 4). Furthermore, the system $(\mathbf{x}_b^s, z_b^s)$ is defined to be right-handed. Accordingly, the linear phase $\overline{\boldsymbol{\xi}}^s\cdot(\mathbf{x}^s-\overline{\mathbf{x}}^s)$ implied by the window function in the $z^s=0$ plane is operative in the $x_{b_1}^s$ direction *but not* in the $x_{b_2}^s$ direction. Consequently, $\overline{\boldsymbol{\xi}}^s$ affects only the $\boldsymbol{\Gamma}_{11}^s$ term in (29) but not the $\boldsymbol{\Gamma}_{22}^s$ term, thereby describing *astigmatic* beams.

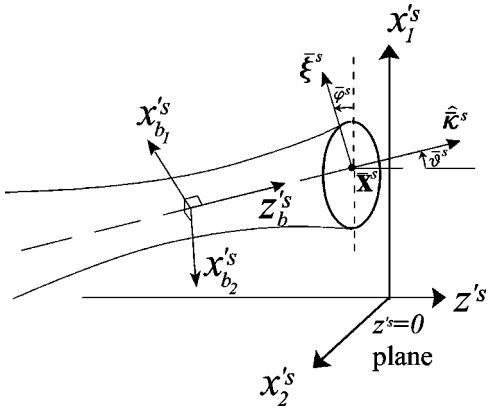

FIG. 4. Scattering propagators' local beam-coordinates; for a given PS spectral parameter $\bar{\mathbf{X}}^s$, the corresponding phase-space scattering propagator $B^s_b(\mathbf{r}';\bar{\mathbf{X}}^s)$ behaves like a collimated beam generated in the $\mathbf{r}'$-domain, whose axis reaches point $\bar{\mathbf{x}}^s$ on the $z'^s=0$ plane along the direction of the beam-axis unit-vector $\hat{\boldsymbol{\kappa}}^s$. The figure depicts the global fixed (x'^s_1,x'^s_2,z'^s) coordinate frame as well as the beam-centered coordinates $(x'^s_{b_1},x'^s_{b_2},z'^s_b)$ (referenced to the $z'^s=0$ plane), which extend along the beam-axis and along the two orthogonal directions perpendicular to the beam-axis.

The parameters of this astigmatic beam field, may be obtained by rewriting the diagonal elements in (29) in the form $\mathbf{\Gamma}=\mathrm{diag}(\Gamma_1,\Gamma_2)$ where $\Gamma^s_{1,2}(z^s_b)=(-z^s_b+Z^s_{1,2}-iF^s_{1,2})^{-1}$ with

$$Z^s_1=-\overline{\zeta}^{s^2}\Gamma^s_r/|\Gamma^s|^2,\quad Z^s_2=-\Gamma^s_r/|\Gamma^s|^2, \tag{32}$$

are identified as the beam *waist* location in the $(z^s_b,x^s_{b_{1,2}})$ plane, and

$$F^s_1=\overline{\zeta}^{s^2}\Gamma^s_i/|\Gamma^s|^2,\quad F^s_2=\Gamma^s_i/|\Gamma^s|^2, \tag{33}$$

are the corresponding *collimation lengths*. Furthermore, the *beam widths* in the $(z^s_b,x^s_{b_{1,2}})$ plane, $D^s_{1,2}$ are found from $\mathrm{Re}\,\Gamma^s(z^s_b)$, giving

$$D^s_{1,2}=\sqrt{F^s_{1,2}/k_o}\sqrt{1+(z^s_b-Z^s_{1,2})^2/F^{s2}_{1,2}}, \tag{34}$$

and the *phase front radius of curvature*, $R^s_{1,2}$ may be obtained from $\mathrm{Im}\,\Gamma^s(z^s_b)$, giving

$$R^s_{1,2}=(Z^s_{1,2}-z^s_b)+F^2_{1,2}/(Z^s_{1,2}-z^s_b). \tag{35}$$

The beam propagator astigmatism is caused by the beam tilt which reduces the effective initial beam width in the x_{b_1} direction. Note that the waist location Z, the collimation length F as well as the phase as a whole, are frequency-independent. However, beam width D is frequency dependent, being proportional to $k_o^{-1/2}$. These properties identify the scattering propagators as ''iso-diffracting'' wave packets.[18]

2. Asymptotic evaluation of the incident propagators

Using Gaussian windows, the PS incident propagators, $B^i_b(\mathbf{r};\bar{\mathbf{X}}^i)$ may be evaluated by inserting free-space Green's function into (18). In the present context it is convenient to express the free-space propagators by the plane-wave representation

$$B^i_b(\mathbf{r};\bar{\mathbf{X}}^i)=\left(\frac{k_o}{2\pi}\right)^2\int d^2\xi\ \ \tilde{w}(\boldsymbol{\xi}-\bar{\boldsymbol{\xi}}^i)\ \ \exp[ik_o(\boldsymbol{\xi}\cdot(\mathbf{x}-\bar{\mathbf{x}}^i)+\zeta z)]. \tag{36}$$

If w is wide on a wavelength scale then the spatial and spectral distributions of $\tilde{w}$ are localized around $\mathbf{x}=\overline{\mathbf{x}}^i$ and $\boldsymbol{\xi}=\overline{\boldsymbol{\xi}}^i$, respectively. Consequently, $B_b^i(\mathbf{r};\overline{\mathbf{X}}^i)$ behaves like a collimated beam whose axis emerges from the $z=0$ plane at $\mathbf{x}=\overline{\mathbf{x}}^i$ with a direction

$$\overline{\boldsymbol{\kappa}}^i=(\overline{\boldsymbol{\xi}}^i,\overline{\zeta}^i),\quad \overline{\zeta}^i=\sqrt{1-|\overline{\boldsymbol{\xi}}^i|^2}, \tag{37}$$

where $|\overline{\boldsymbol{\xi}}^i|^2=\overline{\boldsymbol{\xi}}^i\cdot\overline{\boldsymbol{\xi}}^i$. Next, the general formulation for the scattering process is evaluated for the special case of the Gaussian windows in (25). These windows enable closed form asymptotic evaluation of the PS2PS Green's function, $\Psi_b(\overline{\mathbf{X}}^s,\overline{\mathbf{X}}^i)$, and the scattering cell Λ_b. Via asymptotic evaluation and paraxial approximation, one obtains[11]

$$B_b^i(\mathbf{r};\overline{\mathbf{X}}^i)=\sqrt{\frac{\det\boldsymbol{\Gamma}^i(z_b^i)}{\det\boldsymbol{\Gamma}^i(0)}}\exp\left[ik_o\left(z_b^i+\frac{1}{2}\mathbf{x}_b^i\boldsymbol{\Gamma}^i(z_b^i)\cdot\mathbf{x}_b^i\right)\right], \tag{38}$$

where

$$\boldsymbol{\Gamma}^i(z_b^i)=\begin{bmatrix}(z_b^i+\overline{\zeta}^{i2}/\Gamma^i)^{-1} & 0\\ 0 & (z_b^i+1/\Gamma^i)^{-1}\end{bmatrix}, \tag{39}$$

with $\overline{\zeta}^i=\sqrt{1-\overline{\boldsymbol{\xi}}^i\cdot\overline{\boldsymbol{\xi}}^i}$. In (38), we utilize the beam-coordinates $(x_{b_1}^i,x_{b_2}^i,z_b^i)$ defined, for a given PS point $\overline{\mathbf{X}}^i$, by the transformation in (30) with $(\overline{\vartheta}^s,\overline{\varphi}^s)\to(\overline{\vartheta}^i,\overline{\varphi}^i)$ where $(\overline{\vartheta}^i,\overline{\varphi}^i)$ are the spherical angles associated with the unit-vector

$$\hat{\overline{\boldsymbol{\kappa}}}^i=(\overline{\boldsymbol{\xi}}^i,\overline{\zeta}^i)=(\sin\overline{\vartheta}^i\cos\overline{\varphi}^i,\sin\overline{\vartheta}^i\sin\overline{\varphi}^i,\cos\overline{\vartheta}^i). \tag{40}$$

The parametrization of the beam field in (38) may be obtained in a similar manner to (32)–(35).

The asymptotic beams in (38) facilitate insight into the role of the paraxial approximation: these beams do not satisfy the boundary condition $B^i(\mathbf{r};\overline{\mathbf{X}}^i)|_{z=0}=W^i(\mathbf{x};\overline{\mathbf{X}}^i)$, since near the $z=0$ plane, the paraxial approximation $z_b^i\gg\sqrt{x_{b_1}^{i\,2}+x_{b_2}^{i\,2}}$ is invalid. The paraxially approximated (astigmatic) beam is obtained by projecting the initial window onto the transverse plane $z_b^i=0$ over which the initial effective beam width in the $x_{b_1}^i$ direction is reduced by a factor of $\overline{\zeta}^i$ whereas the width in the $x_{b_2}^i$ direction remains unchanged. Therefore, the paraxial beam boundary conditions on a plane transverse to the beam propagation direction $(z_b^i=0)$ are

$$B^i(\mathbf{r}_b^i;\overline{\mathbf{X}}^i)|_{z_b^i=0}=\exp\left[\frac{i}{2}k_o\mathbf{x}_b^i\quad\boldsymbol{\Gamma}_{\text{parax}}^i\cdot\mathbf{x}_b^i\right], \tag{41}$$

with

$$\boldsymbol{\Gamma}_{\text{parax}}^i=\begin{bmatrix}\Gamma^i/\overline{\zeta}^{i2} & 0\\ 0 & \Gamma^i\end{bmatrix}. \tag{42}$$

Comparing the scattering propagator in (28) to the incident propagator in (38), one finds that they have a similar Gaussian beam type form. They differ mainly in the beam-axis directions: in (40) the beam-axis is directed along the *outgoing* direction (i.e., towards the scattering object) whereas in (31), the scattering propagators are directed *away from the object*. Furthermore, the incident beam is forward propagating (i.e., accumulates positive phase along the beam-axis), whereas the $-z_b^s$ term in (29) implies that the scattering propagators are *back-propagated* into the scattering object domain.

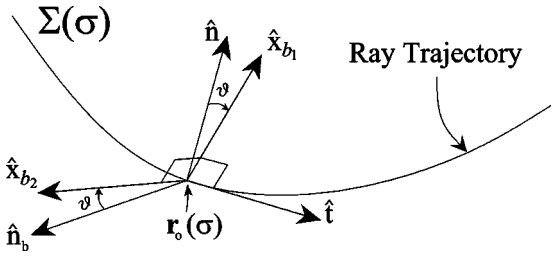

FIG. 5. Local beam-coordinates and ray trajectories; the beam propagator is propagating along ray trajectory Σ. The local orthogonal coordinate system $\mathbf{r}=\mathbf{r}_o(\sigma)+x_1\hat{\mathbf{x}}_1+x_2\hat{\mathbf{x}}_2$, where σ is the arc length along the ray trajectory, is obtained by the rotation transformation in (45).

3. PS2PS mapping

Next, we examine the local scattering cell in the $\mathbf{r}'$ object domain, $\Lambda_b(\mathbf{r}';\overline{\mathbf{X}})$, under the Born approximation. By inserting (38) with (28) into (22), one obtains

$$\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s)=\frac{ik_o^3}{8\overline{\zeta}^s(\pi N^i)^2}\sqrt{\frac{\det\boldsymbol{\Gamma}^i(z_b^i)}{\det\boldsymbol{\Gamma}^i(0)}}\sqrt{\frac{\det\boldsymbol{\Gamma}^s(z_b^s)}{\det\boldsymbol{\Gamma}^s(0)}}$$
$$\times\exp\left[ik_o\left(z_b^i-z_b^s+\frac{1}{2}\mathbf{x}_b^i\boldsymbol{\Gamma}^i(z_b^i)\cdot\mathbf{x}_b^i+\frac{1}{2}\mathbf{x}_b^s\boldsymbol{\Gamma}^s(z_b^s)\cdot\mathbf{x}_b^s\right)\right]. \tag{43}$$

Relation (43) describes a local 3D spatial window; it is centered at the intersection of the incident and scattering propagators axes, where both $\mathbf{x}_b^i$ and $\mathbf{x}_b^s$ are zero, and exhibits a Gaussian decay as the transverse coordinates $\mathbf{x}_b^i$ and $\mathbf{x}_b^s$ increase. The orientation of the cell is determined by the rotation transformation in (30) for incident and scattering propagators, and by the processing parameters Γ^i and Γ^s. For the special case $\Gamma^i=\Gamma^s$, the exponent in (43) contains the sum of $\mathbf{x}_b^i$ and $\mathbf{x}_b^s$. Since both are determined by a rotation transformation of the (30) kind, the result is a new rotation transformation that bisects the incident direction $\hat{\boldsymbol{\kappa}}^i$ in (37) with the scattering direction $\hat{\boldsymbol{\kappa}}^s$ in (31). Therefore, the interaction of the incident spectral beam with the object domain, when parameterized in terms of scattered Gaussian beam propagators, occurs as if each scattered beam were *specularly reflected* from the local medium inhomogeneities (see Fig. 3 and further discussion following (56)).

C. Propagation in the perturbed medium

Next, we consider the propagation of beam propagators (such as B_b^i and B_b^s) in an *inhomogeneous medium* with a wave velocity $v_b(\mathbf{r})$.

1. Local beam-coordinates

An asymptotic solution for general beam-type propagation in an inhomogeneous medium is given in Ref. 3 (see also extension to the time-domain in Refs. 14 and 19). It has been shown there that the field is propagating along a ray trajectory, Σ (see Fig. 5). Denoting σ as the arc length along the ray trajectory, the ray local coordinates are defines by the unit-vectors $\hat{\mathbf{t}}$, $\hat{\mathbf{n}}$, $\hat{\mathbf{n}}_b=\hat{\mathbf{t}}\times\hat{\mathbf{n}}$, denoting the tangent, normal, and bi-normal of Σ at a point $\mathbf{r}_o(\sigma)$ on Σ, respectively. They are related by the Fernet equations[20]

$$\mathbf{r}_o'=\hat{\mathbf{t}},\quad \hat{\mathbf{t}}'=K\hat{\mathbf{n}},\quad \hat{\mathbf{n}}'=-K\hat{\mathbf{t}}+\kappa\hat{\mathbf{n}}_b,\quad \hat{\mathbf{n}}_b'=-\kappa\hat{\mathbf{n}}, \tag{44}$$

where the prime denotes a derivative with respect to σ, K is the curvature of Σ, and κ is its torsion. The ray coordinates are nonorthogonal for $\kappa\neq 0$. A locally orthogonal coordinate system along the ray may be obtain by transverse rotation of the unit-vectors[20] (see Fig. 5)

$$\begin{pmatrix} \hat{\mathbf{x}}_{b_1} \\ \hat{\mathbf{x}}_{b_2} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \hat{\mathbf{n}} \\ \hat{\mathbf{n}}_b \end{pmatrix}, \tag{45}$$

where $\theta(\sigma)$ satisfies

$$\theta'(\sigma) = \kappa(\sigma). \tag{46}$$

Points near the ray may now be expressed as

$$\mathbf{r} = \mathbf{r}_o(\sigma) + n\hat{\mathbf{n}}(\sigma) + n_b\hat{\mathbf{n}}_b(\sigma) = \mathbf{r}_o(\sigma) + x_{b_1}\hat{\mathbf{x}}_{b_1} + x_{b_2}\hat{\mathbf{x}}_{b_2}, \tag{47}$$

where the coordinate frame $(\sigma, x_{b_1}, x_{b_2})$ is locally orthogonal with $dr = \hat{\mathbf{t}}h_\sigma d\sigma + \hat{\mathbf{x}}_{b_1}dx_{b_1} + \hat{\mathbf{x}}_{b_2}dx_{b_2}$, with the Lamé coefficient

$$h_\sigma = 1 - K(\sigma)[x_1\cos\theta + x_2\sin\theta] = 1 - K(\sigma)n. \tag{48}$$

2. Asymptotic evaluation of the scattering propagator

The ray coordinate system may now be applied to the scattering propagators, $B_b^s(\mathbf{r}'; \overline{\mathbf{X}}^s)$. Each propagator arrives at the observation plane to point $\overline{\mathbf{x}}^s$ from a direction $\overline{\boldsymbol{\xi}}^s$; thus, we associate a ray coordinate system to each beam, so that ray parameters σ, x_{b_1} and x_{b_2} are all processing parameters $(\overline{\mathbf{X}}^s)$-dependent, and are denoted as $\sigma^s = \sigma(\overline{\mathbf{X}}^s)$, $\mathbf{x}_b^s = (x_{b_1}(\overline{\mathbf{X}}^s), x_{b_2}(\overline{\mathbf{X}}^s))$, etc. The inhomogeneous medium in the high frequency-localized beam excitation regime may be modelled by the wave speed along the excited ray and its second order transverse derivative matrix $\mathbf{V}_b^{(2)}(\sigma^s)$, whose (ij) elements are $\partial_{x_{b_i}}\partial_{x_{b_i}} v_b|_{\Sigma^s}$. Using the ray coordinate frame, the paraxially approximated scattering propagators may be evaluated in the high frequency regime, giving (see details in Appendix B)

$$B_b^s(\mathbf{r}^s; \overline{\mathbf{X}}^s) = \frac{i}{2k_o\overline{\zeta}^s}\sqrt{\frac{v_b(\sigma^s)}{v_o}\frac{\det\mathbf{Q}_b^s(0)}{\det\mathbf{Q}_b^s(\sigma^s)}}\exp[i\Phi_b^s(\mathbf{r}^s; \overline{\mathbf{X}}^s)], \tag{49}$$

with

$$\Phi_b^s(\mathbf{r}^s; \overline{\mathbf{X}}^s) = -\left[\int_0^{\sigma^s} d\sigma' k_b(\sigma')\right] + \frac{1}{2}k_b(\sigma^s)\mathbf{x}_b^s \quad \boldsymbol{\Gamma}_b^s(\sigma^s)\cdot\mathbf{x}_b^s, \tag{50}$$

where $k_b(\sigma^s) = \omega/v_b(\mathbf{r})|_{\mathbf{r}\in\Sigma^s}$ is the wave number along the excited ray Σ^s. The transverse matrix $\boldsymbol{\Gamma}^s(\sigma^s)$ is a complex symmetric 2×2 matrix with $\mathrm{Im}\,\boldsymbol{\Gamma}^s$ positive definite. One may calculate $\boldsymbol{\Gamma}^s$ by the standard procedure of solving the matrix Riccati equation, setting

$$\boldsymbol{\Gamma}_b^s(\sigma^s) = v_b(\sigma^s)\mathbf{P}_b(\sigma^s)\mathbf{Q}_b^{-1}(\sigma^s), \tag{51}$$

and solving, along Σ^s, the first order system of coupled differential equations

$$\mathbf{Q}_b'(\sigma^s) = v_b(\sigma^s)\mathbf{P}_b(\sigma^s), \quad \mathbf{P}_b'(\sigma^s) = -v_b(\sigma^s)^{-2}\mathbf{V}_b^{(2)}(\sigma^s)\mathbf{Q}_b(\sigma^s), \tag{52}$$

where the prime denotes a derivative with respect to the argument. Relation (52) is subject to the initial conditions

$$\mathbf{Q}_b(0) = \mathbf{I}, \quad \mathbf{P}_b(0) = v_o\boldsymbol{\Gamma}^s. \tag{53}$$

As in the special case of homogeneous background medium (i.e., the Born approximation) in (28), one can show that if $\boldsymbol{\Gamma}^s(0)$ is symmetric with $\mathrm{Im}\,\boldsymbol{\Gamma}^s(0)$ positive definite, then $\boldsymbol{\Gamma}^s(\sigma^s)$ has these

properties for all σ^s, and that $\mathbf{Q}(\sigma^s)\neq 0$ for all σ^s. Following the procedure in (32)–(35), one identifies $\mathrm{Re}\,\mathbf{\Gamma}^s(\sigma^s)$ and $\mathrm{Im}\,\mathbf{\Gamma}^s(\sigma^s)$ as the beam curvature and beam-amplitude matrices, respectively. Note that the special case of the Born approximation in (28), in which the background medium is homogeneous, may be obtained by substituting $v_b(\mathbf{r})=v_o$ into (49)–(53).

The scattering propagators, $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$, are backpropagating along the ray trajectory initiating from the scattered data plane in $z^s=0$, from a processing $\overline{\mathbf{x}}^s$-dependent point, in a processing $\overline{\boldsymbol{\xi}}^s$-dependent direction. The propagator exhibits a Gaussian decay normal to the ray trajectory, i.e., in $\mathbf{x}_b^s$.

3. Asymptotic evaluation of the incident propagators

For the case of the incident propagators, $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$, in (18), each propagator emanates from point $\overline{\mathbf{x}}'$ on the initial distribution plane, in a direction $\overline{\boldsymbol{\xi}}^i$ (see Fig. 3); thus, the ray coordinates associated with each processed beam are denoted accordingly as $\sigma^i=\sigma(\overline{\mathbf{X}}^i)$, etc. As in (49), the inhomogeneous medium may be modeled by the wave number along the excited ray, $k_b(\sigma^i)$, and its second order transverse derivative matrix $\mathbf{V}_b^{(2)}(\sigma^i)$ along the beam-axis. Using the ray coordinate frame, the paraxially approximated scattering propagators may be evaluated in the high frequency regime in a manner similar to (49), giving

$$B_b^i(\mathbf{r};\overline{\mathbf{X}}^i)=\sqrt{\frac{v_b(\sigma^i)}{v_o}\frac{\det\mathbf{Q}_b^i(0)}{\det\mathbf{Q}_b^i(\sigma^i)}}\exp[i\Phi_b^i(\mathbf{r};\overline{\mathbf{X}}^i)] \tag{54}$$

with

$$\Phi_b^i(\mathbf{r};\overline{\mathbf{X}}^i)=\left[\int_0^{\sigma^i}d\sigma' k_b(\sigma')\right]+\frac{1}{2}k_b(\sigma^i)\mathbf{x}_b^i\quad\mathbf{\Gamma}_b^i(\sigma^i)\cdot\mathbf{x}_b^i, \tag{55}$$

where the matrix $\mathbf{\Gamma}_b^i(\sigma^i)$ is found by solving (52) along the incident beam-axis $\sigma^i\in\Sigma^i$ with the initial conditions $\mathbf{Q}_b(0)=\mathbf{I}$ and $\mathbf{P}_b(0)=v_o\mathbf{\Gamma}^i$.

4. PS2PS mapping

Next, we consider the scattering cell under Gaussian windows processing. By inserting $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$ in (49) with $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$ in (54) into (22), we obtain the asymptotic expression for the scattering cell

$$\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s)=\frac{ik_o}{8\pi^2\overline{\zeta}^sN^i}\sqrt{\frac{v_b(\sigma^s)v_b(\sigma^i)/v_o^2}{\det\mathbf{Q}_b^s(\sigma^s)\det\mathbf{Q}_b^i(\sigma^i)}}\exp\{i[\Phi_b^s(\mathbf{r}^s;\overline{\mathbf{X}}^s)+\Phi_b^i(\mathbf{r};\overline{\mathbf{X}}^i)]\}, \tag{56}$$

where Φ_b^s and Φ_b^i are given in (50) and (55), respectively. Relation (56) implies the following: The local scattering cell exhibits Gaussian decay normal to both the incident and scattering ray trajectories (i.e., in $\mathbf{x}_b^i$ and $\mathbf{x}_b^s$). Thus, the window center is located at the intersection of the incident spectral beam $B_b^i(\mathbf{r}';\overline{\mathbf{X}}^i)$ and the scattered beam propagator $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$ axes. Therefore, the location of the scattering cell is resolved by the PS processing parameters $\overline{\mathbf{X}}^s$ and $\overline{\mathbf{X}}^i$, which determine, via (30), the PS propagators ray trajectories (see Fig. 3).

The localization in the object domain as determined by $\Lambda_b(\mathbf{r}';\overline{\mathbf{X}}^i,\overline{\mathbf{X}}^s)$ may be interpreted by using fundamental wave physics. Consider an incident propagator emanating from $z=0$ plane from point $\overline{\mathbf{x}}'$ at angle $\overline{\theta}^i$ along ray Σ^i, arriving at the $z^s=0$ scattering plane at point $\overline{\mathbf{x}}^s$ at angle $\overline{\theta}^s$. In this case, the scattering propagator, $B_b^s(\mathbf{r};\overline{\mathbf{X}}^s)$, corresponding to $\overline{\mathbf{x}}^s$ and $\overline{\theta}^s$, backpropagates along the same ray trajectory $\Sigma^s=\Sigma^i$, and the corresponding scattering cell exhibits Gaussian decay *only* in the transverse coordinates $(\mathbf{x}_{b_1},\mathbf{x}_{b_2})$ and not along the (shared) beam-axis. Therefore, the integration domain in (21) is local *only normal to* Σ^i, which indicates the stationary

contribution to PS spectral distribution at that particular $\overline{\mathbf{X}}^s$ in accord with the Fermat principle. Furthermore, the phase accumulation along Σ^i, $2\int_0^{\sigma^i} d\sigma' k_b(\sigma')$, when introduced into (21), acts as a ''scaled Fourier transform'' operating along the ray trajectory; thus, large contributions to Ψ_b in (21) arise from medium variations *along* Σ in accord with fundamental 1D wave physics.

V. CONCLUDING REMARKS

Inhomogeneous medium Green's function in the phase-space domain were presented, linking the phase-space spectral distributions of the field scattered by a high contrast object to a genetic time-harmonic incident field. Two forms of phase-space Green's function were presented: (a) A *configuration-space to phase-space* Green's function that links induced sources in the object domain to phase-space distributions of the scattered field is obtained by applying PS transform to the scattered field over planar surfaces; and (b) a *phase-space to phase-space* Green's function, which directly links incident- to scattered-phase-space distribution, obtained by applying the PS transform to *both* incident and scattered field distributions, s. The scattering mechanism has been described in terms of local samplings of the object function which are localized in the object domain according to the scattered- and incidence-processing parameters. The special case of Gaussian windows has been considered and asymptotic expressions for the PS Green's functions and scattering cells have been derived for both the Born approximated- and the generic-inhomogeneous medium profiles. The wave phenomenology associated with the PS Green's functions and the scattering mechanism have also been explored.

Equations (20)–(22) establish the building blocks for an *inverse scattering* procedure in which the strong scatterer is found via iterative algorithm where at the nth iteration, the background $v_b(\mathbf{r})=v_n(\mathbf{r})$ is known, and the sampling operation in (20) is inverted to evaluate $O(\mathbf{r})$, from which the next v_{n+1} is found. This operation may be carried out for large scatterers since it can be shown that under appropriate illuminating conditions, the operation in (20) may be reduced to 1D samplings along the (synthesized) scattered ray trajectories.

ACKNOWLEDGMENT

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APPENDIX A: OPERATOR REPRESENTATION OF CS2PS GREEN'S FUNCTION

In order to establish the scattering propagators in (11) as Green's functions, an operator equation associated with the CS2PS is derived hereby. We define the Helmholtz operator $(L_1u)(\mathbf{r})$

$$(L_1u)(\mathbf{r})\equiv[\nabla^2+k_b^2(\mathbf{r})]u(\mathbf{r}), \tag{A1}$$

and the inverse-PS operator $(L_2U)(\overline{\mathbf{X}})$

$$(L_2U)(\overline{\mathbf{X}})\equiv\left(\frac{k_o}{2\pi N^s}\right)^2\int d^4\overline{X}^s \;\; U(\overline{\mathbf{X}},z^s) \;\; W^s(\mathbf{x}^s;\mathbf{X}^s), \tag{A2}$$

where $U(\overline{\mathbf{X}},z^s)$ are PS distributions over planar surfaces of constant z^s. Next, we define the cascade operator $(LU)(\overline{\mathbf{X}})=[L_1(L_2U)(\overline{\mathbf{X}})][\mathbf{r}]$. Using (9), in (1), we identify the operator equation

$$(LU^s)(\overline{\mathbf{X}}^s)=-f(\mathbf{r}), \quad f(\mathbf{r})=k_o^2O(\mathbf{r})u(\mathbf{r}). \tag{A3}$$

The Green's function, B_b^s, associated with the operator Eq. (A3) is obtained by solving

$$(LB_b^s)(\overline{\mathbf{X}}^s) = -\delta(\mathbf{r}-\mathbf{r}') \tag{A4}$$

and the resolvent operator of L, $U^s=(L^{-1}f)(\mathbf{r})$ takes the form in (10), thereby identifying B_b^s in (11) as a Green's function. Furthermore, by substituting (11) into (A3) and inverting the order of integration, one finds that the PS scattering propagators satisfy definition (A4).

APPENDIX B: EVALUATION OF EQ. (49)

In order to establish Eq. (49), we note that generic solution for beam-type wave objects propagating in the background medium $v_b(\mathbf{r})$, along the ray Σ^s, is given by[3,14,19]

$$B_b^s(\mathbf{r}) = A\sqrt{\frac{v_b(\sigma^s)}{v_o}\frac{\det\mathbf{Q}_b(0)}{\det\mathbf{Q}_b(\sigma^s)}}\exp[i\Phi_b(\mathbf{r})], \tag{B1}$$

where A is a constant, and the phase

$$\Phi_b(\mathbf{r}) = \pm\left[\int_0^{\sigma^s} d\sigma' k_b(\sigma')\right] + \frac{1}{2}k_b(\sigma^s)\mathbf{x}_b \quad \mathbf{\Gamma}_b(\sigma^s)\cdot\mathbf{x}_b\,. \tag{B2}$$

Since, according to (11), the scattering propagator $B_b^s(\mathbf{r}';\overline{\mathbf{X}}^s)$ satisfies wave equation (1) with $v(\mathbf{r})=v_b(\mathbf{r})$, we seek for solutions in the form of (B1). Under the paraxial approximation, the initial distribution of the scattering propagator over the $z^s=0$ plane may be replaced by the initial parameter matrix (see discussion following (42))

$$\mathbf{\Gamma}^s_{\text{parax}} = \begin{bmatrix} \Gamma^{s*}/\overline{\zeta^s}^2 & 0 \\ 0 & \Gamma^{s*} \end{bmatrix}, \tag{B3}$$

over the $z_b^s=0$ plane. Note that the projected initial paraxial distribution, which was originally obtained for homogeneous medium, may serve for inhomogeneous propagation as well, as long as the initial plane is embedded in an homogeneous medium, since in the high-frequency limit Bremmer-type reflections are negligible, and the beam-type field is forward propagating along the ray trajectories.[3,14] Therefore, we may use the homogeneous background asymptotic field in (28) with the above-mentioned initial distribution in the general solution (B1) yielding (49). Note that solution (49) satisfies the radiation condition of sources in the $z^s<0$ as exhibited by the propagation phase accumulation of $-\int_0^{\sigma^s} d\sigma' k_b(\sigma')$ for $\sigma^s<0$ (see also Fig. 4).

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Quantizing the line element field

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A metric with signature $(-+++)$ can be constructed from a metric with signature $(++++)$ and a double-sided vector field called the line element field. Some of the classical and quantum properties of this vector field are studied. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738190]

I. INTRODUCTION

The difference between a Lorentzian and a positive definite metric can be expressed as a double-sided vector field U called the line element field. This is done in Ref. 4, p.38, but there only the ratio of vectors in the two spaces is considered; this appears to be the only reference on the line element field and it is from it that the nomenclature is taken. Thus the study of fields or extented objects in Lorentzian space–time is reduced to the study of the same object in a positive definite space and the study of the corresponding line element field. In particlular this can be done for gravity, where the positive defininte action is sometimes called the Euclidean action.[3]

In Sec. II some examples of positive definite metrics are presented and how to change their signature via a vector field is shown; this is successively generalized to vanishing shift metrics and then the general theory, next the first derivatives are studied, and expressed in terms of a contorsion tensor. The second derivatives of the metric are governed by the Riemann tensor which can be expressed by independent terms in the contorsion and Christoffel connection. In Sec. III the Einstein–Hilbert action is decomposed into a positive definite part and a line element field part, the line element field part is varied with repect to both U and $\dot{U}$. The variation with respect to $\dot{U}$ gives the momentum. Quantization is implemented by replacing this momentum by a differential operator to give a modified Klein–Gordon equation. Then the lowest order approximation to the modified Klein–Gordon equation is calculated, and the wave function is calculated for some specific space–times.

Notation used includes the bracket notation of Ref. 4, p. 20,

$$2V_{(a,c)}=V_{a,c}+V_{c,a}=2V_{(a;c)}+2\{^{e}_{ca}\}V_{e}\,,\quad 2V_{[a,c]}=2V_{[a;c]}=V_{a,c}-V_{c,a}\,, \tag{1}$$

the scalars constructed from the expansion and vorticity Ref. 4, p. 82,

$$\omega_{ab}\equiv h^{c}_{a}h^{d}_{b}V_{[c;d]}\,,\quad \theta_{ab}\equiv h^{c}_{a}h^{d}_{b}V_{(c;d)}\,,\quad \sigma_{ab}\equiv\theta_{ab}-\tfrac{1}{3}h_{ab}\theta,$$

$$\theta\equiv\theta_{ab}h^{ab}=V_{a;b}h^{ab}=V^{a}{}_{a}\,,\quad \omega^{2}\equiv\omega^{ab}\omega_{ab}\,,\quad \sigma^{2}\equiv\sigma^{ab}\sigma_{ab}\,, \tag{2}$$

and vector fields

$$\begin{aligned} U_{a}&\quad\text{for a general vector,}\\ V_{a}&\quad\text{for a normalization of this to }\pm1,\\ W_{a}&\quad\text{for a specific vector.}\end{aligned} \tag{3}$$

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II. CURVATURE

A. Relationship between a positive definite metric and a Lorentzian metric

For a given positive definite metric $\overset{-+}{p}_{ab}$ and vector field U_{++a}, one can construct a Lorentzian space–time with covariant metric

$$\overset{-+}{g}_{ab}=-2\frac{\overset{++}{U}_a\overset{++}{U}_b}{\overset{++}{U}^2}+\overset{++}{p}_{ab}, \tag{4}$$

This can be illustrated using the positive definite Schwarzschild metric

$$\overset{++}{ds}^2=+\left(1-\frac{2m}{r}\right)dx_0^2+\left(1-\frac{2m}{r}\right)^{-1}+r^2d\Sigma_2^2,\quad d\Sigma_2^2=d\theta^2+\sin^2\theta d\phi^2,$$

$$\overset{++}{W}_a=\left(\sqrt{1-\frac{2m}{r}},0\right),\quad \overset{++}{W}^a\overset{++}{W}_a=+1, \tag{5}$$

or the positive definite Robertson–Walker metric

$$\overset{++}{ds}^2=+dx_0^2+R^2d\Sigma_3^2,\qquad d\Sigma_3^2=d\chi^2+f^2(\chi)(d\theta^2+\sin^2\theta d\phi^2),\qquad \overset{++}{W}_a=(1,0), \tag{6}$$

then using (4) the space–time metric is recovered. Instead of U it is often convenient to work with the unit vector

$$V_a=\frac{U_a}{\sqrt{\pm U^2}},\qquad U^2=U_aU_b\overset{++}{p}^{ab}, \tag{7}$$

There is a problem of what the contravariant form of $\overset{-+}{g}$, p and U should be. One can generalize (5) and (6) to a positive definite space with shift-free metric ($N_i=0$); being shift-free implies that the metric has no cross $g_{\tau i}$ terms and can be represented thus

$$\overset{++}{p}_{ab}=(q^2,p_{ij}),\qquad \overset{++}{p}^{ab}=\left(\frac{1}{q^2},p^{ij}\right),\qquad \det(\overset{++}{p}_{ab})=q\det(p_{ij}),$$

$$\overset{++}{W}_a=(q,0),\qquad \overset{++}{W}^a=(1/q,0). \tag{8}$$

No cross metric terms $g_{\tau i}=0$, allows W_a to have only one component, if there is a cross term $g_{\tau i}\neq 0$, then either W_a or W^a or both, will have more than one component. Now one can construct a Lorentzian space–time with covariant metric

$$\overset{-+}{g}_{ab}=(-p^2,p_{ij}),\qquad \det(\overset{-+}{g}_{ab})=-\det(\overset{++}{p}_{ab}). \tag{9}$$

Consistency seems to require

$$\overset{-+}{g}^{ab}=-2\overset{++}{V}^a\overset{++}{V}^b+\overset{++}{p}^{ab}=\left(-\frac{1}{p^2},p^{ij}\right). \tag{10}$$

Note that only cross terms in V occur so perhaps $\overset{-+}{V}$ could have been used; (17) shows that this is not the case. Taking $\overset{-+}{V}_a=\overset{++}{V}_a$ and raising using this metric

$$\overset{-+}{W}^a=\left(-\frac{1}{p},0\right),\quad \overset{-+}{W}^2=-1, \tag{11}$$

so that $\overset{-+}{V}$ is a timelike vector. Similarly taking $\overset{-+}{p}_{ab}=\overset{++}{p}_{ab}$ and raising indices using (10) gives

$$\overset{-+}{p}^{ab}=\overset{++}{p}^{ab}. \tag{12}$$

Some products using the above tensors are

$$\overset{-+}{g}{}^{c}{}_{c} \equiv \overset{-+}{g}{}^{ab}\overset{-+}{g}{}_{bc} = \overset{++}{p}{}^{a}{}_{c} - 2\overset{++}{V}{}^{a}\overset{++}{V}{}_{c},$$

$$\overset{++}{p}{}^{ab}\overset{-+}{g}{}_{bc} = 2\overset{-+}{V}{}^{a}\overset{-+}{V}{}_{c} + \overset{-+}{g}{}^{a}{}_{c},$$

$$-\overset{-+}{V}{}_{a} = \overset{-+}{V}{}^{b}\overset{-+}{g}{}_{bc}, \qquad \overset{-+}{V}{}^{a} = \overset{-+}{V}{}^{c}\overset{-+}{g}{}^{a}{}_{c} = -\overset{-+}{V}{}_{c}\overset{++}{p}{}^{ab}, \quad \overset{++}{p}{}^{ac}\overset{-+}{V}{}_{c} = -\overset{-+}{V}{}^{a}. \tag{13}$$

Collecting this together consistency requires

$$\overset{-+}{g}{}^{ab} = -2\frac{\overset{++}{U}{}^{a}\overset{++}{U}{}^{b}}{\overset{++}{U}{}^{2}} + \overset{++}{p}{}^{ab}, \tag{14}$$

and

$$\overset{-+}{V}{}_{a} = \overset{++}{V}{}_{a}, \quad \overset{-+}{V}{}^{a} = -\overset{++}{V}{}^{a}, \quad \overset{-+}{p}{}_{ab} = \overset{++}{p}{}_{ab}, \quad \overset{-+}{p}{}^{ab} = +\overset{++}{p}{}_{ab}. \tag{15}$$

B. Common pitfalls

The above system is new and slips can be made by relying on ones intuition from studying spacetimes using the projection tensor, defined here at (18) below, or confusing the $(-+)$ and $(++)$ spaces. For any metric there is the equation $g_{ab}g^{bc} = \delta^{c}_{a}$, which can be contracted to $g_{ab}g^{ab} =$ dimension of the space $= 4$. The most common pitfall is to use this equation thus

$$4 = g^{a}_{a} \overset{?}{=} -2V_{a}V^{a} + p^{a}_{a} = -2V_{a}V^{a} + 4, \tag{16}$$

suggesting that V is null, contrary to assumption. The correct calculation is

$$4 = \overset{-+}{g}{}^{ab}\overset{-+}{g}{}_{ab} = \left(-2\frac{\overset{++}{U}{}^{a}\overset{++}{U}{}^{b}}{\overset{++}{U}{}^{2}} + p^{ab}\right)\left(-2\frac{\overset{++}{U}{}_{a}\overset{++}{U}{}_{b}}{\overset{++}{U}{}^{2}} + p_{ab}\right) = \left(4\frac{\overset{++}{U}{}^{2}}{\overset{++}{U}{}^{2}} - 2 - 2\right)\frac{\overset{++}{U}{}^{2}}{\overset{++}{U}{}^{2}} + 4, \tag{17}$$

which also serves as showing that $\overset{++}{U}$ rather than $\overset{-+}{U}$ should be used for $\overset{-+}{g}$ in (14). The projection tensor is defined as

$$\overset{-+}{h}{}_{ab} \equiv \overset{-+}{g}{}_{ab} + \frac{\overset{-+}{U}{}_{a}\overset{-+}{U}{}_{b}}{-\overset{-+}{U}{}^{2}} = \overset{++}{p}{}_{ab} - 2\frac{\overset{++}{U}{}_{a}\overset{++}{U}{}_{b}}{\overset{++}{U}{}^{2}} - \frac{\overset{-+}{U}{}_{a}\overset{-+}{U}{}_{b}}{\overset{-+}{U}{}^{2}} = \overset{-+}{p}{}_{ab} + \frac{\overset{-+}{U}{}_{a}\overset{-+}{U}{}_{b}}{\overset{-+}{U}{}^{2}} = \overset{++}{p}{}_{ab} - \frac{\overset{++}{U}{}_{a}\overset{++}{U}{}_{b}}{\overset{++}{U}{}^{2}}, \tag{18}$$

where in this case the indices can be raised and lowered without change of form.

C. First derivatives of the metric

Having formed the metric the next problem is the properties of its first derivatives. To form the connection Γ with g in terms of the connection $\{\}$ with p one has

$$\begin{aligned} 2\overset{g}{\Gamma}_{abc} &\equiv g_{ba,c} + g_{ca,b} - g_{bc,a} \\ &= 2\{_{abc}\} + 4U^{-2}(-U_{a}\{^{e}_{bc}\}U_{e} - U_{a}U_{(b;c)} + U_{b}U_{[c;a]} + U_{c}U_{[b;a]}) \\ &\quad + 4U^{-4}U_{e}(2U_{a}U_{(b}U^{e}_{\ ;c)} - U_{b}U_{c}U^{e}_{\ ;a}), \end{aligned} \tag{19}$$

where in the last two terms the bracket notation 1 for $U_{[a;b]}$ and $U_{(a;b)}$ is used; the covariant derivatives on the rhs of (20) are formed with p. Raising with the metric (10)

$$\overset{g}{\Gamma}{}^{a}_{bc} \equiv \overset{-+}{g}{}^{ad} \overset{g}{\Gamma}_{dbc}, \tag{20}$$

so that

$$\overset{g}{\Gamma}{}^{a}_{bc} = \left\{ \begin{matrix} p \\ a \\ bc \end{matrix} \right\} + \overset{p}{L}{}^{a}{}_{e} \left\{ \begin{matrix} p \\ e \\ bc \end{matrix} \right\} + \overset{p}{K}{}^{a}_{bc}, \tag{21}$$

it is found that $L=0$ implying that the system is covariant. From (21) there is the relation between the covariant derivatives.

$$\overset{++}{V}{}^{-+}_{a;b} = \overset{++}{V}{}^{++}_{a;b} - K^{c}_{ab} \overset{++}{V}{}_{c}, \tag{22}$$

The contorsion tensor K, define by (21), can be expressed in terms of the auxiliary tensors $J\&M$

$$2K^{a}_{bc} = +8U^{-2}U_{(b}J_{c)}{}^{a} + 4U^{-2}U^{a}U_{(bc)} - 2U^{-4}M^{a}_{bc},$$

$$J_{ab} \equiv U_{[a;b]} - 2U^{-2}U_{b}U^{c}U_{[a;c]}, \tag{23}$$

$$M^{a}_{bc} \equiv (U^{2})^{a}U_{b}U_{c} + (U^{2})_{b}U^{a}U_{c} + (U^{2})_{c}U^{a}U_{b} - 2U^{-2}U^{a}U_{b}U_{c}U^{e}(U^{2})_{e},$$

where $(U^{2})_{c} = (U_{a}U^{a})_{c} = 2U^{a}U_{a;c}$. There is no term in the accelerations $\dot{U}^{a}$, $\dot{U}^{b}$, or $\dot{U}^{c}$, M vanishes if U is a constant vector. Some properties of the contorsion K are

$$K^{a}_{ac} = 0, \qquad K^{a}_{ba} = 0, \qquad K^{a}_{bc} = K^{a}_{cb}, \qquad U^{b}U^{c}K^{a}_{bc} = 0,$$

$$U_{a}K^{a}_{bc} = 2U_{bc} - 2U^{-2}(U_{(b}\dot{U}_{c)} + U_{e}U_{(b}U^{e}_{.c)}) + 2U^{-4}U_{b}U_{c}U_{e}\dot{U}^{e}, \tag{24}$$

the dot being formed with the p covariant derivatives; such systems involving a connection and a contorsion occur repeatedly in the study of curvature; for instance, in geometries involving torsion and/or metricity such as the geometries of Weyl and Schouten,[11] the study of a conformal factor, and the study of weak metric perturbations.[9] Alternatively the contorsion can be expressed in terms of the decomposed vector field for a $(-+)$ Lorentzian space–time define θ as in (2) and

$$\omega_{ab} \equiv h_{a}{}^{c}h_{b}{}^{d}V_{[c;d]}, \qquad \theta_{ab} \equiv h_{a}{}^{c}h_{b}{}^{d}V_{(c;d)}, \qquad \sigma_{ab} \equiv \theta_{ab} - \tfrac{1}{3}\theta h_{ab}, \qquad \dot{X}_{abc\ldots} \equiv V^{e}X_{abc\ldots;e}, \tag{25}$$

which allow the covariant derivative of a $(-+)$ space–time to be decomposed

$$U_{a;b} = \theta_{ab} + \omega_{ab} + U^{-2}U_{b}\dot{U}_{a} + U^{-2}U_{a}U^{e}U_{eb} - U^{-4}U_{a}U_{b}U^{e}\dot{U}_{e}, \tag{26}$$

choosing a constant vector field this reduces to Ref. 4, Eq. (4.17). Now Eqs. (24) are in the $(++)$ space and (25) are in a $(-+)$ space–time; they can be related using the projection tensor (18). The projection tensor (18) can be applied to (26) to give the projections of the covariant derivative

$$h^{c}_{a}h^{d}_{b}U_{(c;d)} = U_{(a;b)} - U^{-2}U_{(a}\dot{U}_{b)} - \tfrac{1}{2}U^{-2}U_{(a}(U^{2})_{b)} + \tfrac{1}{2}U^{-4}U_{a}U_{b}(\dot{U}^{2}),$$

$$h^{c}_{a}h^{d}_{b}U_{[c;d]} = U_{[a;b]} - U^{-2}\dot{U}_{[a}U_{b]} - \tfrac{1}{2}U^{-2}U_{[a}(U^{2})_{b]}. \tag{27}$$

To transfer these quantities to the $(++)$ space, the projection tensor (18) shows that it is only necessary to note that the negative quantity $U^2=\overset{-+}{U}_a\overset{-+}{U}{}^a<0$ is changed to the positive quantity $U^2=\overset{++}{U}_a\overset{++}{U}{}^a>0$, and also that the covariant derivative in the expansion is changed using (22). $U_eK^e_{ab}$ is -2 times θ_{ab} so that the sign of θ_{ab} in the $(++)$ space is the negative of the form in (27) and from (25). In particular the expansion (2) becomes

$$-\theta=U^a_{.;a}-\frac{(\dot{U}^2)}{U^2}. \tag{28}$$

Using (24) and (27) the contorsion tensor is found to be

$$J_{ab}=\omega_{ab}-\frac{\dot{U}_{(a}U_{b)}}{U^2}+\frac{U_{(a}(U^2)_{b)}}{2U^2},\qquad K^a_{bc}=\frac{4}{U^2}U_{(b}\omega_{c)}{}^a-\frac{2}{U^2}U^a\theta_{bc}-2\sqrt{U^2}\left(\frac{\dot{U}^a}{\sqrt{U^2}}\right)\frac{U_bU_c}{U^4}. \tag{29}$$

D. Second derivatives of the metric

The second derivatives are governed by the Riemann tensor, the Riemann tensor constructed with a Lorentzian metric can be decomposed into the Riemann tensor constructed with a positive definite metric and the contorsion

$$\overset{g}{R}{}^a{}_{bcd}=\overset{p}{R}{}^a{}_{bcd}+2K^a_{.[d|b|;c]}+2K^a_{.[c|e|}K^e_{.d]b}, \tag{30}$$

such decompositions of the Riemann tensor also happen for several other systems: (1) Weak field gravity requires that the metric be of the form $g_{ab}=\eta_{ab}+w_{ab}$, where η is a flat metric and w is a small adjustment to it, in this case the connection constructed from w is a contorsion tensor, and the analog of (30) is of the form $Rie=\partial K+K\times K$, (2) weakly perturbed gravity requires that the metric be of the form $g=\overline{g}+w$, where $\overline{g}$ is a given background metric and w is a small adjustment to it, again the connection constructed from w is a contorsion tensor, and the analog of (30) is of the form $Rie=R\overline{ie}+\partial K+K\times K$, cf Eq. (111),[4] (3) a metric conformal to another Eq. (2.28)[4] $\hat{g}=\Omega^2g$, gives a contorsion given by the last term of Eq. (2.29),[1] and the analog of (30) is of the form $R\hat{ie}=\Omega^{-2}Rie+\partial K$, (4) different geometries such as those of Weyl and Schouten[11] also have connections which split up into a Christoffel part and a contorsion part and then give equations of the same form as (30). The important thing is that these examples and (30) all have no cross L term in (21), $L=0$ showing that the connection can be split into a Christoffel part and a contorsion part and nothing else.

III. QUANTIZATION

A. The Lagrangian

Contracting the expression for the Riemann tensor (30) and using (9) the Einstein–Hilbert Lagrangian becomes

$$\mathcal{L}_H=\sqrt{-g}\overset{g}{R}=\sqrt{\det(p_{ab})}[\overset{p}{R}+2K^{ab}_{.[b|.|;a]}+2K^a_{.[a|e|}K^{eb]}_{..}{}_b]=\mathcal{L}_1+\mathcal{L}_2+\mathcal{L}_3, \tag{31}$$

$\mathcal{L}_1$ is given by the first term in the square brackets [], and is the positive definite action, sometimes called the Euclidean action and this has previously been studied; $\mathcal{L}_2$ & $\mathcal{L}_3$ are given by the second and third terms in the square bracket [], and are new and they are easiest to describe in terms of the decomposed vector quantities (25) thus

$$\mathcal{L}_2 = -\frac{2}{U^2}(\dot{\theta}-\theta^2) - 2\left(\frac{1}{\sqrt{U^2}}\left(\frac{U^a}{\sqrt{U^2}}\right)^{\circ}\right)_a \equiv l_1 + l_2 + l_3,$$
$$\mathcal{L}_3 = \frac{4\omega^2}{U^2} - \frac{4}{U^4}\left[\left(\frac{U^a}{\sqrt{U^2}}\right)^{\circ} U_a\right]^2 \equiv l_4 + l_5, \qquad \omega^2 \equiv \omega^{ab}\omega_{ab}, \tag{32}$$

where $(U^2)^\circ$ is the absolute derivative of U^2, explicitly $(U^2)^\circ = (U^2)_{;a}U^a$. Expanding (32) $l_5 = 0$. Varying with respect to U,

$$\frac{\delta l_1}{\delta U^c} = -2U^{-2}\theta_c + 2((U^{-2}U^eU^2)_e)_c - 2U^{-2}(U^{-2}U^e)_e(U^2)_c - 4U_c(U^{-2}(^{-2}U^f)_fU^e)_e$$
$$-4U^{-4}(U^{-2}U^e)_e(U^2)^\circ U_c,$$
$$\frac{\delta l_2}{\delta U^c} = 4(U^{-2}\theta)_c + 4U^{-4}\theta(U^2)_c - 8U_c(U^{-4}\theta U^e)_e - 8U^{-6}(U^2)^\circ U_c, \tag{33}$$
$$\frac{\delta l_4}{\delta U^c} = -8(U^{-2}\omega^{ce})_e + 4U^{-2}\omega^{ce}(2\dot{U}_e - U^2(U^2)_e),$$
$$\frac{\delta l_3}{\delta U^c} = \frac{\delta l_5}{\delta U^c} = 0.$$

B. The momentum

In order to produce momenta it is necessary to vary with respect to $\dot{U}^c$

$$\frac{\delta l_1}{\delta \dot{U}^c} = -\frac{4\theta U_c}{U^4}, \qquad \frac{\delta l_2}{\delta \dot{U}^c} = +8\frac{\theta U_c}{U^4}, \qquad \frac{\delta l_3}{\delta \dot{U}^c} = \frac{\delta l_3}{\delta \dot{U}^c} = \frac{\delta l_3}{\delta \dot{U}^c} = 0. \tag{34}$$

Therefore

$$\Pi_a = \frac{\delta}{\delta \dot{U}^a}(l_1 + l_2) = \frac{4\theta U_a}{U^4}. \tag{35}$$

This equation is not fully invertible in terms of the momenta Π thus $U_a = f(\Pi)\Pi_a$, but is partially invertible in terms of both the momenta Π and the vector field U thus $U_a = f(\Pi, U)\Pi_a$,

$$\frac{U_a}{\sqrt{U^2}} = \frac{\Pi_a}{\sqrt{\Pi^2}}, \tag{36}$$

and partially invertible in terms of the expansion θ and momenta Π thus $U_a = f(\Pi, \theta)\Pi_a$,

$$U_a = (4\theta)^{1/3}\Pi^{-4/3}\Pi_a. \tag{37}$$

(35) gives the constraint

$$\lambda = \Pi_c\Pi^c - \frac{16\theta^2}{U^6}. \tag{38}$$

This is the only constraint so that quantization can be achieved via

$$\Pi_a \rightarrow -i\hbar\nabla_a, \tag{39}$$

with U and hence θ remaining unchanged. Plancks constant $\hbar$ is of the same dimensions as action, explicitly $Mass\times Length^2\times Time^{-1}$, so that (39) has introduced a ''mass'' into the system.

C. The modified Klein–Gordon equation

Applying (39) to the constraint gives a modified Klein–Gordon equation

$$\lambda\psi = -\hbar^2\left(\Box + \frac{16\theta^2}{\hbar^2 U^6}\right)\psi = 0. \tag{40}$$

D. Approximation

Defining

$$S \equiv -i\hbar \ln\psi \tag{41}$$

and then substituting S from (41) for ψ everywhere in (40), the modified Klein–Gordon equation (40) becomes

$$-i\hbar S^s_{.a} + S^a S_a - \frac{16\theta^2}{U^6} = 0, \tag{42}$$

expanding in terms of $\hbar$ using

$$S_a = \Pi_a + \hbar\epsilon_a + \mathcal{O}(\hbar^2), \tag{43}$$

the $\hbar^0$ term of (43) is just the constraint (38), the $\hbar^1$ term of (43) is

$$-\imath\Pi^a_{.a} + 2\epsilon_a\Pi^a = 0, \tag{44}$$

For $\theta = 0$, the Lagrangians l_1 and l_2 vanish as does Π, so that to lowest order $\hbar^0$, $S_a = 0$, implying that the wave function ψ is a constant to lowest order, thus for $\theta = 0$ the wave function has no dynamical information corresponding to the classical theory.

U remains unchanged during quantization, but once a solution ϵ to (43) is known, one would hope to be able to calculates the $\hbar^1$ order correction to U and hence g. There is a problem with trying this, as Π is only partially invertible (36) and (37) this cannot be done without an additional assumption. Here this assumption is that θ remains negligible to order $\hbar^1$ in the quantum theory, then it is possible to find the correction to U from (37), denoting the quantum quantities with a ''*'' U becomes

$$U^*_a = (4\theta)^{1/3} S^{4/3} S_a. \tag{45}$$

Substituting for S using (43) and expanding

$$U^*_a = U_a + \frac{\hbar}{4}\frac{U^4}{\theta}\left(\epsilon_a - \frac{8}{3}\frac{U_c\epsilon^c}{U^2}U_a\right) + \mathcal{O}(\hbar^2), \tag{46}$$

with this value of U^* it is now possible to investigate whether the assumption that θ is negligible by noting

$$-\theta^* \equiv U^{*a}_{\ ;a} - U^{*-2}(U^{*2})^\circ = -\theta + \frac{\hbar}{4}\left[\frac{U^4}{\theta}\left(\epsilon^a - \frac{8}{3}U^{-2}U^c\epsilon_c U^a\right)\right]_a + \frac{5\hbar}{6}\left[U^{-2}\left(\frac{U^4\epsilon_a U^a}{\theta}\right)^\circ - \frac{(U^2)^\circ \epsilon_a U^a}{\theta}\right] + \mathcal{O}(\hbar^2). \tag{47}$$

Substituting for U^* the change in the metric is

$$g^*_{ab} = g_{ab} + \frac{\hbar}{\theta}(U_c\epsilon^c U_a U_b - U^2 U_{(a}\epsilon_{b)}) + \mathcal{O}(\hbar^2). \tag{48}$$

The change in the metric can also be directly calculated from the wave function

$$g^*_{ab} - g_{ab} - 2U^{-2}U_aU_b = -2U^{-2}U^*_aU^*_b = -2S^{-4/3}S_aS_b = 2\hbar^2(-i\hbar\ln\psi)^{-4/3}\psi^{-2}\psi_a\psi_b. \tag{49}$$

E. Examples of exact spaces

The modified Klein–Gordon equation (40) can be studied for particular examples, for example, in Robertson–Walker space–time (6) it is

$$\psi_{00} + 3\frac{R_0}{R}\psi_0 + \frac{144}{\hbar^2}\frac{R_0^2}{R^2}\psi - \frac{l(l+2)}{R^2}\psi = 0, \tag{50}$$

where the last term comes from decomposing the ''spatial'' part into spherical harmonics Ref. 9, Sec. IV A. For the Milne universe, which is flat when $k=-1$,[8] $R=t$ and (50) has solution

$$\psi = At^{-1\pm\sqrt{1-\alpha}}, \qquad \alpha = \frac{144}{\hbar^2} - l(l+2), \tag{51}$$

so that g^* is of the form $f\hbar^2/t^2$. For deSitter space Ref. 4, p.125, $R=\exp(\sqrt{\Lambda/3}t)$ and when $l=0$ 50 has solution

$$\psi = A\exp\left(\tfrac{1}{2}\sqrt{3\Lambda}(-1\pm\sqrt{1-16/\hbar^2})t\right), \tag{52}$$

so that g^* is of the form $f\hbar^2$.

IV. CONCLUSION

A. Things not looked at

Things not looked at here include:

(1) Any relationship to analytic continuation, whether for quantum field theory on curved space time or for the energy condition Ref. 4, p. 89;
(2) any classical or quantum detailed mechanism or perturbation whereby a positive definite space could change to a Lorentzian space–time, for example, in the early universe;
(3) the connection with the Kubo–Martin–Schwinger[2] condition where the transformation $\tau \to it$ has thermal properties;
(4) a quantized line element field might fluctuate, this fluctuation could be thought of in terms of the tetrad rather than the metric, leading to fluctuating null cones, compare Penrose,[6]
(5) any comparison with the Toll[12]–Scharnhorst[10] effect, where fluctuations in the quantum electrodynamical vacuum cause fluctuations in the speed of light;
(6) any comparison with the average size of these fluctuations, compare Ellis *et al.*[1] and Yu and Ford;[13]

(7) not only can the difference between the two signatures be thought of as a vector field, also the difference between tensors constructed from the resulting metrics is tensorial, the Bianchi identities will also differ by a tensorial object constructed from the line element field and this gives another way of investigating conservation laws for the two signatures, compare Ref. 5.

B. The classical theory

The transformation between some specific positive definite spaces and Lorentzian spacetime can be achieved via a line element fields 5 and 6. This can be generalized to shift-free and then arbitrary metrics; there is a problem of what the contravariant form of the metric should be, consistency requires (14). Once the Lorenztian metric has been expressed in terms of a positive definite metric and a vector field it is possible to study first derivatives. In (21) $L=0$ so that the Lorentzian connection splits up into the positive definite connection and a contorsion term constructed from the line element field U; this is similar to many other systems, such as those involving Schouten[11] geometries and weak perturbations;[9] that $L=0$ perhaps is not surprising as the decomposition of the Lorentzian metric is covariant. The form of the contorsion tensor (24) involves a lot of terms when expressed solely in terms of U, however, using rotation and shear it takes a simpler form (29). Covariant derivatives in Lorentzian spacetime and the positive definite space are equated via (22), so that the difference is expressible as $V_c K^c_{ab}$ and this is proportional to the expansion of U, changing spaces has the effect of changing the sign of the expansion. Second derivatives of the line element field U can be calculated once the contorsion K is known via (30).

C. The quantum theory

To quantize the system it is necessary to have more information, such as what the Lagrangian and momentum are. Here the vacuum-Einstein–Hilbert Lagrangian is assumed (31), and further that it can be decomposed into a positive definite part and a line element field part which have well-defined and useful variations. Variations with respect to the metric and the line element field (33) can be done, however, of more use is variation with respect to $\dot{U}$ which is taken to give a momentum (35); variations with respect to dotted quantities also occur in the quantization of perfect fluids.[7] The momentum obeys the constraint (38). The two-sided nature of U, the Lorentzian metric is invariant under $U \to -U$; and the ability to use U of different sizes to construct the Lorentzian metric do not seem to lead to further constraints. Quantization can be achieved via (39). The problem with this is that it introduces a mass into the system. The classical theory is just a theory involving length and time, however, Planck's constant has dimensions $Mass \times Length^2 \times Time^{-1}$, so that using it in quantization introduces new quantities of dimension *Mass*. Theories, such as the vacuum-Einstein equations, involving just length and time are usually reversible, in the sense that the sign on the time coordinate can be changed and the field equations still obeyed; however, this is no longer necessarily the case once quantities of dimensions of mass have been introduced, as illustrated by the fact that things fall down not up. This is not only a problem for the theory under study here, similarly using $\hbar$ in quantization of the vacuum-Einstein equations will introduce a mass. The specific wave functions (51) and (52) illustrate the above, of the two terms in the square root one is dimensionless ''1'' and the other is dimensionfull and proportional to $\hbar^{-2}$. A way of avoiding the above is to divide $\hbar$ by the Planck mass or perhaps an arbitrary mass so that objects of dimensions of mass no longer occur in the quantum system; also by analogy with the point particle one could perhaps pre-multiply the line element field Lagrangian by an arbitrary m, but on the analysis so far such an m does not occur naturally, perhaps it might do so in an extended theory which in some way incorporates that U is not necessarily of unit size. Any given Lorentzian metric can be constructed from many different sets of a positive definite metric and a line element field. For example flat space–time can be expressed by the Minkowski metric and this can be constructed from a diagonal metric and unit expansion free line element field; also flat space–time can be expressed by the Milne universe (51) for which U has expansion. In the first case there is no expansion and hence no momentum or quantum theory, in

the second there is with wave function (51). Thus it might be that ''Euclidean'' quantum gravity expresses the full quantum nature of a Lorentzian space–time if the relating line element field is expansion free; however, the main application of such theories is to the early universe where expansion is the most salient feature.

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The relativistic Dirac–Morse Green's function

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Using a recently developed approach for solving the three-dimensional Dirac equation with spherical symmetry, we obtain the two-point Green's function of the relativistic Dirac–Morse problem. This is accomplished by setting up the relativistic problem in such a way that makes comparison with the nonrelativistic problem highly transparent and results in a mapping of the latter into the former. The relativistic bound states energy spectrum is easily obtained by locating the energy poles of the Green's function components in a simple and straightforward manner. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738950]

INTRODUCTION

Despite all the work that has been done over the years on the Dirac equation, its exact solutions for local interaction has been limited to a very small set of potentials. Since the original work of Dirac in the early part of last century up until 1989 only the relativistic Coulomb problem was solved exactly. In 1989, the relativistic extension of the oscillator problem (Dirac–Oscillator) was finally formulated and solved by Moshinsky and Szczepaniak.[1] Recently, and in a series of articles,[2–6] we presented an effective approach for solving the three-dimensional Dirac equation for spherically symmetric potential interaction. The first step in the program started with the realization that the nonrelativistic Coulomb, oscillator, and *S*-wave Morse problems belong to the same class of shape invariant potentials which carries a representation of so(2,1) Lie algebra. Therefore, the fact that the relativistic version of the first two problems (Dirac–Coulomb and Dirac–Oscillator) were solved exactly makes the solution of the third, in principle, feasible. Indeed, the relativistic Dirac–Morse problem was formulated and solved in Ref. 2. The bound state energy spectrum and spinor wave functions were obtained. Taking the nonrelativistic limit reproduces the familiar Schrödinger–Morse problem. Motivated by these findings, the same approach was applied successfully in obtaining solutions for the relativistic extension of yet another class of shape invariant potentials.[3] These included the Dirac–Scarf, Dirac–Rosen–Morse I and II, Dirac–Pöschl–Teller, and Dirac–Eckart potentials. Furthermore, using the same formalism quasiexactly solvable systems at rest mass energies were obtained for a large class of power-law relativistic potentials.[4] Quite recently, Guo *et al.* succeeded in constructing solutions for the relativistic Dirac–Woods–Saxon and Dirac–Hulthén problems using the same approach.[7] In the fourth and last article of the series in our program of searching for exact solutions to the Dirac equation,[5] we found a special graded extension of so(2,1) Lie algebra. Realization of this superalgebra by 2×2 matrices of differential operators acting in the two component spinor space was constructed. The linear span of this graded algebra gives the canonical form of the radial Dirac Hamiltonian. It turned out that the Dirac–Oscillator class, which also includes the Dirac–Coulomb and Dirac–Morse, carries a representation of this supersymmetry.

The central idea in the approach is to separate the variables such that the two coupled first order differential equations resulting from the radial Dirac equation generate Schrödinger-type equations for the two spinor components. This makes the solution of the relativistic problem easily attainable by simple and direct correspondence with well-known exactly solvable nonrelativistic problems. There are two main ingredients in the formulation of the approach that makes it work.

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The first is a unitary transformation of the Dirac equation which, of course, reduces to the identity in the nonrelativistic limit. The second is the introduction, in a natural way, of an auxiliary potential component which is constrained to depend, in a particular way, on the independent potential function of the problem.

The main objective in all previous applications of the approach was in obtaining the discrete energy spectrum and spinor wave functions.[2–7] In this article, however, we demonstrate how to utilize the same approach in generating the two-point Green's function which is an important object of prime significance in the calculation of physical processes where relativistic effects become relevant. The main contribution here is in obtaining the relativistic Green's function for the Dirac–Morse problem, which is then used to give the relativistic bound states energy spectrum in a simple and direct manner. For completeness and clarity of presentation, we start by giving a brief account of how to construct the Green's function of the nonrelativistic problem by transforming that of another (reference) problem which belongs to the same class. We take the three-dimensional isotropic oscillator as the reference problem and use ''point canonical transformation'' (PCT)[8,9] to map it into the Green's function of the nonrelativistic S-wave Morse problem. This is possible because, as stated above, the two problems belong to the same class which carries a representation of the dynamical symmetry group SO(2,1).

MAPPING OF GREEN'S FUNCTION UNDER PCT

The nonrelativistic radial Green's function $\mathcal{G}_\ell(\rho,\rho',\mathcal{E})$ of the three-dimensional isotropic oscillator satisfies the following time-independent Schrödinger equation:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{\ell(\ell+1)}{\rho^2}+\omega^4\rho^2-2\mathcal{E}\right]\mathcal{G}_\ell(\rho,\rho',\mathcal{E})=-2\,\delta(\rho-\rho'), \tag{1}$$

where ℓ is the angular momentum quantum number, ω is the oscillator frequency, and $\mathcal{E}$ is the nonrelativistic energy. The nonrelativistic Green's function of the S-wave Morse problem, on the other hand, satisfies the following equation:[2,9]

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+A^2e^{-2\mu r}-A(2B+\mu)e^{-\mu r}-2E\right]g_\mu(r,r',E)=-2\,\delta(r-r'), \tag{2}$$

where μ is the potential range parameter. A and μ are real and positive. It is to be noted that our definition of the radial Green's function differs by a factor of $(rr')^{-1}$ from other typical definitions. Now, we apply to Eq. (1) the following transformation:

$$\rho=q(r),\quad \mathcal{G}_\ell(\rho,\rho',\mathcal{E})=p(r)g_\mu(r,r',E)p^*(r'). \tag{3}$$

If the result is a mapping into Eq. (2) then this transformation will be referred to as point canonical transformation (PCT). The action of (3), for real functions, on Eq. (1) maps it into the following equation:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(\frac{q''}{q'}-2\frac{p'}{p}\right)\frac{\mathrm{d}}{\mathrm{d}r}+\left(\frac{q''}{q'}\frac{p'}{p}-\frac{p''}{p}\right)+\ell(\ell+1)\left(\frac{q'}{q}\right)^2+(q')^2(\omega^4q^2-2\mathcal{E})\right]g_\mu(r,r',E)$$
$$=-\frac{2(q')^2}{p(r)p(r')}\,\delta(q(r)-q(r')), \tag{4}$$

where the primes on the transformation functions p and q denote derivatives with respect to r. Identifying this with Eq. (2) and using the relation $q'\,\delta(q(r)-q(r'))=\delta(r-r')$ gives $p(r)=\sqrt{\mathrm{d}q/\mathrm{d}r}$ and results in the following constraint on the transformation (3) to be a PCT:

$$A^2e^{-2\mu r}-A(2B+\mu)e^{-\mu r}-2E=(q')^2(\omega^4q^2-2\mathcal{E})+\ell(\ell+1)\left(\frac{q'}{q}\right)^2+\frac{3}{4}\left(\frac{q''}{q'}\right)^2-\frac{1}{2}\frac{q'''}{q'}. \tag{5}$$

This constraint is solved by taking the PCT function $q(r)=e^{-\mu r/2}$, which will result in the following PCT parameter map:

$$\omega^2 \to \frac{2A}{\mu},$$

$$\mathcal{E} \to \frac{4A}{\mu}\left(\frac{B}{\mu}+\frac{1}{2}\right), \tag{6}$$

$$\ell \to \frac{2}{\mu}\sqrt{-2E}-\frac{1}{2}.$$

It should be noted that since PCT is a map of one equation into another, then the above resulting parameter relation is a ''correspondence'' between the parameters of the two problems and not an equality of the parameters. That is we obtain, for example, the correspondence $\ell \to (2/\mu)\sqrt{-2E}-\frac{1}{2}$ but not the equality $\ell=(2/\mu)\sqrt{-2E}-\frac{1}{2}$. In fact, the right-hand-side term is continuous while the left is, of course, not.

Now, the nonrelativistic radial Green's function for the three-dimensional oscillator is well known.[10] It could be written as

$$\mathcal{G}_\ell(\rho,\rho',\mathcal{E})=\frac{\Gamma\left(\frac{2\ell+3}{4}-\mathcal{E}/2\omega^2\right)}{\omega^2\Gamma(\ell+\frac{3}{2})}\frac{1}{\sqrt{\rho\rho'}}\mathcal{M}_{\mathcal{E}/2\omega^2,[(2\ell+1)/4]}(\omega^2\rho_<^2)\mathcal{W}_{\mathcal{E}/2\omega^2,[(2\ell+1)/4]}(\omega^2\rho_>^2), \tag{7}$$

where Γ is the gamma function and $\rho_<$ ($\rho_>$) is the smaller (larger) of ρ and ρ'. $\mathcal{M}_{a,b}$ and $\mathcal{W}_{a,b}$ are the Whittaker functions of the first and second kind, respectively.[11] The two mappings (3) and (6) transform this Green's function into the following one for the nonrelativistic Morse problem:[12]

$$g_\mu(r,r',E)=\frac{\Gamma\left(\frac{1}{\mu}\sqrt{-2E}-B/\mu\right)}{A\Gamma\left(1+\frac{2}{\mu}\sqrt{-2E}\right)}e^{\mu(r+r')/2}\mathcal{M}_{(B/\mu)+(1/2),(1/\mu)\sqrt{-2E}}\left(\frac{2A}{\mu}e^{-\mu r_>}\right)$$

$$\times\mathcal{W}_{(B/\mu)+(1/2),(1/\mu)\sqrt{-2E}}\left(\frac{2A}{\mu}e^{-\mu r_<}\right). \tag{8}$$

The switching of arguments of the Whittaker functions is because $\rho_<$ ($\rho_>$) corresponds to $r_>$ ($r_<$), respectively. Next, we set up the relativistic problem using the approach mentioned above to obtain the relativistic extension of this Green's function for the Dirac–Morse problem.

SOLVING THE DIRAC EQUATION

In atomic units ($m=\hbar=1$) and taking the speed of light $c=\lambda^{-1}$, we write the Hamiltonian for a Dirac spinor coupled to a four-component potential $(A_0,\vec{A})$ as follows:

$$H=\begin{pmatrix} 1+\lambda A_0 & -i\lambda\vec{\sigma}\cdot\vec{\nabla}+i\lambda\vec{\sigma}\cdot\vec{A} \\ -i\lambda\vec{\sigma}\cdot\vec{\nabla}-i\lambda\vec{\sigma}\cdot\vec{A} & -1+\lambda A_0 \end{pmatrix}, \tag{9}$$

where λ is the Compton wavelength scale parameter $\hbar/mc$ and $\vec{\sigma}$ are the three 2×2 Pauli matrices. It is to be noted that this type of coupling does not support an interpretation of $(A_0,\vec{A})$ as the electromagnetic potential unless, of course, $\vec{A}=0$ (e.g., the Coulomb potential). That is, the

wave equation with this Hamiltonian is not invariant under the usual electromagnetic gauge transformation. Imposing spherical symmetry and writing $(A_0,\vec{A})=[\hbar V(r),\hat{r}W(r)]$, where $\hat{r}$ is the radial unit vector, gives the following two component radial Dirac equation:

$$\begin{pmatrix} 1+\hbar^2V(r)-\varepsilon & \hbar\left[\frac{\kappa}{r}+W(r)-\frac{\mathrm{d}}{\mathrm{d}r}\right] \\ \hbar\left[\frac{\kappa}{r}+W(r)+\frac{\mathrm{d}}{\mathrm{d}r}\right] & -1+\hbar^2V(r)-\varepsilon \end{pmatrix}\begin{pmatrix} f^+(r) \\ f^-(r) \end{pmatrix}=0, \tag{10}$$

where ε is the relativistic energy and κ is the spin–orbit quantum number defined as $\kappa=\pm(j+\frac{1}{2})$ for $\ell=j\pm\frac{1}{2}$. $V(r)$ and $W(r)$ are real radial functions referred to as the even and odd components of the relativistic potential, respectively. Equation (10) results in two coupled first order differential equations for the two radial spinor components. Eliminating one component in favor of the other gives a second order differential equation. This will not be Schrödinger-type (i.e., it contains first order derivatives) unless $V=0$. To obtain Schrödinger-type equation in the general case we proceed as follows. A global unitary transformation $\mathcal{U}(\eta)=\exp[(i/2)\hbar\eta\sigma_2]$ is applied to the Dirac equation (10), where η is a real constant parameter and σ_2 is the 2×2 matrix $\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$. The Schrödinger-type requirement relates the two potential components by the linear constraint $V(r)=\zeta[W(r)+\kappa/r]$, where ζ is a real parameter which is related to the transformation parameter η by $\sin(\hbar\eta)=\pm\hbar\zeta$. This results in a Hamiltonian that will be written in terms of only one arbitrary potential function; either the even potential component $V(r)$ or the odd one $W(r)$. Moreover, the solution of the problem is obtained for a given value of κ. The unitary transformation together with the potential constraint map Eq. (10) into the following one, which we choose to write in terms of the even potential component:[2,3]

$$\begin{pmatrix} C-\varepsilon+(1\pm1)\hbar^2V & \hbar\left(\mp\zeta+\frac{C}{\zeta}V-\frac{\mathrm{d}}{\mathrm{d}r}\right) \\ \hbar\left(\mp\zeta+\frac{C}{\zeta}V+\frac{\mathrm{d}}{\mathrm{d}r}\right) & -C-\varepsilon+(1\mp1)\hbar^2V \end{pmatrix}\begin{pmatrix} \phi^+(r) \\ \phi^-(r) \end{pmatrix}=0, \tag{11}$$

where $C=\cos(\hbar\eta)$ and $\left(\begin{smallmatrix} \phi^+ \\ \phi^- \end{smallmatrix}\right)=\mathcal{U}\left(\begin{smallmatrix} f^+ \\ f^- \end{smallmatrix}\right)$. This gives the following equation for one spinor component in terms of the other

$$\phi^{\mp}(r)=\frac{\hbar}{C\pm\varepsilon}\left[-\zeta\pm\frac{C}{\zeta}V(r)+\frac{\mathrm{d}}{\mathrm{d}r}\right]\phi^{\pm}(r). \tag{12}$$

On the other hand, the resulting Schrödinger-type wave equation for the two spinor components reads

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(\frac{C}{\zeta}\right)^2V^2\mp\frac{C}{\zeta}\frac{\mathrm{d}V}{\mathrm{d}r}+2\varepsilon V-\frac{\varepsilon^2-1}{\hbar^2}\right]\phi^{\pm}(r)=0. \tag{13}$$

In all relativistic problems that have been successfully tackled so far, Eq. (13) is solved by correspondence with well-known exactly solvable nonrelativistic problems.[2–7] This correspondence results in two parameter maps (one for each spinor component) relating the relativistic to the nonrelativistic problem. Using these maps and the known solutions (energy spectrum and wave functions) of the nonrelativistic problem one can easily and directly obtain the relativistic energy spectrum and spinor wave functions. An alternative, but equivalent, approach to the one given above is to postulate the one-parameter two-component equation (11) as the relativistic wave equation and show that in the nonrelativistic limit ($\hbar\to0$) the nonrelativistic problem is recovered. However, in this case, one cannot claim that the relativistic problem is a unique extension of the nonrelativistic one.

RELATIVISTIC GREEN'S FUNCTION

Now to the issue at hand—the Green's function. The relativistic 4×4 two-point Green's function $G(\vec{r},\vec{r}',\varepsilon)$ satisfies the inhomogeneous matrix wave equation $(H-\varepsilon)G=-\hbar^2\delta(\vec{r}-\vec{r}')$, where the energy ε does not belong to the spectrum of H. For problems with spherical symmetry, the 2×2 radial component $\mathcal{G}_\kappa(r,r',\varepsilon)$ of G satisfies $(H_\kappa-\varepsilon)\mathcal{G}_\kappa=-\hbar^2\delta(r-r')$, where H_κ is the radial Hamiltonian operator in Eq. (11). Once again, our definition of the radial component of the Green's function differs by a factor of $(rr')^{-1}$ from other typical definitions. We write $\mathcal{G}_\kappa$ as

$$\mathcal{G}_\kappa(r,r',\varepsilon)=\begin{pmatrix}\mathcal{G}_\kappa^{++} & \mathcal{G}_\kappa^{+-}\\ \mathcal{G}_\kappa^{-+} & \mathcal{G}_\kappa^{--}\end{pmatrix}, \tag{14}$$

where $\mathcal{G}_\kappa(r,r',\varepsilon)^\dagger=\mathcal{G}_\kappa(r',r,\varepsilon)$. Let $\Phi=\begin{pmatrix}\phi^+\\ \phi^-\end{pmatrix}$ and $\overline{\Phi}=\begin{pmatrix}\overline{\phi}^+\\ \overline{\phi}^-\end{pmatrix}$ be the regular and irregular solutions of Eq. (13), respectively. Using these two solutions, $\mathcal{G}_\kappa$ could be constructed as

$$\mathcal{G}_\kappa(r,r',\varepsilon)=\frac{1}{\Omega_\kappa(\varepsilon)}[\theta(r'-r)\Phi(r,\varepsilon)\overline{\Phi}^{\mathsf{T}}(r',\varepsilon)+\theta(r-r')\overline{\Phi}(r,\varepsilon)\Phi^{\mathsf{T}}(r',\varepsilon)], \tag{15}$$

where $\theta(r'-r)$ is the Heaviside unit step function and $\Omega_\kappa(\varepsilon)$ is the Wronskian of the regular and irregular solutions,

$$\Omega_\kappa(\varepsilon)=\hbar^{-1}\Phi^{\mathsf{T}}(r,\varepsilon)\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\overline{\Phi}(r,\varepsilon)=\hbar^{-1}[\phi^+(r,\varepsilon)\overline{\phi}^-(r,\varepsilon)-\phi^-(r,\varepsilon)\overline{\phi}^+(r,\varepsilon)] \tag{16}$$

which is independent of r as can be verified by differentiating with respect to r and using Eq. (12). Equation (15) results in the following expressions for the elements of $\mathcal{G}_\kappa$:

$$\mathcal{G}_\kappa^{\pm\pm}(r,r',\varepsilon)=\frac{1}{\Omega_\kappa(\varepsilon)}\phi^\pm(r_<,\varepsilon)\overline{\phi}^\pm(r_>,\varepsilon), \tag{17}$$

$$\mathcal{G}_\kappa^{\pm\mp}(r,r',\varepsilon)=\frac{1}{\Omega_\kappa(\varepsilon)}[\theta(r'-r)\phi^\pm(r,\varepsilon)\overline{\phi}^\mp(r',\varepsilon)+\theta(r-r')\phi^\mp(r',\varepsilon)\overline{\phi}^\pm(r,\varepsilon)]. \tag{18}$$

The equations satisfied by these elements are obtained from $(H_\kappa-\varepsilon)\mathcal{G}_\kappa=-\hbar^2\delta(r-r')$. They parallel Eqs. (12) and (13) for $\phi^\pm$ and read as follows:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(\frac{C}{\zeta}\right)^2V^2\mp\frac{C}{\zeta}\frac{\mathrm{d}V}{\mathrm{d}r}+2\varepsilon V-\frac{\varepsilon^2-1}{\hbar^2}\right]\mathcal{G}_\kappa^{\pm\pm}(r,r',\varepsilon)=-(C\pm\varepsilon)\delta(r-r'), \tag{19}$$

$$\mathcal{G}_\kappa^{\mp\pm}(r,r',\varepsilon)=\frac{\hbar}{C\pm\varepsilon}\left[-\zeta\pm\frac{C}{\zeta}V(r)+\frac{\mathrm{d}}{\mathrm{d}r}\right]\mathcal{G}_\kappa^{\pm\pm}(r,r',\varepsilon). \tag{20}$$

Using the exchange symmetry $r\leftrightarrow r'$ of $\mathcal{G}_\kappa$, then it is sufficient to solve Eq. (20) only for either $\mathcal{G}_\kappa^{-+}$ or $\mathcal{G}_\kappa^{+-}$ depending on the sign in the transformation constraint $\sin(\hbar\eta)=\pm\hbar\zeta$. That is, we write

$$\begin{aligned}\mathcal{G}_\kappa^{-+}(r,r',\varepsilon)=\mathcal{G}_\kappa^{+-}(r',r,\varepsilon)=&\frac{1\pm1}{2}\frac{\hbar}{C+\varepsilon}\left[-\zeta+\frac{C}{\zeta}V(r)+\frac{\mathrm{d}}{\mathrm{d}r}\right]\mathcal{G}_\kappa^{++}(r,r',\varepsilon)\\ &+\frac{1\mp1}{2}\frac{\hbar}{C-\varepsilon}\left[-\zeta-\frac{C}{\zeta}V(r')+\frac{\mathrm{d}}{\mathrm{d}r'}\right]\mathcal{G}_\kappa^{--}(r,r',\varepsilon)\end{aligned} \tag{21}$$

corresponding to $\sin(\hbar\eta)=\pm\hbar\zeta$, respectively. These developments will now be applied to our problem.

DIRAC–MORSE GREEN'S FUNCTION

In this setting, the Dirac–Morse problem is the system described by Eq. (11) with $V(r)=-\mathcal{B}e^{-\mu r}$ and $C=\mathcal{A}/\tau$, where $\tau\mathcal{A}>0$.[2,5,6] The parameters are related by $\tau^2=\mathcal{A}^2+\chi^2\mathcal{B}^2$ with $\zeta=\mathcal{B}/\tau$. Consequently, Eq. (19) for the diagonal elements of the radial Green's function reads as follows:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\mathcal{A}^2e^{-2\mu r}-\mathcal{A}(2\varepsilon\mathcal{B}/\mathcal{A}\pm\mu)e^{-\mu r}-\frac{\varepsilon^2-1}{\chi^2}\right]\mathcal{G}_\mu^{\pm\pm}(r,r',\varepsilon)=-(\mathcal{A}/\tau\pm\varepsilon)\,\delta(r-r'). \tag{22}$$

Comparing this with Eq. (2) gives the following two maps between the relativistic and nonrelativistic problems. The map concerning $\mathcal{G}_\mu^{++}$ is

$$\begin{gathered} g_\mu=2\mathcal{G}_\mu^{++}/(\mathcal{A}/\tau+\varepsilon), \\ A=\mathcal{A} \quad \text{or} \quad A=-\mathcal{A}, \\ B=\varepsilon\mathcal{B}/\mathcal{A} \quad \text{or} \quad B=-\varepsilon\mathcal{B}/\mathcal{A}-\mu, \\ E=(\varepsilon^2-1)/2\chi^2. \end{gathered} \tag{23}$$

The choice $B=\varepsilon\mathcal{B}/\mathcal{A}$ or $B=-\varepsilon\mathcal{B}/\mathcal{A}-\mu$ depends on whether $\mathcal{A}>0$ or $\mathcal{A}<0$, respectively. On the other hand, the map for $\mathcal{G}_\mu^{--}$ is as follows:

$$\begin{gathered} g_\mu=2\mathcal{G}_\mu^{--}/(\mathcal{A}/\tau-\varepsilon), \\ A=\mathcal{A} \quad \text{or} \quad A=-\mathcal{A}, \\ B=\varepsilon\mathcal{B}/\mathcal{A}-\mu \quad \text{or} \quad B=-\varepsilon\mathcal{B}/\mathcal{A}, \\ E=(\varepsilon^2-1)/2\chi^2. \end{gathered} \tag{24}$$

Similarly, the choice $B=\varepsilon\mathcal{B}/\mathcal{A}-\mu$ or $B=-\varepsilon\mathcal{B}/\mathcal{A}$ depends on whether $\mathcal{A}$ is positive or negative, respectively. The two mappings (23) and (24) transform the nonrelativistic Green's function (8) into the following solutions of Eq. (22):

$$\begin{aligned} \mathcal{G}_\mu^{++}=&\frac{\frac{\mathcal{A}}{\tau}+\varepsilon}{2|\mathcal{A}|}\,\frac{e^{\mu(r+r')/2}}{\Gamma(1+2\beta)} \\ &\times\begin{cases}\Gamma(\beta-\alpha)\mathcal{M}_{\alpha+1/2,\beta}\left(\dfrac{2\mathcal{A}}{\mu}e^{-\mu r_>}\right)\mathcal{W}_{\alpha+1/2,\beta}\left(\dfrac{2\mathcal{A}}{\mu}e^{-\mu r_<}\right), & \mathcal{A}>0, \\ \Gamma(1+\beta+\alpha)\mathcal{M}_{-\alpha-1/2,\beta}\left(\dfrac{-2\mathcal{A}}{\mu}e^{-\mu r_>}\right)\mathcal{W}_{-\alpha-1/2,\beta}\left(\dfrac{-2\mathcal{A}}{\mu}e^{-\mu r_<}\right), & \mathcal{A}<0, \end{cases} \end{aligned} \tag{25}$$

$$\mathcal{G}_{\mu}^{--}=\frac{\frac{\mathcal{A}}{\tau}-\varepsilon}{2|\mathcal{A}|}\frac{e^{\mu(r+r')/2}}{\Gamma(1+2\beta)} \times\begin{cases}\Gamma(1+\beta-\alpha)\mathcal{M}_{\alpha-1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r_>}\right)\mathcal{W}_{\alpha-1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r_<}\right), & \mathcal{A}>0,\\ \Gamma(\beta+\alpha)\mathcal{M}_{-\alpha+1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r_>}\right)\mathcal{W}_{-\alpha+1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r_<}\right), & \mathcal{A}<0,\end{cases} \tag{26}$$

where $\alpha=\varepsilon\mathcal{B}/\mu\mathcal{A}$ and $\beta=(1/\mu\lambda)\sqrt{1-\varepsilon^2}$. The off-diagonal elements of $\mathcal{G}_{\mu}$ are obtained by substituting these in Eq. (21), which could be rewritten in terms of the variable $x=(2\mathcal{A}/\mu)e^{-\mu r}$ as

$$\mathcal{G}_{\mu}^{-+}(x,x',\varepsilon)=\mathcal{G}_{\mu}^{+-}(x',x,\varepsilon)=-\frac{\lambda\mu}{\frac{\mathcal{A}}{\tau}+\varepsilon}\frac{1\pm1}{2\sqrt{xx'}}\left(x\frac{\mathrm{d}}{\mathrm{d}x}+\frac{x}{2}+\frac{\mathcal{B}}{\mu\tau}-\frac{1}{2}\right)\sqrt{xx'}\mathcal{G}_{\mu}^{++} -\frac{\lambda\mu}{\frac{\mathcal{A}}{\tau}-\varepsilon}\frac{1\mp1}{2\sqrt{xx'}}\left(x'\frac{\mathrm{d}}{\mathrm{d}x'}-\frac{x'}{2}+\frac{\mathcal{B}}{\mu\tau}-\frac{1}{2}\right)\sqrt{xx'}\mathcal{G}_{\mu}^{--}. \tag{27}$$

Using the differential formulas of the Whittaker functions[11] we obtain the following expressions for the off-diagonal elements of the Dirac–Morse Green's function, depending on the choice of sign in $\sin(\lambda\eta)=\pm\lambda\zeta$, as

$$\begin{aligned}\mathcal{G}_{\mu}^{-+}(r,r',\varepsilon)&=\mathcal{G}_{\mu}^{+-}(r',r,\varepsilon)\\ &=-\frac{\lambda\mathcal{B}}{\mathcal{A}}\left[\left(\frac{1\mp1}{2}\right)\mathcal{G}_{\mu}^{--}+\left(\frac{1\pm1}{2}\right)\mathcal{G}_{\mu}^{++}\right]\pm e^{\mu(r+r')/2}\\ &\quad\times\frac{\lambda\mu}{2\mathcal{A}}\frac{\Gamma(1+\beta-\alpha)}{\Gamma(1+2\beta)}\left[-\theta(r-r')\mathcal{M}_{\alpha-1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r}\right)\mathcal{W}_{\alpha+1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r'}\right)\right.\\ &\quad\left.+(\beta+\alpha)\theta(r'-r)\mathcal{M}_{\alpha+1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r'}\right)\mathcal{W}_{\alpha-1/2,\beta}\left(\frac{2\mathcal{A}}{\mu}e^{-\mu r}\right)\right],\quad \mathcal{A}>0,\end{aligned} \tag{28}$$

$$\begin{aligned}\mathcal{G}_{\mu}^{-+}(r,r',\varepsilon)&=\mathcal{G}_{\mu}^{+-}(r',r,\varepsilon)\\ &=-\frac{\lambda\mathcal{B}}{\mathcal{A}}\left[\left(\frac{1\mp1}{2}\right)\mathcal{G}_{\mu}^{--}+\left(\frac{1\pm1}{2}\right)\mathcal{G}_{\mu}^{++}\right]\pm e^{\mu(r+r')/2}\\ &\quad\times\frac{\lambda\mu}{2\mathcal{A}}\frac{\Gamma(1+\beta+\alpha)}{\Gamma(1+2\beta)}\left[(\beta-\alpha)\theta(r-r')\mathcal{M}_{-\alpha+1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r}\right)\right.\\ &\quad\times\mathcal{W}_{-\alpha-1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r'}\right)-\theta(r'-r)\mathcal{M}_{-\alpha-1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r'}\right)\\ &\quad\left.\times\mathcal{W}_{-\alpha+1/2,\beta}\left(\frac{-2\mathcal{A}}{\mu}e^{-\mu r}\right)\right],\quad \mathcal{A}<0.\end{aligned} \tag{29}$$

One can easily verify that the relativistic bound states energy spectrum of the Dirac–Morse problem[2,5,6] is located at the energy poles of these components of the Green's function. This is simply and directly obtained by taking the argument of the gamma function in the numerator to be equal to $-n$, where $n=0,1,2,\ldots$. That is by taking $\beta-\alpha=-n$ for $\mathcal{A}>0$ and $\beta+\alpha=-n$ for $\mathcal{A}<0$ giving the following spectrum:

$$\varepsilon_n = \frac{\mathcal{A}}{\tau^2}[\mu\lambda^2\mathcal{B}n \pm \sqrt{\tau^2 - (\mu\lambda\mathcal{A}n)^2}], \quad n = 0,1,2,...,n_{\max}, \tag{30}$$

where $n_{\max} \leqslant (1/\mu\lambda)\sqrt{1+(\lambda\mathcal{B}/\mathcal{A})^2}$.

Finally, it might be worthwhile looking at the nonrelativistic limit ($\lambda \to 0$) of the Green's function. One can easily show that in this limit,

$$\varepsilon \approx 1+\lambda^2 E, \quad \alpha \approx \frac{\mathcal{B}}{\mu\mathcal{A}}(1+\lambda^2 E), \quad \beta \approx \frac{1}{\mu}\sqrt{-2E}, \quad \tau \approx \mathcal{A}+\lambda^2\mathcal{B}^2/2\mathcal{A}. \tag{31}$$

Substituting these in formulas (25) and (26) for the diagonal elements of the Green's function shows that their behavior in the limit is $\mathcal{G}_\mu^{++} \approx g_\mu$ and $\mathcal{G}_\mu^{--} \approx \lambda^2 g_\mu$. On the other hand, the off-diagonal elements $\mathcal{G}_\mu^{\pm\mp}$ go to the limit like λ, except for the first term in formulas (28) and (29) which is proportional to $\lambda\mathcal{G}_\mu^{--}$. This term goes to the limit like λ^3. Therefore, the relativistic behavior of the 2×2 radial Green's function could be written symbolically as

$$\mathcal{G}_\mu \sim \begin{pmatrix} 1 & \lambda+\lambda^3 \\ \lambda+\lambda^3 & \lambda^2 \end{pmatrix}. \tag{32}$$

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A technique to identify solvable dynamical systems, and a solvable generalization of the goldfish many-body problem

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A simple approach is discussed which associates to (solvable) matrix equations (solvable) dynamical systems, generally interpretable as (interesting) many-body problems, possibly involving auxiliary dependent variables in addition to those identifying the positions of the moving particles. We then focus on cases in which the auxiliary variables can be altogether eliminated, reobtaining thereby (via this unified approach) well-known solvable many-body problems, and moreover a (solvable) extension of the "goldfish" model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1739297]

I. INTRODUCTION AND MAIN RESULTS

Several decades ago certain many-body problems were introduced and shown to be solvable, first in the quantal context and then as classical dynamical systems (for a review of these results in the classical context, including a capsule account, with appropriate references, of the early history of these developments, see Ref. 15). The seed model[9,23,10] of this development (that over the last few decades featured in many hundreds, perhaps thousands, of papers) is characterized—in the classical context to which our treatment is confined—by the Newtonian equations of motion

$$\ddot{z}_n = 2\,g^2 \sum_{m=1, m\neq n}^{N} (z_n - z_m)^{-3} \tag{1}$$

(the factor 2 in the right-hand side is of course conventional in view of the arbitrariness of the constant g^2, and throughout this paper superimposed dots denote differentiations with respect to the independent variable t, which we always assume to be *real* and we interpret as "time"; the remaining notation is, we trust, self-explanatory).

The Newtonian equations of motion of a related model, usually associated (at least for imaginary values of the constant γ) with the name of Sutherland,[31] reads

$$\ddot{z}_n = 2\,g^2 \sum_{m=1, m\neq n}^{N} \cosh[\,\gamma\,(z_n - z_m)\,]\,\{\gamma^{-1}\sinh[\,\gamma\,(z_n - z_m)\,]\}^{-3} \tag{2}$$

(this model reduces of course to the previous one for $\gamma = 0$).

Another solvable model, to which the honorary name of "goldfish" has been attributed in view of the neatness of its equations of motion[16] (a name also extended to its nonintegrable variants characterized by the presence of arbitrary coupling constants,[20] as well as to its integrable variants characterized by only "nearest-neighbor" interactions[17]), features the Newtonian equations of motion (with velocity-dependent two-body forces)

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$$\ddot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m}, \tag{3}$$

while the Newtonian equations of motion of an, also solvable, variant of it reads

$$\ddot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \dot{z}_n \dot{z}_m \, \gamma \coth[\gamma(z_n - z_m)] \tag{4}$$

(note that the factor 2 in the right-hand side of the last two equations is now essential to guarantee the integrable, indeed solvable, character of these many-body models; of course the second one reduces to the first for $\gamma = 0$). The names of Ruijsenaars and Schneider are appropriately associated with these two latter models, which belong to a hierarchy of integrable dynamical systems introduced by them;[30,15] although actually the two specific models quoted above, (3) and (4), had been shown to be solvable earlier.[11,15]

Solvable variants of the first and third of these models, (1) and (3), characterized by the remarkable property that their *generic* solution is *isochronous* (i.e., completely periodic with a fixed period independent of the initial data), are also well known.[9,1,18,15] The Newtonian equations of motions of these *isochronous* models read, respectively,

$$\ddot{z}_n + \omega^2 z_n = 2 g^2 \sum_{m=1, m\neq n}^{N} (z_n - z_m)^{-3}, \tag{5}$$

$$\ddot{z}_n - i \omega \dot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m}, \tag{6}$$

where the *positive* constant ω characterizes the relevant period T via the standard relation

$$T = \frac{2\pi}{\omega}. \tag{7}$$

The simplest way to obtain these generalized equations, (5) respectively (6)—which of course reduce to (1) respectively (3) for $\omega = 0$—and to thereby demonstrate the origin of their remarkable property of *isochronicity* (as well as showing that their solution is trivially related to the solution of (1) respectively, (3)), is via the following simple change of variables (sometimes called ''the trick'': see, for instance, Refs. 12, 14, 18, 15). First, merely rewrite the original equations (1) respectively (3) with the following, merely notational, change: replace $z_n(t)$ with, say, $\zeta_n(\tau)$, and correspondingly, say, $\dot{z}_n$ with ζ' and $\ddot{z}_n$ with ζ_n'', where the appended primes denote of course differentiations with respect to the new independent variable τ, so that (1) reads

$$\zeta_n'' = 2 g^2 \sum_{m=1, m\neq n}^{N} (\zeta_n - \zeta_m)^{-3}, \tag{8}$$

and likewise (3) read

$$\zeta_n'' = 2 \sum_{m=1, m\neq n}^{N} \frac{\zeta_n' \zeta_m'}{\zeta_n - \zeta_m}. \tag{9}$$

Then, to transform (8) into (5), set

$$z_n(t) = \exp(-i \omega t) \, \zeta_n(\tau), \qquad \tau = \frac{\exp(2 i \omega t) - 1}{2 i \omega}, \tag{10}$$

and likewise to transform (9) into (6) set (even more simply)

$$z_n(t) = \zeta_n(\tau), \quad \tau = \frac{\exp(i\,\omega\,t) - 1}{i\,\omega}. \tag{11}$$

The second of these equations of motion, (6), requires of course that the motion be considered in the *complex* plane, so that (in self-explanatory notation)

$$z_n = x_n + i\,y_n; \tag{12a}$$

but this condition, far from detracting from the ''physical'' significance of this many-body model, allows to interpret it[13,15] as describing the motion of N particles in the horizontal plane (immersed in ordinary, three-dimensional, space), via the introduction of the *real* vectors

$$\mathbf{r}_n = (x_n\,, y_n\,, 0), \tag{12b}$$

since it is easily seen that the *complex* equations of motion (6) become then the following Newtonian (*rotation- and translation-invariant*) equations of motion in the (*real*, horizontal) plane:

$$\ddot{\mathbf{r}}_n - \omega\,\hat{k} \wedge \dot{\mathbf{r}}_n = 2 \sum_{m=1, m\neq n}^{N} r_{nm}^{-2} \cdot [\dot{\mathbf{r}}_n(\dot{\mathbf{r}}_m \cdot \mathbf{r}_{nm}) + \dot{\mathbf{r}}_m(\dot{\mathbf{r}}_n \cdot \mathbf{r}_{nm}) - \mathbf{r}_{nm}(\dot{\mathbf{r}}_n \cdot \dot{\mathbf{r}}_m)]. \tag{13}$$

Here $\hat{k}$ is the unit vector orthogonal to the horizontal plane,

$$\hat{k} = (0, 0, 1), \tag{14a}$$

so that (consistently with the standard definition of vector product in three-dimensional space, see (12b) and (14a))

$$\hat{k} \wedge \mathbf{r}_n = (-y_n\,, x_n\,, 0); \tag{14b}$$

and we use (here and below, see (37)) the short-hand notation

$$\mathbf{r}_{nm} \equiv \mathbf{r}_n - \mathbf{r}_m \tag{15a}$$

so that

$$r_{nm}^2 = (\mathbf{r}_n - \mathbf{r}_m)^2 = r_n^2 + r_m^2 - 2\,(\mathbf{r}_n \cdot \mathbf{r}_m). \tag{15b}$$

After this terse review of results which might by now be considered classical,[15] let us introduce our main findings. First of all—as detailed in the following section—we provide a simple approach that yields directly, in a unified manner, the solution of all the models reported above, and that moreover opens the way to the identification and study of more general solvable models, characterized by equations of motion somewhat analogous to those reported above, although generally also requiring the introduction of additional ''auxiliary variables.'' The study of such models is however postponed to subsequent papers. In this paper we mainly focus on the identification of models which generalize the models described above, with particular attention to those that allow the complete elimination of the auxiliary variables.

The first class of solvable models is characterized by the following Newtonian equations of motion:

$$\ddot{z}_n - a\,\frac{\dot{z}_n^2}{z_n} = -\sum_{m=1, m\neq n}^{N} g_{nm}\,g_{mn}\,(z_n\,z_m)^{2a}\left[\frac{2}{(z_n - z_m)^3} + \frac{a}{z_m\,(z_n - z_m)^2}\right]. \tag{16}$$

Here and throughout a is a constant, and we shall whenever convenient also use (provided $a \neq 1$) the constant α related to it as follows:

$$\alpha = \frac{1}{1-a}, \quad a = \frac{\alpha - 1}{\alpha}. \tag{17}$$

For instance via the change of dependent variables

$$z_n = w_n^{\alpha} \tag{18}$$

the Newtonian equations of motion (16) become

$$\ddot{w}_n = \alpha^{-2} \sum_{m=1, m\neq n}^{N} g_{nm}\, g_{mn}\, w_n^{\alpha-1}\, w_m^{2(\alpha-1)}\, (w_n^{\alpha} - w_n^{\alpha})^{-3} \cdot \left[1 + \alpha - (1-\alpha) \left(\frac{w_n}{w_m} \right)^{\alpha} \right], \tag{19a}$$

$$\ddot{w}_n = \alpha^{-2} \sum_{m=1, m\neq n}^{N} g_{nm}\, g_{mn}\, w_n^{-(\alpha+1)}\, w_m^{-2(\alpha+1)}\, (w_n^{-\alpha} - w_n^{-\alpha})^{-3} \cdot \left[1 - \alpha - (1+\alpha) \left(\frac{w_n}{w_m} \right)^{-\alpha} \right]. \tag{19b}$$

Note the remarkable identity of the right-hand sides of (19a) and (19b), which are obtained from each other via $\alpha \Rightarrow -\alpha$.

In the special case $a = 1$ (corresponding via (17) to $\alpha = \infty$) the formula (18) is replaced by

$$z_n = \exp(2\, \gamma\, w_n), \tag{20}$$

and it is easily seen that (16) then becomes

$$\ddot{w}_n = -2\, (4\, \gamma^2)^{-2} \sum_{m=1, m\neq n}^{N} g_{nm}\, g_{mn} \cosh[\, \gamma\, (w_n - w_m)\,] \{ \gamma^{-1} \sinh[\, \gamma\, (w_n - w_m)\,] \}^{-3}. \tag{21}$$

In these equations of motion, (16), we interpret the quantities $z_n \equiv z_n(t)$ as "particle coordinates" (or alternatively we reserve such an interpretation for the quantities $w_n(t)$, see (18) and (20)), while the "auxiliary variables" $g_{nm} \equiv g_{nm}(t)$ evolve in time according to the following (first-order) equations:

$$\dot{g}_{nm} + g_{nm}\, [F_n - F_m] = -\sum_{\ell=1; \ell\neq n,m}^{N} g_{n\ell}\, g_{\ell m}\, z_{\ell}^{2a} \cdot \{ (z_n - z_{\ell})^{-2} + a\, (z_n - z_{\ell})^{-1}\, z_{\ell}^{-1} - [\, (z_m - z_{\ell})^{-2} + a\, (z_m - z_{\ell})^{-1}\, z_{\ell}^{-1}\,] \}, \quad n \neq m. \tag{22}$$

The quantities F_n in the left-hand side of these evolution equations can be assigned *arbitrarily*, as explicit functions of time or as functions of the dependent variables z_m and $g_{m\ell}$, without spoiling the solvability of the model (16) with (22) nor indeed affecting the time-evolution of the particle coordinates $z_m(t)$ (a proof of this, apparently remarkable but eventually obvious, fact is given in the following section). To (better) exploit this freedom we now set

$$F_n = f_n - \sum_{\ell=1, \ell\neq n}^{N} g_{n\ell}\, z_{\ell}^{2a} [\, (z_n - z_{\ell})^{-2} + a\, (z_n - z_{\ell})^{-1}\, z_{\ell}^{-1}\,], \tag{23}$$

and we thereby rewrite (22) as follows:

$$\dot g_{nm}+g_{nm}[f_n-f_m]-g_{nm}\{g_{nm}z_m^{2a}[(z_n-z_m)^{-2}+a(z_n-z_m)^{-1}z_m^{-1}]-g_{mn}z_n^{2a}[(z_n-z_m)^{-2}$$
$$-a(z_n-z_m)^{-1}z_n^{-1}]\}$$
$$=\sum_{\ell=1;\ell\neq n,m}^{N} z_\ell^{2a}\{(g_{nm}g_{n\ell}-g_{n\ell}g_{\ell m})[(z_n-z_\ell)^{-2}+a(z_n-z_\ell)^{-1}z_\ell^{-1}]$$
$$-(g_{nm}g_{m\ell}-g_{n\ell}g_{\ell m})[(z_m-z_\ell)^{-2}+a(z_m-z_\ell)^{-1}z_\ell^{-1}]\},\quad n\neq m. \tag{24}$$

We now observe that, in the special case $a=0$, these evolution equations simplify to read

$$\dot g_{nm}+g_{nm}[f_n-f_m]-g_{nm}(g_{nm}-g_{mn})(z_n-z_m)^{-2}$$
$$=\sum_{\ell=1;\ell\neq n,m}^{N}\{(g_{nm}g_{n\ell}-g_{n\ell}g_{\ell m})(z_n-z_\ell)^{-2}-(g_{nm}g_{m\ell}-g_{n\ell}g_{\ell m})(z_m-z_\ell)^{-2}\},\quad n\neq m. \tag{25}$$

They therefore admit, for $f_n=0$ (or equivalently for $f_n=f$), the simple solution

$$g_{nm}=i\,g,\quad \dot g=0, \tag{26}$$

whereby the equations of motion (16) (with $a=0$) reproduce the classical model (1) (and of course the same outcome also obtains, up to a merely notational change, from the equations of motion (19) with $\alpha=1$, which corresponds to $a=0$, see (17)).

Likewise, for $a=1$, the equations of motion (24) simplify to read

$$\dot g_{nm}+g_{nm}[f_n-f_m]-g_{nm}(g_{nm}-g_{mn})z_n z_m(z_n-z_m)^{-2}$$
$$=\sum_{\ell=1;\ell\neq n,m}^{N} z_\ell\{(g_{nm}g_{n\ell}-g_{n\ell}g_{\ell m})z_n(z_n-z_\ell)^{-2}$$
$$-(g_{nm}g_{m\ell}-g_{n\ell}g_{\ell m})z_m(z_m-z_\ell)^{-2}\},\qquad n\neq m. \tag{27}$$

They therefore admit, for $f_n=0$ (or equivalently for $f_n=f$), the simple solution

$$g_{nm}=4\,i\,\gamma^2 g,\quad \dot g=0, \tag{28}$$

whereby the equations of motion (21) reproduce (up to a merely notational change) the classical model (2).

And the third case in which the complete elimination of the auxiliary variables g_{nm} can be achieved is for $a=2$, when the evolution equations (24) read

$$\dot g_{nm}+g_{nm}[f_n-f_m]-g_{nm}(z_n-z_m)^{-2}\{g_{nm}z_m^3(2z_n-z_m)-g_{mn}z_n^3(2z_m-z_n)\} \tag{29}$$
$$=\sum_{\ell=1;\ell\neq n,m}^{N} z_\ell^3\{(g_{nm}g_{n\ell}-g_{n\ell}g_{\ell m})(z_n-z_\ell)^{-2}(2z_n-z_\ell)$$
$$-(g_{nm}g_{m\ell}-g_{n\ell}g_{\ell m})(z_m-z_\ell)^{-2}(2z_m-z_\ell)\},\quad n\neq m, \tag{30}$$

hence they admit, for $f_n=i\,g\,z_n^2$, again the solution (26), which yields again, when inserted in (19) with $\alpha=-1$ (which corresponds to $a=2$, see (17)), again the original model (1) (up to the notational replacement of z_n with w_n).

The solvable character of the equations of motion (16) (or, equivalently, (19)) with (22) is exhibited by the following neat result (applicable for any value of the constant a, except $a=1$): the N coordinates $z_n\equiv z_n(t)$ are the N eigenvalues of the $N\otimes N$ matrix

$$U(t)=A\left(1+\frac{B}{\alpha}t\right)^{\alpha}, \tag{31a}$$

where the two constant $N\otimes N$ matrices A, B are given in terms of the initial data by the following formulas:

$$A=\mathrm{diag}[z_n(0)], \tag{31b}$$

$$B_{nm}=\delta_{nm}\frac{\dot{z}_n(0)}{z_n(0)}-(1-\delta_{nm})\frac{g_{nm}(0)\,[z_n(0)\,z_m(0)]^a}{z_n(0)\,[z_n(0)-z_m(0)]}. \tag{31c}$$

In the special case $a=1$ the same prescription applies, except for the replacement of (31a) with

$$U(t)=A\exp(B\,t). \tag{32}$$

These results are demonstrated in the following section, where the formulas suitable to obtain the time evolution of the auxiliary variables $g_{nm}(t)$ are also given. In the special cases identified above in which these variables reduce to a constant independent of the indices n, m and can therefore be essentially eliminated, reproducing thereby, as described above, the classical models (1) and (2), the solutions described here reproduce of course the well-known results originally obtained by Olshanetsky and Perelomov.[26,27,15]

The second class of solvable models is characterized by the Newtonian equations of motion

$$\ddot{z}_n-a\frac{\dot{z}_n^2}{z_n}=\sum_{m=1,m\neq n}^{N}\eta_{nm}\,\eta_{mn}\,\dot{z}_n\,\dot{z}_m\left[\frac{2}{z_n-z_m}+\frac{a}{z_m}\right]. \tag{33a}$$

Here the notation is, we trust, self-explanatory, see above. The auxiliary variables $\eta_{nm}\equiv\eta_{nm}(t)$ evolve now according to the (first-order) equations

$$\begin{aligned}&\dot{\eta}_{nm}+\eta_{nm}\,(1-\eta_{nm}\,\eta_{mn})\left[\frac{\dot{z}_n-\dot{z}_m}{z_n-z_m}-\frac{a}{2}\left(\frac{\dot{z}_n}{z_n}+\frac{\dot{z}_m}{z_m}\right)\right]\\&\quad=-\sum_{\ell=1;\ell\neq n,m}^{N}\dot{z}_\ell\left\{\eta_{n\ell}\,(\eta_{\ell n}\,\eta_{nm}+\eta_{\ell m})\left[(z_n-z_\ell)^{-1}+\frac{a}{2}z_\ell^{-1}\right]\right.\\&\qquad\left.+\eta_{\ell m}\,(\eta_{m\ell}\,\eta_{nm}+\eta_{n\ell})\left[(z_n-z_\ell)^{-1}+\frac{a}{2}z_\ell^{-1}\right]\right\}-\eta_{nm}\,(F_n-F_m),\quad n\neq m.\end{aligned} \tag{33b}$$

We now note that, remarkably, for the assignment $F_n=0$ (or, essentially equivalently, $F_n=F$), the latter equations of motion admit the trivial solution

$$\eta_{nm}=-1, \tag{34}$$

entailing that the equations of motion (33a) become

$$\ddot{z}_n-a\frac{\dot{z}_n^2}{z_n}=\sum_{m=1,m\neq n}^{N}\dot{z}_n\,\dot{z}_m\left[\frac{2}{z_n-z_m}+\frac{a}{z_m}\right]. \tag{35a}$$

The solution of the more general model (33) is described in the following section; in this section we restrict attention to these Newtonian equations of motion, (35a), that obviously can be rewritten in the following form:

$$\ddot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m} + a \sum_{m=1}^{N} \frac{\dot{z}_n \dot{z}_m}{z_m}. \tag{35b}$$

But before reporting the solution of the corresponding initial-value problem, let us interject two remarks.

First we note that clearly, for $a=0$, these equations of motion reproduce the Newtonian equations of motion (3) of the standard goldfish model, while for $a=1$, via (20), they become (4) and for $a=2$, via (18) with $\alpha=-1$, they reproduce again the equations of motion (3) of the standard goldfish model (up to the notational replacement of z_n with w_n).

Next, we apply to them the trick described above, see (11), obtaining thereby the following modified version of these equations of motion:

$$\ddot{z}_n - i\,\omega\,\dot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m} + a \sum_{m=1}^{N} \frac{\dot{z}_n \dot{z}_m}{z_m}, \tag{36}$$

which of course reduce to the previous ones, (35b), when the costant ω vanishes. Let us as well exhibit their reformulation (achieved as above, see the paragraph following (11)) in the guise of the following Newtonian equations of motion of a (*real, rotation-invariant*) N-body problem in the (horizontal) plane:

$$\begin{aligned} \ddot{\mathbf{r}}_n - \omega\,\hat{k}\wedge\dot{\mathbf{r}}_n = {} & 2 \sum_{m=1, m\neq n}^{N} r_{nm}^{-2} \cdot [\dot{\mathbf{r}}_n(\dot{\mathbf{r}}_m \cdot \mathbf{r}_{nm}) + \dot{\mathbf{r}}_m(\dot{\mathbf{r}}_n \cdot \mathbf{r}_{nm}) - \mathbf{r}_{nm}(\dot{\mathbf{r}}_n \cdot \dot{\mathbf{r}}_m)] \\ & + \sum_{m=1}^{N} r_m^{-2}\,(a_1 + a_2\,\hat{k}\wedge) \cdot [\dot{\mathbf{r}}_n(\dot{\mathbf{r}}_m \cdot \mathbf{r}_m) + \dot{\mathbf{r}}_m(\dot{\mathbf{r}}_n \cdot \mathbf{r}_m) - \mathbf{r}_m(\dot{\mathbf{r}}_n \cdot \dot{\mathbf{r}}_m)], \end{aligned} \tag{37}$$

where of course the two *real* "coupling constants" a_1 and a_2 are the real and imaginary parts of a, $a = a_1 + i\,a_2$.

As implied by the treatment detailed in the following section, the solution of the initial-value problem for the Newtonian equations of motion (35) is provided by the following prescription: the particle coordinates $z_n(t)$ are the N eigenvalues of the $N\otimes N$ matrix (31a) (for $a\neq 1$) respectively (32) (for $a=1$), with the constant $N\otimes N$ matrix A given by (31b) and the constant $N\otimes N$ matrix B given by

$$B_{nm} = [z_n(0)]^{-1}\,[\dot{z}_n(0)\,\dot{z}_m(0)]^{1/2}. \tag{38a}$$

But the dyadic character of this matrix entails

$$B^p = b^{p-1}\,B, \quad p = 1, 2, 3, \ldots \tag{38b}$$

with

$$b = \sum_{n=1}^{N} \frac{\dot{z}_n(0)}{z_n(0)}, \tag{39}$$

implying that a more explicit expression of the matrix $U(t)$, the eigenvalues of which yield the particle coordinates $z_n(t)$, can be given in this case than (31a) (for $a\neq 1$) respectively (32) (for $a=1$), namely,

$$U_{nm}(t) = \delta_{nm}\,z_n(0) + b^{-1}\left[\left(1 + \frac{b\,t}{\alpha}\right)^{\alpha} - 1\right][\dot{z}_n(0)\,\dot{z}_m(0)]^{1/2}, \qquad \text{if } a\neq 1, \tag{40a}$$

$$U_{nm}(t) = \delta_{nm}\,z_n(0) + b^{-1}\,[\exp(b\,t) - 1]\,[\dot{z}_n(0)\,\dot{z}_m(0)]^{1/2}, \qquad \text{if } a = 1. \tag{40b}$$

Note that this matrix is written as the sum of two $N\otimes N$ matrices, one diagonal and the other dyadic, both depending remarkably neatly on the data of the initial-value problem (see (39)).

The diligent reader will verify that this prescription reproduces the previously known results[11,15] in the cases ($a=0$, $a=1$, $a=2$, corresponding respectively to $\alpha=1$, $\alpha=\infty$, $\alpha=-1$) when, as discussed above, the model (35) reduces, possibly up to simple changes of dependent variables, to the classical models (3) or (4); while a discussion of the behavior of the solutions of the model (35) for arbitrary values of the constant a, and of the (richer) model (36), is tersely outlined in Sec. III, where we also show how the solution of these models can be reduced after all to the solution of the standard goldfish model. The corresponding, remarkably neat, prescription detailing the solution of the initial-value problem for the (*isochronous* version of the) generalized goldfish model (36) or (37) asserts that *the coordinates* $z_n(t)$ *are the* N *roots of the following algebraic equation in* z:

$$\sum_{n=1}^{N}\frac{\dot z_n(0)}{z-z_n(0)}=b\left\{\left[1+\frac{b\,[\exp(i\,\omega\,t)-1]}{i\,\alpha\,\omega}\right]^{\alpha}-1\right\}^{-1},\qquad \text{if } a\neq 1, \tag{41a}$$

$$\sum_{n=1}^{N}\frac{\dot z_n(0)}{z-z_n(0)}=b\left\{\exp\left[\frac{b\,[\exp(i\,\omega\,t)-1]}{i\,\omega}\right]-1\right\}^{-1},\qquad \text{if } a=1, \tag{41b}$$

with the constant b *defined in terms of the initial data by (39) and of course* α *related to* a *by (17).* Obviously key to the behavior of these solutions $z_n(t)$ is the time evolution of the right-hand sides of these formulas, which, for *positive* ω, is clearly periodic with period T, see (7), in the (not new) $a=1$ case, it is as well periodic with the same period T for *arbitrary* a provided the initial data entail via (39) the inequality

$$\left|1+\frac{i\,b}{\omega}\right|>\left|\frac{b}{\omega}\right|, \tag{42a}$$

namely,

$$\mathrm{Im}(b)<\frac{\omega}{2} \tag{42b}$$

(we assume here for definiteness that ω is *positive*, $\omega>0$), and it is instead periodic for *arbitrary* (but *real*) a with the, generally different, period

$$\tilde T=\frac{T}{\alpha}=(1-a)\,T=\frac{2\,(1-a)\,\pi}{\omega} \tag{43}$$

if the inequality (42) is reversed, $\mathrm{Im}(b)>\omega/2$.

II. THE TECHNIQUE

The point of departure of our treatment is the $N\otimes N$ matrix equation

$$\ddot U=a\,\dot U\,U^{-1}\,\dot U, \tag{44}$$

where a is an arbitrary (scalar) constant. As can be easily verified, for $a\neq 1$ this matrix evolution equation has the *general* solution (31a) with (17) where, in terms of the initial-value problem,

$$A=U(0), \tag{45a}$$

$$B=[U(0)]^{-1}\,\dot U(0), \tag{45b}$$

while in the special case $a=1$ (entailing, via (17), $\alpha=\infty$), $U(t)$ is given by (32).

We now introduce the parametrization of the $N\otimes N$ matrix $U(t)$ in terms of its N eigenvalues $z_n(t)$ and of its diagonalizing $N\otimes N$ matrix $R(t)$:

$$U=R\,Z\,R^{-1}, \tag{46a}$$

$$Z=\mathrm{diag}[z_n]. \tag{46b}$$

Before proceeding to obtain the evolution equations implied by (44) for the diagonal matrix $Z(t)$ and for the diagonalizing matrix $R(t)$, or rather (see below) for the matrix $M(t)$ defined in terms of $R(t)$ by the formula

$$M=R^{-1}\dot{R}, \tag{47}$$

let us note that the formulas (46) define the matrix R only up to multiplication from the right by an *arbitrary* diagonal matrix, say

$$D=\mathrm{diag}[d_n], \tag{48}$$

since replacing in (46a) R with

$$\tilde{R}=R\,D \tag{49}$$

is clearly of no consequence. The corresponding change of the matrix M,

$$\tilde{M}=\tilde{R}^{-1}\dot{\tilde{R}}=D^{-1}\,M\,D+D^{-1}\,\dot{D}, \tag{50a}$$

namely,

$$\tilde{M}_{nn}=M_{nn}+\frac{\dot{d}_n}{d_n}, \tag{50b}$$

$$\tilde{M}_{nm}=d_n^{-1}\,M_{nm}\,d_m\,, \quad n\neq m, \tag{50c}$$

entails essentially that in our parametrization of the $N\otimes N$ matrix $U(t)$ (via (46) with (47)) the N^2 matrix elements of this matrix get replaced by the N elements $z_n(t)$ of the diagonal matrix $Z(t)$ (namely, by the N eigenvalues of the matrix $U(t)$: see (46)) and by the $N(N-1)$ off-diagonal elements $M_{nm}(t)$ (with $n\neq m$) of the $N\otimes N$ matrix $M(t)$, while the N diagonal elements $M_{nn}(t)$ can be arbitrarily adjusted by choosing appropriately the elements $d_n(t)$ of the diagonal matrix $D(t)$, see (50b) (of course, up to a corresponding adjustment of the corresponding off-diagonal elements, see (50c)).

Differentiation with respect to the independent variable t of (46a) yields, using (47),

$$\dot{U}=R\,\{\dot{Z}+[M,Z]\}\,R^{-1}, \tag{51a}$$

$$\ddot{U}=R\,\{\ddot{Z}+[\dot{M},Z]+2\,[M,\dot{Z}]+[M,[M,Z]]\}\,R^{-1}. \tag{51b}$$

Here and throughout we use of course the standard notation $[X,Y]\equiv X\,Y-Y\,X$ for the commutator of two matrices.

Hence insertion of these formulas in the matrix evolution equation (44) yields

$$\ddot{Z}+[\dot{M},Z]+2\,[M,\dot{Z}]+[M,[M,Z]\,]=a\,\{\dot{Z}+[M,Z]\}\,Z^{-1}\,\{\dot{Z}+[M,Z]\}, \tag{52a}$$

namely, by separating the diagonal and off-diagonal terms,

$$\ddot{z}_n - a\frac{\dot{z}_n^2}{z_n} = -\sum_{m=1,m\neq n}^{N} M_{nm}\,M_{mn}\,(z_n - z_m)\left[2 + \frac{a\,(z_n - z_m)}{z_m}\right], \tag{52b}$$

$$\dot{M}_{nm}\,(z_n - z_m) + M_{nm}\left[2\,(\dot{z}_n - \dot{z}_m) - a\,(z_n - z_m)\left(\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m}\right)\right]$$
$$= \sum_{\ell=1;\ell\neq n,m}^{N} M_{n\ell}\,M_{\ell m}\left[(z_n - z_\ell) + (z_m - z_\ell) + \frac{a\,(z_n - z_\ell)\,(z_m - z_\ell)}{z_\ell}\right]$$
$$- M_{nm}\,(z_n - z_m)\,(F_n - F_m), \quad n\neq m, \tag{52c}$$

where we did set

$$M_{nn} \equiv F_n \tag{53}$$

and, consistently with the observation made above, we retain the freedom to assign arbitrarily these N quantities F_n (as given functions of time, or possibly of the dependent variables $z_n(t)$ and $M_{nm}(t)$ with $n\neq m$; see below). Note that the ''source terms'' F_n could be altogether eliminated from the evolution equations (52c) via the transformation

$$M_{nm}(t) = \tilde{M}_{nm}(t)\,\exp\left\{\int_0^t dt'\,[F_m(t') - F_n(t')]\right\}, \tag{54}$$

which entails the replacement of (52b) and (52c) with

$$\ddot{z}_n - a\frac{\dot{z}_n^2}{z_n} = -\sum_{m=1,m\neq n}^{N} \tilde{M}_{nm}\,\tilde{M}_{mn}\,(z_n - z_m)\left[2 + \frac{a\,(z_n - z_m)}{z_m}\right], \tag{55a}$$

$$\dot{\tilde{M}}_{nm}\,(z_n - z_m) + \tilde{M}_{nm}\left[2\,(\dot{z}_n - \dot{z}_m) - a\,(z_n - z_m)\left(\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m}\right)\right]$$
$$= \sum_{\ell=1;\ell\neq n,m}^{N} \tilde{M}_{n\ell}\,\tilde{M}_{\ell m}\left[(z_n - z_\ell) + (z_m - z_\ell) + \frac{a\,(z_n - z_\ell)\,(z_m - z_\ell)}{z_\ell}\right], \quad n\neq m \tag{55b}$$

(namely, just the elimination of the terms involving the quantities F_n and F_m, and a merely notational change). This of course explains why the quantities $F_n(t)$ can be assigned essentially arbitrarily, without affecting the time-evolution of the ''particle coordinates'' $z_n(t)$ (but such an assignment will of course affect the off-diagonal elements of the matrix $M(t)$, as implied by the relation (54)).

Before proceeding further we like to point out that the approach presented here is by no means quite new. Indeed, for the case $a=0$, equations analogous to those reported above, (52), have appeared in the literature quite often, both in analogous, and in somewhat different, contexts, see for instance, Refs. 21, 32, 4, 28, 34, 33, 35, 24, 5, 6, 22, 25, 3, 2.

We now set

$$M_{nm} = (z_n - z_m)^{-2}\,(z_n\,z_m)^a\,g_{nm}, \quad n\neq m, \tag{56}$$

and we thereby obtain, from (52b), the Newtonian equations of motion (16), and from (52c) the evolution equations (22). The results reported in the previous section, regarding the solution of these equations, are thereby justified in the light of the developments reported above (in this section), and they are complemented by the formulas detailing the time evolution of the quantities $g_{nm}(t)$ that are rather obviously implied by (31) and (32) via the relations (46), (47), and (56). Note that the easiest way to get these results is to make the (permissible and convenient) assump-

tion $R(0)=1$, entailing $U(0)=A=\mathrm{diag}[z_n(0)]$ (see (31a), (31b) and (46)), $\dot{U}(0)=A\,B=\dot{Z}(0)+[M(0),Z(0)]$ (see (31a), (51a) and (46b)) and $M_{nm}(0)=[z_n(0)-z_m(0)]^{-2}[z_n(0)\,z_m(0)]^a g_{nm}(0)$ (see (56)).

Likewise, the different assignment (suggested by the structure of the Lax matrix introduced in Ref. 7)

$$M_{nm}=(z_n-z_m)^{-1}(\dot{z}_n\,\dot{z}_m)^{1/2}\,\eta_{nm}\,,\quad n\neq m, \tag{57}$$

yields, from (52b), the Newtonian equations of motion (33a), and from (52c) the evolution equations (33b) (note that, to get them, we must also use (33a)).

These latter developments imply that the solution of the initial-value problem for the model (33) is given by the following simple rule: *the "particle coordinates" $z_n(t)$ are the N eigenvalues of the $N\otimes N$ matrix (31a) (for $a\neq 1$) respectively (32) (for $a=1$), with the constant $N\otimes N$ matrix A given by (31b) and the elements of the constant $N\otimes N$ matrix B reading now*

$$B_{nm}=[z_n(0)]^{-1}\{\delta_{nm}\,\dot{z}_n(0)-(1-\delta_{nm})\,\eta_{nm}(0)\,[\dot{z}_n(0)\,\dot{z}_m(0)]^{1/2}\}. \tag{58}$$

These formulas provide the solution of the initial-value problem of the model (33), as regards the time evolution of the particle coordinates $z_n(t)$; and they clearly imply the corresponding results reported in the previous section for the model (35) (which obtains from (33) via (34)). As for the time-evolution of the auxiliary variable $\eta_{nm}(t)$ in the more general case ((33) without (34)), as above we leave its derivation as an easy task for the diligent reader: again, the easiest way to get these results—as well as those mentioned in the first part of this paragraph—from (46), (47) and (57), is to make the assumption $R(0)=1$, entailing $U(0)=A=\mathrm{diag}[z_n(0)]$ (see (31a), (31b) and (46)), $\dot{U}(0)=A\,B=\dot{Z}(0)+[M(0),Z(0)]$ (see (31a), (51a) and (46b)) and $M_{nm}(0)=[z_n(0)-z_m(0)]^{-1}[\dot{z}_n(0)\,\dot{z}_m(0)]^{1/2}\,\eta_{nm}(0)$ (see (57)).

III. GENERALIZED GOLDFISH MODEL

In this section we discuss tersely the solution, obtained in Sec. II and detailed at the end of Sec. I, of the generalized goldfish model (35), as well as of its *isochronous* version (36); and at the end we show how the generalized goldfish model (35) can be reduced back to the standard goldfish model (3).

Clearly the key function determining the behavior of the solutions of the generalized goldfish model (35) is

$$\beta(\alpha;t)=b^{-1}\left[\left(1+\frac{b\,t}{\alpha}\right)^{\alpha}-1\right]\quad \text{if}\ \ a\neq 1, \tag{59a}$$

$$\beta(\infty;t)=b^{-1}[\exp(b\,t)-1]\quad \text{if}\ \ a=1 \tag{59b}$$

(see (40) with (39)), and likewise the function characterizing the behavior of the solutions of the *isochronous* version (36) (as reported at the end of Sec. I) is $\beta(\alpha;\tau)$ with τ defined by (11) (of course τ reduces to t when ω vanishes, namely when the model (36) reduces to (35)). We leave to the alert reader the amusing task to analyze the various behaviors that may emerge, depending on the values of the constants a (hence α, see (17)) and ω and on the initial data. The more interesting case to consider is of course that characterized by all the variables, and the constants (with the possible exception of ω) being *complex*—also in view of the interpretation of the corresponding motions as taking place in the real horizontal plane. The remarks reported at the end of Sec. I provide a useful hint; the following, completely explicit, solution of the model (35) (immediately extendable to the *isochronous* model (36) via the replacement of t with τ, see (11)) in the $N=2$ case,

$$z_{1,2}(t)=\tfrac{1}{2}\{z_1(0)+z_2(0)-\beta(\alpha;t)\,[\dot z_1(0)+\dot z_2(0)]$$
$$\pm[\{z_1(0)-z_2(0)-\beta(\alpha;t)\,[\dot z_1(0)-\dot z_2(0)]\}^2+4\,[\beta(\alpha;t)]^2\,\dot z_1(0)\,\dot z_2(0)]^{1/2}\} \quad (60)$$

may be useful to explore what tipically happens. But such an analysis is likely to be enlightening (perhaps even amusing) only if it is actually done rather than just read, so we provide no further elaboration here.

Finally let us show how the generalized goldfish model (35) can be reduced back to the standard goldfish model (3). To this end we rewrite (35) as follows:

$$\ddot z_n=2\sum_{m=1,m\neq n}^{N}\frac{\dot z_n\,\dot z_m}{z_n-z_m}+a\,\dot z_n\,r, \quad (61a)$$

with

$$r\equiv r(t)=\sum_{n=1}^{N}\frac{\dot z_n(t)}{z_n(t)}. \quad (61b)$$

Time-differentiation of this formula yields

$$\dot r\equiv\sum_{n=1}^{N}\left[\frac{\ddot z_n}{z_n}-\left(\frac{\dot z_n}{z_n}\right)^2\right], \quad (62a)$$

$$\dot r\equiv a\,r^2-\sum_{n=1}^{N}\left(\frac{\dot z_n}{z_n}\right)^2+2\sum_{n,m=1;m\neq n}^{N}\frac{\dot z_n\,\dot z_m}{(z_n-z_m)\,z_n}, \quad (62b)$$

$$\dot r\equiv a\,r^2-\sum_{n=1}^{N}\left(\frac{\dot z_n}{z_n}\right)^2+\sum_{n,m=1;m\neq n}^{N}\frac{\dot z_n\,\dot z_m}{(z_n-z_m)}\left(\frac{1}{z_n}-\frac{1}{z_m}\right), \quad (62c)$$

$$\dot r\equiv a\,r^2-\sum_{n=1}^{N}\left(\frac{\dot z_n}{z_n}\right)^2-\sum_{n,m=1;m\neq n}^{N}\frac{\dot z_n\,\dot z_m}{z_n\,z_m}, \quad (62d)$$

$$\dot r\equiv(a-1)\,r^2 \quad (62e)$$

(to go from (62a) to (62b) we used (61); from (62b) to (62c), the possibility to exchange the indices m and n; and the next two steps are, we trust, pretty obvious, see (61b)). From the last equation, (62e), we immediately infer (see (61b) and (39), entailing $r(0)=b$)

$$r(t)=\frac{b}{1+(1-a)\,b\,t}. \quad (63)$$

Hence the equations of motion of the generalized goldfish model, see (35) or equivalently (61), can be recast in the following form:

$$\ddot z_n-\frac{a\,b\,\dot z_n}{1+(1-a)\,b\,t}=2\sum_{m=1,m\neq n}^{N}\frac{\dot z_n\,\dot z_m}{z_n-z_m}. \quad (64)$$

And it is now easy to check that via the change of dependent variables

$$z_n(t)=\zeta_n(\tau),\quad \tau=\beta(\alpha;t) \quad (65)$$

with $\beta(\alpha;t)$ defined precisely as above, see (59), one gets for $\zeta_n(\tau)$ just the equations of motion of the standard goldfish model, see (9). (Note moreover that this change of variables, (65) with (59), implies $z_n(0)=\zeta_n(0)$, $\dot{z}_n(0)=\zeta_n'(0)$.) This result provides of course another route to obtain the findings reported above for the generalized goldfish model (35) (see the last paragraph of Sec. II); or one can use the equivalent, but perhaps neater, version[11,15] of the solution of the goldfish model (9) according to which the coordinates $\zeta_n(\tau)$ coincide with the N roots of the following algebraic equation in ζ:

$$\sum_{n=1}^{N} \frac{\zeta_n'(0)}{\zeta-\zeta_n(0)} = \frac{1}{\tau}, \tag{66}$$

which implies via (65), for the generalized goldfish model (35), that the coordinates $z_n(t)$ coincide with the N roots of the following algebraic equation in z:

$$\sum_{n=1}^{N} \frac{\dot{z}_n(0)}{z-z_n(0)} = \frac{1}{\beta(\alpha;t)}, \tag{67}$$

with $\beta(\alpha;t)$ given by (59) with (39); as well as the corresponding result for the *isochronous* generalized goldfish model (36) reported at the end of Sec. I.

IV. OUTLOOK

Clearly the approach described in this paper can be applied more generally, by taking other matrix evolution equations than (44) as point of departure; this will be done in separate papers (for instance, the findings obtained by replacing (44) with the solvable matrix equation

$$\ddot{U}+a\,\dot{U}+bU=0 \tag{68}$$

are reviewed in a joint paper with Jean–Pierre Françoise;[19] and several other solvable matrix evolution equations are under consideration jointly with Mario Bruschi[8]).

Finally let us note that in this paper we focussed on many-body problems defined by *Newtonian* equations of motions (possibly with additional auxiliary variables); we did not discuss the possibility that these equations be embeddable in a *Hamiltonian* (or perhaps in a *quasi-Hamiltonian*[29]) formalism, nor the (possibly related) possibility to ascribe a ''physical'' meaning (possibly as ''spin'' degrees of fredom associated with Euler angles[32]) to the auxiliary variables. Such reformulations open the way to the investigation of these models in a quantal context. These remain as tasks for the future.

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Symmetry classification of KdV-type nonlinear evolution equations

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Group classification of a class of third-order nonlinear evolution equations generalizing KdV and mKdV equations is performed. It is shown that there are two equations admitting simple Lie algebras of dimension three. Next, we prove that there exist only four equations invariant with respect to Lie algebras having nontrivial Levi factors of dimension four and six. Our analysis shows that there are no equations invariant under algebras which are semi-direct sums of Levi factor and radical. Making use of these results we prove that there are three, nine, thirty-eight, fifty-two inequivalent KdV-type nonlinear evolution equations admitting one-, two-, three-, and four-dimensional solvable Lie algebras, respectively. Finally, we perform a complete group classification of the most general linear third-order evolution equation. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The purpose of this article is classifying equations of the form

$$u_t = u_{xxx} + F(x,t,u,u_x,u_{xx}), \tag{1.1}$$

which admit nontrivial Lie (point) symmetries. The standard Korteweg–de Vries (KdV) equation,

$$u_t = u_{xxx} + uu_x,$$

belongs to the family of evolution equations (1.1). Classification of the KdV equation with variable coefficients (vcKdV),

$$u_t = f(x,t)uu_x + g(x,t)u_{xxx}, \quad f \cdot g \neq 0, \tag{1.2}$$

by their symmetries is done in Ref. 1, where it is shown that the vcKdV can admit at most four-dimensional Lie point symmetry group and those having four-dimensional symmetry group can be transformed into the ordinary KdV equation by local point transformations. In Ref. 2, Eq. (1.2) is investigated from the point of view of its integrability. It is shown, in particular, that equations of the form (1.2) with a three-dimensional Lie point symmetry group have a property of ''partially integrability.''

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Our motivation is the same as for classifying vcKdV equations. We start with a rather general class of nonlinear equations generalizing (1.2) for $g_x=0$. Note that any t dependent coefficient of u_{xxx} in (1.1) can be normalized by a reparametrization of time. The main advantage of this classification is that, if we know that the equation under study admits a nontrivial symmetry group, then it is usually possible to apply the whole spectrum of the methods and algorithms of Lie group analysis. This enables us to derive exact analytical solutions of equations that, under study, reveal their integrability properties, find linearizing transformations, etc. Note that the connection between Lie point symmetries and integrability was discussed in Refs. 2, 3.

Recently, a novel generic approach to group classification of low-dimensional partial differential equations (PDEs) has been developed in Ref. 4. The full account of ideas and algorithms applied can be found in the review paper[5] where the approach in question has been applied to classify the most general second-order quasi-linear heat-conductivity equations admitting nontrivial Lie point symmetries. Here we adopt the same approach which basically consists of three steps. We first construct the equivalence group, namely, the most general group of point transformations that transform any equation of the form (1.1) to a (possibly different) equation belonging to the same class. Also, we find the most general element of the symmetry group together with a determining equation for F. As a second step, we realize low-dimensional Lie algebras by vector fields of the above form up to equivalence transformations. To this end, we use various results on the structure of abstract Lie algebras.[6–9] A review of the classification results of nonisomorphic finite-dimensional Lie algebras can be found in Ref. 5. In the last step, after transforming symmetry generators to canonical forms, we proceed to classifying equations that admit nontrivial symmetries. We do this by inserting these generators into the symmetry condition and solving for F.

Let us mention that similar ideas have been used by Winternitz and co-workers for the group classification of several nonlinear partial differential equations[1,10,11] and of discrete dynamical systems.[12–14] Note also that group classification of the nonlinear wave and Schrödinger equations in the same spirit has been done in Refs. 15, 16.

The paper is organized as follows. In Sec. II we present the determining equations for the symmetries and the equivalence group. Section III is devoted to the classification of the equations invariant under low-dimensional symmetry groups. In Sec. IV we perform a classification of linear equations in the class (1.1). A discussion of results and some conclusions are presented in the final section.

II. DETERMINING EQUATIONS AND EQUIVALENCE TRANSFORMATIONS

The Lie algebra of the symmetry group of Eq. (1.1) is realized by vector fields of the form

$$X=\tau(x,t,u)\partial_t+\xi(x,t,u)\partial_x+\phi(x,t,u)\partial_u\,. \tag{2.1}$$

In order to implement the symmetry algorithm we need to calculate the third order prolongation of the field vector field (2.1),[17–19]

$$\mathrm{pr}^{(3)}X=X+\phi^t\partial_{u_t}+\phi^x\partial_{u_x}+\phi^{xx}\partial_{u_{xx}}+\phi^{xxx}\partial_{u_{xxx}}, \tag{2.2}$$

where

$$\phi^t=D_t\phi-u_tD_t\tau-u_xD_t\xi,$$

$$\phi^x=D_x\phi-u_tD_x\tau-u_xD_x\xi,$$

$$\phi^{xx}=D_x\phi^x-u_{xt}D_x\tau-u_{xx}D_x\xi,$$

$$\phi^{xxx}=D_x\phi^{xx}-u_{xxt}D_x\tau-u_{xxx}D_x\xi.$$

Here D_x and D_t denote the total space and time derivatives. In order to find the coefficients of the vector field we require that the prolonged vector field (2.2) annihilate Eq. (1.1) on its solution manifold,

$$\mathrm{pr}^{(3)}X(\Delta)|_{\Delta=0}=0, \quad \Delta=u_t-u_{xxx}-F. \tag{2.3}$$

Equating coefficients of linearly independent terms of invariance criterion (2.3) to zero yields an overdetermined system of linear PDEs (called determining equations). Solving this system we obtain the following assertion.

Proposition 2.1: The symmetry group of the nonlinear equation (1.1) for an arbitrary (fixed) function F is generated by the vector field

$$X=\tau(t)\partial_t+\left(\frac{\dot\tau}{3}x+\rho(t)\right)\partial_x+\phi(x,t,u)\partial_u, \tag{2.4}$$

where the functions $\tau(t)$, $\rho(t)$ and $\phi(x,t,u)$ satisfy the determining equation

$$\begin{aligned}&-3\,u_x\dot\rho-x\,u_x\ddot\tau-9\,u_x\,u_{xx}\,\phi_{uu}-3\,u_x^3\,\phi_{uuu}+3\,\phi_t-9\,u_{xx}\,\phi_{xu}-9\,u_x^2\,\phi_{xuu}-9\,u_x\,\phi_{xxu}-3\,\phi_{xxx}\\&\quad+3(\phi_u-\dot\tau)\,F+(2\,u_{xx}\,\dot\tau-3\,u_{xx}\,\phi_u-3\,u_x^2\,\phi_{uu}-6\,u_x\,\phi_{xu}-3\,\phi_{xx})\,F_{u_{xx}}\\&\quad+(u_x\,\dot\tau-3\,u_x\,\phi_u-3\,\phi_x)\,F_{u_x}-3\,\phi\,F_u-3\,\tau F_t-(3\,\rho+x\,\dot\tau)\,F_x=0.\end{aligned} \tag{2.5}$$

Here the dot over a symbol stands for the time derivative.

If there are no restrictions on F, then (2.5) should be satisfied identically, which is possible only when the symmetry group is a trivial group of identity transformations. Here we shall be concerned with the identification of all specific forms of F for which nontrivial symmetry groups occur. The basic idea is to utilize the fact that for an arbitrarily fixed function F all admissible vector fields form a Lie algebra. This immediately implies the idea of using the classical results on the classification of low-dimensional Lie algebras obtained mostly in the late 1960s.[6–8] Saying it another way, we need to construct a kind of representation theory on low-dimensional Lie algebras generated by Lie vector fields preserving the manifold (2.5).

Our classification is up to equivalence under a group of locally invertible point transformations,

$$\tilde t=T(x,t,u), \quad \tilde x=Y(x,t,u), \quad \tilde u=U(x,t,u), \tag{2.6}$$

that preserve the form of the equation (1.1), but (possibly) change function F into a new one, namely, we have

$$\tilde u_{\tilde t}=\tilde u_{\tilde x\tilde x\tilde x}+\tilde F(\tilde x,\tilde t,\tilde u,\tilde u_{\tilde x},\tilde u_{\tilde x\tilde x}). \tag{2.7}$$

Inserting (2.6) into (1.1) and requiring that the form of the equation be preserved, we arrive at the following assertion.

Proposition 2.2: The maximal equivalence group $\mathcal{E}$ has the form

$$\tilde t=T(t), \quad \tilde x=\dot T^{1/3}x+Y(t), \quad \tilde u=U(x,t,u), \tag{2.8}$$

where $\dot T\neq 0$, $U_u\neq 0$.

We note that the Lie infinitesimal technique can also be used to obtain the equivalence group (2.8). It is straightforward to prove that both approaches produce the same results.

We make use of equivalence transformations (2.8) to transform vector field X into a convenient (canonical) form.

Proposition 2.3: Vector field (2.4) *is equivalent within a point transformation of the form* (2.6) *to one of the following vector fields:*

$$X=\partial_t, \quad X=\partial_x, \quad X=\partial_u. \tag{2.9}$$

Proof: Transformation (2.8) transforms vector field (2.4) into

$$X\to\tilde{X}=\tau(t)\dot{T}(t)\partial_{\tilde{t}}+[\tfrac{1}{3}(\tau\dot{T}^{-1}\ddot{T}+\dot{\tau})(\tilde{x}-Y)+\tau\dot{Y}+\rho\dot{T}^{1/3}]\partial_{\tilde{x}}$$
$$+[\tau U_t+(\tfrac{1}{3}\dot{\tau}x+\rho)U_x+\phi U_u]\partial_{\tilde{u}}. \tag{2.10}$$

There are two cases to consider.

(I) $\phi=0$. Choose $U=U(u)$ so that we have

$$\tilde{X}=\tau(t)\dot{T}(t)\partial_{\tilde{t}}+[\tfrac{1}{3}(\tau\dot{T}^{-1}\ddot{T}+\dot{\tau})(\tilde{x}-Y)+\tau\dot{Y}+\rho\dot{T}^{1/3}]\partial_{\tilde{x}}+\phi U_u\partial_{\tilde{u}}. \tag{2.11}$$

Now if $\tau=0$, then $\rho\neq 0$ (otherwise X would be zero), and we choose $T(t)$ to satisfy

$$\dot{T}=\rho^{-3}.$$

In this case $\tilde{X}$ is transformed into $\partial_{\tilde{x}}$.

If $\tau\neq 0$, then we choose T and Y to satisfy

$$\dot{T}=\tau^{-1}, \quad \tau\dot{Y}+\rho\dot{T}^{1/3}=0.$$

With this choice of T and Y vector field $\tilde{X}$ is transformed into $\partial_{\tilde{t}}$.

(II) $\phi\neq 0$. If $\tau=\rho=0$ then we can choose U to satisfy $\phi U_u=1$ so that we have $\tilde{X}=\partial_{\tilde{u}}$. Otherwise, U can be chosen to satisfy

$$\tau U_t+(\tfrac{1}{3}\dot{\tau}x+\rho)U_x+\phi U_u=0.$$

Hence we recover Case I.

Summing up, the vector field (2.4) is equivalent, up to equivalence under $\mathcal{E}$, to one of the three standard vector fields $\partial_x,\partial_t,\partial_u$. This completes the proof.

III. GROUP CLASSIFICATION OF LINEAR EQUATIONS

To the best of our knowledge no group classification of the most general linear third-order PDE appears in the literature. So we devote this section to the group classification of third-order PDEs:

$$u_t=f_1(x,t)u_{xxx}+f_2(x,t)u_{xx}+f_3(x,t)u_x+f_4(x,t)u+f_5(x,t). \tag{3.1}$$

If we perform the local change of variables $(x,t,u)\to(\tilde{x},\tilde{t},\tilde{u})$ preserving the form of (3.1),

$$\tilde{t}=t, \quad \tilde{x}=F(x,t), \quad u=V(x,t)v(\tilde{x},\tilde{t})+G(x,t), \quad V\neq 0,\ F_x\neq 0, \tag{3.2}$$

we obtain

$$v_{\tilde{t}}=f_1F_x^3v_{\tilde{x}\tilde{x}\tilde{x}}+\{3f_1V^{-1}[V_xF_x^2+VF_xF_{xx}]+f_2F_x^2\}v_{\tilde{x}\tilde{x}}+\{f_1V^{-1}[3V_{xx}F_x+3V_xF_{xx}+VF_{xxx}]$$
$$+f_2V^{-1}[2V_xF_x+Vf_{xx}]+f_3F_x-F_t\}v_{\tilde{x}}+\{f_1V^{-1}V_{xxx}+f_2V^{-1}V_{xx}+f_3V^{-1}V_x+f_4-V^{-1}V_t\}v$$
$$+V^{-1}[f_1G_{xxx}+f_2G_{xx}+f_3G_x+f_4G+f_5-G_t].$$

Now we choose the functions F,V, and G in (3.2) to satisfy constraints,

$$f_1F_x^3=1,$$

$$G_t=f_1G_{xxx}+f_2G_{xx}+f_3G_x+f_4G+f_5,$$

$$3f_1F_x^2V_x+[3f_1F_xF_{xx}+f_2F_x^2]V=0,$$

and thus normalize $f_1(x,t)\to 1$, and set $f_2(x,t)\to 0$, $f_5(x,t)\to 0$.

Thus (3.1) reduces to the following particular form:

$$u_t=u_{xxx}+A(x,t)u_x+B(x,t)u. \tag{3.3}$$

Here A,B are arbitrary smooth functions of x and t.

The most general equivalence transformation preserving the class of equations (3.3), which is a subset of (2.8), reads as

$$\tilde{t}=T(t),\quad \tilde{x}=\dot{T}^{1/3}x+Y(t),\quad \tilde{u}=V(t)u, \tag{3.4}$$

with $\dot{T}\neq 0$, $V\neq 0$.

Performing change of variables (3.4) transforms Eq. (3.3) to become

$$\tilde{u}_{\tilde{t}}=\tilde{u}_{\tilde{x}\tilde{x}\tilde{x}}+\tilde{A}\tilde{u}_{\tilde{x}}+\tilde{B}\tilde{u}, \tag{3.5}$$

where the coefficients $\tilde{A},\tilde{B}$ are expressed in terms of the functions A,B and their derivatives as follows:

$$\begin{aligned}\tilde{A}&=\dot{T}^{-1}(A\dot{T}^{1/3}-\tfrac{1}{3}\ddot{T}\dot{T}^{-2/3}x-\dot{Y}),\\ \tilde{B}&=\dot{T}^{-1}(B+V^{-1}\dot{V}).\end{aligned} \tag{3.6}$$

As Eq. (3.3) is linear, it admits trivial infinite-parameter group having the generator

$$X(\beta)=\beta(x,t)\partial_u,\quad \beta_t=\beta_{xxx}+A\beta_x+B\beta,$$

and the one-parameter group generated by the operator $u\partial_u$. These symmetries give no nontrivial information about the solution structure of the equation under study and therefore are neglected in the sequel.

The nontrivial invariance group of Eq. (3.3) is generated by operators of the form

$$X=\tau(t)\partial_t+(\tfrac{1}{3}\dot{\tau}x+\rho(t))\partial_x+\alpha(t)u\partial_u, \tag{3.7}$$

functions τ,ρ,α,A and B satisfying equations

$$\begin{aligned}&3\dot{\alpha}-3B\dot{\tau}-3\tau B_t-B_x(3\rho+x\dot{\tau})=0,\\ &-3\dot{\rho}-x\ddot{\tau}-2A\dot{\tau}-3\tau A_t-A_x(3\rho+x\dot{\tau})=0.\end{aligned} \tag{3.8}$$

Provided $A=A(x,t)$, $B=B(x,t)$ are arbitrary functions, $\tau=\rho=0$, $\dot{\alpha}=0$. So in this case Eq. (3.3) admits trivial symmetries only.

Transformation (3.4) leaves operator $X_1=u\partial_u$ invariant while transforming operator (3.5) to become

$$X\overset{(3.4)}{\to}\tilde{X}=\tau\dot{T}\partial_{\tilde{t}}+[\tau(\tfrac{1}{3}\ddot{T}\dot{T}^{-2/3}x+\dot{Y})+\dot{T}^{1/3}(\tfrac{1}{3}\dot{\tau}x+\rho)]\partial_{\tilde{x}}+(\tau\dot{V}+\alpha V)u\partial_{\tilde{u}}. \tag{3.9}$$

That is why, if $\tau\neq 0$ in (3.7), then putting

$$\dot{T}=\tau^{-1},\quad Y=-\int^{t}\rho(\xi)\tau^{-4/3}(\xi)d\xi,$$

and taking V as a nonzero solution of the equation

$$\tau\dot{V}+\alpha V=0,$$

in (3.4) transforms (3.9) to the canonical form of the generator of time displacements

$$\widetilde{X}=\partial_{\tilde{t}}.$$

Next, if $\tau=0$, $\rho\neq 0$ in (3.7), then putting $\dot{T}=\rho^{-3}$ in (3.4) yields the operator

$$\widetilde{X}=\partial_{\tilde{x}}+\alpha\tilde{u}\partial_{\tilde{u}}.$$

Finally, if $\tau=\rho=0$, $\dot{\alpha}\neq 0$ in (3.7), we put $T=\alpha$ in (3.4) thus getting the operator

$$\widetilde{X}=\tilde{t}\tilde{u}\partial_{\tilde{u}}.$$

Taking into account the above considerations, we see that there are transformations (3.4), that transform operator (3.7) to one of the following inequivalent forms:

$$\partial_t,\quad \partial_x,\quad \partial_x+f(t)u\partial_u\ \ (\dot{f}\neq 0),\quad tu\partial_u.$$

In what follows, we analyze each of the above operators separately.

Operator $X_1=\partial_t$. The system of determining Eqs. (3.8) for this operator reads as

$$B_t=A_t=0,$$

whence it follows that $A=A(x)$, $B=B(x)$. Inserting these functions into (3.8) yields

$$3\dot{\alpha}-3B\dot{\tau}-B_x(3\rho+x\dot{\tau})=0,$$

$$-3\dot{\rho}-x\ddot{\tau}-2A\dot{\tau}-A_x(3\rho+x\dot{\tau})=0.$$

Analyzing the above system of ordinary differential equations shows that for the case under consideration Eq. (3.3) admits an invariance group whose dimension is higher than one if and only if the following occurs.

(1) $A=mx^{-2}$, $B=nx^{-3}$, $|m|+|n|\neq 0$ with the additional symmetry operator $t\partial_t+\frac{1}{3}x\partial_x$;
(2) $A=0$, $B=\varepsilon x$ $(\varepsilon=\pm 1)$ with the additional symmetry operator $\partial_t+\varepsilon tu\partial_u$;
(3) $A=B\equiv 0$ with the additional symmetry operators $\partial_x, t\partial_t+\frac{1}{3}x\partial_x$.

Operator $X_2=\partial_x$. If Eq. (3.3) is invariant under X_2, then $A=A(t)$, $B=B(t)$. What is more, it follows from (3.6) that there are transformations (3.4), which reduce equation (3.3) to the form (3.5) with $\tilde{A}=\tilde{B}\equiv 0$. So we arrive at the already known case.

Operator $X_3=\partial_x+f(t)u\partial_u$ $(\dot{f}\neq 0)$. If Eq. (3.3) admits operator X_3, then we have $A=0$, $B=\dot{f}x$. Inserting these expressions into (3.8) yields

$$\dot{\rho}=0,\quad \ddot{\tau}=0,\quad \dot{\alpha}=\rho\dot{f},$$
$$3\tau\ddot{f}+4\dot{\tau}\dot{f}=0. \tag{3.10}$$

From the first three equations it follows that $\rho=C_1$, $\tau=C_2t+C_3$, $\alpha=C_1f+C_4$, $C_1,C_2,C_3,C_4\in\mathbb{R}$. Hence we conclude that the last equation of system (3.10) takes the form

TABLE I. Symmetry classification of 3.3.

N	A	B	Symmetry operators
1	$A(x)$	$B(x)$	∂_t
2	0	$\dot{f}(t)x$	$\partial_x+f(t)u\partial_u$, $\dot{f}\neq 0$
3	mx^{-2}, $m\in\mathbb{R}$	nx^{-3}, $n\in\mathbb{R}$, $\lvert m\rvert+\lvert n\rvert\neq 0$	$\partial_t, t\partial_t+\frac{1}{3}x\partial_x$
4	0	εx, $\varepsilon=\pm 1$	$\partial_t, \partial_x+\varepsilon tu\partial_u$
5	0	$-mt^{-4/3}x$, $m\in\mathbb{R}$, $m\neq 0$	$\partial_x+3mt^{-1/3}u\partial_u$, $t\partial_t+\frac{1}{3}x\partial_x$
6	$a\in\mathbb{R}$	0	$\partial_t, \partial_x, t\partial_t+\frac{1}{3}(x-2at)\partial_x$

$$3(C_2t+C_3)\ddot{f}+4C_2\dot{f}=0.$$

Analyzing this equation we see that extension of the symmetry algebra of Eq. (3.3) with $A=0$, $B=\dot{f}x$ is only possible when

$$f=3mt^{-1/3},\quad m\neq 0;$$

$$f=\varepsilon t,\quad \varepsilon=\pm 1.$$

The second case has already been considered. In the first case the basis of nontrivial invariance algebra is formed by the operators $\partial_x+3mt^{-1/3}u\partial_u$, $t\partial_t+\frac{1}{3}x\partial_x$.

Operator $X_4=tu\partial_u$. Inserting the coefficients of this operator into (3.8) leads to the contradiction $3=0$, whence it follows that the operator X_4 cannot be a symmetry operator of Eq. (3.3).

We summarize the above classification results of in Table I, where we give the forms of the functions A and B and basis operators of the nontrivial symmetry algebras of the corresponding equations (3.3).

So the equation $u_t=u_{xxx}$ has the highest symmetry within the class of equations (3.3). Its maximal finite-dimensional symmetry algebra is four-dimensional.

Note that according to Ref. 5 the class of nonlinear equations of the form

$$u_t=F(t,x,u,u_x)u_{xx}+G(t,x,u,u_x),\quad F\neq 0, \tag{3.11}$$

contains five nonlinear equations admitting five-dimensional symmetry algebras. Furthermore, an equation admitting six-dimensional symmetry algebra is equivalent to the heat equation. It is the linear heat conductivity equation $u_t=u_{xx}$ that possess the largest symmetry group within the class of second-order equations (3.11).

This is not the case for the class of third-order PDEs under consideration in the present paper. We shall see that there are examples of nonlinear equations that admits higher symmetry algebras than does the linear equation. For instance, the nonlinear Schwarzian KdV equation (4.14) admits a six-dimensional symmetry algebra.

IV. CLASSIFICATION OF EQUATIONS INVARIANT UNDER SEMI-SIMPLE ALGEBRAS AND ALGEBRAS HAVING NONTRIVIAL LEVI DECOMPOSITIONS

In order to describe equations (1.1) that admit Lie algebras isomorphic to the Lie algebras having nontrivial Levi decomposition, we need, first of all, to describe equations whose invariance algebras are semi-simple.

The lowest order semi-simple Lie algebras are isomorphic to one of the following three-dimensional algebras:

$$\mathrm{sl}(2,\mathbb{R}):[X_1,X_3]=-2X_2,\quad [X_1,X_2]=X_1,\quad [X_2,X_3]=X_3;$$

$$\mathrm{so}(3):[X_1,X_2]=X_3,\quad [X_2,X_3]=X_1,\quad [X_3,X_1]=X_2.$$

Taking into account our preliminary classification we conclude that one of the basis operators reduces to one of the canonical forms $\partial_t,\partial_x,\partial_u$.

First, we study realizations of the algebra so(3) within the class of operators (2.4).

Let $X_1=\partial_t$ and let the operators X_2,X_3 be of the form (2.4). Checking commutation relations $[X_1,X_2]=X_3,[X_3,X_1]=X_2$ we see that

$$X_2=3\alpha\cos t\partial_t+[-\alpha x\sin t+\beta\cos(t+\gamma)]\partial_x+\varphi(x,u)\cos(t+\psi(x,u))\partial_u,$$

$$X_3=-3\alpha\sin t\partial_t-[\alpha x\cos t+\beta\sin(t+\gamma)]\partial_x-\varphi(x,u)\sin(t+\psi(x,u))\partial_u.$$

Here α, β, γ are arbitrary real constants and φ, ψ are arbitrary real-valued smooth functions.

The third commutation relation $[X_2,X_3]=X_1$ implies that $9\alpha^2=-1$. As this equation has no real solutions, there are no realizations of so(3) with $X_1=\partial_t$.

The same assertion holds for the cases when $X_1=\partial_x$ and $X_1=\partial_u$. So the class of operators (2.4) contains no realizations of the algebra so(3). This means that there are no so(3)-invariant equations of the form (1.1).

Theorem 4.1: *There exist no realizations of the algebra* so(3) *in terms of vector fields* (2.4). *Hence no equation of the form* (1.1) *is invariant under* so(3) *algebra.*

Similar reasoning yields that there are three inequivalent realizations of the algebra $\mathrm{sl}(2,\mathbb{R})$ by operators of the form (2.4),

$$\{\partial_t,t\partial_t+\tfrac{1}{3}x\partial_x,-t^2\partial_t-\tfrac{2}{3}tx\partial_x\},$$

$$\{\partial_t,t\partial_t+\tfrac{1}{3}x\partial_x,-t^2\partial_t-\tfrac{2}{3}tx\partial_x-x^3\partial_u\},$$

$$\{\partial_u,u\partial_u,-u^2\partial_u\}.$$

Inserting the coefficients of basis operators of the first realization of the algebra $\mathrm{sl}(2,\mathbb{R})$ into invariance criterion yields the following classifying equations:

$$2u_{xx}F_{u_{xx}}+u_xF_{u_x}-xF_x-3F=0,$$

$$t(2u_{xx}F_{u_{xx}}+u_xF_{u_x}-xF_x-3F)-xu_x=0,$$

from which we get the equation $xu_x=0$. Consequently, the realization in question cannot be invariance algebra of the equation under study.

The two remaining realizations of $\mathrm{sl}(2,\mathbb{R})$ do yield invariance algebras of equation (1.1). The forms of the function F in the corresponding invariant equations read as

$$\{\partial_t,t\partial_t+\tfrac{1}{3}x\partial_x,-t^2\partial_t-\tfrac{2}{3}tx\partial_x-x^3\partial_u\}\quad:\quad F=-x^{-3}[2xu_x+\tfrac{1}{9}x^2u_x^2-G(\omega_1,\omega_2)],$$

$$\omega_1=3u-xu_x,\quad \omega_2=6u-x^2u_{xx};$$

$$\{\partial_u,u\partial_u,-u^2\partial_u\}\quad:\quad F=-\tfrac{3}{2}u_x^{-1}u_{xx}^2+u_xG(x,t).$$

As any semi-simple or simple algebra contains either so(3) or $\mathrm{sl}(2,\mathbb{R})$ (or both) as subalgebra(s),[20] the above result can be utilized to perform the classification of equations (1.1) admitting invariance algebras isomorphic to one having a nontrivial Levi decomposition.

First we turn to the equation

$$u_t = u_{xxx} - \tfrac{3}{2}u_x^{-1}u_{xx}^2 + u_x G(x,t). \tag{4.1}$$

Applying the Lie infinitesimal algorithm we see that the maximal invariance algebra of Eq. (4.1) is spanned by the operators $X_1=\partial_u$, $X_2=u\partial_u$, $X_3=-u^2\partial_u$, and

$$X_4=\tau(t)\partial_t+(\tfrac{1}{3}\dot{\tau}x+\rho(t))\partial_x, \tag{4.2}$$

functions τ, ρ and G satisfying the equation

$$(x\dot{\tau}+3\rho)G_x+3\tau G_t+2\dot{\tau}G+x\ddot{\tau}+3\dot{\rho}=0. \tag{4.3}$$

By direct verification we ensure that the form of basis operators of the realization of $\mathrm{sl}(2,\mathbb{R})$ under study is not altered by the transformations

$$\tilde{t}=T(t),\ \ \tilde{x}=\dot{T}^{1/3}x+Y(t),\ \ \tilde{u}=\gamma u,\ \ \dot{T}\neq 0,\ \ \gamma\neq 0. \tag{4.4}$$

As transformation (4.4) reduces (4.2) to the form

$$X_4 \overset{(4.4)}{\to} \tilde{X}_4=\tau(t)\dot{T}(t)\partial_{\tilde{t}}+[\tfrac{1}{3}(\tau\dot{T}^{-1}\ddot{T}+\tau)(\tilde{x}-Y)+\tau\dot{Y}+\rho\dot{T}^{1/3}]\partial_{\tilde{x}},$$

we can put $X_4=\partial_t$ or $X_4=\partial_x$ within the equivalence relation.

Provided $X_4=\partial_t$, it follows from (4.3) that $G=\tilde{G}(x)$ in (4.1). Next, if $X_4=\partial_x$, then necessarily $G=\tilde{G}(t)$. Consequently, the class of Eqs. (4.1) contains two inequivalent equations:

$$u_t=u_{xxx}-\tfrac{3}{2}u_x^{-1}u_{xx}^2+u_x\tilde{G}(x) \tag{4.5}$$

and

$$u_t=u_{xxx}-\tfrac{3}{2}u_x^{-1}u_{xx}^2+u_x\tilde{G}(t), \tag{4.6}$$

which are invariant under extensions of the algebra $\mathrm{sl}(2,\mathbb{R})$. Namely, they admit algebras $\mathrm{sl}(2,\mathbb{R})\oplus\{\partial_t\}$ and $\mathrm{sl}(2,\mathbb{R})\oplus\{\partial_x\}$, correspondingly. What is more, if the function $\tilde{G}=\tilde{G}(x)$ in (4.5) is arbitrary, the given algebra is maximal (in Lie sense) invariance algebra of Eq. (4.5).

Equation (4.6) is reduced to PDE (4.5) with $\tilde{G}(x)=0$ with the help of the change of variables,

$$\tilde{t}=t,\ \ \tilde{x}=x+\int^t \tilde{G}(\xi)\ \ d\xi,\ \ u=v(\tilde{x},\tilde{t}).$$

Therefore, we can restrict our further considerations to Eq. (4.5), where we need to differentiate between the cases $\tilde{G}=0$ and $\tilde{G}\neq 0$.

Classifying Eq. (4.3) with $G=\tilde{G}(x)$ reads as

$$(x\dot{\tau}+3\rho)\tilde{G}_x+2\dot{\tau}\tilde{G}+x\ddot{\tau}+3\dot{\rho}=0.$$

Hence it follows that there are two cases providing for extension of the symmetry algebra. Namely, the case when $\tilde{G}=0$, which gives rise to two additional symmetry operators $X_5=t\partial_t+\frac{1}{3}x\partial_x$ and $X_6=\partial_x$. Another case of the extension of symmetry of Eq. (4.5) is when $\tilde{G}=\lambda x^{-2}$ $(\lambda\neq 0)$. If this is the case, (4.5) admits the additional operator $X_5=t\partial_t+\frac{1}{3}x\partial_x$.

Now we turn to the equation

$$u_t = u_{xxx} - 2x^{-2}u_x - \tfrac{1}{9}x^{-1}u_x^2 + x^{-3}G(\omega_1,\omega_2),$$
$$\omega_1 = 3u - xu_x, \quad \omega_2 = 6u - x^2u_{xx}. \tag{4.7}$$

First of all, we ensure that the class of PDEs (4.7) does not contain equations whose invariance algebras possess semi-simple subalgebras of the dimension $n>3$.

It is common knowledge[20] that there are four types of abstract simple Lie algebras over the field of real numbers:

- The type A_{n-1} $(n>1)$ contains four real forms of the algebras $\mathrm{sl}(n,\mathbb{C})$: $\mathrm{su}(n)$, $\mathrm{sl}(n,\mathbb{R})$, $\mathrm{su}(p,q)$ $(p+q=n, p\geqslant q)$, $\mathrm{su}^*(2n)$.
- The type B_n $(n>1)$ contains two real forms of the algebra $\mathrm{so}(2n+1,\mathbb{C})$: $\mathrm{so}(2n+1)$, $\mathrm{so}(p,q)$ $(p+q=2n+1, p>q)$.
- The type C_n $(n\geqslant 1)$ contains three real forms of the algebra $\mathrm{sp}(n,\mathbb{C})$: $\mathrm{sp}(n)$, $\mathrm{sp}(n,\mathbb{R})$, $\mathrm{sp}(p,q)$ $(p+q=n, p\geqslant q)$.
- The type D_n $(n>1)$ contains three real forms of the algebra $\mathrm{so}(2n,\mathbb{C})$: $\mathrm{so}(2n)$, $\mathrm{so}(p,q)$ $(p+q=2n,\ p\geqslant q)$, $\mathrm{so}^*(2n)$.

The lowest order classical semi-simple Lie algebras are three-dimensional. The next admissible dimension for classical semi-simple Lie algebras is six. There are four nonisomorphic semi-simple Lie algebras: so(4), so(3,1), so(2,2) and so*(4). As $\mathrm{so}(4)=\mathrm{so}(3)\oplus\mathrm{so}(3)$, $\mathrm{so}^*(4)\sim\mathrm{so}(3)\oplus\mathrm{sl}(2,\mathbb{R})$, and the algebra so(3,1) contains so(3) as a subalgebra, the algebra so(2,2) is the only possible six-dimensional semi-simple algebra that might be invariance algebra of Eq. (4.7). Taking into account that $\mathrm{so}(2,2)\sim\mathrm{sl}(2,\mathbb{R})\oplus\mathrm{sl}(2,\mathbb{R})$ and choosing $\mathrm{so}(2,2)=\{X_1,X_2,X_3\}\oplus\{\tilde{X}_1,\tilde{X}_2,\tilde{X}_3\}$, where X_1,X_2,X_3 form a basis of $\mathrm{sl}(2,\mathbb{R})$, which is invariance algebra of (4.7) and $\tilde{X}_1,\tilde{X}_2,\tilde{X}_3$ are of the form (2.4), we require the commutation relations

$$[X_i,\tilde{X}_j]=0 \quad (i,j=1,2,3)$$

to hold, whence

$$\tilde{X}_j=\lambda_j\partial_u \quad (j=1,2,3),$$

where λ_j are arbitrary real constants. Hence we conclude that the class of operators (2.4) does not contain a realization of so(2,2).

The same result holds for eight-dimensional semi-simple Lie algebras $\mathrm{sl}(3,\mathbb{R})$, su(3), su(2,1).

As $\mathrm{su}^*(4)\sim\mathrm{so}(5,1)$ and the algebra so(5,1) contains so(4) as a subalgebra, the class of operators (2.4) contains no realizations of A_n and D_n $(n>1)$ type algebras that are inequivalent to the algebra $\mathrm{sl}(2,\mathbb{R})$.

The same assertion holds true for B_n $(n>1)$ and C_n $(n\geqslant 1)$ type Lie algebras. Indeed, B_2 type algebras contain so(4) and so(3,1) and what is more,

$$\mathrm{sp}(2,\mathbb{R})\sim\mathrm{so}(3,2)\supset\mathrm{so}(3,1), \quad \mathrm{sp}(1,1)\sim\mathrm{so}(4,1)\supset\mathrm{so}(4), \quad \mathrm{sp}(2)\sim\mathrm{so}(5)\supset\mathrm{so}(4).$$

What remains to be done is to consider the exceptional semi-simple Lie algebras that belong to one of the following five types:[20] G_1,F_4,E_6,E_7,E_8. We consider in some detail G_1 type Lie algebras.

The type G_1 contains one compact real form g_2 and one noncompact real form g_2'. As $g_2\cap g_2'\sim\mathrm{su}(2)\oplus\mathrm{su}(2)\sim\mathrm{so}(4)$ and the algebra so(4) has no realization within the class of operators (2.4), the latter contains no realizations of type G_1.

Summing up, we conclude that class of PDEs (4.7) contains no equations, whose invariance algebras are isomorphic to n-dimensional semi-simple Lie algebras (or contains the latter as subalgebras) under $n>3$.

Consider now Eqs. (4.7), whose invariance algebras has nontrivial Levi factor. First, we turn to equations which are invariant with respect to the Lie algebras that can be decomposed into a direct sum of semi-simple Levi factor and radical, $\mathrm{sl}(2,\mathbb{R})\oplus L$, L being a radical. To this end, we will study possible extensions of the algebra $\mathrm{sl}(2,\mathbb{R})$ by operators (2.4).

Let $\mathrm{sl}(2,\mathbb{R})=\{X_1,X_2,X_3\}$, where X_1,X_2,X_3, form a basis of the invariance algebra of Eq. (4.7). Then it follows from

$$[X_i,Y]=0 \quad (i=1,2,3),$$

Y being an operator of the form (2.4), that $Y=\lambda\partial_u$, $\lambda=\text{const}$. Hence L is the one-dimensional Lie algebra spanned by the operator ∂_u. For Eq. (4.7) to admit the algebra $\mathrm{sl}(2,\mathbb{R})\oplus\{\partial_u\}$, the equation

$$G_{\omega_1}+2G_{\omega_2}=0,$$

has to be satisfied, whence

$$G=\tilde{G}(\sigma), \quad \sigma=x^2u_{xx}-2xu_x.$$

Consequently, an equation of the form (4.7) admits invariance algebra which is the direct sum of semi-simple Levi factor and radical iff it reads as

$$u_t=u_{xxx}-2x^{-2}u_x-\tfrac{1}{9}x^{-1}u_x^2+x^{-3}\tilde{G}(\sigma), \quad \sigma=x^2u_{xx}-2xu_x. \tag{4.8}$$

As Eq. (4.8) contains an arbitrary function of one variable, we can perform direct group classification by a straightforward application of the Lie infinitesimal algorithm. The determining equation for coefficients of the infinitesimal symmetry operator are of the form

(a) $\phi_{uuu}=0$;

(b) $3\phi_{uu}\tilde{G}_\sigma+18\phi_{uu}+9x\phi_{xuu}+\tfrac{1}{3}(x^{-1}\rho-\phi_u)=0$;

(c) $6x^{-1}(\phi_{xu}+x^{-2}\rho)\tilde{G}_\sigma+9x^{-2}\sigma\phi_{uu}+3\rho_t+x\tau_{tt}+6x^{-1}(3\phi_{xu}+2x^{-2}\rho)$
$+9\phi_{xxu}-\tfrac{2}{3}x^{-1}\phi_x=0$;

(d) $[-3x^{-3}(\phi_u+2x^{-1}\rho)\sigma+6x^{-2}\phi_x-3x^{-1}\phi_{xx}]\tilde{G}_\sigma+3x^{-3}(\phi_u+3x^{-1}\rho)\tilde{G}-9x^{-2}\phi_{xu}\sigma$
$+3[\phi_t-\phi_{xxx}+2x^{-2}\phi_x]=0.$

It follows from (a) that

$$\phi=f(x,t)u^2+g(x,t)u+h(x,t), \tag{4.9}$$

where f,g,h are arbitrary smooth functions. Inserting (4.9) into (b) yields

$$6f\tilde{G}_\sigma+36f+18xf_x+\tfrac{1}{3}(x^{-1}\rho-g)-\tfrac{2}{3}fu=0.$$

Taking into account that functions $f,\rho,g,\tilde{G}$ do not depend on u, we get

$$f=0, \ g=x^{-1}\rho.$$

So that equation (c) reduces to

$$3\rho_t+x\tau_{tt}+12x^{-3}\rho+\tfrac{2}{3}x^{-3}\rho u-\tfrac{2}{3}x^{-1}h_x=0.$$

Hence it follows that

$$\rho=0,\ \ h=\tfrac{1}{2}x^3\tau_{tt}+\tilde{h}(t).$$

Finally, inserting the obtained expression for φ into equation (d) gives

$$\tau_{ttt}=0,\ \ \tilde{h}_t=0,$$

whence

$$\tau=C_1t^2+C_2t+C_3,$$

$$\tilde{h}=C_4.$$

Here C_1,C_2,C_3,C_4 are arbitrary (integration) constants.

Summing up, we conclude that the algebra $\mathrm{sl}(2,\mathbb{R})\oplus\{\partial_u\}$ is the maximal invariance algebra admitted by Eq. (4.8). It cannot be extended by specifying the form of an arbitrary function $\tilde{G}(\sigma),\sigma=x^2u_{xx}-2xu_x$.

What remains to be done is classifying Eqs. (4.7), whose invariance algebras are isomorphic to *semi-direct* sums of a semi-simple Levi factor and radical, i.e., whose invariance algebras have the following structure: $\mathrm{sl}(2,\mathbb{R})\in L$. To perform this classification we utilize the classification of these type of Lie algebras obtained by Turkowski.[21]

We choose $\mathrm{sl}(2,\mathbb{R})=\{v_1,v_2,v_3\}$ with

$$v_1=-2t\partial_t-\tfrac{2}{3}x\partial_x,\ \ v_2=\partial_t,\ \ v_3=-t^2\partial_t-\tfrac{2}{3}tx\partial_x-x^3\partial_u.$$

According to Ref. 21, there is only one five-dimensional Lie algebra of the desired form $\mathrm{sl}(2,\mathbb{R})\in L$ with $L=\{e_1,e_2\}$, operators e_1,e_2 satisfying the commutation relations:

$$[e_1,e_2]=0,\ [v_1,e_1]=e_1,\ [v_1,e_2]=-e_2,$$

$$[v_2,e_1]=0,\ [v_2,e_2]=e_1,$$

$$[v_3,e_1]=e_2,\quad [v_3,e_2]=0.$$

As operators e_1,e_2 are necessarily of the form (2.4), we easily get that

$$e_1=|x|^{-3/2}\partial_u,\quad e_2=t|x|^{-3/2}\partial_u.$$

However, checking the invariance criterion for the above realization we find that the algebra in question cannot be invariance algebra of an equation of the form (4.7).

According to Ref. 21, there exist three six-dimensional Lie algebras that are semi-direct sums of semi-simple Levi factor and radical, algebra L being of the form $L=\{e_1,e_2,e_3\}$. Nonzero commutation relations for e_1,e_2,e_3 read as

$$(1)\quad [v_1,e_1]=2e_1,\ [v_2,e_2]=2e_1,\ [v_3,e_1]=e_2,$$

$$[v_1,e_3]=-2e_3,\ [v_2,e_3]=e_2,\ [v_3,e_2]=2e_3;$$

$$(2)\quad [v_1,e_1]=e_1,\ [v_2,e_2]=e_1,\ [v_3,e_1]=e_2,$$

$$[v_1,e_2]=-e_2,\ [e_1,e_2]=e_3;$$

$$(3)\quad [v_1,e_1]=e_1,\ [v_2,e_2]=e_1,\quad [v_3,e_1]=e_2,$$

$$[v_1,e_2]=-e_2,\ [e_1,e_3]=e_1,\ [e_2,e_3]=e_2.$$

Solving the above relations we see that the corresponding realizations cannot be invariance algebras of Eq. (4.7).

Next, we consider seven-dimensional algebras from the Turkowski's classification. According to Ref. 21 there are five inequivalent algebras of the targeted dimension. Four of them contain the above five- and six-dimensional algebras as subalgebras. So we need to consider only the fifth algebra $\mathrm{sl}(2,\mathbb{R})\subset L$, where $L=\{e_1,e_2,e_3,e_4\}$ and the following commutation relations hold:

$$[v_1,e_1]=3e_1,\quad [v_2,e_2]=3e_1,$$

$$[v_3,e_1]=e_2,\quad [v_1,e_2]=e_2,$$

$$[v_2,e_3]=2e_2,\quad [v_3,e_2]=2e_3,$$

$$[v_1,e_3]=-e_3,\quad [v_2,e_4]=e_3,$$

$$[v_3,e_3]=3e_4,\quad [v_1,e_4]=-3e_4.$$

The most general form of operators e_1,e_2,e_3,e_4 satisfying the above relations is as follows:

$$e_1=|x|^{-9/2}\partial_u,\quad e_2=3t|x|^{-9/2}\partial_u,$$

$$e_3=3t^2|x|^{-9/2}\partial_u,\quad e_4=t^3|x|^{-9/2}\partial_u.$$

However, verifying the invariance criterion yields that this algebra cannot be the symmetry algebra of Eq. (4.7).

Thus we proved that the class of PDEs (4.7) contains no equations admitting symmetry algebras of the dimension $n\leqslant 7$, which are semi-direct sums of the Levi factor and radical. It is natural to conjecture that the same assertion holds for an arbitrary n. To prove this fact we need to consider in full details classification of nonlinear equations (1.1), whose invariance algebras are solvable.

Let us sum up the above results as theorems.

Theorem 4.2: *The class of PDEs (1.1) contains two inequivalent equations whose invariance algebra are semi-simple* $(\mathrm{sl}(2,\mathbb{R}))$,

$$u_t=u_{xxx}-\tfrac{3}{2}u_x^{-1}u_{xx}^2+u_xG(x,t);$$

$$u_t=u_{xxx}-x^{-3}[2xu_x+\tfrac{1}{9}x^2u_x^2-G(\omega_1,\omega_2)],$$

$$\omega_1=3u-xu_x,\quad \omega_2=6u-x^2u_{xx}.$$

The maximal invariance algebras of the above equations under arbitrary G read as

$$\mathrm{sl}^1(2,\mathbb{R})=\{\partial_u,u\partial_u,-u^2\partial_u\};$$

$$\mathrm{sl}^2(2,\mathbb{R})=\{\partial_t,t\partial_t+\tfrac{1}{3}x\partial_x,-t^2\partial_t-\tfrac{2}{3}tx\partial_x-x^3\partial_u\}.$$

Theorem 4.3: *Nonlinear equation (1.1) whose invariance algebra is isomorphic to a Lie algebra having nontrivial Levi decomposition is represented by one of the following equations:*

$$u_t=u_{xxx}-\tfrac{3}{2}u_x^{-1}u_{xx}^2+u_x\tilde{G}(x),\quad \mathrm{sl}^1(2,R)\oplus\{\partial_t\};\tag{4.10}$$

$$u_t=u_{xxx}-\tfrac{3}{2}u_x^{-1}u_{xx}^2+\lambda x^{-2}u_x,\quad \lambda\neq 0,\quad \mathrm{sl}^1(2,\mathbb{R})\oplus\{\partial_t,t\partial_t+\tfrac{1}{3}x\partial_x\};\tag{4.11}$$

$$u_t = u_{xxx} - \tfrac{3}{2}u_x^{-1}u_{xx}^2, \quad \mathrm{sl}^1(2,\mathbb{R}) \oplus \{\partial_t, \partial_x, t\partial_t + \tfrac{1}{3}x\partial_x\}; \tag{4.12}$$

$$u_t = u_{xxx} - 2x^{-2}u_x - \tfrac{1}{9}x^{-1}u_x^2 + x^{-3}\tilde{G}(\sigma), \quad \sigma = x^2u_{xx} - 2xu_x, \quad \mathrm{sl}^2(2,\mathbb{R}) \oplus \{\partial_u\}, \tag{4.13}$$

where $\tilde{G}$ is an arbitrary function of x or σ. Moreover, the associated symmetry algebras are maximal.

Note that Eq. (4.12) can be expressed in the form

$$\frac{u_t}{u_x} = \{u;x\}, \tag{4.14}$$

where $\{u;x\}$ denotes the Schwarzian derivative of u with respect to x. It is known that a nonpoint transformation taking this equation into the usual KdV exists.

V. CLASSIFICATION OF EQUATIONS INVARIANT UNDER LOW-DIMENSIONAL SOLVABLE SYMMETRY ALGEBRAS

In this section we apply the strategy summarized in the Introduction to identify representative classes of equations of the form (1.1) invariant under one-, two-, and three-dimensional solvable symmetry algebras. In order to approach this task in a systematic manner we realize all possible inequivalent algebras in terms of vector fields (2.4) under the action of the equivalence group $\mathcal{E}$.

A. Equations with one-dimensional symmetry algebras

We assume that for a given F, Eq. (1.1) is invariant under a one-parameter symmetry group, generated by the vector field (2.4) with coefficients subject to the constraint (2.5). We make use of Proposition 2.3 which characterizes the canonical forms of the vector field X of (2.4). We then substitute the coefficients of the canonical vector field into the determining equation (2.5), which is a first order linear homogeneous PDE for F, and solve the latter in order to construct invariant equations.

According to Proposition 2.3 we have three types of one-dimensional symmetry algebras:

$$A_{1,1}: \quad X_1 = \partial_t, \quad A_{1,2}: X_1 = \partial_x, \quad A_{1,3}: X_1 = \partial_u. \tag{5.1}$$

The corresponding invariant equations will have the form

$$A_{1,1}: \quad u_t = u_{xxx} + F(x,u,u_x,u_{xx}), \tag{5.2a}$$

$$A_{1,2}: \quad u_t = u_{xxx} + F(t,u,u_x,u_{xx}), \tag{5.2b}$$

$$A_{1,3}: \quad u_t = u_{xxx} + F(x,t,u_x,u_{xx}). \tag{5.2c}$$

Theorem 5.1: *There are three inequivalent classes of Eqs. (1.1) invariant under one-parameter symmetry group. Their representatives are given by (5.2).*

B. Equations with two-dimensional symmetry algebras

There are two isomorphy classes of two-dimensional Lie algebras, Abelian and non-Abelian, satisfying the commutation relations $[X_1,X_2] = \kappa X_2$, $\kappa = 0,1$. We denote them by $A_{2,1}$ and $A_{2,2}$.

1. Abelian

We start from each of the one-dimensional cases obtained in (5.1) and add to it vector fields X_2 of the form (2.4) commuting with X_1. We then simplify X_2 by equivalence transformations leaving the vector field X_1 invariant. For further details we refer the reader to Ref. 4. The standardized X_2 and the restricted form of F in (5.2) are then substituted into (2.5). Solving this equation will further restrict the form of the function F. The number of variables of F reduces by

one, three variables in this case. Thus, we find that there exist precisely four classes of two-dimensional Abelian symmetry algebras represented by the following ones:

$$A^1_{2,1}: \quad X_1=\partial_t, \quad X_2=\partial_x, \quad F=F(u,u_x,u_{xx}); \tag{5.3}$$

$$A^2_{2,1}: \quad X_1=\partial_t, \quad X_2=\partial_u, \quad F=F(x,u_x,u_{xx}); \tag{5.4}$$

$$A^3_{2,1}: \quad X_1=\partial_x, \quad X_2=\alpha(t)\partial_x+\partial_u, \quad F=-\dot{\alpha}uu_x+\tilde{F}(t,u_x,u_{xx}); \tag{5.5}$$

$$A^4_{2,1}: \quad X_1=\partial_u, \quad X_2=g(x,t)\partial_u, \quad g_x\neq \text{const}; \tag{5.6}$$

$$F=(g_t-g_{xxx})g_x^{-1}u_x+\tilde{F}(x,t,\omega), \quad \omega=g_{xx}u_x-g_xu_{xx}.$$

2. Non-Abelian

Imposing that X_1 reads as (5.1) and X_2 is in generic form and that they satisfy $[X_1,X_2]=X_2$, we find that five classes of symmetry algebras exist. Those algebras and nonlinear functions F are represented by

$$A^1_{2,2}: \quad X_1=\partial_t, \quad X_2=-t\partial_t-\frac{x}{3}\partial_x,$$

$$F=x^{-3}\tilde{F}(u,\omega_1,\omega_2), \quad \omega_1=xu_x, \quad \omega_2=x^2u_{xx};$$

$$A^2_{2,2}: \quad X_1=-3t\partial_t-x\partial_x, \quad X_2=\partial_x,$$

$$F=t^{-1}\tilde{F}(u,\omega_1,\omega_2), \quad \omega_1=t^{1/3}u_x, \quad \omega_2=t^{2/3}u_{xx};$$

$$A^3_{2,2}: \quad X_1=-u\partial_u, \quad X_2=\partial_u, \quad F=u_x\tilde{F}(x,t,\omega), \quad \omega=u_x^{-1}u_{xx};$$

$$A^4_{2,2}: \quad X_1=\partial_x-u\partial_u, \quad X_2=\partial_u;$$

$$F=e^{-x}\tilde{F}(t,\omega_1,\omega_2), \quad \omega_1=e^xu_x, \quad \omega_2=e^xu_{xx};$$

$$A^5_{2,2}: \quad X_1=\partial_t-u\partial_u, \quad X_2=\partial_u,$$

$$F=u_x\tilde{F}(x,\omega_1,\omega_2), \quad \omega_1=e^tu_x, \quad \omega_2=e^tu_{xx}.$$

Theorem 5.2: *There exist nine classes of two-dimensional symmetry algebras admitted by Eq. (1.1). They are represented by the algebras* $A^1_{2,1},\ldots,A^4_{2,1}$ *and* $A^1_{2,2},\ldots,A^5_{2,2}$.

C. Equations with three-dimensional symmetry algebras

1. Decomposable algebras

A Lie algebra is decomposable if it can be written as a direct sum of two or more Lie algebras $L=L_1\oplus L_2$ with $[L_1,L_2]=0$. There are two types of 3-dimensional decomposable Lie algebras: $A_{3,1}=3A_1=A_1\oplus A_2\oplus A_3$ with $[X_i,X_j]=0$ for $i,j=1,2,3$ and $A_{3,2}=A_{2,2}\oplus A_1$ with $[X_1,X_2]=X_2$, $[X_1,X_3]=0$, $[X_2,X_3]=0$.

We start from the two-dimensional algebras in (5.3) and add a further linearly independent vector field X_3 in the form (2.4) and impose the above commutation relations. We simplify X_3 using equivalence transformations leaving the space $\{X_1,X_2\}$ invariant. We present the following result without proof. We emphasize that there exist several realizations that do not produce invariant equations of the form (1.1):

$$A^1_{3,1}: \quad X_1=\partial_t, \quad X_2=\partial_x, \quad X_3=\partial_u, \quad F=F(u_x,u_{xx});$$

$$A^2_{3,1}: \quad X_1=\partial_t, \quad X_2=\partial_u, \quad X_3=f(x)\partial_u,$$

$$F=-\frac{f'''}{f'}u_x+\tilde{F}(x,\omega), \quad \omega=f''u_x-f'u_{xx};$$

$$A^1_{3,2}: \quad X_1=-t\partial_t-\frac{x}{3}\partial_x, \quad X_2=\partial_t, \quad X_3=\partial_u,$$

$$F=x^{-3}\tilde{F}(\omega_1,\omega_2), \quad \omega_1=xu_x, \quad \omega_2=x^2u_{xx};$$

$$A^2_{3,2}: \quad X_1=-3t\partial_t-x\partial_x, \quad X_2=\partial_x, \quad X_3=\partial_u,$$

$$F=t^{-1}\tilde{F}(\omega_1,\omega_2), \quad \omega_1=tu_x^3, \quad \omega_2=t^2u_{xx}^3;$$

$$A^3_{3,2}: \quad X_1=-3t\partial_t-x\partial_x, \quad X_2=\partial_x, \quad X_3=t^{1/3}\partial_x+\partial_u,$$

$$F=-\tfrac{1}{3}t^{-2/3}uu_x+t^{-1}\tilde{F}(\omega_1,\omega_2), \quad \omega_1=tu_x^3, \quad \omega_2=t^2u_{xx}^3;$$

$$A^4_{3,2}: \quad X_1=\partial_x-u\partial_u, \quad X_2=\partial_u, \quad X_3=e^{-x}f(t)\partial_u, \quad f\neq 0,$$

$$F=-\left(1+\frac{\dot{f}}{f}\right)u_x+e^{-x}\tilde{F}(t,\omega), \quad \omega=e^x(u_x+u_{xx});$$

$$A^5_{3,2}: \quad X_1=\partial_x-u\partial_u, \quad X_2=\partial_u, \quad X_3=\alpha(t)\partial_x, \quad \alpha\neq 0,$$

$$F=-\frac{\dot{\alpha}}{\alpha}u_x\ln(e^xu_x)+u_x\tilde{F}(t,\omega), \quad \omega=u_x^{-1}u_{xx};$$

$$A^6_{3,2}: \quad X_1=\partial_x-u\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_t,$$

$$F=e^{-x}\tilde{F}(\omega_1,\omega_2), \quad \omega_1=e^xu_x, \quad \omega_2=e^xu_{xx};$$

$$A^7_{3,2}: \quad X_1=\partial_t-u\partial_u, \quad X_2=\partial_u, \quad X_3=e^{-t}f(x)\partial_u, \quad f'\neq 0,$$

$$F=-\frac{f'''+f}{f'}u_x+e^{-t}\tilde{F}(x,\omega), \quad \omega=e^t(f''u_x-f'u_{xx});$$

$$A^8_{3,2}: \quad X_1=\partial_t-u\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_x,$$

$$F=e^{-t}\tilde{F}(\omega_1,\omega_2), \quad \omega_1=e^tu_x, \quad \omega_2=e^tu_{xx};$$

$$A^9_{3,2}: \quad X_1=\partial_t-u\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_t+\lambda\partial_x, \quad \lambda\neq 0,$$

$$F=\exp(x/t-\lambda)\tilde{F}(\omega_1,\omega_2),$$

$$\omega_1=\exp(t-x/\lambda)u_x, \quad \omega_2=\exp(t-x/\lambda)u_{xx};$$

$$A^{10}_{3,2}: \quad X_1=\partial_t-u\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_t,$$

$$F=u_x\tilde{F}(x,\omega),\quad \omega=u_x^{-1}u_{xx}.$$

2. Nondecomposable algebras

The isomorphy classes of these algebras are represented by the following list:

$$A_{3,3}:\quad [X_2,X_3]=X_1,\quad [X_1,X_2]=[X_1,X_3]=0;$$

$$A_{3,4}:\quad [X_1,X_3]=X_1,\quad [X_2,X_3]=X_1+X_2;$$

$$A_{3,5}:\quad [X_1,X_3]=X_1,\quad [X_2,X_3]=X_2;$$

$$A_{3,6}:\quad [X_1,X_3]=X_1,\quad [X_2,X_3]=-X_2;$$

$$A_{3,7}:\quad [X_1,X_3]=X_1,\quad [X_2,X_3]=qX_2\quad (0<|q|<1);$$

$$A_{3,8}:\quad [X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1;$$

$$A_{3,9}:\quad [X_1,X_3]=qX_1-X_2,\quad [X_2,X_3]=X_1+qX_2,\quad q>0.$$

Remark: Solvable nondecomposable algebras can be written as semidirect sums of a one-dimensional subalgebra $\{X_3\}$ and an Abelian ideal $\{X_1,X_2\}$. Note that the algebras $A_{3,6}$ and $A_{3,8}$ are isomorphic to $\mathfrak{e}(1,1)$, and $\mathfrak{e}(2)$, respectively. The algebra $A_{3,3}$ is a non-Abelian nilpotent algebra (Heisenberg algebra).

The commutation relations of the algebras in question can be represented in the matrix notation

$$\begin{pmatrix}[X_1,X_3]\\ [X_2,X_3]\end{pmatrix}=J\begin{pmatrix}X_1\\ X_2\end{pmatrix},\quad [X_1,X_2]=0,$$

where J is a 2×2 real matrix that can be taken in Jordan canonical form.

A solvable three-dimensional Lie algebra always possesses a two-dimensional Abelian ideal. We assume that the ideal $\{X_1,X_2\}$ is already of the form (5.3) and add a third element X_3 in the form (2.4) acting on the ideal. Imposing commutation relations and simplifying with equivalence transformations (2.6) (we consider each canonical form of the matrix individually) yield the realizations of solvable Lie algebras together with the corresponding invariant equations.

There exist nine classes of realizations of nilpotent algebras which give rise to invariant equations:

$$A_{3,3}:\quad J=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}. \tag{5.7}$$

$$A_{3,3}^1:\quad X_1=\partial_t,\quad X_2=\partial_u,\quad X_3=t\partial_u+\lambda\partial_x,\quad \lambda>0,$$

$$F=\frac{x}{\lambda}+\tilde{F}(u_x,u_{xx});$$

$$A_{3,3}^2:\quad X_1=\partial_u,\quad X_2=\partial_x,\quad X_3=x\partial_u+b(t)\partial_x,\quad \dot{b}\neq 0,$$

$$F=-\frac{\dot{b}}{2}u_x^2+\tilde{F}(t,u_{xx});$$

$$A_{3,3}^3:\quad X_1=\partial_u,\quad X_2=\partial_x,\quad X_3=x\partial_u+\lambda\partial_t,\quad \lambda\neq 0,$$

$$F=\tilde{F}(t-3\lambda u_x,u_{xx});$$

$$A^4_{3,3}:\quad X_1=\partial_u+3\lambda t^{1/2}\partial_x,\quad X_2=\partial_x,$$

$$X_3=6\lambda t^{3/2}\partial_t+3\lambda t^{1/2}x\partial_x+(x-3\lambda t^{1/2}u)\partial_u,\quad \lambda\neq 0,$$

$$F=-\tfrac{3}{2}\lambda t^{-1/2}uu_x+t^{-2}\tilde{F}(\omega_1,\omega_2),\quad \omega_1=tu_x-\frac{1}{3\lambda}t^{1/2},\quad \omega_2=t^{3/2}u_{xx};$$

$$A^5_{3,3}:\quad X_1=\partial_x,\quad X_2=\partial_t,\quad X_3=t\partial_x+\partial_u,$$

$$F=-uu_x+\tilde{F}(u_x,u_{xx});$$

$$A^6_{3,3}:\quad X_1=\partial_u,\quad X_2=(f(x)-t)\partial_u,\quad X_3=\partial_t,\quad (f'\neq 0),$$

$$F=-(1+f''')(f')^{-1}u_x+\tilde{F}(x,\omega),\quad \omega=f''u_x-f'u_{xx};$$

$$A^7_{3,3}:\quad X_1=\partial_u,\quad X_2=(t-x)\partial_u,\quad X_3=\partial_x,$$

$$F=u_x+\tilde{F}(t,u_{xx});$$

$$A^8_{3,3}:\quad X_1=\partial_u,\quad X_2=-x\partial_u,\quad X_3=\partial_x,$$

$$F=-\tilde{F}(t,u_{xx});$$

$$A^9_{3,3}:\quad X_1=-x^{-1}\partial_u,\quad X_2=\partial_u,\quad X_3=\partial_x-x^{-1}u\partial_u,$$

$$F=3x^{-1}u_{xx}+x^{-1}\tilde{F}(t,\omega),\quad \omega=2u_x+xu_{xx};$$

$$A_{3,4}:\quad J=\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix};\tag{5.8}$$

$$A^1_{3,4}:\quad X_1=\partial_u,\quad X_2=\partial_t,\quad X_3=t\partial_t+\frac{x}{3}\partial_x+(u+t)\partial_u,$$

$$F=3\ln x+\tilde{F}(\omega_1,\omega_2),\quad \omega_1=x^{-2}u_x,\quad \omega_2=x^{-1}u_{xx};$$

$$A^2_{3,4}:\quad X_1=\partial_x,\quad X_2=\partial_u-\tfrac{1}{3}\ln t\partial_x,\quad X_3=3t\partial_t+x\partial_x+u\partial_u,$$

$$F=\frac{1}{3t}uu_x+t^{-2/3}\tilde{F}(u_x,\omega),\quad \omega=t^{1/3}u_{xx};$$

$$A^3_{3,4}:\quad X_1=\partial_u,\quad X_2=\partial_x,\quad X_3=3t\partial_t+x\partial_x+(u+x)\partial_u,$$

$$F=t^{-2/3}\tilde{F}(\omega_1,\omega_2),\quad \omega_1=u_x-\tfrac{1}{3}\ln t,\quad \omega_2=t^{1/3}u_{xx};$$

$$A^4_{3,4}:\quad X_1=\alpha(t)\partial_x+\partial_u,\quad X_2=\partial_x,$$

$$X_3=(\alpha')^{-1}\alpha^2\partial_t+(1+\alpha)x\partial_x+[x+(1-\alpha)u]\partial_u,\quad \alpha'\neq 0,$$

$$\alpha^2\alpha''+(3+\alpha)(\alpha')^2=0,$$

$$F=-\alpha' u u_x+\alpha^{-4}\exp(2\alpha^{-1})\tilde{F}(\omega_1,\omega_2),$$

$$\omega_1=\alpha^3\exp(-\alpha^{-1})u_{xx},\quad \omega_2=\alpha^2 u_x-\alpha;$$

$$A^5_{3,4}:\quad X_1=\partial_u,\quad X_2=(-t+f(x))\partial_u,\quad X_3=\partial_t+u\partial_u,\quad f'\neq 0,$$

$$F=-(1+f''')(f')^{-1}u_x+e^t\tilde{F}(x,\omega),\quad \omega=e^{-t}(f''u_x-f'u_{xx});$$

$$A^6_{3,4}:\quad X_1=\partial_u,\quad X_2=-x\partial_u,\quad X_3=\partial_x+u\partial_u,$$

$$F=e^x\tilde{F}(t,\omega),\quad \omega=e^{-x}u_{xx};$$

$$A_{3,5}:\quad J=\begin{pmatrix}1&0\\0&1\end{pmatrix};\tag{5.9}$$

$$A^1_{3,5}:\quad X_1=\partial_t,\quad X_2=\partial_u,\quad X_3=t\partial_t+\frac{x}{3}\partial_x+u\partial_u,$$

$$F=\tilde{F}(\omega_1,\omega_2),\quad \omega_1=x^{-2}u_x,\quad \omega_2=x^{-1}u_{xx};$$

$$A^2_{3,5}:\quad X_1=\partial_x,\quad X_2=\partial_u,\quad X_3=3t\partial_t+x\partial_x+u\partial_u,$$

$$F=t^{-2/3}\tilde{F}(u_x,t^{1/3}u_{xx});$$

$$A^3_{3,5}:\quad X_1=\partial_u,\ X_2=f(x)\partial_u,\quad X_3=\partial_t+u\partial_u,\ f'\neq 0,$$

$$F=-f'''(f')^{-1}u_x+e^t\tilde{F}(x,\omega),$$

$$\omega=e^{-t}[f''u_x-f'u_{xx}];$$

$$A_{3,6}:\quad J=\begin{pmatrix}1&0\\0&-1\end{pmatrix};\tag{5.10}$$

$$A^1_{3,6}:\quad X_1=\partial_t,\quad X_2=\partial_u,\quad X_3=t\partial_t+\frac{x}{3}\partial_x-u\partial_u,$$

$$F=x^{-6}\tilde{F}(x^4u_x,x^5u_{xx});$$

$$A^2_{3,6}:\quad X_1=\partial_x,\quad X_2=\partial_u+\lambda t^{2/3}\partial_x,\quad X_3=3t\partial_t+x\partial_x-u\partial_u,$$

$$F=-\frac{2\lambda}{3}t^{-1/3}uu_x+t^{-4/3}\tilde{F}(t^{2/3}u_x,tu_{xx});$$

$$A^3_{3,6}:\quad X_1=\partial_u,\quad X_2=e^{2t}f(x)\partial_u,\quad X_3=\partial_t+u\partial_u,\quad f'\neq 0,$$

$$F=(2f-f''')(f')^{-1}u_x+e^t\tilde{F}(x,\omega),\quad \omega=e^{-t}(f''u_x-f'u_{xx});$$

$$A^4_{3,6}:\quad X_1=\partial_u,\quad X_2=e^{2\int f^{-1}x}h(t)\partial_u,\quad X_3=f(t)\partial_x+u\partial_u,\quad fh\neq 0,$$

$$F=-[4f^{-2}-\tfrac{1}{2}hh^{-1}f+f^{-1}f'x]u_x+e^{\int f^{-1}x}\tilde{F}(t,\omega),$$

$$\omega = e^{-f^{-1}x}(2u_x - f u_{xx});$$

$$A_{3,7}: \quad J = \begin{pmatrix} 1 & 0 \\ 0 & q \end{pmatrix}, \quad 0 < |q| < 1; \tag{5.11}$$

$$A^1_{3,7}: \quad X_1 = \partial_t, \quad X_2 = \partial_x, \quad X_3 = t\partial_t + \frac{x}{3}\partial_x, \quad q = 1/3,$$

$$F = u_x^3 \tilde{F}(u, u_x^{-2} u_{xx});$$

$$A^2_{3,7}: \quad X_1 = \partial_t, \quad X_2 = \partial_x, \quad X_3 = t\partial_t + \frac{x}{3}\partial_x + u\partial_u, \quad q = 1/3,$$

$$F = \tilde{F}(\omega_1, \omega_2), \quad \omega_1 = u^{-2/3} u_x, \quad \omega_2 = u^{-1/3} u_{xx};$$

$$A^3_{3,7}: \quad X_1 = \partial_t, \quad X_2 = \partial_u, \quad X_3 = t\partial_t + \frac{x}{3}\partial_x + qu\partial_u, \quad q \neq 0, \pm 1,$$

$$F = x^{3(q-1)} \tilde{F}(\omega_1, \omega_2), \quad \omega_1 = x^{1-3q} u_x, \quad \omega_2 = x^{2-3q} u_{xx};$$

$$A^4_{3,7}: \quad X_1 = \partial_x, \quad X_2 = \partial_u + \lambda t^{(1-q)/3}\partial_x, \quad X_3 = 3t\partial_t + x\partial_x + qu\partial_u,$$

$$q \neq 0, \pm 1, \ \lambda \in \mathbb{R},$$

$$F = \frac{\lambda}{3}(q-1) t^{-(q+2)/3} u u_x + \tilde{F}(\omega_1, \omega_2),$$

$$\omega_1 = t^{-(q-1)/3} u_x, \quad \omega_2 = t^{-(q-2)/3} u_{xx};$$

$$A^5_{3,7}: \quad X_1 = \partial_u, \quad X_2 = e^{(1-q)t} f(x)\partial_u, \quad X_3 = \partial_t + u\partial_u, \quad f' \neq 0, \quad q \neq 0, \pm 1,$$

$$F = [(1-q)f - f'''](f')^{-1} u_x + e^t \tilde{F}(x, \omega),$$

$$\omega = e^{-t}[f'' u_x - f' u_{xx}];$$

$$A^6_{3,7}: \quad X_1 = \partial_u, \quad X_2 = e^{(1-q)f^{-1}(t)x} h(t)\partial_u,$$

$$X_3 = f(t)\partial_x + u\partial_u, \quad f \cdot h \neq 0, \quad q \neq 0, \ \pm 1,$$

$$F = -[(1-q)^2 f^2 + f^{-1} f' x - (1-q)^{-1} f h^{-1} h'] u_x + e^{f^{-1}x} \tilde{F}(t, \omega),$$

$$\omega = e^{-f^{-1}x}[(1-q)u_x - f u_{xx}].$$

Remark: The algebra $A_{3,7}$ has another realization,

$$\{X_1 = \partial_t, X_2 = \partial_x, X_3 = t\partial_t + \tfrac{1}{3}(x + b_0 t)\partial_x + u\partial_u\},$$

that is isomorphic to $A^2_{3,7}$ under the change of basis

$$X_1 \to X_1 + \frac{b_0}{2} X_2, \quad X_2 \to X_2, \quad X_3 \to X_3.$$

Note that its equivalence to the latter is established by the change of variables,

$$\tilde{t}=t, \quad \tilde{x}=x-\tfrac{1}{2}b_0 t, \quad \tilde{u}=u.$$

That is why we have excluded it from the above list:

$$A_{3,8}: \quad J=\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}; \tag{5.12}$$

$$A^1_{3,8}: \quad X_1=\partial_x, \quad X_2=\alpha(t)\partial_x+\partial_u,$$

$$X_3=-\frac{1}{\dot{\alpha}}(1+\alpha^2)\partial_t-\alpha x\partial_x+(\alpha u-x)\partial_u,$$

$$F=-\dot{\alpha}uu_x+(1+\alpha^2)^{-2}\tilde{F}(\omega_1,\omega_2),$$

$$\omega_1=(1+\alpha^2)u_x-\alpha, \quad \omega_2=(1+\alpha^2)^{3/2}u_{xx},$$

where $\alpha(t)$, $\dot{\alpha}\neq 0$ satisfies

$$(1+\alpha^2)\ddot{\alpha}+\alpha\dot{\alpha}^2=0; \tag{5.13}$$

$$A_{3,9}: \quad J=\begin{pmatrix} q & -1 \\ 1 & q \end{pmatrix}, \quad q>0; \tag{5.14}$$

$$A^1_{3,9}: \quad X_1=\partial_x, \quad X_2=\alpha(t)\partial_x+\partial_u,$$

$$X_3=-\frac{1}{\dot{\alpha}}(1+\alpha^2)\partial_t+(q-\alpha)x\partial_x+[(q+\alpha)u-x]\partial_u,$$

$$F=-\dot{\alpha}uu_x+\exp\{2q\arctan\alpha\}(1+\alpha^2)^{-2}\tilde{F}(\omega_1,\omega_2),$$

$$\omega_1=(1+\alpha^2)u_x-\alpha, \quad \omega_2=(1+\alpha^2)^{3/2}\exp\{-q\arctan\alpha\}u_{xx},$$

where $\alpha(t)$, $\dot{\alpha}\neq 0$ satisfies

$$(1+\alpha^2)\ddot{\alpha}+(\alpha-3q)\dot{\alpha}^2=0. \tag{5.15}$$

Remark: $\alpha(t)$ can be obtained implicitly by quadratures as

$$\int^{\alpha}\exp(-3q\arctan\xi)(1+\xi^2)^{1/2}d\xi=c_1t+c_0.$$

Theorem 5.3: *There are thirty-eight inequivalent three-dimensional solvable symmetry algebras admitted by Eq. (1.1).*

VI. EQUATIONS WITH FOUR-DIMENSIONAL SOLVABLE ALGEBRAS

For $\dim L=4$, we proceed exactly in the same manner as above. We start from the already standardized three-dimensional algebras, and add a further linearly independent element X_4, and require that they form a Lie algebra.

A. Decomposable algebras

The list of decomposable four-dimensional Lie algebras consists of the twelve algebras: $4A_1=A_{3,1}\oplus A_1$, $A_{2,2}\oplus 2A_1=A_{3,2}\oplus A_1$, $2A_{2,2}=A_{2,2}\oplus A_{2,2}$, $A_{3,i}\oplus A_1$ $(i=3,4,\ldots,9)$. We preserve the notations of the previous section.

There are four inequivalent realizations of the algebra $2A_{2,2}$ which are invariance algebras of PDEs of the form (1.1). We give these realizations together with the corresponding invariant equations:

$$2A^1_{2,2}:\quad X_1=-t\partial_t-\frac{x}{3}\partial_x,\quad X_2=\partial_t,\quad X_3=\partial_u,\quad X_4=e^u\partial_u,$$

$$F=u_x^3-3u_xu_{xx}+x^{-2}u_x\tilde F(\omega),\quad \omega=x(u_x^{-1}u_{xx}-u_x);$$

$$2A^2_{2,2}:\quad X_1=-3t\partial_t-x\partial_x,\quad X_2=\partial_x,\quad X_3=-u\partial_u+\lambda t^{1/3}\partial_x,\quad X_4=\partial_u,$$

$$F=\frac{\lambda}{3t}\omega_1\ln|\omega_1|+\frac{\omega_1}{t}\tilde F(\omega),\quad \omega_1=t^{1/3}u_x,\quad \omega=t^{1/3}u_x^{-1}u_{xx};$$

$$2A^3_{2,2}:\quad X_1=\partial_x-u\partial_u,\quad X_2=\partial_u,\quad X_3=\frac{1}{\lambda}\partial_t,\quad X_4=\exp(\lambda t)\partial_x,$$

$$F=-\lambda xu_x-\lambda u_x\ln|u_x|+u_x\tilde F(\omega),\quad \omega=u_x^{-1}u_{xx};$$

$$2A^4_{2,2}:\quad X_1=\partial_x-u\partial_u,\quad X_2=\partial_u,\quad X_3=\lambda\partial_t,\quad X_4=e^{\lambda^{-1}t-x}\partial_u,\quad \lambda\neq 0,$$

$$F=(1+\lambda^{-1})u_x+e^{-x}\tilde F(\omega),\quad \omega=e^x(u_x+u_{xx});$$

$$2A^5_{2,2}:\quad X_1=\partial_t-u\partial_u,\quad X_2=\partial_u,\quad X_3=\beta(\partial_x+\gamma\partial_t)-\partial_t,$$

$$X_4=e^{\gamma x-t}\partial_u,\quad \beta\gamma\neq 0,$$

$$F=e^{(\gamma-\beta^{-1})x-t}\tilde F(\omega)-\gamma^{-1}(1+\gamma^3)u_x,$$

$$\omega=e^{t+(\beta^{-1}-\gamma)x}(\gamma u_x-u_{xx}).$$

Equations invariant under the algebra $A_{2,2}\oplus 2A_1=A_{3.2}\oplus A_1$:

$$A^6_{3,2}\oplus\{X_4\}:\quad X_1=\partial_x-u\partial_u,\quad X_2=\partial_u,\quad X_3=\partial_t,\quad X_4=e^{-x}\partial_u,$$

$$F=-u_x+e^{-x}\tilde F(\omega),\quad \omega=e^x(u_x+u_{xx});$$

$$A^6_{3,2}\oplus\{X_4\}:\quad X_1=\partial_x-u\partial_u,\quad X_2=\partial_u,\quad X_3=\partial_t,\quad X_4=\partial_x,$$

$$F=u_x\tilde F(\omega),\quad \omega=u_{xx}u_x^{-1};$$

$$A^7_{3,2}(f=e^{\lambda x},\ \lambda\neq 0)\oplus\{X_4\}:\quad X_1=\partial_t-u\partial_u,\quad X_2=\partial_u,$$

$$X_3=e^{\lambda x-t}\partial_u,\quad X_4=\partial_x+\lambda\partial_t,\quad \lambda\neq 0,$$

$$F=-(\lambda^3+1)\lambda^{-1}u_x+e^{-t+\lambda x}\tilde F(\omega),$$

$$\omega=e^{t-\lambda x}(\lambda u_x-u_{xx});$$

$$A^1_{3.3}\oplus\{X_4\}:\quad X_1=\partial_t,\quad X_2=\partial_u,\quad X_3=t\partial_u+\lambda\partial_x,$$

$$X_4=\partial_t+\lambda^{-1}x\partial_u+\beta\partial_x,\quad \lambda>0,\quad \beta\in\mathbb{R},$$

$$F=\lambda^{-1}x-\beta u_x+\tilde{F}(u_{xx});$$

$$A^3_{3,5}\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=\partial_x,\quad X_3=x\partial_u+\lambda\partial_t,\quad X_4=\partial_t+\beta(\partial_x+\lambda^{-1}t\partial_u),$$

$$\lambda\neq 0,\quad \beta\in\mathbb{R},\quad F=\beta(\lambda^{-1}t-3u_x)+\tilde{F}(u_{xx});$$

$$A^6_{3,5}(f=\lambda^{-1}x,\ \lambda\neq 0)\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=(\lambda^{-1}x-t)\partial_u,$$

$$X_3=\partial_t,\quad X_4=\partial_t+\lambda\partial_x,\quad \lambda\neq 0,$$

$$F=-u_x+\tilde{F}(u_{xx});$$

$$A^9_{3,5}\oplus\{X_4\}:\quad X_1=-x^{-1}\partial_u,\quad X_2=\partial_u,\quad X_3=\partial_x-x^{-1}u\partial_u,\quad X_4=\partial_t,$$

$$F=3x^{-1}u_{xx}+x^{-1}\tilde{F}(\omega),\quad \omega=2u_x+xu_{xx};$$

$$A^1_{3,4}\oplus\{X_4\}:\quad X_1=\partial_u,\ X_2=\partial_t,$$

$$X_3=t\partial_t+\tfrac{1}{3}x\partial_x+(u+t)\partial_u,\quad X_4=x^3\partial_u,$$

$$F=3\ln x-2x^{-2}u_x+\tilde{F}(\omega),\ \omega=x^{-1}u_{xx}-2x^{-2}u_x;$$

$$A^5_{3,4}\ (f=\lambda x,\ \lambda\neq 0)\oplus\{X_4\}:\quad X_1=\partial_u,$$

$$X_2=(-t+\lambda x)\partial_u,\quad X_3=\partial_t+u\partial_u,$$

$$X_4=\partial_x+\lambda\partial_t,\quad \lambda\neq 0,$$

$$F=-\lambda^{-1}u_x+e^{t-\lambda x}\tilde{F}(\omega),\ \omega=e^{-t+\lambda x}u_{xx};$$

$$A^6_{3,4}\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=-x\partial_u,$$

$$X_3=\partial_x+u\partial_u,\quad X_4=\partial_t,$$

$$F=e^x\tilde{F}(\omega),\quad \omega=e^{-x}u_{xx};$$

$$A^1_{3,5}\oplus\{X_4\}:\quad X_1=\partial_t,\quad X_2=\partial_u,$$

$$X_3=t\partial_t+\frac{x}{3}\partial_x+u\partial_u,\quad X_4=x^3\partial_u,$$

$$F=-2x^{-2}u_x+\tilde{F}(\omega),\quad \omega=x^{-1}u_{xx}-2x^{-2}u_x;$$

$$A^1_{3,6}\oplus\{X_4\}:\quad X_1=\partial_t,\quad X_2=\partial_u,$$

$$X_3=t\partial_t+\frac{x}{3}\partial_x-u\partial_u,\quad X_4=x^{-3}\partial_u,$$

$$F=-20x^{-2}u_x+x^{-6}\tilde{F}(\omega),\quad \omega=4x^4u_x-x^5u_{xx},$$

$$A^3_{3,6}(f=e^{-2\beta^{-1}x},\ \beta\neq 0)\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=e^{2(t-\beta^{-1}x)}\partial_u,$$

$$X_3=\partial_t+u\partial_u,\quad X_4=\partial_t+\beta\partial_x,\quad \beta\neq 0,$$

$$F=-(\beta+4\beta^{-2})u_x+e^{t-\beta^{-1}x}\tilde{F}(\omega),$$

$$\omega=e^{-t+\beta^{-1}x}(2u_x+\beta u_{xx});$$

$$A^4_{3,6}(f=h=1)\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=e^{2x}\partial_u,$$

$$X_3=\partial_x+u\partial_u,\quad X_4=\partial_t,$$

$$F=-4u_x+e^{x}\tilde{F}(\omega),\quad \omega=e^{-x}(2u_x-u_{xx});$$

$$A^1_{3,7}\oplus\{X_4\}:\quad X_1=\partial_t,\quad X_2=\partial_x,$$

$$X_3=t\partial_t+\tfrac{1}{3}x\partial_x,\quad X_4=u\partial_u,$$

$$F=u^{-2}u_x^3\tilde{F}(\omega),\quad \omega=u_x^{-2}uu_{xx};$$

$$A^3_{3,7}\oplus\{X_4\}:\quad X_1=\partial_t,\quad X_2=\partial_u,$$

$$X_3=t\partial_t+\frac{x}{3}\partial_x+qu\partial_u,\quad X_4=x^{3q}\partial_u,$$

$$q\neq 0,\ \pm 1,$$

$$F=-(3q-1)(3q-2)x^{-2}u_x+x^{3(q-1)}\tilde{F}(\omega),$$

$$\omega=x^{1-3q}[(3q-1)u_x-xu_{xx}];$$

$$A^5_{3,7}(f=e^{-1(1-q)\beta^{-1}x},\beta\neq 0)\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=e^{(1-q)(t-\beta^{-1}x)}\partial_u,\quad X_3=\partial_t+u\partial_u,$$

$$X_4=\partial_t+\beta\partial_x,\quad \beta\neq 0,\ q\neq 0,\ \pm 1,$$

$$F=-[\beta+(1-q)^2\beta^{-2}]u_x+e^{t-\beta^{-1}x}\tilde{F}(\omega),$$

$$\omega=e^{-t+\beta^{-1}x}[(1-q)u_x+\beta u_{xx}];$$

$$A^6_{3,7}(f=h=1)\oplus\{X_4\}:\quad X_1=\partial_u,\quad X_2=e^{(1-q)x}\partial_u,$$

$$X_3=\partial_x+u\partial_u,\quad X_4=\partial_t,\quad q\neq 0,\ \pm 1,$$

$$F=-(1-q)^2u_x+e^{x}\tilde{F}(\omega),$$

$$\omega=e^{-x}[(1-q)u_x-u_{xx}].$$

Remark: The $A^1_{3,7}\oplus A_1$ invariant equation is

$$u_t = u_{xxx} + \frac{u_x^3}{u^2}\tilde{F}(\omega), \quad \omega = \frac{uu_{xx}}{u_x^2}. \tag{6.1}$$

If, in particular, $\tilde{F} = c\omega^2$, $c = \text{const}$, namely,

$$F = cu_x^{-1}u_{xx}^2, \tag{6.2}$$

the symmetry algebra is further extended by $X_5 = \partial_u$ to a five-dimensional one.

B. Nondecomposable algebras

The set of inequivalent abstract four-dimensional Lie algebras contains ten real nondecomposable Lie algebras $A_{4,i} = \{X_1, X_2, X_3, X_4\}$ $(i = 1,\ldots,10)$.[4,5] They are all solvable and therefore can be written as semidirect sums of a one-dimensional Lie algebra $\{X_4\}$ and a three-dimensional ideal $N = \{X_1, X_2, X_3\}$. For $A_{4,i}$ $(i = 1,\ldots,6)$, N is Abelian, for $A_{4,7}, A_{4,8}, A_{4,9}$ it is of type $A_{3,3}$ (nilpotent), and for $A_{4,10}$ it is of the type $A_{3,5}$. The nonzero commutation relations read as

$$A_{4,1}: \quad [X_2, X_4] = X_1, \quad [X_3, X_4] = X_2;$$

$$A_{4,2}: \quad [X_1, X_4] = qX_1, \quad [X_2, X_4] = X_2,$$

$$[X_3, X_4] = X_2 + X_3, \quad q \neq 0;$$

$$A_{4,3}: \quad [X_1, X_4] = X_1, \quad [X_3, X_4] = X_2;$$

$$A_{4,4}: \quad [X_1, X_4] = X_1, \quad [X_2, X_4] = X_1 + X_2,$$

$$[X_3, X_4] = X_2 + X_3;$$

$$A_{4,5}: \quad [X_1, X_4] = X_1, \quad [X_2, X_4] = qX_2,$$

$$[X_3, X_4] = pX_3, \quad -1 \leqslant p \leqslant q \leqslant 1, \quad pq \neq 0;$$

$$A_{4,6}: \quad [X_1, X_4] = qX_1, \quad [X_2, X_4] = pX_2 - X_3,$$

$$[X_3, X_4] = X_2 + pX_3, \quad q \neq 0, \quad p \geqslant 0;$$

$$A_{4,7}: \quad [X_2, X_3] = X_1, \quad [X_1, X_4] = 2X_1,$$

$$[X_2, X_4] = X_2, \quad [X_3, X_4] = X_2 + X_3;$$

$$A_{4,8}: \quad [X_2, X_3] = X_1, \quad [X_1, X_4] = (1+q)X_1,$$

$$[X_2, X_4] = X_2, \quad [X_3, X_4] = qX_3, \quad |q| \leqslant 1;$$

$$A_{4,9}: \quad [X_2, X_3] = X_1, \quad [X_1, X_4] = 2qX_1,$$

$$[X_2, X_4] = qX_2 - X_3, \quad [X_3, X_4] = X_2 + qX_3, \quad q \geqslant 0;$$

$$A_{4,10}: \quad [X_1, X_3] = X_1, \quad [X_2, X_3] = X_2,$$

$$[X_1, X_4] = -X_2, \quad [X_2, X_4] = X_1.$$

In order to obtain realizations of solvable four-dimensional symmetry algebras of PDEs that belong to the class (1.1), we add X_4 in the generic form (2.4) to the already constructed three-

dimensional symmetry algebras and impose the above commutation relations. Once the algebra is found we insert X_4 into Eq. (2.5) and solve it for the function F. The form of F which is invariant under a three-dimensional algebra is further restricted:

$$A^1_{4,1}: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=\partial_t, \quad X_4=t\partial_x+x\partial_u,$$

$$F=-\tfrac{1}{2}u_x^2+\tilde{F}(u_{xx});$$

$$A^2_{4,1}: \quad X_1=\partial_u, \quad X_2=x\partial_u, \quad X_3=\partial_t, \quad X_4=\partial_x+tx\partial_u,$$

$$F=\tfrac{1}{2}x^2+\tilde{F}(u_{xx});$$

$$A^1_{4,2}: \quad X_1=\partial_t, \quad X_2=\partial_u, \quad X_3=\partial_x, \quad X_4=3t\partial_t+x\partial_x+(x+u)\partial_u,$$

$$F=u_{xx}^2\tilde{F}(e^{u_x}u_{xx});$$

$$A^2_{4,2}: \quad X_1=\partial_x, \quad X_2=\partial_u, \quad X_3=\partial_t, \quad X_4=t\partial_t+\frac{x}{3}\partial_x+(t+u)\partial_u,$$

$$F=\frac{3}{2}\ln|u_x|+\tilde{F}(\omega), \quad \omega=\frac{u_{xx}^2}{u_x};$$

$$A^3_{4,2}: \quad X_1=\partial_t, \quad X_2=\partial_u, \quad X_3=-3q^{-1}\ln x\partial_u,$$

$$X_4=qt\partial_t+\tfrac{1}{3}qx\partial_x+u\partial_u, \quad q\neq 0,$$

$$F=-2x^{-2}u_x+x^{3(q^{-1}-1)}\tilde{F}(\omega), \quad \omega=x^{1-3q^{-1}}u_x+x^{2-3q^{-1}}u_{xx};$$

$$A^4_{4,2}: \quad X_1=x^{3(1-q)}\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_t,$$

$$X_4=t\partial_t+\tfrac{1}{3}x\partial_x+(u+t)\partial_u, \quad q\neq 0,1,$$

$$F=-(2-3q)(1-3q)x^{-2}u_x+3\ln x+\tilde{F}(\omega), \quad \omega=(2-3q)x^{-2}u_x-x^{-1}u_{xx};$$

$$A^1_{4,3}: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=\partial_t, \quad X_4=t\partial_x+u\partial_u,$$

$$F=-u_x\ln|u_x|+u_x\tilde{F}\left(\frac{u_{xx}}{u_x}\right);$$

$$A^2_{4,3}: \quad X_1=\partial_t, \quad X_2=\partial_u, \quad X_3=-3\ln x\partial_u,$$

$$X_4=t\partial_t+\tfrac{1}{3}x\partial_x,$$

$$F=-2x^{-2}u_x+x^{-3}\tilde{F}(\omega), \quad \omega=xu_x+x^2u_{xx};$$

$$A^3_{4,3}: \quad X_1=\partial_u, \quad X_2=e^x\partial_u, \quad X_3=\partial_t,$$

$$X_4=\partial_x+(u+te^x)\partial_u;$$

$$F=-u_x+xe^x+e^x\tilde{F}(\omega), \quad \omega=e^{-x}(u_x-u_{xx});$$

$$A^1_{4,4}: \quad X_1=\partial_u,\ X_2=-3\ln x\,\partial_u,\ X_3=\partial_t,$$

$$X_4=t\partial_t+\tfrac{1}{3}x\partial_x+(u-3t\ln x)\partial_u;$$

$$A^1_{4,5}: \quad X_1=\partial_t, \quad X_2=\partial_x, \quad X_3=\partial_u, \quad X_4=t\partial_t+\frac{x}{3}\partial_x+ku\partial_u, \quad k\neq 0,\ \frac{1}{3},$$

$$F=u_x^{3(1-k)/(1-3k)}\tilde{F}(\omega), \quad \omega=u_x^{(3k-2)/(1-3k)}u_{xx};$$

$$A^2_{4,5}: \quad X_1=\partial_t, \quad X_2=\partial_x, \quad X_3=\partial_u,$$

$$X_4=t\partial_t+\frac{x}{3}\partial_x+\frac{u}{3}\partial_u,$$

$$F=u_{xx}^2\tilde{F}(u_{xx});$$

$$A^3_{4,5}: \quad X_1=\partial_t, \quad X_2=u, \quad X_3=x^{3(q-p)}\partial_u,$$

$$X_4=t\partial_t+\tfrac{1}{3}x\partial_x+qu\partial_u, \quad q\neq p, \quad q\cdot p\neq 0,$$

$$F=-[3(q-p)-1][3(q-p)-2]x^{-2}u_x+x^{3(q-1)}\tilde{F}(\omega),$$

$$\omega=[3(q-p)-1]x^{1-3q}u_x-x^{2-3q}u_{xx};$$

$$A^1_{4,7}: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=x\partial_u-\tfrac{1}{3}\ln t\partial_x, \quad X_4=3t\partial_t+x\partial_x+2u\partial_u,$$

$$F=\frac{1}{6t}u_x^2+t^{-1/3}\tilde{F}(u_{xx});$$

$$A^2_{4,7}: \quad X_1=\partial_u, \quad X_2=x\partial_u+b\partial_x, \quad X_3=-\partial_x,$$

$$X_4=-b^2(b')^{-1}\partial_t+(1-b)x\partial_x+(2u-\tfrac{1}{2}x^2)\partial_u, \quad b=b(t),\ b'\neq 0,$$

$$b^2b''+(b-3)(b')^2=0,$$

$$F=-\tfrac{1}{2}b'u_x^2+b^{-3}e^{-b^{-1}}\tilde{F}(\omega), \quad \omega=b^2u_{xx}-b;$$

$$A^3_{4,7}: \quad X_1=\partial_u, \quad X_2=(\lambda x^3-t)\partial_u, \quad X_3=\partial_t,$$

$$X_4=t\partial_t+\tfrac{1}{3}x\partial_x+(2u-\tfrac{1}{2}t^2+\lambda tx^3)\partial_u, \quad \lambda\neq 0,$$

$$F=-\tfrac{1}{3}\lambda^{-1}(1+6\lambda)x^{-2}u_x+3\lambda x^3\ln x+x^3\tilde{F}(\omega), \quad \omega=2x^{-5}u_x-x^{-4}u_{xx};$$

$$A^4_{4,7}: \quad X_1=\partial_u, \quad X_2=(t-x)\partial_u, \quad X_3=\partial_x,$$

$$X_4=3t\partial_t+(x+2t)\partial_x+\left(xt-\frac{x^2}{2}+2u\right)\partial_u,$$

$$F=-u_x+t^{-1/3}\tilde{F}(\omega)+\frac{t}{4}, \quad \omega=u_{xx}+\frac{1}{3}\ln t;$$

$$A_{4,7}^5: \quad X_1=\partial_u, \quad X_2=-x\partial_u, \quad X_3=\partial_x,$$

$$X_4=3t\partial_t+x\partial_x+\left(2u-\frac{x^2}{2}\right)\partial_u,$$

$$F=t^{-1/3}\tilde{F}(\omega), \quad \omega=u_{xx}+\tfrac{1}{3}\ln t;$$

$$A_{4,7}^6: \quad X_1=-x^{-1}\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_x-x^{-1}u\partial_u,$$

$$X_4=3t\partial_t+x\partial_x+(u+\tfrac{1}{2}x)\partial_u,$$

$$F=3x^{-1}u_{xx}+x^{-1}t^{-1/3}\tilde{F}(\omega), \quad \omega=2u_x+xu_{xx}-\tfrac{1}{3}\ln t;$$

$$A_{4,8}^1: \quad X_1=\partial_x, \quad X_2=\partial_t, \quad X_3=t\partial_x+\partial_u, \quad X_4=t\partial_t+\frac{x}{3}\partial_x-\frac{2}{3}u\partial_u,$$

$$F=-uu_x+u_x^{5/3}\tilde{F}(u_x^{-4/3}u_{xx});$$

$$A_{4,8}^2: \quad X_1=\partial_u, \quad X_2=\partial_t, \quad X_3=t\partial_u+\lambda\partial_x, \quad X_4=t\partial_t+\frac{x}{3}\partial_x+\frac{4}{3}u\partial_u,$$

$$F=\frac{x}{\lambda}+u_x^{1/3}\tilde{F}(\omega), \quad \omega=u_x^{-2/3}u_{xx}, \quad \lambda>0;$$

$$A_{4,8}^3: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=x\partial_u+\lambda t^{(1-q)/3}\partial_x,$$

$$X_4=3t\partial_t+x\partial_x+(1+q)u\partial_u, \quad q\in\mathbb{R},$$

$$F=\frac{\lambda(q-1)}{6}t^{-(2+q)/3}u_x^2+t^{(q-2)/3}\tilde{F}(\omega), \quad \omega=t^{(1-q)/3}u_{xx}, \quad \lambda\neq 0, \quad |q|\neq 1;$$

$$A_{4,8}^4: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=x\partial_u+\lambda\partial_t,$$

$$X_4=3t\partial_t+x\partial_x+4u\partial_u, \quad \lambda\neq 0,$$

$$F=(t-3\lambda u_x)^{1/3}\tilde{F}(\omega), \quad \omega=u_{xx}^3(t-3\lambda u_x)^2;$$

$$A_{4,8}^5: \quad X_1=\partial_u, \quad X_2=(\lambda x^3-t)\partial_u, \quad X_3=\partial_t,$$

$$X_4=qt\partial_t+\tfrac{1}{3}qx\partial_x+(1+q)u\partial_u, \quad \lambda\cdot q\neq 0,$$

$$F=-\tfrac{1}{3}\lambda^{-1}(1+6\lambda)x^{-2}u_x+x^{3q^{-1}}\tilde{F}(\omega), \quad \omega=2x^{-(2+3q^{-1})}u_x-x^{-(1+3q^{-1})}u_{xx};$$

$$A_{4,8}^6: \quad X_1=\partial_u, \quad X_2=(t-x)\partial_u, \quad X_3=\partial_x,$$

$$X_4=3qt\partial_t+q(x+2t)\partial_x+(1+q)u\partial_u,$$

$$F=-u_x+t^{(1/3)(1-2q)q^{-1}}\tilde{F}(\omega), \quad \omega=t^{(1/3)(q-1)q^{-1}}u_{xx};$$

$$A_{4,8}^7: \quad X_1=-x^{-1}\partial_u, \quad X_2=\partial_u, \quad X_3=\partial_x-x^{-1}u\partial_u,$$

$$X_4=3qt+qx\partial_x+u\partial_u, \quad q\neq 0,$$

$$F=3x^{-1}u_{xx}+x^{-1}t^{(1/3)(q-1)q^{-1}}\tilde{F}(\omega), \quad \omega=t^{(1/3)(q-1)q^{-1}}(2u_x+xu_{xx});$$

$$A^8_{4,8}: \quad X_1=\partial_u, \quad X_2=-x\partial_u, \quad X_3=x\partial_x, \quad X_4=3qt\partial_t+qx\partial_x+(1+q)u\partial_u,$$

$$F=t^{(1/3)(1-2q)q^{-1}}\tilde{F}(\omega), \quad \omega=t^{(1/3)(q-1)q^{-1}}u_{xx}.$$

Remarks:

- There exists a realization of $A_{4,6}$:

$$A^1_{4,6}: \quad X_1=\partial_t, \quad X_2=\tan\psi\partial_u, \quad X_3=\partial_u,$$

$$X_4=2t\partial_t+\tfrac{2}{3}x\partial_x+[p+\tan\psi]u\partial_u,$$

$$\psi=\tfrac{3}{2}\ln x, \quad p\in\mathbb{R}.$$

However there are no equations that can be invariant under this algebra.

- The algebra $A^1_{4,8}$ is isomorphic to the KdV algebra which is the semidirect sum of the nilradical (maximal nilpotent ideal) $\mathfrak{h}(2)=\{X_1,X_2,X_3\}$ and the dilation $D=\{X_4\}$:

$$A^1_{4,9}: \quad X_1=\partial_u, \quad X_2=\partial_x, \quad X_3=\alpha(t)\partial_x+x\partial_u,$$

$$X_4=-\frac{(1+\alpha^2)}{\dot{\alpha}}\partial_t+(q-\alpha)x\partial_x+\left(2qu-\frac{x^2}{2}\right)\partial_u, \quad q\in\mathbb{R},$$

$$F=-\tfrac{1}{2}\dot{\alpha}u_x^2+(1+\alpha^2)^{-3/2}\exp(q\arctan\alpha)\tilde{F}(\omega), \quad \omega=(1+\alpha^2)u_{xx}-\alpha,$$

$$(1+\alpha^2)\ddot{\alpha}+(\alpha-3q)\dot{\alpha}^2=0.$$

The function $\alpha(t)$, $\dot{\alpha}\neq 0$ is a solution of the ordinary differential equation (5.15):

$$A^1_{4,10}: \quad X_1=\partial_u, \quad X_2=-\tan x\partial_u, \quad X_3=\partial_t+u\partial_u,$$

$$X_4=\beta\partial_t+\partial_x+u\tan x\partial_u, \quad \beta\in\mathbb{R},$$

$$F=-2u_x-3\tan xu_{xx}+e^{t-\beta x}\sec x\tilde{F}(\omega),$$

$$\omega=e^{\beta x-t}(\cos xu_{xx}-2\sin xu_x).$$

We sum up the above results as a theorem.

Theorem 6.1: *There exist fifty-two inequivalent four-dimensional symmetry algebras admitted by Eq. (1.1). The explicit forms of those algebras as well as the associated invariant equations are given above.*

VII. DISCUSSION AND CONCLUSIONS

In this paper we provide a symmetry classification of the KdV type equations involving an arbitrary function of five arguments. We find that the equivalence classes of invariant equations involve an arbitrary function of four, three, two variables and one variable as soon as the symmetry algebra is one-, two-, three- and four-dimensional, respectively. In particular, we studied symmetries of the most general third order linear evolution equation. What came out from this, to our surprise, is that the symmetry group allowed is four-dimensional at most, while there are

nonlinear equations with symmetry algebras greater than four. This result is in contrast to the second-order evolution equations. It is exactly the linear heat equation that allows for the maximal symmetry algebra.

To complete the classification list, it only remains to obtain the inequivalent equations invariant under solvable algebras of the dimension $\dim L \geqslant 5$. But this would require to going through a large number of isomorphism classes. To give an idea of the complexity of this task let us recall that there are sixty-six classes of nonisomorphic real, solvable Lie algebras of dimension five. For dimension six, there exist ninety-nine classes of them with a nilpotent element. We plan to devote a separate article to study equations admitting higher-dimensional symmetry algebras.

Whenever F is an arbitrary function of its arguments, the symmetry algebras given in the paper are maximal. In particular, if we impose the requirement that function F is be independent of u_{xx} then we find that $\phi = R(t)u + S(x,t)$ in (2.4). In this case, invariance under four-dimensional algebras will force F to depend on an arbitrary constant rather than on an arbitrary function. Then, they may admit symmetry groups of the dimension higher than four. We have analyzed this restricted class of equations and obtained that the only equation whose symmetry algebra is higher than four is the one corresponding to the realization $A^1_{4,1}$ for $\tilde{F} = \text{const}$. On the other hand, for the specific choices of $\tilde{F}$ involving one variable, the equations with four-dimensional symmetry algebras may be invariant under larger symmetry groups. For instance, the particular case of the equation invariant under $A^1_{4,1}$ obtained by setting $\tilde{F} = c u_{xx}^{4/3}$, $c = \text{const}$ admits an additional symmetry group generated by the dilation operator $X_5 = 3t\partial_t + x\partial_x - u\partial_u$.

We only presented representative lists of equivalence classes of invariant equations. All other invariant equations can be recovered from these lists by applying the point transformations (2.6). In other words, an equation in the class (1.1) will have a symmetry group with dimension satisfying $\dim L \leqslant 6$ if and only if it can be transformed to one in the (canonical) equations from the list.

As we mentioned, our classification is performed within point transformations of coordinates. Two equations are equivalent if one can be obtained from the other by a change of variables. On the other hand, consider a special case of (6.2) for $c = -3/4$,[24]

$$u_t = u_{xxx} - \frac{3}{4}\frac{u_{xx}^2}{u_x},$$

which additionally allows a symmetry group generated by $\{\partial_u\}$. Though this equation is equivalent to the third-order linear equation $v_t = v_{xxx}$ under the (no-point) transformation $v = \sqrt{u_x}$, we treat them as inequivalent.

To give a reader an insight into possible applications of the results of this article, we consider a subclass of Eqs. (1.1),

$$u_t = u_{xxx} + uu_x + f(t)u, \tag{7.1}$$

which arises in several physical applications such as the propagation of waves in shallow water of variable depth.

When $f(t)$ is arbitrary, (7.1) admits a two-dimensional Abelian symmetry algebra generated by

$$X_1 = \partial_x, \quad X_2 = \xi(t)\partial_x - \dot{\xi}(t)\partial_u, \quad \xi = \int \exp\left\{\int f(t)\ dt\right\}\ dt. \tag{7.2}$$

By the change of dependent variable $\tilde{u} = u/\dot{\xi}$, the generators are transformed to the realization $A^3_{2,1}$ with $\alpha = -\xi$. The corresponding invariant equation takes the form

$$\tilde{u}_t = \tilde{u}_{xxx} + \dot{\xi}\tilde{u}\tilde{u}_x,$$

which is a particular case of (1.2).

For the special case $f(t)=at^k$ $(a\neq 0)$, the algebra is larger and we have the following possibilities for the algebra to be either three- or four-dimensional.

(1) $(a,k)=(a,-1)$, $a\neq -1$: The equation admits the three-dimensional indecomposable solvable symmetry algebra spanned by

$$X_1=\partial_x,\quad X_2=t^{1+a}\partial_x-(1+a)t^a\partial_u,\quad X_3=t\partial_t+\frac{x}{3}\partial_x-\frac{2}{3}u\partial_u, \tag{7.3}$$

with nonzero commutation relations

$$[X_1,X_3]=-\frac{1}{3}X_1,\quad [X_2,X_3]=-\frac{3a+2}{3}X_2.$$

For $a=-1/3$, the algebra is isomorphic, up to the scaling of basis elements, to $A_{3,5}$, for $-1<a<-\frac{1}{3}$, to $A_{3,7}$.

For $a=-2/3$ it is isomorphic to the decomposable solvable algebra $A_{3,2}$ and a suitable basis is

$$X_1=\partial_x,\quad X_2=t^{1/3}\partial_x-\frac{1}{3}t^{-2/3}\partial_u,\quad X_3=t\partial_t+\frac{x}{3}\partial_x-\frac{2}{3}u\partial_u.$$

With the equivalence transformation

$$\tilde{t}=t,\quad \tilde{x}=x,\quad \tilde{u}=-3t^{2/3}u,$$

the basis elements are transformed, up to scaling, to the realization $A^3_{3,2}$. The transformed equation is

$$\tilde{u}_t=\tilde{u}_{xxx}-\tfrac{1}{3}t^{-2/3}\tilde{u}\tilde{u}_x.$$

This equation belongs to the class corresponding to the realization $A^3_{3,2}$.

We note that a member of (1.2) for $f=1$, $g=t^2$ (see Ref. 1) is equivalent, under appropriate point transformation, to the above equation. Similarly, the particular case $a=-\alpha/(1+\alpha)$, $\alpha\neq 0,1,2$ is equivalent to $f=1$, $g=t^\alpha$ of (1.2). In this case, the symmetry algebra is indecomposable and solvable.

(2) $(a,k)=(-1,-1)$: the spherical KdV (sKdV) equation.

In this case the equation is invariant with respect to a three-dimensional symmetry algebra. We choose its basis to be

$$X_1=\partial_x,\quad X_2=\ln t\partial_x-\frac{1}{t}\partial_u,\quad X_3=t\partial_t+\frac{x}{3}\partial_x-\frac{2}{3}u\partial_u, \tag{7.4}$$

with nonzero commutation relations

$$[X_3,X_1]=-\tfrac{1}{3}X_1,\quad [X_3,X_2]=X_1-\tfrac{1}{3}X_2.$$

It is easy to see that this algebra is isomorphic to $A_{3,4}$. Under the transformation $\tilde{u}=3tu$, the generators are transformed to the realization $A^2_{3,4}$. The sKdV equation takes the form

$$\tilde{u}_t=\tilde{u}_{xxx}+\frac{1}{3t}\tilde{u}\tilde{u}_x,$$

which is a particular case of the equation invariant under the algebra $A^2_{3,4}$.

We note that a member of (1.2) for $f=1$, $g=e^{3t1}$ is equivalent to the case (2), i.e. the sKdV equation.

(3) $(a,k)=(a,0)$: The basis of the symmetry algebra reads as

$$X_1=\partial_x, \qquad X_2=e^{at}(\partial_x-a\partial_u), \quad X_3=\partial_t, \tag{7.5}$$

with nonzero commutation relation $[X_3,X_2]=aX_2$. The algebra is isomorphic to $A_{3,2}$. With the transformation $\tilde{u}=e^{-at}u$ the equation is transformed to a special case of (1.2) for $f=1,g=e^{at}$.

(4) $(a,k)=(-1/2,-1)$: the cylindrical KdV (cKdV) equation.

In this case the symmetry algebra is four-dimensional. In a convenient basis we have

$$X_1=2\sqrt{t}\partial_x-\frac{1}{\sqrt{t}}\partial_u,$$

$$X_2=4t^{3/2}\partial_t+2x\sqrt{t}\partial_x-\left(\frac{x}{\sqrt{t}}+4\sqrt{t}u\right)\partial_u, \tag{7.6}$$

$$X_3=\partial_x, \quad X_4=3t\partial_t+x\partial_x-2u\partial_u,$$

with nonzero commutation relations

$$[X_2,X_3]=-X_1, \quad [X_1,X_4]=-\tfrac{1}{2}X_1, \quad [X_2,X_4]=-\tfrac{3}{2}X_2, \quad [X_3,X_4]=X_3.$$

We see that the symmetry algebra of the cKdV equation is isomorphic to the algebra $A_{4,8}$ with $q=1$. The existence of such an isomorphism is a necessary, but not sufficient condition for a local point transformation to exist, transforming the two equations into each other. Comparing these generators with (2.10) and choosing (2.8) suitably, for example, first transforming the commuting elements $\{X_1,X_3\}$ into $\{\partial_{\tilde{x}},\tilde{t}\partial_{\tilde{x}}+\partial_{\tilde{u}}\}$ and then transforming the remaining ones with the aid of the freedom left in equivalence transformations we arrive at

$$\tilde{t}=2t^{-1/2}, \quad \tilde{x}=t^{-1/2}x, \quad \tilde{u}=tu+\frac{x}{2},$$

which establishes the equivalence of the Lie algebra with basis (7.6) and the cKdV equation to the KdV algebra ($A^1_{4,8}$) and KdV equation. This connection between the KdV and cKdV equations is well-known in the literature.[19]

As a further comparison of the results obtained in the article we consider

$$u_t+u_{xxx}+f(u)u_x^k=0, \quad k>0, \tag{7.7}$$

which is clearly a special case of (1.1). Group classification of this equation is given in a table (see Table II).[22] These results can immediately be derived from those obtained in this paper either directly or performing a change of independent or dependent variables.

Note that the equations that do not appear in the classification list can be recovered from those by suitable point transformations.

A number of integrable KdV type equations can be reproduced by restricting the arbitrary functions contained in invariant equations of this article. For example, the realization $A^2_{3,7}$ is equivalent to $\{\partial_t,\partial_x,t\partial_t+x/3\partial_x-u/3\partial_u\}$ under the transformation $u\to u^{-1/3}$. We have the invariant function

$$F=u^4\tilde{F}(\omega_1,\omega_2), \quad \omega_1=u^{-2}u_x, \quad \omega_2=u^{-3}u_{xx}.$$

Setting $\tilde{F}=\omega_1$ produces the modified KdV (mKdV) equation

TABLE II. Symmetry classification of (7.7).

N	k	$f(u)$	Symmetry generators	Symmetry algebra
1	arb.	arb.	∂_t,∂_x	$A_{2,1}^1$
2	k	u^n	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x+\frac{k-3}{k+n-1}u\partial_u,\quad k+n\neq 1$	$A_{3,7}^2$
3	k	e^u	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x+(k-3)\partial_u$	$A_{3,7}^2$
4	k	1	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x+\frac{k-3}{3(k-1)}u\partial_u,\partial_u,\quad k\neq 1$	$A_{4,3}^1$
5	3	arb.	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x$	$A_{3,7}^1$
6	3	u^{-2}	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x,u\partial_u$	$A_{3,7}^1\oplus A_1$
7	3	1	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x,\partial_u$	$A_{3,7}^1\oplus A_1$
8	1	u^n+c	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x-\frac{2}{n}u\partial_u,\quad n\neq 0$	$A_{3,7}^2$
9	1	u	$\partial_t,\partial_x,t\partial_t+\frac{x}{3}\partial_x-\frac{2}{3}u\partial_u,t\partial_x+\partial_u$	$A_{4,6}^1$
10	1	e^u+c	$\partial_t,\partial_x,t\partial_t+\frac{1}{3}(\partial_x+2ct)\partial_x-\frac{2}{3}\partial_u$	$A_{3,7}^2$
11	1	1	$\partial_t,\partial_x,t\partial_t+\frac{1}{3}(x+2t)\partial_x,u\partial_u,g(x,t)\partial_u$ $g_t+g_{xxx}+g_x=0$	Linear equation ($N=6$ in Table I)

$$u_t=u_{xxx}+u^2u_x. \tag{7.8}$$

Since the maximal symmetry algebra of the mKdV equation is three-dimensional, it is not isomorphic to the KdV algebra. This implies that there is no point transformation, transforming the mKdV equation into KdV equation. In this respect let us mention that there is the well-known nonlocal transformation (Miura transformation),

$$\tilde{u}=u^2\pm\sqrt{6}iu_x,$$

taking the mKdV (7.8) into the KdV equation $\tilde{u}_t=\tilde{u}_{xxx}+\tilde{u}\tilde{u}_x$. Another integrable equation which can be obtained from our classification is[23]

$$u_t=u_{xxx}+3(u_{xx}u^2+3uu_x^2)+3u^4u_x.$$

Its symmetry algebra is isomorphic to $A_{3,7}^2$. Note that this equation can be linearized by a change of dependent variable.

Let us mention that a classification based on higher order symmetries of third order integrable nonlinear equations of the form

$$u_t=u_{xxx}+F(u,u_x,u_{xx}) \tag{7.9}$$

is given in Ref. 24. We should also note that the question of finding PDEs admitting Lie point symmetries is different than finding integrable PDEs. In the latter case one requires the existence of a generalized one as opposed to Lie point symmetries. For the classification of integrable PDEs we refer the reader to Refs. 25–27.

Finally, let us point out that in a very recent work[28] a class of integrable (in the sense of existence of an infinite number of generalized symmetries) third order evolution equations of the

form (7.9) for specific F admitting recursion operators have been analyzed. Among others, the special cases corresponding to $\tilde{F}=3\omega$ and $\tilde{F}=3/2-3\omega$ of (6.1) produce the following equations with 4-dimensional symmetry algebra $A_{3,7}^1\oplus A_1$:

$$u_t=u_{xxx}+3u^{-1}u_xu_{xx},$$

$$u_t=u_{xxx}-3u^{-1}u_xu_{xx}+\tfrac{3}{2}u^{-2}u_x^3,$$

both of which were shown to admit recursion operators. This fact indicates that many equations with relatively large symmetry groups in our classification are among the most probable candidates for being integrable.

We note that the maximal symmetry algebra of the first equation of the above list is infinite-dimensional with basis elements:

$$X_1=\partial_t,\quad X_2=\partial_x,\quad X_3=t\partial_t+\frac{x}{3}\partial_x+\frac{u}{2}\partial_u,$$

$$X(\rho)=\rho(x,t)u^{-1}\partial_u,\quad \rho_t=\rho_{xxx}.$$

The existence of an infinite-dimensional symmetry algebra suggests linearizability of the equation by point transformations and, indeed, it is linearized by the change of dependent variable $v(x,t)=u^2(x,t)/2$.

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$d^3=0$, $d^2=0$ differential calculi on certain noncommutative (super) spaces

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In this paper, we construct a covariant differential calculus on a quantum plane with two-parametric quantum group as a symmetry group. The two cases $d^2=0$ and $d^3=0$ are completely established. We also construct differential calculi $n=2$ and $n=3$ nilpotent on super quantum spaces with one and two-parametric symmetry quantum supergroup. © *2004 American Institute of Physics.*
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I. INTRODUCTION

A noncommutative quantum (super) space[1,2] is an unital, associative algebra with a quantum (super) group as a symmetry group. These objects[3,4] have enriched the arena of mathematics and mathematical physics: they appear in the context of theory of knots and braids,[5] as well as in the study of Yang–Baxter equations.[6] Quantum (super) groups are deformations of the enveloping (super) algebra of classical Lie groups in the sense that one recovers the classical (super) commutator when the deformation parameters go to some particular values. Usually the generators of a quantum (super) group are assumed to commute with the noncommuting coordinates of the corresponding (super) plane. As a consequence, the quantum (super) plane admits a quantum group as a symmetry group with only one parameter: $(GL_q(1/1))GL_q(2)$.[7] More generally, one can obtain a multiparametric quantum (super) group, if one relaxes this property (commutation between space coordinates and group generators), namely, $GL_{p,q}(1/1)$[8] and $GL_{p,q}(2)$,[9] respectively, in the two-dimensional quantum superplane and quantum plane cases.

Many authors[8,10–16] have also studied differential calculus with nilpotency $n=2$ on (super) spaces with one or two-parameter (super) group as symmetry groups. An adequate way leading to generalization of this ordinary differential calculus arises from the graded differential algebra.[17–22] The latter involves a complex parameter that satisfies some conditions allowing to obtain a consistent generalized differential calculus. The most important property of this calculus is that the operator "d" satisfies $\{d^n=0/d^l\neq 0,\ 1\leqslant l\leqslant n-1\}$ and it contains as a consequence, not only first differentials dx^i, $i=1,\ldots,m$, but involves also higher order differentials $d^j x^i$, $j=1,\ldots,n-1$.

In this paper, we construct covariant differential calculus $d^3=0$ on certain quantum (super) spaces with one or two-parametric quantum group as a symmetry groups. We will show that our differential calculus is covariant under the algebra with a quantum group structure. The complex j, which appears in the Leibniz rule, is a third root of unity and will be an interesting and nontrivial aspect of the differential calculus that we will introduce.

This paper is organized as follows:

In Sec. II we start by recalling the two-parameter quantum group acting on a two-dimensional quantum plane. We also establish $n=2$ and $n=3$ covariant differential calculi on this space following the Coquereaux *et al.* approach.[14,15] It will be noticed that some modifications have been brought up to this approach in order to adapt it to the two-parameter quantum group sym-

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metry and the $n=3$ differential calculus. In Sec. III, the same method will be applied to construct the $n=2$, $n=3$ covariant differential calculus on $1+1$-dimensional superspace with one parameter quantum supergroup as a supersymmetry group. In Sec. IV we generalize the results of Sec. III by taking the two-parameter quantum group acting covariantly on the superspace.

II. DIFFERENTIAL CALCULUS ON A TWO-PARAMETRIC QUANTUM PLANE

A. Preliminaries

The two-dimensional quantum plane is an associative algebra generated by two noncommuting coordinates x and y[1,2,14] satisfying the relation

$$xy=q\,yx \quad , \quad q\neq 0,1 \quad (q\in C). \tag{1}$$

In order to have a two-parameter quantum group $\mathrm{GL}_{p,q'}(2)$ as a symmetry group of such a space,[9] one must assume that the coordinates do not commute in general with elements defining this group. Indeed, for a generic element $T=\left(\begin{smallmatrix} a & b \\ c & \mathrm{d}\end{smallmatrix}\right)$ of $\mathrm{GL}_{p,q'}(2)$, the relations between the matrix entries and the coordinates are assumed to be[9]

$$\begin{aligned} x\,a&=q_{11}\,a\,x, \quad y\,a=q_{21}\,a\,y,\\ x\,b&=q_{12}\,b\,x, \quad y\,b=q_{22}\,b\,y,\\ x\,c&=q_{13}\,c\,x, \quad y\,c=q_{23}\,c\,y,\\ x\,\mathrm{d}&=q_{14}\,\mathrm{d}\,x, \quad y\,\mathrm{d}=q_{24}\,\mathrm{d}\,y. \end{aligned} \tag{2}$$

The coordinates x and y transform under T and ${}^tT$ (transposed matrix) as

$$\begin{pmatrix} x\\ y\end{pmatrix}\overset{T}{\to}\begin{pmatrix} x'\\ y'\end{pmatrix}=\begin{pmatrix} a & b\\ c & \mathrm{d}\end{pmatrix}\begin{pmatrix} x\\ y\end{pmatrix},$$

$$\begin{pmatrix} x\\ y\end{pmatrix}\overset{{}^tT}{\to}\begin{pmatrix} x''\\ y''\end{pmatrix}=\begin{pmatrix} a & c\\ b & \mathrm{d}\end{pmatrix}\begin{pmatrix} x\\ y\end{pmatrix}.$$

The requirement that the transformed coordinates obey a similar relation as Eq. (1) (not necessarily with the same deformation parameter q), i.e.,

$$x'y'=\overline{q}\,y'x', \quad \overline{q}\in C, \tag{3}$$

$$x''y''=\bar{\bar{q}}y''x'', \quad \bar{\bar{q}}\in C, \tag{4}$$

and taking account of the defining relations of $\mathrm{GL}_{p,q'}(2)$,[13]

$$\begin{aligned} ab&=p\,ba, \quad c\mathrm{d}=p\,\mathrm{d}c,\\ ac&=q'\,ca, \quad b\mathrm{d}=q'\,\mathrm{d}b,\\ p\,bc&=q'\,cb, \quad a\mathrm{d}-\mathrm{d}a=\left(p-\frac{1}{q'}\right)bc, \end{aligned} \tag{5}$$

for some nonzero p, q' with $pq'\neq -1$, implicates further constraints on the involved parameters:

$$\overline{q}=\bar{\bar{q}}$$

and

$$
\begin{aligned}
&q_{11}=1, \quad q_{21}=qq'^{-1}k,\\
&q_{12}=\bar{q}p^{-1}, \quad q_{22}=q\bar{q}p^{-1}[\bar{q}-(p-q'^{-1})k],\\
&q_{13}=\bar{q}q'^{-1}, \quad q_{23}=q\bar{q}q'^{-1}[\bar{q}-(p-q'^{-1})k],\\
&q_{14}=\bar{q}q'^{-1}k, \quad q_{24}=q\bar{q}^2q'^{-1}p^{-1}[\bar{q}-(p-q'^{-1})k].
\end{aligned}
\tag{6}
$$

One can check that the matrix $T=\left(\begin{smallmatrix} a & b \\ c & \mathrm{d} \end{smallmatrix}\right)$ is indeed an element of the quantum group $\mathrm{GL}_{p,q'}(2)$ and is consistent with Hopf algebra structures.[9] For supplementary properties and results concerning the quantum group $\mathrm{GL}_{p,q'}(2)$ see, for example, Ref. 13.

It is clear that many quantum planes could be associated to this two-parameter quantum group, depending on choices of the q_{ij}'s. In the following, we shall confine our selves to the case $\bar{q}=q$, which corresponds to the standard definition of the quantum plane.

B. Differential calculus with nilpotency $n=2$ ($\mathrm{d}^2=0$)

Our aim in this section, is to construct a differential calculus on the previously defined quantum plane. We proceed using the same approach as the one adopted in Refs. 14, 15, and 20.

We start by defining the exterior differential "d" which satisfies the usual properties, namely,

(i) linearity;

(ii) nilpotency,

$$\mathrm{d}^2=0;$$

(iii) Leibniz rule,

$$\mathrm{d}(uv)=\mathrm{d}(u)v+(-1)^n u\,\mathrm{d}(v),$$

where $u\in\Omega^n$. Ω^n is the space of forms with degree n,

$$\mathrm{d}:\Omega^n\to\Omega^{n+1}.$$

Ω^0 is the algebra of functions defined on the quantum plane. We have also

$$\mathrm{d}(x)=\mathrm{d}x, \quad \mathrm{d}(y)=\mathrm{d}y, \quad \text{and } \mathrm{d}(1)=0. \tag{7}$$

From (2), we deduce

$$
\begin{aligned}
&(\mathrm{d}x)a=q_{11}\,a(\mathrm{d}x), \quad (\mathrm{d}y)a=q_{21}\,a(\mathrm{d}y),\\
&(\mathrm{d}x)b=q_{12}\,b(\mathrm{d}x), \quad (\mathrm{d}y)b=q_{22}\,b(\mathrm{d}y),\\
&(\mathrm{d}x)c=q_{13}\,c(\mathrm{d}x), \quad (\mathrm{d}y)c=q_{23}\,c(\mathrm{d}y),\\
&(\mathrm{d}x)\mathrm{d}=q_{14}\,\mathrm{d}(\mathrm{d}x), \quad (\mathrm{d}y)\mathrm{d}=q_{24}\,\mathrm{d}(\mathrm{d}y).
\end{aligned}
\tag{8}
$$

One can write *a priori* $x\,\mathrm{d}x, x\,\mathrm{d}y, y\,\mathrm{d}x$, and $y\,\mathrm{d}y$ in terms of $(\mathrm{d}x)x, (\mathrm{d}y)x, (\mathrm{d}x)y$, and $(\mathrm{d}y)y$, by means of 16 unknown coefficients.[14] Imposing the covariance of the obtained relations under $\mathrm{GL}_{p,q'}(2)$, and differentiating Eq. (1), permit to fix 15 of the 16 unknown coefficients. The associativity of the expression $(x\,\mathrm{d}x)\mathrm{d}y=x(\mathrm{d}x\,\mathrm{d}y)$ enables us to fix the last unknown parameter.

We notice that in the usual case $\mathrm{Gl}_q(2)$ this approach yields directly the desired differential calculus. However, when $\mathrm{GL}_{p,q'}(2)$ is a symmetry group, we obtain additional conditions on the parameters k and q',

$$q'=q \quad , \quad k=\frac{q'}{p}. \tag{9}$$

Then Eq. (6) becomes

$$q_{11}=q_{13}=1\ ,\quad q_{12}=q_{14}=q_{21}=q_{23}=qp^{-1}\ ,\quad q_{22}=q_{24}=q^2p^{-2}. \tag{10}$$

So, the covariant differential calculus is given by

$$x\,\mathrm{d}x=\frac{1}{pq}\ \mathrm{d}x\,x,\quad x\,\mathrm{d}y=\frac{1}{p}\ \mathrm{d}y\,x,$$

$$y\,\mathrm{d}y=\frac{1}{pq}\ \mathrm{d}y\,y,\quad y\,\mathrm{d}x=\left(\frac{1}{pq}-1\right)\ \mathrm{d}y\,x+\frac{1}{q}\ \mathrm{d}x\,y, \tag{11}$$

$$\mathrm{d}x\,\mathrm{d}y=-\frac{1}{p}\ \mathrm{d}y\,\mathrm{d}x,\quad (\mathrm{d}x)^2=(\mathrm{d}y)^2=0,$$

and the differential algebra is $\Omega_{x,y}^{q,p}=\{x,y,\mathrm{d}x,\mathrm{d}y\}$.

It is remarkable that the differential calculus on the quantum plane with $\mathrm{GL}_q(2)$, as a symmetry group,[11,12,14] can be obtained from the two-parameter one Eq. (11) in the $p\to q$ limit.

As in the ordinary case, the differential operator d can be realized by

$$\mathrm{d}:=\mathrm{d}x\,\partial x+\mathrm{d}y\,\partial y\ .$$

Based on this realization one can construct a gauge field theory on the two-parameter quantum plane. This should be achieved formally as in Ref. 20.

The nilpotent differential calculus can be extended to higher orders, as there is no reason to constrain this one to $n=2$ nilpotency.[17–20,23–27]

In the following section, we generalize the differential calculus on the quantum plane with one-parameter symmetry group[20] to the two-parameter one, this is done by extending the $n=2$ differential calculus obtained here to $n=3$ case.

C. Differential calculus with nilpotency $n=3$ ($\mathrm{d}^3=0$)

Let us introduce the differential operator "d" that satisfies the following conditions:

(i) linearity;

(ii) nilpotency,

$$\mathrm{d}^3=0\ ,\quad \mathrm{d}^2\neq 0;$$

(iii) Leibniz rule,

$$\mathrm{d}(uv)=(\mathrm{d}u)v+(j)^n u\,\mathrm{d}(v).$$

where j is the cubic root of unity: $j=e^{2i\pi/3}$, $1+j+j^2=0$. u is an element of Ω^n, the space of forms with degree n. It is a subspace of the differential algebra $\tilde{\Omega}_{x,y}^{q,p}=\{x,y,\mathrm{d}x,\mathrm{d}y,\mathrm{d}^2x,\mathrm{d}^2y\}$. The new objects d^2x and d^2y which appear are defined by

$$\mathrm{d}(\mathrm{d}x)=\mathrm{d}^2(x)=\mathrm{d}^2x\quad ,\quad \mathrm{d}(\mathrm{d}y)=\mathrm{d}^2(y)=\mathrm{d}^2y,$$

these are "forms" with degree two.

In order to ensure the covariance of the differential calculus under the two-parameter symmetry group $\mathrm{GL}_{p,q'}(2)$, we proceed as in the preceding section. However, instead of the last step where we have used the associativity property, we shall use the independence between the two different 2-forms $z\,\mathrm{d}^2z'$ and $\mathrm{d}z\,\mathrm{d}z'$, where $z,\ z'=x,y$. Below, we will discuss how to recover this property.

The same constraints on q' and k, Eq. (9), are recovered, thus the q_{ij}'s are the same as in Eq. (10). The covariant differential calculus is then given by

$$x\,\mathrm{d}x = j^2\,\mathrm{d}x\,x, \quad x\,\mathrm{d}y = -\frac{jq}{1+qp}\,\mathrm{d}y\,x + \frac{j^2qp-1}{1+qp}\,\mathrm{d}x\,y,$$

$$y\,\mathrm{d}y = j^2\,\mathrm{d}y\,y, \quad y\,\mathrm{d}x = \frac{j^2-qp}{1+qp}\,\mathrm{d}y\,x - \frac{jp}{1+qp}\,\mathrm{d}x\,y,$$

$$x\,\mathrm{d}^2x = j^2\,\mathrm{d}^2x\,x, \quad x\,\mathrm{d}^2y = -\frac{jq}{1+qp}\,\mathrm{d}^2y\,x + \frac{j^2qp-1}{1+qp}\,\mathrm{d}^2x\,y,$$

$$y\,\mathrm{d}^2y = j^2\,\mathrm{d}^2y\,y, \quad y\,\mathrm{d}^2x = \frac{j^2-qp}{1+qp}\,\mathrm{d}^2y\,x - \frac{jp}{1+qp}\,\mathrm{d}^2x\,y, \tag{12}$$

$$\mathrm{d}x\,\mathrm{d}^2x = j\,\mathrm{d}^2x\,\mathrm{d}x, \quad \mathrm{d}x\,\mathrm{d}^2y = -\frac{q}{1+qp}\,\mathrm{d}^2y\,\mathrm{d}x + \frac{jqp-j^2}{1+qp}\,\mathrm{d}^2x\,\mathrm{d}y,$$

$$\mathrm{d}y\,\mathrm{d}^2y = j\,\mathrm{d}^2y\,\mathrm{d}y, \quad \mathrm{d}y\,\mathrm{d}^2x = \frac{j-j^2qp}{1+qp}\,\mathrm{d}^2y\,\mathrm{d}x - \frac{p}{1+qp}\,\mathrm{d}^2x\,\mathrm{d}y,$$

$$\mathrm{d}x\,\mathrm{d}y = q\,\mathrm{d}y\,\mathrm{d}x, \quad \mathrm{d}^2x\,\mathrm{d}^2y = q\,\mathrm{d}^2y\,\mathrm{d}^2x.$$

Moreover, a realization of "d" in terms of partial derivatives,

$$\mathrm{d} = \mathrm{d}x\,\partial_x + \mathrm{d}y\,\partial_y \tag{13}$$

permits us to have $(\mathrm{d}x)^3 = (\mathrm{d}y)^3 = 0$.[20]

We note that the differential algebra $\tilde{\Omega}^{q,p}_{x,y}$, defined above, is not associative. One can check this statement by first assuming that this property (associativity) is preserved, then deriving some inconsistent relations. Especially, one expects, due to this assumption, the two expressions $(x\,\mathrm{d}x)\mathrm{d}y$ and $x(\mathrm{d}x\,\mathrm{d}y)$ to be equal. However, using (12) and successively moving the parentheses, one obtains two expressions which are manifestly not equal, unless $pq = j^2$.

Thus, the differential algebra $\tilde{\Omega}^{q,p}_{x,y}$ is associative only when $pq = j^2$, otherwise it is not.

Another associative 3-nilpotent differential algebra, for $pq = j$, can be constructed basing on the method already mentioned in Sec. II B, with a proper substitution of the differential operator $\mathrm{d}^2 = 0$ with the one $\mathrm{d}^3 = 0$, $(\mathrm{d}^2 \neq 0)$. It follows from this method that the commutation relations between the coordinates and their first order differentials are given (by the first ones) in (11). The first, second, and third differentiations of these relations give rise to the remaining commutation relations between x, y, $\mathrm{d}x$, $\mathrm{d}y$, d^2x, and d^2y.

The results of Ref. 20 (i.e., differential calculus on a reduced quantum plane, respectively, with $q^3 = 1$ and $q^N = 1$) can be recovered as limiting cases of the one obtained here (12); this is done by taking the adequate limit $p \to q$ (respectively, with $q^3 = 1$ and $q^N = 1$).

It is also remarkable that the case $n = 3$ differential calculus was applied to introduce interesting "Higher order gauge theories."[18–20] Indeed, an interesting manner to do this (in the present case) is to pursue the same steps of Ref. 20.

Another important question arises at this step is how to adapt the techniques applied in Secs. II B and II C to the quantum superplane. This will be developed in the next section.

III. DIFFERENTIAL CALCULUS ON A ONE-PARAMETER QUANTUM SUPERPLANE

A. $n = 2$ differential calculus

The $1+1$ dimensional quantum superspace, in Manin's approach,[2,7] is an algebra generated by a bosonic and a fermionic coordinate satisfying the relations

$$x\theta = q\,\theta x, \quad q \neq 0,1, \tag{14}$$

$$\theta^2=0. \tag{15}$$

In analogy with the quantum plane, a symmetry supergroup of this space is $GL_q(1/1)$, and a generic element of this supergroup is a supermatrix: $T=\left(\begin{smallmatrix} a & \beta \\ \gamma & \mathrm{d} \end{smallmatrix}\right)$, where a, d are bosonic elements commuting with x and θ while β, γ are fermionic elements commuting with x, anticommuting with θ and obeying the following relations:

$$\begin{gathered} a\beta=q\,\beta a, \quad \mathrm{d}\beta=q\,\beta\mathrm{d}, \\ a\gamma=q\,\gamma a, \quad \mathrm{d}\gamma=q\,\gamma\mathrm{d} \\ \beta\gamma+\gamma\beta=0, \quad \beta^2=\gamma^2=0, \\ a\mathrm{d}-\mathrm{d}a=(q^{-1}-q)\,\beta\gamma. \end{gathered} \tag{16}$$

These relations can also be obtained by imposing the invariance of Eqs. (14) and (15) under T and ${}^{st}T=\left(\begin{smallmatrix} a & -\gamma \\ \beta & \mathrm{d} \end{smallmatrix}\right)$ (supertranspose).

Many authors studied the differential calculus on this superspace.[8,10,27,28] Here we construct the differential calculus based on the same technique adopted by Couquereaux *et al.*[14] which is used in the preceding section, with however, some modifications to adapt it to this superspace. We introduce an exterior differential operator "d" satisfying the properties:

(i) linearity,

$$\mathrm{d}(\lambda u)=(-1)^{\hat{\lambda}}\,\lambda\,\mathrm{d}(u), \tag{17}$$

where the parity $\hat{\lambda}=0,1$ respectively, if λ is a bosonic or a fermionic element.

(ii) Nilpotency,

$$\mathrm{d}^2=0.$$

(iii) Leibniz rule,

$$\mathrm{d}(uv)=(\mathrm{d}u)v+(-1)^{\hat{u}}(-1)^{\deg u}u(\mathrm{d}v), \tag{18}$$

where $\hat{u}$ is the parity of u and $\deg u$ is the degree of the differential form u.

Note that consistency requires that $\mathrm{d}\theta$ commutes with a, d, β, γ and $\mathrm{d}x$ commutes with a, d and anticommutes with β, γ.

The same method applied in Sec. II B yields

$$\begin{gathered} x\,\mathrm{d}x=q^{-2}\,\mathrm{d}x\,x, \quad x\,\mathrm{d}\theta = q^{-1}\,\mathrm{d}\theta\,x, \\ \theta\,\mathrm{d}\theta=\mathrm{d}\theta\,\theta, \quad \theta\,\mathrm{d}x = (1-q^{-2})\,\mathrm{d}\theta\,x-q^{-1}\,\mathrm{d}x\,\theta, \\ \mathrm{d}x\,\mathrm{d}\theta=q^{-1}\,\mathrm{d}\theta\,\mathrm{d}x, \quad (\mathrm{d}x)^2 = 0, \end{gathered} \tag{19}$$

and the associative differential algebra is denoted $\Omega^q_{x,\theta}=\{x,\theta,\mathrm{d}x,\mathrm{d}\theta\}$.

As in Sec. II C, one can apply the same method to generalize the differential calculus on the superspace to higher orders ($\mathrm{d}^3=0$). This is the aim of the next section.

B. Differential calculus on superspace with nilpotency $n=3$ ($\mathrm{d}^3=0$)

We proceed as in Sec. II C, in order to construct the $n=3$ covariant differential calculus on superspace. We introduce a differential operator "d" satisfying the usual requirements, namely, linearity is the same as in Eq. (17), the nilpotency will be changed to $n=3$ ($\mathrm{d}^3=0$) and the Leibniz rule, Eq. (18) becomes

$$\mathrm{d}(uv)=(\mathrm{d}u)v+(-1)^{\hat{u}}(j)^{\deg u}u(\mathrm{d}v). \tag{20}$$

The resulting differential algebra $\tilde{\Omega}^{q}_{x,\theta}$ is generated by, x, θ, $\mathrm{d}x$, $\mathrm{d}\theta$, d^2x, and $\mathrm{d}^2\theta$ satisfying

$$
\begin{gathered}
x\,\mathrm{d}x = j^2\,\mathrm{d}x\,x, \quad x\,\mathrm{d}\theta = -\frac{jq}{1+q^2}\ \mathrm{d}\theta\,x + \frac{j^2q^2-1}{1+q^2}\ \mathrm{d}x\ \theta, \\
\theta\,\mathrm{d}\theta = \mathrm{d}\theta\ \theta, \quad \theta\,\mathrm{d}x = \frac{q^2-j^2}{1+q^2}\ \mathrm{d}\theta\,x + \frac{jq}{1+q^2}\ \mathrm{d}x\ \theta, \\
\mathrm{d}x\,\mathrm{d}\theta = -q\,\mathrm{d}\theta\,\mathrm{d}x, \quad (\mathrm{d}\theta)^2 = 0, \\
x\,\mathrm{d}^2x = j^2\,\mathrm{d}^2x\,x, \quad x\,\mathrm{d}^2\theta = -\frac{jq}{1+q^2}\ \mathrm{d}^2\theta\,x + \frac{j^2q^2-1}{1+q^2}\ \mathrm{d}^2x\ \theta, \\
\theta\,\mathrm{d}^2\theta = -\mathrm{d}^2\theta\ \theta, \quad \theta\,\mathrm{d}^2x = \frac{j^2-q^2}{1+q^2}\ \mathrm{d}^2\theta\,x - \frac{jq}{1+q^2}\ \mathrm{d}^2x\ \theta, \\
\mathrm{d}x\,\mathrm{d}^2x = j\,\mathrm{d}^2x\,\mathrm{d}x, \quad \mathrm{d}x\,\mathrm{d}^2\theta = \frac{q}{1+q^2}\ \mathrm{d}^2\theta\,\mathrm{d}x + \frac{jq^2-j^2}{1+q^2}\ \mathrm{d}^2x\,\mathrm{d}\theta, \\
\mathrm{d}\theta\,\mathrm{d}^2\theta = j^2\,\mathrm{d}^2\theta\,\mathrm{d}\theta, \quad \mathrm{d}\theta\,\mathrm{d}^2x = \frac{j^2q^2-j}{1+q^2}\ \mathrm{d}^2\theta\,\mathrm{d}x - \frac{q}{1+q^2}\ \mathrm{d}^2x\,\mathrm{d}\theta, \\
\mathrm{d}^2x\,\mathrm{d}^2\theta = q\,\mathrm{d}^2\theta\,\mathrm{d}^2x, \quad (\mathrm{d}^2\theta)^2 = 0.
\end{gathered}
\tag{21}
$$

Let us point out that the differential algebra $\tilde{\Omega}^{q}_{x,\theta}$ is not associative, unless $q=j$. In the case $q\neq j$, one can recover this property by following the same steps mentioned at the end of Sec. II C with the adequate modifications.

IV. DIFFERENTIAL CALCULUS ON A TWO-PARAMETER QUANTUM SUPERPLANE

A. Differential calculus with nilpotency $n=2$ ($\mathrm{d}^2=0$)

In this section, we generalize the results of Sec. III, in the sense that we choose a two-parametric quantum supergroup $\mathrm{GL}_{p,q'}(1/1)$ as a symmetry group for the superplane Eqs. (14) and (15). This group will be introduced using the same method as in Sec. II.[8,9]

The entries of a matrix element $T=\left(\begin{smallmatrix} a & \beta \\ \gamma & \mathrm{d} \end{smallmatrix}\right)$ of $\mathrm{GL}_{p,q'}(1/1)$ satisfy the following nontrivial relations:

$$
\begin{gathered}
a\beta = p\ \ \beta a, \quad \mathrm{d}\beta = p\ \beta\mathrm{d}, \\
a\gamma = q'\ \ \gamma a, \quad \mathrm{d}\gamma = q'\ \gamma\mathrm{d}, \\
p\ \ \beta\gamma + q'\ \ \gamma\beta = 0, \quad \beta^2 = \gamma^2 = 0, \\
a\mathrm{d} - \mathrm{d}a = (q'^{-1} - p)\ \ \beta\gamma.
\end{gathered}
\tag{22}
$$

As it is done in Sec. II this superspace is covariant under T and ${}^{st}T$ (supertranspose), and the analogous of Eq. (2) are

$$
\begin{aligned}
x\,a &= k\,a\,x, \quad \theta\,a = q\bar{q}q'^{-1}p^{-1}k\,a\,\theta,\\
x\,b &= \bar{q}p^{-1}k\,b\,x, \quad \theta\,b = -q\bar{q}^2q'^{-1}p^{-2}k\,b\,\theta,\\
x\,c &= \bar{q}q'^{-1}k\,c\,x, \quad \theta\,c = -q\bar{q}^2q'^{-2}p^{-1}k\,c\,\theta,\\
x\,\mathrm{d} &= \bar{q}^2q'^{-1}p^{-1}k\,\mathrm{d}\,x, \quad \theta\,\mathrm{d} = q\bar{q}^3q'^{-2}p^{-2}k\,\mathrm{d}\,\theta.
\end{aligned}
\tag{23}
$$

We are interested in establishing a covariant differential calculus on this superspace in the case $\bar{q}=\bar{\bar{q}}=q$. To achieve this construction, for $n=2$, we introduce a differential operator "d" satisfying the same properties as in Sec. III B [linearity Eq. (17), nilpotency, and Leibniz rule Eq. (18)]. The associative differential algebra $\Omega^{p,q}_{x,\theta}=\{x,\theta,\mathrm{d}x,\mathrm{d}\theta\}$ is generated by the following relations:

$$
\begin{aligned}
x\,\mathrm{d}x &= (qp)^{-1}\,\mathrm{d}x\,x, \quad x\,\mathrm{d}\theta = p^{-1}\,\mathrm{d}\theta\,x,\\
\theta\,\mathrm{d}\theta &= \mathrm{d}\theta\,\theta, \quad \theta\,\mathrm{d}x = (1-(qp)^{-1})\ \mathrm{d}\theta\,x - q^{-1}\,\mathrm{d}x\,\theta,\\
\mathrm{d}x\,\mathrm{d}\theta &= p^{-1}\,\mathrm{d}\theta\,\mathrm{d}x, \quad (\mathrm{d}x)^2 = 0.
\end{aligned}
\tag{24}
$$

We have used $q'=q$ and $k=q/p$, which, as in Eq. (9), are consequences of the requirement of the covariance of $\Omega^{p,q}_{x,\theta}$ under $\mathrm{GL}_{p,q'}(1/1)$.

As expected, in the limit $p\to q$, we recover $\Omega^{q}_{x,\theta}$ and relations (19).

B. Differential calculus with nilpotency $n=3$ ($\mathrm{d}^3=0$)

The technique used in Secs. II C and III C, allows us to construct the $n=3$ differential algebra $\tilde{\Omega}^{p,q}_{x,\theta}=\{x,\theta,\mathrm{d}x,\mathrm{d}\theta,\mathrm{d}^2x,\mathrm{d}^2\theta\}$,

$$
\begin{aligned}
x\,\mathrm{d}x &= j^2\,\mathrm{d}x\,x, \quad x\,\mathrm{d}\theta = -\frac{jq}{1+qp}\ \mathrm{d}\theta\,x + \frac{j^2qp-1}{1+qp}\ \mathrm{d}x\,\theta,\\
\theta\,\mathrm{d}\theta &= \mathrm{d}\theta\,\theta, \quad \theta\,\mathrm{d}x = \frac{qp-j^2}{1+qp}\ \mathrm{d}\theta\,x + \frac{jp}{1+qp}\ \mathrm{d}x\,\theta,\\
\mathrm{d}x\,\mathrm{d}\theta &= -q\,\mathrm{d}\theta\,\mathrm{d}x, \quad (\mathrm{d}\theta)^2 = 0,\\
x\,\mathrm{d}^2x &= j^2\,\mathrm{d}^2x\,x, \quad x\,\mathrm{d}^2\theta = -\frac{jq}{1+qp}\ \mathrm{d}^2\theta\,x + \frac{j^2qp-1}{1+qp}\ \mathrm{d}^2x\,\theta,\\
\theta\,\mathrm{d}^2\theta &= -\mathrm{d}^2\theta\,\theta, \quad \theta\,\mathrm{d}^2x = \frac{j^2-qp}{1+qp}\ \mathrm{d}^2\theta\,x - \frac{jp}{1+qp}\ \mathrm{d}^2x\,\theta,\\
\mathrm{d}x\,\mathrm{d}^2x &= j\,\mathrm{d}^2x\,\mathrm{d}x, \quad \mathrm{d}x\,\mathrm{d}^2\theta = \frac{q}{1+qp}\ \mathrm{d}^2\theta\,\mathrm{d}x + \frac{jqp-j^2}{1+qp}\ \mathrm{d}^2x\,\mathrm{d}\theta,\\
\mathrm{d}\theta\,\mathrm{d}^2\theta &= j^2\,\mathrm{d}^2\theta\,\mathrm{d}\theta, \quad \mathrm{d}\theta\,\mathrm{d}^2x = \frac{j^2qp-j}{1+qp}\ \mathrm{d}^2\theta\,\mathrm{d}x - \frac{p}{1+qp}\ \mathrm{d}^2x\,\mathrm{d}\theta,\\
\mathrm{d}^2x\,\mathrm{d}^2\theta &= q\,\mathrm{d}^2\theta\,\mathrm{d}^2x, \quad (\mathrm{d}^2\theta)^2 = 0.
\end{aligned}
\tag{25}
$$

The same limit as in Sec. II C, namely, $p\to q$, yields $\tilde{\Omega}^{q}_{x,\theta}$. The differential algebra $\tilde{\Omega}^{p,q}_{x,\theta}$ is not associative. In order to restore this property we proceed as mentioned at the end of Secs. II C and III B.

One physical application of the differential calculi (Secs. III and IV) is to construct a supersymmetric gauge field theory on the quantum superplane (with one or two parameter quantum supergroup as symmetry groups; the latter will be a generalization of the former). However, this is not straightforward, since one should first start by defining a supersymmetric covariant derivative.

V. CONCLUSION

In this paper, we have constructed differential calculi on certain quantum (super) spaces. Namely, the $n=2$ and $n=3$ nilpotent differential calculi on the quantum plane with two parametric quantum group ($\mathrm{GL}_{p,q}(2)$) as a symmetry group was obtained. We have also considered two cases of quantum superplanes related to the one and two-parametric quantum supergroups $\mathrm{GL}_q(1|1)$ and $\mathrm{GL}_{p,q}(1|1)$, as symmetry groups, respectively. The related $n=2$ and $n=3$ differential calculi were also established.

In general, the differential calculus can be applied to formulate gauge field theories.[29–31] As a consequence, the results obtained here permit us to construct gauge theories on the corresponding noncommutative spaces.[32] Indeed, for the quantum space (Sec. II), this can be done using the same techniques of Ref. 20, where the symmetry group is a one parameter.

The noncommutative supersymmetric case (Secs. III and IV) will be treated in the same fashion, with however, more care since it is essential first, to define a covariant supersymmetric derivative.[33,34]

We note that the differential calculus was also applied to derive a corresponding quantum oscillator, where the latter is seen as a representation of the former.[35] It will be interesting to achieve this with the differential calculus in Sec. II, as the resulting quantum oscillator will be two-parameter dependent.

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Soliton lattice and single soliton solutions of the associated Lamé and Lamé potentials

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We obtain the exact nontopological soliton lattice solutions of the associated Lamé equation in different parameter regimes and compute the corresponding energy for each of these solutions. We show that in specific limits these solutions give rise to nontopological (pulse-like) single solitons, as well as to different types of topological (kink-like) single soliton solutions of the associated Lamé equation. Following Manton, we also compute, as an illustration, the asymptotic interaction energy between these soliton solutions in one particular case. Finally, in specific limits, we deduce the soliton lattices, as well as the topological single soliton solutions of the Lamé equation, and also the sine-Gordon soliton solution. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738952]

I. INTRODUCTION

Over the years, extensive research has been carried out seeking the exact soliton solutions of both periodic (e.g., sine-Gordon, double sine-Gordon) and nonperiodic (e.g., ϕ^4, ϕ^6) field theory models. For example, the exactly solvable sine-Gordon (SG) equation[1] and its quasi-exactly solvable (QES) partner, i.e., the double sine-Gordon equation (DSG), have exact single soliton[2,3] as well as soliton lattice[4] solutions.

There have been some advances in the study of the hyperbolic analogues of these problems; the exactly solvable hyperbolic analogue of the SG equation is the sine-hyperbolic Gordon (ShG) equation.[5] This potential has only one minimum and thus does not support (topological) soliton solutions. The hyperbolic analogue of the DSG equation is the double sine-hyperbolic Gordon (DShG) equation, which is a QES double-well potential with exact single soliton and soliton lattice solutions.[6]

However, not much is known regarding the elliptic analogues of these problems. The elliptic generalization of the SG is the Lamé equation[7] but, as far as we are aware of, its single soliton and soliton lattice solutions have not been worked out yet. One would surmise that the elliptic analogue of the DSG equation is the Associated Lamé (AL) equation.[8–10] Nevertheless, we find below that this is not the case. There are many physical contexts in which the Lamé equation arises, such as bond-order and charge density wave systems,[11] nonlinear elasticity,[12] and other contexts, e.g., phase slips in superconductors, magnetoelastic interaction on curved surfaces and symmetric monopoles.[13] The Lamé equation appears in systems with a single periodicity such as a one-dimensional array of identical atoms with a certain strength of the potential. The AL equation would arise from two alternating types of atoms with different strengths of the potential. Moreover, one expects an AL equation in many of the above physical systems in the presence of external—electric, magnetic or stress—fields.

Our goal in the present paper is to obtain the exact single soliton and soliton lattice solutions for both the AL and Lamé elliptic potentials. In particular, we obtain here the soliton lattice

solutions of the AL equation in different parameter regimes corresponding to different shapes of the AL potential. The advantage of this approach is that the corresponding single pulse and topological soliton solutions of the AL equation can be immediately obtained from the lattice solution in suitable limits. Furthermore, the soliton lattices and topological single soliton solutions of the Lamé equation are easily obtained by taking a different appropriate limit. Besides, the asymptotic interaction between the solitons can also be readily obtained by using Manton's formalism.[14]

Our results can be summarized as follows: We show that there are six different soliton lattice solutions of the AL equation for different values of the parameters. From these six solutions we obtain the corresponding AL single soliton solutions. It turns out that while in five cases these are topological (kink-like) single solitons, in one case we have a nontopological (pulse-like) single soliton solution. From the AL soliton lattice solutions, by taking appropriate limits, we also obtain the corresponding Lamé soliton lattices and single soliton solutions (which are also new).

These results will serve as a background for future statistical mechanics studies of the AL and Lamé elliptic potentials. The problem of finding the partition function of the system can be mapped onto the spectral problem of a Schrödinger equation with the potential.[15] Generally speaking, the Schrödinger equations with periodic potentials belong to a class known as Hill's equations,[8] and they lead to a band structure of the energy spectrum of the system. For both the SG and DSG potentials one could calculate (either exact or approximate) statistical and thermodynamical properties[16,17] through a knowledge of the spectral band structure (or, at least, of the band edges) and of their soliton and phonon solutions, respectively. Both AL and Lamé are also periodic potentials with a band structure.[7,9,10] Although we do not pursue this any further here, our results will provide the basis for the thermodynamics of these systems, in particular the contribution of the nonlinear soliton excitations to the specific heat, etc.[15]

The plan of the paper is as follows. In Sec. II we discuss some salient features of the AL potential and consider the limits that lead to the Lamé potential. The readers who are interested only in the single soliton and soliton lattice solutions of the Lamé equation can then directly go to Sec. V. In Sec. III we obtain the nontopological soliton lattice solutions of the AL equation in different regimes in the parameter space and also compute the corresponding energies. In Sec. IV we obtain the topological and pulse single soliton solutions of the AL equation by taking the appropriate limits of the various nontopological solutions obtained in the preceding section. It is worth emphasizing here that in one special case, we obtain two different kinds of topological solutions of the AL equation. As an illustration, in one particular case, we also estimate the asymptotic interaction between these single solitons.[14] (In all the other cases one can follow exactly the same procedure, and thus we will not consider these here.) As a crosscheck on our results, we recover in appropriate limit, the sine-Gordon soliton solution. In Sec. V we show that by taking an appropriate limit in the above results, we can also obtain the (previously not known) kink lattice and the topological single soliton solutions of the Lamé equation. Finally, in Sec. VI we summarize the results obtained in this paper and indicate some open problems.

II. THE ASSOCIATED LAMÉ POTENTIAL

Consider the following family of periodic potentials labeled by a pair of real parameters (p, q):

$$V_{\mathrm{AL}}(\phi,k)=pk^2\,\mathrm{sn}^2(\phi,k)+qk^2\frac{\mathrm{cn}^2(\phi,k)}{\mathrm{dn}^2(\phi,k)}+C=pk^2\,\mathrm{sn}^2(\phi,k)+qk^2\,\mathrm{sn}^2(\phi+K(k),k)+C, \quad (1)$$

that are called *Associated Lamé potentials* (since the corresponding Schrödinger equation is called the Associated Lamé equation).[8–10] Here $\mathrm{sn}(\phi,k)$ and $\mathrm{cn}(\phi,k)$ are, respectively, the sine and cosine amplitude Jacobi elliptic functions of real modulus $k(0\leqslant k\leqslant 1)$ and period $4K(k)$; $\mathrm{dn}(\phi,k)$ is the δ-amplitude Jacobi elliptic function of modulus k and period $2K(k)$; and $K(k)$ denotes the complete elliptic integral of the first kind, see Refs. 18 and 19. We will choose the

constant C in the potential so that the absolute minimum of the potential—with respect to ϕ—equals zero, $V_{\min}=0$. The potential is periodic with period $2K(k)$, except in the limit $p=q$ when the period reduces to $K(k)$, as it is clear from Eq. (1).

The case $q=0$ corresponds to the standard Lamé potential $V_{\mathrm{L}}(\phi,k)$. There are two more cases in which the potential (1) reduces to the Lamé potential. Namely, when $p=0$ and also when $p=q$, as shown below. Therefore in all the calculations below we will admit that $p\neq 0$ and $p\neq q$; the results for the standard Lamé potential will be recovered in the limit $q\to 0$, and we refer to these results whenever the potential reduces to the standard Lamé one. From a physical point of view, if one thinks of a Lamé potential $(p, 0)$ as due to a one-dimensional array of atoms with spacing $2K(k)$ and "strength" p, then the Associated Lamé potential (p,q) results from two alternating types of atoms spaced by $K(k)$ with strengths p and q, respectively. If the two types of atoms are identical (which makes $p=q$), one expects a potential of period $K(k)$.

In addition, when $k\to 0$, and $|p|$, $|q|\to\infty$, so that $|p|k^2\to P=$ finite and $|q|k^2\to Q=$ finite, the potential (1) reduces to the sine-Gordon potential,

$$V_{\mathrm{SG}}=(P\ \mathrm{sign}\,p-Q\ \mathrm{sign}\,q)\sin^2\phi, \tag{2}$$

and the results we present below reduce to the well-known ones for the sine-Gordon potential.

Note that we cannot recover the DSG equation under any limiting condition in the parameter space of the AL equation. Indeed, the only limit where one can get sinusoidal functions from Jacobi elliptic functions of modulus k is the above-mentioned limit $k\to 0$ (of course, with $|p|$, $|q|\to\infty$, so that $|p|k^2\to P=$ finite and $|q|k^2\to Q=$ finite, otherwise the potential trivially becomes a flat one), when one obtains the SG, and *not* the DSG equation.

It is also worth noting that under the transformation $\phi\to\phi+K(k)$ the AL potential (1) $V_{\mathrm{AL}}(p,q)$ goes over into $V_{\mathrm{AL}}(q,p)$ and hence for $p>0$, $q\geqslant 0$, as well as for $p<0$, $q\leqslant 0$, without loss of generality, we shall always consider the case of $p^2>q^2$. Further, instead of considering both the possibilities of $p>0$, $q\leqslant 0$ and $p<0$, $q\geqslant 0$, it suffices to consider just the case of $p>0$, $q\leqslant 0$, but now p^2 can be bigger as well as smaller than q^2.

Finally, consider the case of $p=q$, when, by using the Landen transform[18] and choosing the constant $C=-pk^2$, the AL potential (1) can be written as

$$V_{\mathrm{AL}}(\phi,k)=(1-k')^2V_{\mathrm{L}}\left[(1+k')\phi,\frac{1-k'}{1+k'}\right], \tag{3}$$

where $k'=\sqrt{1-k^2}$ is the complementary elliptic modulus. For the rescaled field $\bar{\phi}=(1+k')\phi$ and in the rescaled space coordinate $\bar{x}=(1+k')x$ the field equations [see next section, Eq. (5)] will remain the same as that for the simple Lamé potential. Note that the $p=q$ case cannot be obtained as a limit of $q\to p$ $(q\neq p)$, since—as already mentioned—when $p=q$ the periodicity of the potential (1) is $K(k)$, while for $p\neq q$ it is $2K(k)$, see also Ref. 9.

III. SOLITON LATTICE SOLUTIONS OF THE AL POTENTIAL

For the scalar field $\phi=\phi(x,t)$ the dynamics is described by the second-order hyperbolic differential equation

$$\frac{\partial^2\phi}{\partial t^2}-\frac{\partial^2\phi}{\partial x^2}=-\frac{\partial V_{\mathrm{AL}}}{\partial\phi}. \tag{4}$$

In the stationary case $\phi=\phi(x)$, this reduces simply to

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}=\frac{\partial V_{\mathrm{AL}}}{\partial\phi}, \tag{5}$$

that can be easily integrated, at least formally, by quadratures. The time-dependent solutions are

immediately obtained from here by Lorentz boosting to velocity v, i.e., $x \to (1-v^2)^{-1/2}(x-vt)$. The physically meaningful solutions (bounded at $x \to \pm\infty$) are given by

$$\pm\sqrt{2}(x-x_0) = \int_{\phi(x_0)}^{\phi(x)} \frac{d\tilde{\phi}}{\sqrt{V_{AL}(\tilde{\phi},k)-A^2}}, \tag{6}$$

where x_0 and $A^2 \equiv |p|k^2a^2$ are the two (suitably chosen) integration constants. Of course, $V_{min} = 0 \leqslant A^2 < V_{max}$, where $V_{min/max}$ is the absolute minimum/maximum of the potential energy with respect to ϕ. In fact, in view of the condition $V_{AL}(\tilde{\phi},k) - A^2 \geqslant 0$, the actual value of A^2 determines the appropriate integration domain in Eq. (6).

Depending on the values of the parameters p and q, the potential $V_{AL}(\phi,k)$ has different behaviors in one period $0 \leqslant \phi < 2K(k)$, and hence the nature of the solutions in Eq. (6) is also different. There are three cases to be considered separately, namely (I) when $p>0$ and $q \geqslant 0$, (II) when $p<0$ and $q \leqslant 0$, and, finally, (III) when $p>0$ and $q \leqslant 0$. Note that in what follows we shall use the shorthand notation $\Gamma \equiv \sqrt{|q|/|p|}$.

A. Case I: $p>0$ and $q \geqslant 0$

As explained above, in this case it is sufficient to consider $0 \geqslant \Gamma < 1$. Note that the case $\Gamma = 0$ corresponds to the standard Lamé potential. Depending on the value of Γ, the potential $V_{AL}(\phi,k)$ can have different behaviors in one period $0 \leqslant \phi < 2K(k)$.

Case I.1: $0 \leqslant \Gamma \leqslant k'$.

Here $0 \leqslant k' = \sqrt{1-k^2} \leqslant 1$ is the complementary elliptic modulus. The potential $V_{AL}(\phi)$ has only one minimum, $V_{min} = 0$ (at $\phi = 0$), and one maximum, $V_{max} = pk^2(1-\Gamma^2)$ [at $\phi = K(k)$], in one period [note that we have chosen $C = -pk^2\Gamma^2$ in Eq. (1) in order to have $V_{min} = 0$]. The plot of the potential V_{AL} as a function of ϕ is given in Fig. 1(a), where the solid and the dashed horizontal lines correspond to two choices of the parameter A^2. Under the change of variable $\tilde{z} = \mathrm{sn}^2(\tilde{\phi},k)$, Eq. (6) can be rewritten as

$$2\sqrt{2pk^4}x = \pm \int_z^1 \frac{d\tilde{z}}{\sqrt{(z_1-\tilde{z})(1-\tilde{z})(\tilde{z}-z_2)(\tilde{z}-0)}}, \tag{7}$$

where $z = \mathrm{sn}^2(\phi,k)$, $x_0 = 0$ for $\phi_0 = K(k)$ (by choice), and $A^2 = pk^2a^2$ with $0 \leqslant a^2 < (1-\Gamma^2)$. The value of a^2 determines the limits of the integration interval in the above equation, through the condition $V(\phi_{1,2}) - pk^2a^2 = 0$; one finds that $z_{1,2} = \mathrm{sn}^2(\phi_{1,2})$ are given by

$$z_{1,2} = \frac{1-\Gamma^2k'^2+a^2k^2}{2k^2}\left[1 \pm \sqrt{1-\frac{4k^2a^2}{(1-\Gamma^2k'^2+a^2k^2)^2}}\right], \tag{8}$$

and $z_1 > 1 > z \geqslant z_2 > 0$. Then the integral in (7) can be evaluated using the formula 3.147(5) of Ref. 18 and one is finally led to the nontopological soliton lattice solution

$$\mathrm{sn}^2(\phi,k) = \frac{[(z_1-z_2)-z_1(1-z_2)\mathrm{sn}^2(y,t)]}{[(x_1-z_2)-(1-z_2)\mathrm{sn}^2(y,t)]}. \tag{9}$$

Here $y = \sqrt{2pk^4(z_1-z_2)}x$ and the period of the lattice $2L = 2K(t)/\sqrt{2pk^4(z_1-z_2)}$ is controlled by the modulus

$$0 < t = \left[\frac{z_1(1-z_2)}{z_1-z_2}\right]^{1/2} \leqslant 1. \tag{10}$$

Note that ϕ oscillates between $K(k)$ and $\mathrm{sn}^{-1}(\sqrt{z_2})$ [respectively, $-K(k)$ and $-\mathrm{sn}^{-1}(\sqrt{z_2})$], i.e., it is indeed a nontopological solution [it does not connect two adjacent degenerate minima of

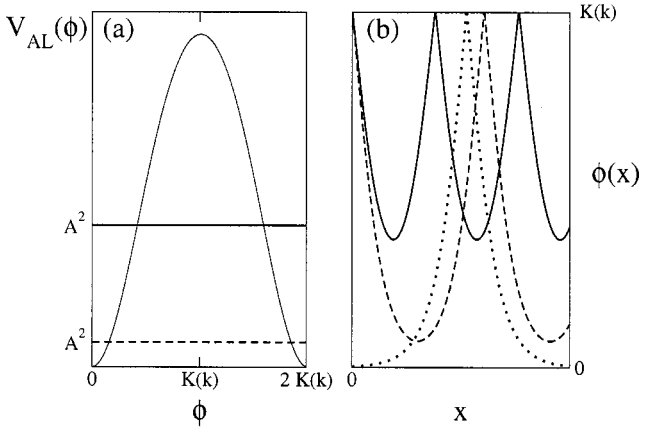

FIG. 1. Case I.1: $0 \leqslant \Gamma \leqslant k'$. (a) The shape of the potential $V_{\mathrm{AL}}(\phi)$. The solid and the dashed horizontal lines correspond to two choices of the integration parameter A^2. (b) The soliton lattice solution [i.e., the field $\phi(x)$] with solid and dashed curves corresponding to the two values of A^2 in (a). The x axis is not labeled because the two lattices have different spatial periods. The dotted curve represents the topological single soliton solution corresponding to $A^2=0$ (for the sake of clarity we have displaced the origin of the x axis for this curve). Note that in (b) and all subsequent figures we have plotted $|\phi(x)|$ modulo $2K(k)$. There are no "cusps" in the actual field $\phi(x)$.

the potential, that are separated by a distance—in the ϕ space—of $2K(k)$]. In Fig. 1(b) we give a plot of the solution (i.e., the field ϕ as a function of x) with solid and dashed curves corresponding to the two choices of A^2 as in Fig. 1(a), while the dotted curve represents the topological single soliton solution (corresponding to $A^2=0$)—see Sec. IV.

We emphasize that there are no "cusps" or slope discontinuities in the actual solutions $\phi(x)$. In order to represent the field in the same range $0<\phi(x)<K(k)$ in Fig. 1(b) and in the subsequent figures we have plotted modulo $2K(k)$ the absolute value of the actual field $\phi(x)$. This is possible because if $\phi(x)$ is a solution then $-\phi(x)$ and $2K(k)-\phi(x)$ are also solutions. Specifically, for solutions that attain the value $K(k)$ such as in Fig. 1(b), the actual field is $\phi(x)$ in $[0,2L]$, $2K(k)-\phi(x)$ in $[2L,4L]$, $\phi(x)$ in $[4L,6L]$, and so on. Similarly, for solutions that attain zero field value such as in Fig. 3(b), the actual field is $\phi(x)$ in $[0,2L]$, $-\phi(x)$ in $[2L,4L]$, $\phi(x)$ in $[4L,6L]$, and so on.

One can compute the energy corresponding to a period $2L$ of this soliton lattice:

$$
\begin{aligned}
E_{\mathrm{SL}} &= \int_{-L}^{L}\left[\frac{1}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)+V_{\mathrm{AL}}(\phi)\right]\mathrm{d}x \\
&= \int_{-L}^{L}[2V_{\mathrm{AL}}(\phi)-A^2]\mathrm{d}x \\
&= 4\int_{0}^{L}V_{\mathrm{AL}}(\phi)\mathrm{d}x-2LA^2 \\
&= 4pk^2\int_{0}^{L}\mathrm{sn}^2[\phi(x),k]\mathrm{d}x+4p^2k^2\Gamma^2\int_{0}^{L}\left\{\frac{\mathrm{cn}^2[\phi(x),k]}{\mathrm{dn}^2[\phi(x),k]}-1\right\}\mathrm{d}x-2Lp^2k^2a^2. \qquad (11)
\end{aligned}
$$

After some algebraic manipulations, using the solution (9) one obtains

$$
\begin{aligned}
E_{\mathrm{SL}} = 2\sqrt{\frac{2p}{z_1-z_2}}\Bigg\{&\left[z_1K(t)-(z_1-1)\Pi\left(\frac{1-z_2}{z_1-z_2},t\right)\right]-\frac{a^2K(t)}{2}\Bigg\} \\
&-\Gamma^2\left[\frac{z_1k'^2}{1-z_1k^2}K(t)-\frac{z_1-1}{1-z_1k^2}\Pi\left(\frac{(1-z_2)(1-z_1k^2)}{(z_1-z_2)k'^2},t\right)\right], \qquad (12)
\end{aligned}
$$

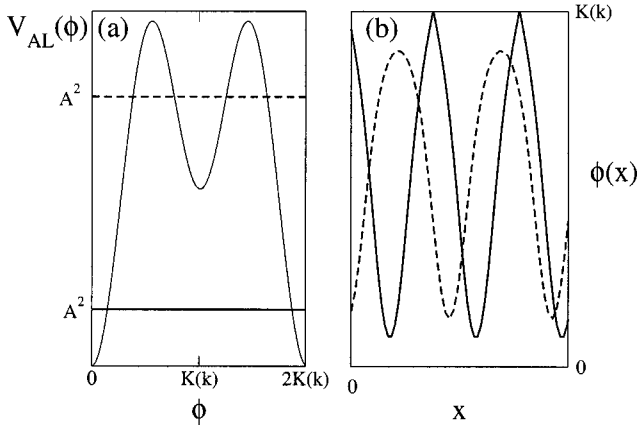

FIG. 2. Case I.2: $k'<\Gamma<1$. (a) The shape of the potential $V_{\mathrm{AL}}(\phi)$. The solid and the dashed horizontal lines correspond to two choices of the integration parameter A^2, namely, Case I.2(i): $V_{\min}\leqslant A^2=pk^2a^2<V^l_{\min}$, i.e., $0\leqslant a^2<1-\Gamma^2$ (solid line); and Case I.2(ii): $V^l_{\min}\leqslant A^2=pk^2a^2<V_{\max}$, i.e., $1-\Gamma^2\leqslant a^2<[(1-\Gamma k')/k]^2$ (dashed line). (b) The soliton lattice solution [i.e., the field $\phi(x)$] with solid and dashed curves corresponding to the two values of A^2 in (a), i.e., respectively, to Case I.2(i) and Case I.2(ii). The x axis is not labeled because the two lattices have different periodicities. We have plotted $|\phi(x)|$ modulo $2K(k)$.

where $\Pi(z_0,t)$ denotes the complete elliptic integral of the third kind.[18,19]

Case I.2: $k'<\Gamma<1$.

The potential $V_{\mathrm{AL}}(\phi)$ has now two minima: $V_{\min}(\phi=0)=0$ and a local minimum $V^l_{\min}[\phi=K(k)]=pk^2(1-\Gamma^2)$, and two symmetric maxima around $\phi=K(k)$, namely, $V_{\max}=pk^2[(1-\Gamma k')/k]^2$ for $\phi=\mathrm{sn}^{-1}[\sqrt{(1-\Gamma k')/k^2}]$, $2K(k)-\mathrm{sn}^{-1}[\sqrt{(1-\Gamma k')/k^2}]$. The plot of the potential $V_{\mathrm{AL}}(\phi)$ as a function of ϕ is given in Fig. 2(a), where the solid and the dashed horizontal lines correspond to the two choices of the integration constant A^2 as explained below. Note that in this case it makes no sense to consider either the limit of the Lamé potential (i.e., $\Gamma\to 0$), or that of the sine-Gordon potential (i.e., $k\to 0$, $pk^2\to P$, $qk^2\to Q$). There are two possible situations, depending on the value of $A^2=pk^2a^2$.

Case I.2(i): $V_{\min}\leqslant A^2=pk^2a^2<V^l_{\min}$, i.e., $0\leqslant a^2<1-\Gamma^2$.

One recovers the same soliton lattice solution as above, Eq. (9), with the same modulus t, Eq. (10), and the same energy per period of the lattice, Eq. (12).

Case I.2(ii): $V^l_{\min}\leqslant A^2=pk^2a^2<V_{\max}$, i.e., $1-\Gamma^2\leqslant a^2<[(1-\Gamma k')/k]^2$. Then the integral (6) becomes

$$2\sqrt{2pk^4}x=\pm\int_{z_2}^{z}\frac{d\tilde{z}}{\sqrt{(1-\tilde{z})(z_1-\tilde{z})(\tilde{z}-z_2)(\tilde{z}-0)}},\tag{13}$$

with $z=\mathrm{sn}^2(\phi,k)$ and $1>z_1\geqslant z>z_2$ [$z_{1,2}$ have the same expressions as above, Eq. (8)]. One can evaluate this integral using the formula 3.147(4) of Ref. 18 and obtain the following nontopological soliton lattice solution

$$\mathrm{sn}^2(\phi,k)=\frac{z_1z_2}{z_1-(z_1-z_2)\mathrm{sn}^2(w,n)},\tag{14}$$

with $w=\sqrt{2pk^4z_1(1-z_2)}x$, and the modulus n given by

$$0<n=\sqrt{\frac{z_1-z_2}{z_1(1-z_2)}}\leqslant 1;\tag{15}$$

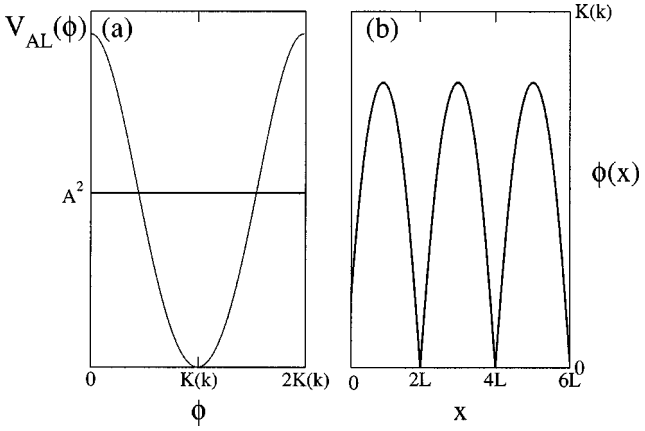

FIG. 3. Case II.1: $0\leqslant\Gamma\leqslant k'$. (a) The shape of the potential $V_{\mathrm{AL}}(\phi)$. The solid horizontal line corresponds to the integration parameter A^2. (b) The soliton lattice solution [i.e., the field $\phi(x)$] corresponding to the value of A^2 in (a). We have plotted $|\phi(x)|$ modulo $2K(k)$.

therefore, the soliton lattice has a spatial period $2L=2K(n)/\sqrt{2pk^4z_1(1-z_2)}$. Note that ϕ varies between $\mathrm{sn}^{-1}(\sqrt{z_1})$ and $\mathrm{sn}^{-1}(\sqrt{z_2})$ [respectively, $-\mathrm{sn}^{-1}(\sqrt{z_1})$ and $-\mathrm{sn}^{-1}(\sqrt{z_2})$] when x varies over one spatial period: indeed, this solution is nontopological.

In Case I.2(ii) in order to compute the energy for one spatial period $2L$, it is useful to shift the potential by $-V^l_{\mathrm{min}}=-pk^2(1-\Gamma^2)$, so that the minimum of the potential explored by the soliton lattice is equal to zero. One finds

$$E_{\mathrm{SL}}=4\int_0^L V_{\mathrm{AL}}(\phi)\mathrm{d}x-2LV^l_{\mathrm{min}}-2Lp^2k^2a^2$$
$$=2\sqrt{\frac{2p^2}{z_1(1-z_2)}}\left[z_2\Pi\left(\frac{z_1-z_2}{z_1},n\right)-\Gamma^2\frac{k'^2z_2}{1-k^2z_2}\Pi\left(\frac{z_1-z_2}{z_1(1-k^2z_2)},n\right)-\frac{a^2+(1-\Gamma^2)}{2}\right]. \tag{16}$$

The plot of the solutions in Case I.2 is given in Fig. 2(b), where the solid line corresponds to the nontopological soliton lattice solution of Case I.2(i), while the dashed line corresponds to the nontopological soliton lattice solution of Case I.2(ii). Note that in the appropriate limits (see Sec. IV) these two types of solutions give birth to a topological [Case I.2(i)] and a nontopological single soliton [Case I.2(ii)] solution, respectively.

B. Case II: $p<0$ and $q\leqslant 0$

As explained above, here again it suffices to focus only on the domain $0\leqslant\Gamma<1$, and we must distinguish between two different behaviors of the potential, depending on the value of Γ.

Case II.1: $0\leqslant\Gamma\leqslant k'$.

The potential $V_{\mathrm{AL}}(\phi,k)$ has only two extrema in $[0,2K(k))$, namely, an absolute maximum $V_{\mathrm{max}}=|p|k^2(1-\Gamma^2)$ for $\phi=0$, and an absolute minimum $V_{\mathrm{min}}=0$ for $\phi=K(k)$ [with the choice of the shift $C=|p|k^2$ in Eq. (1)]. A plot of the potential is given in Fig. 3(a).

One can repeat the integration scheme described in the preceding case. In particular, considering $z=\mathrm{sn}^2(\phi,k)$, Eq. (6) becomes

$$2\sqrt{2|p|k^2}x=\pm\int_0^z\frac{\mathrm{d}\tilde{z}}{\sqrt{(z_1-\tilde{z})(1-\tilde{z})(z_2-\tilde{z})(\tilde{z}-0)}}, \tag{17}$$

where this time

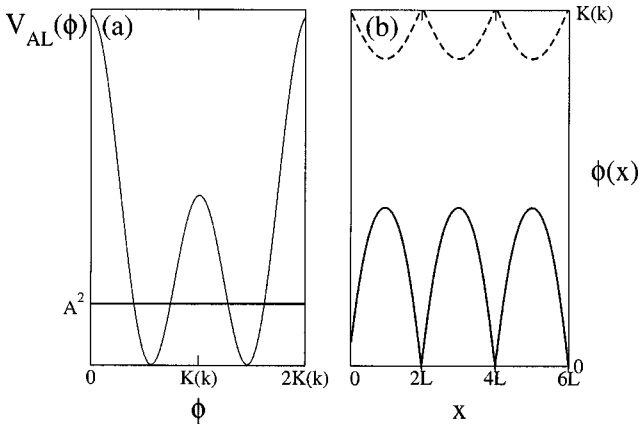

FIG. 4. Case II.2: $k'<\Gamma<1$. (a) The shape of the potential $V_{\mathrm{AL}}(\phi)$. The solid horizontal line corresponds to the integration parameter A^2. (b) The two nontopological soliton lattice solutions [i.e., the field $\phi(x)$] corresponding to the value of A^2 in (a); the solid line represents Solution 1 (see the main text), while the dashed line represents Solution 2. We have plotted $|\phi(x)|$ modulo $2K(k)$.

$$z_{1,2}=\frac{1+k^2-\Gamma^2-a^2k^2}{2k^2}\left[1\pm\sqrt{1-\frac{4k^2(1-\Gamma^2-a^2)}{(1+k^2-\Gamma^2-a^2k^2)^2}}\right], \tag{18}$$

$z_1>1\geqslant z_2>z>0$, and $0\leqslant a^2<(1-\Gamma^2)$. This integral can be evaluated using formula 3.147(2) of Ref. 18 and one obtains the following nontopological soliton lattice:

$$\mathrm{sn}^2(\phi,k)=\frac{z_1z_2\,\mathrm{sn}^2(y,r)}{(z_1-z_2)+z_2\,\mathrm{sn}^2(y,r)}. \tag{19}$$

Here $y=\sqrt{2|p|k^4(z_1-z_2)}x$ and the modulus r that controls the density of solitons in the lattice is given by

$$0<r=\sqrt{\frac{z_2(z_1-1)}{z_1-z_2}}\leqslant 1. \tag{20}$$

The period of the lattice is $2L=2K(r)/\sqrt{2|p|k^4(z_1-z_2)}$ and one notices that ϕ varies between 0 and $\mathrm{sn}^{-1}(\sqrt{z_2})$ [respectively, 0 and $-\mathrm{sn}^{-1}(\sqrt{z_2})$] in one period. A plot of the solution is given in Fig. 3(b).

One can compute the energy for one period $2L$ of this lattice,

$$E_{\mathrm{SL}}=2\sqrt{\frac{2|p|}{z_1-z_2}}\left\{\left[-(z_1-1)K(r)+z_1\Pi\left(-\frac{z_2}{z_1-z_2},r\right)\right]\right.$$
$$\left.-\Gamma^2\left[-\frac{z_1-1}{1-z_1k^2}K(r)+\frac{z_1k'^2}{1-z_1k^2}\Pi\left(-\frac{z_2(1-z_1k^2)}{z_1-z_2},r\right)\right]-\frac{a^2K(r)}{2}\right\}. \tag{21}$$

Case II.2: $k'<\Gamma<1$.

In this case, the potential $V_{\mathrm{AL}}(\phi,k)$ has two maxima and two degenerate minima in one period $0\leqslant\phi<2K(k)$. Namely, an absolute maximum, $V_{\max}=|p|(1-\Gamma k')^2$ (for $\phi=0$); a relative maximum $V^l_{\max}=|p|(\Gamma-k')^2$ [for $\phi=K(k)$]: and two absolute minima $V_{\min}=0$ situated symmetrically around $K(k)$ [for $\phi=\mathrm{sn}^{-1}\sqrt{(1-\Gamma k')/k^2}$, $2K(k)-\mathrm{sn}^{-1}\sqrt{(1-\Gamma k')/k^2}$]. Note that we used a shift $C=|p|(1-2\Gamma k'+\Gamma^2)$ in the expression (1) of the potential. A plot of the potential as a function of ϕ is given in Fig. 4(a).

The very existence of adjacent degenerate minima of the potential separated by different barriers to the right and to the left (on the ϕ axis) implies that in this case one will have two different soliton lattices (and, correspondingly, two different topological single soliton solutions). This is similar to the DSG case.[2–4]

We follow the same type of integration procedure as that described above.

Case II.2(i): When $V_{\min} \leqslant A^2 = |p| k^2 a^2 < V^l_{\max}$, i.e., $0 \leqslant a^2 < (\Gamma - k')^2/k^2$, Eq. (6), under the change of variable $z = \mathrm{sn}^2(\phi, k)$, leads to two different types of solutions.

Solution 1: for $0 < z \leqslant z_2 < z_1 < 1$, one has

$$2\sqrt{2|p|k^4}\,x = \pm \int_0^z \frac{d\tilde{z}}{\sqrt{(1-\tilde{z})(z_1-\tilde{z})(z_2-\tilde{z})(\tilde{z}-0)}}, \tag{22}$$

where now

$$z_{1,2} = \frac{2(1-\Gamma k') - a^2k^2}{2k^2}\left\{1 \pm \sqrt{1 - \frac{4[(1-\Gamma k')^2 - a^2k^2]}{[2(1-\Gamma k') - a^2k^2]^2}}\right\}. \tag{23}$$

Equation (22) can be integrated using formula 3.147(2) of Ref. 18, thus obtaining

$$\mathrm{sn}^2(\phi, k) = \frac{z_2\,\mathrm{sn}^2(w,s)}{(1-z_2) + z_2\,\mathrm{sn}^2(w,s)}, \tag{24}$$

with $w = \sqrt{2|p|k^4 z_1(1-z_2)}\,x$ and the modulus

$$0 < s = \sqrt{\frac{(1-z_1)z_2}{(1-z_2)z_1}} \leqslant 1. \tag{25}$$

It is a nontopological soliton lattice, with ϕ oscillating between 0 and $\mathrm{sn}^{-1}(\sqrt{z_2})$ [respectively, 0 and $-\mathrm{sn}^{-1}(\sqrt{z_2})$]. Its energy for one period $2L = 2K(s)/\sqrt{2|p|k^4 z_1(1-z_2)}$ is given by

$$E_{\mathrm{SL}} = 2\sqrt{\frac{2|p|}{z_1(1-z_2)}}\left\{\left[\frac{(\Gamma-k')^2}{k^2} - \frac{a^2}{2}\right]K(s) + \Pi\left(-\frac{z_2}{1-z_2}, s\right) - \Gamma^2\Pi\left(-\frac{z_2 k'^2}{1-z_2}, s\right)\right\}. \tag{26}$$

Solution 2: for $0 < z_2 < z_1 \leqslant z < 1$ one obtains from Eq. (6),

$$2\sqrt{2|p|k^4} = \pm \int_z^1 \frac{d\tilde{z}}{\sqrt{(1-\tilde{z})(\tilde{z}-z_1)(\tilde{z}-z_2)(\tilde{z}-0)}}, \tag{27}$$

with $z = \mathrm{sn}^2(\phi, k)$ and $z_{1,2}$ given by Eq. (23). This integral can be solved using formula 3.147(7) of Ref. 18, thus leading to the following nontopological pulse-like lattice:

$$\mathrm{sn}^2(\phi, k) = \frac{z_1}{z_1 + (1-z_1)\mathrm{sn}^2(w,s)}, \tag{28}$$

with $w = \sqrt{2|p|k^4 z_1(1-z_2)}\,x$ and the modulus s given by the same expression as above, Eq. (25). Of course, one notices immediately that this soliton lattice is different from the previous one, Eq. (24). In one period $2L = 2K(s)/\sqrt{2|p|k^4 z_1(1-z_2)}$, ϕ oscillates between $\mathrm{sn}^{-1}\sqrt{z_1}$ and $K(k)$ [respectively, $-\mathrm{sn}^{-1}\sqrt{z_1}$ and $-K(k)$].

The energy corresponding to one period $2L$ of this pulse lattice is given by

$$E_{\mathrm{SL}} = s\sqrt{\frac{2|p|}{z_1(1-z_2)}}\left\{\left[\frac{(1-\Gamma k')^2}{k^2} - \frac{a^2}{2}\right]K(s) + \Pi\left(-\frac{1-z_1}{z_1}, s\right) + \Gamma^2\Pi\left(-\frac{1-z_1}{z_1 k'^2}, s\right)\right\}. \tag{29}$$

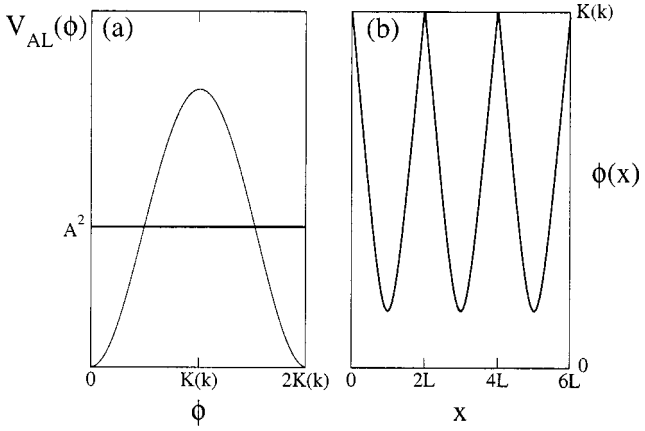

FIG. 5. Case III: $p>0$ and $q\leqslant 0$. (a) The shape of the potential $V_{\mathrm{AL}}(\phi)$. The solid horizontal line corresponds to the integration parameter A^2. (b) The soliton lattice solution [i.e., the field $\phi(x)$] corresponding to the value of A^2 in (a). We have plotted $|\phi(x)|$ modulo $2K(k)$.

A plot of the solutions is given in Fig. 4(b) where the solid and dashed lines correspond, respectively, to the Solution 1 and Solution 2. Therefore, as expected, we obtained two different soliton lattices (with two different limiting cases of topological single solitons). Note that the terms ''large'' and ''small'' applied to the topological solitons do not refer, as usual, to the length of the interval they cover in ϕ space, but to the height of the barrier they ''encounter.''[3]

Case II.2(ii): When $V^{l}_{\max}\leqslant A^2=|p|k^2a^2<V_{\max}$, i.e., $(\Gamma-k')^2/k^2\leqslant a^2<(1-\Gamma k')^2/k^2$ there is no soliton lattice solution.

C. Case III: $p>0$ and $q\leqslant 0$

Unlike the last two cases, here p^2 can be $>$ or $<q^2$. However, it turns out that in this case, whatever the value of $\Gamma=\sqrt{|q|/p}$, the potential $V_{\mathrm{AL}}(\phi)$ has only two extrema in one period $0\leqslant\phi<2K(k)$, namely, an absolute minimum $V_{\min}=0$ for $\phi=0$ and a maximum $V_{\max}=pk^2(1+\Gamma^2)$ for $\phi=K(k)$. Note that we choose $C=pk^2\Gamma^2$ in Eq. (1). A plot of the potential $V_{\mathrm{AL}}(\phi)$ is given in Fig. 5(a). With $z=\mathrm{sn}^2(\phi,k)$, Eq. (6) now becomes

$$2\sqrt{2pk^4}x=\pm\int_z^1\frac{d\tilde{z}}{\sqrt{(z_1-\tilde{z})(1-\tilde{z})(\tilde{z}-z_2)(\tilde{z}-0)}},\tag{30}$$

with

$$z_{1,2}=\frac{(1+\Gamma^2k'^2+a^2k^2)}{2k^2}\left[1\pm\sqrt{1-\frac{4k^2a^2}{(1+\Gamma^2k'^2+a^2k^2)^2}}\right],\tag{31}$$

$z_1>1\geqslant z>z_2>0$. Using the formula 3.147(5) of Ref. 18, one can evaluate the integral in Eq. (30), thus obtaining a nontopological soliton lattice,

$$\mathrm{sn}^2(\phi,k)=\frac{[(z_1-z_2)-z_1(1-z_2)\mathrm{sn}^2(y,t)]}{[(z_1-z_2)-(1-z_2)\mathrm{sn}^2(y,t)]}.\tag{32}$$

Here $y=\sqrt{2pk^4(z_1-z_2)}x$ and the elliptic modulus

$$0<t=\sqrt{\frac{z_1(1-z_2)}{z_1-z_2}}\leqslant 1.\tag{33}$$

In one period $2L=2K(t)/\sqrt{2pk^4(z_1-z_2)}$, ϕ oscillates between $\mathrm{sn}^{-1}\sqrt{z_2}$ and $K(k)$ [respectively, $-K(k)$ and $-\mathrm{sn}^{-1}\sqrt{z_2}$]. A plot of the solution is given in Fig. 5(b).

The energy corresponding to one period $2L$ of this lattice is

$$E_{\mathrm{SL}}=2\sqrt{\frac{2p}{z_1-z_2}}\left\{\left[z_1K(t)-(z_1-1)\Pi\left(\frac{1-z_2}{z_1-z_2},t\right)\right]\right.$$
$$\left.-\Gamma^2k'^2\left[\frac{z_1}{z_1k^2-1}K(t)-\frac{z_1-1}{k'^2(z_1k^2-1)}\Pi\left(-\frac{(1-z_2)(z_1k^2-1)}{k'^2(z_1-z_2)},t\right)\right]-\frac{a^2K(t)}{2}\right\}. \quad (34)$$

IV. SINGLE SOLITON SOLUTIONS OF THE AL POTENTIAL

Having obtained the soliton lattice solutions of the AL problem, it is now straightforward to consider the specific limits of the integration constant A^2 and to obtain the corresponding single soliton solutions of the Associated Lamé potential and compute their energy.

Cases I.1 and I.2(i): The limit of a single soliton (that corresponds to the period of the lattice $L\to\infty$) is obtained for $t\nearrow 1$ [$a^2\searrow 0$; $z_1\to(1-\Gamma^2k'^2)/k^2$ and $z_2\searrow 0$]. One notices that now ϕ can vary continuously between $-K(k)$ and $K(k)$ while x explores the whole real axis; therefore, one obtains a topological single-soliton (kink-like) solution,

$$\mathrm{sn}(\phi,k)=\pm\sqrt{\frac{1-\Gamma^2k'^2}{1-\Gamma^2k'^2+k'^2(1-\Gamma^2)\sinh^2(y^*)}}, \quad (35)$$

where $y^*=\sqrt{2pk^2(1-\Gamma^2k'^2)}x$. The corresponding energy of this single kink-like soliton is obtained from Eq. (12), using the relations

$$\lim_{r\nearrow 1}\Pi(n^2,r)=\lim_{r\nearrow 1}\frac{K(r)}{1-n^2}-\frac{n}{2(1-n^2)}\ln\left(\frac{1+n}{1-n}\right). \quad (36)$$

It may be noted that all the divergences cancel mutually, thus leading to a finite energy of the single soliton:

$$E_{\mathrm{K}}=\sqrt{2p}\left[\ln\left(\frac{\sqrt{1-\Gamma^2k'^2}+k}{\sqrt{1-\Gamma^2k'^2}-k}\right)-\Gamma\ln\left(\frac{\sqrt{1-\Gamma^2k'^2}+(\Gamma k)}{\sqrt{1-\Gamma^2k'^2}-(\Gamma k)}\right)\right]. \quad (37)$$

Following Manton[14] one can compute the asymptotic interaction energy between two solitons in the array, or between a soliton and an antisoliton. As an illustration we will consider this particular soliton solution; for all the other cases one can follow exactly the same procedure.

From Eq. (35) one obtains the asymptotic shape of the soliton, e.g., for $x\to+\infty$:

$$\phi_{\mathrm{as}}\approx\left[\frac{4(1-\Gamma^2k'^2)}{k'^2(1-\Gamma^2)}\right]^{1/2}\exp(-\sqrt{2pk^2(1-\Gamma^2k'^2)}x). \quad (38)$$

Then, if $2L\gg 1$ is the distance between two solitons in the array, according to Ref. 14 the asymptotic interaction energy is

$$U(2L)\approx-\frac{8(2pk^2)^{1/2}(1-\Gamma^2k'^2)^{3/2}}{k'^2(1-\Gamma^2)}\exp(-2L\sqrt{2pk^2(1-\Gamma^2k'^2)}). \quad (39)$$

If one considers now the small parameter $a^2\ll 1$ that measures the distance from the single soliton limit, according to the results in Sec. III we can obtain the asymptotic expression for $2L$ as

$$2L\approx\frac{1}{\sqrt{2pk^2(1-\Gamma^2k'^2)}}\ln\left(\frac{16(1-\Gamma^2k'^2)^2}{a^2k'^2(1-\Gamma^2)}\right), \quad (40)$$

and thus

$$U(a^2) \approx \sqrt{\frac{pk^2}{2(1-\Gamma^2 k'^2)}}\, a^2, \tag{41}$$

that corresponds to a repulsive asymptotic interaction between two solitons in the array. One can consider also the asymptotic interaction energy between a soliton and an antisoliton and obtains simply $U(a^2) \approx -\sqrt{pk^2/[2(1-\Gamma^2 k'^2)]}a^2$, i.e., an attractive interaction.

Sine-Gordon limit: Taking now the limit $k \to 0$, with $|p|, |q| \to \infty$, so that $|p|k^2 \to P =$ finite and $|q|k^2 \to Q =$ finite, in the expressions of the AL single soliton solution, Eq. (35), one obtains the correct kink-like solution of the sine-Gordon potential in Eq. (2), namely,

$$\sin \phi_{\mathrm{SG}} = \pm \operatorname{sech}(y^*), \tag{42}$$

with $y^* = \sqrt{2P(1-\Gamma^2)}x$, and the energy

$$E_{\mathrm{SG}} = 2\sqrt{2P(1-\Gamma^2)}. \tag{43}$$

Case I.2(ii): The single soliton limit $L \to \infty$ [i.e., $n \nearrow 1$; $a^2 \searrow (1-\Gamma^2)$, $z_1 \to 1$, and $z_2 \to (1-\Gamma^2)/k^2$] reads

$$\mathrm{sn}(\phi, k) = \pm \sqrt{\frac{1-\Gamma^2}{1-\Gamma^2+(\Gamma^2-k'^2)\operatorname{sech}^2(\omega^*)}}, \tag{44}$$

with $\omega^* = \sqrt{2pk^2(\Gamma^2-k'^2)}x$. It represents a nonlopological (pulse-like) soliton, with ϕ varying between $K(k)$ and $\mathrm{sn}^{-1}(\sqrt{(1-\Gamma^2)/k^2})$ [respectively, $-K(k)$ and $-\mathrm{sn}^{-1}(\sqrt{(1-\Gamma^2)/k^2})$] when x runs over the real axis, i.e., it does not connect two adjacent degenerate minima of the potential.

Its energy is obtained from Eq. (16) and reads

$$E_{\mathrm{S}} = \sqrt{2p}\left[\Gamma \ln\left(\frac{(\Gamma k)+\sqrt{\Gamma^2-k'^2}}{(\Gamma k)-\sqrt{\Gamma^2-k'^2}}\right) - \ln\left(\frac{k+\sqrt{\Gamma^2-k'^2}}{k-\sqrt{\Gamma^2-k'^2}}\right)\right]. \tag{45}$$

Case II.1: Consider now the single soliton limit $r \nearrow 1$ [$a^2 \searrow 0, z_1 \to (1-\Gamma^2)/k^2$, and $z_2 \to 1$]. One obtains the following topological (i.e., kink-like) soliton:

$$\mathrm{sn}(\phi, k) = \pm \sqrt{\frac{1-\Gamma^2}{k'^2-\Gamma^2+(1-\Gamma^2)\sinh^2(y^*)}}\sinh(y^*), \tag{46}$$

with $y^* = \sqrt{2|p|k^2(k'^2-\Gamma^2)}x$, of energy

$$E_{\mathrm{K}} = 2\sqrt{2|p|}\left[\arctan\left(\frac{k}{k'^2-\Gamma^2}\right) - \Gamma \arctan\left(\frac{(\Gamma k)}{\sqrt{k'^2-\Gamma^2}}\right)\right], \tag{47}$$

where we took the limit $r \nearrow 1$ in Eq. (21) using the relation

$$\lim_{r \nearrow 1} \Pi(-n^2, r) = \lim_{r \nearrow 1} \frac{K(r)}{1+n^2} + \frac{n}{1+n^2}\arctan(n). \tag{48}$$

Note that one can also consider the limit of the sine-Gordon potential in this case and obtain the correct sine-Gordon soliton.

Case II.2(i): Solution 1: large topological kink: Considering the single soliton limit, $s \nearrow 1$ [$a^2 \searrow 0, z_{1,2} \to (1-\Gamma k')/k^2$], one obtains a "large" topological kink, that interpolates between two adjacent minima "across" the large barrier $V_{\max}$ of the potential

$$\mathrm{sn}(\phi,k)=\pm\sqrt{\frac{1-\Gamma k'}{k'(\Gamma-k')+(1-\Gamma k')\tanh^2(\omega^*)}}\tanh(\omega^*), \tag{49}$$

with $\omega^*=\sqrt{2|p|k'(1-\Gamma k')(\Gamma-k')}x$. Its energy is found from Eqs. (26) and (48) as

$$E_{\mathrm{K}}=2\sqrt{2|p|}\left[\arctan\sqrt{\frac{1-\Gamma k'}{k'(\Gamma-k')}}-\Gamma\arctan\sqrt{\frac{k'(1-\Gamma k')}{\Gamma-k'}}\right]. \tag{50}$$

Case II.2(i): Solution 2: small topological kink: Considering now the single soliton limit $s\nearrow 1[a^2\to 0, z_{1,2}\to(1-\Gamma k')/k^2]$, one obtains a "small" topological kink, that interpolates between two adjacent minima "across" the small barrier $V'_{\max}$ of the potential

$$\mathrm{sn}(\phi,k)=\pm\sqrt{\frac{1-\Gamma k'}{1-\Gamma k'+k'(\Gamma-k')\tanh^2(\omega^*)}}, \tag{51}$$

with $\omega^*=\sqrt{2|p|k'(1-\Gamma k')(\Gamma-k')}x$. Its energy is found from Eqs. (29) and (48),

$$E_{\mathrm{K}}=2\sqrt{2|p|}\left[\Gamma\arctan\sqrt{\frac{\Gamma-k'}{k'(1-\Gamma k')}}-\arctan\sqrt{\frac{k'(\Gamma-k')}{1-\Gamma k'}}\right]. \tag{52}$$

Case III: The single soliton limit $t\nearrow 1[a^2\searrow 0, z_1\to(1+\Gamma^2k'^2)/k^2$, and $z_2\to 0]$ represents a topological soliton,

$$\mathrm{sn}(\phi,k)=\pm\sqrt{\frac{(1+k'^2\Gamma^2)}{1+\Gamma^2k'^2+k'^2(1+\Gamma^2)\sinh^2(y^*)}}, \tag{53}$$

with $y^*=\sqrt{2pk^2(1+\Gamma^2k'^2)}x$. Its energy is given by

$$E_{\mathrm{K}}=\sqrt{2p}\left[\ln\left(\frac{\sqrt{1+\Gamma^2k'^2}+k}{\sqrt{1+\Gamma^2k'^2}-k}\right)+2\Gamma\arctan\left(\frac{(\Gamma k)}{\sqrt{1+\Gamma^2k'^2}}\right)\right]. \tag{54}$$

Here again one can consider the limit of the sine-Gordon potential and obtain the correct sine-Gordon soliton of energy $E_{\mathrm{SG}}=2\sqrt{2P(1+\Gamma^2)}$.

V. SOLITON LATTICE AND SINGLE SOLITON SOLUTIONS OF THE LAMÉ POTENTIAL

Let us now consider the standard Lamé potential

$$V_{\mathrm{L}}(\phi,k)=pk^2\,\mathrm{sn}^2(\phi,k). \tag{55}$$

Recall that p is a real parameter and $\mathrm{sn}(\phi,k)$ is the sine amplitude Jacobi elliptic function of real modulus k $(0\leqslant k\leqslant 1)$ and period $4K(k)$, where $K(k)$ denotes the complete elliptic integral of the first kind, see Refs. 18 and 19. As emphasized in Sec. II, the Lamé potential can be obtained from the Associated Lamé potential for special limiting values of the two parameters (p,q) of the latter, Eq. (1).

We shall next demonstrate explicitly that having obtained the AL soliton lattice and single soliton solutions, one can immediately obtain the (previously not known) corresponding solutions of the Lamé problem by taking suitable limits of the appropriate AL solutions.

A. Lamé soliton lattice solutions

Starting from the AL soliton lattice solutions and considering the limit $\Gamma\to 0$, we obtain the two following types of Lamé soliton lattice solutions.

Cases I.1 and III $(p>0)$: These lead to type I Lamé soliton lattice solution. The solution is given by Eq. (9) with simpler forms for z_1, z_2, namely, $z_1=1/k^2$, $z_2=a^2$ $[=A^2/|p|k^2$, see Eq. (6)]:

$$\mathrm{sn}^2(\phi,k)=\frac{(1-k^2a^2)-(1-a^2)\mathrm{sn}^2(y,t)}{(1-k^2a^2)-k^2(1-a^2)\mathrm{sn}^2(y,t)}, \tag{56}$$

where $t=[(1-a^2)/(1-k^2a^2)]^{1/2}$ and $y=\sqrt{2pk^2(1-k^2a^2)}x$. As a result the Lamé soliton lattice energy per period $2L=2K(t)/\sqrt{2pk^2(1-k^2a^2)}$ of the lattice has the simpler form

$$E_{\mathrm{SL}}=2\sqrt{\frac{2pk^2}{1-k^2a^2}}\left[\left(\frac{1}{k^2}-\frac{a^2}{2}\right)K(t)-\frac{k'^2}{k^2}\Pi\left(\frac{k^2(1-a^2)}{1-k^2a^2},t\right)\right], \tag{57}$$

where recall that $\Pi(z_0,t)$ denotes the complete elliptic integral of the third kind.[18,19]

Case II.1 ($p<0$): This produces type II Lamé soliton lattice solution. In this case the solution is in fact the same as that given by Eq. (19), except that now z_1,z_2 take the simpler values $z_1=1/k^2$, $z_2=1-a^2$:

$$\mathrm{sn}^2(\phi,k)=\frac{(1-a^2)\mathrm{sn}^2(y,r)}{1-k^2(1-a^2)+k^2(1-a^2)\mathrm{sn}^2(y,r)}, \tag{58}$$

with $r=[k'^2(1-a^2)/[1-k^2(1-a^2)]^{1/2}$ and $y=\sqrt{2|p|k^2[1-k^2(1-a^2)]}x$. As a result the Lamé soliton lattice energy per period $2L=2K(r)/\sqrt{2|p|k^2[1-k^2(1-a^2)]}$ of the lattice now reads

$$E_{\mathrm{SL}}=2\sqrt{\frac{2|p|k^2}{1-k^2(1-a^2)}}\left[-\left(\frac{k'^2}{k^2}+\frac{a^2}{2}\right)K(r)+\frac{1}{k^2}\Pi\left(-\frac{k^2(1-a^2)}{1-k^2(1-a^2)},r\right)\right]. \tag{59}$$

B. Lamé single soliton solutions

We can now easily obtain the corresponding Lamé topological (kink-like) single soliton solutions, either by taking the appropriate limits of the Lamé soliton lattice solutions, or of the AL single soliton solutions.

Type I ($p>0$)*:* For example, considering $\Gamma=0$ in the expressions for the AL soliton solution as given by Eq. (35), the corresponding Lamé one soliton solution turns out to be

$$\mathrm{sn}(\phi,k)=\frac{1}{\sqrt{1+k'^2\sinh^2(y^*)}}, \tag{60}$$

where $y^*=\sqrt{2pk^2}x$. The corresponding energy is then given by

$$E_{\mathrm{K}}=\sqrt{2p}\ln\left(\frac{1+k}{1-k}\right), \tag{61}$$

where we have used Eq. (37). The asymptotic (repulsive) interaction between two solitons, using Manton's method[14] from Eq. (41), is given by $U(a^2)\simeq\sqrt{p/2}ka^2$.

Type II ($p<0$)*:* Considering $\Gamma=0$ in the expressions for the AL soliton solution as given by Eq. (46) the corresponding Lamé soliton solution turns out to be

$$\mathrm{sn}(\phi,k)=\frac{\sinh(y^*)}{\sqrt{k'^2+\sinh^2(y^*)}}, \tag{62}$$

where $y^*=\sqrt{2|p|k^2k'^2}x$. The corresponding energy is given by

$$E_{\mathrm{K}}=2\sqrt{2|p|}\arctan\left(\frac{k}{k'}\right), \tag{63}$$

where we have used Eq. (47).

VI. CONCLUSION

We have obtained and presented a taxonomy of the exact soliton lattice and single soliton solutions, as well as their corresponding energies, for the Associated Lamé equation[8–10] in various parameter regimes. The class of solutions turns out to be very rich depending on the parameters (p,q) of the AL potential, Eq. (1). In appropriate limits we also obtained the single soliton and soliton lattice solutions of the Lamé equation. The topological and nontopological nature of the different solutions was discussed. As an illustration of Manton's method[14] we also computed, in a particular case, the asymptotic interaction energy between these solitons. In addition to their relevance in the study of nonlinear phenomena, these solutions provide valuable information about domain walls in field theory, materials and many physical systems. It would be worthwhile to study the stability of these solutions, and also the exact thermodynamical properties of these systems.

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On bosonic limits of two recent supersymmetric extensions of the Harry Dym hierarchy

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Two generalized Harry Dym equations, recently found by Brunelli, Das, and Popowicz in the bosonic limit of new supersymmetric extensions of the Harry Dym hierarchy [J. Math. Phys. **44**, 4756 (2003)], are transformed into previously known integrable systems: one, into a pair of decoupled KdV equations, the other one, into a pair of coupled mKdV equations from a bi-Hamiltonian hierarchy of Kupershmidt. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1745128]

I. INTRODUCTION

Integrable supersymmetric differential equations have been attracting much attention in modern mathematical physics and soliton theory (see, e.g., Ref. 1, and references therein). Supersymmetric extensions of known integrable bosonic (or classical) systems are of particular interest, because, if the number N of Grassmann variables is greater than one, those extensions can generate, in their bosonic limits, some new integrable classical systems which generalize the initial ones.

Recently, Brunelli, Das, and Popowicz[2] studied supersymmetric extensions of the Harry Dym hierarchy, and found, as bosonic limits of $N=2$ supersymmetric extensions, the following two new classical generalizations of the Harry Dym equation:

$$w_{0,t}=\tfrac{1}{2}(w_0^{-1/2})_{xxx},$$

$$\begin{aligned} w_{1,t}=\tfrac{1}{64}(&-16w_{1,xxx}w_0^{-3/2}+96w_{1,xx}w_{0,x}w_0^{-5/2}+72w_{1,x}w_{0,xx}w_0^{-5/2}-258w_{1,x}w_{0,x}^2w_0^{-7/2}\\ &-6w_{1,x}w_1^2w_0^{-7/2}+9w_1^3w_{0,x}w_0^{-9/2}-108w_1w_{0,xx}w_{0,x}w_0^{-7/2}+219w_1w_{0,x}^3w_0^{-9/2}), \end{aligned} \tag{1}$$

and

$$w_{0,t}=\tfrac{1}{16}(8(w_0^{-1/2})_{xxx}-6w_{1,x}w_1w_0^{-5/2}+9w_1^2w_{0,x}w_0^{-7/2}),$$

$$\begin{aligned} w_{1,t}=\tfrac{1}{32}(&-8w_{1,xxx}w_0^{-3/2}+48(w_{1,x}w_{0,x})_xw_0^{-5/2}-144w_{1,x}w_{0,x}^2w_0^{-7/2}-6w_{1,x}w_1^2w_0^{-7/2}+9w_1^3w_{0,x}w_0^{-9/2}\\ &+12w_1w_{0,xxx}w_0^{-5/2}-126w_1w_{0,xx}w_{0,x}w_0^{-7/2}+177w_{0,x}^3w_1w_0^{-9/2}), \end{aligned} \tag{2}$$

where w_0 and w_1 are functions of x and t. Note that in system (1), in the seventh term of the right-hand side of its second equation, we have corrected a misprint made in Ref. 2: the degree of w_0 should be $-7/2$ there.

In the present paper, we find chains of transformations which relate these new generalized Harry Dym (GHD) equations (1) and (2) with previously known integrable classical systems. In Sec. II, the GHD equation (1) is transformed into a pair of decoupled KdV equations. In Sec. III, the GHD equation (2) is transformed into a pair of coupled mKdV equations which belongs to the bi-Hamiltonian hierarchy of the modified dispersive water waves equation of Kupershmidt[3] (see also Ref. 4, p. 84). Section IV contains concluding remarks.

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II. TRANSFORMING THE FIRST GHD EQUATION

Unfortunately, there are no generally applicable methods of transforming a given nonlinear system into another one, less complicated or better studied. In order to find necessary transformations, one usually follows the trial and error way in combination with some heuristic considerations. In the present case, we also used this way.

First, the transformation

$$w_0 = u(x,t)^{-2}, \quad w_1 = v(x,t), \quad t \mapsto -4t \tag{3}$$

brings the GHD equation (1) into the following simpler form:

$$u_t = u^3 u_{xxx},$$
$$v_t = u^3 v_{xxx} + 9u^2 v_x u_{xx} + 12u^2 u_x v_{xx} + 27uv u_x u_{xx} + \tfrac{57}{2} v u_x^3 + \tfrac{75}{2} u u_x^2 v_x + \tfrac{9}{8} u^6 v^3 u_x + \tfrac{3}{8} u^7 v^2 v_x. \tag{4}$$

Second, we try to transform x, u, and v in (4) as follows:

$$x = p(y,t), \quad u(x,t) = p_y(y,t), \quad v(x,t) = q(y,t). \tag{5}$$

This is an extension of the transformation used by Ibragimov[5] to relate the original Harry Dym equation with the Schwarzian-modified KdV equation. In the case of scalar evolution equations, the Ibragimov transformation (i.e. (5) with $v = q = 0$) is an essential link in chains of transformations between constant separant equations and nonconstant separant ones.[6,7] Also the transformation (5) appeared recently in Ref. 8, as an essential link in a chain of transformations between a system of symmetrically coupled Harry Dym equations and the Hirota–Satsuma system of coupled KdV equations.

The transformation (5) really works in the present case and relates the system (4) with the system

$$p_t = p_{yyy} - \tfrac{3}{2} p_y^{-1} p_{yy}^2,$$
$$q_t = q_{yyy} + 9p_y^{-1} p_{yyy} q_y + 27 p_y^{-2} p_{yy} p_{yyy} q + 18 p_y^{-2} p_{yy}^2 q_y + 9 p_y^{-1} p_{yy} q_{yy} + \tfrac{3}{2} p_y^{-3} p_{yy}^3 q + \tfrac{3}{8} p_y^6 q^2 q_y + \tfrac{9}{8} p_y^5 p_{yy} q^3. \tag{6}$$

To verify this, one may use the following identities:

$$u\partial_x = \partial_y, \quad u_t = p_{yt} - p_y^{-1} p_{yy} p_t, \quad v_t = q_t - p_y^{-1} q_y p_t. \tag{7}$$

Note that (5) is not an invertible transformation: it maps the system (6) into the system (4), whereas its application in the opposite direction, from (4) to (6), requires one integration by y. We have omitted the terms $\alpha(t)p_y$ and $\alpha(t)q_y$ in the right-hand sides of the first and second equations of (6), respectively, where this arbitrary function $\alpha(t)$ appeared as a ''constant'' of that integration.

Third, we make the transformation

$$f(y,t) = p_y^{-1} p_{yy}, \quad g(y,t) = p_y^3 q, \tag{8}$$

admitted by the system (6) owing to the form of its equations, and obtain the pair of decoupled mKdV equations

$$f_t = (f_{yy} - \tfrac{1}{2} f^3)_y, \quad g_t = (g_{yy} + \tfrac{1}{8} g^3)_y. \tag{9}$$

Needless to say that the pair of Miura transformations

$$a(y,t)=\pm f_y-\tfrac{1}{2}f^2, \quad b(y,t)=\pm\tfrac{1}{2}\mathrm{i}g_y+\tfrac{1}{8}g^2, \tag{10}$$

with independent choice of the $\pm$ signs, relates (9) with the two copies of the KdV equation

$$a_t=a_{yyy}+3aa_y, \quad b_t=b_{yyy}+3bb_y. \tag{11}$$

III. TRANSFORMING THE SECOND GHD EQUATION

We follow the same three-step transformation as used in Sec. II.

First, the transformation (3) brings the GHD equation (2) into the form

$$\begin{aligned} u_t&=u^3u_{xxx}-\tfrac{9}{4}u^7v^2u_x-\tfrac{3}{4}u^8vv_x,\\ v_t&=3u^2vu_{xxx}+u^3v_{xxx}+36uvu_xu_{xx}+12u^2v_xu_{xx}\\ &\quad+12u^2u_xv_{xx}+24vu_x^3+36uu_x^2v_x+\tfrac{9}{4}u^6v^3u_x+\tfrac{3}{4}u^7v^2v_x. \end{aligned} \tag{12}$$

Second, we apply the transformation (5) to the system (12) and obtain

$$\begin{aligned} p_t&=p_{yyy}-\tfrac{3}{2}p_y^{-1}p_{yy}^2-\tfrac{3}{8}p_y^7q^2,\\ q_t&=3p_y^{-1}p_{yyyy}q+24p_y^{-2}p_{yy}p_{yyy}q+12p_y^{-1}p_{yyy}q_y+q_{yyy}-3p_y^{-3}p_{yy}^3q\\ &\quad+\tfrac{27}{2}p_y^{-2}p_{yy}^2q_y+9p_y^{-1}p_{yy}q_{yy}+\tfrac{9}{4}p_y^5p_{yy}q^3+\tfrac{3}{8}p_y^6q^2q_y, \end{aligned} \tag{13}$$

where the terms $\alpha(t)p_y$ and $\alpha(t)q_y$, with arbitrary $\alpha(t)$, have been omitted in the right-hand sides of the first and second equations, respectively.

Third, the transformation (8) relates the system (13) with the following system of coupled mKdV equations:

$$\begin{aligned} f_t&=(f_{yy}-\tfrac{3}{4}gg_y-\tfrac{1}{2}f^3-\tfrac{3}{8}fg^2)_y,\\ g_t&=(g_{yy}+3gf_y-\tfrac{3}{2}f^2g-\tfrac{5}{8}g^3)_y. \end{aligned} \tag{14}$$

The system (14) does not admit any further transformation into a system of coupled KdV equations. It is possible to transform (14) into a system of a KdV–mKdV type, but we will not follow this way. Instead, we notice that the system (14) is invariant under the change of variables $f\mapsto f$, $g\mapsto -g$. Therefore the transformation

$$f=c_1(a+b), \quad g=c_2(a-b), \tag{15}$$

with any nonzero constants c_1 and c_2, relates the system (14) with a system of symmetrically coupled mKdV equations for $a(y,t)$ and $b(y,t)$, which is invariant under $a\mapsto b$, $b\mapsto a$. Systems of symmetrically coupled mKdV equations possessing higher-order generalized symmetries were classified by Foursov.[9] The choice of

$$c_1=1, \quad c_2=\pm\mathrm{i} \tag{16}$$

in the transformation (15) brings the system (14) into the form

$$\begin{aligned} a_t&=(a_{yy}+3aa_y-3ba_y+a^3-6a^2b+3ab^2)_y,\\ b_t&=(b_{yy}+3bb_y-3ab_y+b^3-6b^2a+3ba^2)_y, \end{aligned} \tag{17}$$

which is exactly the case (K) in the Foursov classification.[9]

Foursov[9] proved that the system (17) represents the third-order generalized symmetry of the system of coupled Burgers equations

$$a_t=(a_y+a^2-2ab)_y, \quad b_t=(-b_y+2ab-b^2)_y, \tag{18}$$

and found the bi-Hamiltonian structure of this hierarchy with the Hamiltonian operators

$$P=\begin{pmatrix} 0 & \partial_y \\ \partial_y & 0 \end{pmatrix},$$
$$Q=\begin{pmatrix} -2a\partial_y-a_y & \partial_y^2+(a-b)\partial_y+a_y \\ -\partial_y^2+(a-b)\partial_y-b_y & 2b\partial_y+b_y \end{pmatrix}. \tag{19}$$

In its turn, the system of coupled Burgers equations (18) has a long history. As a system of coupled second-order evolution equations possessing higher-order symmetries, it appeared in the classifications of Mikhailov, Shabat, and Yamilov[10] and Olver and Sokolov.[11] Moreover, the bi-Hamiltonian structure (19) turns out to be not new. Indeed, the transformation

$$a=-r, \quad b=s-r, \quad t\mapsto -\tfrac{1}{2}t \tag{20}$$

relates the system (18) with the modified dispersive water waves equation

$$r_t=\tfrac{1}{2}(-r_y+2rs-r^2)_y,$$
$$s_t=\tfrac{1}{2}(s_y-2r_y-2r^2+2rs+s^2)_y, \tag{21}$$

which was introduced, together with its bi-Hamiltonian structure, by Kupershmidt[3] (see also Ref. 4, p. 84). The bi-Hamiltonian structures of (18) and (21) are related by the transformation (20) as well. For this reason, the system (17) is equivalent to a third-order member of the bi-Hamiltonian hierarchy of the modified dispersive water waves equation (21).

IV. CONCLUSION

In this paper, we found chains of transformations which relate the new GHD equations (1) and (2) of Brunelli, Das, and Popowicz with previously known integrable systems. The transformations (3), (5), (8), and (10) relate the GHD equation (1) with the pair of decoupled KdV equations (11). The transformations (3), (5), (8), (15) with the choice of (16), and (20) relate the GHD equation (2) with a third-order member of the bi-Hamiltonian hierarchy of the modified dispersive water waves equation (21).

It can be observed in the literature (see, e.g., Refs. 5, 6, 7, 10, and references therein) that quite often a newly-found remarkable equation turns out to be related to a well-studied old equation through an explicit chain of transformations. In such a situation, one gets a possibility not to study the new equation directly but to derive its properties from the well-known properties of the corresponding old equation, using the transformations obtained. Now this applies to the new generalized Harry Dym equations of Brunelli, Das, and Popowicz as well.

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Classification of the pseudosymmetric space–times

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The pseudosymmetry condition on a manifold is a generalization of the notion of spaces of constant curvature. A complete algebraic classification of the pseudosymmetric space–times based on the Petrov type of the Weyl tensor and the Segré type of the Ricci tensor is presented. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The most simple generalizations of the flat pseudo-Euclidean space–time, i.e., Minkowski space, are the spaces of constant curvature. For these spaces the sectional curvature K does not depend on the point nor on the tangent plane at any point. Their Riemann tensor is given by

$$R_{\alpha\beta\gamma\mu}=K(g_{\alpha\gamma}g_{\beta\mu}-g_{\alpha\mu}g_{\beta\gamma}),$$

and the space–times of constant curvature are the de Sitter and anti–de Sitter space–times.[1]

Cartan introduced a further generalization by considering the Riemannian spaces for which every local geodesic reflection is an isometry. These are called the locally symmetric spaces and are characterized by the curvature condition

$$\nabla R=0,$$

or equivalently by the property that their sectional curvature is invariant under parallel translation along any curve. The symmetric Riemannian spaces were classified by Cartan[2] and the locally symmetric space–times were classified by Petrov.[3,4]

Of course, the curvature tensor of every locally symmetric space also satisfies the relation $R\cdot R=0$, or in local coordinates:

$$(R\cdot R)_{\alpha\beta\gamma\sigma\mu\nu}=(\nabla_\mu\nabla_\nu-\nabla_\nu\nabla_\mu)R_{\alpha\beta\gamma\sigma}=2R_{\mu\nu\rho[\alpha}R^{\rho}_{\beta]\gamma\sigma}+2R_{\mu\nu\rho[\gamma}R^{\rho}_{\sigma]\alpha\beta}=0.$$

The study of these so-called semisymmetric spaces was initiated by Cartan *et al.* and revitalised by Nomizu,[5] Takagi,[7] and Sekigawa,[6] leading to their classification by Szabó.[8] The semisymmetric spaces are characterized geometrically by the property that the sectional curvature of any plane remains invariant after a parallel translation of the plane along an infinitesimal parallellogram. The semisymmetric space–times were classified by Petrov.[3]

From this notion of semisymmetry we can define a scalar that in general depends on the point in the manifold and two planes, π spanned by $\mathbf{u}$ and $\mathbf{v}$, and $\pi^\star$ spanned by $\mathbf{X}$ and $\mathbf{Y}$, as follows:

$$L(p,\pi,\pi^\star)=\frac{(R\cdot R)(\mathbf{u},\mathbf{v},\mathbf{v},\mathbf{u};\mathbf{X},\mathbf{Y})}{Q(g,R)(\mathbf{u},\mathbf{v},\mathbf{v},\mathbf{u};\mathbf{X},\mathbf{Y})},$$

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whereby $Q(g,R)$ is the (0,6)-Tachibana tensor given in component form as

$$Q(g,R)_{\alpha\beta\gamma\sigma\mu\nu}=2g_{\mu[\alpha}R_{\beta]\nu\gamma\sigma}-2g_{\nu[\alpha}R_{\beta]\mu\gamma\sigma}+2g_{\mu[\gamma}R_{\sigma]\nu\alpha\beta}-2g_{\nu[\gamma}R_{\sigma]\mu\alpha\beta}.$$

The vanishing of this tensor is a necessary and sufficient condition for a space to be of constant curvature;[9] the scalar L is therefore only defined on $U_R=\{x\in\mathcal{M}|Q(g,R)\neq 0 \text{ at } x\}$.

A manifold for which $L(p,\pi,\pi^\star)$ is isotropic, i.e., only depends on the point p, but not on the planes π and $\pi^\star$, is called pseudosymmetric in the sense of Deszcz.[10–12] These spaces are a further generalization of the spaces of constant curvature. We remark that there is no theorem here corresponding to that of Schur, i.e., $L(p)$ is not necessarily constant; there exist ample examples of pseudosymmetric manifolds which are not of constant type.

The pseudosymmetric Einstein space–times were classified in Ref. 13. Here we present the full classification of the pseudosymmetric space–times, showing in particular that they are of the Petrov types D or N or conformally flat.

II. PSEUDOSYMMETRIC SPACE–TIMES

We classify the general pseudosymmetric space–times by using the Newman–Penrose formalism (see, e.g., Ref. 14 for an introduction). Consider a general null tetrad $\{l^\alpha,n^\alpha,m^\alpha,\overline{m}^\alpha\}$, with the relations $l_\alpha n^\alpha=1=-m_\alpha\overline{m}^\alpha$. The space–time metric can then be written as

$$g_{\alpha\beta}=2l_{(\alpha}n_{\beta)}-2m_{(\alpha}\overline{m}_{\beta)}.$$

After projection of the pseudosymmetry condition,

$$R_{\mu\nu\rho[\alpha}R^{\rho}_{\beta]\gamma\sigma}+R_{\mu\nu\rho[\gamma}R^{\rho}_{\sigma]\alpha\beta}-L\{g_{\mu[\alpha}R_{\beta]\nu\gamma\sigma}-g_{\nu[\alpha}R_{\beta]\mu\gamma\sigma}+g_{\mu[\gamma}R_{\sigma]\nu\alpha\beta}-g_{\nu[\gamma}R_{\sigma]\mu\alpha\beta}\}=0,$$

on a general null tetrad, we find 34 algebraic relations between the Ricci and Weyl scalars. The 16 given below will suffice to present the classification, the other 18 relations are automatically satisfied in each of the cases we will consider:

$$2\Psi_0(\Psi_2-\Lambda)-2(\Psi_1)^2=L\Psi_0, \tag{1}$$

$$2\Psi_4(\Psi_2-\Lambda)-2(\Psi_3)^2=L\Psi_4, \tag{2}$$

$$\Phi_{02}(\overline{\Psi}_1-\Phi_{10})-\Phi_{01}(\overline{\Psi}_2+2\Lambda)+\Phi_{00}\Phi_{12}=L\Phi_{01}, \tag{3}$$

$$\Psi_3\Phi_{20}-\Psi_4\Phi_{10}=0, \tag{4}$$

$$\Phi_{01}\Phi_{22}+\Phi_{02}(\Psi_3-\Phi_{21})-\Phi_{12}(\Psi_2+2\Lambda)=L\Phi_{12}, \tag{5}$$

$$\Psi_3\Phi_{22}-\Psi_4\Phi_{12}=0, \tag{6}$$

$$2\Psi_1\Psi_3+\Psi_0\Psi_4-3\Psi_2(\Psi_2+2\Lambda)=3L\Psi_2, \tag{7}$$

$$2\Psi_3\Phi_{01}-2\Phi_{11}(\Psi_{22}+2\Lambda)-\Phi_{02}\Phi_{20}+\Phi_{00}\Phi_{22}=2L\Phi_{11}, \tag{8}$$

$$\Psi_3\Phi_{21}-\Psi_4\Phi_{11}=0, \tag{9}$$

$$\Psi_0\Phi_{20}+2\Psi_1\Phi_{10}-3\Psi_2\Phi_{00}=0, \tag{10}$$

$$\overline{\Psi}_0\Phi_{02}-2\Phi_{01}\Phi_{10}-\Phi_{00}(\overline{\Psi}_2-2\Phi_{11}+2\Lambda)=L\Phi_{00}, \tag{11}$$

$$\Psi_0\Phi_{22}+2\Psi_1\Phi_{12}-3\Psi_2\Phi_{02}=0, \tag{12}$$

$$\Psi_0\Phi_{22}-\Psi_1\Phi_{12}+\overline{\Psi}_3\Phi_{01}-\overline{\Psi}_4\Phi_{00}=0, \tag{13}$$

$$\overline{\Psi}_4\Phi_{00}+2\Phi_{01}\Phi_{12}-\Phi_{02}(\overline{\Psi}_2+2\Phi_{11}+2\Lambda)=L\Phi_{02}, \tag{14}$$

$$\Psi_4\Phi_{02}+2\Psi_3\Phi_{12}-3\Psi_2\Phi_{22}=0, \tag{15}$$

and

$$\Psi_4\Phi_{02}-2\Phi_{12}\Phi_{21}-\Phi_{22}(\Psi_2-2\Phi_{11}+2\Lambda)=L\Phi_{22}. \tag{16}$$

The above relations hold for a general null tetrad. For each Petrov type there exists a preferred tetrad, adapted to the principal null directions of the Weyl tensor, which makes a number of Weyl scalars zero.

If the space–time is of Petrov type I, we can find a null tetrad such that $\Psi_0=\Psi_4=0$ and $\Psi_1\neq 0$, $\Psi_2\neq 0$, and $\Psi_3\neq 0$. But from (1) and (2) we then find the contradiction $\Psi_1=\Psi_3=0$.

In a Petrov type II space–time we can construct a null tetrad such that $\Psi_0=\Psi_1=\Psi_4=0$, $\Psi_2\neq 0$, and $\Psi_3\neq 0$. But then again we find a contradiction with (2).

If the space–time is of Petrov type D we can choose l^α and n^α along the two double degenerate null directions such that $\Psi_0=\Psi_1=\Psi_3=\Psi_4=0$ and $\Psi_2\neq 0$. Equations (1)–(16) are then satisfied if and only if $\Phi_{0i}=\Phi_{2i}=0$ and $L=-(\Psi_2+2\Lambda)$. This is only possible when Ψ_2 is real.

In a Petrov type III space–time we can always construct a null tetrad such that $\Psi_0=\Psi_1=\Psi_2=\Psi_4=0$ and $\Psi_3\neq 0$. But then Eq. (2) gives again a contradiction.

If the space–time is of Petrov type N we can find a null tetrad such that $\Psi_0=\Psi_1=\Psi_2=\Psi_3=0$ and $\Psi_4\neq 0$. The pseudosymmetry relations (1)–(16) are satisfied if and only if $\Phi_{0i}=\Phi_{1i}=0$ and $L=-2\Lambda$.

A space–time is conformally flat, i.e., Petrov type O, if $\Psi_i=0$, $\forall i=0,\ldots,4$. Equations (1)–(16) then reduce to

$$2\Phi_{00}(\Phi_{11}-\Lambda)-2\Phi_{01}\Phi_{10}=L\Phi_{00}, \tag{17}$$

$$\Phi_{00}\Phi_{12}-\Phi_{02}\Phi_{10}-2\Phi_{01}\Lambda=L\Phi_{01}, \tag{18}$$

$$2\Phi_{01}\Phi_{12}-2\Phi_{02}(\Phi_{11}+\Lambda)=L\Phi_{02}, \tag{19}$$

$$\Phi_{00}\Phi_{22}-\Phi_{02}\Phi_{20}-4\Phi_{11}\Lambda=2L\Phi_{11}, \tag{20}$$

$$\Phi_{01}\Phi_{22}-\Phi_{02}\Phi_{21}-2\Phi_{12}\Lambda=L\Phi_{12}, \tag{21}$$

$$2\Phi_{22}(\Phi_{11}-\Lambda)-2\Phi_{12}\Phi_{21}=L\Phi_{22}. \tag{22}$$

In summary we have the following:

Theorem II.1: (i) Petrov type I, II, and III space–times are not pseudosymmetric.

(ii) A Petrov type D space–time is pseudosymmetric iff w.r.t. the principal null tetrad the Ricci tensor has the form $R_{\alpha\beta}=2R_{12}l_{(\alpha}n_{\beta)}+2R_{34}m_{(\alpha}\overline{m}_{\beta)}$ (i.e., the Segré type is [(1,1)(11)]) and $L=-(\Psi_2+2\Lambda)$ with real Ψ_2.

(iii) A Petrov type N space–time is pseudosymmetric iff w.r.t. the principal null tetrad the Ricci tensor has the form $R_{\alpha\beta}=R_{22}l_\alpha l_\beta+R_{12}g_{\alpha\beta}$ (i.e., the Segré type is [2,(11)]) and $L=-2\Lambda$.

(iv) A Petrov type O space–time is pseudosymmetric iff the Ricci tensor satisfies the relations (17)–(22).

For $L=0$ the above theorem yields the classification of the semisymmetric space–times (see e.g., Ref. 3, p. 350 for an alternative way of classifying the semisymmetric space–times).

Theorem II.2: (i) Petrov type I, II, III space–times are not semisymmetric.

(ii) A Petrov D space–time is semisymmetric iff w.r.t. the principal null tetrad the Ricci tensor has the form $R_{\alpha\beta}=2R_{12}l_{(\alpha}n_{\beta)}+2R_{34}m_{(\alpha}\overline{m}_{\beta)}$ (i.e., the Segré type is $[(1,1)(11)]$) and real $\Psi_2=-2\Lambda$.

(iii) A Petrov type N space–time is semisymmetric iff w.r.t. the principal null tetrad the Ricci tensor has the form $R_{\alpha\beta}=R_{22}l_\alpha l_\beta$ (i.e., the Segré type is $[(1,111)]$).

(iv) A Petrov type O space–time is semisymmetric iff the Ricci tensor satisfies the relations (17)–(22) with $L=0$.

Using the Segré type of the Ricci tensor we obtain information about the possible matter content of the pseudosymmetric space–times. We hereafter consider only the physically most relevant cases of vacuum, Einstein, perfect fluid, and electromagnetic (non-)null Maxwell fields.

Corollary II.1: (i) Every vacuum Petrov type D space–time with real Ψ_2 w.r.t. the principal null tetrad is pseudosymmetric (e.g., the Schwarzschild and Kantowski–Sachs metrics). Every Petrov type D non-null Maxwell field ($R_{12}=R_{34}$) is pseudosymmetric and also every Petrov type D Einstein space ($R_{12}=-R_{34}$) is pseudosymmetric. Petrov type D perfect fluids and electromagnetic null fields are not pseudosymmetric.

(ii) A Petrov type N Einstein space–time ($R_{22}=0$) is pseudosymmetric. Space–times of Petrov type N vacuum, perfect fluid or electromagnetic (non)-null field, are not pseudosymmetric ($\Lambda\neq 0$).

(iii) Einstein and perfect fluid (e.g., Robertson–Walker) conformally flat space–times are pseudosymmetric. In the latter case the proportionality factor equals $L=-\frac{1}{3}\rho$, ρ being the energy density. Electromagnetic (non-)null Petrov type O space–times are not pseudosymmetric.

Because a Petrov type D vacuum space–time is only pseudosymmetric if Ψ_2 is real this excludes the Kinnersley class[15] II.E. The metrics in the Kinnersley classes I (i.e. the NUT space–times), II.F, III.A, and IV.A are all pseudosymmetric. In the other classes only those with real nonvanishing Weyl scalar are pseudosymmetric. As such, for example, the Kerr metric, which belongs to Kinnersley class II.A, is readily seen to be not pseudosymmetric (as mentioned already in Ref. 13, although we would like to point out here that the calculations done there for this latter fact were not correct).

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Calculation of the self force using the extended-object approach

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We present the extended-object approach for the explanation and calculation of the self-force phenomenon (often called ''radiation-reaction force''). In this approach, one considers a charged extended object of a finite size ϵ that accelerates in a nontrivial manner, and calculates the total force exerted on it by the electromagnetic field (whose source is the charged object itself). We show that at the limit $\epsilon \to 0$ this overall electromagnetic field yields a universal result, independent of the object's shape, which agrees with the standard expression for the self force acting on a point-like charge. Previous implementation of this approach ended up with expressions for the total electromagnetic force that include $O(1/\epsilon)$ terms which do not have the form required by mass-renormalization. (In the special case of a spherical charge distribution, this $\propto 1/\epsilon$ term was found to be 4/3 times larger than the desired quantity.) We show here that this problem was originated from a too naive definition of the notion of ''total electromagnetic force'' used in previous analyses. We then derive the correct notion of total electromagnetic force. This completely cures the problematic $O(1/\epsilon)$ term, for any object's shape, and yields the correct self force at the limit $\epsilon \to 0$. In particular, for a spherical charge distribution, the above ''4/3 problem'' is resolved. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1737052]

I. INTRODUCTION AND SUMMARY

When an electrically charged particle accelerates (nonuniformly) in flat space–time, it exerts a force on itself. This force, known as the *self force* (or ''radiation-reaction force''), results from the particle's interaction with its own electromagnetic field. Early investigations by Abraham[1] and Lorentz,[2] in the case of nonrelativistic motion, showed that the self force is proportional to the time derivative of the acceleration. Later, Dirac[3] obtained the covariant relativistic expression for the self force:

$$f^{\mu}_{\rm self} = \tfrac{2}{3} q^2 (\dot{a}^{\mu} - a^2 u^{\mu}) \ , \tag{1}$$

where q is the electrical charge, u^{μ} and a^{μ} denote the four-velocity and four-acceleration, respectively, an overdot denotes a proper-time derivative, and $a^2 \equiv a^{\mu} a_{\mu}$.[4] Dirac derived this expression by considering the momentum flux through a ''world-tube'' surrounding the particle's worldline, and demanding energy–momentum conservation.

The fact that a particle can exert a force on itself is obviously intriguing. One of the ways to make sense of this phenomenon is by considering a charged, rigid, extended object of finite size ϵ. A model of a continuously charged, finite-size object has the obvious advantage that the electromagnetic field is everywhere regular, allowing (in principle) an almost straightforward calculation of all electromagnetic forces involved (this is of course not the case when a point-like charge is considered, as the field is singular at the particle's location). On physical grounds, one would expect that an extended object of a sufficiently small size will behave like a point-like particle.

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(One should expect finite-size correction terms, which may depend on the object's shape, but one would hope these corrections would become negligible for a sufficiently small object.)

For a finite-size extended object, each charge element exerts an electromagnetic force on each other charge element. Then, roughly speaking, the overall electromagnetic force that the charged object exerts on itself is the sum of the contributions of all mutual forces between all pairs of the object's charge elements. In the case of a static object this sum always vanishes. However for an accelerating object this sum generically does not vanish due to the energy–momentum exchange between the charged object and the electromagnetic field. In particular, the electromagnetic radiation field carries energy and momentum away from the object to infinity (hence the name "radiation-reaction force").

Recognizing that the overall mutual electromagnetic force does not vanish, one is tempted to identify this overall force with the notion of the self force acting on a charged particle. Thus, one would hope that at the limit where the object's size is taken to zero, a universal result (independent of the object's size and shape) will be obtained, which will coincide with Eq. (1). Many attempts have been made to derive this extended-object total force. Two types of models have been considered: objects that are continuously charged,[2,5–7] and objects with a finite number of discrete charges.[7] The simplest model of a discretely charged rigid object is the "dumbbell," i.e., a fixed-length rod with two point charges located at its two edges. The previous analyses of both the continuous and discrete models revealed that indeed the overall electromagnetic force does not generally vanish. But these analyses also indicated a fundamental difficulty (which we shortly explain), which made it impossible to derive the universal small-size limit of this force. The goal of this paper is to provide a simple resolution to this difficulty.

Let $f^{\mu}_{\rm sum}$ denote the sum of (or, in the continuous model, the double-integral over) all mutual electromagnetic forces, acting on all charge elements at a particular moment. (By "particular moment" we refer here to a hypersurface of simultaneity in the particle's rest frame; see the following.) We would like to explore how $f^{\mu}_{\rm sum}$ depends on ϵ. For all types of electrically charged objects, the small-ϵ dependence of $f^{\mu}_{\rm sum}$ is found to be of the form

$$f^{\mu}_{\rm sum}=c^{\mu}_{-1}/\epsilon+c^{\mu}_{0}+O(\epsilon)\,. \tag{2}$$

The $O(\epsilon)$ term will not concern us here, as it vanishes at the limit $\epsilon\to 0$. The coefficients c^{μ}_{0} and c^{μ}_{-1} depend on the object's worldline, but are (by definition) independent of ϵ.

The $O(\epsilon^{-1})$ term is the problematic term, as it diverges at the limit of interest, i.e., $\epsilon\to 0$. Obviously, the small-object limit does not make sense if we do not know how to handle the problematic term c_{-1}/ϵ.

Now, there is a standard procedure of *mass-renormalization*, often used for eliminating such $O(\epsilon^{-1})$ terms. However, the very nature of this procedure requires that the undesired $O(\epsilon^{-1})$ term will be of the form $-ca^{\mu}$, where c is a parameter that is independent of the time and the state of motion (though it may depend on the object's size and shape): A force term of the form $a^{\mu}\cdot$const can be dropped, because it is experimentally indistinguishable from an inertial term in the equation of motion (see Sec. II). In order for the whole theory to make sense (assuming that interaction energy equally contributes to the inertial mass), the constant c must be equal to the object's electrostatic energy, which we denote $E_{\rm es}$. (Recall that the latter scales like ϵ^{-1}.)

The problem is that the term c^{μ}_{-1}/ϵ is actually *not* equal to $-E_{\rm es}a^{\mu}$—and, furthermore, generally it is not in the form $-ca^{\mu}$, nor is it even in the direction of a^{μ}. In the special case of a spherical charge distribution, several authors found[2,5–7] that the term c^{μ}_{-1}/ϵ indeed takes the form $-ca^{\mu}$, but with $c=(4/3)E_{\rm es}$. This is the well-known "4/3 problem." In this special case the mass-renormalization procedure still makes sense from the operational point of view (because any force term of the form $-ca^{\mu}$ is experimentally indistinguishable from an inertial term), though the logical consistency of the theory may be questioned. The situation is worse, however, when the charge distribution is asymmetric. In such a situation one generally finds that the problematic term c^{μ}_{-1}/ϵ is not even in the direction of a^{μ}. Clearly, this type of divergent term cannot be removed by mass renormalization. A simple demonstration of this situation was given by Griffiths and Owen,[7]

who considered a one-directional motion of a dumbbell. They found that when the dumbbell is oriented perpendicular to the direction of motion, then $c^{\mu}_{-1}/\epsilon = -E_{\rm es}a^{\mu}$ as desired. However, if the dumbbell is co-directed with the motion, then $c^{\mu}_{-1}/\epsilon = -ca^{\mu}$ with $c = 2E_{\rm es}$. Furthermore, if the dumbbell is oriented in any other direction, the term c_{-1}/ϵ will not be co-directed with a^{μ}. Clearly, in such a generic situation the problematic term c^{μ}_{-1}/ϵ cannot be removed by mass renormalization. As a consequence, the limit $\epsilon \to 0$ of $f^{\mu}_{\rm sum}$ does not make a physical sense. We note that this problem arises even if the object's motion is treated in a fully relativistic manner[8]—as long as the quantity $f^{\mu}_{\rm sum}$ is considered.

It should be noted that in the case of a spherical charge distribution there is another ''4/3 problem'': When the object is in slow motion, the electromagnetic-field momentum turns out to be 4/3 times the electromagnetic-field energy times the velocity.[2] We may refer to this problem as the ''inertial 4/3 problem'' (as opposed to the ''mass-renormalization 4/3 problem''). We shall not address this problem here. The relation between these two ''4/3 problems'' is not completely clear. Poincaré[10] introduced the nonelectromagnetic internal stresses in order to resolve the inertial 4/3 problem. On the other hand, the analysis presented in the following clearly indicates that no consideration of the nonelectromagnetic internal forces is required for solving the mass-renormalization 4/3 problem.[11]

In this paper we shall provide a simple and natural solution to the above-mentioned mass-renormalization problem. We shall show that the overall mutual electromagnetic force is *not* the quantity $f^{\mu}_{\rm sum}$ (i.e., the naive sum or integration over all mutual forces); By employing simple energy–momentum considerations we show that the overall mutual electromagnetic force, which we denote $f^{\mu}_{\rm mutual}$, is the sum (or integral) over all mutual forces, each multiplied by a certain kinematic factor representing the proper-time lapse of each charge element between two ''moments'' (i.e., between two neighboring hypersurfaces of simultaneity; see Sec. II). This kinematic factor is of the form $1+O(\epsilon)$; and the $O(\epsilon)$ correction (when multiplying the mutual forces $\propto \epsilon^{-2}$) leads to a difference between $f^{\mu}_{\rm sum}$ and $f^{\mu}_{\rm mutual}$, proportional to ϵ^{-1}, which is exactly the amount required to correct the problematic term c^{μ}_{-1}/ϵ. Namely, when $f^{\mu}_{\rm mutual}$ is expanded in powers of ϵ, it takes a form similar to Eq. (2), but with an $O(1/\epsilon)$ term which is precisely of the form $-E_{\rm es}a^{\mu}$. This $O(1/\epsilon)$ term is naturally removed by mass renormalization.

After we have eliminated the problematic $O(\epsilon^{-1})$ term in Eq. (2), we are left with the regular term c^{μ}_{0}. It is this term which should yield the desired expression for the self force. With the anticipation that the self force should be universal, one would expect c^{μ}_{0} to depend only on the object's total charge q, and not on the way it is distributed. In fact, the very nature of the self-force phenomenon—the force that a charge exerts on itself—suggests that the self force must be proportional to q^2. For continuous charge distributions, the term c^{μ}_{0} is indeed found to be $\propto q^2$ and it can be brought to the form (1). However, for discrete charge distributions c^{μ}_{0} is found to depend on the charge distribution. This is best demonstrated in the simplest discrete model, the dumbbell. In this case, c^{μ}_{0} (like the mutual forces) is proportional to the product q_+q_-, rather than to $q^2 = (q_+ + q_-)^2$, where q_+ and q_- denote the two edge charges. This apparent inconsistency has an obvious origin: The overall force exerted on the dumbbell by the electromagnetic field includes not only the mutual forces between different charges, but also the forces that each of the individual charges exerts *on itself* (which we shall refer to as the ''partial self force,'' to distinguish it from the ''overall self force'' acting on the dumbbell). Obviously, it would be inconsistent to neglect these partial self forces: By universality considerations, one may view each of the point charges as a very small extended charged object; And, the result of our analysis, namely, $c^{\mu}_{0} \neq 0$, should apply to each of these individual charged objects as well, therefore, these forces cannot be ignored. Note that the partial self forces do not depend on the other charges in the extended object, so they are by definition independent of ϵ. Therefore they do not affect the divergent term $O(\epsilon^{-1})$, but merely add to the term c^{μ}_{0}. The need to include these partial self forces might appear disturbing, as these quantities are initially unknown. However, basic considerations imply that the self force acting on each charged object must be proportional to the square of its charge. This observation provides us with the required expression for the partial self forces (more precisely, the relation of the latter to the overall self forces). The inclusion of the partial self forces leads to a universal expression for

the overall electromagnetic force acting on the dumbbell (or on any other discrete charge distribution), which is indeed proportional to the square of the total charge as desired, and which coincides with Eq. (1). We further show in Sec. IV that for a continuous charge distribution the contribution of the partial self forces vanishes. Therefore, in the continuous case the quantity c_0^μ (i.e., the properly weighted integral of the mutual electromagnetic forces) directly yields the desired universal expression for the self force, Eq. (1).

The overall mutual force $f^\mu_{\rm mutual}$ may naturally be viewed as the sum (or double-integral) of the contributions of all *pairs* of charge element. The contribution of each such pair is the sum of the two mutual forces, each weighted by the above-mentioned kinematic factor. In summing these two forces, the dominant $O(\epsilon^{-2})$ term always cancels out (leaving a weaker divergence $\propto\epsilon^{-1}$ that is in turn handled by mass-renormalization). This leading-order cancellation occurs for each pair separately, suggesting that the fundamental element in any extended-object model is the single pair of charges. Once the single-pair system is well understood, the analysis of any charge distribution will follow quite immediately—essentially by summing (or double-integrating) over all pairs of charge elements. We shall therefore start by analyzing the *dumbbell model*, i.e., a pair of point-like charges separated by a fixed-length rod. Then we shall consider a discrete system with an arbitrary number N of charges. Then, taking the infinitesimal limit (in which $N\to\infty$), we shall analyze the case of continuous charge distribution. In all cases the object (and the charge distribution) is regarded as rigid, and we allow it to move (nonrotationally) along an arbitrary worldline. For both the discrete and continuous cases, we obtain the same universal result: After calculating the overall mutual electromagnetic force $f^\mu_{\rm mutual}$, mass-renormalizing it, and then taking the limit $\epsilon\to0$, we recover the desired expression (1) for the self force.

We should mention here previous analyses which seemingly overcame the mass-renormalization 4/3 problem in the spherical case. First, Fermi[16] carried out an extended-object analysis of a different type: Instead of summing the contributions of all mutual forces, he constructed an effective relativistic Hamiltonian of a charged rigid body, and derived the equation of motion from this Hamiltonian. It seems that no ''4/3 problem'' is encountered in this method. Later, Nodvick used a similar method[17] and obtained the correct expression for the self force (note, however, that these analyses[16,17] only considered spherically symmetric distributions, whereas we are treating here an arbitrary charge distribution). Also, after this work was completed, we became aware of a previous work by Pearle,[12] in which he analyzed the case of a spherically symmetric charged object. In this analysis he took into account the above-mentioned kinematic weighting factor which expresses the proper-time lapse of each charge element. Then, in a fairly complicated calculation he obtained the correct $O(1/\epsilon)$ term, namely, $-E_{\rm es}a^\mu$, thereby overcoming the 4/3 problem in the case of spherical charge distribution. We believe that our analysis is simpler, more transparent, and it is also much more general; In particular, the analysis presented here resolves the mass-renormalization problem for *any* type of charge distribution.

An outline of the analysis given here was published recently, focusing on the case of dumbbell-like charge distribution.[18] Here we present the full calculations, and also analyze in detail extended objects with an arbitrary number of point charges, as well as continuously charged extended objects (these cases were only briefly mentioned in Ref. 18).

In Sec. II we analyze the dumbbell model, i.e., the case of two point-like charges. We first formulate the dumbbell's relativistic kinematics. Then we calculate the mutual forces, obtain their sum $f^\mu_{\rm sum}$, and (following Griffiths and Owen[7]) demonstrate the severe mass-renormalization directionality problem discussed earlier. Then we use energy–momentum considerations to construct the correct expression for the overall mutual electromagnetic force $f^\mu_{\rm mutual}$. We show that the latter is free of the mass-renormalization problem. In Sec. III we extend the analysis to a system with an arbitrary number of point-like charges. Finally, in Sec. IV we consider the case of a continuous charge distribution. In all three cases we obtain, at the limit $\epsilon\to0$, the universal result (1).

II. A CHARGED DUMBBELL

A. The general approach

We consider a dumbbell made of a rigid rod with two point charges located at its two edges. The forces acting on the dumbbell (or on its parts) may be schematically divided into several types:

(1) Electromagnetic forces: the forces exerted on the two charges by the electromagnetic field they produce.
(2) The ''other internal forces:'' the inter-atomic (or ''elastic'') forces that are responsible for the dumbbell's rigidity.
(3) External forces: forces exerted on the dumbbell by external fields.[19]

The electromagnetic forces acting on the two charges are divided into two types: (i) mutual electromagnetic forces, i.e., forces that one charge exerts on the other one [more precisely, it is the force that the electromagnetic field produced by one charge (in the sense of the retarded Lienard–Wiechert solution) exerts on the other charge]; and (ii) the self forces that each of the two charges exerts on itself, which we shall refer to as the ''partial self forces'' (to be distinguished from the overall self force acting on the dumbbell). The justification and necessity of including the partial self forces in our analysis is discussed in the following, but two remarks should be made already at this stage: First, the partial self forces are not relevant to the mass-renormalization problem, as they only affect the term c_0^μ (above), not the problematic term c_1^μ/ϵ. Second, these partial self forces are very significant for a system of two charges (they contribute at least as much as the mutual forces do), but they become less important in a system including a large number N of point charges (assuming that the magnitude of the individual charges scales line $1/N$). This is because the number of mutual forces scales like N^2, whereas the number of partial self forces scales like N. Most important, the contribution of partial self forces vanishes at the continuum limit, as we discuss in Sec. IV.

In Newtonian theory it is usually presumed that the sum of any pair of mutual forces will always vanish; however, when electromagnetic interactions are concerned, this presumption does not hold. Its failure may be attributed to the long range of the electrodynamical interaction between two charges. It is this long range which is responsible for the electromagnetic radiative phenomena (which transport energy and momentum away from the interacting charges). On the other hand, the nonelectromagnetic internal forces are assumed here to be of ''short range.'' [20] Hence, it will be assumed that upon summation these forces will always cancel out (except for a ''mass-renormalization like'' term, which is the interaction energy associated with these forces, multiplied by the four-acceleration). For this reason, the nonexternal forces that are relevant to the calculations to follow are only the electromagnetic ones, namely, (i) the two mutual forces between the two charges, and (ii) the two ''partial self forces.''

B. Dumbbell's structure and kinematics

The dumbbell consists of two point charges situated at the edges of a rigid rod of a proper length 2ϵ. We shall assume that ϵ is small compared to $1/a$, where a denotes the norm of the acceleration vector. Throughout this section we shall use the subscripts ''$+$'' or ''$-$'' to denote the quantities associated with the two dumbbell's edges. The two electric charges are therefore denoted q_+ and q_-, respectively, and the total charge is $q \equiv q_+ + q_-$. We do *not* require the two charges to be equal. We assume that ϵ is time-independent and that the dumbbell moves in a nonrotational manner (see the following).

We take the dumbbell's central point (i.e., half way between the two edges) to represent the dumbbell's motion. The worldline of this representative point is denoted $z^\mu(\tau)$, where τ is the proper time along the central worldline. The four-velocity and four-acceleration of the central worldline are defined in the usual manner, $u^\mu \equiv \dot{z}^\mu$ and $a^\mu \equiv \dot{u}^\mu$, where an overdot denotes differ-

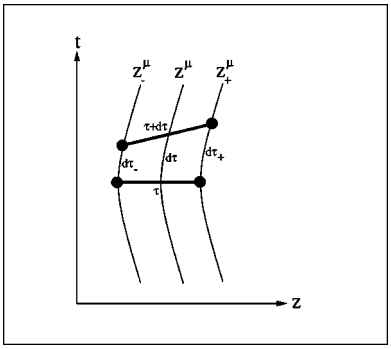

FIG. 1. A space–time diagram describing the dumbbell's kinematics. t is the time coordinate (in some inertial reference frame), and z schematically represents a spatial coordinate. The dumbbell is represented by a straight bold line, with the black points representing the two edge points $z^\mu_\pm$. Two such bold lines are shown, representing the dumbbell's location in space–time at two moments separated by an infinitesimal time interval $d\tau$. The three thin solid lines are the worldlines of the central point z^μ and the two edge points $z^\mu_\pm$.

entiation with respect to τ. We denote the two rod's edges by $z^\mu_+(\tau)$ and $z^\mu_-(\tau)$. At any given moment (by "moment" we mean here a hypersurface of simultaneity in the momentary rest frame of the central point) the two rod's edges are located at (see Fig. 1)

$$z^\mu_\pm(\tau) \equiv z^\mu(\tau) \pm \epsilon w^\mu(\tau) \ , \tag{3}$$

where $w^\mu(\tau)$ is a unit spatial vector, satisfying

$$w_\mu w^\mu = 1, \quad w^\mu u_\mu = 0. \tag{4}$$

The time evolution of w^μ is completely determined by its role here as a vector representing a nonrotating rod: (i) As a unit vector, its norm should be time-independent (corresponding to a rod of fixed length), which implies $\dot{w}^\mu w_\mu = 0$; (ii) as a spatial vector w^μ should be normal to the worldline at all times. Differentiating the second equation in (4) we obtain

$$\dot{w}^\mu u_\mu = -w_\mu a^\mu \ . \tag{5}$$

(iii) Since we assume that w^μ is nonrotating in the momentary rest frame of $z^\mu(\tau)$, $\dot{w}^\mu$ should be free of any spatial component, i.e.,

$$\dot{w}^\mu = c(\tau) u^\mu \ , \tag{6}$$

where $c(\tau)$ is some (yet unspecified) scalar. The last demand, combined with the second equation in (4), guarantees that restriction (i) is satisfied. Substituting Eq. (6) in (5) we find

$$c(\tau) = w_\mu a^\mu \ .$$

We thus arrive at the evolution law

$$\dot{w}^\mu = u^\mu a^\nu w_\nu = u^\mu a_w \ , \tag{7}$$

where we have introduced the scalar $a_w \equiv w_\lambda a^\lambda$. This is in fact an implementation of the more general Fermi–Walker transport law (see, e.g., Ref. 21), $\dot{e}^\mu = (u^\mu a^\nu - u^\nu a^\mu) e_\nu$, to a spatial vector w^μ.

Next, we calculate the four-velocities and accelerations of the dumbbell's edges. We denote the proper times along the worldlines of the two rods' edges $z^\mu_\pm$ by $\tau_\pm$, respectively. Note that

generally τ_+ and τ_- differ from τ (and from each other). The four-velocities of the two charges are defined in the usual manner, $u_\pm^\mu \equiv dz_\pm^\mu/d\tau_\pm$. Differentiating Eq. (3), with respect to $\tau_\pm$, we obtain

$$u_\pm^\mu = (u^\mu \pm \epsilon \dot{w}^\mu)\frac{d\tau}{d\tau_\pm} = \left[(1 \pm \epsilon a_w)\frac{d\tau}{d\tau_\pm}\right]u^\mu \quad . \tag{8}$$

Taking the norm of the two sides of this equation, recalling that both u^μ and $u_\pm^\mu$ are of unit norm, we find that the term in square brackets is just unity, namely,

$$\frac{d\tau_\pm}{d\tau} = 1 \pm \epsilon a_w \quad . \tag{9}$$

It now immediately follows that

$$u_\pm^\mu = u^\mu \quad . \tag{10}$$

These are the two key features of the rod's kinematics.

Equation (10) indicates that in the rest frame of the dumbbell's central point, the two edges (and similarly any other point on the dumbbell) are at rest as well. We can therefore identify this reference frame as the rest frame of the entire dumbbell. Since at any moment there exists a reference frame in which the entire dumbbell is momentarily at rest, it is justified to view this type of motion as a rigid motion.

We denote by $a_\pm^\mu$ the four-accelerations of the two edge points, namely, $a_\pm^\mu = du_\pm^\mu/d\tau_\pm$. From Eqs. (9) and (10) it immediately follows that

$$a_\pm^\mu = \frac{a^\mu}{1 \pm \epsilon a_w} \quad . \tag{11}$$

C. Mutual forces

At the heart of the dumbbell's model are the mutual forces acting between the two charges. To determine these forces, we need an expression for the retarded electromagnetic field tensor $F_{\mu\nu}$ that a single point charge q moving on an arbitrary worldline $z^\mu(\tau)$ produces at a nearby point $z^\mu + \hat{\epsilon}\hat{w}^\mu$, where $\hat{\epsilon}$ is a small positive number ($\hat{\epsilon} = 2\epsilon$), and $\hat{w}^\mu$ is a unit spatial vector satisfying $\hat{w}^\mu \hat{w}_\mu = 1, \hat{w}^\mu u_\mu = 0$. Later we shall apply the limit $\epsilon \to 0$, and therefore we shall only need an expression for $F_{\mu\nu}$ valid up to zero order in $\hat{\epsilon}$. Such an expression was derived by Dirac:[3]

$$\begin{aligned} F_{\mu\nu} &\cong \frac{q}{\sqrt{(1+\hat{\epsilon}a_{\hat{w}})}}\left[\left(\frac{u_\mu \hat{w}_\nu}{\hat{\epsilon}^2} + \frac{a_\mu u_\nu}{2\hat{\epsilon}} + \frac{a^2 u_\mu \hat{w}_\nu}{8} - \frac{\dot{a}_\mu \hat{w}_\nu}{2} - \frac{a_{\hat{w}} a_\mu u_\nu}{2} - \frac{2}{3}\dot{a}_\mu u_\nu\right) - (\mu \leftrightarrow \nu)\right] \\ &\cong q\left[\left(\frac{u_\mu \hat{w}_\nu}{\hat{\epsilon}^2} + \frac{a_\mu u_\nu - a_{\hat{w}} u_\mu \hat{w}_\nu}{2\hat{\epsilon}} - \frac{2}{3}\dot{a}_\mu u_\nu + \hat{Z}_{\mu\nu}\right) - (\mu \leftrightarrow \nu)\right], \end{aligned} \tag{12}$$

where $a_{\hat{w}} \equiv a_\lambda \hat{w}^\lambda$,

$$\hat{Z}_{\mu\nu} \equiv \frac{a^2 u_\mu \hat{w}_\nu}{8} - \frac{\dot{a}_\mu \hat{w}_\nu}{2} + \frac{3a_{\hat{w}}^2 u_\mu \hat{w}_\nu}{8} - \frac{3a_{\hat{w}} a_\mu u_\nu}{4}, \tag{13}$$

$a^2 \equiv a_\mu a^\mu$, and throughout this paper the "$\cong$" symbol denotes an equality up to $O(\epsilon)$ correction terms. $\hat{Z}_{\mu\nu}$ is the collection of all terms that are proportional to $\hat{\epsilon}^0$ and to an odd power of $\hat{w}$. Such terms will cancel out when summing the contributions of the two charges (see the following). The electromagnetic field $F_+^{\mu\nu}$ that the charge q_- produces at the location of charge q_+ is obtained by substituting in Eqs. (12) and (13) $q \to q_-$, $a \to a_-$, $\dot{a} \to da_-/d\tau_-$, $\hat{w}^\mu \to w^\mu$, $a_{\hat{w}} \to a_-^\lambda w_\lambda$, and

$\hat{\epsilon}\to 2\epsilon$ (the four-velocity is unchanged, as $u^\mu_\pm = u^\mu$). The electromagnetic field $F^{\mu\nu}_-$ that the charge q_+ produces at the location of the charge q_- is obtained in a similar manner, by substituting in these equations $q\to q_+$, $a\to a_+$, $\dot{a}\to \mathrm{d}a_+/\mathrm{d}\tau_+$, $\hat{w}^\mu\to -w^\mu$, $a_{\hat{w}}\to -a^\lambda_+ w_\lambda$, and $\hat{\epsilon}\to 2\epsilon$. Let us denote by f^μ_+ (f^μ_-) the Lorentz force that the charge "−" ("+") exerts on the other charge "+" ("−"):

$$f^\mu_\pm = q_\pm F^{\mu\nu}_\pm u_\nu .$$

By virtue of Eq. (12) this becomes

$$f^\mu_\pm \cong q_+ q_- u_\nu \left[\left(\pm\frac{u^\mu w^\nu}{4\epsilon^2} + \frac{a^\mu_\mp u^\nu - (a^\lambda_\mp w_\lambda) u^\mu w^\nu}{4\epsilon} - \frac{2}{3}\dot{a}^\mu_\mp u^\nu \pm Z^{\mu\nu}_\pm \right) - (\mu\leftrightarrow\nu) \right], \tag{14}$$

where

$$Z^{\mu\nu}_\pm \equiv \frac{a^2_\mp u^\mu w^\nu}{8} - \frac{\dot{a}^\mu_\mp w^\nu}{2} + \frac{3(a^\lambda_\mp w_\lambda)^2 u^\mu w^\nu}{8} - \frac{3(a^\lambda_\mp w_\lambda) a^\mu_\mp u^\nu}{4},$$

and $\dot{a}^\mu_\mp \equiv \mathrm{d}a^\mu_\mp/\mathrm{d}\tau_\mp$. Next we re-express $f^\mu_\pm$ in terms of the acceleration a^μ and proper time τ of the central point (rather than those of the source charges). To this end we use Eq. (11), and expand $a^\mu_\mp$ in ϵ. Since the acceleration does not appear in the $O(\epsilon^{-2})$ term, it is sufficient to carry out this expansion up to first order in ϵ:

$$a^\mu_\mp = a^\mu(1 \pm \epsilon a_w) + O(\epsilon^2) .$$

Note that $\dot{a}^\mu_\mp$ only appears in the $O(\epsilon^0)$ term, hence it can be replaced by $\dot{a}^\mu$. [The same holds for all factors $a^\mu_\mp$ and $a^2_\mp$ that appear in the $O(\epsilon^0)$ term.] We find

$$f^\mu_\pm \cong q_+ q_- u_\nu \left[\left(\pm\frac{u^\mu w^\nu}{4\epsilon^2} + \frac{a^\mu u^\nu - a_w u^\mu w^\nu}{4\epsilon} - \frac{2}{3}\dot{a}^\mu u^\nu \pm Z^{\mu\nu} \right) - (\mu\leftrightarrow\nu) \right], \tag{15}$$

where

$$Z^{\mu\nu} \equiv Z^{\mu\nu}_\pm(a^\mu_\mp \to a^\mu) + \frac{a_w a^\mu u^\nu - a^2_w u^\mu w^\nu}{4}.$$

Note that $Z^{\mu\nu}$ is $O(\epsilon^0)$, and is the same for the two charges. Recalling that $u^\nu u_\nu = -1$, $w^\nu u_\nu = a^\nu u_\nu = 0$, and $\dot{a}^\nu u_\nu = -a^2$ (the latter identity is obtained by differentiating $a^\nu u_\nu = 0$), we find

$$f^\mu_\pm \cong q_+ q_- \left[\pm\frac{w^\mu}{4\epsilon^2} - \frac{a^\mu + w^\mu a_w}{4\epsilon} + \frac{2}{3}(\dot{a}^\mu - a^2 u^\mu) \pm Z^\mu \right], \tag{16}$$

where $Z^\mu \equiv u_\nu(Z^{\mu\nu} - Z^{\nu\mu})$.

D. Naive sum of the mutual forces

Next we calculate the sum of the two mutual forces, i.e., the quantity f^μ_{sum}:

$$f^\mu_{\mathrm{sum}} \equiv f^\mu_+ + f^\mu_- \cong -\frac{q_+ q_-}{2\epsilon}(a^\mu + w^\mu a_w) + \frac{4}{3} q_+ q_- (\dot{a}^\mu - a^2 u^\mu) . \tag{17}$$

This quantity would be the simplest candidate for the dumbbell's self force; However, as already discussed in the previous section, it suffers from a serious problem: The first term on the right-hand side is proportional to $1/\epsilon$, and hence diverges at the limit of interest, $\epsilon\to 0$. The usual way to eliminate such an undesired $O(\epsilon^{-1})$ term is by the procedure of *mass renormalization* (see the

following); However, from the very nature of this procedure, it will only be applicable if the term to be removed is of the form $a^\mu \cdot \text{const}$ (a constant that scales like $1/\epsilon$). Instead, in Eq. (17) the term $a^\mu + w^\mu a_w$ is orientation-dependent. Furthermore, this term is *not* co-directed with a^μ. This difficulty was observed by Griffiths and Owen.[7,22] [Note that adding the two "partial self forces" would not change this situation, as it does not affect the $O(\epsilon^{-1})$ term—see the following.]

E. Energy–momentum balance

The above-mentioned pathology of the $O(1/\epsilon)$ term clearly indicates that f^μ_{sum} is not a valid candidate for the dumbbell's self force. The reason is that f^μ_{sum} does not correctly represent the overall mutual force. To understand the reason for this, we shall now employ simple considerations of energy–momentum conservation. These considerations will indicate the appropriate way to sum the two mutual forces, in order to obtain the correct expression for the overall mutual force.

Let us denote the total dumbbell's four-momentum, at a given moment τ, by $p^\mu(\tau)$. This quantity is to be obtained by integrating the appropriate components of the dumbbell's stress–energy tensor over the hypersurface of simultaneity, which we denote σ. Recalling that u^ν is normal to σ, we may write this integral as

$$p^\mu \equiv -\int_\sigma T^{\mu\nu}_{(\text{dumb})} u_\nu d^3\sigma . \tag{18}$$

Here $d^3\sigma$ is a volume element, and $T^{\mu\nu}_{(\text{dumb})}$ denotes the dumbbell's stress–energy tensor, *not including* the electromagnetic field. The integration is performed over the entire volume of the dumbbell (the integrand vanishes off the dumbbell).

It is worth emphasizing two points here: First, the integration is carried out over a *hypersurface of simultaneity*, i.e., a constant-time hypersurface in a Lorentz frame where the dumbbell is instantaneously at rest, and *not* over a hypersurface $t = \text{const}$ of some fixed Lorentz frame. This is the natural covariant way to define the time-dependent four-momentum of a rigid body.[23] Second, we choose not to include the electromagnetic stress–energy tensor in p^μ, because the electromagnetic contribution is not well localized: It is partly scattered throughout the space in the form of electromagnetic waves. The nonelectromagnetic part, however, is by assumption well-localized, and hence monitoring $p^\mu(\tau)$ will provide us with the desired information concerning the dumbbell's motion. Note that the external field (i.e., the above-mentioned "external force") is also not included in $T^{\mu\nu}_{(\text{dumb})}$.

From energy–momentum conservation it follows that $p^\mu(\tau)$ will only change due to external forces acting on the dumbbell (if such exist), and due to energy–momentum exchange between the dumbbell and the electromagnetic field. The electromagnetic energy–momentum exchange is manifested by the electromagnetic forces acting on the two charges. In an infinitesimal time interval $\mathrm{d}\tau$, the change in $p^\mu(\tau)$ will be given by

$$\mathrm{d}p^\mu = \mathrm{d}p^\mu_+ + \mathrm{d}p^\mu_- + \mathrm{d}p^\mu_{\text{ext}} , \tag{19}$$

where $\mathrm{d}p^\mu_{\text{ext}}$ is the contribution of the external force, and $\mathrm{d}p^\mu_\pm$ denote the contributions from the electromagnetic forces acting on the two charges.[24] Let us denote these electromagnetic forces by $f^\mu_{(\text{em})\pm}$. As discussed earlier, $f^\mu_{(\text{em})\pm}$ includes both the mutual electromagnetic force $f^\mu_\pm$, and the partial self force acting on the $\pm$ charge, which we denote $\hat{f}^\mu_\pm$:

$$f^\mu_{(\text{em})\pm} = f^\mu_\pm + \hat{f}^\mu_\pm . \tag{20}$$

Note that simple consistency considerations require us to include the partial self forces in the analysis: Our calculation shows (as many previous analyses did) that there is a nonvanishing self force acting on a charged object (the dumbbell, in our specific model); this force is found to be universal (at the limit of small ϵ), namely it is independent of the object's size and orientation. It must therefore apply to *any* sufficiently small charged object—and, in particular, to the two point

charges q_+ and q_-. Later we shall employ a simple argument to quantitatively relate the two partial self forces $\hat{f}^\mu_\pm$ to the overall self force acting on the dumbbell. (It should be emphasized that the calculation below yields a nonvanishing overall self force even if one does not take into account the partial self forces; Nevertheless the resultant expression for the self force would be incorrect in such a case, due to the inconsistency.) Note that the need for adding the partial self forces is also made obvious from the following observation: Without the partial self forces, the overall mutual electromagnetic force is proportional to the product q_+q_-, whereas the overall self force of the dumbbell (like that of any charged particle) must be proportional to $q^2=(q_+ + q_-)^2$. Adding the partial self forces compensates for this difference exactly, as we show in the following.

Let us now calculate dp^μ_+, the energy–momentum exchange of the "+" charge with the electromagnetic field, between the two hypersurfaces of simultaneity τ and $\tau+d\tau$. An observer located at the "+" charge will measure a proper-time interval $d\tau_+$ between these two hypersurfaces. Therefore, the amount of electromagnetic energy–momentum transfer is $dp^\mu_+ = f^\mu_{(\mathrm{em})+}d\tau_+$. Similar considerations will apply of course to the other charge "−"; therefore,

$$dp^\mu_\pm = f^\mu_{(\mathrm{em})\pm}d\tau_\pm . \tag{21}$$

Combining Eqs. (19), (21), and (20), we obtain

$$dp^\mu = (f^\mu_+ + \hat{f}^\mu_+)d\tau_+ + (f^\mu_- + \hat{f}^\mu_-)d\tau_- + dp^\mu_{\mathrm{ext}} . \tag{22}$$

Defining the overall force acting on the system to be $f^\mu \equiv dp^\mu/d\tau$, we find

$$f^\mu \cong \left[\left\{ f^\mu_+ \frac{d\tau_+}{d\tau} + f^\mu_- \frac{d\tau_-}{d\tau} \right\} + (\hat{f}^\mu_+ + \hat{f}^\mu_-)\right] + f^\mu_{\mathrm{ext}} . \tag{23}$$

Note that since the external force is presumably regular (i.e., it is well-behaved at the limit of small ϵ), and $d\tau_\pm/d\tau \to 1$ at the limit $\epsilon \to 0$, we can simply take $dp^\mu_{\mathrm{ext}} \cong f^\mu_{\mathrm{ext}}d\tau$. For the same reason, since the partial self forces are presumably regular, too, we can ignore the factors $d\tau_\pm/d\tau$ multiplying $\hat{f}^\mu_\pm$. It is only the mutual force $f^\mu_\pm$, which includes negative powers of ϵ, that requires one to make the distinction between $d\tau$ and $d\tau_\pm$.

The overall mutual electromagnetic force f^μ_{mutual} is the term in curly braces in Eq. (23):

$$f^\mu_{\mathrm{mutual}} = f^\mu_+ \frac{d\tau_+}{d\tau} + f^\mu_- \frac{d\tau_-}{d\tau} . \tag{24}$$

Using Eqs. (9) and (16), and again neglecting terms that vanish as $\epsilon \to 0$, we find

$$f^\mu_\pm \frac{d\tau_\pm}{d\tau} = (1 \pm \epsilon a_w) f^\mu_\pm \cong q_+q_- \left[\pm \frac{w^\mu}{4\epsilon^2} - \frac{a^\mu}{4\epsilon} + \frac{2}{3}(\dot{a}^\mu - a^2u^\mu) \pm \tilde{Z}^\mu \right],$$

where

$$\tilde{Z}^\mu = Z^\mu - \frac{a_w(a^\mu + w^\mu a_w)}{4} .$$

It now follows that

$$f^\mu_{\mathrm{mutual}} \cong -\frac{q_+q_-}{2\epsilon}a^\mu + \frac{4}{3}q_+q_-(\dot{a}^\mu - a^2u^\mu) . \tag{25}$$

The overall electromagnetic contribution to the total force f^μ acting on the dumbbell (not including the external force) is the term in square brackets in Eq. (23), i.e., the sum of f^μ_{mutual} and

the two partial self forces. We shall refer to it as the "bare self force" (because subsequently we shall apply to it the mass-renormalization procedure, to obtain the "renormalized self force"), and denote it f^{μ}_{bare}. It is given by

$$f^{\mu}_{\text{bare}} = f^{\mu}_{\text{mutual}} + (\hat{f}^{\mu}_{+} + \hat{f}^{\mu}_{-}) = -\frac{q_+ q_-}{2\epsilon} a^{\mu} + \frac{4}{3} q_+ q_- (\dot{a}^{\mu} - a^2 u^{\mu}) + (\hat{f}^{\mu}_{+} + \hat{f}^{\mu}_{-}) + O(\epsilon) . \tag{26}$$

F. Mass renormalization and the renormalized self force

In Eq. (26) [like in Eq. (25)] the $O(1/\epsilon)$ term has the desired form $-E_{\text{es}} a^{\mu}$, where E_{es} is the dumbbell's electrostatic energy (at rest):

$$E_{\text{es}} \equiv q_+ q_- / 2\epsilon .$$

This is exactly the type of $O(1/\epsilon)$ term that is cured by mass renormalization, as we now briefly discuss.

The expression for the self force is to be used for predicting the dumbbell's motion, through an equation of motion of the form $m_{\text{bare}} a^{\mu} = f^{\mu}$, where f^{μ} refers to the total force acting on the dumbbell, i.e., $f^{\mu} = f^{\mu}_{\text{bare}} + f^{\mu}_{\text{ext}}$. (In the following we shall further discuss the justification to this equation of motion.) Similarly, m_{bare} refers to the so-called "bare mass," i.e., the total dumbbell's energy (in the momentary rest frame) *not including the electromagnetic/electrostatic interaction energy*. We now add the term $E_{\text{es}} a^{\mu}$ to both sides of the equation of motion. Defining the "renormalized mass" m_{ren} and "renormalized self force" f^{μ}_{ren} by

$$m_{\text{ren}} \equiv m_{\text{bare}} + E_{\text{es}} , \quad f^{\mu}_{\text{ren}} \equiv f^{\mu}_{\text{bare}} + E_{\text{es}} a^{\mu} , \tag{27}$$

the equation of motion now takes the form

$$m_{\text{ren}} a^{\mu} = f^{\mu}_{\text{ren}} + f^{\mu}_{\text{ext}} .$$

This is the "renormalized equation of motion." Note that m_{ren} is nothing but the total dumbbell's energy (including the electrostatic interaction) while at rest. This is in fact the measured physical mass of the dumbbell. To simplify the notation, we shall hereafter omit the suffix "ren," denoting the renormalized mass by m and the "renormalized self force" by f^{μ}_{self}. The equation of motion now reads

$$m a^{\mu} = f^{\mu}_{\text{self}} + f^{\mu}_{\text{ext}} ,$$

where

$$f^{\mu}_{\text{self}} \equiv f^{\mu}_{\text{bare}} + E_{\text{es}} a^{\mu} = \tfrac{4}{3} q_+ q_- (\dot{a}^{\mu} - a^2 u^{\mu}) + (\hat{f}^{\mu}_{+} + \hat{f}^{\mu}_{-}) + O(\epsilon) . \tag{28}$$

Now that we eliminated the problematic $O(1/\epsilon)$ term, we can safely take the limit $\epsilon \to 0$. It is at this limit where we expect to obtain the universal expression for the self force. In this limit all the $O(\epsilon)$ correction terms vanish, and we find

$$f^{\mu}_{\text{self}} = \tfrac{4}{3} q_+ q_- (\dot{a}^{\mu} - a^2 u^{\mu}) + (\hat{f}^{\mu}_{+} + \hat{f}^{\mu}_{-}) . \tag{29}$$

As it stands, Eq. (29) provides a single relation for three unknowns, $\hat{f}^{\mu}_{\pm}$ and f^{μ}_{self}. In order to extract from it the expression for f^{μ}_{self}, we need to relate the latter to the two partial self forces $\hat{f}^{\mu}_{\pm}$. Since the self force is the force that a charge experiences due to its own field, it must be proportional (for a prescribed worldline) to q^2, where q is the particle's charge. In the limit of interest, $\epsilon \to 0$, the trajectories of the two charges $\pm$, and also that of the dumbbell itself (i.e., the repre-

sentative point), all converge to the same worldline. Therefore, the two partial self forces $\hat{f}^{\mu}_{\pm}$ will be given by $\hat{f}^{\mu}_{\pm}=(q^2_{\pm}/q^2)f^{\mu}_{\rm self}$, where $q=q_+ + q_-$ is the dumbbell's total charge. Substituting this in Eq. (29), rewriting it as

$$\frac{4}{3}q_+q_-(\dot{a}^{\mu}-a^2u^{\mu})=f^{\mu}_{\rm self}-(\hat{f}^{\mu}_{+}+\hat{f}^{\mu}_{-})=\left[1-\frac{q^2_+}{q^2}-\frac{q^2_-}{q^2}\right]f^{\mu}_{\rm self}\,, \tag{30}$$

and noting that the term in square brackets is nothing but $2q_+q_-/q^2$, we finally obtain the desired expression for the self force:

$$f^{\mu}_{\rm self}=\tfrac{2}{3}q^2(\dot{a}^{\mu}-a^2u^{\mu}). \tag{31}$$

This agrees with Dirac's[3] expression (1).

To summarize, let us formulate all elements of the above-mentioned construction of $f^{\mu}_{\rm self}$ by a single mathematical expression. This expression takes the form

$$f^{\mu}_{\rm self}=\frac{q^2}{2q_+q_-}\lim_{\epsilon\to 0}\left[(1+\epsilon a_w)f^{\mu}_{+}+(1-\epsilon a_w)f^{\mu}_{-}+\frac{q_+q_-}{2\epsilon}a^{\mu}\right]. \tag{32}$$

This involves the following manipulations, which are all justified (and necessitated) by simple physical considerations: (i) the proper-time weighting of the two mutual force (the factors $(1\pm\epsilon a_w)$); (ii) mass renormalization (the last term in the square brackets); (iii) the inclusion of the partial self forces (the factor $q^2/2q_+q_-$); and (iv) taking the limit $\epsilon\to 0$. This expression yields a universal, orientation-independent, result, which conforms with the well-known expression (1) for the self force.

Finally, we briefly discuss the justification of the (''bare'') equation of motion $m_{\rm bare}a^{\mu}=f^{\mu}$ in our case. We have *defined* the total force f^{μ} as the proper-time derivative of the dumbbell's nonelectromagnetic energy–momentum p^{μ}. Let us transform to a Lorentz frame in which the dumbbell is momentarily at rest. In this frame Eq. (18) reads

$$p^{\mu}\equiv\int_{t=\rm const}T^{\mu 0}_{\rm (dumb)}d^3x^i\,, \tag{33}$$

where x^i denotes the three spatial Cartesian coordinates. For simplicity let us approximate the dumbbell's stress–energy by that of a continuous matter (plus, possibly, arbitrary number of point masses situated at fixed locations on the dumbbell). Since the matter that composes each element of the dumbbell is momentarily at rest, $T^{i0}_{\rm (dumb)}$ vanishes, and hence $p^i=0$. The dumbbell's energy in the rest frame is

$$p^0\equiv\int_{t=\rm const}T^{00}_{\rm (dumb)}d^3x^i\quad\text{(rest frame)}. \tag{34}$$

This is by definition the dumbbell's bare mass. Thus, in the momentary rest frame we have $p^{\mu}=(m_{\rm bare},0,0,0)$. Rewriting this in a covariant form (valid in any Lorentz frame), we obtain

$$p^{\mu}=m_{\rm bare}u^{\mu}\,.$$

Since the dumbbell is approximated as rigid, its composition does not change in time, hence $m_{\rm bare}$ is time-independent. Differentiating now p^{μ} with respect to proper time, we obtain the desired equation of motion

$$f^{\mu}=m_{\rm bare}a^{\mu}\,.$$

Recall that this is the ''bare'' equation of motion. After mass renormalization, we obtain the equation of motion in its final, renormalized form:[25]

$$ma^{\mu}=f^{\mu}_{\text{self}}+f^{\mu}_{\text{ext}}=\tfrac{2}{3}q^{2}(\dot{a}^{\mu}-a^{2}u^{\mu})+f^{\mu}_{\text{ext}}\ . \tag{35}$$

III. EXTENDED OBJECT WITH *N* POINT CHARGES

In this section we shall consider a rigid extended object with an arbitrary number N of point charges located on it. The charges are denoted q_i, where hereafter Roman indices like $i,j,\ldots$ run from 1 to N. The total charge is $q=\Sigma_i q_i$. We shall calculate the overall self force acting on the object by a natural extension of the method used earlier in the dumbbell case.

A. Extended object kinematics

We start by describing the extended object kinematics. We choose (quite arbitrarily) a representative point inside this object and denote its worldline by $z^{\mu}(\tau)$, and its four-velocity and four-acceleration by $u^{\mu}\equiv \mathrm{d}z^{\mu}/\mathrm{d}\tau$ and $a^{\mu}\equiv \mathrm{d}u^{\mu}/\mathrm{d}\tau$, respectively, where τ is the proper time along this worldline.

The location of a charge i at each moment τ is given by[27]

$$z^{\mu}_{i}(\tau)\equiv z^{\mu}(\tau)+\epsilon_i w^{\mu}_{i}(\tau), \tag{36}$$

where $\epsilon_i\geqslant 0$ is the distance of the charge i from the representative point, and $w^{\mu}_{i}(\tau)$ is a unit spatial vector normal to $u^{\mu}(\tau)$. We denote the proper time of this worldline by τ_i and its four-velocity and four-acceleration by $u^{\mu}_{i}\equiv \mathrm{d}z^{\mu}_{i}/\mathrm{d}\tau_i$ and $a^{\mu}_{i}\equiv \mathrm{d}u^{\mu}_{i}/\mathrm{d}\tau_i$, respectively.

Since the object is rigid, and it moves in a nonrotational manner, the time evolution of the spatial vectors w^{μ}_{i} is given by the Fermi–Walker transport,

$$\dot{w}^{\mu}_{i}=(u^{\mu}a_{\nu}-u_{\nu}a^{\mu})w^{\nu}_{i}=u^{\mu}a_{\nu}w^{\nu}_{i}. \tag{37}$$

Repeating the above-presented dumbbell kinematic calculations, we again find that

$$\frac{\mathrm{d}\tau_i}{\mathrm{d}\tau}=1+\epsilon_i a_{\mu}w^{\mu}_{i} \tag{38}$$

and

$$u^{\mu}_{i}=u^{\mu}\ . \tag{39}$$

Again, the last equality implies that in the momentary rest frame of the representative point, all charges are (momentarily) at rest too. One also finds that

$$a^{\mu}_{i}=\frac{a^{\mu}}{1+\epsilon_i a_{\nu}w^{\nu}_{i}}. \tag{40}$$

We shall be interested in the limit in which the object's size is taken to be arbitrarily small, but its shape (including the location of the charges) is unchanged in this limiting process. To describe this limit mathematically, let $\epsilon>0$ denote the object's size, e.g., its ''radius'' (i.e., half the maximal distance between pairs of object's points). We now define

$$\epsilon_i\equiv\epsilon\alpha_i\ .$$

The parameters α_i are thus dimensionless numbers of order unity or smaller. The above-noted limiting process is thus described by $\epsilon\to 0$ with all parameters α_i kept fixed.

In the calculations to follow we shall make use of the results that were obtained in Sec. II in the dumbbell case. Recall, however, that in the latter case the representative point was chosen at

half the distance between the two charges. This cannot be done in the present case (as long as $N>2$). In order to allow the implementation of the dumbbell results to our case, we shall also need to consider, for each pair of charges i,j, the worldline of the central point between these two charges, which we denote z^μ_{ij}:

$$z^\mu_{ij}(\tau)\equiv\tfrac{1}{2}[z^\mu_i(\tau)+z^\mu_j(\tau)]=z^\mu(\tau)+\tfrac{1}{2}[\epsilon_i w^\mu_i+\epsilon_j w^\mu_j]\,.$$

Obviously there exists a number $\epsilon_{ij}\geqslant 0$ and a unit vector w^μ_{ij} such that $\epsilon_{ij}w^\mu_{ij}=(1/2)(\epsilon_i w^\mu_i+\epsilon_j w^\mu_j)$. Then ϵ_{ij} is the distance of this central point from the representative point, and (for $\epsilon_{ij}>0$) w^μ_{ij} is a vector normal to u^α which satisfies the Fermi–Walker transport law, as one can easily verify. We denote the proper time along the worldline $z^\mu_{ij}(\tau)$ by τ_{ij}, and the four-velocity and four-acceleration by $u^\mu_{ij}\equiv \mathrm{d}z^\mu_{ij}/\mathrm{d}\tau_{ij}$ and $a^\mu_{ij}\equiv \mathrm{d}u^\mu_{ij}/\mathrm{d}\tau_{ij}$, respectively. Obviously all the above-mentioned kinematic relations satisfied by the point charge $z^\mu_i(\tau)$, e.g., Eqs. (38)–(40), are also satisfied by a central point $z^\mu_{ij}(\tau)$. Of particular importance for the analysis to follow is the relation

$$a^\mu_{ij}\frac{\mathrm{d}\tau_{ij}}{\mathrm{d}\tau}=a^\mu\,, \tag{41}$$

which follows from Eqs. (38) and (40) (with "i" replaced by "ij").

Let us finally emphasize that, for a particular pair i,j, the three points z^μ_i, z^μ_j, and z^μ_{ij} satisfy all the dumbbell's kinematic relations satisfied by the three dumbbell's points z^μ_+, z^μ_-, and z^μ, correspondingly. This will allow us to apply all the above-mentioned dumbbell results to any pair i,j, though with the dumbbell's central point z^μ replaced by z^μ_{ij} (and τ by τ_{ij}, etc.). The dumbbell's length $\hat{\epsilon}=2\epsilon$ is of course replaced by the distance between the charges i and j, which we denote $\hat{\epsilon}_{ij}$.

B. Calculation of the self force

To derive the self force acting on the extended object we shall use energy–momentum considerations similar to those of Sec. II. The four-momentum of the extended object $p^\mu(\tau)$ is defined just as in the dumbbell case, by the integral (18) over a hypersurface of simultaneity. In analogy with Eq. (19), we now have

$$\mathrm{d}p^\mu=\sum_{i=1}^{N}\mathrm{d}p^\mu_i+\mathrm{d}p^\mu_{\mathrm{ext}}\,, \tag{42}$$

where $\mathrm{d}p^\mu_i$ denotes the contribution from all the electromagnetic forces (sourced by all object's charges) acting on the ith charge, and $\mathrm{d}p^\mu_{\mathrm{ext}}$ denotes the contribution from the overall external force. The electromagnetic energy–momentum exchange with the charge i is

$$\mathrm{d}p^\mu_i=f^\mu_{(\mathrm{em})i}\mathrm{d}\tau_i\,,$$

where $f^\mu_{(\mathrm{em})i}$ is the overall electromagnetic forces acting on the charge i, given by

$$f^\mu_{(\mathrm{em})i}=\hat{f}^\mu_i+\sum_{\substack{j=1\\ j\neq i}}^{N}f^\mu_{j\to i}\,.$$

Here $f^\mu_{j\to i}$ denotes the electromagnetic force that the charge j exerts on the charge i, and $\hat{f}^\mu_i$ denotes the partial self force acting on this charge. Therefore,

$$\mathrm{d}p^\mu=\mathrm{d}p^\mu_{\mathrm{ext}}+\sum_{i=1}^{N}\hat{f}^\mu_i\mathrm{d}\tau_i+\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}f^\mu_{j\to i}\mathrm{d}\tau_i\,.$$

Since the external force is presumably well behaved as $\epsilon \to 0$ (it is essentially independent of ϵ), we can use $\mathrm{d}p^{\mu}_{\mathrm{ext}} \cong f^{\mu}_{\mathrm{ext}} \mathrm{d}\tau$, without bothering which proper time exactly one should use. For the same reason we may replace $\mathrm{d}\tau_i$ multiplying the partial self force by $\mathrm{d}\tau$. Defining the overall force acting on the object to be

$$f^{\mu} = \frac{\mathrm{d}p^{\mu}}{\mathrm{d}\tau},$$

we obtain

$$f^{\mu} \cong \left[\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathrm{d}\tau_i}{\mathrm{d}\tau} f^{\mu}_{j \to i} + \sum_{i=1}^{N} \hat{f}^{\mu}_{i} \right] + f^{\mu}_{\mathrm{ext}}. \tag{43}$$

The overall mutual force is the term including the double-sum over i and j:

$$f^{\mu}_{\mathrm{mutual}} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathrm{d}\tau_i}{\mathrm{d}\tau} f^{\mu}_{j \to i} = \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathrm{d}\tau_{ij}}{\mathrm{d}\tau} \left[\frac{\mathrm{d}\tau_i}{\mathrm{d}\tau_{ij}} f^{\mu}_{j \to i} + \frac{\mathrm{d}\tau_j}{\mathrm{d}\tau_{ij}} f^{\mu}_{i \to j} \right]. \tag{44}$$

Consider the last term in square brackets, for a particular pair of charges i,j. This pair satisfies a ''dumbbell kinematics''; namely, the kinematic relations between the worldlines of the three points z^{μ}_i, z^{μ}_j, and z^{μ}_{ij} are exactly the same as those satisfied by the three dumbbell's points z^{μ}_{+}, z^{μ}_{-}, and z^{μ}, correspondingly. This allows us to apply the dumbbell's results to this new two-charge system. In particular, Eqs. (24) and (25) now yield

$$\frac{\mathrm{d}\tau_i}{\mathrm{d}\tau_{ij}} f^{\mu}_{j \to i} + \frac{\mathrm{d}\tau_j}{\mathrm{d}\tau_{ij}} f^{\mu}_{i \to j} \cong - \frac{q_i q_j}{\hat{\epsilon}_{ij}} a^{\mu}_{ij} + \frac{4}{3} q_i q_j (\dot{a}^{\mu}_{ij} - a^2_{ij} u^{\mu}),$$

where $\hat{\epsilon}_{ij}$ is the distance between the two charges, and $\dot{a}^{\mu}_{ij} \equiv \mathrm{d}a^{\mu}_{ij}/\mathrm{d}\tau_{ij}$. Note that $\hat{\epsilon}_{ij}$, like all other object's distances, scales like ϵ (the object's size). Since the last term at the right-hand side is of order ϵ^0, we are allowed to replace τ_{ij} and a^{μ}_{ij} by the corresponding representative-point quantities, τ and a^{μ} (which we cannot do when treating the other term, the one proportional to $1/\hat{\epsilon}_{ij}$). With the aid of Eq. (41) we obtain

$$\frac{\mathrm{d}\tau_{ij}}{\mathrm{d}\tau} \left[\frac{\mathrm{d}\tau_i}{\mathrm{d}\tau_{ij}} f^{\mu}_{j \to i} + \frac{\mathrm{d}\tau_j}{\mathrm{d}\tau_{ij}} f^{\mu}_{i \to j} \right] \cong - \frac{q_i q_j}{\hat{\epsilon}_{ij}} a^{\mu} + \frac{4}{3} q_i q_j (\dot{a}^{\mu} - a^2 u^{\mu}).$$

Notice that in the last expression all kinematic quantities are those associated with the representative point, and the only reference to the two charges is through q_i, q_j, and $\hat{\epsilon}_{ij}$. Substituting this result back in Eq. (44) we obtain

$$f^{\mu}_{\mathrm{mutual}} \cong - E_{\mathrm{es}} a^{\mu} + \frac{2}{3} \left(\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} q_i q_j \right) (\dot{a}^{\mu} - a^2 u^{\mu}), \tag{45}$$

where

$$E_{\mathrm{es}} \equiv \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_i q_j}{\hat{\epsilon}_{ij}}. \tag{46}$$

This last expression is exactly the electrostatic energy of the system of N charges (the factor 1/2 corresponds to the fact that every pair i,j appears twice in this sum).

The overall (bare) self force f^{μ}_{bare} is the term in square brackets in Eq. (43), which we write as

$$f^{\mu}_{\text{bare}} = f^{\mu}_{\text{mutual}} + \sum_{i=1}^{N} \hat{f}^{\mu}_{i} = -E_{\text{es}} a^{\mu} + \frac{2}{3}\left(\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \right)(\dot{a}^{\mu} - a^2 u^{\mu}) + \sum_{i=1}^{N} \hat{f}^{\mu}_{i} + O(\epsilon) . \qquad (47)$$

Implementing now the mass-renormalization procedure, given by Eq. (27), and then taking the limit $\epsilon \to 0$, we obtain the renormalized self force:

$$f^{\mu}_{\text{self}} = \frac{2}{3}\left(\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \right)(\dot{a}^{\mu} - a^2 u^{\mu}) + \sum_{i=1}^{N} \hat{f}^{\mu}_{i} . \qquad (48)$$

To factor out the partial self forces, we again use the fact that the self force is quadratic in the charge, namely,

$$\hat{f}^{\mu}_{i} = (q_i^2/q^2) f^{\mu}_{\text{self}} ,$$

where $q \equiv \Sigma_i q_i$ is the total charge. Transferring all partial self forces to the left-hand side and then multiplying by q^2, we obtain

$$\left[q^2 - \sum_{i=1}^{N} q_i^2 \right] f^{\mu}_{\text{self}} = \frac{2}{3} q^2 \left[\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \right](\dot{a}^{\mu} - a^2 u^{\mu}) .$$

Noting that the two terms in square brackets are equal, we obtain the self force in its final form:

$$f^{\mu}_{\text{self}} = \frac{2}{3} q^2 (\dot{a}^{\mu} - a^2 u^{\mu}) . \qquad (49)$$

The equation of motion is given by Eq. (35), just as in the dumbbell case.

IV. CONTINUOUSLY CHARGED EXTENDED OBJECT

In this section we shall consider a rigid extended object which is continuously charged. Again, we denote the object's size (e.g., its "radius") by ϵ. Let (X,Y,Z) be a system of comoving Cartesian coordinates that parametrize the three-dimensional hypersurface of simultaneity, and let $\overline{R} \equiv (X,Y,Z)$. The representative point (an arbitrary point of the object) is taken to be, e.g., at $\overline{R} = 0$. Note that the worldline of any point of fixed $\overline{R}$ satisfies all the kinematic relations described in Sec. III. The charge distribution is denoted $\rho(X,Y,Z)$. We assume that the charge distribution is fixed (in the object's frame), i.e., $\rho(X,Y,Z)$ is independent of the proper time τ.

The calculation of the self force proceeds in full analogy with the discrete case discussed in Sec. III, with the discrete charge q_i replaced by the infinitesimal charge element $\mathrm{d}q \equiv \rho \mathrm{d}X\, \mathrm{d}Y\, \mathrm{d}Z$, and with the summations replaced by integrals. There is a remarkable difference between the two cases, though: In the discrete case, the demand for consistency required us to take into account the partial self forces. No such partial self forces appear in the continuous case (see the following). This makes the continuous case simpler and more elegant.

One can follow all the considerations and calculations of Sec. III, up to Eq. (47). In the continuous variant of this equation, the double-sum becomes a double-integral:

$$\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \to \int \int \rho(\overline{R}_1)\rho(\overline{R}_2) d^3\overline{R}_1 d^3\overline{R}_2 = q^2 , \qquad (50)$$

where $q \equiv \int \rho(\overline{R}) d^3\overline{R}$ is the total charge. On the other hand, the term including the partial self forces has only one summation. This term disappears in the continuous case: At the limit $N \to \infty$ (in which the individual charges scale like $1/N$) the magnitude of the individual partial self forces

scales like $q_i^2 \propto 1/N^2$, whereas their number only scales like N. Therefore, the overall contribution of the partial self forces scales like $1/N \to 0$.[28] (This is to be contrasted with the situation of the mutual electromagnetic forces: The magnitude of the mutual forces scales like $1/N^2$ too, but their number scales like N^2, so the overall mutual force attains a nonvanishing value at the limit $N \to \infty$.) The integral analog of Eq. (47) is thus

$$f^{\mu}_{\text{bare}} = -E_{\text{es}} a^{\mu} + \tfrac{2}{3} q^2 (\dot{a}^{\mu} - a^2 u^{\mu}) + O(\epsilon) , \tag{51}$$

where E_{es} is the integral analog of Eq. (46):

$$E_{\text{es}} \equiv \frac{1}{2} \int \int \frac{\rho(\bar{R}_1)\rho(\bar{R}_2)}{|\bar{R}_1 - \bar{R}_2|} d^3\bar{R}_1 d^3\bar{R}_2 . \tag{52}$$

Note that E_{es} is the electrostatic energy of the continuous charge distribution.

The mass-renormalization (27) now removes the irregular term $E_{\text{es}} a^{\mu}$ in Eq. (51), and (after taking the limit $\epsilon \to 0$) one arrives at the final expression for the self force:

$$f^{\mu}_{\text{self}} = \tfrac{2}{3} (\dot{a}^{\mu} - a^2 u^{\mu}) . \tag{53}$$

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$O(1/\epsilon)$ term of $f^{\mu}_{\rm sum}$ is the "4/3 problem." However, for generic nonsymmetric distributions, the integrated force will not be co-directed with a^{μ}.

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Hydrodynamic reductions of multidimensional dispersionless PDEs: The test for integrability

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A $(d+1)$-dimensional dispersionless PDE is said to be integrable if its n-component hydrodynamic reductions are locally parametrized by $(d-1)n$ arbitrary functions of one variable. The most important examples include the four-dimensional heavenly equation descriptive of self-dual Ricci-flat metrics and its six-dimensional generalization arising in the context of sdiff(Σ^2) self-dual Yang–Mills equations. Given a multidimensional PDE which does *not* pass the integrability test, the method of hydrodynamic reductions allows one to effectively reconstruct additional differential constraints which, when added to the equation, make it an integrable system in fewer dimensions. As an example of this phenomenon we discuss the second commuting flow of the dispersionless KP hierarchy. Considered separately, this is a four-dimensional PDE which does *not* pass the integrability test. However, the method of hydrodynamic reductions generates additional differential constraints which reconstruct the full $(2+1)$-dimensional dispersionless KP hierarchy. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738951]

I. INTRODUCTION

We address the problem of integrability of multidimensional dispersionless PDEs of the form

$$F(u,u_i,u_{ij})=0, \tag{1}$$

where u is a (vector-) function of $d+1$ independent variables. For definiteness, let us consider $(3+1)$-dimesional PDEs in four independent variables t,x,y,z. Equations of this type naturally arise in mechanics, mathematical physics, general relativity, and differential geometry. Let us look for exact solutions of (1) of the form $u=u(R^1,\ldots,R^n)$ where the Riemann invariants $R^1,\ldots,R^n$ solve a triple of commuting diagonal systems

$$R^i_t=\lambda^i(R)\ R^i_x, \quad R^i_y=\mu^i(R)\ R^i_x, \quad R^i_z=\eta^i(R)\ R^i_x. \tag{2}$$

Notice that the number of Riemann invariants is allowed to be arbitrary. Thus, the original multidimensional equation (1) is decoupled into a collection of commuting $(1+1)$-dimensional systems in Riemann invariants. In some cases one first needs to rewrite the original PDE (1) in a quasilinear form to make the method work: see examples in Sec. II. Solutions of this type, known as nonlinear interactions of n planar simple waves, were investigated in gas dynamics and magnetohydrodynamics.[32,4,29] Later, they appeared in the context of the dispersionless KP hierarchy.[14–16,18,24,25,3] We will call a multidimensional equation integrable if it possesses sufficiently many n-component reductions of the form (2) for arbitrary n (the precise definition follows). Exact solutions arising within this approach can be viewed as dispersionless analogues of n-gap solutions.

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Partial classification results of $(2+1)$-dimensional integrable systems of hydrodynamic type (the integrability is understood in the above sense) were obtained in our recent publications.[12,13] Integrable second order PDEs of the form $u_{tt}=f(u_{xx},u_{xt},u_{xy})$ were classified in Ref. 28. Particularly interesting examples arise in the theory of self-dual and Einstein–Weyl spaces,[30,8–11] in the context of the Dirichlet boundary problem in multiconnected domains,[22] and the Whitham averaging procedure (in particular, the dispersionless limit) applied to $(2+1)$-dimensional solitonic PDEs.[20,21,34]

We recall, see Ref. 33, that the requirement of commutativity of the flows (2) is equivalent to the following restrictions on their characteristic speeds:

$$\frac{\partial_j\lambda^i}{\lambda^j-\lambda^i}=\frac{\partial_j\mu^i}{\mu^j-\mu^i}=\frac{\partial_j\eta^i}{\eta^j-\eta^i}, \tag{3}$$

$i\neq j$, $\partial_j=\partial/\partial_{R^j}$; no summation. Once these conditions are met, the general solution of (2) is given by the implicit generalized hodograph formula[33]

$$v^i(R)=x+\lambda^i(R)t+\mu^i(R)\ y+\eta^i(R)z, \quad i=1,\ldots,n, \tag{4}$$

where $v^i(R)$ are characteristic speeds of the general flow commuting with (2), that is, the general solution of the linear system

$$\frac{\partial_j v^i}{v^j-v^i}=\frac{\partial_j\lambda^i}{\lambda^j-\lambda^i}=\frac{\partial_j\mu^i}{\mu^j-\mu^i}=\frac{\partial_j\eta^i}{\eta^j-\eta^i}. \tag{5}$$

Substituting $u(R^1,\ldots,R^n)$ into (1) and using (2) one arrives at an over-determined system for $\lambda^i(R),\mu^i(R),\eta^i(R)$, and $u(R)$ as functions of the Riemann invariants R^i. This system implies, in particular, that the characteristic speeds λ^i,μ^i, and η^i satisfy an algebraic relation which can be interpreted as the dispersion relation for the system (1).

One can show that the requirement of existence of nontrivial three-component reductions is already sufficiently restrictive implying, in particular, the existence of n-component reductions for arbitrary n.[12] This phenomenon is similar to the well-known three-soliton condition in the Hirota bilinear approach[19] (recall that two-soliton solutions exist for arbitrary PDEs transformable to Hirota's bilinear form and, therefore, cannot detect the integrability), and the condition of three-dimensional consistency in the classification of discrete integrable systems on quad-graphs.[1] One can show that the maximum number of n-component reductions a $(d+1)$-dimensional PDE may possess is parametrized, modulo changes of variables $R^i\to f^i(R^i)$, by $(d-1)n$ arbitrary functions of one variable. Therefore, we propose the following.

Definition: A $(d+1)$-dimensional PDE is said to be integrable if its n-component reductions are locally parametrized by $(d-1)n$ arbitrary functions of one variable.

One of the most important examples of PDEs in four dimensions which are integrable in this sense is the second heavenly equation,

$$\theta_{tx}+\theta_{zy}+\theta_{xx}\theta_{yy}-\theta_{xy}^2=0,$$

descriptive of self-dual Einstein spaces[30] (see Example 2 of Sec. II). Its equivalent first heavenly form was discussed in the recent publication[11] where it was shown that n-component reductions are parametrized by $2n$ arbitrary functions of a single variable. It would be interesting to compare these reductions with the solitonic reductions of Ref. 7. The requirement of existence of n-component reductions parametrized by $2n$ arbitrary functions of one variable appears to be very strong, indeed, the heavenly equation is the only nonlinear PDE of the form

$$\theta_{tx}+\theta_{zy}=f(\theta_{xx},\theta_{xy},\theta_{yy}),$$

which passes the integrability test (see the Appendix).

An interesting six-dimensional integrable generalization of the heavenly equation,

$$\theta_{t\tilde{t}}+\theta_{z\tilde{z}}+\theta_{tx}\theta_{zy}-\theta_{ty}\theta_{zx}=0,$$

arises in the context of sdiff(Σ^2) self-dual Yang–Mills equations.[31] Its n-component reductions are parametrized by $4n$ arbitrary functions of a single variable (Example 5 of Sec. III). We would like to thank M. Dunajski for drawing our attention to this equation.

Another integrable example is the six-dimensional system

$$m_t=n_x+nm_r-mn_r, \quad n_z=m_y+mn_s-nm_s,$$

see Sec. III. Its n-component reductions depend on $4n$ arbitrary functions of one variable. Under the additional constraints $m_r=n_r=0$, $s=x$, $z=t$, this system is descriptive of hyperCR Einstein–Weyl structures;[6] it was investigated in a series of recent publications.[27,9,26]

In the Example 3 of Sec. II we apply our method to the four-dimensional PDE

$$F_{xz}=F_{xx}F_{xy}+F_{yt},$$

which is the second flow of the dispersionless KP (dKP) hierarchy

$$F_{xt}=\tfrac{1}{2}F_{xx}^2+F_{yy},$$

$$F_{xz}=F_{xx}F_{xy}+F_{yt},$$

see, e.g., Ref. 5. It is demonstrated that, considered separately, this equation is *not* integrable (as a four-dimensional PDE), the fact which is not at all surprising. What is more important, the method of hydrodynamic reductions allows one to effectively reconstruct the differential constraint $F_{xt}=\frac{1}{2}F_{xx}^2+F_{yy}$ which, when added to the equation, generates the $(2+1)$-dimensional dKP hierarchy.

Although the method of hydrodynamic reductions provides an infinity of (implicit) solutions parametrized by arbitrarily many functions of one variable, the question of solving the initial value problem for integrable multidimensional dispersionless PDEs remains open. A detailed investigation of the behavior and singularity structure of solutions describing nonlinear interactions of planar simple waves is beyond the scope of this paper.

II. EXAMPLES

In this section we list some examples of multidimensional PDEs which are integrable in the sense of hydrodynamic reductions.

Example 1: Let us consider the first two flows of the dispersionless KP hierarchy,

$$F_{xt}=\tfrac{1}{2}F_{xx}^2+F_{yy},$$

$$F_{xz}=F_{xx}F_{xy}+F_{yt}, \tag{6}$$

which, in the new variables

$$F_{xx}=u, \quad F_{xy}=v, \quad F_{yy}=w, \quad F_{yt}=s, \quad F_{xt}=\tfrac{1}{2}u^2+w, \quad F_{xz}=uv+s,$$

assume the quasilinear form

$$\begin{aligned} &u_y=v_x, \quad v_y=w_x, \quad v_t=s_x, \quad w_t=s_y, \quad u_t=(\tfrac{1}{2}u^2+w)_x, \quad u_z=(uv+s)_x,\\ &v_t=(\tfrac{1}{2}u^2+w)_y, \quad v_z=(uv+s)_y, \quad s_x=(\tfrac{1}{2}u^2+w)_y, \quad (\tfrac{1}{2}u^2+w)_z=(uv+s)_t. \end{aligned} \tag{7}$$

Notice that u satisfies the dispersionless KP equation,

$$(u_t - uu_x)_x = u_{yy}.$$

Looking for reductions in the form $u=u(R^1,\ldots,R^n)$, $v=v(R^1,\ldots,R^n)$, $w=w(R^1,\ldots,R^n)$, $s=s(R^1,\ldots,R^n)$ where the Riemann invariants R^i satisfy (2), and substituting into (7), one readily obtains

$$\partial_i v = \mu^i \partial_i u, \quad \partial_i s = \lambda^i \mu^i \partial_i u, \quad \partial_i w = (\mu^i)^2 \partial_i u, \tag{8}$$

along with the dispersion relations

$$\lambda^i = u + (\mu^i)^2, \quad \eta^i = v + 2u\mu^i + (\mu^i)^3. \tag{9}$$

The compatibility condition $\partial_i \partial_j v = \partial_j \partial_i v$ implies

$$\partial_i \partial_j u = \frac{\partial_j \mu^i}{\mu^j - \mu^i} \partial_i u + \frac{\partial_i \mu^j}{\mu^i - \mu^j} \partial_j u, \tag{10}$$

while the commutativity condition (3) results in

$$\partial_j \mu^i = \frac{\partial_j u}{\mu^j - \mu^i}. \tag{11}$$

The substitution of (11) into (10) implies the Gibbons–Tsarev system for $u(R)$ and $\mu^i(R)$,

$$\partial_j \mu^i = \frac{\partial_j u}{\mu^j - \mu^i}, \quad \partial_i \partial_j u = 2 \frac{\partial_i u \partial_j u}{(\mu^j - \mu^i)^2}, \tag{12}$$

$i \neq j$, which was first derived in Refs. 15 and 16 in the context of hydrodynamic reductions of Benney's moment equations. For any solution μ^i, u of the system (12) one can reconstruct λ^i, η^i and v, s, w by virtue of the relations (9) and (10), which are automatically consistent. The general solution of the system (12) depends, modulo reparametrizations $R^i \to f^i(R^i)$, on n arbitrary functions of one variable, thus manifesting the fact that PDEs (6) constitute a $(2+1)$-dimensional integrable system.

Example 2: The so-called second heavenly equation,

$$\theta_{tx} + \theta_{zy} + \theta_{xx}\theta_{yy} - \theta_{xy}^2 = 0, \tag{13}$$

is descriptive of self-dual Ricci-flat metrics.[30] Introducing the variables $\theta_{xx}=u$, $\theta_{xy}=v$, $\theta_{yy}=w$, $\theta_{tx}=p$, $\theta_{zy}=v^2-uw-p$, one can rewrite (13) in a quasilinear form,

$$\begin{gathered} u_y = v_x, \quad u_t = p_x, \quad v_y = w_x, \quad v_t = p_y, \\ v_z = (v^2 - uw - p)_x, \quad w_z = (v^2 - uw - p)_y. \end{gathered} \tag{14}$$

Hydrodynamic reductions are sought in the form $u=u(R^1,\ldots,R^n)$, $v=v(R^1,\ldots,R^n)$, $w=w(R^1,\ldots,R^n)$, $p=p(R^1,\ldots,R^n)$ where the Riemann invariants $R^1,\ldots,R^n$ solve a triple of commuting hydrodynamic type systems (2). The substitution into (14) implies

$$\partial_i p = \lambda^i \partial_i u, \quad \partial_i v = \mu^i \partial_i u, \quad \partial_i w = (\mu^i)^2 \partial_i u, \tag{15}$$

along with the dispersion relation

$$\lambda^i = 2v\mu^i - w - u(\mu^i)^2 - \mu^i \eta^i. \tag{16}$$

Substituting λ^i into the commutativity conditions (3), and taking into account that the compatibility conditions for the relations $\partial_i p = \lambda^i \partial_i u$, $\partial_i v = \mu^i \partial_i u$ imply

$$\partial_i\partial_j u=\frac{\partial_j\mu^i}{\mu^j-\mu^i}\partial_i u+\frac{\partial_i\mu^j}{\mu^i-\mu^j}\partial_j u,$$

one arrives at the following system:

$$\partial_j\mu^i=\frac{(\mu^j-\mu^i)^2}{\eta^j-\eta^i+u(\mu^j-\mu^i)}\partial_j u,\quad \partial_j\eta^i=\frac{(\mu^j-\mu^i)(\eta^j-\eta^i)}{\eta^j-\eta^i+u(\mu^j-\mu^i)}\partial_j u,$$

$$\partial_i\partial_j u=2\frac{\mu^j-\mu^i}{\eta^j-\eta^i+u(\mu^j-\mu^i)}\partial_i u\partial_j u. \tag{17}$$

Solving equations (17) for μ^i,η^i and u, determining λ^i from (16) and calculating p,v,w from Eqs. (15) [which are automatically compatible by virtue of (17)], one obtains the general n-component hydrodynamic reduction of the heavenly equation. Moreover, the commutativity conditions will also be satisfied identically.

We emphasize that the system (17) is in involution and its general solution depends on $3n$ arbitrary functions of one variable. Indeed, one can arbitrarily prescribe the restrictions of μ^i and η^i to the R^i-coordinate line. This gives $2n$ arbitrary functions. Moreover, one can arbitrarily prescribe the restriction of u to each of the coordinate lines, which provides extra n arbitrary functions. However, since reparametrizations $R^i\to f^i(R^i)$ leave the system (17) invariant, one concludes that general n-component reductions are locally parametrized by $2n$ arbitrary functions of one variable. This supports the evidence that the heavenly equation (13) is a true four-dimensional integrable PDE.

Obviously, the same method applies to other equivalent forms of the heavenly equation (13). For instance, hydrodynamic reductions of the first heavenly equation

$$\Omega_{xy}\Omega_{zt}-\Omega_{xt}\Omega_{zy}=1$$

were investigated in detail in Ref. 11. Another possibility is to work with the evolutionary form[17] of the heavenly equation,

$$\psi_{tt}=\psi_{xy}\psi_{zt}-\psi_{xt}\psi_{zy}.$$

In both cases one can derive analogues of equations (17) which, although involutive, look somewhat more complicated.

The requirement of existence of n-component reductions (parametrized by $2n$ arbitrary functions of one variable) is very strong indeed: as demonstrated in the Appendix, the heavenly equation (13) is the only nonlinear PDE of the form

$$\theta_{tx}+\theta_{zy}+f(\theta_{xx},\theta_{xy},\theta_{yy})=0,$$

which passes the integrability test.

Remark: The heavenly equation (and equivalent forms thereof) belongs to the class of special Monge–Ampére equations which can be defined as follows. Consider a function $u(x^1,\dots x^k)$ and introduce a $k\times k$ symmetric matrix $U=|u_{ij}|$ of its second partial derivatives. A special Monge–Ampere equation with constant coefficients is a PDE of the form

$$M_0+M_1+\cdots+M_k=0,$$

where M_l is a constant-coefficient linear combination of all distinct $l\times l$ minors of U, $0\leqslant l\leqslant k$. Here, for instance, M_0 is a constant, $M_k=\det U=\mathrm{Hess}\,u$, etc. Equivalently, this PDE can be obtained by equating to zero a constant-coefficient k-form in $2k$ variables x^i,u_i. It is an interesting problem to classify integrable PDEs within this class, in particular, for $k=4$. We emphasize that the case $k=3$ is understood completely: one can show that, for $k=3$, any special Monge–

Ampére equation is either linearizable by a contact transformation (in this case it is automatically integrable by the method of hydrodynamic reductions), or contact equivalent to either of the three nondegenerate forms,[23,2]

$$\mathrm{Hess}\, u = 1, \quad \mathrm{Hess}\, u = u_{11} + u_{22} + u_{33}, \quad \mathrm{Hess}\, u = u_{11} + u_{22} - u_{33}.$$

We have verified directly that these three PDEs are *not* integrable by the method of hydrodynamic reductions.

Example 3: Let us consider the second flow of the dispersionless KP hierarchy,

$$F_{xz} = F_{xx}F_{xy} + F_{yt}, \tag{18}$$

see Example 1. The question is: should it be regarded as a four-dimensional integrable PDE? We will see that the answer to this question is negative, moreover, the method of hydrodynamic reductions applied to this equation reconstructs additional differential constraints which, when added to (18), generate the $(2+1)$-dimensional dKP hierarchy. In the new variables

$$F_{xx} = u, \quad F_{xy} = v, \quad F_{yy} = w, \quad F_{yt} = s, \quad F_{xt} = p, \quad F_{xz} = uv + s,$$

Eq. (18) assumes the quasilinear form

$$\begin{gathered} u_y = v_x, \quad v_y = w_x, \quad v_t = s_x, \quad w_t = s_y, \quad u_t = p_x, \quad u_z = (uv+s)_x, \\ v_t = p_y, \quad v_z = (uv+s)_y, \quad s_x = p_y, \quad p_z = (uv+s)_t. \end{gathered} \tag{19}$$

Looking for reductions in the form $u = u(R^1, \ldots, R^n)$, $v = v(R^1, \ldots, R^n)$, $w = w(R^1, \ldots, R^n)$, $s = s(R^1, \ldots, R^n)$, $p = p(R^1, \ldots, R^n)$, where the Riemann invariants R^i satisfy (2), and substituting into (19), one readily obtains

$$\partial_i v = \mu^i \partial_i u, \quad \partial_i s = \lambda^i \mu^i \partial_i u, \quad \partial_i w = (\mu^i)^2 \partial_i u, \quad \partial_i p = \lambda^i \partial_i u, \tag{20}$$

along with the dispersion relation

$$\eta^i = v + u\mu^i + \mu^i \lambda^i. \tag{21}$$

The compatibility condition $\partial_i \partial_j v = \partial_j \partial_i v$ implies

$$\partial_i \partial_j u = \frac{\partial_j \mu^i}{\mu^j - \mu^i} \partial_i u + \frac{\partial_i \mu^j}{\mu^i - \mu^j} \partial_j u, \tag{22}$$

while the commutativity condition (3) results in

$$\partial_j \mu^i = \frac{\mu^j + \mu^i}{\lambda^j - \lambda^i} \partial_j u, \quad \partial_j \lambda^i = \frac{\mu^j + \mu^i}{\mu^j - \mu^i} \partial_j u. \tag{23}$$

The substitution of (23) into (22) implies the over-determined system for $\mu^i(R)$, $\lambda^i(R)$, and $u(R)$,

$$\begin{gathered} \partial_j \mu^i = \frac{\mu^j + \mu^i}{\lambda^j - \lambda^i} \partial_j u, \quad \partial_j \lambda^i = \frac{\mu^j + \mu^i}{\mu^j - \mu^i} \partial_j u, \\ \partial_i \partial_j u = 2 \frac{\mu^j + \mu^i}{(\mu^j - \mu^i)(\lambda^j - \lambda^i)} \partial_i u \partial_j u, \end{gathered} \tag{24}$$

$i \neq j$, which is analogous to the system (17). There is one crucial difference: the system (24) is *not* in involution. Calculating compatibility conditions $\partial_k(\partial_j \mu^i) - \partial_j(\partial_k \mu^i) = 0$, $\partial_k(\partial_j \lambda^i) - \partial_j(\partial_k \lambda^i) = 0$, and $\partial_k(\partial_j \partial_i u) - \partial_j(\partial_k \partial_i u) = 0$, one arrives at extra relations

$$[(\mu^i)^2(\lambda^k-\lambda^j)+(\mu^k)^2(\lambda^j-\lambda^i)+(\mu^j)^2(\lambda^i-\lambda^k)]$$
$$\times[\mu^k\mu^j(\lambda^k-\lambda^j)+\mu^i\mu^j(\lambda^j-\lambda^i)+\mu^i\mu^k(\lambda^i-\lambda^k)]=0. \tag{25}$$

Thus, there are two cases to consider.

Case 1: Equating to zero the first set of square brackets in (25),

$$(\mu^i)^2(\lambda^k-\lambda^j)+(\mu^k)^2(\lambda^j-\lambda^i)+(\mu^j)^2(\lambda^i-\lambda^k)=0,$$

one obtains $\lambda^i=a(\mu^i)^2+b$. The substitution of this ansatz into (24) implies $(\mu^i)^2\partial_j a+\partial_j b=\partial_j u$, so that $a=\alpha$, $b=u+\beta$ where α,β are arbitrary constants. Thus, $\lambda^i=\alpha(\mu^i)^2+u+\beta$. Substituting λ^i into the equation $\partial_i p=\lambda^i\partial_i u$ and using (20) one obtains, upon elementary integration, $p=\frac{1}{2}u^2+\beta u+\alpha w+\gamma$. Expressed in terms of second derivatives of F, this constraint reads

$$F_{xt}=\tfrac{1}{2}F_{xx}^2+\beta F_{xx}+\alpha F_{yy}+\gamma.$$

One can show that the constants α,β,γ are not essentials and can be reduced to $\alpha=1,\beta=\gamma=0$. Thus, the method of hydrodynamic reductions applied to the PDE (18) reconstructs the first flow of the dKP hierarchy, $F_{xt}=\frac{1}{2}F_{xx}^2+F_{yy}$.

Case 2: Equating to zero the second set of square brackets in (25),

$$\mu^k\mu^j(\lambda^k-\lambda^j)+\mu^i\mu^j(\lambda^j-\lambda^i)+\mu^i\mu^k(\lambda^i-\lambda^k)=0,$$

one obtains $\lambda^i=(a/\mu^i)+b$. The substitution of this ansatz into (24) implies $\partial_j a+\mu^j\partial_j u+\mu^i(\partial_j b+\partial_j u)=0$, so that $a=-v+\alpha$, $b=-u+\beta$ where α,β are arbitrary constants. Thus, $\lambda^i=[(\alpha-v)/\mu^i]+\beta-u$. Substituting λ^i into the equation $\partial_i s=\lambda^i\mu^i\partial_i u$ and using (20) one has, upon elementary integration, $s=-uv+\alpha u+\beta v+\gamma$. Expressed in terms of second derivatives of F, this constraint reads

$$F_{xx}F_{xy}+F_{yt}=\alpha F_{xx}+\beta F_{xy}+\gamma.$$

Again, the constants α,β,γ are not essentials and can be reduced to zero. The resulting constraint $F_{yt}+F_{xx}F_{xy}=0$ characterizes stationary points of the flow (18). We have checked that this constraint is integrable in the sense of hydrodynamic reductions [as a $(2+1)$-dimensional PDE].

In any case, we conclude that Eq. (18) is *not* integrable as a four-dimensional PDE. This is manifested by the fact that the system (24), which governs hydrodynamic reductions, is not in involution.

Example 4: Let us consider the system

$$m_t=n_x, \quad n_z=m_y+mn_x-nm_x, \tag{26}$$

which, in the limit $z=t$, has been extensively investigated in Refs. 27, 9, and 26. Looking for reductions in the form $m=m(R^1,\ldots,R^n)$, $n=n(R^1,\ldots,R^n)$ where the Riemann invariants R^i satisfy (2), one obtains

$$\partial_i n=\lambda^i\partial_i m, \quad \mu^i=\lambda^i\eta^i-m\lambda^i+n.$$

The commutativity conditions (3) imply

$$\partial_j\eta^i=\partial_j m, \quad \partial_i\partial_j m=0,$$

hence, up to reparametrizations $R^i\to\varphi^i(R^i)$, one has

$$m=\sum_k R^k, \quad \eta^i=f^i(R^i)+\sum_k R^k,$$

where $f^i(R^i)$ are arbitrary functions of a single variable. The characteristic speeds λ^i solve the linear system

$$\frac{\partial_j \lambda^i}{\lambda^j - \lambda^i} = \frac{1}{f^j(R^j) - f^i(R^i)}.$$

We refer to Ref. 27 for the general formula for λ^i and further discussion of this example in the $(2+1)$-dimensional limit $z=t$. Thus, n-component hydrodynamic reductions of the system (26) are parametrized by $2n$ arbitrary functions of one variable [n functions $f^i(R^i)$ plus n functions in the general solution of the linear system for λ^i]. Therefore, the four-dimensional system (26) is integrable. Notice that it can be obtained as the condition of commutativity of two vector fields,

$$[\partial_z - m\partial_x - \lambda\partial_x, \quad \partial_y - n\partial_x - \lambda\partial_t] = 0,$$

$\lambda = \text{const}$, compare with Ref. 9. Some further multidimensional generalizations of this example are discussed in Sec. III.

Example 5: The six-dimensional generalization of the heavenly equation,

$$\theta_{t\tilde{t}} + \theta_{z\tilde{z}} + \theta_{tx}\theta_{zy} - \theta_{ty}\theta_{zx} = 0, \tag{27}$$

has been proposed in Ref. 31. Introducing the variables $\theta_{tx}=a$, $\theta_{zy}=b$, $\theta_{ty}=p$, $\theta_{zx}=q$, $\theta_{z\tilde{z}}=r$, $\theta_{t\tilde{t}}=pq-ab-r$, one can rewrite (27) in a quasilinear form,

$$\begin{gathered} a_y = p_x, \quad a_z = q_t, \quad b_t = p_z, \quad b_x = q_y, \quad b_{\tilde{z}} = r_y, \quad q_{\tilde{z}} = r_x, \\ p_{\tilde{z}} = (pq - ab - r)_y. \end{gathered} \tag{28}$$

Hydrodynamic reductions are sought in the form $a=a(R^1,\ldots,R^n)$, $b=b(R^1,\ldots,R^n)$, $p=p(R^1,\ldots,R^n)$, $q=q(R^1,\ldots,R^n)$, $r=r(R^1,\ldots,R^n)$, where the Riemann invariants $R^1,\ldots,R^n$ solve the commuting equations

$$R^i_x = \lambda^i(R)\ R^i_z, \quad R^i_y = \mu^i(R)\ R^i_z, \quad R^i_{\tilde{z}} = \eta^i(R)\ R^i_z, \quad R^i_t = \beta^i(R)\ R^i_z, \quad R^i_{\tilde{t}} = \gamma^i(R)\ R^i_z.$$

The substitution into (28) implies

$$\partial_i p = \beta^i \partial_i b, \quad \partial_i r = \frac{\eta^i}{\mu^i}\partial_i b, \quad \partial_i q = \frac{\lambda^i}{\mu^i}\partial_i b, \quad \partial_i a = \frac{\lambda^i \beta^i}{\mu^i}\partial_i b, \tag{29}$$

along with the dispersion relation

$$\eta^i = \beta^i \mu^i q + \lambda^i p - \beta^i \lambda^i b - \mu^i a - \beta^i \gamma^i. \tag{30}$$

Substituting η^i into the commutativity conditions

$$\frac{\partial_j \lambda^i}{\lambda^j - \lambda^i} = \frac{\partial_j \mu^i}{\mu^j - \mu^i} = \frac{\partial_j \eta^i}{\eta^j - \eta^i} = \frac{\partial_j \beta^i}{\beta^j - \beta^i} = \frac{\partial_j \gamma^i}{\gamma^j - \gamma^i},$$

and taking into account that the compatibility conditions for the relations $\partial_i p = \beta^i \partial_i b$ imply

$$\partial_i \partial_j b = \frac{\partial_j \beta^i}{\beta^j - \beta^i}\partial_i b + \frac{\partial_i \beta^j}{\beta^i - \beta^j}\partial_j b,$$

one arrives at the following system:

$$\frac{\partial_j\beta^i}{\beta^j-\beta^i}=\frac{\partial_j\lambda^i}{\lambda^j-\lambda^i}=\frac{\partial_j\mu^i}{\mu^j-\mu^i}=\frac{\partial_j\gamma^i}{\gamma^j-\gamma^i}=\frac{\lambda^i-\lambda^j\mu^i/\mu^j}{q(\mu^j-\mu^i)+b(\lambda^i-\lambda^j)+\gamma^i-\gamma^j}\,\partial_j b,$$
$$\partial_i\partial_j b=\frac{\lambda^i(1+\mu^j/\mu^i)-\lambda^j(1+\mu^i/\mu^j)}{q(\mu^j-\mu^i)+b(\lambda^i-\lambda^j)+\gamma^i-\gamma^j}\,\partial_i b\,\partial_j b. \tag{31}$$

Solving equations (31) for β^i, λ^i, μ^i, γ^i, and b, determining η^i from the dispersion relation (30) and calculating p,r,q,a from Eqs. (29) [which are automatically compatible by virtue of (31)], one obtains the general n-component reduction of Eq. (27). The commutativity conditions will be satisfied identically. We have checked that the system (31) is in involution and its general solution depends, up to reparametrizations $R^i\to\varphi^i(R^i)$, on $4n$ arbitrary functions of one variable.

III. MULTIDIMENSIONAL LINEARLY DEGENERATE SYSTEMS OF HYDRODYNAMIC TYPE

In the recent publication,[13] we gave a complete characterization of two-component $(2+1)$-dimensional integrable systems of hydrodynamic type,

$$\begin{pmatrix} v\\ w\end{pmatrix}_t+A(v,w)\begin{pmatrix} v\\ w\end{pmatrix}_x+B(v,w)\begin{pmatrix} v\\ w\end{pmatrix}_y=0,$$

which possess infinitely many hydrodynamic reductions. The integrability conditions constitute a complicated overdetermined system of second order PDEs for 2×2 matrices A and B. In the particular case when the matrix A is assumed to be linearly degenerate,

$$A=\begin{pmatrix} w & 0\\ 0 & v\end{pmatrix}, \tag{32}$$

these conditions imply

$$B=\begin{pmatrix} \dfrac{f(w)}{w-v}-\alpha w^2 & \dfrac{f(v)}{w-v}\\[2ex] \dfrac{f(w)}{v-w} & \dfrac{f(v)}{v-w}-\alpha v^2\end{pmatrix},$$

where f is a cubic polynomial, $f(v)=\alpha v^3+\beta v^2+\gamma v+\delta$, and $\alpha,\beta,\gamma,\delta$ are arbitrary constants. A remarkable property of this example is that *any* matrix in the linear pencil $B+\mu A$ is also linearly degenerate [that is, reduces to the diagonal form (32) after an appropriate change of dependent variables]. Explicitly, one has

$$B=\delta B_1+\gamma B_2+\beta B_3+\alpha B_4=\delta\begin{pmatrix} \dfrac{1}{w-v} & \dfrac{1}{w-v}\\[2ex] \dfrac{1}{v-w} & \dfrac{1}{v-w}\end{pmatrix}+\gamma\begin{pmatrix} \dfrac{w}{w-v} & \dfrac{v}{w-v}\\[2ex] \dfrac{w}{v-w} & \dfrac{v}{v-w}\end{pmatrix}+\beta\begin{pmatrix} \dfrac{w^2}{w-v} & \dfrac{v^2}{w-v}\\[2ex] \dfrac{w^2}{v-w} & \dfrac{v^2}{v-w}\end{pmatrix}$$
$$+\alpha\begin{pmatrix} \dfrac{vw^2}{w-v} & \dfrac{v^3}{w-v}\\[2ex] \dfrac{w^3}{v-w} & \dfrac{wv^2}{v-w}\end{pmatrix}.$$

Let us introduce the $(5+1)$-dimensional system,

$$\begin{pmatrix} v \\ w \end{pmatrix}_t + A\begin{pmatrix} v \\ w \end{pmatrix}_x + B_1\begin{pmatrix} v \\ w \end{pmatrix}_y + B_2\begin{pmatrix} v \\ w \end{pmatrix}_z + B_3\begin{pmatrix} v \\ w \end{pmatrix}_s + B_4\begin{pmatrix} v \\ w \end{pmatrix}_r = 0.$$

Notice that an arbitrary linear combination of matrices A and B_1, B_2, B_3, B_4 is linearly degenerate. In the new variables $m=v+w$, $n=vw$, this system reduces to

$$m_t + n_x + nm_r - mn_r = 0, \quad n_t + mn_x - nm_x + m_y + n_z + mn_s - nm_s = 0,$$

taking a fully symmetric form

$$m_{\tilde{t}} = n_{\tilde{x}} + nm_{\tilde{r}} - mn_{\tilde{r}}, \quad n_{\tilde{z}} = m_{\tilde{y}} + mn_{\tilde{s}} - nm_{\tilde{s}}, \tag{33}$$

after the obvious linear change of independent variables. In the limit $\tilde{s}=\tilde{x}$, $m_{\tilde{r}}=n_{\tilde{r}}=0$ it reduces to the system (26) from Example 4. Notice that the system (33) arises as the condition of commutativity of two vector fields,

$$[\partial_{\tilde{z}} - m\partial_{\tilde{s}} - \lambda\partial_{\tilde{x}} + \lambda m\partial_{\tilde{r}}, \quad \partial_{\tilde{y}} - n\partial_{\tilde{s}} - \lambda\partial_{\tilde{t}} + \lambda n\partial_{\tilde{r}}] = 0.$$

Let us demonstrate that the system (33) possesses enough hydrodynamic reductions and, therefore, should be regarded as an integrable system in $5+1$ dimensions. Looking for reductions in the form $m=m(R^1,\ldots,R^n)$, $n=n(R^1,\ldots,R^n)$ where the Riemann invariants R^i solve five commuting systems,

$$R^i_{\tilde{t}} = \lambda^i(R)\ R^i_{\tilde{x}}, \quad R^i_{\tilde{y}} = \mu^i(R)\ R^i_{\tilde{x}}, \quad R^i_{\tilde{z}} = \eta^i(R)\ R^i_{\tilde{x}}, \quad R^i_{\tilde{r}} = \beta^i(R)\ R^i_{\tilde{x}}, \quad R^i_{\tilde{s}} = \gamma^i(R)\ R^i_{\tilde{x}},$$

and substituting into (33), we obtain

$$(\lambda^i - n\beta^i)\partial_i m = (1-m\beta^i)\partial_i n, \quad (\eta^i - m\gamma^i)\partial_i n = (\mu^i - n\gamma^i)\partial_i m.$$

Setting $\partial_i n = \varphi^i \partial_i m$, one obtains expressions for λ^i and μ^i in the form

$$\lambda^i = n\beta^i + (1-m\beta^i)\varphi^i, \quad \mu^i = n\gamma^i + (\eta^i - m\gamma^i)\varphi^i,$$

as well as the consistency condition

$$\partial_i\partial_j m = \frac{\partial_j \varphi^i}{\varphi^j - \varphi^i}\partial_i m + \frac{\partial_i \varphi^j}{\varphi^i - \varphi^j}\partial_j m.$$

Inserting the expressions for λ^i and μ^i into the commutativity conditions

$$\frac{\partial_j \lambda^i}{\lambda^j - \lambda^i} = \frac{\partial_j \mu^i}{\mu^j - \mu^i} = \frac{\partial_j \eta^i}{\eta^j - \eta^i} = \frac{\partial_j \beta^i}{\beta^j - \beta^i} = \frac{\partial_j \gamma^i}{\gamma^j - \gamma^i},$$

one ends up with the following equations for η^i, β^i, γ^i, φ^i, and m:

$$\frac{\partial_j \eta^i}{\eta^j - \eta^i} = \frac{\partial_j \beta^i}{\beta^j - \beta^i} = \frac{\partial_j \gamma^i}{\gamma^j - \gamma^i} = \frac{\beta^i \eta^i - \gamma^i}{(1-m\beta^j)(\eta^i - m\gamma^i) - (1-m\beta^i)(\eta^j - m\gamma^j)}\partial_j m,$$

$$\frac{\partial_j \varphi^i}{\varphi^j - \varphi^i} = \frac{\beta^i \eta^j - \gamma^i + m(\gamma^i\beta^j - \gamma^j\beta^i)}{(1-m\beta^j)(\eta^i - m\gamma^i) - (1-m\beta^i)(\eta^j - m\gamma^j)}\partial_j m, \tag{34}$$

$$\partial_i\partial_j m = \frac{\gamma^j - \gamma^i + \beta^i\eta^j - \beta^j\eta^i + 2m(\gamma^i\beta^j - \gamma^j\beta^i)}{(1-m\beta^j)(\eta^i - m\gamma^i) - (1-m\beta^i)(\eta^j - m\gamma^j)}\partial_i m \partial_j m.$$

It has been verified directly that this system is in involution and its general solution depends, modulo reparametrizations $R^i \to f^i(R^i)$, on $4n$ arbitrary functions of one variable, thus manifesting the integrability of the $(5+1)$-dimensional system (33).

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APPENDIX A: HYDRODYNAMIC REDUCTIONS

Here we apply the method of hydrodynamic reductions to the classification of integrable PDEs of the form

$$\theta_{tx}+\theta_{zy}=f(\theta_{xx},\theta_{xy},\theta_{yy}). \tag{A1}$$

Introducing new variables $\theta_{xx}=u$, $\theta_{xy}=v$, $\theta_{yy}=w$, $\theta_{tx}=p$, $\theta_{zy}=f(u,v,w)-p$, one rewrites (A1) in the quasilinear form

$$\begin{gathered} u_y=v_x, \quad u_t=p_x, \quad v_y=w_x, \quad v_t=p_y, \\ v_z=(f(u,v,w)-p)_x, \quad w_z=(f(u,v,w)-p)_y. \end{gathered} \tag{A2}$$

Hydrodynamic reductions are sought in the form $u=u(R^1,\ldots,R^n)$, $v=v(R^1,\ldots,R^n)$, $w=w(R^1,\ldots,R^n)$, $p=p(R^1,\ldots,R^n)$ where the Riemann invariants $R^1,\ldots,R^n$ solve a triple of commuting hydrodynamic type systems (2). The substitution into (A2) implies

$$\partial_i p=\lambda^i \partial_i u, \quad \partial_i v=\mu^i \partial_i u, \quad \partial_i w=(\mu^i)^2 \partial_i u, \tag{A3}$$

along with the dispersion relation

$$\lambda^i=f_u+f_v\mu^i+f_w(\mu^i)^2-\mu^i\eta^i. \tag{A4}$$

Substituting λ^i into the commutativity conditions (3), and taking into account that the compatibility conditions for the relations (A3) imply

$$\partial_i\partial_j u=\frac{\partial_j\mu^i}{\mu^j-\mu^i}\partial_i u+\frac{\partial_i\mu^j}{\mu^i-\mu^j}\partial_j u,$$

one arrives at the following system:

$$\begin{gathered} \partial_j\mu^i=\frac{S_{ij}}{f_w(\mu^j-\mu^i)+\eta^i-\eta^j}\partial_j u, \quad \partial_j\eta^i=\frac{\eta^j-\eta^i}{\mu^j-\mu^i}\frac{S_{ij}}{f_w(\mu^j-\mu^i)+\eta^i-\eta^j}\partial_j u, \\ \partial_i\partial_j u=\frac{2}{\mu^j-\mu^i}\frac{S_{ij}}{f_w(\mu^j-\mu^i)+\eta^i-\eta^j}\partial_i u\partial_j u; \end{gathered} \tag{A5}$$

here

$$S_{ij}=f_{uu}+(\mu^i+\mu^j)f_{uv}+((\mu^i)^2+(\mu^j)^2)f_{uw}+\mu^i\mu^j f_{vv}+\mu^i\mu^j(\mu^i+\mu^j)f_{vw}+(\mu^i)^2(\mu^j)^2 f_{ww}.$$

Compatibility conditions for the system (A5) are of the form

$$\partial_k(\partial_j\mu^i)-\partial_j(\partial_k\mu^i)=(\cdots)\ \partial_j u\partial_k u, \quad \partial_k(\partial_j\eta^i)-\partial_j(\partial_k\eta^i)=(\cdots)\ \partial_j u\partial_k u,$$

$$\partial_k(\partial_j\partial_i u)-\partial_j(\partial_k\partial_i u)=(\cdots)\ \partial_j u\partial_k u,$$

where dots $(\cdots)$ denote complicated rational expressions in μ^i, μ^j, μ^k and η^i, η^j, η^k whose coefficients are functions of the derivatives of f up to third order. Equating these rational expressions to zero one arrives at the following system for f:

$$f_{uu}=f_{ww}=f_{uv}=f_{wv}=f_{vv}-2\,f_{uw}=f_{vvv}=0.$$

Up to elementary changes of variables, the general nonlinear solution of this system corresponds to the second heavenly equation (13).

APPENDIX B: CONCLUDING REMARKS

We have demonstrated that the requirement of existence of sufficiently many n-component reductions can be used as the effective criterion providing the test for integrability of multidimensional dispersionless PDEs. We believe that using the approach outlined in this paper along with the available computer algebra packages (we have used Mathematica 5.0), one can obtain complete lists of multidimensional integrable systems within various particularly interesting classes, hyperbolic systems of hydrodynamic type being one of them. Partial classification results can be found in Refs. 12, 13, and 28. The main problems arising here are the complexity of integrability conditions (making difficult their geometric analysis), and the volume of symbolic calculations required.

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2D conformal field theories and holography

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It is known that the chiral part of any 2D conformal field theory defines a 3D topological quantum field theory: quantum states of this TQFT are the CFT conformal blocks. The main aim of this paper is to show that a similar CFT/TQFT relation exists also for the full CFT. The 3D topological theory that arises is a certain ''square'' of the chiral TQFT. Such topological theories were studied by Turaev and Viro; they are related to 3D gravity. We establish an operator/state correspondence in which operators in the chiral TQFT correspond to states in the Turaev–Viro theory. We use this correspondence to interpret CFT correlation functions as particular quantum states of the Turaev–Viro theory. We compute the components of these states in the basis in the Turaev–Viro Hilbert space given by colored 3-valent graphs. The formula we obtain is a generalization of the Verlinde formula. The later is obtained from our expression for a zero colored graph. Our results give an interesting ''holographic'' perspective on conformal field theories in two dimensions. © *2004 American Institute of Physics.*
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I. INTRODUCTION

To put results of this paper in a somewhat general context we recall that any conformal field theory (CFT) defines a topological quantum field theory (TQFT), see Refs. 1–4. The TQFT arises by extracting a modular tensor category from the CFT chiral vertex operator algebra. Then, as explained in Ref. 5, any modular category gives rise to a 3D TQFT. The TQFT can be (partially) described by saying that its Hilbert space is the space of (holomorphic) conformal blocks of the CFT. The canonical example of such CFT/TQFT correspondence is the well-known relation between Wess–Zumino–Witten (WZW) and Chern–Simons (CS) theories. Let us emphasize that this is always a relation between the holomorphic sector of the CFT (or its chiral part) and a TQFT. As such it is not an example of a holographic correspondence, in which correlation functions (comprising both the holomorphic and antiholomorphic sectors) of CFT on the boundary would be reproduced by some theory in bulk.

It is then natural to ask whether there is some 3D theory that corresponds to the *full* CFT. A proposal along these lines was put forward some time ago by Verlinde,[6] who argued that a relation must exist between the quantum Liouville theory (full, not just the chiral part) and 3D gravity. Recently one of us presented[7] some additional arguments in favor of this relation, hopefully somewhat clarifying the picture. The main goal of the present paper is to demonstrate that such a relation between the full CFT and a certain 3D theory exists for a large class of CFT's. Namely, we show that given a CFT there is a certain 3D field theory, which is a TQFT, and which is a rather natural spin-off of the corresponding ''chiral'' TQFT. The TQFT in question is not new, it is

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the one defined by Turaev–Viro,[8] and described in great detail in Ref. 5. This paper is thus aimed at a clarification of the relation between the Turaev–Viro (TV) 3D TQFT's and CFT's in two dimensions.

The point that given a CFT there exists a relation between the full CFT and some 3D TQFT is to some extent contained in recent works on boundary conformal field theory, see Refs. 2, 3, 4, 9, and references therein, and also a more recent paper.[10] As is emphasized, e.g., in Ref. 4, the full CFT partition function on some Riemann surface X (possibly with a boundary) is equal to the chiral CFT partition function on the double $\tilde{X}$. There is then a certain ''connecting'' 3D manifold $\tilde{M}$ whose boundary $\partial\tilde{M}$ is the double $\tilde{X}$. Using the chiral CFT/TQFT relation one obtains a 3D TQFT in $\tilde{M}$ that reproduces the chiral partition function on $\tilde{X}$, and thus the full partition function on X. This formalism turns out to be very useful for analyzing the case when X has a boundary.

Our analysis was motivated by the above picture, but the logic is somewhat different. Instead of working with the chiral TQFT in the connecting 3-manifold $\tilde{M}$ we work directly with a 3-manifold M whose boundary is X, and the Turaev–Viro TQFT on M. The two approaches are clearly related as the TV theory is a ''square'' of the chiral TQFT. However, bringing the Turaev–Viro TQFT into the game suggests some new interpretations and provides new relations. Thus, most notably, we establish an operator/state correspondence in which the chiral TQFT operators correspond to states in the TV theory, and the trace of an operator product corresponds to the TV inner product. We use this to interpret the CFT correlators as quantum states of TV theory. Then, using the fact that a basis in the Hilbert space of TV theory on X is given by colored trivalent graph states, we will characterize the CFT correlation functions by finding their components in this basis. Thus, the relation that we demonstrate is about a 3D TQFT on a 3-manifold M and a CFT on the boundary X of M. It is therefore an example of a holographic correspondence, while this is not obviously so for the correspondence based on a chiral TQFT in the connecting manifold $\tilde{M}$.

The holography discussed may be viewed by some as trivial, because the three-dimensional theory is topological. What makes it interesting is that it provides a very large class of examples. Indeed, there is a relation of this type for any CFT. Importantly, this holography is not limited to any AdS type background, although a very interesting subclass of examples (not considered in this paper, but see Ref. 7) is exactly of this type.

As the relation chiral CFT/TQFT is best understood for the case of a rational CFT, we shall restrict our analysis to this case. Our constructions can also be expected to generalize to nonrational and even noncompact CFT's with a continuous spectrum, but such a generalization is non-trivial, and is not attempted in this paper. Even with noncompact CFT's excluded, the class of CFT's that is covered by our considerations, namely, rational CFT, is still very large. To describe the arising structure in its full generality we would need to introduce the apparatus of category theory, as it was done, e.g., in Ref. 5. In order to make the exposition as accessible as possible we shall not maintain the full generality. We demonstrate the CFT/TQFT holographic relation using a compact group WZW CFT (and CS theory as the corresponding chiral TQFT) as an example.

We shall often refer to the TV TQFT as ''gravity.'' For the case of chiral TQFT being the Chern–Simons theory for a group $G=\mathrm{SU}(2)$ this ''gravity'' theory is just the usual 3D Euclidean gravity with positive cosmological constant. However, the theory can be associated to any CFT. The reader should keep in mind its rather general character.

In order to describe the holographic correspondence in detail we will need to review (and clarify) the relation between CS theory and gravity (or between the Reshetikhin–Turaev–Witten and Turaev–Viro invariants) for a 3-manifold with boundary. We found that the expositions of this relation available in the literature (see Refs. 5, 11) are rather brief and sketchy. This paper provides a more detailed account and obtains new results. In particular, the operator/state correspondence established in this paper is new.

Finally, we would like to emphasize that the approach presented in this paper is not equivalent to that of Refs. 2, 3, 4, 9, even though it was motivated by these papers. Thus, most of our discussion only concerns the diagonal-type partition functions, while Ref. 4 is applicable to the

more general case. It would be of interest to study the relation to Refs. 2, 3, 4, 9 in more detail, and also extend the approach presented here to modular invaraint partition functions of other types. We shall not attempt this in the present paper.

The paper is organized as follows: In Sec. II we review the quantization of Chern–Simons theory. Section III is devoted to the Turaev–Viro theory. We then review the definition of 3-manifold invariants in Sec. IV, and some facts on the Verlinde formula in Sec. V. The new material starts in Sec. VI, where we discuss the CS/TV operator/state correspondence and the arising relation between the CS and TV Hilbert spaces. In Sec. VII we interpret the CFT partition function as a TV quantum state, and compute components of this state in a natural basis in the TV Hilbert space given by graphs. We conclude with a discussion.

II. CHERN–SIMONS THEORY

This section is a rather standard review of CS theory. We discuss the CS phase space, the Hilbert space that arises as its quantization, review the Verlinde formula, and a particular basis in the CS Hilbert space that arises from a pant decomposition. The reader may consult, e.g., Refs. 12 and 5 for more details.

A. Action

The Chern–Simons (CS) theory is a three-dimensional TQFT of Witten-type. The CS theory for a group G is defined by the following action functional:

$$S^{-}_{\mathrm{CS}}[A]=\frac{k}{4\pi}\int_M \mathrm{Tr}\left(A\wedge dA+\frac{2}{3}A\wedge A\wedge A\right)-\frac{k}{4\pi}\int_{\partial M} dz\wedge d\bar{z}\,\mathrm{Tr}(A_z A_{\bar{z}}). \tag{2.1}$$

Here M is a three-dimensional manifold and A is a connection on the principal G-bundle over M. For the case of a compact G that we consider in this paper the action is gauge invariant (modulo 2π) when k is an integer. The second term in (2.1) is necessary to make the action principle well-defined on a manifold with boundary. To write it one needs to choose a complex structure on ∂M. As ∂M is a 2D Riemann surface, complex structures on it are same as conformal structures. Thus, one has to make a choice of the conformal structure. Then the term in (2.1) is the one relevant for fixing $A_{\bar{z}}$ on the boundary. Another possible choice of boundary condition is to fix A_z. The corresponding action is:

$$S^{+}_{\mathrm{CS}}[A]=\frac{k}{4\pi}\int_M \mathrm{Tr}\left(A\wedge dA+\frac{2}{3}A\wedge A\wedge A\right)+\frac{k}{4\pi}\int_{\partial M} dz\wedge d\bar{z}\,\mathrm{Tr}(A_z A_{\bar{z}}). \tag{2.2}$$

B. Partition function

The partition function arises (formally) by considering the path integral for (2.1). For a closed M it can be given a precise meaning through the surgery representation of M and the Reshetikhin–Turaev–Witten (RTW) invariant of links. Before we review this construction, let us discuss the formal path integral for the case when M has a boundary. For example, let the manifold M be a handlebody H. Its boundary $X=\partial H$ is a (connected) Riemann surface. Recall that TQFT assigns a Hilbert space to each connected component of ∂M, and a map between these Hilbert spaces to M. The map can be heuristically thought of as given by the path integral. For a manifold with a single boundary component, which is the case for a handlebody H, TQFT on H gives a map $\mathcal{F}:\mathcal{H}^{\mathrm{CS}}_X\to\mathbb{C}$ mapping the CS Hilbert space of X into $\mathbb{C}$. This map can be obtained from the following Hartle–Hawking (HH) type state:

$$\mathcal{F}(\underline{A})=\int_{A_{\bar{z}}=\underline{A}}\mathcal{D}A\; e^{iS^{-}_{\mathrm{CS}}[A]}. \tag{2.3}$$

The path integral is taken over connections in H with the restriction of A on X fixed. More precisely, with the choice of boundary term in the action as in (2.1), one fixes only the antiholomorphic part $\underline{A}=A_{\bar{z}}$ of the connection on X, as defined by an auxiliary complex structure. The result of the path integral (2.3) is the partition function of CS theory on H. It can be thought of as a particular quantum state $\mathcal{F}(\underline{A})$ in the CS Hilbert space $\mathcal{H}_X^{\mathrm{CS}}$. The inner product in $\mathcal{H}_X^{\mathrm{CS}}$ is (formally) defined as

$$\langle \Psi_1|\Psi_2\rangle=\int_{\mathcal{A}}\mathcal{D}\underline{A}\overline{\mathcal{D}\underline{A}}\; e^{-(k/\pi)\int_{\partial\mathcal{M}}d^2z\,\mathrm{Tr}(\underline{A}_z\underline{A}_{\bar{z}})}\overline{\Psi_1(\underline{A})}\Psi_2(\underline{A}). \tag{2.4}$$

Here $d^2z=dz\wedge d\bar{z}/2i$ is the real measure on the boundary. The above mentioned map $\mathcal{F}:\mathcal{H}_X^{\mathrm{CS}}\to\mathbb{C}$ is given by

$$\mathcal{F}(\Psi)=\langle\mathcal{F}|\Psi\rangle=\int_{\mathcal{A}}\mathcal{D}\underline{A}\overline{\mathcal{D}\underline{A}}\; e^{-(k/\pi)\int_{\partial\mathcal{M}}dz^2\,\mathrm{Tr}(\underline{A}_z\underline{A}_{\bar{z}})}\overline{\mathcal{F}(\underline{A})}\Psi(\underline{A}). \tag{2.5}$$

The state $\mathcal{F}(\underline{A})\in\mathcal{H}_X^{\mathrm{CS}}$ depends only on the topological nature of the 3-manifold and a framing of M.

C. Phase space

To understand the structure of the CS Hilbert space $\mathcal{H}^{\mathrm{CS}}$ it is natural to use the Hamiltonian description. Namely, near the boundary the manifold has the topology $X\times\mathbb{R}$. Then the phase space $\mathcal{P}^{\mathrm{CS}}$ of CS theory based on a group G is the moduli space of flat G-connections on X modulo gauge transformations:

$$\mathcal{P}_X^{\mathrm{CS}}\sim\mathcal{A}/\mathcal{G}. \tag{2.6}$$

It is finite dimensional.

Let X be a (connected) Riemann surface of type (g,n) with $g\geqslant 0$, $n>0$, $2g+n-2>0$. Denote the fundamental group of X by $\pi(X)$. The moduli space $\mathcal{A}$ can then be parametrized by homomorphisms $\phi:\pi(X)\to G$. The phase space is, therefore, isomorphic to

$$\mathcal{P}_X^{\mathrm{CS}}\sim\mathrm{Hom}(\pi(X),G)/G, \tag{2.7}$$

where one mods out by the action of the group at the base point. The fundamental group is generated by $m_i, i=1,\ldots,n$ and $a_i,b_i, i=1,\ldots,g$ satisfying the following relation:

$$m_1\cdots m_n[a_1,b_1]\cdots[a_g,b_g]=1. \tag{2.8}$$

Here $[a,b]=aba^{-1}b^{-1}$. The dimension of the phase space can now be seen to be

$$\dim\mathcal{P}_X^{\mathrm{CS}}=(2g+n-2)\dim G. \tag{2.9}$$

The fact that (2.7) is naturally a Poisson manifold was emphasized in Ref. 13. The Poisson structure described in Ref. 13 is the same as the one that comes from CS theory. For the case of a compact X the space (2.7) is actually a symplectic manifold. For the case when punctures are present the symplectic leaves are obtained by restricting the holonomy of $\underline{A}$ around punctures to lie in some conjugacy classes in the group. An appropriate power of the symplectic structure can be used as a volume form on the symplectic leaves. Their volume turns out to be finite. One thus expects to get finite dimensional Hilbert spaces upon quantization.

D. Hilbert space

The Hilbert space $\mathcal{H}_X^{\mathrm{CS}}$ was understood[12,14] to be the same as the space of conformal blocks of the chiral Wess–Zumino–Witten (WZW) theory on a genus g-surface with n vertex operators

inserted. Let us fix irreducible representations $\mathbf{R}=\{\rho_1,\ldots,\rho_n\}$ of G labeling the punctures. The dimension of each of $\mathcal{H}_X^{\mathrm{CS}}$ can be computed using the Verlinde formula:[15,16]

$$\dim \mathcal{H}_X^{\mathrm{CS}}=\sum_\rho \frac{S_{\rho_1\rho}\cdots S_{\rho_n\rho}}{S_{0\rho}\cdots S_{0\rho}}(S_{0\rho})^{2-2g}. \tag{2.10}$$

The sum is taken over irreducible representations ρ, $S_{\rho\rho'}$ is the modular S-matrix, see (4.3) below for the case of SU(2), and $S_{0\rho}=\eta\dim_\rho$, where η is given by (4.2).

E. Pant decomposition

The states from $\mathcal{H}_X^{\mathrm{CS}}$ can be understood as the HH type states given by the path integral over a handlebody H with Wilson lines in representations $\mathbf{R}$ intersecting the boundary X transversally at n points. A convenient basis in $\mathcal{H}_X^{\mathrm{CS}}$ can be obtained by choosing a pant decomposition of X. A pair of pants is a sphere with 3 holes (some of them can be punctures). A Riemann surface X of type (g,n) can be represented by $2g+n-2$ pants glued together. For example, the surface of type (0,4) with 4 punctures can be obtained by gluing together 2 spheres each with 2 punctures and one hole. Note that a pant decomposition is not unique. Different pant decompositions are related by simple ''moves.'' A pant decomposition can be conveniently encoded in a tri-valent graph Δ with $2g+n-2$ vertices and $3g+2n-3$ edges. Each vertex of Δ corresponds to a pair of pants, and each internal edge corresponds to two holes glued together. Open-ended edges of Δ end at punctures. We shall call such edges ''loose.'' There are exactly n of them. The graph Δ can be thought of as a 1-skeleton of the Riemann surface X, or as a Feynman diagram that corresponds to the string world-sheet X. The handlebody H can be obtained from Δ as its regular neighborhood $U(\Delta)$, so that Δ is inside H and the loose edges of Δ end at the punctures. Let us label the loose edges by representations $\mathbf{R}$ and internal edges by some other (non-null) irreducible representations. It is convenient to formalize the labeling of Δ in a notion of *coloring* ϕ. A coloring ϕ is the map

$$\phi: E_\Delta \to \mathcal{I}, \quad \phi(e)=\rho_e\in\mathcal{I} \tag{2.11}$$

from the set E_Δ of edges of Δ to the set $\mathcal{I}$ of (non-null) irreducible representations of the quantum group G. The loose edges are colored by representations from $\mathbf{R}$. The CS path integral on H with the spin network Δ^ϕ inserted is a state in $\mathcal{H}_X^{\mathrm{CS}}$. See below for a definition of spin networks. Changing the labels on the internal edges one gets states that span the whole $\mathcal{H}_X^{\mathrm{CS}}$. Different choices of pant decomposition of H (and thus of Δ) lead to different bases in $\mathcal{H}_X^{\mathrm{CS}}$.

F. Inner product

The inner product (2.4) of two states of the type described can be obtained by the following operation. Let one state be given by the path integral over H with Δ^ϕ inserted and the other by H with $\Delta^{\phi'}$ inserted, where both the graph and/or the coloring may be different in the two states. Let us invert orientation of the first copy of H and glue $-H$ to H across the boundary (using the identity homomorphism) to obtain some 3D space $\tilde{H}$ without boundary. We will refer to $\tilde{H}$ as the *double* of H. For H being a handlebody with g handles the double $\tilde{H}$ has the topology of a connected sum:

$$\tilde{H}\sim \#_{g-1} S^2\times S^1. \tag{2.12}$$

The loose ends of Δ are connected at the punctures to the loose ends of Δ' to obtain a colored closed graph $\Delta^\phi\cup\Delta^{\phi'}$ inside $\tilde{H}$. The inner product (2.4) is given by the CS path integral over $\tilde{H}$ with the spin network $\Delta^\phi\cup\Delta^{\phi'}$ inserted. This path integral is given by the RTW evaluation of $\Delta^\phi\cup\Delta^{\phi'}$ in $\tilde{H}$, see below for a definition of the RTW evaluation.

III. GRAVITY

The material reviewed in this section is less familiar, although is contained in the literature. We give the action for Turaev–Viro theory, discuss the phase space, then introduce certain important graph coordinatization of it, define spin networks, and describe the TV Hilbert space. A useful reference for this section is the book of Turaev (Ref. 5 and Ref. 17).

A. Action

What we refer to as ''gravity'' arises as a certain ''square'' of CS theory. We will also refer to this gravity theory as Turaev–Viro (TV) theory, to have uniform notations (CS-TV).

To see how the TV theory (gravity) arises from CS theory, let us introduce two connection fields A and B. Consider the corresponding CS actions $S_{\mathrm{CS}}[A], S_{\mathrm{CS}}[B]$. Introduce the following parametrization of the fields:

$$A=\mathbf{w}+\left(\frac{\pi}{k}\right)\mathbf{e}, \quad B=\mathbf{w}-\left(\frac{\pi}{k}\right)\mathbf{e}. \tag{3.1}$$

Here $\mathbf{w}$ is a G-connection, and $\mathbf{e}$ is a one-form valued in the Lie algebra of G. The TV theory action is essentially given by the difference $S^{-}_{\mathrm{CS}}[A]-S^{+}_{\mathrm{CS}}[B]$, plus a boundary term such that the full action is

$$S_{\mathrm{TV}}[\mathbf{w},\mathbf{e}]=\int_M \mathrm{Tr}\left(\mathbf{e}\wedge\mathbf{f}(\mathbf{w})+\frac{\Lambda}{12}\mathbf{e}\wedge\mathbf{e}\wedge\mathbf{e}\right). \tag{3.2}$$

The boundary condition for this action is that the restriction $\underline{\mathbf{w}}$ of $\mathbf{w}$ on $X=\partial M$ is kept fixed. Here Λ is the ''cosmological constant'' related to k as $k=2\pi/\sqrt{\Lambda}$. For $G=\mathrm{SU}(2)$ the TV theory is nothing else but the Euclidean gravity with positive cosmological constant Λ. We emphasize, however, that the theory is defined for other groups as well. Moreover, it also exists as a square of a chiral TQFT for any TQFT, that is even in cases when the chiral TQFT is not a CS theory.

B. Path integral

Similarly to CS theory, one can consider HH type states given by the path integral on a manifold with a single boundary component. Thus, for a manifold being a handlebody H we get the TV partition function:

$$\mathcal{T}(\underline{\mathbf{w}})=\int_{\mathbf{w}|_X=\underline{\mathbf{w}}}\mathcal{D}\mathbf{w}\mathcal{D}\mathbf{e}\ e^{iS_{\mathrm{TV}}[\mathbf{w},\mathbf{e}]}. \tag{3.3}$$

The integral is taken over both $\mathbf{w}$,$\mathbf{e}$ fields in the bulk with the restriction $\underline{\mathbf{w}}$ of the connection fixed on the boundary. The TV partition function $\mathcal{T}(\underline{\mathbf{w}})$ is thus a functional of the boundary connection. It can also be interpreted as a particular state in the TV Hilbert space $\mathcal{H}^{\mathrm{TV}}_X$.

States from $\mathcal{H}^{\mathrm{TV}}_X$ are functionals of the boundary connection. The inner product on this space can be formally defined by the formula

$$\langle\Psi_1|\Psi_2\rangle=\frac{1}{\mathrm{Vol}\,\mathcal{G}}\int_{\mathcal{A}}\mathcal{D}\underline{\mathbf{w}}\ \overline{\Psi_1(\underline{\mathbf{w}})}\Psi_2(\underline{\mathbf{w}}) \tag{3.4}$$

similar to (2.4). Note, however, that the measure in (3.4) is different from that in (2.4). We shall see this below when we describe how to compute TV inner products in practice.

C. Relation between TV and CS states

Formally, the following relation between TV and CS states exists. As one can easily check, the difference of two CS actions in the parametrization (3.1) is given by

$$S^-_{\rm CS}[A]-S^+_{\rm CS}[B]=S_{\rm TV}[\mathbf{w},\mathbf{e}]+\frac{1}{2}\int_{\partial\mathcal{M}}{\rm Tr}(\mathbf{e}\wedge\mathbf{w})-\frac{k}{2\pi}\int_{\partial\mathcal{M}}dz\wedge d\bar{z}\,{\rm Tr}\left(\mathbf{w}_z\mathbf{w}_{\bar{z}}+\left(\frac{\pi}{k}\right)^2\mathbf{e}_z\mathbf{e}_{\bar{z}}\right). \tag{3.5}$$

Therefore,

$$e^{iS^-_{\rm CS}[A]-iS^+_{\rm CS}[B]-(k/\pi)\int_{\partial\mathcal{M}}d^2z\,{\rm Tr}(A_{\bar{z}}B_z)}=e^{iS_{\rm TV}[\mathbf{w},\mathbf{e}]+(2\pi/k)\int_{\partial\mathcal{M}}dz^2\,{\rm Tr}(\mathbf{e}_z\mathbf{e}_{\bar{z}})}. \tag{3.6}$$

Here $d^2z=dz\wedge d\bar{z}/2i$ is the real measure on $\partial\mathcal{M}$. Note that the last term in the exponential on the left hand side is the same as in the CS inner product (2.4). From this expression one can read off a prescription for obtaining the TV state $\mathcal{T}(\underline{\mathbf{w}})$. Indeed, let us integrate the left-hand side over bulk A,B, keeping A^-_z,B_z fixed on the boundary. Let us denote the result by $\Phi(A^-_z,B_z)$. We have

$$\Phi(A^-_z,B_z)=\Psi(A^-_z)\overline{\Psi}(B_z)\;e^{-(k/\pi)\int_{\partial\mathcal{M}}d^2z\,{\rm Tr}(A_{\bar{z}}B_z)}. \tag{3.7}$$

To get $\mathcal{T}(\mathbf{w})$ one must take $\Phi(A^-_z,B_z)$ in the parametrization (3.1), multiply the result by an exponential factor and integrate over the restriction $\underline{\mathbf{e}}$ of $\mathbf{e}$ on the boundary:

$$\mathcal{T}(\underline{\mathbf{w}})=\int\mathcal{D}\underline{\mathbf{e}}\;e^{-(2\pi/k)\int_{\partial\mathcal{M}}dz^2\,{\rm Tr}(\underline{\mathbf{e}_z\mathbf{e}_{\bar{z}}})}\;\Phi\left(\underline{\mathbf{w}}_{\bar{z}}+\left(\frac{\pi}{k}\right)\underline{\mathbf{e}}_{\bar{z}},\underline{\mathbf{w}}_z-\left(\frac{\pi}{k}\right)\underline{\mathbf{e}}_z\right). \tag{3.8}$$

The functional $\Phi(A^-_z,B_z)$ is a vector in the Hilbert space $\mathcal{H}^{\rm CS}\otimes\overline{\mathcal{H}^{\rm CS}}$. We should view (3.8) as a transform between this Hilbert space and $\mathcal{H}^{\rm TV}$. This transform will play an important role in what follows. Below we shall see how the result of the transform (3.8) can be found in practice.

D. Phase space

The TV phase space is basically two copies of $\mathcal{P}^{\rm CS}$, but with an unusual polarization. The polarization on $\mathcal{P}^{\rm TV}$ is given by $\mathbf{e}$, $\mathbf{w}$, which are canonically conjugate variables. Note that there is no need to choose a complex structure in order to define this polarization.

It turns out to be very convenient to think of $\mathcal{P}^{\rm TV}$ as some deformation of the cotangent bundle $T^*(\mathcal{A}/\mathcal{G})$ over the moduli space $\mathcal{A}/\mathcal{G}$ of flat connections on X. Note, however, that the TV connection $\underline{\mathbf{w}}$ on the boundary is not flat, so the configuration space for TV theory is not really the moduli space of flat connections. One does get $\mathcal{A}/\mathcal{G}$ as the configurational space in an important limit $k\to\infty$, in which the $\mathbf{e}^{\wedge 3}$ term drops from the action (3.2). Thus, it is only in this limit that the TV phase space is the cotangent bundle $T^*(\mathcal{A}/\mathcal{G})$. For a finite k the TV phase space is compact (as consisting of two copies of $\mathcal{P}^{\rm CS}$), while $T^*(\mathcal{A}/\mathcal{G})$ is not. We will see, however, that it is essentially correct to think of $\mathcal{P}^{\rm TV}$ as a deformation of $T^*(\mathcal{A}/\mathcal{G})$ even in the finite k case. The compactness of $\mathcal{P}^{\rm TV}$ will manifest itself in the fact that after the quantization the range of eigenvalues of $\mathbf{e}$ is bounded from above.

These remarks being made we write

$$\mathcal{P}^{\rm TV}\sim T^*_k(\mathcal{A}/\mathcal{G}), \tag{3.9}$$

where T^*_k is certain compact version of the cotangent bundle. The phase space becomes the usual cotangent bundle in the $k\to\infty$ limit. We will not need any further details on spaces T^*_k. As we shall see the quantization of $\mathcal{P}^{\rm TV}$ is rather straightforward once the quantization of the cotangent bundle is understood.

We note that the dimension

$$\dim\mathcal{P}^{\rm TV}=2(2g+n-2)\dim G \tag{3.10}$$

is twice the dimension of the phase space of the corresponding CS theory, as required. A convenient parametrization of the cotangent bundle phase space can be obtained by using graphs.

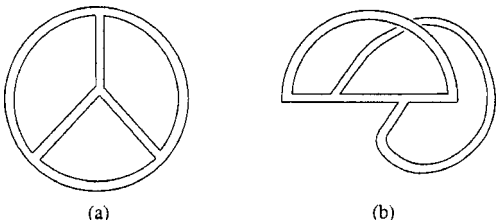


FIG. 1. A fat graph Γ for the (a) sphere with 4 punctures; (b) torus with one puncture.

E. Graphs

The graphs one considers are similar to those that arise in the Penner coordinatization[18] of the moduli space of punctured Riemann surfaces. Namely, given X, introduce a trivalent closed fat graph Γ with the number F of faces equal to the number n of punctures. Such a graph can be obtained by triangulating the surface X using punctures as vertices, and then constructing a dual graph. What arises is exactly a graph Γ. See Fig. 1 for examples of Γ. Note that different triangulations lead to different graphs, so Γ is by no means unique.

Because the graph is trivalent $3V=2E$, where V is the number of vertices and E is the number of edges. We also have the Euler characteristics relation:

$$F-E+V=2-2g. \tag{3.11}$$

We thus get that the number E of edges of Γ is $E=3(2g+n-2)$.

Note that the graph Γ does not coincide with the graph Δ introduced in the previous section. There is, however, a simple relation between them that is worth noting. Let us, as in the previous section, form the double $\tilde{H}=H\cup -H$. It is a closed 3-manifold obtained by gluing two copies of the handlebody H across the boundary X. Let us take a graph Δ in H, and another copy of Δ in $-H$. These graphs touch the boundary $\partial H=X$ at the punctures. Gluing these two copies of Δ at the punctures one obtains a closed graph $\Delta\cup\Delta$ in $\tilde{H}$. It is a trivalent graph with $2(2g+n-2)$ vertices and $3(2g+n-2)$ edges. Now consider the regular neighborhood $U(\Delta\cup\Delta)$ of $\Delta\cup\Delta$ in $H\cup -H$. This is a handlebody, whose boundary is of genus

$$G=2g+n-1. \tag{3.12}$$

The surface $\partial U(\Delta\cup\Delta)$ can be obtained by taking two copies of X, removing some small disks around the punctures, and identifying the resulting circular boundaries to get a closed surface without punctures. We have the following:

Lemma: The surface $\partial U(\Delta\cup\Delta)$ *is a Heegard surface for* $H\cup -H$. *The complement of* $U(\Delta\cup\Delta)$ *in* $H\cup -H$ *is a handlebody that is the regular neighborhood* $U(\Gamma)$ *of the graph* Γ *on* X.

Proof: The complement of $U(\Delta\cup\Delta)$ in $H\cup -H$ can be seen to be the cylinder $X\times[0,1]$ with n holes cut in it. So, it is indeed a handlebody of genus (3.12). Its 1-skeleton that can be obtained by choosing a pant decomposition is the trivalent graph Γ.

F. Graph connections

Given Γ equipped with an arbitrary orientation of all the edges, one can introduce what can be called graph connections. Denote the set of edges e of Γ by E. We use the same letter both for the set E of edges and for its dimension. A graph connection $\mathbf{A}$ is an assignment of a group element to every edge of the graph:

$$\mathbf{A}:E\to G, \quad \mathbf{A}(e)=\mathbf{g}_e\in G. \tag{3.13}$$

One can also introduce a notion of graph gauge transformations. These act at vertices of Γ. A gauge transformation is parametrized by V group elements. Let us introduce:

$$\mathbf{H}: V \to G, \quad \mathbf{H}(v) = \mathbf{h}_v \in G. \tag{3.14}$$

Here V is the set of vertices of Γ. For an edge $e \in E$ denote by $s(e)$ (source) the vertex from which e originates, and by $t(e)$ (target) the vertex where e ends. The action of a gauge transformation $\mathbf{H}$ on a graph connection $\mathbf{A}$ is now as follows:

$$\mathbf{A}^{\mathbf{H}}(e) = \mathbf{h}_{s(t)}^{-1}\, \mathbf{g}_e\, \mathbf{h}_{s(e)}. \tag{3.15}$$

The space of graph connections modulo graph gauge transformations can now be seen to be isomorphic to $G^{\otimes E}/G^{\otimes V}$. Its dimension is given by (2.9). We thus get a parametrization of the CS phase space $\mathcal{P}^{\mathrm{CS}}$ based on a graph Γ:

$$\mathcal{P}^{\mathrm{CS}} \sim G^{\otimes E}/G^{\otimes V}. \tag{3.16}$$

The TV phase space is the cotangent bundle

$$\mathcal{P}^{\mathrm{TV}} \sim T_k^*(G^{\otimes E}/G^{\otimes V}). \tag{3.17}$$

As we shall see, it is rather straightforward to quantize the noncompact, $k \to \infty$ version of $\mathcal{P}^{\mathrm{TV}}$, that is the cotangent bundle. The quantum states are given by spin networks.

G. Spin networks

To quantize the cotangent bundle $T^*(\mathcal{A}/\mathcal{G})$ one introduces a Hilbert space of functionals on the moduli space of flat connections. A complete set of such functionals is given by spin networks. These functions will thus form (an over-complete) basis in the Hilbert space of TV theory. They also serve as observables for CS quantum theory, see below.

Before we define these objects, let us introduce some convenient notations. Denote the set of irreducible representations ρ of the quantum group G by $\mathcal{I}$. Introduce a coloring $\psi: E \to \mathcal{I}, \psi(e) = \rho_e$ of the edges of Γ with irreducible representations of G. A spin network Γ^{ψ} is a functional on the space of graph connections:

$$\Gamma^{\psi}: G^{\otimes E} \to \mathbb{C}. \tag{3.18}$$

Given a connection $\mathbf{A}$ the value of $\Gamma^{\psi}(\mathbf{A})$ is computed as follows. For every edge e take the group element $\mathbf{g}_e$ given by the graph connection in the irreducible representation ρ_e. One can think of this as a matrix with two indices: one for the source $s(e)$ and the other for the target $t(e)$. Multiply the matrices for all the edges of Γ. Then contract the indices at every tri-valent vertex using an intertwining operator. The normalization of intertwiners that we use is specified in the Appendix. The definition we gave is applicable to $G = \mathrm{SU}(2)$. In this case the trivalent intertwiner is unique up to normalization. For other gauge groups one in addition has to label the vertices of Γ with intertwiners, so that a spin network explicitly depends on this labeling. The functional (3.18) so constructed is invariant under the graph gauge transformations (3.14) and is thus a functional on the moduli space of flat connections modulo gauge transformations. As such it is an element of the Hilbert space of TV theory. It is also an observable on the CS phase space (3.16).

H. Quantization

We can define the Hilbert space $\mathcal{H}^{\mathrm{TV}}$ of Turaev–Viro theory to be the space of gauge-invariant functionals $\Psi(\underline{\mathbf{w}})$ on the configurational space $G^{\otimes E}/G^{\otimes V}$. This gives a quantization of the $k \to \infty$ limit, but a modification for the case of finite k is straightforward. As we discussed above, a complete set of functionals on $G^{\otimes E}/G^{\otimes V}$ is given by spin networks. We denote the state corresponding to a spin network Γ^{ψ} by $|\Gamma^{\psi}\rangle$. They form a basis of states in $\mathcal{H}^{\mathrm{TV}}$:

$$\mathcal{H}^{\mathrm{TV}} = \mathrm{Span}\{|\Gamma^{\psi}\rangle\}. \tag{3.19}$$

One can construct certain momenta operators, analogs of $\mathbf{e} \sim \partial/\partial \underline{\mathbf{w}}$ in the continuum theory. Spin networks are eigenfunctions of these momenta operators. To specialize to the case of finite k one has to replace all spin networks by quantum ones. That is, the coloring of edges of Γ must use irreducible representations of the quantum group, which there is only a finite set.

The spin network states $|\Gamma^{\psi}\rangle$ form an overcomplete basis in $\mathcal{H}^{\mathrm{TV}}$, in that the TV inner product between differently colored states is nonzero. However, these states do give a partition of unity in that

$$\sum_{\psi} \left(\prod_{e \in E_{\Gamma}} \dim_{\rho_e} \right) |\Gamma^{\psi}\rangle\langle\Gamma^{\psi}| \tag{3.20}$$

is the identity operator in $\mathcal{H}^{\mathrm{TV}}$. This will become clear from our definition of the TV inner product, and the definition of the TV invariant in the next section.

It seems from the way we have constructed the Hilbert space $\mathcal{H}^{\mathrm{TV}}$ that it depends on the graph Γ. This is not so. Choosing Γ differently one gets a different basis in the same Hilbert space. To describe an effect of a change of Γ it is enough to give a rule for determining the inner products between states from two different bases.

I. Inner product

The inner product on $\mathcal{H}^{\mathrm{TV}}$ is given (formally) by the integral (3.4) over boundary connections. To specify the measure in this integral, one has to consider the path integral for the theory. Namely, consider a 3-manifold $X \times [-1,1]$ over X, which is a 3-manifold with two boundary components, each of which is a copy of X. The TV path integral over $X \times [-1,1]$ gives a kernel that should be sandwiched between the two states whose inner product is to be computed. Thus, the measure in (3.4) is defined by the TV path integral. The measure, in particular, depends on the level k.

In practice the inner product of two states Γ^{ψ} $\Gamma^{\psi'}$, where both the graphs and the coloring may be different, is computed as the TV invariant for the manifold $X \times [-1,1]$ with Γ^{ψ} on $X \times \{-1\}$ and $\Gamma^{\psi'}$ on $X \times \{1\}$. Further details on the TV inner product are given in the next section.

IV. 3-MANIFOLD INVARIANTS

In this section we review the definition of RTW and TV invariants. The main references for this section are Refs. 19 and 20.

A. Reshetikhin–Turaev–Witten invariant

The RTW invariant of a closed 3-manifold (with, possibly, Wilson loops or spin networks inserted) gives a precise meaning to the CS path integral for this manifold. The definition we give is for M without insertions, and is different from, but equivalent to the original definition in Ref. 21. We follow Roberts.[19]

Any closed oriented 3-manifold M can be obtained from S^3 by a surgery on a link in S^3. Two framed links represent the same manifold M if and only if they are related by isotopy or a sequence of Kirby moves, that is either handle-slides or blow-ups, see Refs. 19 or 22 for more detail. Let L be a link giving the surgery representation of M. Define $\Omega L \in \mathbb{C}$ to be the evaluation of L in S^3 with a certain element Ω inserted along all the components of L, paying attention to the framing. The element Ω is defined as follows, see Ref. 19. It is an element of $\mathcal{H}_T^{\mathrm{CS}}$, where T is the torus, and is given by

$$\Omega = \eta \sum_{\rho} \dim_{\rho} R_{\rho}. \tag{4.1}$$

The sum is taken over all irreducible representations $\rho \in \mathcal{I}$, the quantity $\dim_\rho$ is the quantum dimension, and R_ρ is the state in $\mathcal{H}_T^{\mathrm{CS}}$ obtained by inserting the 0-framed unknot in the ρ's representation along the cycle that is noncontractible inside the solid torus having T as its boundary. The quantity η is given by

$$\eta^{-2} = \sum_\rho \dim_\rho^2. \tag{4.2}$$

For example, for $G = \mathrm{SU}(2)$ $\eta = \sqrt{2/k}\sin(\pi/k) = S_{00}$, where

$$S_{ij} = \sqrt{\frac{2}{k}}\sin\left(\frac{(i+1)(j+1)\pi}{k}\right), \quad k \geqslant 3. \tag{4.3}$$

With the normalization chosen, the S^3 value of a 0-framed unknot with Ω attached is η^{-1}, while ± 1 framed unknots with Ω attached give certain unit modulus complex numbers $r^{\pm 1}$. For $G = \mathrm{SU}(2)$ $r = \exp(-i\pi/4 - 2\pi i(3+k^2)/4k)$.

Let us now continue with the definition of the RTW invariant. Define by $\sigma(L)$ the signature of the 4-manifold obtained by attaching 2-handles to the 4-ball B^4 along $L \subset S^3 = \partial B^4$. Define

$$I(M) = \eta r^{-\sigma(L)}\, \Omega L. \tag{4.4}$$

This is the RTW invariant of the manifold M presented by L. We use the normalization of Roberts,[19] in which the RTW invariant satisfies $I(S^3) = \eta, I(S^2 \times S^1) = 1$, as well as the connected sum rule $I(M_1 \# M_2) = \eta^{-1} I(M_1) I(M_2)$.

B. Turaev–Viro invariant

The original Turaev–Viro invariant is defined[8] for triangulated manifolds. A more convenient presentation[20] uses standard 2-polyhedra. Another definition is that of Roberts.[19] It uses a handle decomposition of M. We first give the original definition of Turaev and Viro.

Let T be a triangulation of 3D manifold M. We are mostly interested in case that M has a boundary. Denote by V_T the number of vertices of T, and by $\{e\},\{f\},\{t\}$ collections of edges, faces and tetrahedra of T. Choose a coloring μ of all the edges, so that $\mu(e) = \rho_e$ is the color assigned to an edge e. The Turaev–Viro invariant is defined as

$$\mathrm{TV}(M, T|_{\partial M}, \mu|_{\partial M}) = \eta^{2V_T} \sum_\mu \prod_{e \notin \partial M} \dim_{\rho_e} \prod_t (6j)_t. \tag{4.5}$$

Here $(6j)_t$ is the $6j$-symbol constructed out of 6 colors labeling the edges of a tetrahedron t, and the product is taken over all tetrahedra t of T. The product of dimensions of representations labelling the edges is taken over all edges that do not lie on the boundary. The sum is taken over all colorings μ keeping the coloring on the boundary fixed. The invariant depends on the restriction $T|_{\partial M}$ of the triangulation to the boundary ∂M, and on the coloring $\mu|_{\partial M}$ of this restriction. The invariant is independent of an extension of $T|_{\partial M}$ inside M.

Note that the TV invariant is constructed in such a way that for a closed 3-manifold $M = M_1 \cup M_2$ obtained by gluing two manifolds M_1, M_2 with a boundary across the boundary the invariant $\mathrm{TV}(M)$ is easily obtained once $\mathrm{TV}(M_{1,2}, T_{1,2}|_{\partial M_{1,2}}, \mu_{1,2}|_{\partial M_{1,2}})$ are known. One has to triangulate the boundary of $M_{1,2}$ in the same way $T_1|_{\partial M_1} = T_2|_{\partial M_2}$, multiply the invariants for $M_{1,2}$, multiply the result by the dimensions of the representations labelling the edges of $T_{1,2}|_{\partial M_{1,2}} = T|_{\partial M}$, and sum over these representations. The result is $\mathrm{TV}(M)$:

$$\mathrm{TV}(M) = \sum_{\mu|_{\partial M}} \left(\prod_{e \in \partial M} \dim_{\rho_e} \right) \mathrm{TV}(M_1, T|_{\partial M}, \mu|_{\partial M}) \mathrm{TV}(M_2, T|_{\partial M}, \mu|_{\partial M}). \tag{4.6}$$

This, together with the definition of the TV inner product as the TV invariant for $X\times I$ establishes that (3.20) is indeed the identity operator in $\mathcal{H}^{\mathrm{TV}}$.

C. Roberts invariant

We shall now introduce the more general invariant of Roberts. We consider the case without boundary.

Consider a handle decomposition D of M. The canonical example to have in mind is the handle decomposition coming from a triangulation T of M. A thickening of the corresponding dual complex T^* then gives a handle decomposition. The vertices of the dual complex (baricenters of tetrahedra of the triangulation) correspond to 0-handles, edges of T^* (faces of T) correspond to 1-handles, faces of T^* (edges of T) give 2-handles, and 3-cells of T^* (vertices of T) give 3-handles. The union of 0- and 1-handles is a handlebody. Choose a system of meridian disks for it, one meridian disk for every 1-handle. Now specify the system of attaching curves for 2-handles. If the handle decomposition came from a triangulation there are exactly 3 attaching curves along each 1-handle. Frame all meridian and attaching curves using the orientation of the boundary of the handlebody. Denote the corresponding link by $C(M,D)$. Insert the element Ω on all the components of $C(M,D)$, paying attention to the framing, and evaluate $C(M,D)$ in S^3. This gives the Roberts invariant for M:

$$\mathrm{R}(M)=\eta^{d_3+d_0}\Omega C(M,D). \tag{4.7}$$

Here d_3,d_0 are the numbers of 3- and 0-handles correspondingly. Note that to evaluate $\Omega C(M,D)$ in S^3 one needs to first specify an embedding. The result of the evaluation does not depend on the embedding, see Ref. 19. Moreover, the invariant does not depends on a handle decomposition D and is thus a true invariant of M.

When the handle decomposition D comes from a triangulation T the Roberts invariant (4.7) coincides with the Turaev–Viro invariant (4.5). An illustration of this fact is quite simple and uses the 3-fusion (A2), see Ref. 19 for more detail.

Lemma (Roberts): The described above system $C(M,D)$ of meridian and attaching curves for a handle decomposition D of M gives a surgery representation of $M\#-M$.

This immediately implies the theorem of Turaev and Walker:

$$\mathrm{TV}(M)=\eta\, I(M\#-M)=|I(M)|^2. \tag{4.8}$$

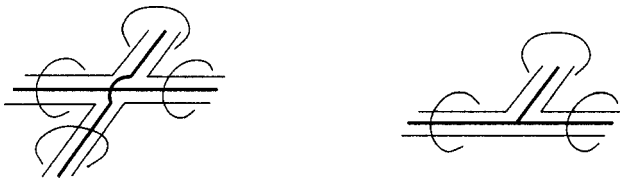
Below we shall see an analog of this relation for a manifold with boundary. All the facts mentioned make it clear that the TV invariant is a natural spin-off of the CS (RTW) invariant.

D. TV inner product

Recall that the Turaev–Viro inner product between the graph states $|\Gamma^{\psi}\rangle$ was defined in the previous section as the TV path integral on $X\times I$. The TV path integral is rigorously defined by the TV invariant (4.5). Here we describe how to compute the inner product in practice. The prescription we give is from Ref. 20, Sec. 4.d. We combine it with the chain-mail idea of Roberts[19] and give this chain-mail prescription.

The product $\langle\Gamma^{\psi}|\Gamma^{\psi'}\rangle$ is obtained by a certain face model on X. Namely, consider the 3-manifold $X\times I$, where I is the interval $[-1,1]$. Put Γ^{ψ} on $X\times\{-1\}$ and $\Gamma^{\psi'}$ on $X\times\{1\}$. Both graphs can be projected onto $X=X\times\{0\}$, keeping track of under- and upper-crossings. By using an isotopy of X the crossings can be brought into a generic position of double transversal crossing of edges. We thus get a graph on X, with both 3 and 4-valent vertices. The 3-valent vertices come from those of $\Gamma^{\psi},\Gamma^{\psi'}$, and 4-valent vertices come from edge intersections between the two graphs. The inner product is given by evaluation in S^3 of a certain chain-mail that can be constructed from $\Gamma^{\psi},\Gamma^{\psi'}$. Namely, let us take one 0-framed link for every face, and one 0-framed link around every edge of the graph $\Gamma^{\psi}\cup\Gamma^{\psi'}$ on X. We get the structure of links at vertices as is shown

in the following drawings:



(4.9)

Denote by $C(\Gamma,\Gamma')$ the obtained collection of links. The inner product is given by

$$\langle \Gamma^{\psi}|\Gamma^{\psi'}\rangle = \eta^{V_\Gamma + V_{\Gamma'} + V_{\rm int}}(\Gamma^{\psi}\cup\Gamma^{\psi'}.\,\Omega C(\Gamma\cup\Gamma')). \tag{4.10}$$

Here $V_\Gamma, V_{\Gamma'}$ are the numbers of 3-valent vertices of graphs Γ,Γ' correspondingly, and $V_{\rm int}$ is the number of 4-valent vertices coming from intersections. The expression in brackets must be evaluated in S^3. Using the 3-fusion (A2) one can easily convince oneself that (4.10) coincides with the prescription given in Ref. 20.

We would also like to note an important relation for the TV inner product that expresses it as the RTW evaluation:

$$\langle \Gamma^{\psi}|\Gamma^{\psi'}\rangle = I(X\times S^1,\Gamma^{\psi},\Gamma^{\psi'}). \tag{4.11}$$

The evaluation is to be carried out in the 3-manifold $X\times S^1$. This relation that does not seem to have appeared in the literature. A justification for it comes from our operator/state correspondence, see below. Let us also note that a direct proof of a particular subcase of (4.11) corresponding to one of the graphs being zero colored is essentially given by our proof in the Appendix of the main theorem of Sec. VII. We decided not to attempt a direct proof of (4.11) in its full generality.

Turaev theorem: Let us note the theorem 7.2.1 from Ref. 5. It states that the TV invariant for H with the spin network Γ^{ψ} on $X=\partial H$ equals the RTW evaluation of Γ^{ψ} in $H\cup -H$:

$$\mathrm{TV}\,(H,\Gamma^{\psi}) = I(H\cup -H,\Gamma^{\psi}). \tag{4.12}$$

This is an analog of (4.8) for a manifold with a single boundary, and is somewhat analogous to our relation (4.11) for the TV inner product.

V. VERLINDE FORMULA

The purpose of this somewhat technical section is to review some facts about the Verlinde formula for the dimension of the CS Hilbert space. Considerations of this section will motivate a more general formula given in Sec. VII for the CFT partition function projected onto a spin network state. This section can be skipped on the first reading.

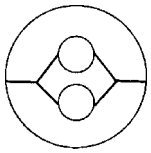
A. Dimension of the CS Hilbert space

Let us first obtain a formula for the dimension of the CS Hilbert space that explicitly sums over all different possible states. This can be obtained by computing the CS inner product. Indeed, as we have described in Sec. II, a basis in $\mathcal{H}_X^{\rm CS}$ is given by spin networks Δ^{ϕ}. With our choice of the normalization of the 3-valent vertices the spin network states $|\Delta^{\phi}\rangle$ are orthogonal but not orthonormal. Below we will show that the dimension can be computed as

$$\dim \mathcal{H}_X^{\rm CS} = \sum_{\phi}\left(\prod_{\text{int } e}\dim_{\rho_e}\right)\langle\Delta^{\phi}|\Delta^{\phi}\rangle = \sum_{\phi}\left(\prod_{\text{int } e}\dim_{\rho_e}\right) I(H\cup -H,\Delta^{\phi}\cup\Delta^{\phi}), \tag{5.1}$$

where the sum is taken over the colorings of the internal edges. The coloring of the edges of Δ that end at punctures are fixed.

To evaluate $\Delta^{\phi}\cup\Delta^{\phi}$ we proceed as follows. Let us project the graph $\Delta\cup\Delta$ to X. We note that there is a canonical way to do this projection so that there are exactly two 3-valent vertices of $\Delta\cup\Delta$ on each pair of pants, and there are exactly two edges of $\Delta\cup\Delta$ going through each boundary circle of a pair of pants. For example, the part of $\Delta\cup\Delta$ projected on a pair of pants with no punctures looks like



(5.2)

One gets a similar structure when projecting on a pair of pants with punctures. In that case the two holes in the center are replaced by punctures and loose edges of Δ are connected at the punctures to the loose edges of the other copy of Δ.

Let us now form a link L_{Δ} whose components are circles along which one glues the pant boundaries together. There are $3g+n-3$ such circles, in one-to-one correspondence with internal edges of Δ. We push all components of L_{Δ} slightly out of X. Using the prescription of the Appendix of Ref. 20 for computing the RTW evaluation of M with a graph inserted, one obtains

$$I(H\cup -H,\Delta^{\phi}\cup\Delta^{\phi})=\eta^{3g+n-3}(\Delta^{\phi}\cup\Delta^{\phi}.\Omega L_{\Delta}). \tag{5.3}$$

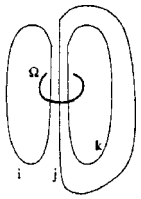
The evaluation on the right-hand side is to be taken in S^3. This relation establishes (5.1). Indeed, there are exactly two edges of $\Delta\cup\Delta$ linked by every component of L_{Δ}. Using the 2-fusion we get them connected at each pair of pants, times the factor of $\eta^{-1}/\dim_{\rho_e}$. The factors of η are canceled by the prefactor in (5.3), and the factors of $1/\dim_{\rho_e}$ are canceled by the product of dimensions in (5.1). What remains is the sum over the colorings of the internal edges of the product of N_{ijk} for every pair of pants. This gives the dimension. This argument also shows that the states $|\Delta^{\phi}\rangle$ with different coloring ϕ are orthogonal.

B. Computing the dimension: Verlinde formula

The sum over colorings of the internal edges in (5.3) can be computed. This gives the Verlinde formula. Let us sketch a simple proof of it, for further reference.

We first observe that, using the 3-fusion, the Verlinde formula for the 3-punctured sphere can be obtained as a chain-mail. Namely,

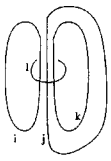
$$\eta^{-1}N_{ijk}=$$



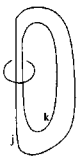
(5.4)

The Verlinde formula for N_{ijk} can be obtained by using the definition (4.1) of Ω and the recoupling identity (A4) of the Appendix. The computation is as follows:

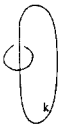
$$\eta^{-1}N_{ijk}=\eta\sum_{l}\dim_l$$



$$=\sum_{l}S_{il}$$



$$=\sum_{l}\frac{S_{il}S_{jl}}{\eta\dim_l}$$



$$=\eta^{-1}\sum_{l}\frac{S_{il}S_{jl}S_{kl}}{S_{0l}}. \tag{5.5}$$

This is the Verlinde formula (2.10) for the case of a 3-punctured sphere. We have used the fact that $\eta\dim_l=S_{0l}$. The above proof of the Verlinde formula for N_{ijk} is essentially that from Ref. 12.

The general Verlinde formula (2.10) can be obtained using a pant decomposition of X and taking a sum over labelings of the internal edges of Δ of the product of N_{ijk} one for every pair of pants. To get (2.10) one just has to use the unitarity $\Sigma_l S_{il} S_{jl} = \delta_{ij}$ of the S-matrix.

C. Verlinde formula using graph Γ: No punctures

Here we find a different representation of the Verlinde dimension. It was noticed in Ref. 23 that the Verlinde formula can be obtained using a certain gauge theory on a graph on X. Here we reinterpret this result using a chain-mail. We first derive a formula for a Riemann surface without punctures. It is obtained by starting from a graph Γ corresponding to a surface with some number n of punctures. Then a sum is carried over the labels at the punctures, so the end result depends only on the genus g, but not on n.

Consider a fat trivalent graph Γ that represents $X_{g,n}$. Let us form a chain-mail $C(\Gamma)$ as follows. Let us introduce a curve for every face of the fat graph Γ, and a linking curve around every $3(2g+n-2)$ edges of Γ, so that the obtained structure of curves at each 3-valent vertex is as in (4.9). Insert the element Ω along each component of $C(\Gamma)$, and evaluate the result in S^3. What is evaluated is just the chain-mail for Γ, no spin network corresponding to Γ is inserted. We get the following result:

Theorem (Boulatov): *The dimension of the Hilbert space of CS states on X_g is equal:*

$$\dim \mathcal{H}_{X_g}^{\mathrm{CS}} = \eta^{V_\Gamma} \Omega C(\Gamma). \tag{5.6}$$

The expression on the right-hand side is independent of the graph Γ that is used to evaluate it.

To prove this formula we use the 2-strand fusion. We get that all of the n different colorings on the links of Γ become the same. Denote by ρ the corresponding representation. The result is then obtained by a simple counting. Each $3(2g+n-2)$ of links around edges introduces the factor of $\eta^{-1}/\dim_\rho$. Every $2(2g+n-2)$ vertices of Γ gives a factor of $\dim_\rho$. Each of n faces of Γ gives another factor of $\eta \dim_\rho$. All this combines, together with the prefactor to give

$$\dim \mathcal{H}_{X_g}^{\mathrm{CS}} = \sum_\rho (\eta \dim_\rho)^{2-2g}, \tag{5.7}$$

which is the Verlinde formula (2.10) for the case with no punctures.

VI. OPERATOR/STATE CORRESPONDENCE

This section is central to the paper. Here we discuss a one-to-one correspondence between observables of CS theory and quantum states of TV theory. The fact that the algebra of observables in CS theory is given by graphs is due to Refs. 24 and 25, see also references below. The notion of the connecting 3-manifold $\tilde{M}$ is from Refs. 4 and 9. The operator/state correspondence of this section, as well as the arising relation between the CS and TV Hilbert spaces, although to some extent obvious, seems new.

A. CS observables and relation between the Hilbert spaces

We have seen that a convenient parametrization of the moduli space $\mathcal{A}/\mathcal{G}$ is given by the graph Γ connections. An expression for the CS Poisson structure in terms of graph connections was found in Ref. 24. A quantization of the corresponding algebra of observables was developed in Refs. 25–29 (see also Ref. 30 for a review). As we have seen in Sec. III a complete set of functionals on $\mathcal{A}/\mathcal{G}$ is given by spin networks. Spin networks thus become operators $\hat{\Gamma}^\psi$ in the CS Hilbert space $\mathcal{H}_X^{\mathrm{CS}}$. We therefore get a version of an operator/state correspondence, in which TV states correspond to observables of CS theory.

The fact that a CS/TV operator/state correspondence must hold follows from the relation between the phase spaces of the two theories. Namely, as we have seen in Sec. III, the TV phase

space is given by two copies of the phase space of Chern–Simons theory: $\mathcal{P}^{\mathrm{TV}}=\mathcal{P}^{\mathrm{CS}}\otimes\overline{\mathcal{P}}^{\mathrm{CS}}$, where the two copies have opposite Poisson structures. This means that in the quantum theory the following relation must hold:

$$\mathcal{H}_X^{\mathrm{TV}}\sim\mathcal{H}_X^{\mathrm{CS}}\otimes\mathcal{H}_{-X}^{\mathrm{CS}}\sim\mathrm{End}\,(\mathcal{H}_X^{\mathrm{CS}}). \tag{6.1}$$

Thus, the TV Hilbert space is isomorphic to the direct product of two copies of $\mathcal{H}^{\mathrm{CS}}$. The above isomorphism is given formally by the formula (3.8). We shall denote it by **I**. It identifies the TV spin network states $|\Gamma^{\psi}\rangle$ with the CS spin network observables $\hat{\Gamma}^{\psi}$. This statement deserves some explanation. The TV spin network states are wave functionals of the connection $\underline{\mathbf{w}}$: $\mathcal{T}(\underline{\mathbf{w}})=\mathcal{T}(A_z+B_z, A_{\bar{z}}+B_{\bar{z}})$, whereas Chern–Simons states are functionals $\Psi(A_z, B_{\bar{z}})$. Thus, the isomorphism (6.1) can be understood as a change of polarization. Being a change of polarization it intertwines the operator algebras acting on the two sides of (6.1). The polarization we have chosen for the TV Viro model is the one for which $\hat{\mathbf{e}}\sim(\hat{A}-\hat{B})$ acts trivially on the TV vacuum state. Using the intertwinning property of **I** this means that $\mathbf{I}(|0\rangle_{\mathrm{TV}})$ is commuting with all CS operators $\hat{\Gamma}^{\psi}$. It is therefore proportional to the identity in $\mathrm{End}\,(\mathcal{H}_X^{\mathrm{CS}})$. It follows from here that the operator that corresponds to the TV state $|\Gamma^{\psi}\rangle$ is the CS spin network operator:

$$\mathbf{I}(|\Gamma^{\psi}\rangle_{\mathrm{TV}})=\hat{\Gamma}^{\psi}\mathbf{I}(|0\rangle_{\mathrm{TV}})\propto\hat{\Gamma}^{\psi}. \tag{6.2}$$

Thus, the described isomorphism (6.1) given by the change of polarization indeed identifies TV graph states with the CS spin network operators.

Another important fact is as follows. Being a change of polarization, the isomorphism (6.1) preserves the inner product. Since the inner product on the right-hand side of (6.1) is just the CS trace, we get an important relation:

$$\mathrm{Tr}_{\mathrm{CS}}(\hat{\Gamma}\hat{\Gamma}')=\langle\Gamma|\Gamma'\rangle_{\mathrm{TV}}. \tag{6.3}$$

In other words, the trace of the product of operators in the CS Hilbert space is the same as the inner product in the TV theory. This relation is central to the operator/state correspondence under consideration. Let us now describe the isomorphism (6.1) more explicitly.

B. Connecting manifold $\tilde{M}$

A very effective description of the above operator/state correspondence uses the ''connecting manifold'' $\tilde{M}$. It is a 3-manifold whose boundary is the Schottky double $\tilde{X}$ of the Riemann surface X. Recall that the Schottky double of a Riemann surface X is another Riemann surface $\tilde{X}$. For the case of a closed X, the surface $\tilde{X}$ consists of two disconnected copies of X, with all moduli replaced by their complex conjugates in the second copy. For X with a boundary (the case not considered in this paper, but of relevance to the subject of boundary CFT, see, e.g., Refs. 4, 9) the double $\tilde{X}$ is obtained by taking two copies of X and gluing them along the boundary. Consider a 3-manifold

$$\tilde{M}=\tilde{X}\times[0,1]/\sigma, \tag{6.4}$$

where σ is an antiholomorphic map such that $\tilde{X}/\sigma=X$, and σ reverses the ''time'' direction. See, e.g., Ref. 4 for more detail on the construction of $\tilde{M}$. The manifold $\tilde{M}$ has a boundary $\partial\tilde{M}=\tilde{X}$, and the original surface X is embedded into $\tilde{M}$. For the case of a closed X, relevant for this paper, the manifold $\tilde{M}$ has the topology $X\times I$, where I is the interval $I=[0,1]$, see Fig. 2.

Consider the RTW evaluation of a spin network Γ^{ψ} in $\tilde{M}$. It gives a particular state in $\mathcal{H}_{\tilde{X}}^{\mathrm{CS}}$:

$$I(\tilde{M},\Gamma^{\psi})\in\mathcal{H}_{\tilde{X}}^{\mathrm{CS}}. \tag{6.5}$$

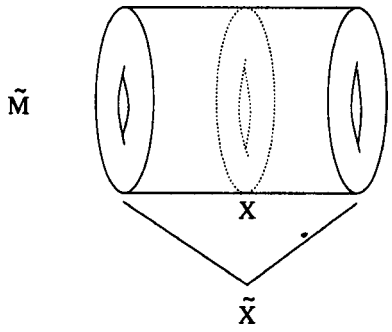


FIG. 2. The manifold $\tilde{M}$.

However, we have

$$\mathcal{H}^{\mathrm{CS}}_{\tilde{X}} \sim \mathcal{H}^{\mathrm{CS}}_{X} \otimes \mathcal{H}^{\mathrm{CS}}_{-X} \sim \mathrm{End}(\mathcal{H}^{\mathrm{CS}}_{X}). \tag{6.6}$$

Thus (6.5) gives an operator in $\mathcal{H}^{\mathrm{CS}}_{X}$ for every graph state $|\Gamma^{\psi}\rangle \in \mathcal{H}^{\mathrm{TV}}_{X}$.

C. Operator product

In the realization described the product of two operators $\hat{\Gamma}^{\psi}, \hat{\Gamma}^{\psi'}$ is an element of $\mathcal{H}^{\mathrm{CS}}_{\tilde{X}}$ obtained by evaluating in $\tilde{M}$ both Γ^{ψ} and $\Gamma^{\psi'}$:

$$I(\tilde{M}, \Gamma^{\psi}, \Gamma^{\psi'}) \in \mathcal{H}^{\mathrm{CS}}_{\tilde{X}}. \tag{6.7}$$

D. Trace

The trace of an operator $\hat{\Gamma}^{\psi}$ is obtained by gluing the two boundaries of $\tilde{M}$ to form a closed manifold of the topology $X \times S^1$:

$$\mathrm{Tr}_{\mathrm{CS}}(\hat{\Gamma}^{\psi}) = I(X \times S^1, \Gamma^{\psi}). \tag{6.8}$$

One can similarly obtain the trace of an operator product:

$$\mathrm{Tr}_{\mathrm{CS}}(\hat{\Gamma}^{\psi} \hat{\Gamma}^{\psi'}) = I(X \times S^1, \Gamma^{\psi}, \Gamma^{\psi\prime}). \tag{6.9}$$

In view of (6.3), the above relation establishes (4.11).

E. Identity operator

It is easy to see that the operator/state correspondence defined by (6.5) is such that the zero colored graph Γ^0 corresponds to the identity operator in the CS Hilbert space:

$$\hat{\Gamma}^0 = \hat{I}. \tag{6.10}$$

Indeed, insertion of Γ^0 into $\tilde{M}$ is the same as $\tilde{M}$ with no insertion, whose RTW evaluation gives the identity operator in $\mathcal{H}^{\mathrm{CS}}$.

F. Matrix elements

We recall that a basis in $\mathcal{H}^{\mathrm{CS}}_{X}$ is obtained by choosing a pant decomposition of X, or, equivalently, choosing a trivalent graph Δ, with a coloring ϕ. The matrix elements $\langle \Delta^{\phi} | \hat{\Gamma}^{\psi} | \Delta^{\phi'} \rangle$ are obtained by the following procedure. Take a handlebody H with a graph Δ^{ϕ} in it, its loose ends

ending at the punctures. The boundary of H is X, so that we can glue H from the left to $\tilde{M}$. One similarly takes $-H$ with $\Delta^{\phi'}$ in it, and glues it to $\tilde{M}$ from the right. One connects the punctures on the boundary of H to those on the boundary of $-H$ by strands inside $\tilde{M}$. What one gets is a closed manifold of the topology $H\cup -H$, with closed graphs $\Delta^{\phi}\cup\Delta^{\phi'}$ and Γ^{ψ} sitting inside it. The matrix elements are obtained as the evaluation:

$$\langle\Delta^{\phi}|\hat{\Gamma}^{\psi}|\Delta^{\phi'}\rangle = I(H\cup -H, \Delta^{\phi}\cup\Delta^{\phi'}, \Gamma^{\psi}). \tag{6.11}$$

VII. CFT PARTITION FUNCTION AS A STATE

Here we interpret the CFT partition function (correlator) as a particular state in the Hilbert space of TV theory. We also compute components of this state in the basis of states given by spin networks.

A. CFT partition function

The partition function of any CFT holomorphically factorizes. To understand this holomorphic factorization, and the relation to the chiral TQFT, it is most instructive to consider the partition function as a function of an external connection. Namely, let CFT be the WZW model coupled to an external connection (gauged model), and consider its partition function $Z_X^{\mathrm{CFT}}[\mathbf{m},\overline{\mathbf{m}},\mathbf{z},\overline{\mathbf{z}},\underline{A}_z,\underline{A}_{\bar{z}}]$ on X. Note that no integration is carried over $\underline{A}$ yet. Thus, the above quantity is not what is usually called the gauged WZW partition function. The later is obtained by integrating over $\underline{A}$. The introduced partition function depends on the moduli (both holomorphic and antiholomorphic) $\mathbf{m},\overline{\mathbf{m}}$, on positions of insertions of vertex operators coordinatized by $\mathbf{z},\overline{\mathbf{z}}$, and on both the holomorphic and anti-holomorphic components of the connection $\underline{A}$ on X. The partition function holomorphically factorizes according to

$$Z_X^{\mathrm{CFT}}[\mathbf{m},\overline{\mathbf{m}},\mathbf{z},\underline{\mathbf{z}},\underline{A}_z,\underline{A}_{\bar{z}}] = \sum_i \Psi_i[\mathbf{m},\mathbf{z},\underline{A}_z]\overline{\Psi}_i[\overline{\mathbf{m}},\overline{\mathbf{z}},\underline{A}_{\bar{z}}]. \tag{7.1}$$

Here $\Psi_i[\mathbf{m},\mathbf{z},\underline{A}_z]$ are the (holomorphic) conformal blocks with respect to the affine Lie algebra (in the case of WZW theories that we consider). The conformal blocks can be thought of as forming a basis in the Hilbert space $\mathcal{H}_X^{\mathrm{CS}}$ of CS theory on X. More precisely, there is a fiber bundle over the moduli space $\mathcal{M}_{g,n}$ of Riemann surfaces of type (g,n) with fibers isomorphic to $\mathcal{H}_{X_{g,n}}^{\mathrm{CS}}$. The conformal blocks are (particular) sections of this bundle, see Ref. 31 for more detail. Note that the sum in (7.1) is finite as we consider a rational CFT. As was explained in Ref. 14, the usual CFT partition function is obtained by evaluating (7.1) on the "zero" connection. The formula (7.1) then gives the factorization of the usual partition function, with $\Psi_i[\mathbf{m},\mathbf{z},0]$ being what is usually called the Virasoro conformal blocks.

Instead of evaluating (7.1) on the zero connection one can integrate over $\underline{A}$. The result is the partition function of the gauged model, which gives the dimension of the CS Hilbert space:

$$\dim \mathcal{H}_X^{\mathrm{CS}} = \frac{1}{\mathrm{Vol}\,\mathcal{G}}\int_{\mathcal{A}} \mathcal{D}\underline{A}\; Z_X^{\mathrm{CFT}}[\mathbf{m},\overline{\mathbf{m}},\mathbf{z},\overline{\mathbf{z}},\underline{A}_z,\underline{A}_{\bar{z}}]. \tag{7.2}$$

The value of the integral on the right-hand side is independent of moduli (or positions of insertion points).

A particular basis of states in $\mathcal{H}_X^{\mathrm{CS}}$ was described in Sec. II and is given by states $|\Delta^{\phi}\rangle$. Let us use these states in the holomorphic factorization formula (7.1). We can therefore think of the partition function (correlator) as an operator in the CS Hilbert space:

$$\hat{Z}_X^{\mathrm{CFT}} = \sum_{\phi}\left(\prod_{\mathrm{int}\,e}\dim_{\rho_e}\right)|\Delta^{\phi}\rangle\otimes\langle\Delta^{\phi}|. \tag{7.3}$$

The dimension of the CS Hilbert space is obtained by taking the CS trace of the above operator, which gives (5.1).

The CFT partition function (7.3) is the simplest possible modular invariant (the diagonal) that can be constructed out of the chiral CFT data. There are other possible modular invariants, and it is an ongoing effort to try to understand and classify different possibilities, see, e.g., the recent paper.[10] In this paper we only consider and give a TV interpretation of the simplest invariant (7.3). Our TV interpretation might prove useful also for the classification program, but we do not pursue this.

B. CFT partition function as a state

The formula (7.3) for the partition function, together with the operator/state correspondence of the previous section imply that Z_X^{CFT} can be interpreted as a particular state in the TV Hilbert space. We introduce a special notation for this state:

$$|Z_X^{\mathrm{CFT}}\rangle \in \mathcal{H}_X^{\mathrm{TV}}. \tag{7.4}$$

In order to characterize this state we first of all note that $\hat{Z}_X^{\mathrm{CFT}}$ is just the identity operator in $\mathcal{H}_X^{\mathrm{CS}}$:

$$\hat{Z}_X^{\mathrm{CFT}} = \hat{I}. \tag{7.5}$$

The representation (7.3) gives the decomposition of the identity over a complete basis of states in $\mathcal{H}_X^{\mathrm{CS}}$. Using (6.10) we see that the state $|Z_X^{\mathrm{CFT}}\rangle$ is nothing else but the spin network state with zero coloring, together with a set of strands labeled with representations $\mathbf{R}$ and taking into account the punctures:

$$|Z_X^{\mathrm{CFT}}\rangle = |\Gamma^0, \mathbf{R}\rangle. \tag{7.6}$$

Another thing that we are interested in is the components of $|Z_X^{\mathrm{CFT}}\rangle$ in the basis of spin networks $|\Gamma^\psi\rangle$. In view of (4.11) we have

$$\langle \Gamma^\psi | Z_X^{\mathrm{CFT}}\rangle = I(X\times S^1, \mathbf{R}, \Gamma^\psi). \tag{7.7}$$

The evaluation in $X\times S^1$ is taken in the presence of n links labeled by representations $\mathbf{R}$. Note that all the dependence on the moduli of X is lost in (7.7). However, the coloring ψ of Γ can be thought of as specifying the ''geometry'' of X, see more on this below.

C. Zero colored punctures

Here, to motivate the general formula to be obtained below, we deduce an expression for (7.7) for the case where the colors at all punctures are zero. In this case there is no extra links to be inserted in $X\times S^1$, and (7.7) reduces to $\langle \Gamma^\psi | \Gamma^0\rangle$. This can be evaluated using the prescription (4.10). One immediately obtains

$$\langle \Gamma^\psi | \Gamma^0\rangle = \eta^{V_\Gamma}(\Gamma^\psi . \Omega C(\Gamma)) = \eta^{2-2g} \sum_{\{\rho_f\}} \prod_{f\in F_\Gamma} \dim_{\rho_f} \prod_{v\in V_\Gamma} (6j)_v . \tag{7.8}$$

Here $C(\Gamma)$ is the chain-mail for Γ, as defined in the formulation of the theorem (5.6). In the last formula the sum is taken over irreducible representations labeling the faces of the fat graph Γ, the product of $6j$-symbols is taken over all vertices of Γ, and the $6j$-symbols $(6j)_v$ are constructed out of three representations labeling the edges incident at v, and three representations labeling the faces adjacent at v. The last formula is obtained using the 3-fusion recoupling identity (A2).

D. Verlinde formula

The dimension of the CS Hilbert space can be obtained as the inner product of $|Z_X^{\mathrm{CFT}}\rangle$ with the "vacuum" state $|\Gamma^0\rangle \in \mathcal{H}_X^{\mathrm{TV}}$, which corresponds to the spin network with zero (trivial representation) coloring on all edges:

$$\dim \mathcal{H}_X^{\mathrm{CS}} = \langle \Gamma^0 | Z_X^{\mathrm{CFT}} \rangle. \tag{7.9}$$

Expression (7.9) gives an unusual perspective on the Verlinde formula: it appears as a particular case of a more general object (7.7).

E. General formula

Here we find the result of the evaluation (7.7). As we have just explained, (7.7) must reduce to the Verlinde formula (2.10) when the graph Γ has zero colors. We have seen in Sec. V that, at least for the case with no punctures, the Verlinde formula can be obtained from the chain-mail $C(\Gamma)$ with no graph Γ inserted. We have also seen in (7.8) that for the case with no punctures the quantity (7.7) is given by the evaluation of $C(\Gamma)$ together with the graph. Thus, a natural proposal for (7.7) is that it is given by the evaluation (5.6), with the graph Γ added, and with an additional set of curves taking into account the punctures. This results in:

Main Theorem: *The CFT partition function (correlator), interpreted as a state of TV theory, projected onto a spin network state is given by*

$$\langle \Gamma^{\psi} | Z_X^{\mathrm{CFT}} \rangle = \eta^{2-2g-n} \sum_{\{\rho_f\}} \prod_{f \in F_\Gamma} S_{\rho_i \rho_{f_i}} \prod_{v \in V_\Gamma} (6j)_v \,. \tag{7.10}$$

A proof is given in the Appendix.

VIII. DISCUSSION

Thus, the CFT partition function (correlator) receives the interpretation of a state of TV theory. This state is the TV "vacuum" given in (7.6) by the graph with zero coloring. Thus, quite a nontrivial object from the point of view of the CFT, the partition function receives a rather simple interpretation in the TV theory.

We note that, apart from the partition function state $|Z_{\mathrm{CFT}}\rangle$, there is another state in $\mathcal{H}^{\mathrm{TV}}$ with a simple CS interpretation. This is the state that can be denoted as

$$|H\rangle \in \mathcal{H}^{\mathrm{TV}}. \tag{8.1}$$

It arises as the TV partition function for a handlebody H. The TV invariant (4.5) for a manifold with boundary has the interpretation of the TV inner product of $|H\rangle$ with a spin network state:

$$\mathrm{TV}(H, \Gamma^{\psi}) = \langle H | \Gamma^{\psi} \rangle. \tag{8.2}$$

In view of the Turaev theorem (4.12),

$$\langle H | \Gamma^{\psi} \rangle = I(H \cup -H, \Gamma^{\psi}). \tag{8.3}$$

From this, and the relation (6.11) for the matrix elements it can be seen that the state $|H\rangle$ corresponds in CS theory to the operator

$$\hat{H} = |\Delta^0\rangle \otimes \langle \Delta^0|, \tag{8.4}$$

which is just the projector on the CS "vacuum" state Δ^0, given by the zero colored pant decomposition graph Δ. We note that the TV state $|H\rangle$ has a rather nontrivial expression when decomposed into the spin network basis. Thus, the described relation between CS and TV theories (the operator/state correspondence) is a nontrivial duality in that simple objects on one side correspond

to nontrivial objects on the other: CFT correlators, nontrivial from the point of view of CS, are the TV ''vacuum'' states; the nontrivial TV handlebody state $|H\rangle$ is a rather trivial ''vacuum'' projector on the CS side.

We would like to emphasize that the CFT partition function state $|Z_X^{\rm CFT}\rangle$ does not coincide with the TV partition function state $|H\rangle$ on a handlebody H. However, the state $|Z_X^{\rm CFT}\rangle$ can be interpreted as a certain sum of TV handlebody states, provided a certain generalization of the Turaev theorem (4.12) holds. An attempt to prove this generalized Turaev theorem would lead us too far, so we shall formulate it as a conjecture:

Conjecture 1: Let $\mathrm{TV}((H,\Delta^\phi),\Gamma^\psi)$ *denote the Turaev–Viro invariant for a manifold H with a spin network* Δ^ϕ *inserted in it, and a spin network* Γ^ψ *on the boundary. This invariant can be evaluated as the RTW invariant for the double* $H\cup -H$*:*

$$\mathrm{TV}((H,\Delta^\phi),\Gamma^\psi)=\mathrm{I}((H,\Delta^\phi)\cup -(H,\Delta^\phi),\Gamma^\psi). \tag{8.5}$$

The justification for this conjecture is the theorem (4.12), which is nothing but (8.5) with no graph Δ insertion. Let us now introduce a set of states $|H,\phi\rangle$ obtained as the TV partition function inside a handlebody H with a spin network Δ^ϕ inserted inside. From the point of view of CS theory these states are just the projection operators:

$$\hat{H}^\phi=|\Delta^\phi\rangle\langle\Delta^\phi|. \tag{8.6}$$

Indeed, let us compute the TV inner product between the state $|H,\Delta^\phi\rangle$ and a spin network state $|\Gamma^\psi\rangle$:

$$\langle H,\phi|\Gamma^\psi\rangle=\mathrm{TV}((H,\Delta^\phi),\Gamma^\psi). \tag{8.7}$$

If the above conjecture holds this equals to the right hand side of (8.5). The later, on the other hand, is equal to

$$\langle\Delta^\phi|\hat{\Gamma}^\psi|\Delta^\phi\rangle. \tag{8.8}$$

This implies (8.6). Using relation (8.6) the CFT partition function as a state in TV Hilbert space can be represented as a sum of HH-type TV states obtained as the TV partition function over a handlebody with spin network insertion:

$$|Z_{\rm CFT}\rangle=\sum_\phi\left(\prod_{\mathrm{int}\,e}\dim_{\rho_e}\right)|H,\phi\rangle. \tag{8.9}$$

This formula should be contrasted with the usual AdS/CFT prescription, which states that the CFT partition function on the boundary is obtained as a sum of gravity partition functions on all manifolds H that have X as a boundary. In other words, one must sum over all ways to fill in the surface X so that the resulting 3-manifold H is non-singular inside. As we see, the ''holography'' arising in our context is different. Instead of taking a sum over all nonsingular manifolds H that have X as the boundary, in (8.9) one takes some fixed H, but sums over all labelings of the graph Δ sitting inside H. The graph Δ is a 1-skeleton of H; it can be thought of as a singularity inside the handlebody. Thus, to obtain the CFT partition function (modular invariant) one sums over labelings of the singularity inside H. This is a finite sum. The sum over different ways to fill in X is, on the other hand, infinite. It would be of interest to find if there is any relation between these two sums. If no such relation exists then the holographic prescription (8.9) predicted by our analysis is different from the AdS/CFT one.

Thus, we have seen that there are two TV states that correspond to CFT modular invariants: one is the TV vacuum (7.6) that gives the diagonal modular invariant, the other is the handlebody state $|H\rangle$ that gives the trivial modular invariant (8.4). An interesting question is what other states

in TV give CFT modular invariants. An answer to this question may be instrumental in understanding the structure of rational CFT's, see the recent paper[10] for a discussion along these lines.

Let us now discuss a physical interpretation of the formula (7.10). We note that the object (7.7) can be interpreted as the CFT partition function on a surface X whose ''geometry'' is specified by the state $|\Gamma^{\psi}\rangle$. This ''geometry'' should not be confused with the conformal geometry of X, on which the usual CFT partition function depends. Once the state $|Z_X^{\mathrm{CFT}}\rangle$ is projected onto $|\Gamma^{\psi}\rangle$ the dependence on the moduli of X is traded for the dependence on the coloring ψ of Γ. All the dependence on the moduli is encoded in the spin network states. Let us first discuss the dependence on the ''geometry'' as specified by the colored graph Γ^{ψ}, and then make comments as to the dependence of $|\Gamma^{\psi}\rangle$ on the moduli.

To understand the spin network Γ^{ψ} as specifying the ''geometry'' of X we recall, see Sec. III, that $|\Gamma^{\psi}\rangle$ are eigenstates of the ''momentum'' operators $\mathbf{e}\sim\partial/\partial\underline{\mathbf{w}}$. In this sense they are states of particular configuration of the **e** field on the boundary. To understand this in more detail let us consider the TV partition function $\mathrm{TV}(H,\Gamma^{\psi})$. Let us take the simple example of the 4-punctured sphere. Thus, we take $H=B^3$, a 3-ball. We will put all representations at the punctures to be trivial. In view of the Turaev theorem (4.12), $\mathrm{TV}(B^3,\Gamma^{\psi})=I(S^3,\Gamma^{\psi})$. Thus, for $X=S^2$, the TV invariant is given simply by the evaluation of the spin network Γ^{ψ} in S^3. In our simple example of the 4-punctures sphere this evaluation is a single $6j$-symbol. Let us now restrict ourselves to the case $G=\mathrm{SU}(2)$. As we have mentioned above, the TV theory in this case is nothing else but 3D gravity with positive cosmological constant. On the other hand, it is known that the quantum $(6j)$-symbol has, for large k and large spins, an asymptotic of the exponential of the classical Einstein–Hilbert action evaluated inside the tetrahedron:

$$(6j)\sim e^{iS_{\mathrm{TV}}[\mathrm{tet}]}+\mathrm{c.c.} \tag{8.10}$$

This fact was first observed[32] by Ponzano and Regge for the classical $(6j)$-symbol. In that case one evaluates the classical gravity action inside a flat tetrahedron. The action reduces to a boundary term (the usual integral of the trace of the extrinsic curvature term), which for a tetrahedron is given by the so-called Regge action:

$$S_{\mathrm{TV}}[\mathrm{tet},\Lambda=0]\sim\sum_e l_e\theta_e, \tag{8.11}$$

where the sum is taken over the edges of the tetrahedron, and l_e,θ_e are the edge length and the dihedral angle at the edge correspondingly. Dihedral angles are fixed once all the edge length are specified. Ponzano and Regge observed that the $(6j)$-symbol has the asymptotic of (8.10) with the action given by (8.11) if spins labeling the edges are interpreted as the length of edges. A similar (8.10) interpretation is true for the $\mathrm{SU}_q(2)$ $(6j)$-symbol, as was shown in Ref. 33. The gravity action in this case is that with a positive cosmological constant $\Lambda=(k/2\pi)^2$, and is evaluated in the interior of tetrahedron in S^3 whose edge length are given by spins. To summarize, in these examples the $(6j)$-symbol gets the interpretation of the exponential of the classical gravity action evaluated inside a tetrahedron embedded in either $\mathbb{R}^3$ or S^3, depending on whether one takes the classical limit $k\to\infty$ or considers a quantum group with finite k. The tetrahedron itself is fixed once all edge length are specified. The edge length are essentially given by the spins. We also note that the graph Γ in this example is the dual graph to the triangulated boundary of the tetrahedron in question.

Thus, the TV partition function (given by a single $(6j)$-symbol) inside a 4-punctured sphere (tetrahedron) has the interpretation of the gravity partition function inside the tetrahedron with its boundary geometry (edge length) fixed by the spins. This interpretation of Γ^{ψ} is valid also for other surfaces. One should think of Γ^{ψ} as specifying the geometry **e** on X. The TV invariant is, in the semi-classical limit of large representations, dominated by the exponential of the classical action evaluated inside the handlebody. The geometry inside is completely determined by the

geometry of the surface, in other words, the spins. The interpretation is valid not only for SU(2), but also for other groups. In such a general case the notion of ''geometry'' is more complicated, as described by the field **e** and the TV action (3.2).

The bottom line is that the TV spin network states $|\Gamma^{\psi}\rangle$ should be thought of as specifying the ''geometry'' of X. The quantity (7.10) then receives the interpretation of the CFT partition function on a surface X whose ''geometry'' is specified by Γ^{ψ}.

The other question is how the states $|\Gamma^{\psi}\rangle$ depend on the moduli of the surface. The fact that the graph Γ is the same as the one used in the Penner[18] coordinatization of the moduli space suggests that this dependence may be not very complicated. In fact, we believe that for the groups $SL(2,\mathbb{R})$ or $SL(2,\mathbb{C})$ that are relevant in the description of the moduli spaces, the dependence is rather simple: the described above ''geometry'' in this case must coincide with the usual conformal geometry of the surface. An argument for this is as follows. In the Penner coordinatization of the moduli space, or in any of its versions[34,35] the moduli are given by prescribing a set of real numbers: one for each edge of the graph Γ. The numbers specify how two ideal triangles are glued together across the edge, see Refs. 34, 35 for more detail. For the case when $G=\mathrm{SL}_q(2,\mathbb{R})$, as is relevant for, e.g., Liouville theory, see Ref. 36, the representations are also labeled by a single real number. We believe that the Penner coordinates and the representations that label the edges are simply dual to each other, in the sense of duality between the conjugacy classes of elements in the group and its irreducible representations. A similar proposal for the relation between the SL(2) spin and length was made in Ref. 6. Thus, there is some hope that the dependence $|\Gamma^{\psi}\rangle$ on the moduli can be understood rather explicitly, at least for some groups. Having this said we note that considerations of the present paper do not immediately generalize to the case of noncompact groups, relevant for the description of the moduli spaces. It is an outstanding problem to develop a noncompact analog of the Verlinde formula, not speaking of the formula (7.10). Thus, at this stage of the development of the subject considerations of this paragraph remain mere guesses. However, progress along these lines may be instrumental in developing a better technique for integrating over the moduli spaces, and thus, eventually, for a better understanding of the structure of string theory.

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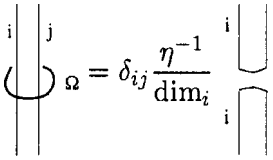
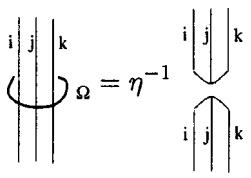
APPENDIX A: SOME RECOUPLING IDENTITIES

The 2-fusion identity:



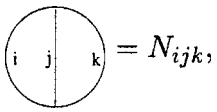
$$= \delta_{ij}\frac{\eta^{-1}}{\dim_i} \tag{A1}$$

The 3-fusion identity:



$$= \eta^{-1} \tag{A2}$$

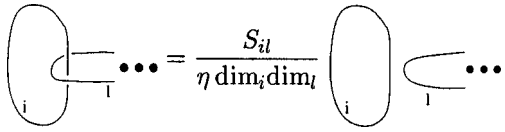
The 3-vertex is normalized so that



$$= N_{ijk}, \tag{A3}$$

where N_{ijk} is the multiplicity with which the trivial representation appears in the tensor product of i,j,k. For SU(2) this is either zero or one. In order to obtain (A1) from (A2) it is necessary to take into account the normalization (A3).

Another recoupling identity uses the modular S-matrix:



(A4)

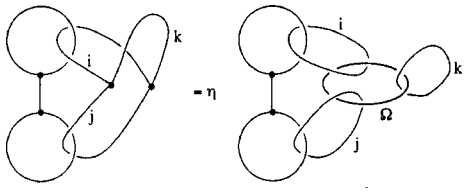
The dots on the right-hand side mean that the open ends can be connected (in an arbitrary way) to a larger graph.

APPENDIX B: PROOF

Here we give a proof of the main theorem.

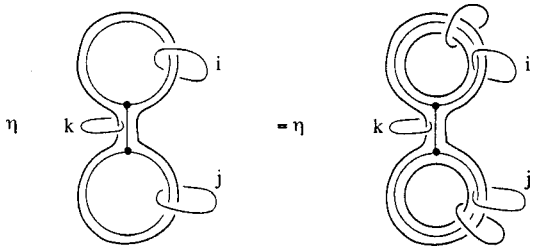
1. Genus zero case

We start by working out the simplest case of the 3-punctured sphere. We choose Γ to be given by a dumbbell. We thus need to compute the following evaluation:



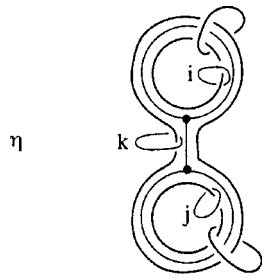
(B1)

Here we have used the observation (5.4) to replace two trivalent vertices of $\Delta \cup \Delta$ by a link with Ω inserted. Let us now slide the curve along which Ω is inserted to go all around the graph Γ, thus making one of the curves of the chain-mail $C(\Gamma)$. In the next step we add two more curves from $C(\Gamma)$ that go around punctures, and at the same time add two meridian curves with Ω inserted. This addition of two pairs of Ω linked does not change the evaluation in view of the killing property of Ω. The steps of sliding the Ω and adding two new pairs of curves is shown here:



(B2)

The last step is to use the sliding property of Ω to slide the links labeled i,j inside Γ:

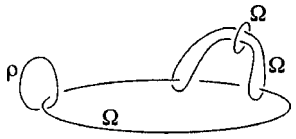


(B3)

One can now use the recoupling identity (A4) to remove the curves i,j,k at the expense of introducing a factor of $\eta^{-1}S_{ii'}/\dim_{i'}$ and similarly for other loops. Here i' is the representation on the loop from $C(\Gamma)$ going around the puncture i. The element Ω on that loop must be expanded to (4.1). The factor $\eta\dim_{i'}$ from that expansion is canceling the factor we got when removing the loop i. What is left is the S-matrix element $S_{ii'}$, with no extra factors. One can now use the 3-fusion identity (A2) to get the formula (7.10). One uses the 3-fusion 2 times, which produces η^{-2}. This combines with the factor of η in (B1)–(B3) to give η^{-1}, as prescribed by (7.10) for the case $g=0,n=3$. One can easily extend this proof to the case $g=0$ arbitrary number of punctures. To understand the general case, we first find a surgery representation for $X\times S^1$.

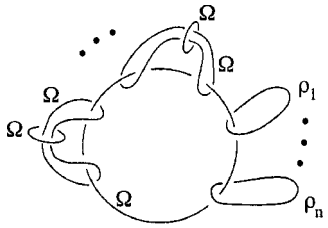
2. Surgery representation for $X\times S^1$

Let us first understand the genus one case. A surgery representation for $X_{1,1}\times S^1$ is given by the following link:



(B4)

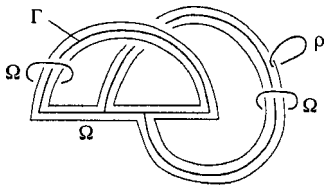
One must insert the element Ω into all components, and evaluate in S^3. Representing all the Ω's as the sum (4.1) and using the recoupling identity (A4) it is easy to show that (B4) gives the correct expression $\eta I(L)=\Sigma_{\rho'}S_{\rho\rho'}/S_{0\rho'}$ for the dimension. The same surgery representation was noticed in Ref. 37. The generalization to higher genus and to a larger number of punctures is straightforward. It is given by the following link:



(B5)

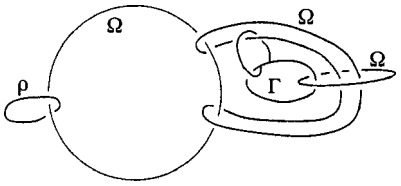
3. General case

We will work out only the (1,1) case. General case is treated similarly. We first note that the formula (7.10) for the (1,1) case can be obtained as the result of the following evaluation:



(B6)

This link is to be evaluated in S^3 and, as usual, the result multiplied by the factor of η. This gives (7.10) specialized to the case (1,1). It is now a matter of patience to verify that by the isotropy moves in S^3 the above link can be brought to the form:



(B7)

This is the correct surgery representation for $X_{1,1}\times S^1$ with the graph Γ inside. Thus, (7.10) indeed gives the evaluation $I(X\times S^1,\Gamma^{\psi})$, which, in view of (7.7), proves the theorem.

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On the Leibniz bracket, the Schouten bracket and the Laplacian

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The Leibniz bracket of an operator on a (graded) algebra is defined and some of its properties are studied. A basic theorem relating the Leibniz bracket of the commutator of two operators to the Leibniz bracket of them is obtained. Under some natural conditions, the Leibniz bracket gives rise to a (graded) Lie algebra structure. In particular, those algebras generated by the Leibniz bracket of the divergence and the Laplacian operators on the exterior algebra are considered, and the expression of the Laplacian for the product of two functions is generalized for arbitrary exterior forms. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738188]

I. INTRODUCTION

In mathematical physics, some operators of interest are not derivations of the underlying algebraic structures. Their complement to the Leibniz rule of derivation defines then a product, called the Leibniz bracket. The Leibniz bracket of a linear operator on an algebra is thus a bilinear form that gives rise to a new algebra, called the Leibniz algebra. Leibniz algebras present interesting properties, and this work concerns them.

In particular, if the Leibniz bracket of an operator (its adjoint action) is a derivation, the operator is of degree odd and its square vanishes or is also a derivation, then the Leibniz bracket is a Lie bracket.

This is the case, for example, in the antibracket formalism context,[1] for the exterior derivative considered as a second order differential operator on the differential forms of finite codimension: the antibracket can then be defined as the corresponding Leibniz bracket, and some of its known properties are simple consequences of the general results obtained here.

A similar situation occurs for the divergence operator over the exterior algebra, for which the Leibniz bracket is nothing but the Schouten[2,3] bracket (in another different context, an equivalent result has been obtained by Koszul[4]). The expression obtained here relating the Schouten bracket to the divergence operator is of interest in mathematical physics. It allows, for example, to express Maxwell equations in terms of Schouten bracket and to study *proper variations* of Maxwell fields.[5,6] It has been also used to express the electromagnetic field equations in a non linear theory which solves, in part, an old problem concerning the existence and physical multiplicity of null electromagnetic fields in general relativity.[6,7]

The Leibniz bracket of the commutator of two operators admits a simple expression: It is the commutator of the Leibniz bracket of every one of them with respect to the operation defined by the Leibniz bracket of the other one. For the Laplacian operator, which *appears* as the (graded) commutator of the divergence and the exterior derivative, the above expression may be applied directly to it, giving the following interesting result: The Leibniz bracket of the Laplace operator

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acting over the exterior algebra equals the Leibniz bracket of the exterior derivative acting over the Schouten algebra. This gives an interesting generalization to the exterior algebra of the well known expression for the Laplacian of a product of functions, and it has been applied in the analysis of harmonic coordinates in General Relativity.[8]

II. LEIBNIZ ALGEBRA OF A GRADED OPERATOR

(a) Let $\mathcal{E}=\oplus\mathcal{E}_a$ be a commutative graded group and $\circ:\mathcal{E}\times\mathcal{E}\to\mathcal{E}$ an operation verifying $\mathcal{E}_a\circ\mathcal{E}_b\subseteq\mathcal{E}_{a+b+k}$. Although it is always possible to regraduate $\mathcal{E}$ so that k vanishes, we shall retain the above graduation to avoid confusion when using different operations, as we shall do; such a k will be called the *degree* of the operation $\circ$ (with respect to this graduation).

The known properties (and concepts) on a graded group $\mathcal{E}$ concerning an operation $\circ$ of degree zero admit an equivalent form, depending generically on the degree k, when an arbitrary graduation is considered. Thus, the k-graded operation $\circ$ is *commutative* (resp. *anticommutative*) if it verifies $A\circ B=\epsilon(-1)^{(a+k)(b+k)}B\circ A$ with $\epsilon=1$ (resp. $\epsilon=-1$), and it is *associative* if $A\circ(B\circ C)=(A\circ B)\circ C$.

If $\mathcal{E}$ is a module and $\circ$ is bilinear, $(\mathcal{E},\circ)$ is said a k-*graded algebra*. A *derivation of degree* r is a r-graded endomorphism **D** on $\mathcal{E}$, $\mathbf{D}(\mathcal{E}_a)\subseteq\mathcal{E}_{a+r}$, verifying the Leibniz rule $\mathbf{D}(A\circ B)=\mathbf{D}A\circ B+(-1)^{(a+k)r}A\circ\mathbf{D}B$. An anticommutative k-graded algebra $(\mathcal{E},[,])$ verifying the Jacobi identity $\oint(-1)^{(a+k)(c+k)}[[A,B],C]=0$ is said a k-*graded Lie algebra*. Jacobi identity states, equivalently, that the (a+k)-graded endomorphism ad$A$, ad$A(B)=[A,B]$, is a derivation on $(\mathcal{E},[,])$. If $(\mathcal{E},\circ)$ is a k-graded associative algebra, the commutator defines a k-graded Lie algebra.

Let $\mathcal{E}$ be a graded group, $\circ$ a k-graded operation and **P** a p-graded operator. When **P** does not satisfy the Leibniz rule, its ''deviation'' interests us. So we give the following definition: the *Leibniz bracket* $\mathrm{L}_{\mathbf{P}}\langle\circ\rangle$ of **P** with respect to $\circ$ is the (p+k)-graded operation given by

$$\mathcal{L}_{\mathbf{P}}\langle\circ\rangle(A,B)=A\circ\mathbf{P}(B)+(-1)^{p(a+k)}[\mathbf{P}(A)\circ B-\mathbf{P}(A\circ B)]. \tag{1}$$

Of course, **P** verifies the Leibniz rule iff the Leibniz bracket $\mathcal{L}_{\mathbf{P}}\langle\circ\rangle$ vanishes identically.

The Leibniz bracket of a linear operator with respect to a bilinear operation is a bilinear operation, so that: *when* $(\mathcal{E},\circ)$ *is a k-graded algebra and* **P** *is a p-graded endomorphism*, $(\mathcal{E},\mathcal{L}_{\mathbf{P}}\langle\circ\rangle)$ *is a* $(k+p)$*-graded algebra*. We call it the *Leibniz algebra* of **P** on $(\mathcal{E},\circ)$. If **P** and **Q** are, respectively, p- and q-graded endomorphisms, their commutator $[\mathbf{P},\mathbf{Q}]=\mathbf{PQ}-(-1)^{pq}\mathbf{QP}$ is a (p+q)-graded endomorphism. Then, taking into account that $\mathcal{L}_{\mathbf{P}}\langle\circ\rangle$ and $\mathcal{L}_{\mathbf{Q}}\langle\circ\rangle$ are, respectively, (p+k)- and (q+k)-graded bilinear operations, and applying successively relation (1), one obtains the fundamental result:

Theorem 1: *In a k-graded algebra* $(\mathcal{E},\circ)$*, the Leibniz bracket of the commutator of two endomorphisms is related to the Leibniz bracket of every one of them by*

$$\mathcal{L}_{[\mathbf{P},\mathbf{Q}]}\langle\circ\rangle=\mathcal{L}_{\mathbf{Q}}\langle\mathcal{L}_{\mathbf{P}}\langle\circ\rangle\rangle-(-1)^{pq}\mathcal{L}_{\mathbf{P}}\langle\mathcal{L}_{\mathbf{Q}}\langle\circ\rangle\rangle. \tag{2}$$

In Marx's style:[9] The Leibniz bracket of the commutator [**P**, **Q**] of two endomorphisms **P** and **Q** on the algebra $(\mathcal{E},\circ)$ equals the graded difference between the Leibniz bracket of **Q** on the Leibniz algebra $(\mathcal{E},\mathcal{L}_{\mathbf{P}}\langle\circ\rangle)$ of **P** and the Leibniz bracket of **P** on the Leibniz algebra $(\mathcal{E},\mathcal{L}_{\mathbf{Q}}\langle\circ\rangle)$ of **Q**.

In particular, as $\mathbf{P}^2=\mathbf{P}\cdot\mathbf{P}$ is a 2p-graded operator, it follows that *for any odd-graded operator* **P**, *one has*

$$\mathcal{L}_{\mathbf{P}^2}\langle\circ\rangle=\mathcal{L}_{\mathbf{P}}\langle\mathcal{L}_{\mathbf{P}}\langle\circ\rangle\rangle\ , \tag{3}$$

Let us note that $\mathcal{L}_{\mathbf{P}}\langle x\rangle$ may be thought as *an operator* $\mathcal{L}_{\mathbf{P}}$ *over any operation x on* $\mathcal{E}$. In this sense, theorem 1 says that $\mathcal{L}_{[\mathbf{P},\mathbf{Q}]}\langle x\rangle=[\mathcal{L}_{\mathbf{Q}},\mathcal{L}_{\mathbf{P}}]\langle x\rangle$, and relation (3) says that $\mathcal{L}_{\mathbf{P}^2}\langle x\rangle=(\mathcal{L}_{\mathbf{P}})^2\langle x\rangle$.

Theorem 1 shows directly the well known result that if **P** and **Q** are derivations on $(\mathcal{E},\circ)$, so is [**P**, **Q**]. Also, from (3), it follows:

Lemma 1: The square $\mathbf{P}^2$ *of an endomorphism* **P** *of odd degree is a derivation on* $(\mathcal{E},\circ)$ *iff* **P** *is a derivation on* $(\mathcal{E},\mathcal{L}_{\mathbf{P}}\langle\circ\rangle)$.

On the other hand, if the operation $\circ$ is commutative or anticommutative, i.e., $A\circ B=\epsilon(-1)^{(a+k)(b+k)}B\circ A$, one can find the following result:

$$\mathcal{L}_{\mathbf{P}}\langle\circ\rangle(A,B)=\epsilon(-1)^{(a+k+p)(b+k+q)+p}\mathcal{L}_{\mathbf{P}}\langle\circ\rangle(B,A), \tag{4}$$

that is to say, *for a k-graded commutative (resp. anticommutative) algebra* $(\mathcal{E},\circ)$, *the* $(k+p)$*-graded Leibniz algebra* $(\mathcal{E},\mathcal{L}_{\mathbf{P}}\langle\circ\rangle)$ *is commutative (resp. anticommutative) if* $\mathbf{P}$ *is even-graded, and it is anticommutative (resp. commutative) if* $\mathbf{P}$ *is odd-graded.*

Let us denote, for simplicity, $\{A,B\}_{\mathbf{P}}=\mathcal{L}_{\mathbf{P}}\langle\circ\rangle(A,B)$. Then, when $(\mathcal{E},\circ)$ is a k-graded associative algebra and $\mathbf{P}$ an endomorphism, one has

$$\{A,B\circ C\}_{\mathbf{P}}-\{A,B\}_{\mathbf{P}}\circ C=(-1)^{p(b+k)}[\{A\circ B,C\}_{\mathbf{P}}-A\circ\{B,C\}_{\mathbf{P}}]. \tag{5}$$

(b) Let $(\mathcal{F},\circ)$ be a 0-graded associative and commutative algebra generated by its submodule $\mathcal{F}_1$, $\{,\}_{\mathbf{P}}$ be the Leibniz bracket of the p-graded endomorphism $\mathbf{P}$ on $(\mathcal{F},\circ)$, $\{A,B\}_{\mathbf{P}}\equiv\mathcal{L}_{\mathbf{P}}\langle\circ\rangle(A,B)$, and $\mathrm{ad}\{A\}_{\mathbf{P}}$ be the adjoint of A in the Leibniz algebra $(\mathcal{F},\{,\}_{\mathbf{P}})$, i.e., $\mathrm{ad}\{A\}_{\mathbf{P}}(B)\equiv\{A,B\}_{\mathbf{P}}$.

From the commutativity of $(\mathcal{F},\circ)$ and relation (4), Eq. (5) may be written $\{C,B\}_{\mathrm{ad}\{A\}_{\mathbf{P}}}=(-1)^{ca}\{A,B\}_{\mathrm{ad}\{C\}_{\mathbf{P}}}$. Then, it follows: *for any p-graded endomorphism* $\mathbf{P}$ *in* $(\mathcal{F},\circ)$, *one has*

$$\mathrm{ad}\{C\}_{\mathrm{ad}\{A\}_{\mathbf{P}}}=(-1)^{ca+a+p}\mathrm{ad}\{A\}_{\mathrm{ad}\{C\}_{\mathbf{P}}}. \tag{6}$$

In particular, $\mathrm{ad}\{A\}_{\mathbf{P}}$ obeys the Leibniz rule on the set $\{C\}\times\mathcal{F}$ iff $\mathrm{ad}\{C\}_{\mathbf{P}}$ does it on the set $\{A\}\times\mathcal{F}$. Thus, iff $\mathrm{ad}\{X\}_{\mathbf{P}}$ is a derivation for every $X\in\mathcal{F}_1$, $\mathrm{ad}\{A\}_{\mathbf{P}}$ verifies the Leibniz rule on $\mathcal{F}_1\times\mathcal{F}$. But an endomorphism that verifies the Leibniz rule on $\mathcal{F}_1\circ\mathcal{F}$ is a derivation on $(\mathcal{F},\circ)$, so that one has:

Lemma 2: If $\mathrm{ad}\{X\}_{\mathbf{P}}$ *is a derivation on* $(\mathcal{F},\circ)$ *for any X of* $\mathcal{F}_1$, *then* $\mathrm{ad}\{A\}_{\mathbf{P}}$ *is a derivation on* $(\mathcal{F},\circ)$ *for every A of* $\mathcal{F}$.

If $\mathbf{P}$ is a derivation on its induced Leibniz algebra $(\mathcal{F},\{,\}_{\mathbf{P}})$, the Leibniz rule may be written $[\mathbf{P},\mathrm{ad}\{A\}_{\mathbf{P}}]=\mathrm{ad}\{\mathbf{P}(A)\}_{\mathbf{P}}$. Then, applying theorem 1 it follows that $\mathrm{ad}\{A\}_{\mathbf{P}}$ is a derivation on $(\mathcal{F},\{,\}_{\mathbf{P}})$ when $\mathrm{ad}\{A\}_{\mathbf{P}}$ and $\mathrm{ad}\{\mathbf{P}(A)\}_{\mathbf{P}}$ are derivations on $(\mathcal{F},\circ)$. From this result and lemma 2 one has:

Lemma 3: If $\mathrm{ad}\{X\}_{\mathbf{P}}$ *is a derivation on* $(\mathcal{F},\circ)$ *for any* $X\in\mathcal{F}_1$ *and if* $\mathbf{P}$ *is a derivation on* $(\mathcal{F},\{,\}_{\mathbf{P}})$, *then* $\mathrm{ad}\{A\}_{\mathbf{P}}$ *is a derivation on* $(\mathcal{F},\{,\}_{\mathbf{P}})$ *for any* $A\in\mathcal{F}$.

For p odd, lemma 1 states that $\mathbf{P}$ is a derivation on $(\mathcal{F},\{,\}_{\mathbf{P}})$ iff $\mathbf{P}^2$ do it on $(\mathcal{F},\circ)$. On the other hand, it follows from relation (4) that $(\mathcal{F},\{,\}_{\mathbf{P}})$ is a p-graded anticommutative algebra. But under this condition Jacobi identity says equivalently that $\mathrm{ad}\{A\}_{\mathbf{P}}$ is a derivation on $(\mathcal{F},\{,\}_{\mathbf{P}})$. All that and lemma 3 lead to the following result:

Theorem 2: *For p odd, if* $\mathbf{P}^2$ *and* $\mathrm{ad}\{X\}_{\mathbf{P}}$, *for any X in* $\mathcal{F}_1$, *are derivations on* $(\mathcal{F},\circ)$ *then the Leibniz algebra* $(\mathcal{F},\{,\}_{\mathbf{P}})$ *is a p-graded Lie algebra.*

III. SCHOUTEN BRACKET, DIVERGENCE OPERATOR, AND LAPLACIAN

(a) Let Λ^p (resp. $\Lambda^{\star p}$) be the set of p-forms (*resp.* p-tensors) over the differential manifold M, that is to say, the set of completely antisymmetric covariant (resp. contravariant) tensor fields. Then, $\Lambda=\oplus\Lambda^p$ (resp. $\Lambda^\star=\oplus\Lambda^{\star p}$) with the exterior product $\wedge$ is a 0-graded associative and commutative algebra over the function ring $\chi=\chi(M)$: the *exterior covariant algebra* (*resp. exterior contravariant algebra*). We shall denote by α,β,γ the elements of Λ, and by A,B,C those of $\Lambda^\star$, with corresponding degrees a,b,c.

Denote the interior product $i(A)\beta$, $[i(A)\beta]_{\underline{b-a}}=(1/a!)A^q\beta_{a,\underline{b-a}}$ if $a\leqslant b$, by (A,β) and put $(\beta,A)=(-1)^{a(b-a)}(A,\beta)$. When $X\in\Lambda^1$, one has the usual interior product $i(X)$ which is a derivation of degree -1 on $(\Lambda,\wedge)$. Moreover, one has

$$(\gamma,A\wedge B)=((A,\gamma),B)+(-1)^{ab}((B,\gamma),A)\quad\text{if } c=a+b-1, \tag{7}$$

$$(A\wedge B,\gamma)=(B,(A,\gamma)),\quad (\gamma,A\wedge B)=((\gamma,B),A)\quad \text{if } c\geqslant a+b. \tag{8}$$

Suppose now that M is a n-dimensional and oriented manifold, and let η be a (covariant) volume element, $\eta^\star$ being its (contravariant) dual: $\eta_{p,n-p}\eta^{\star p',n-p}=\epsilon(n-p)^{-1}\delta_p^{p'}$, $\epsilon=\pm 1$. Then, the Hodge operators are given by $*A=(\eta,A)$, $*\alpha=(\eta^\star,\alpha)$ and verify $**A=\epsilon(-1)^{a(n-a)}A$. Therefore, if $a+b\leqslant n$,

$$*(A\wedge B)=(*B,A),\qquad *A\wedge\beta=*(\beta,A)\ . \tag{9}$$

The set of real numbers $\mathcal{R}$ being a sub-ring of the set of functions χ, $(\Lambda,\wedge)$ and $(\Lambda^\star,\wedge)$ are χ-algebras and $\mathcal{R}$-algebras. The exterior differentiation d is a 1-graded $\mathcal{R}$-derivation on $(\Lambda,\wedge)$, and the codifferentiation (divergence up to sign) is a (-1)-graded $\mathcal{R}$-endomorphism given by $\delta=\epsilon(-1)^{na}*d*$. Then, from (9) it follows,

$$\delta(A,\beta)=(\delta A,\beta)+(-1)^r(A,d\beta),\quad r=a-b>0. \tag{10}$$

(b) It is known that for $X,Y\in\Lambda^{\star 1}$, $\delta(X\wedge Y)=(\delta X)Y-(\delta Y)X-L_XY$, where L_X denotes the Lie derivative operator with respect to the vector field X. So that the operator δ is not a derivation on $(\Lambda^\star,\wedge)$. Thus, it is possible to consider the Leibniz bracket $\{\ ,\ \}_\delta$ of the codifferential operator on the exterior contravariant algebra $(\Lambda^\star,\wedge)$,

$$(-1)^a\{A,B\}_\delta=\delta A\wedge B+(-1)^aA\wedge\delta B-\delta(A\wedge B)\ . \tag{11}$$

Taking into account relations (7), (8), and (10), it is not difficult to show that, for any (a+b−1)-form γ, one has

$$(-1)^a i(\{A,B\}_\delta)\gamma=(d(\gamma,B),A)+(-1)^{ab}(d(\gamma,A),B)-(d\gamma,A\wedge B)\ . \tag{12}$$

The Schouten bracket $\{\ ,\}$ of two contravariant tensors[2] is a first order differential concomitant that generalize the Lie derivative.[3] For p-tensors (antisymmetric contravariant tensors) this bracket is defined by its action over the closed forms,[10] $i(\{A,B\})\gamma=(d(\gamma,B),A)+(-1)^{ab}(d(\gamma,A),B)$. Comparing this relation and (12), it follows $\{A,B\}=(-1)^a\{A,B\}_\delta$, and one has the following form of the Koszul[4] result:

Theorem 3: *The Schouten bracket is, up to a graded factor, the Leibniz bracket of the operator* δ *on the exterior contravariant algebra* $(\Lambda^\star,\wedge)$: $\{,\}=(-1)^a\{,\}_\delta$. *Explicitly*:

$$\{A,B\}=\delta A\wedge B+(-1)^aA\wedge\delta B-\delta(A\wedge B), \tag{13}$$

This result justifies that we name *Leibniz–Schouten bracket* the Leibniz bracket $\{,\}_\delta$ of the operator δ on the exterior contravariant algebra. Is is worth pointing out that both, the Schouten bracket and the Leibniz–Schouten bracket, define on the exterior contravariant algebra two *equivalent* structures of (-1)-graded algebra, which we name, respectively, *Schouten algebra* and *Leibniz–Schouten algebra*. Althought equivalent, it is to be noted that the Schouten algebra does *not* satisfies the standard writing of a Lie algebra properties, meanwhile the Leibniz-Schouten algebra does. Let us see that.

It is not difficult to see that $\forall X\in\Lambda^{\star 1}$, $\forall A\in\Lambda^{\star p}$, one has $\{X,A\}=L_XA$; that shows how the Schouten bracket generalizes the Lie derivative. Let us write $\{A,B\}\equiv L_AB$, $\forall A,B\in\Lambda^\star$; as it is known, $L_X, X\in\Lambda^{\star 1}$, is a derivation and δ is a (-1)-graded endomorphism on the 0-graded associative and commutative algebra $(\Lambda^{\star p},\wedge)$ such that $\delta^2=0$. As a consequence, the Leibniz–Schouten bracket $\{,\}_\delta$ satisfies the hypothesis of theorem 2 and so *the Leibniz–Schouten algebra* $(\Lambda^\star,\{,\}_\delta)$ *is a* (-1)*-graded Lie algebra*, that is, $\{\Lambda^{\star a},\Lambda^{\star b}\}_\delta\subseteq\Lambda^{\star a+b-1}$ and

$$\{A,B\}_\delta=-(-1)^{(a-1)(b-1)}\{B,A\}_\delta,\qquad \oint(-1)^{(a-1)(c-1)}\{\{A,B\}_\delta,C\}_\delta=0. \tag{14}$$

The Schouten bracket {,} also satisfies $\{\Lambda^{\star a},\Lambda^{\star b}\}\subseteq\Lambda^{\star a+b-1}$, and the properties of the Leibniz–Schouten Lie algebra (14) can equivalently be written in terms of the Schouten bracket as

$$\{A,B\}=(-1)^{ab}\{B,A\},\qquad \oint(-1)^{ac}\{\{A,B\},C\}=0\,. \tag{15}$$

Let us note that these last relations (15) satisfied by the Schouten algebra do not reduce, by any regraduation, to the standard ones of a Lie algebra.

Jacobi identity equivalently states, the following generalization for the Lie derivative with respect to the Lie bracket:

$$L_{\{A,B\}}=-(-1)^{a}[L_A,L_B].$$

Also, from lemmas 1 and 2 and taking into account the properties of the codifferential operator, it follows that: *(i) The codifferential operator δ is a $\mathcal{R}$-derivation on the Leibniz–Schouten algebra*:

$$-\delta\{A,B\}=\{\delta A,B\}+(-1)^{a}\{A,\delta B\}.$$

(ii) The operator L_A is a $\mathcal{R}$-derivation on the exterior contravariant algebra:

$$L_A(B\wedge C)=L_AB\wedge C+(-1)^{b(a-1)}B\wedge L_AC.$$

The property (i) gives the generalization of the commutator of the codifferential and Lie derivative operators:

$$[\delta,L_A]\equiv\delta L_A+(-1)^{a}L_A\delta=-L_{\delta A}\,.$$

On the other hand, Eq. (10) may be written $[i(\beta),\delta]=i(d\beta)$. But $i(\omega)$ is a derivation on $(\Lambda^{\star},\wedge)$ for any 1-form ω. Then, taking into account theorem 1, we have $\mathcal{L}_{i(\omega)}\langle\{\,\}_{\delta}\rangle=\mathcal{L}_{i(d\omega)}\langle\wedge\rangle$. In particular, when ω is a closed 1-form, then $i(\omega)$ is a derivation on the Leibniz–Schouten algebra.

(c) Suppose now M endowed with a (pseudo-)Riemannian metric g, allowing to identify $(\Lambda,\wedge)$ and $(\Lambda^{\star},\wedge)$. The Laplacian operator is then the *graded* commutator of the differential and codifferential operators:

$$\Delta=[d,\delta]\equiv d\delta+\delta d\ .$$

It is known that Δ is not a derivation on the exterior algebra. From theorem 1 its Leibniz bracket is given by:

Theorem 4: *The Leibniz bracket of the Laplacian operator on the exterior algebra equals the Leibniz bracket of the exterior derivative on the Leibniz–Schouten algebra*: $\mathcal{L}_{\Delta}\langle\wedge\rangle=\mathcal{L}_{d}\langle\{\,\}_{\delta}\rangle$. *Explicitly*:

$$\Delta\alpha\wedge\beta+\alpha\wedge\Delta\beta-\Delta(\alpha\wedge\beta)=\{d\alpha,\beta\}+(-1)^{a}\{\alpha,d\beta\}+d\{\alpha,\beta\}, \tag{16}$$

where α and β are arbitrary a- and b-forms, respectively.

This theorem gives the generalization to the exterior algebra of the expression for the Laplacian of a product of functions: $\Delta f.h+f.\Delta h-\Delta(f.h)=2(df,dh)$.

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Slater sum for the one-dimensional sech^2 potential in relation to the kinetic energy density

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In earlier work on the one-dimensional sech^2 potential energy [I. A. Howard and N.H. March, Int. J. Quantum Chem. **91**, 119 (2003)] it has been shown that both electron density $\rho(x)$ and kinetic energy $t(x)$ are low-order polynomials in the potential $V(x)$, for a small number of bound states. Here all attention is focused on the continuum states for the sech^2 potential with a single bound state. The tool employed is the Slater sum, which satisfies a partial differential equation. This is first solved explicitly for the bound state, and then the solution is generalized to apply to the continuum. Again, considerable simplification is exhibited for this specific choice of potential. A brief discussion is included of a central sech$^2(r)$ potential. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1745126]

I. BACKGROUND AND OUTLINE

March and Murray,[1,2] in early work on the properties of Fermions moving independently in a one-body potential $V(r)$, calculated the canonical density matrix $C(\mathbf{r},\mathbf{r}_0,\beta)$ by perturbation theory to all orders in V, with the unperturbed state described by plane waves. $C(\mathbf{r},\mathbf{r}_0,\beta)$ can be written exactly in terms of the eigenfunctions $\psi_i(\mathbf{r})$ and the corresponding eigenvalues ϵ_i of the Hamiltonian

$$H_{\mathbf{r}} = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \tag{1.1}$$

as

$$C(\mathbf{r},\mathbf{r}_0,\beta) = \sum_{all\ i} \psi_i(\mathbf{r})\psi_i^*(\mathbf{r}_0)\exp(-\beta\epsilon_i): \quad \beta = (k_B T)^{-1}. \tag{1.2}$$

Here, we shall mainly be concerned with the one-dimensional counterpart, i.e., a potential energy $V(x)$, but of the very specific form

$$\frac{2m}{\hbar^2}V(x) = -2\gamma^2\,\mathrm{sech}^2(\gamma x). \tag{1.3}$$

In a quite different context, Montroll[3] has utilized this potential (1.3) in discussing electronic band structure via a quantum network model.

In Montroll's study,[3] as well as in the book of Landau and Lifshitz,[4] it was recognized that this potential energy (1.3) generates a single bound state, with wave function

$$\psi(x) = \sqrt{\frac{\gamma}{2}}\,\mathrm{sech}(\gamma x) \tag{1.4}$$

corresponding to electron density $\rho(x)$ given by

$$\rho(x) = \frac{\gamma}{2}\,\mathrm{sech}^2(\gamma x) = -\frac{m}{2\gamma\hbar^2}V(x), \tag{1.5}$$

where in the last step Eq. (1.3) has been utilized. This result has been generalized to include a few bound states by two of us,[5] the kinetic energy density $t(x)$ being shown, as with $\rho(x)$, to be a low-order polynomial in this sech^2 potential $V(x)$. In density-functional parlance, this therefore constitutes a specific example of the Legendre transform of the single-particle kinetic energy. As Nagy and March[6] pointed out recently, the perturbation theory of March and Murray[2] and the subsequent derivation by Stoddart and March[7] of the kinetic energy density $t(\mathbf{r})$ in particular, already constitute an example of the Legendre transform of the single-particle kinetic energy.

However, to date these results[2,7] have only been summed to all orders in $V(\mathbf{r})$ for the harmonic oscillator potential, as in the investigation of Sondheimer and Wilson.[8] So it remains of interest to investigate whether one can solve explicitly for the sech^2 potential. In particular, one wishes to handle the entire continuous spectrum, as well as the bound states, generated by this potential.

Before outlining the present study, a referee has asked us to emphasize the importance of the Slater sum, which is the focus of this work. The Slater sum is the diagonal element of the canonical density matrix defined in Eq. (1.2). In turn, the canonical density matrix is determined by the Laplace transform of the one-particle (or Dirac) density matrix. Thus the Slater sum is directly given by the Laplace transform of the (diagonal) density. The role and importance of the Fermion density is well-known. Simple model systems have significance in that exact relations derived for them can often be applied to more complicated systems, at least in an approximate fashion.

The outline of the present article is then as follows: In Sec. II, the partial differential equation satisfied by the one-dimensional Slater sum $S(x,\beta)$ is set out, as follows from the early study of March and Murray,[1] and particular solutions are generated for the potential (1.3). Section III then utilizes these results to obtain the kinetic energy density $t(x)$, which is indeed conveniently presented in Legendre transform manner. Section IV constitutes a summary, with some proposals for future work. In an Appendix, but more formally now, a brief discussion is given of the central potential sech$^2(\gamma r)$.

II. PARTIAL DIFFERENTIAL EQUATION SATISFIED BY THE SLATER SUM

As mentioned above, defining the Slater sum $S(x,\beta)$ in one dimension as $C(x,x_0,\beta)|_{x_0=x}$, the Bloch equation

$$H_x C = -\frac{\partial C}{\partial \beta} \tag{2.1}$$

was shown by March and Murray[1] to be expandable around its diagonal $x=x_0$ to yield a partial differential equation for $S(x,\beta)$ for a general one-dimensional potential $V(x)$ as

$$\frac{1}{8}\frac{\partial^3 S(x,\beta)}{\partial x^3} - \frac{\partial^2 S(x,\beta)}{\partial x \partial \beta} - V(x)\frac{\partial S(x,\beta)}{\partial x} - \frac{1}{2}\frac{\partial V}{\partial x}S(x,\beta) = 0. \tag{2.2}$$

Below, for initial orientation which will lead into the solution of Eq. (2.2) for the sech^2 potential (1.3), we shall make use of the explicit continuum wave functions given in convenient form by Montroll[3] in the very different problem of the quantum theory of periodic networks. He classifies the wave functions of the potential $V(x)$ in Eq. (1.3) into symmetrical forms $\psi_s(x)$ and antisymmetrical forms $\psi_a(x)$. One can now use his results to form explicitly $\psi_s^2(x)+\psi_a^2(x)$, which evidently appears in the Slater sum from the definition (1.2) of $C(\mathbf{r},\mathbf{r}_0,\beta)$ with $\mathbf{r}_0$ put equal to $\mathbf{r}$ and motion restricted to the x-axis only. To obtain $\psi_s^2(x)+\psi_a^2(x)$, we first note with Montroll[3] that the general solution of the Schrödinger equation in the continuum is given by

$$\psi(x)=\mathcal{N}[\cos(kx+\delta)-(\gamma/k)\sin(kx+\delta)\tanh(\gamma x)], \tag{2.3}$$

where $E=k^2/2$ is the energy of the state.

Choosing $\delta=0$ in Eq. (2.3) yields the symmetric wave functions $\psi_s(x)$ while $\delta=\pi/2$ generates the antisymmetric forms. One then finds after a short calculation that $\psi_s^2+\psi_a^2$ takes the form

$$\psi_s^2+\psi_a^2=a^2(\gamma,k)[1+(\gamma/k)^2\tanh^2(\gamma x)]. \tag{2.4}$$

Inserting Eq. (2.4) into the definition of the Slater sum $S(x,\beta)$ set out above, one finds

$$S_c(x,\beta)=\sum_{all\ k>0} a^2(\gamma,k)[1+(\gamma/k)^2\tanh^2(\gamma x)]\exp\left(-\frac{\beta k^2}{2}\right), \tag{2.5}$$

where the subscript c on $S(x,\beta)$ indicates that in the form (2.5) one is summing only over continuum (c) states. This form (2.5) is important, in that it tells us that $S_c(x,\beta)$ has the general "shape"

$$\begin{aligned} S_c(x,\beta)&=F(\gamma,\beta)+\tanh^2(\gamma x)\sum_{all\ k>0} a^2(\gamma,k)(\gamma/k)^2\exp\left(-\frac{\beta k^2}{2}\right)\\ &\equiv F(\gamma,\beta)+G(\gamma,\beta)\tanh^2(\gamma x). \end{aligned} \tag{2.6}$$

Our task below must therefore be to find the explicit forms of the two functions $F(\gamma,\beta)$ and $G(\gamma,\beta)$ in Eq. (2.6). But already, one sees here the appearance of the sech^2 potential (1.3), since

$$\tanh^2(\gamma x)=1-\mathrm{sech}^2(\gamma x) \tag{2.7}$$

and hence Eq. (2.6) can be rewritten as

$$S_c(x,\beta)=[F(\gamma,\beta)+G(\gamma,\beta)]+\frac{G(\gamma,\beta)}{\gamma^2}V(x). \tag{2.8}$$

Equation (2.8) shows similarity of shape with the bound-state result (1.5) for the particle density, which corresponds to a bound-state contribution $S_b(x,\beta)$ to the Slater sum of

$$S_b(x,\beta)=\psi^2(x)\exp(-\beta\epsilon_0) \tag{2.9}$$

with ϵ_0 the bound-state energy $-\gamma^2/2$. Indeed, using Eq. (1.5) one finds

$$S_b(x,\beta)\propto\exp(\gamma^2\beta/2)V(x). \tag{2.10}$$

However one has to be wary, as in Eq. (2.8), that the potential again enters, via γ, in the "proportionality constant" in Eq. (2.10). Returning to Eq. (2.8), since $V(x)\to 0$ as $x\to\pm\infty$, we can see on physical grounds in Eq. (2.8) that $S_c(x,\beta)$ must tend to the well-known result for the partition function per unit length (in one dimension) for free electrons. This, in the units employed in Eq. (2.2) ($\hbar=m=1$), is

$$\lim_{x\to\pm\infty} S_c(x,\beta)=(2\pi\beta)^{-1/2}, \tag{2.11}$$

which shows from Eq. (2.8) that the γ dependence appearing in F and G separately must cancel in the sum $F+G=(2\pi\beta)^{-1/2}$. This is an important simplification to be utilized below.

Before turning to the main task of the present study, namely, the solution of the partial differential equation (2.2) subject to the appropriate physical boundary conditions, one should stress that while $S_b(x,\beta)$ in Eq. (2.10) and $S_c(x,\beta)$ in Eq. (2.8) must separately be solutions, $S_b(x,\beta)$ in Eq. (2.10) is much the simpler to handle, as the solution is a product of a function solely of x and one dependent only on β. Let us therefore take that as the starting point for discussing the solutions of Eq. (2.2).

A. Solutions of Eq. (2.2) for $S(x,\beta)$ obtained by the method of separation of variables

In such a separable solution for $S(x,\beta)$, let us write

$$S(x,\beta)=X(x)B(\beta). \tag{2.12}$$

Inserting this form into Eq. (2.2), but for the present retaining a general one-dimensional potential energy $V(x)$, we can write, after dividing the result obtained by $X'(x)B(\beta)$ where $X'=\partial X/\partial x$, etc.:

$$\frac{1}{8}\frac{X'''}{X'}-\frac{\partial}{\partial\beta}\ln B-V(x)-\frac{1}{2}\frac{V'X}{X'}=0. \tag{2.13}$$

This Eq. (2.13) shows, as yet for general $V(x)$, that separable solutions can be obtained, with separation constant κ such that $X(x)$ and $B(\beta)$ separately satisfy the ordinary differential equations

$$\frac{1}{8}\frac{X'''}{X'}-V(x)-\frac{1}{2}\frac{V'X}{X'}=\text{const}=\kappa \tag{2.14}$$

and

$$\frac{\partial}{\partial\beta}\ln B=\kappa, \tag{2.15}$$

the difference of these two equations (2.14) and (2.15) plainly satisfying Eq. (2.13). Without specifying $V(x)$, the general solution of the differential equation (2.15) is clearly

$$B(\beta)=A\exp(\kappa\beta), \tag{2.16}$$

where A is an arbitrary ''constant.'' To obtain the particular ''bound state'' Slater sum in Eq. (2.10) one must choose, now for the sech^2 potential (1.3), the separation constant $\kappa=\gamma^2/2$. Inserting this value into Eq. (2.14) one must plainly have, from Eq. (2.10), a particular solution $X=\text{const}\times V(x)\propto\text{sech}^2(\gamma x)$.

B. Particular solution for continuum Slater sum having the ''shape'' of Eq. (2.8)

Having established the ''shape'' of the continuum Slater sum $S_c(x,\beta)$, but now for the potential (1.3) alone as

$$S_c(x,\beta)=(2\pi\beta)^{-1/2}+\frac{G(\gamma,\beta)}{\gamma^2}V(x) \tag{2.17}$$

the question that remains is to find $G(\gamma,\beta)$, if that is possible, by direct substitution of Eq. (2.17) into the general partial differential equation (2.2). One then finds straightforwardly that

$$\frac{1}{8}\frac{G}{\gamma^2}V'''(x)-\frac{1}{\gamma^2}\frac{\partial G}{\partial\beta}V'(x)-\frac{3}{2}\frac{G}{\gamma^2}V(x)V'(x)-\frac{1}{2}(2\pi\beta)^{-1/2}V'(x)=0. \tag{2.18}$$

This, on rearrangement, reads

$$\frac{1}{\gamma^2}\frac{\partial G}{\partial\beta}-\frac{G}{\gamma^2}\left[\frac{V'''/V'}{8}-\frac{3}{2}V\right]+\frac{1}{2}(2\pi\beta)^{-1/2}=0. \tag{2.19}$$

Thus, the question posed above resolves into whether the square bracket in Eq. (2.19) is independent of x. This does indeed prove to be the case when $V(x)$ is inserted from Eq. (1.3). The resulting first-order ordinary differential equation may be integrated to yield

$$\begin{aligned}G(\gamma,\beta)&=-\frac{\gamma^2}{2}\exp\left(\frac{\gamma^2\beta}{2}\right)\left[\int_0^\beta\frac{1}{(2\pi\beta)^{1/2}}\exp\left(-\frac{\gamma^2\beta}{2}\right)d\beta+f(\gamma)\right]\\&=\left[-\frac{\gamma}{2}\operatorname{erf}\left(\frac{\gamma}{2}\sqrt{2\beta}\right)-\frac{\gamma^2 f(\gamma)}{2}\right]\exp\left(\frac{\gamma^2\beta}{2}\right),\end{aligned} \tag{2.20}$$

where $f(\gamma)$ is a constant of integration, and thus from (2.17),

$$S_c(x,\beta)=(2\pi\beta)^{-1/2}-\left[\frac{f(\gamma)}{2}+\frac{1}{2\gamma}\operatorname{erf}\left(\frac{\gamma}{2}\sqrt{2\beta}\right)\right]\exp\left(\frac{\gamma^2\beta}{2}\right)V(x). \tag{2.21}$$

In Appendix B, contact is made with a direct calculation of the local density of states in the continuum at $x=0$, namely, $\partial\rho_c(0,E)/\partial E$. Using the Laplace transform relation

$$S_c(x,\beta)=\int_0^\infty\frac{\partial\rho_c(x,E)}{\partial E}\exp(-\beta E)\,dE \tag{2.22}$$

and inserting Eq. (B9) into the right-hand side yields the result (2.17) with $G(\gamma,\beta)$ given in Eq. (2.20) and $f(\gamma)=-1/\gamma$, so that we can write

$$S_c(x,\beta)=(2\pi\beta)^{-1/2}-\frac{1}{2\gamma}\operatorname{erfc}\left(\frac{\gamma}{2}\sqrt{2\beta}\right)\exp\left(\frac{\gamma^2\beta}{2}\right)V(x). \tag{2.23}$$

The Slater sum is plotted in Fig. 1 for representative values of β and γ. We turn finally to discuss how the kinetic energy density $t(x)$ may be obtained from the Slater sum $S_c(x,\beta)$.

III. DERIVATION OF KINETIC ENERGY DENSITY FROM UNIFORM FERMI GAS RESULT IN ONE DIMENSION FOR THE sech^2 POTENTIAL

Returning to the Bloch equation (2.1), and inserting the one-body Hamiltonian

$$H_x=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V(x), \tag{3.1}$$

use of Eq. (1.2) in one dimension enables one to write almost immediately

$$-\frac{\partial S_c}{\partial\beta}=-\frac{1}{2}\sum_{k>0}\psi_k(x)\frac{\partial^2\psi_k^*(x)}{\partial x^2}\exp\left(\frac{\beta k^2}{2}\right)+V(x)S_c \tag{3.2}$$

or

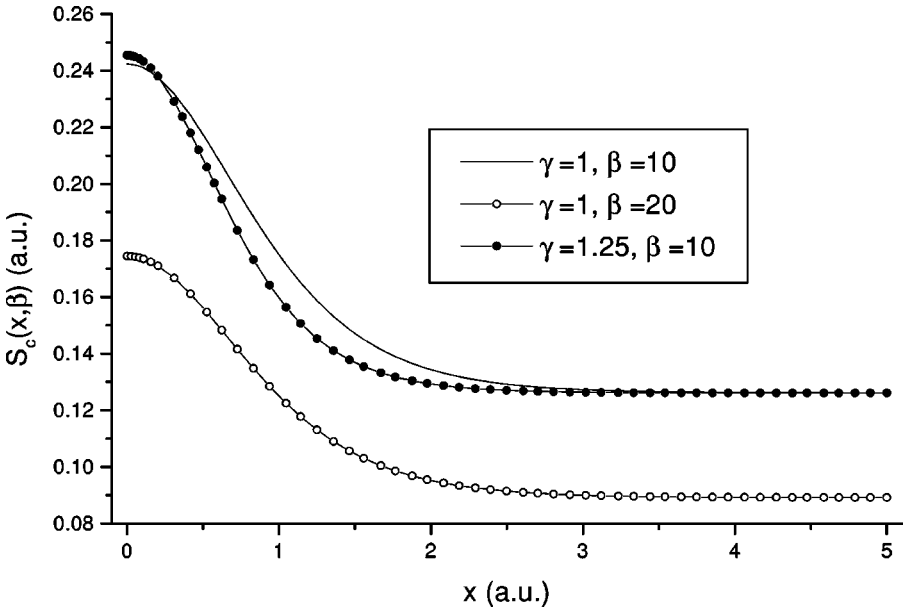

FIG. 1. Continuum Slater sum of Eq. (2.23) as a function of x for selected values of β and potential parameter γ in Eq. (1.3).

$$-\frac{\partial S_c}{\partial \beta} = t_c(x,\beta) + V(x) S_c\,, \tag{3.3}$$

which serves to define a ''kinetic energy density'' $t_c(x,\beta)$ which is related to the desired $t(x,E)$ by a Laplace inversion paralleling Eq. (2.22). But from Eqs. (3.3) and (2.23) one has

$$t_c(x,\beta) = \frac{1}{2\beta}\frac{1}{(2\pi\beta)^{1/2}} - V(x)\left[\frac{1}{2}\frac{3}{(2\pi\beta)^{1/2}} - \frac{\gamma}{4}\mathrm{erfc}\left(\frac{\gamma}{2}\sqrt{2\beta}\right)\exp\left(\frac{\gamma^2\beta}{2}\right)\right]$$
$$+\frac{1}{2\gamma}\mathrm{erfc}\left(\frac{\gamma}{2}\sqrt{2\beta}\right)\exp\left(\frac{\gamma^2\beta}{2}\right)V^2(x). \tag{3.4}$$

In Fig. 2 we plot this kinetic energy density for the β and γ of Fig. 1. Writing explicitly the analogous equation to (2.22), but now for the kinetic energy densities, one has

$$t_c(x,\beta) = \int_0^\infty \frac{\partial t_c(x,E)}{\partial E}\exp(-\beta E)\,dE \tag{3.5}$$

and one then obtains from Eq. (3.4) the kinetic energy change Δt from the one-dimensional Fermi gas, the result being given in Eq. (B3) of Appendix B.

IV. SUMMARY AND PROPOSALS FOR FUTURE STUDY

The main achievements of the present investigation are as follows: (i) the explicit solution of the partial differential equation (2.2) for the (continuum c) Slater sum $S_c(x,\beta)$ given in Eqs. (2.17) and (2.23); (ii) the analogous result (B9) for the continuum density of states and the consequent result (B8) for the total density $\rho(0,E)$ in the continuum, both now at the origin $x=0$; (iii) the kinetic energy density $t_c(x,\beta)$ in the continuum, defined by Eqs. (3.3) and (3.2), and given in Eq. (3.4); and (iv) the corresponding result for $t_c(x,E)$ exhibited in Eq. (B3).

In the future we believe it would be interesting to extend the calculations presented here explicitly to the three-dimensional $\mathrm{sech}^2(\gamma r)$ potential, the route to follow being indicated in

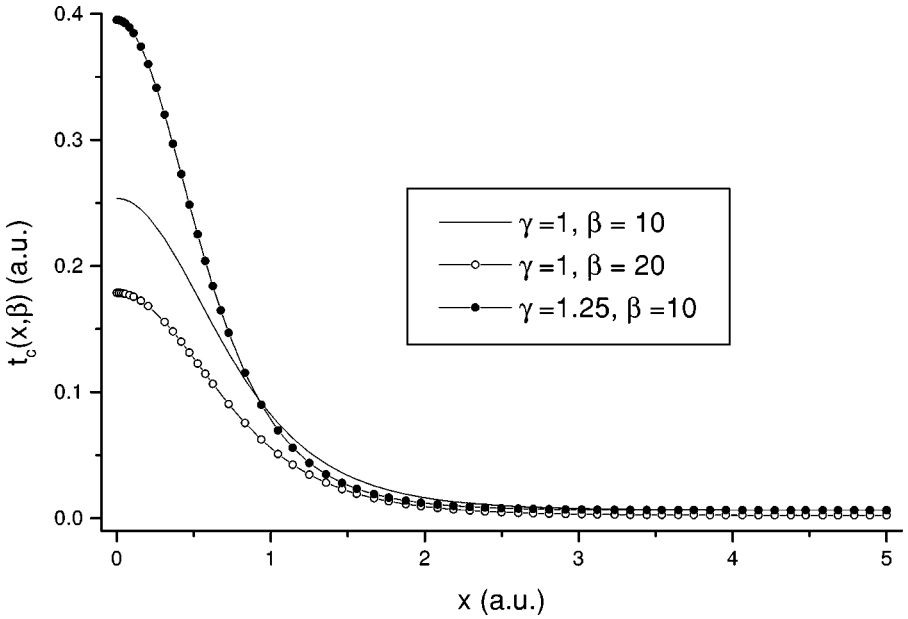

FIG. 2. Statistical mechanical kinetic energy density $t_c(x,\beta)$ of Eq. (3.4), for the same values of β and γ as in Fig. 1.

Appendix A. Furthermore, since separable solutions of Eq. (2.2) can be found for arbitrary $V(x)$, study of the ordinary differential equation (2.14) would seem worthwhile for a wider class of potentials. The progress here on the kinetic energy density $t[V(\mathbf{r})]$ may lead to partial summations to infinite order of the Stoddart–March perturbation series for $t[V(\mathbf{r})]$ measured relative to the Fermi gas value $t_0 = c_k \rho_\infty^{5/3}$, where ρ_∞ is the density of the unperturbed system, and c_k is known from the homogeneous Fermi assembly.

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APPENDIX A: THE THREE-DIMENSIONAL sech^2 POTENTIAL

For the three-dimensional analog of the potential $V(x)$ above, we can also study the density of states in the continuum for the case of zero angular momentum, $l=0$. The three-dimensional March–Murray equation ((4.12) in Ref. 1) for the density of states $N_s = \partial \rho_s / \partial E$ is

$$\frac{1}{8}\frac{\partial^3 (r^2 N_s)}{\partial r^3} - \frac{r^2 N_s}{2}\frac{\partial V}{\partial r} + (E-V)\frac{\partial (r^2 N_s)}{\partial r} = 0. \tag{A1}$$

Taking the potential to be $V(r) = -\gamma^2 \operatorname{sech}^2(\gamma r)$, we find the solution for energies $E = k^2/2$ to be of the form

$$\begin{aligned} N_s(r) = &[C_1 \cos^2(I_{k,\gamma}(r)) + C_2 \sin(I_{k,\gamma}(r))\cos(I_{k,\gamma}(r)) + C_3 \sin^2(I_{k,\gamma}(r))] \\ &\times ((\gamma^2 + k^2)\cosh(2\gamma r) - \gamma^2 + k^2)/r^2, \end{aligned} \tag{A2}$$

where

$$I_{k,\gamma}(r)=\frac{k}{\gamma}\ln[\cosh(\gamma r)+\sqrt{\cosh^2(\gamma r)-1}]+\frac{1}{2}\arctan\left[2\gamma k\frac{\cosh(\gamma r)\sqrt{\cosh^2(\gamma r)-1}}{(k^2-\gamma^2)\cosh^2(\gamma r)+\gamma^2}\right] \quad \text{(A3)}$$

and C_1, C_2, and C_3 are constants.

APPENDIX B: KINETIC ENERGY DENSITY DEVIATION FROM UNIFORM ELECTRON GAS RESULT

From Eq. (2.4) it can be seen that the total density $\rho(x)$ in the continuum will have the form $\rho(x)\equiv B(\gamma)+C(\gamma)\tanh^2(\gamma x)$. Note that $\rho(x\to 0)\equiv\rho(0)=B$ and $\rho(x\to\infty)\equiv\rho_\infty=B+C$, so that we may also write $\rho(x)=\rho(0)+(\rho_\infty-\rho(0))\tanh^2(\gamma x)$.

If we consider $\overline{t}=(t+t_G)/2$, the average of the gradient (t_G) and Laplacian (t) forms of the kinetic energy density, then the one-dimensional form of the differential virial theorem is, with $\Delta t=t-t_0$: $t_0=c_k\rho_\infty^3$,

$$\Delta\overline{t}'=-\frac{\rho}{2}\frac{\partial V}{\partial x}, \quad \text{(B1)}$$

so that for our potential,

$$\Delta\overline{t}=-\int^x\frac{\rho}{2}\frac{\partial V}{\partial x}dx=\frac{\gamma^2}{2}\left[\rho_\infty+\frac{(\rho(0)-\rho_\infty)}{2}\operatorname{sech}^2(\gamma x)\right]\operatorname{sech}^2(\gamma x),$$

$$=-\frac{1}{2}V(x)\left[\rho_\infty-\frac{(\rho(0)-\rho_\infty)}{2\gamma^2}V(x)\right] \quad \text{(B2)}$$

the constant of integration being chosen so that $\Delta\overline{t}(x\to\pm\infty)\to 0$. Expressing this in terms of the Laplacian $\psi\nabla^2\psi$ form of the kinetic energy density Δt, we have

$$\Delta t=\Delta\overline{t}-\frac{\rho''}{8}=\frac{\gamma^2}{2}[(2\rho_\infty-\rho(0))+2(\rho(0)-\rho_\infty)\operatorname{sech}^2(\gamma x)]\operatorname{sech}^2(\gamma x)$$

$$=\frac{\gamma^2}{2(\rho(0)-\rho_\infty)}(\rho-\rho_\infty)(2\rho-\rho(0)), \quad \text{(B3)}$$

so that the excess total kinetic energy due to the inhomogeneity, $T=\int_{-\infty}^{\infty}\Delta t(x)dx$, is

$$T=\frac{\gamma}{3}(\rho(0)+2\rho_\infty). \quad \text{(B4)}$$

Because Δt is local in ρ, we can write the functional derivative $\delta T/\delta\rho$ as simply $\partial t/\partial\rho$, so that

$$\frac{\delta T}{\delta\rho}=\frac{\partial t}{\partial\rho}=\frac{\gamma^2}{2(\rho_\infty-\rho(0))}(-4\rho(x)+\rho(0)+2\rho_\infty). \quad \text{(B5)}$$

The one-dimensional counterpart of March and Murray's[1] Eq. (4.12) for s-states gives

$$\frac{\rho'''}{8}-\frac{\rho}{2}\frac{\partial V}{\partial x}-V\rho'+\int_0^E E\frac{\partial^2\rho}{\partial x\partial E}dE=0. \quad \text{(B6)}$$

Inserting $\rho(x)$ and differentiating with respect to E, we find

$$(\gamma^2+2E)\frac{\partial\rho(0)}{\partial E}-2E\frac{\partial\rho_\infty}{\partial E}=0. \quad \text{(B7)}$$

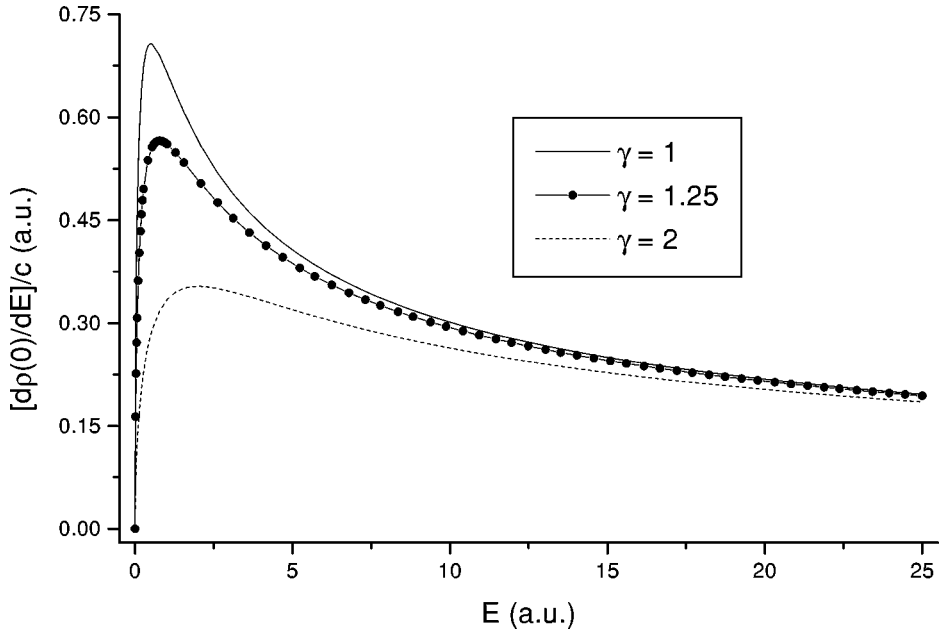

FIG. 3. Local density of states $[\partial\rho(0)/\partial E]/c$ at the origin $x=0$, as given in Eq. (B9), for selected values of γ.

Here $\partial\rho(0)/\partial E$ and $\partial\rho_\infty/\partial E$ are the density of states at the origin and at infinity (i.e., in the region of the uniform electron gas), respectively. But we know that for a uniform electron gas in one dimension, $\partial\rho_\infty/\partial E = c/\sqrt{E}$, where c is a constant; therefore

$$\rho(0,E) = 2c\left[\sqrt{E} - \frac{\gamma}{\sqrt{2}}\arctan\left(\frac{\sqrt{2E}}{\gamma}\right)\right] \tag{B8}$$

and

$$\frac{\partial\rho(0,E)}{\partial E} = \frac{2c\sqrt{E}}{\gamma^2 + 2E}. \tag{B9}$$

If $\gamma\to 0$, $V(x)\to 0$, and so $\rho(x)\to\rho(0)$ everywhere; then $\partial\rho(0,E)/\partial E \to c/\sqrt{E}$ as expected. The behavior of $\partial\rho(0)/\partial E$ is depicted in Fig. 3. Note also that if we subtract from $\rho(x)$ the spatially uniform density ρ_∞, we can integrate over all space to find the total number Δn of electrons in the nonuniform contribution to $\rho(x)$ as $\Delta n(E) = 2[\rho(0,E) - \rho_\infty(E)]/\gamma$. It is known that the potential $V(x)$ has a single bound state,[4] with associated density $\rho_b(x) = (\gamma/2)[1 - \tanh^2(\gamma x)]$ and energy level $E_b = -\gamma/2$. Thus by considering the density $\rho(x)\to(\rho(0) + \gamma/2) + (\rho_\infty - (\rho(0) + \gamma/2))\tanh^2(\gamma x)$ we include both bound and continuum states; all of our arguments above hold, down through Eq. (B5), with replacement of $\rho(0)$ by $(\rho(0) + \gamma/2)$. Equation (B6), however, holds only for the continuum states.

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Calculation of correlation function of the director fluctuations in cholesteric liquid crystals by WKB method

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The spatial correlation functions of the thermal fluctuations in systems with smoothly varying structure are calculated by means of the WKB method. As a particular physical problem we consider the behavior of director fluctuations in cholesteric liquid crystals possessing one-dimensional spatial periodicity. The problem leads to the solution of set of two second order differential equations with periodic coefficients. It is shown that in this physical system there exist regions where the WKB approximation is not valid. The analysis of these regions is similar to that of the turning points in quantum mechanics. Contrary to standard approach in our problem the turning point has fourth-order singularity and only decaying solutions have physical sense. We find WKB solutions for normal modes of director fluctuations in cholesteric liquid crystals far from the turning point as well as in its vicinity. We obtain that two fluctuating modes interact in the vicinity of the turning point, but any of these modes does not produce another. The amplitudes of modes change in such a way the product of amplitudes is constant. As a result we obtain explicit expressions for spatial correlation function in cholesteric liquid crystals with the large pitch which are valid in the entire domain. Finally we discuss the use of the correlation function in light scattering experiments. [DOI: 10.1063/1.1705717]

I. INTRODUCTION

In many physical situations such as those occurring in the vicinity of the second order phase transitions, the threshold effects, the turbulence flow, etc. the influence of fluctuations is crucial. In these systems fluctuations are not small and their interaction is essential. Various approaches were developed for describing the behavior of such systems.[1–3]

However there are some obstacles in calculations of fluctuations even in the simplest Gaussian approximation. Formally calculation of the fluctuation spatial correlation function in homogeneous systems requires the matrix conversion. There exists no standard approach for this problem in the case of inhomogeneous systems. Particularly this problem appears in physics of liquid crystals—liquids in which ordering of orientation can be established.[4] This ordering exists due to interaction with surfaces of a cell or due to external electric or magnetic fields. Depending on types of molecules and geometry of the cells the structure of liquid crystals can be both simple (spatially homogeneous) and rather complex [spiral and cubic structures in cholesteric liquid crystals (CLC) in the ordered and blue phases; twist-cells in nematic liquid crystals (NLC); various structures in spherical droplets of liquid crystals, etc]. As far as the energy of the orientation melting in liquid crystals is small the thermal fluctuations in these systems are large, and the correlation length of

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the spatial correlation function is not small either. These fluctuations noticeably influence physical properties of liquid crystals and first of all their optical properties. Since liquid crystals with complex spatial structure are intensively used in recent developments of various technical devices of information mapping, the problem of accurate account of thermal fluctuations and, first of all spatial correlation functions become important.

The methods of calculation of correlation functions in infinite uniform systems is well developed.[1–5] For restricted uniform systems with finite or infinite anchoring energy this problem was investigated in detail with the aid of various approaches for obtaining of the correlation functions: an expansion over eigenfunctions,[6,7] a method of the path integrals,[6,8] a method of the self-conjugate operators.[9,10] Meanwhile for systems with regular spatial structure such detailed investigations so far have not been carried out. Typical object is the cholesteric liquid crystal in the ordered phase, in this system the direction of primary orientation of molecules periodically varies along some axis and the correlation length of orientation fluctuations is comparable with the period of the structure. The problem of calculation of fluctuations in cholesterics was first analyzed by Lubensky[11] and later discussed in Refs. 12–14. The problem was solved with an assumption, that the correlation length is greater than the pitch, which allowed to reduce the problem to calculation of fluctuations in spatially homogeneous anisotropic media. In the medium with smoothly varying properties the problem of calculation of fluctuations was not yet considered. As long as the regular structure of the fluctuating system varies smoothly we use here the Wentzel–Kramers–Brillouin (WKB) approximation.[15,16] We generalize this approximation to the vector case. It is found that in our problem only damping solutions have the physical meaning. In terms of the WKB method using the damping solutions only is the specific character of the considered problem. Calculation of the fluctuating modes provided us to obtain the correlation matrix. The analysis of the obtained solution showed that there exist the regions where the WKB approximation is inapplicable. There are turning points in these regions. The method of analysis in the vicinity of these points is similar to that for the turning points in quantum mechanics.[15,16] Similar problems are known for the wave propagation theory, e.g., caustic[17] or the modes transformation,[18] and in the theory of elasticity, e.g., in the case of the Timoshenko beams.[19]

In particular, we find that two fluctuating modes interact in the vicinity of the turning point, but any of these modes does not produce another. The amplitudes of modes change in such a way the product of amplitudes is constant. It is shown that such unusual character of amplitudes behavior results from the exponential decreasing of the WKB solutions and it is consistent with general conservation law which takes place for solutions of second-order differential equations.

The paper is organized as follows. In Sec. II the basic equations describing CLC fluctuations are presented. In Sec. III the description of the WKB approach for the problem to be considered is given. In Sec. IV we calculate the correlation function of the director fluctuations far from the turning point. In Secs. V and VI the correlation function in the vicinity of the turning point is considered. In Conclusions (Sec. VII) we discuss physical consequences of the obtained results, in particular, in the light scattering problems. We consider conservation laws for WKB solutions in relaxation systems in Appendix.

II. BASIC EQUATIONS

Let us consider the cholesteric liquid crystal with the pitch directed along the z axis. Equilibrium vector of the director $\mathbf{n}^0$ in such system rotates in the (x,y) plane

$$\mathbf{n}^0(\mathbf{r})=\mathbf{n}^0(z)=(\cos\phi,\sin\phi,0), \tag{2.1}$$

where $\phi=p_0z+\phi_0$, ϕ_0 is the initial phase. The free energy of CLC has the form

$$F=F_0+\frac{1}{2}\int \mathrm{d}\mathbf{r}\{K_{11}(\nabla\cdot\mathbf{n})^2+K_{22}[\mathbf{n}\cdot(\nabla\times\mathbf{n})+p_0]^2+K_{33}(\mathbf{n}\times(\nabla\times\mathbf{n}))^2\}, \tag{2.2}$$

where F_0 is the energy of a homogeneous system, K_{ll}, $l=1,2,3$ are Frank modules, $d=2\pi/p_0$ is the pitch, $\mathbf{n}$ is the vector of the director. The distribution Eq. (2.1) minimizes the free energy Eq. (2.2).

We are interested in fluctuations of the director in CLC. Let us present the vector director as

$$\mathbf{n}(\mathbf{r})=\mathbf{n}^0(\mathbf{r})+\delta\mathbf{n}(\mathbf{r}), \tag{2.3}$$

where $\delta\mathbf{n}$ is the fluctuation of the director. In the quadratic in $\delta\mathbf{n}$ approximation the contribution of the director fluctuations to the free energy has the form

$$\delta F=\frac{1}{2}\int d\mathbf{r}\{K_{11}(\nabla\cdot\delta\mathbf{n})^2+K_{22}(\mathbf{n}^0\cdot(\nabla\times\delta\mathbf{n}))^2+K_{33}[(\delta\mathbf{n}\cdot\nabla)\mathbf{n}^0+(\mathbf{n}^0\cdot\nabla)\delta\mathbf{n}]^2\}. \tag{2.4}$$

Here we take into account the relations: $\nabla\cdot\mathbf{n}^0=0$; $\nabla\times\mathbf{n}^0=-p_0\mathbf{n}^0$, which follow from Eq. (2.1). Since $|\mathbf{n}|=|\mathbf{n}^0|=1$, in the quadratic approximation the relation $\mathbf{n}^0\cdot\delta\mathbf{n}=0$ is valid. Vector $\delta\mathbf{n}=(\delta n_x,\delta n_y,\delta n_z)$ can be parametrized in the form

$$\delta n_x=-u_1\sin\phi,\quad \delta n_y=u_1\cos\phi,\quad \delta n_z=u_2. \tag{2.5}$$

The functions u_1 and u_2 determine the director fluctuations in the plane (x,y) and along the z axis, respectively. Substituting Eq. (2.5) to Eq. (2.4) we get

$$\begin{aligned}\delta F=\frac{1}{2}\int d\mathbf{r}\{&K_{11}(-\sin\phi\partial_x u_1+\cos\phi\partial_y u_1+\partial_z u_2)^2+K_{22}[\cos\phi(\partial_y u_2-\partial_z(u_1\cos\phi))\\&+\sin\phi(\partial_z(-u_1\sin\phi)-\partial_x u_2)]^2+K_{33}[(-u_2p_0\sin\phi+\cos\phi\partial_x(-u_1\sin\phi)\\&+\sin\phi\partial_y(-u_1\sin\phi))^2+(u_2p_0\cos\phi+\cos\phi\partial_x(u_1\cos\phi)+\sin\phi\partial_y(u_1\cos\phi))^2\\&+(\cos\phi\partial_x u_2+\sin\phi\partial_y u_2)^2]\},\end{aligned} \tag{2.6}$$

where $\partial_l\equiv\partial/\partial l$, $l=x,y,z$.

We investigate the behavior of the correlation function

$$G_{kl}(\mathbf{r},\mathbf{r}_1)=\langle u_k(\mathbf{r})u_l(\mathbf{r}_1)\rangle, \tag{2.7}$$

where $k,l=1,2$, the brackets $\langle\cdots\rangle$ mean the statistical average. Due to CLC symmetry with respect to shifts in the (x,y) plane we have

$$G_{kl}(\mathbf{r},\mathbf{r}_1)=G_{kl}(\mathbf{r}_\perp-\mathbf{r}_{1\perp};z,z_1), \tag{2.8}$$

where $\mathbf{r}_\perp=(x,y)$. The correlation function of the director fluctuations

$$g_{\alpha\beta}(\mathbf{r}_{1\perp}-\mathbf{r}_{2\perp};z_1,z_2)=\langle\delta n_\alpha(\mathbf{r}_{1\perp},z_1)\delta n_\beta(\mathbf{r}_{2\perp},z_2)\rangle \tag{2.9}$$

is connected with the correlation matrix of scalar values $u_{1,2}$ by relationship

$$g_{\alpha\beta}(\mathbf{r}_\perp;z_1,z_2)=\sum_{k,l=1}^{2}G_{kl}(\mathbf{r}_\perp;z_1,z_2)h_\alpha^{(k)}(z_1)h_\beta^{(l)}(z_2), \tag{2.10}$$

where

$$\mathbf{h}^{(1)}(z)=(-\sin\phi(z),\cos\phi(z),0),\quad \mathbf{h}^{(2)}=(0,0,1). \tag{2.11}$$

Since CLC in the plane orthogonal to the z axis is spatially homogeneous it is convenient to use the two-dimensional Fourier transformation

$$u_\beta(\mathbf{r}) = \frac{1}{4\pi^2}\int \mathrm{d}^2\mathbf{q}\exp(i\mathbf{q}\cdot\mathbf{r}_\perp)u_\beta(\mathbf{q},z),$$

$$u_\beta(\mathbf{q},z) = \int \mathrm{d}^2\mathbf{r}_\perp \exp(-i\mathbf{q}\cdot\mathbf{r}_\perp)u_\beta(\mathbf{r}). \tag{2.12}$$

Then the distortion energy (2.6) has the form

$$\delta F = \frac{1}{4\pi^2}\int \mathrm{d}^2\mathbf{q}\,\delta F_q, \tag{2.13}$$

where

$$\delta F_q = \frac{1}{2}\int \mathrm{dz}\{K_{11}|\partial_z u_2 + i(-\sin\phi q_x + \cos\phi q_y)u_1|^2 + K_{22}|-\partial_z u_1 + iu_2(\cos\phi q_y - \sin\phi q_x)|^2$$
$$+ K_{33}[|u_2 p_0 + i(\cos\phi q_x + \sin\phi q_y)u_1|^2 + |u_2|^2(\cos\phi q_x + \sin\phi q_y)^2]\}. \tag{2.14}$$

We present the function δF_q as a quadratic form

$$\delta F_q = \frac{1}{2}\int \mathbf{u}^*(\mathbf{q},z)\hat{A}(\mathbf{q},z)\mathbf{u}(\mathbf{q},z)\mathrm{dz}, \tag{2.15}$$

where

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

is the two-dimensional vector and superscript "*" denotes the complex conjugation. The $\hat{A}$ matrix represents the differential operator of the second order.

For convenience we direct the x axis along the $\mathbf{q}$ vector, so that $q_x = q$ and $q_y = 0$. In this case the $\hat{A}$ matrix has the form

$$\hat{A} = K_{11}\begin{pmatrix} q^2\sin^2\phi & iq\sin\phi\partial_z \\ iq\partial_z\sin\phi & -\partial_z^2 \end{pmatrix} + K_{22}\begin{pmatrix} -\partial_z^2 & -iq\partial_z\sin\phi \\ -iq\sin\phi\partial_z & q^2\sin^2\phi \end{pmatrix}$$
$$+ K_{33}\begin{pmatrix} q^2\cos^2\phi & -ip_0 q\cos\phi \\ ip_0 q\cos\phi & q^2\cos^2\phi + p_0^2 \end{pmatrix}, \tag{2.16}$$

where $\partial_z \equiv \partial/\partial z$. As the probability of fluctuations $w_q \sim \exp[-\delta F_q/k_B T]$, where k_B is the Boltzmann constant, T is the temperature, the calculation of the correlation function is reduced to an inversion of the matrix $\hat{A}$. This procedure is equivalent to the solution of the equation

$$\hat{A}(\mathbf{q},z)\hat{G}(\mathbf{q},z,z_1) = k_B T\delta(z-z_1)\hat{I}, \tag{2.17}$$

where $\delta(z-z_1)$ is the delta function, $\hat{I}$ is the unit matrix of the second rank.

Equation (2.17) should be supplemented by the boundary conditions. In boundless CLC the principle of correlation decay in the infinity limit, $\hat{G}(\mathbf{q},z,z_1)\to 0$ at $z\to\pm\infty$, may be used as such a condition.

Since $u_{1,2}(\mathbf{r})$ are real the correlation function in $(\mathbf{q},z)$ representation satisfies the symmetry relationship

$$G_{kl}(\mathbf{q},z,z_1) = G_{lk}^*(\mathbf{q},z_1,z). \tag{2.18}$$

Taking into account Eq. (2.16) the problem is reduced to the solution of a set of two inhomogeneous differential equations of the second order, Eq. (2.17), with periodic coefficients. General solution of this equation set satisfies the Floquet theorem. According to this theorem the solution has the form of a product of two matrix functions depending on z and z_1. One of them is periodical with a period of $2\pi/p_0$ and another one is exponential. The procedure of determining the exponents and the Fourier harmonics of the periodical function is presented for instance in Ref. 20. Director fluctuations in CLC were calculated by this method in Ref. 11. In this work large-scale fluctuations, $q/p_0 \ll 1$, were considered when the Fourier-harmonic contribution decreases rapidly with the increasing of the harmonic number. Several lowest harmonics of the correlation function were calculated. From the physical point of view the limit $q/p_0 \ll 1$ corresponds to the smecticlike liquid crystal. This conclusion was supported by the result of Ref. 11 where three-dimensional Fourier component of the correlation function similarly to smectics has the form $\hat{G}(\mathbf{q},k_\parallel) \sim (k_\parallel^2 + c_0 q^4)^{-1}$, where c_0 is a constant.

In this work we are concerned of the opposite case, $p_0/q \to 0$, when CLC is close to nematic liquid crystal. Such situation corresponds to CLC with a large pitch. Complication of the problem from the point of view of the usual approach[11] is related to the fact that the wide spectrum of harmonics contributes to the correlation function. In this case the method based on the Floquet theorem[21] is not effective and the WKB approximation with the large parameter $\Omega = q/p_0 \gg 1$ seems to be more promising.

III. APPLICATION OF THE WKB METHOD TO SOLUTION OF THE PROBLEM

Equation (2.17) and the condition of correlation decay at $z \to \pm\infty$ determine the Green's function. Since for $z \neq z_1$ Eq. (2.17) becomes homogeneous we start with solution of homogeneous equations at $z > z_1$ and $z < z_1$. Then, using the conditions of function continuity and a jump of the derivative we construct the Green's function.

In what follows it is convenient to introduce the dimensionless variable $\xi = p_0 z$. Then the system of homogeneous equations is presented as

$$\left[-\begin{pmatrix} K_{22} & 0 \\ 0 & K_{11} \end{pmatrix} \frac{d^2}{d\xi^2} + i\Omega (K_{11} - K_{22}) \sin\phi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{d}{d\xi} + \begin{pmatrix} \Omega^2 (K_{11} \sin^2\phi + K_{33} \cos^2\phi) & -i\Omega \cos\phi (K_{22} + K_{33}) \\ i\Omega \cos\phi (K_{11} + K_{33}) & \Omega^2 (K_{22} \sin^2\phi + K_{33} \cos^2\phi) + K_{33} \end{pmatrix} \right] \mathbf{u}(\xi) = 0. \quad (3.1)$$

This system has four linearly independent solutions. Due to boundary conditions for $\hat{G}$, we use linearly independent solutions of Eq. (3.1) for construction of two matrices, $\hat{u}_1(\xi)$ and $\hat{u}_2(\xi)$, so that $\hat{u}_1(\xi) \to \hat{0}$ at $\xi \to +\infty$ and $\hat{u}_2(\xi) \to \hat{0}$ at $\xi \to -\infty$.

The Green's function is sought in the form

$$\hat{G}(\xi,\xi_1) = \begin{cases} \hat{u}_1(\xi)\hat{v}_1(\xi_1) & \text{at } \xi > \xi_1, \\ \hat{u}_2(\xi)\hat{v}_2(\xi_1) & \text{at } \xi < \xi_1, \end{cases} \quad (3.2)$$

where $\hat{v}_1$ and $\hat{v}_2$ are 2×2 matrices depending on ξ_1 only. For determination of eight elements of these matrices we use the conditions of the Green's function continuity and of the first derivative jump at the point $\xi = \xi_1$,

$$\hat{G}(\xi_1 + 0, \xi_1) = \hat{G}(\xi_1 - 0, \xi_1),$$
$$\hat{K}\left[\left.\frac{d\hat{G}}{d\xi}\right|_{\xi=\xi_1-0} - \left.\frac{d\hat{G}}{d\xi}\right|_{\xi=\xi_1+0} \right] = \frac{k_B T}{p_0} \hat{I}, \quad (3.3)$$

where

$$\hat{K}=\begin{pmatrix} K_{22} & 0 \\ 0 & K_{11} \end{pmatrix}.$$

Substituting Eq. (3.2) into Eq. (3.3) we obtain the system of eight equations for the elements of the $\hat{v}_{1,2}$ matrices

$$\begin{aligned} \hat{u}_1(\xi_1)\hat{v}_1(\xi_1)-\hat{u}_2(\xi_1)\hat{v}_2(\xi_1)=0, \\ \hat{u}_1'(\xi_1)\hat{v}_1(\xi_1)-\hat{u}_2'(\xi_1)\hat{v}_2(\xi_1)=-k_BTp_0^{-1}\hat{K}^{-1}. \end{aligned} \tag{3.4}$$

Solution of this system is

$$\hat{v}_j=k_BTp_0^{-1}\hat{u}_j^{-1}(\hat{u}_2'\hat{u}_2^{-1}-\hat{u}_1'\hat{u}_1^{-1})^{-1}\hat{K}^{-1}, \quad j=1,2. \tag{3.5}$$

Substituting Eq. (3.5) into Eq. (3.2) we get the Green's function in the form

$$\hat{G}(\xi,\xi_1)=\frac{k_BT}{p_0}\times\begin{cases} \hat{u}_1(\xi)\hat{u}_1^{-1}(\xi_1)(\hat{u}_2'\hat{u}_2^{-1}-\hat{u}_1'\hat{u}_1^{-1})^{-1}(\xi_1)\hat{K}^{-1} & \text{at } \xi\geqslant\xi_1, \\ \hat{u}_2(\xi)\hat{u}_2^{-1}(\xi_1)(\hat{u}_2'\hat{u}_2^{-1}-\hat{u}_1'\hat{u}_1^{-1})^{-1}(\xi_1)\hat{K}^{-1} & \text{at } \xi<\xi_1. \end{cases} \tag{3.6}$$

Note that the choice of the $\hat{u}_1$ and $\hat{u}_2$ matrices is ambiguous due to arbitrariness in the normalization of the $\hat{u}_1$ and $\hat{u}_2$ columns. But this ambiguity is not essential in Eq. (3.6). Note also that the calculation of the Green's function using the solutions of the homogeneous equations does not require the large parameter Ω.

We construct the solutions of the homogeneous equation set (3.1) by the WKB method. For this purpose it is convenient to reduce Eq. (3.1) to a system of four equations of the first order. Introducing the **v** vector

$$\mathbf{v}=\frac{1}{i\Omega}\frac{\mathrm{d}}{\mathrm{d}\xi}\mathbf{u}, \tag{3.7}$$

we may present Eq. (3.1) in the form

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\boldsymbol{\Psi}=(i\Omega\hat{B}+\hat{C})\boldsymbol{\Psi}. \tag{3.8}$$

Here we use the following notations:

$$\boldsymbol{\Psi}=\begin{pmatrix}\mathbf{u}\\ \mathbf{v}\end{pmatrix}, \quad \hat{B}=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ b_1 & 0 & 0 & b_3 \\ 0 & b_2 & b_4 & 0 \end{pmatrix}, \quad \hat{C}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & c_1 & 0 & 0 \\ c_2 & c_3 & 0 & 0 \end{pmatrix}, \tag{3.9}$$

where

$$b_1=-(K_{11}\sin^2\phi+K_{33}\cos^2\phi)K_{22}^{-1}, \quad b_3=(K_{11}-K_{22})\sin\phi K_{22}^{-1},$$

$$b_2=-(K_{22}\sin^2\phi+K_{33}\cos^2\phi)K_{11}^{-1}, \quad b_4=(K_{11}-K_{22})\sin\phi K_{11}^{-1},$$

$$c_1=-(K_{22}+K_{33})\cos\phi K_{22}^{-1}, \quad c_2=(K_{11}+K_{33})\cos\phi K_{11}^{-1}, \quad c_3=-iK_{33}(K_{11}\Omega)^{-1}.$$

We accept as an initial condition the value of $\boldsymbol{\Psi}$ in $\xi=\xi_0$. Then the solution of Eq. (3.8) can be presented in the form

$$\mathbf{\Psi}(\xi)=\hat{M}(\xi,\xi_0)\mathbf{\Psi}(\xi_0), \tag{3.10}$$

where $\hat{M}(\xi,\xi_0)$ is the matrix of evolution satisfying the initial condition $\hat{M}(\xi_0,\xi_0)=\hat{I}$. We calculate this matrix taking into account terms of the first and the second order with respect to the Ω parameter. Substituting Eq. (3.10) into equation set (3.8), we get the equation for the matrix of evolution $\hat{M}(\xi,\xi_0)$,

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\hat{M}(\xi,\xi_0)=(i\Omega\hat{B}+\hat{C})\hat{M}(\xi,\xi_0). \tag{3.11}$$

For solution of this set of equations it is convenient to introduce a new variable chosen in such a way that in principal order over the Ω parameter the equation set becomes diagonal. To do so we present $\hat{M}(\xi,\xi_0)$ as

$$\hat{M}(\xi,\xi_0)=\hat{U}(\xi)\hat{H}(\xi,\xi_0), \tag{3.12}$$

where $\hat{H}(\xi,\xi_0)$ is a new variable, $\hat{H}(\xi_0,\xi_0)=\hat{U}^{-1}(\xi_0)$. The choice of the $\hat{U}$ matrix will be discussed later. Substituting Eq. (3.12) into Eq. (3.11) we get

$$\frac{\mathrm{d}\hat{H}}{\mathrm{d}\xi}=\left(i\Omega\hat{U}^{-1}\hat{B}\hat{U}+\hat{U}^{-1}\hat{C}\hat{U}-\hat{U}^{-1}\frac{\mathrm{d}\hat{U}}{\mathrm{d}\xi}\right)\hat{H}. \tag{3.13}$$

Let us select $\hat{U}(\xi)$ so that the matrix $\hat{U}^{-1}\hat{B}\hat{U}$ becomes diagonal

$$\hat{U}^{-1}\hat{B}\hat{U}=\hat{\Lambda}, \tag{3.14}$$

where the diagonal matrix $\hat{\Lambda}$ is composed of eigenvalues of the $\hat{B}$ matrix. The columns of the $\hat{U}$ matrix are eigenvectors of the $\hat{B}$ matrix. Then the equation (3.13) for the $\hat{H}$ matrix can be written in the form

$$\frac{\mathrm{d}\hat{H}}{\mathrm{d}\xi}=i\Omega\left[\hat{\Lambda}+\frac{i}{\Omega}\left(\hat{U}^{-1}\frac{\mathrm{d}\hat{U}}{\mathrm{d}\xi}-\hat{U}^{-1}\hat{C}\hat{U}\right)\right]\hat{H}. \tag{3.15}$$

In zero approximation we omit the term of the $1/\Omega$ order in the right-hand side of Eq. (3.15). Then Eq. (3.15) is transformed to a set of independent equations

$$\frac{\mathrm{d}\hat{H}_{(0)}}{\mathrm{d}\xi}=i\Omega\hat{\Lambda}\hat{H}_{(0)}. \tag{3.16}$$

Its solution is

$$\hat{H}_{(0)}(\xi,\xi_0)=\exp\left[i\Omega\int_{\xi_0}^{\xi}\hat{\Lambda}(\xi')\mathrm{d}\xi'\right]\hat{U}^{-1}(\xi_0). \tag{3.17}$$

In order to solve Eq. (3.15) in the first approximation we present $\hat{H}(\xi,\xi_0)$ in the form

$$\hat{H}(\xi,\xi_0)=\hat{U}_{(1)}(\xi)\hat{H}_{(1)}(\xi,\xi_0), \tag{3.18}$$

where $\hat{H}_{(1)}(\xi_0,\xi_0)=\hat{U}_{(1)}^{-1}(\xi_0)\hat{U}^{-1}(\xi_0)$, and obtain the equation for $\hat{H}_{(1)}(\xi,\xi_0)$,

$$\frac{\mathrm{d}\hat{H}_{(1)}}{\mathrm{d}\xi}=i\Omega\left\{\hat{U}_{(1)}^{-1}\left[\hat{\Lambda}+\frac{i}{\Omega}\left(\hat{U}^{-1}\frac{\mathrm{d}\hat{U}}{\mathrm{d}\xi}-\hat{U}^{-1}\hat{C}\hat{U}\right)\right]\hat{U}_{(1)}+\frac{i}{\Omega}\hat{U}_{(1)}^{-1}\frac{\mathrm{d}\hat{U}_{(1)}}{\mathrm{d}\xi}\right\}\hat{H}_{(1)}. \tag{3.19}$$

Let us choose the $\hat{U}_{(1)}(\xi)$ matrix so that

$$\hat{U}_{(1)}^{-1}\left[\hat{\Lambda}+\frac{i}{\Omega}\left(\hat{U}^{-1}\frac{d\hat{U}}{d\xi}-\hat{U}^{-1}\hat{C}\hat{U}\right)\right]\hat{U}_{(1)}=\hat{\Lambda}_{(1)}, \tag{3.20}$$

where $\hat{\Lambda}_{(1)}$ is a diagonal matrix composed of eigenvalues of the matrix in square brackets of Eq. (3.20). Then Eq. (3.19) can be written as

$$\frac{d\hat{H}_{(1)}}{d\xi}=\left(i\Omega\hat{\Lambda}_{(1)}-\hat{U}_{(1)}^{-1}\frac{d\hat{U}_{(1)}}{d\xi}\right)\hat{H}_{(1)}. \tag{3.21}$$

For $\Omega\gg 1$ the matrix $\hat{\Lambda}+i\Omega^{-1}(\hat{U}^{-1}\hat{U}'-\hat{U}^{-1}\hat{C}\hat{U})$ is close to $\hat{\Lambda}$, so that matrices $\hat{\Lambda}$ and $\hat{\Lambda}_{(1)}$ are close to each other and $\hat{U}_{(1)}$ matrix is close to the unit one, i.e.,

$$\hat{U}_{(1)}(\xi)\approx\hat{I}+i\Omega^{-1}\hat{V}(\xi),\quad \hat{U}_{(1)}^{-1}(\xi)\approx\hat{I}-i\Omega^{-1}\hat{V}(\xi). \tag{3.22}$$

These expressions allow to get the condition of the WKB method applicability,

$$|V_{lm}|\ll\Omega.$$

Substituting (3.22) into Eq. (3.20), for $\hat{\Lambda}_{(1)}$ and $\hat{V}$ we get

$$(\hat{\Lambda}_{(1)})_{ll}\approx i\mu_l+\frac{i}{\Omega}\left(\hat{U}^{-1}\frac{d\hat{U}}{d\xi}-\hat{U}^{-1}\hat{C}\hat{U}\right)_{ll}, \tag{3.23}$$

$$V_{lm}\approx\frac{1}{i(\mu_m-\mu_l)}\left(\hat{U}^{-1}\frac{d\hat{U}}{d\xi}-\hat{U}^{-1}\hat{C}\hat{U}\right)_{lm},\quad l\neq m, \tag{3.24}$$

where $\mu_l=\Lambda_{ll}/i$. It follows from Eqs. (3.23) and (3.24) that the second term in brackets (3.21) is of the $1/\Omega^2$ order, so that it may be omitted in the first approximation. So we get

$$\hat{H}_{(1)}(\xi,\xi_0)\approx\exp\left[i\Omega\int_{\xi_0}^{\xi}\hat{\Lambda}_{(1)}(\xi')d\xi'\right]\hat{U}_{(1)}^{-1}(\xi_0)\hat{U}^{-1}(\xi_0). \tag{3.25}$$

If we omit terms of the $1/\Omega$ order in the $\hat{U}_{(1)}$ and $\hat{U}_{(1)}^{-1}$ matrices the evolution matrix $\hat{M}(\xi,\xi_0)$ in the first approximation has the form

$$\hat{M}(\xi,\xi_0)\approx\hat{U}(\xi)\widehat{\mathrm{diag}}\left\{\exp\left[-\int_{\xi_0}^{\xi}(\Omega\mu_l(x)+(\hat{U}^{-1}(x)\hat{U}'(x)-\hat{U}^{-1}(x)\hat{C}(x)\hat{U}(x))_{ll})dx\right]\right\}\hat{U}^{-1}(\xi_0). \tag{3.26}$$

This formula is a vector analogue of the classical WKB approximation.

According to Eq. (3.26) vector $\boldsymbol{\Psi}$ has the form

$$\boldsymbol{\Psi}(\xi)\approx\hat{U}(\xi)\widehat{\mathrm{diag}}\left\{\exp\left[-\int_{\xi_0}^{\xi}(\Omega\mu_l(x)+(\hat{U}^{-1}(x)\hat{U}'(x)-\hat{U}^{-1}(x)\hat{C}(x)\hat{U}(x))_{ll})dx\right]\right\}$$
$$\times\hat{U}^{-1}(\xi_0)\boldsymbol{\Psi}(\xi_0), \tag{3.27}$$

where $i\mu_l$ are eigenvalues of the $\hat{B}$ matrix and the columns of the $\hat{U}$ matrix are eigenvectors of the $\hat{B}$ matrix. Note that this expression for the $\mathbf{\Psi}$ vector is not valid, if the eigenvalues of the $\hat{B}$ matrix are becoming close to each other. Indeed, as it is seen from Eq. (3.24) in this case V_{lm} becomes large and condition of the WKB method validity, $|V_{lm}| \ll \Omega$, is violated.

Equation (3.27) allows to get the solution of Eq. (3.8) for any boundary conditions. The solution of Eq. (3.8) in the form (3.27) can be considered as a linear combination of four linearly independent vectors representing the columns of the evolution matrix $\hat{M}(\xi,\xi_0)$, with four factors representing the elements of the $\mathbf{\Psi}(\xi_0)$ vector. In what follows it is convenient to use $\hat{M}(\xi,\xi_0)\hat{U}(\xi_0)$ instead of the $\hat{M}(\xi,\xi_0)$ matrix and $\hat{U}^{-1}(\xi_0)\mathbf{\Psi}(\xi_0)$ instead of the $\mathbf{\Psi}(\xi_0)$ vector.

The solutions $\mathbf{u}$ which represent the first and the second components of the $\mathbf{\Psi}(\xi)$ vector are necessary for construction of the Green's function. The columns of the $\hat{u}_{1,2}(\xi)$ matrices are vectors constructed of first two elements of columns of the $\hat{M}(\xi,\xi_0)\hat{U}(\xi_0)$ matrix or linear combinations of these vectors.

IV. CALCULATION OF THE CORRELATION FUNCTION

In order to get the Green's function, i.e., the correlation function, in an explicit form we calculate the matrix of evolution. For this purpose it is necessary to calculate the eigenvalues and eigenvectors of the $\hat{B}$ matrix. The eigenvalues are determined from the relation

$$\det(\hat{B} - i\mu\hat{I}) = 0, \tag{4.1}$$

which represents the biquadratic equation. The solutions of this equation are

$$\begin{gathered} \mu_l = \sqrt{\sin^2\phi + K_{33}K_{ll}^{-1}\cos^2\phi}, \quad l = 1,2, \\ \mu_3 = -\mu_1, \quad \mu_4 = -\mu_2. \end{gathered} \tag{4.2}$$

Eigenvectors $\boldsymbol{\psi}_l$ satisfy the relation $\hat{B}\boldsymbol{\psi}_l = i\mu_l\boldsymbol{\psi}_l$. The matrix $\hat{U} = (\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \boldsymbol{\psi}_3, \boldsymbol{\psi}_4)$ composed of these vectors has the form

$$\hat{U} = \begin{pmatrix} -i\sin\phi\mu_1^{-1} & 1 & i\sin\phi\mu_1^{-1} & -1 \\ -1 & -i\sin\phi\mu_2^{-1} & -1 & -i\sin\phi\mu_2^{-1} \\ \sin\phi & i\mu_2 & \sin\phi & i\mu_2 \\ -i\mu_1 & \sin\phi & i\mu_1 & -\sin\phi \end{pmatrix}. \tag{4.3}$$

There is an arbitrariness in the choice of the $\boldsymbol{\psi}_l$ vectors due to normalizing factors. But it is possible to show, that solution (3.27) does not depend on normalizing conditions of the eigenvectors. Further we calculate the inverse matrix $\hat{U}^{-1}$,

$$\hat{U}^{-1} = \frac{-1}{2K_{33}\cos^2\phi} \begin{pmatrix} iK_{11}\mu_1\sin\phi & K_{22}\mu_2^2 & K_{22}\sin\phi & -iK_{11}\mu_1 \\ -K_{11}\mu_1^2 & iK_{22}\mu_2\sin\phi & iK_{22}\mu_2 & K_{11}\sin\phi \\ -iK_{11}\mu_1\sin\phi & K_{22}\mu_2^2 & K_{22}\sin\phi & iK_{11}\mu_1 \\ K_{11}\mu_1^2 & iK_{22}\mu_2\sin\phi & iK_{22}\mu_2 & -K_{11}\sin\phi \end{pmatrix}. \tag{4.4}$$

In the $\hat{C}$ matrix we neglect the term of the $1/\Omega$ order since it has order of smallness higher than the approximation (3.27) for the matrix of evolution. Then we have

$$(\hat{U}^{-1}\hat{C}\hat{U})_{ll} = (-1)^{l+1}(K_{11} - K_{22})(2K_{33})^{-1}\tan\phi, \quad l = 1,...,4. \tag{4.5}$$

It is convenient to present the diagonal elements of $\hat{U}^{-1}(d\hat{U}/\mathrm{d}\xi)$ matrix in the form

$$\left(\hat{U}^{-1}\frac{d\hat{U}}{d\xi}\right)_{ll}=\frac{1}{2}\frac{(\cos\phi/\mu_l)'}{\cos\phi/\mu_l}+\frac{1}{2}\frac{(\cos\phi)'}{\cos\phi}-\frac{K_{11}-K_{22}}{2K_{33}}\frac{(\cos\phi)'}{\cos\phi}(-1)^{l+1},\quad l=1,...,4. \tag{4.6}$$

From Eqs. (4.5) and (4.6) we get

$$\int_{\xi_0}^{\xi}\left(\hat{U}^{-1}\hat{C}\hat{U}-\hat{U}^{-1}\frac{d\hat{U}}{d\xi'}\right)_{ll}d\xi'=-\frac{1}{2}\ln\frac{\mu_l(\xi_0)|\cos\phi|}{\mu_l(\xi)|\cos(\xi_0+\phi_0)|}-\frac{1}{2}\ln\frac{|\cos\phi|}{|\cos(\xi_0+\phi_0)|}. \tag{4.7}$$

Thus we found all expressions entering Eq. (3.27). Using expression (4.7) it is possible to write the evolution matrix in the form

$$\hat{M}(\xi,\xi_0)=\hat{U}(\xi)\frac{|\cos(\xi_0+\phi_0)|}{|\cos\phi|}\widehat{\mathrm{diag}}\left\{\sqrt{\frac{\mu_l(\xi)}{\mu_l(\xi_0)}}\exp\left(-\int_{\xi_0}^{\xi}\Omega\mu_l\,d\xi'\right)\right\}\hat{U}^{-1}(\xi_0). \tag{4.8}$$

For determination of the correlation function it is necessary to construct the matrices $\hat{u}_1(\xi)$ and $\hat{u}_2(\xi)$. Selecting the solutions for the $\mathbf{\Psi}(\xi)$ vector, Eq. (3.10), which displays the required behavior at the infinity we obtain

$$\hat{u}_1(\xi)=\begin{pmatrix}-i\sin\phi\mu_1^{-1} & 1\\ -1 & -i\sin\phi\mu_2^{-1}\end{pmatrix}\exp(\hat{\Phi}_-),$$

$$\hat{u}_2(\xi)=\begin{pmatrix}i\sin\phi\mu_1^{-1} & -1\\ -1 & -i\sin\phi\mu_2^{-1}\end{pmatrix}\exp(\hat{\Phi}_+), \tag{4.9}$$

where

$$\exp(\hat{\Phi}_\pm)=\frac{|\cos(\xi_0+\phi_0)|}{|\cos\phi|}\widehat{\mathrm{diag}}\left\{\sqrt{\frac{\mu_l(\xi)}{\mu_l(\xi_0)}}\exp\left(\pm\int_{\xi_0}^{\xi}\Omega\mu_l\,d\xi'\right)\right\},\quad l=1,2. \tag{4.10}$$

It is easy to check that under this choice of the $\hat{u}_{1,2}(\xi)$ matrices the conditions $\hat{u}_1(\xi)\to\hat{0}$ at $\xi\to+\infty$ and $\hat{u}_2(\xi)\to\hat{0}$ at $\xi\to-\infty$ are valid. Substituting the $\hat{u}_{1,2}(\xi)$ matrices, Eq. (4.9), into expression for the correlation function, Eq. (3.6), and neglecting terms of the $1/\Omega$ order in non-exponential factors we get the correlation function in the form

$$\begin{aligned}\hat{G}(\xi,\xi_1)=&\frac{k_BT}{2qK_{33}\cos\phi(\xi_1)\cos\phi(\xi)}\begin{pmatrix}\mathrm{sign}(\xi-\xi_1)\sin\phi(\xi) & \mathrm{sign}(\xi-\xi_1)i\mu_2(\xi)\\ -i\mu_1(\xi) & \sin\phi(\xi)\end{pmatrix}\\ &\times\begin{pmatrix}\dfrac{\exp\left(-\Omega\left|\int_{\xi}^{\xi_1}\mu_1\,d\xi'\right|\right)}{\sqrt{\mu_1(\xi)\mu_1(\xi_1)}} & 0\\ 0 & \dfrac{\exp\left(-\Omega\left|\int_{\xi}^{\xi_1}\mu_2\,d\xi'\right|\right)}{\sqrt{\mu_2(\xi)\mu_2(\xi_1)}}\end{pmatrix}\\ &\times\begin{pmatrix}\mathrm{sign}(\xi_1-\xi)\sin\phi(\xi_1) & i\mu_1(\xi_1)\\ \mathrm{sign}(\xi_1-\xi)i\mu_2(\xi_1) & -\sin\phi(\xi_1)\end{pmatrix}.\end{aligned} \tag{4.11}$$

This expression has a simple structure. It is composed of a diagonal matrix and two matrices which turn the coordinate frame in ξ and ξ_1 points.

It is convenient to split the $\hat{G}$ matrix into two parts, associated with two modes μ_1 and μ_2. We have

$$\hat{G}(\mathbf{q};z_1,z_2)=\hat{G}^{(1)}(\mathbf{q};z_1,z_2)+\hat{G}^{(2)}(\mathbf{q};z_1,z_2), \tag{4.12}$$

where

$$\hat{G}^{(j)}(\mathbf{q};z_1,z_2)=\frac{k_BT}{2qK_{33}\cos\phi(z_1)\cos\phi(z_2)}\exp\left(-q\left|\int_{z_1}^{z_2}\mu_j(z)\mathrm{d}z\right|\right)\hat{W}^{(j)}(\mathbf{q};z_1,z_2), \tag{4.13}$$

$$\hat{W}^{(1)}(\mathbf{q},z_1,z_2)=\begin{pmatrix} -\dfrac{\sin\phi(z_1)\sin\phi(z_2)}{\sqrt{\mu_1(z_1)\mu_1(z_2)}} & i\,\mathrm{sign}(z_1-z_2)\sin\phi(z_1)\dfrac{\sqrt{\mu_1(z_2)}}{\sqrt{\mu_1(z_1)}} \\ i\,\mathrm{sign}(z_1-z_2)\sin\phi(z_2)\dfrac{\sqrt{\mu_1(z_1)}}{\sqrt{\mu_1(z_2)}} & \sqrt{\mu_1(z_1)\mu_1(z_2)} \end{pmatrix}, \tag{4.14}$$

$$\hat{W}^{(2)}(\mathbf{q},z_1,z_2)=-\begin{pmatrix} -\sqrt{\mu_2(z_1)\mu_2(z_2)} & i\,\mathrm{sign}(z_1-z_2)\sin\phi(z_2)\dfrac{\sqrt{\mu_2(z_1)}}{\sqrt{\mu_2(z_2)}} \\ i\,\mathrm{sign}(z_1-z_2)\sin\phi(z_1)\dfrac{\sqrt{\mu_2(z_2)}}{\sqrt{\mu_2(z_1)}} & \dfrac{\sin\phi(z_1)\sin\phi(z_2)}{\sqrt{\mu_2(z_1)\mu_2(z_2)}} \end{pmatrix}. \tag{4.15}$$

Here $\cos\phi=\mathbf{q}\cdot\mathbf{n}^0/q$, $\sin\phi=\sqrt{q^2-(\mathbf{q}\cdot\mathbf{n}^0)^2}/q$ are presented in the form independent on the coordinate frame choice.

Figure 1 shows the correlation matrix components, G_{11} and G_{12}, in arbitrary units. These functions are obtained from Eqs. (4.12)–(4.15). Here G_{12} is imaginary. Both components decrease exponentially with the distance $\xi-\xi_1$. For $\xi=\xi_1$ the component G_{11} has a peak and the value of this peak increases with the growth of ξ. When we approach the point $\phi=\xi+\phi_0=\pi/2$ the functions G_{11} and G_{12} tend to infinity.

We analyze the behavior of the expression (4.12) for $p_0\to 0$. In this limit Eq. (4.12) describes the nematic liquid crystal. If we set $p_0=0$, then $\phi(z)\equiv\phi_0$ and Eq. (4.12) takes the form

$$\begin{aligned}\hat{G}(\mathbf{q};z-z_1)=&\frac{k_BT\exp(-q\mu_1|z-z_1|)}{2qK_{33}\cos^2\phi_0}\begin{pmatrix} -\mu_1^{-1}\sin^2\phi_0 & i\,\mathrm{sign}(z-z_1)\sin\phi_0 \\ i\,\mathrm{sign}(z-z_1)\sin^2\phi_0 & \mu_1 \end{pmatrix}\\ &+\frac{k_BT\exp(-q\mu_2|z-z_1|)}{2qK_{33}\cos^2\phi_0}\begin{pmatrix} \mu_2 & -i\,\mathrm{sign}(z-z_1)\sin\phi_0 \\ -i\,\mathrm{sign}(z-z_1)\sin\phi_0 & -\mu_2^{-1}\sin^2\phi_0 \end{pmatrix}.\end{aligned} \tag{4.16}$$

Note, that there is an indeterminacy in Eq. (4.16) at $\phi_0\to\pi/2$, which can be easily removed. It results in the finite expression for $\phi_0=\pi/2$. Therefore the correlation function has no singularities in the vicinity of this point.

Performing Fourier transform over the $z-z_1$ variable in Eq. (4.16) and using Eq. (2.10) we obtain well-known De Gennes expression[4] for the correlation function of the director fluctuations in NLC,

$$g_{\alpha\beta}(\mathbf{k})=k_BT\sum_{l=1,2}\frac{e_{l\alpha}(\mathbf{k})e_{l\beta}(\mathbf{k})}{K_{33}(\mathbf{n}^0\cdot\mathbf{k})^2+K_{ll}(k^2-(\mathbf{n}^0\cdot\mathbf{k})^2)}, \tag{4.17}$$

where $\mathbf{k}=(\mathbf{q},q_z)$, $\mathbf{e}_l\perp\mathbf{n}^0$, $|\mathbf{e}_l|=1$, $\mathbf{e}_1\perp\mathbf{e}_2$, $\mathbf{e}_1\parallel\mathbf{k}-\mathbf{n}^0(\mathbf{n}^0\cdot\mathbf{k})$.

It is interesting to compare our result, Eq. (4.12) for the correlation function $\hat{G}(\mathbf{q};z_1,z_2)$, which is valid for $q\gg p_0$ (“nematiclike” CLC), to the results for the opposite case $q\ll p_0$ (“smec-

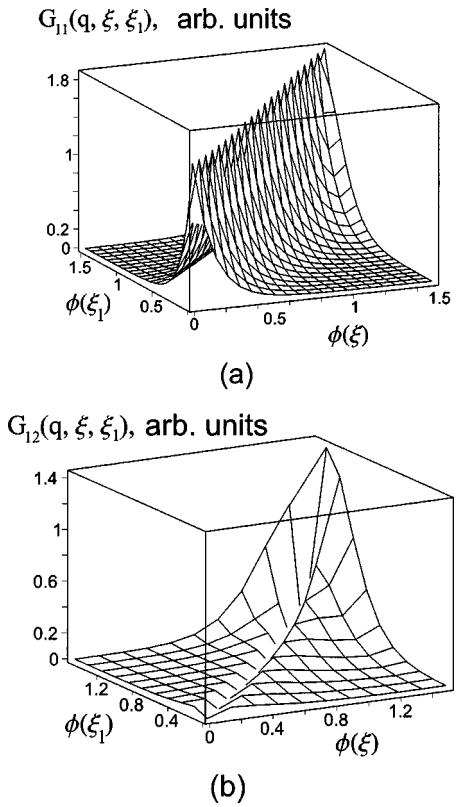

FIG. 1. The $G_{11}(\mathbf{q},\xi,\xi_1)$ (a) and $G_{12}(\mathbf{q},\xi,\xi_1)$ (b) components of the correlation function as a function of ξ and ξ_1 expressed in the same arbitrary units. Here $K_{11}=5.0\times10^{-6}$ dyne, $K_{22}=3.0\times10^{-6}$ dyne, $K_{33}=7.0\times10^{-6}$ dyne.

ticlike'' CLC).[11] For simplicity we consider the case, where all three elastic constants (the Frank modules) are equal $K_{11}=K_{22}=K_{33}=K$. We are interested in behavior of $\hat{G}(\mathbf{q};z_1,z_2)$ as a function of the wave vector module q and the z_1-z_2 variable.

According to Eq. (4.12) all components of the correlation function $\hat{G}$ for the case $q\gg p_0$ behave as

$$G_{kl}(\mathbf{q};z_1,z_2)\sim q^{-1}\exp(-q|z_1-z_2|). \tag{4.18}$$

On the other hand, three-dimensional Fourier-components of the correlation function in the case $q\ll p_0$ have the form[12]

$$\tilde{G}_{11}(\mathbf{q},q_z)=\frac{2p_0^2k_BT}{K(2p_0^2q_z^2+q^2q_z^2+q^4)},$$
$$\tilde{G}_{22}(\mathbf{q},q_z)=\frac{k_BT}{K(p_0^2+q^2+q_z^2)},\quad \tilde{G}_{12}=\tilde{G}_{21}=0. \tag{4.19}$$

Expressions (4.19) have been obtained by averaging over many pitches. Therefore the modes u_1 and u_2 here do not correlate (nondiagonal elements of the correlation function are equal to zero). It differs from our approach which takes into account almost local fluctuations. However if we average Eq. (4.12) over many pitches, the matrices $\hat{W}^{(1)}$ and $\hat{W}^{(2)}$ become diagonal and we obtain $G_{12}=G_{21}=0$ as well.

Note, in this limit the director fluctuations in the plane normal to the pitch axis ($\tilde{G}_{11}$) behaves as the layer-displacement fluctuations in smectic-A liquid crystals.[4] Fluctuations along the pitch axis ($\tilde{G}_{22}$) have the form similar to the director fluctuation in nematic, Eq. (4.17), but they are bounded by the cholesteric pitch [the term p_0^2 in the denominator of $\tilde{G}_{22}$ in Eq. (4.19)].

In $(\mathbf{q},z)$-representation Eq. (4.19) has the form

$$\tilde{G}_{11}(\mathbf{q};z_1-z_2)\propto\frac{2p_0^2}{q^2\sqrt{2p_0^2+q^2}}\exp\left(-\frac{q^2|z_1-z_2|}{\sqrt{2p_0^2+q^2}}\right),$$

$$\tilde{G}_{22}(\mathbf{q};z_1-z_2)\propto\frac{1}{\sqrt{p_0^2+q^2}}\exp(-\sqrt{p_0^2+q^2}|z_1-z_0|). \tag{4.20}$$

Let analyze the behavior of expressions (4.18) and (4.20) in the intermediate range $q\simeq p_0$. Although both formulas are not valid in this range we consider extrapolation,

$$G_{kk}(p_0;z_1,z_2)\sim\frac{1}{p_0}\exp(-p_0|z_1-z_2|),$$

$$\tilde{G}_{11}(p_0;z_1,z_2)\sim\frac{2}{\sqrt{3}p_0}\exp\left(-\frac{p_0}{\sqrt{3}}|z_1-z_2|\right), \tag{4.21}$$

$$\tilde{G}_{22}(p_0;z_1,z_2)\sim\frac{1}{\sqrt{2}p_0}\exp(-\sqrt{2}p_0|z_1-z_2|).$$

It can be seen the mode amplitudes are of the similar order, but the exponents are different. Thus, their asymptotic behaviors for the cases $q\gg p_0$ and $q\ll p_0$ do not match in the range $q\simeq p_0$.

An extrapolation of the expressions (4.20) into the range $q\gg p_0$ gives

$$\begin{aligned}\tilde{G}_{11}(\mathbf{q};z_1-z_2)&\sim p_0^2q^{-3}\exp(-q|z_1-z_2|),\\ \tilde{G}_{22}(\mathbf{q};z_1-z_2)&\sim q^{-1}\exp(-q|z_1-z_2|).\end{aligned} \tag{4.22}$$

It is curious that exponential factors in Eqs. (4.22) and (4.18) coincide. But the nonexponential factors for the u_1 mode corresponding to the fluctuations in the plane perpendicular to the pitch axis (G_{11} and $\tilde{G}_{11}$) are different. The first mode is more sensitive to the pitch and its behavior significantly differs for the cases $q\ll p_0$ and $q\gg p_0$. The factors for the u_2 mode corresponding to the fluctuations along the pitch axis (G_{22} and $\tilde{G}_{22}$) coincide. It is conceivable that expression for $\tilde{G}_{22}$ is applicable in a wider domain over the q variable (just as for $q\ll p_0$, so $q\simeq p_0$, $q\gg p_0$).

Equation (4.11) loses its sense if $\cos\phi=0$ in the point ξ or ξ_1 or if the point ξ_* with $\cos\phi(\xi_*)=0$ lies between ξ and ξ_1. It follows from the fact that eigenvalues of the $\hat{B}$ matrix at these conditions coincide. As it follows from Eq. (3.24) if the values μ_l and μ_m approach each other the function V_{lm} increases and the condition of the WKB applicability, $|V_{lm}|\ll\Omega$, could be violated.

According to Eq. (4.2) $\mu_1=\mu_2=1$, $\mu_3=\mu_4=-1$ at the point $\phi=\pi/2$, and so in the vicinity of $\phi=\pi/2$ the WKB method becomes invalid.

Let us now estimate the applicability region of the WKB method. For this purpose we introduce a new variable $\zeta=p_0z+\phi_0-\pi/2=\phi-\pi/2$ and expand μ_l in a series near the $\zeta=0$ point

$$\mu_l\approx1-C_l\zeta^2/2,\quad l=1,2,$$

$$\mu_3=-\mu_1,\quad \mu_4=-\mu_2,\quad C_l=1-K_{33}/K_{ll}. \tag{4.23}$$

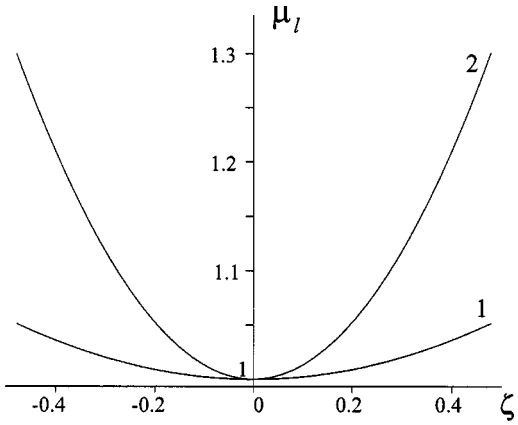

FIG. 2. The behavior of μ_1 (curve 1) and μ_2 (curve 2) in the vicinity of the $\zeta=0$ point. Here $K_{11}=2.0\times10^{-6}$ dyne, $K_{22}=0.8\times10^{-6}$ dyne, $K_{33}=2.9\times10^{-6}$ dyne.

Figure 2 shows schematically the behavior of the μ_1 and μ_2 values in the neighborhood of the turning point. Note that values $\mu_1(\xi)$ and $\mu_2(\xi)$ do not intersect but can only touch each other.

Matrix element V_{12} near the turning point, $\zeta=0$, can be estimated as

$$V_{12}\sim\zeta^{-3}(1+O(\zeta^2)).$$

Then the condition of the WKB method applicability has the form

$$\Omega|\zeta|^3\gg1. \tag{4.24}$$

It means that Eq. (4.11) is valid when $\Omega|\zeta|^3\gg1$, $\Omega|\zeta_1|^3\gg1$ and there are no points between points ζ and ζ_1 where μ_1 and μ_2 coincide.

The analysis of the correlation function behavior in the vicinity of the turning point represents a rather complicated mathematics problem. In what follows two cases will be considered:

(i) one or both variables ξ, ξ_1 are near the point $\cos\phi=0$;
(ii) ξ and ξ_1 are in the region where the WKB method is valid but between them there is the point with $\cos\phi=0$.

In both cases it is necessary to obtain the solution of Eq. (3.8) in a neighborhood of the degeneration point, $\cos\phi=0$.

V. VICINITY OF THE TURNING POINT AND CONNECTION FORMULAS FOR WKB SOLUTIONS

The problem of turning points and of matching WKB solutions has been investigated thoroughly. For scalar problems which have the form $Y''-\Gamma(X)Y=0$ one of the two following methods is usually applied. The first one is the complex plane method. The method solves the problem by contour integration in complex plane around a turning point. The method permits to match WKB solutions, but the contour of integration intersects the so-called Stokes lines where analytical extension of the WKB solutions is broken. The second and most common method is the method of model equations. In the vicinity of the turning point X_0, where $\Gamma(X_0)=0$, the function $\Gamma(X)$ is expanded over $X-X_0$. The resulting model equation depends on the $\Gamma(X)$ behavior in the vicinity of the turning point X_0. If the behavior is linear (simple turning point) we have the Airy equation and the solution is a linear combination of the Airy functions.[22] In the case $\Gamma(X)\sim(X-X_0)^m$, $m\geqslant2$ (multiple turning point of the mth order) the solution of the model equation can be expressed in terms of modified Bessel function of the second kind $K_{1/(m+2)}$. Then the solution of the model equation is used for matching WKB solutions to the left and to the right of the turning point.

Our problem has some distinctions from usual situation. First, the WKB solutions are exponentially increasing and exponentially decreasing. It involves additional difficulties for matching as it requires to consider exponentially small variable in the presence of exponentially large variable. Second, the difference of eigenvalues μ_1 and μ_2 is quadratic over $X-X_0$ in the vicinity of the turning point, which means that the turning point is of the fourth order. Third, our problem is a set of two differential equations of the second order. This multimode character is the main difficulty. For contour integration method there are six Stokes lines and we have problems with analytical extension of WKB solutions. For the second method the problem is that the model equation method gives equation of the fourth order in the vicinity of the turning point. Model equations of the fourth order and their solutions are investigated much less than the model equations of the second order.

In such a situation it is more convenient to analyze the set of four equations of the first order instead of the set of two equations of the second order. We have previously used this approach to construct the WKB solutions far from the turning point in Sec. IV [see Eq. (3.8)]. In this case peculiar character of the turning point is manifested in the nondiagonal normal form of the arising 4×4 matrix in this point, as in Eqs. (3.13) and (3.20). Instead it contains Jordan blocks. Next we expand the equations in the vicinity of the singular point and match the solutions of corresponding model equations to the WKB solutions. The 4×4 problem splits into several independent sets of the lower order separately for each Jordan block. Each of these sets produces a more simpler model equation. This approach for asymptotic solution of systems of linear differential equations was developed and applied in Refs. 23–25. As we shall see later in our problem we have two 2×2 Jordan blocks. Therefore we come to two model equations of the second order instead of the model equation of the fourth order.

It is more convenient to seek the solution for the $\mathbf{\Psi}$ vector, rather than for the matrix of evolution, $\hat{M}$. For this purpose we expand Eq. (3.8) in a series near the point $\zeta=0$,

$$\left[i\hat{B}(0)+\frac{i}{2}\hat{B}''(0)\zeta^2+\frac{i}{24}\hat{B}^{IV}(0)\zeta^4+\frac{1}{\Omega}\hat{C}'(0)\zeta+\cdots\right]\mathbf{\Psi}(\zeta)=\frac{1}{\Omega}\frac{\mathrm{d}\mathbf{\Psi}}{\mathrm{d}\zeta}. \tag{5.1}$$

The direct iterative solution of Eq. (5.1) is difficult due to existence of two small parameters, $1/\Omega$ and ζ. Therefore it is convenient to introduce a new ''stretched'' variable $\tau=\Omega^{1/3}\zeta$. We have

$$\left[i\hat{B}(0)+\frac{i}{2}\Omega^{-2/3}\tau^2\hat{B}''(0)+\Omega^{-4/3}\left(\frac{i}{24}\tau^4\hat{B}^{IV}(0)+\tau\hat{C}'(0)\right)+\cdots\right]\mathbf{\Psi}(\tau)=\Omega^{-2/3}\frac{\mathrm{d}\mathbf{\Psi}}{\mathrm{d}\tau}. \tag{5.2}$$

The terms of this equation represent series over the small parameter $\Omega^{-2/3}$, though τ is not a small parameter in contrast to ζ. Solution of this equation corresponding to μ_1 and μ_2 is sought in the form

$$\mathbf{\Psi}_1(\tau)=\exp(-\Omega^{2/3}\mu_1(0)\tau)(\mathbf{\Psi}_1^{(0)}(\tau)+\Omega^{-2/3}\mathbf{\Psi}_1^{(1)}(\tau)+\Omega^{-4/3}\mathbf{\Psi}_1^{(2)}(\tau)+\cdots), \tag{5.3}$$

where $\mu_1(0)=\mu_2(0)=1$. Substitution of $\mathbf{\Psi}_1(\tau)$ (5.3) into Eq. (5.2) reduces the latter in zero approximation to the equation for the eigenvector

$$\hat{B}(0)\mathbf{\Psi}_1^{(0)}=i\mu_1(0)\mathbf{\Psi}_1^{(0)}. \tag{5.4}$$

Solution of this equation has the form

$$\mathbf{\Psi}_1^{(0)}=\boldsymbol{\chi}_1\beta(\tau), \tag{5.5}$$

where $\boldsymbol{\chi}_1$ is the eigenvector,

$$\boldsymbol{\chi}_1=(1,-i,i,1)^T, \tag{5.6}$$

and $\beta(\tau)$ is an arbitrary function of τ. Here the superscript "T" denotes transposition.

In the first approximation we have

$$(\hat{B}(0)-i\mu_1(0)\hat{I})\mathbf{\Psi}_1^{(1)}=(-i\beta'(\tau)\hat{I}-\tfrac{1}{2}\tau^2\beta(\tau)\hat{B}''(0))\boldsymbol{\chi}_1\equiv\mathbf{R}^{(1)}, \tag{5.7}$$

where $\mathbf{R}^{(1)}$ is the four-component vector. The determinant of the equation set (5.7) is equal to zero, since $i\mu_1$ is the eigenvalue of the $\hat{B}$ matrix. The solvability condition for such systems implies that the right-hand side of Eq. (5.7) should be orthogonal to the adjoint vector $\boldsymbol{\chi}_2$, which determines by the condition

$$(\hat{B}(0)-i\mu_1(0)\hat{I})\boldsymbol{\chi}_2=\boldsymbol{\chi}_1. \tag{5.8}$$

As a solution of this equation it is possible to take

$$\boldsymbol{\chi}_2=\left(0,\frac{K_{11}+K_{22}}{K_{11}-K_{22}},1,\frac{2iK_{22}}{K_{11}-K_{22}}\right)^T. \tag{5.9}$$

Note, that at such choice of $\boldsymbol{\chi}_2$ the orthogonality condition, $\boldsymbol{\chi}_1\cdot\boldsymbol{\chi}_2=0$, is valid. It is easy to check that the solvability condition of the equation $\mathbf{R}^{(1)}\cdot\boldsymbol{\chi}_2=0$ is fulfilled automatically and is not reduce to any conditions for the $\beta(\tau)$ function. Therefore for determination of the $\beta(\tau)$ function it is necessary to take into account the solvability condition for the second approximation.

As a first step it is necessary to find the $\mathbf{\Psi}_1^{(1)}$ vector. We shall seek it as a linear combination of two eigenvectors, $\boldsymbol{\chi}_1$ and $\boldsymbol{\chi}_3$, and corresponding adjoint vectors, $\boldsymbol{\chi}_2$ and $\boldsymbol{\chi}_4$. Here $\boldsymbol{\chi}_3$ is the eigenvector corresponding to the eigenvalue $i\mu_3(0)$

$$\boldsymbol{\chi}_3=(-1,-i,i,-1)^T,\quad \boldsymbol{\chi}_4=\left(0,-\frac{K_{11}+K_{22}}{K_{11}-K_{22}},-1,\frac{2iK_{22}}{K_{11}-K_{22}}\right)^T. \tag{5.10}$$

Vectors $\boldsymbol{\chi}_l$, $l=1,...,4$ can be considered as a basis. If we expand $\mathbf{R}^{(1)}$ over this basis, $\mathbf{R}^{(1)}=\Sigma_{k=1}^{4}\mathrm{d}_k(\tau)\boldsymbol{\chi}_k$, the condition of solvability has the form $(\hat{P}^{-1}\mathbf{R}^{(1)})_2=\mathrm{d}_2(\tau)=0$, where

$$\hat{P}=(\boldsymbol{\chi}_1,\boldsymbol{\chi}_2,\boldsymbol{\chi}_3,\boldsymbol{\chi}_4). \tag{5.11}$$

We seek $\mathbf{\Psi}_1^{(1)}$ as a linear combination of vectors $\boldsymbol{\chi}_l$, $l=1,...,4$

$$\mathbf{\Psi}_1^{(1)}=\sum_{k=1}^{4}a_k(\tau)\boldsymbol{\chi}_k. \tag{5.12}$$

It is possible to assume that $a_1=0$ since $\mathbf{\Psi}_1^{(0)}$ already contains the $\boldsymbol{\chi}_1$ vector and the coefficient a_1 is related to the normalization condition of the $\mathbf{\Psi}_1$ vector, which can be selected arbitrarily.

If we substitute $\mathbf{\Psi}_1^{(1)}$ in the form (5.12) to the first approximation (5.7) and multiply the right- and left-hand sides of the obtained equation by $\hat{P}^{-1}$ we obtain a system of four equations connecting three factors a_2, a_3, and a_4. The second of the obtained equations is the solvability condition of the first approximation. Since this equation represents an identity, we consider

$$a_2=-i\beta'+i\beta\tau^2A_2,\quad -2ia_3+a_4=i\beta\tau^2A_2,\quad -ia_4=\beta\tau^2A_3, \tag{5.13}$$

where

$$A_2=A_1\frac{K_{11}+K_{22}}{K_{22}},\quad A_3=A_1\frac{K_{11}-K_{22}}{K_{22}},\quad A_1=\frac{K_{11}+K_{22}-2K_{33}}{8K_{11}}. \tag{5.14}$$

Solutions of these equations are

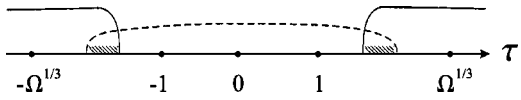

FIG. 3. Regions where the WKB solution and the solution near the turning point are applicable for the τ variable. The solid line shows the regions where the WKB solution is valid. The dotted line shows the vicinity of the turning point. As it can be seen at $1 \ll |\tau| \ll \Omega^{1/3}$ both solutions are applicable (shaded regions).

$$a_2 = -i\beta' + i\beta\tau^2 A_2, \quad a_3 = -\beta\tau^2 A_1, \quad a_4 = i\beta\tau^2 A_3. \tag{5.15}$$

The equation for the second approximation has the form

$$(\hat{B}(0) - i\mu_1(0)\hat{I})\boldsymbol{\Psi}_1^{(2)} = -i\boldsymbol{\Psi}_1^{(1)\prime} - \tfrac{1}{2}\tau^2\hat{B}''(0)\boldsymbol{\Psi}_1^{(1)} + (i\tau\hat{C}'(0) - \tfrac{1}{24}\tau^4\hat{B}^{IV}(0))\boldsymbol{\Psi}_1^{(0)} = \mathbf{R}^{(2)}. \tag{5.16}$$

The solvability condition for the second approximation has the same form as that for the first approximation, $(\hat{P}^{-1}\mathbf{R}^{(2)})_2 = 0$. Substituting to this condition the expressions for $\boldsymbol{\Psi}_1^{(0)}$ and $\boldsymbol{\Psi}_1^{(1)}$, we obtain

$$-ia_2' - \frac{1}{2}\tau^2\left(\hat{P}^{-1}\hat{B}''(0)\sum_{k=2}^{4} a_k\boldsymbol{\chi}_k\right)_2 + \beta(\tau)\left[\hat{P}^{-1}\left(i\tau\hat{C}'(0) - \frac{1}{24}\tau^4\hat{B}^{IV}(0)\right)\boldsymbol{\chi}_1\right]_2 = 0. \tag{5.17}$$

Let us calculate the coefficients of this equation and substitute the expressions (5.15) for the a_k coefficients into (5.17). Then we have

$$\beta''(\tau) - \beta'(\tau)\tau^2\tfrac{1}{2}(C_1 + C_2) - \beta(\tau)\tau\tfrac{1}{2}(C_1 + C_2 - \tfrac{1}{2}C_1C_2\tau^3) = 0. \tag{5.18}$$

In usual cases inequalities $K_{22} < K_{11} < K_{33}$ take place, hence it follows according to Eq. (4.23) $C_1 < 0$, $C_2 < 0$, and $C_1 > C_2$. These conditions do not impose any restrictions on the generality of the obtained results. Then solution of Eq. (5.18) can be written in the form

$$\beta(\tau) = \sqrt{\tau}\exp(C_3\tau^3)[F_1K_{1/6}(C_4\tau^3 e^{-3\pi i}) + F_2K_{1/6}(C_4\tau^3)], \tag{5.19}$$

where $F_{1,2}$ are constants, $K_{1/6}(a)$ is the modified Bessel function of the second kind,

$$C_3 = (C_1 + C_2)/12, \quad C_4 = (C_1 - C_2)/12. \tag{5.20}$$

It is possible to present the solution of Eq. (5.18) as a linear combination of other Bessel functions. The choice $K_{1/6}(a)$ hereinafter will be convenient for matching the solutions inside and outside the turning point vicinity.

Note, that in the vicinity of the zero the solution (5.19) has no singularities such as a pole. Thus, in the zero approximation the solution $\boldsymbol{\Psi}_1(\tau)$ has the form

$$\boldsymbol{\Psi}_1(\tau) = \sqrt{\tau}\exp(-\Omega^{2/3}\tau + C_3\tau^3)[F_1K_{1/6}(C_4\tau^3 e^{-3\pi i}) + F_2K_{1/6}(C_4\tau^3)]\boldsymbol{\chi}_1. \tag{5.21}$$

Since the WKB approximation is valid for $|\zeta|\Omega^{1/3} \gg 1$, in the region $\Omega^{-1/3} \ll |\zeta| \ll 1$ (or $1 \ll |\tau| \ll \Omega^{1/3}$) both the WKB approximation and the solution near the turning point are valid (Fig. 3). Equating these solutions we can get the relation between constants entering these solutions.

Primarily we consider the WKB solution in the regions $1 \ll |\tau| \ll \Omega^{1/3}$. From the solution (3.10), where $\hat{M}(\xi, \xi_0)$ is described by Eq. (4.8), we select two solutions corresponding to μ_1 and μ_2. For this purpose we put third and fourth components of the $\hat{U}^{-1}(\xi_0)\boldsymbol{\Psi}(\xi_0)$ vector equal to zero and expand all functions depending on ξ in series in the vicinity of the point $\phi = \pi/2$ ($\tau = 0$). As a result the solution in the considered region has the form

$$\mathbf{\Psi}(\tau)=B_1\mathbf{\Phi}_1(\tau)+B_2\mathbf{\Phi}_2(\tau), \tag{5.22}$$

where

$$\mathbf{\Phi}_1(\tau)=\Phi_{01}(\tau)\left(-i\left(1+\frac{C_1-1}{2\Omega^{2/3}}\tau^2\right),-1,1-\frac{\tau^2}{2\Omega^{2/3}},-i\left(1-\frac{C_1\tau^2}{2\Omega^{2/3}}\right)\right)^T,$$

$$\mathbf{\Phi}_2(\tau)=\Phi_{02}(\tau)\left(1,-i\left(1+\frac{C_2-1}{2\Omega^{2/3}}\tau^2\right),i\left(1-\frac{C_2\tau^2}{2\Omega^{2/3}}\right),1-\frac{\tau^2}{2\Omega^{2/3}}\right)^T, \tag{5.23}$$

$$\Phi_{0j}(\tau)=\frac{\sqrt{i}\Omega^{1/3}}{|\tau|}\left(1-\frac{C_j\tau^2}{4\Omega^{2/3}}\right)\exp\left(-\Omega^{2/3}\tau+\frac{1}{6}C_j\tau^3\right),\quad j=1,2.$$

Note, that constant factors B_1 and B_2 can differ in regions $\tau>0$ and $\tau<0$ since the regions of the WKB method applicability, $|\tau|\gg 1$, do not intersect. In what follows we shall denote the coefficients B_1 and B_2 at $\tau>0$ and $\tau<0$ as $B_l^{(+)}$ and $B_l^{(-)}$, respectively, $l=1, 2$.

Now we consider the solution (5.21), which is valid near the turning point, at $|\tau|\gg 1$. For this purpose we get its asymptotic behavior at $\tau\to\pm\infty$ in the zero approximation. Actually the problem consists in searching of the Bessel function $K_{1/6}(a)$ asymptotics. At $a\to\infty$ its asymptotics has the form[20]

$$K_{1/6}(a)\sim\sqrt{\pi/(2a)}\exp(-a). \tag{5.24}$$

This formula is valid for $|\arg a|<3\pi/2$. This condition is fulfilled for the second term in (5.21) at $\tau\to+\infty$. The same asymptotics can be used for the first term, but for $\tau\to-\infty$, as in this case $\tau=|\tau|e^{i\pi}$, and argument of the total expression appears to be equal to zero. Thus we have

$$K_{1/6}(C_4\tau^3e^{-3\pi i})\underset{\tau\to-\infty}{\sim}C_5|\tau|^{-3/2}\exp(-C_4|\tau|^3),$$

$$K_{1/6}(C_4\tau^3)\underset{\tau\to+\infty}{\sim}C_5\tau^{-3/2}\exp(-C_4\tau^3), \tag{5.25}$$

where

$$C_5=\sqrt{\pi/(2C_4)}. \tag{5.26}$$

For deriving the rest two asymptotic behaviors, $K_{1/6}(C_4\tau^3e^{-3\pi i})$ at $\tau\to+\infty$ and $K_{1/6}(C_4\tau^3)$ at $\tau\to-\infty$, we use the relation[20]

$$K_\nu(ae^{im\pi})=e^{-im\pi\nu}K_\nu(a)-i\pi\frac{\sin(m\pi\nu)}{\sin(\pi\nu)}I_\nu(a), \tag{5.27}$$

where m is integer, $I_\nu(a)$ is the modified Bessel function of the first kind, which has an asymptotics $I_\nu(a)\underset{a\to+\infty}{\sim}\exp(a)/\sqrt{2\pi a}$. Supposing $m=-3$ and $m=3$, we get the asymptotic behavior of the first and the second term, respectively. Thus we have

$$K_{1/6}(C_4\tau^3e^{-3\pi i})\underset{\tau\to+\infty}{\sim}2iC_5\tau^{-3/2}\exp(C_4\tau^3),$$

$$K_{1/6}(C_4\tau^3)\underset{\tau\to-\infty}{\sim}-2iC_5|\tau|^{-3/2}\exp(C_4|\tau|^3). \tag{5.28}$$

Substituting asymptotics (5.25) and (5.28) in the expression (5.21) for $\mathbf{\Psi}_1(\tau)$ we get

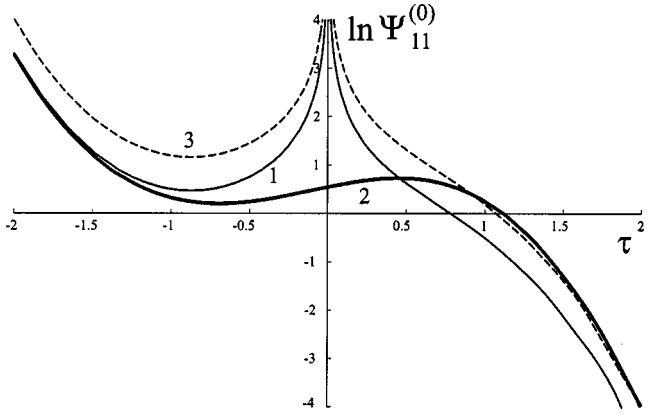

FIG. 4. The first component of the vector $\Psi_1^{(0)}(\tau)$ (curve 2) in the vicinity of the turning point. This curve is obtained by the numerical solution of Eq. (5.2) for $K_{11}=10^{-6}$ dyne, $K_{22}=0.5\times10^{-6}$ dyne, $K_{33}=4.0\times10^{-6}$ dyne. Curves 1 and 3 are the WKB solution and doubled WKB solution, respectively.

$$\mathbf{\Psi}_1(\tau)=C_5|\tau|^{-1}\exp(-\Omega^{2/3}\tau)(1,-i,i,1)^T\times\begin{cases}2iF_1\exp(C_1\tau^3/6)+F_2\exp(C_2\tau^3/6) & \text{at } \tau\to+\infty,\\ iF_1\exp(C_1\tau^3/6)+2F_2\exp(C_2\tau^3/6) & \text{at } \tau\to-\infty.\end{cases} \tag{5.29}$$

Matching solutions (5.29) with the WKB solutions (5.22), (5.23), we obtain two systems of two equations, connecting the factors $B_l^{(\pm)}$, $l=1,2$ with the factors F_1 and F_2

$$-\Omega^{1/3}i^{1/2}B_1^{(+)}=2F_1C_5,\quad -\Omega^{1/3}i^{1/2}B_1^{(-)}=F_1C_5,$$

$$\Omega^{1/3}i^{1/2}B_2^{(+)}=F_2C_5,\quad \Omega^{1/3}i^{1/2}B_2^{(-)}=2F_2C_5. \tag{5.30}$$

Equation (5.30) gives the relation between factors $B_l^{(\pm)}$, $l=1,2$ (connection formulas),

$$B_1^{(+)}=2B_1^{(-)},\quad B_2^{(+)}=B_2^{(-)}/2. \tag{5.31}$$

So, passing by the turning point the mode amplitudes vary. Thus the modes interact, but any of these modes does not produced another.

Figure 4 illustrates the solution of Eq. (5.2). The dependence of the first component $\Psi_{11}^{(0)}$ of the vector $\Psi_1^{(0)}(\tau)$ is presented in the vicinity of the turning point. This dependence corresponds to behavior of the correlation function $G_{11}(\tau,\tau_1)$ for fixed $\tau_1<\tau$. The curve 1 presents the WKB solution diverging at the turning point $\tau=0$. Curve 2 was obtained by numerical solution of Eq. (5.2). Curve 3 illustrates formula (5.31) connecting solution amplitudes before and after the turning point. This curve was obtained by doubling the WKB solution. One can see that to the left of the turning point the numerical solution coincides with the WKB solution and to the right of this point—with the doubled WKB solution.

Note, that the modes do not interact in the zero approximation over the $\Omega^{-2/3}$ parameter. If we take into account the terms of the next order we can get the contributions determined by the mode interaction.

Similarly it is possible to obtain the solution $\mathbf{\Psi}_3(\tau)$ corresponding to μ_3 and μ_4 near the turning point

$$\mathbf{\Psi}_3(\tau)=\sqrt{\tau}\exp(\Omega^{2/3}\tau-C_3\tau^3)[F_3K_{1/6}(C_4\tau^3e^{-3\pi i})+F_4K_{1/6}(C_4\tau^3)](-1,-i,i,-1)^T. \tag{5.32}$$

We select two WKB solutions, corresponding to μ_3 and μ_4 for deriving the connection formulas similar to Eq. (5.31). For this purpose it is enough to set $\hat{U}^{-1}(\xi_0)\Psi(\xi_0)=(0,0,B_3,B_4)^T$. Acting similarly in the case of values μ_1 and μ_2 we obtain the connection formulas

$$B_3^{(+)}=B_3^{(-)}/2, \quad B_4^{(+)}=2B_4^{(-)}. \tag{5.33}$$

In the Appendix we demonstrate that the multiplicative conditions $B_3^{(+)}B_4^{(+)}=B_3^{(-)}B_4^{(-)}$, $B_1^{(+)}B_2^{(+)}=B_1^{(-)}B_2^{(-)}$ are corollaries from conservation law for relaxation system.

Note, that we considered the case $\phi=\pi/2$ only. Actually the developed approach allows to describe all turning points $\phi=\pi/2+2\pi m$, where m is integer. The turning points $\phi=-\pi/2+2\pi m$ should be considered separately. The reason is that the expansion of the $\hat{B}$ matrix in the vicinity of these turning points has another form. But it may be shown that the relation between amplitudes conserves. It is natural since the points $\phi(z)=\pi/2$ and $\phi(z)=-\pi/2$ refer to opposite directions of the director, $\mathbf{n}^0$ and $-\mathbf{n}^0$, which are equivalent for CLC.

VI. CORRELATION FUNCTION NEAR THE TURNING POINTS

First we consider the case, when both points ξ and ξ_1 lie in the regions, where the WKB method is valid, but between them there is one turning point $\xi_*=\pi/2-\phi_0$. Let us consider for definiteness $\xi>\xi_*$, and $\xi_1<\xi_*$, i.e., $\xi>\xi_1$. In this case expression for the Green's function (3.6) still holds. Since Eq. (3.6) contains the $\hat{u}_1$ matrix in both points ξ and ξ_1, it is necessary to take the expression for this matrix which is valid on each side of the turning point, i.e., it is necessary to take into account connection formulas, Eqs. (5.31).

These formulas mean, that on passing through the turning point the amplitudes of the solutions corresponding to μ_1 and μ_2 increase and decrease twice, respectively. Therefore the $\hat{u}_1$ matrix for $|\xi-\xi_*|\gg\Omega^{-1/3}$ can be written in the form

$$\hat{u}_1(\xi)=\begin{cases}\hat{\tilde{u}}_1(\xi) & \text{at } \xi<\xi_*,\\ \hat{\tilde{u}}_1(\xi)\hat{s} & \text{at } \xi>\xi_*,\end{cases} \tag{6.1}$$

where $\hat{\tilde{u}}_1(\xi)$ is described by Eq. (4.9) and the matrix

$$\hat{s}=\begin{pmatrix}2 & 0\\ 0 & 1/2\end{pmatrix}$$

describes the transformation of amplitudes on passing through the turning point. Then Eq. (3.6) is written as

$$\hat{G}(\xi,\xi_1)=k_BTp_0^{-1}\hat{\tilde{u}}_1(\xi)\hat{s}\hat{\tilde{u}}^{-1}(\xi_1)(\hat{u}_2'\hat{u}_2^{-1}-\hat{\tilde{u}}_1'\hat{\tilde{u}}_1^{-1})^{-1}(\xi_1)\hat{K}^{-1}. \tag{6.2}$$

This expression differs from Eq. (4.11) by an insertion of the diagonal matrix $\hat{s}$

$$\hat{G}(\xi,\xi_1)=\frac{k_BT}{2qK_{33}\cos\phi(\xi_1)\cos\phi(\xi)}\begin{pmatrix}\sin\phi(\xi) & i\mu_2(\xi)\\ -i\mu_1(\xi) & \sin\phi(\xi)\end{pmatrix}$$
$$\times\begin{pmatrix}\dfrac{2\exp\left(-\Omega\int_{\xi_1}^{\xi}\mu_1\,d\xi'\right)}{\sqrt{\mu_1(\xi)\mu_1(\xi_1)}} & 0\\ 0 & \dfrac{\exp\left(-\Omega\int_{\xi_1}^{\xi}\mu_2\,d\xi'\right)}{2\sqrt{\mu_2(\xi)\mu_2(\xi_1)}}\end{pmatrix}\begin{pmatrix}-\sin\phi(\xi_1) & i\mu_1(\xi_1)\\ -i\mu_2(\xi_1) & -\sin\phi(\xi_1)\end{pmatrix}. \tag{6.3}$$

The case $\xi<\xi_1$ can be considered in a similar way. The new matrix $\hat{u}_2(\xi)$ is constructed with the aid of connection formulas (5.33). However there is a simpler way to obtain $\hat{G}(\xi,\xi_1)$ for $\xi<\xi_1$. It is enough to apply the symmetry property Eq. (2.18),

$$\hat{G}(\xi,\xi_1)=\hat{G}^{*T}(\xi_1,\xi).$$

If there are several turning points between ξ and ξ_1 the Green's function will contain a set of $\hat{s}$ matrices with the number in this set being equal to the number of the turning points.

Now we consider the case, when the point ξ lies in the vicinity of the turning point ξ_* and the point ξ_1 is situated far from this turning point, i.e., in the region, where the WKB method is valid. For definiteness we consider again $\xi>\xi_1$. In order to find the Green's function, it is necessary to expand the expression (4.9) for the $\hat{u}_1(\xi)$ matrix in the vicinity of the turning point. It can be made, using solution (5.21) for the $\mathbf{\Psi}_1$ function and the second set of equations in (5.30). This set describes the relation between constants which enter to the WKB solution and to the solution near the turning point. From Eq. (5.21) for the $\hat{u}_1$ matrix in the vicinity of the turning point we get

$$\hat{u}_1(\tau)=\sqrt{\tau}\exp(-\Omega^{2/3}\tau+C_3\tau^3)\begin{pmatrix} K_{1/6}(C_4\tau^3e^{-3\pi i}) & K_{1/6}(C_4\tau^3) \\ -iK_{1/6}(C_4\tau^3e^{-3\pi i}) & -iK_{1/6}(C_4\tau^3)\end{pmatrix}\begin{pmatrix} F_1 & 0 \\ 0 & F_2\end{pmatrix}. \quad (6.4)$$

It is necessary to choose F_1 and F_2, so that Eq. (6.4) is consistent with the expression (4.9) for the $\hat{u}_1$ matrix. For this purpose we choose $B_1^{(-)}$ and $B_2^{(-)}$ as

$$B_l^{(-)}=\frac{|\cos(\xi_0+\phi_0)|}{\sqrt{i\mu_l(\xi_0)}}\exp\left(-\Omega\int_{\xi_0}^{\xi_*}\mu_l\,d\xi'\right), \quad l=1,2. \quad (6.5)$$

This choice on the one hand reduces to Eq. (4.9) for the $\hat{u}_1(\xi)$ matrix and on the other hand it is consistent with the solution (5.23) in the regions $1\ll|\tau|\ll\Omega^{1/3}$. From Eqs. (6.5) and (5.30) we obtain F_1 and F_2 in the form

$$F_l=\frac{(-1)^l}{l}\Omega^{1/3}\frac{|\cos(\xi_0+\phi_0)|}{C_5\sqrt{\mu_l(\xi_0)}}\exp\left(-\Omega\int_{\xi_0}^{\xi_*}\mu_l\,d\xi'\right), \quad l=1,2. \quad (6.6)$$

Substituting expression (6.4) for $\hat{u}_1(\xi)$ and expressions (4.9) for $\hat{u}_1(\xi_1)$, $\hat{u}_2(\xi_1)$ into Eq. (3.6) we obtain the correlation function in the form

$$\begin{aligned}\hat{G}(\xi,\xi_1)=&\frac{ik_BT\Omega^{1/6}}{2C_5qK_{33}\cos\phi(\xi_1)\sqrt{\xi-\xi_*}}\exp\{-\Omega[\xi-\xi_*-C_3(\xi-\xi_*)^3]\}\\ &\times\begin{pmatrix} -K_{1/6}(C_4\Omega(\xi-\xi_*)^3e^{-3\pi i}) & 0 \\ 0 & \frac{1}{2}K_{1/6}(C_4\Omega(\xi-\xi_*)^3)\end{pmatrix}\\ &\times\begin{pmatrix} \dfrac{\exp\left(-\Omega\int_{\xi_1}^{\xi_*}\mu_1\,d\xi'\right)}{\sqrt{\mu_1(\xi_1)}} & 0 \\ 0 & \dfrac{\exp\left(-\Omega\int_{\xi_1}^{\xi_*}\mu_2\,d\xi'\right)}{\sqrt{\mu_2(\xi_1)}}\end{pmatrix}\begin{pmatrix} -\sin\phi(\xi_1) & i\mu_1(\xi_1) \\ -i\mu_2(\xi_1) & -\sin\phi(\xi_1)\end{pmatrix}.\end{aligned} \quad (6.7)$$

Finally we consider the case when both points ξ and ξ_1 are in the vicinity of the turning point. On the one hand, this case is more complicate since for calculation of $\hat{u}_1$ and $\hat{u}_2$ matrices it is necessary to take into account the terms of the higher orders, otherwise these matrices are degenerate. On the other hand, this case is more simple as soon as there is no need to match the WKB solutions and solutions in the vicinity of the turning point.

Let us construct the $\hat{u}_1$ matrix in the vicinity of the turning point taking into account the correction $\mathbf{\Psi}_1^{(1)}$ (the $\hat{u}_2$ matrix can be constructed similarly). Note, that two first components of the $\mathbf{\Psi}_1$ vector are used for the $\hat{u}_1$ construction. We denote $\mathbf{w}_1=((\Psi_1)_1,(\Psi_1)_2)$. Using expressions (5.15) and (5.19), we get

$$\mathbf{w}_1(\tau)=\beta(\tau)\begin{pmatrix}1\\-i\end{pmatrix}+\Omega^{-2/3}\begin{pmatrix}A_1\beta(\tau)\tau^2\\ i[A_5\beta(\tau)\tau^2-A_4\beta'(\tau)]\end{pmatrix}, \tag{6.8}$$

where A_1 was defined in Eq. (5.14) and

$$A_4=(K_{11}+K_{22})/(K_{11}-K_{22}),\quad A_5=A_1(3K_{11}+K_{22})/(K_{11}-K_{22}). \tag{6.9}$$

The function $\beta(\tau)$ in Eq. (5.19) contains two arbitrary constants F_1 and F_2. Let

$$\hat{u}_1(\tau)=(\mathbf{w}_1(\tau;F_1=1,F_2=0),\mathbf{w}_1(\tau;F_1=0,F_2=1)). \tag{6.10}$$

Such choice of the constants F_1 and F_2 gives the linear independence of the columns of the $\hat{u}_1(\tau)$ matrix. The components of the $\hat{u}_1(\tau)$ matrix have the form

$$\begin{aligned}
(\hat{u}_1)_{11}(\tau)&=\Theta^{(+)}(\tau)K_{1/6}(C_4\tau^3e^{-3\pi i})(1+\Omega^{-2/3}\tau^2A_1),\\
(\hat{u}_1)_{12}(\tau)&=-i\Theta^{(+)}(\tau)K_{1/6}(C_4\tau^3e^{-3\pi i})\\
&\quad\times\{1+\Omega^{-2/3}A_4\ln[\sqrt{\tau}\exp(C_3\tau^3)K_{1/6}(C_4\tau^3e^{-3\pi i})]'_\tau-\Omega^{-2/3}\tau^2A_5\},\\
(\hat{u}_1)_{21}(\tau)&=\Theta^{(+)}(\tau)K_{1/6}(\tau)K_{1/6}(C_4\tau^3)(1+\Omega^{-2/3}\tau^2A_1),\\
(\hat{u}_1)_{22}(\tau)&=-i\Theta^{(+)}(\tau)K_{1/6}(C_4\tau^3)\\
&\quad\times\{1+\Omega^{-2/3}A_4\ln[\sqrt{\tau}\exp(C_3\tau^3)K_{1/6}(C_4\tau^3)]'_\tau-\Omega^{-2/3}\tau^2A_5\},
\end{aligned} \tag{6.11}$$

where

$$\Theta^{(+)}(\tau)=\exp(-\Omega^{2/3}\tau)\sqrt{\tau}\exp(C_3\tau^3). \tag{6.12}$$

For calculation of the $\hat{u}_2(\tau)$ matrix it is necessary to construct the corrections of the next order for obtaining $\mathbf{\Psi}_3(\tau)$, Eq. (5.32). This procedure is similar to procedure fulfilled for $\mathbf{\Psi}_1(\tau)$. Therefore we present the result for $\hat{u}_2(\tau)$ only

$$\begin{aligned}
(\hat{u}_2)_{11}(\tau)&=-\Theta^{(-)}(\tau)K_{1/6}(C_4\tau^3e^{-3\pi i})(1+\Omega^{-2/3}\tau^2A_1),\\
(\hat{u}_2)_{12}(\tau)&=-i\Theta^{(-)}(\tau)K_{1/6}(C_4\tau^3e^{-3\pi i})\\
&\quad\times\{1-\Omega^{-2/3}A_4\ln[\sqrt{\tau}\exp(-C_3\tau^3)K_{1/6}(C_4\tau^3e^{-3\pi i})]'_\tau-\Omega^{-2/3}\tau^2A_5\},\\
(\hat{u}_2)_{21}(\tau)&=-\Theta^{(-)}(\tau)K_{1/6}(C_4\tau^3)(1+\Omega^{-2/3}\tau^2A_1),\\
(\hat{u}_2)_{22}(\tau)&=-i\Theta^{(-)}(\tau)K_{1/6}(C_4\tau^3)\\
&\quad\times\{1-\Omega^{-2/3}A_4\ln[\sqrt{\tau}\exp(-C_3\tau^3)K_{1/6}(C_4\tau^3)]'_\tau-\Omega^{-2/3}\tau^2A_5\},
\end{aligned} \tag{6.13}$$

where

$$\Theta^{(-)}(\tau)=\exp(\Omega^{2/3}\tau)\sqrt{\tau}\exp(-C_3\tau^3). \tag{6.14}$$

For calculation of the correlation function $\hat{G}(\xi,\xi_1)$ we can now use the expression (3.6) for $\xi > \xi_1$.

VII. CONCLUSIONS

In the present paper we developed the scheme for calculation of the thermal fluctuations in the system with smooth inhomogeneities. We take into account the nonlocal fluctuations in the explicit form. The WKB approximation was applied for the first time to calculate the spatial correlation functions in systems with smooth inhomogeneities. We consider the system with one-dimensional periodicity. As an illustration the director fluctuations in cholesteric liquid crystal were considered.

We construct the correlation function of the director fluctuations in $(\mathbf{q},z)$-representation. Now we will illustrate the application of this function for solving the problem of light scattering in CLC. The light is scattered by the fluctuations of the permittivity tensor $\delta\hat{\varepsilon}(\mathbf{r})$. These fluctuations are connected with the director fluctuations $\delta\mathbf{n}$ by the formula[4]

$$\delta\varepsilon_{\alpha\beta}(\mathbf{r})=\varepsilon_a[n^0_\beta(z)\,\delta n_\alpha(\mathbf{r})+n^0_\alpha(z)\,\delta n_\beta(\mathbf{r})], \tag{7.1}$$

where ε_a is the difference between permittivities along and across equilibrium director. From Eq. (7.1) we obtain the connection for the correlation function of the permittivity fluctuations $\hat{\mathcal{G}}(\mathbf{r}_{1\perp}-\mathbf{r}_{2\perp};z_1,z_2)=\langle\delta\hat{\varepsilon}(\mathbf{r}_1)\delta\hat{\varepsilon}^*(\mathbf{r}_2)\rangle$ and the correlation function of the director fluctuations $\hat{g}(\mathbf{r}_{1\perp}-\mathbf{r}_{2\perp};z_1,z_2)$, Eq. (2.9),

$$\begin{aligned}\mathcal{G}_{\alpha\beta\gamma\delta}(\mathbf{r}_\perp;z,z_1)=\varepsilon_a^2[&n^0_\alpha(z)n^0_\gamma(z_1)g_{\beta\delta}(\mathbf{r}_\perp;z,z_1)+n^0_\alpha(z)n^0_\delta(z_1)g_{\beta\gamma}(\mathbf{r}_1;z,z_1)\\&+n^0_\beta(z)n^0_\gamma(z_1)g_{\alpha\delta}(\mathbf{r}_\perp;z,z_1)+n^0_\beta(z)n^0_\delta(z_1)g_{\alpha\gamma}(\mathbf{r}_\perp;z,z_1)].\end{aligned} \tag{7.2}$$

Using Eq. (7.2) and Eq. (2.10) it is not difficult to express $\hat{\mathcal{G}}$ via obtained correlation matrix $\hat{G}(\mathbf{r}_{1\perp}-\mathbf{r}_{2\perp};z_1,z_2)$, Eq. (2.7).

For solving the problem of light scattering in addition to the correlation function of the permittivity fluctuations normal light waves in the medium $\mathbf{E}(\mathbf{r})$ and the field of a point source (the Green's function of the wave equation) $\hat{T}(\mathbf{r},\mathbf{r}_1)$ are required. These problems are considered in Refs. 26–29. In these studies the vector WKB method corresponding to approximation of geometrical optics in anisotropic inhomogeneous medium is applied for electromagnetic field. According to Refs. 26–29 the presence of large-scale inhomogeneities results in the amplitude and the phase of the field adiabatically following to the local medium characteristics. Moreover the Green's function as well as the fluctuation correlation function depends not only on the difference of spatial coordinates but on their absolute values.

Below we shall describe the general procedure for calculation of the single light scattering intensity in the medium with one-dimensional inhomogeneities which characteristic scale d is much larger than the wavelength of light λ, $d \gg \lambda$. In such medium the single light scattering intensity in the $\mathbf{r}$ point is given by

$$I^{(s)}_{(i)}\propto\int_{V_{sc}}\hat{T}(\mathbf{r},\mathbf{r}_1)\hat{T}^*(\mathbf{r},\mathbf{r}_2)\langle\delta\hat{\varepsilon}(\mathbf{r}_1)\,\delta\hat{\varepsilon}^*(\mathbf{r}_2)\rangle\mathbf{E}^{(i)}(\mathbf{r}_1)\mathbf{E}^{(i)*}(\mathbf{r}_2)\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2, \tag{7.3}$$

where V_{sc} is a scattering volume.

We use the approximation of geometrical optics for incident and scattered fields. Let introduce local (depending on z) wave vectors of incident $\mathbf{k}^{(i)}(z)=(\mathbf{k}^{(i)}_\perp,k^{(i)}_z(z))$ and scattered $\mathbf{k}^{(s)}(z)=(\mathbf{k}^{(s)}_\perp,k^{(s)}_z(z))$ light. The corresponding polarization vectors are $\mathbf{e}^{(i)}(\mathbf{k}^{(i)}_\perp,z)$ and $\mathbf{e}^{(s)}(\mathbf{k}^{(s)}_\perp,z)$. Here the components of the wave vectors transversal to the z axis $\mathbf{k}^{(i,s)}_\perp$ are constants since our system is uniform in planes normal to the z axis. Then for the incident field we obtain

$$\mathbf{E}^{(i)}(\mathbf{r})=E^{(i)}(\mathbf{k}_\perp^{(i)},z)\mathbf{e}^{(i)}(\mathbf{k}_\perp^{(i)},z)\exp\left[i\left(\mathbf{k}_\perp^{(i)}\cdot\mathbf{r}_\perp+\int_{z_0}^{z}k_z^{(i)}(z')\mathrm{d}z'\right)\right], \tag{7.4}$$

where $E^{(i)}$ is the amplitude of the incident wave. For the propagator of the scattered field in the far zone $r\gg r_1$ we get

$$T_{\alpha\beta}(\mathbf{r},\mathbf{r}_1)=\sum_{s=1,2}t^{(s)}(\mathbf{r};z_1,\mathbf{k}_\perp^{(s)})e_\alpha^{(s)}(\mathbf{k}_\perp^{(s)},z)e_\beta^{(s)}(\mathbf{k}_\perp^{(s)},z_1)\exp\left[-i\left(\mathbf{k}_\perp^{(s)}\cdot\mathbf{r}_{1\perp}+i\int_0^{z_1}k_z^{(s)}(z')\mathrm{d}z'\right)\right]. \tag{7.5}$$

Here $t^{(s)}(\mathbf{r};z_1,\mathbf{k}_\perp^{(s)})\propto 1/r$ as function of variable $\mathbf{r}$, whereas $E^{(i)}(\mathbf{k}_\perp^{(i)},z)$ and $t^{(s)}(\mathbf{r};z,\mathbf{k}_\perp^{(s)})$ have the characteristic scale d over variable z. Equations (7.4) and (7.5) are valid for $k_z^{(i,s)}\mathrm{d}\gg 1$.

Then by substituting Eqs. (7.4) and (7.5) in Eq. (7.3) and performing integration over $\mathbf{r}_{1,2\perp}$ we obtain for the light scattering intensity

$$I_{(i)}^{(s)}\propto\frac{I^{(i)}S_\perp}{r^2}\int_0^L\mathrm{d}z_1\int_0^L\mathrm{d}z_2\,H(z_1;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})H^*(z_2;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})e_\alpha^{(s)}(z_1)e_\gamma^{(s)}(z_2)$$
$$\times\mathcal{G}_{\alpha\beta\gamma\delta}(\mathbf{Q}_{sc\perp};z_1,z_2)e_\beta^{(i)}(z_1)e_\delta^{(i)}(z_2)\exp\left(i\int_{z_1}^{z_2}Q_{scz}(z')\mathrm{d}z'\right), \tag{7.6}$$

where $\mathbf{Q}_{sc\perp}=\mathbf{k}_\perp^{(s)}-\mathbf{k}_\perp^{(i)}$, $Q_{scz}(z)=k_z^{(s)}(z)-k_z^{(i)}(z)$, $I^{(i)}$ is the intensity of the incident wave, $S_\perp$ is the square of the sample cross section, $H(z_j;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})=E^{(i)}(\mathbf{k}_\perp^{(i)},z_j)t^{(s)}(\mathbf{r};z_j,\mathbf{k}_\perp^{(s)})$. Here we have assumed that the sample with the width L occupies the layer $0\leqslant z\leqslant L$ and the transversal sizes of the sample are sufficiently large in comparison to the wavelength λ, $\sqrt{S_\perp}\gg\lambda$.

The exponential factor in expression (7.6) is a rapidly oscillating function. The $\hat{\mathcal{G}}(\mathbf{Q}_{sc\perp};z_1,z_2)$ function is associated with the function $\hat{G}(\mathbf{Q}_{sc\perp};z_1,z_2)$. As we can see from Eqs. (4.12) and (4.13) the function $\hat{G}(\mathbf{q};z_1,z_2)$ contains rapidly damping exponential factors $\exp(-q|\int_{z_1}^{z_2}\mu_j(z)dz|)$. The factors $H(z_1;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})$ and $H^*(z_2;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})$ are slowly varying as compared to the exponential factors. Let us use the differed $z_-=z_1-z_2$ and summary $z_+=(z_1+z_2)/2$ variables instead of z_1,z_2 $(0\leqslant z_+\leqslant L,|z_-|\leqslant|L-2|z_+-L/2\|)$, and the saddle-point technique for the variable z_-. The vicinity of the point $z_-=0$ gives the main contribution into the integral. Then in all smooth factors (the factors H, H^* and all nonexponential factors in $\hat{\mathcal{G}}$) we can set $z_1=z_2=z_+$ and expand exponents in the vicinity of the line $z_-=0$ up to the first nonzero terms (the first order terms over z_-). We have

$$I_{(i)}^{(s)}\propto\frac{I_0^{(i)}S_\perp}{r^2}\int\mathrm{d}z_+\int\mathrm{d}z_-|H(z_+;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})|^2e_\alpha^{(s)}(z_+)e_\gamma^{(s)}(z_+)\mathcal{G}_{\alpha\beta\gamma\delta}(\mathbf{Q}_{sc\perp};z_-,z_+)e_\beta^{(i)}(z_+)$$
$$\times e_\delta^{(i)}(z_+)\exp[iQ_{scz}(z_+)z_-]$$
$$=\frac{I_0^{(i)}S_\perp}{r^2}\int_0^L|H(z;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})|^2e_\alpha^{(s)}(z)e_\gamma^{(s)}(z)\mathcal{G}_{\alpha\beta\gamma\delta}(\mathbf{Q}_{sc\perp};Q_{scz}(z),z)e_\beta^{(i)}(z)e_\delta^{(i)}(z)\mathrm{d}z. \tag{7.7}$$

We are investigating the problem of light scattering in CLC with the pitch exceeding the wavelength of light λ significantly in detail in Ref. 30 with taking into account anisotropy of CLC and wave refraction effects. Here we restrict our consideration by general consequences of Eq. (7.7). Substituting Eqs. (2.10) and (2.11) into Eq. (2.9) we obtain from Eq. (7.2) the single light scattering intensity in the form

$$I_{(i)}^{(s)}\propto\frac{I_0^{(i)}S_\perp}{r^2}\sum_{k,l=1,2}\int_0^L G_{kl}(\mathbf{Q}_{sc\perp},Q_{scz}(z),z)\mathcal{H}_{kl}(z;\mathbf{k}_\perp^{(i)},\mathbf{k}_\perp^{(s)})\mathrm{d}z, \tag{7.8}$$

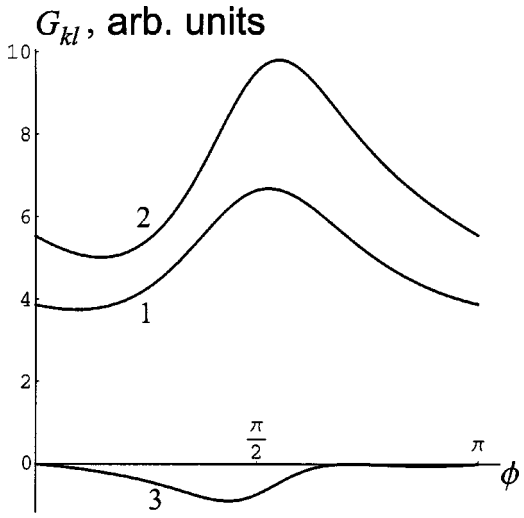

FIG. 5. The $G_{kl}(\mathbf{Q}_{sc\perp}, Q_{scz}(z), z)$ components of the correlation function as functions of $\phi = 2\pi z/d + \phi_0$ (G_{11}, curve 1; G_{22}, curve 2; and G_{12}, curve 3). The components are calculated for the ordinary incident and extraordinary scattered waves. Angles between the z axis and the wave vectors $\mathbf{k}^{(i)}$ and $\mathbf{k}^{(s)}$ outside of the CLC are equal to $\pi/4$ and $\pi/8$, respectively. Angle between $\mathbf{k}_\perp^{(i)}$ and $\mathbf{k}_\perp^{(s)}$ is equal to $\pi/16$. Permittivities are $\varepsilon_\perp = 2.0$, $\varepsilon_a = 0.5$. The Frank modules are $K_{11} = 3.0 \times 10^{-6}$ dyne, $K_{22} = 2.0 \times 10^{-6}$ dyne, $K_{33} = 5.0 \times 10^{-6}$ dyne.

where $\mathcal{H}_{kl}(z; \mathbf{k}_\perp^{(i)}, \mathbf{k}_\perp^{(s)})$ are the functions arising from angular and polarization factors. These functions have the characteristic scale over z of the order of the pitch d.

Figure 5 presents the dependencies $G_{kl}(\mathbf{Q}_{sc\perp}, Q_{scz}(z), z)$ on the $\phi = 2\pi z/d + \phi_0$ variable, $0 \leqslant \phi \leqslant \pi$. In terms of the z variable it corresponds to one period of the helix. One can see that all components contribute to the light scattering intensity. The figure shows that vicinity of $\phi = \pi/2$ brings larger contribution than the other regions to the light scattering intensity. Evidently, this effect is connected with the turning point $\phi = \pi/2$. The components of the correlation function in Fig. 5 were calculated by Eq. (4.13). As we have seen in Secs. V and IV there is a narrow region near the turning point $\phi = \pi/2$ where we should use Eq. (6.7) instead of Eq. (4.13).

Let us discuss the influence of this narrow region near the turning points on the light scattering. In integral Eq. (7.7) over z_- variable the main input to the scattering intensity comes from the range $|z_-| \sim \lambda \ll d$. Note, that for $|z_1 - z_2| \ll d$ the equilibrium director $\mathbf{n}^0$ variation in the space is negligible, $\mathbf{n}^0(z_1) = \mathbf{n}^0(z_2)$. It means that for this scale over variable $z_- = z_1 - z_2$ correlation function of CLC locally coincides with one of NLC. But the characteristic scale over variable $z_+ = (z_1 + z_2)/2$ is equal to d and distinction between CLC and NLC correlation functions still retains. As we have seen in Sec. IV the divergences in $\hat{G}^{(1)}$ and $\hat{G}^{(2)}$ [Eq. (4.12)] for $\phi \to \pi/2$ related by the presence of the turning point cancel each other for the case of NLC [Eq. (4.16)]. Therefore in all geometries of light scattering when at least one of the conditions $|Q_{sc\perp}|d \gg 1$ and $|Q_{scz}|d \gg 1$ is correct Eq. (4.13) is valid. The first of these conditions $Q_{sc\perp} = q \gg p_0$ is the condition of validity for WKB method. Hence for entire region where our results for correlation function are valid we can use Eq. (4.13) for calculation of the light scattering intensity in Eq. (7.8).

Our approach provides to consider nonlocal fluctuations in the inhomogeneous media. This approach is universal for any physical systems with smoothly varying structure and properties. For example, this problem exists in calculations of the order parameter fluctuations in the vicinity of the second order phase transition in inhomogeneous electric and magnetic fields and near liquid-vapor critical point in presence of the gravitational effects. The occurrence of the turning points is not obligatory in such problems. If turning points exist, the considered scheme allows to take them into account in the framework of developed approach.

In the present work we investigate the correlation functions for boundless system. In this case as a boundary condition we use the principle of correlation decay. For this reason exponentially

decreasing solutions contribute to the correlation function only. We suppose the calculation of correlation function of fluctuations in restricted CLC will be the next step in investigation of fluctuations in CLC and twist cells of NLC. In restricted systems an additional input appears in the free energy associated with anchoring effects. In this case we should consider both decreasing and increasing solutions in the correlation function. In restricted CLC our WKB method is perspective for use with method of path integrals[6,8] and method of self-conjugation operators.[9,10]

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APPENDIX: CONSERVATION LAW IN RELAXATION SYSTEMS

Now it is essential to clarify the sense of Eqs. (5.31) and (5.33) using the simplest relaxation model described by equation

$$Y''-\Gamma(X)Y=0, \tag{A1}$$

where $\Gamma(X)$ is a positive function. Multiplying Eq. (A1) by Y^* and the conjugate equation by Y we obtain

$$Y''Y^*-\Gamma(X)YY^*=0, \quad Y^{*\prime\prime}Y-\Gamma(X)YY^*=0.$$

Subtracting term by term we have

$$Y''Y^*-Y^{*\prime\prime}Y=(Y'Y^*-Y^{*\prime}Y)'=0.$$

So we arrive at a conservation law for Eq. (A1),

$$\mathrm{Im}(Y'Y^*)=\mathrm{const}. \tag{A2}$$

The exact solution of Eq. (A1) can be written in the form

$$Y(X)=A_1(X)W_1(X)+A_2(X)W_2(X), \tag{A3}$$

where

$$W_{1,2}(X)=\Gamma(X)^{-1/4}\exp\left(\pm\int_{X_0}^{X}\sqrt{\Gamma(X')}\mathrm{d}X'\right) \tag{A4}$$

are WKB solutions, and $A_{1,2}(X)$ are amplitude functions. For eliminating the arbitrariness in the choice of the $A_{1,2}(X)$ functions we use the subsidiary condition

$$A_1'(X)W_1(X)+A_2'(X)W_2(X)=0. \tag{A5}$$

We substitute solution (A3) into Eq. (A2) and take into account identity $W_1'W_2-W_1W_2'=2$. As long as the $W_{1,2}(X)$ functions are real we obtain from Eq. (A5) the resulting conservation law,

$$\mathrm{Im}[A_1^*(X)A_2(X)]=\mathrm{const}. \tag{A6}$$

Let us denote the limit amplitudes of the WKB solutions for $X\to-\infty$ as $A_{1,2}^{(-)}$ and for $X\to+\infty$ as $A_{1,2}^{(+)}$. Equation (A6) is fulfilled for $A_1^{(-)}=A_1^{(+)}$ and $A_2^{(-)}=A_2^{(+)}$. This situation takes place in the

absence of turning points. Note, that this equation is also fulfilled for the case when $\mathrm{Re}\,A_j\,\mathrm{Im}\,A_j=0$ for both $j=1,2$. The very situation takes place due to passing by the turning point. If we draw the analogy to our multimode problem and apply Eq. (5.30) we obtain

$$A_1^{(+)}=2iF_1C_5,\quad A_2^{(+)}=F_2C_5,\quad A_1^{(-)}=iF_1C_5,\quad A_2^{(-)}=2F_2C_5.$$

This yields the relation

$$A_1^{(-)}A_2^{(-)}=A_1^{(+)}A_2^{(+)}.$$

Thus, in an equation of this type the amplitudes may vary with their product remains conserved.

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Canonical decompositions of *n*-qubit quantum computations and concurrence

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The two-qubit canonical decomposition $SU(4)=[SU(2)\otimes SU(2)]\Delta[SU(2)\otimes SU(2)]$ writes any two-qubit unitary operator as a composition of a local unitary, a relative phasing of Bell states, and a second local unitary. Using Lie theory, we generalize this to an n-qubit decomposition, the concurrence canonical decomposition (CCD) $SU(2^n)=KAK$. The group K fixes a bilinear form related to the concurrence, and in particular any unitary in K preserves the tangle $|\overline{\langle\phi|}\times(-i\sigma_1^y)\cdots(-i\sigma_n^y)|\phi\rangle|^2$ for n even. Thus, the CCD shows that any n-qubit unitary is a composition of a unitary operator preserving this n-tangle, a unitary operator in A which applies relative phases to a set of GHZ states, and a second unitary operator which preserves the tangle. As an application, we study the extent to which a large, random unitary may change concurrence. The result states that for a randomly chosen $a\in A\subset SU(2^{2p})$, the probability that a carries a state of tangle 0 to a state of maximum tangle approaches 1 as the even number of qubits approaches infinity. Any $v=k_1ak_2$ for such an $a\in A$ has the same property. Finally, although $|\overline{\langle\phi|}(-i\sigma_1^y)\cdots(-i\sigma_n^y)|\phi\rangle|^2$ vanishes identically when the number of qubits is odd, we show that a more complicated CCD still exists in which K is a symplectic group. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Entanglement is a unique feature of quantum systems that plays a key role in quantum information proccessing. Much effort has gone into describing the entanglement present in the state of a quantum system composed of two or more measurably distinct subsystems. Because different amounts of entanglement may be shared among the various partitions of the tensor factors of the Hilbert state space, there is no single measure of entanglement that captures all nonlocal correlations for many-particle systems. Rather, the number of partitions of the tensor factors grows exponentially with the number of factors themselves. Thus, it is reasonable to guess that same is true for the number of useful entanglement measures. In fact, the situation is yet more complicated. Certain definitions create uncountably many entanglement types, which thus may not be associated to countable collections of partitions or monotones.

Nevertheless, it is interesting to consider how much entanglement is created by a given unitary evolution U of an n-qubit state space. To achieve this in a limited context, we focus on a single multi-qubit entanglement measure, the n-concurrence.[25] Using Lie theory, we may decompose a unitary operator acting on n qubits into a form such that the entangling power of the unitary with respect to this measure is manifest.

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The n-tangle and its square root, the n-concurrence, are two of several proposed multiqubit entanglement measures. Others include polynomial invariants which involve moments of the reduced state eigenvalues,[1] the Schmidt measure[6] which is related to the minimum number of terms in the product state expansion of a state, the Q measure,[16] which is related to the average purity each qubit's reduced state, and distances between a state and its multipartite twirled image.[5] A further measure makes use of hyperdeterminants;[17] this powerful technique makes computation difficult in more than six qubits. The *concurrence* C_n is originally introduced in the two-qubit case.[9] It is generalized to a measure on two systems of arbitrarily many dimensions in Ref. 19 and extends to n-qubits.[25]

We now consider the quantitative expression for the concurrence. Suppose a quantum state space of data for a quantum computer. Specifically, fix n as the number of qubits, $N=2^n$. Throughout, we use $|j\rangle$ not to denote the state of a qubit but rather as an abbreviated multiqubit state via binary form. For example, in three qubits $|5\rangle=|101\rangle=|1\rangle\otimes|0\rangle\otimes|1\rangle$. We write $\mathcal{H}_n=\mathrm{span}_{\mathbb{C}}\{|j\rangle;\ 0\leqslant j\leqslant N-1\}$ for the n-qubit Hilbert state space. Then the concurrence is a map $C_n:\mathcal{H}_n\rightarrow[0,\infty)$ given by $C_n(|\psi\rangle)=|\overline{\langle\psi|}(-i\sigma_1^y)\cdots(-i\sigma_n^y)|\psi\rangle|$. Note that the expression inside the complex norm is in general not real. A related entanglement measure $\tau_n=C_n^2$ is known as the *n-tangle* when n is even.[27] For $\langle\psi|\psi\rangle=1$, the n-tangle of a state $|\psi\rangle$ assumes real values in the range $0\leqslant\tau_n\leqslant 1$. It is moreover an entanglement monotone,[23] as any good measure should be. This means in particular that $\tau_n:\mathcal{H}_n\rightarrow[0,\infty)$ vanishes on full tensor products of local states, and moreover that $\tau_n(v_1\otimes v_2\otimes\cdots\otimes v_n|\psi\rangle)=\tau_n(|\psi\rangle)$ for any $v_1\otimes v_2\otimes\cdots\otimes v_n\in\otimes_1^n SU(2)$. We show in Appendix C that the n-concurrence is also an entanglement monotone.

The n-concurrence only detects certain kinds of entanglement. Specifically, while it returns zero on all separable states, it may also return zero on certain nonseparable states. We illustrate the monotone's behavior by example. First, the n-partite Greenberger–Horne–Zeilinger (GHZ) state $|\mathrm{GHZ}_n\rangle=(1/\sqrt{2})(|0_1\cdots 0_n\rangle+|1_1\cdots 1_n\rangle)$ has maximal n-concurrence while $C_n(|\mathrm{GHZ}_{n-1}\rangle\otimes|0\rangle_n)=0$. As a second example, the generalized $|W\rangle$ state given by $|W\rangle=(1/\sqrt{n})(|10\cdots 0\rangle+|010\cdots 0\rangle+\cdots+|0\cdots 01\rangle)$ has zero n-concurrence despite being entangled. States with subglobal entanglement can also assume maximal n-concurrence; $C_n(|\mathrm{GHZ}_n\rangle)=C_n(|\mathrm{GHZ}_{n/2}\rangle\otimes|\mathrm{GHZ}_{n/2}\rangle)=1$. Generally, the n-concurrence seeks out superpositions between a state and its binary bit flip.

We extend these definitions by introducing a complex bilinear form, the *concurrence form* $\mathcal{C}_n:\mathcal{H}_n\times\mathcal{H}_n\rightarrow\mathbb{C}$. Here, complex bilinear means the function is linear when restricted to each variable. The antisymmetric concurrence form $\mathcal{C}_n(-,-)$ is nonzero even in the case n is odd, although of course $C_{2p-1}\equiv 0$ since $\mathcal{C}_{2p-1}(|\psi\rangle,|\psi\rangle)=-\mathcal{C}_{2p-1}(|\psi\rangle,|\psi\rangle)=0$.

Definition I.1: The concurrence form $\mathcal{C}_n:\mathcal{H}_n\times\mathcal{H}_n\rightarrow\mathbb{C}$ is given by $\mathcal{C}_n(|\psi\rangle,|\phi\rangle)=\overline{\langle\psi|}(-i\sigma_1^y)\times(-i\sigma_2^y)\cdots(-i\sigma_n^y)|\phi\rangle$. Note the complex conjugation of the lead bra is required for complex linearity (rather than antilinearity) in the first variable. The concurrence quadratic form is $Q_n^C(|\psi\rangle)=\mathcal{C}_n(|\psi\rangle,|\psi\rangle)$, so that $C_n(|\psi\rangle)=|Q_n^C(|\psi\rangle)|=\sqrt{\tau_n(|\psi\rangle)}$. Note that Q_n^C is a complex quadratic polynomial on the vector space $\mathcal{H}_n$.

The main technique of this paper is to build a new matrix decomposition of the Lie group of global phase normed quantum computations $SU(N)$. It is optimized for the study of the concurrence and n-tangle and generalizes the two-qubit canonical decomposition,[4,10,13–15,26]

$$SU(4)=[SU(2)\otimes SU(2)]\Delta[SU(2)\otimes SU(2)]. \tag{1}$$

Here, the commutative group Δ applies relative phases to a "magic basis"[2,4,9,10,14] of phase-shifted Bell states. This two-qubit canonical decomposition is used to the study of the entanglement capacity of two-qubit operations,[26] to build efficient (small) circuits in two qubits,[4,20,24] and to classify which two-qubit unitary operators require fewer than average multiqubit interactions.[20,24]

The canonical decomposition is itself an example of the $G=KAK$ metadecomposition theorem of Lie theory (Ref. 8, Theorem 8.6, Sec. VII.8). This theorem produces a decomposition of an input semisimple Lie group G given two further inputs:

(1) a Cartan involution (Ref. 8, Sec. X.6.3, p. 518) $\theta:\mathfrak{g}\to\mathfrak{g}$ for $\mathfrak{g}=\mathrm{Lie}(G)$. By definition, θ satisfies (i) $\theta^2=\mathbf{1}$ and (ii) $\theta[X,Y]=[\theta X,\theta Y]$ for all $X,Y\in\mathfrak{g}$. We write $\mathfrak{g}=\mathfrak{p}\oplus\mathfrak{k}$ for the decomposition of $\mathfrak{g}$ into the $+1$ and -1 eigenspace of θ;
(2) a commutative subalgebra $\mathfrak{a}\subset\mathfrak{p}$ which is maximal commutative in $\mathfrak{p}$.

Then write $K=\exp\mathfrak{k}$, $A=\exp\mathfrak{a}$, where for linear $G\subset GL(n,\mathbb{C})$ the exponential coincides with the matrix power series on each of the Lie subalgebras $\mathfrak{k}$, $\mathfrak{a}$. The theorem asserts then that $G=KAK=\{k_1ak_2;k_1,k_2\in K,a\in A\}$.

For example, the canonical decomposition of $SU(4)$ arises as follows. Take $\theta:\mathfrak{su}(4)\to\mathfrak{su}(4)$ by $\theta(X)=(-i\sigma_1^y)(-i\sigma_2^y)\overline{X}(-i\sigma_1^y)(-i\sigma_2^y)$ and

$$\mathfrak{a}=\mathrm{span}_{\mathbb{R}}\{i|0\rangle\langle 0|-i|1\rangle\langle 1|-i|2\rangle\langle 2|+i|3\rangle\langle 3|,\ i|0\rangle\langle 3|+i|3\rangle\langle 0|,\ i|1\rangle\langle 2|+i|2\rangle\langle 1|\}. \quad (2)$$

We extend this particular construction to n-qubits.

Definition I.2: Let $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)$. Define $\theta:\mathfrak{su}(2^n)\to\mathfrak{su}(2^n)$ by $\theta(X)=S^{-1}\overline{X}S=(-1)^nS\overline{X}S$. Then $\mathfrak{k}$ denotes the $+1$-eigenspace of θ while $\mathfrak{p}$ denotes the -1-eigenspace. Finally, in case n is even, we define

$$\begin{aligned}\mathfrak{a}=\mathrm{span}_{\mathbb{R}}(\{\ & i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|-i|j+1\rangle\langle j+1|-i|N-j-2\rangle\langle N-j-2|;\\ & 0\leqslant j\leqslant 2^{n-1}-2\}\sqcup\{i|j\rangle\langle N-j-1|+i|N-j-1\rangle\langle j|;0\leqslant j\leqslant 2^{n-1}-1\},),\\ & \text{in case } n \text{ even,}\end{aligned} \quad (3)$$

with $A=\exp\ \mathfrak{a}$. In case n odd, we drop the second set:

$$\begin{aligned}\mathfrak{a}=\mathrm{span}_{\mathbb{R}}(\{\ & i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|-i|j+1\rangle\langle j+1|-i|N-j-2\rangle\langle N-j-2|;\\ & 0\leqslant j\leqslant 2^{n-1}-2\}), \quad \text{in case } n \text{ odd.}\end{aligned} \quad (4)$$

Modulo checks reserved for the body, the *concurrence canonical decomposition* (CCD) in n-qubits is the resulting matrix decomposition $SU(2^n)=KAK$. Note that n may be even or odd.

In n-qubits, it is certainly *not* the case that K is the Lie group of local unitaries. Nonetheless, we prove momentarily by direct computation that the local unitary group $SU(2)\otimes SU(2)\otimes\cdots\otimes SU(2)\subset K$, with strict containment in $n\geqslant 3$ qubits by a dimension count. Moreover, for $n=2p$ an even number of qubits the concurrence canonical decomposition is computable via an algorithm familiar from the two-qubit case[4] (see Appendix A). The following theorem provides the key to interpreting this extended canonical decomposition.

Theorem I.3: *Let $K=\exp\mathfrak{k}$ for $\mathfrak{k}$ the $+1$-eigenspace of the Cartan involution $\theta(X)=S^{-1}\overline{X}S$. Then K is the symmetry group of the concurrence form $\mathcal{C}_n$. Specifically, for $u\in SU(N)$,*

$$(u\in K)\Leftrightarrow[\mathcal{C}_n(u|\phi\rangle,u|\psi\rangle)=\mathcal{C}_n(|\phi\rangle,|\psi\rangle),\quad \text{for every } |\phi\rangle,|\psi\rangle\in\mathcal{H}_n]. \quad (5)$$

Moreover, for n even the concurrence form is symmetric. In the even case, it restricts to the usual dot product on the $\mathbb{R}$-span of a collection of n concurrence one states, and this $\mathbb{R}$ subspace of $\mathcal{H}_n$ is preserved by K. On the other hand, for n odd $\mathcal{C}_n$ is antisymmetric, i.e. a two-form. Thus,

$$K\cong Sp(N/2),\quad \textit{if } n \textit{ is an odd number of qubits;}$$

$$K\cong SO(N),\quad \textit{if } n \textit{ is an even number of qubits.}$$

Remark I.4: Bremner *et al.* (Ref. 3, Theorem 5) observe symplectic Lie algebras independently in a context related to the above. We explore this in more detail in a future manuscript. ◇

This interpretation allows for an extension of prior work on the entangling capacity of two-qubit unitaries.[26] Here is the precise result.

Definition I.5: The *concurrence capacity* of a given n-qubit unitary operator $v \in SU(N)$ is defined by $\kappa(v) = \max\{C_n(v|\psi\rangle);\ C_n(|\psi\rangle) = 0, \langle\psi|\psi\rangle = 1\}$.

Corollary I.6 (of I.3): Let $u = k_1 a k_2$ be the n-qubit canonical decomposition of $u \in SU(N)$. Then $\kappa(u) = \kappa(a)$.

Given the CCD, the function κ is properly viewed as a function on the A factor rather than on the entire group of phase-normalized unitaries $SU(N)$. Finally, a careful analysis of $\kappa(a)$ for randomly chosen a in A produces the following, perhaps surprising, result.

Theorem I.7: *Suppose the number of qubits is even, i.e., $n = 2p$. Then for large p almost all $a \in A$ have maximal concurrence capacity. Specifically, suppose we choose $a \in A$ at random per the probability density function given by the unit normalized Haar measure da. Then*

$$\lim_{p\to\infty} \text{Probability}[\kappa(a) = 1] = \lim_{p\to\infty} da(\{a \in A; \kappa(a) = 1\}) = 1. \tag{6}$$

We rephrase this result colloquially. Suppose we think of those states $|\psi\rangle$ in even qubits with $\tau_n(|\psi\rangle) = 1$ as GHZ-like. Then as the even number of qubits grows large, almost every unitary evolution will be able to produce such a maximally concurrent GHZ-like state from some input state of 0 concurrence.

Notation and contents: We provide some samples of our notation for the reader's convenience. Throughout, n is a number of qubits and $N = 2^n$. For $v = \Sigma_{j,k=0}^{N-1} v_{j,k}|k\rangle\langle j|$, we have the adjoint $v^\dagger = \Sigma_{j,k=0}^{N-1} \overline{v}_{k,j}|k\rangle\langle j|$. We also require the transpose operation, most easily visualized in matrix form as $(v_{j,k})^T = (v_{k,j})$. Equivalently, $v^T = \Sigma_{j,k=0}^{N-1} v_{j,k}|j\rangle\langle k|$. Thus $v^\dagger = \overline{v^T}$. Recall also the convention of collapsing the binary for an integer inside the ket of a computational basis state. We use lower rather than upper case letters for most operators to avoid confusing them with Lie groups denoted by capital letters. The older term *scholium* is used to refer to a corollary of the proof of a theorem or proposition rather than its formal statement. Besides these conventions, we follow the notations of either Refs. 18 or 8.

The paper is structured as follows. In Sec. II, we verify that the conventions of Definition I.2 are appropriate for invoking the $G = KAK$ theorem. Having verified that the matrix decomposition exists, Sec. II further describes *entanglers* and *finaglers*, loosely similarity matrices which rotate the CCD onto more standard KAK decompositions of $SU(N)$. In Sec. III, we discuss the concurrence capacity and prove the properties of this capacity asserted above. The three appendixes consecutively (i) provide an algorithm for computing the CCD given a matrix $v \in SU(N)$, exclusively in the case n is even, (ii) argue that any two normalized states $|\phi\rangle$, $|\psi\rangle$ with identical concurrence must have $k|\phi\rangle = |\psi\rangle$ for some k in the symmetry group K, and (iii) prove that the concurrence $C_n(-)$ is an entanglement monotone.

II. ENTANGLERS, FINAGLERS, AND CARTAN INVOLUTIONS OF $\mathfrak{su}(N)$

This section has two goals. First, we show our KAK decomposition is well-defined, by noting that θ is a Cartan involution, checking by direct computation that $\mathfrak{a}$ is Abelian, and arguing that $\mathfrak{a}$ is maximal commutative. Second, we prove Theorem I.3. There are generally two approaches to the theorem. We could recall standard Cartan involutions and KAK decompositions from the literature. We will shortly construct similarity matrices E_0 and F_0 which rotate the standard $G = KAK$ decompositions of $SU(N)$ onto the CCD, and we could simply appeal to these matrices and the standard structures. Alternately, (many) intrinsic computations would suffice to check the required properties for $G = KAK$. The present approach is a compromise. The argument that the CCD $SU(N) = KAK$ is well-defined is intrinsic, except for a single appeal to classification. On the other hand, the classification of the K groups uses similarity matrices. As such, it is ultimately a change of basis in the n-qubit state space $\mathcal{H}_n$.

A. Properties of the CCD $SU(N)=KAK$

The following proposition is not used in the sequel. However, we include a direct proof due to its importance in guiding the choice of θ. It simplifies an older argument and arose from correspondence with Zanardi.

Proposition II.1: Let K be as in Definition I.2. Then there is an inclusion $SU(2)\otimes SU(2)\otimes\cdots\otimes SU(2)\subset K$.

Proof: Recall $i\sigma^x=i|0\rangle\langle 1|+i|1\rangle\langle 0|$, $i\sigma^y=|0\rangle\langle 1|-|1\rangle\langle 0|$, and $i\sigma^z=i|0\rangle\langle 0|-i|1\rangle\langle 1|$ forms a basis of $\mathfrak{su}(2^1)$. For the statement of the proposition, it suffices to check $\mathrm{Lie}[\otimes_1^n SU(2)]=\mathrm{span}\{i\sigma_j^x,i\sigma_j^y,i\sigma_j^z;\ 1\leqslant j\leqslant n\}\subset\mathfrak{k}$. We further recall the last item of Lemma II.2, as well as the fact that the complex conjugates of the Pauli matrices are $\overline{i\sigma^x}=-i\sigma^x$, $\overline{i\sigma^y}=i\sigma^y$, and $\overline{i\sigma^z}=-i\sigma^z$. Then we wish to show that θ fixes every σ_j^x, σ_j^y, and σ_j^z. For this,

$$(-1)^n S\ \overline{(i\sigma_j^x)}S=(-1)^n S(-i\sigma_j^x)S=(-1)^n S^2(i\sigma_j^x)=(i\sigma_j^x),$$

$$(-1)^n S\overline{(i\sigma_j^y)}S=(-1)^n S(i\sigma_j^y)S=(-1)^n S^2(i\sigma_j^y)=(i\sigma_j^y),$$

$$(-1)^n S\overline{(i\sigma_j^z)}S=(-1)^n S(-i\sigma_j^z)S=(-1)^n S^2(i\sigma_j^z)=(i\sigma_j^z).$$

Hence each such infinitesimal unitary is in the $+1$ eigenspace of θ. This concludes the proof. □

We next note that θ is a Cartan involution. Indeed, direct computation shows that $\theta^2=\mathbf{1}$. Moreover,

$$[\theta X,\theta Y]=(S^{-1}\overline{X}S)(S^{-1}\overline{Y}S)-(S^{-1}\overline{Y}S)(S^{-1}\overline{X}S)=S^{-1}\overline{(XY-YX)}S=\theta[X,Y]. \tag{7}$$

Thus we need the following to complete the argument that $SU(N)=KAK$ of Definition I.2 is well-defined: (i) $\mathfrak{a}\subset\mathfrak{p}$, (ii) $\mathfrak{a}$ is commutative, and (iii) no larger subalgebra of $\mathfrak{p}$ containing $\mathfrak{a}$ is commutative.

Lemma II.2: Let #j denote the number of 1's in the binary expansion of j. Let $S=(-i\sigma_1^y)\times(-i\sigma_2^y)\cdots(-i\sigma_n^y)$ be as in Definition I.2. Then (i) $S|j\rangle=(-1)^{\#j}|N-j-1\rangle$, (ii) $\langle j|S=(-1)^{n-\#j}\langle N-j-1|$, and (iii) $S\sigma_j^x=-\sigma_j^x S$, $S\sigma_j^y=\sigma_j^y S$, and $S\sigma_j^z=-\sigma_j^z S$. Note that (ii) refers to a composition of linear maps.

Sketch: For (i), compute. For (ii), consider $\langle j|S|k\rangle$ for $|k\rangle$ varying over all computational basis states. Then apply (i) for (ii). For (iii), distinct Pauli matrices anticommute, while S itself is a tensor. □

Lemma II.3: Let $\mathfrak{a}$ be as in Definition I.2. Then $\mathfrak{a}\subset\mathfrak{p}$.

Proof: There are two coordinate computations to complete in this case. For the first, momentarily extend the definition of θ to $\tilde{\theta}$ acting on $\mathfrak{u}(N)$ by the same formula. Then

$$\begin{aligned}\tilde{\theta}&[i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|]\\&=(-1)^n S(-i|j\rangle\langle j|-i|N-j-1\rangle\langle N-j-1|)S\\&=(-1)^{n+1}i[(-1)^n|N-j-1\rangle\langle N-j-1|+(-1)^n|j\rangle\langle j|]\\&=-i|j\rangle\langle j|-i|N-j-1\rangle\langle N-j-1|.\end{aligned}$$

Thus $i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|$ is in the -1-eigenspace of $\tilde{\theta}$, so that the elements of the first set of the definition of $\mathfrak{a}$ are contained in $\mathfrak{p}$. For the second basis set in case n even,

$$\begin{aligned}
&\theta[i|j\rangle\langle N-j-1|+i|N-j-1\rangle\langle j|]\\
&\quad=S[(-i)|j\rangle\langle N-j-1|+(-i)|N-j-1\rangle\langle j|]S\\
&\quad=[(-1)^{\#j+[n-(n-\#j)]}(-i)|N-j-1\rangle\langle j|+(-1)^{n-\#j+(n-\#j)}(-i)|j\rangle\langle N-j-1|]\\
&\quad=(-i)|N-j-1\rangle\langle j|+(-i)|j\rangle\langle N-j-1|.
\end{aligned}$$

Thus $i|j\rangle\langle N-j-1|+i|N-j-1\rangle\langle j|\in\mathfrak{p}$, in case n even. □

Proposition II.4: Recall $\mathfrak{a}$ *from Definition I.2. Then* $\mathfrak{a}$ *is commutative.*

Proof: Throughout, $0\leqslant j,k\leqslant N/2-1$, $N=2^n$. The following three computations of Lie brackets suffice:

$$\begin{aligned}
&[i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|,i|k\rangle\langle k|+i|N-k-1\rangle\langle N-k-1|]\\
&\quad=-|j\rangle\langle j|k\rangle\langle k|-|N-j-1\rangle\langle N-j-1|N-k-1\rangle\langle N-k-1|\\
&\qquad+|k\rangle\langle k|j\rangle\langle j|+|N-k-1\rangle\langle N-k-1|N-j-1\rangle\langle N-j-1|;
\end{aligned}$$

$$\begin{aligned}
&[(-i)^{n+1}|j\rangle\langle N-j-1|+i^{n-1}|N-j-1\rangle\langle j|,(-i)^{n+1}|k\rangle\langle N-k-1|+i^{n-1}|N-k-1\rangle\langle k|]\\
&\quad=-|j\rangle\langle N-j-1|N-k-1\rangle\langle k|-|N-j-1\rangle\langle j|k\rangle\langle k|\\
&\qquad+|k\rangle\langle N-k-1|N-j-1\rangle\langle j|+|N-k-1\rangle\langle k|j\rangle\langle N-j-1|;
\end{aligned}$$

$$\begin{aligned}
&[i|j\rangle\langle j|+i|N-j-1\rangle\langle N-j-1|,(-i)^{n+1}|k\rangle\langle N-k-1|+i^{n-1}|N-k-1\rangle\langle k|]\\
&\quad=(-i)^n|j\rangle\langle j|k\rangle\langle N-k-1|+i^n|N-j-1\rangle\langle N-j-1|N-k-1\rangle\langle k|\\
&\qquad-(-i)^n|k\rangle\langle N-k-1|N-j-1\rangle\langle N-j-1|-i^n|N-k-1\rangle\langle k|j\rangle\langle j|.
\end{aligned}$$

Each of the final expressions is zero in case $j\neq k$ and also zero in case $j=k$. Thus, $\mathfrak{a}$ is commutative. □

The arguments above almost complete the proof that the CCD $SU(N)=KAK$ is well-defined. In the abstract, one also needs a fairly large coordinate computation which verifies $\mathfrak{a}$ is maximal commutative. This would verify that for any $X\in\mathfrak{p}$ with $[X,H]=0$ for all $H\in\mathfrak{a}$, one must in fact have $X\in\mathfrak{a}$.

Rather than complete that task, we instead appeal to the Cartan classification (Ref. 8, p. 518, Table V). Ostensibly a classification of globally symmetric spaces, this classification also describes all possible Cartan involutions of any real semisimple group G up to Lie isomorphism. For $G=SU(N)$, there are three overall possibilities grouped as type **AI**, **AII**, and **AIII**. For each, the *rank* refers to the dimension of any maximal commutative subalgebra $\mathfrak{a}$ of $\mathfrak{p}$. This dimension may not vary by subalgebra, since any two such $\mathfrak{a}_1$, $\mathfrak{a}_2$ must have $k\mathfrak{a}_1k^{-1}=\mathfrak{a}_2$ for some $k\in K$. We now excerpt from the table the possibilities for $G=SU(N)$:

Type	Domain $\mathfrak{g}$ of $\theta:\mathfrak{g}\to\mathfrak{g}$	Isomorphism representative of K	Rank
AI	$\mathfrak{su}(N)$	$SO(N)$	$N-1$
AII	$\mathfrak{su}(N)$	$Sp(N/2)$	$N/2-1$
AIII	$\mathfrak{su}(N)$	$S[U(p)\oplus U(q)],p+q=N$	$\min(p,q)$

Suppose then for the moment that the number of qubits n is even. No type **AIII** Cartan involution admits an $\mathfrak{a}$ of dimension $N-1$. Indeed, if $p+q=N$, then $\min(p,q)\leqslant N/2<N-1$. The same is true of type **AII** involutions, i.e., $N-1>N/2-1$. Hence we see that A must be maximal, and for n even the Cartan involution θ must have type **AI**.

What remains is to prove that $\mathfrak{a}$ is maximal in $\mathfrak{p}$ in case n odd. This follows by a dimension count *if* the Cartan involution is type **AII**. We thus postpone noting this point until after the proof of Theorem I.3. See Remark II.19.

As an aside, type **AIII** involutions do not appear in this work but have been used in quantum circuit design. Indeed, the CS-decomposition[7,21] is an example of a *KAK* decomposition arising from a type **AIII** involution. Elements within the appropriate K group may be interpreted as products of computations on the last $n-1$ lines with computations on these lines controlled on the first qubit.

B. Entanglers

In the two-qubit case, the following computation E has the following property:

$$E=(1/\sqrt{2})\begin{pmatrix}1 & i & 0 & 0\\ 0 & 0 & 1 & i\\ 0 & 0 & -1 & i\\ 1 & -i & 0 & 0\end{pmatrix} \text{ satisfies } E^{\dagger}[SU(2)\otimes SU(2)]E=SO(4). \tag{8}$$

Using more Lie theory terminology, recall the adjoint representation of G on $\mathfrak{g}$ given by $\mathrm{Ad}(g)\times[X]=gXg^{-1}$. Then we may restate $\{\mathrm{Ad}(E^{\dagger})\}[SU(2)\otimes SU(2)]=SO(4)$. This provides a physical interpretation for the low dimensional isomorphism $\mathfrak{su}(2)\oplus\mathfrak{su}(2)\cong\mathfrak{so}(4)$. We would like entanglers for the concurrence canonical decomposition.

Definition II.5: Let $\theta_{\mathbf{AI}}:\mathfrak{su}(2^n)\to\mathfrak{su}(2^n)$ denote the usual type **AI** Cartan involution $\theta_{\mathbf{AI}}(X)=\overline{X}$ associated to $SO(N)\subset SU(N)$. We say $E\in SU(2^n)$ is an entangler iff the following diagram commutes:

$$\begin{array}{ccc}\mathfrak{su}(N) & \xrightarrow{\theta_{\mathrm{AI}}} & \mathfrak{su}(N)\\ {\scriptstyle \mathrm{Ad}(E)}\downarrow & & \downarrow{\scriptstyle \mathrm{Ad}(E)}\\ \mathfrak{su}(N) & \xrightarrow{\theta} & \mathfrak{su}(N)\end{array}. \tag{9}$$

In particular as both groups are connected, we must have $\mathrm{Ad}(E)[SO(N)]=K$.

We next prove the surprising fact that there are no entanglers when n is odd. For this, we need to recall the central subgroup $\mathcal{Z}[SU(N)]=\{v\in SU(N); vuv^{\dagger}=u \text{ for all } u\in SU(N)\}$. The center is in fact the set of all phase computations corresponding to the Nth roots of unity:

$$\mathcal{Z}[SU(N)]=\{\xi\mathbf{1};\xi^N=1\} \quad (\text{Ref. 8, pp. 310, 516}). \tag{10}$$

With this fact recalled from the literature, we have the following lemma.

Lemma II.6: Suppose that for $v\in SU(N)$, $[\mathrm{Ad}(v)](X)=vXv^{\dagger}=X$ for every $X\in\mathfrak{su}(N)$. Then $v=\xi\mathbf{1}$ for some $\xi\in\mathbb{C}$ with $\xi^N=1$. (Hence $\xi=e^{2\pi ik/N}$,$0\leqslant k\leqslant N-1$.)

Proof: Recall that $\exp:\mathfrak{su}(N)\to SU(N)$ is onto. Thus each $u\in SU(N)$ may be written as $\exp X$ for some X. Thus, consider the one-parameter-subgroup (Ref. 8 p. 104) $\gamma:\mathbb{R}\to SU(N)$ given by $t\mapsto v[\exp(tX)]v^{\dagger}$. This has derivative $(d\gamma/dt)\big|_{t=0}=vXv^{\dagger}=X$, and by uniqueness of one-parameter-subgroups (Ref. 8, p. 103, Corollary 1.5) $v\exp(tX)v^{\dagger}=\exp(tX)$ for all t. Taking $t=1$, we see $vuv^{\dagger}=u$ for a generic $u\in SU(N)$. □

Proposition II.7: If the number of qubits n is odd, then there does not exist an entangler $E\in U(N)$.

Proof: Assume by way of contradiction that there does exist an entangler E for n odd. Then for all $X\in\mathfrak{su}(N)$, we have the following equation:

$$(EE^T)\overline{X}(EE^T)^{\dagger} = E\theta_{\mathbf{AI}}[E^{\dagger}XE]E^{\dagger}=\theta(X)=S\overline{X}S^{-1}. \tag{11}$$

Since we may vary $Y=\overline{X}$ over $\mathfrak{su}(N)$ as well, this implies that $S^{-1}EE^T$ satisfies the hypothesis of Lemma II.6. Thus $S^{-1}EE^T=\xi\mathbf{1}$ for $\xi^N=1$ or $EE^T=(\xi\mathbf{1})S$. The contradiction for EE^T is always a complex symmetric matrix while $(\xi\mathbf{1})S$ is not a complex symmetric matrix when n is odd. □

Scholium II.8: For an even number of qubits n, the matrix $E\in U(N)$ is an entangler iff $EE^T=(\xi\mathbf{1})S$, where $\xi^N=1$.

There are many possible entanglers. Indeed, even in two-qubits other choices have been used.[15,26] One possibility given n even is to take the $n/2$ fold tensor product $E\otimes E\otimes\cdots\otimes E$. However, we prefer the following choice as a standard instead, since it highlights the mapping of the computational basis to Greenberger–Horne–Zeilinger states.

Definition II.9: Suppose n is even, and write $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)=\Sigma_{j=0}^{N/2-1}\varepsilon_j(|j\rangle\times\langle N-j-1|+|N-j-1\rangle\langle j|)$, with $\varepsilon_j=(-1)^{\#j}$, where $\#j$ is the number of 1's in the binary expression for j. The standard entangler E_0 in n-qubits is then given by

$$E_0=\frac{1}{\sqrt{2}}\sum_{j=0}^{N/2-1}|j\rangle\langle 2j|+i|j\rangle\langle 2j+1|+\varepsilon_j(|N-j-1\rangle\langle 2j|-i|N-j-1\rangle\langle 2j+1|). \tag{12}$$

Proposition II.10: The standard entangler E_0 is an entangler.

Proof: First, we omit due to reasons of space a set of row operations which verifies that $\det(E_0)=1$. Then we may write out an expression for E_0^T by reversing the indices in each bra-ket pair:

$$E_0^T=\frac{1}{\sqrt{2}}\sum_{k=0}^{N/2-1}|2k\rangle\langle k|+i|2k+1\rangle\langle k|+\varepsilon_k(|2k\rangle\langle N-k-1|-i|2k+1\rangle\langle N-k-1|). \tag{13}$$

Then Scholium II.8 shows that the following computation suffices to prove that E is an entangler:

$$\begin{aligned}E_0E_0^T=&\frac{1}{2}\sum_{j=0}^{N/2-1}|j\rangle\langle j|+\varepsilon_j|j\rangle\langle N-j-1|+i^2|j\rangle\langle j|+\varepsilon_j|j\rangle\langle N-j-1|+\varepsilon_j|N-j-1\rangle\langle j|\\&+\varepsilon_j^2|N-j-1\rangle\langle N-j-1|+\varepsilon_j(|N-j-1\rangle\langle j|+i^2\varepsilon_j^2|N-j-1\rangle\langle N-j-1|)\\=&\sum_{j=0}^{N/2-1}\varepsilon_j(|j\rangle\langle N-j-1|+|N-j-1\rangle\langle j|)\\=&(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y).\end{aligned} \tag{14}$$

This concludes the coordinate computation. □

In the next section, we will also make use of the following lemma. The computation is similar.

Lemma II.11: $E_0^TE_0$ is diagonal and real. In fact, $E_0^TE_0=|0\rangle\langle 0|-|1\rangle\langle 1|+|2\rangle\langle 2|-|3\rangle\langle 3|+\cdots$.

Proof: Computing the reversed product:

$$\begin{aligned}E_0^TE_0=&\frac{1}{2}\sum_{j=0}^{N/2-1}|2j\rangle\langle 2j|+i|2j+1\rangle\langle 2j|+i|2j\rangle\langle 2j+1|-|2j+1\rangle\langle 2j+1|\\&+\varepsilon_j^2|2j\rangle\langle 2j|-i\varepsilon_j^2|2j\rangle\langle 2j+1|-i\varepsilon_j^2|2j+1\rangle\langle 2j|+i^2\varepsilon_j^2|2j+1\rangle\langle 2j+1|\\=&\sum_{j=0}^{N/2-1}|2j\rangle\langle 2j|-|2j+1\rangle\langle 2j+1|.\end{aligned} \tag{15}$$

This concludes the proof. □

Example II.12: Although this example is large, we explicitly describe the standard four-qubit entangler:

$$E_0=(1/\sqrt{2})\begin{pmatrix}
1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & i & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & i & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & i & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & i\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & i\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -i & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -i & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & i & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & -1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & -1 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & -i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}. \tag{16}$$

Note that the antidiagonal pattern mirrors $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)$ and that each computational basis state maps to a relative phase of a GHZ state. ◇

C. Finaglers

There do not exist entanglers when the number of qubits n is odd, because $\mathfrak{k}\cong\mathfrak{sp}(N/2)$ rather than $\mathfrak{so}(N)$. See the as yet unproven Theorem I.3. Yet the fairly abstract embedding K of $Sp(N/2)$ into $SU(N)$ might be made more standard. This is indeed possible, and we call the any matrix which rotates K to the standard $Sp(N/2)$ a finagler.

Definition II.13: Let $\theta_{\mathbf{AII}}:\mathfrak{su}(N)\to\mathfrak{su}(N)$ be the standard Cartan involution (Ref. 8, p. 445) fixing $\mathfrak{sp}(N/2)$, i.e., $\theta_{\mathbf{AII}}(X)=(-i\sigma^y\otimes\mathbf{1}_{N/2})X^T(-i\sigma^y\otimes\mathbf{1}_{N/2})=(-i\sigma^y\otimes\mathbf{1}_{N/2})^{-1}\overline{X}(-i\sigma^y\otimes\mathbf{1}_{N/2})$. Then a finagler F is any $F\in SU(2^n)$ which causes the following diagram to commute:

$$\begin{array}{ccc}
\mathfrak{su}(N) & \xrightarrow{\theta_{\mathrm{AII}}} & \mathfrak{su}(N)\\
{\scriptstyle \mathrm{Ad}(F)}\downarrow & & \downarrow{\scriptstyle \mathrm{Ad}(F)}\\
\mathfrak{su}(N) & \xrightarrow{\theta} & \mathfrak{su}(N)
\end{array}. \tag{17}$$

If $F\in SU(N)$, then we say F finagles iff F is a finagler.

Proposition II.14: F is a finagler iff $F(-i\sigma^y\otimes\mathbf{1}_{N/2})^TF^T=(\xi\mathbf{1})(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)=(\xi\mathbf{1})S$, $\xi^N=1$.

Proof: For convenience, label $\Sigma=-i\sigma^y\otimes\mathbf{1}_{N/2}$. ($F$ finagles)$\Leftrightarrow[F\Sigma^{-1}(\overline{F^\dagger XF})\Sigma F^\dagger=S^{-1}\overline{X}S\ \forall X\in\mathfrak{su}(N)]\Leftrightarrow[F\Sigma^TF^T=(\xi\mathbf{1})S,\xi^N=1]$. Note that the second equivalence uses Lemma II.6. □

Example II.15: In three qubits, we see the following computation is a finagler by direct computation:

$$F=(1/\sqrt{2})\begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \end{pmatrix}. \tag{18}$$

Unlike entanglers, it is possible for $F=\overline{F}$. The finagler maps computational basis states to GHZ states. ◇

Definition II.16: Fix n an odd number of qubits. Let $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)=\Sigma_{j=0}^{N/2-1}\iota_j(|N-j-1\rangle\langle j|-|j\rangle\langle N-j-1|)$ with $\iota_j=\pm 1$. The standard finagler F_0 is defined to be the following linear operator:

$$F_0=\sum_{j=0}^{N/2-1}|j\rangle\langle j|+|N-j-1\rangle\langle j|+\iota_j(|j\rangle\langle N/2+j|-|N-j-1\rangle\langle N/2+j|). \tag{19}$$

Note that the standard finagler is real.

Proposition II.17: The standard finagler F_0 finagles.

Proof: We again omit the column operations verifying $\det(F_0)=1$, as this would take several pages. Thus, let $\Sigma=-i\sigma^y\otimes\mathbf{1}_{N/2}$ be expanded as $\Sigma=\Sigma_{j=0}^{N/2-1}|j\rangle\langle N/2+j|-|N/2+j\rangle\langle j|$. We have the following equation:

$$F_0\Sigma=\frac{1}{\sqrt{2}}\sum_{j=0}^{N/2-1}|j\rangle\langle N/2+j|+|N-j-1\rangle\langle N/2+j|-\iota_j(|j\rangle\langle j|-|N-j-1\rangle\langle j|). \tag{20}$$

Moreover, $F_0^T=(1/\sqrt{2})\,\Sigma_{j=0}^{N/2-1}|j\rangle\langle j|+|j\rangle\langle N-j-1|+\iota_j(|N/2+j\rangle\langle j|-|N/2+j\rangle\langle N-j-1|)$. Thus we see that

$$\begin{aligned}(F_0\Sigma)F_0^T=&\frac{1}{2}\sum_{j=0}^{N/2-1}\iota_j(|j\rangle\langle j|-|j\rangle\langle N-j-1|+|N-j-1\rangle\langle j|-|N-j-1\rangle\langle N-j-1|)\\&-\iota_j(|j\rangle\langle j|+|j\rangle\langle N-j-1|-|N-j-1\rangle\langle j|-|N-j-1\rangle\langle N-j-1|)\\=&\sum_{j=0}^{N/2-1}\iota_j(|N-j-1\rangle\langle j|-|j\rangle\langle N-j-1|).\end{aligned} \tag{21}$$

This concludes the proof. □

We also briefly review how $Sp(N/2)$ embeds into $SU(N)$. By one standard definition of the group (Ref. 8, p. 446),

$$\mathfrak{sp}(N/2)=\left\{\begin{pmatrix} X_1 & X_2 \\ X_3 & -X_1^T \end{pmatrix};X_j=\overline{X_j},X_{2,3}\ \text{symmetric}\right\}. \tag{22}$$

Another standard definition (Ref. 11, pp. 34–36) uses a symmetry in matrices of quaternions. Note that the matrices of Eq. (22) are not elements of $\mathfrak{su}(N)$. Rather, the $+1$ eigenspace of $\theta_{\mathbf{AII}}(X)=\Sigma^{-1}\overline{X}\Sigma$ is

$$\mathfrak{sp}(N/2)=\left\{\begin{pmatrix} V & W \\ -W^\dagger & \overline{V}\end{pmatrix}; V\in\mathfrak{u}(N/2), W=W^T \text{ is complex symmetric}\right\}. \tag{23}$$

[For example, $Sp(4)\subset SU(8)$; this is 36 dimensional. For W includes two real symmetric matrices with 10 dimensions each, while $\mathfrak{u}(4)$ is 16 dimensional.] One may verify that this is also a copy of $\mathfrak{sp}(N/2)$, so that $\mathfrak{k}$ is a copy of $\mathfrak{sp}(N/2)$ as well. Also, note that for $k\in K$, in particular $k\in\otimes_1^n SU(2)$, we expect $FkF^\dagger$ to be in the *copy of* $Sp(N/2)$ *above* rather than to be a real matrix in an orthogonal subgroup of $SU(N)$. Finally, note that exponentiating the Lie algebra above is not the best way to write out a closed form for elements of the global group $Sp(N/2)$. Rather, we have a block form:

$$\begin{aligned} Sp(N/2)&=\{V\in SU(N); V^T\Sigma V=\Sigma\}\\ &=\left\{\begin{pmatrix} A & B\\ C & D\end{pmatrix}\in SU(N);\ \begin{matrix} A^TC \text{ is symmetric}, B^TD \text{ is symmetric}\\ A^TD-C^TB=\mathbf{1}\end{matrix}\right\}. \end{aligned} \tag{24}$$

D. *K* is the symmetry group of the concurrence form

We are now in a position to provide the physical interpretation of K. Namely, K is the symmetry group of the concurrence bilinear form, as stated in Theorem I.3.

Proof of Theorem I.3: We first prove that $v\in K$ iff $\mathcal{C}_n(v|\phi\rangle, v|\psi\rangle)=\mathcal{C}_n(|\phi\rangle,|\psi\rangle)$ for all $|\phi\rangle$, $|\psi\rangle\in\mathcal{H}_n$. Let $X=\log v$. Since $X\in\mathfrak{su}(N)$, X is anti-Hermitian, i.e., $X=-X^\dagger=-\overline{X^T}$. Finally, recall $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)$. Thus in mathematical notation, we have for $w,x\in\mathcal{H}_n$ the concurrence form given by $\mathcal{C}_n(w,x)=w^TSv$. Hence

$$(X=S^{-1}\overline{X}S)\Leftrightarrow(SX=\overline{X}S)\Leftrightarrow(SX=-X^TS)\Leftrightarrow(X^TS+SX=0)\Leftrightarrow(v^TSv=S). \tag{25}$$

Now the first item is equivalent to $v\in K$ while the last is equivalent to $\mathcal{C}(vw,vx)=(w^Tv^T)S(vx)=w^T(v^TSv)x=w^TSx=\mathcal{C}(w,x)$ for all $w,x\in\mathcal{H}_n$.

We next prove that for n odd, $K\cong Sp(N/2)$. To do so, it suffices to show n odd implies $\mathcal{C}_n$ is a nondegenerate two-form on $\mathcal{H}_n$. We first show $\mathcal{C}_n(x,w)=-\mathcal{C}_n(w,x)$ for any $w,x\in\mathcal{H}_n$. Noting that the transpose of a 1×1 matrix is again the same matrix, we realize that $\mathcal{C}_n$ is a two-form as follows:

$$\mathcal{C}_n(w,x)=w^TSx=[w^TSx]^T=x^TS^Tw=-x^TSw=-\mathcal{C}_n(x,w). \tag{26}$$

Moreover, consider the tensor expression for S. We see that no eigenvalues of S are zero, and hence the form is nondegenerate. Thus, we must have $K\cong Sp(N/2)$.

Suppose now that n is even. We finally prove $K\cong SO(N)$. It suffices to construct a real vector space $V_{\mathbb{R}}\subset\mathcal{H}_n$ so that the following properties hold:

- $K\cdot V_{\mathbb{R}}\subseteq V_{\mathbb{R}}$;
- The restriction of $\mathcal{C}_n$ to $V_{\mathbb{R}}\times V_{\mathbb{R}}$ is the usual dot product in the coordinates of a given basis.

Consider then $V_{\mathbb{R}}=\mathrm{span}_{\mathbb{R}}\{E_0|j\rangle;\ 0\leqslant j\leqslant N-1\}$, for E_0 the standard entangler of Definition II.9. Since E_0 is an entangler, certainly $K\cdot V_{\mathbb{R}}\subset V_{\mathbb{R}}$ since K acts on this real vector space by (real) orthogonal maps. Moreover, consider the concurrence on $V_{\mathbb{R}}$. For w,x in the $\mathbb{R}$ span of the computational basis, we have E_0w, E_0x generic vectors in $V_{\mathbb{R}}$. Then

$$\mathcal{C}_n(E_0w,E_0x)=(E_0w)^TS(E_0x)=w^TE_0^TSE_0x=w^TE_0^TE_0E_0^TE_0x=w^T\mathbf{1}x=w\cdot x, \tag{27}$$

with the fourth equality by Lemma II.11. Hence in an even number of qubits, K fixes a real inner product on a real vector subspace of $\mathcal{H}_n$. Thus $K \cong SO(N)$. □

Scholium II.18: For n even, for E_0 the standard entangler of Definition II.9, for any $|\phi\rangle$, $|\psi\rangle \in \mathcal{H}_n$, we have $\mathcal{C}_n(E_0|\phi\rangle, E_0|\psi\rangle) = \overline{\langle\phi|\psi\rangle}$.

Remark II.19: Note that independent of any discussion of the algebra $\mathfrak{a}$ in n an odd number of qubits, we have shown that the Cartan involution θ has type **AII**. Hence any commutative $N/2-1$ dimensional subalgebra of $\mathfrak{p}$ must be maximal, and the concurrence canonical decomposition $SU(N)=KAK$ is well-defined for n odd. ◇

Remark II.20: Similar to Scholium II.18, note that the standard (real) finagler F_0 of Definition II.16 translates between the concurrence and the more standard two-form $(w,x) \mapsto w^T[(-i\sigma^y) \otimes \mathbf{1}_{N/2}]x$. Indeed, $F_0^{-1} = F_0^T$ since F_0 is orthogonal. Moreover, let w,x be in the real span of the computational basis states $\{|j\rangle;\ 0 \leqslant j \leqslant N-1\}$. Then we may view $\{F_0|j\rangle;\ 0 \leqslant j \leqslant N-1\}$ as a finagled basis, and the pullback of the concurrence from the finagled to the computational basis is the model two-form. Indeed, labeling $\Sigma = (-i\sigma^y) \otimes \mathbf{1}_{N/2}$, $F_0 \Sigma F_0^T = S$ and F_0 real imply $\Sigma = F_0^T S F_0$. Hence $\mathcal{C}_n(F_0 w, F_0 x) = (F_0 w)^T S (F_0 x) = w^T \Sigma x$. ◇

E. Cartan involution in coordinates

We finally present the Cartan involution in coordinates and provide some sample calculations. Let $X \in \mathfrak{su}(N)$, say with $X = \Sigma_{j,k=0}^{N-1} x_{j,k}|k\rangle\langle j|$. We now compute explicitly $\theta(X)$ so as to arrive at coefficient expressions for $\mathfrak{p}$, $\mathfrak{k}$.

$$\theta(X) = (-1)^n \sum_{j,k=0}^{N-1} \overline{x_{j,k}} S|k\rangle\langle j|S = (-1)^{n+n-\#k+\#j} \sum_{j,k=0}^{N-1} \overline{x_{j,k}}|N-k-1\rangle\langle N-j-1|.$$

Consequently, we have the following characterizations:

- $X = \Sigma_{j,k=0}^{N-1} x_{j,k}|k\rangle\langle j| \in \mathfrak{p}$ iff $[(X \in \mathfrak{su}(N))$ and $(x_{N-1-k,N-1-j} = (-1)^{\#j+\#k+1}\overline{x_{k,j}})]$;
- $X = \Sigma_{j,k=0}^{N-1} x_{j,k}|k\rangle\langle j| \in \mathfrak{k}$ iff $[(X \in \mathfrak{su}(N))$ and $(x_{N-1-k,N-1-j} = (-1)^{\#j+\#k}\overline{x_{k,j}})]$.

This moreover produces the following description of $\mathfrak{k}$.

$$\begin{aligned}\mathfrak{k} = \mathrm{span}_{\mathbb{R}}\{&|k\rangle\langle j| - |j\rangle\langle k| + (-1)^{\#j+\#k}|N-k-1\rangle\langle N-j-1| - (-1)^{\#j+\#k}|N-j-1\rangle\langle N-k-1|\} \\ &\sqcup \{i|k\rangle\langle j| + i|j\rangle\langle k| + (-1)^{\#k+\#j+1} i|N-j-1\rangle\langle N-k-1| + (-1)^{\#j+\#k+1} i|N-k-1\rangle \\ &\times \langle N-j-1|\} \sqcup \{i|j\rangle\langle j| - i|N-j-1\rangle\langle N-j-1|\}. \end{aligned} \tag{28}$$

Remark II.21: We *warn* the reader that the above expression does not allow one to count dimensions. Several repetitions occur from set to set, and moreover the expressions may vanish in case $j = N-k-1$. ◇

F. Example in the two-qubit case

Recall the subalgebra $[\mathbf{1} \otimes \mathfrak{su}(2)] \oplus [\mathfrak{su}(2) \otimes \mathbf{1}]$ of infinitesimal transformations by $SU(2) \otimes SU(2) \subseteq SU(4)$. We show how the above equation (28) recovers this subalgebra in the case of $n=2$ qubits.

We begin by plugging $k=0$, $j=1$. Expanding into binary (or writing out the matrix) makes clear this is a tensor, and moreover a tensor by an identity matrix. Recall again that both are required to be in the Lie algebra of $SU(2) \otimes SU(2)$:

$$\begin{aligned}|0\rangle\langle 1| - |1\rangle\langle 0| - |3\rangle\langle 2| + |2\rangle\langle 3| &= |00\rangle\langle 01| - |01\rangle\langle 00| - |11\rangle\langle 10| + |10\rangle\langle 11| \\ &= (|0\rangle\langle 0| + |1\rangle\langle 1|) \otimes (|0\rangle\langle 1| - |1\rangle\langle 0|). \end{aligned} \tag{29}$$

One may similarly analyze the following matrices:

$$
\begin{aligned}
&i|0\rangle\langle 1|+i|1\rangle\langle 0|+i|3\rangle\langle 2|+i|2\rangle\langle 3|,\\
&|0\rangle\langle 2|-|2\rangle\langle 0|-|3\rangle\langle 1|+|1\rangle\langle 3|,\\
&i|0\rangle\langle 2|+i|2\rangle\langle 0|+i|3\rangle\langle 1|+i|1\rangle\langle 3|.
\end{aligned}
\tag{30}
$$

Note that for the next four expressions, substitution returns a 0 matrix:

$$
\begin{aligned}
&|0\rangle\langle 3|-|3\rangle\langle 0|+|3\rangle\langle 0|-|0\rangle\langle 3|,\\
&i|0\rangle\langle 3|+i|3\rangle\langle 0|-i|3\rangle\langle 0|-i|0\rangle\langle 3|,\\
&|1\rangle\langle 2|-|2\rangle\langle 1|+|2\rangle\langle 1|-|1\rangle\langle 2|,\\
&i|1\rangle\langle 2|+i|2\rangle\langle 1|-i|2\rangle\langle 1|-i|1\rangle\langle 2|.
\end{aligned}
\tag{31}
$$

Further substitution yields the following:

$$
\begin{aligned}
&|1\rangle\langle 3|-|3\rangle\langle 1|+|2\rangle\langle 0|-|0\rangle\langle 2|,\\
&i|1\rangle\langle 3|+i|3\rangle\langle 1|+i|2\rangle\langle 0|+i|0\rangle\langle 2|,\\
&|2\rangle\langle 3|-|3\rangle\langle 2|-|1\rangle\langle 0|+|0\rangle\langle 1|,\\
&i|2\rangle\langle 3|+i|3\rangle\langle 2|+i|1\rangle\langle 0|+i|0\rangle\langle 1|.
\end{aligned}
\tag{32}
$$

Finally, we consider the diagonal matrices in $\mathfrak{k}$:

$$
\begin{aligned}
&i|0\rangle\langle 0|-i|3\rangle\langle 3|,\\
&i|1\rangle\langle 1|-i|2\rangle\langle 2|.
\end{aligned}
\tag{33}
$$

Note that the $\mathbb{R}$ span of these two matrices coincides with $\mathbb{R}(i\sigma_z^1)\oplus\mathbb{R}(i\sigma_z^2)$.

The Cartan involution formalism thus works, although in a cumbersome way. We next explore the answer it returns in the three-qubit case.

G. Example in the three-qubit case, $K=Sp(4)$

We now describe explicitly the output of Eq. (28) in three qubits. The corresponding real Lie algebra is thirty-six dimensional, which implies by the Cartan classification that K is an abstract copy of $Sp(4)$. A copy of $SO(8)$ would rather be 28 dimensional.

The simplest way to organize the three qubit computation is to appeal to separation. We say a term $|k\rangle\langle j|$ has separation $|k-j|$ and extend linearly. In Eq. (28), each matrix described has a well-defined separation:

$$
\begin{aligned}
&\text{Separation } 0 && i|0\rangle\langle 0|-i|7\rangle\langle 7|\\
&\text{Total } 4 && i|1\rangle\langle 1|-i|6\rangle\langle 6|,\\
&&& i|2\rangle\langle 2|-i|5\rangle\langle 5|,\\
&&& i|3\rangle\langle 3|-i|4\rangle\langle 4|,
\end{aligned}
\tag{34}
$$

$$
\begin{aligned}
&\text{Separation } 1 && |0\rangle\langle 1|-|1\rangle\langle 0|-|7\rangle\langle 6|+|6\rangle\langle 7|\\
&\text{Total } 8 && i|0\rangle\langle 1|+i|1\rangle\langle 0|+i|7\rangle\langle 6|+i|6\rangle\langle 7|,\\
&&& |1\rangle\langle 2|-|2\rangle\langle 1|+|6\rangle\langle 5|-|5\rangle\langle 6|,\\
&&& i|1\rangle\langle 2|+i|2\rangle\langle 1|-i|6\rangle\langle 5|-i|5\rangle\langle 6|,\\
&&& |2\rangle\langle 3|-|3\rangle\langle 2|-|5\rangle\langle 4|+|4\rangle\langle 5|,\\
&&& i|2\rangle\langle 3|+i|3\rangle\langle 2|+i|5\rangle\langle 4|+i|4\rangle\langle 5|,\\
&&& |3\rangle\langle 4|-|4\rangle\langle 3|,\quad i|3\rangle\langle 4|+i|4\rangle\langle 3|,
\end{aligned}
\tag{35}
$$

$$
\begin{aligned}
&\text{Separation } 2 && |0\rangle\langle 2|-|2\rangle\langle 0|-|7\rangle\langle 5|+|5\rangle\langle 7|\\
&\text{Total } 6 && |0\rangle\langle 2|+i|2\rangle\langle 0|+i|7\rangle\langle 5|+i|5\rangle\langle 7|,\\
&&& |1\rangle\langle 3|-|3\rangle\langle 1|-|6\rangle\langle 4|+|4\rangle\langle 6|,\\
&&& i|1\rangle\langle 3|+i|3\rangle\langle 1|+i|6\rangle\langle 4|+i|4\rangle\langle 6|,\\
&&& |2\rangle\langle 4|-|4\rangle\langle 2|+|5\rangle\langle 3|-|3\rangle\langle 5|,\\
&&& i|2\rangle\langle 4|+i|4\rangle\langle 2|-i|5\rangle\langle 3|-i|3\rangle\langle 5|
\end{aligned}
\tag{36}
$$

$$\begin{aligned}
&\text{Separation 3} \quad |0\rangle\langle 3|-|3\rangle\langle 0|+|7\rangle\langle 4|-|4\rangle\langle 7| \\
&\text{Total 6} \quad i|0\rangle\langle 3|+i|3\rangle\langle 0|-i|7\rangle\langle 4|-i|4\rangle\langle 7|, \\
&\qquad |1\rangle\langle 4|-|4\rangle\langle 1|+|6\rangle\langle 3|-|3\rangle\langle 6|, \\
&\qquad i|1\rangle\langle 4|+i|4\rangle\langle 1|-i|6\rangle\langle 3|-i|3\rangle\langle 6|, \\
&\qquad |2\rangle\langle 5|-|5\rangle\langle 2|, \quad i|2\rangle\langle 5|+i|5\rangle\langle 2|, \qquad (37)
\end{aligned}$$

$$\begin{aligned}
&\text{Separation 4} \quad |0\rangle\langle 4|-|4\rangle\langle 0|-|7\rangle\langle 3|+|3\rangle\langle 7| \\
&\text{Total 4} \quad i|0\rangle\langle 4|+i|4\rangle\langle 0|+i|7\rangle\langle 3|+i|3\rangle\langle 7|, \\
&\qquad |1\rangle\langle 5|-|5\rangle\langle 1|-|6\rangle\langle 2|+|2\rangle\langle 6|, \\
&\qquad i|1\rangle\langle 5|+i|5\rangle\langle 1|+i|6\rangle\langle 2|+i|2\rangle\langle 6|, \qquad (38)
\end{aligned}$$

$$\begin{aligned}
&\text{Separation 5} \quad |0\rangle\langle 5|-|5\rangle\langle 0|+|7\rangle\langle 2|-|2\rangle\langle 7| \\
&\text{Total 4} \quad i|0\rangle\langle 5|+i|5\rangle\langle 0|-i|7\rangle\langle 2|-i|2\rangle\langle 7|, \\
&\qquad |1\rangle\langle 6|-|6\rangle\langle 1|, \\
&\qquad i|1\rangle\langle 6|+i|6\rangle\langle 1|, \qquad (39)
\end{aligned}$$

$$\begin{aligned}
&\text{Separation 6} \quad |0\rangle\langle 6|-|6\rangle\langle 0|+|7\rangle\langle 1|-|1\rangle\langle 7| \\
&\text{Total 2} \quad i|0\rangle\langle 6|+i|6\rangle\langle 0|-i|7\rangle\langle 1|-i|1\rangle\langle 7|, \qquad (40)
\end{aligned}$$

$$\begin{aligned}
&\text{Separation 7} \quad |0\rangle\langle 7|-|7\rangle\langle 0| \\
&\text{Total 2} \quad i|0\rangle\langle 7|+i|7\rangle\langle 0|. \qquad (41)
\end{aligned}$$

Thus we see a total of $4+8+6+6+4+4+2+2=36$ real dimensions in $\mathfrak{k}$. Now by the Cartan classification (Ref. 8, p. 518), the Cartan involution θ must be either type **AI** fixing an abstract copy of $SO(28)$, type **AIII** fixing some $S[U(p)\oplus U(q)]$ for $p+q=2^n$, or else type **AII** fixing an abstract copy of $Sp(4)$. Since only $Sp(4)$ is thirty-six dimensional, we see $\mathfrak{k}\cong\mathfrak{sp}(4)$ and $K\cong Sp(4)$.

III. APPLICATIONS TO CONCURRENCE CAPACITY

In this section we focus on an application of the concurrence canonical decomposition $SU(N)=KAK$ of Definition I.2 when the number of qubits n is even. Namely, we study how a given computation $v\in SU(N)$ may change the concurrence of the quantum data state. Since we have the concurrence $C_n(|\psi\rangle)=|\overline{\langle\psi|}(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)|\psi\rangle|$ with the n-tangle $\tau_n=C_n^2$ for n even, there are immediate applications to the n-tangle as well.

Let $v\in SU(N)$. Recall from Definition I.5 that the concurrence capacity is defined as

$$\kappa(v)=\max\{C_n(v|\psi\rangle);C_n(|\psi\rangle)=0,\langle\psi|\psi\rangle=1\}. \qquad (42)$$

Since we vary over all $C_n(|\psi\rangle)=0$, we see that for $k\in K$ we have $\kappa(vk)=\kappa(v)$ by symmetry. Immediately $\kappa(kv)=\kappa(v)$. Thus, for $v=k_1ak_2$ the C.C. decomposition of any $v\in SU(N)$, we have $\kappa(v)=\kappa(k_1ak_2)=\kappa(a)$.

We next describe the concurrence capacity of any $a\in A$. The formalism makes strong use of entanglers to translate between $\mathcal{C}_n$ and $(w,x)\mapsto w^Tx$.

Definition III.1: The *concurrence spectrum* $\lambda_c(v)$ of $v\in SU(N)$ is the spectrum of $E_0^\dagger vE_0(E_0^\dagger vE_0)^T$, for E_0 the standard entangler of Definition II.9. Note that the spectrum is the set of eigenvalues since $\mathcal{H}_n$ is finite dimensional. The *convex hull* $\mathrm{CH}[\lambda_c(v)]$ of $\lambda_c(v)$ is the set of all line segments joining all points of $\lambda_c(v)$, i.e.,

$$\mathrm{CH}[\lambda_c(v)]=\left\{\sum_{z_j\in\lambda_c(v)} t_jz_j;0\leqslant t_j\leqslant 1,\sum_{j=0}^{\#\lambda_c(v)} t_j=1\right\}. \qquad (43)$$

These definitions allow us then to prove the following general results regarding concurrence capacity. The techniques closely follow those in prior work.[26]

Lemma III.2: Let $v \in SU(N)$, *with* CCD $v = k_1 a k_2$ *for* $a = E_0 d E_0^\dagger$ *for* d *diagonal in* $SU(N)$*:*

- $\lambda_c(v) = \lambda_c(a) = \{d_j^2; d = \Sigma_{j=0}^{N-1} d_j |j\rangle\langle j|\}$.
- $\kappa(v) = \kappa(a) = \max\{|\Sigma_{j=0}^{N-1} a_j^2 d_j^2|; |\psi\rangle = \Sigma_{j=0}^{N-1} a_j |j\rangle, \langle\psi|\psi\rangle = 1, \overline{\langle\psi|}\,|\psi\rangle = 0\}$.
- $(\kappa(v) = \kappa(a) = 1) \Leftrightarrow (0 \in \mathrm{CH}[\lambda_c(v)] = \mathrm{CH}[\lambda_c(a)])$.

Proof: For the first item, recall $v = k_1 a k_2$. Thus the following expression results from expanding Definition III.1:

$$E_0^\dagger v E_0 (E_0^\dagger v E_0)^T = [(E_0^\dagger k_1 E_0)(E_0^\dagger a E_0)(E_0^\dagger k_2 E_0)][(E_0^\dagger k_2 E_0)^T (E_0^\dagger a E_0)^T (E_0^\dagger k_1 E_0)^T]. \quad (44)$$

Label the elements of $SO(N)$ by $o_1 = (E_0^\dagger k_1 E_0)$, $o_2 = (E_0^\dagger k_2 E_0)$, and put $d = E_0^\dagger a E_0$ diagonal. Then the above reduces to $o_1 d o_2 o_2^T d^T o_1^T = o_1 d^2 o_1^{-1}$, with spectrum identical to d.

For the next item, compare the two-qubit case [Ref. 26, Eq. (41)] and recall Scholium II.18. Suppose $C_n(|\varphi\rangle) = 0$. Then per Scholium II.18, for $|\psi\rangle = E_0^\dagger |\varphi\rangle$ we have $0 = \mathcal{C}_n(E_0 E_0^\dagger |\varphi\rangle, E_0 E_0^\dagger |\varphi\rangle) = \overline{\langle\psi|}\,|\psi\rangle$. Now for $\kappa(a)$, take $|\psi\rangle = E_0^\dagger |\varphi\rangle$. We then maximize over expressions $\mathcal{C}_n(a|\varphi\rangle, a|\varphi\rangle) = \mathcal{C}_n(E_0 E_0^\dagger a E_0 |\psi\rangle, E_0 E_0^\dagger a E_0 |\psi\rangle) = \mathcal{C}_n(E_0 d |\psi\rangle, E_0 d |\psi\rangle) = \overline{\langle\psi|} d^2 |\psi\rangle$.

The final item makes use of the Schwarz inequality. For the concurrence capacity to be maximal, there is by compactness of the set of normalized kets some normalized $|\psi\rangle$ with $C_n(|\Phi\rangle) = 1$. For $|\psi\rangle = \Sigma_{j=0}^{N-1} a_j |j\rangle$,

$$1 = \left| \sum_{j=0}^{N-1} a_j^2 d_j^2 \right| \leqslant \sum_{j=0}^{N-1} |a_j^2 d_j^2| = \sum_{j=0}^{N-1} |a_j|^2 = 1. \quad (45)$$

The Schwarz *equality* further requires some $z \in \mathbb{C}$, $z^- z = 1$, so that $a_j^2 d_j^2 = |a_j|^2 z, \forall j$. Now since $\overline{\langle\psi|}\,|\psi\rangle = 0$,

$$0 = \sum_{j=0}^{N-1} a_j^2 = \sum_{j=0}^{N-1} |a_j|^2 \overline{d_j^2} z. \quad (46)$$

Multiplying through by $\overline{z}$ and taking the complex conjugate, we see $0 \in \mathrm{CH}[\lambda_c(v)]$. □

As already noted in the Introduction, the concurrence capacity κ is properly thought of as a function of A rather than a function of $SU(N)$. This is advantageous from a computational standpoint, because in order to calculate $\kappa(v)$ one need minimize over a function involving $N-1$ real parameters in A versus N^2-1 parameters describing a general $v \in SU(N)$. We next consider typical values for a large number of qubits. To do so, we need to be able to randomly choose an element of A.

Definition III.3: Consider the following coordinate map on the commutative group A:

$$[0,2\pi]^{N-1} \to A \text{ by } (t_0, t_2, \ldots, t_{N-2}) \mapsto \exp E_0 \left(\sum_{j=0}^{N-2} i t_j |j\rangle\langle j| - i t_j |j+1\rangle\langle j+1| \right) E_0^\dagger. \quad (47)$$

The Haar measure on da is the group multiplication invariant measure $da = (2\pi)^{-N+1} dt_0\ dt_2\ \cdots\ dt_{N-2}$. This is the pushforward of the independent product of uniform measures $dt_j/(2\pi)$ on each $[0,2\pi]$.

Recall that for $p = 2n$, Theorem I.7 asserts that according to da, almost all $a \in A$ have $\kappa(a) = 1$ for p large. Specifically, we assert

$$\lim_{p \to \infty} da(\{a \in A; \kappa(a) = 1\}) = 1. \quad (48)$$

We prove this assertion shortly, but we first need a lemma.

Lemma III.4: Label as uniform distribution on the circle a distribution whose pullback to $[0,2\pi]$ *under* $t\mapsto e^{2\pi i t}$ *is uniform, and similarly say two random variables* Z_1, Z_2 *on* $\{z\bar{}z=1\}$ *are independent iff their pullbacks to* $[0,2\pi]\times[0,2\pi]$ *are. Then suppose* Z_1 *is any random variable on the circle, and let* Z_2 *be independent to* Z_1 *and uniform. Then* Z_1Z_2 *is uniform.*

Proof: Consider the random variable $T=-i\log Z_1-i\log Z_2 \bmod 2\pi$ on $[0,2\pi]$. Let $f_1(t)$ be the pullback probability density function of the nonuniform random variable Z_1 to $[0,2\pi]$. We let $F_T(t)=\mathrm{Prob}(T\leqslant t)$ be the cumulative density function. Then

$$F_T(t)=\frac{1}{2\pi}\int_0^{2\pi}\mathrm{Prob}(-i\log Z_2\in[s,s+t])f_1(s)ds=\frac{1}{2\pi}\int_0^{2\pi}tf_1(s)ds=t/(2\pi). \tag{49}$$

Since $F_T(t)=t/(2\pi)$, we see that T is uniform. Hence Z_1Z_2 is uniform. □

Proof of Theorem I.7: First, let us check that $\{\kappa(a)=1\}$ is da-measurable. To see this, note that the concurrence spectrum $\lambda_c(a)$ may be expressed in terms of the coordinates t_j as follows:

$$d_0^2=\mathrm{e}^{2it_0},d_1=\mathrm{e}^{2it_1-2it_0},d_2^2=\mathrm{e}^{2it_2-2it_1},\cdots d_j^2=\mathrm{e}^{2it_j-2it_{j-1}},\ldots,d_{N-1}^2=\mathrm{e}^{-2it_{N-2}}. \tag{50}$$

Thus Lemma III.2 induces a measurable condition on the t_j.

Continuing the proof, by direct calculation Z^2 is a uniform random variable on the circle $\{z\bar{}z=1\}$ given that Z is such. Thus note that d_0^2, d_2^2, $d_4^2,\ldots,d_{N-1}^2$ are $p=N/2$ independent, uniform random variables by Lemma III.4. It suffices to show that $\ell+1=p$ independent, random variables on the circle have 0 in their convex hull as $\ell\mapsto\infty$. Relabel $d_0^2=Z_0$, $d_2^2=Z_1,\ldots,d_{N-1}^2=Z_\ell$.

Without loss of generality, say $Z_0=1$. Let C_2 be the event that no $Z_1,Z_2,\ldots,Z_\ell$ is in the second quadrant $\{z=x+iy;x<0,y>0\}$, with C_3 similar for the third quadrant $\{x<0,y<0\}$. Let D be the event that 0 is in the convex hull of Z_0, $Z_1,\ldots,Z_\ell$. Then $(\mathrm{NOT}\ C_2\cap\mathrm{NOT}\ C_3)\subset D$. Then $\mathrm{Prob}(\mathrm{NOT}\ C_2\cap\mathrm{NOT}\ C_3)\leqslant\mathrm{Prob}(D)$, and

$$1-\mathrm{Prob}(D)\leqslant 1-\mathrm{Prob}(\mathrm{NOT}\ \ C_2\ \ \mathrm{and}\ \ \mathrm{NOT}\ \ C_3)=\mathrm{Prob}(C_2\ \ \mathrm{or}\ \ C_3)=(1/2)^\ell. \tag{51}$$

Hence as $\ell\to\infty$, $\mathrm{Prob}(D)$ goes to 1. Hence the probability $\mathrm{CH}[\lambda_c(v)]$ contains 0 limits to 1. □

IV. CONCLUSIONS AND ONGOING WORK

We have shown that there exists a generalized canonical decomposition of unitary operators on n qubits which may be used to study changes in the concurrence entanglement monotone. This decomposition closely resembles the older two-qubit decomposition when n is even, and it may be used to study the concurrence-entanglement capacity of generic unitary operators. The main result is that such a generic unitary operator is almost always perfectly entangling with respect to the concurrence monotone when the number of qubits is large and even.

Ongoing work would attempt to extend the dynamical viewpoint taken in this paper. Specifically, the unitary operator describes the dynamics of a quantum data state, and the present techniques allow us to quantitatively study the dynamics of the concurrence entanglement measure. Similarly, we would wish to study the dynamics of this concurrence capacity of quantum computations in naturally defined families or sequences of such computations. As a separate topic, we might also study the failure of the concurrence function itself by quantifying how entangled with respect to other measures a quantum state with zero concurrence may be.

APPENDIX A: COMPUTING THE CCD WHEN THE NUMBER OF QUBITS IS EVEN

This appendix recalls how to compute the canonical decomposition in an even number $n=2p$ of qubits. Note that other arguments in the case $n=2$[10,14] may be found in the literature, and that the present treatment is a straightforward genearlization of a matrix-oriented treament in the two-qubit case (Ref. 4, Appendix A). It is included for completeness.

The overall structure of the algorithm contains two steps.

(1) Produce an algorithm for computing the decomposition $SU(N)=SO(N)\ D\ SO(N)$ for D the diagonal subgroup of $SU(N)$. We will refer to this decomposition as the *unitary* SVD *decomposition* henceforth.
(2) Recall E_0, the standard entangler of Definition II.9. Given a $v\in SU(N)$ for which we wish to compute the CCD, compute first the unitary SVD $E_0^\dagger v E_0 = o_1 d o_2$. Then we have a CCD given by

$$v=(E_0 o_1 E_0^\dagger)(E_0 d E_0^\dagger)(E_0 o_2 E_0^\dagger)=k_1 a k_2, \tag{A1}$$

since $k_1=E_0 o_1 E_0^\dagger\in K$, $k_2=E_0 o_2 E_0^\dagger\in K$, and $a=E_0 d E_0^\dagger\in A$.

Note that the unitary SVD decomposition exists due to *KAK* metadecomposition theorem, taking as inputs $G=SU(N)$, $\theta_{\mathbf{AI}}(X)=\overline{X}$, and $\mathfrak{a}$ the diagonal subalgebra of $\mathfrak{su}(N)$.

Before continuing to Step 1, we first prove a lemma. It is useful in computing particular instances of the unitary SVD.

Lemma A.1: For any $p\in SU(N)$ with $p=p^T$, there is some $o\in SO(N)$ such that $p=odo^T$ with d a diagonal, determinant one matrix.

Proof: We first show the following:

$\forall\ a,b$, symmetric real $N\times N$ matrices with $ab=ba$; there is some $o\in SO(N)$ such that oao^T and obo^T are diagonal.

It suffices to construct a basis which is simultaneously a basis of eigenvectors for both a and b. Thus, say V_λ is the λ eigenspace of b. For $x\in V_\lambda$, $b(ax)=a(bx)=\lambda ax$, i.e., $x\mapsto ax$ preserves the eigenspace. Now find eigenvectors for a restricted to V_λ, which remains symmetric. Thus we may find the desired $o\in SO(N)$, making choices of orderings and signs on an eigenbasis as appropriate for a determinant one.

Given the above, write $p=a+ib$. Now $\mathbf{1}=pp^\dagger=p\overline{p}=(a+ib)(a-ib)=(a^2+b^2)+i(ba-ab)$. Since the imaginary part of $\mathbf{1}$ is $\mathbf{0}$, we conclude that $ab=ba$. Hence a single o exists per the last paragraph which diagonalizes the real and imaginary parts. □

Suppose then that $v=o_1 d o_2$ is the unitary SVD of some $v\in SU(N)$. For convenience, we also label $v=po_3$ the type **AI** Cartan decomposition (Ref. 8, Theorem 1.1.iii, p. 252) (Ref. 11, Theorem 6.31.c). This is a generalized polar decomposition in which $p=p^T$, $k\in SO(N)$. Note that it is equivalent via Lemma A.1 to compute $v=pk$, as the unitary SVD follows by $v=(o_1 d o_1^T)k=o_1 d o_2$. Continuing to the algorithm for Step 1:

- Compute p^2 as follows: $p^2=pp^T=po_3o_3^Tp^T=vv^T$.
- Apply Lemma A.1 to p^2. Thus $p^2=o_1 d^2 o_1^T$ for $o_1\in SO(N)$.
- Choose square roots entrywise in d^2 to form d. Be careful to ensure $\det d=1$.
- Compute $p=o_1 d o_1^T$.
- Thus $o_3=p^\dagger v$, and $v=p(o_3)=o_1 d o_1^T o_3=o_1 d o_2$.

This concludes the algorithm for computing the unitary SVD of Step 1.

Step 2 is almost follows given the inline description. The reader may produce algorithms outputting E_0.

Another question is computational efficiency. This is ongoing work, but we note immediately that an implementation of the spectral theorem of Lemma A.1 is required. This will be difficult with current technologies in 16+ qubits. Moreover, in the range of 50 to 60 qubits an even spread of the concurrence spectrum $\lambda_c(v)$ of Definition III.1 would make certain elements indistinguishable at 16-digit precision.

APPENDIX B: CONCURRENCE LEVEL SETS AND *K* ORBITS

Mathematically, related measures are often easier to use than C_n. For example, the concurrence quadratic form $Q_n^C(|\psi\rangle)=\mathcal{C}_n(|\psi\rangle,|\psi\rangle)$ with $C_n(|\psi\rangle)=|Q_n^C(|\psi\rangle)|$ has smaller level sets than

C_n itself. Moreover, it turns out that the normalized states within these level sets $[Q_n^C]^{-1}(\{z\}) = \{|\psi\rangle; Q_n^C(|\psi\rangle) = z\}$ are naturally orbits of the group K, which must then be false for C_n.

Suppose throughout $n=2p$ is an even number of qubits. For a vector $v \in \mathbb{C}^N$, put $Q_{\mathbf{AI}}(v) = v^T v$, noting that $Q_{\mathcal{C}}(E_0 v) = Q_{\mathbf{AI}}(v)$. Moreover, for $O \in SO(N)$, we have the following:

$$Q_{\mathbf{AI}}(O \cdot v) = Q_{\mathcal{C}}[E_0 O E_0^\dagger \cdot (E_0 v)]. \tag{B1}$$

Thus we may study level sets of $Q_{\mathbf{AI}}$ under $SO(N)$ rather than study level sets of $Q_{\mathcal{C}}$ under K. Now if $v = v_1 + iv_2$ is a decomposition into real and imaginary parts of a complex vector, note that $Q_{\mathbf{AI}}(v_1 + iv_2) = v^T v = (|v_1|^2 - |v_2|^2) + 2i(v_1 \cdot v_2)$.

Lemma B.1: Label $S^{2N-1} = \{|\psi\rangle; \langle\psi|\psi\rangle = 1\}$. *We have the following orbit decompositions of the level sets* $Q_{\mathbf{AI}}^{-1}(\alpha) \cap S^{2N-1}$ *for any fixed* $\alpha \in \mathbb{C}$.

(1) Let t *be real, and let* $v \in Q_{\mathbf{AI}}^{-1}(t) \cap S^{2N-1}$. *Then* $Q_{\mathbf{AI}}^{-1}(t) \cap S^{2N-1} = [SO(N) \cdot v]$.

(2) Let α *be complex, and let* $v \in Q_{\mathbf{AI}}^{-1}(\alpha) \cap S^{2N-1}$. *Then* $Q_{\mathbf{AI}}^{-1}(\alpha) \cap S^{2N-1} = [SO(N) \cdot v]$.

Proof: For the first item, write $v = v_1 + iv_2$. Then $v_1 \cdot v_2$ is zero as a set of real vectors. Consider the subset of $\mathbb{R}^{2N}$ given by $|v_1|^2 - |v_2|^2 = t$. Suppose now we have another pair of orthogonal vectors w_1, w_2 with $|w_1|^2 - |w_2|^2 = t$ and $|w_1|^2 + |w_2|^2 = 1$. Then $|w_1|^2 = |v_1|^2 = (1 - t)/2$, thus $|v_2|^2 = |w_2|^2$ so that there is some $O \in SO(N)$ with $O \cdot v_1 = w_1$, $O \cdot v_2 = w_2$.

For the second item, suppose $\alpha = e^{i\phi} t$ for some $t \in \mathbb{R}$. Now if $v \in Q_{\mathbf{AI}}^{-1}(\alpha)$, then note that we have $Q_{\mathbf{AI}}(e^{-i\phi/2} v) = e^{-i\phi} Q_{\mathbf{AI}}(v) = e^{-i\phi} \alpha = t$. Conversely, if $w \in Q_{\mathbf{AI}}^{-1}(t)$ we have $e^{i\phi/2} w \in Q_{\mathbf{AI}}^{-1}(\alpha)$. Having established bijective phase maps between the two level sets, it must also be the case that the level set of α forms a single $SO(N)$ orbit. □

Corollary B.2: The restricted action of K to the normalized kets in any concurrence level set is transitive. Specifically, suppose $\alpha \in \mathbb{C}$, *with* $|\psi\rangle$ *normalized with* $Q_{\mathcal{C}}(|\psi\rangle) = \alpha$. *Then label* $S^{2N-1} = \{\langle\phi|\phi\rangle = 1\}$ *the set of normalized kets. Per Eq. (B1), we have* $K \cdot |\psi\rangle = Q_{\mathcal{C}}^{-1}(\alpha) \cap S^{2N-1}$.

We restate the result colloquially. Should any two normalized states $|\phi\rangle$, $|\psi\rangle$ have the same concurrence, then there is some global phase $e^{i\theta}$ so that $|\phi\rangle = e^{i\theta} k |\psi\rangle$ for $k \in K = E_0 SO(N) E_0^\dagger$.

APPENDIX C: CONCURRENCE IS AN ENTANGLEMENT MONOTONE

The n-tangle, defined to be $\tau_n(|\psi\rangle) = C_n(|\psi\rangle)^2$ has been proposed[25] as a measure of an n-qubit entanglement for n even. The n-tangle of a state $|\psi\rangle$, like the n-concurrence, assumes real values in the range $0 \leqslant \tau_n \leqslant 1$ and has been shown to be an entanglement monotone, meaning τ_n is a convex function on density matrices and is nonincreasing under local operations and classical communication (LOCC). Most of our arguments focus on constructions more directly related to the concurrence C_n rather than the n-tangle $\tau_n = (C_n)^2$. Therefore, for completeness, we show that the n-concurrence is, in fact, a good measure of entanglement. The monotonicity property of a function is established by considering its action on mixtures of quantum states encoded within Hermitian density matrices ρ with tr $\rho = 1$. See, e.g., Ref. 18.

Definition C.:1 The n-concurrence can be defined on mixed states ρ using the convex roof extension:

$$C_n(\rho) = \min\left\{ \sum_k \lambda_k C_n(|\psi^k\rangle); \quad \rho = \sum_k \lambda_k |\psi^k\rangle\langle\psi^k|, |\psi\rangle^k \in \mathcal{H}_n, \quad \langle\psi^k|\psi^k\rangle = 1 \right\}. \tag{C1}$$

This minimization is over all pure state ensemble decompositions of the state $\rho = \Sigma_k \lambda_k |\psi^k\rangle\langle\psi^k|$.

This definition is quite intricate. We point out the following remarkable result, not used in the sequel.

Theorem C.2 (Uhlmann[22,25]): *We may express* $C_n(\rho)$ *in closed form as follows:*

$$C_n(\rho) = \max\{0, \lambda_0 - \lambda_1 \cdots - \lambda_{N-1}\}. \tag{C2}$$

Here, the λ_k are the square roots of the eigenvalues (in nonincreasing order) of the product $\rho\tilde{\rho}$ where $\tilde{\rho}=S\overline{\rho}S^{-1}$.

The necessary and sufficient conditions for a function on quantum states to be a entanglement monotone are delineated in Ref. 23. For the n-concurrence, they can be summarized as follows:

- $C_n \geqslant 0$, and $C_n(\rho)=0$ if ρ is fully separable.
- C_n is a convex function, i.e., $C_n(p\rho_1+(1-p)\rho_2)\leqslant pC_n(\rho_1)+(1-p)C_n(\rho_2), \forall p\in[0,1]$ and ρ_1,ρ_2 Hermitian matrices of trace one.
- C_n is nonincreasing under LOCC. Specifically, $C_n(\rho)\geqslant \Sigma_j p_j C_n(\rho_j)$, where $\rho_j=A_j\rho A_j^\dagger/p_j$ are the states conditioned on the outcome j of a positive operator valued measurement (POVM) which occurs with probability $p_j=\mathrm{Tr}[A_j^\dagger A_j\rho]$.

Before proving this, we first establish the useful fact that the n-concurrence is invariant under permutations of the qubits. Defining Π_n to be the set of unitary operators corresponding to permutations on n qubits, we have the following.

Proposition C.3: For n even, $C_n(P|\psi\rangle)=C_n(|\psi\rangle)\forall P\in\Pi_n$.

Proof: Any permutation P on n elements can be written as a finite composition of transpositions on pairs of elements. Hence it suffices to show invariance under a single swap operation. Writing the swap operator between qubits j and k as

$$S_{jk}=\frac{\mathbf{1}_j\otimes\mathbf{1}_k+\sigma_j^x\otimes\sigma_k^x+\sigma_j^y\otimes\sigma_k^y+\sigma_j^z\otimes\sigma_k^z}{2}, \tag{C3}$$

we have for any state $|\psi\rangle$,

$$C_n(S_{jk}|\psi\rangle)=|\overline{\langle\psi|S_{jk}^\dagger}SS_{jk}|\psi\rangle|=|\overline{\langle\psi|}S_{jk}SS_{jk}|\psi\rangle|=|\overline{\langle\psi|}SS_{jk}^2|\psi\rangle|=C_n(|\psi\rangle). \tag{C4}$$

Here we have used the fact that S_{jk} is real symmetric and unitary, and in the third equality we use the fact that $[\sigma_j^y\otimes\sigma_k^y,\sigma_j^l\otimes\sigma_k^l]=0$ for $\sigma^l\in\{\sigma^x,\sigma^y,\sigma^z\}$. This proposition necessarily implies that $\Pi_n^+\subsetneq K$, where Π_n^+ is the set of unitary permutation matrices on n objects with $+1$ determinant, i.e., permutations composed of an even number of transpositions. □

Lemma C.4: $C_n(\rho)$ is an entanglement monotone.

Sketch: For the first condition, one first checks that $0\leqslant C_n\leqslant 1$ using the eigenvalue decomposition of the matrix $S=(-i\sigma_1^y)(-i\sigma_2^y)\cdots(-i\sigma_n^y)$. Then any separable state can be realized by stochastic local unitaries acting on the fiducial separable state $|0\rangle_n=|0_1\cdots 0_n\rangle$. Now, $C_n(|0\rangle_n)=0$ and C_n is invariant under local unitaries per Proposition II.1 and Theorem I.3. To generalize from pure states to density matrices, recall Definition C.1.

The second condition is shown by writing the minimal ensemble decompositions for ρ_1 and ρ_2 separately as

$$p\min_{\{\lambda_k,|\psi^k\rangle\}|\Sigma\lambda_k|\psi^k\rangle\langle\psi^k|=\rho_1}\sum_k\lambda_k C_n(|\psi^k\rangle)+(1-p)\min_{\{\beta_k,|\phi^k\rangle\}|\Sigma\beta_k|\phi^k\rangle\langle\phi^k|=\rho_2}\sum_k\beta_k C_n(|\phi^k\rangle). \tag{C5}$$

These are not necessarily the minimal decompositions for the composite state $\rho=pp_1+(1-p)p_2$, therefore, $C_n(p\rho_1+(1-p)\rho_2)\leqslant pC_n(\rho_1)+(1-p)C_n(\rho_2)$.

Finally, we show that the n-concurrence is on average nonincreasing under LOCC. First, because of permutation symmetry of the concurrence we can consider operations on one particular qubit of the n qubit system, say the first. An arbitrary, trace perserving, completely positive map on a quantum system can written in the Krauss decompostion[12] as $S(\rho)=\Sigma_j A_j\rho A_j^\dagger$ where the positive Krauss operators satisfy the sum rule $\Sigma_j A_j^\dagger A_j=\mathbf{1}$. The map can be composed of multiple operations with two operators at a time so we consider only two operators A_0 and A_1 acting on the first qubit. By the polar decomposition theorem, the operators can be written as $A_j=u_j b_j$, where $b_j=\sqrt{A_j^\dagger A_j}$ is positive and u_j is defined to be $\mathbf{1}$ on the kernel $\mathcal{K}$ of A_j and $A_j|A_j|^{-1}$ on $\mathcal{K}^\perp$.

Physically, the map $S(\rho)$ corresponds to a generalized measurement on ρ followed by a unitary operation conditioned on the measurement. Because of the sum rule, which corresponds to trace preservation, we can write $A_0 = w_o \cos gX$ and $A_1 = w_1 \sin gX$ for $g \in \mathbb{R}$ and X a positive operator with unit trace. These operators are expressed in simpler form by diagonalizing X, viz., $A_0 = u_o d_o v$ and $A_1 = u_1 d_1 v$, where $u_j, v \in SU(2)$ and d_j are real diagonal matrices with elements (q,r) and $(\sqrt{1-q^2}, \sqrt{1-r^2})$. The average concurrence of a state ρ after the 2 outcome POVM is

$$p_0 C_n(\rho_0) + p_1 C_n(\rho_1) = p_0 \min_{\{\lambda_k, |\psi^k\rangle\} | \Sigma \lambda_k |\psi^k\rangle\langle\psi^k| = \rho} \sum_k \lambda_k C_n(A_0 |\psi^k\rangle / \sqrt{p_0}) + p_1 \min_{\{\beta_k, |\phi^k\rangle\} | \Sigma \beta_k |\phi^k\rangle\langle\phi^k| = \rho} \sum_k \beta_k C_n(A_1 |\phi^k\rangle / \sqrt{p_1}). \tag{C6}$$

States conditioned on the first outcome satisfy

$$C_n(A_0|\psi\rangle/\sqrt{p_0}) = |\overline{\langle\psi|} v^T d_0^T u_0^T S u_0 d_0 v |\psi\rangle| / p_0 = qr C_n(v|\psi\rangle)/p_0 = qr C_n(|\psi\rangle)/p_0, \tag{C7}$$

where in the second equality we have used $u_0^T(-i\sigma^y)u_0 = -i\sigma^y$, and the third equality follows by invariance of concurrence under local unitaries. Similarly, $C_n(A_1|\phi\rangle/\sqrt{p_1}) = \sqrt{(1-q^2)(1-r^2)} C_n(|\phi\rangle)/p_1$. The result is

$$\begin{aligned} p_0 C_n(\rho_0) + p_1 C_n(\rho_1) &= qr \min_{\{\lambda_k, |\psi^k\rangle\} | \Sigma \lambda_k |\psi^k\rangle\langle\psi^k| = \rho} \sum_k \lambda_k C_n(|\psi^k\rangle) \\ &\quad + \sqrt{(1-q^2)(1-r^2)} \min_{\{\beta_k, |\phi^k\rangle\} | \Sigma \beta_k |\phi^k\rangle\langle\phi^k| = \rho} \sum_k \beta_k C_n(|\phi^k\rangle) \\ &= (qr + \sqrt{(1-q^2)(1-r^2)}) C_n(\rho) \leqslant C_n(\rho), \end{aligned} \tag{C8}$$

with equality iff $q = r$. □

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[27] It is not clear how to recover the celebrated 3-tangle from this construction. By this definition we will see that $\tau_n \equiv 0$ for all odd n, so references to τ_n in the present paper will suppose that is not the case.

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Properties of continuous Fourier extension of the discrete cosine transform and its multidimensional generalization

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A versatile method is described for the practical computation of the exact discrete Fourier transforms (DFT), both the direct and the inverse ones, of a continuous function g given by its values g_j at the points of a uniform grid F_N generated by conjugacy classes of elements of finite adjoint order N in the fundamental region F of compact semisimple Lie groups. The present implementation of the method is for the groups SU(2), when F is reduced to a one-dimensional segment, and for $\mathrm{SU}(2)\times\mathrm{SU}(2)\times\cdots\times\mathrm{SU}(2)$ in multidimensional cases. This simplest case turns out to be a version of the discrete cosine transform (DCT). Implementations, abbreviated as DGT for *Discrete Group Transform*, based on simple Lie groups of higher ranks, are to be considered separately. DCT is often taken to be simply a specific type of the standard DFT. Here we show that the DCT is very different from the standard DFT when the properties of the *continuous extensions* of the two inverse discrete transforms are studied. The following properties of the continuous extension of DCT (called CEDCT) from the discrete $t_j \in F_N$ to all $t \in \mathsf{F}$ are proven and exemplified. Like the standard DFT, the DCT also returns the exact values of $\{g_j\}$ on the $N+1$ points of the grid. However, unlike the continuous extension of the standard DFT:

(a) The CEDCT function $f_N(t)$ closely approximates $g(t)$ *between* the points of the grid as well;
(b) for increasing N, the derivative of $f_N(t)$ converges to the derivative of $g(t)$;
(c) for CEDCT the principle of locality is valid.

In this article we also use the continuous extension of the two-dimensional (2D) DCT, $\mathrm{SU}(2)\times\mathrm{SU}(2)$, to illustrate its potential for interpolation as well as for the data compression of 2D images. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The decomposition of functions integrable on a finite segment into Fourier series of trigonometric functions of one variable is a well known method (e.g., Refs. 1 and 2) whose theoretical and practical aspects have been thoroughly investigated during the last two centuries in connection with its numerous applications in science and engineering. It is natural to question whether any attempt to add something to it is not in fact a reinvention of what has been found before.

Our general goal, which goes beyond this paper, is to elaborate a new decomposition method of functions of n variables into Fourier series using orbit functions of compact semisimple Lie groups,[3,4] with the idea of (i) making it accessible to users who are not specialists in Lie theory, (ii) underlining the versatility of its practical implementations, and (iii) most importantly, demonstrating the fertility of the underlying theme of this approach. One can find complete answers to

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limited questions (like the values of a finite number of Fourier coefficients) replacing the Lie group by a suitably chosen set of its discrete elements. The choice of the discrete elements is clearly crucial.

In the context of our goal, the SU(2) case results in the simplest example of the new method, even though that is the case where the potential advantages of the method based on the symmetry groups could be most limited. Remarkably, however, in this low dimensional space the discrete Fourier transform on the SU(2) group results in one type of discrete cosine transforms discovered in 1974,[5] or more exactly the DCT-1 (see Refs. 6 and 7). Its comparison with the standard method is both misleading and revealing. It is misleading because of its apparent similarity (see Ref. 13) to the well known Discrete Fourier transform abbreviated as DFT (e.g., Refs. 8–10). Nevertheless it is revealing, since it can help to understand better the underlying reasons why for many practical applications the DCT is proven significantly more efficient than the DFT. In this paper we consider the concept of *continuous extension* of the discrete transform, and show that the convergence properties of the continuous extension of the inverse DCT, abbreviated here as CEDCT, match very closely the properties of the canonical (*continuous*) Fourier transform (CFT) of smooth functions. Meanwhile continuous extension of the inverse DFT (hereafter CEDFT) does not result in any reasonable function. Note that for the sake of simplicity, if the ''inverse'' is not explicitly used, we will henceforth adopt DFT and DCT (or DGT in a more general sense) abbreviations for both direct and inverse Fourier transforms.

In Sec. II we present some pertinent information on the Fourier analysis on the SU(2) group, which also demonstrates the general formalism used for the Fourier transforms on Lie groups. We show that in practice the Fourier transform of a class function of SU(2) is reduced to the decomposition of a discrete function $\{g_k | k=0,1,\ldots,N\}$ defined on a N-interval grid of variable $t \in [0,T_0]$ onto the series of $(N+1)$ cosine functions (including $\cos 0=1$) of harmonic order $n=j/2\leqslant N/2$. The basis for the DCT series is thus composed of the first N *half*-order harmonics of $\cos(2\pi t/T_0)$, i.e., $\cos(2\pi nt/T_0)=\cos(\pi jt/T_0)$ with $j=0,1,\ldots,N$. The harmonic order of these functions formally is either integer for j even, *or* half-integer for odd j. This approach is compared to the standard method of DFT where the given $\{g_k\}$ is decomposed into the trigonometric polynomials of $e^{(i\,2\pi\,nt/T_0)}$ of the *full* harmonic order $n\leqslant N$. In Sec. II we also define the continuous extension of a discrete transform onto the segment $[0,T_0]$. We then compare CEDCT and CEDFT, and show that although both DCT and DFT formally belong to the group of *exact* discrete transforms, rather surprisingly, only the CEDCT converges with increasing N to the continuous function $g(t\in[0,T_0])$ which originates the grid function $\{g_k\}$. We explain this difference comparing CEDCT and CEDFT from the point of view of Shannon sampling theorem.

In Sec. III we prove some important properties of CEDCT. These properties closely resemble those of the canonical CFT polynomials, such as the principle of *locality* of CEDCT. This property can ensure, in particular, that numerical computation errors or uncertainties in one segment of the interval $[0,T_0]$ would not dramatically affect the transform results in a distant segment. Another important property proven in Sec. III is that, similar to the CFT polynomials, the term-by-term derivative series of the continuous extension of an N-interval DCT converges to $g'(t)$ with the increase of N. Note that all these properties hold for any function $g(t)$ with bounded second derivative. In particular, they are also valid when $g_0\neq g_N$, which is not the case for standard DFT.

In Sec. IV we extend the formalism of one-dimensional DGT on SU(2), or the DCT, for decomposition of multidimensional functions. We bring examples of approximation of two-dimensional discrete functions/images by two-dimensional CEDCTs.

Finally, let us also point out that additional examples of exploitation of our method are found in the Proceedings of 3 recent meetings on the numerical methods.[11,12,34–36]

II. FOURIER ANALYSIS ON SU(2)

The Lie group SU(2) can be realized as a set of all 2×2 unitary matrices A, with $\det A=1$. A complex valued *class function* f on SU(2) is any map of SU(2) onto the complex number space $\mathbb{C}$

which is invariant under conjugation, i.e., $f:\mathrm{SU}(2)\to\mathbb{C}$, and $f(B^{-1}AB)=f(A)$ for all $A,B\in\mathrm{SU}(2)$. Since the defining two-dimensional representation of SU(2) is faithful, we can use it in order to describe the pertinent discrete elements of SU(2).

Any unitary matrix can be diagonalized by a unitary transformation. Therefore, every element of SU(2) is conjugate to at least one diagonal matrix in the defining two-dimensional representation. All the elements which can be simultaneously diagonalized form a maximal torus T of SU(2). Since all maximal tori are SU(2)-conjugate, we can write

$$\mathsf{T}=\left\{ x(\theta)=\begin{pmatrix} e^{2\pi i\theta} & 0 \\ 0 & e^{-2\pi i\theta}\end{pmatrix} \;\middle|\; 0\leqslant\theta\leqslant 1\right\}. \tag{1}$$

Furthermore, using $B=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)\in\mathrm{SU}(2)$, we have $Bx(\theta)B^{-1}=x(-\theta)$. Therefore, every element of SU(2) is conjugate to just one element in the subset $F\subset T$, where

$$\mathsf{F}=\left\{ x(\theta)=\begin{pmatrix} e^{2\pi i\theta} & 0 \\ 0 & e^{-2\pi i\theta}\end{pmatrix} \;\middle|\; 0\leqslant\theta\leqslant \frac{1}{2}\right\}. \tag{2}$$

Trace functions, otherwise called *characters*, play an important role in SU(2). For any element $x(\theta)$ of (1) we have $\mathrm{tr}\,x(\theta)=2\cos(2\pi\theta)$. In general, $\mathrm{tr}\,x(\theta)$ is a class function because for all $B\in\mathrm{SU}(2)\Rightarrow\mathrm{tr}\{B^{-1}xB\}=\mathrm{tr}\,x$. Let $R=R(\mathrm{SU}(2))$ denote a complex algebra generated by the character functions of SU(2). It is well known that R has a linear basis consisting of characters of all finite dimensional irreducible representations of SU(2).

With each irreducible representation of a semisimple Lie group, in particular SU(2), one associates a set of weights (weight system) of the representation,[3,4] which is a union of orbits of weights under the action of the Weyl group, W. In physics the SU(2)-weights are known as projections of the angular momenta which have integer and half-integer eigenvalues. In mathematics one usually prefers to deal with the doubles of the angular momenta in order to avoid nonintegers.

The Weyl group of SU(2) is very simple. It is of order 2, its 2 elements being generated by reflection r. It acts on any element $m\in\mathbb{R}$ of the one-dimensional space $\mathbb{R}$ of the ''projections of angular momenta'' in the straightforward way: $r(m)=-m$. The finite dimensional irreducible representations of SU(2) and of its Lie algebra su(2) are well known. The ''angular momentum states,'' the basis vectors of representation spaces, are eigenvectors of the ''diagonal'' generator of SU(2). Unlike the common normalization of that generator in physics, we normalize it so that its eigenvalues are twice the usual projections of angular momenta. The set of the eigenvalues $\Omega(l)$ is the weight system of the representation l. The weight system of an irreducible representation consists of $l+1$ weights,

$$\Omega(l)=\{m\omega|m\in\{-l,-l+2,\ldots,l-2,l\}\},$$

where l is the highest weight (''twice the angular momentum'') of the representation;[31] l is used to specify the representation. Note that all the elements of $\Omega(l)$ have the same parity.

A W-orbit of a weight m thus consists of one or two elements:

$$Wm=\begin{cases}\{m,-m\} & \text{for } m\neq 0\\ \{0\} & \text{for } m=0.\end{cases}$$

The character $\chi(\theta)$ is a function of conjugacy classes of the elements of SU(2). Every class is represented by one value of θ within $0\leqslant\theta\leqslant\frac{1}{2}$. The values of the character of an irreducible representation l can be written as the sum of values of the orbit functions $\Phi_m(\theta)$,

$$\chi_l(\theta)=\sum_m^l \Phi_m(\theta)=\Phi_l(\theta)+\Phi_{l-2}(\theta)+\cdots+\begin{cases}\Phi_1(\theta), & l \text{ odd}\\ \Phi_0(\theta), & l \text{ even.}\end{cases} \tag{3}$$

$$\Phi_m(\theta)=\begin{cases} e^{2\pi i m\theta}+e^{-2\pi i m\theta} & \text{for } m>0 \\ 1 \quad \text{for } m=0 \end{cases}, \quad \text{and } 0\leqslant\theta\leqslant\frac{1}{2}. \tag{4}$$

Only for the one- and two-dimensional representations, $l=0$ and 1, respectively, the character consists of a single orbit function. Note that $\Phi_m(\theta)$ is symmetric (antisymmetric) with respect to the midpoint of its range of θ for m even (odd).

The decomposition of irreducible characters (3) into the sum of orbit functions is given by a triangular matrix. Hence it is invertible. Therefore, the orbit functions $\{\Phi_m(\theta),\ m=0,1,2,\ldots\}$ also form a basis in the space of class functions $f(\theta)$ of SU(2). Using (4), it implies that

$$f(\theta)=\sum_{m=0}^{\infty} a_m\,\Phi_m(\theta) \quad =a_0+2\sum_{m=1}^{\infty} a_m\cos(2\pi m\theta), \quad 0\leqslant\theta\leqslant\frac{1}{2}. \tag{5}$$

There are two properties of the expansion (5) which we want to underline:
(i) It can be reduced to the familiar case of the standard Fourier decomposition of $f(\theta)$ in the interval $\theta\in[-1/2,1/2]$, if one makes an even extension $f(\theta)=f(-\theta)$ for $t\in[-1/2,0]$.
(ii) Although $f(\theta)$ is being expanded into a series of functions which are periodic within the range $0\leqslant\theta\leqslant1$, the actual range of θ in (5) makes periodic only the cosines with even values of m, i.e., $m=2k$. Their arguments vary over the range $\{0,2k\pi\}$, i.e., over an integer multiple of 2π.

A. Discrete Fourier transform on SU(2)

The discrete Fourier transform differs from (5) by the fact that the independent variable θ takes only finite number of values within its range of variation. Fixing a rational value of θ, one fixes an element of finite order (EFO) belonging to the SU(2) torus T. Every conjugacy class of EFO in SU(2) is represented by an element of T with $0\leqslant\theta\leqslant\frac{1}{2}$. In SU(2) one can be explicit, see Refs. 14 or 15 (Sec. IV) for all other compact simple Lie groups.

Let T_N denote the set of all elements of T whose adjoint order divides N, where N is a positive integer. The adjoint order is the order of an element given by matrices of irreducible representations of SU(2) of odd dimensions (i.e., l even). There are exactly $(N+1)$ SU(2)-conjugacy classes of such elements. Taking the unique diagonal matrix as representative of each conjugacy class, in representations of dimensions 2 and 3 we have the following set of matrices

$$\mathsf{T}_N^{(2)}=\left\{ x_{N,k}=\begin{pmatrix} e^{2\pi ik/2N} & 0 \\ 0 & e^{-2\pi ik/2N} \end{pmatrix} \;\middle|\; k=0,1,\ldots,N \right\},$$

$$\mathsf{T}_N^{(3)}=\left\{ x_{N,k}=\begin{pmatrix} e^{2\pi ik/N} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-2\pi ik/N} \end{pmatrix} \;\middle|\; k=0,1,\ldots,N \right\}.$$

The trace functions of each of these matrices, of size $(l+1)\times(l+1)$, are the characters $\chi_l(\theta)$ of the representation l. The characters can be used for decomposition of the class functions on SU(2), and generally on compact simple Lie groups.

A more suitable basis for such a decomposition consists of orbit functions.[3,4] It makes possible (*practical*) decomposition of class functions on groups of high ranks, such as E_8.[16–18] In the case of SU(2), the orbit functions are also much closer to the familiar set of exponentials $\exp(2\pi im\theta)$ used in the standard Fourier analysis.

Note that the elements $x_{N,k}$ are equidistant in the fundamental region $\mathsf{F}=\{\theta\in[0,1/2]\}$ of the Weyl group W. The number of elements of the W-conjugacy class $m=k/N$ is denoted by $C_{N,k}$ and is given by

$$C_{N,k}=\begin{cases} 1 & \text{if } k=0,N \\ 2 & \text{otherwise.} \end{cases} \tag{6}$$

The following definition of a sesquilinear form $\langle f,g\rangle_N$ in the space R of class functions f and g on SU(2) is a crucial step for our method:

$$\langle f,g\rangle_N=\sum_{k=0}^{N} C_{N,k} f(x_{N,k})\,\overline{g(x_{N,k})}\,, \tag{7}$$

where the overline stands for complex conjugation. It is known,[3,15] and it can be verified by direct computation, that the set of orbit functions $\{\Phi_k|k=0,\ldots,N\}$ is orthogonal on the discrete equidistant N-interval grid with respect to this form. More precisely, we have

$$\frac{\langle \Phi_k,\Phi_m\rangle_N}{\langle \Phi_m,\Phi_m\rangle_N}=\delta_{km},\quad \text{for}\quad 0\leqslant k,m\leqslant N.$$

For further convenience and for comparison of the results with the conventional Fourier series, let us instead of orbit functions $\Phi_m(\theta)$ defined by (4) consider the functions $\psi_m(\theta)=\cos(2\pi m\theta)$ for all $m\geqslant 0$. Then one can easily verify that for $0\leqslant k,m\leqslant N$

$$\langle \psi_k,\psi_m\rangle_N=\sum_{j=0}^{N} C_{N,j}\cos\frac{\pi jk}{N}\cos\frac{\pi jm}{N}=\frac{2N}{C_{N,k}}\delta_{km}. \tag{8}$$

The method proposed here for decomposition of the class functions into series of orbit functions is based on the discrete orthogonality relation (8).

Let $f(\theta)\in R$ be a class function that can be decomposed into a *finite* series of orbit functions:

$$f(\theta)=\sum_{m=0}^{N} a_m\,\psi_m(\theta)\quad (0\leqslant\theta\leqslant\tfrac{1}{2})\,. \tag{9}$$

This can be compared with the general case of infinite series (5) and with the discrete Fourier transform (2) in Ref. 19.

Our goal now is to find the expansion coefficients $\{a_m\}$. In order to use the orthogonality property (8), we form a system of $(N+1)$ linear equations for $\{a_m\}$, restricting θ to the discrete set of its values $\{\theta_k=k\Delta\theta\,|k=0,\ldots,N\}$, with $\Delta\theta=1/2N$:

$$f_k\equiv f(\theta_k)=\sum_{m=0}^{N} a_m\psi_m(\theta_k)=\sum_{m=0}^{N} a_m\cos\frac{\pi mk}{N}. \tag{10}$$

After multiplication of (10) by $C_{N,k}\,\psi_{jk}$ and summing over k, we arrive at $\Sigma_{m=0}^{N} a_m\langle\psi_m,\psi_j\rangle_N$. Then, given (8), we find

$$a_j=\sum_{k=0}^{N} D_N^{jk} f_k\quad \text{for}\quad j=0,\ldots,N, \tag{11}$$

where

$$D_N^{jk}=\frac{C_{N,j}\,C_{N,k}}{2N}\cos\frac{\pi kj}{N}. \tag{12}$$

Here D_N^{jk} are the elements of $(N+1)\times(N+1)$ matrix D_N of the DGT on SU(2). It is easily reduced to the transform matrix of the discrete cosine transform of the type DCT-1 after renormalization by a factor $\sqrt{2C_{N,j}\,C_{N,k}/N}$. The matrix D_N is independent of the values $\{f_k\}$ of the class function which is being decomposed. It is therefore possible to compute D_N in advance for any predefined value of the positive integer N, and use it repeatedly whenever it is needed.

Examples of the transform matrices D_N for the lowest values of N are the following:

$$D_1=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix},\quad D_2=\frac{1}{2}\begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} \\ 1 & 0 & -1 \\ \frac{1}{2} & -1 & \frac{1}{2} \end{pmatrix},\quad D_3=\frac{1}{3}\begin{pmatrix} \frac{1}{2} & 1 & 1 & \frac{1}{2} \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ \frac{1}{2} & -1 & 1 & -\frac{1}{2} \end{pmatrix},$$

$$D_4=\frac{1}{4}\begin{pmatrix} \frac{1}{2} & 1 & 1 & 1 & \frac{1}{2} \\ 1 & \sqrt{2} & 0 & -\sqrt{2} & -1 \\ 1 & 0 & -2 & 0 & 1 \\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1 \\ \frac{1}{2} & -1 & 1 & -1 & \frac{1}{2} \end{pmatrix}. \tag{13}$$

Introducing single-column matrices $A_N=\{a_j\}$ and $F_N=\{f_N(t_k)\}$, and a square matrix $\Psi_N=\{\cos(\pi jk/N)|j,k=0,\ldots,N\}$, Eqs. (10) and (11) can be written in the matrix form,

$$F_N=\Psi_N A_N \quad \text{and} \quad A_N=D_N F_N, \quad \text{where} \quad D_N=\Psi_N^{-1}. \tag{14}$$

The matrix D_N, being the inverse of Ψ_N, formally solves the problem of discrete Fourier transform on SU(2).

B. Continuous extension of the discrete Fourier transforms

Let a continuous function $g(t)$ be the origin for the discrete function $\{g_k=g(t_k)\}$ defined at the $(N+1)$ points $t_k=kT_0/N$, $k=0,1,\ldots,N$, of the interval $[0,T_0]$. The DCT of $\{g_k\}$ with the use of the transform matrix (12) results in the discrete function $\{a_j\}$ in the frequency space. This is an exact (''lossless'') discrete transform, since it allows unambiguous recovery of all $N+1$ values of $\{g_k\}$ by applying the inverse DCT in the form of (10). We recall that the standard discrete Fourier transform, i.e., DFT, has the same property.

It seems then natural to ask if it is possible to recover the originating function $g(t)$ by a Fourier series not only at the grid points $\{t_k\}$, but also on the entire continuous segment $[0,T_0]$. In order to answer this question, let us consider the continuous extension of the discrete transform between the grid points, which can be formulated as follows.

Proposition: Let $g(t)$ be a complex valued function of $t\in[0,T_0]$, taking values $g_k=g(t_k)$ on an equidistant point grid $\{t_k=kT_0/N\,|k=0,1,\ldots,N\}$. The function

$$f_N(t)=\sum_{j=0}^{N} a_j \cos(\pi jt/T_0), \qquad t\in[0,T_0], \tag{15}$$

with the discrete transform coefficients

$$a_j=\sum_{k=0}^{N} \frac{C_{N,j}C_{N,k}}{2N} g_k \cos\frac{\pi jk}{N}, \tag{16}$$

is the continuous Fourier extension of the inverse DCT of $\{g_k\}$. It is exact in the sense that $f(t_k)=g_k$ at all $N+1$ points of the grid.

The proof of this proposition is obvious if one recalls that (15) and (16) are reduced, respectively, to (10) and (11) after substitution $t=2\theta T_0$ with $\theta\in[0,\frac{1}{2}]$.

Similar to DCT, one can also continuously extend to all points of the segment $[0,T_0]$ any other types of discrete transforms, in particular the DFT, resulting in CEDFT.

Below we address two important questions. First, how well the CEDCT approximates any "reasonably behaved" (e.g., continuous) function $g(t)$ on the interval $[0,T_0]$ between the points of the grid. The second question is how it compares with the CEDFT. At last, we will also briefly address the question of the possible use of CEDCT in practical applications, in particular, for purposes of smooth representation of compressed images.

In order to provide a partial answer to the first question, we consider two examples.

Example 1: Let us take a Gaussian function

$$g(t)=\exp[-\tfrac{1}{2}(t/\sigma)^2], \quad t\in[0,1], \tag{17}$$

with the dispersion $\sigma=1/3$, and choose $N=3$. Thus we have chosen a rather coarse grid relative to the dispersion: The width of its intervals $1/N$ is equal to the dispersion. The coefficients (11) are readily calculated using D_3 from (13):

$$A_3=\begin{pmatrix} a_0\\ a_1\\ a_2\\ a_3\end{pmatrix}=\frac{1}{3}\begin{pmatrix} 0.5+e^{-0.5}+e^{-2}+0.5\,e^{-4.5}\\ 1+e^{-0.5}-e^{-2}-e^{-4.5}\\ 1-e^{-0.5}-e^{-2}+e^{-4.5}\\ 0.5+e^{-0.5}+e^{-2}+0.5\,e^{-4.5}\end{pmatrix}=\begin{pmatrix} 0.415\,807\\ 0.486\,695\\ 0.089\,748\\ 0.007\,750\end{pmatrix}. \tag{18}$$

The corresponding CEDCT function (15) reads

$$f_3(t)=a_0+a_1\cos(\pi t)+a_2\cos(2\pi t)+a_3\cos(3\pi t), \tag{19}$$

where the coefficients are given by (18).

Now we are in a position to compare (17) with (19). At the grid points $t_k=k/3$ the functions coincide, $f_3(t_k)=g(t_k)$ (which is easily verified). One may then expect large deviations of $f_3(t)$ from $g(t)$ around intermediate points of the grid, i.e., $t=1/6$, $1/2$, and $5/6$:

$$\begin{pmatrix} f_3(1/6)\\ f_3(1/2)\\ f_3(5/6)\end{pmatrix}=\begin{pmatrix} 0.882\,171\\ 0.326\,059\\ 0.039\,191\end{pmatrix} \quad\leftrightarrow\quad \begin{pmatrix} g(5/6)\\ g(1/2)\\ g(1/6)\end{pmatrix}=\begin{pmatrix} 0.882\,497\\ 0.324\,652\\ 0.043\,937\end{pmatrix}.$$

A good agreement between $f_3(t)$ and $g(t)$ is apparent even for $t=5/6$ where $g(t)$ becomes very small.

Example 2: DCT approximation for a more complicated function is found in Fig. 1, where we show $f_N(t)$, $N=10$ and 14, for the function $g(t)$ composed of two Gaussians,

$$g(t)=A_1e^{-((t-t_1)/\sigma_1)^2/2}+A_2e^{-((t-t_2)/\sigma_2)^2/2}, \tag{20}$$

with amplitudes $A_1=2$, $A_2=1.5$, narrow dispersions $\sigma_1=\sigma_2=0.05$, and centered at $t_1=0.42$, $t_2=0.56$.

For comparison, in Fig. 1 we show by dashed lines the approximations to $g(t)$ provided by the trigonometric CFT polynomials where the transform coefficients are calculated by exact integrations. Recall that for a real function $g\to\mathbb{R}$ the CFT polynomials of the harmonic order K are given by the series[32] (see, e.g., Ref. 2):

$$P_K(t)=\sum_{j=-K}^{K} c_j\,e^{i2\pi jt/T_0}=c_0+2\,\mathrm{Re}\sum_{j=1}^{K} c_j\,e^{i2\pi jt/T_0}, \tag{21}$$

where

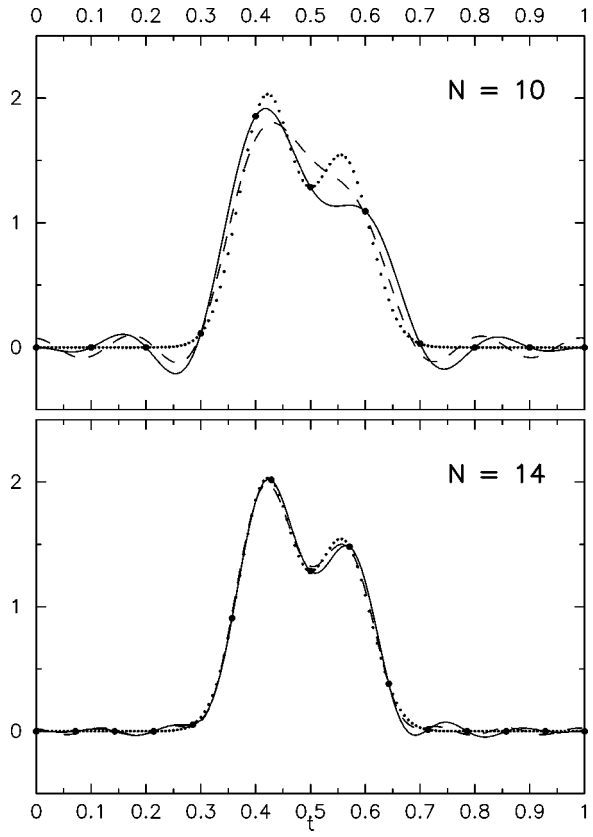

FIG. 1. Approximation of an analytic function (20), shown by the dotted lines, with the CEDCT function $f_N(t)$ (solid lines) for the discrete interval numbers $N=10$ and $N=14$. The big dots show the values of the grid function $\{g_k \equiv g(t_k)\}$ for $\{k=0,\ldots,N\}$. For comparison we also show by dashed lines the approximation of $g(t)$ by the exact CFT polynomials of (21) with $K=N/2$. It gives polynomials of the same harmonic maximum order as the ones in the DCT. The parameters in (20) are $A_1=2$, $A_2=1.5$, $\sigma_1=\sigma_2=0.05$, $t_1=0.42$, $t_2=0.56$.

$$c_j=\frac{1}{T_0}\int_0^{T_0} g(t)\, e^{-i2\pi jt/T_0}\, \mathrm{d}t. \tag{22}$$

In order to compare approximations to $g(t)$ that can be provided by series (15) and (21) of the same order for the highest harmonics, for the series $P_K(t)$ in Fig. 1 we put $K=N/2$.

Figure 1 illustrates that the DCT is really an exact discrete Fourier transform, i.e., that $f_N(t_j)=g(t_j)$ for all $0\leqslant j\leqslant N+1$. Remarkably, its continuous extension $f_N(t\in[0,T_0])$ approximates $g(t)$ practically as well as the accurate CFT trigonometric Fourier series $P_K(t)$ of the same harmonic order, i.e., $K=N/2$. In the case of Gaussian-type functions, CEDGT series approximates the original function $g(t)$ reasonably well even in the case of narrow structures with dispersions as small as $\sigma\approx T_0/1.5N$.

C. Comparing with standard DFT

First, let us recall some properties of the standard exploitation of the discrete Fourier transform. Further details can be found in many books (e.g., see Refs. 8–10).

The standard DFT is formally derived from an approximate calculation of the integral coefficients c_j for the trigonometric Fourier series, using a simple rule of rectangles for integration of c_j in (22) when the function g is given on the N-interval equidistant grid, $g(t)\rightarrow\{g_k|k=0,\ldots,N\}$. This leads to DFT coefficients

$$u_j = \frac{1}{N} \sum_{k=0}^{N-1} g_k e^{-i(2\pi/N)kj}, \tag{23}$$

where $1/N$ is the length of the sampling interval Δt (assuming for simplicity $T_0 = 1$).

A crucial feature of this definition of DFT consists in the fact that the system of Eqs. (23) for the first N coefficients $\{u_j | j = 0,\ldots,N-1\}$ can be inverted with respect to $\{g_k | k = 0,\ldots,N-1\}$. Such a possibility is based on the observation that the matrices with matrix elements

$$M_{jk} = \frac{1}{N} e^{-i(2\pi/N)kj} \quad \text{and} \quad (M^{-1})_{jk} = e^{i(2\pi/N)kj},$$

are inverse to each other. Therefore, the *inverse* DFT is

$$g_k = \sum_{j=0}^{N-1} u_j e^{i(2\pi/N)kj}. \tag{24}$$

Thus, the discrete sets $\{u_j\}$ and $\{g_k\}$ represent a pair of exact (*lossless*) direct and inverse transforms (e.g., see Ref. 10) in the form of Fourier series, which is generally treated as the exact *solution* to the problem of Fourier transform of discrete functions given on the equidistant grid.

We argue below, however, that there are significant reasons to suggest that the real (and not only formal) exact solution to the problem of discrete Fourier transform of a grid function is provided by the DCT transform pair given by (16) and (10). It retains all the ''good'' properties of the DFT:

(i) it is easy and fast to compute;

(ii) it is a lossless discrete transform, with the exact inverse DCT at all $(N+1)$ points of the grid (even if $g_0 \neq g_N$, unlike for DFT).

However, in addition to these properties, the continuous extension of DCT, $f_N(t)$ in (15), converges to the originating continuous function $g(t)$ with increasing N, as illustrated in the previous section, and as it is proved in the next Section. Only the continuous extension of the DCT, and not the DFT, reveals properties characteristic to the canonical continuous Fourier transform series.

It is worth noting here that the very good convergence properties seem to be a common feature for the discrete Lie group transforms, as we also demonstrate on the example of SU(3) group in our recent paper, Ref. 34. The basic mathematics of DGT has been formulated[15] for any dimension $n < \infty$. In fact there are as many different variants of the method one could use, as there are different semisimple compact Lie groups of rank n, and then within each variant the choice of the points of the grid is also far from unique, except for the lowest cases like SU(2). It then provides an opportunity to make a choice of appropriate DGT in situations where the choice of symmetry is dictated by the experimental data.

The absence of the convergence property for the continuous extension of the DFT given by (24) is not easy to anticipate because CEDFT looks like a Fourier polynomial, or a cutoff of an ''ordinary'' Fourier expansion:

$$h_N(t) = \sum_{j=0}^{N-1} u_j e^{2i\pi jt}. \tag{25}$$

Similar to CEDCT, it satisfies the equality $h_N(t_k) = g_k$ on the grid points $t_k = k/N$ for[33] all $k \leqslant N-1$. The fact that their continuous extensions CEDGT and CEDFT behave quite differently is illustrated in Example 3. It has rarely been emphasized that $h_N(t)$ *does not* approximate the initial function $g(t)$ between the grid points, and it does not converge at all to any continuous function (except for a trivial case of $g(t) = \text{const}$) with increasing N. It is worth citing in this regard Ref. 9, p. 87: ''The DFT is a Fourier representation of finite length sequence which is itself a sequence rather than a continuous function.''

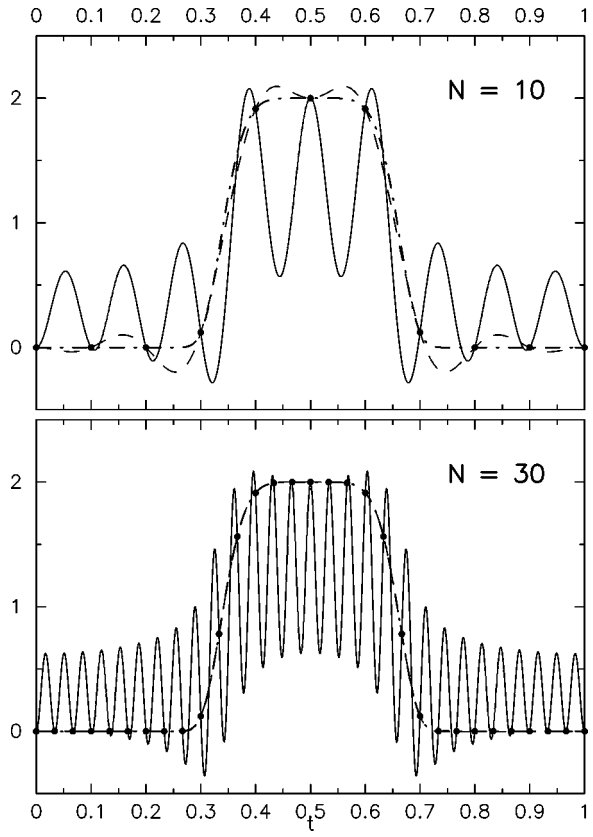

FIG. 2. Behaviors of the Fourier series $h_N(t)$ and $f_N(t)$, given by Eq. (25) and (15). Solid lines represent the CEDFT, and dashed lines show the CEDCT. Big dots show the values of the grid function $\{g_k|k=0,\ldots,N\}$ originated from an analytic function $g(t)$ which is given by Eq. (26), and is shown by the dot–dashed line.

Example 3: Let $h_N(t)$ be the CEDFT of N-interval grid function arising from a sampling of the continuous function

$$g(t)=Ae^{-(t-t_0)^6/a^6}, \tag{26}$$

with $A=2$ and parameter $a=0.15$. Here we have chosen a large value, 6, for the power in the exponent in order to illustrate a case with gradients significantly larger than in the case of Gaussian functions.

Solid lines in Fig. 2 correspond to continuous DFT extensions $h_N(t)$, and the dashed lines show the DCT extension $f_N(t)$. Although $h_N(t)$ passes through all g_k at $t=t_k$ (shown as full dots), similar to $f_N(t)$, its behavior in between shows profound oscillations due to the presence in (25) of high-frequency Fourier components, $\nu_j=j$ (for $T_0=1$), with values of $N/2\leqslant j\leqslant N-1$ comparable to N. These oscillations in CEDFT do not decrease with increasing N. But they quickly disappear in CEDCT series where the harmonic order of the maximum frequency mode does not exceed $J_{\mathrm{Ny}}\equiv N/2$. Note that this mode corresponds to the so called Nyquist frequency $N/2$ which plays a fundamental role in the digital signal processing theory.

D. Shannon sampling theorem and DCT and DFT

Nonconverging behavior of CEDFT appears puzzling especially in the light of Nyquist–Shannon sampling theorem[20,21] for a continuous band-limited signal which states

Every continuous band-limited analog signal $X(t)$ *can be reconstructed fully from its discrete samples* $X_n = X(n\Delta t)$, *provided the sampling rate* $1/\Delta t$ *exceeds twice the maximum frequency* ν_{max} *contained in* $X(t)$.

The sampling rate $1/\Delta t = 2\nu_{\max}$ corresponds to the sampling at the rate of 2 points per period $T_{\min} = 1/\nu_{\max}$, which is the Nyquist rate. Shannon formula[21] provides exact interpolation between the sampling points for unlimited time sequence:

$$X(t) = \sum_{n=-\infty}^{\infty} X_n \frac{\sin(t - n\Delta t)\pi/\Delta t}{(t - n\Delta t)\pi/\Delta t}. \tag{27}$$

It should be emphasized here that Shannon interpolation is *not* a Fourier-type interpolation, but is based on *sinc* function $\sin(t)/t$. In case of limited time interval $t \in [0,1]$, hence limited number of points $X_n \to g_n$ with $n = 0,\ldots,N$, the truncated version $X_N(t)$ of the sequence (27) provides an approximate interpolation to the original $g(t)$ converging in the limit of $N \gg J_{\mathrm{Ny}}$.

The reason for oscillatory behavior of CEDFT can be understood if we note that for any large N the harmonics $\exp(-2i\pi jt)$ with frequencies $j > N/2$ strongly vary and change the sign within any single narrow interval $\Delta t = 1/N$. The use of rectangular integration rule in (22) cannot provide any reasonable similarity between the canonical CFT coefficients c_j in (22) and their standard DFT ''approximations'' u_j in (23). Effectively, the ''fine tuning'' between the coefficients for high-order harmonics intrinsic to the continuous Fourier transform is lost. Moreover, the DFT coefficients (23) with harmonic order exceeding J_{Ny} are no more declining for higher j, which is a normal general trend for both DCT and CFT coefficients. In fact, the well known property of DFT coefficients at $j > J_{\mathrm{Ny}}$ is that they fully ''recover'' the low-order coefficients in complex conjugate form as

$$u_j = \overline{u}_{N-j}. \tag{28}$$

This notion allows us to understand different behaviors of continuous extensions of DFT and DCT in the view of Nyquist–Shannon sampling theorem. Indeed, for any N one can consider CEDCT as a continuous band-limited function with maximum frequency formally equal to frequency J_{Ny}/T_0. This function is formally sampled at the Nyquist rate. However, for large N the DCT coefficients $|a_j|$ for large order harmonics rapidly drop (see Ref. 13). It leaves the CEDCT with an effective bandwith of order of the bandwidth ν_g of the original function $g(t)$. Thus, we can say that at large N the set $\{g_j \mid j = 0,1,\ldots,N\}$ samples CEDCT with a rate much higher than the Nyquist rate. Therefore, one could also say that ''$g(t)$ provides a good reconstruction to CEDCT.''

Meanwhile, because of the relation (28), large frequency harmonics do not disappear from DFT at any large N. The maximum bandwidth of CEDFT is $\nu_{\max} = (N-1)$. Therefore the sampling rate of $\{g_j\}$ is 2 times less than the Nyquist rate which is needed to have sufficient information about the CEDFT function. In a definite sense, $g(t)$ represents an example of a ''low-frequency alias'' to CEDFT. In the next section we will see that elimination of high-order harmonics from the DFT sequence allows construction of a reasonable continuous interpolation for $g(t)$ based on DFT coefficients.

E. Comments on fast Fourier transform

There is a number of ways to make a more accurate approximation for the high-frequency Fourier transform coefficients c_j than the rectangular integration can provide. Despite this, the standard version of DFT defined by (23) and (24) for the direct and inverse discrete transforms has been widely used since the pioneering paper by Cooley and Tukey,[22] where the first algorithms for fast calculation of this DFT had been developed. Different algorithms for such *fast Fourier transform* (FFT) computations allow an increase of the speed of practical calculations of DFTs by one or two orders of magnitude. A direct ''head-on'' algorithm for calculations of $\{u_j \mid j = 0,\ldots,N$

$-1\}$ would require about N^2 multiplications and additions. Meanwhile, for special values of N, FFT algorithms significantly reduce the required number of elementary operations, e.g., down to $\sim N \log_2 N$ in case of $N=2^n$.

The discussion of various FFT algorithms, extensively developed by many authors (e.g., Refs. 23–26), is outside the scope of this article. Here we only note that the FFT methods are fundamentally exploiting the property of the standard DFT coefficients (23) that u_j can be reduced to a power-law series of a single complex element $W_N=\exp(-i2\pi/N)$ as $u_j=N^{-1}\Sigma g_k W_N^{jk}$. This would not be possible if more accurate integration methods for the high-order harmonics were used. It should be also noted, however, that the DCT does allow application of FFT methods since it can be formally reduced (with insignificant differences) to $2N$-point DFT of an even function $g(-t)=g(t)$ (see Ref. 13). A number of efficient FFT-based algorithms have been developed for DCT (e.g., Refs. 27–30) including algorithms competing with FFT but specific to DCT (see Ref. 13 for details).

A simple modification could significantly improve behaviors of continuous extensions of the discrete transforms based on the use of standard DFT coefficients (23), but not without a penalty. Because the reason for strong oscillations of CEDFT is the use of frequencies exceeding the Nyquist frequency J_{Ny}/T_0, one can try to eliminate first these terms from the discrete transform construction (24). Using (28), in the case of even $N=2K$, the sum in (24) is reduced to

$$g_k=u_0+\sum_{j=1}^{K-1}\left(u_j e^{i2\pi j\,k/N}+\overline{u}e^{-i2\pi j\,k/N}\right)\ +u_{N/2}(-1)^k. \tag{29}$$

In the case of odd $N=2K+1$ the last term disappears. However, the attractiveness of DFT retains mostly to the cases of even N $(=2^p)$, for which very effective FFT algorithms are developed. Meanwhile, it is impossible to ''continuously extend'' the modified DFT sequence (29) by substituting $k/N\rightarrow t/T_0$, unless one neglects the last term with flipping argument $(-1)^k$. The resulting function is similar to the series (21) truncated to harmonics of order $j\leqslant N/2$, but it uses the DFT coefficients u_j:

$$s_K(t)=u_0+2\ \mathrm{Re}\sum_{j=1}^{K} u_j e^{i2\pi jt/T}, \tag{30}$$

where the coefficients u_j are defined by (23). Here we use K equal to $J_{\mathrm{Ny}}=N/2$. But one also can take $K<N/2$, and still $s_K(t)$ will be converging to $g(t)$ for $K\rightarrow\infty$.

In Fig. 3 we show that the function $s_K(t)$ with $K=N/2$ (dashed curves) can indeed approximate $g(t)$ practically as well as the DCT extension $f_N(t)$. But in this case the penalty is a loss of the ''exactness'' property for such modified DFT sequence. Because we had to drop the last term in (29) out, $s_K(t)$ can be equal to g_k at the grid points $t=t_k$ only within the accuracy of the term $u_{N/2}$. Therefore, (30) cannot represent an exact solution to the problem of discrete Fourier transform. Meanwhile, the series $f_N(t)$ both satisfies that condition, and rapidly converges to $g(t)$ with increasing N.

For comparison, we also show in Fig. 3 (dot–dashed line) the function $s_K(t)$ calculated for $K=6<N/2=8$. In this case the approximation errors $[s_K(t)-g(t)]$ are larger than the ones when $K=8$, because the order of high frequency harmonics becomes important for the approximation of features with a dispersion $\sigma\leqslant T/2K$.

III. LOCALIZATION AND DIFFERENTIABILITY OF CEDCT

In this section we prove the properties *localization* and *differentiability* of the CEDCT which are analogous to the properties of the canonical CFT polynomials (21) (e.g., see Ref. 2).

Derive first a useful formula for an N-interval CEDGT (15) of a grid function $\{g_k\}$. Using (16), and assuming for simplicity $T_0=1$, i.e., $t\in[0,1]$, (15) is reduced to

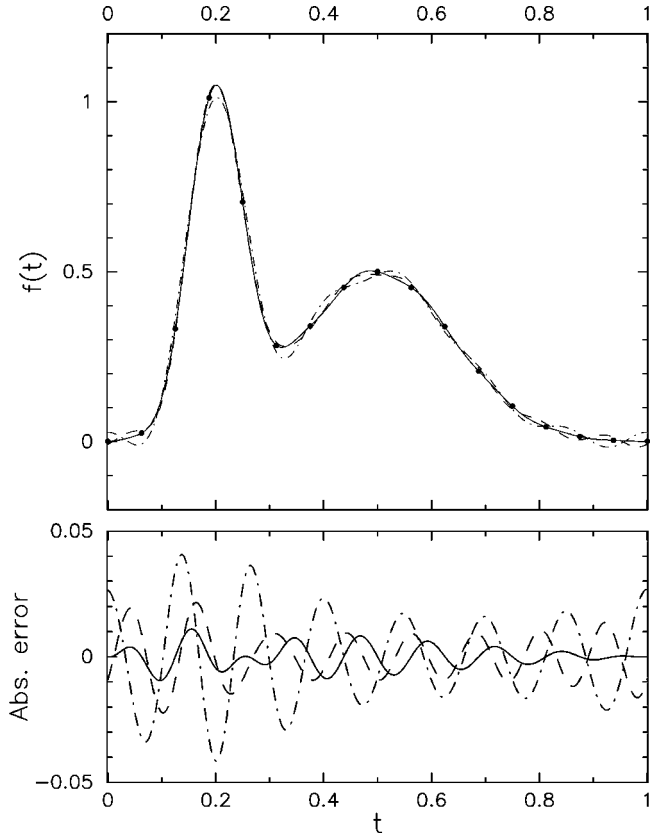

FIG. 3. Approximation of an analytic function $g(t)$ composed of two Gaussians, (20), with the CEDCT function $f_N(t)$ of (15) with $N=16$ (*solid lines*) and the Fourier series $s_K(t)$ of (30) that uses only the first $K\sim N/2$ coefficients $\{u_j|j\leqslant K\}$ of the standard DFT (23). The dashed line is for $K=N/2=8$, and the dot–dashed line corresponds to $K=6$. The full dots in the upper panel correspond to $\{g_k|k=0,\ldots,N\}$. The lower panel shows the corresponding errors of the approximation to $g(t)$ by these 3 types of discrete Fourier transforms. The dispersions in (20) are assumed to be $\sigma_1=0.07$ and $\sigma_2=0.2$.

$$f_N(t)=\frac{1}{2N}\sum_{j=0}^{N}\sum_{k=0}^{N} C_{N,k}C_{N,j}\cos(\pi jt)\cos(\pi jt_k)\,g_k, \tag{31}$$

where $t_k\equiv k/N$. Using $2\cos\alpha\cos\beta=\cos(\alpha+\beta)+\cos(\alpha-\beta)$, the terms containing index j can be re-written as a sum of two geometric series:

$$\sum_{j=0}^{N} C_{N,j}\cos(\pi jt)\cos(\pi jt_k)=(-1)^k\cos(\pi Nt)-1+\mathrm{Re}\left(\sum_{j=0}^{N-1} e^{i\pi(t+t_k)j}+\sum_{j=0}^{N-1} e^{i\pi(t-t_k)j}\right).$$

Summing up the series, one gets a compact expression for CEDGT:

$$f_N(t)=\sum_{k=0}^{N}\frac{(-1)^kC_{N,k}}{2N}\frac{\sin(\pi Nt)\sin(\pi t)}{\cos\pi t_k-\cos\pi t}g_k\equiv\sum_{k=0}^{N}A_{N,k}(t)\,g_k,\quad\text{for}\quad t\in[0,1]. \tag{32}$$

The values of $f_N(t)$ for any $t\to t_n=n/N$ are found by applying the Lipshitz rule for the ratio of infinitesimals of a smooth function. For (32) it results in $f_N(t_n)=g_n$ for all $n=0,\ldots,N$, as expected.

Using (32), below we prove that the *localization principle*, known (see Ref. 2) for the CFT series (21) also holds for the CEDCT. The localization lemma can be formulated as follows:

Localization Lemma: Let the set of N-interval grid functions $\{g_k\}$*, with various* N*, be originated from a smooth function* $g(t)$ *with a bounded derivative* $g'(t)$ *on the interval [0,1]. Then at any given* $t\in[0,1]$ *and for any small* $\Delta>0$ *and* $\epsilon>0$ *there exists* $N_{\epsilon,\Delta}$ *such that for all* $N>N_{\epsilon,\Delta}$ *the behavior of the continuous extension of the discrete group transform* $f_N(t)$ *is defined within the accuracy* ϵ *only by the values of* $g(t)$ *in the* Δ*-neighborhood of* t*, i.e.:*

for any $\epsilon,\Delta>0$ $\exists N_{\epsilon,\Delta}$ *such that for all* $N>N_{\epsilon,\Delta}\Rightarrow$

$$\left| f_N(t)-\sum_{\{k'\}} A_{N,k'}(t)g_{k'}\right|<\epsilon, \quad \text{with all } k' \text{ within} \quad t-\Delta<\frac{k'}{N}<t+\Delta.$$

Proof: From (16), using (8), it follows that the DGT coefficients of any constant function $g_1(t)=\text{const}$ are equal to $a_k^{(1)}=\delta_{k0}\times\text{const}$, i.e., that all coefficients except for $a_0^{(1)}=\text{const}$ are equal to 0. Thus the convergence properties of the CEDGT of any function $g(t)$ are the same as the properties of the function $g(t)+\text{const}$. So taking into account that the function is bounded, it is sufficient to prove the Lemma, while generally assuming that $g(t)$ is positive on the interval [0,1].

Let us split the sum in (32) into 3 parts corresponding to

$$\begin{aligned} S_-&=\sum_{k=0}^{K_t-K_\Delta-1} A_{N,k}\,g_k,\\ S_+&=\sum_{k=K_t+K_\Delta+1}^{N} A_{N,k}\,g_k,\\ S_\Delta&=\sum_{k=K_t-K_\Delta}^{K_t+K_\Delta} A_{N,k}\,g_k, \end{aligned} \tag{33}$$

where $K_t=[Nt]$ and $K_\Delta=[N\Delta]$ are the integer parts of the respective products. If any of the points $t\pm\Delta$ is outside the interval [0,1], then only 2 sub-series are left. In all cases, only S_Δ of these sub-sums is defined by $g(t)$ in the close neighborhood of t. The localization Lemma for (32) then implies that the *non-local* sums, S_+ and S_-, are reduced with increasing N to absolute values below any small ϵ.

Indeed, on the basis of (32), for any fixed Δ each of those non-local sums represents a series of bound-value elements with alternating signs, which can be then combined into pairs of consequetive elements of order $O(1/N^2)$ each. Considering for example the sum S_-, and using the Taylor series decomposition for $g_{k+1}\equiv g(t_{k+1})=g_k+g'(t_k)/N+o(1/N)$ each pair of elements $A_{N,k}g_k+A_{N,k+1}g_{k+1}$ starting with even $k\geqslant 2$ can be reduced to

$$\frac{\sin(\pi Nt)\sin(\pi t)}{N^2}\left[\frac{g'(t_k)}{\cos\pi t_k-\cos\pi t}-\frac{g_k\sin\pi t_k}{(\cos\pi t_k-\cos\pi t)^2}+o(1/N^2)\right].$$

The expression in the square brackets is bounded with some absolute value independent of N as far as g' is bounded and $|t_k-t|>\Delta$, therefore, $A_{N,k}g_k+A_{N,k+1}g_{k+1}\sim O(1/N^2)$. The number of such pairs in S_- or S_+ is increasing $\propto N$. Therefore taking also into account that in the sums S_- and S_+ each of the limited number of elements left out from such pairing process (e.g., in case of $C_{N,k}=1$ for $k=0,N$) is only of order $O(1/N)$, we conclude that both series S_- or S_+ tend to zero with the increase of N. This proves the localization Lemma. ■

A very important property of the CEDGT series $f_N(t)$ is the possibility of its term-by-term differentiation such that the resulting series converges with increasing N to the derivative $g'(t)$. Note that while being well-known for the CFT series (21), this property is not trivial for finite (N-)element discrete Fourier transforms. Recall that although in trigonometric polynomials in the form of (15) or (30) each individual term, being $\propto 1/N$, decreases to 0 at large N, their derivatives over t corresponding to a high-order harmonics, say $j>N/2$, become of order $j/N\sim 1$, and therefore, might not necessarily vanish with increasing N. Thus, a "fine tuning" of the entire discrete-

transform based series is needed in order to provide convergence of the series produced by its term-by-term differentiation.

Theorem: *Let $g(t)$ be a smooth function with bounded second derivative on the interval $t \in [0,T_0]$, which originates the N-interval grid function $\{g_k | k=0,1,\ldots,N\}$. Then the function $f'_N(t)$ produced by the term-by-term differentiation of the continuous extension of the discrete Fourier transform on SU(2), $f_N(t)$, converges with increasing N to $g'(t)$ at any $t \in (0,T_0)$.*

Proof: As earlier, we put $T_0=1$ for simplicity of the formulas below. Because the series $f_N(t)$ given by (31) contains a finite number of elements, it is obvious that its derivative f'_N can be summed up to the series produced by the term-by-term differentiation of (32).

Consider first the derivative $f'_N(t)$ at any *rational* t_0 in the open interval (0,1). In that case we can choose N such that $t_0=m/N$, and it then makes sense to choose all further subdivisions of the interval $[0,1]$ such that t_0 will be always kept as a knot of the grid, i.e., $t_0=m_1/N_1$ for all $N_1 > N$, i.e., choosing $N_1=aN$ with some integer $a>1$. Using the Lipshitz rule, the derivative of (32) at $t_0=m/N$ is reduced to

$$f'_N(t_0)=\frac{\pi}{2}\sin \pi t_0 \sum_{k=0}^{N\ (k\neq m)} (-1)^{k-m} C_{N,k}\, U_k(t_0) \quad + \quad \frac{\pi \cos \pi t_0}{2 \sin \pi t_0} g_m, \tag{34}$$

$$U_k(t_0)=\frac{g_k}{\cos \pi t_k - \cos \pi t_0}, \quad \text{where} \quad t_k=k/N. \tag{35}$$

Let us choose some small Δ, such that both $(t_0 \pm \Delta) \in (0,1)$, and then split the sum in (34) into 3 sub-series S'_+, S'_- and S'_Δ as in (33), where the number $K_t=m$ for $t=t_0=m/N$. It is convenient for further analysis to choose K_Δ as the maximum integer which satisfies the condition $K_\Delta/N \leqslant \Delta$ and is of the same parity as m. Then the indices of both the last element in the series S'_- and the first element in S'_+, $m-K_\Delta-1$ and $m+K_\Delta+1$, respectively, are odd.

Recall that for any smooth function $U(t)$ with a bounded second derivative on the equidistant grid we have

$$2U_k=U_{k-1}+U_{k+1}+U''_k N^{-2}+o(N^{-2}) \quad , \tag{36}$$

which follows from the familiar Taylor series decomposition $g(t+x)=g(t)+g'(t)\,x+0.5\,g''(t)\,x^2+o(x^2)$ in the $x=\pm 1/N$ vicinity of t. Applying (36) to $U(t)=g(t)/[\cos \pi t - \cos \pi t_0]$ at all $t=t_k$ in (34) and (35) with k odd (i.e., $k=2j-1 | 1 \leqslant j \leqslant (m-K_\Delta)/2$), and given (6), the series S'_- is reduced to

$$S'_-=(-1)^m \frac{\pi \sin \pi t_0}{2}\left(-U_{m-K_\Delta}+N^{-2} \sum_{j=1}^{(m-K_\Delta)/2} U''_{2j-1} \right)+o(N^{-1}). \tag{37}$$

The first term on the right-hand side is exactly one half of the first term in the localized sum S_Δ, but with a negative sign. The second term is of order $O(N^{-1})$. A more precise estimate of this term can be derived if we note that for large N the sum

$$\frac{2}{N} \sum_{j=1}^{(m-K_\Delta)/2} U_{2j-1} \to \int_0^{t_0-\Delta} U''(t)\mathrm{d}t = U'(t_0-\Delta)-U'(0) \tag{38}$$

is bounded for any given Δ, as far as $g''(t)$ is bounded. Note that the estimate of (38) implies only that $U''(t)$ is integrable. This suggests that in principle the conditions of the validity of the differentiation Theorem can be relaxed, requiring that $g''(t)$ be an integrable function on $[0,1]$, but not necessarily bounded.

Applying the same approach to S'_+, we find

$$S'_- + S'_+ = \frac{\pi \sin \pi t_0}{2}(-1)^{m+1}(U_{m-K_\Delta} + U_{m+K_\Delta}) + O_1, \tag{39}$$

with $O_1 \sim O(N^{-1})$. Note that in the case of an odd N, the residual O_1 also includes the difference between the last term, $k=N$, and one *half* of the $k=(N-1)$-th term, which is of order $U'_N \sin(\pi t_0)/N$. Here we take into account that $C_{N,N-1} = 2\, C_{N,N}$ from (6). Thus, for any ϵ we can choose N_ϵ such that for all $N > N_\epsilon$ the residual in (39) is $O_1 < \epsilon/2$. Then (34) is reduced with accuracy $< \epsilon/2$ to a summation of elements localized around, and symmetric with respect to, the point $t_0 = m/N$:

$$f'_N(t_0) = \pi \sin \pi t_0 \sum_{j=1}^{K_\Delta - 1} (-1)^j (U_{m-j} + U_{m+j}) + \frac{\pi \sin \pi t_0}{2}(-1)^{K_\Delta}(U_{m-K_\Delta} + U_{m+K_\Delta})$$

$$+ \frac{\pi \cos \pi t_0}{2 \sin \pi t_0} g_m + O_1(\epsilon/2). \tag{40}$$

Here we take into account that K_Δ is chosen to be of the same parity with m. Introducing now $r_j = j/N$ which is $\leqslant \Delta$ for $j \leqslant K_\Delta$, we have

$$\sin \pi t_0 (U_{m-j} + U_{m+j}) = g_m \frac{\cos \pi t_0}{\sin \pi t_0} - \frac{2}{\pi} g'_m + O_{2,j} \quad ,$$

where, keeping the largest order terms, the residual $O_{2,j}$ is reduced to

$$O_{2,j} \simeq \left(g_m - \frac{2}{\pi} g'_m + \frac{2 \sin^2 \pi t_0}{\pi^2} g''_m \right) \left(\frac{\pi r_j}{2 \sin \pi t_0} \right)^2 \quad . \tag{41}$$

Substituting these 2 relations into (40), and recalling that $g'_m \equiv g'(t_0 = m/N)$, it is easily shown that for both even and odd m and K_Δ one has

$$f'_N(t_0) = g'(t_0) + O_1(\epsilon/2) + O_2(\Delta^2), \tag{42}$$

where the residual O_2 represents the sum of residuals $O_{2,j}$, i.e., $O_2 \Sigma_{\{j\}} O_{2,j}$. Because of the sign alteration term $(-1)^j$ in (40), this sum does not increase with increasing N beyond the absolute value of $O_{2,j}$ at $r_j = \Delta$ in (41). It follows then that for any small $\epsilon > 0$ we can first choose an interval Δ proportional to $\sqrt{\epsilon} \sin \pi t_0$ (depending also on g, g', g'') such that $|O_2| < \epsilon/2$. Then we can choose a number N_ϵ such that $|O_1| < \epsilon/2$. Hence $|O_1 + O_2| < \epsilon$ for all $N > N_\epsilon$. This proves the differentiation Theorem. ■

Note that in the derivation of (38) which has allowed principal clipping of both end-terms in the localized (40) exactly by one half, the symmetry properties of the SU(2) DGT series expressed in the term $C_{N,k}$ have been fully exploited.

Another notice is that, along with the continuous DGT extension of $\{g_k\}$, the *localization Lemma is also valid for its term-by-term derivative* $f'_N(t)$. This property is actually proven by the localized structure of the sum in the construction (40).

Example 4: In Fig. 4 we show interpolations which are provided by the CEDCT series (15) (dashed curves) for the function

$$g(t) = e^{-3t} + \tfrac{1}{2} e^{-((t-0.5)/0.1)^2}, \tag{43}$$

and its first derivative $g'(t)$ (bottom panels). For comparison, we also show approximations provided by the continuous extension of the truncated DFT series (30) with $K = N/2$ (thin solid curves), and by the Shannon's interpolation formula (27) (heavy 3-dot–dashed curves). Recall that the use of the standard CEDFT series (25) for calculations of derivatives does not make any sense as far as CEDFT does not converge (see Fig. 2). Although both the truncated DFT series $s_N(t)$ and the Shannon's interpolation series $X(t)$ do converge to $g(t)$ with increasing N, as shown on the

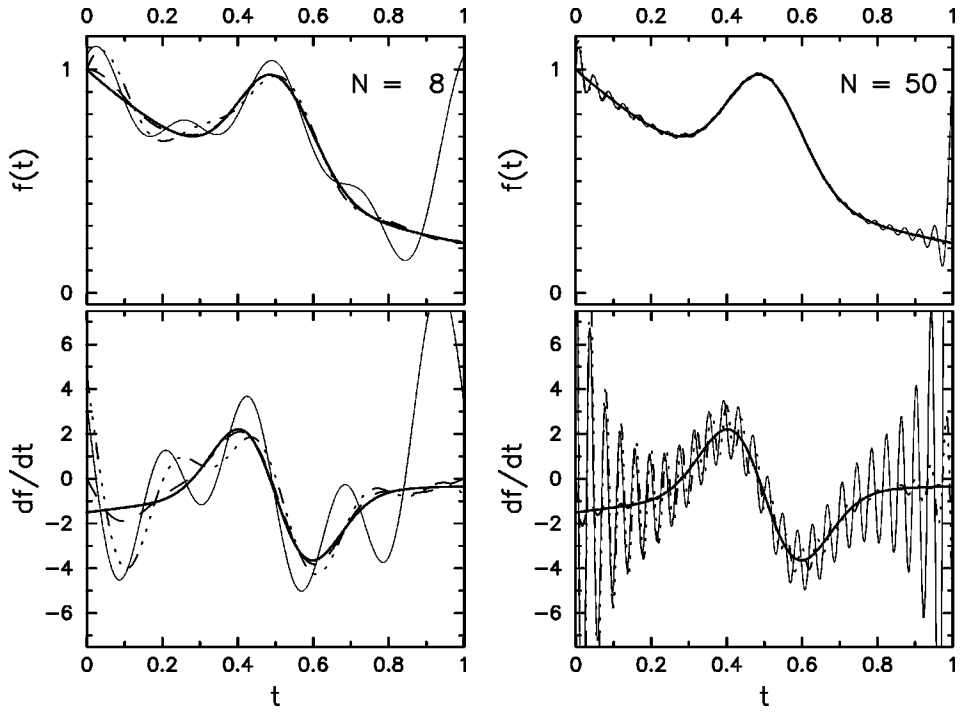

FIG. 4. The CEDCT series $f_N(t)$ (*dashed curves, top panels*) and the derivatives $f'_N(t)$ (*dashed curves, bottom panels*) for an analytic function $g(t)$ of Eq. (43) and its derivative $g'(t)$ (*heavy solid curves*) in the case of $N=8$ and $N=50$. For comparison, we also show the approximations provided by Shannon interpolation formula (27) with $N+1$ points (3-dot–dashed curves), and by truncated DFT series $s_K(t)$ of Eq. (30) and its derivative $s'_K(t)$ with $K=N/2$ (thin solid curves). Note that both $s_K(t)$ and $X_N(t)$ converge with $N\to\infty$ at all $t\in(0,1)$, but their derivatives do not.

top right-side panel, their derivatives reveal profound oscillations at any large N. Meanwhile, $f'_N(t)$ shown by solid lines on the two bottom panels of Fig. 4 already provides a rather good approximation to $g'(t)$ at rather small values of N.

At the end of this section we would like to note, albeit without any proof or demonstration in this paper, that our numerical calculations show that the second derivative of CEDGT also appears to converge to $g''(t)$ if the derivatives $g'(0)=g'(T_0)=0$ is satisfied.

IV. MULTIDIMENSIONAL FOURIER TRANSFORM

Being a transform with separable variables, the multidimensional DCT is easily reduced to the product of one-dimensional DCTs, which is widely used, for example, for effective 2D-image processing (e.g., see Refs. 7 and 13). Although the multidimensional DCT is well known, in this section we will first formulate it in terms of discrete Fourier transform on the $\mathrm{SU}(2)\times\cdots\times\mathrm{SU}(2)$ group. Then we will briefly discuss the convergence properties of the continuous extension of 2D discrete cosine transforms.

The generalization of the transform formulas for decomposition of functions of n variables, $G(x_1,\ldots,x_n)$, into the Fourier series of orbit functions of $[\mathrm{SU}(2)]^n$ group is straightforward. Let us consider first the case of $n=2$, i.e., when a function $G\to G(x,y)$ defined in the region $\mathsf{F}_\mathsf{n}=\{0\leqslant x\leqslant 1,\ 0\leqslant y\leqslant 1\}$ (i.e., assuming normalized variables $x\to x/X_0$, $y\to y/Y_0$) is to be decomposed into the series of the orbit functions $\Phi_{mn}(x,y)$ of the symmetry group $\mathrm{SU}(2)\times\mathrm{SU}(2)$. In this case $\Phi_{mn}(x,y)=\Phi_m(x)\,\Phi_n(y)$. Using for convenience again the functions $\psi_m(x)=\cos(\pi m x)$ instead of $\Phi_m(x)$, we can write

$$\Psi_{mn}(x,y)=\psi_m(x)\,\psi_n(y)=\cos(\pi m x)\cos(\pi n y)\,, \tag{44}$$

where $(x,y)\in F$. For a uniform rectangular grid $\{x_j,y_k\}$ defined in the region F such that

$$\{x_j = j/M,\ \ y_k = k/N \ \ | j = 0,1,\ldots,M;\quad k = 0,1,\ldots,N\},$$

the functions Ψ_{mn} are orthogonal in the following bilinear form

$$\langle \Psi_{mn}, \Psi_{pq} \rangle_{M,N} = \sum_{j=0}^{M} \sum_{k=0}^{N} C_{M,j} C_{N,k} \Psi_{m,n}(x_j, y_k) \Psi_{pq}(x_j, y_k) = \frac{4MN}{C_{M,j}\, C_{N,k}} \delta_{mp}\, \delta_{nq}, \tag{45}$$

which follows directly from (8).

Let $G(x,y) \to \mathbb{R}$ be a continuous function originating a two-dimensional grid function $G_{jk} = G(x_j, y_k)$ on the grid $\{x_j, y_k\}$. Then the decomposition of G into the Fourier series on SU(2) $\times$ SU(2) group corresponds to solving the system of equations

$$G_{jk} = \sum_{m=0}^{M} \sum_{n=0}^{N} A_{mn}\, \Psi_{mn}(x_j, y_k) \equiv \sum_{m=0}^{M} \sum_{n=0}^{N} A_{mn} \cos\frac{\pi m j}{M} \cos\frac{\pi n k}{N}, \tag{46}$$

with $\{0 \leqslant j \leqslant M,\, 0 \leqslant k \leqslant N\}$, with respect to the coefficients A_{mn}. This can be easily achieved using the orthogonality relation (45), if we multiply (46) by $C_{M,j} C_{N,k} \Psi_{pq}(x_j, y_k)$ and take the sum over $\{j,k\}$. Thus we find the coefficients A_{mn} of the discrete Fourier transform (46),

$$A_{mn} = \sum_{j=0}^{M} \sum_{k=0}^{N} D_M^{mj} D_N^{nk} G_{jk}. \tag{47}$$

The matrix D_N is defined as before by (12),

$$D_N^{ab} = \frac{C_{N,a} C_{N,b}}{2N} \cos\frac{\pi a b}{N}, \quad N, a, b \in \mathbb{Z},$$

with the weights $C_{N,a}$, $C_{N,b}$ given by (6).

In this way the coefficients A_{mn} of the two-dimensional DGT are found for any grid function $\{G_{jk}\}$ with bounded values at the grid points $(x_j, y_k) \in \mathsf{F}$. Thus we can formulate the following proposition:

Proposition: Let $G_{jk} = G(x_j, y_k)$ be values of a bounded function $G(x,y)$ on the rectangular grid points

$$x_j = jX_0/M, \quad y_k = kY_0/N; \quad j \in \{0,1,\ldots,M\}, \quad k \in \{0,1,\ldots,N\}.$$

A trigonometric function given by finite Fourier series

$$F_{MN}(x,y) = \sum_{m=0}^{M} \sum_{n=0}^{N} A_{mn} \cos\frac{\pi m x}{X_0} \cos\frac{\pi n y}{Y_0}, \tag{48}$$

with

$$A_{mn} = \sum_{j=0}^{M} \sum_{k=0}^{N} \frac{C_{M,m} C_{M,j} C_{N,n} C_{N,k}}{4MN} G_{jk} \cos\frac{\pi m j}{M} \cos\frac{\pi n k}{N}, \tag{49}$$

continuously extends the discrete inverse Fourier transform of the grid function $\{G_{jk}\}$ onto the entire rectangular area $(x \in [0,X_0], y \in [0,Y_0])$, and satisfies the equality

$$F_{MN}(x_j, y_k) = G_{jk} \quad \textit{for all} \quad j \in \{0,1,\ldots,M\}, \quad k \in \{0,1,\ldots,N\}.$$

Furthermore, if $G(x,y)$ is continuous, then $F_{MN}(x,y)$ converges to $G(x,y)$ for $M,N \to \infty$.

Since for any fixed $y_0 \in [0,Y_0]$ or $x_0 \in [0,X_0]$ the series $F_{MN}(x,y_0)$ or $F_{MN}(x_0,y)$, respectively, are reduced to one-dimensional CEDCT/CEDGT series along the x or y axes considered in

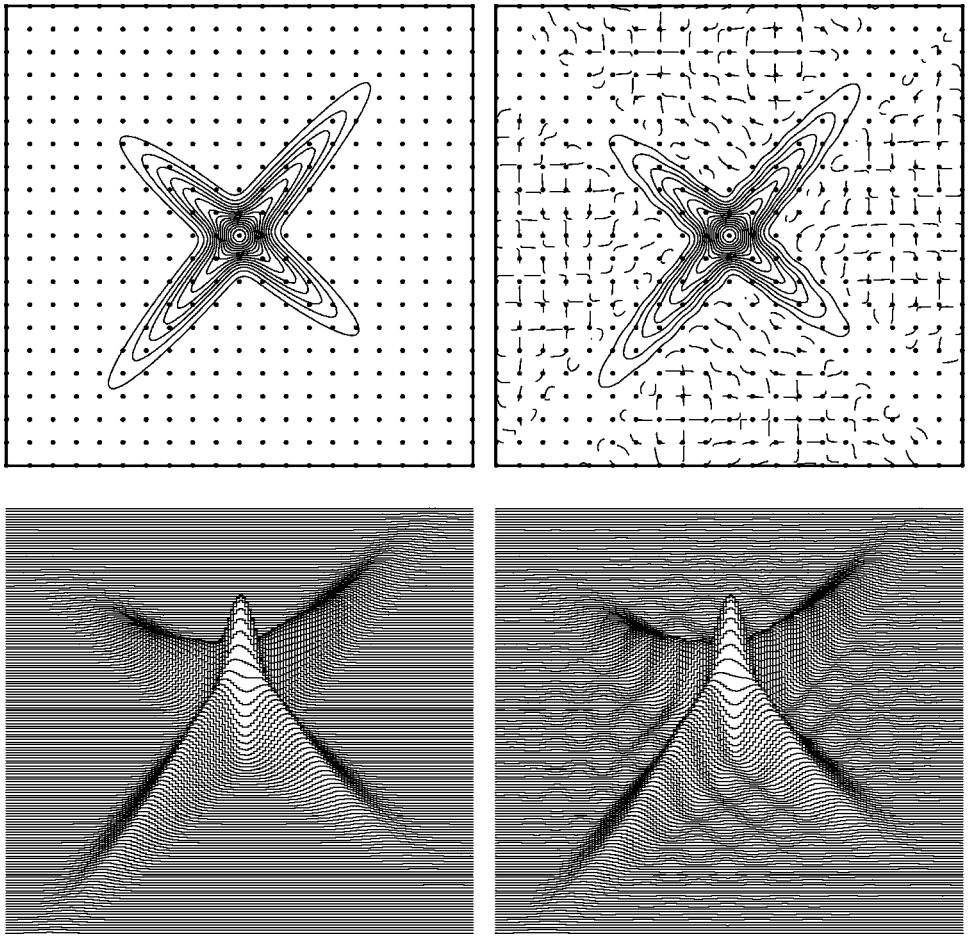

FIG. 5. Contour plots (upper panels) and visual "3D" images (lower panels) of an analytic function $G(x,y)$ (right side) and its approximation by two-dimensional SU(2)×SU(2) CEDGT/DCT series $F_{MN}(x,y)$ (left side) with $M=N=20$. $G(x,y)$ is composed of a sum of 2 two-dimensional Gaussian ellipsoids, each in the form of (50), and with dispersions $\sigma_{\perp,1}=\sigma_{\perp,2}=0.025=1/2N$. The dashed lines on the left bottom panel show the contour level $F_{MN}(x,y)=-0.001$.

the previous section, it is obvious that the continuous extension $F_{MN}(x,y)$ of 2D DGT on the SU(2)×SU(2) group (i.e., the two-dimensional DCT) not only converges with increasing (M,N) to $G(x,y)$, but also that it has properties of *locality* and *differentiability* similar to the one-dimensional CEDGT on ordinary SU(2) group.

Example 5: The upper panels in Fig. 5 show the contour plots of a function $G(x,y)$ defined in the square region $F=[0,1]\times[0,1]$ and composed of two two-dimensional Gaussian functions, each of type

$$e^{-(x'-x_0)^2/2\sigma_\parallel^2-(y'-y_0)^2/2\sigma_\perp^2}, \tag{50}$$

where $\sigma_\parallel \geqslant \sigma_\perp$, but with directions of the major axes x_1' and x_2' perpendicular to each other. For both Gaussians we have taken the transverse dispersions to be $\sigma_{1,\perp}=\sigma_{2,\perp}=0.025$, which is exactly 2 times smaller than the grid's cell size $\Delta x=\Delta y=1/20$ for the chosen $M=N=20$. The contour plots shown on the upper panels in Fig. 5 illustrate that even in the case of a grid with cell size this large compared with $\sigma_\perp$, the continuous extension of the two-dimensional DGT series reconstructs Gaussian-fast smooth structures reasonably well.

This is also apparent on the bottom panels of Fig. 5 where we show the three-dimensional images for the same analytic function $G(x,y)$ (left panel) and its approximation in the form of

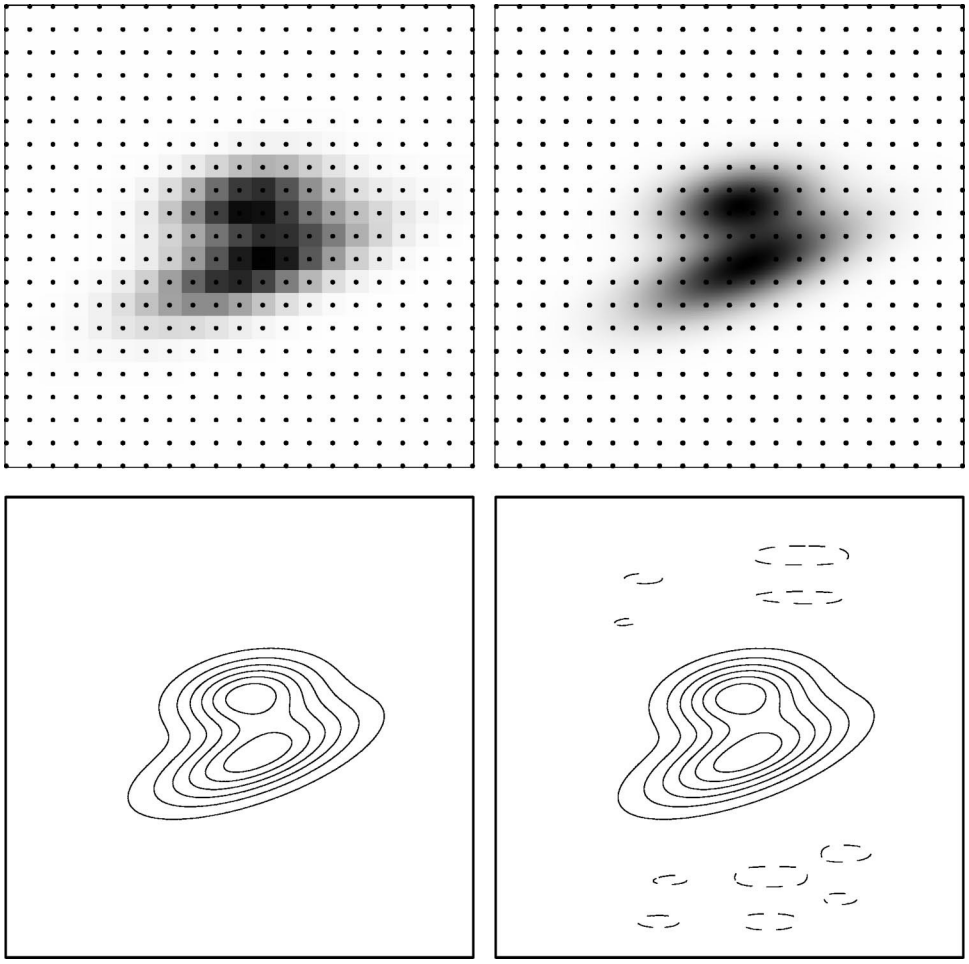

FIG. 6. **Upper panels**: The images, in terms of brightness distributions, corresponding to the grid function $\{G_{j,k}\}$ given on $M=N=20$ square grid (on the left), and its reconstruction by two-dimensional CEDCT series $F_{M,N}(x,y)$ (on the right). **Lower panels**: Contour plots of the analytic function $G(x,y)$ originating $\{G_{j,k}\}$ (on the left), and of its approximation by $F_{M,N}(x,y)$ (on the right). The original function $G(x,y)$ is composed of two-dimensional Gaussian distributions with transverse dispersions for both $\sigma_\perp = 1/N = 0.05$, an angle between long axes of the ellipsoids equal to 20°, and a small separation between their peak positions.

two-dimensional continuous DGT extension $F_{MN}(x,y)$ (right panel). Note that any waviness that can be seen in the approximated function would disappear from the images had we taken $N, M \geqslant 1/\sigma_\perp$ for the same functions.

Example 6: The latter case is chosen in Fig. 6 where the upper panels show, in terms of brightness distribution, the original grid function produced by 2 Gaussians with $\sigma_{1,\perp}=\sigma_{2,\perp} = 0.05 = 1/N$, for $N=M=20$, and its reconstruction in the form of two-dimensional continuous DGT extension (on the right). The major axes of the ellipsoids are inclined at a small angle (20°) to each other. For comparison, on the bottom left panel we show the contour plot of the exact (i.e., originating) function $G(x,y)$, and the bottom right panel shows its approximation by two-dimensional CEDGT. It is obvious that the reconstructed CEDGT image not only recovers the directions of the ellipsoids and their maxima, but it practically coincides with the exact image. Note that the dashed contours on both Figs. 5 and 6 show a level slightly below zero, $F_{MN} = -0.001$.

Generalization of the proposition for an n-dimensional DGT of a function $G(x_1,\ldots,x_n)$ on $[\mathbf{SU}(2)]^n$ group is straightforward:

Proposition: Let $G_{j_1\cdots j_n}=G(x_{1,j_1},\ldots,x_{n,j_n})$ *be values of a bounded function* $G(x^{(1)},\ldots,x^{(n)})$ *given on the rectangular* $(M_1,\ldots,M_n)$*-interval grid points*

$$\{x^{1,j_1}=j_1X_1/M_1,\ldots,x^{n,j_n}=j_nX_n/M_n,\quad j_k=0,1,\ldots,M_k:\quad k=0,1,\ldots,n\}.$$

A continuous function given by finite Fourier series

$$F_{M_1\cdots M_n}(x_1,\ldots,x_n)=\sum_{m_1=0}^{M_1}\cdots\sum_{m_n=0}^{M_n}A_{m_1\cdots m_n}\cos\frac{\pi m_1x_1}{X_1}\cdot\cdots\cdot\cos\frac{\pi m_nx_n}{X_n},\tag{51}$$

where

$$A_{m_1\cdots m_n}=\sum_{j_1=0}^{M_1}\cdots\sum_{j_n=0}^{M_n}\frac{C_{M_1,m_1}C_{M_1,j_1}\cdot\cdots\cdot C_{M_n,m_n}C_{M_n,j_n}}{2^nM_1\cdot\cdots\cdot M_n}\times G_{j_1\cdots j_n}\cos\frac{\pi m_1j_1}{M_1}\cdot\cdots\cdot\cos\frac{\pi m_nj_n}{M_n},\tag{52}$$

satisfies the equality

$$F_{M_1\cdots M_n}(x_{j_1},\ldots,x_{j_n})=G_{j_1\cdots j_n}\quad\text{,for all}\quad j_k\in\{0,1,\ldots,M_k\}\quad\text{and}\quad k\in\{0,1,\ldots,n\}.$$

Furthermore, if $G(x_1,\ldots,x_n)$ *is continuous, then* $F_{M_1\cdots M_n}(x_1,\ldots,x_n)$ *converges to* $G(x_1,\ldots,x_n)$ *with* $M_1,\ldots,M_n\to\infty$.

The proof of this proposition is readily obtained by the method of induction on the SU(2) factors of the group.

A. An example of CEDCT application to real images

In order to demonstrate the potential of the above suggested approach of *continuous extension* of the inverse multidimensional discrete group transforms for purposes of natural interpolation of discrete images between the grid points, as well as for the possibility of data compression and smooth representation of the compressed images, we have chosen a 56×140 pixel fragment of the well known image "Lena." The original fragment shown on Fig. 7(a) is strongly enlarged ("zoomed") in order to make visible the granularity of the image at its resolution limits. The grayscale color coding of the fragment contains all 256 intensity levels, from $g=0$ (*black*) to $g=255$ (*white*).

In Fig. 7(b) we show the continuous extension of the original image. It is constructed by subdividing each of the initial intervals Δx and Δy into 3 subintervals. This procedure increases the density of the grid points (pixels) by a factor $3\times3=9$. Calculations are done dividing first the initial 56×140 pixel fragment into ten 28×28 pixel subfragments, then calculating the CEDCT for each of these sub-fragments. It allows us to demonstrate, on the next two panels, the effects of CEDCT image reconstruction at the block edges after some image compression is done. Because the continuous extension of the inverse DCT can formally extend the values of the initial intensity distribution function to values $F_{MN}(x,y)$ beyond the limits $[0,255]$ used for the intensity coding, we have linearly renormalized the values of $F_{NN}\to\widetilde{F}_{NN}\in[0,255]$. The positive impact of the higher resolution achieved by the use of CEDCT in Fig. 7(b), as compared with the original image in Fig. 7(a), is apparent.

Note that the harmonic order of the cosine functions $\cos(\pi nx/X_0)$ and $\cos(\pi my/Y_0)$ used in CEDCT corresponds to the modes $0\leqslant m,n\leqslant50$. In Fig. 7(c) we show the continuous extension of the image obtained after application of the simplest "low-pass compression" procedure (see, e.g., Ref. 13), putting the DCT coefficients $A_{mn}\to0$ for all high-order modes with either m or n exceeding $n_{\max}=19$. This procedure generally removes the high-frequency "noise" from the image, and compresses the image by a factor $(29/20)^2\approx2$. No visual degradation of the CEDCT image is apparent. It is noteworthy that although the exactness property of the transform in Fig. 7(c) is lost, the edges of the 10 individual blocks, or the sub-fragments, cannot be visually

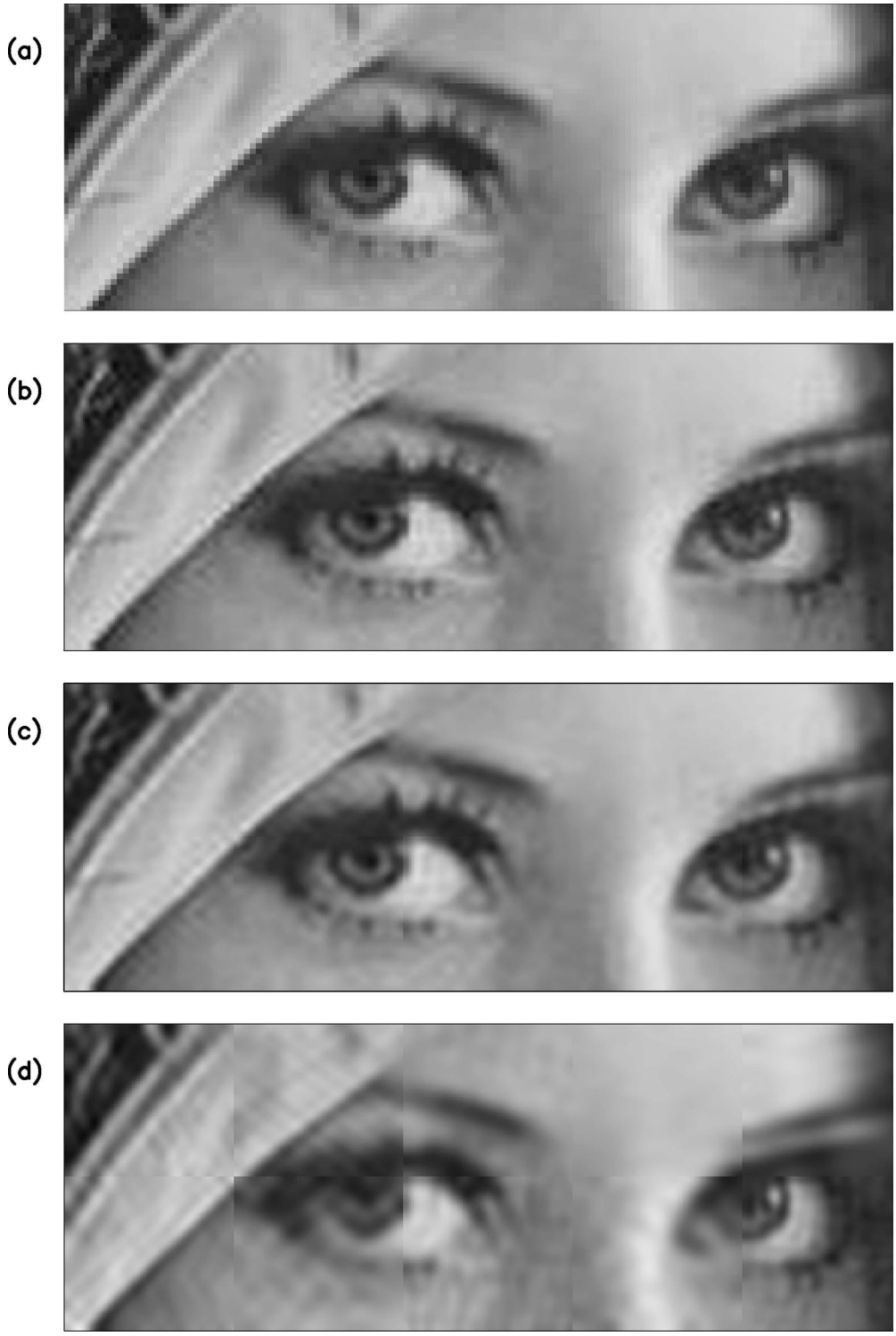

FIG. 7. **(a)** Zoomed 56×140-pixel fragment of the original image ''Lena''; **(b)** CEDCT image calculated with the 3×3 higher resolution, i.e., corresponding to 168×420 pixels; For our calculations the image was first subdivided into 10 square blocks of 28×28 size. **(c)** The picture in the same 168×420 pixel representation compressed by a factor of 2. The compression is reached by retaining in (48) only the first $0 \leqslant m,n \leqslant 19$ DCT coefficients A_{mn}, and discarding all higher-order terms. **(d)** The picture compressed by a factor of 10; the compression is achieved by discarding all cosine terms with $|A_{mn}| \leqslant 0.05\, A_{\max}$ (see text).

distinguished. The block edges become noticeable only in Fig. 7(d), where we have applied again the CEDCT approach for visualization of the image compressed now by a factor of 10. The compression in Fig. 7(d) is effectively reached by keeping in CEDCT series only 10% of the cosine terms with the large-value coefficients A_{mn}, and discarding all terms with small-value A_{mn}. For Fig. 7(b) it has corresponded to the assumption $A_{mn}\to 0$ if $|A_{mn}|\leqslant 0.05\,A_{\max}$, where $A_{\max}$ is the maximum absolute value of the coefficients $\{A_{mn}|\}$ (*excluding* A_{00}). Obviously, the image in Fig. 7(d) still remains smooth and quite recognizable.

We would like to note here that it has not been our aim in this paper to reach the goal of the best possible image compression. We believe, however, that through this paper our examples demonstrate the high potential of the developed approach of *continuous extensions* of DCT, and of the DGTs generally, as considered in the next Paper II for the SU(3) group (in preparation), for purposes of practical applications, and in particular for image processing and compression.

V. SUMMARY

We have shown that:

1. A discrete Fourier transform of a grid function $\{g_k|k=0,1,\ldots,N\}$ on the orbit functions of Lie groups, abbreviated DGT, in the case of SU(2) is reduced to the well known discrete cosine transform, namely, to DCT-I, which is a known type of exact discrete transforms, like the standard DFT sequence.
2. The principal difference between these 2 types of discrete Fourier transforms consists in the fact that DCT is based on the functions $\cos(k\pi t/T_0)$ corresponding to $k\leqslant N$ trigonometric harmonics of both integer and half-integer orders, $n=k/2\leqslant N/2$, whereas the DFT utilizes trigonometric functions of integer n only, but extending to orders $n\leqslant N$. This results in vital differences in the subsequent properties of DFT and DCT (or DGT generally).
3. If the function $g(t)$ originating $\{g_k\}$ is a continuous function of $t\in[0,T_0]$, then the continuous extension of the (*inverse*) DCT sequence results in the function $f_N(t)$ which converges to the original $g(t)$ with increasing N at all t. This property does not hold for the continuous extension of the standard DFT sequence, which shows profound oscillations between the points of the grid. Note that potentially this feature implies significantly smaller vulnerability of DCT to the truncation/approximation errors in the process of filtering as compared with the standard DFT. Therefore, it could be the reason for the superior general performance of the DCT compared with the DFT (see Ref. 5).
4. Similar to canonical *continuous* Fourier transform polynomials with coefficients calculated by exact integrations, the CEDCT series satisfies the principle of *locality*. This property insures, in particular, that the computation errors connected, e.g., with noise or uncertainties in one segment of the data will not significantly affect the reconstructed CEDCT image on the distant segment of data. This property of DCT may become important especially in the process of lossy data compression when the property of exactness of the *discrete* transform is not necessarily preserved.
5. Similar to the canonical CFT, the CEDCT series $f_N(t)$ can be differentiated term by term, so that for the (*first*) derivative series $\lim_{N\to\infty} f'_N(t)\to g'(t)$ for all $t\in(0,T_0)$ provided that the second derivative of $g(t)$ is a continuous (or just an integrable) function on the interval $[0,T_0]$. For CEDCT this property is valid both when $g(0)=g(T_0)$ and $g(0)\neq g(T_0)$. It does not necessarily hold for continuous extensions of other types of discrete transforms, which might be converging, like $s_k(t)$ in (30) or Shannon interpolation $X_N(t)$, but which produce nonconverging derivative series, as demonstrated in Fig. 4.

The derivative series $f'_N(t)$ satisfies the localization principle along with $f_N(t)$.

6. In the case of an n-dimensional function defined on the knots of a rectangular n-dimensional grid, the DGT Fourier decomposition can be performed using the orbit functions of $[\mathrm{SU}(2)]^n$ group. Such Fourier series are effectively reduced to the n-fold convolution of one-dimensional DGT on SU(2) alongside n independent (rectangular) axes. Therefore they have nice properties of *convergence*, *localization*, and *differentiability* of their continuous DGT extensions similar to the one-dimensional CEDCT.

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Superconformal primary fields on a graded Riemann sphere

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Primary superfields for a two-dimensional Euclidean superconformal field theory are constructed as sections of a sheaf over a graded Riemann sphere. The transformation law is found to be the same as that of an O(N) extended primary field. The construction is then applied to the $N=3$ Neveu–Schwarz case. Various quantities in the $N=3$ theory are calculated, such as elements of the super-Möbius group, and the two-point function. Applications of the construction to calculate three-point functions and fusion rules in a manifestly supersymmetric fashion are discussed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1739295]

I. INTRODUCTION

Two-dimensional conformal field theory has many applications in statistical mechanics and string theory. It also has a very rich algebraic nature, in a sense due to the symmetry algebra being infinite-dimensional. Exactly how this works in the bosonic case is extremely well understood.[13]

The supersymmetrization of two-dimensional conformal field theory is something that has been studied heavily from a string theory approach.[16] The string is described by a two-dimensional conformal field theory, and the supersymmetrization of the conformal field theory essentially admits fermions onto the string. This has mostly been studied from a Lagrangian point of view, where the Lagrangian exhibits the classical symmetries. Canonical quantization can then be used to then obtain the quantum algebra.

In bosonic conformal field theory there is a way, using the high degree of symmetry, to obtain the quantum algebra by algebraic means, rather than from a Lagrangian. Extending this to a theory with one or two Grassmann variables has been covered extensively in the literature. Adding more supersymmetry to the theory has been studied, e.g., Refs. 29, 8, 9, but in nowhere near as much depth as the $N=1,2$ theories.

In two-dimensional conformal field theory, it is found that one can always find a conformal transformation that maps the two-dimensional theory to a two dimensional theory that is flat. In the Euclidean case, the conformal transformations that map the plane to itself are precisely the holomorphic and antiholomorphic transformations of the plane to itself. One can therefore build Euclidean two-dimensional conformal field theory on a complex plane.[17] To get a more ''global'' picture of what is going on, the theory can then be conformally mapped to the Riemann sphere. Many of the properties of the conformal field theory can then be described by the properties of the Riemann sphere. The question then becomes how to build a theory on a ''super-Riemann sphere,''[14,15] and how the properties of this object can be related to the properties of a superconformal field theory. In this note, the question is addressed, with particular attention payed to the $N=3$ case.

Superconformal algebras in the classical case look like derivations on a polynomial ring in $\{z,z^{-1},\theta_i\}$, where the θ_i are anticommuting ''coordinates,'' that preserve a differential form. This can be combined with the theory of extended graded manifolds, with the manifold in question being the Riemann sphere, to give a suitable setting for superconformal field theory (Secs. II–IV).

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One can then use this setting to construct and calculate various quantities in the field theory. The $N=3$ Neveu–Schwarz case is studied in detail (Secs. V–X).

II. THE GRADED RIEMANN SPHERE

In this section, a Riemann sphere is considered, and how one can generalize it to the superconformal case. It should be mentioned that there are strictly speaking two approaches, which give rise to the same structure.[28,5,4] Here, the algebraic structure,[23,24] known as a Graded Manifold (of the extended type) will mostly be used. In some instances, it will become necessary to transfer to the analytic point of view, namely Supermanifolds.[26]

First consider an ordinary Riemann sphere. Rather than consider it as a geometric object, one could consider it as a collection of open sets, U_i, and consider the functions $f:U_i\to\mathbb{C}$ that are holomorphic in each open set, denoted $f(U_i)$. Each $f(U_i)$ is a ring under addition in $\mathbb{C}$, and pointwise multiplication. Given an open subset $V\subseteq U$, one can construct a nonsingular ring homomorphism $\rho_{UV}:f(U)\to f(V)$. These ring homomorphisms become the fundamental tools to work with. They give a way of comparing $f(U_i)|_{U_i\cap U_j}$ and $f(U_j)|_{U_i\cap U_j}$ and allow one to construct a sheaf of rings over the Riemann sphere, denoted $\mathcal{A}_0$.[23,18] One can see that each $f(U_i)$ will be a subring of $\mathbb{C}[z,z^{-1}]$. One can then consider derivations on each $f(U_i)$, denoted $\mathrm{Der}(U_i)$ which are $\mathbb{C}$-linear maps from $f(U_i)$ to $f(U_i)$ that obey the Leibniz rule. $\mathrm{Der}(U_i)$ then forms a rank one module over $f(U_i)$. The map ρ_{UV} induces a map $\rho_{UV*}^{-1}:\mathrm{Der}(U)\to\mathrm{Der}(V)$. One can use these ρ_{UV*} to construct a sheaf of abelian groups, namely the tangent sheaf, denoted $\mathcal{D}^1\mathcal{A}_0$. It is, locally, a rank one $\mathcal{A}_0$-module. A section of it can be written locally as $g(z)(\partial/\partial z)$. On each U_i, one can also consider the $\mathcal{A}_0$ linear maps of $\mathrm{Der}(U_i)$ into $\mathcal{A}_0$, denoted $\Omega^1(U_i)$. This is also a rank one $f(U_i)$-module, and the ρ_{UV*} induce a map $\rho_{UV}^*:\Omega^1(U)\to\Omega^1(V)$. Once again, the ρ_{UV}^* can be used to construct a sheaf, denoted $\mathcal{D}_1\mathcal{A}_0$. It is locally a rank one $\mathcal{A}_0$-module. Locally, a section can be written as $dzg(z)$. One can define the conformal condition as demanding that $\rho_{UV}:z'\mapsto z$, for z',z local coordinates in U,V respectively, as having the property $\rho_{UV}^*dz'=dz\kappa(z)$ for some $\kappa\in\mathcal{A}_0$. Given this construction, a basis of infinitesimal transformations can be written down, namely $z'=z+az^{n+1}$ corresponding to a space of vector fields, which gives rise to the Witt algebra. Phrasing the structure of a Riemann sphere in this way gives the most natural generalization to a graded Riemann sphere.

Similarly, an extended graded manifold can be defined, where each ring associated to each open set is no longer a subring of $\mathbb{C}[z,z^{-1}]$, but a larger ring containing Grassmann generators. The ring is no longer over $\mathbb{C}$, but over a complex, finitely generated unital Grassmann algebra, $B_{L'}$. Each ring associated to each open set is now a subring of

$$B_{L'}[z,z^{-1},\theta_1,\ldots,\theta_N]. \tag{1}$$

It is worth noting that this is a slightly more general requirement than that of a graded manifold. In the graded manifold case, the ring is often still taken to be over $\mathbb{C}$, and so would look like

$$\mathbb{C}[z,z^{-1},\theta_1,\ldots,\theta_N], \tag{2}$$

which, as a ring, is contained in (1). This can be seen by constructing a map $\pi:B_{L'}\mapsto\mathbb{C}$ by projecting onto the unital element in $B_{L'}$. The map defines an important quantity, namely the "body" of an element of a grassmann algebra. The approach of looking at an algebra over $B_{L'}$ rather than $\mathbb{C}$, as far as the author is aware, was first introduced in Ref. 28. The ring (1) is the Neveu–Schwarz ring. This gives rise to a sheaf, denoted by $\mathcal{A}_N$ for some positive integer N. The only condition on the ring associated to each open set, is that it be "holomorphic in z." This is, in fact, quite a subtle analytic condition, a discussion of which will be postponed for a few paragraphs. Derivations are now replaced by the sheaf of graded derivations, $\mathcal{D}^1\mathcal{A}_N$ which is a left $\mathcal{A}_N$ module. Accordingly, there is the sheaf of graded one-forms, $\mathcal{D}_1\mathcal{A}_N$, which are $\mathcal{A}_N$ linear maps of $\mathcal{D}^1\mathcal{A}_N$ into $\mathcal{A}_N$. $\mathcal{D}_1\mathcal{A}_N$ is a right $\mathcal{A}_N$ module. For full details of this construction of derivations and one-forms, see Ref. 23.

There is now a question of a preserved one-form. The basis of differentials is now given by $(dz, d\theta_i)$. Rather than the one-form coming for free, it must now be defined. This one-form will define a generalized conformal structure.[19] Define the one form[9] $\omega = dz - \Sigma_i d\theta_i \theta_i$. A transformation $(z, \theta_i) \mapsto (z', \theta_i')$ is superconformal iff it is invertible and $\omega' = \omega\kappa(z, \theta_i)$ for $\kappa \in \mathcal{A}_N$. All homomorphisms between open sets with intersection are demanded to be superconformal. An alternative basis for $\mathcal{D}_1\mathcal{A}_N$ is $(\omega, d\theta_i)$, which gives a corresponding dual basis of $\mathcal{D}^1\mathcal{A}_N$, namely (∂, D_i). Here, $\partial = \partial/\partial z$, and $D_i = (\partial/\partial\theta_i) + \theta_i(\partial/\partial z)$. This is a convenient basis to work with. It can be readily shown from the superconformal condition, that

$$D_i z' - \sum_j \theta_j' D_i \theta_j' = 0, \tag{3}$$

$$\kappa = \partial z' + \sum_j \theta_j' \partial \theta_j'. \tag{4}$$

From here on summations are dropped, and summation convention should be assumed. In particular, considering infinitesimal transformations, once the z' transformation is known, all the θ_i' transformations can almost be deduced. In the $N=1$ case, there is a $\mathbb{Z}_2$ ambiguity. For higher N this ambiguity becomes a continuous group, often interpreted as a gauge group in the physics literature.[1,2] κ can also be given by a slightly different expression. The relation $[D_i, D_k] = 2\delta_{ik}\partial$, where the commutator is graded, and (3), are useful in showing that $\det(D_i\theta_j')^2 = (\partial z' + \theta_i' \partial\theta_i')^N = \kappa^N$. This is an expression in a Grassmann ring over $\mathbb{C}$, so it is not obvious that one can divide or take Nth roots. If the coordinate transformation on the intersection of two open neighborhoods $(z, \theta_i) \mapsto (z', \theta_i')$ involves a scale factor κ, the inverse transformation will induce a scale factor κ', with $\kappa\kappa' = \kappa'\kappa = 1$. Thus, κ has a unique[32] inverse, and both κ and κ' have a component that is pure complex number, i.e., they have a nonzero "body." Since an extended graded manifold framework is being used, this is not as trivial a fact as it might seem. Nth roots of κ can now be defined, as the binomial expansion around the "body," $\epsilon(\kappa)$. This expansion is finite due to the nilpotency of $\kappa - \epsilon(\kappa)$. One finds that $\omega' = \omega(\det(D_i\theta_j'))^{2/N}\zeta^2$, where ζ is an Nth root of unity. Calculating the corresponding transformation on the basis of $\mathcal{D}^1\mathcal{A}_N$, one finds that $D_i' = (D_i'\theta_j)D_j$, and that $(D_i\theta_j')^{-1} = (D_i'\theta_j)$.

There is a subtle point about the superconformal transformation. The map

$$z' = z, \quad \theta_i' = -\theta_i \tag{5}$$

is superconformal. If one restricts to transformations $z' = z'(z)$ and uses the superconformal condition to deduce how the θ_i can transform, the choice of possible minus manifests itself as a choice of spin structure. Considering the transformation (5), one can ask what functions of (1) are invariant under it. A basis can be chosen for this ring, namely $\{z^n, z^n\theta_i, \ldots, z^n\theta_1\theta_2, \ldots, \theta_N\}$, for $n \in \mathbb{Z}$. Without the minus sign, all these basis elements are transformed to themselves. With the minus sign, one finds that those elements with an odd number of θ_i obtain a minus sign. Thus, only a subring is invariant. One can enlarge the invariant subring by introducing square roots and choosing the minus sign in the square root whenever one has an odd number of θ_i in a basis element. Consider now a subring of

$$B_{L'}[z^{1/2}, z^{-(1/2)}, \theta_1, \ldots, \theta_N], \tag{6}$$

which has as a basis $\{z^n, z^{n+(1/2)}\theta_i, z^n\theta_i\theta_j, z^{n+(1/2)}\theta_i\theta_j\theta_k, \ldots\}$ $n \in \mathbb{Z}$ and choose the negative square root under a superconformal transformation. Now all the basis elements are mapped to themselves under a superconformal transformation. This is the Ramond ring. It should be noted that with the analytic definition of functions that are "holomorphic in z" that will be used here

(see below), the Ramond ring introduces a branch cut. It should also be noted that this construction can easily be extended to the case when some of the θ_i have a minus sign in the transformation, and some do not.

Already the need for a more analytic idea of what is going on is apparent. This will be particularly important when the question of contour integration arises. Full details of this approach can be found in Refs. 28, 26. Many details are not mentioned here. Consider now a Grassmann algebra generated by L generators, B_L. This algebra can be given a Banach algebra structure, with the resulting topology being Hausdorff. This splits into an even and odd part, $B_L = B_{L0} \oplus B_{L1}$ as a vector space over $\mathbb{C}$. Now the θ coordinates take values in B_{L1} and z in B_{L0}. In particular, z can now have a nilpotent even part $s(z)$ (the soul), but must have a proper complex number part $\epsilon(z)$ (the body). Using the fact that a body exists, a "superdifferentiable" [26] function can be constructed. For $L' = \{\text{the smallest integer not smaller than } L/2\}$, a continuation can be specified, namely a continuation $Z_{L',L} : C^\infty(\epsilon(U), B_{L'}) \to G^\infty(U, B_L)$ for U open in B_L. The algebra $B_{L'}$ can be associated to the algebra B_L by the inclusion map $\iota_{L',L} : B_{L'} \to B_L$ which is the algebra homomorphism that maps the generators β_i to L' of the generators in B_L, and the unit in $B_{L'}$ to the unit in B_L. Note, $f(z)$ may be even or odd,

$$Z_{L',L}(f)(z) = \sum_{i=0}^{L} \frac{1}{i!} \iota_{L',L}(f^{(i)}(\epsilon(z))) \times s(z)^i, \tag{7}$$

where $f^{(i)}$ denotes the ith derivative. Now consider functions of the variables (z, θ_i) that can be written as

$$F(z, \theta_i) = Z_{L',L}(f_0)(z) + \sum_{i=1}^{N} Z_{L',L}(f_i)(z)\,\theta_i + \cdots = \sum_{\mu=0}^{2^L - 1} Z_{L',L}(f_\mu)(z)\,\theta_\mu . \tag{8}$$

The statement that $F(z, \theta_i)$ is holomorphic in z is the statement all the $f_\mu(w)$, are holomorphic in the complex variable w. These are examples of GH^∞ functions. For a sheaf to be GH^∞, its restriction maps, ρ_{UV}, must also be GH^∞.

An interesting sheaf to look at is that formed by the one-form ω. It shares similar properties to the one-form dz on an ordinary Riemann sphere. Call the sections of this line bundle on the Riemann sphere $\mathcal{O}_0(1)$. If the change of coordinates on an intersection from one open set to another is $z \mapsto f(z)$, then the transition function for an element of $\mathcal{O}_0(1)$ is $f'(z)$. In conformal field theory, a primary field of weight h can be thought of as a section of $\mathcal{O}_0(h) = \mathcal{O}_0(1)^{\otimes h}$, where h is a positive integer. In the super case, this gives something similar. It should be pointed out that ω will not give a line bundle. This would require the typical fiber to be a free $B_{L'}$ module of rank one, rather than a line. As a result, it must be regarded as a sheaf. This gives rise to a sheaf of sections, $\mathcal{O}_N(1)$. On an intersection, the function $(\det D_i \theta'_j)^{2/N} \zeta^2$ is the sheaf's homomorphism. This should be compared to the transition functions on a line bundle. "Uncharged" primary superfields[12] can then be thought of as sections of $\mathcal{O}_N(h) = \mathcal{O}_N(1)^{\otimes h}$. It should be noted that now tensor products are taken over a graded ring, $\mathcal{A}_N$, so care must be taken with signs in the tensor product. For example, consider a tensor product between two graded left-$\mathcal{A}_N$ modules. Then

$$f_1 \otimes p f_2 = (-1)^{p f_1} p f_1 \otimes f_2 ,$$

where $p \in \mathcal{A}_N$, and exponents of (-1) give the parity of the associated element. Similar formulas should be used if one of the two modules, or both are right-$\mathcal{A}_N$ modules, with the obvious modifications in the exponent of (-1).

There are other interesting sheaves also present. If one accepts the Berezin prescription for integration, then the integration "measure" on the graded Riemann sphere is $\omega \otimes_i D_i$, which has a transformation rule $(\det D_i \theta'_j)^{((2/N)-1)} \zeta^2$. As was first noticed in Ref. 29, there is also a O(N) group present. This can be regarded as a sheaf in the following way. Since the $\{D_i\}$, $i = 1,\ldots,N$, transform amongst themselves, one can consider the sheaf of supercovariant derivatives. Then the

transformation law on intersections of open sets is $D_i' = (D_i' \theta_j) D_j$. Since the superderivatives transform into one another, one can consider the sheaf of supercovariant derivatives. Call the sections of this sheaf $\mathcal{C}_N$. The matrices $D_i \theta_j'$ enjoy the following property:

$$(D_i \theta_j')(D_k \theta_j') = \delta_{ik}(\partial z' + \theta_j' \partial \theta_j') = \delta_{ik} \kappa = \delta_{ik} (\det D_i \theta_j')^{2/N} \zeta^2. \tag{9}$$

The right-hand side can be though of as an $N \times N$ identity matrix multiplying the scale factor of the superconformal transformation. Consider now a sheaf whose sections are $\mathcal{O}(-\frac{1}{2}) \otimes \mathcal{C}_N$. Constructing $\mathcal{O}(-\frac{1}{2})$ requires taking a square root, and is very analogous to taking the square root of a line bundle. Hence, the choice of sign can be thought of as choosing a spin structure. The group homomorphisms on an intersection of open sets in this sheaf are given by

$$M_{ij} = \frac{(D_i \theta_j')}{\sqrt{\kappa}} \tag{10}$$

and the sheaf itself is an $\mathcal{A}_N$-module of rank N. Recall that on intersections, κ has an inverse κ', and so $\kappa^{-(1/2)}$ is well defined on this intersection. There is still a question of a sign. Keeping in mind that $\theta_j' = \pm \theta_j$ is a superconformal transformation, it is really the θ_j that one would want to account for different spin structures, rather than $\mathcal{O}(-\frac{1}{2})$. Therefore, it seems reasonable to choose a plus sign for $\kappa^{-(1/2)}$. Regarding the new homomorphism M_{ij} as a matrix acting on a free module of rank N, it can be thought of as an element of $\mathrm{O}(N)$, with the entries being even Grassmann elements. The new sheaf then gives rise to a fundamental representation of $\mathrm{O}(N)$, and the M_{ij} the coefficients of a matrix with basis E^{ij}. Call this sheaf $\mathcal{G}_N$. This can give rise to other sheaves which are also $\mathrm{O}(N)$ representations.

The manner in which this is done parallels what is often done for vector bundles, in particular frame bundles and spin bundles. The reason this treatment can be applied is that $\mathcal{G}_N$ almost looks like a vector bundle, the only hinderance being that the ''typical fiber'' would be a $B_{L'}$ module rather than a vector space. Rather than an Abelian group of rank N being associated to each open set, one can instead associate a group element of $\mathrm{O}(N)$, just as is done with frame bundles with principal bundles, and retain the same M_{ij}. This gives rise to a sheaf $\tilde{\mathcal{G}}_N$. Considering, now a different representation ρ of $\mathrm{O}(N)$ gives rise to a sheaf homomorphism (albeit of non-Abelian groups)

$$\sigma: (\mathbb{P}_1, \tilde{\mathcal{G}}_N) \to (\mathbb{P}_1, \tilde{\mathcal{G}}_N^{\rho}), \tag{11}$$

where the group homomorphisms are now given by $M_{ij} \rho(E^{ij})$. Since the representation ρ has a vector space V associated to it, one can consider the sheaf which has the group homomorphisms given by $M_{ij} \rho(E^{ij})$, and stalk V, and denote the sections of this sheaf by $\mathcal{R}(G_N)$. An $\mathrm{O}(N)$-extended primary superfield, first introduced in Ref. 29, can then be defined as a section of $\mathcal{O}_N(h) \otimes \mathcal{R}(G_N)$.

III. CONTOUR INTEGRATION

Since one wishes to do conformal field theory in the setting presented above, a sensible question to ask is what closed contour integrals will look like, given the set of analytic functions (7). All functions on a given open set look like

$$f(z) = Z_{L',L}(f_0)(z) = \sum_{i=0}^{L} \frac{1}{i!} \iota_{L',L}(f_0^{(i)}(\epsilon(z))) s(z)^i, \tag{12}$$

where $f_0 \in C^{\infty}(\mathcal{U}, B_{L'})$. This should be compared to the usual notion of a Taylor expansion, around $\epsilon(z)$. Note that if $L' = 0$, $B_{L'} = \mathbb{C}$, and H^{∞} functions are retrieved. In the following, the $\iota_{L',L}$ will

be suppressed (for clarity). It is a linear map, so one can see that the following workings are unaffected. The contour integral $\oint_{C_z} f(z)dz$ needs to be considered. By the definition above, if z is an ordinary complex number (i.e., has no soul), one finds

$$f(z)=\sum_{i=0}^{L}\frac{1}{i!}f_0^{(i)}(\epsilon(z))s(z)^i=f_0(z). \tag{13}$$

If the even coordinate, w, were to have soul as well as body, it would give an element of an even Grassmann algebra over a complex field, when evaluated at a point. Hence one can consider w itself as being parametrized by a complex number z. Now consider a parametrization $w=g(z)=b(z)+u(z)$, where $\epsilon(w)=b(z)$, $s(w)=u(z)$,

$$f(w)=\sum_{i=0}^{L}\frac{1}{i!}f_0^{(i)}(\epsilon(w))s(w)^i=\sum_{i=0}^{p}\frac{1}{i!}(f_0^{(i)}\circ b)(z)u(z)^i=(f\circ g)(z), \tag{14}$$

where $p<L$ is the integer such that $u(z)^p\neq 0$, $u(z)^{p+1}=0$. Using the definition of a contour integral given in Ref. 27, with $C_w=g(C_z)$,

$$\begin{aligned}\oint_{C_w} f(w)dw &= \oint_{C_z}(f\circ g)(z)g'(z)dz\\ &= \oint_{C_z}\left(\sum_{i=0}^{p}\frac{1}{i!}(f_0^{(i)}\circ b)(z)u(z)^i\right)\left(\frac{d}{dz}b(z)+\frac{d}{dz}u(z)\right)dz\\ &= \oint_{C_z}\left(\frac{d}{dz}b(z)\right)(f_0\circ b)(z)+\sum_{i=1}^{p}\frac{1}{i!}\left(\frac{d}{dz}b(z)\right)(f^{(i)}\circ b)(z)u(z)^i\\ &\quad+\sum_{i=0}^{p}\frac{1}{i!}(f^{(i)}\circ b)(z)u(z)^i\left(\frac{d}{dz}u(z)\right)dz.\end{aligned} \tag{15}$$

All that has be done above is put all the definitions in and split up some summations. Note in the first summation, the chain rule can be used on the function $b(z)$, and in the second summation, the chain rule can be used on $u(z)$, giving

$$\begin{aligned}\oint_{C_w} f(w)dw &= \oint_{C_z}\left(\frac{d}{dz}b(z)\right)(f_0\circ b)(z)+\sum_{i=1}^{p}\frac{1}{i!}\left(\frac{d}{dz}(f^{(i-1)}\circ b)(z)\right)u(z)^i\\ &\quad+\sum_{i=0}^{p}\frac{1}{(i+1)!}(f^{(i)}\circ b)(z)\frac{d}{dz}(u(z)^{i+1})\quad dz\\ &= \oint_{C_z}\left(\frac{d}{dz}b(z)\right)(f_0\circ b)(z)+\sum_{i=1}^{p}\frac{1}{i!}\frac{d}{dz}((f^{(i-1)}\circ b)(z)\cdot u(z)^i)\\ &\quad+\frac{1}{(p+1)!}(f^{(p)}\circ b)(z)\frac{d}{dz}(u(z)^{p+1})\quad dz.\end{aligned} \tag{16}$$

The last term is in fact zero, due to the nilpotency of $u(z)$. The term under the summation is a total derivative. As such, integrated around a closed contour, it vanishes identically. All that remains is

$$\oint_{C_w} f(w)dw = \oint_{C_z} (f_0 \circ b)(z) b'(z) dz. \tag{17}$$

Thus, the contour integral can formally be treated as an integral in a normal complex number. It should be noted that all that has been used in this calculation is the chain rule and product rule over C^∞ functions.

IV. THE PRESERVED ONE-FORM AND RAMOND FIELDS

Whilst generalizing the bosonic setting in the previous sections, it was found that rather than a preserved one-form coming for free, it had to be specified. One could ask, what happens if another one-form is specified. In Ref. 21, other one-forms were considered. It was found that if one wanted a $\mathbb{Z}$-graded algebra, a one-form of the form $dz - d\theta_i f(z)\theta_i$ had to have $f(z) = z^n$. By making a change of variables,[21] then shows that one only need consider the cases $n = 0,1$.

Consider, now, a different preserved one-form, namely $\omega = dz - d\theta_i z \theta_i$. The dual derivations to (ω, θ_i) are (∂, D_i), where $D_i = (\partial/\partial\theta_i) + z\theta_i(\partial/\partial z)$. Now one finds that $[D_i, D_j] = 2\delta_{ij} z\partial$. Requiring that under a transformation, $\omega' = \omega\kappa(z, \theta_i)$ yields

$$D_j z' - z' \theta_i' D_j \theta_i' = 0, \tag{18}$$

$$\kappa = \partial z' + z' \theta_i' \partial \theta_i' = \left(\frac{z'}{z}\right) (\det D_i \theta_j')^{2/N} \zeta^2, \tag{19}$$

$$D_i' = (D_i' \theta_j) D_j, \tag{20}$$

$$(D_i \theta_j')(D_k \theta_j') = \delta_{ik} (\det D_i \theta_j')^{2/N} \zeta^2. \tag{21}$$

One can ask what an element of $\mathcal{O}_N(h)$ may transform like, and what is the algebra of infinitesimal transformations associated to it. Consider the case $N = 1$. The field has a transformation rule under $(z, \theta) \mapsto g(z, \theta) = (z', \theta')$,

$$(U_g^{-1} \Phi U_g)(z', \theta') = \Phi'(z', \theta') = \Phi(z, \theta) \left(\left(\frac{z'}{z}\right) (D\theta')^2 \right)^{-h}. \tag{22}$$

The superconformal condition, namely preserving the new one-form w, imposes two types of transformation, a bosonic and a fermionic one. On the coordinates, (z, θ), the infinitesimal transformations are given by

$$\begin{gathered} (z, \theta) \mapsto \left(z + a z^{n+1}, \theta + a \frac{n}{2} z^n \theta \right) \quad \text{and} \\ (z, \theta) \mapsto (z + \epsilon \theta z^{r+1}, \theta - \epsilon z^r), \end{gathered} \tag{23}$$

where $r, n \in \mathbb{Z}$. These provide a basis for all infinitesimal transformations. Each one induces a transformation on the field, (22), with $a(n) = a z^{n+1}$, $\epsilon(r) = \epsilon \theta z^{r+1}$,

$$\begin{aligned} \delta_{a(n)} \Phi(z, \theta) &= -a \left(z^{n+1} \partial_z + \frac{n}{2} z^n \theta \partial_\theta + h(n+1) z^n \right) \Phi(z, \theta), \\ \delta_{\epsilon(r)} \Phi(z, \theta) &= -\epsilon (\theta z^{r+1} \partial_z - z^r \partial_\theta + h(2r+1) \theta z^r) \Phi(z, \theta), \end{aligned} \tag{24}$$

where $n, r \in \mathbb{Z}$. These differential operators give rise to commutation relations

$$[\delta_{a_1(m)},\delta_{a_2(n)}]=(m-n)\delta_{a_2a_1(m+n)},$$

$$[\delta_{\epsilon_1(r)},\delta_{\epsilon_2(s)}]=2\delta_{\epsilon_2\epsilon_1(r+s)}, \tag{25}$$

$$[\delta_{a(m)},\delta_{\epsilon(r)}]=\left(\frac{m}{2}-r\right)\delta_{\epsilon a(m+r)}.$$

This gives a representation of the Ramond algebra. Note that no branch cut has been introduced. Another thing to note is that $\delta_{a(0)}$ gives a l_0 operator, which says that θ scales like a field of weight zero, rather than a field of weight half. As a result, the expansion of $\Phi(z,\theta)$ is now taken to be

$$\Phi(z,\theta)=\phi_0(z)+\theta\phi_1(z)=\sum_{m\in\mathbb{Z}}\phi_{0m}z^{-m-h}+\theta\sum_{m\in\mathbb{Z}}\phi_{1m}z^{-m-h}.$$

Using this expansion, and writing the transformation of a field as

$$(U_g\Phi U_g^{-1})(z,\theta)=\Phi(z',\theta')\left(\left(\frac{z'}{z}\right)(D\theta')^2\right)^h \qquad U_g=\exp(a_nL_n+\epsilon_rG_r) \tag{26}$$

one can find the action of the algebra on the modes of Φ as[33]

$$[L_n,\phi_{0m}]=((h-1)n-m)\phi_{0m+n},\quad [L_n,\phi_{1m}]=((h-\tfrac{1}{2})n-m)\phi_{1m+n},$$

$$[G_r,\phi_{0m}]=\phi_{1m+r},\quad [G_r,\phi_{1m}]=((2h-1)r-m)\phi_{0m+r}.$$

These are precisely the commutation relations one obtains from the $N=1$ Ramond OPEs from the usual method of introducing a branch cut.[25] Rewriting the commutation relations (25) in a more familiar way, and inserting the unique central extension,[21] the algebra can be written down

$$\begin{aligned}[L_m,L_n]&=(m-n)L_{m+n}+\frac{C}{6}m(m^2-1)\delta_{m+n,0},\\ [L_m,G_r]&=\left(\frac{m}{2}-r\right)G_{m+r},\quad [G_r,G_s]=2L_{r+s}+\frac{2C}{3}\left(r^2-\frac{1}{4}\right)\delta_{r+s,0}.\end{aligned} \tag{27}$$

Influenced by the form of the infinitesimal changes (24), OPEs can be postulated that give the above commutation relations, which read as

$$L(w)\phi_0(z)\sim\left(\frac{\partial}{(w-z)}+\frac{h}{(w-z)^2}\right)\phi_0(z),$$

$$L(w)\phi_1(z)\sim\left(\frac{\partial}{(w-z)}+\frac{h+\frac{1}{2}}{(w-z)^2}-\frac{1}{2z(w-z)}\right)\phi_0(z),$$

$$G(w)\phi_0(z)\sim\frac{1}{z(w-z)}\phi_1(z),$$

$$G(w)\phi_1(z)\sim\left(\frac{\partial}{(w-z)}+\frac{2h}{(w-z)^2}-\frac{h}{z(w-z)}\right)\phi_0(z), \tag{28}$$

$$L(w)L(z)\sim\frac{C}{(w-z)^4}+\frac{2L(z)}{(w-z)^2}+\frac{\partial L(z)}{(w-z)},$$

$$L(w)G(z)\sim\frac{\partial G(z)}{(w-z)}+\frac{3G(z)}{2(w-z)^2}-\frac{G(z)}{2z(w-z)},$$

$$G(w)G(z)\sim\frac{2zL(z)}{(w-z)}+\frac{2C}{3}\left(\frac{2z}{(w-z)^3}+\frac{1}{(w-z)^2}-\frac{1}{4z(w-z)}\right), \tag{29}$$

where $L(z)=\Sigma_n L_n z^{-n-2}$, $G(z)=\Sigma_r G_r z^{-r-1}$, $z,r\in\mathbb{Z}$. This final set of OPEs demonstrate the drawbacks of the more abstract construction used in this paper of a Conformal Field Theory (namely via a section of a sheaf over some manifold), compared to the more usual approach of a free field realization. One can calculate the infinitesimal transformations of the field (the section obtained), and show the transformations close as a Lie algebra. One then has to ''work backwards'' and try and construct OPEs and central charge terms that agree with the transformations and lie algebras calculated. It would be interesting to see if the Ramond field (22) could be realized via a free field realization where usually one finds central terms and OPEs are explicitly calculable.

V. CLASSICAL $N=3$ ALGEBRA

Consider now that case of preserving the usual one-form, $dz-d\theta_i\theta_i$, with three Grassmann variables. The superconformal condition is then (3). Using a notation of $Z=(z,\theta_i)$, and writing a superconformal transformation as $Z\mapsto g(Z)$, a representation of the group can be constructed via $\mathcal{A}_3$, namely $U_g f(Z)=(f\circ g^{-1})(Z)$. The infinitesimal transformations can be calculated, and a Lie superalgebra constructed. The infinitesimal transformations take the form of vector fields acting on functions.

The most general infinitesimal transformation on the z coordinate is

$$z\mapsto z+af(z,\theta_1,\theta_2,\theta_3)+\epsilon h(z,\theta_1,\theta_2,\theta_3)$$

for f (h) some even (odd) function, and a (ϵ) infinitesimal and of even (odd) parity. The functions f have analogs for transformations in the θ_i coordinates. Breaking up f into superfield components gives eight different types of transformation.

$$z\mapsto z+a(z)+\alpha_i(z)\theta_i+\tfrac{1}{2}a_{ij}(z)\theta_i\theta_j+\alpha_{123}(z)\theta_1\theta_2\theta_3. \tag{30}$$

The possible transformations are forced into only these eight types, and not some mix between them, by the superconformal condition.

An infinitesimal transformation most generally reads

$$z'=z+\delta z,\quad \theta_j'=\theta_j+\delta\theta_j. \tag{31}$$

On substituting into (3), one finds that the superconformal condition reads

$$D_i\delta z=\delta\theta_i+\sum_{j=1}^{3}\theta_j D_i\delta\theta_j, \tag{32}$$

i.e., three equations, with three unknowns once δz has been specified. A basis for the infinitesimal z transformations is easily found, which is $\delta z=\epsilon\theta_1\theta_2\theta_3 z^{n+(1/2)}$, $\delta z=a\theta_i\theta_j z^{n+1}$ for $i<j$, $\delta z=\epsilon\theta_i z^{n+(1/2)}$, and $\delta z=az^{n+1}$. Given these eight types of transformation, precisely what the corresponding $\delta\theta_i$ are, modulo possible $\delta\theta_i$ if $\delta z=0$, can be calculated explicitly. The case when $\delta z=0$ is taken care of by the t_n^i generators below. Using this procedure, the infinitesimal genera-

tors of the $N=3$ algebra can be calculated. The results are quite hefty, but the actual transformations give an intuitive idea of what each element of the algebra actually does. Summation convention is used in the following:

$$z\mapsto z+az^{n+1},$$

$$\theta_i\mapsto\theta_i+a\tfrac{1}{2}(n+1)\theta_i z^n, \tag{33}$$

$$\Rightarrow l_m=-z^m\left(z\frac{\partial}{\partial z}+\frac{1}{2}(m+1)\theta_i\frac{\partial}{\partial\theta_i}\right)$$

gives a vector field corresponding to an infinitesimal transformation when only $a(z)$ is nonzero in (30). There are then the three single θ terms, which can be found by considering the case when only one $\alpha_i(z)$ is nonzero,

$$z\mapsto z-\epsilon\theta_1 z^{r+(1/2)},$$

$$\theta_1\mapsto\theta_1+\epsilon z^{r+(1/2)},$$

$$\theta_2\mapsto\theta_2-\epsilon(r+\tfrac{1}{2})\theta_1\theta_2 z^{r-(1/2)},$$

$$\theta_3\mapsto\theta_3-\epsilon(r+\tfrac{1}{2})\theta_1\theta_3 z^{r-(1/2)}$$

gives rise to the vector field

$$g_r^1=z^{r-(1/2)}\left(z\theta_1\frac{\partial}{\partial z}-z\frac{\partial}{\partial\theta_1}+\left(r+\frac{1}{2}\right)\theta_1\theta_2\frac{\partial}{\partial\theta_2}+\left(r+\frac{1}{2}\right)\theta_1\theta_3\frac{\partial}{\partial\theta_3}\right).$$

Similarly

$$g_r^i=z^{r-(1/2)}\left(z\theta_i\frac{\partial}{\partial z}-z\frac{\partial}{\partial\theta_i}+\left(r+\frac{1}{2}\right)\theta_i\theta_j\frac{\partial}{\partial\theta_j}\right).$$

It is worth noting that if one were not working on an extended graded manifold, but on a graded manifold (cf. (1), (2)), then one would not be able to obtain the above vector field. The same statement holds for ψ_r below.

There are three double θ terms, e.g., $\theta_1\theta_2$ gives t_n^3,

$$z\mapsto z,$$

$$\theta_1\mapsto\theta_1+a\theta_2 z^{n+1},$$

$$\theta_2\mapsto\theta_2-a\theta_1 z^{n+1},$$

$$\theta_3\mapsto\theta_3+a(n+1)\theta_1\theta_2\theta_3 z^n.$$

A similar calculation applies to t_n^1 and t_n^2,

$$t_m^i=z^{m-1}\left(z\epsilon_{ijk}\theta_j\frac{\partial}{\partial\theta_k}-m\theta_1\theta_2\theta_3\frac{\partial}{\partial\theta_i}\right).$$

These transformations leave the z component unaltered, and as such have sometimes been interpreted in the physics literature[2] as a gauge group. The final term is similarly calculated, and is the three θ transformation

$$\psi_r=-z^{r-(1/2)}\left(\theta_1\theta_2\theta_3\frac{\partial}{\partial z}+\frac{1}{2}\epsilon_{ijk}\theta_i\theta_j\frac{\partial}{\partial\theta_k}\right).$$

These vector fields, similarly calculated in Refs. 20, 7 then give rise to the commutation relations for the $N=3$ algebra without central extension,

$$[t^i_m,t^j_n]=-\epsilon_{ijk}t^k_{m+n},\quad [t^i_m,\psi_s]=0,\quad [t^i_m,g^j_r]=\delta_{ij}m\psi_{r+m}-\epsilon_{ijk}g^k_{r+m},$$

$$[l_m,\psi_s]=-\left(\frac{m}{2}+s\right)\psi_{m+s},\quad [l_m,t^i_n]=-nt^i_{m+n},\quad [g^i_r,\psi_s]=t^i_{r+s},$$

$$[l_m,g^i_r]=\left(\frac{m}{2}-r\right)g^i_{r+m},\quad [g^i_r,g^j_s]=2\delta_{ij}l_{r+s}+\epsilon_{ijk}(r-s)t^k_{r+s},$$

$$[l_m,l_n]=(m-n)l_{m+n},\quad [\psi_m,\psi_n]=0. \tag{34}$$

Note in particular that the t^i_n form an su(2) loop algebra, which will be enhanced by a central extension in the quantum case to give an affine su(2) algebra. One implication of this is that the representation theory will have to be very different to that of the $N=2$ case, where a u(1) loop algebra appeared. The highest weight state must also be an su(2) highest weight state. Since U(1) is Abelian, all its irreducible representations are one dimensional. The upshot of this is that the OPE can be easily adapted by including one more quantum number. Since SU(2) is non-Abelian, it will be seen that su(2) generators will appear in the OPE.

VI. QUANTUM $N=3$ ALGEBRA

The quantum $N=3$ algebra was calculated from a Lagrangian approach, and canonically quantized in Refs. 1 and 2. Whilst this section may look very technical, it should be stressed that essentially the same procedure is being used as in the well documented bosonic case, where the starting point is a section of a sheaf, namely $\mathcal{O}_0(h)$. One plays the same game, but now uses the section $\mathcal{O}_N(h)\otimes\mathcal{R}(G_N)$. Since it is defined covariantly, one can then write down how it transforms. This then gives rise to infinitesimal transformations $\delta\Phi$, which close as a Lie algebra. These relations can be written in terms of an operator $\mathbb{T}$ acting on Φ, giving an OPE. From the $\delta\Phi$, an ansatz for the OPE of $\mathbb{T}$ with itself can be inferred. The action of the quantum algebras on primary fields is inherent in the $\mathbb{T}\Phi$ OPE. The commutation relations of the quantum algebra are then inherent in the $\mathbb{T}\mathbb{T}$ OPE as the modes. What must be checked from the first OPE, is that the primary superfield does indeed yield a highest weight vector.

Recall that for a primary field in the bosonic case, one performs a diffeomorphism from the Riemann sphere to itself that obeys the conformal condition, and looks at how the primary field transforms. More precisely, one considers, a diffeomorphism f,

$$\begin{aligned} f&:\mathbb{P}_1\to\mathbb{P}_1\\ z&\mapsto f(z)=z' \end{aligned} \tag{35}$$

with the conformal condition

$$(f^*dz)=dz\,\kappa(z). \tag{36}$$

One then calculates how $\phi\in\mathcal{O}(h)$ transforms under a pullback, where ϕ in local coordinates is $\phi(z)dz^{\otimes h}$,

$$(f^*\phi)(z)=\kappa^h(\phi\circ f)(z)dz^{\otimes h}=\left(\frac{dz'}{dz}\right)^h\phi(z')dz^{\otimes h}=:\phi'(z)dz^{\otimes h} \tag{37}$$

yielding the transformation law

$$(U_g \phi U_g^{-1})(z) = \left(\frac{dz'}{dz}\right)^h \phi(z') = \phi'(z). \tag{38}$$

For the graded case, one has to consider an invertible sheaf morphism

$$\begin{aligned} f&:(\mathbb{P}_1, \mathcal{A}_N) \to (\mathbb{P}_1, \mathcal{A}_N), \\ Z = (z, \theta_i) &\mapsto Z' = (z', \theta_i'), \end{aligned} \tag{39}$$

such that f (as well as f^{-1}) has a GH^∞ action on the functions $\mathcal{A}_N$, and obeys the conformal condition

$$(f^* \omega) = \omega \kappa(Z). \tag{40}$$

The transformation rule for the components of $\Phi \in \mathcal{O}_N(h) \otimes \mathcal{R}(G_N)$ under a pullback are then given by

$$\Phi'(Z) = \kappa^h \frac{(D_i \theta_j')}{\sqrt{\kappa}} g^{ij} (\Phi \circ f)(Z). \tag{41}$$

The g^{ij} are, up to a discrete subgroup, a representation of the Lie group O(N). The g^{ij} explicitly realize the map (11). This formula matches that found in Ref. 29 for how a primary superfield transforms. One now writes down the transformation law as

$$(U_g \Phi U_g^{-1})(Z) = \kappa^h \frac{(D_i \theta_j')}{\sqrt{\kappa}} g^{ij} \Phi(Z') \tag{42}$$

and parametrize the group action infinitesimally by

$$\begin{aligned} U_g &= \exp(a_n L_n + \alpha_r^i G_r^i + b_n^i T_n^i + \beta_r \psi_r), \\ Z' &= \exp(a_n l_n + \alpha_r^i g_r^i + b_n^i t_n^i + \beta_r \psi_r) Z, \end{aligned}$$

in a completely analogous way to (26), to obtain the commutators of the super-Virasoro operators on a primary field. For the $N=3$ case this yields (45). One must now work backward to try and construct an OPE between a stress-energy tensor and primary superfield that yield these commutators.

For the $N=3$ case, the stress-energy tensor will be weight $\frac{1}{2}$, and have superfield decomposition[34]

$$\mathbb{T}(Z) = \theta_1 \theta_2 \theta_3 L(z) + \tfrac{1}{2} \epsilon_{ijk} \theta_i \theta_j G^k(z) + \theta_i T^i(z) + \psi(z). \tag{43}$$

An OPE for $N=3$ is found in Ref. 8, that, on contour integration, gives rise to the infinitesimal transformations of a primary superfield.[29] With $Z_1 = (w, \chi_i)$, $Z_2 = (z, \theta_i)$, this reads

$$\begin{aligned} \mathbb{T}(Z_1)\Phi(Z_2) \sim{}& \frac{h \theta_{12,1} \theta_{12,2} \theta_{12,3}}{Z_{12}^2} \Phi(Z_2) + \frac{\theta_{12,1} \theta_{12,2} \theta_{12,3}}{Z_{12}} \partial_w \Phi(Z_2) + \frac{\epsilon_{ijk} \theta_{12,i} \theta_{12,j} D_{2,k}}{4 Z_{12}} \Phi(Z_2) \\ &+ \frac{\theta_{12,i} J_i}{Z_{12}} \Phi(Z_2), \end{aligned} \tag{44}$$

where

$$D_{2,i} = \frac{\partial}{\partial \theta_i} + \theta_i \frac{\partial}{\partial z}, \quad Z_{12} = (w - z - \chi_i \theta_i), \quad \theta_{12,i} = (\chi_i - \theta_i),$$

where the J_i form an su(2) algebra.[35] The field, $\Phi(Z)$, now also lives in an su(2) representation, say $\mathcal{V}$. It is in fact an su(2) highest weight. $\mathbb{T}$ can then be thought of as being an endomorphism of $\mathcal{V}$, e.g., explicitly with su(2) indices $\mathbb{T}(Z_1)^a{}_b\Phi(Z_2)^b$. This OPE is effectively a non-abelian version of the q term appearing in the $N=2$ case. In its place, another quantum number appears, which is the J_3 eigenvalue. On the representation space, the action of T_0^i on a highest weight state is identified with that of J_i. The OPE can be split up into θ components, according to (43), and modes be taken of each of the operators, $L(z), G^i(z), T^i(z), \psi(z)$, giving the formulas (45), as required. Note in particular, how the classical algebra appears in the relations again. The extra terms are the h terms, which will give the L_0 eigenvalue h. The other extra terms, the J_i, will give an action of su(2) on the primary field, and hence on the highest weight, which we know must be required from the classical analysis (34), where an su(2) loop algebra appeared,

$$
\begin{aligned}
[L_m,\Phi(Z)] &= z^m\left(h(m+1)+z\partial_z+\frac{1}{2}(m+1)\theta_i\partial_{\theta_i}+\frac{1}{2z}m(m+1)\epsilon_{ijk}\theta_i\theta_jJ_k\right)\Phi(Z),\\
[G_s^i,\Phi(Z)] &= -z^{(s-(1/2))}\left(h\left(s+\frac{1}{2}\right)\theta_i+\frac{1}{2}\theta_iz\partial_z-\frac{1}{2}z\partial_{\theta_i}+\frac{1}{2}\left(s+\frac{1}{2}\right)\theta_i\theta_j\partial_{\theta_j}+\left(s+\frac{1}{2}\right)(\epsilon_{ijk}\theta_jJ_k)\right.\\
&\quad\left.-\frac{1}{z}\left(s^2-\frac{1}{4}\right)\theta_1\theta_2\theta_3J_i\right)\Phi(Z),\\
[T_m^i,\Phi(Z)] &= z^{(m-1)}\left(\frac{mh}{2}\epsilon_{ijk}\theta_j\theta_k-\epsilon_{ijk}\frac{1}{2}z\theta_j\partial_{\theta_k}+\frac{1}{2}m\theta_1\theta_2\theta_3\partial_{\theta_i}+zJ_i-m(\theta_i\theta_kJ_k)\right)\Phi(Z),\\
[\psi_s,\Phi(Z)] &= z^{(s-(1/2))}\left(-\frac{h}{z}\left(s-\frac{1}{2}\right)\theta_1\theta_2\theta_3+\frac{1}{2}\theta_1\theta_2\theta_3\partial_z+\frac{1}{4}\epsilon_{ijk}(\theta_i\theta_j\partial_{\theta_k}-\theta_iJ_i)\right)\Phi(Z).
\end{aligned}
\tag{45}
$$

Note that

$$
[L_{-1},\Phi(Z)]=\partial_z\Phi(Z),\quad [G^i_{-(1/2)},\Phi(Z)]=\tfrac{1}{2}(\partial_{\theta_i}-\theta_i\partial_z)\Phi(Z). \tag{46}
$$

In particular, L_{-1} acts as a translation in z and $G^i_{-(1/2)}$ as a supertranslation in the respective θ_i direction. This allows vertex operators to be used, and an operator-state mapping employed.[22,36,17] In the bosonic theory, vertex operators are characterized uniquely by their action on a vacuum $|0\rangle$, which is annihilated by the raising operators, $\{L_n : n\geqslant -1\}$. The vacuum cannot be invariant under the whole symmetry algebra without implying vanishing of the central extension. This generalizes to $N=3$, so that now $|0\rangle$ is annihilated by $\{L_n, G^i_r, T^i_m, \psi_s : n\geqslant -1, r\geqslant -\frac{1}{2}, m\geqslant 0, s\geqslant \frac{1}{2}\}$. To get the state associated to any vertex operator $\Phi(Z)$, one looks at $\lim_{Z\to 0}\Phi(Z)|0\rangle$. Given this, it can be seen from the relations (45) that the action of the raising operators on $|\Phi\rangle$ is zero, e.g., for $\{L_m : m>0\}$

$$
\lim_{Z\to 0}[L_m,\Phi(Z)]|0\rangle=0.
$$

The action of L_0 is given by

$$
[L_0,\Phi(Z)]=(h+z\partial_z+\tfrac{1}{2}(\theta_1\partial_{\theta_1}+\theta_2\partial_{\theta_2}+\theta_3\partial_{\theta_3}))\Phi(Z)\Rightarrow\lim_{Z\to 0}[L_0,\Phi(Z)]|0\rangle=h|\Phi\rangle=L_0|\Phi\rangle. \tag{47}
$$

The action of T_0^i is given by

$$
\begin{aligned}
[T_0^1,\Phi(Z)] &= (\tfrac{1}{2}\theta_3\partial_{\theta_2} - \tfrac{1}{2}\theta_2\partial_{\theta_3} + J_1)\Phi(Z),\\
[T_0^2,\Phi(Z)] &= (\tfrac{1}{2}\theta_1\partial_{\theta_3} - \tfrac{1}{2}\theta_3\partial_{\theta_1} + J_2)\Phi(Z),\\
[T_0^3,\Phi(Z)] &= (\tfrac{1}{2}\theta_2\partial_{\theta_1} - \tfrac{1}{2}\theta_1\partial_{\theta_2} + J_3)\Phi(Z),\\
\Rightarrow \lim_{Z\to 0}[T_0^i,\Phi(Z)]|0\rangle &= \lim_{Z\to 0}(J_i\Phi)(Z)|0\rangle = J_i|\Phi\rangle = T_0^i|\Phi\rangle,
\end{aligned}
\tag{48}
$$

where the vacuum is T_0^i invariant.

Hence, on the highest weight state, the T_0^i can be identified with the J_i, so that T_0^3 gives rise to the q eigenvalue, and $J^+ = J_0^1 + iJ_0^2$ annihilates $|\Phi\rangle$. As can be seen, $\Phi(Z)$ is associated to a vector $|\Phi\rangle$, which is a highest weight of the $N=3$ field.

Rather than work explicitly with (45), one could simply consider what the infinitesimal transformations of the field are under an infinitesimal superconformal map

$$(z,\theta_i)\mapsto(z+\delta z,\theta_i+\delta\theta_i). \tag{49}$$

This is useful to check closure as a Lie algebra. It is useful to introduce the quantity $\nu(z)=\delta z + \theta_i\delta\theta_i$. The transformation reads

$$
\begin{aligned}
\delta\Phi(Z) &= h(\partial_z\nu(Z))\Phi(Z) + \nu(Z)\partial_z\Phi(Z) + \frac{1}{2}\sum_{j=1}^{3}(D_j\nu(Z))(D_j\Phi(Z))\\
&\quad + ((J_3D_1D_2 + J_1D_2D_3 + J_2D_3D_1)(\nu(Z)))\Phi(Z)\\
&= \frac{2h}{3}(D_1\delta\theta_1 + D_2\delta\theta_2 + D_3\delta\theta_3)\Phi(Z) + (\delta z)\partial_z\Phi(Z) + \sum_{j=1}^{3}(\delta\theta_j)\partial_{\theta_j}\Phi(Z)\\
&\quad + ((D_1\delta\theta_2 - D_2\delta\theta_1)J_3 + (D_2\delta\theta_3 - D_3\delta\theta_2)J_1 + (D_3\delta\theta_1 - D_1\delta\theta_3)J_2)\Phi(Z).
\end{aligned}
\tag{50}
$$

The infinitesimal transformations form a Lie algebra, which can be calculated explicitly from (50),

$$
\begin{aligned}
[\delta_{\nu_1},\delta_{\nu_2}]\Phi(Z) &= \delta_{\nu_3}\Phi(Z),\\
\nu_3 &= \nu_2(\partial_z\nu_1) - \nu_1(\partial_z\nu_2) + \frac{1}{2}\sum_{i=1}^{3}(D_i\nu_2)(D_i\nu_1).
\end{aligned}
\tag{51}
$$

It is worth noting that the algebra closes if and only if the J_i satisfy the commutation relations $[J_i,J_j] = -\frac{1}{2}\epsilon_{ijk}J_k$.

This can then be used to construct an ansatz for an OPE of $\mathbb{T}(Z_1)\mathbb{T}(Z_2)$ (52), and then the modes calculated to give the commutators of the quantum theory (53),

$$\mathbb{T}(Z_1)\mathbb{T}(Z_2) = \frac{c}{Z_{12}} + \frac{\theta_{12,1}\theta_{12,2}\theta_{12,3}}{2Z_{12}^2}\mathbb{T}(Z_2) + \frac{\theta_{12,1}\theta_{12,2}\theta_{12,3}}{Z_{12}}\partial_w\mathbb{T}(Z_2) + \frac{\epsilon_{ijk}\theta_{12,i}\theta_{12,j}D_{2,k}}{4Z_{12}}\mathbb{T}(Z_2). \tag{52}$$

The first term gives rise to the central extension in the algebra, and arises in precisely the same way as the bosonic case. This OPE shows explicitly that $\mathbb{T}(Z)$ is a weight $\frac{1}{2}$ field, although not primary. Since the central charge does not appear for the super-Möbius subalgebra, $\mathbb{T}$ can be thought of as a quasiprimary superfield, in the trivial representation of su(2). The modes of this

can then be calculated to give the $N=3$ algebra. Note that when the classical algebra expressions appear in (45), there are extra factors of $\frac{1}{2}$ appearing in (45). This corresponds to the extra factors of $\frac{1}{2}$ appearing in (53) when compared to the classical algebra,

$$[T^i_m,T^j_n]=-\tfrac{1}{2}\epsilon_{ijk}T^k_{m+n}+mc\,\delta_{ij}\delta_{m+n,0},\quad [T^i_m,\psi_s]=0,$$

$$[T^i_m,G^j_r]=\tfrac{1}{2}(\delta_{ij}m\psi_{r+m}-\epsilon_{ijk}G^k_{r+m}),\quad [L_m,\psi_s]=-\left(\frac{m}{2}+s\right)\psi_{m+s},$$

$$[L_m,T^i_n]=-nT^i_{m+n},\quad [G^i_r,\psi_s]=\tfrac{1}{2}T^i_{r+s},\quad [L_m,G^i_r]=\left(\frac{m}{2}-r\right)G^i_{r+m}, \tag{53}$$

$$[G^i_r,G^j_s]=\tfrac{1}{2}\delta_{ij}L_{r+s}+\tfrac{1}{2}\epsilon_{ijk}(r-s)T^k_{r+s}-c(r^2-\tfrac{1}{4})\delta_{r+s,0}\delta_{ij},$$

$$[L_m,L_n]=(m-n)L_{m+n}-cm(m^2-1)\delta_{m+n,0},\ [\psi_r,\psi_s]=c\,\delta_{r+s,0},$$

which agrees with Ref. 2.

VII. THE NEVEU–SCHWARZ ALGEBRA AND ITS VERMA MODULE

The $N=3$ Neveu–Schwarz algebra is given by the above commutation relations where $m\in\mathbb{Z}$, $r\in\mathbb{Z}+\frac{1}{2}$. The basis can be changed so that the above relations are more useful for representation theory. Consider a change of variables

$$\begin{gathered}T^+_m=2(iT^1_m-T^2_m),\quad T^-_m=2(iT^1_m+T^2_m),\quad T^H_m=-2iT^3_m,\\ G^+_r=4(G^2_r-iG^1_r),\quad G^-_r=4(G^2_r+iG^1_r),\quad G^H_r=8iG^3_r,\quad k=-4c.\end{gathered} \tag{54}$$

Then, the commutation relations become, for $x\in\{H,\pm\}$,[37]

$$[T^+_m,T^-_n]=2T^H_{m+n}+2km\,\delta_{m+n,0},\quad [T^H_m,T^\pm_n]=\pm T^\pm_{m+n},\quad [T^\pm_m,T^\pm_n]=0,$$

$$[T^H_m,T^H_n]=km\,\delta_{m+n,0},\quad [T^\pm_m,G^\pm_r]=0,\quad [T^\mp_m,G^\pm_r]=-G^H_{r+m}\pm 8m\psi_{r+m},$$

$$[T^\pm_m,G^H_r]=-2G^\pm_{m+r},\quad [T^H_m,G^H_r]=8m\psi_{m+r},\quad [T^H_m,G^\pm_r]=\pm G^\pm_{r+m},$$

$$[\psi_s,G^\pm_r]=\mp T^\pm_{r+s},\quad [\psi_s,G^H_r]=-2T^H_{r+s},\quad [G^\pm_r,G^\pm_s]=0,\quad [T^x_m,\psi_s]=0,$$

$$[G^H_r,G^H_s]=-32L_{r+s}-16k(r^2-\tfrac{1}{4})\delta_{r+s,0},\quad [G^\pm_r,G^H_s]=8(r-s)T^\pm_{r+s}, \tag{55}$$

$$[G^+_r,G^-_s]=16L_{r+s}+8k(r^2-\tfrac{1}{4})\delta_{r+s,0}+8(r-s)T^H_{r+s},$$

$$[L_m,\psi_s]=-\left(\frac{m}{2}+s\right)\psi_{m+s},\quad [L_m,T^x_n]=-nT^x_{m+n},\quad [\psi_r,\psi_s]=-\frac{k}{4}\delta_{r+s,0},$$

$$[L_m,G^x_r]=\left(\frac{m}{2}-r\right)G^x_{r+m},$$

$$[L_m,L_n]=(m-n)L_{m+n}+\frac{k}{4}m(m^2-1)\delta_{m+n,0}.$$

On the representations considered here, the algebra obeys hermiticity conditions[38]

$$(\psi_r)^\dagger = -\psi_{-r}, \quad (T_m^+)^\dagger = T_{-m}^-, \quad (T_m^-)^\dagger = T_{-m}^+, \quad (T_m^H)^\dagger = T_{-m}^H,$$
$$(G_r^H)^\dagger = -G_{-r}^H, \quad (L_n)^\dagger = L_{-n}, \quad (G_r^+)^\dagger = G_{-r}^-, \quad (G_r^-)^\dagger = G_{-r}^+. \tag{56}$$

The highest weight conditions on a vector $|\phi\rangle$ are then

$$T_m^x|\phi\rangle = 0, \quad G_r^x|\phi\rangle = 0, \quad L_m|\phi\rangle = 0, \quad \psi_r|\phi\rangle = 0, \quad T_0^+|\phi\rangle = 0 \tag{57}$$

for $m,r>0$. The Cartan subalgebra is spanned by the elements L_0, T_0^H, such that $L_0|\phi\rangle = h|\phi\rangle$, $T_0^H|\phi\rangle = q|\phi\rangle$. The algebra of raising operators, i.e., the algebra spanned by the elements giving the highest weight conditions, is generated by T_0^+, $G_{1/2}^-$, $\psi_{1/2}$. Thus, a vector $|\chi\rangle$ with the properties $T_0^+|\chi\rangle = 0$, $G_{1/2}^-|\chi\rangle = 0$ and $\psi_{1/2}|\chi\rangle = 0$ will obey the highest weight conditions. Consider the Verma module $V(h,q)$ for a highest weight $|\phi\rangle$, with $L_0|\phi\rangle = h|\phi\rangle$, $T_0^H|\phi\rangle = q|\phi\rangle$. A vector $|\chi\rangle \neq |\phi\rangle$ in the module defines a singular vector. The module itself admits a decomposition

$$V(h,q) = \bigoplus_{(m\geqslant 0)} \bigoplus_{(n\leqslant m/2)} V_{m,n}, \tag{58}$$

where $m \in \mathbb{Z}$ and $n \in \mathbb{Z}/2$. This can be seen from the root structure (55), and the highest weight conditions. An example of a singular vector occurs when $(h,q,k) = (-\frac{1}{2}, -1, k)$. Under such conditions, a singular vector exists in $V_{1/2,0}$,

$$|\chi\rangle = T_0^- G_{-(1/2)}^+ |\phi\rangle. \tag{59}$$

VIII. THE SUPER MÖBIUS GROUP

One might ask how exactly does the theory of the Möbius group generalize. In the bosonic case, the lie algebra of the group can be obtained by finding the globally defined vector fields on the Riemann sphere. The Riemann sphere can be considered as a pair of complex planes with transition function $w = \frac{1}{z}$ between them. In the graded Riemann sphere case, one can choose a homomorphism between rings of functions given by $(w, \chi_i) = (1/z, \theta_i\sqrt{-1}/z)$. The South pole is $Z_s = (z, \theta_i) = (0,0,0,0)$, and the North pole given by $Z_n = (1/z, \theta_i\sqrt{-1}/z) = (0,0,0,0)$. One can then ask what are the globally defined graded vector fields. A basis of vector fields was calculated in Sec. V. It can be seen that many of them are divergent at the origin, or South pole. One must then check which vector fields are well behaved at both poles. As an example, consider the vector field (33). This is clearly divergent for $m<-1$ at the south pole. To find out what l_n looks like at the north pole, one uses the techniques of graded one-forms and vector fields[23] to find

$$l_m = w^{-m+1}\frac{\partial}{\partial w} - \frac{1}{2}(m-1)w^{-m}\chi_j\frac{\partial}{\partial \chi_j}, \tag{60}$$

which is divergent for $m>1$ at the North pole. Thus, one can conclude that $\{l_1, l_0, l_{-1}\}$ are globally defined. Similarly, one finds that the only other globally defined vector fields are $\{g_{1/2}^r, g_{-(1/2)}^r, t_0^i\}$. From the commutation relations, (34) it can be seen that the vector fields form a closed subalgebra, namely osp(3,2). One can then write down formal group elements by exponentiation.

$$
\begin{gathered}
\exp(\lambda l_1):(z,\theta_i)\mapsto \frac{1}{1-\lambda z}(z,\theta_i),\\
\exp(\lambda l_0):(z,\theta_i)\mapsto (e^{\lambda}z,e^{\lambda/2}\theta_i),\\
\exp(\lambda l_{-1}):(z,\theta_i)\mapsto (z+\lambda,\theta_i),\\
\exp(\epsilon g^j_{-(1/2)}):(z,\theta_i)\mapsto (z-\epsilon\theta_j,\theta_i,\theta_j+\epsilon),\quad i\neq j,\\
\exp(\epsilon g^j_{1/2}):(z,\theta_i)\mapsto \frac{1}{1+\epsilon\theta_j}(z,\theta_i,\theta_j+\epsilon z),\quad i\neq j,\\
\exp(\lambda_i t^i_0):(z,\theta_i)\mapsto (z,M_{ij}(\lambda)\theta_j),\quad M_{ij}(\lambda)\in \mathrm{SO}(3).
\end{gathered}
\tag{61}
$$

In particular, the $g^i_{-(1/2)}$ give supersymmetry generators, the $g^i_{1/2}$ give special superconformal transformations, and the t^i_0 give an R-symmetry. Writing these transformations as $Z\mapsto Z'$, the corresponding transformations on the field become

$$
\begin{gathered}
e^{\lambda L_0}\Phi(Z)e^{-\lambda L_0}=e^{\lambda h}\Phi(Z'),\quad e^{\lambda L_{-1}}\Phi(Z)e^{-\lambda L_{-1}}=\Phi(Z'),\\
e^{\epsilon G^i_{-1/2}}\Phi(Z)e^{-\epsilon G^i_{-1/2}}=\Phi(Z'),\\
e^{\rho G^i_{1/2}}\Phi(Z)e^{-\rho G^i_{1/2}}=\frac{1}{(1+\epsilon\theta_i)^h}e^{-2\rho\epsilon_{ijk}\theta_j J_k}\Phi(Z'),\\
e^{\lambda T^i_0}\Phi(Z)e^{-\lambda T^i_0}=e^{\lambda J_i}\Phi(Z'),\\
e^{\lambda L_1}\Phi(Z)e^{-\lambda L_1}=\frac{1}{(1-\lambda z)^h}e^{(\lambda/(1-\lambda z)\,\epsilon_{ijk}\theta_i\theta_j J_k)}\Phi\left(\frac{z}{(1-\lambda z)},\frac{\theta_i}{(1-\lambda z)}\right).
\end{gathered}
\tag{62}
$$

Using these formal group elements, any two points, $V=(v,\beta_i)$ and $U=(u,\alpha_i)$ say, can be mapped to the North and South poles, respectively. In a conformal field theory formalism, usually the South pole is where the ''in vacuum'' sits, and the North pole where the ''out vacuum'' sits. The formal group element corresponding to this map is given by

$$
(z,\theta_i)\mapsto(z',\theta'_i)=\frac{\left(z-u,\theta_i-\alpha_i+\left(\frac{\alpha_i-\beta_i}{v-u}\right)(z-u)\right)}{\left(1+\frac{(\alpha-\beta)\cdot\theta}{v-u}\right)-\left(1+\frac{\alpha\cdot\beta}{v-u}\right)\left(\frac{z-u}{v-u}\right)},
\tag{63}
$$

where $\alpha\cdot\beta=\Sigma_{i=1}^3\alpha_i\beta_i$.

To obtain this transformation, one can use $g^i_{-(1/2)}$ to send α^i to 0, l_{-1} to move u to 0, $g_{1/2}$ to send β_i to 0 when $z=v$, and l_1 to send v to ∞. It is worth noting, that the only operators that have not been used are the t^i_0 and l_0. This degree of freedom is essentially a (complex) scale factor, and an SO(3) action on the θs. Thus, the even ''coordinate'' of the third point can be sent anywhere one wishes, but one cannot quite do the same with the odd ''coordinates'' of the third point. It should also be noted, that this construction should generalize to osp(N,2), i.e., with an arbitrary number of odd coordinates.

The formal group element found (63) implies that a correlation function of the form

$$
\langle 0|\Phi_1(V)\Phi_2(Z)\Phi_3(U)0\rangle
\tag{64}
$$

can be superconformally mapped to a more typical presentation of the three-point function in conformal field theory,

$$\langle 0|\Phi_1(\infty)\Phi_2(Z')\Phi_3(0)0\rangle=\langle \phi_1|\Phi_2(Z')\phi_3\rangle. \tag{65}$$

IX. THE TWO-POINT FUNCTION

In conformal field theory it is known that global conformal invariance is sufficient to solve for the two point function. This is indeed also the case for $N=1,2$.[31] In this section, global $N=3$ invariance is used to solve for the two-point function. This becomes quite a bit more complicated than $N\leqslant 2$, calculationally, due to the presence of non-Abelian R-symmetry, manifested by the presence of su(2) generators in the theory. More precisely, the primary fields are $\mathcal{A}_N\otimes \mathrm{End}\mathcal{H}\otimes\mathcal{V}$ valued, where $\mathcal{V}$ is an su(2) representation and $\mathcal{H}$ is the Hilbert space that $|0\rangle$ belongs to. The super-Virasoro operators are valued in $\mathrm{End}\mathcal{H}\otimes\mathrm{End}\mathcal{V}$.

The most convenient basis to work in is a ''charged'' basis, where elements can be classified by their su(2) charge, namely their T_0^3 eigenvalue. The basis is given by

$$\begin{gathered}\theta^+=2(i\theta_1-\theta_2),\quad J^+=2(iJ_1-J_2),\\ \theta^-=2(i\theta_1+\theta_2),\quad J^-=2(iJ_1+J_2),\\ \theta^H=i\theta_3,\quad J^H=-2iJ_3.\end{gathered} \tag{66}$$

The primary field Φ itself is the highest weight in an su(2) representation, i.e., carries an su(2) representation index, so that

$$\begin{gathered}J^+\Phi(Z)=(J^+)^A{}_B\Phi^B(Z)=0,\\ J^H\Phi(Z)=(J^H)^A{}_B\Phi^B(Z)=q\Phi^A(Z).\end{gathered} \tag{67}$$

In the following, $\Phi_i(Z)$ has conformal weight h_i and spin q_i. The action of the twelve globally defined generators on $\Phi(Z)$ can then be given in Lie algebra form. The infinitesimal transformations are

$$\begin{gathered}[L_{-1},\Phi]=\partial_z\Phi,\quad [G^{\pm}_{-(1/2)},\Phi]=\pm(\theta^{\pm}\partial_z+8\partial_{\theta^{\mp}})\Phi,\\ [G^H_{-(1/2)},\Phi]=-4(\theta^H\partial_z+\partial_{\theta^H})\Phi,\quad [T_0^H,\Phi]=(\theta^-\partial_{\theta^-}-\theta^+\partial_{\theta^+}+J^H)\Phi,\\ [L_0,\Phi]=(h+z\partial_z+\tfrac{1}{2}(\theta^+\partial_{\theta^+}+\theta^-\partial_{\theta^-}+\theta^H\partial_{\theta^H}))\Phi,\\ [T_0^{\pm},\Phi]=(\mp\tfrac{1}{2}\theta^{\pm}\partial_{\theta_H}\pm 4\theta^H\partial_{\theta^{\mp}}+J^{\pm})\Phi,\\ [L_1,\Phi]=(2hz+z(z\partial_z+\theta^+\partial_{\theta^+}+\theta^-\partial_{\theta^-}+\theta^H\partial_{\theta^H})+\tfrac{1}{8}\theta^+\theta^-J^H+\tfrac{1}{4}\theta^+\theta^HJ^--\tfrac{1}{4}\theta^-\theta^HJ^+)\Phi,\\ [G^{\pm}_{1/2},\Phi]=(\pm 2h\theta^{\pm}\pm\theta^{\pm}z\partial_z\pm 8z\partial_{\theta^{\mp}}\pm\theta^{\pm}\theta^H\partial_{\theta^H}+\theta^+\theta^-\partial_{\theta^{\mp}}+2\theta^HJ^{\pm}+\theta^{\pm}J^H)\Phi,\\ [G^H_{1/2},\Phi]=(-8h\theta^H-4\theta^Hz\partial_z-4z\partial_{\theta^H}-4\theta^H\theta^-\partial_{\theta^-}-4\theta^H\theta^+\partial_{\theta^+}+\theta^-J^+-\theta^+J^-)\Phi.\end{gathered} \tag{68}$$

Note that under the T_0^H operator, θ^+ and θ^- are ''charged,'' i.e., they possess a nonzero T_0^H eigenvalue. The two point function, $\langle 0|\Phi_1(Z_1)\Phi_2(Z_2)0\rangle=\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle$ is, as a function, a function of $Z_1=(z,\theta_i)$ and $Z_2=(w,\chi_i)$. Since the Φ_i are also highest weight vectors of su(2) representations, $\mathcal{V}_i$, the two point function is an element of $\mathcal{V}_1\otimes\mathcal{V}_2$. The L_{-1} condition on the two-point function reads

$$\mathcal{L}_{-1}\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle=(\partial_z+\partial_w)\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle=0 \tag{69}$$

implying that $\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle$ is a function of $(z-w)$ and θ_i,χ_i. Applying the $G^x_{-(1/2)}$ conditions yields similar equations to (69). These conditions show that $\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle$ is a function of

$$\begin{gathered}(\theta^- - \chi^-),\quad (\theta^H - \chi^H),\quad (\theta^+ - \chi^+),\\ s = (z-w+\tfrac{1}{8}(\theta^-\chi^+ + \theta^+\chi^-) + \theta^H\chi^H).\end{gathered} \tag{70}$$

The L_0 condition gives a scaling condition, from which the most general form of the two point function can be seen to be

$$\begin{aligned}\langle\Phi_1(Z_1)\Phi_2(Z_2)\rangle = \frac{a}{s^{h_1+h_2}} + \frac{\epsilon_+(\theta^+ - \chi^+)}{s^{h_1+h_2+1/2}} + (\text{two similar terms}) + \frac{b_{+H}(\theta^+ - \chi^+)(\theta^H - \chi^H)}{s^{h_1+h_2+1}}\\ + (\text{two similar terms}) + \frac{\eta(\theta^+ - \chi^+)(\theta^- - \chi^-)(\theta^H - \chi^H)}{s^{h_1+h_2+3/2}}.\end{aligned} \tag{71}$$

The T_0^H condition includes su(2) elements. It is worth writing this condition out explicitly, to illustrate the action of the elements. Putting in all the tensor products between su(2) representations explicitly, the condition reads

$$((\mathbb{I}\otimes\mathbb{I})(\theta^-\partial_{\theta^-} - \theta^+\partial_{\theta^+} + \chi^-\partial_{\chi^-} - \chi^+\partial_{\chi^+}) + J^H\otimes\mathbb{I} + \mathbb{I}\otimes J^H)\langle\Phi_1(Z_1)\otimes\Phi_2(Z_2)\rangle = 0, \tag{72}$$

where

$$\begin{aligned}(J^H\otimes\mathbb{I} + \mathbb{I}\otimes J^H)\langle\Phi_1(Z_1)\otimes\Phi_2(Z_2)\rangle &= \langle(J^H\Phi_1)(Z_1)\otimes\Phi_2(Z_2)\rangle + \langle\Phi_1(Z_1)\otimes(J^H\Phi_2)(Z_2)\rangle\\ &= (q_1+q_2)\langle\Phi_1(Z_1)\otimes\Phi_2(Z_2)\rangle.\end{aligned} \tag{73}$$

This condition gives three possible cases

$$\begin{gathered}q_1+q_2 = 0 \Rightarrow \text{only } (a, \epsilon_H, b_{+-}, \eta) \text{ nonzero},\\ q_1+q_2 = 1 \Rightarrow \text{only } (\epsilon_+, b_{+H}) \text{ nonzero},\\ q_1+q_2 = -1 \Rightarrow \text{only } (\epsilon_-, b_{-H}) \text{ nonzero}.\end{gathered} \tag{74}$$

Replacing H with $+$ in (73), it can be seen that $J^+\otimes\mathbb{I} + \mathbb{I}\otimes J^+$ annihilates $\langle\Phi_1(Z_1)\otimes\Phi_2(Z_2)\rangle$. The T_0^+ condition then gives—if $q_1+q_2=-1$, then $\epsilon_-, b_{-H}=0$—if $q_1+q_2=0$, then $\epsilon_+, b_{+H}=0$—and gives no extra conditions if $q_1+q_2=1$. Thus, the $q_1+q_2=-1$ case is irrelevant. J^- is an operator that can cause calculational difficulties. The T_0^- condition can be used to relate $\langle(J^-\Phi_1)\Phi_2\rangle$ and $\langle\Phi_1(J^-\Phi_2)\rangle$.

Consider now the L_1 condition. This contains a term like

$$\theta^+\theta^H\langle(J^-\Phi_1)\Phi_2\rangle + \chi^+\chi^H\langle\Phi_1(J^-\Phi_2)\rangle.$$

The T_0^- condition can be used to relate this to a term of the form

$$(\theta^+\theta^H - \chi^+\chi^H)\langle(J^-\Phi_1)\Phi_2\rangle.$$

Thus the condition implies that all those terms that cannot be factored by $(\theta^+\theta^H - \chi^+\chi^H)$ are zero. A similar condition arises for the $G^x_{1/2}$ conditions. After much tedious algebra, one finds that

$$\langle \Phi_1(Z_1)\Phi_2(Z_2)\rangle = \begin{cases} \dfrac{a}{s^{h_1+h_2}} & \text{if} \quad h_1=h_2, \quad q_1=q_2=0, \\ \dfrac{b_{+H}(\theta^+-\chi^+)(\theta^H-\chi^H)}{s^{h_1+h_2+1}} & \text{if} \quad h_1=h_2, \quad q_1+q_2=1, \\ \qquad q_1,q_2\neq 0 & \\ 0 \quad \text{otherwise.} & \end{cases} \tag{75}$$

This has important applications to fusion. Considering the three-point function

$$\mathcal{F}_{123}=\langle \Phi_1(Z_1)\Phi_2(Z_2)\Phi_3(Z_3)\rangle,$$

where $\Phi_1(Z_1)$ is a "probe field," i.e., one can choose its (h,q) parameters, call them (h_1,q_1). $\Phi_2(Z_2)$ and $\Phi_3(Z_3)$ will have an OPE, which schematically looks like (i.e., omitting pole structure and other factors)

$$\Phi_2(Z_2)\Phi_3(Z_3)\sim\sum_n \Psi_n(Z_3) \tag{76}$$

that may be unknown, namely one may not know the (h,q) of the Ψ_n. One can ask if the OPE between $\Phi_2(Z_2)$ and $\Phi_3(Z_3)$ can be deduced if one knows the values of $\mathcal{F}_{123}$, for all h_1 and q_1. From (75), one can see that for $\langle \Phi_1(Z_1),\Psi_n(Z_3)\rangle$ to be nonzero, a unique (h_1,q_1) must be chosen. This choice determines the (h,q) of $\Psi_n(Z_3)$. Thus one can make the statement that knowing when the three point function $\mathcal{F}_{123}$ vanishes is equivalent to knowing what $\Psi_n(Z_3)$ are in (76). These then give rise to the fusion rules.

One should note that global conformal invariance of the theory almost fixes three super coordinates, as can be seen from (63). In the mapping from (64) to (65) one can map V and U to the North and South poles. One can also map z' from $Z'=(z',\theta_i')$ in (65), to wherever desired, using L_0. There is not enough freedom to move the θ_i' wherever desired. Thus, one would expect that the three-point function could also be computed, up to an arbitrary function in θ_i'. After expanding this function into components, this can be seen as being computable up to some arbitrary constants.

X. OTHER APPLICATIONS

This section is strictly speaking a list of things that could be done, in the $N=3$ theory. Since most of these things are very calculationally intensive, the author has not checked the details.

An interesting question is analyzing the constraints that singular vectors give on three-point functions. If $|\chi\rangle$ is a singular vector in a module with highest weight $|\phi_1\rangle$, then what does the requirement that

$$\langle \phi_3|\Phi(Z)\chi\rangle$$

vanish imply about

$$\langle \phi_3|\Phi(Z)\phi_1\rangle.$$

Algebraically, this is in fact quite difficult, and the author has not managed to accomplish this. The main complication is that the composition between primary fields in the correlator are a tensor product between su(2) representations $\mathcal{V}$ and $\mathcal{V}'$ and an End$\mathcal{H}$ composition. This means that the only super-Virasoro operators that can be transferred across the tensor product are those that have End$\mathcal{V}$ part proportional to the identity. The most obvious case where this applies is where all the

fields have $q=0$, i.e., they are all su(2) singlets. Following Refs. 11 and 30, the lowering operators acting appearing in $|\chi\rangle$ can be rewritten in terms of operators that have commutator with a primary field in (z,θ_i) given by a polynomial in (z,θ_i), namely

$$\begin{aligned}
\mathcal{L}_m &= -L_m + \frac{1}{z}L_{m+1} + \frac{1}{16z}(\theta^+ G^-_{m+(1/2)} - \theta^- G^+_{m+(1/2)} + 2\theta^H G^H_{m+(1/2)}) \\
&\quad + \frac{m+1}{4z}(\theta^-\theta^H T^+_m - \theta^+\theta^H T^-_m - \theta^+\theta^- T^H_m), \\
\mathcal{G}^\pm_r &= -G^\pm_r + \frac{1}{z}G^\pm_{r+1} - \frac{2\theta^H}{z}T^\pm_{r+(1/2)} - \frac{\theta^\pm}{z}T^H_{r+(1/2)}, \\
\mathcal{G}^H_r &= -G^H_r + \frac{1}{z}G^H_{r+1} - \frac{\theta^-}{z}T^+_{r+(1/2)} + \frac{\theta^+}{z}T^-_{r+(1/2)}, \\
\mathcal{T}^\pm_m &= -T^\pm_m + \frac{1}{z}T^\pm_{m+1} - \frac{\theta^\pm}{z}\psi_{m+(1/2)}, \\
\mathcal{T}^H_m &= -T^H_m + \frac{1}{z}T^H_{m+1} + \frac{2\theta^H}{z}\psi_{m+(1/2)}, \\
\mathcal{P}_r &= -\psi_r + \frac{1}{z}\psi_{r+1}.
\end{aligned} \tag{77}$$

One then finds

$$\begin{aligned}
&[\mathcal{L}_m,\Phi(Z)] = hz^m, \quad [\mathcal{G}^\pm_r,\Phi(Z)] = \pm 2h\theta^\pm z^{r-(1/2)}, \\
&[\mathcal{G}^H_r,\Phi(Z)] = -8h\theta^H z^{r-(1/2)}, \quad [\mathcal{T}^\pm_m,\Phi(Z)] = \pm h\theta^\pm\theta^H z^{m-1}, \\
&[\mathcal{T}^H_m,\Phi(Z)] = -\tfrac{1}{4}h\theta^+\theta^- z^{m-1}, \quad [\mathcal{P}_r,\Phi(Z)] = \tfrac{1}{8}h\theta^+\theta^-\theta^H z^{r-(3/2)}.
\end{aligned} \tag{78}$$

Now one can commute the operators from $|\chi\rangle$ past Φ without introducing differential operators. The operators $\mathcal{L}_m$, etc., may now be re-expanded in terms of L_m, etc. Some of these operators will annihilate $\langle\phi_3|$. Those that do not, and are not diagonal, must be processed using the descent equations on $|\Phi(Z)\phi_1\rangle$.[6] This then yields a set of polynomial equations giving conditions on the weights of the primary fields.

From a differential equation point of view, the question of singular vectors may not be such a difficult problem. As in Ref. 6, the lowering operators can be written as contour integrals, e.g.,

$$\begin{aligned}
L_{-k}(z) &= \frac{1}{2\pi i}\oint dw L(z)(w-z)^{1-k}, \\
G_{-r}(z) &= \frac{1}{2\pi i}\oint dw G(z)(w-z)^{(1/2)-r}, \quad \text{etc.}
\end{aligned} \tag{79}$$

The condition of a singular vector, $\mathcal{N}|\phi_3\rangle$, where $\mathcal{N}$ are some lowering operators, can be written as

$$\langle\Phi_1(Z_1)\Phi_2(Z_2)(\mathcal{N}\Phi_3)(Z_3)\rangle = 0.$$

This then gives rise, via (79) and the OPE, to a differential equation on the three point function. One would expect the three point function to look like a product of powers of differences, as in the

case of the two point function, e.g., $s,(\theta^+-\chi^+)$. As in the bosonic case, this should give rise to a polynomial in the h_i,q_i of the fields concerned. The difference now, is that the presence of J^- operators will give independent equations, e.g., $\mathcal{F}_{123}\in\mathcal{V}_1\otimes\mathcal{V}_2\otimes\mathcal{V}_3$, hence $(\mathbb{I}\otimes\mathbb{I}\otimes J^-)\mathcal{F}$ is linearly independent of $(\mathbb{I}\otimes\mathbb{I}\otimes\mathbb{I})\mathcal{F}$. Other than this, the calculations should proceed precisely as in the bosonic case.

XI. CONCLUSIONS

Starting from a graded Riemann sphere, a superconformal field theory was constructed. The construction roughly parallels that of the bosonic case, namely defining sections of a line bundle on a Riemann sphere, and rewriting the infinitesimal transformations of these sections as operator product expansions. Two ways were used to introduce a Ramond field, one by introducing a branch cut, the other by altering the preserved one-form. This suggests that looking at various sheaves on a graded Riemann sphere may be a potentially useful way of realizing fields in a superconformal field theory.

The super OPEs, together with an understanding of how the symmetries act on the graded Riemann sphere, were sufficient to compute the $N=3$ two-point function, up to multiplicative constants. In addition, it was illustrated how, in principle, the $N=3$ three point function and conditions given by singular vectors on the three point function could be calculated. It should be pointed out that the method of calculation was entirely in superfield formalism, and hence manifestly supersymmetric.

The only case that has really been studied here is the $N=3$ case, based on a Riemann surface of genus zero. How this generalizes to higher genus is an interesting question. An even more interesting question, is the $N=4$ case. Processing the $N=4$ theory through this machinery, does not produce the full OPE of the theory. There is a log term missing from the OPE corresponding to a U(1) charge. A question then arises, how to extend the framework of a graded Riemann sphere to incorporate this log term. Many parts of the $N=4$ theory will in fact look like the $N=3$ theory,[3] since the $N=4$ currents arising from R-symmetry are a pair of commuting su(2) currents.

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[32] Assume otherwise, so that $\kappa\kappa'=1=\kappa'\kappa$, and $\kappa\kappa''=1=\kappa''\kappa$. Subtracting and factorizing gives $(\kappa'-\kappa'')\kappa=0=\kappa(\kappa'-\kappa'')$. Using either inverse on these equations shows $\kappa'-\kappa''=0$.
[33] The commutators are graded, i.e., $[A,B]=AB-(-1)^{p(A)p(B)}BA$.
[34] $\epsilon_{123}=1$ and ϵ is antisymmetric in all its indices. Summation convention is used over repeated indices.
[35] The commutation relations are $[J_i,J_j]=-\frac{1}{2}\epsilon_{ijk}J_k$. These are precisely the commutation relations of the subalgebra formed by the $\frac{1}{2}t_0^i$.
[36] In the bosonic case, a vertex operator is characterized uniquely by its action on a vacuum, and can be defined by $\phi(z)|0\rangle=\exp(zL_{-1})|\phi\rangle$. On a supercomplex plane, this can be generalized to $\Phi(Z)|0\rangle=\exp(zL_{-1})\exp(\theta_1 G^1_{-(1/2)})\cdots\exp(\theta_N G^N_{-(1/2)})|\Phi\rangle$, giving the operator associated with a state.
[37] The author thanks M. Dörrzapf for checking these relations.
[38] More precisely, these come from an ungraded involution on the algebra. On any representation of the algebra that admits a Hermitian contragredient form, this involution then gives the adjoint with respect to that form.

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Cyclic statistics in three dimensions

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The existence of anyons in two-dimensional systems is a well-known example of nonpermutation group statistics. In higher dimensions, however, it is expected that statistics is dictated solely by representations of the permutation group. Using basic elements from representation theory we show that this expectation is false in three-dimensions for a certain nongravitational system. Namely, we demonstrate the existence of "cyclic," or $\mathbb{Z}_n$, *nonpermutation group* statistics for a system of $n>2$ identical, unknotted rings embedded in $\mathbb{R}^3$. We make crucial use of a theorem due to Goldsmith in conjunction with the Fuchs–Rabinovitch relations for the automorphisms of the free product group on n elements. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1738189]

I. INTRODUCTION

It is a well-established fact that the topology of the configuration space of a classical system can have a nontrivial effect on its quantization. A simple illustration of this is found in the sum-over-histories quantization of a particle on a circle wherein the set of paths with fixed initial and final positions fall into classes labeled by the winding number m.[1] The full partition function is expressed as a sum of partitions over these different classes of paths, each multiplied by an overall phase $e^{im\theta}$, where $\theta\in[0,2\pi]$ labels the unitary irreducible representations of the fundamental group $\mathbb{Z}$ of the circle. Each choice of θ thus leads to an inequivalent quantization of the system. In general, inequivalent quantizations of a classical system are labeled by the unitary irreducible representations of the fundamental group of the configuration space. Indeed, several phenomena of physical interest ranging from the quantum statistics of point particles, to a Hamiltonian interpretation of the QCD theta angle, to spinorial states in quantum gravity, can be attributed to such inequivalent quantizations.[2–6]

The particular phenomenon of interest to us in this paper is the emergence of quantum statistics in systems of n identical objects. For spatial dimensions $d>2$, the fundamental group of the configuration space of such systems contains the permutation group on n elements S_n as a subgroup. For typical systems, the unitary irreducible representations of S_n and its permutation subgroups are sufficient to determine quantum statistics. For $n=2$, $d>2$, for example, the permutation group S_2 generated by the exchange operation $\mathcal{E}$ has two inequivalent unitary irreducible representations: The trivial one ($\mathcal{E}\rightarrow 1$) corresponds to bose statistics and the nontrivial one ($\mathcal{E}\rightarrow -1$) corresponds to fermi statistics. For $n>2$, $d>2$, S_n has nonabelian unitary irreducible representations which give rise to parastatistics. In dimension $d=2$, however, statistics is dictated by a nonpermutation infinite discrete group called the braid group B_n, rather than the finite group S_n. The resulting statistics is referred to as "anyonic" and plays a central role in the study of two-dimensional systems.[5,6]

Since the permutation group S_n is always a subset of the fundamental group of the configuration space for $d>2$, it is generally believed that quantum statistics is dictated by a nonpermutation group only in two-dimensions. However, for $d>2$ quantum statistics does not merely depend on the existence of the permutation group S_n as a subgroup of the fundamental group

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$\pi_1(\mathcal{Q}_n)$ of the configuration space $\mathcal{Q}_n$, but more crucially on how it "sits" in $\pi_1(\mathcal{Q}_n)$.[7] Typically, for a system of n identical objects, $\pi_1(\mathcal{Q}_n)$ has the semidirect product structure $P \ltimes S_n$, with $\ltimes$ the semidirect product and P a normal subgroup. Standard representation theory[7,8] then tells us that quantum statistics is determined not by unitary irreducible representations of S_n, but rather those of the little groups (or stability subgroups) $\mathcal{R} \subseteq S_n$ with respect to the action of S_n on the space of representations of P.

For most systems the little groups are themselves permutation subgroups S_m of S_n, with $m \leqslant n$. This can be traced to the fact that the normal subgroup P is generated only by the "internal" symmetry groups K of each object and is simply the product of n copies of K. Representation theory then tells us that the little group $\mathcal{R}$ must be a permutation subgroup of S_n.[7,8] For example, consider a system of 3 identical extended solitons which are allowed to possess spin, i.e., a 2π rotation of the soliton is nontrivial (see Ref. 9 for an example). The permutation group on 3 elements, S_3 is a subgroup of $\pi_1(\mathcal{Q}_3) = P \ltimes S_3$, where for concreteness, P can be identified with the spin subgroup $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$, each $\mathbb{Z}_2$ factor representing the spin subgroup of a single soliton. Even though the solitons are classically identical, one can construct the representation $\{1/2,1/2,0\}$ of P in which two of the solitons are spin half and the third one is spin zero, thus rendering it quantum mechanically distinguishable from the others. As one might expect, the little group $\mathcal{R} \subseteq S_3$ associated with P is S_2 and not S_3, thus implying 2 rather than 3 particle quantum statistics.

In this paper, we will explicitly construct a nongravitational example in which the normal subgroup P does not have a simple product structure, and thus does indeed admit nonpermutation little groups $\mathcal{R} \subset S_n$. Namely, we will construct quantum sectors for a system of n closed, identical unknotted rings embedded in $\mathbb{R}^3$, for which $\mathcal{R}$ is a cyclic group, so that the associated quantum statistics is *cyclic*. An analogy was made between this system and that of n $\mathbb{R}P^3$ geons in $3+1$ canonical quantum gravity by the authors of Ref. 10; drawing on earlier results of Ref. 2 they demonstrated the existence of quantum sectors exhibiting indeterminate statistics when $n=2$. [A reanalysis of these sectors for 2 $\mathbb{R}P^3$ geons shows that this ambiguity is due to the lack of a canonical exchange operator (Ref. 7). Such indeterminate statistics have also been found for a system of two particles on $\mathbb{R}P^3$.] In Ref. 7 a rigorous analysis of the quantum sectors for a system of n topological geons in $3+1$ canonical quantum gravity was carried out and the existence of sectors obeying cyclic, or $\mathbb{Z}_n$ statistics was demonstrated for a system of n $\mathbb{R}P^3$ geons. Here, we will employ techniques developed in Ref. 7 to demonstrate the existence of cyclic statistics (an analogue of cyclic statistics in five-dimensions has been constructed in Ref. 12) for the system of $n \geqslant 3$ closed rings embedded in $\mathbb{R}^3$. Rings can appear in a wide class of physical systems, ranging from closed string theory, to cosmic strings, to closed superconducting flux tubes, to name a few. Recently, the existence of ring-like solitons was shown for certain nonlinear sigma models.[11] The existence of kinematical sectors exhibiting novel statistics in such systems may therefore have nontrivial physical implications.

The inequivalent quantizations for this system of rings are determined by the unitary irreducible representations of the so-called *motion group* $\mathcal{G}$ which we present in Sec. II. Using a theorem due to Goldsmith,[13] combined with the Fuchs–Rabinovitch relations for the automorphisms of the free product group on n elements,[14] we show that $\mathcal{G}$ has a nested semidirect product structure. In Sec. III, using Mackey's theory of induced representations,[8] we construct quantum sectors which exhibit cyclic statistics in a system of $n > 2$ rings. We end with some brief remarks in Sec. IV on the question of modeling cyclic statistics using string Lagrangians with topological terms.

Since the spin of the rings we consider is trivial, the sectors obeying cyclic statistics clearly violate the spin-statistics connection. In Ref. 15 a spin-statistics correlation was shown to hold when the configuration space is expanded to allow the creation and annihilation of rings, thus excluding nonpermutation group statistics. However, first quantized systems with ring-like structures could very well occur in condensed matter systems; as suggested in Ref. 10, the rings can be stabilized against creation and annihilation by carrying conserved charges. Whether sectors obeying cyclic statistics are physically realized or not is, of course, ultimately a question for experiment to decide.

II. THE MOTION GROUP FOR A SYSTEM OF *n* RINGS

We consider the system of n identical, nonintersecting, infinitely thin, unknotted, unlinked, unoriented rings, $C=C_1\cup C_2\cup\cdots\cup C_n$ in $\mathbb{R}^3$, which cannot be destroyed or created. The configuration space $\mathcal{Q}_n$ for this system of rings is the space of embeddings of C in $\mathbb{R}^3$ quotiented by an appropriate group of symmetries called the *motion group* $\mathcal{G}$ which we will define below. An obvious example of a symmetry is the exchange of a pair of identical rings. The fundamental group of $\mathcal{Q}_n$ for this system is isomorphic to the motion group $\mathcal{G}$. This group is nontrivial for all $n\geqslant 1$, and has been extensively studied by Dahm and Goldsmith.[13]

Since the configuration space $\mathcal{Q}_n$ is multiply connected, on quantization, the Hilbert space splits into inequivalent quantum sectors. A systematic study of such quantum sectors can be found in Ref. 4. The wave functions $\psi:\tilde{\mathcal{Q}}_n\rightarrow\mathbb{C}$, where $\tilde{\mathcal{Q}}_n$ is the universal cover of $\mathcal{Q}_n$, so that $\pi_1(\mathcal{Q}_n)$ acts nontrivially on ψ. Since physically measurable quantities like inner products should only be functions on the classical configuration space $\mathcal{Q}_n$, the action of $\pi_1(\mathcal{Q}_n)$ on ψ must be represented as a "phase," which can be nonabelian for $n\geqslant 2$. Thus, at every point $q\in\mathcal{Q}_n$, ψ is valued in the carrier spaces of the unitary irreducible representations of $\pi_1(\mathcal{Q}_n)$. The inequivalent unitary irreducible representations of $\pi_1(\mathcal{Q}_n)$ then correspond to inequivalent quantum sectors.

The motion group $\mathcal{G}$ for this system of rings is defined as follows.[13] Let $H(\mathbb{R}^3)$ denote the space of continuous maps or homeomorphisms of $\mathbb{R}^3$ into itself and $H(\mathbb{R}^3,C)$ the subspace of homeomorphisms which leave C invariant. Let $H_\infty(\mathbb{R}^3)$ and $H_\infty(\mathbb{R}^3,C)$ be subspaces of $H(\mathbb{R}^3)$ and $H(\mathbb{R}^3,C)$, respectively, consisting of homeomorphisms with compact support. A *motion* is then defined as a path h_t in $H_\infty(\mathbb{R}^3)$ such that h_0 is the identity map from $\mathbb{R}^3$ to itself and $h_1=H_\infty(\mathbb{R}^3,C)$. The product of two motions can then be defined and the inverse g^{-1} of the motion g is the path $g_{(1-t)}\circ g_1^{-1}$.[13] Two motions h,h' are taken to be equivalent if $h'^{-1}h$ is homotopic to a path which lies entirely in $H_\infty(\mathbb{R}^3,C)$. The motion group $\mathcal{G}$ is then the set of equivalence classes of motions of C in $\mathbb{R}^3$ with multiplication induced by "$\circ$" (for brevity of expression we will henceforth refer to an equivalence class of motions as a motion).

We will use Hendricks' definition of a rotation[16] to describe the generators of the motion group. A 3-ball $\mathbb{B}^3\subset\mathbb{R}^3$ will be said to be rotated by an angle α in the following sense: take a collar neighborhood $S^2\times[0,1]$ of $\partial\mathbb{B}^3\approx S^2$ and let the S^2's be differentially rotated from 0 to α with $S^2\times\{0\}=\partial\mathbb{B}^3$ rotated by α and $S^2\times\{1\}$ not rotated at all. The rotation by an angle α of a solid torus $U=\mathbb{B}^2\times S^1$ in the direction of its noncontractible circle S^1 is similarly defined as a differential rotation of a collar neighborhood $T^2\times[0,1]$ of $\partial U\approx T^2$, with $T^2\times\{0\}=\partial U$ rotated by α and $T^2\times\{1\}$ not rotated at all.

$\mathcal{G}$ is generated by three types of motions which are quite easily visualized.[13] The first is the flip motion f_i which corresponds to "flipping" the ith ring (in the case of oriented rings, this motion yields a configuration distinct from the first and is not a symmetry). This motion corresponds to a rotation by π of an open ball in $\mathbb{R}^3$ containing C_i, about an axis lying in the plane of C_i. Since the rings are embedded in three dimensions, $f_i^2=e$, so that each flip generates a $\mathbb{Z}_2$ subgroup. Next is the exchange motion e_i which exchanges the ith ring with the $(i+1)$th ring. This can be thought of as a π rotation of a solid torus in $\mathbb{R}^3$ containing both C_i and C_{i+1} (but no others). These motions generate the permutation group S_n. Finally, one has the slide motion s_{ij} which requires a slightly more detailed description. A point in the configuration space (i.e., $\mathbb{R}^3-C$ modulo the action of the motion group) is itself a multiply connected space with $\pi_1(\mathbb{R}^3-C)$ isomorphic to the free product group on n generators $F(x_1,x_2\ldots,x_n)\approx\mathbb{Z}*\mathbb{Z}*\cdots*\mathbb{Z}$, each factor of $\mathbb{Z}$ isomorphic to the fundamental group of a single ring in $\mathbb{R}^3$. s_{ij} is then the motion of C_i along one of these $\mathbb{Z}$ factors, specifically, the generator of $\mathbb{Z}\subset\pi_1(\mathbb{R}^3-C)$ passing through C_j. Again, one can define the slide using a rotation: Consider a solid torus containing C_i and "threading" C_j, without intersecting it. A slide is then a 2π rotation of this solid torus. The existence of slide motions is key to the present analysis, and is what makes the analogy with the system of topological geons explicit.

We denote the three subgroups generated by the flips, the exchanges and the slides as $\mathcal{F}$, S_n and $\mathcal{S}$, respectively. We will also need to identify the subgroup $\tilde{\mathrm{G}}$ generated by only the flips and

the exchanges. The structure of S_n is known: It is simply the permutation group on n elements. However, the structures of $\mathcal{F}$ and $\mathcal{S}$ need to be deduced, as does information on how these groups sit in $\mathcal{G}$. While the generators of $\mathcal{G}$ have been known for some years, its explicit structure in terms of these subgroups has not been obtained until now.

Definition: A group G is said to be a semidirect group $P \ltimes K$ if (a) $\forall g \in G$, $\exists p \in P$ and $k \in K$ such that $g = pk$ (b) P is normal in G and (c) $P \cap K = e$. For every fixed $k \in K$, $p \to kpk^{-1}$ generates an automorphism α_k of P. G is said to have a nested semidirect product structure if further, either K or P or both, themselves are semidirect product groups.

We now show that $\mathcal{G}$ has the nested semidirect product structure

$$\mathcal{G} = \mathcal{S} \ltimes (\mathcal{F} \ltimes S_n). \tag{1}$$

We also show that $\mathcal{S}$ is the nonabelian group made up of the free product group on $n(n-1)$ generators

$$\underbrace{\mathbb{Z} * \mathbb{Z} * \cdots * \mathbb{Z}}_{n(n-1)}, \tag{2}$$

subject to the conditions

$$s_{ij} s_{kl} = s_{kl} s_{ij}, \quad s_{ij} s_{kj} = s_{kj} s_{ij}, \quad s_{ik} s_{jk} s_{ij} = s_{ij} s_{ik} s_{jk}. \tag{3}$$

$\mathcal{F}$, on the other hand, can be shown to be the abelian group isomorphic to the direct product group of the $\mathbb{Z}_2$ flips of each ring

$$\mathcal{F} = \underbrace{\mathbb{Z}_2 \times \mathbb{Z}_2 \times \cdots \times \mathbb{Z}_2}_{n}. \tag{4}$$

For brevity of notation we define the exchange action π_i on the set of n integers labeling the n rings as follows: For $1 \leqslant j \leqslant n$, $\pi_i : j \to \pi_i(j)$ where $\pi_i(j) = j$ for $j \neq i, i+1$, $\pi_i(i) = i+1$ and $\pi_i(i+1) = i$. Here when $i = n$, $i+1$ is identified with 1.

Lemma: $\mathcal{G}$ has the nested semidirect product structure (1). Thus, $\mathcal{S}$ is normal in $\mathcal{G}$ and $\mathcal{F}$ is normal in the subgroup $\tilde{\mathrm{G}} \subset \mathcal{G}$ generated by the flips and the permutations. The automorphisms of $\mathcal{S}$ generated by $\tilde{\mathrm{G}}$ and those of $\mathcal{F}$ generated by S_n are given by the Fuchs–Rabinovitch relations, induced by the Dahm isomorphism $D : \mathcal{G} \to \overline{\mathcal{G}} \subseteq Aut(F(x_1, \ldots, x_n))$ where $Aut(F(x_1, \ldots, x_n))$ is the group of automorphisms of $F(x_1, \ldots, x_n)$. Moreover, $\mathcal{S}$ is isomorphic to the group (2) subject to the conditions (3), and $\mathcal{F}$ is isomorphic to the group (4).

Proof: The induced action of the motion group on $\pi_1(\mathbb{R}^3 - C)$ has been examined by Goldsmith,[13] and provides us with a crucial step in deducing the structure of $\mathcal{G}$. As noted earlier, $\pi_1(\mathbb{R}^3 - C)$ is isomorphic to $F(x_1, \ldots, x_n)$, the free product group on n-generators, x_i, $i = 1, \ldots, n$. In Ref. 13 the "Dahm" homomorphism $D : \mathcal{G} \to Aut(F(x_1, \ldots, x_n))$ is defined where $Aut(F(x_1, \ldots, x_n))$ is the group of automorphisms of $F(x_1, \ldots, x_n)$. For each motion $g \in \mathcal{G}$, D induces an automorphism of $F(x_1, \ldots, x_n)$. The following theorem then states:

Goldsmith's Theorem:[13] The group of motions $\mathcal{G}$ of the trivial n-component link C in $\mathbb{R}^3$ is generated by the following types of motions:

(1) f_i or flips. Turn the ith ring over. This induces the automorphism $\phi_i : x_i \to x_i^{-1}$, $x_k \to x_k$, $k \neq i$, of $F(x_1, \ldots, x_n)$.
(2) e_i or exchange. Interchange the ith and the $(i+1)$th rings. The induced automorphism of $F(x_1, \ldots, x_n)$ is $\epsilon_i : x_i \to x_{i+1}, x_{i+1} \to x_i$ and $x_k = x_k$ for $k \neq i, i+1$.
(3) s_{ij} or slides. Pull the ith ring through the jth ring. This induces the automorphism $\sigma_{ij} : x_i \to x_j x_i x_j^{-1}$, $x_k \to x_k$, $k \neq i$, of $F(x_1, \ldots, x_n)$.

Moreover, the Dahm homomorphism, $D : \mathcal{G} \to Aut(F(x_1, \ldots, x_n))$ is an isomorphism onto the subgroup $\overline{\mathcal{G}}$ of $Aut(F(x_1, \ldots, x_n))$ generated by ϕ_i, ϵ_i and σ_{ij}, where $1 \leqslant i, j \leqslant n, i \neq j$.

Let us denote the subgroups of $\overline{\mathcal{G}}$ generated by the automorphisms σ_{ij}, ϕ_i and ϵ_i as $\overline{\mathcal{S}}$, $\overline{\mathcal{F}}$ and $\overline{\mathrm{S}_n}$, respectively. We may now employ the Fuchs–Rabinovitch relations for $Aut(F(x_1,\ldots,x_n))$ which provides a complete set of relations for the generators of $\overline{\mathcal{G}}$.[14] For $\pi_1(\mathbb{R}^3-C)=\mathbb{Z}*\mathbb{Z}*\cdots*\mathbb{Z}$, in particular, these relations are simple and imply that $\overline{\mathcal{G}}\subset Aut(F(x_1,\ldots,x_n))$ has the nested semidirect product structure

$$\overline{\mathcal{G}}=\overline{\mathcal{S}}\ltimes(\overline{\mathcal{F}}\ltimes\overline{\mathrm{S}_n})=\overline{\mathcal{S}}\ltimes\bar{\bar{\mathrm{G}}}, \tag{5}$$

where $\bar{\bar{\mathrm{G}}}=\overline{\mathcal{F}}\ltimes\overline{\mathrm{S}_n}$. In particular, the generators ϵ_i of $\overline{\mathrm{S}_n}$ generate the following automorphisms of $\overline{\mathcal{F}}$:

$$\epsilon_i\phi_j\epsilon_i^{-1}=\phi_{\pi_i(j)}, \tag{6}$$

and the generators ϵ_i and ϕ_i of $\bar{\bar{\mathrm{G}}}$ generate the following automorphisms of $\overline{\mathcal{S}}$:

$$\begin{aligned}\epsilon_i\sigma_{jk}\epsilon_i^{-1}&=\sigma_{\pi_i(j)\pi_i(k)},\\ \phi_i\sigma_{jk}\phi_i^{-1}&=\sigma_{jk},\forall k\neq i,\\ \phi_i\sigma_{ji}\phi_i^{-1}&=\sigma_{ji}^{-1}.\end{aligned} \tag{7}$$

Moreover, these relations imply that $\overline{\mathcal{S}}$ is the free product group on $n(n-1)$ generators $\mathbb{Z}*\mathbb{Z}*\cdots*\mathbb{Z}$ subject to the conditions $\sigma_{ij}\sigma_{kl}=\sigma_{kl}\sigma_{ij}$, $\sigma_{ij}\sigma_{kj}=\sigma_{kj}\sigma_{ij}$, and $\sigma_{ik}\sigma_{jk}\sigma_{ij}=\sigma_{ij}\sigma_{ik}\sigma_{jk}$ while $\overline{\mathcal{F}}$ is the abelian direct product group made up of n factors of $\mathbb{Z}_2$, $\overline{\mathcal{F}}=\mathbb{Z}_2\times\mathbb{Z}_2\times\cdots\times\mathbb{Z}_2$. Since D is an isomorphism with $D(\mathcal{S})\subseteq\overline{\mathcal{S}}$, $D(\mathcal{F})\subseteq\overline{\mathcal{F}}$ and $D(S_n)\subseteq\overline{\mathrm{S}_n}$, this means that $\mathcal{S}\approx\overline{\mathcal{S}}$, $\mathcal{F}\approx\overline{\mathcal{F}}$ and $S_n\approx\overline{\mathrm{S}_n}$. From (5), it is then obvious that $\mathcal{G}$ itself has the nested semidirect product structure (1). The automorphisms of S_n on $\mathcal{F}$ and of $\tilde{\mathrm{G}}$ on $\mathcal{S}$, respectively, are given by (6) and (7) and induced by the isomorphism $D:\mathcal{G}\rightarrow\overline{\mathcal{G}}$. Moreover, $\mathcal{S}$ is the free product group on $n(n-1)$ generators $\mathbb{Z}*\mathbb{Z}*\cdots*\mathbb{Z}$ subject to the relations (3) and $\mathcal{F}$ is given by (4). □

While the structure of the motion group can be completely deduced from the Dahm homomorphism and the Fuchs–Rabinovitch relations, it is instructive to examine this group without recourse to $Aut(F(x_1,\ldots,x_n))$. Using just the definition of the motion group we now illustrate the following properties of $\mathcal{G}$: (a) $\mathcal{S}$ is normal in $\mathcal{G}$ and satisfies the relations (3) and (b) that $\mathcal{F}$ is normal in $\tilde{\mathrm{G}}$.

By definition, an element of the motion group is a homotopy equivalence class of paths in the space of homeomorphisms with compact support. Two homeomorphisms h_1 and h_2 with compact support on the regions U_1 and U_2 commute if $U_1\cap U_2=\phi$ and hence so do the corresponding motions. It is, therefore, useful to isolate the "minimal" neighborhoods in which homeomorphisms representing the generators of the motion group act so as to determine which two motions commute.

Let U_i denote an open ball neighborhood of C_i in $\mathbb{R}^3$ which contains no other C_j, $j\neq i$, and let U_{ij} denote an open ball neighborhood of $C_i\cup C_j$ containing no other C_k, $k\neq i,j$, etc. We will refer to the U_i as "exclusive" neighborhoods and the $U_{ij}, U_{ijk},\ldots$, etc. as "common" neighborhoods. The flip motion f_i is then defined by a homotopy equivalence class of paths in $H_\infty(\mathbb{R}^3)$ which include a "model" path made up of homeomorphisms with support only on U_i, i.e., a path in $H_\infty(\mathbb{R}^3)$ along which C_i is flipped without disturbing any of the other rings. Next, the exchange motion e_i is defined by a homotopy equivalence class of paths including a model path made up of homeomorphisms with support only on $U_{i(i+1)}$, i.e., the ith and the $(i+1)$th ring are exchanged without disturbing the other rings. Finally, the slides s_{ij} are defined by a homotopy equivalence class of paths including a model path with support only on U_{ij}, i.e., a path in which the other rings are not disturbed.

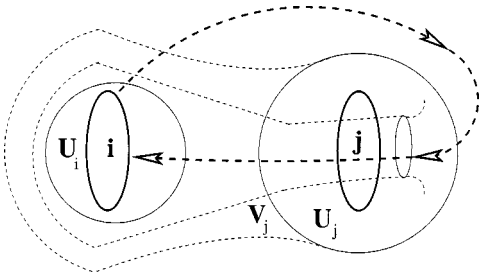

FIG. 1. Under the slide s_{ij} C_i "tunnels" through the neighborhood U_j of C_j and maps it onto the region V_j, shown by dashed lines. V_j, therefore, "encloses" C_i without containing it, i.e., $U_i \cap V_j = \phi$.

Now, the set of exclusive neighborhoods $\{U_i\}$ remains invariant when acted upon by the subgroup $\tilde{\mathrm{G}}$ generated by the flips and by the exchanges. This is obvious for $\mathcal{F}$, since each flip f_i acts within an exclusive neighborhood. For S_n, while the exchange e_i has compact support on $U_{i(i+1)}$, its action can be considered as a pure exchange of U_i with U_{i+1}. Thus, one can consider as a model path for the exchange, a localized π rotation in $U_{i(i+1)}$ which exchanges U_i with U_{i+1}. This, however, is not the case with the slides s_{ij}. While the set $\{U_k\}$ for $k \neq j$ remains invariant under the slide s_{ij} of C_i through C_j, the exclusive neighborhood U_j does not. The nonlocal action of the slide takes U_j into a set V_j which "encloses" C_i even though it does not contain it, i.e., there exists a U_i such that $U_i \cap V_j = \phi$ (see Fig. 1). Thus, V_j is not an exclusive neighborhood of C_j. This feature leads to subtleties in what follows.

Since the exchanges and the flips leave the set $\{U_i\}$ invariant, model paths are sufficient to see that $\mathcal{F}$ is normal in $\tilde{\mathrm{G}}$, i.e., for all $\tilde{g} \in \tilde{\mathrm{G}}$, $i \leqslant n$, $\tilde{g} f_i \tilde{g}^{-1} \in \mathcal{F}$. To show this, it is sufficient to take $\tilde{g}$ to be an exchange. For the motion $e_i f_j e_i^{-1}$ with $j \neq i, i+1$, the model paths for e_i and f_j have compact support on $U_{i(i+1)}$ and U_j, respectively, where $U_{i(i+1)} \cap U_j = \phi$. Hence the motions commute, so that $e_i f_j e_i^{-1} = f_j$. Now consider the motion $e_i f_i e_i^{-1}$. The model paths for e_i^{-1} exchange U_i with U_{i+1}. One can then use a model path for the motion f_i which acts on some $U'_{i+1} \subset U_{i+1}$ so that the final exchange e_i which exchanges U_{i+1} with U_i does not disturb the action of f_i on U'_{i+1}. Thus, $e_i f_i e_i^{-1} = f_{i+1}$. Similarly, $e_i f_{i+1} e_i^{-1} = f_i$.

However, model paths are insufficient when one wants to deal with the slides. Let us consider a motion whose model path involves homeomorphisms with support only on the compact region U. The homotopy class of paths defining this motion also includes the nonmodel, or "gregarious" paths, which involve homeomorphisms with nontrivial compact support on $\mathbb{R}^3 - U$. In other words, gregarious paths *can* disturb the other rings; they can contain homeomorphisms with nontrivial support on neighborhoods of rings left undisturbed by the model path. Consider the motion f_i for simplicity. A model path for f_i has support only on U_i and corresponds to a π rotation about an axis in the plane of C_i. A gregarious path on the other hand can be constructed piecewise as follows: (a) Rotate C_i by $\pi/3$, about an axis $\hat{x}$ in its plane; (b) flip another C_j, $j \neq i$; (c) rotate C_i by a further $\pi/3$ about $\hat{x}$ in the same sense as before; (d) flip C_j again; (e) and complete with a further $\pi/3$ rotation of C_i about $\hat{x}$ in the same sense as before. Such a path clearly corresponds to the motion f_i, but involves homeomorphisms of $\mathbb{R}^3$ in $H_\infty(\mathbb{R}^3)$ which have nontrivial support on the ring C_j, $j \neq i$.

Both model and gregarious paths are necessary to demonstrate that $\mathcal{S}$ is normal in $\mathcal{G}$. $\mathcal{S}$ is a normal subgroup of $\mathcal{G}$ if $\forall g \in \mathcal{G}$ and $\forall i,j \leqslant n$ $g s_{ij} g^{-1} \in \mathcal{S}$. It is sufficient to take g to be a generator of S_n or $\mathcal{F}$.

We begin with the exchanges. Let us examine the motion $e_k s_{ij} e_k^{-1}$ by considering only model paths in the appropriate homotopy class. For $k \neq i,j$ $e_k s_{ij} e_k^{-1} = s_{ij}$, since the homeomorphisms that make up model paths for e_k and s_{ij} have compact supports on U_k and U_{ij} with $U_k \cap U_{ij} = \phi$. Model paths are, however, insufficient to show that $e_k s_{ij} e_k^{-1}$ is also a slide for $k = i$, $i-1$, j or $j-1$. Consider the motion $e_j s_{ij} e_j^{-1}$ with $k = j$, $i \neq j, j+1$. e_j^{-1} swaps U_j with U_{j+1} by a π rotation of a torus containing both U_j and U_{j+1}. Next, s_{ij} rotates by 2π a solid torus containing

C_i and threading C_{j+1}, thus mapping U_{j+1} into a nonexclusive neighborhood V_{j+1}. A model path for the final exchange e_j would rotate by π a solid torus containing new exclusive neighborhood U'_{j+1} of C_{j+1} and U_i. $U_{i(j+1)}$ in which the slide acts, is not left invariant by this final exchange, making the resultant motion difficult to unravel. Instead, we use the following gregarious path to perform the final exchange: consider a path in $H_\infty(\mathbb{R}^3)$ where $U_{i(j+1)}$ and U_j are swapped by performing an appropriate π rotation in the common neighborhood $U_{ij(j+1)}$ of C_i, C_j and C_{j+1}. The final exchange motion is then completed by merely moving C_i back to its original position. $U_{i(j+1)}$ is thus left undisturbed so that the full motion is the slide $s_{i(j+1)}$. A use of a similar gregarious path for the final exchange shows that $e_{(j-1)}s_{ij}e^{-1}_{(j-1)}=s_{i(j-1)}$, $e_i s_{ij} e_i^{-1} = s_{(i+1)j}$ and $e_{(i-1)}s_{ij}e^{-1}_{(i-1)}=s_{(i-1)j}$.

Next, consider the flips. The motion $f_k s_{ij} f_k^{-1}$ can again be examined using only model paths for $k\neq j$, and we can see that it is s_{ij}. This is because the model path for f_k has compact support only on U_k which is undisturbed by the slide even when $k=i$. However, the use of model paths is insufficient to examine the motion $f_j s_{ij} f_j^{-1}$: not only does U_j not remain an exclusive neighborhood under the slide s_{ij}, but the f_j moves the points in U_j relative to each other. Rather than consider just a single gregarious path, following Ref. 7, we use a particular set of homotopy equivalent paths. Let κ be the generator of $\pi_1(\mathbb{R}^3-C)$ through C_j about which the slide s_{ij} takes C_i. We define the paths γ_α as follows: (a) perform a "part" inverse flip corresponding to a $(\pi-\alpha)$ rotation of C_j about $\hat{x}$ (b) slide C_i through C_j along κ^{-1} (c) finish the inverse flip f_j^{-1} of C_j by a rotation α about $\hat{x}$ and (d) finally, perform the flip f_j of C_j about $\hat{x}$. γ_0 then corresponds to the model path for the motion $f_j s_{ij} f_j^{-1}$ while the path γ_π corresponds to the slide s_{ij}^{-1}. Since α is a continuous parameter $\alpha\in[0,\pi]$, the γ_α provide a homotopy map from γ_0 to γ_π, which implies that $f_j s_{ij} f_j^{-1}=s_{ij}^{-1}$ (it is perhaps a useful exercise for the reader to see why a similar argument cannot be used to find a set of homotopic paths between $s_{ij}f_j s_{ij}^{-1}$ and an element of $\mathcal{F}$).

Thus, the slide subgroup $\mathcal{S}$ is a normal subgroup of $\mathcal{G}$.

We can also demonstrate that the relations (3) are satisfied by $\mathcal{S}$, using just the definition of the motion group. The first of these relations is clearly satisfied by the generators of $\mathcal{S}$, since the model paths corresponding to the slides s_{ij} and s_{kl} involve homeomorphisms with compact support only on U_{ij} and U_{kl} where $U_{ij}\cap U_{kl}=\phi$. It takes a little more work to show that the other two relations are also satisfied by the generators of $\mathcal{S}$.

Consider the motion $s_{ij}s_{kj}s_{ij}^{-1}$. s_{ij} and s_{kj} are slides of the two rings C_i and C_k through a third ring C_j. These slides are obtained by 2π rotations of the solid tori $V_{ij}\approx B^2\times S^1$ and $V_{kj}\approx B^2\times S^1$ which thread through C_j, with $V_{ij}\cap V_{kj}=\phi$. Define the paths γ_α as follows: (a) A rotation by $-\alpha$ of V_{ij}; (b) a 2π rotation of V_{kj}; (c) a $-(2\pi-\alpha)$ rotation of V_{ij} and finally; (d) a 2π rotation of V_{ij}. γ_0 then defines a model path for the motion $s_{ij}s_{kj}s_{ij}^{-1}$, and $\gamma_{2\pi}$ corresponds to the slide s_{kj}. Since α is a continuous parameter, γ_0 is homotopic to $\gamma_{2\pi}$ and hence also corresponds to s_{kj}. Notice that by keeping $V_{ij}\cap V_{kj}=\phi$ we prevent a mixing of their rotations and hence the deformations of the neighborhood U_j by s_{ij} and by s_{kj}.

Next, consider the motion $s_{ij}s_{ik}s_{jk}s_{ij}^{-1}$. Although this looks considerably more complicated than the previous motion, the two elements of $\mathcal{S}$ involved, $s_{ik}s_{jk}$ and s_{ij}, have compact supports on nonintersecting neighborhoods. Namely, the element $s_{ik}s_{jk}$ corresponds to sliding C_j through a generator ρ of π_1 of C_k and then sliding C_i through the same generator. Under this action, $U_j\rightarrow U_j$ and $U_i\rightarrow U_i$, while U_k is now mapped to a region V_k which now "encloses" both C_i and C_j. Thus, there exists a path in $H_\infty(\mathbb{R}^3)$ corresponding to the motion $s_{ik}s_{jk}$ made up of homeomorphisms which leave the common neighborhood U_{ij} undisturbed. Since there is a model path corresponding to the slide s_{ij} which has compact support only on U_{ij}, this means that the two motions $s_{ik}s_{jk}$ and s_{ij} indeed commute. Thus, the generators of $\mathcal{S}$ satisfy all the relations (3).

Remark: In Ref. 10 a set of relations for the generators in the $n=2$ case was given: $f_i^2=\mathcal{E}^2=(f_i\mathcal{E})^4=(f_i\mathcal{E}s_j\mathcal{E})^2=e$ where $i=1,2$ and the slides s_i generate $\mathcal{S}$, the flips f_i generate $\mathcal{F}$ and the exchange $\mathcal{E}$ generates S_2. These follow in a straightforward manner from the relations presented above.

III. CYCLIC STATISTICS

The inequivalent quantum sectors for our system of n identical rings are labeled by the unitary irreducible representations of $\pi_1(\mathcal{Q}_n)\approx\mathcal{G}$. The group $\mathcal{G}$ represents a "gauge" symmetry and the action of the individual motions $g\in\mathcal{G}$ on $\mathbb{R}^3-C$ can be used to interpret the associated quantum phases.

Let us begin by considering the simplest case, namely a single ring for which the motion group $\pi_1(\mathcal{Q})$ is simply $\mathcal{F}=\mathbb{Z}_2$. Let ψ_1 be a wave function on $\tilde{\mathcal{Q}}$ with localized support along the fibre $\{\tilde{q}_1,\tilde{q}_2\}$ at $q\in\mathcal{Q}$, generated by the action of the flip f, i.e., $\tilde{q}_1\rightarrow\tilde{q}_2=f\circ\tilde{q}_1$. Under the action of f, $\psi_1\rightarrow\psi_2$, which is also localized on the fibre at q. Since wave functions take values in the carrier spaces of the irreducible representations of $\pi_1(\mathcal{Q})$, $\psi_2=\Delta(f)\circ\psi_1$, where Δ is a unitary irreducible representation of $\mathcal{F}=\mathbb{Z}_2$. Δ can be either the trivial representation $\Delta(f)=1$ or the nontrivial one with $\Delta(f)=-1$, the associated quantum sectors corresponding to either an "unoriented" quantum ring in which $\psi_2=\psi_1$ or an "oriented" quantum ring in which $\psi_2=-\psi_1$. (Recall that classically, the rings are unoriented, since flips are a symmetry of the classical configuration space.) When there are two rings, i.e., $n=2$, the motion group includes the permutation group $S_2=\mathbb{Z}_2$ which gives rise to nontrivial quantum statistics. Consider a wave function ψ which is localized along the fibre of a configuration where the two rings are well-separated and identical: Under an exchange operation ψ, therefore, picks up a phase of ±1 corresponding to bosonic/fermionic quantum statistics (see Refs. 2, 4, and 7 for a more detailed discussion of quantum phases and statistics for extended objects). As we will presently demonstrate, for $n>2$ the existence of the slide subgroup in $\pi_1(\mathcal{Q}_n)$ gives rise to an unexpected complexity in the structure of the phases acquired by the wave function under the action of the permutation group.

As mentioned in the introduction, the quantum statistics of a system is not solely determined by S_n, but rather by the unitary irreducible representations of its stability subgroup $\mathcal{R}\subseteq S_N$ associated with its action on the unitary irreducible representations of the normal subgroup $\mathcal{S}\ltimes\mathcal{F}$ of $\mathcal{G}$. This follows from Mackey's theory of induced representations for semidirect product groups $P\ltimes K$.[8] In this construction, one begins with the space of unitary irreducible representations $\hat{P}$ of the normal subgroup P. The subgroup K has the (not necessarily free) action on $\hat{P}$

$$\Delta(p)\rightarrow\tilde{\Delta}(p)=\Delta(kpk^{-1}), \tag{8}$$

where $\Delta\in\hat{P}$, $p\in P$ and $k\in K$. Starting with a particular $\Delta_1\in\hat{P}$ one obtains an orbit $\mathcal{O}=\{\Delta_1,\Delta_2,\ldots,\Delta_r\}$ of the K action on $\hat{P}$, and the little group $\mathcal{R}$ associated with $\mathcal{O}$. The full unitary irreducible representation of $P\ltimes K$ is then built up by taking the direct product of (a) $[\Delta_1\oplus\Delta_2\oplus\cdots\oplus\Delta_r]$ with (b) a unitary irreducible representation of $\mathcal{R}$. For example, if one starts with the trivial representation of P, then the orbit consists of a single point and $\mathcal{R}=K$. The unitary irreducible representations of $P\ltimes K$ that can be constructed from this orbit are just the unitary irreducible representations of K. On the other hand, one may find an orbit of K in $\hat{P}$ with $\mathcal{R}=e$. The full unitary irreducible representation is then simply the sum of the unitary irreducible representations in the orbit, $\oplus_i\Delta_i$. The action of the subgroup K is then reduced to a canonical map which permutes the carrier spaces $\mathbb{H}_i$ of Δ_i[7] (as discussed in Ref. 7 for $n\geqslant4$ the possibility of projective statistics exists when $\pi_1(Q)$ has a semidirect product structure).

We now illustrate the importance of the little group in determining quantum statistics with a simple example. Because of the nested semidirect product structure of the motion group, we may begin by first representing the slides trivially. We thus need to find only the unitary irreducible representations of the subgroup $\tilde{\mathrm{G}}=\mathcal{F}\ltimes S_n$. Since $\mathcal{F}\approx\mathbb{Z}_2\times\mathbb{Z}_2\times\cdots\times\mathbb{Z}_2$ with n $\mathbb{Z}_2$ factors, it is trivial to list its unitary irreducible representations, i.e., $\Delta\equiv(k_1,k_2,\ldots,k_n)$, with $k_i=\pm1$. For example, for $n=3$, let us start with the unitary irreducible representation $\Delta_1=(-,-,+)$ of the normal subgroup $\mathcal{F}$ of $\tilde{\mathrm{G}}$. This choice corresponds to two of the rings being identical and oriented, while the third is unoriented and hence distinguishable from the others. The action of S_3 on Δ_1

generates the orbit $\{\Delta_1,\Delta_2,\Delta_3\}\equiv\{(-,-,+),(+,-,-),(-,+,-)\}$ in $\hat{\mathcal{F}}$ whose associated little group is S_2. The resulting unitary irreducible representation of $\tilde{\mathrm{G}}$ is then $\{\Delta_1\oplus\Delta_2\oplus\Delta_3\}\otimes\Gamma$, where Γ is a unitary irreducible representation of S_2. Under a two particle exchange Γ provides either a bosonic $(+1)$ or a fermionic (-1) phase. Since one of the three rings has been rendered quantum mechanically distinguishable from the other two, one obtains an appropriate two ring statistics. The action of the remaining elements of S_3, namely the cyclic elements, is canonical: They merely permute the carrier spaces $\mathbb{H}_i$ of the Δ_i. This general structure continues to hold for all n, and is illustrative for the case of primary interest here when the slides are nontrivially represented.

Before proceeding to construct a quantum sector exhibiting cyclic statistics for $n\geqslant 3$, let us consider the simplest case with the slides nontrivially represented, namely when $n=2$. For $n=2$, the slide subgroup is generated by the two slides s_1,s_2, the flip subgroup $\mathcal{F}$ by the two flips f_1,f_2 and the permutation group S_2 by the exchange $\mathcal{E}$. The following example demonstrates a peculiar feature which will reappear for $n>2$, whereby slides render a pair of ''locally identical'' rings distinguishable. Let us start with the abelian unitary irreducible representation of $\mathcal{S}$, $\Omega_1(s_1)=1,\Omega_1(s_2)=-1$. The action of f_j on Ω_1 is $\Omega_1(s_i)\rightarrow\tilde{\Omega}_1(s_i)=\Omega_1(f_j s_i f_j^{-1})=\Omega_1(s_i)$ and is hence contained in the little group $\mathcal{R}$ of $\tilde{\mathrm{G}}$. Under the action of $\mathcal{E}$, $\Omega_1(s_i)\rightarrow\tilde{\Omega}_1(s_i)=\Omega_1(\mathcal{E}s_i\mathcal{E}^{-1})=\Omega_1(s_j)\neq\Omega_1(s_i)$ where $j\neq i$, so that $S_2\subseteq\mathcal{R}$. Thus, the two rings are quantum mechanically distinguishable even if $\mathcal{F}$ is trivially represented. This is very unusual, since indistinguishability of a collection of objects is often thought of as a local, intrinsic property of each object. However, in this representation, it is the nonlocal action of slides which renders the two rings distinguishable: The rings slide through each other differently. Thus, there exists a wave function ψ localized along the fibre of a configuration of two well-separated identical rings such that under the action of s_1, $\psi\rightarrow\psi$ and under that of s_2, $\psi\rightarrow-\psi$. This quantum lifting of indistinguishability by slides is key to the existence of nonpermutation group statistics for $n>2$.

We are now ready to demonstrate cyclic statistics for the case of $n=3$ rings. The slide subgroup $\mathcal{S}$ is generated by the six generators s_{ij}, $i,j=1,2,3$, $i\neq j$, the flip subgroup $\mathcal{F}$ is generated by the 3 elements f_1,f_2,f_3, and the permutations form the nonabelian subgroup S_3. We start with the following abelian unitary irreducible representation Ω_1 of $\mathcal{S}$:

$$\Omega_1(s_{12})=\Omega_1(s_{23})=\Omega_1(s_{31})=-1,\quad \Omega_1(s_{21})=\Omega_1(s_{32})=\Omega_1(s_{13})=1. \tag{9}$$

Consider the action of $\tilde{\mathrm{G}}$ on Ω_1. The action of a flip f_k on Ω_1 for $k=i$ or j is: $\Omega_1(s_{ij})\rightarrow\Omega_1(f_k s_{ij} f_k^{-1})=\Omega_1^{-1}(s_{ij})=\Omega_1(s_{ij})$, while the action of f_k, $k\neq i,j$ is trivial. Thus, $\mathcal{F}$ lies in the stability subgroup of $\tilde{\mathrm{G}}$. Single exchanges e_i however, do not leave Ω_1 invariant: For example, $\Omega_1(s_{i(i+1)})\rightarrow\Omega_1(e_i s_{i(i+1)}e_i^{-1})=\Omega_1(s_{(i+1)i})=-\Omega_1(s_{i(i+1)})$ (where $(i+1)$ is defined mod 3). However, a pair of exchanges does leave Ω_1 invariant! A pair of exchanges, say $z=e_2e_3$, generates the cyclic subgroup Z_3 of S_3. Under the action of e_2e_3 the slides $\{s_{12},s_{23},s_{31}\}\rightarrow\{s_{23},s_{31},s_{12}\}$, and $\{s_{21},s_{32},s_{13}\}\rightarrow\{s_{32},s_{13},s_{21}\}$, thus leaving Ω_1 invariant. Therefore, the stability subgroup associated to Ω_1 is $\mathcal{F}\ltimes\mathbb{Z}_3$. The remaining elements of $\mathcal{F}\ltimes S_3$, namely e_1,e_2, and e_3 generate the two element orbit $\mathcal{O}\equiv\{\Omega_1,\Omega_2\}$ in $\hat{\mathcal{S}}$ the space of unitary irreducible representations of $\mathcal{S}$, where

$$\Omega_2(s_{12})=\Omega_2(s_{23})=\Omega_2(s_{31})=1,\quad \Omega_2(s_{21})=\Omega_2(s_{32})=\Omega_2(s_{13})=-1. \tag{10}$$

The associated unitary irreducible representation of $\mathcal{G}$ is therefore nonabelian, and can be symbolically expressed as

$$(\Omega_1\oplus\Omega_2)\otimes\mathcal{T}, \tag{11}$$

where $\mathcal{T}$ is a unitary irreducible representation of the stability subgroup $\mathcal{F}\ltimes\mathbb{Z}_3$.

Let us for simplicity consider the case when $\mathcal{F}$ is trivially represented in $\mathcal{T}$, so that $\mathcal{T}$ is a unitary irreducible representation of $\mathbb{Z}_3$. $\mathbb{Z}_3$ has two nontrivial inequivalent unitary irreducible

representations (a) $z \to e^{2\pi i/3}$ and (b) $z \to e^{4\pi i/3}$. Thus, wave functions ψ_a, ψ_b on $\tilde{\mathcal{Q}}_3$ take values in the (two-dimensional) carrier spaces $\mathbb{H}_a$ and $\mathbb{H}_b$ of the corresponding quantum sectors. If $\psi_{a,b}$ are localized along the fibre of a configuration of well separated identical rings, under the action of the cyclic permutations they pick up the respective phases $\psi_a \to e^{2\pi i/3}\psi_a$ and $\psi_b \to e^{4\pi i/3}\psi_b$. Thus, these sectors exhibit a cyclic, nonpermutation group, statistics: the rings are identical *only* when permuted by a cyclic combination, and *not* under pair-wise exchange! This is indeed a very curious behavior and is again linked to the nonlocality of slide motions: even though the flips are all trivially represented the slides render the rings pair-wise distinguishable but cyclically indistinguishable. We say that the rings obey $\mathbb{Z}_3$ *cyclic statistics*.

The case for arbitrary $n>2$ follows in a straightforward manner. Namely, we can always isolate a pair of nontrivial subsets from the set of slide generators $\{s_A\}$ and $\{s_B\}$ which are invariant under $\mathbb{Z}_n$. There is a small difference in the construction in the even $n=2m$ and odd $n=2m+1$ cases. For $n=2m$, $\mathbb{Z}_{2m}$ contains the subgroup $\mathbb{Z}_2$; if z is the generator of $\mathbb{Z}_{2m}$ with $z^{2m}=e$, then z^m generates a $\mathbb{Z}_2$ subgroup corresponding to m commuting exchanges. One can then see that the two sets of generators $\{s_A\}$ and $\{s_B\}$ which are invariant under $\mathbb{Z}_{2m}$ have cardinality $2m(m-1)$ and $2m^2$, respectively. For $n=2m+1$, Z_2 is not a subgroup of $\mathbb{Z}_{2m+1}$. Hence the two sets of generators $\{s_A\}$ and $\{s_B\}$ each have cardinality $m(2m+1)$. One can thus obtain $\mathbb{Z}_n$ cyclic statistics for arbitrary $n>2$.

We end this section by commenting on the possibility that sectors with more complicated nonpermutation group statistics may exist. To construct the above cyclic statistics sectors we started with very simple abelian unitary irreducible representations of the slide subgroup. It is conceivable that if one instead started with a nonabelian unitary irreducible representation of $\mathcal{S}$ (with certain symmetries) that the stability subgroup $\mathcal{F}\ltimes K$ associated with it is such that K is nonabelian and a nonpermutation subgroup of S_n. Such a sector would then exhibit a *nonabelian, nonpermutation* group statistics. Our current work provides a framework in which to probe such questions.

IV. REMARKS

Anyonic statistics in $2+1$ dimensions can be modeled by adding a Chern Simon's term to the n particle Lagrangian.[17] In Ref. 10 a stringy generalization of this was developed to obtain nontrivial phases from the action of the motion group, namely a $B\wedge F$ topological term made up of an abelian gauge field and an axion field was added to the n string Lagrangian along with an interaction term. Similar systems have subsequently been studied in Ref. 18. In Ref. 10 it was shown that even though the statistical phases are trivial (i.e., bosonic) the action of the slide subgroup is nontrivial, giving rise to fractional quantum phases. Since slides involve the motion of one ring through a nontrivial generator of the fundamental group of another ring, these fractional phases correspond to Aharnov–Bohm phases rather than to fractional quantum statistics. Indeed, slides can occur between nonidentical particles as well and hence the interpretation of such phases as statistics in Ref. 18 seems questionable. Since cyclic statistics occur in nonabelian sectors of the system, it would be interesting to construct appropriate nonabelian generalizations of Ref. 10 which exhibit this behavior. We leave this problem to future investigations.

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Position and momentum observables on $\mathbb{R}$ and on $\mathbb{R}^3$

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We characterize all position and momentum observables on $\mathbb{R}$ and on $\mathbb{R}^3$. We study some of their operational properties and discuss their covariant joint observables.
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I. INTRODUCTION

In the traditional presentation of quantum mechanics, observables are represented by self-adjoint operators or, equivalently, by spectral measures. It is widely recognized that this concept is too narrow. Indeed, spectral measures correspond to measurements with perfect accuracy, never found in real experiments. A less restrictive mathematical formulation of a quantum mechanical observable is a normalized positive operator measure. This generalization allows one, among many other things, to describe measurements with limited accuracy. (For a review of positive operator measures in quantum mechanics, see Refs. 4, 10, 15.)

In this paper we take covariance and invariance with respect to suitable symmetry groups as the defining properties of an observable. For example, a position observable on $\mathbb{R}$ is defined to be an observable which is covariant under space translations and invariant under momentum boosts. We characterize all position and momentum observables on $\mathbb{R}$ and on $\mathbb{R}^3$.

In Sec. II we study position and momentum observables on $\mathbb{R}$. In Sec. II A the definitions are given and in Sec. II B we characterize the structure of position and momentum observables. In Sec. II C we investigate the ability of a position observable to discriminate states, that is, the state distinction power. Another relevant property, the limit of resolution, is studied in Sec. II D. In Sec. II E we consider a covariant joint observable of position and momentum in phase space and derive a lower bound for the product of their limits of resolution. Section III is devoted to studying position and momentum observables in $\mathbb{R}^3$. The corresponding definitions are formulated in Sec. III A, and a complete classification of position and momentum observables in $\mathbb{R}^3$ is given in Sec. III B.

Concluding this section we fix some notations. Let $\mathcal{H}$ be a complex separable Hilbert space and $\mathcal{L}(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$. A positive operator $T \in \mathcal{L}(\mathcal{H})$ of trace one is called a *state* and the set of all states is denoted by $\mathcal{S}(\mathcal{H})$. A positive operator A bounded from above by the unit operator I is called an *effect* and the set of all effects is denoted by $\mathcal{E}(\mathcal{H})$. We say that the null operator O and the unit operator I are *trivial effects*. Let Ω be a nonempty set and $\mathcal{A}$ a σ-algebra of subsets of Ω. A set function $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ is an *operator measure*, if it is σ-additive with respect to the strong (or Ref. 12, p. 318, equivalently, weak) operator topology.

We call an operator valued measure E an *observable* if $E(X) \in \mathcal{E}(\mathcal{H})$ for all $X \in \mathcal{A}$ and

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$E(\Omega)=I$. If an observable E has projections as its values, that is, $E(X)^*=E(X)=E(X)^2$ for all $X\in\mathcal{A}$, it is called a *sharp observable*. For an observable $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ and a state $T\in\mathcal{S}(\mathcal{H})$, we let p_T^E denote the probability measure on Ω defined by

$$p_T^E(X)=\mathrm{tr}[TE(X)],\quad X\in\mathcal{A}.$$

The number $p_T^E(X)$ is interpreted as the probability of having an outcome in X when the system is in the state T and the observable E is measured.

We denote by $\mathcal{B}(\mathbb{R}^n)$ the Borel σ-algebra of $\mathbb{R}^n$. The Fourier transform of any $f\in L^1(\mathbb{R}^n)$ is denoted by $\hat{f}$. We set also $\hat{f}=\mathcal{F}(f)$ to denote the Fourier–Plancherel transform of any $f\in L^2(\mathbb{R}^n)$ and $\hat{\mu}=\mathcal{F}(\mu)$ is the Fourier–Stieltjes transform of any complex Borel measure μ on $\mathbb{R}^n$.

II. POSITION AND MOMENTUM OBSERVABLES ON $\mathbb{R}$

A. Definitions

Let us consider a nonrelativistic particle living in the one-dimensional space $\mathbb{R}$ and fix $\mathcal{H}=L^2(\mathbb{R})$. Let U and V be the one-parameter unitary representations on $\mathcal{H}$ related to the groups of space translations and momentum boosts. They act on $\varphi\in\mathcal{H}$ as

$$[U(q)\varphi](x)=\varphi(x-q),$$

$$[V(p)\varphi](x)=e^{ipx}\varphi(x).$$

Let P and Q be the self-adjoint operators generating U and V, that is, $U(q)=e^{-iqP}$ and $V(p)=e^{ipQ}$ for every $q,p\in\mathbb{R}$. We denote by Π_P and Π_Q the spectral decompositions of the operators P and Q, respectively. They have the form

$$[\Pi_Q(X)\varphi](x)=\chi_X(x)\varphi(x),$$

$$\Pi_P(X)=\mathcal{F}^{-1}\Pi_Q(X)\mathcal{F}.$$

The sharp observable Π_Q has the property that, for all $q,p\in\mathbb{R}$ and $X\in\mathcal{B}(\mathbb{R})$,

$$U(q)\Pi_Q(X)U(q)^*=\Pi_Q(X+q), \tag{1}$$

$$V(p)\Pi_Q(X)V(p)^*=\Pi_Q(X). \tag{2}$$

Equation (1) means that Π_Q is covariant under translations, whereas (2) shows that Π_Q is invariant under momentum boosts. Hence, these relations suggest to call Π_Q a position observable. As the kinematical meaning of the observable Π_Q is solely in the relations (1) and (2), we take these symmetry properties as the definition of a general position observable. The observable Π_Q is called the *canonical position observable*.

Definition 1: An observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is a *position observable on* $\mathbb{R}$ if, for all $q,p\in\mathbb{R}$ and $X\in\mathcal{B}(\mathbb{R})$,

$$U(q)E(X)U(q)^*=E(X+q), \tag{3}$$

$$V(p)E(X)V(p)^*=E(X). \tag{4}$$

We will denote by $\mathcal{POS}_{\mathbb{R}}$ the set of all position observables on $\mathbb{R}$.

In an analogous way we define a momentum observable to be an observable which is covariant under momentum boosts and invariant under translations.

Definition 2: An observable $F:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is a *momentum observable on* $\mathbb{R}$ if, for all $q,p\in\mathbb{R}$ and $X\in\mathcal{B}(\mathbb{R})$,

$$U(q)F(X)U(q)^*=F(X), \tag{5}$$

$$V(p)F(X)V(p)^*=F(X+p). \tag{6}$$

Since $\mathcal{F}U(q)=V(-q)\mathcal{F}$ and $\mathcal{F}V(p)=U(p)\mathcal{F}$, the sharp observable $\Pi_P=\mathcal{F}^{-1}\Pi_Q\mathcal{F}$ satisfies (5) and (6). It is called the *canonical momentum observable*. Moreover, an observable E is a position observable if and only if $\mathcal{F}^{-1}E\mathcal{F}$ is a momentum observable. Therefore, in the following we will restrict ourselves to the study of position observables, the results of Secs. II B, II C, and II D being easily converted to the case of momentum observables.

Remark 1: In some articles an observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ satisfying the covariance condition (1) (and not necessarily the invariance condition (2)) is called a (generalized) position observable. In this paper we say that such an observable is a *localization observable*. These are characterized in Refs. 7 and 16. In Sec. II B it is shown, especially, that every position observable is commutative. However, there exist noncommutative localization observables. Hence, the set $\mathcal{POS}_{\mathbb{R}}$ is a proper subset of all localization observables.

B. The structure of position observables

Let $\rho:\mathcal{B}(\mathbb{R})\to[0,1]$ be a probability measure. For any $X\in\mathcal{B}(\mathbb{R})$, the map $q\mapsto\rho(X-q)$ is bounded and measurable, and hence the equation

$$E_\rho(X)=\int \rho(X-q)\ \ d\Pi_Q(q) \tag{7}$$

defines a bounded positive operator. The map

$$\mathcal{B}(\mathbb{R})\ni X\mapsto E_\rho(X)\in\mathcal{L}(\mathcal{H})$$

is an observable. It is straightforward to verify that the observable E_ρ satisfies the covariance condition (3) and the invariance condition (4), hence it is a position observable on $\mathbb{R}$. Denote by δ_t the Dirac measure concentrated at t. The observable E_{δ_0} is the canonical position observable Π_Q. We may also write

$$\Pi_Q(X)=\int \delta_0(X-q)\ \ d\Pi_Q(q) \tag{8}$$

and comparing (7) to (8) we note that E_ρ is obtained when the sharply concentrated Dirac measure δ_0 is replaced by the probability measure ρ. The observable E_ρ admits an interpretation as an imprecise, or fuzzy, version of the canonical position observable Π_Q. (See Refs. 1–3 for further details.)

Proposition 1: Any position observable E on $\mathbb{R}$ is of the form $E=E_\rho$ for some probability measure $\rho:\mathcal{B}(\mathbb{R})\to[0,1]$.

The proof of Proposition 1 is given in Appendix A.

Besides covariance (1) and invariance (2), the canonical position observable Π_Q has still more symmetry properties. Namely, let $\mathbb{R}_+$ be the set of positive real numbers regarded as a multiplicative group. It has a family of unitary representations $\{A_t|t\in\mathbb{R}\}$ acting on $\mathcal{H}$, and given by

$$[A_t(a)f](x)=\frac{1}{\sqrt{a}}f(a^{-1}(x-t)+t).$$

It is a direct calculation to verify that for all $a\in\mathbb{R}_+$, $X\in\mathcal{B}(\mathbb{R})$,

$$A_0(a)\Pi_Q(X)A_0(a)^*=\Pi_Q(aX).$$

We adopt the following terminology.

Definition 3: We say that an observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is *covariant under dilations* if there exists a unitary representation A of $\mathbb{R}_+$ such that for all $a\in\mathbb{R}_+$ and $X\in\mathcal{B}(\mathbb{R})$,

$$A(a)E(X)A(a)^*=E(aX). \tag{9}$$

The canonical position observable Π_Q is not the only position observable which is covariant under dilations. An observable $E_{\delta_t}, t\in\mathbb{R}$, is a translated version of Π_Q, namely, for any $X\in\mathcal{B}(\mathbb{R})$,

$$E_{\delta_t}(X)=\Pi_Q(X-t)=U(t)^*\Pi_Q(X)U(t).$$

Since $A_{-t}(a)=U(t)^*A_0(a)U(t)$, the observable E_{δ_t} is covariant under dilations, with, for example, $A=A_{-t}$.

Proposition 2: Let E be a position observable on $\mathbb{R}$. The following conditions are equivalent:

(a) *E is covariant under dilations;*
(b) *$\|E(U)\|=1$ for every nonempty open set $U\subset\mathbb{R}$;*
(c) *$E=E_{\delta_t}$ for some $t\in\mathbb{R}$;*
(d) *E is a sharp observable.*

Proof: Let E be covariant under dilations. In a similar way as in Ref. 8, Lemma 3, it can be shown that $\|E(U)\|=1$ for all nonempty open sets U, and so, (a) implies (b). Assume then that (b) holds. For any nonempty open set U we get

$$1=\|E(U)\|=\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(x+U). \tag{10}$$

It follows that $\operatorname{supp}(\rho)$ contains only one point. Indeed, assume on the contrary that $\operatorname{supp}(\rho)$ contains two points $x_1\neq x_2$ and denote $U=\{x\in\mathbb{R}\,|\,|x|<\frac{1}{4}|x_1-x_2|\}$. Since x_1+U and x_2+U are neighborhoods of x_1 and x_2, respectively, we have $m_i:=\rho(x_i+U)>0$ for $i=1,2$. Then, for any $x\in\mathbb{R}$, $\rho(x+U)\leqslant 1-\min(m_1,m_2)$. This is in contradiction with (10). Hence, (b) implies (c). As previously mentioned, (c) implies (a). Clearly, (c) also implies (d). Since (d) implies (b) the proof is complete. □

The dilation covariance means that the observable in question has no scale dependence. A realistic position measurement apparatus has a limited accuracy and hence it cannot define a position observable which is covariant under dilations. Thus, sharp position observables are not suitable to describe nonideal situations.

Remark 2: If A is a unitary representation of $\mathbb{R}_+$ satisfying Eq. (9) with $E=E_{\delta_t}$, then there exists a measurable function $\beta:\mathbb{R}\to\mathbb{T}$ ($\mathbb{T}=$ the complex numbers of modulus 1) such that

$$[A(a)f](x)=\frac{1}{\sqrt{a}}\beta(x+t)\overline{\beta(a^{-1}(x+t))}f(a^{-1}(x+t)-t).$$

In particular, A is equivalent to A_{-t}. See Appendix B for more details.

C. State distinction power of a position observable

Definition 4: Let E_1 and E_2 be observables on $\mathbb{R}$. The *state distinction power* of E_2 is greater than or equal to E_1 if for all $T,T'\in\mathcal{S}(\mathcal{H})$,

$$p_T^{E_2}=p_{T'}^{E_2}\Rightarrow p_T^{E_1}=p_{T'}^{E_1}.$$

In this case we denote $E_1\sqsubseteq E_2$. If $E_1\sqsubseteq E_2\sqsubseteq E_1$ we say that E_1 and E_2 are *informationally equivalent* and denote $E_1\sim E_2$. If $E_1\sqsubseteq E_2$ and $E_2\not\sqsubseteq E_1$, we write $E_1\sqsubset E_2$.

Example 1: An observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is *trivial* if $p_T^E=p_{T'}^E$ for all states $T,T'\in\mathcal{S}(\mathcal{H})$. This implies that a trivial observable E is of the form $E(X)=\lambda(X)I, X\in\mathcal{B}(\mathbb{R})$, for some probability measure λ. The state distinction power of any observable E' is greater than or equal to that of the trivial observable E. Clearly there is no trivial position observable on $\mathbb{R}$.

Example 2: An observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is called *informationally complete* if $p_T^E\neq p_{T'}^E$ whenever $T\neq T'$. The state distinction power of an informationally complete observable is greater than or equal to that of any other observable E_1 on $\mathbb{R}$. It is easy to see that there is no informationally complete position observable. Namely, let ψ be a unit vector, $p\neq 0$ a real number, and denote $\psi'=V(p)\psi$. Then the states $T=|\psi\rangle\langle\psi|$ and $T'=|\psi'\rangle\langle\psi'|$ are different but for any position observable E_ρ, $p_T^{E_\rho}=p_{T'}^{E_\rho}$ since $V(p)$ commutes with all the effects $E_\rho(X), X\in\mathcal{B}(\mathbb{R})$.

We will next think of $\sim$ as a relation on the set $\mathcal{POS}_\mathbb{R}$. The relation $\sim$ is clearly reflexive, symmetric and transitive, and hence it is an equivalence relation. We denote the equivalence class of a position observable E by $[E]$ and the space of equivalence classes as $\mathcal{POS}_\mathbb{R}/\sim$. The relation $\sqsubseteq$ induces a partial order in the set $\mathcal{POS}_\mathbb{R}/\sim$ in a natural way.

Let E_ρ be a position observable and T a state. The probability measure $p_T^{E_\rho}$ is the convolution of the probability measures $p_T^{\Pi_Q}$ and ρ,

$$p_T^{E_\rho}=p_T^{\Pi_Q}*\rho. \tag{11}$$

It is clear from (11) that for all $T,T'\in\mathcal{S}(\mathcal{H})$,

$$p_T^{\Pi_Q}=p_{T'}^{\Pi_Q}\Rightarrow p_T^{E_\rho}=p_{T'}^{E_\rho},$$

and hence $E_\rho\sqsubseteq\Pi_Q$. We conclude that $[\Pi_Q]$ is the only maximal element of the partially ordered set $\mathcal{POS}_\mathbb{R}/\sim$.

It is shown in Ref. 14, Proposition 5, that a position observable E_ρ belongs to the maximal equivalence class $[\Pi_Q]$ if and only if $\mathrm{supp}(\hat{\rho})=\mathbb{R}$. The following proposition characterizes the equivalence classes completely.

Proposition 3: Let ρ_1,ρ_2 be probability measures on $\mathbb{R}$ and E_{ρ_1},E_{ρ_2} the corresponding position observables. Then

$$E_{\rho_1}\sqsubseteq E_{\rho_2}\Leftrightarrow\mathrm{supp}(\hat{\rho}_1)\subseteq\mathrm{supp}(\hat{\rho}_2). \tag{12}$$

Proof: Taking the Fourier transform of Eq. (11), we get

$$\mathcal{F}(p_T^{E_\rho})=\mathcal{F}(p_T^{\Pi_Q})\mathcal{F}(\rho). \tag{13}$$

Since the Fourier transform is injective, it is clear from the above relation that $\mathrm{supp}(\hat{\rho}_1)\subseteq\mathrm{supp}(\hat{\rho}_2)$ implies $E_{\rho_1}\sqsubseteq E_{\rho_2}$.

Conversely, suppose $\mathrm{supp}(\hat{\rho}_1)\nsubseteq\mathrm{supp}\,(\hat{\rho}_2)$. As $\hat{\rho}_i$, $i=1,2$, are continuous functions and $\hat{\rho}_i(\xi)=\overline{\hat{\rho}_i(-\xi)}$, there exists a closed interval $[2a,2b]$, with $0\leqslant a<b$, such that $[2a,2b]\cup[-2b,-2a]\subseteq\mathrm{supp}\,(\widehat{\rho}_1)$ and $([2a,2b]\cup[-2b,-2a])\cap\mathrm{supp}(\hat{\rho}_2)=\varnothing$. Define the functions

$$h_1=\frac{1}{\sqrt{2(b-a)}}(\chi_{[a,b]}-\chi_{[-b,-a]}),$$

$$h_2=\frac{1}{\sqrt{2(b-a)}}(\chi_{[a,b]}+\chi_{[-b,-a]}),$$

and for $i=1,2$, denote

$$h_i^*(\xi) := \overline{h_i(-\xi)}.$$

Define

$$f_i = \mathcal{F}^{-1}(h_i),$$

and let T_i be the one-dimensional projection $|f_i\rangle\langle f_i|$. We then have

$$dp^{\Pi_Q}_{T_i}(x) = |f_i(x)|^2 dx = |(\mathcal{F}^{-1}h_i)(x)|^2 dx = \mathcal{F}^{-1}(h_i * h_i^*)(x)dx,$$

and

$$\begin{aligned}\mathcal{F}(p^{\Pi_Q}_{T_i}) &= \mathcal{F}\mathcal{F}^{-1}(h_i * h_i^*) \\ &= h_i * h_i^* \\ &= \frac{1}{2(b-a)}(2\chi_{[a,b]} * \chi_{[-b,-a]} + (-1)^i \chi_{[-b,-a]} * \chi_{[-b,-a]} + (-1)^i \chi_{[a,b]} * \chi_{[a,b]}).\end{aligned}$$

Since

$$\operatorname{supp}(\chi_{[a,b]} * \chi_{[-b,-a]}) = [a-b, b-a],$$

$$\operatorname{supp}(\chi_{[a,b]} * \chi_{[a,b]}) = [2a, 2b],$$

$$\operatorname{supp}(\chi_{[-b,-a]} * \chi_{[-b,-a]}) = [-2b, -2a],$$

an application of (13) shows that

$$\mathcal{F}(p^{E_{\rho_1}}_{T_1}) \neq \mathcal{F}(p^{E_{\rho_1}}_{T_2}),$$

$$\mathcal{F}(p^{E_{\rho_2}}_{T_1}) = \mathcal{F}(p^{E_{\rho_2}}_{T_2}),$$

or in other words, $E_{\rho_1} \not\sqsubseteq E_{\rho_2}$. □

Remark 3: It follows from the above proposition that $E_1 \sqsubset E_2 \Leftrightarrow \operatorname{supp}(\hat{\rho}_1) \subset \operatorname{supp}(\hat{\rho}_2)$, and hence the set $\mathcal{POS}_{\mathbb{R}}/\sim$ has no minimal element. Indeed, if ρ_2 is a probability measure, there always exists a probability measure ρ_1 such that $\operatorname{supp}(\hat{\rho}_1) \subset \operatorname{supp}(\hat{\rho}_2)$. In fact, since $\hat{\rho}_2$ is continuous, $\hat{\rho}_2(\xi) = \overline{\hat{\rho}_2(-\xi)}$ and $\hat{\rho}_2(0) = \rho_2(\mathbb{R}) \neq 0$, there exists $a > 0$ such that the closed interval $[-a, a]$ is strictly contained in $\operatorname{supp}(\hat{\rho}_2)$. If we define $h = (1/\sqrt{a})\,\chi_{[-(a/2),(a/2)]}$, $f = \mathcal{F}^{-1}h$, then $d\rho_1(x) := |f(x)|^2 dx$ is a probability measure, and $\operatorname{supp}(\hat{\rho}_1) = \operatorname{supp}(h * h) = [-a, a]$.

D. Limit of resolution of a position observable

Let $\Pi : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ be a sharp observable. For any nontrivial projection $\Pi(X)$, there exist states $T, T' \in \mathcal{S}(\mathcal{H})$ such that $p^{\Pi}_T(X) = 1$ and $p^{\Pi}_{T'}(X) = 0$. We may say that $\Pi(X)$ is a *sharp property* and it is *real* in the state T.

In general, an observable E has effects as its values which are not projections and, hence, not sharp properties. An effect $B \in \mathcal{E}(\mathcal{H})$ is called *regular* if its spectrum extends both above and below $\frac{1}{2}$. This means that there exist states $T, T' \in \mathcal{S}(\mathcal{H})$ such that $\operatorname{tr}[TB] > \frac{1}{2}$ and $\operatorname{tr}[T'B] < \frac{1}{2}$. In this sense regular effects can be seen as *approximately realizable properties*, see Ref. 4, Sec. II.2.1. The observable E is called regular if all the nontrivial effects $E(X)$ are regular.

It is shown in Ref. 14, Proposition 4 that if a probability measure ρ is absolutely continuous with respect to the Lebesgue measure, then the position observable E_ρ is not regular. Here we modify the notion of regularity to get a quantification of sharpness, or resolution, of position observables.

For any $x\in\mathbb{R}, r\in\mathbb{R}_+$, we denote the interval $[x-(r/2), x+(r/2)]$ by $I_{x;r}$. We also denote $I_r=I_{0;r}$. Let $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ be an observable and $\alpha>0$. We say that E is *α-regular* if all the nontrivial effects $E(I_{x;r})$, $x\in\mathbb{R}$, $r\geqslant\alpha$, are regular.

Definition 5: Let $E:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ be an observable. We denote

$$\gamma_E=\inf\{\alpha>0|E \text{ is } \alpha\text{-regular}\}$$

and say that γ_E is the *limit of resolution of E*.

It follows directly from definitions that the limit of resolution of a regular observable is 0. Especially, the limit of resolution of canonical position observables is 0.

Example 3: Let E be a trivial observable (see Example 1). For any $X\in\mathcal{B}(\mathbb{R})$, we have either $E(X)\geqslant\frac{1}{2}I$ or $E(X)\leqslant\frac{1}{2}I$. Hence, $\gamma_E=\infty$.

Proposition 4: A position observable E_ρ is α-regular if and only if

$$\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(I_{x,\alpha})>\tfrac{1}{2}. \tag{14}$$

Proof: An effect $E_\rho(X)$ is regular if and only if $\|E_\rho(X)\|>\frac{1}{2}$ and $\|E_\rho(\mathbb{R}\backslash X)\|>\frac{1}{2}$. Since the norm of the multiplicative operator $E_\rho(X)$ is $\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(X-x)$, we conclude that $E_\rho(X)$ is regular if and only if

$$\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(X-x)>\tfrac{1}{2} \quad\text{and}\quad \operatorname{ess\,inf}_{x\in\mathbb{R}}\rho(X-x)<\tfrac{1}{2}.$$

Thus, E_ρ is α-regular if and only if, for all $r\geqslant\alpha$,

$$\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(I_{x;r})>\tfrac{1}{2} \quad\text{and}\quad \operatorname{ess\,inf}_{x\in\mathbb{R}}\rho(I_{x;r})<\tfrac{1}{2}.$$

The second condition is always satisfied and the first is equivalent to (14). □

Corollary 1: A position observable E_ρ has a finite limit of resolution and

$$\gamma_{E_\rho}=\inf\{\alpha>0|\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(I_{x;\alpha})>\tfrac{1}{2}\}. \tag{15}$$

Example 4: Let us consider the case in which the probability measure has Gaussian distribution, that is,

$$d\rho(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-[(x-\bar{x})^2/2\sigma^2]}dx.$$

By Proposition 4 the position observable E_ρ is α-regular if, for each $r\geqslant\alpha$,

$$\frac{1}{2}<\int_{I_{\bar{x};r}}\frac{1}{\sigma\sqrt{2\pi}}e^{-[(x-\bar{x})^2/2\sigma^2]}dx=\frac{1}{\sqrt{2\pi}}\int_{-r/2\sigma}^{r/2\sigma}e^{-(x^2/2)}dx.$$

It follows that the limit of resolution γ_{E_ρ} is proportional to the standard deviation σ and $\gamma_{E_\rho}\approx 1.36\sigma$.

E. Covariant joint observables of position and momentum observables

Let $E_1, E_2:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ be two observables. An observable $G:\mathcal{B}(\mathbb{R}^2)\to\mathcal{L}(\mathcal{H})$ is their *joint observable* if for all $X,Y\in\mathcal{B}(\mathbb{R})$,

$$E_1(X)=G(X\times\mathbb{R}),$$

$$E_2(Y)=G(\mathbb{R}\times Y).$$

In this case E_1 and E_2 are the *margins* of G.

For all $(q,p)\in\mathbb{R}^2$, we denote

$$W(q,p)=e^{-iqP+ipQ}=e^{iqp/2}U(q)V(p).$$

The mapping $W:(q,p)\mapsto W(q,p)$ is an irreducible projective representation of the phase space translation group $\mathbb{R}^2$ in $\mathcal{H}$. An observable $G:\mathcal{B}(\mathbb{R}^2)\to\mathcal{L}(\mathcal{H})$ is called a *covariant phase space observable* if for all $(q,p)\in\mathbb{R}^2$ and $Z\in\mathcal{B}(\mathbb{R}^2)$,

$$W(q,p)G(Z)W(q,p)^*=G(Z+(q,p)).$$

It is proved in Ref. 6, Sec. III A that all covariant phase space observables are of the form

$$G_T(Z)=\frac{1}{2\pi}\int_Z W(q,p)TW(q,p)^*\ dqdp \tag{16}$$

for some $T\in\mathcal{S}(\mathcal{H})$.

The margins of a covariant phase space observable G_T are position and momentum observables. Indeed, let $\Sigma_i\lambda_i|\varphi_i\rangle\langle\varphi_i|$ be the spectral decomposition of T. A straightforward calculation shows that

$$G_T(X\times\mathbb{R})=\int \rho(X-q)\ d\Pi_Q(q)=E_\rho(X), \tag{17}$$

where $d\rho(q)=e(q)dq$ and $e(q)=\Sigma_i\lambda_i|\varphi_i(-q)|^2$. Similarly,

$$G_T(\mathbb{R}\times Y)=\int \nu(Y-p)\ d\Pi_P(p)=F_\nu(Y), \tag{18}$$

where $d\nu(p)=f(p)dp$ and $f(p)=\Sigma_i\lambda_i|\hat{\varphi}_i(-p)|^2$.

The following proposition is a direct consequence of the previously mentioned results.

Proposition 5: A position observable E_ρ [a momentum observable F_ν] is a margin of a phase space observable if and only if the probability measure ρ [prob. measure ν] is absolutely continuous with respect to the Lebesgue measure.

As noted in Example 4, the limit of resolution of a position observable E_ρ with ρ having Gaussian distribution is proportional to the standard deviation σ of ρ. This shows, in particular, that there exists a position observable which is a margin of a phase space observable and which has an arbitrary small positive limit of resolution. However, we next show that if position and momentum observables have a covariant phase space observable as their joint observable, then the product of limit of resolutions has a lower bound.

Proposition 6: Let E_ρ be a position observable and F_ν a momentum observable. If E_ρ and F_ν have a covariant phase space observable as their joint observable, then

$$\gamma_{E_\rho}\cdot\gamma_{F_\nu}\geqslant 3-2\sqrt{2}. \tag{19}$$

Proof: Since E_ρ and F_ν have a covariant phase space observable as a joint observable there is a vector valued function $\theta\in L^2(\mathbb{R},\mathcal{H})$ such that $d\rho(q)=\|\theta(q)\|^2_{\mathcal{H}}dq$ and $d\nu(p)=\|\hat{\theta}(p)\|^2_{\mathcal{H}}dp$.

By Proposition 4 the observable E_ρ is α-regular if and only if

$$\operatorname{ess\,sup}_{x\in\mathbb{R}}\rho(I_{x;\alpha})>1/2.$$

Since the map $x\mapsto\rho(I_{x;\alpha})$ is continuous, this is equivalent to

$$\sup_{x\in\mathbb{R}}\rho(I_{x;\alpha})=\sup_{x\in\mathbb{R}}\int_{I_{x;\alpha}}\|\theta(x)\|_{\mathcal{H}}^2 dx>1/2.$$

By the same argument, F_ν is β-regular if and only if

$$\sup_{\xi\in\mathbb{R}}\nu(I_{\xi;\beta})=\sup_{\xi\in\mathbb{R}}\int_{I_{\xi;\beta}}\|\hat{\theta}(\xi)\|_{\mathcal{H}}^2 d\xi>1/2.$$

Using Ref. 11, Theorem 2 extended to the case of vector valued functions, we find

$$\alpha\cdot\beta\geqslant 3-2\sqrt{2},$$

and hence (19) follows. □

III. POSITION AND MOMENTUM OBSERVABLES ON $\mathbb{R}^3$

A. Definitions

In this section $\mathcal{H}=L^2(\mathbb{R}^3)$. Let $Q_i, i=1,2,3$, denote the multiplication operator on $\mathcal{H}$ given by $[Q_i f](\mathbf{x})=x_i f(\mathbf{x})$, where x_i is the ith component of $\mathbf{x}$. By P_i we mean the operator $\mathcal{F}^{-1}Q_i\mathcal{F}$ and we denote $\mathbf{Q}=(Q_1,Q_2,Q_3)$, $\mathbf{P}=(P_1,P_2,P_3)$. The space translation group $\mathbb{R}^3$ has a unitary representation $U(\mathbf{q})=e^{-i\mathbf{q}\cdot\mathbf{P}}$ and similarly, the momentum boost group has a representation $V(\mathbf{p})=e^{i\mathbf{p}\cdot\mathbf{Q}}$. It is an immediate observation that the sharp observables $\Pi_{\mathbf{Q}}$ and $\Pi_{\mathbf{P}}$ on $\mathbb{R}^3$, associated with the representations V and U, respectively, satisfy the obvious covariance and invariance conditions, analogous to (3)–(6). Let D be the representation of the rotation group SO(3) in $\mathcal{H}$ defined as

$$[D(R)f](\mathbf{x})=f(R^{-1}\mathbf{x}).$$

It is straightforward to verify that the sharp observables $\Pi_{\mathbf{Q}}$ and $\Pi_{\mathbf{P}}$ are covariant under rotations, that is, for all $R\in\mathrm{SO}(3)$ and $X\in\mathcal{B}(\mathbb{R}^3)$,

$$D(R)\Pi_{\mathbf{Q}}(X)D(R)^*=\Pi_{\mathbf{Q}}(RX),$$

$$D(R)\Pi_{\mathbf{P}}(X)D(R)^*=\Pi_{\mathbf{P}}(RX).$$

These observations motivate the following definitions:

Definition 6: An observable $E:\mathcal{B}(\mathbb{R}^3)\to\mathcal{L}(\mathcal{H})$ is a *position observable on* $\mathbb{R}^3$ if, for all $\mathbf{q},\mathbf{p}\in\mathbb{R}^3$, $R\in\mathrm{SO}(3)$ and $X\in\mathcal{B}(\mathbb{R}^3)$,

$$U(\mathbf{q})E(X)U(\mathbf{q})^*=E(X+\mathbf{q}), \tag{20}$$

$$V(\mathbf{p})E(X)V(\mathbf{p})^*=E(X), \tag{21}$$

$$D(R)E(X)D(R)^*=E(RX). \tag{22}$$

We will denote by $\mathcal{POS}_{\mathbb{R}^3}$ the set of all position observables on $\mathbb{R}^3$.

Definition 7: An observable $F:\mathcal{B}(\mathbb{R}^3)\to\mathcal{L}(\mathcal{H})$ is a *momentum observable on* $\mathbb{R}^3$ if, for all $\mathbf{q},\mathbf{p}\in\mathbb{R}^3$, $R\in\mathrm{SO}(3)$ and $X\in\mathcal{B}(\mathbb{R}^3)$,

$$U(\mathbf{q})F(X)U(\mathbf{q})^*=F(X),$$

$$V(\mathbf{p})F(X)V(\mathbf{p})^*=F(X+\mathbf{p}),$$

$$D(R)F(X)D(R)^*=F(RX).$$

B. Structure of position observables on $\mathbb{R}^3$

We say that a probability measure ρ on $\mathbb{R}^3$ is rotation invariant if for all $X \in \mathcal{B}(\mathbb{R}^3)$ and $R \in \mathrm{SO}(3)$,

$$(R \cdot \rho)(X) := \rho(R^{-1}X) \equiv \rho(X).$$

The set of rotation invariant probability measures on $\mathbb{R}^3$ is denoted by $M(\mathbb{R}^3)^+_{1,\mathrm{inv}}$. Using the isomorphism $\mathbb{R}^3\backslash\{0\} \simeq \mathbb{R}_+ \times S^2$ and the disintegration of measures, the restriction of any measure $\rho \in M(\mathbb{R}^3)^+_{1,\mathrm{inv}}$ to the subset $\mathbb{R}^3\backslash\{0\}$ can be written in the form

$$d\rho|_{\mathbb{R}^3\backslash\{0\}}(\mathbf{r}) = d\rho_{\mathrm{rad}}(r)\, d\rho_{\mathrm{ang}}(\Omega),$$

where ρ_{rad} is a finite measure on $\mathbb{R}_+$ with $\rho_{\mathrm{rad}}(\mathbb{R}_+) = 1 - \rho(\{0\})$, and ρ_{ang} is the SO(3)-invariant measure on the sphere S^2 normalized to 1.

Given a rotation invariant probability measure ρ, the formula

$$E_\rho(X) = \int \rho(X - \mathbf{q})\; d\Pi_{\mathbf{Q}}(\mathbf{q}), \quad X \in \mathcal{B}(\mathbb{R}^3), \tag{23}$$

defines a position observable on $\mathbb{R}^3$.

Proposition 7: Any position observable E on $\mathbb{R}^3$ is of the form $E = E_\rho$ for some $\rho \in M(\mathbb{R}^3)^+_{1,\mathrm{inv}}$.

Proof: It is shown in Appendix A that if E satisfies Eqs. (20), (21), then E is given by Eq. (23) for some probability measure ρ in $\mathbb{R}^3$. If $\varphi \in C_c(\mathbb{R}^3)$, let

$$E(\varphi) = \int_{\mathbb{R}^3} \varphi(\mathbf{x})\, dE(\mathbf{x}).$$

For all $f \in L^2(\mathbb{R}^3)$, define the measure

$$d\mu_f(\mathbf{x}) = |f(\mathbf{x})|^2 d\mathbf{x}.$$

We then have

$$\langle f \,|\, E(\varphi) f \rangle = (\mu_f * \rho)(\varphi).$$

From (22) it then follows

$$(\mu_{D(R)f} * \rho)(\varphi) = (\mu_f * \rho)(R^{-1} \cdot \varphi), \tag{24}$$

where $(R^{-1} \cdot \varphi)(\mathbf{x}) = \varphi(R\mathbf{x})\ \forall \mathbf{x} \in \mathbb{R}^3$. Rewriting explicitly (24), we then find

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} \varphi(\mathbf{x}+\mathbf{y}) |f(R^{-1}\mathbf{x})|^2 d\mathbf{x} d\rho(\mathbf{y}) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} (R^{-1} \cdot \varphi)(\mathbf{x}+\mathbf{y}) |f(\mathbf{x})|^2 d\mathbf{x} d\rho(\mathbf{y}).$$

With some computations, setting $\psi(\mathbf{x}) = (R^{-1} \cdot \varphi)(-\mathbf{x})$, this gives

$$\int_{\mathbb{R}^3} (\psi * |f|^2)(-\mathbf{y}) d(R^{-1} \cdot \rho)(\mathbf{y}) = \int_{\mathbb{R}^3} (\psi * |f|^2)(-\mathbf{y}) d\rho(\mathbf{y}). \tag{25}$$

Letting ψ and f vary in $C_c(\mathbb{R}^3)$, the functions $\psi * |f|^2$ span a dense subset of $C_0(\mathbb{R}^3)$. From Eq. (25), it then follows that $R^{-1} \cdot \rho = \rho$. □

Proposition 8: Let E be a position observable on $\mathbb{R}^3$. The following facts are equivalent:

(a) $\|E(U)\|=1$ *for every nonempty open set* $U\subset\mathbb{R}$*;*
(b) E *is a sharp observable;*
(c) $E=\Pi_{\mathbf{Q}}$.

Proof: It is clear that (c)⇒(b)⇒(a). Hence, it is enough to show that (a) implies (c). As in the proof of Proposition 2, it follows from (a) that $\rho=\delta_{\mathbf{t}}$ for some $\mathbf{t}\in\mathbb{R}^3$. However, the probability measure $\delta_{\mathbf{t}}$ is rotation invariant if and only if $\mathbf{t}=\mathbf{0}$. This means that $E=\Pi_{\mathbf{Q}}$. □

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APPENDIX A: TRANSLATION COVARIANT AND BOOST INVARIANT OBSERVABLES IN DIMENSION *n*

Let $N=\mathbb{R}^{n+1}$ and $H=\mathbb{R}^n$, with the usual structure of additive Abelian groups. Denote with (p,t), $p\in\mathbb{R}^n$, $t\in\mathbb{R}$, an element of N. Let H act on N as

$$\alpha_q(p,t)=(p,t+q\cdot p),\quad q\in H,(p,t)\in N.$$

The Heisenberg group is the semidirect product $G=N\times_{\alpha}H$ (see Ref. 13). We will denote an element $nq\in G$, with $n=(p,t)\in N$ and $q\in H$, as $((p,t),q)$.

Let W be the following irreducible unitary representation of G acting in $L^2(\mathbb{R}^n)$

$$[W((p,t),q)f](x)=e^{-i(t-p\cdot x)}f(x-q).$$

Clearly, $W((0,0),q)=U(q)$, $W((p,0),0)=V(p)$, and $W((0,t),0)=e^{-it}$. The groups H and G/N are naturally identified. With such an identification, the canonical projection $\pi:G\to G/N$ is

$$\pi((p,t),q)=q,$$

and an element $((p,t),q)\in G$ acts on $q_0\in H$ as

$$((p,t),q)[q_0]=\pi(((p,t),q)((0,0),q_0))=q+q_0.$$

An observable E based on $\mathbb{R}^n$ and acting in $L^2(\mathbb{R}^n)$ then satisfies the analogs of Eqs. (3), (4) in dimension n if, and only if, for all $X\in\mathcal{B}(\mathbb{R})$ and $((p,t),q)\in G$,

$$W((p,t),q)E(X)W((p,t),q)^*=E(X+q),\tag{A1}$$

i.e., if and only if E is a W-covariant observable based on G/N. By virtue of the Generalized Imprimitivity Theorem (see Refs. 5 and 9), E is W-covariant if and only if there exists a representation σ of N and an isometry L intertwining W with the induced representation $\mathrm{ind}_N^G(\sigma)$ such that

$$E(X)=L^*P(X)L$$

for all $X\in\mathcal{B}(\mathbb{R}^n)$, where P is the canonical projection valued measure of the induced representation. Since $\mathrm{ind}_N^G(\sigma)\subset\mathrm{ind}_N^G(\sigma')$ (as imprimitivity systems) if $\sigma\subset\sigma'$ (as representations), it is not restrictive to assume that such σ has constant infinite multiplicity, so that there exists a positive Borel measure μ_σ on $\hat{N}=\mathbb{R}^{n+1}$ and an infinite dimensional Hilbert space $\mathcal{H}$ such that σ is the diagonal representation acting in $L^2(\mathbb{R}^{n+1},\mu_\sigma;\mathcal{H})$, i.e.,

$$[\sigma(p,t)\phi](h,k)=e^{ih\cdot p}e^{ikt}\phi(h,k).$$

Denote with $\gamma_{h,k}$, $h\in\mathbb{R}^n$, $k\in\mathbb{R}$ the following character of N:

$$\gamma_{h,k}(p,t)=e^{ih\cdot p}e^{ikt}.$$

The action of H on $\hat{N}$ is given by

$$(q\cdot\gamma_{h,k})(p,t)=\gamma_{h,k}(\alpha_{-q}(p,t))=e^{i(h-kq)\cdot p}e^{ikt},$$

or in other words

$$q\cdot\gamma_{h,k}=\gamma_{h-kq,k}.$$

If $k\neq 0$, the orbit passing through $\gamma_{h,k}$ is

$$\mathcal{O}_{\gamma_{h,k}}=\mathbb{R}^n\times\{k\}$$

and the corresponding stability subgroup is

$$H_{\gamma_{h,k}}=\{0\}.$$

From the Mackey Machine it follows that the representations

$$\rho_{h,k}:=\mathrm{ind}_N^G(\gamma_{h,k})$$

are irreducible if $k\neq 0$, $\rho_{h,k}$ and $\rho_{h',k'}$ are inequivalent if $k\neq k'$ and, fixed $k\neq 0$, $\rho_{h,k}$ and $\rho_{h',k}$ are equivalent.

The representation $\rho:=\mathrm{ind}_N^G(\sigma)$ acts on $L^2(\mathbb{R}^n,dx;L^2(\mathbb{R}^{n+1},\mu_\sigma;\mathcal{H}))$ according to

$$[\rho((p,t),q)f](x)=\sigma(p,t-p\cdot x)f(x-q).$$

Using the fact that σ acts diagonally in $L^2(\mathbb{R}^{n+1},\mu_\sigma;\mathcal{H})$ and the identification $L^2(\mathbb{R}^n,dx;L^2(\mathbb{R}^{n+1},\mu_\sigma;\mathcal{H}))\cong L^2(\mathbb{R}^n\times\mathbb{R}^{n+1},dx\otimes d\mu_\sigma(x);\mathcal{H})$, we find that ρ acts on $L^2(\mathbb{R}^n\times\mathbb{R}^{n+1},dx\otimes d\mu_\sigma(x);\mathcal{H})$ as

$$[\rho((p,t),q)f](x,h,k)=e^{ih\cdot p}e^{ik(t-p\cdot x)}f(x-q,h,k).$$

Write $\mu_\sigma=\mu_{\sigma_1}+\mu_{\sigma_2}$, where $\mu_{\sigma_1}\perp\mu_{\sigma_2}$ and $\mu_{\sigma_2}(\mathcal{O}_{\gamma_{0,-1}})=0$, and let $\sigma=\sigma_1\oplus\sigma_2$ be the corresponding decomposition of σ. We then have

$$\mathrm{ind}_N^G(\sigma)=\mathrm{ind}_N^G(\sigma_1)\oplus\mathrm{ind}_N^G(\sigma_2),$$

where the two representations in the sum are disjoint and the sum is a direct sum of imprimitivity systems. Since $W\simeq\mathrm{ind}_N^G(\gamma_{0,-1})$, it is not restrictive to assume $\sigma=\sigma_1$, i.e., that μ_σ is concentrated in the orbit $\mathcal{O}_{\gamma_{0,-1}}=\mathbb{R}^n\times\{-1\}\cong\mathbb{R}^n$. Let T be the following unitary operator in $L^2(\mathbb{R}^n\times\mathbb{R}^n,dx\otimes d\mu_\sigma(x);\mathcal{H})$:

$$[Tf](x,h)=f(x+h,h).$$

If we define the representation $\hat{\rho}$, given by

$$[\hat{\rho}((p,t),q)f](x,h)=e^{-i(t-p\cdot x)}f(x-q,h),$$

then T intertwines $\hat{\rho}$ with ρ. Since $\hat{\rho}\simeq W\otimes I_{L^2(\mathbb{R}^n,\mu_\sigma;\mathcal{H})}$ and W is irreducible, every isometry intertwining W with $\hat{\rho}$ has the form

$$[\tilde{L}f](x,h)=f(x)\varphi(h) \quad \forall f\in L^2(\mathbb{R}^n)$$

for some $\varphi\in L^2(\mathbb{R}^n,\mu_\sigma;\mathcal{H})$ with $\|\varphi\|_{L^2}=1$. The most general isometry L intertwining W with ρ has then the form $L=T\tilde{L}$ for some choice of φ, and the corresponding observable is given by

$$\begin{aligned}\langle g\,|\,E(X)f\rangle &=\langle g\,|\,L^*P(X)Lf\rangle\\ &=\langle T\tilde{L}g\,|\,P(X)T\tilde{L}f\rangle\\ &=\int_{\mathbb{R}^{2n}}\chi_X(x)f(x+h)\overline{g(x+h)}\langle\varphi(h),\varphi(h)\rangle dx\,d\mu_\sigma(h).\end{aligned}$$

It follows that

$$[E(X)f](x)=f(x)\int_{\mathbb{R}^n}\chi_X(x-h)\|\varphi(h)\|^2 d\mu_\sigma(h)=f(x)\int_{\mathbb{R}^n}\chi_X(x-h)d\mu(h),$$

where $d\mu(h)=\|\varphi(h)\|^2 d\mu_\sigma(h)$ is a probability measure on $\mathbb{R}^n$.

APPENDIX B: SUPPLEMENT TO REMARK 2

Let $A'(a)=U(t)A(a)U(t)^*$. Then, $A'(a)\Pi_Q(X)A'(a)^*=\Pi_Q(aX)$. Denote with Π_Q^+ the restriction of Π_Q to the Borel subsets of $\mathbb{R}_+$. Then, $S_0=(A_0,\Pi_Q^+,L^2(0,+\infty))$ and $S=(A',\Pi_Q^+,L^2(0,+\infty))$ are transitive imprimitivity systems of the group $\mathbb{R}_+$ based on $\mathbb{R}_+$. Using the Mackey Imprimitivity Theorem, there exists a Hilbert space $\mathcal{K}$ such that $S=\mathrm{ind}_{\{1\}}^{\mathbb{R}_+}(I_\mathcal{K})$, where $I_\mathcal{K}$ is the trivial representation of $\{1\}$ acting in $\mathcal{K}$. Since $S_0=\mathrm{ind}_{\{1\}}^{\mathbb{R}_+}(1)$, we have the isomorphism of intertwining operators $\mathcal{C}(1,I_\mathcal{K})\simeq\mathcal{C}(S_0,S)$, and hence there exists an isometry $W_1:L^2(0,+\infty)\to L^2(0,+\infty)$ intertwining S_0 with S. In particular, $W_1\Pi_Q^+=\Pi_Q^+W_1$, and hence there exists a measurable function $\beta_1:\mathbb{R}_+\to\mathbb{T}$ such that

$$[W_1f](x)=\beta_1(x)f(x) \quad \forall f\in L^2(0,+\infty).$$

It follows that W_1 is unitary. Reasoning as above, one finds a unitary operator W_2 intertwining the restrictions of A_0 and A' to $L^2(-\infty,0)$, with

$$[W_2f](x)=\beta_2(x)f(x) \quad \forall f\in L^2(-\infty,0),$$

for some measurable function $\beta_2:\mathbb{R}_-\to\mathbb{T}$. Then, $\tilde{W}=W_1\oplus W_2$ is unitary on $L^2(-\infty,+\infty)$, and $A(a)=U(t)^*\tilde{W}A_0(a)\tilde{W}^*U(t)$ has the claimed form for all $a\in\mathbb{R}_+$.

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3-geometries and the Hamilton–Jacobi equation

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In the first part of this work we show that on the space of solutions of a certain class of systems of three second-order PDE's, $u_{\alpha\alpha}=\Upsilon(\alpha,\beta,u,u_\alpha,u_\beta)$, $u_{\beta\beta}=\Psi(\alpha,\beta,u,u_\alpha,u_\beta)$ and $u_{\alpha\beta}=\Omega(\alpha,\beta,u,u_\alpha,u_\beta)$, a three-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the three-dimensional Hamilton–Jacobi equation, $g^{ab}u_{,a}u_{,b}=1$ holds. Furthermore, we remark that this structure is invariant under a subset of contact transformations. In the second part, we obtain analogous results for a certain class of third-order ordinary differential equation (ODE's), $u'''=\Lambda(s,u,u',u'')$. In both cases, we apply our general results to the cental force problem. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In the early years of the 20th century, while studying the structure and transformation properties of second- and third-order ODE's, Lie, Tresse, Wünschmann[1–4] among others, discovered that there was a rich differential geometry induced on the solution spaces of the differential equations by the equations themselves. This work was greatly developed and generalized by Cartan and Chern[5–9] in the 1930–1940s. Robert Bryant,[10] in more recent years, studied the geometry associated with fourth-order ODE's. Paul Tod[11] showed how third-order ODE's could generate three-dimensional Einstein–Weyl metrics.

With a totally different motivation and from a different point of view originating with General Relativity, Frittelli, Kozameh and Newman, in a series of papers[12–17] came to the same set of issues and problems. Rather than starting with given differential equations, the point of view of these authors began with three- and four-dimensional conformal Lorentzian manifolds, already containing a metric. They then studied families of complete solutions to the eikonal equation on these manifolds. From these solutions, by the elimination of the space–time coordinates, the differential equations of Cartan and Chern were reobtained. However, from this point of view, unwittingly, the Cartan–Chern work was generalized from ODE's to pairs of second-order PDE's whose solution spaces could be identified with any four-dimensional manifold with a conformal Lorentzian metric. In particular, they showed that the Einstein equations could be reformulated in terms of pairs of second-order PDE's.

Later, with Kamran and Nurowski,[18–22] this work was connected with the Cartan–Chern work for both the equivalence problem for differential equations under a variety of transformations and with the theory of Cartan normal conformal connections. With this consideration one saw how the differential equations (both the third-order equation and the pair of second-order equations) had to lie in a restricted class defined by the vanishing of the so-called Wünschmann (or generalized Wünschmann) equation.

An underlying unifying theme in many of the discussions was the existence of the eikonal equation and families of complete solutions. These solutions could be obtained either via the given

third-order ODE or pair of second-order PDE's or alternatively from the solutions to the eikonal equation on the given conformal background space.

In a recent work,[23] we turned to the geometry associated with a new class of second-order ODE's. The connecting link with the earlier work is that now we used the time-independent two-dimensional Hamilton–Jacobi equation rather than the eikonal equation to obtain this new class. We showed (via two different procedures) that, in the solution spaces of the ODE's, either a two-dimensional Riemannian or Lorentzian metric can be constructed in a natural way and that the metric structure associated with each differential equation is preserved when the equation is transformed by a subset of contact transformations (namely canonical transformations).

The aim of the present work is to generalize our previous result to the three-dimensional time-independent Hamilton–Jacobi equation. In Sec. II we begin with a three-dimensional manifold, $\mathcal{M}$, with no further structure and then investigate arbitrary two-parameter families of surfaces on $\mathcal{M}$ given by $u=constant=Z(x^a,\alpha,\beta)$. (The x^a are local coordinates on $\mathcal{M}$ and α and β parametrize the families and take values on $\mathcal{S}^2$, $\mathcal{S}^1\times\mathcal{R}$ or on $\mathcal{R}^2$.) More specifically, we then ask when do such families of surfaces define a three-dimensional metric, $g_{ab}(x^a)$, such that

$$g^{ab}\nabla_a Z(x^a,\alpha,\beta)\nabla_b Z(x^a,\alpha,\beta)=1. \tag{1}$$

We will show that the $u=Z(x^a,\alpha,\beta)$ must also satisfy a system of three second-order PDE's

$$\begin{aligned}\partial_{\alpha\alpha}Z&=\Upsilon(u,v,w,\alpha,\beta),\\ \partial_{\beta\beta}Z&=\Psi(u,v,w,\alpha,\beta),\\ \partial_{\alpha\beta}Z&=\Omega(u,v,w,\alpha,\beta),\end{aligned} \tag{2}$$

with

$$v\equiv\partial_\alpha Z,\quad \text{and}\quad w\equiv\partial_\beta Z,$$

and where Υ, Ψ, and Ω are restricted to satisfy certain "Wünschmann-type" conditions.

Here ∂ denotes partial derivative. Observe that in the solutions $u=Z(x^a,\alpha,\beta)$, the x^a are three constants of integration for Eqs. (2) while the "α" and "β" are two integration constants for Eq. (1).

Before proceeding we make the following important remark:

Remark 1: The time-independent Hamilton–Jacobi equation for a particle, with mass m and energy E, in a three-dimensional Riemannian space under the influence of a potential and the eikonal equation describing the evolution of the light rays in a three-dimensional isotropic optical medium characterized by its index of refraction, i.e., either of

$$\begin{aligned}g^{*ab}\nabla_a S(x^a,\alpha,\beta)\nabla_b S(x^a,\alpha,\beta)&=E-V(x^a),\\ g^{*ab}\nabla_a S(x^a,\alpha,\beta)\nabla_b S(x^a,\alpha,\beta)&=n(x^a),\end{aligned}$$

can be rewritten in the form of Eq. (1) by dividing the equations by either $E-V(x^a)$ or by $n(x^a)$ and simultaneously rescaling the metric by the same factors.

This action has the effect of changing certain properties of solutions to the Hamilton–Jacobi (H-J) equation. Normally for the three-dimensional H-J equation a complete integral contains three constants of integration, where one of them is E. In our case, after the conformal rescaling, E is hidden as a *fixed* constant in the metric g^{ab} and the solution will depend now on only two parameters, α and β. With an abuse of language, we will refer to $u=Z(x^a,\alpha,\beta)$ as a "restricted complete" integral to the H-J equation. In Sec. II we also show that any two arbitrary restricted complete integrals of the same H-J equation are connected via a special contact transformation. This result allows one to establish that if two systems of three second-order PDE's are connected

via that special contact transformation then in their spaces of solutions the same three-dimensional metric can be constructed. Finally, our result is applied to the central force problem in spherical polar coordinates.

In Sec. III we present analogous results for a certain class of third-order ODE's. That is, we begin with a three-dimensional manifold, $\mathcal{M}$, with no further structure and then investigate arbitrary one-parameter families of surfaces on $\mathcal{M}$ given by $u=constant=Z(x^a,s)$. (The x^a are local coordinates on $\mathcal{M}$ and s parametrizes the families and takes values on $\mathcal{S}^1$ or on $\mathcal{R}^1$.) More specifically, we ask when do such families of surfaces define a three-dimensional metric, $g_{ab}(x^a)$, such that

$$g^{ab}\nabla_a Z(x^a,s)\nabla_b Z(x^a,s)=1. \tag{3}$$

We will show that the $u=Z(x^a,s)$ must also satisfy a third-order ODE,

$$u'''=\Lambda(s,u,u',u''), \tag{4}$$

where Λ is restricted to satisfy a certain ''Wünschmann-type'' condition.

Here the prime denotes ''s'' derivatives. Observe that in the solutions $u=Z(x^a,s)$, which we will refer to as a one-parameter family of solutions to the Hamilton–Jacobi equation, the x^a, are three constant of integration for Eq. (4) while the ''s'' is an integration constant for Eq. (3). In this section it is also remarked that the three-metric is invariant when the third-order ODE is transformed by a subclass of contact transformations. Finally, these results are also applied to the central force problem in spherical polar coordinates.

II. THE SYSTEM OF PDE's CASE

In this section we prove that in the space of solutions of a certain class of systems of three second-order PDE's, a three-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the solutions satisfy the three-dimensional H-J equation. We start with a three-dimensional manifold $\mathcal{M}$ [with local coordinates $x^a=(x^0,x^1,x^2)$] and assume we are given a two-parameter set of functions $u=Z(x^a,\alpha,\beta)$, the parameters α and β can take values on $\mathcal{S}^2$, $\mathcal{S}^1\times\mathcal{R}$ or on $\mathcal{R}^2$. We also assume that for fixed values of the parameters α and β the level surfaces

$$u=constant=Z(x^a,\alpha,\beta), \tag{5}$$

locally foliate the manifold $\mathcal{M}$ and that $u=Z(x^a,\alpha,\beta)$ satisfies the H-J equation

$$g^{ab}(x^a)\nabla_a Z(x^a,\alpha,\beta)\nabla_b Z(x^a,\alpha,\beta)=1 \tag{6}$$

for some unknown metric $g_{ab}(x^a)$.

Remark 2: If g^{ab} contains the E simply as a number or fixed parameter it will appear in the solution to the H-J equation. i.e., $u=Z(x^a,E,\alpha,\beta)$.

The basic idea now is to solve Eq. (6) for the components of the metric in terms of $\nabla_a Z(x^a,\alpha,\beta)$. To do so, we will consider a number of parameter derivatives of the condition (6), and then by manipulation of these derivatives, obtain both the three-dimensional metric and the three partial differential equations defining the surfaces plus the conditions they must satisfy. We will refer to them as the Wünschmann-type conditions.

Remark 3: The notation is as follows: there will be two types of differentiation, one is with respect to the local coordinates, x^a, of the manifold $\mathcal{M}$, denoted by ∇_a or ''comma a,'' the other is with respect to the parameters α and β, denoted by ∂_α and ∂_β.

From the assumed existence of $u=Z(x^a,\alpha,\beta)$, we define three parametrized scalars θ^i in the following way:

$$\theta^0 = u \equiv Z(x^a, \alpha, \beta),$$

$$\theta^1 = v \equiv \partial_\alpha Z(x^a, \alpha, \beta), \tag{7}$$

$$\theta^2 = w \equiv \partial_\beta Z(x^a, \alpha, \beta).$$

Remark 4: For each value of α and β Eqs. (7) can be thought of as a coordinate transformation between the x^a's and (u, v, w).

We also define the following three important scalars

$$\Upsilon^* = \partial_{\alpha\alpha} Z(x^a, \alpha, \beta),$$

$$\Psi^* = \partial_{\beta\beta} Z(x^a, \alpha, \beta), \tag{8}$$

$$\Omega^* = \partial_{\alpha\beta} Z(x^a, \alpha, \beta).$$

In what follows we will assume that Eqs. (7) can be solved for the x^a's; that is,

$$x^a = X^a(u, v, w, \alpha, \beta),$$

so that Eqs. (8) can be rewritten as

$$\partial_{\alpha\alpha} Z = \Upsilon(u, v, w, \alpha, \beta),$$

$$\partial_{\beta\beta} Z = \Psi(u, v, w, \alpha, \beta), \tag{9}$$

$$\partial_{\alpha\beta} Z = \Omega(u, v, w, \alpha, \beta).$$

This means that the two-parameter family of level surfaces, Eq. (5), can be obtained as solutions to the system of three second-order PDE's (9). Note that (Υ, Ψ, Ω) satisfy the integrability conditions, $\Upsilon_{,\beta} = \Omega_{,\alpha}$ and $\Omega_{,\beta} = \Psi_{,\alpha}$.

The solution space of Eqs. (9) is three-dimensional. This can be seen in the following way. The system of PDE's (9) is equivalent to the vanishing of the three one-forms, ω^i,

$$\omega^0 = du - v\, d\alpha - w\, d\beta,$$

$$\omega^1 = dv - \Upsilon\, d\alpha - \Omega\, d\beta, \tag{10}$$

$$\omega^2 = dw - \Omega\, d\alpha - \Psi\, d\beta.$$

A simple calculation, using the integrability conditions on (Υ, Ψ, Ω), leads to $d\omega^i = 0$ (*modulo* ω^i) from which, via the Frobenius Theorem, the solution space of Eqs. (9) is three-dimensional.

From the three scalars, θ^i, we have their associated gradient basis $\theta^i{}_{,a}$ given by

$$\theta^i{}_{,a} = \nabla_a \theta^i = \{Z_{,a}, \partial_\alpha Z_{,a}, \partial_\beta Z_{,a}\}, \tag{11}$$

and its dual vector basis $\theta_i{}^a$, so that

$$\theta_i{}^a \theta^j{}_{,a} = \delta_i{}^j, \quad \theta_i{}^a \theta^i{}_{,b} = \delta_b{}^a. \tag{12}$$

Definition 1: The total α and β derivatives of a function $F = F(u, v, w, \alpha, \beta)$ are defined by

$$D_\alpha F \equiv F_\alpha + F_u v + F_v \Upsilon + F_w \Omega,$$

$$D_\beta F \equiv F_\beta + F_u w + F_v \Omega + F_w \Psi, \tag{13}$$

respectively.

It is easier to search for the components of the three-dimensional metric in the gradient basis rather than in the original coordinate basis. Furthermore, it is preferable to use the contravariant components rather than the covariant components of the metric; that is, we want to determine

$$g^{ij}(x^a,s)=g^{ab}(x^a)\,\theta^i{}_{,a}\,\theta^j{}_{,b}\,. \tag{14}$$

The metric components and the Wünschmann-type conditions, for this case, are obtained by repeatedly operating with ∂_α and ∂_β on Eq. (6), that is, by definition, on

$$g^{00}=g^{ab}Z_{,a}Z_{,b}=1. \tag{15}$$

Applying ∂_α to Eq. (15) yields $\partial_\alpha g^{00}=2g^{ab}\partial_\alpha Z,_a Z,_b=0$, i.e.,

$$g^{10}=0. \tag{16}$$

In the same way we obtain that $\partial_\beta g^{00}=2g^{ab}\partial_\beta Z,_a Z,_b=0$ and thus,

$$g^{20}=0. \tag{17}$$

A direct computation shows that

$$\partial_{\alpha\alpha}(g^{00}/2)=g^{ab}\partial_{\alpha\alpha}Z,_a Z,_b+g^{ab}\partial_\alpha Z,_a\partial_\alpha Z,_b=g^{ab}\Upsilon,_a Z,_b+g^{11}=0. \tag{18}$$

Since, by the assumed linear independence of $(Z,_a,\partial_\alpha Z,_a,\partial_\beta Z,_a)$,

$$\Upsilon,_a=\Upsilon_u Z,_a+\Upsilon_v\partial_\alpha Z,_a+\Upsilon_w\partial_\beta Z,_a\,, \tag{19}$$

Eq. (18), using Eqs. (16), (17), and (19), is equivalent to

$$g^{11}=-\Upsilon_u\,. \tag{20}$$

In exactly the same way we find that

$$\begin{aligned}\partial_{\alpha\beta}(g^{00}/2)&=\Omega_u+g^{21}=0,\\ \partial_{\beta\beta}(g^{00}/2)&=\Psi_u+g^{22}=0.\end{aligned} \tag{21}$$

Therefore, the final result is

$$(g^{ij})=\begin{pmatrix}1 & 0 & 0\\ 0 & -\Upsilon_u & -\Omega_u\\ 0 & -\Omega_u & -\Psi_u\end{pmatrix}. \tag{22}$$

Remark 5: We require that $\det(g^{ij})=\Delta$ *be different from zero, with*

$$\Delta\equiv(\Upsilon_u\Psi_u-\Omega_u^2). \tag{23}$$

The metricity or Wünschmann-type conditions are obtained from the conditions $\partial_{\alpha\alpha\alpha}g^{00}=0$, $\partial_{\beta\alpha\alpha}g^{00}=0$, $\partial_{\beta\beta\alpha}g^{00}=0$, and $\partial_{\beta\beta\beta}g^{00}=0$. A direct computation shows that they are equivalent to

$$\begin{aligned}\Upsilon_{u\alpha}+\Upsilon_{uu}v+\Upsilon_{uv}\Upsilon+\Upsilon_{uw}\Omega&=2(\Upsilon_v\Upsilon_u+\Upsilon_w\Omega_u),\\ \Upsilon_{u\beta}+\Upsilon_{uu}w+\Upsilon_{uv}\Omega+\Upsilon_{uw}\Psi&=2(\Omega_v\Upsilon_u+\Omega_w\Omega_u),\\ \Omega_{u\beta}+\Omega_{uu}w+\Omega_{uv}\Omega+\Omega_{uw}\Psi&=\Omega_v\Omega_u+\Omega_w\Psi_u+\Psi_v\Upsilon_u+\Psi_w\Omega_u\,,\end{aligned} \tag{24}$$

$$\Psi_{u\beta}+\Psi_{uu}w+\Psi_{uv}\Omega+\Psi_{uw}\Psi=2(\Psi_v\Omega_u+\Psi_w\Psi_u).$$

Summarizing: (a) If we start from a restricted complete integral, $u=Z(x^a,\alpha,\beta)$ to the H-J equation, (6), then it satisfies the system of three second-order PDE's (9), with Υ, Ψ and Ω satisfying the Wünschmann-type conditions (24); in other words, in the solution space of Eqs. (9) there is the naturally defined metric,

$$ds^2=\left[u_{,a}u_{,b}-\frac{1}{\Delta}(\Psi_u v_{,a}v_{,b}-\Omega_u(v_{,a}w_{,b}+w_{,a}v_{,b})+\Upsilon_u w_{,a}w_{,b})\right]dx^a dx^b, \tag{25}$$

where Δ is defined by Eq. (23). (b) If we start with a system of three second-order PDE's (9), where Υ, Ψ, and Ω satisfy Eqs. (24) and the integrability conditions, then in its solution space there exist a natural three-dimensional metric given by Eq. (25). Though it might appear as if the metric components depend on the parameters (α,β), the Wünschmann-type conditions guarantees that they do not. Furthermore, the solutions $u=Z(x^a,\alpha,\beta)$ satisfy the H-J equation

$$g^{ab}\nabla_a Z(x^a,\alpha,\beta)\nabla_b Z(x^a,\alpha,\beta)=1$$

with the just determined metric, Eq. (25).

Remark 6: From the results presented above we conclude that solving the three-dimensional H-J equation is equivalent to solving a system of three second-order PDE's.

In some of the earlier work on the eikonal equation in three and four dimensional Lorentzian spaces, it was proved that the conformal Lorentzian metrics associated with third-order ODE's and pairs of second order PDE's satisfying the Wünschmann condition and generalized Wünschmann condition, is preserved when the differential equation is transformed by a contact transformation. For our present case, there is an analogous result given by the following:

Theorem 1: *Let Eqs. (9) be a system of three second-order PDE's, with* Υ, Ψ, *and* Ω *satisfying the conditions* (24) *and let*

$$\begin{aligned}
\partial_{\overline{\alpha}\overline{\alpha}}\overline{Z}&=\overline{\Upsilon}(\overline{u},\overline{v},\overline{w},\overline{\alpha},\overline{\beta}),\\
\partial_{\overline{\beta}\overline{\beta}}\overline{Z}&=\overline{\Psi}(\overline{u},\overline{v},\overline{w},\overline{\alpha},\overline{\beta}),\\
\partial_{\overline{\alpha}\overline{\beta}}\overline{Z}&=\overline{\Omega}(\overline{u},\overline{v},\overline{w},\overline{\alpha},\overline{\beta}),
\end{aligned} \tag{26}$$

be a system of three second-order PDE's locally equivalent to Eqs. (9) under the subset of contact transformations generated by the generating function

$$H(\alpha,\beta,u,\overline{\alpha},\overline{\beta},\overline{u})=\overline{u}-u-G(\alpha,\beta,\overline{\alpha},\overline{\beta}). \tag{27}$$

Then under this subset of contact transformations the metric given by Eq. (25) is preserved.

The proof of this theorem is exactly as that presented in Ref. 18 for a system of two second-order PDE's such that in its space of solutions is living a four-dimensional conformal Lorentzian metric, g^{ab}, such that $g^{ab}u_{,a}u_{,b}=0$ holds. Here we only justify the form of the generating function (27). We first review the definition of a general contact transformation.

Theorem 2: *Every contact transformation which is not a prolonged point transformation is determined in terms of a generating function* $H(\alpha,\beta,u,\overline{\alpha},\overline{\beta},\overline{u})$ *by solving the following five implicit equations for* $\overline{\alpha}$, $\overline{\beta}$, $\overline{u}$, $\overline{v}=\partial_{\overline{\alpha}}\overline{u}$, $\overline{w}=\partial_{\overline{\beta}}\overline{u}$:

$$\begin{aligned}
&H(\alpha,\beta,u,\overline{\alpha},\overline{\beta},\overline{u})=0,\\
&H_\alpha+vH_u=0,\quad H_{\overline{\alpha}}+\overline{v}H_{\overline{u}}=0,\\
&H_\beta+wH_u=0,\quad H_{\overline{\beta}}+\overline{w}H_{\overline{u}}=0.
\end{aligned} \tag{28}$$

The generating function $H(\alpha,\beta,u,\overline{\alpha},\overline{\beta},\overline{u})$ *is an arbitrary smooth function, subject only to the solubility of Eqs. (28) for* $\overline{\alpha}$, $\overline{\beta}$, $\overline{u}$, $\overline{v}$, $\overline{w}$.

For a proof of this theorem see, for example, Olver.[24]

Without loss of generality one can take

$$H=\overline{u}-\overline{V}(u,\alpha,\beta,\overline{\alpha},\overline{\beta}), \tag{29}$$

so that the contact transformation has the form

$$\begin{aligned}
\overline{u}&=\overline{V}(u,\alpha,\beta,A(\alpha,\beta,u,v,w),B(\alpha,\beta,u,v,w)),\\
\overline{\alpha}&=A(\alpha,\beta,u,v,w),\\
\overline{\beta}&=B(\alpha,\beta,u,v,w),\\
\overline{v}&=\overline{V}_{\overline{\alpha}}(u,\alpha,\beta,A(\alpha,\beta,u,v,w),B(\alpha,\beta,u,v,w)),\\
\overline{w}&=\overline{V}_{\overline{\beta}}(u,\alpha,\beta,A(\alpha,\beta,u,v,w),B(\alpha,\beta,u,v,w)),
\end{aligned} \tag{30}$$

where $A(\alpha,\beta,u,v,w)$ and $B(\alpha,\beta,u,v,w)$ are obtained by solving

$$\begin{aligned}
\overline{V}_{\alpha}+v\overline{V}_{u}&=0,\\
\overline{V}_{\beta}+w\overline{V}_{u}&=0,
\end{aligned} \tag{31}$$

for $\overline{\alpha}$ and $\overline{\beta}$ in terms of α, β u, v, and w.

As was pointed out earlier, for each value of α and β, the three-parameter family of solutions

$$u=Z(x^a,\alpha,\beta), \tag{32}$$

of (9) is also a two-parameter family of solutions of Eq. (6), i.e., are ''restricted complete'' integrals of Eq. (6). We now invoke the envelope construction to take one restricted complete integral of Eq. (6) into another such solution. Consider the function $\overline{u}=\overline{Z}(x^a,\overline{\alpha},\overline{\beta})$ defined by

$$\overline{u}=\overline{V}(u,\alpha,\beta,\overline{\alpha},\overline{\beta}), \tag{33}$$

where u is defined by Eq. (32) and α and β are defined implicitly as functions of x^a, $\overline{\alpha}$ and $\overline{\beta}$ by the envelope condition[18,25]

$$\begin{aligned}
\overline{V}_{u}v+\overline{V}_{\alpha}&=0,\\
\overline{V}_{u}w+\overline{V}_{\beta}&=0.
\end{aligned} \tag{34}$$

Note that although Eqs. (34) have the same form as Eqs. (31), they involve the variables x^a, α, and β. Using both Eqs. (33) and (34), we have that

$$\overline{u}_{,a}=\overline{V}_{u}u_{,a}\,. \tag{35}$$

By direct substitution of $\overline{u}_{,a}$ into the H-J equation, Eq. (6), we see that it is a new restricted complete integral if and only if $\overline{V}_{u}^{2}=1$. That is, $\overline{u}=\overline{V}(u,\alpha,\beta,\overline{\alpha},\overline{\beta})$ has the form $\overline{u}=\pm u+G(\alpha,\beta,\overline{\alpha},\overline{\beta})$. For simplicity, taking the positive sign, we have that if $u(x^a,\alpha,\beta)$ is a restricted complete integral of Eq. (6) then

$$\overline{u}=u+G(\alpha,\beta,\overline{\alpha},\overline{\beta}), \tag{36}$$

where α and β are defined implicitly as a function of x^a, $\overline{\alpha}$, and $\overline{\beta}$ by the envelope conditions

$$v+G_\alpha=0,$$

$$w+G_\beta=0, \tag{37}$$

is a new restricted complete integral of Eq. (6). Equations (36) and (37) define a particular subset of the contact transformations given by contact transformations

$$\overline{u}=u+G(\alpha,\beta,\overline{\alpha},\overline{\beta}), \tag{38}$$

$$v=-G_\alpha, \tag{39}$$

$$w=-G_\beta, \tag{40}$$

$$\overline{v}=G_{\overline{\alpha}}, \tag{41}$$

$$\overline{w}=G_{\overline{\beta}}. \tag{42}$$

The generating function for this set of contact transformations is given by

$$H(\alpha,\beta,u,\overline{\alpha},\overline{\beta},\overline{u})=\overline{u}-u-G(\alpha,\beta,\overline{\alpha},\overline{\beta})=0, \tag{43}$$

thus justifying our choice of the generating function, Eq. (27).

As an example we apply our results to the central force problem in spherical polar coordinates, $x^a=(r,\theta,\phi)$. For this problem the time-independent Hamilton–Jacobi equation is given by

$$\left(\frac{1}{2m(E-V)}\right)\left(u_{,r}^2+\frac{u_{,\theta}^2}{r^2}+\frac{u_{,\phi}^2}{r^2\sin^2\theta}\right)=1, \tag{44}$$

where m is the mass, $V(r)$ the potential energy, and E is the total energy of the particle, respectively. By the method of separation of variables one finds that a complete solution to Eq. (44) can be written in the following form

$$u=Z(x^a,E,\alpha,\beta)=\int\sqrt{2m(E-V)-\frac{\beta^2}{r^2}}\,dr+\int\sqrt{\beta^2-\frac{\alpha^2}{\sin^2\theta}}\,d\theta+\alpha\phi, \tag{45}$$

where α and β are two constants of separation. For this problem, α, is the magnitude of the total angular momentum and β is the value of the angular momentum about the polar axis. In this case, our restricted complete integral is obtained from Eq. (45) by fixing E. Now we obtain the system of three second-order PDE's associated with this restricted complete integral. A direct computation shows that

$$v=\partial_\alpha Z=\int\frac{-\alpha\,d\theta}{\sin^2\theta\sqrt{\beta^2-\dfrac{\alpha^2}{\sin^2\theta}}}+\phi,$$

$$w=\partial_\beta Z=\int\frac{-\beta dr}{r^2\sqrt{2m(E-V)-\dfrac{\beta^2}{r^2}}}+\int\frac{\beta\,d\theta}{\sqrt{\beta^2-\dfrac{\alpha^2}{\sin^2\theta}}}. \tag{46}$$

By using Eqs. (45) and (46), one sees that the Jacobian of the coordinate transformation, $\theta^i = \theta^i(x^a, \alpha, \beta)$, for this case, is given by

$$J = \frac{\partial(u,v,w)}{\partial(r,\theta,\phi)} = \frac{-2m(E-V)\beta}{\sqrt{\beta^2 - \dfrac{\alpha^2}{\sin^2\theta}}\sqrt{2m(E-V) - \dfrac{\beta^2}{r^2}}}. \tag{47}$$

Therefore, β cannot be zero.

Using Eqs. (46), we see that for the central force problem in spherical polar coordinates

$$\begin{aligned} \partial_{\alpha\alpha} Z &= -\beta^2 \mathcal{F}(\theta,\alpha,\beta), \\ \partial_{\beta\beta} Z &= -\mathcal{G}(r,\beta) - \alpha^2 \mathcal{F}(\theta,\alpha,\beta), \\ \partial_{\alpha\beta} Z &= \alpha\beta \mathcal{F}(\theta,\alpha,\beta), \end{aligned} \tag{48}$$

where

$$\begin{aligned} \mathcal{F}(\theta,\alpha,\beta) &= \int \frac{d\theta}{\sin^2\theta\left(\beta^2 - \dfrac{\alpha^2}{\sin^2\theta}\right)^{3/2}}, \\ \mathcal{G}(r,\beta) &= \int \frac{2m(E-V)dr}{r^2\left(2m(E-V) - \dfrac{\beta^2}{r^2}\right)^{3/2}}. \end{aligned} \tag{49}$$

On the other hand, Eqs. (45) and (46) imply that

$$\begin{aligned} r &= R(u,v,w,\alpha,\beta), \\ \theta &= \Theta(u,v,w,\alpha,\beta). \end{aligned} \tag{50}$$

Therefore, the system of three second-order PDE's for the central force problem in spherical polar coordinates is given by

$$\begin{aligned} \partial_{\alpha\alpha} Z = \Upsilon &= -\beta^2 \mathcal{F}(\Theta(u,v,w,\alpha,\beta),\alpha,\beta), \\ \partial_{\beta\beta} Z = \Psi &= -\mathcal{G}(R(u,v,w,\alpha,\beta),\beta) - \alpha^2 \mathcal{F}(\Theta(u,v,w,\alpha,\beta),\alpha,\beta), \\ \partial_{\alpha\beta} Z = \Omega &= \alpha\beta \mathcal{F}(\Theta(u,v,w,\alpha,\beta),\alpha,\beta). \end{aligned} \tag{51}$$

Since $u(x^a,\alpha,\beta)$ given by Eq. (45) with E fixed is a restricted complete integral to the H-J equation (44), then Υ, Ψ, and Ω given in Eqs. (51) satisfy Eqs. (24) and, therefore, a three-dimensional metric can be defined in the space of solutions of Eqs. (51). By comparison of Eqs. (6) and (44) it is clear what that metric should be. However, here we show the steps to explicitly obtain this metric by the procedure developed in earlier. What is remarkable is that this metric can be obtained without the evaluation of the integrals that arose in this problem. As we can see from Eq. (25), to obtain the three-dimensional metric, g_{ab}, associated with this problem, we need to compute: $\theta^i{}_{,a} = (u_{,a}, v_{,a}, w_{,a})$, Υ_u, Ψ_u, Ω_u, and Δ. By using Eqs. (45) and (46), we have that

$$u_{,a}=\left(\sqrt{2m(E-V)-\frac{\beta^2}{r^2}},\quad \sqrt{\beta^2-\frac{\alpha^2}{\sin^2\theta}},\alpha\right),$$

$$v_{,a}=\left(0,\frac{-\alpha}{\sin^2\theta\sqrt{\beta^2-\frac{\alpha^2}{\sin^2\theta}}},\quad 1\right), \tag{52}$$

$$w_{,a}=\left(\frac{-\beta}{r^2\sqrt{2m(E-V)-\frac{\beta^2}{r^2}}},\quad \frac{\beta}{\sqrt{\beta^2-\frac{\alpha^2}{\sin^2\theta}}},\quad 0\right).$$

From Eq. (47) we have that these three vectors are linearly independent when β is different from zero.

Since, for example,

$$\Psi_u=(\partial\Psi/\partial r)(\partial r/\partial u)+(\partial\Psi)/\partial\theta)(\partial\theta/\partial u),$$

then to compute Υ_u, Ψ_u, Ω_u, and Δ we need to obtain $(\partial\theta/\partial u)$ and $(\partial r/\partial u)$. From Eqs. (45) and (46), via implicit derivations, we obtain that

$$\frac{\partial r}{\partial u}=\frac{\sqrt{2m(E-V)-\frac{\beta^2}{r^2}}}{2m(E-V)},$$

$$\frac{\partial\theta}{\partial u}=\frac{\sqrt{\beta^2-\frac{\alpha^2}{\sin^2\theta}}}{2mr^2(E-V)}. \tag{53}$$

By using the definition of Δ given by Eqs. (23), (51), and (53), a direct computation shows that

$$\frac{\Upsilon_u}{\Delta}=-2mr^2(E-V)+\beta^2,$$

$$\frac{\Psi_u}{\Delta}=-2mr^2(E-V)\sin^2\theta+\alpha^2, \tag{54}$$

$$\frac{\Omega_u}{\Delta}=\frac{\alpha[2mr^2(E-V)-\beta^2]}{\beta}.$$

Finally, substituting Eqs. (52) and (54) into Eq. (25) we obtain the three-dimensional metric living in the solution space of the PDE's (51);

$$ds^2=g_{ab}dx^a dx^b=2m(E-V)(dr^2+r^2d\theta^2+r^2\sin^2\theta d\phi^2), \tag{55}$$

the desired result.

In the special case of the Kepler problem with energy equal to zero, i.e., for $V=-k/r$ and $E=0$, we have for the three PDE's.

$$\partial_{\alpha\alpha}Z=\frac{\beta\cot(\partial_\beta Z+\arccos\epsilon)}{\alpha^2-\beta^2},$$

$$\partial_{\beta\beta}Z=\frac{\alpha^2\cot(\partial_\beta Z+\arccos\epsilon)}{\beta(\alpha^2-\beta^2)}+\frac{4}{Z-\alpha\partial_\alpha Z-\beta\partial_\beta Z}, \tag{56}$$

$$\partial_{\alpha\beta}Z=\frac{\alpha\cot(\partial_\beta Z+\arccos\epsilon)}{\beta^2-\alpha^2},$$

where

$$\epsilon=\left(\frac{4\beta^2-(Z-\alpha\partial_\alpha Z-\beta\partial_\beta Z)^2}{4\beta^2+(Z-\alpha\partial_\alpha Z-\beta\partial_\beta Z)^2}\right). \tag{57}$$

III. THE THIRD-ORDER ODE's CASE

In this section we prove that in the solution space of a certain class of third-order ODE's a three-dimensional definite or indefinite metric, g_{ab}, can be constructed directly from the solutions such that the three-dimensional time-independent H-J equation holds. We begin with a three-dimensional manifold $\mathcal{M}$ (with local coordinates $x^a=(x^0,x^1,x^2)$) and assume we are given a one-parameter set of functions $u=Z(x^a,s)$; the parameter s can take values on $\mathcal{S}^1$ or on $\mathcal{R}$. We also assume that for a fixed value of the parameter s, the level surfaces

$$u=constant=Z(x^a,s), \tag{58}$$

locally foliate the manifold $\mathcal{M}$ and that $u=Z(x^a,s)$ satisfies the H-J equation

$$g^{ab}\nabla_a Z(x^a,s)\nabla_b Z(x^a,s)=1, \tag{59}$$

for some unknown metric $g_{ab}(x^a)$. That is, $u=Z(x^a,s)$, is a one-parameter family of solutions to the three-dimensional time-independent H-J equation.

The basic idea now is to solve Eq. (59) for the components of the metric in terms of $\nabla_a Z(x^a,s)$. To do so, we will consider a number of parameter derivatives of the condition (59), and then by manipulation of these derivatives, obtain both the three-dimensional metric and the ODE defining the surfaces and the Wünschmann-type condition it must satisfy.

Remark 7: The notation is as follows: as in the previous section, there will be two types of differentiation, one is with respect to the local coordinates, x^a, of the manifold $\mathcal{M}$, denoted by ∇_a or "comma a," the other is with respect to the parameter s, denoted by a prime or by ∂_s.

We first note that the one-parameter family of "level" surfaces, Eq. (58), can be obtained as solutions to the third-order ODE

$$u'''=\Lambda(u,u',u'',s) \tag{60}$$

by first calculating

$$u'''(x^a,s)\equiv\Lambda^*(x^a,s) \tag{61}$$

and then by inverting the relations

$$u=Z(x^a,s),$$

$$u'=Z'(x^a,s),$$

$$u''=Z''(x^a,s),$$

obtaining

$$x^a = X^a(u,u',u'',s). \tag{62}$$

The three x^a can be eliminated in Λ^* yielding Eq. (60).

Remark 8: Eq. (62) can be thought of as an "s" dependent coordinate transformation between x^a and (u,u',u'').

We define three parametrized scalars:

$$\theta^i = \{\theta^0,\theta^1,\theta^2\} \equiv \{u,u',u''\} = \{Z(x^a,s),Z'(x^a,s),Z''(x^a,s)\}, \tag{63}$$

which for each value of s form a coordinate system intrinsically adapted to the surfaces.

From the three scalars, θ^i, we have their associated gradient basis $\theta^i{}_{,a}$ given by

$$\theta^i{}_{,a} = \nabla_a \theta^i = \{Z_{,a},\partial Z_{,a},\partial^2 Z_{,a}\}, \tag{64}$$

and its dual vector basis $\theta_i{}^a$, so that

$$\theta_i{}^a \theta^j{}_{,a} = \delta_i^j, \quad \theta_i{}^a \theta^i{}_{,b} = \delta_b{}^a. \tag{65}$$

Definition 2: The total s derivative of a function $F = F(s,u,u',u'')$ *is defined by*

$$DF \equiv F_s + F_u u' + F_{u'} u'' + F_{u''} \Lambda. \tag{66}$$

As in the previous section, it is easier to search for the components of the three-dimensional metric in the gradient basis rather than in the original coordinate basis. Furthermore, it is preferable to use the contravariant components rather than the covariant components of the metric; that is, we are interested in

$$g^{ij}(x^a,s) = g^{ab}(x^a)\,\theta^i{}_{,a}\,\theta^j{}_{,b}\,. \tag{67}$$

The metric components and the Wünschmann-type condition, for this case, are obtained by repeatedly operating with ∂_s on Eq. (59), that is, on

$$g^{00} = g^{ab} Z_{,a} Z_{,b} = 1. \tag{68}$$

Applying ∂_s on Eq. (68) yields

$$\partial_s(g^{ab} Z_{,a} Z_{,b}) = 2 g^{ab} Z'_{,a} Z_{,b} = 2 g^{10} = 0, \tag{69}$$

where we have used that $\partial_s g^{ab} = 0$. Applying ∂_s on Eq. (69) we obtain

$$\partial_s^2(g^{00}/2) = g^{ab} Z''_{,a} Z_{,b} + g^{ab} Z'_{,a} Z'_{,b} = 0, \tag{70}$$

which is equivalent to $g^{11} = -g^{20}$. In the same manner we find that

$$\partial_s^3(g^{00}/2) = g^{ab} Z'''_{,a} Z_{,b} + 2 g^{ab} Z''_{,a} Z'_{,b} + g^{ab} Z'_{,a} Z''_{,b} = g^{ab} \Lambda_{,a} Z_{,b} + 3 g^{ab} Z''_{,a} Z'_{,b} = 0. \tag{71}$$

Since

$$\Lambda_{,a} = \Lambda_u Z_{,a} + \Lambda_{u'} Z'_{,a} + \Lambda_{u''} Z''_{,a}\,, \tag{72}$$

then Eq. (71) is equivalent to

$$g^{21} = -\tfrac{1}{3}[\Lambda_u + \Lambda_{u''} g^{20}]. \tag{73}$$

In the same way we find that

$$\partial_s^4(g^{00}/2)=D\Lambda_u-\tfrac{1}{3}\Lambda_u\Lambda_{u''}+[D\Lambda_{u''}-\tfrac{1}{3}(\Lambda_{u''})^2-3\Lambda_{u'}]g^{20}+3g^{22}=0, \tag{74}$$

$$\partial_s^5(g^{00}/2)=-W^{(1)}[\Lambda]-g^{20}W^{(2)}[\Lambda]=0, \tag{75}$$

where

$$W^{(1)}[\Lambda]\equiv-D^2\Lambda_u-\tfrac{1}{3}\Lambda_uD\Lambda_{u''}+\tfrac{7}{3}\Lambda_{u''}D\Lambda_u+4\Lambda_u\Lambda_{u'}-\tfrac{4}{9}\Lambda_u(\Lambda_{u''})^2, \tag{76}$$

$$W^{(2)}[\Lambda]\equiv-\tfrac{4}{9}(\Lambda_{u''})^3+2\Lambda_{u''}D\Lambda_{u''}-2\Lambda_{u'}\Lambda_{u''}-D^2\Lambda_{u''}+3D\Lambda_{u'}-6\Lambda_u. \tag{77}$$

Remark 9: Observe that $W^{(2)}[\Lambda]$ is the standard Wünschmann invariant for third-order ODE's, which is an invariant under a general contact transformation.

From Eq. (75) one sees that there are, at this point, four different possible cases to look at:

(a) $W^{(1)}[\Lambda]\neq0$, $W^{(2)}[\Lambda]\neq0$; in this case the three-dimensional metric can be completely reconstructed;
(b) $W^{(1)}[\Lambda]=0$, $W^{(2)}[\Lambda]\neq0$; in this case we obtain a degenerate metric, which must be excluded by the assumption of the H-J equation. See Remark 10 below, for the proof;
(c) $W^{(1)}[\Lambda]=0$, $W^{(2)}[\Lambda]=0$; in this case the metric is not completely determined. See the conjecture below;
(d) The case of $W^{(2)}[\Lambda]=0$ with nothing said about $W^{(1)}[\Lambda]$ arises not with the H-J equation but with the time dependent three-dimensional eikonal equation. It leads to a conformal metric on the solution space.[12–17] As this case has been extensively studied, nothing further will be said here about it.

We thus consider only the first case which leads to the final result

$$g^{ij}(x^a,s)=h^{ij}(x^a,s)+g_c^{ij}(x^a,s), \tag{78}$$

where

$$(h^{ij})=\begin{pmatrix}1&0&0\\0&0&-\tfrac{1}{3}\Lambda_u\\0&-\tfrac{1}{3}\Lambda_u&-\tfrac{1}{3}D\Lambda_u+\tfrac{1}{9}\Lambda_u\Lambda_{u''}\end{pmatrix}, \tag{79}$$

$$(g_c^{ij})=g^{20}\begin{pmatrix}0&0&1\\0&-1&-\tfrac{1}{3}\Lambda_{u''}\\1&-\tfrac{1}{3}\Lambda_{u''}&-\tfrac{1}{3}D\Lambda_{u''}+\tfrac{1}{9}\Lambda_{u''}^2+\Lambda_{u'}\end{pmatrix}, \tag{80}$$

with

$$g^{20}=-\left(\frac{W^{(1)}[\Lambda]}{W^{(2)}[\Lambda]}\right). \tag{81}$$

The Wünschmann-type condition, which is obtained from $\partial_s^6(g^{00}/2)=0$, is

$$D\left(\frac{W^{(1)}[\Lambda]}{W^{(2)}[\Lambda]}\right)=\left(\frac{2}{3}\right)\left(\frac{\Lambda_{u''}W^{(1)}[\Lambda]}{W^{(2)}[\Lambda]}-\Lambda_u\right). \tag{82}$$

Remark 10: When $W^{(1)}[\Lambda]=0$, using Eqs. (81) and (82), one sees from

$$\det(g^{ij}) = -\frac{\Lambda_u^2}{9} + \frac{g^{20}}{3}[D\Lambda_u - \Lambda_u\Lambda_{u''}] + \frac{(g^{20})^2}{3}\left[D\Lambda_{u''} - \frac{2}{3}(\Lambda_{u''})^2 - 3\Lambda_{u'}\right] + (g^{20})^3 \quad (83)$$

that $\det(g^{ij})=0$. *This implies a degenerate metric thus excluding this case*.

Summarizing, we conclude the following: If Λ is such that $W^{(1)}[\Lambda]\neq 0$, $W^{(2)}[\Lambda]\neq 0$ and satisfies the Wünschmann-type condition (82), then in the solution space of the ODE, $u''' = \Lambda(u,u',u'',s)$, there is defined either a three-dimensional Riemannian or Lorentzian metric given by

$$ds^2 = g_{ab}dx^a dx^b = g_{ij}\theta^i{}_{,a}\theta^j{}_{,b}dx^a dx^b, \quad (84)$$

with (g^{ij}) given by Eqs. (78)–(81). Furthermore the solution satisfies the H-J equation with this metric. One can think of the ODE and the H-J equation as dual to each other; each being satisfied by the same function but with respect to different variables.

In earlier work on the eikonal equation in three-dimensional Lorentzian spaces, it was proved that the conformal Lorentzian metric associated with a third-order ODE satisfying the Wünschmann condition, is preserved when the differential equation is transformed by a contact transformation. For our present case, there is an analogous result given by the following:

Theorem 3: *Let Eq. (60) be a third-order ODE, with* Λ *satisfying the condition* (82) *with* $W^{(1)}[\Lambda]\neq 0$, $W^{(2)}[\Lambda]\neq 0$ *and let*

$$\overline{u}''' = \overline{\Lambda}(\overline{u},\overline{u}',\overline{u}'',\overline{s}), \quad (85)$$

be a third-order ODE locally equivalent to Eq. (60) under the subset of contact transformations generated by the generating function

$$H(s,u,\overline{s},\overline{u}) = \overline{u} - u - G(s,\overline{s}). \quad (86)$$

Then under this subset of contact transformations the metric given by Eqs. (78)–(81) is preserved.

The proof of this theorem is exactly as that presented in Ref. 18 for the third-order ODE case such that a conformal Lorentzian metric, g^{ab}, lives on its space of solutions is living, such that the eikonal equation $g^{ab}u_a u_b = 0$ is satisfied. The justification of this choice of generating function (86) is the same as that given in the previous section.

We return to the example from the previous section of the central force problem but now with only one parameter, s, in the solution. We see that ODE's can be constructed from the two-parameter solution, Eq. (45), i.e., from

$$u = Z(x^a,E,\alpha,\beta) = \int \sqrt{2m(E-V) - \frac{\beta^2}{r^2}}\,dr + \int \sqrt{\beta^2 - \frac{\alpha^2}{\sin^2\theta}}\,d\theta + \alpha\phi, \quad (87)$$

by choosing α and β as functions of s. To illustrate what can occur we take three different cases:

(a) $(\alpha = s, \beta = \beta_0) \Rightarrow W^{(1)}[\Lambda]=0$ and $W^{(2)}[\Lambda]=0$;
(b) $(\alpha = \alpha_0, \beta = s) \Rightarrow W^{(1)}[\Lambda]=0$ and $W^{(2)}[\Lambda]=0$;
(c) $(\alpha = as, \beta = s), \Rightarrow W^{(1)}[\Lambda]=0$, the three vectors $\theta^i{}_{,a}$ are not linearly independent;
(d) $(\alpha = s^2, \beta = s), \Rightarrow W^{(1)}[\Lambda]\neq 0$, $W(2)[\Lambda]\neq 0$.

Conjecture: Whenever one has a third-order ODE, $u''' = \Lambda(u,u',u'',s)$, *so that* $W^{(1)}[\Lambda]=0$ *and* $W^{(2)}[\Lambda]=0$ *then the equation came from a solution where the one-parameter entered the solution as a Killing trajectory; i.e., the change in the solution as "s" evolves can be undone by dragging the metric along the Killing trajectory*.

For case (d) the metric can be found (after a lengthy calculation) from the solution

$$u(x^a,s)=\int \sqrt{2m(E-V(r))-\frac{s^2}{r^2}}\,dr+\int s\sqrt{1-s^2\csc^2\theta}\,d\theta+s^2\phi \tag{88}$$

by the following steps:

$$u'=\int \frac{-s\,dr}{r^2\sqrt{2m(E-V(r))-\frac{s^2}{r^2}}}+\int \frac{(1-2s^2\csc^2\theta)d\theta}{\sqrt{1-s^2\csc^2\theta}}+2s\phi,$$

$$u''=\int \frac{-2m(E-V)dr}{r^2\left[2m(E-V(r))-\frac{s^2}{r^2}\right]^{3/2}}+\int \frac{s\csc^2\theta(2s^2\csc^2\theta-3)d\theta}{(1-s^2\csc^2\theta)^{3/2}}+2\phi. \tag{89}$$

The ODE becomes

$$u'''=-[\mathcal{H}(r,s)+\mathcal{J}(\theta,s)], \tag{90}$$

where

$$\mathcal{H}(r,s)=\int \frac{6sm(E-V)dr}{r^4\left[2m(E-V(r))-\frac{s^2}{r^2}\right]^{5/2}},$$

$$\mathcal{J}(\theta,s)=\int \frac{3\csc^2\theta d\theta}{(1-s^2\csc^2\theta)^{5/2}}. \tag{91}$$

By inverting, we, in principle, find

$$r=R(u,u',u'',s),$$

$$\theta=\Theta(u,u',u'',s),$$

$$\phi=\Phi(u,u',u'',s), \tag{92}$$

from which

$$u'''=\Lambda=-[\mathcal{H}(R(u,u',u'',s),s)+\mathcal{J}(\Theta(u,u',u'',s),s)]. \tag{93}$$

This leads after much work to

$$\frac{W^{(1)}[\Lambda]}{W^{(2)}[\Lambda]}=\frac{-2mr^2(E-V)+s^4\csc^2\theta}{2mr^2[2mr^2(E-V)-s^2](E-V)(s^2\csc^2\theta-1)} \tag{94}$$

and finally to

$$u_{,a}=\left(\frac{\sqrt{2mr^2(E-V)-s^2}}{r},s\sqrt{1-s^2\csc^2\theta},s^2\right),$$

$$u'_{,a}=\left(\frac{-s}{r\sqrt{2mr^2(E-V)-s^2}},\frac{1-2s^2\csc^2\theta}{\sqrt{1-s^2\csc^2\theta}},2s\right), \tag{95}$$

$$u''_{,a}=\left(\frac{-2mr(E-V)}{(2mr^2(E-V)-s^2)^{3/2}},\frac{s\csc^2\theta(2s^2\csc^2\theta-3)}{(1-s^2\csc^2\theta)^{3/2}},2\right),$$

and the metric (first in tetrad components)

$$
\begin{aligned}
g^{00} &= 1, \\
g^{20} &= \frac{2mr^2(E-V) - s^4 \csc^2\theta}{2mr^2[2mr^2(E-V)-s^2](E-V)(s^2\csc^2\theta - 1)}, \\
g^{21} &= \frac{2s\sin^2\theta}{mr^2(E-V)[2s^2+\cos(2\theta)-1]^2} + \frac{s}{[2mr^2(E-V)-s^2]^2}, \\
g^{22} &= \frac{2mr^2(E-V)}{[2mr^2(E-V)-s^2]^3} + \frac{3s^2\sin^2\theta - 4\sin^4\theta}{2mr^2(E-V)[s^2-\sin^2\theta]^3},
\end{aligned}
\tag{96}
$$

and then the final form,

$$
ds^2 = g_{ab}dx^a dx^b = 2m(E-V)[dr^2 + r^2 d\theta^2 + r^2\sin^2\theta d\phi^2]. \tag{97}
$$

IV. CONCLUSIONS

In this work, we have shown that the ideas and procedures developed in our recent paper[23] on the two-dimensional time-independent H-J equation can be generalized to the three-dimensional time-independent H-J equation. The results presented in this work show that solving the three-dimensional time-independent H-J equation is equivalent to solving a system of three second-order PDE's or a third-order ODE.

We point out that, though we have used, in the present work, only the three-dimensional time-independent H-J equation, this can be generalized. In a future paper we will present the results for the four-dimensional H-J equation.

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Distributive and analytic properties of lattice sums

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We use sums over Bessel functions of the first kind to derive a convenient form of the Poisson summation identity relating sums over direct lattices in two dimensions to sums over reciprocal lattices. After three simple examples of the use of the identity, we consider sums over complex powers of the radial distance to lattice points, and also sums incorporating factors $\exp(4im\varphi_p)$ depending on angles of lattice points. We study the distribution of zeros of lattice sums, and show two which seemingly obey the Riemann hypothesis, and a third which does not. We provide a reflection formula for angular lattice sums, and a Macdonald function sum for the lowest order angular lattice sum. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1755861]

I. INTRODUCTION

The study of lattice sums is an old problem in physics, dating back to investigations of the Madelung constant,[1] and to the foundations of the Lorentz–Lorenz equation.[2] Such sums may be divided into various types, for example, according to dimensionality, governing equation and whether the summand is a function of distance only, or of distance and angles.

Here, we will investigate two-dimensional lattice sums, and will show the interest of combining knowledge of sums related to the Helmholtz equation with sums related to the Laplace equation. The former type of sum is naturally linked with the Bloch Theorem, and phase-modulated sums, and depends on both a wavenumber and wavevector. We will show that these extra parameters enable one to deduce interesting connections between lattice sums for the Laplace equation. These take the form of connections between sums over the direct and reciprocal lattices, and are particularly interesting when the two coincide, for example for the square lattice. These connections have been remarked before, for example, by Hardy and Titchmarsh[3] and Kober,[4] but these early investigations were hampered by lack of access to numerical and symbolic algebra tools.

We commence by showing that a sum over Bessel functions of the first kind over a lattice is equivalent to a sum of delta functions over the reciprocal lattice. This relation can be integrated over wavenumber to give a convenient form of the Poisson summation formula connecting sums over the direct lattice with sums over the reciprocal lattice. After three simple examples of this formula, we move to the consideration of complex powers of distance in the plane. This is a rich topic, connected with, but not restricted to, the Epstein zeta function. Potter and Titchmarsh[5] have speculated that the complex zeros of certain Epstein functions obey the Riemann hypothesis, while others do not. We provide an example of a lattice sum already studied by Kober,[4] which may be represented as the sum of two terms, with the original term and one of its components seemingly obeying the Riemann hypothesis, while the second component does not. We also provide a reflection formula for angular lattice sums, and a Macdonald function sum for the lowest order angular lattice sum.

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The main results of this paper are, firstly, a concise formula linking a general class of sums over a direct lattice with related sums over its reciprocal lattice (Sec. III). Second, we illustrate the utility of considering lattice sums incorporating a phase modulation term characterized by a Bloch factor in establishing links between unmodulated lattice sums (Secs. IV–VI). Third, we identify functions other than the zeta function which seem to obey the Riemann hypothesis (Secs. IV, VI, and the Appendix). In particular, we exhibit an example of two different functions which seemingly obey the hypothesis, while their difference does not. We also give numerical evidence bearing on the Lindelöf hypothesis for these functions.

II. THE BASIC DISTRIBUTIVE SUM

Lattice sums $S_l(k,\mathbf{k}_0)$ are defined by

$$S_l(k,\mathbf{k}_0)=\sum_{p\neq 0} H_l^{(1)}(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}$$

$$=\sum_{p\neq 0} J_l(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}+i\sum_{p\neq 0} Y_l(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}$$

$$\overset{\text{def}}{=}S_l^J(k,\mathbf{k}_0)+iS_l^Y(k,\mathbf{k}_0). \tag{1}$$

Here $\mathbf{k}_0$ is the Bloch vector, k is a wavenumber and $\mathbf{R}_p$ is a lattice vector, written in polar form (R_p,φ_p). Note that k will be regarded as an extra parameter over which we can integrate to derive the formula in Sec. III linking sums over the direct lattice with sums over the reciprocal lattice. This will leave the Bloch vector as an essential tool in derivation of later results. In what follows, we assume the lattice to be square with lattice constant d, although our methods are applicable to other lattices.

We evaluate the sums $S_l^J(k,\mathbf{k}_0)$ as follows. First we have the Poisson summation formula

$$\sum_p e^{-i\mathbf{R}_p\cdot\mathbf{s}}=\left(\frac{2\pi}{d}\right)^2\sum_h \delta(\mathbf{s}-\mathbf{K}_h),$$

where $\mathbf{K}_h$, $h\in\mathbb{Z}^2$, are the reciprocal lattice vectors. Hence with $\mathbf{s}=\mathbf{k}-\mathbf{k}_0$ we have

$$1+\sum_{p\neq 0} e^{-i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{R}_p}=\left(\frac{2\pi}{d}\right)^2\sum_h \delta(\mathbf{k}-\mathbf{k}_0-\mathbf{K}_h). \tag{2}$$

Next we substitute the Bessel function expansion

$$e^{-i\mathbf{R}_p\cdot\mathbf{k}}=\sum_{l=-\infty}^{\infty}(-i)^l J_l(kR_p)e^{il(\varphi_p-\theta)}$$

into Eq. (2), where $\theta=\arg\mathbf{k}$, to get

$$1+\sum_{l=-\infty}^{\infty}(-i)^l e^{-il\theta}\sum_{p\neq 0} J_l(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}=\left(\frac{2\pi}{d}\right)^2\sum_h \delta(\mathbf{k}-\mathbf{k}_0-\mathbf{K}_h)$$

$$=\left(\frac{2\pi}{d}\right)^2\sum_h \frac{\delta(k-Q_h)\,\delta(\theta-\theta_h)}{k}, \tag{3}$$

where

$$Q_h=|\mathbf{k}_0+\mathbf{K}_h|,\qquad \theta_h=\arg\mathbf{Q}_h. \tag{4}$$

Multiplying both sides of Eq. (3) by $e^{in\theta}$ and integrating from 0 to 2π yields

$$\delta_{n,0}+(-i)^l S_l^J(k,\mathbf{k}_0)\,\delta_{n,l}=\frac{2\pi}{kd^2}\sum_h\ \delta(k-Q_h)e^{in\theta_h}, \tag{5}$$

so that

$$S_l^J(k,\mathbf{k}_0)=-\delta_{l,0}+\frac{2\pi i^l}{kd^2}\sum_h\ \delta(k-Q_h)e^{il\theta_h}. \tag{6}$$

For the $S_l^Y(k,\mathbf{k}_0)$ terms, we use a Green's function $G(\mathbf{r},\mathbf{r}';\omega,\mathbf{k}_0)$ which satisfies the inhomogeneous equation

$$\nabla^2 G+k^2 G=\sum_p\ \delta(\mathbf{r}-\mathbf{r}_s-\mathbf{R}_p), \tag{7}$$

from which we can derive (following Chin, Nicorovici, and McPhedran[6])

$$\begin{aligned} S_l J_l(k\xi)&=-H_0^{(1)}(k\xi)\,\delta_{l,0}-\frac{4i^{l+1}}{d^2}\sum_h\ \frac{J_l(Q_h\xi)}{Q_h^2-k^2}e^{il\theta_h}\\ &=-H_0^{(1)}(k\xi)\,\delta_{l,0}-\frac{4i^{l+1}}{d^2}\sum_h\ \frac{J_l(Q_h\xi)}{2Q_h}\left(\frac{1}{Q_h+k}+\frac{1}{Q_h-k}\right)e^{il\theta_h}, \end{aligned} \tag{8}$$

where $\xi=|\mathbf{r}-\mathbf{r}'|$. Using the Plemelj formula

$$\frac{1}{x-i0}=i\pi\delta(x)+\mathcal{P}\left(\frac{1}{x}\right), \tag{9}$$

we rewrite this equation as

$$\begin{aligned} S_l J_l(k\xi)&=-J_0(k\xi)\,\delta_{l,0}-iY_0(k\xi)\,\delta_{l,0}\\ &\quad-\frac{4i^{l+1}}{d^2}\sum_h\ \frac{J_l(Q_h\xi)}{2Q_h}\left(\frac{1}{Q_h+k}+i\pi\delta(k-Q_h)+\mathcal{P}\frac{1}{Q_h-k}\right)e^{il\theta_h}. \end{aligned} \tag{10}$$

Comparing Eqs. (10) and (6), we find

$$S_l^Y J_l(k\xi)=-Y_0(k\xi)\,\delta_{l,0}-\frac{4i^l}{d^2}\sum_h\ \frac{J_l(Q_h\xi)}{2Q_h}\left(\frac{1}{Q_h+k}+\mathcal{P}\frac{1}{Q_h-k}\right)e^{il\theta_h}. \tag{11}$$

The interpretation of Eqs. (6) and (11) is that the S_l^J are distributive lattice sums, with their distributive nature being concentrated around light lines, which are the trajectories $Q_h=k$ in the Brillouin zone. The S_l^Y are singular at light lines, exhibiting first order poles at each.

It is an elementary consequence of their definition (1) that the S_l^J all integrate to zero across the Brillouin zone. Hence,

$$\frac{1}{A_{BZ}}\int_{BZ}\sum_h\ \delta(k-Q_h)e^{il\theta_h}d^2\mathbf{k}_0=\frac{kd^2}{2\pi}\,\delta_{l,0}. \tag{12}$$

The only nonzero value of the right-hand side occurs for $l=0$, and is the density of states in free space subject to a period cell which is a square with side d. Hence, we see that S_0^J is associated with the free-space spectral density of states for the lattice.

III. A GENERAL EXPRESSION FOR LATTICE SUMS

We start with Eq. (6), which we multiply by a real or complex function of wavenumber $f(k)$:

$$\sum_{p\neq 0} f(k)J_l(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = -f(k)\,\delta_{l,0} + \frac{2\pi i^l}{d^2}\sum_h \frac{f(Q_h)}{Q_h}\,\delta(k-Q_h)e^{il\theta_h}. \tag{13}$$

Integrating this expression over k,

$$\sum_{p\neq 0}\left[\int_0^\infty f(k)J_l(kR_p)dk\right]e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = -\left[\int_0^\infty f(k)dk\right]\delta_{l,0} + \frac{2\pi i^l}{d^2}\sum_h \frac{f(Q_h)}{Q_h}e^{il\theta_h}, \tag{14}$$

and changing the variable in the first integration, yields

$$\sum_{p\neq 0}\left[\int_0^\infty \frac{1}{R_p}f\left(\frac{x}{R_p}\right)J_l(x)dx\right]e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = -\left[\int_0^\infty f(k)dk\right]\delta_{l,0} + \frac{2\pi i^l}{d^2}\sum_h \frac{f(Q_h)}{Q_h}e^{il\theta_h}. \tag{15}$$

The companion result to (12) is then

$$\frac{1}{A_{BZ}}\int_{BZ}\sum_h \frac{f(Q_h)}{Q_h}e^{il\theta_h}d^2\mathbf{k}_0 = \frac{d^2}{2\pi}\,\delta_{l,0}\left[\int_0^\infty f(k)dk\right]. \tag{16}$$

To apply Eqs. (14) or (15), we need choices of the function f for which, ideally, the two integrals are evaluable in closed form, and, certainly, for which they converge (in the normal sense, or in the sense of generalized functions). One convenient list of integrals is given in Chap. 11 of Abramowitz and Stegun.[7] As a first example, with

$$f(k) = k^{l+1}e^{-a^2k^2}, \tag{17}$$

from Eq. (11.4.29)[7] where $\mathrm{Re}(a^2)>0$, we obtain

$$\sum_{p\neq 0} R_p^l e^{-R_p^2/(4a^2)}e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = -\,\delta_{l,0} + \frac{2^{l+2}a^2\pi i^l}{d^2}\sum_h (a^2Q_h)^l e^{-a^2Q_h^2}e^{il\theta_h}. \tag{18}$$

This is analogous to the theta function transformation,[8] but is more general. It contains the extra distance and angle terms for $l\neq 0$, and a phase modulation present through the Bloch factor $\exp(i\mathbf{k}_0\cdot\mathbf{R}_p)$ on the left-hand side. The occurrence of $\mathbf{k}_0$ on the right-hand side is implicit via the definition of Q_h in Eq. (4). The form of (18) for $l=0$ is

$$\sum_{p\neq 0} e^{-R_p^2/(4a^2)}e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = -1 + \frac{4a^2\pi}{d^2}\sum_h e^{-a^2Q_h^2}e^{il\theta_h}. \tag{19}$$

Figure 1 shows the real and imaginary parts of the right-hand side of this relation for a particular value of a. Note the sign reversal around the edge of the Brillouin zone, and the fourfold symmetry of the function consequent on the choice of the square array for study. Note also that, as is often the case with sums connected by the Poisson summation formula, the left-hand side of Eq. (18) converges rapidly when $\mathrm{Re}(1/a^2)$ is large and positive, whereas its right-hand side converges rapidly when $\mathrm{Re}(a^2)$ is large and positive. Since both series have a common region of convergence, we were able to test Eqs. (18) and (19) numerically in particular cases.

As a second example, we use Eq. (11.4.44),[7] putting

$$f(k) = \frac{k^{l+1}}{(k^2+z^2)^{\mu+1}}, \tag{20}$$

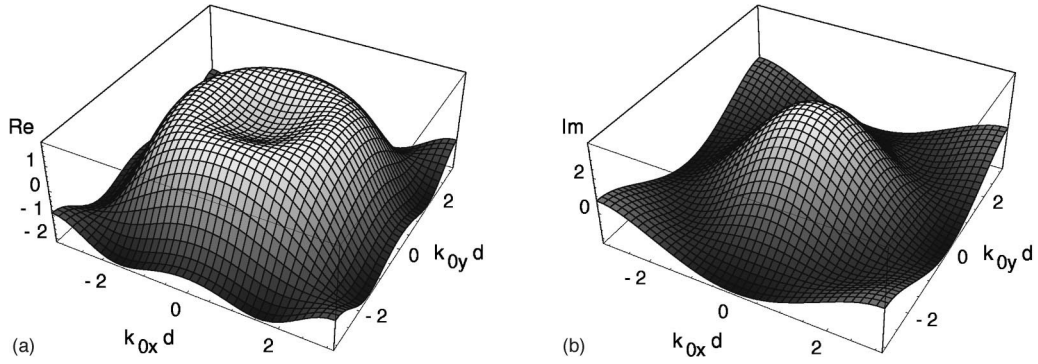

FIG. 1. Real part (left) and imaginary part (right) of Eq. (19) as a function of $k_{0x}d$ and $k_{0y}d$, for $a=0.5+0.3i$.

where $\mathrm{Re}(z)>0$, $l<2\mathrm{Re}(\mu)+3/2$, and find

$$\sum_{p\neq 0}\frac{R_p^{\mu}z^{l-\mu}}{2^{\mu}\Gamma(\mu+1)}K_{l-\mu}(R_pz)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}=-\frac{\delta_{l,0}}{2\mu z^{2\mu}}+\frac{2\pi i^l}{d^2}\sum_h\frac{Q_h^l e^{il\theta_h}}{(Q_h^2+z^2)^{\mu+1}}. \tag{21}$$

An example of the behavior of this sum is given in Fig. 2, for integer μ. For noninteger μ (real or complex), both sides of Eq. (21) exhibit branch-cut behavior. Note that the rapidity of the convergence of the left-hand side of Eq. (21) is governed by the magnitude of $\mathrm{Re}(z)$, while that of the right-hand side is governed by $\mathrm{Re}(2\mu)+2-l$. The nonzero value of l is reflected in the angular dependence in Fig. 2, which of course is different for real and imaginary parts.

As a third example, we choose $f(k)=J_{l-1}(kd)$ which leads to the discontinuous integral [Eq. (11.4.42)[7]]:

$$\int_0^{\infty}J_{l-1}(kd)J_l(kR_p)dk=\begin{cases}\dfrac{d^{l-1}}{R_p^l} & \text{if } R_p>d,\\[2ex] \dfrac{1}{2d} & \text{if } R_p=d,\end{cases} \tag{22}$$

for $l>0$. Hence,

$$d^l\sum_{R_p\neq 0}\frac{e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}}{R_p^l}=\sigma_l(\mathbf{k}_0)=\frac{d^l}{2}\sum_{R_p=d}\frac{e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}}{R_p^l}+\frac{2\pi i^l}{d}\sum_h\frac{J_{l-1}(Q_hd)e^{il\theta_h}}{Q_h}. \tag{23}$$

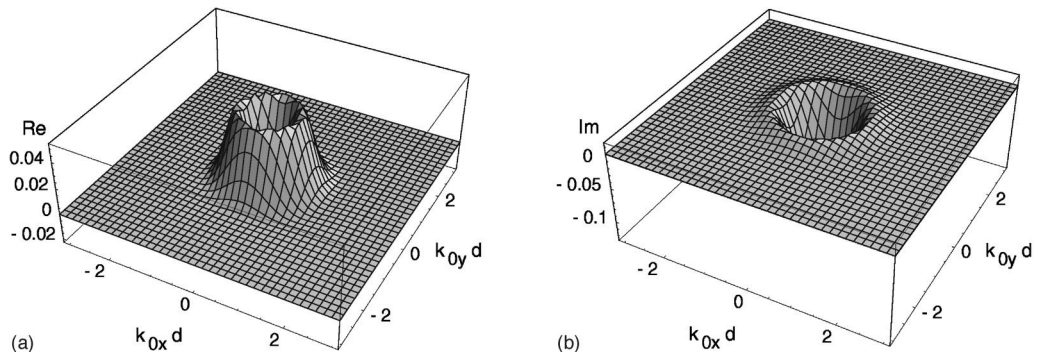

FIG. 2. Real part (left) and imaginary part (right) of Eq. (21) as a function of $k_{0x}d$ and $k_{0y}d$, for $l=2$, $\mu=5$, $z=2.18+0.82i$, $d=1$.

Here, the sums $\sigma_l(\mathbf{k}_0)$ (written here in nondimensional form) have been considered previously by McPhedran and Nicorovici,[9] who provide the following alternative expression for them:

$$\sigma_l(\mathbf{k}_0)=(2\pi i)^l\left\{\frac{1}{(2l)!!}\left[\frac{l}{\pi}\kappa^{l-2}-\kappa^l\right]+\sum_{m\geqslant 1}^{\infty}\mathcal{S}_{l-4m,4m,l}(\kappa)e^{-4im\theta_0}\right\}e^{il\theta_0}. \tag{24}$$

Here, $\kappa=k_0d/2\pi$ and

$$\mathcal{S}_{l,4m,n}(\xi)=\frac{1}{d^n}\sum_{K_h\neq 0}\frac{J_l(K_h\xi)}{K_h^n}e^{i4m\psi_h}. \tag{25}$$

McPhedran and Nicorovici[9] provide graphs of $\sigma_1,\ldots,\sigma_6$ across the first Brillouin zone. Note that, from (24), σ_1 has a first-order singularity as $k_0\to 0$.

IV. POWERS OF RADIAL DISTANCE

We now consider the applications of Eqs. (14) and (16) to complex powers s of the radial distance. The analysis is more difficult than in Sec. III, principally because of the occurrence of an undefined integral which arises in a straightforward application of (14). We will use raising and lowering operators to remove this difficulty.

We rely on results obtained using the methods of the theory of distributions from Chap. 7 of Jones,[10] and in particular

$$\int_{-\infty}^{\infty}r^{\beta}e^{-i\boldsymbol{\alpha}\cdot\mathbf{x}}d\mathbf{x}=2\pi\int_0^{\infty}r^{\beta+1}J_0(\alpha r)dr=\frac{(\frac{1}{2}\beta)!2^{\beta+2}\pi}{(-\frac{1}{2}\beta-1)!\alpha^{\beta+2}}, \tag{26}$$

valid when $\beta\neq 2m$ and $\beta\neq -2-2m$ $(m=0,1,2,\ldots)$. Hence, if $s\neq 2m-1$ or $-1-2m$,

$$\int_0^{\infty}r^sJ_0(\alpha r)dr=\frac{\Gamma(\frac{1}{2}+\frac{1}{2}s)2^s}{\Gamma(\frac{1}{2}-\frac{1}{2}s)\alpha^{1+s}}. \tag{27}$$

By differentiation under the integral sign in (27), and use of Bessel function recurrence relations, we obtain Weber's integral:

$$\int_0^{\infty}r^sJ_l(\alpha r)dr=\frac{\Gamma\left(\dfrac{1+l+s}{2}\right)2^s}{\Gamma\left(\dfrac{1+l-s}{2}\right)\alpha^{1+s}}, \tag{28}$$

provided $1+l\pm s$ is not a negative even integer.

Hence, if we put

$$f(k)=k^s \tag{29}$$

in Eq. (14), we obtain for nonzero l,

$$2^s\Gamma\left(\frac{l+1+s}{2}\right)\sum_{p\neq 0}\frac{e^{i\mathbf{k}_0\cdot\mathbf{R}_p}e^{il\varphi_p}}{R_p^{1+s}}=\frac{2\pi i^l}{d^2}\Gamma\left(\frac{l+1-s}{2}\right)\left(\frac{e^{il\theta_0}}{k_0^{1-s}}+\sum_{h\neq 0}\frac{e^{il\theta_h}}{Q_h^{1-s}}\right). \tag{30}$$

For $l=0$, we can write the result formally:

$$2^s\Gamma\left(\frac{1+s}{2}\right)\sum_{p\neq 0}\frac{e^{i\mathbf{k}_0\cdot\mathbf{R}_p}}{R_p^{1+s}}=\Gamma\left(\frac{1-s}{2}\right)\int_0^{\infty}k^sdk+\frac{2\pi}{d^2}\Gamma\left(\frac{1-s}{2}\right)\left(\frac{1}{k_0^{1-s}}+\sum_{h\neq 0}\frac{1}{Q_h^{1-s}}\right), \tag{31}$$

but the expression (31) is nugatory because of the presence of the first integral on the right-hand side. Hence, we approach the case $l=0$ by a different argument.

A. Definition of phased lattice sums

Let us extend the definition of (23) to nonintegral powers of the distance

$$\sigma_{1+s}^{m}(\mathbf{k}_0)=d^{1+s}\sum_{p\neq 0}\frac{\exp(im\varphi_p)}{R_p^{1+s}}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}. \tag{32}$$

Here, the lattice sum subscript $1+s$ is taken to be real or complex, while the superscript m must be integral, if the angular factor $\exp(im\varphi_p)$ is to be continuous at $\varphi_p=2\pi$. Note that the Bloch sums $\sigma_{1+s}^{m}(\mathbf{k}_0)$ are absolutely convergent if $\mathrm{Re}(s)>1$, conditionally convergent if $\mathrm{Re}(s)=1$, and divergent otherwise. We seek their analytic continuations across the whole complex plane of s, and knowledge of their poles and zeros. Further, note that in the region of absolute convergence, $\sigma_{1+s}^{m}(\mathbf{k}_0)$ is zero for the square array unless m is a multiple of four. Also, the sums for positive and negative m are equivalent. In what follows, we will use the compact notation $\sigma_{1+s}^{(m)}$ for $\sigma_{1+s}^{m}(0)$.

We expand the phase factor in (32) in terms of its Bessel function series, and obtain

$$\sigma_{1+s}^{m}(\mathbf{k}_0)=i^m e^{im\theta_0}d^{1+s}\sum_{n}\sum_{p\neq 0}\frac{J_{m+4n}(k_0R_p)e^{4in\varphi_p}}{R_p^{1+s}}. \tag{33}$$

We re-express (33) in terms of the dimensionless lattice sums studied by Nicorovici *et al.*:[11]

$$\sigma_{1+s}^{m}(\mathbf{k}_0)=i^m(2\pi)^{1+s}e^{im\theta_0}\sum_{n}\mathcal{S}_{m+4n,4n,1+s}(\kappa)e^{4in\theta_0}, \tag{34}$$

where $\kappa=k_0d/(2\pi)$ and

$$\mathcal{S}_{m+4n,4n,1+s}(\kappa)=\sum_{h\neq 0}\frac{J_{m+4n}(\kappa K_h d)e^{4in\psi_h}}{(K_h d)^{1+s}} \tag{35}$$

is expressed as a reciprocal lattice sum.

The treatment of the sums $\mathcal{S}$ in Ref. 11 separates the sums with $n=0$ from those with $n\neq 0$. In the first case, the Weber–Schafheitlin integral[7] is used in connection with the Poisson summation formula to give

$$\mathcal{S}_{m,0,1+s}(\kappa)=\kappa^{s-1}\frac{2^{-(s+1)}\Gamma((m-s+1)/2)}{\pi\Gamma((m+s+1)/2)}+\sum_{p\neq 0}\frac{d^{m-s+1}\kappa^m\Gamma((m-s+1)/2)}{2^{s+1}\pi R_p^{m-s+1}\Gamma(m+1)\Gamma((s+1-m)/2)}$$
$$\times{}_2F_1\left(\frac{m-s+1}{2},\frac{m-s+1}{2};m+1;\frac{\kappa^2d^2}{R_p^2}\right). \tag{36}$$

Expanding the hypergeometric function, we obtain

$$\mathcal{S}_{m,0,1+s}(\kappa)=\kappa^{s-1}\frac{2^{-(s+1)}\Gamma((m-s+1)/2)}{\pi\Gamma((m+s+1)/2)}+\frac{\kappa^m\sin\pi(s+1-m)/2}{\pi^2 2^{s+1}}$$
$$\times\sum_{l=0}^{\infty}\frac{[\Gamma((m-s+1)/2+l)]^2}{(m+l)!\,l!}\kappa^{2l}\sigma_{2l+m+1-s}^{(0)}. \tag{37}$$

The conditions required in the manipulations leading to (37) were $\mathrm{Re}(m-s-1)>0$, $\mathrm{Re}(s)>-1/2$ and $\kappa<1$. As far as the last is concerned, κ does not exceed $1/\sqrt{2}$ in the Brillouin zone. As

far as the first two are concerned, we shall see that the right-hand side of the expression (37) provides an analytic continuation of the left-hand side for all integral values of m and complex values of s.

The sums $\sigma^{(0)}_{2l+m+1-s}$ were evaluated analytically by Hardy,[12–14] in a form valid throughout the complex plane

$$\sigma^{(0)}_{1+s}=d^{1+s}\sum_{p\neq 0}\frac{1}{R_p^{1+s}}=4\zeta\left(\frac{1+s}{2}\right)\beta\left(\frac{1+s}{2}\right). \tag{38}$$

Here, $\zeta(s)$ is the Riemann zeta function [Eq. (23.2.1) in Ref. 7], while

$$\beta(s)=\sum_{n=0}^{\infty}(-1)^n(2n+1)^{-s}=2^{-s}\Phi(-1,s,1/2)=\frac{1}{4^s}\left(\zeta\left(s,\frac{1}{4}\right)-\zeta\left(s,\frac{3}{4}\right)\right) \tag{39}$$

is the Catalan beta function [Eq. (23.2.21) in Ref. 7], which may be defined in terms of the Lerch phi function and the Hurwitz zeta function, respectively. We will need the following reflection formula[13]

$$\pi^{-(1+s)/2}\zeta\left(\frac{1+s}{2}\right)\beta\left(\frac{1+s}{2}\right)\Gamma\left(\frac{1+s}{2}\right)=\pi^{-(1-s)/2}\zeta\left(\frac{1-s}{2}\right)\beta\left(\frac{1-s}{2}\right)\Gamma\left(\frac{1-s}{2}\right). \tag{40}$$

We consider next the sums $\mathcal{S}$ with $n\neq 0$. The treatment from Ref. 11 again uses the Weber–Schafheitlin integral, and gives (if $s\neq l-1$)

$$\mathcal{S}_{l,4m,s+1}(\kappa)=\frac{1}{2^{s+1}\pi\Gamma(1-w+4m)\Gamma(w-4m)}\sum_{q=0}^{\infty}\frac{\Gamma(w+q)\Gamma(w-4m+q)}{q!(q+l)!}\sigma^{(4m)}_{2q+l-s+1}\kappa^{2q+l}, \tag{41}$$

where $w=2m+(l+1-s)/2$.

We now return to (34):

$$\sigma^0_{1+s}(\mathbf{k}_0)=(2\pi)^{1+s}\left[\mathcal{S}_{0,0,1+s}(\kappa)+2\sum_{n=1}^{\infty}\mathcal{S}_{4n,4n,1+s}(\kappa)\cos(4n\theta_0)\right]. \tag{42}$$

Using (37) and (41), this gives

$$\begin{aligned}\sigma^0_{1+s}(\mathbf{k}_0)=(2\pi)^{1+s}\Bigg\{&\frac{\kappa^{s-1}\Gamma((1-s)/2)}{\pi 2^{s+1}\Gamma((1+s)/2)}+\frac{\sin\pi(s+1)/2}{\pi^2 2^{s+1}}\sum_{l=0}^{\infty}\left[\frac{\Gamma((2l+1-s)/2)}{l!}\right]^2\kappa^{2l}\sigma^{(0)}_{2l+1-s}\\&+2\sum_{n=1}^{\infty}\frac{\cos 4n\theta_0}{2^{s+1}\pi\Gamma((1-s)/2)\Gamma((1+s)/2)}\\&\times\sum_{q=0}^{\infty}\frac{\Gamma(4n+q+(1-s)/2)\Gamma(q+(1-s)/2)}{q!(q+4n)!}\sigma^{(4n)}_{2q+4n-s+1}\kappa^{2q+4n}\Bigg\}.\end{aligned} \tag{43}$$

The term in κ^{s-1} in fact cancels the second term on the right-hand side of (31). This suggests the identification

$$\frac{2\pi}{d^2}\frac{\Gamma\left(\frac{1-s}{2}\right)}{2^s\Gamma\left(\frac{1+s}{2}\right)}\sum_{h\neq 0}\frac{1}{Q_h^{1-s}}=\left(\frac{2\pi}{d}\right)^{1+s}\left\{\frac{\sin\pi(s+1)/2}{\pi^2 2^{s+1}}\sum_{l=0}^{\infty}\left[\frac{\Gamma((2l+1-s)/2)}{l!}\right]^2\kappa^{2l}\sigma^{(0)}_{2l+1-s}\right.$$
$$+2\sum_{n=1}^{\infty}\frac{\cos 4n\theta_0}{2^{s+1}\pi\Gamma((1-s)/2)\Gamma((1+s)/2)}$$
$$\left.\times\sum_{q=0}^{\infty}\frac{\Gamma(4n+q+(1-s)/2)\Gamma(q+(1-s)/2)}{q!(q+4n)!}\sigma^{(4n)}_{2q+4n-s+1}\kappa^{2q+4n}\right\}. \tag{44}$$

Let us define a nondimensional lattice sum over the reciprocal lattice by analogy with (32):

$$\rho^0_{1-s}(\mathbf{k}_0)=\left(\frac{2\pi}{d}\right)^{1-s}\sum_{h\neq 0}\frac{1}{Q_h^{1-s}}. \tag{45}$$

Then, from (44),

$$\rho^0_{1-s}(\mathbf{k}_0)=\sigma^{(0)}_{1-s}+\sum_{l=1}^{\infty}\left[\frac{\Gamma((2l+1-s)/2)}{l!\Gamma((1-s)/2)}\right]^2\kappa^{2l}\sigma^{(0)}_{2l+1-s}+2\sum_{n=1}^{\infty}\frac{\cos 4n\theta_0}{(\Gamma((1-s)/2))^2}$$
$$\times\sum_{q=0}^{\infty}\frac{\Gamma(4n+q+(1-s)/2)\Gamma(q+(1-s)/2)}{q!(q+4n)!}\sigma^{(4n)}_{2q+4n-s+1}\kappa^{2q+4n}. \tag{46}$$

If we examine the various terms in (46), we see that the part independent of θ_0 is defined for all complex values of s, while in the part dependent on θ_0 convergence is limited by the term $\sigma^{(4)}_{5-s}$ to the region $\mathrm{Re}(s)<3$.

Note that Eq. (46) can be obtained directly from the definition (45). The inverse power of the distance is expanded via the expression (22.9.3) from Abramowitz and Stegun,[7] while the ultraspherical functions occurring in the expansion are expressed using (22.3.12).

B. Raising and lowering operators

We can transform the angular and radial variations in these sums using the following raising and lowering operators:

$$\mathcal{R}=\frac{-i}{d}\left(\frac{\partial}{\partial k_{0x}}+i\frac{\partial}{\partial k_{0y}}\right)=\frac{-i}{2\pi}e^{i\theta_0}\left(\frac{\partial}{\partial\kappa}+\frac{i}{\kappa}\frac{\partial}{\partial\theta_0}\right) \tag{47}$$

and

$$\mathcal{L}=\frac{-i}{d}\left(\frac{\partial}{\partial k_{0x}}-i\frac{\partial}{\partial k_{0y}}\right)=\frac{-i}{2\pi}e^{-i\theta_0}\left(\frac{\partial}{\partial\kappa}-\frac{i}{\kappa}\frac{\partial}{\partial\theta_0}\right). \tag{48}$$

Then, by direct differentiation, we find

$$\mathcal{L}\sigma^m_{1+s}(\mathbf{k}_0)=\sigma^{m-1}_s(\mathbf{k}_0),\quad \mathcal{R}\sigma^m_{1+s}(\mathbf{k}_0)=\sigma^{m+1}_s(\mathbf{k}_0). \tag{49}$$

Again by direct differentiation,

$$\mathcal{L}\rho^m_{1-s}(\mathbf{k}_0)=\frac{(m-s-1)}{2\pi i}\rho^{m-1}_{2-s}(\mathbf{k}_0),\quad \mathcal{R}\rho^m_{1-s}(\mathbf{k}_0)=\frac{-(m+1-s)}{2\pi i}\rho^{m+1}_{2-s}(\mathbf{k}_0). \tag{50}$$

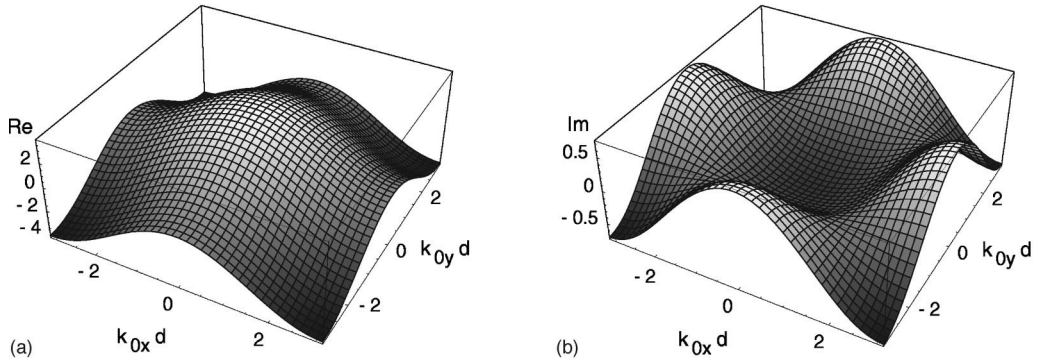

FIG. 3. Real part (left) and imaginary part (right) of $\sigma^0_{1+s}(k_{0x},k_{0y})$, for $s=4.128+5.073i$.

Let us rewrite Eq. (30):

$$2^s\Gamma((l+1+s)/2)\sigma^l_{1+s}(\mathbf{k}_0)=(2\pi)^s i^l\Gamma((l+1-s)/2)[e^{il\theta_0}\kappa^{s-1}+\rho^l_{1-s}(\mathbf{k}_0)]. \tag{51}$$

Then, we can verify using (49) and (50) that $\mathcal{L}$ transforms l in this equation to $l-1$ and s to $s-1$. If we apply $\mathcal{L}$ to (51) with $l=1$, we obtain

$$\Gamma((1+s)/2)\sigma^0_{1+s}(\mathbf{k}_0)=\pi^s\Gamma((1-s)/2)[\kappa^{s-1}+\rho^0_{1-s}(\mathbf{k}_0)]. \tag{52}$$

This is Eq. (31), with the nugatory integral replaced by zero.

Hence, if $\mathrm{Re}(s)>1$, we have in the limit as $\kappa\to 0$ in (52):

$$\begin{aligned}\Gamma((1+s)/2)\sigma^0_{1+s}(0)&=4\Gamma((1+s)/2)\beta((1+s)/2)\zeta((1+s)/2)\\&=\pi^s\Gamma((1-s)/2)\rho^0_{1-s}(0)\\&=4\pi^s\Gamma((1-s)/2)\beta((1-s)/2)\zeta((1-s)/2).\end{aligned} \tag{53}$$

The equality of the left- and right-hand sides of (53) is guaranteed by the reflection formula (40). If $\mathrm{Re}(s)<1$, we know from (46) that $\rho^0_{1-s}(\mathbf{k}_0)$ continues to behave continuously at the center of the Brillouin zone, while $\sigma^0_{1+s}(\mathbf{k}_0)$ develops a singularity there.

We give an example of the behavior of σ^0_{1+s} across the Brillouin zone in Fig. 3. The value of s chosen permits rapid direct evaluation of the sum using the definition (32). We can also use (46) and (52), with the two methods agreeing to the accuracy of the determination of the lattice sums $\sigma^{(4n)}_{2q+4n-s+1}$. For the latter, we need to use the Macdonald function series for the sums with $n=1$ derived in the Appendix. We note in Fig. 3 that the real and imaginary parts of σ^0_{1+s} are fourfold symmetric, and their normal derivatives are zero both at the edges of the Brillouin zone, and on the lines $k_{0x}=0$ and $k_{0y}=0$.

From the definition of $\sigma^m_{1+s}(\mathbf{k}_0)$, we see that

$$\int_{BZ}\sigma^m_{1+s}(\mathbf{k}_0)d^2\mathbf{k}_0=0. \tag{54}$$

Using the Laplacian operator with respect to $\mathbf{k}_0$, we note that

$$\nabla^2\sigma^m_{1+s}(\mathbf{k}_0)=-d^2\sigma^m_{s-1}(\mathbf{k}_0). \tag{55}$$

Using this, we see that the property (54) is guaranteed if the normal derivative vanishes at the edge of the Brillouin zone:

$$\int_{BZ}\sigma_{1+s}^{m}(\mathbf{k}_0)d^2\mathbf{k}_0=\frac{1}{d^2}\int_{BZ}\nabla^2\sigma_{3+s}^{m}(\mathbf{k}_0)d^2\mathbf{k}_0=\frac{1}{d^2}\int_{BBZ}\frac{\partial\sigma_{3+s}^{m}(\mathbf{k}_0)}{\partial n}dl, \tag{56}$$

with the last integral running over the boundary of the Brillouin zone, of which dl denotes an element of length, and the partial derivative is taken along the outward normal to the boundary.

We can deduce an interesting relation from (51), if we assume $\mathrm{Re}(s)>1$ and let $\kappa\to 0$:

$$\Gamma\left(\frac{4l+1+s}{2}\right)\sigma_{1+s}^{4l}(0)=\pi^s\Gamma\left(\frac{4l+1-s}{2}\right)\rho_{1-s}^{4l}(0). \tag{57}$$

This suggests the following reflection formula:

$$\frac{1}{\pi^{(4l+1+s)/2}}\Gamma\left(\frac{4l+1+s}{2}\right)\sigma_{1+s}^{(4l)}=\frac{1}{\pi^{(4l+1-s)/2}}\Gamma\left(\frac{4l+1-s}{2}\right)\sigma_{1-s}^{(4l)}, \tag{58}$$

so that, if we define the function

$$G_{4l}\left(\frac{s}{2}\right)=\frac{1}{\pi^{(4l+1+s)/2}}\Gamma\left(\frac{4l+1+s}{2}\right)\sigma_{1+s}^{(4l)}, \tag{59}$$

then G_{4l} is even in s. In the Appendix we comment on verifications of this formula for the case $l=1$.

V. LATTICE SUM IDENTITIES

We commence with (32). We evaluate the partial derivative of this with respect to k_{0x}, set $k_{0x}=\pi/d$, and put $\mathbf{R}_p=(X_p,Y_p)$. The result is, for a sum of even order,

$$\left.\frac{\partial\sigma_{1+s}^{2m}}{\partial k_{0x}}\right|_{k_{0x}=\pi/d}=id^{1+s}\sum_{p\neq 0}\frac{X_p e^{2im\varphi_p}}{R_p^{1+s}}e^{i(\pi X_p/d+k_{0y}Y_p)}. \tag{60}$$

We evaluate the contribution to this sum from four points in the lattice at equal distances from the origin: (X_p,Y_p), $(-X_p,-Y_p)$, $(-X_p,Y_p)$ and $(X_p,-Y_p)$. These collectively give

$$\frac{-4X_p\, i\, d^{1+s}}{R_p^{1+s}}e^{i\pi X_p/d}\sin(k_{0y}Y_p)\sin(2m\varphi_p). \tag{61}$$

Hence, we arrive at two lattice sum identities:

$$\left.\frac{\partial\sigma_{1+s}^{0}}{\partial k_{0x}}\right|_{k_{0x}=\pi/d}=0 \tag{62}$$

and

$$\left.\frac{\partial}{\partial k_{0x}}[\sigma_{1+s}^{2m}+\sigma_{1+s}^{-2m}]\right|_{k_{0x}=\pi/d}=0. \tag{63}$$

These identities hold for all values of k_{0y} ranging from $-\pi/d$ to π/d.

We will concentrate here on (62). We note that this guarantees that the integral of σ_{1+s}^{0} over the Brillouin zone is zero [see (55) and (56)]. Using (46) and (52), (62) becomes

$$\frac{(s-1)}{2}\kappa^{s-3}+\sum_{l=1}^{\infty} l\left[\frac{\Gamma((2l+1-s)/2)}{l!\Gamma((1-s)/2)}\right]^2\kappa^{2l-2}\sigma^{(0)}_{2l+1-s}$$
$$+2\sum_{n=1}^{\infty}\sum_{q=0}^{\infty}\frac{\Gamma((8n+2q+1-s)/2)\Gamma((2q+1-s)/2)q}{q!(q+4n)![\Gamma((1-s)/2)]^2}\sigma^{(4n)}_{2q+4n+1-s}\kappa^{2q+4n-2}\cos(4n\theta_0)$$
$$+8\sum_{n=1}^{\infty}\sum_{q=0}^{\infty}\frac{\Gamma((8n+2q+1-s)/2)\Gamma((2q+1-s)/2)n}{q!(q+4n)![\Gamma((1-s)/2)]^2}\sigma^{(4n)}_{2q+4n+1-s}\kappa^{2q+4n-1}$$
$$\times\cos((4n-1)\theta_0)=0. \tag{64}$$

This identity is to be applied for

$$\kappa^2=(\tfrac{1}{4}+\kappa_y^2),\quad \kappa\cos\theta_0=\tfrac{1}{2},\quad \kappa_y\in[-\tfrac{1}{2},\tfrac{1}{2}]. \tag{65}$$

The sums in (64) are of hypergeometric form and converge absolutely provided $\kappa<1$, where of course the largest value of κ encountered in the Brillouin zone is $1/\sqrt{2}$. However, the sums do converge more slowly and become increasingly badly conditioned numerically as $|s|$ increases, due to the gamma function ratios in them. If we put $\kappa_y=0$ in (64), we obtain

$$\sigma^{(0)}_{1-s}=\frac{\Gamma((-1-s)/2)}{2^{s-1}\Gamma((1-s)/2)}-\sum_{l=2}^{\infty}\left(\frac{\Gamma((2l-s-1)/2)}{\Gamma((1-s)/2)}\right)^2\frac{\sigma^{(0)}_{2l-1-s}}{l!(l-1)!2^{2l-2}}$$
$$-\sum_{n=1}^{\infty}\sum_{q=0}^{\infty}\frac{\Gamma((8n+2q-1-s)/2)\Gamma((2q-1-s)/2)}{(\Gamma((1-s)/2))^2q!(q+4n)!2^{2q+4n-2}}(2q+4n)\sigma^{(4n)}_{2q+4n-1-s}. \tag{66}$$

This equation is also obtainable from the symmetry property that σ^1_{1+s} is zero for $\kappa_x=1/2$ and $\kappa_y=0$.

The convergence of the series on the right-hand side of (66) may be accelerated somewhat by re-expressing nearest neighbor terms in their original form. Let us define

$$\tilde{\sigma}^{(4n)}_{2q+4n+1-s}=\sigma^{(4n)}_{2q+4n+1-s}-d^{2q+4n+1-s}\sum_{p\in\mathcal{N}}\frac{e^{4in\varphi_p}}{R_p^{2q+4n+1-s}}, \tag{67}$$

where $\mathcal{N}$ denotes a set of nearest neighbors of the origin. For $2q+4n$ large, the sums $\tilde{\sigma}^{(4n)}_{2q+4n+1-s}$ can be evaluated by direct summation:

$$\tilde{\sigma}^{(4n)}_{2q+4n+1-s}=d^{2q+4n+1-s}\sum_{p\in\bar{\mathcal{N}}}\frac{e^{4in\varphi_p}}{R_p^{2q+4n+1-s}}, \tag{68}$$

where $\bar{\mathcal{N}}$ denotes the complement of $\mathcal{N}$ in the lattice. Then (66) can be rewritten

$$\tilde{\sigma}^{(0)}_{1-s}=\frac{-1}{(s+1)2^{s-2}}-\sum_{l=2}^{\infty} l\left(\frac{\Gamma((2l-s-1)/2)}{l!\Gamma((1-s)/2)}\right)^2\frac{\tilde{\sigma}^{(0)}_{2l-1-s}}{2^{2l-2}}$$
$$-\sum_{n=1}^{\infty}\sum_{q=0}^{\infty}\frac{\Gamma((8n+2q-1-s)/2)\Gamma((2q-1-s)/2)}{(\Gamma((1-s)/2))^2q!(q+4n)!2^{2q+4n-2}}(2q+4n)\tilde{\sigma}^{(4n)}_{2q+4n-1-s}$$
$$-\frac{4}{s+1}\sum_{h\in NN}\frac{h_x+1/2}{[(h_x+1/2)^2+h_y^2]^{(1-s)/2}}. \tag{69}$$

Numerical studies has shown that (69) is numerically better-conditioned than (66). However, both become less and less useful as $\mathrm{Im}(s)$ increases in the region where $\mathrm{Re}(s)$ is close to zero, with the

summations generating larger and larger initial terms which have to be cancelled by later terms. Thus, it seems that the lattice sum identities described here have more analytic than numeric interest.

VI. PROPERTIES OF THE SUM $\sigma^{(0)}$

We start with the expansion (A3) from the Appendix, which we consider for the square array $(d_1=d_2)$, and write in symmetric form:

$$G_0(s)=f_1(s)+8\sum_{p_1,p_2=1}^{\infty}\left(\frac{p_2}{p_1}\right)^s K_s(2\pi p_1 p_2)\overset{\text{def}}{=}f_1(s)+f_2(s), \tag{70}$$

where

$$f_1(s)=2\zeta(2s+1)\frac{\Gamma(s+1/2)}{\pi^{s+1/2}}+2\zeta(2s)\frac{\Gamma(s)}{\pi^s}. \tag{71}$$

Equation (70) links three analytic functions, all of which are even functions of s, are real on $\mathrm{Re}(s)=0$ and also real on $\mathrm{Im}(s)=0$. Note that $G_0(s)$ has $s=\pm 1/2$ as its only poles, and these have residue ± 1 respectively. The same property applies to $f_1(s)$, while $f_2(s)$ is regular in the finite part of the plane. Our purpose here is to provide numerical and analytical data on the order of these three functions, and on the distribution of their zeros.

A. Lindelöf analysis

We start with the order of $\zeta(s)$ and $\beta(s)$. Writing the argument of each in the standard form $s=\sigma+it$, we wish to know their behavior as $t\to\infty$, as a function of σ. We write

$$\zeta(\sigma+it)=O(t^{\mu(\sigma)}),\quad \beta(\sigma+it)=O(t^{\nu(\sigma)}), \tag{72}$$

where we are interested in the smallest values μ and ν for which the order assignments are valid. As discussed by Titchmarsh,[15] Lindelöf's hypothesis is that

$$\mu(\sigma)=\begin{cases}\frac{1}{2}-\sigma & \text{for } \sigma\leqslant\frac{1}{2},\\ 0 & \text{for } \sigma>\frac{1}{2},\end{cases} \tag{73}$$

where $\mu(\sigma)$ is continuous, nonincreasing, convex downwards and never negative. Glasser[13] has provided order estimates for $\beta(s)$.

Our procedure will be numerical, and so we are in a position to investigate somewhat stronger statements than the order of each function—i.e., typically we will seek both powers and coefficients of the leading term. Our first investigation will be into the asymptotics of locally smoothed functions, to establish statements which we will denote

$$|\zeta(\sigma+it)|\bar{\sim}C_\zeta t^{\mu(\sigma)},\quad |\beta(\sigma+it)|\bar{\sim}C_\beta t^{\nu(\sigma)}, \tag{74}$$

using the bar over the asymptotic sign to denote a leading term on average.

To investigate numerically the order of the smoothed functions $\zeta(\sigma+it)$ and $\beta(\sigma+it)$, we plot the logarithm of the absolute value of the function in question, as a function of t, divided by t^p, for a test power p. To smooth the plot somewhat, we average the result over a significant number of neighboring points. The value of p is chosen to deliver as flat a plot as possible, and then C is obtained using a growing average over all the points on the first graph. This procedure is illustrated in Fig. 4, for $\sigma=0.3$. The results are in keeping with Lindelöf's hypothesis, and furthermore indicate that the exponents for ζ and β are equal to computational accuracy.

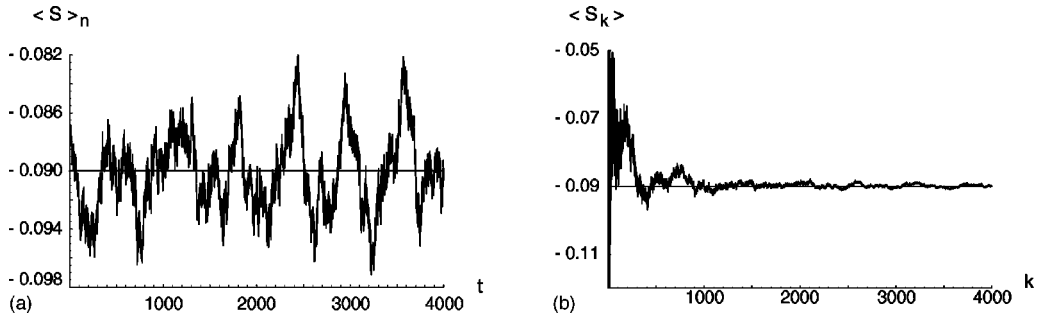

FIG. 4. Averages of the sequence $S=\{S(t)\mid t=1,\ldots,4800\}$, where $S(t)=\log(|\beta(0.3+i\,t)|)/t^{0.20}$. Left: the moving average $\langle S\rangle_n(t)=(S(t)+S(t+1)+\cdots+S(t+n))/n$, with $n=800$. Right: the averages of the sequences $S_k=\{S(t)\mid t=1,\ldots,k\}$ for $k=1,\ldots,4000$. Its values near the end of the sample give the value (-0.090) reported in Table I.

Table I shows the numerical estimates for the coefficients C, for $\sigma\leqslant 0.5$. Above this limit, the coefficients are unity to computational accuracy. The coefficients in fact bear a constant ratio (around 58.7), to the accuracy of their determination. We thus have the augmented Lindelöf hypothesis:

$$\mu(\sigma)=\nu(\sigma)=\begin{cases}\frac{1}{2}-\sigma & \text{for } \sigma\leqslant\frac{1}{2},\\ 0 & \text{for } \sigma>\frac{1}{2}.\end{cases} \tag{75}$$

Note that the truth of the Riemann hypothesis implies that of the Lindelöf hypothesis, but not the contrary.[15]

Assuming $C_\zeta=1$ and $C_\beta=1$ for $\sigma\geqslant 1/2$, we can use the reflection formulas for these functions to arrive at

$$C_\beta=\left(\frac{2}{\pi}\right)^{1/2-\sigma},\quad C_\zeta=\left(\frac{1}{\pi}\right)^{1/2-\sigma},\quad \sigma\leqslant 1/2. \tag{76}$$

This result is illustrated in Table I, where the difference between numerical results and the formulas (76) evidently illustrates the accuracy of the former.

Our second numerical procedure is to find the minimum value of the modulus of a function such as $\log(|\zeta(1/2+\delta+it)|/t^\mu)$, for t ranging over N equally spaced values between $n-1/2$ and $n+1/2$. This minimum value is plotted as a function of n, and the exponent μ chosen to yield as flat a graph as possible, for a range of values of δ. The exponent values resulting for both ζ and β are again found to be equal, and in accord with (75).

If we consider $G_0(s)$, using (75) and (76), we have

TABLE I. The coefficients of the leading terms in ζ and β.

σ	$\log C_\zeta$	(76)	$\log C_\beta$	(76)
−3.0	−6.431	−6.433	−1.579	−1.581
−2.0	−4.594	−4.595	−1.128	−1.129
−1.0	−2.760	−2.756	−0.677	−0.677
0.0	−0.920	−0.919	−0.226	−0.226
0.1	−0.737	−0.735	−0.181	−0.181
0.2	−0.553	−0.551	−0.135	−0.135
0.3	−0.370	−0.368	−0.090	−0.090
0.4	−0.186	−0.184	−0.043	−0.045
0.5	<0.005	0	<0.015	0

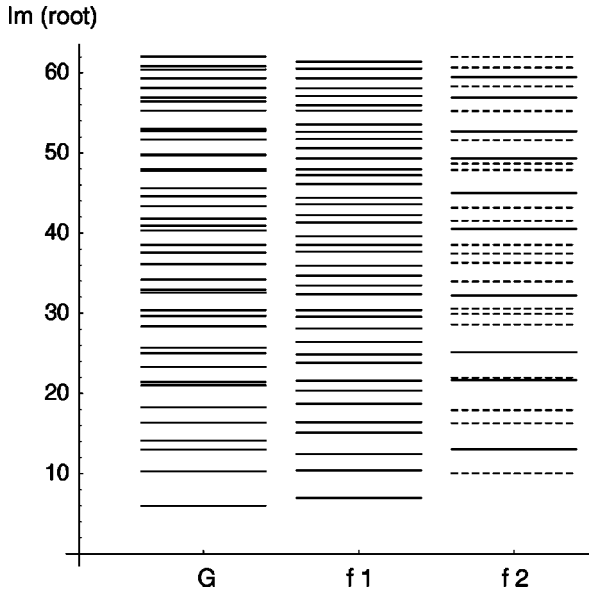

FIG. 5. Imaginary parts of the roots of $G(s)$, $f_1(s)$ and $f_2(s)$. For the first two, all roots have $\mathrm{Re}(s)=0$, while for the third function, those with this property are indicated by dashed lines, and those off the line by solid lines. Note that the roots off the critical line come in pairs, with equal imaginary parts and opposite real parts.

$$|G_0(\sigma+it)| \sim 4\left|\frac{\Gamma(1/2+\sigma+it)}{\pi^{1/2+\sigma+it}}\right| \sim 4\sqrt{2}\left(\frac{t}{\pi}\right)^{\sigma} e^{-\pi t/2}, \tag{77}$$

for $\sigma>0$ and $t>0$. Since $G_0(s)$ is even, (77) holds for with $|\sigma|$ replacing σ.

B. Distributions of zeros

We next consider the distributions of zeros of G_0, f_1, and f_2. We have numerically determined the zeros up to modulus of the argument around 60 using an algorithm based on the argument principle.[16] We have found that the zeros of G_0 and f_1 both lie on the line $\mathrm{Re}(s)=0$, while those of f_2 are mixed, with some lying on the critical line and others not. The imaginary parts of the roots found are shown in Fig. 5, while the roots of f_2 are shown in Fig. 6. Note that about half the roots of f_2 shown lie on $\mathrm{Re}(s)=0$. The roots of $G_0(s)$ are associated with those of $\beta(s+1/2)$ and $\zeta(s+1/2)$, with the former having around twice the density of roots of the latter. It is to be noted that the zeros of $f_1(s)$ occur for points where the arguments of the two zeta functions do not have $\mathrm{Re}(s)=1/2$. At these points, if we write

$$f_1(s)=f_1^+(s)+f_1^-(s), \quad f_1^+(s)=2\zeta(1+2s)\frac{\Gamma(1/2+s)}{\pi^{1/2+s}},$$

$$f_1^-(s)=2\zeta(1-2s)\frac{\Gamma(1/2-s)}{\pi^{1/2-s}}, \tag{78}$$

then we find the roots exhibited have the property that

$$\mathrm{Re}(f_1^+)=0=\mathrm{Re}(f_1^-), \quad \mathrm{Im}(f_1^+)=-\mathrm{Im}(f_1^-). \tag{79}$$

Given that the function $f_2(s)$ has zeros off the critical line, it is interesting to compare the order of this function with that of $G_0(s)$. Using the same method as described in the previous sub-section, we have verified that the function $f_2(\sigma+it)\exp(\pi t/2)$ scales as t^{σ} for large and positive σ. In Fig. 7 we compare the asymptotic order for the two functions $G_0(\sigma$

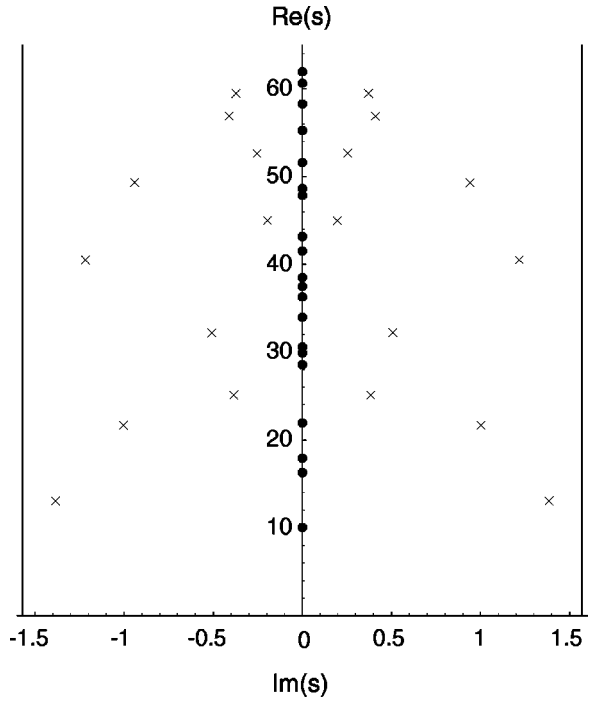

FIG. 6. Distribution of the lowest roots of $f_2(s)$ for $\mathrm{Re}(s) \in [-\pi/2, \pi/2]$ (the limits of this interval are shown by the lateral vertical lines. The roots on the imaginary axis are marked by dots.

$+it)\exp(\pi t/2)/t^{\sigma}$ or $4\sqrt{2}/\pi^{\sigma}$, from (77), and $f_2(\sigma+it)\exp(\pi t/2)/t^{\sigma}$. Note the change in the behavior of f_2 at $\sigma=1$, in contrast with the smoothly varying G_0. We can conclude that $f_2(s)$ does not behave asymptotically in the same way as $G_0(s)$, and thus that the presence of zeros of the former off the critical line is not in contradiction with the Lindelöf hypothesis.

VII. CONCLUSIONS

We have exhibited here some analytic properties of lattice sums in two dimensions, concentrating on results for the square lattice. The properties we have exhibited are interesting, and indicate that there is much yet to be understood about these sums. Their link with the Riemann hypothesis is one topic which merits further exploration. We have seen that the Catalan beta function shares many of the properties of the Riemann zeta function, and is connected to it in Hardy's formula for radial lattice sums over the square lattice. This suggests the exploration of

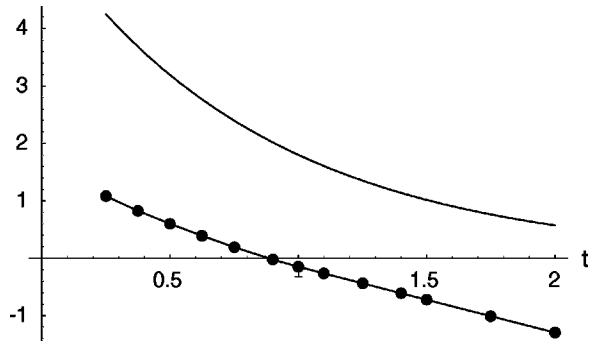

FIG. 7. Continuous line: $|G_0(\sigma+it)| \sim 4\sqrt{2}/\pi^{\sigma}$—see (77). Line with points: the asymptotic estimate for the limit of $f_2(\sigma+it)\exp(\pi t/2)/t^{\sigma}$ for large t, as a function of σ.

radial lattice sums for other arrays, and of angular lattice sums, in the light of the properties we have shown for $\sigma_{1+s}^{(4)}$. This may result in the identification of other analytic functions sharing essential characteristics with the zeta function.

We might call such functions ''complementary zeta functions.'' Characteristics required of them would be the existence of a reflection formula, reduction to a form even about the critical line, and numerical evidence for the confinement of zeros to the critical line. Evidence we have presented for the square array shows that $G_0(s)$ and $G_4(s)$ may well belong to this family, and we conjecture that, for general m, $G_{4m}(s)$ will also belong to it. Of course, it will be interesting to investigate other two-dimensional lattices to see whether similar functions occur for them.

ACKNOWLEDGMENTS

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APPENDIX: RECTANGULAR AND ANGULAR ARRAY SUMS

We now consider sums over inverse powers of the distance from the origin for the rectangular array, with periods d_1 and d_2 along the x and y axes, respectively. The result will be a rapidly convergent Macdonald function series of the type derived by Kober.[4] Given the series, by successive differentiation with respect to the periods d_1 and d_2, one can obtain Macdonald function series for angular lattice sums. We illustrate the procedure by deriving the series for $\sigma_{1+s}^{(4)}$.

We consider the nondimensionalized sum:

$$\sigma_{1+s}^{(0)}=(d_1d_2)^{(1+s)/2}\sum_{p\neq 0}\frac{1}{(p_1^2d_1^2+p_2^2d_2^2)^{(1+s)/2}}. \tag{A1}$$

The procedure we follow is based on that of Glasser.[17] We represent the inverse power of the distance as a Mellin transform, apply Jacobi's transformation from the theory of theta functions, and separate out the terms from the axes $p_1=0$ and $p_2=0$, before using Hobson's integral

$$\int_0^\infty t^{s-1}e^{-pt}e^{-q/t}dt=2\left(\frac{q}{p}\right)^{(s/2)}K_s(2\sqrt{qp}). \tag{A2}$$

The result is

$$\begin{aligned}\sigma_{1+s}^{(0)}(d_1,d_2)=&2\zeta(1+s)\left(\frac{d_1}{d_2}\right)^{(1+s)/2}+2\frac{\Gamma(s/2)}{\Gamma((s+1)/2)}\sqrt{\pi}\zeta(s)\left(\frac{d_2}{d_1}\right)^{(s-1)/2}\\&+\frac{8\pi^{(1+s)/2}}{\Gamma((1+s)/2)}\left(\frac{d_1}{d_2}\right)^{1/2}\sum_{p_1=1}^{\infty}\sum_{p_2=1}^{\infty}\left(\frac{p_2}{p_1}\right)^{s/2}K_{s/2}\left(\frac{2\pi d_1p_1p_2}{d_2}\right).\end{aligned} \tag{A3}$$

Note the apparent asymmetry between d_1 and d_2 in this formula arises from the arbitrary choice as to whether the Jacobi transform applies to p_1 or to p_2. An alternative and equivalent expression arises if d_1,p_1 and d_2,p_2 are interchanged. As a numerical example of (A2), if we choose $s=3.43+4.68i$, $d_1=1.0$, $d_2=0.73$, we can use direct summation of the left-hand side to obtain $3.300\,85+1.380\,22i$, and either form of the right-hand side to obtain as a rapidly convergent series the same value. Putting $d_1=d_2$ in (A3), we obtain Kober's result.[4]

The next step is to take the partial derivative of (A3) with respect to d_1. Using the Macdonald function recurrence relations, this gives

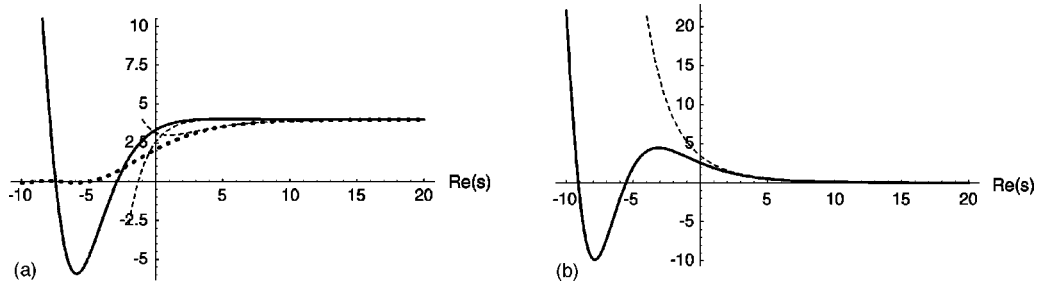

FIG. 8. Left: real part of $\sigma_{1+s}^{(4)}$ for (dotted curve) $\mathrm{Im}(s)=0$ and (solid curve) $\mathrm{Im}(s)=5$. Right: the corresponding imaginary part for $\mathrm{Im}(s)=5$. Dashed lines correspond to the nearest neighbor expansion (A7).

$$d_1^{(1+s)/2}d_2^{(1+s)/2}\sum_{p\neq 0}\frac{p_1^2}{(p_1^2d_1^2+p_2^2d_2^2)^{(1+s)/2}}$$
$$=2\frac{\Gamma(s/2)}{\Gamma((s+1)/2)}\sqrt{\pi}\zeta(s-2)\left(\frac{d_2}{d_1}\right)^{(s-1)/2}$$
$$+\frac{8\pi^{(1+s)/2}}{\Gamma((1+s)/2)}\left(\frac{d_1}{d_2}\right)^{1/2}\sum_{p_1=1}^{\infty}\sum_{p_2=1}^{\infty}\frac{p_2^{s/2}}{p_1^{s/2-2}}K_{s/2}\left(\frac{2\pi d_1p_1p_2}{d_2}\right). \tag{A4}$$

For $s=5.43+4.68i$, $d_1=1.0$, $d_2=0.73$, both the left-hand and right-hand sides of (A4) give the value $0.432\,88-0.761\,512i$. A second relation involving p_2^2 in the numerator rather than p_1^2 follows by interchanging p_1,d_1 and p_2,d_2.

We now take the partial derivative of (A3) with respect to d_2. The result is

$$d_1^{(1+s)/2}d_2^{(1+s)/2}\sum_{p\neq 0}\frac{p_1^2p_2^2}{(p_1^2d_1^2+p_2^2d_2^2)^{(1+s)/2}}$$
$$=\frac{\Gamma(s/2-1)}{\Gamma((s+1)/2)}\sqrt{\pi}\zeta(s-4)\left(\frac{d_2}{d_1}\right)^{(s-5)/2}$$
$$+\frac{4\pi^{(s-1)/2}}{\Gamma((1+s)/2)}\left(\frac{d_1^3}{d_2^3}\right)^{1/2}\sum_{p_1=1}^{\infty}\sum_{p_2=1}^{\infty}\frac{p_2^{s/2-1}}{p_1^{s/2-3}}$$
$$\times K_{s/2-1}\left(\frac{2\pi d_1p_1p_2}{d_2}\right)-\frac{8\pi^{(s+1)/2}}{\Gamma((1+s)/2)}\left(\frac{d_1^5}{d_2^5}\right)^{1/2}$$
$$\times\sum_{p_1=1}^{\infty}\sum_{p_2=1}^{\infty}\frac{p_2^{s/2}}{p_1^{s/2-4}}K_{s/2-2}\left(\frac{2\pi d_1p_1p_2}{d_2}\right). \tag{A5}$$

For $s=7.43+4.68i$, $d_1=1.0$, $d_2=0.73$, both the left-hand and right-hand sides of (A4) give the value $-0.053\,880\,1-0.146\,562i$.

The final step is to use these relations to evaluate

$$\sigma_{1+s}^{(4)}=(d_1d_2)^{(1+s)/2}\sum_{p\neq 0}\frac{e^{4i\varphi_p}}{R_p^{1+s}}=(d_1d_2)^{(1+s)/2}\sum_{p\neq 0}\frac{1}{R_p^{1+s}}-8(d_1d_2)^{(5+s)/2}\sum_{p\neq 0}\frac{p_1^2p_2^2}{R_p^{5+s}}. \tag{A6}$$

For $s=7.43+4.68i$, $d_1=1.0$, $d_2=0.73$, both the left-hand and right-hand sides of (A6) give the value $5.986\,87+4.832\,69i$. A second check on (A5) is to use it to evaluate $\sigma_4^{(4)}$, for $d_1=d_2$. The value obtained is $3.151\,200\,2$, to be compared with the value obtained by hand ($3.151\,204$) by Lord Rayleigh,[2] using hyperbolic series.

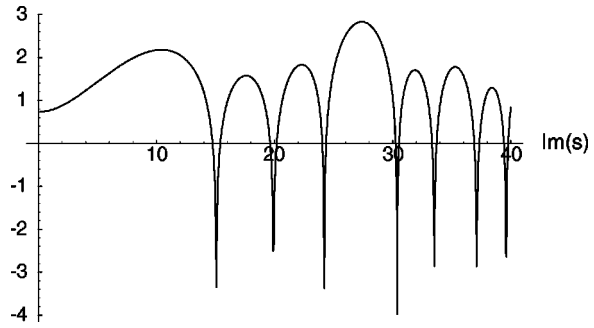

FIG. 9. The logarithm of the absolute value of $\sigma_{1+s}^{(4)}$ on the critical line $\mathrm{Re}(s)=0$, for $d_1=d_2$.

Figure 8 shows the behavior of $\sigma_{1+s}^{(4)}$, with $d_1=d_2$, as a function of the real part of its argument, for two constant values of the imaginary part. For $\mathrm{Im}(s)=0$, this sum has zeros at $\mathrm{Re}(s)=-5,-7,-9,\ldots$, corresponding to the poles of the factor $\Gamma((5+s)/2)$ present in the denominator of the second term in (A5), which coincide with the later poles of the factor $\Gamma((1+s)/2)$ in the first term. Note from Fig. 8 how the value of the sum tends towards the nearest-neighbor contribution (4) as $\mathrm{Re}(s)$ increases. The first three terms in its nearest-neighbor expansion, useful when $\mathrm{Re}(s)$ is sufficiently positive (say greater than 5), are

$$\sigma_{1+s}^{(4)}(d_1,d_1)=4\left(1-\frac{1}{2^{(1+s)/2}}+\frac{1}{2^{1+s}}+\cdots\right). \tag{A7}$$

Figure 9 shows the behavior of the logarithm of the absolute value of $\sigma_{1+s}^{(4)}$ along the critical line $\mathrm{Re}(s)=0$. The first seven zeros of this function are evident. Note that the sum is not real on the critical line. However, numerical investigations have verified that the function $G_4(s)$ of (59) is an even function of s, in keeping with (58), and is real on $\mathrm{Re}(s)=0$. It is also real on $\mathrm{Im}(s)=0$, but has no zeros on this line.

This function plays the same role for $\sigma_{1+s}^{(4)}(d_1,d_1)$ as does the function

$$G_0\left(\frac{s}{2}\right)=\frac{\sigma_{1+s}^{(0)}(d_1,d_1)\Gamma((1+s)/2)}{\pi^{(1+s)/2}}=4\,\frac{\zeta((1+s)/2)\beta((1+s)/2)\Gamma((1+s)/2)}{\pi^{(1+s)/2}} \tag{A8}$$

for the radial sum $\sigma_{1+s}^{(0)}$.

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Existence of the Bogoliubov $S(g)$ operator for the $(:\phi^4:)_2$ quantum field theory

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We prove the existence of the Bogoliubov $S(g)$ operator for the $(:\phi^4:)_2$ quantum field theory for coupling functions g of compact support in space and time. The construction is nonperturbative and relies on a theorem of Kisyński. It implies almost automatically the properties of unitarity and causality for disjoint supports in the time variable. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND SUMMARY

Recent progress in perturbative quantum field theory for the Stückelberg–Bogoliubov–Epstein–Glaser $S(g)$ operator[1,2] in non-Abelian gauge theories[3] (see also Ref. 4), revived interest in a long-standing problem: is it possible to construct $S(g)$ *nonperturbatively* in quantum field theory? This question is of obvious relevance to theories where the (dimensionless) coupling constant is large ($\gtrsim 1$), e.g., strong interactions, for which perturbation theory is not expected to be asymptotic.

For certain super-renormalizable theories—the $(:P(\phi):)_2$ theories—there exists, for weak coupling, a construction of the true (LSZ–Haag–Ruelle) scattering operator, due to Osterwalder and Séneor[5] and Eckmann, Epstein, and Fröhlich,[6] one of the crowning achievements of constructive quantum field theory which started with the pioneering work on the particle structure of weakly coupled $P(\phi)_2$ model by Glimm, Jaffe, and Spencer.[7] The method of proof was, however, perturbative: the perturbation series for the scattering operator was shown to be asymptotic.

In contrast to the true scattering operator, $S(g)$ is, in perturbation theory, the generating functional for the time-ordered products of Wick polinomials. However, on the basis of Ref. 8 one might expect that, in the present massive case, defining

$$g_\varepsilon(x) \equiv g(\varepsilon x), \quad g \in \mathcal{S}(\mathbb{R}^2)$$

the (adiabatic) limit

$$S\Psi \equiv \lim_{\varepsilon \to 0} \; S(g_\varepsilon)\Psi \tag{1.1}$$

exists, $\forall \quad \Psi \in \mathcal{D}$, where $\mathcal{D}$ is a Poincaré-invariant dense set in Fock space $\mathcal{F}$. Thus we expect that the physical S-matrix elements are obtainable as

$$(\Phi, S\Psi) \equiv \lim_{\varepsilon \to 0} \quad (\Phi, S(g_\varepsilon)\Psi), \tag{1.2}$$

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with $\Phi \in \mathcal{F}$, $\Psi \in \mathcal{D}$, where $g(0)>0$ should be identified with the coupling constant. In Ref. 4 an algebraic construction of the adiabatic limit was performed for perturbative QED.

A natural nonperturbative approach to construct $S(g)$ for the $(:\phi^4:)_2$ theory (and hopefully for any super-renormalizable QFT) consists in proving the existence of a (unique) solution of the evolution (propagator) equation ($\hbar=1$),

$$i\frac{\partial U(t,s)}{\partial t}\Psi=\tilde{H}(t)U(t,s)\Psi, \tag{1.3}$$

with

$$\tilde{H}(t)\equiv H_g(t)+M\mathbf{1}, \tag{1.4}$$

where M is a constant introduced in order to make $\tilde{H}(t)$ a positive operator (see Sec. II) and

$$H_g(t)\equiv H_0+V_g(t). \tag{1.5}$$

In (1.3) $U(t,s)$ is a two-parameter family of unitary operators on (symmetric) Fock space $\mathcal{F}$. H_0 is the free field Hamiltonian corresponding to a zero-time scalar field $\phi(x,0)$ of mass m,[9,10] and, formally, for

$$g\in\mathcal{D}(\mathbb{R}^2), \quad g\geqslant 0, \tag{1.6}$$

let

$$V_g(t)=\int \mathrm{d}x\, g(x,t):\phi^4(x,0):. \tag{1.7}$$

Above, $\mathcal{D}$ denotes the Schwartz space of infinitely differentiable functions of compact support. The operators in (1.3) are expected to satisfy the propagator conditions:

$$U(t,s)U(s,r)=U(t,r), \quad -\infty<r\leqslant s\leqslant t<\infty,$$

$$U(t,t)=\mathbf{1}, \quad \forall \quad t\in\mathbb{R}. \tag{1.8}$$

The vector Ψ is supposed to belong to the domain $D(\tilde{H}(s))$ (dense in $\mathcal{F}$) such that

$$U(t,s)D(\tilde{H}(s))\subset D(\tilde{H}(t)). \tag{1.9}$$

Above and elsewhere in this paper $D(A)$ denotes the domain of an operator A.

Under assumptions (1.3) and (1.9), defining the ''Dirac (or interaction) picture propagator'' by

$$U^D(t,s)\equiv e^{i(H_0+M)t}U(t,s)e^{-i(H_0+M)s}, \tag{1.10}$$

it follows that

$$i\frac{\partial U^D(t,s)}{\partial t}\Psi=H_g^D(t)U^D(t,s)\Psi, \tag{1.11}$$

for $\Psi\in e^{i(H_0+M)s}D(H_g(s))$, which is a dense set in $\mathcal{F}$ for every s, where

$$H_g^D(t)\equiv e^{iH_0t}V_g(t)e^{-iH_0t}. \tag{1.12}$$

One may then define

$$S(g)\equiv s-\lim_{\substack{t\to+\infty\\ s\to-\infty}} U^D(t,s), \tag{1.13}$$

if the above limit exists; $S(g)$ is expected to satisfy

(i) $S(g)^{-1}=S(g)^*$ (*unitarity);*
(ii) $S(g_1+g_2)=S(g_1)S(g_2)$ if
$(ii.a)$ supp $g_1>$supp g_2 and/or
$(ii.b)$ supp $g_1\sim$supp g_2 (*causality),*
where "$\sim$" means "spacelike to," i.e., $(x-y)^2=(t_1-t_2)^2-(x_1-x_2)^2<0$, $\forall\ (t_1,x_1)\in$supp g_1 and $\forall\ (t_2,x_2)\in$supp g_2;
(iii) there exists a unitary representation $U(a,\Lambda)$ of the Poincaré group on $\mathcal{F}$—the scalar field representation of mass m—such that

$$U(a,\Lambda)S(g)U(a,\Lambda)^{-1}=S(\{a,\Lambda\}g),$$

where

$$(\{a,\Lambda\}g)(x)=g(\Lambda^{-1}(x-a))$$

(*Lorentz covariance*).

The main difficulty to proving (1.3)–(1.9) is that $D(H_g(t))$ is, for each $g\in\mathcal{D}(\mathbb{R}^2)$, time-dependent. In Sec. II we state the basic existence theorem we employ, which is due to Kisyński[11] (see also Ref. 12). In Sec. III we prove our central existence theorem for $S(g)$, as well as properties (i) and $(ii.a)$. In Sec. IV we provide a brief summary of the remarkable results of Ref. 11, establishing a concrete link between them and our conditions in Sec. III. We leave the conclusion and open problems to Sec. V. The Appendix summarizes some of the basics elements of the construction of Refs. 11 and 13 for the convenience of the reader.

II. THE BASIC EXISTENCE THEOREM

The Hamiltonian of the $(:\phi^4:)_2$ theory[14] is given by (1.5), where

$$H_0=\int \omega(k)a^*(k)a(k)\mathrm{d}k, \tag{2.1}$$

with

$$\omega(k)=(k^2+m^2)^{1/2}, \tag{2.2}$$

is the free field Hamiltonian on symmetric Fock space $\mathcal{F}$, with

$$[a(k),a^*(k')]=\delta(k-k'). \tag{2.3}$$

The self-interaction V_g is given by (1.7), with the $t=0$ scalar free field of mass m:

$$\phi(x)=\frac{1}{(4\pi)^{1/2}}\int e^{-ikx}[a^*(k)+a(-k)]\omega(k)^{-1/2}\mathrm{d}k. \tag{2.4}$$

Thus V_g may be written[14]

$$V_g(t)=\sum_{j=0}^{4}\binom{4}{j}\int a^*(k_1)\cdots a^*(k_j)a(-k_{j+1})\cdots a(-k_4)\tilde{g}\left(\sum_{i=1}^{4}k_i,t\right)\prod_{i=1}^{4}\omega(k_i)^{-1/2}\mathrm{d}k_i, \tag{2.5}$$

where

$$\tilde{g}(k,t)\equiv\int \mathrm{d}x\, e^{ikx}g(x,t). \tag{2.6}$$

The number operator N is defined by

$$N=\int \mathrm{d}k\, a^*(k)a(k). \tag{2.7}$$

By (Ref. 14 Lemma 2.2)

$$\|(N+\mathbf{1})^{-j/2}\ \ V_g(t)\ \ (N+\mathbf{1})^{-(4-j)/2}\|\leqslant\ \text{const}\ \ \|W\|_{L^2},\quad |j|\leqslant 4, \tag{2.8}$$

where

$$W(k,t)\equiv\tilde{g}\left(\sum_{i=1}^{4}k_i,t\right)\prod_{i=1}^{4}\omega(k_i)^{-1/2}. \tag{2.9}$$

The above-mentioned lemma just uses the Fock space definitions of the creation and annihilation operators and the Schwartz inequality. We need two theorems due to Glimm and Jaffe, which we state as adapted to our case:

Theorem II.1 (Ref. 14): (**a**) *$H(t)$ is self-adjoint on the domain*

$$D(H(t))=D(H_0)\cap D(V_g(t)), \tag{2.10}$$

where $D(V_g(t))$ is the domain of the unique self-adjoint closure of $V_g(t)$ on the domain

$$D_0=\bigcap_{n=0}^{\infty}D(H_0^n). \tag{2.11}$$

(**b**) *$H(t)$ is essentially self-adjoint on D_0.*

Theorem II.2 (Ref. 10): *For each $g\in\mathcal{D}(\mathbb{R}^2)$, there exists $0<M_g<\infty$ such that*

$$H_g(t)\geqslant -M_g\mathbf{1} \tag{2.12}$$

as a bilinear form on $D_0\times D_0$.

By Theorem II.2 and (**b**) of Theorem II.1, $H(t)$ is a semi-bounded self-adjoint operator, and thus defining

$$M=M_g+c, \tag{2.13}$$

for some $c>0$, then

$$\tilde{H}(t)=H_g(t)+M\mathbf{1}\geqslant c\mathbf{1} \tag{2.14}$$

is a positive self-adjoint operator. Let $\mathcal{F}_{+2}=D(H_0)$ endowed with the Hilbert space structure given by

$$f_{+2}(x,y)=\langle(H_0+1)x,(H_0+1)y\rangle \tag{2.15}$$

and denote $\sqrt{f_{+2}(x,x)}$ by $\|x\|_{+2}$. By the Riesz lemma we may associate $\mathcal{F}_{+2}$ and the space $\mathcal{F}_{-2}$ of continuous conjugate linear functions on $\mathcal{F}_{+2}$. While we consider $\mathcal{F}$ isomorphic to its conjugate dual space $\mathcal{F}^*$, the isomorphism being the identity, the isomorphism of $\mathcal{F}_{+2}$ with $\mathcal{F}_{-2}$ is given by the operator $(H_0+1)^2$, because

$$\|v\|_{-2}=\sup\{|\langle w,v\rangle|\ :\ \|w\|_{+2}\leqslant 1\}.$$

Since $f_{+2}(x,y)=\langle x,(H_0+1)^2y\rangle$, we have

$$\|(H_0+1)^2y\|_{-2}=\sup\{|\langle w,(H_0+1)^2y\rangle| : \|w\|_{+2}=\sqrt{\langle w,(H_0+1)^2w\rangle}\leqslant 1\}=\|(H_0+1)y\|=\|y\|_{+2},$$

from which we also have, for $y\in\mathcal{F}$,

$$\|y\|_{-2}=\|(H_0+1)^{-1}y\|, \tag{2.16}$$

which explains the notation $\mathcal{F}_{-2}$. Clearly $\|x\|\leqslant\|x\|_{+2}$ for $x\in\mathcal{F}_{+2}$, and by (2.16), $\|y\|_{-2}\geqslant\|y\|$ for $y\in\mathcal{F}$. Thus, under the above conditions:

$$\mathcal{F}_{+2}\subset\mathcal{F}\subset\mathcal{F}_{-2}. \tag{2.17}$$

A bounded operator $\mathbf{B}$ from $\mathcal{F}_{+2}$ to $\mathcal{F}_{-2}$ is thus such that, for some constant c,

$$\|\mathbf{B}\psi\|_{-2}\leqslant c\|\psi\|_{+2}, \quad \psi\in\mathcal{F}_{+2}, \tag{2.18}$$

or, by (2.15) and (2.16),

$$\|(H_0+1)^{-1}\mathbf{B}\psi\|\leqslant c\|(H_0+1)\psi\|, \quad \psi\in\mathcal{F}_{+2}, \tag{2.19}$$

or

$$\|(H_0+1)^{-1}\mathbf{B}(H_0+1)^{-1}\phi\|\leqslant c\|\phi\|, \quad \phi\in\mathcal{F}. \tag{2.20}$$

Now, by (2.14), we may define $\tilde{H}(t)^{1/2}$, and, by (2.8) for $x\in\mathcal{F}_{+2}$, the closed sesquilinear form

$$S(x,y)=\langle\tilde{H}(t)^{1/2}x,\tilde{H}(t)^{1/2}y\rangle, \tag{2.21}$$

which is, by the form representation theorem,[15] the form of the operator $\tilde{H}(t)$. In Sec. III we show the explicit connection of (2.21) to the basic theorem of Kisyński,[11] which we state in the form of Theorems II.23 and II.24 of Ref. 12, with slight changes.

In the theorem stated below, $\mathcal{F}_{\pm2}$ have been defined in (2.15)–(2.17).

Theorem II.3: *Let (2.17) hold and $\tilde{H}(t)$ $(-T\leqslant t\leqslant S)$ be a one-parameter family of strictly positive [i.e., satisfying (2.14)] self-adjoint operators on $\mathcal{F}$. Suppose that $\tilde{H}(t):\mathcal{F}_{+2}\to\mathcal{F}_{-2}$ are bounded and twice differentiable, with a continuous second derivative, in the $\|\cdot\|_{-2,2}$-norm (2.18). Then there exists a two-parameter family $U(t,s)$ of unitary propagators satisfying (1.3), (1.8), and (1.9).*

III. THE CENTRAL EXISTENCE THEOREM

We now use Theorem II.3 in order to prove our main

Theorem III.1: *The $(:\phi^4:)_2$ theory, as defined by (1.5), (1.6), (1.7), (2.1), and (2.2), satisfies a stronger condition than the hypothesis of Theorem II.3: $H_g(\cdot)$ is infinitely differentiable as an operator from $\mathcal{F}_{+2}$ to $\mathcal{F}_{-2}$.*

In order to prove Theorem III.1 we first show a useful auxiliary result.

Lemma III.1: Let W be defined by (2.9). Then there exists $r>1$ such that

$$\|W(\cdot,t)\|_2\leqslant\text{const}\ \ \|g(\cdot,t)\|_r, \tag{3.1}$$

where

$$\|g(\cdot,t)\|_r=\left(\int_{-\infty}^{+\infty}\mathrm{d}k|\tilde{g}(k,t)|^r\right)^{1/r}. \tag{3.2}$$

Proof: We have

$$\|W(\cdot,t)\|_2^2=\int_{-\infty}^{+\infty}\mathrm{d}k_1\omega(k_1)^{-1}\cdot\int_{-\infty}^{+\infty}\mathrm{d}k_2\omega(k_2)^{-1}\cdot\int_{-\infty}^{+\infty}\mathrm{d}k_3\omega(k_3)^{-1}$$
$$\cdot\int_{-\infty}^{+\infty}\mathrm{d}k'|\tilde{g}(k',t)|^2\omega\left(k'-\sum_{i=1}^{3}k_i\right)^{-1} \tag{3.3}$$

by the change of variable $k'=\Sigma_{i=1}^{3}k_i$. Introducing further the variables K_1,K_2,K_3 such that

$$K_1=k_1+k_2+k_3,$$

$$K_2=k_1+k_2,$$

$$K_3=k_1,$$

so that $k_3=K_1-K_2$ and $k_2=K_2-K_3$, we write (3.3) as

$$\|W(\cdot,t)\|_2^2=(\omega^{-1}*(\omega^{-1}*(\omega^{-1}*(\omega^{-1}*|\tilde{g}|^2))))(0), \tag{3.4}$$

where the convolution is defined as usual by

$$(f*g)(k)=\int_{-\infty}^{+\infty}\mathrm{d}k_1 f(k-k_1)g(k_1).$$

Consider, now, the quantity associated to the right-hand side of (3.3):

$$I(q,t)\equiv\int_{-\infty}^{+\infty}\mathrm{d}k_1\ \ \omega(k_1-q)^{-1}\cdot\int_{-\infty}^{+\infty}\mathrm{d}k_2\ \ \omega(k_2)^{-1}\cdot\int_{-\infty}^{+\infty}\mathrm{d}k_3\ \ \omega(k_3)^{-1}$$
$$\cdot\int_{-\infty}^{+\infty}\mathrm{d}k'\ \ |\tilde{g}(k',t)|^2\omega\left(k'-\sum_{i=1}^{3}k_i\right)^{-1}. \tag{3.5}$$

Since $g\in\mathcal{D}(\mathbb{R})$ this function is differentiable, hence continuous, in q for any compact subset containing the origin, which implies that $I(0,t)\leqslant\|I(\cdot,t)\|_\infty$ (where $\|\cdot\|_\infty$-norm is with respect to the q-variable).

We now apply Young's inequality[16]

$$\|f*g\|_r\leqslant C_{rpq}\|f\|_p\|g\|_q$$

with C_{rpq} a constant and

$$\frac{1}{p}+\frac{1}{q}=1+\frac{1}{r}$$

to (3.4), starting with $r=\infty$. Above,

$$\|f\|_p=\left(\int_{-\infty}^{+\infty}\mathrm{d}k|f(k)|^p\right)^{1/p}.$$

We thus obtain

$$\|W(\cdot,t)\|_2^2\leqslant C_{2r_1r_2}\|\omega^{-1}\|_{r_1}\ \ \|(\omega^{-1}*(\omega^{-1}*(\omega^{-1}*|\tilde{g}|^2)))\|_{r_2}$$

with $r_1^{-1}+r_2^{-1}=1$, and so on, up to (indicating all the constants resulting from the Young's inequality by C')

$$\|W(\cdot,t)\|_2^2 \leqslant C' \|\omega^{-1}\|_{r_1} \ \|\omega^{-1}\|_{r_3} \ \|\omega^{-1}\|_{r_5} \ \|\omega^{-1}\|_{r_7} \ \||\tilde{g}|^2\|_{r_8} \tag{3.6}$$

with $r_3^{-1}+r_4^{-1}=1+r_2^{-1}$, $r_5^{-1}+r_6^{-1}=1+r_4^{-1}$, $r_7^{-1}+r_8^{-1}=1+r_6^{-1}$. We require $r_i>1$, for $i=1,3,5,7$, so that $\|\omega^{-1}\|_{r_i}<\infty$, the choice $r_1=r_2=2$, $r_3=r_4=\frac{4}{3}$, $r_5=r_6=\frac{8}{7}$, $r_7=r_8=\frac{16}{15}$ is, for instance, possible. By (3.6)

$$\|W(\cdot,t)\|_2^2 \leqslant C \||\tilde{g}|^2\|_r \tag{3.7}$$

with

$$r>1. \tag{3.8}$$

Above

$$\| \ |\tilde{g}|^2 \ \|_r = \left(\int_{-\infty}^{+\infty} \mathrm{d}k |\tilde{g}(k,t)|^{2r} \right)^{1/r}. \tag{3.9}$$

obtaining finally, (3.7). □

Proof of III.1: By (2.8),

$$\|(N+\mathbf{1})^{-1} V_g(t) (N+\mathbf{1})^{-1}\| \leqslant \text{const} \|W\|_{L^2} \tag{3.10}$$

and, by (2.2), $\omega(k) \geqslant m\mathbf{1}$; hence

$$\|(H_0+\mathbf{1})^{-1}(N+\mathbf{1})\| \leqslant d_1, \quad \|(N+\mathbf{1})(H_0+\mathbf{1})^{-1}\| \leqslant d_2,$$

for constants d_1 and d_2. Hence, by (3.10) and (3.1),

$$\|(H_0+\mathbf{1})^{-1} V_g(t) (H_0+\mathbf{1})^{-1}\| \leqslant \text{const} \|g(\cdot,t)\|_r \tag{3.11}$$

with $r>1$: *a fortiori* this holds for $H_g(\cdot)$ by (1.5), hence

$$\|(H_0+\mathbf{1})^{-1} H_g(t) (H_0+\mathbf{1})^{-1}\| \leqslant \text{const} \|g(\cdot,t)\|_r. \tag{3.12}$$

By (2.20) and Theorem II.3 we only need to prove that the left-hand side of (3.12) is three times differentiable. We shall prove that

$$\left\| (H_0+\mathbf{1})^{-1} \left(\frac{H_g(t+h)-H_g(t)}{h} - H_g'(t) \right) (H_0+\mathbf{1})^{-1} \right\| \to 0 \qquad \text{as} \qquad h \to 0, \tag{3.13}$$

where

$$H_g'(t) = H_0 + V_{g'}(t) \tag{3.14}$$

with

$$V_{g'}(t) = \int \mathrm{d}x : \phi^4(x,0) : g'(x,t) \tag{3.15}$$

and

$$g'(x,t) \equiv \frac{\partial g(x,t)}{\partial t}.$$

We now prove (3.13). By (3.12)

$$J \equiv \left\| (H_0+\mathbf{1})^{-1}\left(\frac{H_g(t+h)-H_g(t)}{h}-H_g'(t)\right)(H_0+\mathbf{1})^{-1}\right\|$$
$$\leqslant \text{const}\left[\int_{-\infty}^{\infty} \mathrm{d}k \left| \int \mathrm{d}x\, e^{-ikx}\left(\frac{g(x,t+h)-g(x,t)}{h}-g'(x,t)\right)\right|^r\right]^{1/r}. \tag{3.16}$$

We now write the integral on the right-hand side of (3.16) as

$$\int_{-\infty}^{\infty} \mathrm{d}k\{\cdots\} = \int_{-\infty}^{1} \mathrm{d}k\{\cdots\} + \int_{-1}^{1} \mathrm{d}k\{\cdots\} + \int_{1}^{\infty} \mathrm{d}k\{\cdots\}$$

and estimate the last integral above

$$J_+ \equiv \int_1^{\infty} \mathrm{d}k \left| \int \mathrm{d}x\, e^{-ikx}\left(\frac{g(x,t+h)-g(x,t)}{h}-g'(x,t)\right)\right|^r$$
$$\leqslant \int_1^{\infty} \frac{\mathrm{d}k}{k^{2r}} \left| \int \mathrm{d}x\, e^{-ikx}\left(\frac{\partial_x^2 g(x,t+h)-\partial_x^2 g(x,t)}{h}-\partial_x^2 g'(x,t)\right)\right|^r, \tag{3.17}$$

where we have used two partial integrations and $\partial_x \equiv \partial/\partial x$. Let now

$$V(x,t) \equiv \partial_x^2 g(x,t). \tag{3.18}$$

Now V is also an infinitely differentiable function of compact support and

$$V(x,t+h) = V(x,t) + hV'(x,t) + \frac{h^2}{2!}V''(x,t+t_h^*(x)) \tag{3.19}$$

by Taylor's formula with remainder, where $0<t_h^*(x)<h$. Putting (3.19) into (3.17) we get

$$J_+ \leqslant c_r' h^r \left(\int_{-\infty}^{\infty} \mathrm{d}x |V''(x,t+t_h^*(x))|\right)^r \leqslant c_r \quad h^r (\sup_{x,t} |V''(x,t)|)^r,$$

where c_r' and c_r are constants depending on r. The estimate of $J_- \equiv \int_{-\infty}^{-1}\{\cdots\}$ is similar. The estimate of $J_1 \equiv \int_{-1}^{1}\{\cdots\}$ follows along the same lines, but in this case we should not introduce the partial integrations in order to avoid divergences at $k=0$. Then, we obtain

$$J \leqslant \text{const}\, h[A_r(\sup_{x,t}|g''(x,t)|)^r + B_r(\sup_{x,t}|V''(x,t)|)^r]^{1/r}$$

with A_r and B_r constants depending on r. Then we have (3.13).

We now notice that the bounds (3.12) *continue to hold* for $H_g'(t)$ with $\|g(\cdot,t)\|_r$ replaced by $\|g'(\cdot,t)\|_r$ on the right-hand side of (3.12). Thus the same proof applies to $H_g'(t)$, $H_g''(t)$, ... and in fact $H_g(t)$ is infinitely differentiable as an operator from $\mathcal{F}_{+2}$ to $\mathcal{F}_{-2}$. □

Proposition III.1: The $S(g)$ matrix for the $(:\phi^4)_2$ theory, as defined in (1.13), is unitary and it satisfies the causality condition for disjoint supports [condition $(ii.a)$—Sec. I].

Proof: The unitarity follows directly from the existence theorems. For the proof of causality it is convenient to explicitly dispose of the dependence of the propagators on the function g. Let $\text{supp}_t g_1 > \text{supp}_t g_2$ and suppose $\text{supp}_t g_1 \subset (r,+\infty)$ and $\text{supp}_t g_2 \subset (-\infty,r)$, where supp_t stands for the support in the time variable. Then, for $t>r>s$ we have

$$U^D_{(g_1+g_2)}(t,s) = U^D_{(g_1+g_2)}(t,r)\,U^D_{(g_1+g_2)}(r,s) \tag{3.20}$$

but

$$i\frac{\partial}{\partial t}U^D_{(g_1+g_2)}(t,r)\Psi = H^D_{(g_1+g_2)}(t)U^D_{(g_1+g_2)}(t,r)\Psi = H^D_{g_1}(t)U^D_{(g_1+g_2)}(t,r)\Psi$$

and, by the uniqueness of the solutions of the above equation, we have $U^D_{(g_1+g_2)}(t,r) = U^D_{g_1}(t,r)$. Analogously, we have $U^D_{(g_1+g_2)}(r,s) = U^D_{g_2}(r,s)$. This, together with (3.20) imply that

$$U^D_{(g_1+g_2)}(t,s) = U^D_{g_1}(t,r)U^D_{g_2}(r,s)$$

from this equation and the fact that $U^D_{g_1}(t,s) = U^D_{g_1}(t,r)$ and $U^D_{g_2}(r,s) = U^D_{g_2}(t,s)$ due to the support properties of g_1 and g_2, we finally have

$$U^D_{(g_1+g_2)}(t,s) = U^D_{g_1}(t,s)U^D_{g_2}(t,s). \tag{3.21}$$

Then, by (3.21) and the definition (1.13), we obtain

$$S(g_1+g_2) = S(g_1)S(g_2).$$

□

IV. THE RELATION BETWEEN KISYŃSKI'S THEORY AND THEOREM III.1

Let us now briefly summarize (without proof) some steps in Kisyński's proof of Theorem II.3. First of all, we will state a crucial auxiliary theorem. Let X be a Banach space with the norm $\|\cdot\|$ and $A(t)$, $t\in[-T_1,T_2]$ $(T_1,T_2>0)$, a family of linear operators in X. Consider the following conditions:

(a) there exists a family $\|\cdot\|_t$, $t\in[-T_1,T_2]$, of norms in X equivalent to $\|\cdot\|$ such that $|\,\|\Psi\|_t - \|\Psi\|_s\,| \leqslant k\,\|\Psi\|_s\,|t-s|$ with $k=\text{const}$, $-T_1\leqslant s,t\leqslant T_2$ and $\Psi\in X$;
(b) for all $t\in[-T_1,T_2]$ the set $D(A(t))$ is dense in X;
(c) there exists a constant $\lambda_0\geqslant 0$ such that $R(\lambda-\epsilon A(t))=X$ and $\|(\lambda-\epsilon A(t))\Psi\|_t \geqslant (\lambda-\lambda_0)\|\Psi\|_t$ for $\epsilon=\pm 1$, $\lambda>\lambda_0$, $t\in[-T_1,T_2]$ and $\Psi\in D(A(t))$;
(d) there exists a family $R(t)$, $t\in[-T_1,T_2]$, of invertible bounded linear operators in X, such that $R(t)$ is twice weakly continuously differentiable in $[-T_1,T_2]$ and $(R(t))^{-1}D(A(t)) = Y = \text{const}\ \forall t\in[-T_1,T_2]$;
(e) $(R(t))^{-1}A(t)R(t)$ is weakly continuously differentiable.

Above $R(A)$ stands for the range of the operator A. Then we have:

Theorem IV.1 (Ref. 11, Theorem 4.4): *Let the conditions* (a)–(e) *be satisfied. Then there exists a two-parameter family of propagators* $U(t,s)$, $-T_1\leqslant s,t\leqslant T_2$, *such that*

$$\Psi(t)\equiv U(t,s)\Psi(s), \quad \Psi(s)\in D(A(s)),$$

is the unique solution of the problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = A(t)\Psi(t) \tag{4.1}$$

with initial data $\Psi(s)$. *The bounded propagators* $U(t,s)$ *are strongly continuous on* $-T_1\leqslant s,t\leqslant T_2$ *and satisfy*

$$U(t,t)=1\ , \quad \forall\ \ t\in[-T_1,T_2], \tag{4.2}$$

$$U(t,s)U(s,r)=U(t,r), \quad \text{for} -T_1\leqslant r,s,t\leqslant T_2, \tag{4.3}$$

$$U(t,s)D(A(s))=D(A(t)), \quad \text{for} -T_1\leqslant s,t\leqslant T_2, \tag{4.4}$$

besides, $\forall\ s\in[-T_1,T_2]$ *and* $\Psi\in D(A(s))$ *the function* $U(t,s)\Psi$ *is continuously differentiable (in the sense of the norm) in* X*, satisfying*

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t,s)\Psi=A(t)U(t,s)\Psi. \tag{4.5}$$

The method of proof of this theorem is to reduce the problem to the case where we have an operator with constant domain by making use of the properties of $R(t)$ [for an outline of Kisyński's solution of the problem (4.1) with $D(A(t))=\text{const}$ see the Appendix].

Let us now consider Kisyński's approach to the abstract Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t)=-iA(t)\Psi(t),\quad -T_1\leqslant t\leqslant T_2, \tag{4.6}$$

where $\Psi\in\mathcal{H}$, with $\mathcal{H}$ a Hilbert space and $A(t)$ an operator in $\mathcal{H}$ defined as follows. Consider the condition:

(i) Let $\mathcal{H}$ be a Hilbert space, $\mathcal{H}_+$ a dense subset of $\mathcal{H}$ and, $\forall\ t\in[-T_1,T_2]$, let $\langle\cdot,\cdot\rangle_t^+$ be a scalar product defined on $\mathcal{H}_+$ which makes it a Hilbert space $\mathcal{H}_+^t$ algebraically and topologically contained in $\mathcal{H}$. Assume that $\langle\cdot,\cdot\rangle_t^+$ is n times $(n\geqslant 1)$ continuously differentiable on $[-T_1,T_2]$.

If condition (i) is satisfied we have

Lemma IV.1 (Ref. 11, Lemma 7.2): *The equality*

$$\langle\Phi,\Psi\rangle_t^+=\langle\Phi,Q(t)\Psi\rangle_{-T_1}^+,\quad \Phi,\Psi\in\mathcal{H}_+,\quad t\in[-T_1,T_2] \tag{4.7}$$

defines a bounded n *times weakly continuously differentiable operator* $Q(t)$ *on* $\mathcal{H}_+^{-T_1}$*. For all fixed* $t\in[-T_1,T_2]$*,* $Q(t)$ *is Hermitian with* $\inf Q(t)>0$ *in* $\mathcal{H}_+^{-T_1}$*.*

Another consequence of condition (i) is that we can define an operator $J_{-T_1}(t)$ by means of the equality (Ref. 11, Lemma 7.4)

$$\langle\Phi,\Psi\rangle=\langle\Phi,J_{-T_1}(t)\Psi\rangle_t^+,\quad \Phi\in\mathcal{H}_+,\quad \Psi\in\mathcal{H} \tag{4.8}$$

with $J_{-T_1}(t)$ a positive Hermitian operator in $\mathcal{L}(\mathcal{H})$ such that $J_{-T_1}(t)\mathcal{H}_+$ is a dense subset of $\mathcal{H}_+^t$. Then, defining

$$\|\Psi\|_t^-\equiv\|J_{-T_1}(t)\Psi\|_t^+,\quad \Psi\in\mathcal{H}, \tag{4.9}$$

it follows that the completion $\mathcal{H}_-^t=\mathcal{H}_-^{-T_1}\equiv\mathcal{H}_-$ of $\mathcal{H}$ in the norm $\|\cdot\|_t^-$ contains $\mathcal{H}$ algebraically and topologically (Ref. 11, Lemma 7.5).

Finally, we can define an operator $A(t)$ by means of the form $\langle\cdot,\cdot\rangle_t^+$ according to the following lemma:

Lemma IV.2 (Ref. 11, Lemma 7.7): *For all* $t\in[-T_1,T_2]$*,*

$$D(A(t))=\left\{\Psi\in\mathcal{H}_+:\ \sup_{\Phi\in\mathcal{H}_+,\,\|\Phi\|\leqslant 1}\{|\langle\Phi,\Psi\rangle_t^+|\}<+\infty\right\}, \tag{4.10}$$

$$\langle\Phi,A(t)\Psi\rangle\equiv\langle\Phi,\Psi\rangle_t^+,\quad \Psi\in D(A(t)) \tag{4.11}$$

define an inversible self-adjoint positive operator $A(t)$ *in* $\mathcal{H}$*, with*

$$D(A(t))=(Q(t))^{-1}D(A(-T_1)) \tag{4.12}$$

and

$$A(t)=(J_{-T_1}(t))^{-1}=A(-T_1)Q(t). \tag{4.13}$$

Then the operator $A(t)$ is shown to satisfy the Schrödinger equation (4.6) and the propagators of problem (4.6) satisfy the properties enumerated in Theorem II.3 (Ref. 11, Theorem 8.1). In order to prove his Theorem 8.1 for the operator $A(t)$, as defined above, Kisyński made use of Theorem IV.1 identifying $R(t)=(Q(t))^{-1}$. Let us now show that the $(:\phi^4:)_2$ theory satisfies the necessary conditions for Theorem II.3. In fact, all we need to show is that condition (i) is satisfied. However for the benefit of clarity we will explicitly display the main operators introduced in Kisyński's proof and some of its properties.

The Hilbert space $\mathcal{H}$ in (i) should be identified with the symmetric Fock space $\mathcal{F}$ (as defined in Sec. II) and $\mathcal{F}_{+2}=D(H_0)$ is a dense subset of $\mathcal{F}$. Then, taking the closure $\mathcal{F}^t_{+2}$ of $\mathcal{F}_{+2}$ in the norm induced by the scalar product $\langle\cdot,\cdot\rangle^+_t$, which is related to the operator $\tilde{H}(t)$ [see Eq. (2.14)] by means of the form (2.21), i.e.,

$$\langle\Phi,\Psi\rangle^+_t\equiv S(\Phi,\Psi)=\langle\tilde{H}(t)^{1/2}\Phi,\tilde{H}(t)^{1/2}\Psi\rangle, \tag{4.14}$$

we can show the following:

Proposition IV.1: $\mathcal{F}^t_{+2}$ is a Hilbert space such that

$$\mathcal{F}^t_{+2}\subset\mathcal{F} \tag{4.15}$$

algebraically and topologically.

Proof: That $\mathcal{F}^t_{+2}$ is a Hilbert space follows immediately from the fact that the form defined in (4.14) is closed (see, e.g., Ref. 15). The property that $\mathcal{F}^t_{+2}\subset\mathcal{F}$ algebraically is trivial. So, it remains to show that (4.15) holds topologically. This is achieved by showing that for $\{f_n\}_{n=1}^{\infty}\in\mathcal{F}_{+2}$ and $f\in\mathcal{F}_{+2}$ such that

$$\|f_n-f\|\to 0 \tag{4.16}$$

we have

$$\|f_n-f\|^+_t\to 0.$$

To show this, set

$$\begin{aligned}(\|f_n-f\|^+_t)^2&=\langle(f_n-f),(f_n-f)\rangle^+_t=\langle(f_n-f),\tilde{H}(t)(f_n-f)\rangle\\&=\langle(H_0+\mathbf{1})(f_n-f),(H_0+\mathbf{1})^{-1}\tilde{H}(t)(H_0+\mathbf{1})^{-1}(H_0+\mathbf{1})(f_n-f)\rangle.\end{aligned}$$

The Schwarz inequality applied to the last term above yields

$$\|f_n-f\|^+_t\leqslant\|(H_0+\mathbf{1})^{-1}\tilde{H}(t)(H_0+\mathbf{1})^{-1}\|\ \ \|(H_0+\mathbf{1})(f_n-f)\|^2.$$

The first term on the right-hand side is bounded due to (3.12). The second term on the right-hand side converges since $H_0+\mathbf{1}$ is a self-adjoint operator (hence closed) and, by hypothesis, (4.16) holds. Then the proof of the proposition is complete. □

In addition, it follows straightforwardly from (4.14) and Theorem III.1 that $\langle\cdot,\cdot\rangle^+_t$ is n times (infinitely, in fact) continuously differentiable. Then it is proved that condition (i) is satisfied and Theorem II.3 follows as proved in Ref. 11 and summarized above.

Now we turn to explicitly show the properties of $Q(t)$ in our case. From (4.14) and the definition

$$\langle\Phi,\Psi\rangle^+_t\equiv\langle\Phi,Q(t)\Psi\rangle^+_{-T_1}$$

we obtain that $Q(t)$ is the operator

$$Q(t)=(\tilde{H}(-T_1))^{-1}\tilde{H}(t). \tag{4.17}$$

Proposition IV.2: $Q(t)$, as defined in (4.17), is a (strictly) positive Hermitian operator in $\mathcal{F}_{+2}$ and it is infinitely weakly differentiable.

Proof: It follows directly from the properties of the scalar product $\langle\cdot,\cdot\rangle_t^+$ that $Q(t)$ is infinitely weakly differentiable.

For Φ, $\Psi\in\mathcal{F}_{+2}$, we have

$$(\langle\Phi,Q(t)\Psi\rangle_{-T_1}^+)^*=\langle Q(t)\Psi,\Phi\rangle_{-T_1}^+=\langle\tilde{H}(-T_1)^{-1}\tilde{H}(t)\Psi,\tilde{H}(-T_1)\Phi\rangle=\langle\tilde{H}(t)\Psi,\Phi\rangle, \tag{4.18}$$

where we have used (4.17). We then have that

$$\begin{aligned}(\langle\Phi,Q(t)\Psi\rangle_{-T_1}^+)^*&=\langle\Psi,\tilde{H}(-T_1)(\tilde{H}(-T_1))^{-1}\tilde{H}(t)\Phi\rangle\\&=\langle\Psi,\tilde{H}(-T_1)Q(t)\Phi\rangle=\langle\Psi,Q(t)\Phi\rangle_{-T_1}^+,\end{aligned} \tag{4.19}$$

which proves that $Q(t)$ is Hermitian.

In order to prove that $Q(t)$ is strictly positive on $\mathcal{F}_{+2}$, we must remember that, since $\mathcal{F}_{+2}^t\subset\mathcal{F}_{+2}$ $\forall$ t algebraically and topologically, it follows that the norms $\|\cdot\|_{-T_1}^+$ and $\|\cdot\|_t^+$ are equivalent, i.e., there exists $a_t\geqslant 1$ such that $a_t^{-1}\|\cdot\|_{-T_1}^+\leqslant\|\cdot\|_t^+\leqslant a_t\|\cdot\|_{-T_1}^+$. Then, for $\Psi\in\mathcal{F}_{+2}$,

$$\langle\Psi,Q(t)\Psi\rangle_{-T_1}^+=(\|\Psi\|_t^+)^2\geqslant a_t^{-2}(\|\Psi\|_{-T_1}^+)^2, \tag{4.20}$$

from which it follows that $\inf Q(t)>0$ and the proof is complete. □

V. CONCLUSION: OPEN PROBLEMS

The problem of the nonperturbative construction of $S(g)$ for the $(:\phi^4:)_2$ quantum field theory was addressed in Ref. 17 using Yosida's approach, which requires that the domain of $H_g(t)$ be time-independent. For test functions $g(x,t)=h_1(x)\cdot f_1(t)$, i.e., of the product form, this condition is satisfied, but already for a sum of two products, e.g., $g(x,t)=h_1(x)\cdot f_1(t)+h_2(x)\cdot f_2(t)$, with f_1 and f_2 having disjoint supports, this is no longer true, and thus the results of Ref. 17 are incomplete. The present approach does not suffer from this inconvenience, and g is allowed to be an arbitrary infinitely differentiable function of compact support. Moreover, the use of a scale of spaces makes the theory very flexible, being applicable to more singular super-renormalizable theories, as well as to four-dimensional theories with an ultraviolet cutoff. It is a very challenging problem to discover a possibility of ''renormalization'' of the exponentials of the type (A7) in the latter, in analogy to the interesting approach of Barata[18] and Gentile[19] to the study of certain two-level systems.

There are, however, open problems even to finish this program for the present $(:\phi^4:)_2$ theory: proof of causality for space-like supports $(ii.b)$ and proof of Lorentz covariance (iii). For this purpose, the method outlined in Ref. 17 seems natural: the above properties would follow from a proof of Faris's product formula[20] under the assumptions of Theorem IV 1. We shall return to this problem in the future.

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APPENDIX

Let us consider the problem (4.1) for the case in which $D(A(t))=\text{const}$. The notation is as in the first part of Sec. IV.

Consider the following conditions (in what follows $t\in[-T_1,T_2]$, unless otherwise specified):

(i) there exists a family $\|\cdot\|_t$, of norms in X such that $a^{-1}\|\Psi\|\leqslant\|\Psi\|_t\leqslant\|\Psi\|_s\leqslant a\|\Psi\|$, $a\geqslant 1$, for $-T_1\leqslant s\leqslant t\leqslant T_2$ and $\Psi\in X$;
(ii) Y is a dense subset of X with $D(A(t))=Y$;
(iii) for all $\lambda>0$ and $\Psi\in Y$ we have $R(\lambda-A(t))=X$ and $\|(\lambda-A(t))\Psi\|_t\geqslant\lambda\|\Psi\|_t$;
(iv) $A(t)$ is weakly continuously differentiable.

Theorem A.1 (Ref. 11, Theorem 3.0): *Let the conditions (i)–(iv) be satisfied. Then, there exists a unique solution of the problem (4.1) and the corresponding propagator $U(t,s)$ is strongly continuous in $-T_1\leqslant s\leqslant t\leqslant T_2$ and satisfies the properties (4.2), (4.3), (4.4), and (4.5).*

Now we shall explain some aspects of Kisyński's proof of this theorem. Consider the family of equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t)=A_n(t)\Phi(t),\quad \Phi(0)=\Phi_0,\quad n=1,2,\ldots, \tag{A1}$$

with

$$A_n(t)=nA(t)(n-A(t))^{-1}. \tag{A2}$$

The set Y supplied with the norm $\|\|\cdot\|\|_t=\|((1-A(t))\cdot\|$ is a Banach space algebraically and topologically contained in X. Then, from (i) and (iv), it follows that $A(t)\in\mathcal{L}(Y,X)$ is a weakly continuously differentiable operator, which, by the Banach–Steinhaus theorem, implies $\|A(t)\Phi\|\leqslant C\|\|\Phi\|\|_0$ for $\Phi\in Y$ and some constant C (the equivalence of the norms $\|\|\cdot\|\|_t$ was used). So, by using (i) and (iii), it follows that

$$\|\Phi-n(n-A(t))^{-1}\Phi\|=\frac{1}{n}\|(1-A(t)/n)^{-1}(A(t)\Phi)\|\leqslant\frac{Ca^2}{n}\|\|\Phi\|\|_0, \tag{A3}$$

which implies that $n(n-A(t))^{-1}$ converges strongly and uniformly to 1. Therefore, the sequence of bounded operators $A_n(t)$ converges strongly to $A(t)$. The operators $A_n(t)$ are weakly continuously differentiable, therefore they satisfy a Lipschitz condition in the sense of the norm. Hence, it follows that $A_n(t)$ is continuous in the sense of the norm and Yosida's method[13] guarantees the existence and the uniqueness of the evolution operators $U_n(t,s)$ of Eq. (A1) satisfying the properties equivalent to (4.2)–(4.5). Besides, $U_n(t,s)$ satisfy[11]

$$\|U_n(t,s)\|\leqslant M. \tag{A4}$$

Before proceeding we will consider Eq. (A1) perturbed by the bounded (in X) weakly continuous operator

$$B(t)=-\frac{\mathrm{d}A(t)}{\mathrm{d}t}(1-A(t))^{-1},$$

that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t)=(A_n(t)+B(t))\Phi(t),\quad \Phi(0)=\Phi_0. \tag{A5}$$

The evolution operator of (A5), denoted $H_n(t,s)$, is given by

$$H_n(t,s)=(1-A(t))U_n(t,s)(1-A(s))^{-1}.$$

Then, it follows that $H_n(t,s)\in\mathcal{L}(X)$ is weakly continuously differentiable in $-T_1\leqslant s,t\leqslant T_2$, satisfying

$$\|H_n(t,s)\|\leqslant D. \tag{A6}$$

Next we subdivide the segment $[-T_1,T_2]$ into K equal intervals. Then, the conditions ($T\equiv T_1+T_2$)

$$U_{nK}(t,s)=\exp\left\{(t-s)A_n\left(-T_1+\frac{i-1}{K}T\right)\right\}, \tag{A7}$$

$-T_1+((i-1)/K)\,T\leqslant s,t\leqslant -T_1+(i/K)\,T,\ i=1,\ldots,K,$ and

$$U_{nK}(t,s)U_{nK}(s,r)=U_{nK}(t,s),\quad -T_1\leqslant r,s,t\leqslant T_2, \tag{A8}$$

define a unique family of operators $U_{nK}(t,s)\in\mathcal{L}(X)$ continuous in the sense of the norm such that

$$\|U_{nK}(t,s)\|\leqslant a^2. \tag{A9}$$

The operators $U_{nK}(t,s)$ satisfy

$$\frac{\partial}{\partial s}U_{nK}(t,s)=-U_{nK}(t,s)A_n\left(-T_1+\frac{T}{K}\left[\frac{Ks}{T}\right]\right),$$

where $[(Ks)/T]$ stands for the integer part of $(Ks)/T$. Besides, for fixed K, $U_{nK}(t,s)$, $n=1,2,\ldots$, is a sequence uniformly strongly convergent in $-T_1\leqslant s\leqslant t\leqslant T_2$.

Then, by integrating $(\partial/\partial\tau)\,U_{nK}(t,\tau)U_n(\tau,s)$ we obtain

$$U_n(t,s)-U_{nK}(t,s)=\int_s^t U_{nK}(t,\tau)\left(A_n(\tau)-A_n\left(-T_1+\frac{T}{K}\left[\frac{K\tau}{T}\right]\right)\right)U_n(\tau,s)\,\mathrm{d}\tau. \tag{A10}$$

We have[11]

$$\left\|A_n(\tau)\Phi-A_n\left(-T_1+\frac{T}{K}\left[\frac{K\tau}{T}\right]\right)\Phi\right\|\leqslant\frac{\text{const}}{K}\||\Phi|\|_0. \tag{A11}$$

Then, since

$$U_n(t,s)=(1-A(t))^{-1}H_n(t,s)(1-A(s))$$

and $(1-A(s))\in\mathcal{L}(Y,X)$ and $(1-A(t))^{-1}\in\mathcal{L}(X,Y)$ are weakly differentiable, we obtain, by using (A6),

$$\||U_n(t,s)\Phi|\|_0\leqslant\text{const}\||\Phi|\|_0, \tag{A12}$$

for $\Phi\in Y$ and $-T_1\leqslant s\leqslant t\leqslant T_2$. Then, from (A9), (A10), (A11), and (A12), it follows that

$$\|U_n(t,s)\Phi-U_{nK}(t,s)\Phi\|\leqslant\frac{\mathrm{L}}{K}\||\Phi|\|_0, \tag{A13}$$

with $L=\text{const}$.

Now, for $\Phi\in Y$ we have

$$\begin{aligned}\|U_n(t,s)\Phi - U_m(t,s)\Phi\| &\leqslant \|U_n(t,s)\Phi - U_{nK}(t,s)\Phi\| + \|U_{mK}(t,s)\Phi - U_m(t,s)\Phi\| \\ &\quad + \|U_{nK}(t,s)\Phi - U_{mK}(t,s)\Phi\| \\ &\leqslant 2\frac{L}{K}\|\|\Phi\|\|_0 + \|U_{nK}(t,s)\Phi - U_{mK}(t,s)\Phi\|. \end{aligned} \tag{A14}$$

The first term on the right-hand side may be made arbitrarily small for large K. After this, one chooses n and m so large that the second term becomes arbitrarily small for all $-T_1 \leqslant s \leqslant t \leqslant T_2$, since the sequence $U_{nK}(t,s)$ is uniformly strongly convergent. Since Y is dense in X, and from (A4), (A14) implies that the convergence is in all of X, in the triangle $-T_1 \leqslant s \leqslant t \leqslant T_2$. Then, it follows directly from the properties of $U_n(t,s)$ that $U(t,s) = s - \lim_{n\to\infty} U_n(t,s)$ is the evolution operator of (4.1) for constant domain.[11]

Remark: The proof outlined above is valid for $-T_1 \leqslant s \leqslant t \leqslant T_2$. However, by substituting the conditions (i) and (iii) above by the conditions (a) and (c) in Theorem IV.1 the proof can be extended for the square $-T_1 \leqslant s,t \leqslant T_2$.

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Killing initial data revisited

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Considering the Killing vector fields on a Lorentzian manifold in terms of their lapse and shift along a space-like hypersurface, we give a new definition of the Killing Initial Data (KID) of Beig and Chruściel [Class. Quantum Grav. **14-1A**, A83 (1996)]. We define, on these new KID's, the bracket operation induced by the usual Lie bracket of Killing vector fields on the Lorentzian manifold, and study the conditions for our new KID's to form a Lie algebra. The interesting fact is that these conditions only depend on data along the hypersurface. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1755862]

I. INTRODUCTION AND NOTATIONS

The starting point of this work is the paper of Beig and Chruściel, Killing Initial Data,[1] where they studied properties of Killing vector fields on a Lorentzian manifold $(\overline{M},\overline{g})$ of dimension $n+1$. Let (M,g,k) be a space-like hypersurface, with induced metric g and second fundamental form k. Then they raised the following issue: If we decompose any vector field $\overline{X}$ in terms of a lapse function N and a shift vector X, that is to say, $\overline{X}=X+N\partial_t$, where ∂_t denotes the unit normal to M, how can we deduce that $\overline{X}$ is Killing only thanks to information along (M,g,k)?

For convenience, we are going to consider a tubular neighborhood $]-\epsilon,+\epsilon[\times M$ of M, $\epsilon>0$, and write $\overline{g}$ in Gaussian normal coordinates, that is to say,

$$\overline{g}=-dt^2+g_t,$$

where g_{t_0} is the Riemannian metric on the slice of equation $\{t=t_0\}$ induced by $\overline{g}$. Such coordinates will be chosen so that $M=\{t=0\}$, and then the Killing equations for $\overline{X}=X+N\partial_t$ are

$$\mathcal{L}_X g=-2Nk, \tag{1}$$

$$\partial_t N=0, \tag{2}$$

$$\partial_t X=\nabla N, \tag{3}$$

where $\mathcal{L}$ is the Lie derivative. Taking ∂_t of (1) we find

$$\mathcal{L}_X k+HessN=N(Ric+(trk)k-2(k\circ k))-N\overline{Ric}_{|TM\otimes TM}, \tag{4}$$

where $\circ$ is the composition of 2-tensors:

$$(k\circ k)_{ij}=k_{ip}k_{rj}g^{rp}.$$

In order to define "candidate Killing vector fields" they decided to call Killing Initial Data (KID), any couple $(N,X)\in C^\infty(M)\times\Gamma(TM)$ satisfying (1) and (4). Then, noticing that the space

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of Killing fields on $\overline{M}$ was closed under the usual bracket on $\overline{M}$, they wondered whether they could define a bracket {,} on the space of KID's with the same stability property.

Still reasoning from the decomposition of Killing fields in terms of lapse and shift, they gave a natural bracket {,} on the space of KID's, constructed from the usual bracket of Killing vector fields on $\overline{M}$. The important fact is that the conditions, in order to make KID's closed under {,}, involve a geometric quantity which is distinct from the constraints [part of Ricci curvature of $\overline{g}$ which is solely determined by the data (M,g,k)].

As a matter of fact, from a Cauchy point of view, a slightly different definition of KID's (that we will call new KID's) is more natural that the one used in Ref. 1. Both coincide in the vacuum and cosmological cases but they are not identical in general. The present work singles out the necessary and sufficient conditions under which the new KID's form a Lie algebra. The result obtained here is much more satisfactory, as the resulting conditions for the Lie algebra structure only involve objects naturally defined by a initial data set: The energy density and the momentum density.

Let us denote by G the Einstein tensor, and let us focus on the vacuum $(G=0)$ or cosmological $(G=\Lambda\overline{g},\ \Lambda$ constant) cases for a moment. If we call $L^\star$ the adjoint of the linearized constraints map, then being a KID exactly means belonging to Ker$L^\star$. More precisely, according to Ref. 2, it is possible to give an explicite correspondence between KID's and solutions of $L^\star=0$:

$$(N,X) \quad \text{KID} \Leftrightarrow L^\star(N,X^\flat)=0,$$

where $^\flat$ is the canonical isomorphism from TM to $T^\star M$ with respect to g. We will use the symbol $^\sharp$ to denote its inverse.

As a consequence, it leads us to adopt, in general, that is to say for *any Einstein tensor* G, the following:

Definition: Our new "candidate Killing vector fields" are the $(N,X)\in C^\infty(M)\times\Gamma(TM)$ *such as*

$$L^\star(N,X^\flat)=0.$$

Thus, using the same bracket as in Ref. 1, we study the conditions so that the space of our ''new KID's'' is a Lie algebra.

We will adopt the following definitions and conventions.[3,4] The Einstein tensor G of $\overline{g}$, is by definition

$$G=\overline{Ric}-\tfrac{1}{2}\overline{Scal}\,\overline{g}, \tag{5}$$

where $\overline{Ric}$ and $\overline{Scal}$ are the Ricci curvature and the scalar curvature of $\overline{g}$.

Let us define the constraint map as

$$\Phi(g,k)=\begin{pmatrix} Scal+(trk)^2-|k|^2 \\ -2(\delta k+dtrk)\end{pmatrix}, \quad (g,k)\in\mathcal{M}\times\Gamma(S^2T^\star M),$$

where $\mathcal{M}$ denotes the space of Riemannian metrics on M, *Scal* is the scalar curvature of g, norm and trace have to be taken with respect to g, and δ is the divergence operator acting on symmetric tensors, that is to say,

$$\delta S=-\sum_{i=1}^{n} D_{e_i}S(e_i,.,\ldots,.),$$

where D is the Levi-Civita connexion of (M,g), $(e_i)_{i=1}^n$ is any orthonormal basis at the point, and S is any symmetric tensor. We also define the adjoint of δ denoted by $\delta^\star$ which is

$$\delta^\star\beta(X,Y)=\tfrac{1}{2}(D_X\beta(Y)+D_Y\beta(X)),$$

for any 1-form β. For later use we define the Hessian and the Laplacian of a function f as follows:

$$Hess(f)=Ddf, \quad \Delta f=\delta df=-tr_g Hess(f).$$

If we denote at $t=0$

$$2G_{|TM\otimes TM}=\tau, \quad 2G(\partial_t,\partial_t)=\psi, \quad 2G(\partial_t,.)=\omega,$$

then the following equations, known as the constraints equations, are satisfied on M:

$$\begin{pmatrix} Scal+(trk)^2-|k|^2 \\ -2(\delta k+dtrk) \end{pmatrix}=\begin{pmatrix} \psi \\ \omega \end{pmatrix}.$$

If one defines

$$E(f,\alpha)=Hess(f)-f(Ric+2(trk)k-2(k\circ k))+\mathcal{L}_{\alpha^\sharp}k+(\delta\alpha)k,$$

then the expression of $L^\star$ is

$$\begin{pmatrix} L_1^\star(f,\alpha) \\ L_2^\star(f,\alpha) \end{pmatrix}=\begin{pmatrix} E(f,\alpha)-tr(E(f,\alpha))g-(\frac{1}{2}\langle L_2^\star(f,\alpha),k\rangle+\frac{1}{2}\langle\alpha,\omega\rangle+f\psi)g \\ -2(\delta^\star\alpha+fk)+2tr(\delta^\star\alpha+2fk)g \end{pmatrix},$$

where $(f,\alpha)\in C^\infty(M)\times\Gamma(T^\star M)$ are the dual infinitesimal deformations for Φ at the point (g,k) and $\langle,\rangle$ denotes the scalar product extended to all tensors.

Finally a direct computation leads us to

$$L^\star(f,\alpha)=0\Leftrightarrow\begin{cases} \mathcal{L}_X k+HessN=N(Ric+(trk)k-2(k\circ k))+\dfrac{1}{2(1-n)}(\omega(X)+2N\psi)g \\ \mathcal{L}_X g+2Nk=0, \end{cases}$$

if we denote $f=N$, $\alpha=X^\flat$. These relations, and the equivalence above will be used implicitly throughout the text, so that we can write elements of $\mathrm{Ker}L^\star$ in terms of (N,X) or in terms of (f,α).

II. LIE ALGEBRA STRUCTURE OF Ker$L^\star$

The motivation for the definition of the bracket lies on the Lie structure of the Killing fields on the Lorentzian manifold $\overline{M}$. Let us take two Killing fields $\overline{X_i}=X_i+N_i\partial_t$ $(i=1,2)$, their bracket, using (2)–(4), is

$$[\overline{X_1},\overline{X_2}]=[X_1,X_2]+N_1\nabla N_2-N_2\nabla N_1+(\mathcal{L}_{X_1}N_2-\mathcal{L}_{X_2}N_1)\partial_t.$$

Definition: We define $\{,\}$ *on* $C^\infty(M)\times\Gamma(TM)$ *as*

$$\{(N_1,X_1),(N_2,X_2)\}:=(\mathcal{L}_{X_1}N_2-\mathcal{L}_{X_2}N_1,[X_1,X_2]+N_1\nabla N_2-N_2\nabla N_1).$$

Proposition: $\{,\}$ *satisfies the Jacobi identity on* $KerL_2^\star\subset C^\infty(M)\times\Gamma(TM)$.

Proof: It relies on computations which are the same as in Ref. 1.

From now on, $\odot$ will denote the symmetric product of 1-forms, that is to say,

$$\theta_1\odot\theta_2(U,V)=\tfrac{1}{2}(\theta_1(U)\theta_2(V)+\theta_1(V)\theta_2(U)),$$

for any 1-forms θ_i, $i=1,2$. The main result of this note is then:

Theorem: *The* $\mathbb{R}$*-vector space* $KerL^\star \subset C^\infty(M) \times \Gamma(TM)$ *with the bracket* $\{,\}$*, is a Lie algebra if and only if the following conditions are satisfied:*

$$\text{(i)} \quad N_1\omega(X_2) = N_2\omega(X_1),$$

$$\text{(ii)} \quad \omega \odot (N_2 \mathrm{d}N_1 - N_1 \mathrm{d}N_2) = 0,$$

$$\text{(iii)} \quad \mathrm{d}\omega(X_1, X_2) + \mathrm{d}\psi(N_2X_1 - N_1X_2) = 0,$$

$\forall (N_1X_1), (N_2X_2) \in KerL^\star$, along (M, g, k, ω, ψ).

Remark: We have to underline that the existence of nontrivial solutions of $L^\star = 0$ prevents the level-sets of the constraints map from being manifolds. So it could appear important to be able to give information about Ker$L^\star$ only depending on the constraints which caracterize the level-sets. This provides another interest for this new definition of KID's.

Corollary: If $\psi = constant$ *and* $\omega = 0$*, then* $(KerL^\star, \{,\})$ *is a Lie algebra.*

Applications of the Corollary: The first remark concerns the vacuum and cosmological cases. The corollary points out a result that was already known thanks to the KID's. This is a consequence of the simple fact that, in both cases, being a KID in the sense of Ref. 1, is equivalent to be a solution of the equation $L^\star = 0$.

Second, we can hope, thanks to the following example, that this theorem could have good applications. Indeed let us consider the case of perfect fluid-pure matter for the stress-energy tensor. Then

$$T = (\rho + p)\xi \otimes \xi + p\overline{g},$$

where $v = \xi^\flat$ is the unitary and time-like speed vector of fluid particule. If we assume moreover that $\xi = dt$, so that

$$T = \rho dt^2 + p g_t .$$

If we make the assumption that ρ only depends on t, the conditions of our theorem are satisfied, whereas the conditions for the KID's are not if we do not make any assumption on the function p. This shows that the conditions of our theorem are adapted to the geometric constraints (ψ and ω), whereas the conditions of Ref. 1 are less, because of the role of τ in their expression.

III. PROOF OF THE THEOREM

(i) Let us take 2 couples $(N_1X_1), (N_2X_2)$ satisfying $L^\star(N_i, X_i^\flat) = 0$ $(i = 1,2)$. Then one finds

$$\begin{aligned} &\mathcal{L}_{[X_1,X_2]+N_1\nabla N_2 - N_2\nabla N_1} g + 2(\mathcal{L}_{X_1}N_2 - \mathcal{L}_{X_2}N_1)k \\ &\quad = 2N_1(\mathcal{L}_{X_2}k + Hess N_2) - 2N_2(\mathcal{L}_{X_1}k + Hess N_1) \\ &\quad = \frac{1}{(1-n)}(N_1\omega(X_2) - N_2\omega(X_1)), \end{aligned}$$

and the first condition follows.

(ii) Still in order to make Ker$L^\star$ closed under $\{,\}$, the following equation has to hold:

$$\begin{aligned} 0 = {} & \mathcal{L}_{N_1\nabla N_2 - N_2\nabla N_1}k + [Hess, \mathcal{L}_{X_1}]N_2 - [Hess, \mathcal{L}_{X_2}]N_1 + (N_2\mathcal{L}_{X_1} - N_1\mathcal{L}_{X_2})(Ric + (trk)k \\ & - 2(k \circ k)) + \frac{1}{(1-n)}(N_2\mathcal{L}_{X_1} - N_1\mathcal{L}_{X_2})(\psi g) + \frac{1}{2(1-n)}(\mathcal{L}_{X_1}(\omega(X_2)g) - \mathcal{L}_{X_2}(\omega(X_1)g)) \\ & - \frac{1}{2(1-n)}\omega([X_1, X_2] + N_1\nabla N_2 - N_2\nabla N_1)g = \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} + \mathrm{V} + \mathrm{VI}. \end{aligned} \tag{6}$$

From this point, we will assume that condition (i) holds. For convenience, we are going to compute this expression in several steps. We will use the notation $\{(N_1,X_1)\leftrightarrow(N_2,X_2)\}$ which means that we rewrite the beginning of the expression replacing (N_1,X_1) by (N_2,X_2).

$$\mathrm{I}=D_{N_1\nabla N_2}k+2\mathrm{d}N_1\odot i_{\nabla N_2}k+N_1(k\circ HessN_2+HessN_2\circ k)-\{(N_1,X_1)\leftrightarrow(N_2,X_2)\},$$

$$\mathrm{II}=2N_2\delta^\star(i_{\nabla N_1}k)+2\mathrm{d}N_2\odot i_{\nabla N_1}k-D_{N_2\nabla N_1}k-N_2(HessN_1\circ k+k\circ HessN_1)$$
$$-\{(N_1,X_1)\leftrightarrow(N_2,X_2)\}.$$

Three terms are involved in III:
First of all:

$$(N_2\mathcal{L}_{X_1}-N_1\mathcal{L}_{X_2})(Ric)=-N_2\Delta N_1k+2N_2D_{\nabla N_1}k-2N_2\delta^\star(i_{\nabla N_1}k)$$
$$-(N_2trk)\mathcal{L}_{X_1}k-\omega\odot(N_2\mathrm{d}N_1)-\{(N_1,X_1)\leftrightarrow(N_2,X_2)\}.$$

Second:

$$(N_2\mathcal{L}_{X_1}-N_1\mathcal{L}_{X_2})(k\circ k)=N_2(k\circ\mathcal{L}_{X_1}k+\mathcal{L}_{X_1}k\circ k)-\{(N_1,X_1)\leftrightarrow(N_2,X_2)\}.$$

And finally, taking the trace of $L_1^\star(f,\alpha)=0$, we find

$$\mathcal{L}_{X_i}(trk)+2\langle k,\delta^\star X_i^\flat\rangle-\Delta N_i=N_i(Scal+(trk)^2-2|k|^2)+[n/2(1-n)](\omega(X_i)+2N_i\psi),$$

but reminding that $\langle k,\delta^\star X_i^\flat\rangle=\langle k,\delta^\star\alpha_i\rangle=-f_i|k|^2=-N_i|k|^2$, this equation is equivalent to

$$\mathcal{L}_{X_i}(trk)=\Delta N_i+N_i\left(Scal+(trk)^2+\frac{n}{(1-n)}\psi\right)+\frac{n}{2(1-n)}\omega(X_i).$$

We use this information in order to compute the last term of III:

$$(N_2\mathcal{L}_{X_1}-N_1\mathcal{L}_{X_2})((trk)k)=trk(N_2\mathcal{L}_{X_1}-N_1\mathcal{L}_{X_2})k+(N_2\Delta N_1-N_1\Delta N_2)k.$$

Thus it follows:

$$\mathrm{III}=2N_2(D_{\nabla N_1}k-\delta^\star(i_{\nabla N_1}k)-k\circ\mathcal{L}_{X_1}k-\mathcal{L}_{X_1}k\circ k-\tfrac{1}{2}\omega\odot\mathrm{d}N_1)-\{(N_1,X_1)\leftrightarrow(N_2,X_2)\}.$$

Finally, we have a look at the terms involving ψ and ω in the expression of (6). After some easy computations, the remainig terms are

$$(1-n)\mathrm{IV}=\mathrm{d}\psi(N_2X_1-N_1X_2)g+\psi(N_2\mathcal{L}_{X_1}g-N_1\mathcal{L}_{X_2}g)=\mathrm{d}\psi(N_2X_1-N_1X_2)g,$$

$$2(1-n)\mathrm{V}=((D_{X_1}\omega)(X_2)-(D_{X_2}\omega)(X_1)+\omega([X_1,X_2]))g+2(N_2\omega(X_1)-N_1\omega(X_2))k$$
$$=(2\mathrm{d}\omega(X_1,X_2)+\omega([X_1,X_2]))g.$$

Finally, when we add all terms of (6) together, still assuming that condition (i) holds, (6) becomes

$$0=-\omega\odot(N_2\mathrm{d}N_1-N_1\mathrm{d}N_2)$$
$$+\frac{1}{(1-n)}\left(\mathrm{d}\omega(X_1,X_2)+\mathrm{d}\psi(N_2X_1-N_1X_2)+\frac{1}{2}\omega(N_2\nabla N_1-N_1\nabla N_2)\right)g. \qquad (7)$$

Now, taking the trace of (7), it follows:

$$\omega(N_2\nabla N_1 - N_1\nabla N_2) = \frac{2n}{(2-3n)}(\mathrm{d}\omega(X_1,X_2) + \mathrm{d}\psi(N_2X_1 - N_1X_2)). \tag{8}$$

And finally we obtain

$$\omega\odot(N_2\mathrm{d}N_1 - N_1\mathrm{d}N_2) = \frac{2}{(2-3n)}(\mathrm{d}\omega(X_1,X_2) + \mathrm{d}\psi(N_2X_1 - N_1X_2))g. \tag{9}$$

And the proof is complete: The fact that the rank of the left member of (9) is 2 whereas the rank of the right one is $n \geqslant 3$, entails that both vanish. The corollary is straightforward since the conditions of our theorem are clearly satisfied. □

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On quantum error-correction by classical feedback in discrete time

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We consider the problem of correcting the errors incurred from sending quantum information through a noisy quantum environment by using classical information obtained from a measurement on the environment. For discrete time Markovian evolutions, in the case of fixed measurement on the environment, we give criteria for quantum information to be perfectly corrigible and characterize the related feedback. Then we analyze the case when perfect correction is not possible and, in the qubit case, we find optimal feedback maximizing the channel fidelity. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1758320]

I. INTRODUCTION

Error correction is a key problem in quantum information processing. Without it, decoherence would easily destroy all hopes for quantum computation and quantum cryptography.

Two important approaches have been devoloped to combat decoherence. The usual theory of quantum error-correction[1,2] redundantly encodes the original quantum information in a larger quantum system by a unitary operation which maps the initial Hilbert space into the code space, a subspace of the Hilbert space associated to this larger system. After encoding, the larger system is subjected to noise and then a measurement is performed on the system to diagnose the type of error which occurred. Finally, on the basis of the outcome, a restoring operation is performed to return the system to the original state in the code space.

Another approach,[3–7] based on feedback control, has been developed for systems which are continuously monitored during their noisy evolution.[8] It employs the result of this continuous measurement to determine the errors occurred and, on this basis, perform corrections in real time to protect states which are known to lie initially within a certain code space. The continuous measurement can be performed introducing an additional interaction to the evolution of the system or preferably by simply observing the environment after its interaction with the system. Up to now there is no general theory for quantum feedback control, but some correction schemes have been considered and have dealt only with Hamiltonian feedback.

Taking from feedback control the idea of a correction scheme based on a measurement performed not on the system but on the environment, we have analyzed in an earlier publication[9] the different possible behaviors of a channel with respect to the existence of a measurement allowing perfect correction of information, quantum or classical. No code space is introduced and, for every initial state, the aim is to find proper measurement and restoring operations, not necessarily unitary, to recover the initial information or at least optimally restore it.

Here we develop the analysis in Ref. 9 to evolutions composed of many time steps. We consider quantum information carried by a system undergoing a discrete time Markovian evolution (multistep channel $T=T^{(n)}\circ\cdots\circ T^{(1)}$) and allow correction operations between any two sub-

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sequent steps: every time we perform a measurement on the environment and a restoring operation on the system. We take the measurments on the environment as given and we look for the best restoring operations choosen on the basis of all the outcomes observed so far. First we give conditions for quantum information to be perfectly corrigible and characterize the related feedback. It turns out that classical feedback is not useful because perfect correction of quantum information is possible only if a unique correction at the end would suffice. Then we analyze the case when perfect correction is not possible and, in the qubit case, we find optimal feedback maximizing the channel fidelity. Similarly to the case of perfect correction, but more surprisingly, classical feedback is still useless if quantum information is carried by one qubit because again a unique restoring operation performed at the end of the evolution guarantees the same performance of correction. Anyway classical feedback is shown to be helpful when the quantum carrier has a higher dimensional Hilbert space.

Every section of the paper considers first the case of quantum information sent through a single-step channel, so that it is possible only one correction after this noisy evolution just as in Ref. 9, and then the case of a multistep channel, so that classical feedback is possible during the noisy evolution. In Sec. II, we set up the framework and the basic correction scheme. In Sec. III, for a given channel and given measurements on the environment, we prove the basic criteria for the existence of a scheme perfectly correcting quantum information, and we characterize the related feedback. In Sec. IV we look for optimal correction scheme when it is not be possible to achieve a complete correction of errors. In Sec. V we briefly discuss the transposition of this approach to continuous time and the difficulties which arise in this case.

II. THE CORRECTION SCHEME

We consider quantum information carried by a quantum system with finite dimensional Hilbert space $\mathcal{H}$. We work in the Schrödinger picture, so the action of the noisy *channel*, which corrupts the information transforming each input density operator ρ on $\mathcal{H}$ to a different output density operator $T(\rho)$ on $\mathcal{H}$, is given by a completly positive, trace preserving, linear map $T:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$, where $\mathcal{L}(\mathcal{H})$ denotes the space of all linear operators on $\mathcal{H}$. A channel T is not physically reversible, i.e., there is no channel R such that $R\circ T=\mathrm{id}$, unless T is a unitary channel $T(\rho)=u\,\rho\,u^*$, with $u\in\mathcal{U}(\mathcal{H})$, the group of unitary operators on $\mathcal{H}$.

A. Single-step channel

Every channel can be described as the result of a unitary coupling to an environment, followed by the discard of the environment after the interaction. Nevertheless, the initial information carried by $\mathcal{H}$ is then shared with the environment and indeed, if we controlled perfectly the combined system, then we could recover the initial quantum information simply by reversing the global evolution, so restoring perfectly the input state ρ. We do not hypothesize this, but we assume that our control on the environment is good enough to have its initial state pure and to be able to perform any measurement on it after the interaction with $\mathcal{H}$. The measurement of an observable X on the environment decomposes the channel T into an *instrument*, a family of completely positive maps T_x giving the (non-normalized) output states $T_x(\rho)$ of the subensembles of systems selected according to the result "x" of this measurement: the probability of observing x is $\mathbb{P}(X=x)=\mathrm{tr}T_x(\rho)$, the normalized output state for the corresponding subensemble is $T_x(\rho)/\mathrm{tr}T_x(\rho)$, and the expectation in that subensemble of a self-adjoint $A\in\mathcal{L}(\mathcal{H})$ is $\mathrm{tr}(T_x(\rho)A)/\mathrm{tr}T_x(\rho)$. Ignoring the result of the measurement one recovers the original channel

$$T=\sum_x T_x. \tag{1}$$

Of course, the result x of the measurement gives classical information about the environment after the interaction, and hence also about $\mathcal{H}$ before the interaction. The idea for the correction scheme is to employ this information to select a proper restoring channel: we introduce a family of channels $R^{(x)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$, where $R^{(x)}$ can depend in an arbitrary way on x. After correction,

the state of the subensemble for which the measurement has given the result x, will be $R^{(x)}(T_x(\rho))$ up to the normalization factor $\mathrm{tr}(T_x(\rho))$. The overall corrected channel is built from these conditional operations by ignoring the intermediate information x, and is the sum of these contributions:

$$T_{\mathrm{corr}}=\sum_x R^{(x)}\circ T_x. \tag{2}$$

The goodness of the scheme in restoring quantum information depends on how T_{corr} can be brought close to the ideal channel on $\mathcal{H}$, i.e., id.

Whether or not we can find a good correction scheme in principle depends not only on the noisy channel T, but also on the set of decompositions (1) obtainable by a measurment on the environment, which usually depends on the particular coupling which induces the noisy evolution T. Anyway the assumption of a pure environment overcomes this problem because it guarantees that every decomposition of T into c.p. summands T_x can be realized by a measurement on the environment. Moreover, in order to correct quantum information, the preferable docompositions are the finest ones, those for which no proper refinement is possible. Therefore we shall consider the non refinable decompositions given by the Kraus representations of T:

$$T(\rho)=\sum_x t_x\,\rho\,t_x^*, \quad \text{where } \sum_x t_x^* t_x=\mathbb{1}. \tag{3}$$

In the following we shall assume that a decomposition (3) is given, that it is associated to the measurement of an observable X, and for it we shall consider the problem of perfectly correcting quantum information or, if this is not possible, optimally restoring it.

B. Multistep channel

We are especially interested in multistep channels, where the noisy evolution T is given by n Markovian steps:

$$T=T^{(n)}\circ\cdots\circ T^{(1)}, \tag{4}$$

where $T^{(k)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ are n possibly different channels. In this case we assume to be able to perform a measurement at each step, so that every $T^{(k)}$ is decomposed into

$$T^{(k)}(\rho)=\sum_{x_k} t_{x_k}^{(k)}\,\rho\,t_{x_k}^{(k)*}, \quad \text{where } \sum_{x_k} t_{x_k}^{(k)*} t_{x_k}^{(k)}=\mathbb{1}, \tag{5}$$

the channel T is decomposed into

$$T(\rho)=\sum_{x_1,\ldots,x_n} t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)*}\cdots t_{x_n}^{(n)*}, \tag{6}$$

and the probability of observing $(x_1,\ldots,x_n)$ is $\mathbb{P}(X_1=x_1,\ldots,X_n=x_n)=\mathrm{tr}\,t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)*}\cdots t_{x_n}^{(n)*}$.

We also assume to be able to interfere in the evolution of the system after each step by appling a restoring channel selected according to the whole information gathered so far. For every $k=1,\ldots,n$, we introduce a family of channels $R^{(x_1,\ldots,x_k)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$, where $R^{(x_1,\ldots,x_k)}$ can depend in an arbitrary way on $(x_1,\ldots,x_k)$ and it is applied after the measurement of X_k so that the overall corrected channel turns out to be

$$T_{\mathrm{corr}}(\rho)=\sum_{x_1,\ldots,x_n} R^{(x_1,\ldots,x_n)}(t_{x_n}^{(n)}\cdots R^{(x_1)}(t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)*})\cdots t_{x_n}^{(n)*}). \tag{7}$$

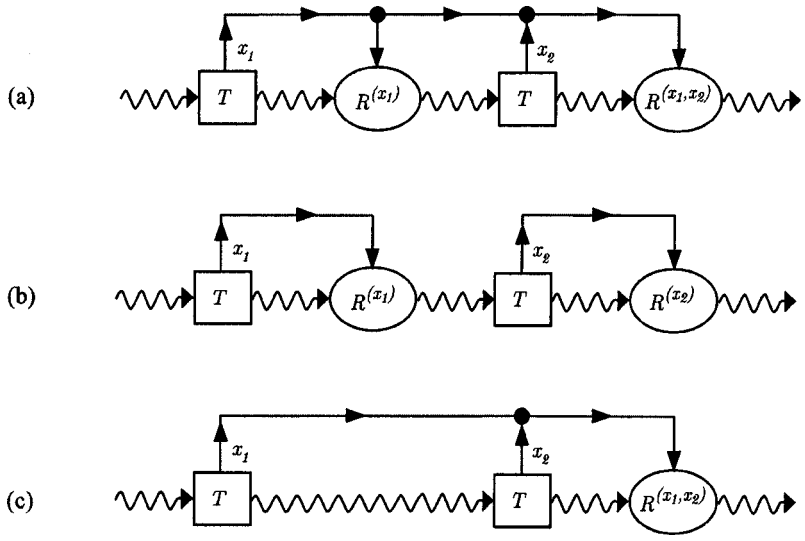

FIG. 1. Different error correction schemes for multiple channels. (a) represents the most general case. In (b) only the information from the immediately preceding step is used. In (c) only one correction is done at the end.

So the classical information obtained by the measurement process on the environment is fedback to modify the evolution of the system $\mathcal{H}$. Notice that this general scheme includes the special cases (compare Fig. 1):

(b) $R^{(x_1,\ldots,x_k)}=R^{(x_k)}$ for every $k=1,\ldots,n$, i.e., every restoring channel is selected according only to the last observation x_k;

(c) $R^{(x_1,\ldots,x_k)}=\mathrm{id}$ for every $k=1,\ldots,n-1$, i.e., the information given by the measurement on the environment is gathered during the evolution, but every correction is deferred after it.

In the following we shall assume that a decomposition (6) is fixed, that it is associated with a measurement process, and, given this, we shall consider the problem of perfect or optimal correction of quantum information.

III. PERFECT CORRECTION OF QUANTUM INFORMATION

Given a channel T with a fixed decomposition (3) or (6), our scheme can perfectly correct quantum information if one can find restoring channels R such that

$$T_{\mathrm{corr}}=\mathrm{id}\,.$$

A. Single-step channel

Let us improve the criterion given in Ref. 9.

Propostion 1: Let $T:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ be a channel over a finite dimensional Hilbert space $\mathcal{H}$. Given a Kraus decomposition $T(\rho)=\Sigma_x t_x\,\rho\,t_x^*$, the following are equivalent:

(a) there exists a family of channels $R^{(x)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ perfectly restoring quantum information;

(b) $t_x^* t_x=p_x\mathbb{1}$ for all x, with $p_x\geqslant 0$, $\Sigma_x p_x=1$;

(b′) $t_x=\sqrt{p_x}\,u_x$ for all x, with $u_x\in\mathcal{U}(\mathcal{H})$, $p_x\geqslant 0$, $\Sigma_x p_x=1$;

(b″) $T(\rho)=\Sigma_x p_x\,u_x\,\rho\,u_x^*$ is a convex combination of unitary channels;

(c) $\mathbb{P}(X=x)=\mathrm{tr}\,t_x\,\rho\,t_x^*$ is independent of the input state ρ.

When these conditions hold, then the restoring channels in (a) have to be

$$R^{(x)}(\rho)=u_x^*\,\rho\,u_x\,, \tag{8}$$

and the probability law of the outcome is

$$\mathbb{P}(X=x)=p_x\,. \tag{9}$$

Proof: (a)⇒(b). Let $R^{(x)}$ be channels such that $\Sigma_x R^{(x)}(t_x\,\rho\,t_x^*)=\rho$ for every state ρ. Then for every x, by the ''No information without perturbation'' Theorem, $R^{(x)}(t_x\,\rho\,t_x^*)=p_x\,\rho$, for some $p_x\geqslant 0$, $\Sigma_x p_x=1$. Therefore $\mathrm{tr}t_x^*t_x\,\rho=\mathrm{tr}t_x\,\rho\,t_x^*=\mathrm{tr}R^{(x)}(\mathrm{tr}t_x\,\rho\,t_x^*)=p_x$ for all ρ, and so $t_x^*t_x=p_x\,\mathbb{1}$.

(b)⇔(b′)⇔(b″). These conditions are clearly all equivalent because $\dim\mathcal{H}<\infty$.

(b′)⇒(c). $\mathbb{P}(X=x)=\mathrm{tr}t_x\,\rho\,t_x^*=\mathrm{tr}\sqrt{p_x}\,u_x^*\,\rho\,\sqrt{p_x}\,u_x=p_x$ for every ρ, so (b′) implies (c), and Eq. (9), too.

(c)⇒(a). $\mathrm{tr}\,t_x^*t_x\,\rho=\mathrm{tr}\,t_x\,\rho\,t_x^*=\mathbb{P}(X=x)$ which does not depend on ρ and so $t_x^*t_x=\mathbb{P}(X=x)\,\mathbb{1}$. Then $t_x=\sqrt{\mathbb{P}(X=x)}\,u_x$, where u_x is unitary because $\dim\mathcal{H}<\infty$, and the channels $R^{(x)}(\rho)=u_x^*\,\rho\,u_x$ perfectly restore quantum information.

Now we have to show that conditions (a), (b), and (c) imply (8). Consider a family of channels $R^{(x)}$ restoring quantum information, with $R^{(x)}(\rho)=\Sigma_j r_j^{(x)}\,\rho\,r_j^{(x)*}$ and $\Sigma_j r_j^{(x)*}r_j^{(x)}=\mathbb{1}$. Then

$$\sum_{x,j} r_j^{(x)}\,t_x\,\rho\,t_x^*\,r_j^{(x)*}=\rho\,,\quad \forall\ \rho\,,$$

and using again the ''No information without perturbation'' Theorem we have

$$r_j^{(x)}\,t_x=\sqrt{p_{x,j}}\,\mathrm{e}^{\mathrm{i}\theta(x,j)}\,\mathbb{1}\,,\quad \forall\ x,j,$$

for some probability law $p_{x,j}$ and some real function θ. Using (b′), we get

$$r_j^{(x)}=\sqrt{\frac{p_{x,j}}{p_x}}\,\mathrm{e}^{\mathrm{i}\theta(x,j)}\,u_x^*\propto u_x^*\quad \forall\ j,$$

i.e., fixed $R^{(x)}$, all the Kraus oprators $r_j^{(x)}$ have to be proportional to the same unitary operator u_x^*, and (8) holds. □

Let us remark that condition (b) gives a simple criterion for the existence of channels R perfectly restoring quantum information based directly on the Kraus operators of T. Moreover it clarifies the structure of channels which allow perfect correction with our scheme: the measurement on the environment has to decompose T into a convex combination of unitary channels, so that the overall evolution can be seen as an average of reversible evolutions $\rho\mapsto u_x\,\rho\,u_x^*$, which occur randomly with probability p_x; the measurement detects the transformation occurred and $R^{(x)}(\rho')=u_x^*\,\rho'\,u_x$ restores the initial state ρ. This means also, by condition (c), that the measurement on the environment is completely uninformative about the system $\mathcal{H}$: the output x can be interpreted as classical information about ''what happened'' to the system $\mathcal{H}$, but it gives no information about the input system because it is independent of its state. And the uninformative character of the observation, if associated to a Kraus decomposition of T, is sufficient for perfect correction. Moreover, if perfect correction is possible, the restoring channels R have to be unitary.

Here every channel T with a decomposition satisfying condition (b) will be called *corrigible*.

Just to show how useful can be a suitable measurement on the environment, let us remark that our scheme can perfectly correct quantum information sent through a depolarizing channel, which is known to destroy all quantum information and for which no ordinary quantum error correcting code works (it has zero quantum and classical capacity). Indeed, set $N=\dim\mathcal{H}$, the depolarizing channel $T(\rho)=(1/N)\mathbb{1}$ admits the Kraus representation

$$T(\rho)=\sum_{x,y=1}^{N} t_{x,y}\,\rho\,t_{x,y}^*\,,\quad t_{x,y}=\frac{1}{N}\sum_{z=1}^{N}\mathrm{e}^{(2\pi\mathrm{i}/N)\,zy}\,|z+x\rangle\langle z|=\frac{1}{N}u_{x,y}\,,$$

with unitary operators $u_{x,y}$, where $\{|z\rangle\}_{z\in\mathbb{Z}_N}$ denotes a basis labeled cyclically so that addition in $|z+x\rangle$ is modulo N.

B. Multistep channel

Let us consider now perfect correction for multistep channels.

Propostion 2: Let $T=T^{(n)}\circ\cdots\circ T^{(1)}$, *with every* $T^{(k)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$, *be a multistep channel over a finite dimensional Hilbert space* $\mathcal{H}$. *Given the Kraus decompositions* $T^{(k)}(\rho)=\Sigma_{x_k}t^{(k)}_{x_k}\rho\, t^{(k)*}_{x_k}$, *T.F.A.E.*

(a) there exists a family of channels $R^{(x_1)},R^{(x_1,x_2)},\ldots,R^{(x_1,\ldots,x_n)}$ *perfectly restoring quantum information*;

(b) every channel $T^{(k)}(\rho)=\Sigma_{x_k}t^{(k)}_{x_k}\rho\, t^{(k)*}_{x_k}$ *is corrigible, i.e., for all* x_k *we have* $t^{(k)}_{x_k}=\sqrt{p^{(k)}_{x_k}}\,u^{(k)}_{x_k}$, *with* $u^{(k)}_{x_k}\in\mathcal{U}(\mathcal{H})$, $p^{(k)}_{x_k}\geqslant 0$, $\Sigma_{x_k}p^{(k)}_{x_k}=1$;

(c) $\mathbb{P}(X_1=x_1,\ldots,X_n=x_n)=\mathrm{tr}\,t^{(n)}_{x_n}\cdots t^{(1)}_{x_1}\rho\, t^{(1)*}_{x_1}\cdots t^{(n)*}_{x_n}$ *is independent of the input state* ρ.

When these conditions hold, then for every $k=1,\ldots,n$ *the restoring channels in (a) have to be*

$$R^{(x_1,\ldots,x_k)}(\rho)=v^{(x_1,\ldots,x_k)}\rho\, v^{(x_1,\ldots,x_k)*},\quad v^{(x_1,\ldots,x_k)}\in\mathcal{U}(\mathcal{H}),\tag{10}$$

with

$$v^{(x_1,\ldots,x_n)}=u^{(1)*}_{x_1}v^{(x_1)*}\cdots v^{(x_1,\ldots,x_{n-1})*}u^{(n)*}_{x_n},\tag{11}$$

and the probability law of the outcome process is always

$$\mathrm{tr}\,R^{(x_1,\ldots,x_n)}(t^{(n)}_{x_n}\cdots R^{(x_1)}(t^{(1)}_{x_1}\rho\, t^{(1)*}_{x_1})\cdots t^{(n)*}_{x_n})=\prod_{k=1}^{n}p^{(k)}_{x_k}.\tag{12}$$

Therefore, as long as we are interested in perfect correction of quantum information, the multistep structure of the channel and the possibility of applying feedback during the evolution do not help: perfect correction is possible if and only if every step is corrigible and, in this case, it is enough to make a unique correction at the end. Indeed only unitary corrections are allowed, otherwise the original information would be corrupted by the feedback itself, and then the first $n-1$ unitaries $v^{(x_1,\ldots,x_k)}$ can be chosen arbitrarly, also $v^{(x_1,\ldots,x_k)}=\mathbb{1}$, provided that the whole evolution is reversed by the last one (Eq. (11)). Again, the channel is corrigible if and only if the measured process is uninformative; moreover its probabilistic law, which cannot be modified by the unitary feedback, is that of a sequence of independent random variables.

The proof of Proposition 2 goes via a more general result about the composition of n channels when each channel is decomposed according to a measurement and, not only each channel itself, but also its decomposition, may depend on the previous observations. Therefore, denoted by x_k the outcomes of the measurement at the kth step, we want to consider the evolution of a quantum system sent through a sequence of channels on $\mathcal{L}(\mathcal{H})$,

$$T^{(x_1,\ldots,x_{k-1})}(\rho)=\sum_{x_k}t^{(x_1,\ldots,x_{k-1})}_{x_k}\rho\, t^{(x_1,\ldots,x_{k-1})*}_{x_k},\quad \sum_{x_k}t^{(x_1,\ldots,x_{k-1})*}_{x_k}t^{(x_1,\ldots,x_{k-1})}_{x_k}=\mathbb{1},\tag{13}$$

where for the first step, $k=1$, we denote by "0" the empty string of prior results, so we write

$$T^{(0)}(\rho)=\sum_{x_1}t^{(0)}_{x_1}\rho\, t^{(0)*}_{x_1},\quad \sum_{x_1}t^{(0)*}_{x_1}t^{(0)}_{x_1}=\mathbb{1}.$$

Then the total evolution is

$$T(\rho)=\sum_{x_1,\ldots,x_n}t^{(x_1,\ldots,x_{n-1})}_{x_n}\cdots t^{(0)}_{x_1}\rho\, t^{(0)*}_{x_1}\cdots t^{(x_1,\ldots,x_{n-1})*}_{x_n},\tag{14}$$

and the next Proposition holds.

Propostion 3: Given a finite dimensional Hilbert space $\mathcal{H}$, let $T:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ be a channel (14) resulting from the application of n decomposed channels $T^{(x_1,\ldots,x_{k-1})}$ (13). If $T=\mathrm{id}$, then

(a) every channel $T^{(x_1,\ldots,x_{k-1})}(\rho)=\Sigma_{x_k}t_{x_k}^{(x_1,\ldots,x_{k-1})}\,\rho\,t_{x_k}^{(x_1,\ldots,x_{k-1})^*}$ is corrigible;

*(b) a channel $T^{(x_1,\ldots,x_{k-1})}$ is unitary if later channels and their decomositions do not depend on the value x_k observed at the k*th *step.*

Proof: If $T=\mathrm{id}$, then

$$t_{x_n}^{(x_1,\ldots,x_{n-1})}\cdots t_{x_1}^{(0)}=\sqrt{p(x_1,\ldots,x_n)}\,\mathrm{e}^{\mathrm{i}\theta(x_1,\ldots,x_n)}\,\mathbb{1},\quad\forall\ x_1,\ldots,x_n, \tag{15}$$

where p is the joint probability law of the outcomes, independent of ρ, and θ is a real function.

(a) Using the normalization property of Kraus operators, we can immediately show that $T^{(0)}$ is corrigible:

$$\begin{aligned}t_{x_1}^{(0)^*}t_{x_1}^{(0)}&=\sum_{x_2,\ldots,x_n}t_{x_1}^{(0)^*}t_{x_2}^{(x_1)^*}\cdots t_{x_n}^{(x_1,\ldots,x_{n-1})^*}t_{x_n}^{(x_1,\ldots,x_{n-1})}\cdots t_{x_2}^{(x_1)}t_{x_1}^{(0)}\\&=\sum_{x_2,\ldots,x_n}p(x_1,\ldots,x_n)\,\mathbb{1}=p(x_1)\,\mathbb{1},\end{aligned}$$

where $p(x_1)$ is the probability of observing x_1 at the first step. Now, since $t_{x_1}^{(0)}=\sqrt{p(x_1)}\,u_{x_1}^{(0)}$ for some unitary $u_{x_1}^{(0)}$, we can fix x_1 and find that $T^{(x_1)}$ is corrigible:

$$\begin{aligned}t_{x_2}^{(x_1)^*}t_{x_2}^{(x_1)}&=\frac{1}{p(x_1)}u_{x_1}^{(0)}t_{x_1}^{(0)^*}t_{x_2}^{(x_1)^*}t_{x_2}^{(x_1)}t_{x_1}^{(0)}u_{x_1}^{(0)^*}\\&=\frac{1}{p(x_1)}u_{x_1}^{(0)}\sum_{x_3,\ldots,x_n}t_{x_1}^{(0)^*}t_{x_2}^{(x_1)^*}\cdots t_{x_n}^{(x_1,\ldots,x_{n-1})^*}t_{x_n}^{(x_1,\ldots,x_{n-1})}\cdots t_{x_2}^{(x_1)}t_{x_1}^{(0)}u_{x_1}^{(0)^*}\\&=\frac{1}{p(x_1)}\sum_{x_3,\ldots,x_n}p(x_1,\ldots,x_n)\,\mathbb{1}=p(x_2|x_1)\,\mathbb{1},\end{aligned}$$

where $p(x_2|x_1)$ is the probability of observing x_2 at the second step conditioned upon the observation of x_1 at the first step. Again we have $t_{x_2}^{(x_1)}=\sqrt{p(x_2|x_1)}\,u_{x_2}^{(x_1)}$ for some unitary $u_{x_2}^{(x_1)}$ and, repeating the same argument, we find for every k

$$t_{x_k}^{(x_1,\ldots,x_{k-1})}=\sqrt{p(x_k|x_1,\ldots,x_{k-1})}\,u_{x_k}^{(x_1,\ldots,x_{k-1})},\quad u_{x_k}^{(x_1,\ldots,x_{k-1})}\in\mathcal{U}(\mathcal{H}), \tag{16}$$

where $p(x_k|x_1,\ldots,x_{k-1})$ is the probability of observing x_k at the kth step conditioned upon the observation of $(x_1,\ldots,x_{k-1})$ during the previous steps. Equation (16) gives the polar decomposition of $t_{x_k}^{(x_1,\ldots,x_{k-1})}$, which in this case is unique.

(b) Combining Eqs. (15) and (16) we get

$$t_{x_k}^{(x_1,\ldots,x_{k-1})}=\sqrt{p(x_k|x_1,\ldots,x_{k-1})}\,\mathrm{e}^{\mathrm{i}\theta(x_1,\ldots,x_n)}\,u_{x_{k+1}}^{(x_1,\ldots,x_k)^*}\cdots u_{x_n}^{(x_1,\ldots,x_{n-1})^*}\,u_{x_1}^{(0)^*}\cdots u_{x_{k-1}}^{(x_1,\ldots,x_{k-2})^*},$$

where, because of the uniqueness of the polar decomposition of $t_{x_k}^{(x_1,\ldots,x_{k-1})}$,

$$\mathrm{e}^{\mathrm{i}\theta(x_1,\ldots,x_n)}\,u_{x_{k+1}}^{(x_1,\ldots,x_k)^*}\cdots u_{x_n}^{(x_1,\ldots,x_{n-1})^*}\,u_{x_1}^{(0)^*}\cdots u_{x_{k-1}}^{(x_1,\ldots,x_{k-2})^*}=u_{x_k}^{(x_1,\ldots,x_{k-1})},$$

which therefore has to be independent of $x_{k+1},\ldots,x_n$. If moreover $(x_1,\ldots,x_{k-1})$ is such that for all $m>k$ the operators $t_{x_m}^{(x_1,\ldots,x_{m-1})}$ do not depend on x_k, then the same is true for the unitary

operator $u_{x_{k+1}}^{(x_1,\ldots,x_k)^*}\cdots u_{x_n}^{(x_1,\ldots,x_{n-1})^*}\,u_{x_1}^{(0)^*}\cdots u_{x_{k-1}}^{(x_1,\ldots,x_{k-2})^*}$ and so the Kraus operators $t_{x_k}^{(x_1,\ldots,x_{k-1})}$ are all proportional to a same unitary operator $u^{(x_1,\ldots,x_{k-1})}$ and $T^{(x_1,\ldots,x_{k-1})}(\rho)=u^{(x_1,\ldots,x_{k-1})}\,\rho\,u^{(x_1,\ldots,x_{k-1})^*}$.

Proof of Proposition 2:

(a)⇒(b). Let $R^{(x_1,\ldots,x_{k-1})}(\rho)=\Sigma_{j_k} r_{j_k}^{(x_1,\ldots,x_{k-1})}\,\rho\,r_{j_k}^{(x_1,\ldots,x_{k-1})^*}$, where $\Sigma_{j_k} r_{j_k}^{(x_1,\ldots,x_{k-1})^*} r_{j_k}^{(x_1,\ldots,x_{k-1})}=\mathbb{1}$.

If $\Sigma_{\substack{x_1,\ldots,x_n\\ j_1,\ldots,j_n}} r_{j_n}^{(x_1,\ldots,x_n)}\,t_{x_n}^{(n)}\cdots r_{j_1}^{(x_1)}\,t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)^*}\,r_{j_1}^{(x_1)^*}\cdots t_{x_n}^{(n)^*}\,r_{j_n}^{(x_1,\ldots,x_n)^*}=\rho$ for every ρ, then this decomposition of the ideal channel is associated to a probability measure $p(x_1,j_1,\ldots,x_n,j_n)$ and Proposition 3 directly implies $t_{x_k}^{(k)}=\sqrt{p(x_k|x_1,j_1,\ldots,x_{k-1},j_{k-1})}\,u_{x_k}^{(x_1,j_1,\ldots,x_{k-1},j_{k-1})}$, where $u_{x_k}^{(x_1,j_1,\ldots,x_{k-1},j_{k-1})}$ is unitary and where $p(x_k|x_1,j_1,\ldots,x_{k-1},j_{k-1})=p_{x_k}^{(k)}$ and $u_{x_k}^{(x_1,j_1,\ldots,x_{k-1},j_{k-1})}=u_{x_k}^{(k)}$ because $t_{x_k}^{(k)}$ does not depend on $(x_1,j_1,\ldots,x_{k-1},j_{k-1})$.

(b)⇒(c). If $t_{x_k}^{(k)}=\sqrt{p_{x_k}^{(k)}}\,u_{x_k}^{(k)}$, with $u_{x_k}^{(k)}\in\mathcal{U}(\mathcal{H})$, $p_{x_k}^{(k)}\geqslant 0$, $\Sigma_{x_k}p_{x_k}^{(k)}=1$, then for every ρ

$$\mathbb{P}(X_1=x_1,\ldots,X_n=x_n)=\operatorname{tr} t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)^*}\cdots t_{x_n}^{(n)^*}=\prod_{k=1}^{n} p_{x_k}^{(k)}.$$

(c)⇒(a). According to (c), $\operatorname{tr} t_{x_1}^{(1)^*}\cdots t_{x_n}^{(n)^*}t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}\,\rho=\operatorname{tr} t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}\,\rho\,t_{x_1}^{(1)^*}\cdots t_{x_n}^{(n)^*}$ $=\mathbb{P}(X_1=x_1,\ldots,X_n=x_n)$ does not depend on ρ and so one gets $t_{x_1}^{(1)^*}\cdots t_{x_n}^{(n)^*}t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}$ $=\mathbb{P}(X_1=x_1,\ldots,X_n=x_n)\,\mathbb{1}$. Then, with the same argument used in the proof of property (a) of Proposition 3,

$$t_{x_k}^{(k)}=\sqrt{\mathbb{P}(X_k=x_k|X_1=x_1,\ldots,X_{k-1}=x_{k-1})}\,u_{x_k}^{(x_1,\ldots,x_{k-1})},$$

where $u_{x_k}^{(x_1,\ldots,x_{k-1})}$ is unitary, and where actually $\mathbb{P}(X_k=x_k|X_1=x_1,\ldots,X_{k-1}=x_{k-1})$ $=\mathbb{P}(X_k=x_k)$ and $u_{x_k}^{(x_1,\ldots,x_{k-1})}=u_{x_k}^{(k)}$ because $t_{x_k}^{(k)}$ is independent of $(x_1,\ldots,x_{k-1})$. Then the channels $R^{(x_1,\ldots,x_k)}(\rho)=u_{x_k}^{(k)^*}\,\rho\,u_{x_k}^{(k)}$ perfectly restore quantum information.

When (a), (b), and (c) hold, all the restoring channels R in (a) satisfy (10) by Proposition 3, and of course for every choice of $v^{(x_1,\ldots,x_k)}$, $k=1,\ldots,k-1$, the channel $R^{(x_1,\ldots,x_n)}$ defined by (11) can perfectly restore quantum information. Finally Eq. (12) directly follows from condition (b) and Eq. (10). □

IV. OPTIMAL RECOVERY OF QUANTUM INFORMATION

When perfect correction of quantum information is not possible, we would like the restoring channels R which bring the corrected channel T_{corr} as close as possible to id, in some sense. We look for channels R which maximize the *channel fidelity* of the corrected channel, $\mathcal{F}(T_{\text{corr}})$. For a channel $T:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$, $T(\rho)=\Sigma_x t_x\,\rho\,t_x^*$, $\dim\mathcal{H}=N$, denoted by Ω a maximally entangled unit vector in $\mathcal{H}\otimes\mathcal{H}$, the channel fidelity

$$\mathcal{F}(T)=\langle\Omega,T\otimes\mathrm{id}(|\Omega\rangle\langle\Omega|)\,\Omega\rangle=\frac{1}{N^2}\sum_x |\operatorname{tr} t_x|^2$$

measures how well T preserves quantum information, reaching 1 if and only if $T=\mathrm{id}$.

A. Single-step channel

Let us recall what was found in Ref. 9 for the single-step case. Given T, chosen a Kraus decomposition (3) and the restoring channels $R^{(x)}$,

$$R^{(x)}(\rho)=\sum_j r_j^{(x)}\,\rho\,r_j^{(x)*},\quad \sum_j r_j^{(x)*}r_j^{(x)}=\mathbb{1},$$

we are interested in

$$\mathcal{F}(T_{\mathrm{corr}})=\frac{1}{N^2}\sum_{x,j}|\mathrm{tr}\,r_j^{(x)}\,t_x|^2, \tag{17}$$

and we want to maximize it with respect to all possible families $\{R^{(x)}\}$.

Propostion 4: Let $T:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ be a channel over a finite dimensional Hilbert space $\mathcal{H}$. Fixed a Kraus decomposition $T(\rho)=\Sigma_x t_x\,\rho\,t_x^*$, for every family of channels $R^{(x)}:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ let T_{corr} be the corresponding overall corrected channel (2). Then

$$\mathcal{F}(T_{\mathrm{corr}})\leqslant\frac{1}{N^2}\sum_x(\mathrm{tr}|t_x|)^2. \tag{18}$$

Moreover equality holds if and only if

$$T_{\mathrm{corr}}(\rho)=\sum_x|t_x|\,\rho\,|t_x|, \tag{19}$$

and it can always be attained choosing

$$R^{(x)}(\rho)=u_x^*\,\rho\,u_x, \tag{20}$$

where u_x is a unitary operator in the polar decomposition $t_x=u_x|t_x|$.

Proof: Inequality (18) follows from (17) because the Cauchy–Schwarz inequality for the Hilbert–Schmidt inner product gives

$$\begin{aligned}\sum_j|\mathrm{tr}\,r_j^{(x)}\,t_x|^2&=\sum_j|\mathrm{tr}(r_j^{(x)}\,u_x|t_x|^{1/2}|t_x|^{1/2})|^2\\&\leqslant\sum_j\mathrm{tr}(|t_x|^{1/2}u_x^*r_j^{(x)*}r_j^{(x)}u_x|t_x|^{1/2})\,\mathrm{tr}|t_x|=(\mathrm{tr}|t_x|)^2.\end{aligned} \tag{21}$$

Equality holds in (18) if and only if equality holds in (21) for every x, which occurs if and only if $r_j^{(x)}\,u_x|t_x|^{1/2}=\lambda_{xj}|t_x|^{1/2}$, $\lambda_{xj}\in\mathbb{C}$, for every x and j. Then $r_j^{(x)}\,t_x=\lambda_{xj}|t_x|$ and (19) holds. The opposite implication is obvious.

Finally, if $R^{(x)}$ are chosen according to (20), then T_{corr} is given by (19) and equality holds in (18). □

The structure of the optimal restoring channels (20) obtained by maximizing $\mathcal{F}(T_{\mathrm{corr}})$, is just what one could expect. When a measurement on the environment has given the result x, we deal with a subensemble of systems undergone the state transformation $\rho\mapsto t_x\,\rho\,t_x^*=u_x|t_x|\,\rho\,|t_x|u_x^*$, which can be seen as a composition of $\rho\mapsto|t_x|\,\rho\,|t_x|$ followed by $\rho\mapsto u_x\,\rho\,u_x^*$. Unless we are in the trivial case $|t_x|\propto\mathbb{1}$, only the second transformation is physically reversible, and this is just what the channel (20) does. Therefore $\mathcal{F}(T_{\mathrm{corr}})$ can be maximized considering only unitary feedback, even if sometimes non unitary feedback could work as well (for example, every time the polar decomposition of t_x is not unique).

B. Multistep channel

Given a multistep channel T, decomposed according to (6), we allow corrections also before the evolution stops and so we want to maximize the channel fidelity of T_{corr} over all possible families $R^{(x_1)},R^{(x_1,x_2)},\ldots,R^{(x_1,\ldots,x_n)}$ in (7). We are interested in the optimal feedback, of course, and we want to compare the maximum attainable fidelity with

(1) the maximum fidelity obtainable only with a unique correction at the end, which is, by Proposition 4,

$$\mathcal{F}(T'_{\mathrm{corr}}) = \frac{1}{N^2} \sum_{x_1,\ldots,x_n} (\mathrm{tr}|t^{(n)}_{x_n} \cdots t^{(1)}_{x_1}|)^2 , \tag{22}$$

where T'_{corr} denotes the corrected channel

$$T'_{\mathrm{corr}}(\rho) = |t^{(n)}_{x_n} \cdots t^{(1)}_{x_1}| \, \rho \, |t^{(n)}_{x_n} \cdots t^{(1)}_{x_1}| ;$$

(2) the fidelity obtainable applying step by step the feedback suggested by Proposition 4, chosen on the basis of the whole avaible information; the corrected evolution associated to the observation of $(x_1,\ldots,x_n)$ would be

$$\rho \mapsto t^{(1)}_{x_1} \rho \, t^{(1)*}_{x_1} \mapsto |t^{(1)}_{x_1}| \, \rho \, |t^{(1)}_{x_1}| \mapsto t^{(2)}_{x_2} |t^{(1)}_{x_1}| \, \rho \, |t^{(1)}_{x_1}| \, t^{(2)*}_{x_2} \mapsto |t^{(2)}_{x_2} |t^{(1)}_{x_1}|| \, \rho \, |t^{(2)}_{x_2} |t^{(1)}_{x_1}|| \mapsto \cdots$$

$$\mapsto |t^{(n)}_{x_n} \cdots |t^{(2)}_{x_2}| t^{(1)}_{x_1}||| \, \rho \, |t^{(n)}_{x_n} \cdots |t^{(2)}_{x_2}| t^{(1)}_{x_1}||| := T''_{\mathrm{corr}}(\rho) , \tag{23}$$

with fidelity

$$\mathcal{F}(T''_{\mathrm{corr}}) = \frac{1}{N^2} \sum_{x_1,\ldots,x_n} (\mathrm{tr}|t^{(n)}_{x_n} \cdots |t^{(2)}_{x_2}| t^{(1)}_{x_1}|||)^2 . \tag{24}$$

Quite surprisingly, these two strategies are equivalent, and optimal, in the qubit case ($\dim \mathcal{H} = 2$), but in the general case ($\dim \mathcal{H} \geqslant 3$) there is no relationship between them, and neither of them gives the optimal correction.

1. Qubit multistep channels

Propostion 5: Let $\dim \mathcal{H} = 2$ *and* $T = T^{(n)} \circ \cdots \circ T^{(1)}$ *be a multistep channel, with every* $T^{(k)} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$. *Fixed the Kraus decompositions* $T^{(k)}(\rho) = \Sigma_{x_k} t^{(k)}_{x_k} \rho \, t^{(k)*}_{x_k}$, *for every family of channels* $R^{(x_1)}, R^{(x_1,x_2)}, \ldots, R^{(x_1,\ldots,x_n)}$, *let* T_{corr} *be the corresponding overall corrected channel (7). Then*

$$\mathcal{F}(T_{\mathrm{corr}}) \leqslant \frac{1}{4} \sum_{x_1,\ldots,x_n} (\mathrm{tr}|t^{(n)}_{x_n} \cdots t^{(1)}_{x_1}|)^2 . \tag{25}$$

Moreover equality can always be attained choosing

$$R^{(x_1,\ldots,x_k)}(\rho) = v^{(x_1,\ldots,x_k)} \rho \, v^{(x_1,\ldots,x_k)*} , \quad v^{(x_1,\ldots,x_k)} \in \mathcal{U}(\mathcal{H}) , \quad \forall \;\; k = 1,\ldots,n , \tag{26}$$

with $v^{(x_1,\ldots,x_n)} = w^{(x_1,\ldots,x_n)*}$, *where* $w^{(x_1,\ldots,x_n)}$ *is a unitary operator in the polar decomposition* $t^{(n)}_{x_n} v^{(x_1,\ldots,x_{n-1})} \cdots v^{(x_1)} t^{(1)}_{x_1} = w^{(x_1,\ldots,x_n)} |t^{(n)}_{x_n} v^{(x_1,\ldots,x_{n-1})} \cdots v^{(x_1)} t^{(1)}_{x_1}|$.

Proof: The key property in a two-dimensional Hilbert space is that for every operator A

$$(\mathrm{tr}|A|)^2 = \mathrm{tr}(|A|^2) + 2 \det|A| , \quad \text{where} \quad \det|A| = |\det A| \leqslant \tfrac{1}{2} \mathrm{tr}(|A|^2) .$$

Then, for every family of channels $R^{(x_1,\ldots,x_{k-1})}(\rho) = \Sigma_{j_k} r^{(x_1,\ldots,x_{k-1})}_{j_k} \rho \, r^{(x_1,\ldots,x_{k-1})*}_{j_k}$, $\Sigma_{j_k} r^{(x_1,\ldots,x_{k-1})*}_{j_k} r^{(x_1,\ldots,x_{k-1})}_{j_k} = \mathbb{I}$,

$$\begin{aligned}
\mathcal{F}(T_{\mathrm{corr}}) &= \frac{1}{4}\sum_{\substack{x_1,\dots,x_n\\ j_1,\dots,j_n}} |\operatorname{tr} r_{j_n}^{(x_1,\dots,x_n)}\, t_{x_n}^{(n)}\cdots r_{j_1}^{(x_1)}\, t_{x_1}^{(1)}|^2 \\
&\leqslant \frac{1}{4}\sum_{\substack{x_1,\dots,x_n\\ j_1,\dots,j_{n-1}}} (\operatorname{tr}|t_{x_n}^{(n)}\, r_{j_{n-1}}^{(x_1,\dots,x_{n-1})}\cdots r_{j_1}^{(x_1)}\, t_{x_1}^{(1)}|)^2 \\
&= \frac{1}{2}+\frac{1}{2}\sum_{\substack{x_1,\dots,x_n\\ j_1,\dots,j_{n-1}}} |\det t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}|\cdot|\det r_{j_{n-1}}^{(x_1,\dots,x_{n-1})}|\cdot|\det r_{j_1}^{(x_1)}| \\
&\leqslant \frac{1}{2}+\frac{1}{2}\sum_{x_1,\dots,x_n} |\det t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}| \\
&= \frac{1}{4}\sum_{x_1,\dots,x_n} (\operatorname{tr}|t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}|)^2 .
\end{aligned}$$

Analogously for every family of unitary channels $R^{(x_1,\dots,x_k)}(\rho)=v^{(x_1,\dots,x_k)}\,\rho\, v^{(x_1,\dots,x_k)*}$, with $v^{(x_1,\dots,x_n)}=w^{(x_1,\dots,x_n)*}$,

$$\begin{aligned}
\mathcal{F}(T_{\mathrm{corr}}) &= \frac{1}{4}\sum_{x_1,\dots,x_n} (\operatorname{tr}|t_{x_n}^{(n)}\, v^{(x_1,\dots,x_{n-1})}\cdots v^{(x_1)}\, t_{x_1}^{(1)}|)^2 \\
&= \frac{1}{2}+\frac{1}{2}\sum_{x_1,\dots,x_n} |\det t_{x_n}^{(n)}\, v^{(x_1,\dots,x_{n-1})}\cdots v^{(x_1)}\, t_{x_1}^{(1)}| \\
&= \frac{1}{2}+\frac{1}{2}\sum_{x_1,\dots,x_n} |\det t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}| = \frac{1}{4}\sum_{x_1,\dots,x_n} (\operatorname{tr}|t_{x_n}^{(n)}\cdots t_{x_1}^{(1)}|)^2 .
\end{aligned}$$

□

2. Higher dimensional two-step channels

When $\dim\mathcal{H}\geqslant 3$ there is no general relationship between the two fidelities (22) and (24). Consider on $\mathbb{C}^3$ the multistep channels $T=T^{(2)}\circ T^{(1)}$ and $S=S^{(2)}\circ S^{(1)}$, where

$$T^{(1)}(\rho)=T^{(2)}(\rho)=\sum_{x=1}^{2} t_x\,\rho\, t_x^*, \quad S^{(1)}(\rho)=S^{(2)}(\rho)=\sum_{x=1}^{2} s_x\,\rho\, s_x^*,$$

$$|t_1|^2=|s_1|^2=\begin{pmatrix} 1/6 & 0 & 0\\ 0 & 1/3 & 0\\ 0 & 0 & 1/2\end{pmatrix}, \quad |t_2|^2=|s_2|^2=\begin{pmatrix} 5/6 & 0 & 0\\ 0 & 2/3 & 0\\ 0 & 0 & 1/2\end{pmatrix},$$

$$t_1=u\,|t_1|, \quad t_2=|t_2|, \quad s_1=v\,|s_1|, \quad s_1=u\,|s_1|,$$

where

$$u=\begin{pmatrix} 0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}, \quad \text{and} \quad v=\frac{1}{\sqrt{3}}\begin{pmatrix} e^{2i\pi/3} & e^{-2i\pi/3} & 1\\ e^{-2i\pi/3} & e^{2i\pi/3} & 1\\ 1 & 1 & 1\end{pmatrix}.$$

Then since the absolute values of the Kraus operators coincide, the single-step corrected versions of T and S are the same. Moreover, since these absolute values commute, the iterated absolute values factorize, i.e.,

$$|t_{x_n}^{(n)}\cdots|t_{x_2}^{(2)}\,|t_{x_1}^{(1)}|||=|t_{x_n}^{(n)}|\cdots|t_{x_2}^{(2)}|\cdot|t_{x_1}^{(1)}|. \tag{27}$$

Hence the greedy strategy of correcting for maximal fidelity at every step, using all available information, gives the same result for these channels as the product of the single-step corrected channels. In particular, S and T are equivalent in this respect, and $\mathcal{F}(T''_{\mathrm{corr}})=\mathcal{F}(S''_{\mathrm{corr}})$ (see last line in the table below).

On the other hand, we can leave the system undisturbed, and only make an optimal correction at the end, again using all available information. Finally, we may optimize fidelity over all correction schemes. Numerically this achieved by an iteration, developed in Ref. 10, which efficiently determines the maximum of a general positive linear functional on channels. In the case at hand this is the overall channel fidelity as a function of the correcting channels R. Since we can correct the unitaries u and v immediately in every step, it is clear that the channels S and T once again give the same corrected fidelities. The results are summarized in the following:

Channel fidelities	T	S
Optimal correction	0.9584	0.9584
Final correction only	0.9556	0.9576
	$<$	$>$
Optimal correction at each step	0.9570	0.9570

Hence, in contrast to the case of perfect corrigibility, it may help to perform corrections on the way, rather than a single correction at the end (column T). Perhaps surprisingly, the optimal correction at the intermediate steps requires some foresight, and depends on what is to follow: otherwise the strategy of correcting for highest fidelity using all available information, which is clearly optimal in the last step, would also have to be optimal in the intermediate steps (compare first and last line). Even leaving out the intermediate correction altogether may be better (column S).

3. Higher dimensional many-step channels

We noted that in the previous example the correction scheme for T''_{corr} is equivalent to multiplying the one-step corrected channels. That is, whether this correction step may use all available information or just the information from the last step, leads to the same corrected channel. We showed this by noting that the absolute values of all Kraus operators involved commute. This will be true in any dimension if there are only two Kraus operators, as in the example. Here we just note that this equality is not a general fact. In fact using random channels one quickly finds examples (3 Hilbert space dimensions, 3 Kraus operators, and 4 time steps), in which using all information or just information from the last step give different results. Surprisingly, once again the comparison may be either way: sometimes using only one-step information is *better* than using all information. Of course, this is only possible because the greedy strategy is not optimal in the first place.

V. OUTLOOK

We would like to spend some words about the quantum error-correction in *continuous* time. Our aim would be to generalize this correction scheme for quantum information corrupted by a noisy Markovian evolution assigned by a Quantum Dynamical Semigroup. The present analysis for a multistep channel $T=(T^{(1)})^n$ would provide the intervalwise treatment, but it is not easy to take the limit to continuous time. The well established theory of continuous measurements[11] gives the possible decompositions (unravelings) of the channel according to the observed trajectoies, but a continuous time formulation of general non-Hamiltonian feedback is missing. There is no general description of the evolution conditioned on the observed process if a feedback depending on the whole measurement record is added. And also if the feedback is supposed to depend only on the present observation, the measured current, still there is no general description for non-Hamiltonian feedback. A theory exists only for Hamiltonian feedback simply proportional to the measured currents.[12] Anyway a preliminary study of perfect correction in this framework leads to the same conclusions of Proposition 2: perfect correction is possible if and only if the measured

process is uninformative and in this case a unique correction at the end suffices. It is also possible to characterize the Linblad generator of semigroups allowing such perfect correction and, as pointed out by Luc Bouten, these semigroups are just the ones admitting an essentially commutative dilation.[13]

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Inverse scattering problem in nuclear physics—Optical model

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We consider the inverse scattering problem for the Schrödinger operator with optical potential introduced in nuclear physics to study the scattering of nucleons by nuclei. We show that the corresponding spin–orbit interaction and the complex matrix potential can be uniquely reconstructed from the scattering amplitude at fixed energy. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1753665]

I. INTRODUCTION

The optical model is an operator phenomenologically or empirically introduced in nuclear physics to study the scattering of nucleons by nuclei. The model corresponds to the Schrödinger operator with a complex potential and it was first effectively used by Feshbach, Porter, and Weisskopf[9] to reproduce with great success the experimental results on the scattering of neutrons. Since then this optical model has been improved and accepted as a fundamental tool in nuclear physics. Usually the spin–orbit interaction is included and the following form of the Hamiltonian is adopted:

$$\begin{gathered} H=-\Delta+V, \\ V=W(x)+a(x)\sigma\cdot(x\times p)+U_c(x), \quad p=-i\nabla_x, \\ W(x)=c_1F(r;R_1,\alpha_1)+i\left\{c_2F(r;R_2,\alpha_2)-c_3\frac{\mathrm{d}}{\mathrm{d}r}F(r;R_2,\alpha_2)\right\}, \\ a(x)=c_4\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}F(r;R_3,\alpha_3), \end{gathered} \tag{1.1}$$

where $F(r;R,\alpha)$ is the so-called Woods–Saxon potential having the following form:

$$F(r;R,\alpha)=\left(1+\exp\left(\frac{r-R}{\alpha}\right)\right)^{-1},$$

and $U_c(x)$ is the Coulomb interaction. Here $\sigma\cdot x=\Sigma_{i=1}^3\sigma_i x_i$ and $\sigma=(\sigma_1,\sigma_2,\sigma_3)$ is the vector of Pauli spin matrices, that is, they are the 2×2 Hermitian matrices satisfying the following commutation relations:

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$$\sigma_1\sigma_2 = i\sigma_3, \quad \sigma_2\sigma_3 = i\sigma_1, \quad \sigma_3\sigma_1 = i\sigma_2. \tag{1.2}$$

A standard representation of the Pauli matrices is

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.3}$$

The original problem of scattering nucleons should be dealt with by the N body Schrödinger operator, in which many scattering channels appear. Usually the elastic process is dominant, and in order to ignore the inelastic processes, physicists introduced the complex two-body potential so that these inelastic scattering processes are regarded to be absorbed into the background. This is the origin of the terminology *optical* in analogy to the scattering and absorption of light by materials. By suitably adjusting constants c_i (which are usually energy-dependent) and R_i, α_i, the cross section calculated by this model is known to reproduce very well the experimental data (see, e.g., Feshbach[8] or Roy and Nigam[18]).

Let us consider the operator (1.1) in $(L^2(\mathbf{R}^3))^2$, where

$$V = a(x)\sigma\cdot(x\times p) + W(x), \tag{1.4}$$

and $a(x)$, $W(x)$ satisfy the following assumptions:

(A.1) $a(x)$ is a complex-valued C^∞-function on $\mathbf{R}^3$ such that for some $\delta_0 > 0$,

$$|\partial_x^\alpha \ a(x)| \leqslant C_\alpha e^{-\delta_0|x|} \quad \forall\, \alpha.$$

(A.2) $W(x)$ is a 2×2-matrix valued function on $\mathbf{R}^3$ with complex entries such that for some $\delta_0 > 0$,

$$|W(x)| \leqslant Ce^{-\delta_0|x|}.$$

In Sec. II, we shall show that under these assumptions, there is a discrete set $\mathcal{E}_0$ in a neighborhood of $(0,\infty)$ such that for $E \in (0,\infty)\backslash\mathcal{E}_0$, there exists a solution $\psi(x,E,\omega)$, $\omega \in S^2$, of the Schrödinger equation

$$(-\Delta + V)\psi(x,E,\omega) = E\psi(x,E,\omega)$$

having the following asymptotic expansion:

$$\psi(x,E,\omega) \sim e^{i\sqrt{E}\omega\cdot x} + \frac{e^{i\sqrt{E}r}}{r} f(E;\theta,\omega), \quad \theta = x/r, \quad r = |x| \to \infty.$$

The 2×2-matrix valued function $f(E;\theta,\omega)$ of $\theta,\omega \in S^2$ is the scattering amplitude. The main theorem of this paper is the following one.

Theorem 1.1: *For each fixed energy $E \in (0,\infty)\backslash\mathcal{E}_0$, one can uniquely reconstruct the perturbations $a(x), W(x)$ from the scattering amplitude $f(E;\theta,\omega)$.*

The Born approximation at high energies is not valid in the case considered in this paper since the perturbation is energy dependent so that it is natural to consider the fixed energy problem.

There has been considerable works in recent years in studying inverse scattering problem at fixed energy for the case of the Schrödinger equation associated to a potential, that is the two-body problem. To solve this problem one can use Faddeev's Green function[7] and the direction dependent Faddeev's Green's function (see Ref. 12 for a review and references) or the method of constructing complex geometrical optics solutions initiated by Calderón[3] and the connection to the Dirichlet-to-Neumann map (see Ref. 22 for a review and references). The problem considered here is more closely related to the case of the Schrödinger equation in the presence of a magnetic field studied in Ref. 5 or 16. An important ingredient in those articles is the reduction to the case of a lower order perturbation of the Laplacian by exponentiating with a pseudodifferential operator. We

use a similar method to deal with the main difficulty in the optical model, which is the reconstruction of the spin–orbit interaction $a(x)\sigma\cdot(x\times p)$. Namely by making semi-classical analysis type arguments (Lemma 5.1) and using the commutation relations of the Pauli spin matrices, we reconstruct $a(x)$ using the complex Born approximation of the scattering amplitude. We shall also use the gauge invariance of the scattering amplitude and introduce an auxiliary magnetic field to reconstruct the complex potential $W(x)$.

For earlier results on the scattering theory for non-self-adjoint Schrödinger operators see, e.g., Refs. 15, 19, 14, and 4 from the mathematical side, and Refs. 2 and 21 from the physical side.

Some remarks on the notations. For two Banach spaces X and Y, $\mathbf{B}(X;Y)$ denotes the set of all bounded operators from X to Y. For $x\in\mathbf{R}^3$, $\langle x\rangle=(1+|x|^2)^{1/2}$. C's denote various constants.

II. RESOLVENT ESTIMATES AND THE SCATTERING AMPLITUDE

We shall derive in this section the analytic continuation of the resolvent of $-\Delta+V$ and introduce the scattering amplitude.

A. Resolvent estimates

Let $H_0=-\Delta$ in $(L^2(\mathbf{R}^3))^2$. For $a\in\mathbf{R}$, we define

$$f\in\mathcal{H}_a\Leftrightarrow\|f\|_{\mathcal{H}_a}=\|e^{a|x|}f(x)\|_{L^2(\mathbf{R}^3)}<\infty. \tag{2.1}$$

Then, by passing to the Fourier transformation and by shifting the path of $|\xi|$-integration, for any $\delta>0$ $R_0(z)=(H_0-z)^{-1}$ defined for $\mathrm{Im}\,z>0$ has an analytic continuation across $(0,\infty)$ into the region

$$\Omega_\delta=\{z;\mathrm{Im}\ \ z>0\}\cup\{z;\mathrm{Re}\,\sqrt{z}>0,\ \ 0\geqslant\mathrm{Im}\ \ \sqrt{z}>-\delta\} \tag{2.2}$$

as a $\mathbf{B}(\mathcal{H}_\delta;\mathcal{H}_{-\delta})$-valued function. We denote this operator by $R_0^{(+)}(z)$. This is actually the integral operator with kernel $e^{i\sqrt{z}|x-y|}/(4\pi|x-y|)$.

For a technical reason, which will be explained in Sec. VI, we include also a magnetic field $b(x)$. Let $H=H_0+V$, where

$$V=V(-i\nabla_x), \tag{2.3}$$

$$V(\xi)=(2b(x)\cdot\xi-i\,\mathrm{div}\,b(x)+|b(x)|^2)I+a(x)\sigma\cdot(x\times\xi)+W(x), \tag{2.4}$$

I being the 2×2 identity matrix. We shall assume that

(A.1) $a(x)\in C^\infty(\mathbf{R}^3;\mathbf{C}),b(x)\in C^\infty(\mathbf{R}^3;\mathbf{R}^3)$ *and for some* $\delta_0>0$

$$|\partial_x^\alpha a(x)|+|\partial_x^\alpha b(x)|\leqslant C_\alpha e^{-\delta_0|x|},\quad\forall\alpha.$$

(A.2) $W(x)$ *is a* $M_2(\mathbf{C})$*-valued function such that for some* $\delta_0>0$,

$$|W(x)|\leqslant Ce^{-\delta_0|x|}.$$

These assumptions imply that for $0<\delta<\delta_0/2$, $R_0^{(+)}(z)V$ is a $\mathbf{B}(\mathcal{H}_{-\delta};\mathcal{H}_{-\delta})$-valued analytic function on Ω_δ and is compact for each z. We define $\mathcal{E}_0$ to be the set

$$\mathcal{E}_0=\{z\in\Omega_\delta;-1\in\mathrm{spec}_p(R_0^{(+)}(z)V)\}. \tag{2.5}$$

Here $\mathrm{spec}_p(A)$ denotes the point spectrum of the operator A.

Lemma 2.1: (1) There exists $C>0$ *such that*

$$\mathcal{E}_0\cap\{i\tau;\tau>C\}=\varnothing.$$

(2) $\mathcal{E}_0$ *is discrete in* Ω_δ.

Proof: Suppose $i\tau \in \mathcal{E}_0$ and let u be the associated eigenvector. Since $R_0^{(+)}(i\tau) \in \mathbf{B}(L^2;H^2)$, we have $u \in H^2$. Since $(-\Delta + V - i\tau)u = 0$, we then have

$$\|u\|_{H^1}^2 = ((1-\Delta)u,u) \leqslant C(\|u\|_{H^{1/2}}^2 + \tau\|u\|_{L^2}^2),$$

which implies $\|u\|_{H^1} \leqslant C\sqrt{\tau}\|u\|_{L^2}$. Using the equation $u = -R_0^{(+)}(i\tau)Vu$, we then have

$$\|u\|_{L^2} \leqslant \frac{C}{\tau}\|u\|_{H^1} \leqslant \frac{C}{\sqrt{\tau}}\|u\|_{L^2}.$$

Therefore $u = 0$ for large $\tau > 0$. This proves (1). Assertion (2) follows from the analytic Fredholm theorem (Ref. 17, p. 204). □

We define

$$R(z) = (1 + R_0^{(+)}(z)V)^{-1}R_0^{(+)}(z), \quad z \in \Omega_\delta \backslash \mathcal{E}_0. \tag{2.6}$$

The following theorem is easily proved.

Theorem 2.2: *(1) $R(z)$ is a $\mathbf{B}(\mathcal{H}_\delta;\mathcal{H}_{-\delta})$-valued analytic function on $\Omega_\delta \backslash \mathcal{E}_0$.*
(2) $R(z) = (H-z)^{-1}$ for $z \in \{z;\mathrm{Im}\ z > 0\} \cap (\Omega_\delta \backslash \mathcal{E}_0)$.
(3) For $z \in \Omega_\delta \backslash \mathcal{E}_0$,

$$R(z) = R_0^{(+)}(z) - R_0^{(+)}(z)VR(z). \tag{2.7}$$

For $s \in \mathbf{R}$, $L^{2,s}$ is defined by

$$u \in L^{2,s} \Leftrightarrow \|u\|_s = \|(1+|x|)^s u(x)\|_{L^2(\mathbf{R}^3)} < \infty.$$

Since $R_0^{(+)}(E) = (-\Delta - E - i0)^{-1} \in \mathbf{B}(L^{2,s};L^{2,-s})$ for $s > 1/2$ and $E > 0$ (see, e.g., Ref. 19), it follows from (2.6) that

$$R(E) \in \mathbf{B}(L^{2,s};L^{2,-s}), \quad s > 1/2, \quad E \in (0,\infty) \backslash \mathcal{E}_0. \tag{2.8}$$

In fact, let A_1 and A_2 be $R_0^{(+)}(E)V$ acting on $\mathcal{H}_{-\delta}$ and $L^{2,-s}$, respectively. Then it is easy to see that

$$-1 \in \mathrm{spec}_p(A_1) \Leftrightarrow -1 \in \mathrm{spec}_p(A_2). \tag{2.9}$$

B. Scattering amplitudes

Theorem 2.3: *For $E \in (0,\infty) \backslash \mathcal{E}_0$ and $\omega \in S^2$, there exists a unique solution ψ of the equation*

$$(-\Delta + V - E)\psi = 0$$

such that $u = \psi - e^{i\sqrt{E}\omega \cdot x}$ satisfies the radiation condition

$$\left(\frac{\partial}{\partial r} - i\sqrt{E}\right)u \in L^{2,-\alpha}, \quad 0 < \alpha < 1/2.$$

Such ψ is represented as

$$\psi(x,E,\omega) = e^{i\sqrt{E}\omega \cdot x} - R(E)Ve^{i\sqrt{E}\omega \cdot x}. \tag{2.10}$$

Proof: To show existence, we have only to put ψ as in (2.9). To show the uniqueness, we note that the difference of two such solutions satisfies

$$(-\Delta-E)u=-Vu,\quad \left(\frac{\partial}{\partial r}-i\sqrt{E}\right)u\in L^{2,-\alpha}.$$

Then $u=-R_0^{(+)}(E)Vu$. Hence if $u\neq 0$, $-1\in \mathrm{spec}_p(A_1)$. □

Using the resolvent equation (2.7), we have

$$\psi(x,E,\omega)\sim e^{i\sqrt{E}\omega\cdot x}+\frac{e^{i\sqrt{E}r}}{r}f(E;\theta,\omega),\quad \theta=x/r \tag{2.11}$$

as $r=|x|\to\infty$, where

$$f(E;\theta,\omega)=-\frac{1}{4\pi}\int_{\mathbf{R}^3}e^{-i\sqrt{E}\theta\cdot x}Ve^{i\sqrt{E}\omega\cdot x}\mathrm{d}x+\frac{1}{4\pi}\int_{\mathbf{R}^3}e^{-i\sqrt{E}\theta\cdot x}VR(E)Ve^{i\sqrt{E}\omega\cdot x}\mathrm{d}x. \tag{2.12}$$

We introduce the following notation for 2×2-matrices $f(x),g(x)$:

$$\langle f,g\rangle=\int_{\mathbf{R}^3}f(x)^*g(x)\mathrm{d}x. \tag{2.13}$$

Then $f(E;\theta,\omega)$ is written as

$$f(E;\theta,\omega)=-\frac{1}{4\pi}\int_{\mathbf{R}^3}e^{-i\sqrt{E}(\theta-\omega)\cdot x}V(\sqrt{E}\omega)\mathrm{d}x+\frac{1}{4\pi}\langle V^*(\sqrt{E}\theta)e^{i\sqrt{E}\theta\cdot x},R(E)V(\sqrt{E}\omega)e^{i\sqrt{E}\omega\cdot x})\rangle, \tag{2.14}$$

where

$$V^*(\xi)=2b(x)\cdot\xi+\overline{a(x)}\sigma\cdot(x\times\xi)-i\sigma\cdot(x\times\overline{\nabla a(x)})+|b(x)|^2+W(x)^*. \tag{2.15}$$

III. DIRECTION DEPENDENT GREEN OPERATORS

The aim of this section is to construct Green operators for $-\Delta+V$ depending on a direction $\gamma\in S^2$.

A. Unperturbed operator

For $\epsilon>0$, we let

$$D_\epsilon=\{z\in\mathbf{C};\mathrm{Im}\,z>0,|\mathrm{Re}\,z|<\epsilon/2\}. \tag{3.1}$$

We fix an arbitrary direction $\gamma\in S^2$.

Theorem 3.1: *(1) For any $\delta>0$ and $E>0$, there exists an $\epsilon>0$ and a $\mathbf{B}(\mathcal{H}_\delta;\mathcal{H}_{-\delta})$-valued analytic function $U_{\gamma,0}(E,z)$ defined on D_ϵ such that*

$$(-\Delta-2iz\gamma\cdot\nabla+z^2-E)U_{\gamma,0}(E,z)=I.$$

(2) When $z\to t\in(-\epsilon/2,\epsilon/2)$, $U_{\gamma,0}(E,z)$ has a boundary value $U_{\gamma,0}(E,t)$. Moreover

$$U_{\gamma,0}(E,t)\in\mathbf{B}(L^{2,s};L^{2,-s}),\quad s>1/2.$$

(3) For $\tau>0$,

$$U_{\gamma,0}(E,i\tau)f(x)=(2\pi)^{-3/2}\int_{\mathbf{R}^3}\frac{e^{ix\cdot\xi}\hat{f}(\xi)}{(\xi+i\tau\gamma)^2-E}\mathrm{d}\xi,$$

$\hat{f}$ being the Fourier transform of f. If f is rapidly decreasing, the integral is absolutely convergent.

(4) For $0<s<1$, $U_{\gamma,0}(E,i\tau)\in\mathbf{B}(L^{2,s};L^{2,s-1})$, *and*

$$\|U_{\gamma,0}(E,i\tau)\|_{\mathbf{B}(L^{2,s};L^{2,s-1})}\leqslant C_s/\tau,\quad \tau>1.$$

Proof: For the proof see Ref. 13, Theorem 2.10. The last assertion (4) is proved in the same way as in Sylvester–Uhlmann,[20] Lemma 3.1. □

We next observe a relation between this direction dependent Green operator and the $\bar{\partial}$-operator. For $\zeta\in\mathbf{C}^3$, Im $\zeta\neq 0$, let

$$\tilde{G}(\zeta)f(x)=(2\pi)^{-3/2}\int_{\mathbf{R}^3}\frac{e^{ix\cdot\xi}\hat{f}(\xi)}{\xi^2+2\zeta\cdot\xi}\mathrm{d}\xi. \tag{3.2}$$

For $\eta\in S^2$ such that $\eta\cdot\gamma=0$, let $p(\tau)=\sqrt{E+\tau^2}\,\eta$ and $\zeta(\tau)=p(\tau)+i\tau\gamma$. Then

$$e^{-ip(\tau)\cdot x}U_{\gamma,0}(E,i\tau)e^{ip(\tau)\cdot x}=\tilde{G}(\zeta(\tau)). \tag{3.3}$$

We also define

$$M_\gamma(\tau)=\tau\tilde{G}(\zeta(\tau)), \tag{3.4}$$

$$N_\gamma f=(2\pi)^{-3/2}\int_{\mathbf{R}^3}\frac{e^{ix\cdot\xi}\hat{f}(\xi)}{2\xi\cdot(\eta+i\gamma)}\mathrm{d}\xi. \tag{3.5}$$

Lemma 3.2: (1) For $0<s<1$ *and* $\tau>0$,

$$M_\gamma(\tau)\in\mathbf{B}(L^{2,s};L^{2,s-1}).$$

(2) For $f\in L^{2,s}$, $0<s<1$,

$$M_\gamma(\tau)f\to N_\gamma f$$

in $L^{2,s-1}$ *as* $\tau\to\infty$.

The proof is the same as the one in Ref. 20, Proposition 3.6 and Ref. 13, Theorem 4.6.

B. Perturbed operator

Let $p=-i\nabla_x$. For $\zeta\in\mathbf{C}^3$, we let

$$H_0(\zeta)=(p+\zeta)^2, \tag{3.6}$$

and

$$H(\zeta)=(p+b(x)+\zeta)^2+a(x)\sigma\cdot(x\times(p+\zeta))+W(x)=H_0(\zeta)+V(p+\zeta), \tag{3.7}$$

where V is defined by (2.4).

Our aim is to construct a direction dependent Green operator for $H(z\gamma)-E$. The main difficulty comes from the term $2b(x)\cdot(p+z\gamma)+a(x)\sigma\cdot(x\times(p+z\gamma))$, which we are going to eliminate by introducing a suitable pseudodifferential operator (ΨDO). Namely by using the identity

$$(H(z\gamma)-E)SU_{\gamma,0}(E,z)S^{-1}=1+([H_0(z\gamma),S]+V(p+z\gamma)S)U_{\gamma,0}(E,z)S^{-1},$$

we seek S in such a way that the right-hand side is invertible.

Before entering into the technical details, we explain the idea in the background. Let us suppose for the sake of simplicity that $b(x)=0$. If S is a ΨDO belonging to $\mathcal{S}^0$ to be introduced below, the natural choice is to assume that the symbol $S(x,\xi)$ of S satisfies

$$2(\xi+z\gamma)\cdot\nabla_x S(x,\xi)+ia(x)\sigma\cdot(x\times(\xi+z\gamma))S(x,\xi)=0.$$

In general when one considers inverse scattering problems at a fixed energy for systems of partial differential equations, one often encounters the equation $\zeta\cdot\nabla_x S=B(x,\zeta)S$, where ζ is a complex vector satisfying some conditions and $B(x,\zeta)$ is a matrix coming from the lower part of the equation. This sort of Cauchy-Riemann type equation is difficult to solve for systems (see Ref. 6 for a recent review). It is trivial to solve for scalar equations like in the case of the Schrödinger equation in the presence of a magnetic field. However, in our case it is sufficient to solve the equation

$$2(\xi+z\gamma)\cdot\nabla_x\psi+ia(x)=0,$$

and put $S=e^C$, $C=\psi(x,D_x)\sigma\cdot(x\times(D_x+z\gamma))$, $D_x=-i\nabla_x$. This is due to the fact that at the level of symbols, C solves

$$2i(\xi+z\gamma)\cdot\nabla_x C=a(x)\sigma\cdot(x\times(\xi+z\gamma))=:B(x,\xi+z\gamma),$$

and the symbol of C commutes with $B(x,\xi+z\gamma)$. (See Lemma 3.3 below.) Now the above equation for ψ is just the one we encounter in considering the inverse scattering problem for the scalar Schrödinger operator in a magnetic field, and the solution plays a significant role only near the zeros of $(\xi+z\gamma)^2-E$. With these remarks in mind, let us return to the construction of the perturbed direction dependent Green operator.

For a sufficiently small $\epsilon>0$, let $\chi_0(t)\in C^\infty(\mathbf{R})$ be such that $\chi_0(t)=1$ if $|t|<\epsilon/2$, $\chi_0(t)=0$ if $|t|>\epsilon$ and let

$$\chi(\xi+i\tau\gamma)=\chi_0\left(\frac{|(\xi+i\tau\gamma)^2-E|^2}{E+\tau^2+|\xi|^2}\right). \tag{3.8}$$

Note that on the support of $\chi(\xi+i\tau\gamma)$,

$$|\xi^2+2i\tau\gamma\cdot\xi-\tau^2-E|\leqslant\epsilon(E+\tau^2+|\xi|^2). \tag{3.9}$$

Let us put

$$\varphi(x,\xi+i\tau\gamma)=-(2\pi)^{-3/2}\chi(\xi+i\tau\gamma)\int_{\mathbf{R}^3}e^{ix\cdot k}\frac{\hat{b}(k)\cdot(\xi+i\tau\gamma)}{k\cdot(\xi+i\tau\gamma)}\mathrm{d}k, \tag{3.10}$$

$$\psi(x,\xi+i\tau\gamma)=-(2\pi)^{-3/2}\chi(\xi+i\tau\gamma)\int_{\mathbf{R}^3}e^{ix\cdot k}\frac{\hat{a}(k)}{2k\cdot(\xi+i\tau\gamma)}\mathrm{d}k. \tag{3.11}$$

For $m\in\mathbf{R}$, let $\mathcal{S}^m$ be the class of ΨDO's with symbol $p(x,\xi;\tau)$ satisfying

$$|\partial_x^\alpha\partial_\xi^\beta\ p(x,\xi;\tau)|\leqslant C_{\alpha\beta}\langle x\rangle^{-1}(\tau+|\xi|)^{m-|\beta|}\quad\forall\alpha,\beta,\quad\tau>1.$$

We use the same notation $\mathcal{S}^m$ to denote the associated class of symbols.

Lemma 3.3: (1) $\varphi(x,\xi+i\tau\gamma)\in\mathcal{S}^0,\psi(x,\xi+i\tau\gamma)\in\mathcal{S}^{-1}$.

(2) We have

$$2i(\xi+i\tau\gamma)\cdot\nabla_x\varphi(x,\xi+i\tau\gamma)=2\chi(\xi+i\tau\gamma)b(x)\cdot(\xi+i\tau\gamma),$$

$$2i(\xi+i\tau\gamma)\cdot\nabla_x[\psi(x,\xi+i\tau\gamma)\sigma\cdot(x\times(\xi+i\tau\gamma))]=\chi(\xi+i\tau\gamma)a(x)\quad\sigma\cdot(x\times(\xi+i\tau\gamma)).$$

The assertion (2) follows from a direct computation. The assertion (1) is proved in the Appendix.

Let $\varphi_0(\tau),\psi_0(\tau)$ be ΨDO's with symbol $\varphi(x,\xi+i\tau\gamma),\psi(x,\xi+i\tau\gamma)$ and let

$$A(\tau)=\varphi_0(\tau)+\psi_0(\tau)\sigma\cdot(x\times(p+i\tau\gamma)),\quad S(\tau)=e^{A(\tau)}. \tag{3.12}$$

Lemma 3.4: Let

$$K(\tau)=([H_0(i\tau\gamma),S(\tau)]+V(p+i\tau\gamma)S(\tau))U_{\gamma,0}(E,i\tau)S(\tau)^{-1}. \tag{3.13}$$

Then for $1/2<s<1$ *and large* $\tau>0$,

$$\|K(\tau)\|_{\mathbf{B}(L^{2,s};L^{2,s})}\leqslant C_s/\tau.$$

Proof: For two operators $P_1(\tau)$ and $P_2(\tau)$ we write

$$P_1(\tau)\sim P_2(\tau), \tag{3.14}$$

if they satisfy for large $\tau>0$,

$$\|P_1(\tau)-P_2(\tau)\|_{\mathbf{B}(L^{2,s};L^{2,s})}\leqslant C_s/\tau. \tag{3.15}$$

Let $L>\sup_{-1/2<s<1,1<\tau}\|A(\tau)\|_{\mathbf{B}(L^{2,s};L^{2,s})}$. Then we have

$$e^{A(\tau)}=\frac{1}{2\pi i}\int_{|z|=L}e^z(z-A(\tau))^{-1}\mathrm{d}z. \tag{3.16}$$

Therefore we have

$$[H_0(i\tau\gamma),e^{A(\tau)}]=\frac{1}{2\pi i}\int_{|z|=L}e^z(z-A(\tau))^{-1}[H_0(i\tau\gamma),A(\tau)](z-A(\tau))^{-1}\mathrm{d}z. \tag{3.17}$$

Since $A(\tau)\in S^0$ by Lemma 3.3 (1), by the symbolic calculus we have

$$[H_0(i\tau\gamma),A(\tau)]=P_1(\tau)+P_2(\tau), \tag{3.18}$$

where $\|P_2(\tau)\|_{\mathbf{B}(L^{2,s-1};L^{2,s})}\leqslant C_s$, and $P_1(\tau)$ is the ΨDO with symbol

$$-2\chi(\xi+i\tau\gamma)b(x)\cdot(\xi+i\tau\gamma)-\chi(\xi+i\tau\gamma)a(x)\sigma\cdot(x\times(\xi+i\tau\gamma)). \tag{3.19}$$

Let $Q(\tau)$ be the ΨDO with symbol $\chi(\xi+i\tau\gamma)$. By (3.18) and (3.19), we have

$$[H_0(i\tau\gamma),A(\tau)]=-Q(\tau)R(\tau)+P_3(\tau), \tag{3.20}$$

where $\|P_3(\tau)\|_{\mathbf{B}(L^{2,s-1};L^{2,s})}\leqslant C_s$, and

$$R(\tau)=2b(x)\cdot(p+i\tau\gamma)+a(x)\sigma\cdot(x\times(p+i\tau\gamma)). \tag{3.21}$$

Let us note that

$$[Q(\tau),A(\tau)]\in\mathcal{S}^{-1}, \tag{3.22}$$

$$[R(\tau),A(\tau)]\in\mathcal{S}^0, \tag{3.23}$$

$$\|(1-Q(\tau))U_{\gamma,0}(E,i\tau)\|_{\mathbf{B}(L^{2,s};L^{2,s})}\leqslant C_s/\tau^2. \tag{3.24}$$

The estimate (3.24) follows from Theorem 3.1 (3). Then in view of Theorem 3.1 (4), we have

$$[H_0(i\tau\gamma),S(\tau)]U_{\gamma,0}(E,i\tau)\sim-\frac{1}{2\pi i}\int_{|z|=L}e^z(z-A(\tau))^{-1}R(\tau)Q(\tau)(z-A(\tau))^{-1}\mathrm{d}zU_{\gamma,0}(E,i\tau)$$

$$\sim-R(\tau)\frac{1}{2\pi i}\int_{|z|=L}e^z(z-A(\tau))^{-2}\mathrm{d}zU_{\gamma,0}(E,i\tau)$$

$$=-R(\tau)e^{A(\tau)}U_{\gamma,0}(E,i\tau).$$

It then follows that

$$K(\tau)\sim(-R(\tau)+V(p+i\tau\gamma))S(\tau)U_{\gamma,0}(E,i\tau)S(\tau)^{-1}\sim 0. \tag{3.25}$$

This proves the lemma. □

With the aid of Lemma 3.4, we define the modified direction dependent Green operator for large $\tau>0$ by

$$L_\gamma(\tau)=S(\tau)U_{\gamma,0}(E,i\tau)S(\tau)^{-1}(1+K(\tau))^{-1}. \tag{3.26}$$

By definition it satisfies

$$(H(i\tau\gamma)-E)L_\gamma(\tau)=I. \tag{3.27}$$

We define $\mathcal{E}_\gamma(E)$ to be the set of $z\in\overline{D_\epsilon}$ such that

$$-1\in\mathrm{spec}_p(U_{\gamma,0}(E,z)V(p+z\gamma)).$$

Lemma 3.5: (1) $\mathcal{E}_\gamma(E)\cap\{z;\mathrm{Im}\,z>0\}$ *is discrete.*
(2) $\mathcal{E}_\gamma(E)\cap\mathbf{R}$ *is a closed set of measure zero.*
(3) There exists a constant $C>0$ *such that*

$$i\tau\notin\mathcal{E}_\gamma(E)\quad\text{if}\quad\tau>C.$$

Proof: We have only to show the last assertion. The assertions (1) and (2) follow from the analytic Fredholm theorem and the well-known Riesz' theorem on boundary values of analytic functions (see, e.g., Ref. 11, p. 52). Let $K_1(\tau)=U_{\gamma,0}(E,i\tau)V(p+i\tau\gamma)$. Since $K_1(\tau)$ is compact, we have only to show that $\mathrm{Ran}(1+K_1(\tau))$ is dense in $L^{2,-s},1/2<s<1$ for large $\tau>0$. For $f\in C_0^\infty(\mathbf{R}^3)$, let $u=L_\gamma(\tau)(H_0(i\tau\gamma)-E)f$. Then we have $(H_0(i\tau\gamma)-E)(u-f+K_1(\tau)u)=0$. Since $u-f+K_1(\tau)u\in L^{2,-s},1/2<s<1$, we have $u-f+K_1(\tau)u=0$ by virtue of Theorem 2.2 of Agmon–Hörmander.[1] □

Let us define for $z\notin\mathcal{E}_\gamma(E)$,

$$U_\gamma(E,z)=(1+U_{\gamma,0}(E,z)V(p+z\gamma))^{-1}U_{\gamma,0}(E,z). \tag{3.28}$$

Theorem 3.6. *(1) As a* $\mathbf{B}(\mathcal{H}_\delta;\mathcal{H}_{-\delta})$*-valued function,* $U_\gamma(E,z)$ *is meromorphic on* D_ϵ.
(2) When $z\to t\in(-\epsilon/2,\epsilon/2)\backslash\mathcal{E}_\gamma(E)$, $U_\gamma(E,z)$ *converges to* $U_\gamma(E,t)$ *and*

$$U_\gamma(E,t)\in\mathbf{B}(L^{2,s};L^{2,-s})\quad s>1/2.$$

(3) For large $\tau>0$,

$$U_\gamma(E,i\tau)=L_\gamma(\tau).$$

Proof: We show the last assertion. We have only to show that the equation $(H(i\tau\gamma)-E)u=0,u\in L^{2,-s}$, has only a trivial solution for large $\tau>0$. Since $(H_0(i\tau\gamma)-E)u=-V(p+i\tau\gamma)u\in L^{2,s}$, we have by the uniqueness theorem of Agmon–Hörmander, $u=-U_{\gamma,0}(E,i\tau)V(p+i\tau\gamma)u$. Therefore $u=0$ by using Lemma 3.5 (3). □

IV. FADDEEV SCATTERING AMPLITUDE

The Faddeev theory, which we have rewritten in Ref. 12, is transferred without any essential change to the non-self-adjoint case. For $E>0$, let

$$\mathcal{F}_0(E)f(\omega)=(2\pi)^{-3/2}(E/4)^{1/4}\int_{\mathbf{R}^3}e^{-i\sqrt{E}\omega\cdot x}f(x)\mathrm{d}x. \tag{4.1}$$

As is well known $\mathcal{F}_0(E)\in\mathbf{B}(L^{2,s};L^2(S^2))$ if $s>1/2$. Then for $E\notin\mathcal{E}_0$, the scattering amplitude is written as, up to a constant depending only on E,

$$A(E)=\mathcal{F}_0(E)(V-VR(E)V)\mathcal{F}_0(E)^*. \tag{4.2}$$

The scattering amplitude $f(E;\theta,\omega)$ from (2.12) is the integral kernel of $A(E)$. Let for $t\in(-\epsilon/2,\epsilon/2)\backslash\mathcal{E}_\gamma(E)$,

$$R_\gamma(E,t)=e^{it\gamma\cdot x}U_\gamma(E,t)e^{-it\gamma\cdot x}. \tag{4.3}$$

Then the Faddeev scattering amplitude is defined by

$$A_\gamma(E,t)=\mathcal{F}_0(E)(V-VR_\gamma(E,t)V)\mathcal{F}_0(E)^*. \tag{4.4}$$

The following two theorems are proved in the same way as in Theorems 7.1 and 7.3 of Ref. 12.

Theorem 4.1: *Let $F_\gamma(E,t)$ be the operator of multiplication by the characteristic function of the set $\{\omega\in S^2;\gamma\cdot\omega\geqslant t/\sqrt{E}\}$. Then*

$$A_\gamma(E,t)=A(E)+2\pi iA(E)F_\gamma(E,t)A_\gamma(E,t).$$

Theorem 4.2: *Let $K=2\pi iA(E)F_\gamma(E,t)$. Then*

$$t\in\mathcal{E}_\gamma(E)\Leftrightarrow 1\in\mathrm{spec}_p(K).$$

Let us give a brief sketch of the proof of the above theorems. Let

$$T_\gamma=2\pi i\mathcal{F}_0(E)^*F_\gamma(E,t)\mathcal{F}_0(E). \tag{4.5}$$

Then we have (Ref. 12, Lemma 6.4)

$$R_\gamma=R-(1-RV)T_\gamma(1-VR_\gamma), \tag{4.6}$$

where $R_\gamma=R_\gamma(E,t),R=R(E)$. The eigenoperator $\mathcal{F}(E)$ and the Faddeev eigenoperator $\mathcal{F}_\gamma(E,t)$ are defined by

$$\mathcal{F}(E)=\mathcal{F}_0(E)(1-V^*R(E)^*), \tag{4.7}$$

$$\mathcal{F}_\gamma(E,t)=\mathcal{F}_0(E)(1-V^*R_\gamma(E,t)^*). \tag{4.8}$$

Then by the resolvent equation (4.6) we have

$$\mathcal{F}_\gamma(E,t)^*=\mathcal{F}(E)^*+(1-RV)T_\gamma V\mathcal{F}_\gamma(E,t)^*.$$

Using (4.5) we get

$$\mathcal{F}_\gamma(E,t)^*=\mathcal{F}(E)^*+2\pi i\mathcal{F}(E)^*F_\gamma(E,t)A_\gamma(E,t).$$

Multiplying this by $\mathcal{F}_0(E)V$, we obtain Theorem 4.1.

To prove Theorem 4.2 we note the following operator equation:

$$1+R_{\gamma,0}(E,t)V=(1+R_0(E+i0)V)(1-\tilde{K}), \tag{4.9}$$

$$\tilde{K}=(1-R(E)V)T_\gamma V, \tag{4.10}$$

where $R_0(z)=(-\Delta-z)^{-1}$, $R_{\gamma,0}(E,t)=e^{it\gamma\cdot x}U_{\gamma,0}(E,t)e^{-it\gamma\cdot x}$. In fact, this follows from the formula

$$R_{\gamma,0}(E,t)=R_0(E+i0)-T_\gamma$$

(Ref. 12, Lemma 6.3) and the resolvent equation.

Since $E\notin\mathcal{E}_0$, $1+R_0(E+i0)V$ is invertible. Therefore

$$t\in\mathcal{E}_\gamma(E)\Leftrightarrow 1\in \mathrm{spec}_p(\tilde{K}). \tag{4.11}$$

Letting

$$S_1=2\pi i(1-R(E)V)\mathcal{F}_0(E)^*F_\gamma(E,t),$$

$$S_2=\mathcal{F}_0(E)V,$$

we have

$$\tilde{K}=S_1S_2,\quad K=S_2S_1.$$

Therefore

$$1\in\mathrm{spec}_p(\tilde{K})\Leftrightarrow 1\in\mathrm{spec}_p(K). \tag{4.12}$$

This proves Theorem 4.2.

It follows from Theorems 4.1 and 4.2 that for $t\in(-\epsilon/2,\epsilon/2)\backslash\mathcal{E}_\gamma(E)$,

$$A_\gamma(E,t)=(1-K)^{-1}A(E). \tag{4.13}$$

We have thus constructed the Faddeev scattering amplitude $A_\gamma(E,t)$ from the scattering amplitude $A(E)$. The kernel of $A_\gamma(E,t)$ is written as, up to a constant depending only on E,

$$A_\gamma(E,t;\theta',\theta)=\int_{\mathbf{R}^3}e^{-i\sqrt{E}(\theta'-\theta)\cdot x}V(\sqrt{E}\,\theta)\mathrm{d}x-\langle V^*(\sqrt{E}\,\theta')e^{i\sqrt{E}\theta'\cdot x},R_\gamma(E,t)V(\sqrt{E}\,\theta)e^{i\sqrt{E}\theta\cdot x}\rangle, \tag{4.14}$$

where $V^*(\xi)$ is defined by (2.15). We now put

$$\sqrt{E}\,\theta=\sqrt{E-t^2}\,\omega+t\gamma,\quad \sqrt{E}\,\theta'=\sqrt{E-t^2}\,\omega'+t\gamma, \tag{4.15}$$

where $\omega,\omega'\in S^2,\omega\cdot\gamma=\omega'\cdot\gamma=0$. Then the above kernel is rewritten as

$$\int_{\mathbf{R}^3}e^{-i\sqrt{E-t^2}(\omega'-\omega)\cdot x}V(\sqrt{E}\,\theta)\mathrm{d}x-\langle V^*(\sqrt{E}\,\theta')e^{i\sqrt{E-t^2}\omega'\cdot x},U_\gamma(E,t)V(\sqrt{E}\,\theta)e^{i\sqrt{E-t^2}\omega\cdot x}\rangle, \tag{4.16}$$

which we denote by $B_\gamma(\omega',\omega;t)$. Since $U_\gamma(E,t)$ is a boundary value of a meromorphic function, $B_\gamma(\omega',\omega;t)$ is uniquely extended to a meromorphic function on D_ϵ.

V. RECONSTRUCTION OF THE SPIN–ORBIT INTERACTION

In this section we reconstruct the spin–orbit term from $B_\gamma(\omega',\omega;t)$ defined by (4.16). Our intention is to consider the case without magnetic field $b(x)$. However, since we shall use an auxiliary magnetic field in the next section, we include $b(x)$ until Lemma 5.5.

As has been noted above, $B_\gamma(\omega',\omega;t)$ is meromorphically extended to D_ϵ. By Theorem 3.6 (3), for large $\tau>0$, $B_\gamma(\omega',\omega;i\tau)$ has the following expression:

$$B_\gamma(\omega',\omega;i\tau)=\int e^{-i\sqrt{E+\tau^2}(\omega'-\omega)\cdot x}V(\sqrt{E}\,\theta)\mathrm{d}x - \langle V^*(\sqrt{E}\,\theta')e^{i\sqrt{E+\tau^2}\omega'\cdot x},L_\gamma(\tau)V(\sqrt{E}\,\theta)e^{i\sqrt{E+\tau^2}\omega\cdot x}\rangle, \tag{5.1}$$

where

$$\sqrt{E}\,\theta=\sqrt{E+\tau^2}\,\omega+i\tau\gamma,\quad \sqrt{E}\,\theta'=\sqrt{E+\tau^2}\,\omega'+i\tau\gamma.$$

For $\xi\in\mathbf{R}^3$, we take $\gamma,\eta\in S^2$ such that $\xi\cdot\gamma=\xi\cdot\eta=\eta\cdot\gamma=0$, and put

$$\omega=\omega(\tau)=\left(1-\frac{|\xi|^2}{4\tau^2}\right)^{1/2}\eta-\frac{\xi}{2\tau},\quad \omega'=\omega(\tau)'=\left(1-\frac{|\xi|^2}{4\tau^2}\right)^{1/2}\eta+\frac{\xi}{2\tau},$$

$$p(\tau)=\sqrt{E+\tau^2}\,\omega(\tau),\quad p(\tau)'=\sqrt{E+\tau^2}\,\omega(\tau)',$$

$$\zeta(\tau)=p(\tau)+i\tau\gamma,\quad \zeta(\tau)'=p(\tau)'+i\tau\gamma.$$

We split $B_\gamma(\omega(\tau)',\omega(\tau);i\tau)$ into two parts:

$$B_\gamma(\omega(\tau)',\omega(\tau);i\tau)=B_\gamma^{(1)}(\tau)+B_\gamma^{(2)}(\tau), \tag{5.2}$$

$$B_\gamma^{(1)}(\tau)=\int e^{-i(p(\tau)'-p(\tau))\cdot x}V(\zeta(\tau))\mathrm{d}x, \tag{5.3}$$

$$B_\gamma^{(2)}(\tau)=-\langle V^*(\zeta(\tau)')e^{ip(\tau)'\cdot x},L_\gamma(\tau)V(\zeta(\tau))e^{ip(\tau)\cdot x}\rangle. \tag{5.4}$$

Noting that

$$p(\tau)'-p(\tau)=\xi+O(\tau^{-1}),$$

$$\zeta(\tau)/\tau=\eta+i\gamma+O(\tau^{-1}),$$

we have by (2.4)

$$\lim_{\tau\to\infty}B_\gamma^{(1)}(\tau)/\tau=\int e^{-ix\cdot\xi}\{2b(x)\cdot(\eta+i\gamma)+a(x)\sigma\cdot(x\times(\eta+i\gamma))\}\mathrm{d}x. \tag{5.5}$$

To compute $B_\gamma^{(2)}(\tau)$, we rewrite it as follows:

$$B_\gamma^{(2)}(\tau)=-\langle V^*(\zeta(\tau)')e^{i(p(\tau)'-p(\tau))\cdot x},U(\tau)^{-1}L_\gamma(\tau)U(\tau)V(\zeta(\tau))\rangle, \tag{5.6}$$

where

$$U(\tau)=e^{ip(\tau)\cdot x}. \tag{5.7}$$

By (3.3) and (3.26), the term $U(\tau)^{-1}L_\gamma(\tau)U(\tau)$ is rewritten as

$$U(\tau)^{-1}L_\gamma(\tau)U(\tau)=U(\tau)^{-1}S(\tau)U(\tau)\cdot\tilde{G}(\zeta(\tau))\cdot U(\tau)^{-1}S(\tau)^{-1}(1+K(\tau))^{-1}U(\tau).$$

Let $A(\tau)$ be from (3.12) and put

$$B(\tau)=U(\tau)^{-1}A(\tau)U(\tau). \tag{5.8}$$

Then we have by virtue of (3.12)

$$U(\tau)^{-1}S(\tau)^{-1}U(\tau)=e^{-B(\tau)}. \tag{5.9}$$

Lemma 5.1: Let

$$\Psi(x,\xi+\zeta(\tau))=\varphi(x,\xi+\zeta(\tau))+\psi(x,\xi+\zeta(\tau))\sigma\cdot(x\times(\xi+\zeta(\tau))),$$

and let $P(\tau)$ be the ΨDO with symbol $e^{-\Psi(x,\xi+\zeta(\tau))}$. Then

$$e^{-B(\tau)}-P(\tau)\in\mathcal{S}^{-1}.$$

Proof: Modulo $\mathcal{S}^{-1}$, $B(\tau)$ is a ΨDO with symbol $\Psi(x,\xi+\zeta(\tau))$. Therefore for large $|z|$, $(z-B(\tau))^{-1}$ is a ΨDO with symbol $(z-\Psi(x,\xi+\zeta(\tau)))^{-1}$ modulo $\mathcal{S}^{-1}$. Since for large M,

$$e^{-B(\tau)}=\frac{1}{2\pi i}\int_{|z|=M}e^{-z}(z-B(\tau))^{-1}\mathrm{d}z,$$

$e^{-B(\tau)}$ is a ΨDO with symbol $e^{-\Psi(x,\xi+\zeta(\tau))}$, modulo $\mathcal{S}^{-1}$. □

We put

$$\eta=e_1,\quad \gamma=e_2,\quad \eta\times\gamma=e_3, \tag{5.10}$$

$$\Psi_\infty(x)=f+g\sigma\cdot(x\times(e_1+ie_2)), \tag{5.11}$$

$$f=-(2\pi)^{-3/2}\int_{\mathbf{R}^3}e^{ix\cdot k}\frac{\hat{b}(k)\cdot(e_1+ie_2)}{k_1+ik_2}\mathrm{d}k, \tag{5.12}$$

$$g=-(2\pi)^{-3/2}\int_{\mathbf{R}^3}e^{ix\cdot k}\frac{\hat{a}(k)}{2(k_1+ik_2)}\mathrm{d}k, \tag{5.13}$$

where $k_j=k\cdot e_j, x_j=x\cdot e_j$ and $\tilde{a}(\xi_1,\xi_2,x_3)$ is the partial Fourier transform with respect to x_1,x_2 of $a(x)$. We also let

$$f_0(x)=2b(x)\cdot(e_1+ie_2)+a(x)\sigma\cdot(x\times(e_1+ie_2)). \tag{5.14}$$

Lemma 5.2:

$$\lim_{\tau\to\infty}\frac{1}{\tau}B_\gamma^{(2)}(\tau)=-\int_{\mathbf{R}^3}e^{-ix\cdot\xi}f_0e^{\Psi_\infty}N_\gamma(e^{-\Psi_\infty}f_0)\mathrm{d}x.$$

Proof: First we note

$$U(\tau)^{-1}(1+K(\tau))^{-1}U(\tau)V(\zeta(\tau))/\tau\to f_0(x). \tag{5.15}$$

Let

$$\chi_1(\xi+i\tau\gamma)=\chi_0\left(\frac{2|(\xi+i\tau\gamma)^2-E|}{E+\tau^2+|\xi|^2}\right),\quad \chi_2(\xi+i\tau\gamma)=1-\chi_1(\xi+i\tau\gamma),$$

$\chi_0(t)$ being as in (3.8), and let Q_j be the ΨDO with symbol $\chi_j(\xi+i\tau\gamma)$. On the support of $\chi_2(\xi+i\tau\gamma)$, we have

$$|(\xi+i\tau\gamma)^2-E|\geqslant\frac{\epsilon}{4}(E+\tau^2+|\xi|^2).$$

So we have

$$\|U_{\gamma,0}(E,i\tau)Q_2\|_{\mathbf{B}(L^2;L^2)}\leqslant C/\tau^2.$$

Therefore as an operator in $\mathbf{B}(L^{2,s};L^{2,s-1})$,$0<s<1$,

$$U_{\gamma,0}(E,i\tau)=U_{\gamma,0}(E,i\tau)Q_1+O(\tau^{-2}). \tag{5.16}$$

On the other hand, by Lemma 5.1, we have

$$\tilde{Q}_1U(\tau)^{-1}S(\tau)^{-1}U(\tau)=\tilde{Q}_1e^{-B(\tau)}\sim\tilde{Q}_1P(\tau), \tag{5.17}$$

and $\tilde{Q}_1P(\tau)$ converges strongly to $e^{-\Phi_\infty(x)}$.

Similarly $U(\tau)^{-1}S(\tau)U(\tau)$ converges strongly to $e^{\Psi_\infty(x)}$. Furthermore by Lemma 3.2,

$$\tau\tilde{G}(\zeta(\tau))\to N_\gamma.$$

These facts prove Lemma 5.2. □

Our next aim is to compute $N_\gamma(e^{-\Psi_\infty}f_0)$. Let us note that putting $\bar{\partial}=\frac{1}{2}(e_1+ie_2)\cdot\nabla_x$, we have

$$4i\bar{\partial}\Psi_\infty=f_0. \tag{5.18}$$

Since $\bar{\partial}\Psi_\infty$ and Ψ_∞ commute, we also have

$$\bar{\partial}e^{\Psi_\infty}=(\bar{\partial}\Psi_\infty)e^{\Psi_\infty}. \tag{5.19}$$

Lemma 5.3:

$$\int_{\mathbf{R}^3}e^{-ix\cdot\xi}f_0e^{\Psi_\infty}N_\gamma e^{-\Psi_\infty}f_0\mathrm{d}x=4i\int_{\mathbf{R}^3}e^{-ix\cdot\xi}(\bar{\partial}e^{\Psi_\infty})(e^{-\Psi_\infty}-1)\mathrm{d}x.$$

Proof: The left-hand side is equal to

$$\int_{\mathbf{R}^3}e^{-ix\cdot\xi}4i(\bar{\partial}\Psi_\infty)e^{\Psi_\infty}N_\gamma e^{-\Psi_\infty}4i(\bar{\partial}\Psi_\infty)\mathrm{d}x=16\int_{\mathbf{R}^3}e^{-ix\cdot\xi}(\bar{\partial}e^{\Psi_\infty})N_\gamma(\bar{\partial}e^{-\Psi_\infty})\mathrm{d}x.$$

Using

$$N_\gamma\bar{\partial}e^{-\Psi_\infty}=\frac{i}{4}(e^{-\Psi_\infty}-1),$$

which follows from Liouville's theorem, we get the lemma. □

Lemma 5.4:

$$\int_{\mathbf{R}^3}e^{-ix\cdot\xi}f_0e^{\Psi_\infty}N_\gamma e^{-\Psi_\infty}f_0\mathrm{d}x=0.$$

Proof: By integration by parts, we have

$$\int_{x_1^2+x_2^2<r^2} e^{-ix\cdot\xi}(\overline{\partial}e^{\Psi_\infty})(e^{-\Psi_\infty}-1)\mathrm{d}x_1\,\mathrm{d}x_2$$

$$=\frac{1}{2}\int_{x_1^2+x_2^2=r^2} e^{-ix\cdot\xi}(x_1+ix_2)(1-e^{\Psi_\infty})\mathrm{d}\theta-\int_{x_1^2+x_2^2<r^2} e^{-ix\cdot\xi}e^{\Psi_\infty}\overline{\partial}e^{-\Psi_\infty}\mathrm{d}x_1\,\mathrm{d}x_2\equiv(I)-(II).$$

The second term is written as

$$(II)=-\int_{x_1^2+x_2^2<r^2} e^{-ix\cdot\xi}\overline{\partial}\Psi_\infty\mathrm{d}x_1\,\mathrm{d}x_2=-\frac{1}{2}\int_{x_1^2+x_2^2=r^2} e^{-ix\cdot\xi}(x_1+ix_2)\Psi_\infty\mathrm{d}\theta.$$

On the other hand, $e^{\Psi_\infty}=1+\Psi_\infty+O(|x|^{-2})$. Therefore

$$(I)\sim-\frac{1}{2}\int_{x_1^2+x_2^2=r^2} e^{-ix\cdot\xi}(x_1+ix_2)\Psi_\infty\mathrm{d}\theta.$$

□

Using (5.5) and Lemmas 5.2, 5.4, one can compute

$$\int_{\mathbf{R}^3} e^{-ix\cdot\xi}\{2b(x)\cdot(\eta+i\gamma)+a(x)\sigma\cdot(x\times(\eta+i\gamma))\}\mathrm{d}x \tag{5.20}$$

form the scattering amplitude.

Here let us recall the following formulas for spin matrices, which are proved by using the commutation relations:

$$(\sigma\cdot\xi)(\sigma\cdot\eta)=\xi\cdot\eta+i\sigma\cdot(\xi\times\eta), \tag{5.21}$$

$$[\sigma\cdot(x\times(e_1+ie_2)),\sigma\cdot e_3]=2ix_3\sigma\cdot(e_1+ie_2). \tag{5.22}$$

We now reconstruct $a(x)$. We take $b(x)\equiv 0$. Then by (5.20) and (5.22), one can recover

$$\int e^{-ix\cdot\xi}a(x)x_3\mathrm{d}x.$$

Since $\xi=(0,0,\xi_3)$, one can recover

$$\int_{\mathbf{R}^3} a(x_1,x_2,x_3)\mathrm{d}x_1\,\mathrm{d}x_2.$$

Choosing the direction of ξ arbitrarily, one can reconstruct $a(x)$ by the inversion formula of the Radon transform (see, e.g., Ref. 10).

VI. RECONSTRUCTION OF THE COMPLEX POTENTIAL

A. Gauge invariance

In the previous section we constructed the spin–orbit term $a(x)\sigma\cdot(x\times p)$ from the scattering amplitude of the operator

$$-\Delta+V(p),\quad V(p)=a(x)\sigma\cdot(x\times p)+W(x).$$

To reconstruct $W(x)$ we shall make use of the gauge invariance.

Let $\psi(x)$ be the solution of

$$(-\Delta+V(p)-E)\psi=0 \tag{6.1}$$

having the asymptotic expansion

$$\psi \sim e^{i\sqrt{E}\omega\cdot x} + \frac{e^{i\sqrt{E}r}}{r} f(E;\theta,\omega), \quad \theta = x/r, \quad r = |x| \to \infty. \tag{6.2}$$

Let $c(x) = \exp(-|x|^2)$ and $\psi_\lambda(x) = e^{i\lambda c(x)}\psi(x)$, λ being a large parameter. Then ψ_λ satisfies

$$((p-b_\lambda)^2 + V(p-b_\lambda) - E)\psi_\lambda = 0 \tag{6.3}$$

with $b_\lambda(x) = \lambda\nabla c(x)$. Since $c(x)$ is exponentially decreasing, ψ_λ has the same asymptotic expansion as in (6.2). This means that the family of operators $\{(p-b_\lambda)^2 + V(p-b_\lambda); \lambda > 0\}$ has the same scattering amplitude. One should also note that due to the unitary equivalence, the sets of exceptional points $\mathcal{E}_0$ and $\mathcal{E}_\gamma(E)$ are independent of $\lambda > 0$.

B. Reconstruction of the complex potential

We use the same notation as in Sec. V with b replaced by $b_\lambda = \lambda\nabla c(x)$. Let

$$V_1(\xi) = 2b_\lambda\cdot\xi + a\sigma\cdot(x\times\xi),$$

$$V_2 = -i\,\mathrm{div}\, b_\lambda - |b_\lambda|^2 - a\sigma\cdot(x\times b_\lambda) + W.$$

Then

$$V(\zeta(\tau) - b_\lambda) \simeq \tau V_1(\eta + i\gamma) - V_1(\xi/2) + V_2,$$

$$V^*(\zeta(\tau)' - b_\lambda) \simeq \tau V_1^*(\eta - i\gamma) + V_1^*(\xi/2) + V_2^*.$$

Recall that we already know $a(x)$ and $b_\lambda(x)$.

We first show that up to known terms

$$B_\gamma^{(1)}(\tau) + B_\gamma^{(2)}(\tau) \simeq \int_{\mathbf{R}^3} e^{-ix\cdot\xi} W(x)\mathrm{d}x - \langle e^{-ix\cdot\xi} V_1^*(\eta - i\gamma), e^{\Psi_\infty} N_\gamma e^{-\Psi_\infty}(-V_1(\xi/2) + V_2)\rangle$$
$$- \langle e^{-ix\cdot\xi}(V_1^*(\xi/2) + V_2), e^{\Psi_\infty} N_\gamma e^{-\Psi_\infty} V_1(\eta + i\gamma)\rangle.$$

In fact,

$$B_\gamma^{(1)}(\tau) \simeq \tau\int_{\mathbf{R}^3} e^{-ix\cdot\xi} V_1(\eta + i\gamma)\mathrm{d}x - \int_{\mathbf{R}^3} e^{-ix\cdot\xi} V_1(\xi/2)\mathrm{d}x + \int_{\mathbf{R}^3} e^{-ix\cdot\xi} V_2 \mathrm{d}x.$$

Up to a known term, this is equal to $\int e^{-ix\cdot\xi} W(x)\mathrm{d}x$.

Next we note that

$$B_\gamma^{(2)}(\tau) \sim -\tau^2\langle V_1^*(\eta - i\gamma)e^{ip(\tau)'x}, L_\gamma(\tau) V_1(\eta + i\gamma)e^{ip(\tau)x}\rangle - \tau\langle V_1^*(\eta - i\gamma)e^{ip(\tau)'x}, L_\gamma(\tau)$$
$$\times(-V_1(\xi/2) + V_2)e^{ip(\tau)x}\rangle - \tau\langle (V_1^*(\xi/2) + V_2^*)e^{ip(\tau)'x}, L_\gamma(\tau) V_1(\eta + i\gamma)e^{ip(\tau)x}\rangle.$$

Since

$$L_\gamma(\tau) = S(\tau) U_{\gamma,0}(E, i\tau) S(\tau)^{-1}(1 - K(\tau)) + O(\tau^{-3}),$$

the first term is a known term. Applying

$$L_\gamma(\tau) = S(\tau) U_{\gamma,0}(E, i\tau) S(\tau)^{-1} + O(\tau^{-2}),$$

and arguing in the same way as in the proof of Lemma 5.2, we get

$$B_\gamma^{(2)}(\tau)\simeq -\langle e^{-ix\cdot\xi}V_1^*(\eta-i\gamma),e^{\Psi_\infty}N_\gamma e^{-\Psi_\infty}(-V_1(\xi/)+V_2)\rangle-\langle e^{-ix\cdot\xi}(V_1^*(\xi/2)+V_2^*),e^{\Psi_\infty}N_\gamma e^{-\Psi_\infty}V_1(\eta+i\gamma)\rangle.$$

The right-hand side is equal to

$$-\int e^{ix\cdot\xi}(\overline{\partial}e^{\Psi_\infty})N_\gamma e^{-\Psi_\infty}(-V_1(\xi/2)+V_2)\mathrm{d}x+\int e^{ix\cdot\xi}(V_1(\xi/2)+V_2)e^{\Psi_\infty}N_\gamma(\overline{\partial}e^{-\Psi_\infty})\mathrm{d}x$$

$$=\int e^{ix\cdot\xi}(N_\gamma\overline{\partial}e^{\Psi_\infty})e^{-\Psi_\infty}(-V_1(\xi/2)+V_2)\mathrm{d}x+\int e^{ix\cdot\xi}(V_1(\xi/2)+V_2)e^{\Psi_\infty}(N_\gamma\overline{\partial}e^{-\Psi_\infty})\mathrm{d}x,$$

where we have used (7.6). Since

$$N_\gamma e^{\pm i\Psi_\infty}=\frac{i}{4}(e^{\pm i\Psi_\infty}-1),$$

this is equal to

$$\frac{i}{4}\int e^{ix\cdot\xi}(1-e^{\Psi_{-\infty}})(-V_1(\xi/2)+V_2)\mathrm{d}x+\frac{i}{4}\int e^{ix\cdot\xi}(V_1(\xi/2)+V_2)(1-e^{\Psi_\infty})\mathrm{d}x.$$

Since $\Psi_\infty=-i\lambda c(x)+g$, by the stationary phase method, the term containing $e^{\pm i\Psi_\infty}$ vanishes as $\lambda\to\infty$. Here one must note that $b_\lambda(0)=0$. What remains is

$$\frac{i}{2}\int e^{ix\cdot\xi}V_2\mathrm{d}x.$$

Up to a known term this is equal to $i/2\int e^{ix\cdot\xi}W\,\mathrm{d}x$. We have thus reconstructed $\hat{W}(\xi)$.

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APPENDIX

We summarize here basic properties of the $\overline{\partial}$-operator used in this paper. Note that we define $\overline{\partial}=(\partial/\partial x_1+i\partial/\partial x_2)/2$.

Theorem 7.1: *If* $|f(z)|\leqslant C(1+|z|)^{-1-\epsilon}$ *for some* $C,\epsilon>0$, *the solution of the equation* $\overline{\partial}u=f$ *satisfying* $u(z)\to 0$ *as* $|z|\to\infty$ *is unique and is given by*

$$u(z)=\frac{1}{2\pi i}\int_{\mathbf{C}}\frac{f(\zeta)}{\zeta-z}\mathrm{d}\zeta\wedge\mathrm{d}\overline{\zeta}=\frac{1}{\pi}\int_{\mathbf{R}^2}\frac{f(x_1-y_1,x_2-y_2)}{y_1+iy_2}\mathrm{d}y_1\mathrm{d}y_2.$$

Using the identity

$$\frac{1}{\zeta-z}=-\frac{1}{z}\sum_{k=0}^{n}\left(\frac{\zeta}{z}\right)^k+\frac{1}{\zeta-z}\left(\frac{\zeta}{z}\right)^{n+1}$$

we have if $(1+|z|)^n f(z)\in L^1(\mathbf{C})$,

$$u(z)=-\frac{1}{2\pi i}\sum_{k=0}^{n}z^{-k-1}\int_{\mathbf{C}}\zeta^k f(\zeta)\mathrm{d}\zeta\wedge\mathrm{d}\overline{\zeta}+\frac{1}{2\pi i}z^{-n-1}\int_{\mathbf{C}}\frac{\zeta^{n+1}f(\zeta)}{\zeta-z}\mathrm{d}\zeta\wedge\mathrm{d}\overline{\zeta}.$$

In particular we have

Theorem 7.2. *If* $|f(z)| \leqslant C(1+|z|)^{-3-\epsilon}$, *the above solution satisfies*

$$(x_1+ix_2)u(z)=\frac{1}{\pi}\int_{\mathbf{R}^2} f(y_1,y_2)\mathrm{d}y_1\mathrm{d}y_2+O(|x|^{-1}).$$

From this theorem it follows that

$$u(x)=(2\pi)^{-1}\int_{\mathbf{R}^2}\frac{e^{ix\cdot k}\hat{f}(k)}{k_1+ik_2}\mathrm{d}k \tag{A1}$$

satisfies

$$(x_1+ix_2)u(x)=\frac{i}{2\pi}\int_{\mathbf{R}^2} f(y)\mathrm{d}y+O(|x|^{-1}), \tag{A2}$$

if $|f(y)| \leqslant C(1+|y|)^{-3-\epsilon}$.

For $f \in \mathcal{S}(\mathbf{R}^3)$, let

$$Nf(x)=(2\pi)^{-3/2}\int_{\mathbf{R}^3}\frac{e^{ix\cdot\xi}\hat{f}(\xi)}{2(\xi_1+i\xi_2)}\mathrm{d}\xi. \tag{A3}$$

Then we have

$$\frac{1}{2}\left(\frac{\partial}{\partial x_1}+i\frac{\partial}{\partial x_2}\right)Nf=\frac{i}{4}f, \tag{A4}$$

$$Nf(x)=\frac{i}{4\pi}\int_{\mathbf{R}^2}\frac{f(y_1,y_2,x_3)}{x_1-y_1+i(x_2-y_2)}\mathrm{d}y, \tag{A5}$$

$$\int_{\mathbf{R}^3}(Nf(x))g(x)\mathrm{d}x=-\int_{\mathbf{R}^3} f(x)(Ng(x))\mathrm{d}x. \tag{A6}$$

Let us prove Lemma 3.3 (1). We first note that $|\xi^2+2i\tau\gamma\cdot\xi-\tau^2-E| \leqslant \epsilon(E+\tau^2+|\xi|^2)$ implies there exists a constant $C>0$ such that

$$C^{-1}\tau \leqslant |\xi| \leqslant C\tau, \quad |\gamma\cdot\frac{\xi}{|\xi|}| \leqslant C\epsilon, \tag{A7}$$

for large $\tau>0$. Therefore we have only to show the following lemma.

Lemma 7.3: Let $m \in \mathbf{R}$. *Suppose* $f(x,\xi;\tau)$ *satisfies*

$$|\partial_x^\alpha\partial_\xi^\beta f(x,\xi;\tau)| \leqslant C_{\alpha\beta}\langle x\rangle^{-3-|\alpha|}(\tau+|\xi|)^{m-|\beta|} \quad \forall\alpha,\beta$$

for ξ, τ *satisfying the condition (7.7). Then*

$$g(x,\xi;\tau)=(2\pi)^{-3/2}\int_{\mathbf{R}^3} e^{ix\cdot k}\frac{\hat{f}(k,\xi;\tau)}{k\cdot(\xi+i\tau\gamma)}\mathrm{d}k$$

satisfies

$$|\partial_x^\alpha\partial_\xi^\beta g(x,\xi;\tau)| \leqslant C_{\alpha\beta}\langle x\rangle^{-1}(\tau+|\xi|)^{m-1-|\beta|} \quad \forall\alpha,\beta,$$

for ξ, τ *satisfying the condition (7.7).*

Proof: We make the linear change of variables $p=Ak$, where

$$p_1=\frac{\xi}{\tau}\cdot k,\ p_2=\gamma\cdot k, p_3=\left(\frac{\xi}{\tau}\times\gamma\right)\cdot k.$$

Then letting $f_A(x,\xi;\tau)=f({}^tAx,\xi;\tau)$, we have

$$g({}^tAx,\xi;\tau)=\frac{i}{2\pi\tau}\int_{\mathbf{R}^2}\frac{f_A(x_1-y_1,x_2-y_2,x_3,\xi;\tau)}{y_1+iy_2}\mathrm{d}y,$$

whose derivative is estimated as follows:

$$|\partial_x^\alpha\partial_\xi^\beta g({}^tAx,\xi;\tau)|\leqslant C_{\alpha\beta}(\tau+|\xi|)^{m-1-|\beta|}\int_{\mathbf{R}^2}\frac{(1+|x'-y|+|x_3|)^{-3}}{|y|}\mathrm{d}y,$$

where $x'=(x_1,x_2)$. The integral over the region $\{|y|<|x'|/2\}$ is estimated as

$$\int_{|y|<|x'|/2}\frac{(1+|x'-y|+|x_3|)^{-3}}{|y|}\mathrm{d}y\leqslant C(1+|x|)^{-2}.$$

The integral over the region $\{|y|>|x'|/2\}$ is estimated as

$$\int_{|y|>|x'|/2}\frac{(1+|x'-y|+|x_3|)^{-3}}{|y|}\mathrm{d}y\leqslant\frac{C}{|x'|}\int_{\mathbf{R}^2}(1+|y|+|x_3|)^{-3}\mathrm{d}y\leqslant\frac{C}{|x'|(1+|x^3|)}.$$

If $|x'|>1$, this is dominated from above by $C(1+|x|)^{-1}$. If $|x'|\leqslant 1$, we estimate in the following manner:

$$\int_{|x'|/2<|y|<1}\frac{(1+|x'-y|+|x_3|)^{-3}}{|y|}\mathrm{d}y\leqslant C(1+|x_3|)^{-3}\int_{|y|<1}\frac{\mathrm{d}y}{|y|}\leqslant C(1+|x_3|)^{-3}\leqslant C(1+|x|)^{-3},$$

$$\int_{|y|>1}\frac{(1+|x'-y|+|x_3|)^{-3}}{|y|}\mathrm{d}y\leqslant C\int_{|y|<1}(1+|x'-y|+|x_3|)^{-3}\mathrm{d}y$$
$$\leqslant C(1+|x_3|)^{-1}\leqslant C(1+|x|)^{-1}.$$

We have thus proven

$$|\partial_x^\alpha\partial_\xi^\beta g({}^tAx,\xi;\tau)|\leqslant C_{\alpha\beta}\langle x\rangle^{-1}(\tau+|\xi|)^{m-1-|\beta|}.$$

From this we can conclude the lemma. □

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On an integrable hierarchy derived from the isentropic gas dynamics

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In this paper we study a new hierarchy of equations derived from the system of isentropic gas dynamics equations where the pressure is a nonlocal function of the density. We show that the hierarchy of equations is integrable. We construct the two compatible Hamiltonian structures and show that the first structure has three distinct Casimirs while the second has one. The existence of Casimirs allows us to extend the flows to local ones. We construct an infinite series of commuting local Hamiltonians as well as three infinite series (related to the three Casimirs) of nonlocal charges. We discuss the zero curvature formulation of the system where we obtain a simple expression for the nonlocal conserved charges, which also clarifies the existence of the three series from a Lie algebraic point of view. We point out that the nonlocal hierarchy of Hunter–Zheng equations can be obtained from our nonlocal flows when the dynamical variables are properly constrained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1756699]

I. INTRODUCTION

The dynamics of a gas are described by the equations[1]

$$\begin{aligned} &u_t+uu_x+\frac{1}{\rho}P_x=0,\\ &\rho_t+(\rho u)_x=0,\\ &s_t+us_x=0, \end{aligned} \tag{1}$$

where u,ρ,s denote, respectively, the velocity, density, and entropy while P represents the pressure. Here the pressure, in general, can have a functional dependence of the form

$$P=P(\rho^{(n)},s^{(n)}),$$

where $n\in\mathbb{Z}$ and

$$\rho^{(n)}=(\partial^n\rho),\quad s^{(n)}=(\partial^n s).$$

For an isentropic gas (s constant), the equations in (1) take the forms

$$\begin{aligned} &u_t+uu_x+\frac{1}{\rho}P=0,\\ &\rho_t+(\rho u)_x=0, \end{aligned} \tag{2}$$

and have been well studied in the literature for the cases where the pressure is a local monomial of the density, i.e., it has the simple form $P=P(\rho^{(0)})$. For example, for $P=\rho^{\gamma}$, $\gamma\neq 0,1$, Eq. (1) is known as the polytropic gas equations, and for the choice $P=-1/\rho$, the system is called the Chaplygin gas. This class of systems are known to be Hamiltonian systems of hydrodynamic type[2] and are integrable. Various properties associated with such systems have been derived in the past several years.[3–5]

In this paper, we will study a new class of Hamiltonian equations derived from the isentropic gas dynamics system (2) where the pressure is a nonlocal function of the density. In particular, we will choose for the pressure $P(v^{(-1)})=-\frac{1}{2}(\partial^{-1}v)^2$, where $v\equiv\rho$ (we make this identification to be consistent with the conventional choice in the literature), leading to the dynamical equations

$$\begin{aligned} u_t&=-uu_x+(\partial^{-1}v),\\ v_t&=-(uv)_x. \end{aligned} \tag{3}$$

As we will show later, this system of equations is Hamiltonian (in fact, bi-Hamiltonian). In fact, let us note here that the simple first order action

$$S=\int \mathrm{d}t\,\mathrm{d}x\left[(\partial^{-1}u)v_t-\frac{1}{2}u^2v-\frac{1}{2}(\partial^{-1}v)^2\right], \tag{4}$$

generates the dynamical equations in (3) as Euler–Lagrange equations and leads to one of the Hamiltonian structures to be discussed in the next section. In this first order representation, the dynamical equations have a nonlocal form.

One can, of course, take the time derivative of the first equation in (3) to obtain a local representation of the form

$$\begin{aligned} u_{tt}&=-(uu_x)_t+uv,\\ v_t&=-(uv)_x. \end{aligned} \tag{5}$$

This is a second order representation involving only the second time derivative of u and cannot be given a Hamiltonian description. In fact, even a Lagrangian description for this system is not easily obtained. One can, of course, make the system of equations completely second order in which case a Lagrangian formulation is possible. However, since the properties of integrability are best discussed within the Hamiltonian formulation, we will not pursue a Lagrangian description. Sometimes a redefinition of variables can also convert a nonlocal equation into a local one. Indeed, with the identification $z=(\partial^{-1}v)$, the set of equations (3) take the local form

$$u_t=-uu_x+z,\quad z_t=-uz_x, \tag{6}$$

and can be described by a simple first order action of the form

$$S=\int \mathrm{d}t\,\mathrm{d}x\left[zu_t-\frac{1}{2}(u^2z_x+z^2)\right], \tag{7}$$

which shows that the system is Hamiltonian. (The Hamiltonian structure in these new variables can be easily seen to be the canonical one.) However, description of the system in these variables makes the connection with the gas dynamics less transparent.

Although the system of equations in (3), (5), and (6) are equivalent, since we are interested in the integrability properties within the Hamiltonian description, we will study the system in detail in the form described in (3) keeping in mind the mapping to the Hunter–Zheng equation that we will discuss later in the paper. We will show that the hierarchy of equations associated with this system is integrable. The system (3) is bi-Hamiltonian[6,7] (possesses two compatible Hamiltonian

structures) and the infinite set of (nonlocal) charges can be constructed recursively. The two Hamiltonian structures of the system possess nontrivial Casimirs (distinguished functionals) leading to three distinct infinite series of nonlocal charges and allowing us to extend the flows to local ones.[8,9] As a result, we can also construct recursively an infinite set of local conserved charges associated with the system which are in involution. The zero curvature formulation for both the local and the nonlocal equations of the hierarchy can be given in terms of the Lie algebra valued potentials belonging to $SL(2)\otimes U(1)$ (Ref. 10) and generate the nonlocal charges in a compact form. However, we have not yet succeeded in finding a scalar Lax description for the local equations and, consequently, the relation between the local conserved charges and a Lax operator remains an open question. Finally, we show that the hierarchy of equations associated with (3) reduce to the nonlocal hierarchy of Hunter–Zheng equations[11] when properly constrained, whereas the local equations become trivial (they do not go over to the hierarchy of Harry Dym equations[12]). We note that even though we do not yet know of a physical system corresponding to Eqs. (3) or (6), the nice integrability properties that emerge make it worth studying it in its own right. Furthermore, from its relation with the Hunter–Zheng equation, it is quite likely that such a system of equations would find application in a physical problem.

This paper is organized as follows. In Sec. II, we show that the system is bi-Hamiltonian. We obtain the two Hamiltonian structures associated with the Hamiltonian description of Eq. (3). We prove Jacobi identity as well as the compatibility of the two structures using the method of prolongation. We comment on the relation between these structures and the known Lie algebras. The bi-Hamiltonian nature of the system is sufficient to guarantee the integrability of the system. We construct the recursion operator and obtain the first few charges recursively. We show that the two Hamiltonian structures have nontrivial Casimirs which allows us to construct three distinct series of nonlocal charges associated with the three different Casimirs of the first Hamiltonian structure. The Casimir of the second Hamiltonian structure, on the other hand, allows us to extend the flows to local ones. In this case, the recursion operator can be inverted and allows us to construct the infinite set of local charges associated with the system recursively. By construction these charges are in involution. We also describe briefly the matrix Lax description for the system. In Sec. III, we present the zero curvature description of both the local as well as the nonlocal hierarchies of equations based on the Lie algebra $SL(2)\otimes U(1)$. We obtain the nonlocal charges associated with the system from the zero curvature which also clarifies from a different perspective why there are three distinct series of nonlocal charges. In Sec. IV, we summarize our results as well as present some open problems. In particular, we point out how the nonlocal hierarchy of equations associated with (3) reduce to the nonlocal hierarchy of Hunter–Zheng equations. In spite of having a zero curvature formulation of the system, we have not succeeded in obtaining a scalar Lax description for the local equations which remains an interesting open problem.

II. BI-HAMILTONIAN STRUCTURE

In this section, we will show that Eq. (3) is a bi-Hamiltonian system with an infinite number of conserved charges. From the structure of the equations, it is easy to construct the first few conserved charges of the system which take the forms

$$H_1=\int \mathrm{d}x\, v,$$

$$H_2=\int \mathrm{d}x\, uv, \tag{8}$$

$$H_3=\int \mathrm{d}x \left[\frac{1}{2}u^2v+\frac{1}{2}(\partial^{-1}v)^2\right].$$

From the structure of the conserved charges in (8), we see that Eq. (3) can be written in the Hamiltonian forms as

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \mathcal{D}_1 \begin{pmatrix} \delta H_3/\delta u \\ \delta H_3/\delta v \end{pmatrix} = \mathcal{D}_2 \begin{pmatrix} \delta H_2/\delta u \\ \delta H_2/\delta v \end{pmatrix},$$

where we have defined

$$\mathcal{D}_1 = \begin{pmatrix} 0 & -\partial \\ -\partial & 0 \end{pmatrix}, \quad \mathcal{D}_2 = \begin{pmatrix} \partial^{-1} & -u_x \\ u_x & -(v\,\partial + \partial v) \end{pmatrix}. \tag{9}$$

The skew symmetry of these Hamiltonian structures is manifest. The proof of the Jacobi identity for these structures as well as their compatibility can be shown through the standard method of prolongation[7] which we describe briefly. Introducing the matrix univector

$$\vec{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix},$$

we can construct the two bivectors associated with the two structures $\mathcal{D}_1$ and $\mathcal{D}_2$ as

$$\Theta_{\mathcal{D}_1} = \frac{1}{2}\int dx\,\{\vec{\theta}^{\,T} \wedge \mathcal{D}_1 \vec{\theta}\} = -\int dx\; \theta_1 \wedge \theta_{2x},$$

$$\Theta_{\mathcal{D}_2} = \frac{1}{2}\int dx\,\{\vec{\theta}^{\,T} \wedge \mathcal{D}_2 \vec{\theta}\} = \frac{1}{2}\int dx\,[\,\theta_1 \wedge (\partial^{-1}\theta_1) - 2v\;\theta_2 \wedge \theta_{2x} - 2u_x\,\theta_1 \wedge \theta_2].$$

Using the prolongation relations for any vector field $\tilde{\mathbf{v}}$,

$$\begin{aligned} \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_1\vec{\theta}}(u) &= -\theta_{2x}, \\ \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_1\vec{\theta}}(v) &= -\theta_{1x}, \\ \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_2\vec{\theta}}(u) &= (\partial^{-1}\theta_1) - u_x\,\theta_2, \\ \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_2\vec{\theta}}(v) &= u_x\,\theta_1 - v\;\theta_{2x} - (v\;\theta_2)_x, \end{aligned} \tag{10}$$

it is straightforward to show that the prolongations of the bivectors $\Theta_{\mathcal{D}_1}$ and $\Theta_{\mathcal{D}_2}$ vanish,

$$\mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_2\vec{\theta}}(\Theta_{\mathcal{D}_1}) = \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_2\vec{\theta}}(\Theta_{\mathcal{D}_2}) = 0,$$

implying that $\mathcal{D}_1$ and $\mathcal{D}_2$ satisfy Jacobi identity. Furthermore, using (10), it also follows that

$$\mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_1\vec{\theta}}(\Theta_{\mathcal{D}_2}) + \mathbf{pr}\,\tilde{\mathbf{v}}_{\mathcal{D}_2\vec{\theta}}(\Theta_{\mathcal{D}_1}) = 0.$$

This shows that $\mathcal{D}_1$ and $\mathcal{D}_2$ are compatible, namely, not only are $\mathcal{D}_1$ and $\mathcal{D}_2$ genuine Hamiltonian structures, any arbitrary linear combination of them is as well. As a result, the dynamical equations in (3) correspond to a bi-Hamiltonian system and, consequently, are integrable.[6,7]

It is worth making a few remarks about these Hamiltonian structures. We note that the first Hamiltonian structure is the standard structure that arises in systems of hydrodynamic type (for example, in polytropic gas dynamics[4,5]). It is the second Hamiltonian structure which normally has some interesting connection with Lie algebras. The Lie algebra structure of $\mathcal{D}_2$ is not quite manifest in the form given in (9). However, with a change of basis

$$\tilde{u} = u_x, \quad \tilde{v} = v - \tfrac{1}{2}u_x^2 = v - \tfrac{1}{2}\tilde{u}^2,$$

it follows that the second structure can be written as

$$\tilde{\mathcal{D}}_2=\begin{pmatrix} -\partial & 0 \\ 0 & -(\tilde{v}\partial+\partial\tilde{v}) \end{pmatrix}.$$

We recognize this to be the Lie algebra of $\mathrm{SL}(2)\otimes\mathrm{U}(1)$ without the central charge [for SL(2)]. This is similar to the algebra in the case of the two boson hierarchy where there is a central charge present in the SL(2) algebra.[10] It is also clear from this analysis that we can naturally assign the scaling dimensions $[\tilde{v}]=[v]=2$, $[\tilde{u}]=[u]+1=1$, $[x]=-1$ (with these assignments $[t]=-1$ for nonlocal equations and $[t]=0$ for local ones as will be clear later), which will be useful later in connection with the zero curvature formulation of the system. For completeness, we also note that in this new basis, the first Hamiltonian structure takes the form

$$\tilde{\mathcal{D}}_1=\begin{pmatrix} 0 & -\partial^2 \\ \partial^2 & -(\tilde{u}_x\partial+\partial\tilde{u}_x) \end{pmatrix}.$$

We will, however, continue to use, for simplicity, the variables u,v which are conventional in the study of such systems.

For the bi-Hamiltonian system such as in (3), we can naturally define an associated hierarchy of commuting flows through the relation

$$\begin{pmatrix} u \\ v \end{pmatrix}_t=\mathcal{D}_1\begin{pmatrix} \delta H_{n+1}/\delta u \\ \delta H_{n+1}/\delta v \end{pmatrix}=\mathcal{D}_2\begin{pmatrix} \delta H_n/\delta u \\ \delta H_n/\delta v \end{pmatrix}, \quad n=1,2,\ldots .$$

The gradients of the successive Hamiltonians in the hierarchy can be related through the recursion operator as

$$\begin{pmatrix} \delta H_{n+1}/\delta u \\ \delta H_{n+1}/\delta v \end{pmatrix}=R^{\dagger}\begin{pmatrix} \delta H_n/\delta u \\ \delta H_n/\delta v \end{pmatrix}, \tag{11}$$

where we have defined

$$R=\mathcal{D}_2\mathcal{D}_1^{-1}=\begin{pmatrix} u_x\partial^{-1} & -\partial^{-2} \\ 2v+v_x\partial^{-1} & -u_x\partial^{-1} \end{pmatrix}. \tag{12}$$

It is interesting to note that, in this case, we can invert the recursion operator to write

$$R^{-1}=\begin{pmatrix} -\frac{1}{2}\partial z\partial^{-1}zu_x\partial & \frac{1}{2}\partial z\partial^{-1}z \\ -\partial^2-\frac{1}{2}\partial^2 zu_x\partial^{-1}u_xz\partial & \frac{1}{2}\partial^2u_xz\partial^{-1}z \end{pmatrix}, \tag{13}$$

where we have defined

$$z=(v-\tfrac{1}{2}u_x^2)^{-1/2}.$$

This will be useful later in the construction of the local flows associated with the system. Using Eqs. (11) and (12), we can write the relations for the gradients explicitly as

$$\frac{\delta H_{n+1}}{\delta u}=-\partial^{-1}u_x\frac{\delta H_n}{\delta u}+(2v-\partial^{-1}v_x)\frac{\delta H_n}{\delta v},$$

$$\frac{\delta H_{n+1}}{\delta v}=-\partial^{-2}\frac{\delta H_n}{\delta u}+\partial^{-1}u_x\frac{\delta H_n}{\delta v}, \quad n=1,2,\ldots . \tag{14}$$

These can be explicitly integrated to give the infinite set of (nonlocal) Hamiltonians

$$H_1=\int \mathrm{d}x\, v,$$

$$H_2=\int \mathrm{d}x\, uv,$$

$$H_3=\int \mathrm{d}x\left[\frac{1}{2}u^2v+\frac{1}{2}(\partial^{-1}v)^2\right],$$

$$H_4=\int \mathrm{d}x\left[\frac{1}{6}u^3v-uv\,(\partial^{-2}v)-\frac{1}{2}u\,(\partial^{-1}v)^2\right],$$

$$H_5=\int \mathrm{d}x\left[\frac{1}{24}u^4v+\frac{1}{2}u^2\left(-v\,(\partial^{-2}v)-\frac{1}{2}(\partial^{-1}v)^2\right)-\frac{1}{2}(\partial^{-1}v)^2(\partial^{-2}v)\right.$$
$$\left.+\frac{1}{2}(\partial^{-1}(u_x(\partial^{-1}v)))^2\right],\quad \ldots. \tag{15}$$

The corresponding flows (the first few) have the forms

$$u_{t_1}=-u_x,\quad v_{t_1}=-v_x,$$

$$u_{t_2}=-uu_x+(\partial^{-1}v),\quad v_{t_2}=-(uv)_x, \tag{16}$$

$$u_{t_3}=-\tfrac{1}{2}u^2u_x+u(\partial^{-1}v)+\partial^{-1}(u_{xx}(\partial^{-2}v)),$$

$$v_{t_3}=-uvu_x-\tfrac{1}{2}u^2v_x+2v(\partial^{-1}v)+v_x(\partial^{-2}v),\ldots.$$

We note that, with the dimensionalities of the variables described earlier, all the conserved charges in (15) have the same canonical dimension of 1 and by construction they are all in involution.

To further understand the properties of this hierarchy, let us note that the first Hamiltonian structure in (9) has three Casimirs

$$H_1=\int \mathrm{d}x\, v,$$

$$H_1^{(1)}=-\int \mathrm{d}x\, u_x\to 0,$$

$$H_1^{(2)}=\int \mathrm{d}x\, u,$$

such that

$$\mathcal{D}_1\begin{pmatrix}\delta H_1/\delta u\\ \delta H_1/\delta v\end{pmatrix}=\mathcal{D}_1\begin{pmatrix}\delta H_1^{(1)}/\delta u\\ \delta H_1^{(1)}/\delta v\end{pmatrix}=\mathcal{D}_1\begin{pmatrix}\delta H_1^{(2)}/\delta u\\ \delta H_1^{(2)}/\delta v\end{pmatrix}=0. \tag{17}$$

We remark here that the Casimir $H_1^{(1)}$ is trivial much like in the case of the Hunter–Zheng equation.[11] The existence of Casimirs would normally imply that the series of recursive flows cannot be extended to negative values of n. However, in the present case, it is not very hard to check that the second Hamiltonian structure $\mathcal{D}_2$ also has a Casimir of the form

$$H_{-1}=2\int \mathrm{d}x\left(v-\frac{1}{2}u_x^2\right)^{1/2},$$

such that

$$\mathcal{D}_2\begin{pmatrix}\delta H_{-1}/\delta u\\ \delta H_{-1}/\delta v\end{pmatrix}=0. \tag{18}$$

As a consequence, the hierarchy of flows in (16) can be extended to negative values of n.[8] We note that the Casimir in (18) is conserved under the flows of (16).

For negative values of n, the gradients of the Hamiltonians will satisfy a recursion relation involving R^{-1} given in (13), and take the explicit forms

$$\begin{aligned}\frac{\delta H_n}{\delta v}&=\frac{1}{2}\left(v-\frac{1}{2}u_x^2\right)^{-1/2}\partial^{-1}\left(v-\frac{1}{2}u_x^2\right)^{-1/2}\left(\partial\frac{\delta H_{n+1}}{\delta u}-u_x\partial^2\frac{\delta H_{n+1}}{\delta v}\right),\\ \frac{\delta H_n}{\delta u}&=\frac{1}{2}\partial u_x\left(v-\frac{1}{2}u_x^2\right)^{-1/2}\partial^{-1}\left(v-\frac{1}{2}u_x^2\right)^{-1/2}\left(\partial\frac{\delta H_{n+1}}{\delta u}-u_x\partial^2\frac{\delta H_{n+1}}{\delta v}\right)-\partial^2\frac{\delta H_{n+1}}{\delta v}\\ &=\partial u_x\frac{\delta H_n}{\delta v}-\partial^2\frac{\delta H_{n+1}}{\delta v},\quad n=-2,-3,\ \ldots\quad .\end{aligned} \tag{19}$$

The corresponding conserved charges can now be recursively constructed and have the forms

$$\begin{aligned}H_{-1}&=2\int \mathrm{d}x\left(v-\frac{1}{2}u_x^2\right)^{1/2},\\ H_{-2}&=-\int \mathrm{d}x\,u_{xx}\left(v-\frac{1}{2}u_x^2\right)^{-1/2},\\ H_{-3}&=-\frac{1}{12}\int \mathrm{d}x\,(v_{xx}+2u_{xx}^2-u_xu_{xxx})\left(v-\frac{1}{2}u_x^2\right)^{-3/2},\\ H_{-4}&=-\frac{1}{8}\int \mathrm{d}x\,(v_{xx}u_{xx}-v_xu_{xxx})\left(v-\frac{1}{2}u_x^2\right)^{-5/2},\\ H_{-5}&=-\int \mathrm{d}x\left[\frac{5}{64}\left(u_{xx}^2+\left(v-\frac{1}{2}u_x^2\right)_{xx}\right)^2-\frac{1}{24}\left(\left(v-\frac{1}{2}u_x^2\right)_{xx}\right)^2-\frac{5}{192}(v_x-u_xu_{xx})\left(v-\frac{1}{2}u_x^2\right)_{xxx}\right.\\ &\quad\left.-\frac{1}{8}u_{xx}u_{xxxx}\left(v-\frac{1}{2}u_x^2\right)\right]\left(v-\frac{1}{2}u_x^2\right)^{-7/2},\quad \ldots .\end{aligned} \tag{20}$$

The dynamical equations following from these (the first few) take the forms

$$\begin{aligned}u_{t_{-1}}&=-[(v-\tfrac{1}{2}u_x^2)^{-1/2}]_x,\quad v_{t_{-1}}=-[u_x(v-\tfrac{1}{2}u_x^2)^{-1/2}]_{xx},\\ u_{t_{-2}}&=-\tfrac{1}{2}[u_{xx}(v-\tfrac{1}{2}u_x^2)^{-3/2}]_x,\qquad v_{t_{-2}}=-\tfrac{1}{2}[v_x(v-\tfrac{1}{2}u_x^2)^{-3/2}]_{xx},\quad \ldots .\end{aligned} \tag{21}$$

We note that these flows and the Hamiltonians for negative n are completely local. The Hamiltonians involve increasing number of derivatives of the variables, unlike the conserved charges in the polytropic gas where they are pure polynomials of the dynamical variables. Similarly, the local dynamical equations become increasingly more nonlinearly dispersive as n becomes more nega-

tive. Thus, this hierarchy of equations is very different from the usual polytropic gas systems.[4,5] Nonetheless, all these local charges are in involution (having been constructed from compatible Hamiltonian structures). We note here that, with the dimensionalities for the variables described earlier, all the local charges in (20) have the scaling dimension 0.

The three Casimirs in (17) can be easily checked to be conserved under the flows (21). In fact, we can also construct nonlocal charges from $H_1^{(1)}$ recursively and they take the forms

$$\begin{aligned} H_1^{(1)} &= -\int \mathrm{d}x\, u_x \to 0, \\ H_2^{(1)} &= -\int \mathrm{d}x\, (\partial^{-1} v), \\ H_3^{(1)} &= \int \mathrm{d}x\ \partial^{-1}(u_x(\partial^{-1} v)), \\ H_4^{(1)} &= \int \mathrm{d}x\ \partial^{-1}\left[-\frac{1}{2}(\partial^{-1} v)^2 - u_x\, \partial^{-1}(u_x(\partial^{-1} v))\right], \quad \ldots . \end{aligned} \tag{22}$$

All these charges have the dimensionality 0 and are in involution. [Note that we can obtain $H_2^{(1)}$ from the trivial Casimir $H_1^{(1)}$ using the recursion relation (14) with the prescription $(\partial^{-1} 0) = -1$, for more details see Ref. 8 and references therein.] Similarly, $H_1^{(2)}$ also leads to the following series of nonlocal charges which are related recursively:

$$\begin{aligned} H_1^{(2)} &= \int \mathrm{d}x\, u, \\ H_2^{(2)} &= -\int \mathrm{d}x \left[\frac{1}{2}u^2 + (\partial^{-2} v)\right], \\ H_3^{(2)} &= \int \mathrm{d}x \left[\frac{1}{6}u^3 + \partial^{-2}(u_x(\partial^{-1} v)) + v\,(\partial^{-2} u)\right], \\ H_4^{(2)} &= \int \mathrm{d}x \left[-\frac{1}{24}u^4 - \frac{1}{2}(\partial^{-2} v)^2 - \frac{1}{2}\partial^{-2}(\partial^{-1} v)^2 - \frac{1}{2}v(\partial^{-2} u^2) + v\ \partial^{-1}(u_x(\partial^{-2} u))\right. \\ &\quad \left. - \partial^{-2}(u_x \partial^{-1}(u_x(\partial^{-1} v)))\right], \end{aligned} \tag{23}$$

The scaling dimensions for this set of charges turn out to be -1. They are all conserved under the local flows of (21) and are in involution. The meaning of the three series of nonlocal charges is quite clear from the point of view of the existence of three Casimirs. However, in the next section, we will see within the context of the zero curvature formulation that the three series are related to the fact that the Lie algebra of SL(2) (related to the second Hamiltonian structure of the system) has three generators. We remark here that nonlocal flows can also be derived from the set of charges in (22) and (23), but we do not get into that.

To close this section, we note that a bi-Hamiltonian system of evolution equations,

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = K_n[u,v],$$

is known[13,14] to have a natural Lax description of the form

$$\frac{\partial \mathbb{M}}{\partial t}=[\mathbb{M},\mathbb{B}],$$

where, we can identify

$$\mathbb{M}\equiv R,$$

$$\mathbb{B}\equiv \mathbb{K}_n'.$$

Here $\mathbb{K}_n'$ represents the matrix Fréchet derivative of K_n, defined by

$$\mathbb{K}_n'\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}=\frac{\mathrm{d}}{\mathrm{d}\epsilon}K_n[u+\epsilon w_1, v+\epsilon w_2]\Big|_{\epsilon=0}.$$

In this way, we can obtain a matrix Lax description ($\mathbb{M}$,$\mathbb{B}$ are matrix operators) for the nonlocal as well as the local equations. However, such a Lax description is not very useful since it does not directly lead to conserved charges. Therefore, we do not give details of this and study the zero curvature formulation for this system in the next section.

III. ZERO CURVATURE

To construct the zero curvature for the local as well as the nonlocal equations, let us recall some of the features of our system of equations. We note that the second Hamiltonian structure corresponds to the Lie algebra of $\mathrm{SL}(2)\otimes\mathrm{U}(1)$ so that the zero curvature condition can be based on this algebra. Furthermore, the canonical dimensions of the variables are given by $[u]=0$, $[v]=2$, $[x]=-1$, $[t]=0$ (for local flows). Since the canonical dimension of t is zero, for a zero curvature condition of the form

$$\partial_t \mathbb{A}_1-\partial_x \mathbb{A}_0-[\mathbb{A}_0,\mathbb{A}_1]=0, \tag{24}$$

we note that multiplication with the matrix $\mathbb{A}_0$ must preserve the canonical dimensions of the elements of any matrix and, therefore, will have the unique form

$$\mathbb{A}_0=\begin{pmatrix} [\ ]=0 & [\ ]=-1 \\ [\ ]=1 & [\ ]=0 \end{pmatrix}, \tag{25}$$

where [ ] represents the dimensionality of the matrix element. It follows from (24) that the matrix $\mathbb{A}_1$ will have the form (since $[\partial]=1$)

$$\mathbb{A}_1=\begin{pmatrix} [\ ]=1 & [\ ]=0 \\ [\ ]=2 & [\ ]=1 \end{pmatrix}. \tag{26}$$

Following the procedure in Ref. 10 which describes the general construction of zero curvature based on $\mathrm{SL}(2)\otimes\mathrm{U}(1)$, and recalling the dimensionalities of our matrices in (25) and (26), let us choose

$$\mathbb{A}_0=\begin{pmatrix} -\lambda B_x+\frac{\lambda^2}{2}(-(\partial^{-1}A)+2u_xB) & -B \\ \frac{\lambda^3}{2}(-A+\lambda Bv) & -\frac{\lambda^2}{2}(\partial^{-1}A) \end{pmatrix},$$

$$\mathbb{A}_1=\begin{pmatrix} \lambda u_x & -\dfrac{1}{\lambda} \\ \dfrac{\lambda^3}{2}v & 0 \end{pmatrix}, \tag{27}$$

where λ represents a dimensionless spectral parameter and A,B are arbitrary functions of the dynamical variables as well as the spectral parameter. The zero curvature condition (24), in this case, leads to the dynamical equations

$$u_t=\lambda(-(\partial^{-1}A)+u_xB)-B_x,$$

$$v_t=\lambda(-u_xA+(v\partial+\partial v)B)-A_x. \tag{28}$$

Since the dynamical variables are independent of the spectral parameter, it is clear that the functions A,B must depend on λ for this equation to be meaningful. Let us make a Taylor expansion in λ of the form (recall that for the local flows n is negative)

$$A=\sum_{j=-1}^{-|n|}\lambda^{j+|n|}A_j, \quad B=\sum_{j=-1}^{-|n|}\lambda^{j+|n|}B_j, \tag{29}$$

with

$$A_{-1}=(u_x(v-\tfrac{1}{2}u_x^2)^{-1/2})_x, \quad B_{-1}=(v-\tfrac{1}{2}u_x^2)^{-1/2}. \tag{30}$$

Substituting (29) and (30) into (28), we obtain

$$\begin{gathered}\mathcal{D}_2\begin{pmatrix}A_j\\B_j\end{pmatrix}=\mathcal{D}_1\begin{pmatrix}A_{j+1}\\B_{j+1}\end{pmatrix}, \quad j=-1,-2,\ldots,-|n|+1, \\ \begin{pmatrix}u_t\\v_t\end{pmatrix}=\mathcal{D}_1\begin{pmatrix}A_{n+1}\\B_{n+1}\end{pmatrix}.\end{gathered} \tag{31}$$

It is clear now that if we identify

$$A_j=\frac{\delta H_j}{\delta u}, \quad B_j=\frac{\delta H_j}{\delta v}, \tag{32}$$

then (31) gives the dynamical equations of the hierarchy (for any n), the two Hamiltonian structures of the system as well as the recursion relations between the conserved charges given in (19). The first local flow for $n=-1$, for example, takes the form

$$u_t=-[(v-\tfrac{1}{2}u_x^2)^{-1/2}]_x,$$

$$v_t=-[u_x(v-\tfrac{1}{2}u_x^2)^{-1/2}]_{xx},$$

which coincides with the first flow in (21).

For the nonlocal equations (n positive) let us choose

$$\mathbb{A}_0=\begin{pmatrix} -B_x+\dfrac{1}{2\lambda}(-(\partial^{-1}A)+2u_xB) & -B \\ \dfrac{1}{2\lambda}\left(-A+\dfrac{1}{\lambda}vB\right) & -\dfrac{1}{2\lambda}(\partial^{-1}A) \end{pmatrix},$$

$$\mathbb{A}_1=\begin{pmatrix} \frac{1}{\lambda}u_x & -1 \\ \frac{1}{2\lambda^2}v & 0 \end{pmatrix}.$$

The zero curvature condition (24), in this case, gives

$$u_t=(-(\partial^{-1}A)+u_xB)-\lambda B_x,$$

$$v_t=(-u_xA+(v\partial+\partial v)B)-\lambda A_x.$$

Using a Taylor expansion of the type in (29) (here n is positive), namely,

$$A=\sum_{j=1}^{n}\lambda^{n-j}A_j, \quad B=\sum_{j=1}^{n}\lambda^{n-j}B_j,$$

with

$$A_1=0, \quad B_1=1,$$

we obtain

$$\mathcal{D}_1\begin{pmatrix}A_{j+1}\\ B_{j+1}\end{pmatrix}=\mathcal{D}_2\begin{pmatrix}A_j\\ B_j\end{pmatrix}, \quad j=1,2,\ldots,n-1,$$

$$\begin{pmatrix}u_t\\ v_t\end{pmatrix}=\mathcal{D}_2\begin{pmatrix}A_n\\ B_n\end{pmatrix}.$$

Once again, with the identification in (32), it is easy to see that this leads to the dynamical nonlocal equations of the hierarchy. For $n=1$, for example, it gives the chiral boson equation of (16).

As we have seen, the zero curvature formulation is quite nice in that it not only gives the dynamical equations, but also leads to the two Hamiltonian structures of the system as well as the recursion relation for the conserved charges. It can also give the nonlocal charges (if present) of the system.[15] For example, let us consider the matrix $\mathbb{A}_1$ in (27). Then, it is straightforward to show that as a result of the zero curvature condition (24),

$$Z=P(e^{-\int_{-\infty}^{\infty}dx\,\mathbb{A}_1}),$$

is conserved. Here "P" stands for path ordering of the exponential. This path ordered exponential can be expanded as

$$Z=-\int_{-\infty}^{\infty}dx\,\mathbb{A}_1+\int_{-\infty}^{\infty}dx\,\mathbb{A}_1(\partial^{-1}\mathbb{A}_1)-\int_{-\infty}^{\infty}dx\,\mathbb{A}_1(\partial^{-1}(\mathbb{A}_1(\partial^{-1}\mathbb{A}_1))+\cdots,$$

and each term of the expansion will be individually conserved. (Actually, the coefficient of each independent power of λ would be conserved. However, as we will see below, each term in the expansion leads to different powers of λ for the matrix elements, as a result of which each term in the expansion is individually conserved.) We can work out explicitly the first few terms in the expansion to see that

$$\int_{-\infty}^{\infty} dx\, \mathbb{A}_1 = \begin{pmatrix} \lambda \int_{-\infty}^{\infty} dx\, u_x & -\frac{1}{\lambda}\int_{-\infty}^{\infty} dx \\ \frac{\lambda^3}{2}\int_{-\infty}^{\infty} dx\, v & 0 \end{pmatrix} = \begin{pmatrix} 0 & c \\ \frac{\lambda^3}{2}\int_{-\infty}^{\infty} dx\, v & 0 \end{pmatrix},$$

$$\int_{-\infty}^{\infty} dx\, \mathbb{A}_1(\partial^{-1}\mathbb{A}_1) = \begin{pmatrix} \lambda^2 \int_{-\infty}^{\infty} dx \left(u_x(\partial^{-1}u_x) - \frac{1}{2}\left(\partial^{-1}\left(v - \frac{1}{2}u_x^2\right)\right)\right) & -\int_{-\infty}^{\infty} dx\, u_x(\partial^{-1}1) \\ \frac{\lambda^4}{2}\int_{-\infty}^{\infty} dx\, v(\partial^{-1}u_x) & -\frac{\lambda^2}{2}\int_{-\infty}^{\infty} dx\, v(\partial^{-1}1) \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{\lambda^2}{2}\int_{-\infty}^{\infty} dx(\partial^{-1}v) & \int_{-\infty}^{\infty} dx\, u \\ \frac{\lambda^4}{2}\int_{-\infty}^{\infty} dx\, uv & \frac{\lambda^2}{2}\int_{-\infty}^{\infty} dx\, (\partial^{-1}v) \end{pmatrix},$$

$$\int_{-\infty}^{\infty} dx\, \mathbb{A}_1(\partial^{-1}(\mathbb{A}_1(\partial^{-1}\mathbb{A}_1)))$$

$$= -\int_{-\infty}^{\infty} dx\, (\partial^{-1}\mathbb{A}_1)(\mathbb{A}_1(\partial^{-1}\mathbb{A}_1))$$

$$= -\begin{pmatrix} -\frac{\lambda^3}{2}\int_{-\infty}^{\infty} dx\, \partial^{-1}(u_x(\partial^{-1}v)) & \lambda\int_{-\infty}^{\infty} dx\left[\frac{1}{2}u^2 + (\partial^{-2}v)\right] \\ -\frac{\lambda^5}{2}\int_{-\infty}^{\infty} dx\left[\frac{1}{2}u^2 v + \frac{1}{2}(\partial^{-1}v)^2\right] & \frac{\lambda^3}{2}\int_{-\infty}^{\infty} dx\, \partial^{-1}(u_x(\partial^{-1}v)) \end{pmatrix}.$$

These are indeed the three series of nonlocal charges for our system (up to multiplicative constants). The origin of the three infinite series of charges can be understood in this approach in the following manner. We note that our zero curvature condition is based on the Lie algebra SL(2) $\otimes$U(1) and that the potential $\mathbb{A}_1$ belongs to this algebra. However, the Abelian (U(1)) part of the potential is not subjected to path ordering and, consequently, does not contribute to nonlocal charges. On the other hand, SL(2) has three generators and the charges projected along any of the generators must be conserved. Consequently, the system possesses three infinite series of nonlocal charges.

IV. CONCLUSION

In this paper, we have studied a new system of equations derived from a gas dynamics with the pressure given by a nonlocal function of the density and have shown that the hierarchy of equations is integrable. We have shown that the system possesses two compatible Hamiltonian structures and have constructed an infinite number of (nonlocal) conserved charges recursively. The second Hamiltonian structure of this system corresponds to the centerless SL(2)$\otimes$U(1) algebra. We have shown that the first Hamiltonian structure of the system possesses three nontrivial Casimirs while the second Hamiltonian structure has one. This allows us to extend the nonlocal flows into local ones corresponding to negative flows of the hierarchy. We have constructed an infinite series of commuting local charges associated with the system recursively. This local system of equations possesses three infinite series of nonlocal charges and we have constructed them from the three Casimirs of the first Hamiltonian structure recursively. We have given the zero curvature formulation for the system of local as well as nonlocal equations based on the Lie algebra SL(2)$\otimes$U(1). This brings out naturally the two Hamiltonian structures of the system

as well as the recursion relations between the conserved charges. The zero curvature formulation also leads to the three infinite series of conserved nonlocal charges of the system in a simple manner and relates their existence to the fact that the Lie algebra of SL(2) has three generators.

There are some other interesting features of this system that we would like to discuss briefly. We note that the nonlocal hierarchy of flows associated with the Hunter–Zheng equation can be obtained from (16) when the dynamical variables are constrained as

$$u=(\partial^{-2}w), \quad v=\tfrac{1}{2}(\partial^{-1}w)^2=\tfrac{1}{2}u_x^2. \tag{33}$$

Under this reduction, the three series of nonlocal charges go over to the ones associated with the Hunter–Zheng equation. However, under this reduction, the local flows of the hierarchy become trivial and do not go over to the Harry Dym equation.

Another interesting issue that remains open is the construction of a scalar Lax representation for the system of local equations. (We do not expect to find a scalar Lax representation for the nonlocal flows.) It is well known that given the zero curvature formulation of a system, one can easily go over to a scalar Lax description and vice versa.[16,17] In this case, however, in spite of the fact that we have a zero curvature formulation, we have not been able to find a scalar Lax description for this system. We have discussed the standard matrix Lax description, but finding a scalar Lax operator remains an open question that deserves further study.

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Deformed Harry Dym and Hunter–Zheng equations

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We study the deformed Harry Dym and Hunter–Zheng equations with two arbitrary deformation parameters. These reduce to various other known models in appropriate limits. We show that both these systems are bi-Hamiltonian with the same Hamiltonian structures. They are integrable and belong to the same hierarchy corresponding to positive and negative flows. We present the Lax pair description for both the systems and construct the conserved charges of negative order from the Lax operator. For the deformed Harry Dym equation, we construct the nonstandard Lax representation for two special classes of values of the deformation parameters. In general, we argue that a nonstandard description will involve a pseudodifferential operator of infinite order. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The search for exactly solvable equations has acquired enormous importance since the nonlinear Kortweg–de Vries equation was shown to be integrable.[1,2] Exactly solvable equations, linear or nonlinear, constitute a very special class of dynamical systems with many interesting properties. The significance of determining new integrable systems, as well as studying their properties and solutions, can not be overestimated. The structure of integrable systems (or partial differential equations) is highly restrictive and, in general does not allow for deformations. In particular, the presence of arbitrary constant parameters (which cannot be transformed away by some symmetry) is quite rare. One notable exception is the two boson equation,[3] which has an arbitrary constant parameter present, is known to be integrable. Different values of this parameter reduce the model to other known soluble models. In this paper, we propose a new system of equations, with two arbitrary constant parameters, that is exactly soluble and reduces to various other known physical models in different limits of these parameters.

Let us recall that the Harry Dym (HD) equation,[4,5]

$$u_t = (u_{xx}^{-1/2})_x, \tag{1}$$

and the Hunter–Zheng (HZ) equation,[6]

$$(u_t + u u_x)_x = \tfrac{1}{2} u_x^2, \tag{2}$$

are known to be integrable and, in fact, belong to the same hierarchy corresponding to negative and positive order flows, respectively.[7] The HD equation has interest in the study of the Saffman–Taylor problem which describes the motion of a two-dimensional interface between a viscous and

a nonviscous fluid.[8] The HZ equation, on the other hand, arises in the study of massive nematic liquid crystals and in the study of shallow water waves.[6] In this paper we will show that the following system of two equations,

$$u_t=\sqrt{2}\left(\frac{1-\lambda u_{xx}}{\sqrt{2u_{xx}-\alpha-\lambda u_{xx}^2}}\right)_x \tag{3}$$

and

$$u_{xxt}=\alpha u_x-2u_xu_{xx}-uu_{xxx}+\frac{\lambda}{6}(u_x^3)_{xx}, \tag{4}$$

are integrable for arbitrary values of the constant parameters α,λ. Furthermore, they belong to the same hierarchy corresponding to the negative and positive flows respectively, much like the HD and the HZ equations. It is interesting to note from (4) that when $\alpha\neq 0$, it can be scaled to unity through the scaling $x\to x/\alpha$, $u\to u/\alpha$. Therefore, looking at (4) alone, it would appear that there are only two meaningful values for α, namely, $\alpha=0,1$. Similarly, under a scaling $t\to t/\alpha^{3/2}$, $x\to x/\alpha$, $u\to u/\alpha$, the parameter α in the dHD equation (3) can be scaled to unity when it is not zero. However, there is no scaling which will scale α to unity (when it is nonzero) simultaneously in both the equations and, consequently, if the two systems belong to the same hierarchy, α has to be thought of as an arbitrary parameter.

We note that, for $\alpha=\lambda=0$, Eqs. (3) and (4) reduce, respectively, to the HD equation (1) and the HZ equation (2). For lack of a better name, we will refer to (3) as the deformed Harry Dym equation (dHD) and (4) as the deformed Hunter–Zheng equation (dHZ). (The name ''generalized Harry Dym'' equation has already been used earlier in the context of a multicomponent Harry Dym equation.[9]) For $\alpha\neq 0$ and $\lambda=0$ equation (4) was studied by Alber *et al.*[10] and its solutions contain solitons of the type known as umbilic solitons. Equation (4) with $\alpha=1$ and $\lambda\neq 0$ has appeared more recently in the literature[11] as describing short capillary-gravity waves and its solutions are known to become multivalued in a finite amount of time. While a matrix Lax pair for this system was provided in Ref. 11 and solubility of the model was argued based on a map to the sine-Gordon equation, interesting properties, such as the bi-Hamiltonian structure, the infinite number of conserved charges were not discussed at all. Our results clarify these aspects and provide direct support for the integrability of this new system. The deformed equation (3) for arbitrary α and $\lambda\neq 0$ is truly a new integrable system (which to the best of our knowledge has not been studied in the literature) and leads to the above mentioned models in different limits. This can, therefore, be considered as a very rich system, much like the two boson hierarchy.

Our paper is organized as follows: In Sec. II, we obtain the first Hamiltonian structure of the dHD and dHZ equations. In Sec. III, a second Hamiltonian structure, compatible with the first one, is obtained. We show that both the dHD and dHZ equations are bi-Hamiltonian and, therefore, integrable and belong to the same hierarchy corresponding to negative and positive flows. In Sec. IV, we present a Lax pair description of both the system of equations and construct the conserved charges of negative order from the Lax operator. We obtain a nonstandard Lax description for the dHD equation for the special values of the deformation parameters $\lambda=0,\lambda=-3/\alpha$. We argue that, for general values of the parameters, a nonstandard Lax description will involve a pseudodifferential operator of infinite order. In Sec. V we present our conclusions.

II. dHZ AND dHD AS HAMILTONIAN SYSTEMS

To describe the dHD and the dHZ equations in a compact manner, let us introduce the following notation. Let us define

$$F_{(\alpha,\lambda)}^2\equiv 2u_{xx}-\alpha-\lambda u_{xx}^2,\quad A\equiv\frac{1-\lambda u_{xx}}{F}. \tag{5}$$

Then, it follows from the definitions in (5) that

$$\kappa \equiv (1-\alpha\lambda) = \lambda F^2 + (1-\lambda u_{xx})^2 = (\lambda + A^2)F^2,$$

$$\frac{F_x}{F^3} = -\frac{1}{\kappa} A A_x, \tag{6}$$

$$\frac{u_{xxx}}{F^3} = -\frac{1}{\kappa} A_x.$$

These and other relations following from these prove very useful in the analysis of the two systems.

Given the dHZ equation (4), we obtain from the definition in (5) that

$$F_t = -\left[F\left(u - \frac{\lambda}{2} u_x^2 \right) \right]_x. \tag{7}$$

Similarly, in terms of the new variables in (5), the dHD equation (3) can be written as

$$u_t = \sqrt{2}\, A_x, \tag{8}$$

and it follows that, under the evolution of dHD,

$$\begin{aligned} F_t &= \sqrt{2}\, A\, A_{xxx}, \\ A_t &= -\sqrt{2}\, \kappa \frac{A_{xxx}}{F^3}. \end{aligned} \tag{9}$$

It is now straightforward to note from Eqs. (7) and (9) that

$$H_{-1} = \sqrt{2} \int dx\, F \tag{10}$$

is conserved under both the dHD and dHZ flows.

The dHZ equation can be obtained from a variational principle, $\delta \int dt dx\, \mathcal{L}$, with the Lagrangian density

$$\mathcal{L} = \frac{1}{2} u_x u_t + \frac{\alpha}{2} u^2 + \frac{1}{2} u u_x^2 - \frac{\lambda}{24} u_x^4. \tag{11}$$

This is a first order Lagrangian density and, consequently, the Hamiltonian structure can be readily read out, or we can use, for example, Dirac's theory of constraints[12] to obtain the Hamiltonian and the Hamiltonian operator associated with (11). The Lagrangian is degenerate and the primary constraint is obtained to be

$$\Phi = \pi - \tfrac{1}{2} u_x, \tag{12}$$

where $\pi = \partial \mathcal{L} / \partial u_t$ is the canonical momentum. The total Hamiltonian can be written as

$$H_T = \int dx (\pi u_t - \mathcal{L} + \beta \Phi) = \int dx \left[-\frac{\alpha}{2} u^2 - \frac{1}{2} u u_x^2 + \frac{\lambda}{24} u_x^4 + \beta \left(\pi - \frac{1}{2} u_x \right) \right], \tag{13}$$

where β is a Lagrange multiplier field. Using the canonical Poisson bracket relation

$$\{ u(x), \pi(y) \} = \delta(x-y), \tag{14}$$

with all others vanishing, it follows that the requirement of the primary constraint to be stationary under time evolution,

$$\{\Phi(x),H_T\}=0,$$

determines the Lagrange multiplier field β in (13) and the system has no further constraints.

Using the canonical Poisson bracket relations (14), we can now calculate

$$K(x,y)\equiv\{\Phi(x),\Phi(y)\}=\tfrac{1}{2}\partial_y\delta(x-y)-\tfrac{1}{2}\partial_x\delta(x-y). \tag{15}$$

This shows that the constraint (12) is second class and that the Dirac bracket between the basic variables has the form

$$\{u(x),u(y)\}_D=\{u(x),u(y)\}-\int dz\,dz'\{u(x),\Phi(z)\}J(z,z')\{\Phi(z'),u(y)\}=J(x,y),$$

where J is the inverse of the Poisson bracket of the constraint (15),

$$\int dz\,K(x,z)J(z,y)=\delta(x-y)\,.$$

This last relation determines

$$\partial_x J(x,y)=\delta(x-y),$$

or

$$J(x,y)=\mathcal{D}_1\delta(x-y),$$

where

$$\mathcal{D}_1=\partial^{-1}, \tag{16}$$

and can be thought of as the alternating step function in the coordinate space. We can now set the constraint (12) strongly to zero in (13) to obtain

$$H_2\equiv -H_T=\int dx\left(\frac{\alpha}{2}u^2+\frac{1}{2}uu_x^2-\frac{\lambda}{24}u_x^4\right). \tag{17}$$

Therefore, the dHZ equation can be written in the Hamiltonian form

$$u_t=\mathcal{D}_1\frac{\delta H_2}{\delta u},$$

with $\mathcal{D}_1$ and H_2 given by (16) and (17), respectively.

From the results in Ref. 7 we know that the HD and HZ equations belong to the same hierarchy of equations. Here, too, we will see that both the dHD and the dHZ equations belong to the same hierarchy. In particular, we note that

$$u_t=\mathcal{D}_1\frac{\delta H_{-1}}{\delta u},$$

with H_{-1}, given by (10), yields the deformed Harry Dym equation (8). As a result, the dHD equation also is Hamiltonian with the same Hamiltonian structure of the dHZ equation in (16) and, consequently, has a Lagrangian description given by

$$\mathcal{L}=\tfrac{1}{2}u_x u_t-\sqrt{2}\,F.$$

The reader can easily check that H_2 is also conserved by both the dHD and dHZ equations, much like H_{-1}. Note that for $\alpha=\lambda=0$, these two charges reduce to the corresponding ones in the HD and HZ systems.

III. dHD AND dHZ AS BI-HAMILTONIAN SYSTEMS

It is well known that a system can be shown to be integrable if it is bi-Hamiltonian.[13,14] This corresponds to the system having a Hamiltonian description with two distinct Hamiltonian structures that are compatible. Therefore, we try to see if the dHD and the dHZ equations can be described as bi-Hamiltonian systems. For this, we have to find a second Hamiltonian description for the two systems.

In order to determine a second Hamiltonian structure for the two systems, we recall[7] that, when $\alpha=\lambda=0$, the corresponding H_{-1} is a Casimir of the second Hamiltonian structure for the HD and HZ systems, namely,

$$\mathcal{D}_2^{(\alpha=\lambda=0)}=\partial^{-2}u_{xx}\,\partial^{-1}+\partial^{-1}u_{xx}\,\partial^{-2} \tag{18}$$

satisfies

$$\mathcal{D}_2^{(\alpha=\lambda=0)}\frac{\delta H_{-1}^{(\alpha=\lambda=0)}}{\delta u}=0.$$

Since we know H_{-1} for the deformed systems which is a generalization of $H_{-1}^{(\alpha=\lambda=0)}$, we look for a Hamiltonian structure for which it is a Casimir. With some work, it can be determined that H_{-1} given in (10) is a Casimir of

$$\mathcal{D}_2\equiv\mathcal{D}_2^{(\alpha,\lambda)}=\tfrac{1}{2}(\partial^{-2}F^2\,\partial^{-1}+\partial^{-1}F^2\,\partial^{-2})+\lambda\,\partial^{-2}u_{xxx}\,\partial^{-1}u_{xxx}\partial^{-2}. \tag{19}$$

Note that this structure reduces to (18) when $\alpha=\lambda=0$. The skew symmetry of this Hamiltonian structure is manifest. The proof of the Jacobi identity for this structure as well as its compatibility with $\mathcal{D}_1$ in (16) can be determined through the standard method of prolongation described in Ref. 14, which we discuss briefly.

Performing the change of variables

$$w=u_{xx},$$

the Hamiltonian structures (16) and (19) assume the forms

$$\mathcal{D}_1=\partial^3,$$

$$\mathcal{D}_2=\tfrac{1}{2}(F^2\partial+\partial F^2)+\lambda w_x\,\partial^{-1}w_x.$$

We can construct the two bivectors associated with the two structures as

$$\Theta_{\mathcal{D}_1}=\frac{1}{2}\int dx\,\{\theta\wedge\mathcal{D}_1\theta\}=\frac{1}{2}\int dx\;\theta\wedge\theta_{xxx},$$

$$\Theta_{\mathcal{D}_2}=\frac{1}{2}\int dx\,\{\theta\wedge\mathcal{D}_2\theta\}=\frac{1}{2}\int dx\,\{-\alpha\;\theta\wedge\theta_x+2w\;\theta\wedge\theta_x-\lambda\;w^2\theta\wedge\theta_x+\lambda\;w_x\;\theta\wedge(\partial^{-1}w_x\;\theta)\}.$$

Using the prolongation relations,

$$\begin{aligned}
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(w)=\theta_{xxx},\\
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(w^2)=2w\,\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(w),\\
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(w_x)=(\,\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(w))_x,\\
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(w)=-\alpha\,\theta_x+2w\,\theta_x-\lambda\,w^2\theta_x+w_x\,\theta-\lambda\,ww_x\,\theta+\lambda w_x(\partial^{-1}w_x\,\theta),\\
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(w^2)=2w\;\,\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(w),\\
&\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(w_x)=(\,\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(w))_x,
\end{aligned}\tag{20}$$

it is straightforward to show that the prolongation of the bivector $\Theta_{\mathcal{D}_2}$ vanishes,

$$\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(\Theta_{\mathcal{D}_2})=0,$$

implying that $\mathcal{D}_2$ satisfies Jacobi identity. Using (20), it also follows that

$$\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_1\theta}(\Theta_{\mathcal{D}_2})+\mathbf{pr}\,\mathbf{v}_{\mathcal{D}_2\theta}(\Theta_{\mathcal{D}_1})=0,$$

showing that $\mathcal{D}_1$ and $\mathcal{D}_2$ are compatible. Namely, not only are $\mathcal{D}_1,\mathcal{D}_2$ genuine Hamiltonian structures, any arbitrary linear combination of them is as well. Any physical system that is Hamiltonian with respect to these two structures, therefore, defines a pencil system and is integrable. It is worth pointing out here that when $\alpha=\lambda=0$, the second Hamiltonian structure (18) represents the centerless Virasoro algebra[15] (with dimension zero operators). The structure in (19) appears to be a highly nonlocal generalization of this algebra, but we are not familiar with any study of such an algebra in the literature.

To show that the dHD and dHZ are bi-Hamiltonian systems, we note that the charges

$$H_1=\int dx\,u_x^2, \tag{21}$$

$$H_{-2}=\frac{1}{2\kappa}\int dx\,FA_x^2 \tag{22}$$

are also conserved by both the dHZ and dHD equations. While the charge in (21) is the unmodified charge of the HD and HZ systems (this seems to be a simple coincidence), the charge in (22) is a true generalization of the corresponding charge of the HD and HZ systems. With these charges, it is easy to see that the dHZ equation can be written in a truly bi-Hamiltonian form

$$u_t=\mathcal{D}_1\frac{\delta H_2}{\delta u}=\mathcal{D}_2\frac{\delta H_1}{\delta u}.$$

Similarly, the dHD equation can also be written in the bi-Hamiltonian form

$$u_t=\mathcal{D}_1\frac{\delta H_{-1}}{\delta u}=\mathcal{D}_2\frac{\delta H_{-2}}{\delta u}.$$

Thus, we see that both the dHD as well as dHZ systems are bi-Hamiltonian with the same two compatible Hamiltonian structures and are, therefore, integrable.

IV. THE LAX REPRESENTATION

When a system is bi-Hamiltonian, we can naturally define a hierarchy of commuting flows through the relation

$$u_t = K_n[u] = \mathcal{D}_1 \frac{\delta H_{n+1}}{\delta u} = \mathcal{D}_2 \frac{\delta H_n}{\delta u}, \quad n = 0,1,2,\ldots . \tag{23}$$

In the present case, both the Hamiltonian structures have Casimirs. We have already seen that H_{-1} is a Casimir of $\mathcal{D}_2$ and it can be checked that the trivial Hamiltonian

$$H_0 = \int dx\, u_{xx} \tag{24}$$

formally defines the Casimir of $\mathcal{D}_1$ (namely, if we write formally $\delta H_0 / \delta u = \partial^2$, it is annihilated by $\mathcal{D}_1$). As a result, the system of flows can be extended to both positive and negative integer values for n. In this way, we see that much like in the HD and HZ systems,[7] the dHD and dHZ systems also belong to the same hierarchy corresponding to the negative and positive flows.

Let us introduce the recursion operator following from the two Hamiltonian structures as

$$R = \mathcal{D}_2 \mathcal{D}_1^{-1}.$$

Then, it follows from (23) that

$$K_{n+1} = R\, K_n,$$

and

$$\frac{\delta H_{n+1}}{\delta u} = R^{\dagger} \frac{\delta H_n}{\delta u}, \tag{25}$$

where

$$R^{\dagger} = \partial^{-1} u_{xx}\, \partial^{-1} + (-\alpha + u_{xx})\, \partial^{-2} - \lambda\, u_{xx}\, \partial^{-1} u_{xx}\, \partial^{-1} \tag{26}$$

is the adjoint of R. The conserved charges for the hierarchy can, of course, be determined in principle recursively from (25). However, in practice, integrating the recursion relation is highly nontrivial. Therefore, we look for a Lax representation for the system of dHD and dHZ equations which will allow us to construct the conserved charges directly.

It is well known[16,17] that for a bi-Hamiltonian system of evolution equations, $u_t = K_n[u]$, a natural Lax description

$$\frac{\partial M}{\partial t} = [M, B],$$

is easily obtained where, we can identify

$$M \equiv R^{\dagger},$$

$$B \equiv K_n'.$$

Here K_n' represents the Fréchet derivative of K_n, defined by

$$K_n'[u]\, v = \frac{d}{d\epsilon} K_n[u + \epsilon v]\bigg|_{\epsilon = 0}.$$

For the dHD and dHZ system of equations in (3) and (4), respectively, we have

$$B^{\mathrm{dHD}} \equiv K_{-2} = \sqrt{2}\, \kappa\, \partial^2 F^{-3} \partial,$$

$$B^{\mathrm{dHZ}} \equiv K_1 = (-\alpha + u_{xx})\,\partial^{-1} + \partial\left(u - \frac{\lambda}{2}u_x^2\right).$$

The two systems have the same $M = R^{\dagger}$ given in (26). It can now be checked that

$$\frac{\partial M}{\partial t} = [M, B^{\mathrm{dHD}}],$$

$$\frac{\partial M}{\partial t} = [M, B^{\mathrm{dHZ}}], \tag{27}$$

do indeed generate the dHD and the dHZ equations and, thereby, provide a Lax pair for the system.

One of the advantages of a Lax representation is that they directly give the conserved charges of the system. From the structure of (27), it follows that $\mathrm{Tr}\, M^{(2n+1)/2}$ are conserved, where "Tr" represents Adler's trace.[18] We note that

$$\mathrm{Tr}\, M^{(2n+1)/2} = 0, \quad n \geqslant 1,$$

$$\mathrm{Tr}\, M^{1/2} = \int dx\, F,$$

$$\mathrm{Tr}\, M^{-(1/2)} = -\frac{1}{2\kappa}\int dx\, F A_x^2, \tag{28}$$

$$\mathrm{Tr}\, M^{-(3/2)} = \frac{3}{\kappa}\int dx \left(4\frac{A_{xx}^2}{F} + \frac{1}{\kappa}F A_x^4\right),$$

$$\vdots.$$

The first two nontrivial charges correspond respectively to H_{-1}, H_{-2} given in Eqs. (10) and (22), constructed earlier by brute force. In fact, all H_{-n-1} with positive $n \geqslant 0$ can be constructed from $\mathrm{Tr}\, M^{-[(2n-1)/2]}$ and by construction (namely, because of the nature of (27)), they are conserved under both the dHD and dHZ flows. Unfortunately, as is clear from (28), this procedure does not yield the charges H_n with positive integer values. These are, in general, nonlocal and even in the HD and HZ case, construction of these charges relies primarily on the recursion relation (25). It remains an interesting question to construct these charges in a more direct manner.

The Harry Dym equation has a Gelfand–Dikii representation for the Lax pair, while the HZ equation does not. We will now discuss the existence of such a Lax representation for the dHD equation. A spectral problem associated with the dHD equations can be obtained from the recursion relation (25) (see Ref. 19, and references therein) as follows. Introducing a spectral parameter μ and defining

$$\psi^2(x,t,\mu) = \sum_{n=0}^{\infty} \mu^n \frac{\delta H_n}{\delta u},$$

we note that the recursion relation (25) can be written compactly as (recall that H_0 is a Casimir of $\mathcal{D}_1$)

$$(\mathcal{D}_1 - \mu\mathcal{D}_2)\,\psi^2 = 0,$$

or

$$(1-\mu R^{\dagger})\,\psi^2=0, \tag{29}$$

which defines an eigenvalue problem for the eigenfunction ψ^2 with eigenvalue $1/\mu$. A linear eigenvalue problem can be derived from this if we can factorize the operator $(1-\mu R^{\dagger})$.

Let us note that the operator $R^{\dagger}$ in (26) can be rewritten in the form

$$R^{\dagger}=\tfrac{1}{2}[\partial^{-1}(F^2_{(\alpha,\lambda)}+X)\partial^{-1}+(F^2_{(\alpha,\lambda)}+X)\partial^{-2}], \tag{30}$$

where

$$X=\sum_{n=1} X_n\partial^{-n},$$

and the coefficients X_n can be determined recursively to be

$$X_1=0,$$

$$X_2=\frac{\lambda}{4}u^2_{xxx},$$

$$X_3=-\tfrac{1}{2}X_{2,x},$$

$$\vdots.$$

When $\lambda=0$, it follows that $X=0$ and that $F^2_{(\alpha,\lambda=0)}$ is a simple function. In this case, the eigenvalue problem (29) can be factorized as

$$(1-R^{\dagger})\,\psi^2=2\,\partial^{-1}\phi^{-2}\,\partial\,\phi^3\left(\partial^2-\frac{\mu}{4}F^2_{(\alpha,\lambda=0)}\right)\phi=0,$$

where we have identified

$$\phi^2=(\partial^{-2}\psi^2).$$

This shows that if the linear equation

$$\left(\partial^2-\frac{\mu}{4}F^2_{(\alpha,\lambda=0)}\right)\phi=0$$

is satisfied, then (29) will hold and this identifies the Lax operator for the system to be

$$L=\frac{1}{F^2_{(\alpha,\lambda=0)}}\,\partial^2.$$

In fact, it can be readily checked that when $\lambda=0$, the hierarchy of dHD equations can be obtained from the non-standard Lax equation

$$\frac{\partial L}{\partial t_n}=4\sqrt{2}[L,(L^{(2n-1)/2})_{\geqslant 2}].$$

The conserved quantities for this system can be obtained from $\mathrm{Tr}\,L^{(2n-1)/2}$, $n=0,1,2,\ldots$.

On the other hand, when $\lambda\neq 0$, the coefficients X_n are nontrivial and X represents a pseudo-differential operator. The factorization, in such a case, is not so simple and, in principle would involve an infinite series of terms. For arbitrary values of κ, the terms in the series can possibly be determined recursively. However, this is not very interesting. We simply note here that for the

special value $\kappa=4$, the infinite series of terms seems to have a simpler compact form and the Lax operator, in such a case, has the form

$$L_{\kappa=4}=\frac{1}{F}\partial\frac{1}{F}\partial-\frac{1}{4}A_x\partial^{-1}A_x\partial,$$

and, in this case, the hierarchy of dHD equations can be obtained from the nonstandard Lax representation

$$\frac{\partial L_{\kappa=4}}{\partial t_n}=4\sqrt{2}[L_{\kappa=4},(L_{\kappa=4}^{(2n-1)/2})_{\geqslant 2}].$$

The conserved quantities, in this case, also follow from $\mathrm{Tr}\,L_{\kappa=4}^{(2n-1)/2}$ and up to multiplicative factors, they have the forms given in (28) with $\kappa=4$. A simple Lax description for arbitrary λ, however, remains an open question.

V. CONCLUSION

In this paper, we have studied the general system of dHD and dHZ equations. We have shown that both these systems are bi-Hamiltonian and, therefore, integrable and belong to the same hierarchy corresponding to negative and positive flows. The Lax pair for the two system of equations have been derived and conserved charges corresponding to negative integer values follow from the Lax operator. A simple construction of the charges for positive integer values remains an open question. For $\lambda=0$, we have constructed a nonstandard Lax representation for the dHD equation, which involves a purely differential Lax operator. For arbitrary values of λ, we have argued that a nonstandard Lax representation will necessarily involve a Lax operator which is a pseudodifferential operator of infinite order. For the particular case of $\kappa=4$, however, this takes a simpler compact form.

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Expansion around half-integer values, binomial sums, and inverse binomial sums

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I consider the expansion of transcendental functions in a small parameter around rational numbers. This includes in particular the expansion around half-integer values. I present algorithms which are suitable for an implementation within a symbolic computer algebra system. The method is an extension of the technique of nested sums. The algorithms allow in addition the evaluation of binomial sums, inverse binomial sums and generalizations thereof. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1758319]

I. INTRODUCTION

The expansion of higher transcendental functions[1,2] occurs frequently in many areas of science. In particular, one encounters these functions in the calculation of higher order corrections to scattering processes in particle physics. In a previous publication we considered the expansion of transcendental functions in a small parameter around integer values.[3,4] The restriction to integer values is in general sufficient for the evaluation of loop integrals arising in massless quantum field theories. However, the inclusion of particle masses in loop integrals[5–13] or the evaluation of phase space integrals[14–20] can lead to half-integer values. It is therefore desirable to extend the algorithm of Refs. 3, 4 to include at least half-integer values. Here I report on algorithms for the expansion of transcendental functions around rational number p/q, where p and q are integers. In particular this includes the half-integer case.

Each term in the expansion is expressed through multiple polylogarithms.[21,22] Compared to the pure integer case, the extension to rational numbers p/q introduces naturally the qth roots of unity in the arguments of the polylogarithms. All algorithms are based on manipulations of a special form of nested sums. These nested sums are generalizations of Euler–Zagier sums[23,24] or harmonic sums.[25–29] The algorithms presented here can be implemented into a symbolic computer algebra system like Form[27,30] or GiNaC.[31]

As a spin-off, the methods presented here allow the evaluation of binomial sums,[5,6] inverse binomial sums[5,7–9,32,33] and generalizations thereof. Inverse binomial sums are sometimes evaluated with the help of log-sine integrals.[10,11] In the Appendix, I compare the log-sine approach with the one presented here.

This paper is organized as follows: Sec. II recalls the definition and main properties of nested sums and multiple polylogarithms. It is a brief summary of Ref. 3. Section III introduces roots of unity and gives the basic algorithms for the expansion around rational numbers. Section IV treats binomial sums and generalizations thereof. Section V deals with inverse binomial sums and generalizations thereof. Section VI gives some simple applications to massive loop integrals and phase space integrals. Finally, Section VII contains a summary and the conclusions. The Appendix compares this approach to log-sine integrals and collects some important relations for polylogarithms of low weight.

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II. A SUMMARY OF KNOWN PROPERTIES OF NESTED SUMS

In this section I shortly review properties of particular forms of nested sums, which are called Z-sums and S-sums. Details can be found in Ref. 3. Z-sums are defined by

$$Z(n;m_1,\ldots,m_k;x_1,\ldots,x_k)=\sum_{n\geqslant i_1>i_2>\cdots>i_k>0}\frac{x_1^{i_1}}{i_1^{m_1}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}} \tag{1}$$

and form a Hopf algebra. If the sums go to infinity ($n=\infty$) the Z-sums are identical to multiple polylogarithms (note that we use here the reversed notation for multiple polylogs and multiple zeta values as compared to Refs. 3, 21):[21]

$$Z(\infty;m_1,\ldots,m_k;x_1,\ldots,x_k)=\mathrm{Li}_{m_1,\ldots,m_k}(x_1,\ldots,x_k). \tag{2}$$

For $x_1=\cdots=x_k=1$ the definition reduces to the Euler–Zagier sums:[23,24]

$$Z(n;m_1,\ldots,m_k;1,\ldots,1)=Z_{m_1,\ldots,m_k}(n). \tag{3}$$

For $n=\infty$ and $x_1=\cdots=x_k=1$ the sum is a multiple ζ-value:[22]

$$Z(\infty;m_1,\ldots,m_k;1,\ldots,1)=\zeta_{m_1,\ldots,m_k}. \tag{4}$$

The multiple polylogarithms contain as the notation already suggests as subsets the classical polylogarithms $\mathrm{Li}_n(x)$,[34] as well as Nielsen's generalized polylogarithms[35]

$$S_{n,p}(x)=\mathrm{Li}_{n+1,1,\ldots,1}(x,\underbrace{1,\ldots,1}_{p-1}), \tag{5}$$

the harmonic polylogarithms[36]

$$H_{m_1,\ldots,m_k}(x)=\mathrm{Li}_{m_1,\ldots,m_k}(x,\underbrace{1,\ldots,1}_{k-1}) \tag{6}$$

and two-dimensional harmonic polylogarithms.[37] The usefulness of the Z-sums lies in the fact, that they interpolate between multiple polylogarithms and Euler–Zagier sums. In addition, the interpolation is compatible with the algebra structure.

In addition to Z-sums, it is sometimes useful to introduce as well S-sums. S-sums are defined by

$$S(n;m_1,\ldots,m_k;x_1,\ldots,x_k)=\sum_{n\geqslant i_1\geqslant i_2\geqslant\cdots\geqslant i_k\geqslant 1}\frac{x_1^{i_1}}{i_1^{m_1}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}} \tag{7}$$

and form an algebra. The S-sums reduce for $x_1=\cdots=x_k=1$ (and positive m_i) to harmonic sums:[27]

$$S(n;m_1,\ldots,m_k;1,\ldots,1)=S_{m_1,\ldots,m_k}(n). \tag{8}$$

The S-sums are closely related to the Z-sums, the difference being the upper summation boundary for the nested sums: $(i-1)$ for Z-sums, i for S-sums. It is advantageous to introduce both Z-sums and S-sums, since some properties are more naturally expressed in terms of Z-sums while others are more naturally expressed in terms of S-sums. One can easily convert from one notation to the other.

Basic manipulations involving nested sums are:
Conversion:

$$Z(n;\ldots)\to S(n;\ldots),$$

$$S(n;\ldots)\to Z(n;\ldots). \tag{9}$$

Multiplication:

$$\begin{aligned} Z(n;\ldots)Z(n;\ldots)&\to Z(n;\ldots),\\ S(n;\ldots)S(n;\ldots)&\to S(n;\ldots). \end{aligned} \tag{10}$$

Convolution:

$$\sum_{i=1}^{n-1} \frac{x^i}{i^m} Z(i-1;\ldots) \frac{y^{n-i}}{(n-i)^{m'}} Z(n-i-1;\ldots)\to Z(n-1;\ldots). \tag{11}$$

Conjugation:

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i;\ldots)\to S(n;\ldots). \tag{12}$$

Conjugation and convolution:

$$-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i;\ldots) \frac{y^{n-i}}{(n-i)^{m'}} S(n-i;\ldots)\to S(n-1;\ldots). \tag{13}$$

These algorithms are described in Ref. 3. It is worth to recall some technical steps to evaluate the conjugation in Eq. (12), since the same pattern of steps will be used in Sec. IV. To evaluate the conjugation it is convenient to introduce yet another type of sum as follows:

$$B(n;N;m_1,\ldots,m_k;x_1,\ldots,x_k)=\sum_{i_1=n+1}^{N} \sum_{i_2=i_1+1}^{N} \cdots \sum_{i_k=i_{k-1}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}} \frac{x_2^{i_2}}{i_2^{m_2}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}. \tag{14}$$

These B-sums can be used to express S-sums with upper summation limit n in terms of S-sums with upper summation limit N:

$$\begin{aligned} S(n;m_1,\ldots,m_k;x_1,\ldots,x_k)=&S(N;m_1,\ldots,m_k;x_1,\ldots,x_k)\\ &-S(N;m_2,\ldots,m_k;x_2,\ldots,x_k)B(n;N;m_1;x_1)\\ &+S(N;m_3,\ldots,m_k;x_3,\ldots,x_k)B(n;N;m_1,m_2;x_1,x_2)\\ &-\cdots+(-1)^k B(n;N;m_1,\ldots,m_k;x_1,\ldots,x_k). \end{aligned} \tag{15}$$

Equation (15) also allows us to express a B-sum recursively in terms of S-sums $S(N;\ldots)$ and $S(n;\ldots)$:

$$\begin{aligned} B(n;N;m_1,\ldots,m_k;x_1,\ldots,x_k)=&(-1)^k S(n;m_1,\ldots m_k;x_1,\ldots,x_k)\\ &-(-1)^k S(N;m_1,\ldots m_k;x_1,\ldots,x_k)\\ &+(-1)^k S(N;m_2,\ldots m_k;x_2,\ldots,x_k)B(n;N;m_1;x_1)-\cdots\\ &+(-1)^k S(N;m_k;x_k)B(n;N;m_1,\ldots,m_{k-1};x_1,\ldots,x_{k-1}). \end{aligned} \tag{16}$$

Finally, it is convenient to introduce raising and lowering operators as follows:

$$(\mathbf{x}^+)^m \cdot 1 = \frac{1}{m!}\ln^m(x),$$

$$\mathbf{x}^+ \cdot f(x) = \int_0^x \frac{dx'}{x'} f(x'), \tag{17}$$

$$\mathbf{x}^- \cdot f(x) = x\frac{d}{dx} f(x).$$

It is understood that in the second line only functions which are integrable at $x=0$ are considered. With the help of raising operators a B-sum $B(n;\infty;\dots)$ may be expressed as follows:

$$B(n;\infty;m_1,\dots,m_k;x_1,\dots,x_k)$$

$$= (\mathbf{x_k}^+)^{m_k}(\mathbf{x_{k-1}}^+)^{m_{k-1}}\cdots(\mathbf{x_1}^+)^{m_1}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_1\dots x_k}{1-x_1\dots x_k}(x_1\cdots x_k)^n. \tag{18}$$

Some important integrals related to the raising operators are

$$\mathbf{x_1}^+[1-(1-x_1x_2)^n] = \sum_{i=1}^{n}\frac{1}{i}[1-(1-x_1x_2)^i],$$

$$\mathbf{x_1}^+\frac{x_1x_2}{1-x_1x_2}[1-(1-x_0x_1x_2)^n]$$

$$= -(1-x_0)^n\sum_{i=1}^{n}\frac{1}{i}\left(\frac{1}{1-x_0}\right)^i[1-(1-x_0x_1x_2)^i]$$

$$+(1-(1-x_0)^n)\sum_{i=1}^{N}\frac{(x_1x_2)^i}{i}+\mathbf{x_1}^+\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N(1-(1-x_0)^n). \tag{19}$$

To evaluate the conjugation in Eq. (12) one first converts the S-sum to B-sums and introduces then the raising operators. This allows to perform all sums explicitly and one is left with the integrals corresponding to the raising operators. With the help of Eq. (19) one can systematically perform these integrals and convert them back into nested sums.

The basic manipulations in Eqs. (9)–(13) are the building blocks to reduce the following two generic types of sums to single Z-sums:
Type A:

$$\sum_{i=1}^{n}\frac{x^i}{(i+c)^m}\frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)}\cdots\frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)}Z(i+o-1,m_1,\dots,m_l,x_1,\dots,x_l); \tag{20}$$

Type B:

$$\sum_{i=1}^{n-1}\frac{x^i}{(i+c)^m}\frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)}\cdots\frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)}Z(i+o-1,m_1,\dots,m_l,x_1,\dots,x_l)$$

$$\times\frac{y^{n-i}}{(n-i+c')^{m'}}\frac{\Gamma(n-i+a_1'+b_1'\varepsilon)}{\Gamma(n-i+c_1'+d_1'\varepsilon)}\cdots\frac{\Gamma(n-i+a_{k'}'+b_{k'}'\varepsilon)}{\Gamma(n-i+c_{k'}'+d_{k'}'\varepsilon)}$$

$$\times Z(n-i+o'-1,m_1',\dots,m_{l'}',x_1',\dots,x_{l'}'). \tag{21}$$

Here, all a_j, a'_j, c_j, and c'_j are integers, c,c', are non-negative integers, and o,o' are integers. For sums of type A the upper summation limit n may extend to Infinity. In the rest of the paper I relax the condition on a_j, a'_j, c_j and c'_j to allow for rational numbers. Reference 3 contains in addition two generic types (labeled type C and D in Ref. 3) involving a conjugation. These types do not allow an extension to rational numbers along the lines of this paper. The conjugation is however related to two other important types of sums, which are generalizations of binomial and inverse binomial sums. They are treated in Secs. IV and V of this paper.

III. ALGORITHMS FOR THE EXPANSION AROUND RATIONAL NUMBERS

In this section I extend the algorithms for the expansion of transcendental functions towards the expansion around rational numbers. Sec. III A introduces roots of unity. Roots of unity are useful for the refinement algorithm in Sec. III B, which allows us to express an S-sum $S(n;\ldots)$ as a combination of S-sums, whose upper summation limit is an integer multiple of n. Section III C treats the expansion of Euler's Gamma function around rational numbers. Finally, in Sec. III D all pieces are assembled and the algorithms for the expansion of functions of type A and B around rational numbers are given. A restriction on these algorithms is given by the fact, that rational numbers have to appear in the same place in the numerator and in the denominator. This restriction is relaxed in Sec. IV (a rational number only in the numerator) and Sec. V (a rational number only in the denominator).

A. Roots of unity

We define a short-hand notation for the roots of unity:

$$r_q^p = \exp\left(\frac{2\pi i p}{q}\right). \tag{22}$$

Here, q is a positive integer and p is a non-negative integer. We will need a few properties of the qth roots of unity. Powers of the qth roots of unity are periodic modulo q:

$$(r_q^p)^{j+q} = (r_q^p)^j. \tag{23}$$

Sums of powers of the qth roots of unity yield

$$\sum_{p=0}^{q-1} (r_q^p)^m = \begin{cases} q, & m = 0 \bmod q, \\ 0, & m \neq 0 \bmod q. \end{cases} \tag{24}$$

If $m = 0 \bmod q$, the proof of the relation is trivial. In the case $m \neq 0 \mod q$ we may assume that $0 < m < q$ (due to the periodicity). Then $r_q^m \neq 1$ and we have

$$\sum_{p=0}^{q-1} (r_q^p)^m = \sum_{p=0}^{q-1} (r_q^m)^p = \frac{1-(r_q^m)^q}{1-r_q^m} = 0. \tag{25}$$

From Eq. (24) we obtain immediately

$$\frac{1}{q}\sum_{l=0}^{q-1} (r_q^l)^{m+p} = \begin{cases} 1, & \text{for} \quad m = nq-p, \\ 0, & \text{otherwise.} \end{cases} \tag{26}$$

Since this sum occurs frequently, we introduce the notation

$$\delta_{p,q}(m) = \frac{1}{q}\sum_{l=0}^{q-1} (r_q^l)^{m+p}. \tag{27}$$

Equation (26) will be useful to convert sums with upper summation limit n to sums with upper summation limit $(q\cdot n)$. Note that $\delta_{p,q}(m)$ is idempotent:

$$\delta_{p,q}(m)\cdot\delta_{p,q}(m)=\delta_{p,q}(m) \qquad \text{for all integer } m. \tag{28}$$

Some examples for the half-integer case are

$$\begin{aligned}\delta_{0,2}(n)&=\tfrac{1}{2}[1+(-1)^n],\\ \delta_{1,2}(n)&=\tfrac{1}{2}[1-(-1)^n].\end{aligned} \tag{29}$$

B. Refinements of *S*-sums

An S-sum $S(n;m_1,\ldots;x_1,\ldots)$ with upper summation limit n can be expressed as a combination of S-sums with upper summation limit $(q\cdot n)$, where q is a positive integer. The algorithm proceeds recursively in the depth of the S-sum. For the empty sum one has

$$S(n)=S(q\cdot n). \tag{30}$$

For a S-sum of the form

$$S(n;m_1,m_2,\ldots;x_1,x_2,\ldots)=\sum_{i=1}^{n}\frac{x_1^i}{i^{m_1}}S(i;m_2,\ldots;x_2,\ldots) \tag{31}$$

the algorithm converts first the subsum $S(i;m_2,\ldots;x_2,\ldots)$ to a combination of subsums $S(q\cdot i;\ldots)$. Finally, the outermost sum is converted according to

$$\begin{aligned}\sum_{i=1}^{n}\frac{x^i}{i^m}S(q\cdot i;\ldots)&=q^m\sum_{i=1}^{q\cdot n}\delta_{0,q}(i)\frac{1}{i^m}(x^{1/q})^iS(i;\ldots)\\ &=q^{m-1}\sum_{p=0}^{q-1}\sum_{i=1}^{q\cdot n}\frac{1}{i^m}(r_q^px^{1/q})^iS(i;\ldots).\end{aligned} \tag{32}$$

This completes the algorithm for the conversion of S-sums $S(n;\ldots)$ to $S(q\cdot n;\ldots)$. As an example we have

$$\begin{aligned}S(n;1,1;x_1,x_2)=&S(2n;1,1;\sqrt{x_1},\sqrt{x_2})+S(2n;1,1;\sqrt{x_1},-\sqrt{x_2})\\ &+S(2n;1,1;-\sqrt{x_1},\sqrt{x_2})+S(2n;1,1;-\sqrt{x_1},-\sqrt{x_2}).\end{aligned} \tag{33}$$

Note that as a consequence of the refinement algorithm one obtains relations like

$$\mathrm{Li}_m(x^2)=2^{m-1}[\mathrm{Li}_m(x)+\mathrm{Li}_m(-x)]. \tag{34}$$

C. Expansion of the gamma function

For the expansion of the gamma function around positive integer values one has the well-known formula

$$\frac{\Gamma(n+1+\varepsilon)}{\Gamma(1+\varepsilon)}=\Gamma(n+1)\exp\left(-\sum_{k=1}^{\infty}\varepsilon^k\frac{(-1)^k}{k}S_k(n)\right). \tag{35}$$

For the expansion around rational numbers one finds

$$\frac{\Gamma\left(n+1-\frac{p}{q}+\varepsilon\right)}{\Gamma\left(1-\frac{p}{q}+\varepsilon\right)} = \frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma\left(1-\frac{p}{q}\right)} \exp\left(-\sum_{k=1}^{\infty} \varepsilon^k \frac{(-q)^k}{k} \sum_{j=1}^{qn} \frac{\delta_{p,q}(j)}{j^k}\right)$$

$$= \frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma\left(1-\frac{p}{q}\right)} \exp\left(-\frac{1}{q}\sum_{l=0}^{q-1} (r_q^l)^p \sum_{k=1}^{\infty} \varepsilon^k \frac{(-q)^k}{k} S(q\cdot n;k;r_q^l)\right). \quad (36)$$

Here, n and q are positive integers and p is an integer with $0 \leqslant p < q$ and $\gcd(p,q)=1$. For the case $p=0$ and $q=1$ this reduces to the formula Eq. (35). Equation (36) is derived as follows: One starts from the expansion of the logarithm of the Gamma function:

$$\ln\Gamma\left(n+1-\frac{p}{q}+\varepsilon\right) = \ln\Gamma\left(n+1-\frac{p}{q}\right) + \sum_{k=1}^{\infty} \frac{\varepsilon^k}{k!} \psi^{(k-1)}\left(n+1-\frac{p}{q}\right). \quad (37)$$

Here $\psi^{(k-1)}(x)$ is the polygamma function defined as

$$\psi^{(k-1)}(x) = \frac{d^k}{dx^k} \ln\Gamma(x). \quad (38)$$

From the recurrence formula for the polygamma function

$$\psi^{(k-1)}(x+1) - \psi^{(k-1)}(x) = -\Gamma(k)\left(-\frac{1}{x}\right)^k \quad (39)$$

one obtains

$$\psi^{(k-1)}\left(n+1-\frac{p}{q}\right) = \psi^{(k-1)}\left(1-\frac{p}{q}\right) - \Gamma(k)(-1)^k \sum_{i=1}^{n} \left(\frac{1}{i-\frac{p}{q}}\right)^k. \quad (40)$$

The sum in the last term of Eq. (40) is then rewritten in terms of S-sums with upper summation limit $(q\cdot n)$ with the help of Eq. (26).

D. Expansion around rational numbers

In this section we generalize the algorithms A and B, which expand the transcendental sums in Eqs. (20) and (21) around integers to algorithms for the expansion around rational numbers. In the following we will always assume that q_j is a positive integer and that p_j is an integer with $0 \leqslant p_j < q_j$ and $\gcd(p_j,q_j)=1$. We restrict ourselves here to ratios of Gamma function of the form

$$\frac{\Gamma\left(n+a_j-\frac{p_j}{q_j}+b_j\varepsilon\right)}{\Gamma\left(n+c_j-\frac{p_j}{q_j}+d_j\varepsilon\right)}, \quad (41)$$

where n, a_j, and b_j are integers. Here the same fraction p_j/q_j occurs in the numerator and the denominator. In products of these ratios, different fractions are allowed, like, for example, in

$$\frac{\Gamma(n+a_1-\frac{1}{2}+b_1\varepsilon)}{\Gamma(n+c_1-\frac{1}{2}+d_1\varepsilon)}\frac{\Gamma(n+a_2-\frac{2}{3}+b_2\varepsilon)}{\Gamma(n+c_2-\frac{2}{3}+d_2\varepsilon)}. \tag{42}$$

The restriction to ratios of the form (41) ensures that the prefactors $\Gamma(n+1-p/q)$ from the expansion of the Gamma function in Eq. (36) cancel between the numerator and the denominator. The restriction in Eq. (41) will be relaxed in Secs. IV and V. We now consider sums of the type A and B, where we allow the substitutions

$$\begin{aligned} a_j &\to a_j-\frac{p_j}{q_j}, \quad c_j \to c_j-\frac{p_j}{q_j}, \\ a_j' &\to a_j'-\frac{p_j'}{q_j'}, \quad c_j' \to c_j'-\frac{p_j'}{q_j'}, \\ c &\to c-\frac{p_0}{q_0}, \quad c' \to c'-\frac{p_0'}{q_0'}, \end{aligned} \tag{43}$$

in Eqs. (20) and (21). For example, a sum of type A involving rational numbers is of the form

$$\sum_{i=1}^{n}\frac{x^i}{\left(i+c-\frac{p_0}{q_0}\right)^m}\frac{\Gamma\left(i+a_1-\frac{p_1}{q_1}+b_1\varepsilon\right)}{\Gamma\left(i+c_1-\frac{p_1}{q_1}+d_1\varepsilon\right)}\cdots\frac{\Gamma\left(i+a_k-\frac{p_k}{q_k}+b_k\varepsilon\right)}{\Gamma\left(i+c_k-\frac{p_k}{q_k}+d_k\varepsilon\right)}S(i+o,m_1,\ldots,x_1,\ldots), \tag{44}$$

where c_0 is a non-negative integer, o and all a_j, c_j are integers. When dealing with rational numbers it is more convenient to work with S-sums instead of Z-sums and we replaced the Z-sum in Eq. (20) by a S-sum in Eq. (44). Due to the conversion algorithm the two formulations are equivalent.

The algorithms for the expansion in ε of these sums starts by reducing the offsets o and o' in the subsums $S(i+o;m_1,\ldots;x_1,\ldots)$ and $S(n-i+o';m_1',\ldots;x_1',\ldots)$ to zero. Then, using the identity

$$\Gamma(x+1)=x\Gamma(x) \tag{45}$$

for the gamma function, the ratios of the gamma functions are brought to the form

$$\frac{\Gamma\left(i+1-\frac{p_j}{q_j}+b_j\varepsilon\right)}{\Gamma\left(i+1-\frac{p_j}{q_j}+d_j\varepsilon\right)} \quad \text{or} \quad \frac{\Gamma\left(n-i+1-\frac{p_j'}{q_j'}+b_j'\varepsilon\right)}{\Gamma\left(n-i+1-\frac{p_j'}{q_j'}+d_j'\varepsilon\right)}. \tag{46}$$

They are then expanded in ε, using Eq. (36). This yields S-sums with upper summation limit $(q_j\cdot i)$ or $(q_j'\cdot(n-i))$. Now, let $q=\mathrm{lcm}(q_0,q_1,\ldots,q_k)$ be the least common multiple of q_0, $q_1,\ldots,q_k$ and let $q'=\mathrm{lcm}(q_0',q_1',\ldots,q_k')$ be the least common multiple of $q_0',q_1',\ldots,q_k'$ Using the refinement algorithm we can convert any occuring S-sum $S(q_j i;\ldots)$ to S-sums with upper summation limit $(q\cdot i)$. Similar any S-sum $S(q_j'(n-i);\ldots)$ is converted to S-sums $S(q'(n-i);\ldots)$. Products of S-sums are then converted into single S-sums with the help of the multiplication algorithm. After partial fractioning one arrives at the following forms:

$$\text{Type A:} \quad \sum_{i=1}^{n} \frac{x^i}{\left(i+c-\frac{p_0}{q_0}\right)^m} S(qi;\dots),$$
$$\text{Type B:} \quad \sum_{i=1}^{n-1} \frac{x^i}{\left(i+c-\frac{p_0}{q_0}\right)^m} S(qi;\dots)S(q'(n-i);\dots), \tag{47}$$

where q_0 divides q. For sums of type A one then reduces the offset c to zero and one arrives at sums of the form

$$\sum_{i=1}^{n} \frac{x^i}{\left(i-\frac{p_0}{q_0}\right)^m} S(qi,\dots). \tag{48}$$

Using Eq. (26) this sum can be written as

$$\sum_{i=1}^{n} \frac{x^i}{\left(i-\frac{p_0}{q_0}\right)^m} S(qi,\dots) = q^m x^{p/q} \sum_{i=1}^{qn} \delta_{p,q}(i) \frac{(x^{1/q})^i}{i^m} S(i+p;\dots)$$
$$= q^{m-1} \sum_{l=0}^{q-1} (r_q^l x^{1/q})^p \sum_{i=1}^{qn} \frac{(r_q^l x^{1/q})^i}{i^m} S(i+p;\dots), \tag{49}$$

where $p=p_0 q/q_0$ is an integer with $0 \leqslant p < q$. Finally, reducing the offset p of the subsum $S(i+p;\dots)$ to zero, one arrives at S-sums with upper summation limit (qn).

For sums of type B one first refines the subsums $S(qi;\dots)$ and $S(q'(n-i);\dots)$ to $S(\hat{q}i;\dots)$ and $S(\hat{q}(n-i);\dots)$, respectively. Here $\hat{q}=\mathrm{lcm}(q,q')$ is the least common multiple of q and q'. The next step consists in rewriting

$$\sum_{i=1}^{n-1} \frac{x^i}{\left(i+c-\frac{p_0}{q_0}\right)^m} S(qi;\dots)S(q(n-i);\dots)$$
$$= q^m x^{p/q} \sum_{i=1}^{qn-q} \delta_{p,q}(i) \frac{(x^{1/q})^i}{(i+qc)^m} S(i+p;\dots)S(qn-i-p;\dots), \tag{50}$$

which brings us back to the integer case.

This completes the necessary modifications for the extension towards the expansion around rational numbers for the algorithm A and B.

IV. BINOMIAL SUMS AND GENERALIZATIONS

Here we study sums of the form

$$\frac{1}{\Gamma\left(1-\frac{p}{q}\right)} \sum_{n=1}^{\infty} \frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma(n+1)} \frac{x_0^n}{n^{m_0}} S(n;m_1,\dots,m_k;x_1,\dots,x_k). \tag{51}$$

This relaxes the condition (41) and allows one unbalanced fraction

$$\frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma(n+1)}. \tag{52}$$

A special case of the form in Eq. (51) are binomial sums

$$\sum_{n=1}^{\infty}\binom{2n}{n}\frac{z^n}{n^{m_0}}S(n;m_1,\ldots,m_k;x_1,\ldots,x_k), \tag{53}$$

which are obtained by setting $p=1$, $q=2$, $x_0=4z$ in Eq. (51) and by noting the identity

$$\binom{2n}{n}=4^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(\frac{1}{2})\Gamma(n+1)}. \tag{54}$$

Binomial sums have been studied in Refs. 5 and 6. The evaluation of the sums in Eq. (51) follows the same pattern of steps as the evaluation of the conjugation in Eq. (12), as given in Ref. 3. Due to Eq. (15) we may replace in Eq. (51) the S-sum $S(n;\ldots)$ with S-sums $S(\infty;\ldots)$ and B-sums $B(n;\infty;\ldots)$ and it is sufficient to study sums of the form

$$\begin{aligned}&\frac{1}{\Gamma\left(1-\frac{p}{q}\right)}\sum_{n=1}^{\infty}\frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma(n+1)}\frac{x_0^n}{n^{m_0}}B(n;\infty;m_1,\ldots,m_k;x_1,\ldots,x_k)\\&\quad=-(\mathbf{x_k}^+)^{m_k}(\mathbf{x_{k-1}}^+)^{m_{k-1}}\cdots(\mathbf{x_1}^+)^{m_1}(\mathbf{x_0}^+)^{m_0}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_1\cdots x_k}{1-x_1\cdots x_k}\\&\qquad\times[1-(1-x_0x_1\cdots x_k)^{-(1-(p/q))}].\end{aligned} \tag{55}$$

To derive the r.h.s. of Eq. (55) we first introduced the raising operators $\mathbf{x}_+$, then performed explicitly all geometric sums from $B(n;\infty;0,\ldots,0;x_1,\ldots,x_k)$ and finally performed the remaining sum with the help of the hypergeometric summation formula

$$\frac{1}{\Gamma\left(1-\frac{p}{q}\right)}\sum_{n=1}^{\infty}\frac{\Gamma\left(n+1-\frac{p}{q}\right)}{\Gamma(n+1)}x^n=-[1-(1-x)^{-(1-p/q)}]. \tag{56}$$

We then perform succesivly the integrations corresponding to the raising operators. Due to the appearance of rational numbers in the exponent, the set in Eq. (19) is no longer sufficient and has to be supplemented with additional equations. Nevertheless, the principle stays the same: Each integration preserves the structure, such that multiple integrations can be performed iteratively. To reduce m_0 we have

$$\mathbf{x_0}^+[1-(1-x_0x_1)^{-(1-p/q)}]=q\sum_{n=1}^{\infty}\frac{1}{n}[\delta_{0,q}(n)-\delta_{q-p,q}(n)][1-(1-x_0x_1)^{n/q}],$$

$$\mathbf{x_0^+}\,\delta_{q-p,q}(n)[1-(1-x_0x_1)^{n/q}]$$

$$=q\,\delta_{q-p,q}(n)\sum_{i=1}^{\infty}\frac{1}{i}[\,\delta_{0,q}(i)-\delta_{q-p,q}(i)][1-(1-x_0x_1)^{i/q}]$$

$$+q\,\delta_{q-p,q}(n)\sum_{i=1}^{n}\frac{1}{i}\,\delta_{q-p,q}(i)[1-(1-x_0x_1)^{i/q}]. \tag{57}$$

To reduce $m_1,m_2,\ldots,m_k$ we have in the general case $x_0\neq 1$:

$$\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}[1-(1-x_0x_1x_2)^{-(1-p/q)}]$$

$$=-q(1-x_0)^{-(1-(p/q))}\left\{\sum_{n=1}^{\infty}\frac{1}{n}[\,\delta_{0,q}(n)-\delta_{q-p,q}(n)]\left(\frac{1}{1-x_0}\right)^{n/q}[1-(1-x_0x_1x_2)^{n/q}]\right\}$$

$$+[1-(1-x_0)^{-(1-(p/q))}]\sum_{n=1}^{N}\frac{1}{n}(x_1x_2)^n$$

$$+\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N[1-(1-x_0)^{-(1-(p/q))}], \tag{58}$$

$$\mathbf{x_1^+}\,\delta_{q-p,q}(n)\frac{x_1x_2}{1-x_1x_2}[1-(1-x_0x_1x_2)^{n/q}]$$

$$=-q(1-x_0)^{n/q}\delta_{q-p,q}(n)\left\{\sum_{i=1}^{\infty}\frac{1}{i}[\,\delta_{0,q}(i)-\delta_{q-p,q}(i)]\left(\frac{1}{1-x_0}\right)^{i/q}[1-(1-x_0x_1x_2)^{i/q}]\right.$$

$$\left.+\sum_{i=1}^{n}\frac{1}{i}\,\delta_{q-p,q}(i)\left(\frac{1}{1-x_0}\right)^{i/q}[1-(1-x_0x_1x_2)^{i/q}]\right\}$$

$$+\,\delta_{q-p,q}(n)[1-(1-x_0)^{n/q}]\sum_{i=1}^{N}\frac{1}{i}(x_1x_2)^i+\delta_{q-p,q}(n)\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N[1-(1-x_0)^{n/q}].$$

In the special case $x_0=1$ we have instead

$$\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}[1-(1-x_1x_2)^{-(1-(p/q))}]$$

$$=\frac{1}{1-\dfrac{p}{q}}[1-(1-x_1x_2)^{-(1-(p/q))}]+\sum_{n=1}^{N}\frac{1}{n}(x_1x_2)^n+\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N, \tag{59}$$

$$\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}[1-(1-x_1x_2)^{n/q}]=-\frac{q}{n}[1-(1-x_1x_2)^{n/q}]+\sum_{i=1}^{N}\frac{1}{i}(x_1x_2)^i+\mathbf{x_1^+}\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N.$$

Equations (58) and (59) introduce an arbitrary integer N. It is worth noting that Eqs. (58) and (59) hold for any integer N. We will take the limit $N\to\infty$ in the end. It is clear that in this limit terms of the form

$$(\mathbf{x}^+)^m\frac{x}{1-x}x^N=\sum_{i=N+1}^{\infty}\frac{x^i}{i^m} \tag{60}$$

can be neglected. Some examples are

$$\frac{1}{\Gamma(\frac{1}{2})}\sum_{n=1}^{\infty}\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}\frac{x^n}{n}=2\ln 2-2\ln(1+\sqrt{1-x}),$$

$$\frac{1}{\Gamma(\frac{1}{2})}\sum_{n=1}^{\infty}\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}\frac{x^n}{n^2}=2[\ln 2\ln(1+\sqrt{1-x})+\ln 2\ln(1-\sqrt{1-x})-\mathrm{Li}_{11}(-\sqrt{1-x},1)$$
$$-\mathrm{Li}_{11}(\sqrt{1-x},-1)-\mathrm{Li}_2(-1)-(\ln 2)^2],$$

$$\frac{1}{\Gamma(\frac{1}{2})}\sum_{n=1}^{\infty}\sum_{j=1}^{n}\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}\frac{x^n}{n}\frac{y^j}{j}$$
$$=2\ \mathrm{Li}_{11}\left(\sqrt{1-x},-\sqrt{\frac{1-xy}{1-x}}\right)+2\ \mathrm{Li}_{11}\left(-\sqrt{1-x},\sqrt{\frac{1-xy}{1-x}}\right)$$
$$-2\ \mathrm{Li}_{11}\left(\sqrt{1-x},-\frac{1}{\sqrt{1-x}}\right)-2\ \mathrm{Li}_{11}\left(-\sqrt{1-x},\frac{1}{\sqrt{1-x}}\right)$$
$$+4\ \mathrm{Li}_2(-\sqrt{1-xy})-4\ \mathrm{Li}_2(-1)+2\ln\frac{1+\sqrt{1-x}}{1-\sqrt{1-x}}\ln\frac{1+\sqrt{\frac{1-xy}{1-x}}}{1+\frac{1}{\sqrt{1-x}}}. \tag{61}$$

V. INVERSE BINOMIAL SUMS AND GENERALIZATIONS

In this section I consider sums with one unbalanced rational number in the denominator. Examples of these type are sums of the form

$$\Gamma\left(1-\frac{p}{q}\right)\sum_{n_1=1}^{\infty}\frac{\Gamma(n_1+a)}{\Gamma\left(n_1+b-\frac{p}{q}\right)}x_1^{n_1}$$
$$\times\sum_{n_2=1}^{n_1-1}\frac{x_2^{n_2}}{(n_1-n_2)^{m_1}}\cdots\sum_{n_{k-1}=1}^{n_{k-2}-1}\frac{x_{k-1}^{n_{k-1}}}{(n_{k-2}-n_{k-1})^{m_{k-2}}}\sum_{n_k=1}^{n_{k-1}-1}\frac{x_k^{n_k}}{(n_{k-1}-n_k)^{m_{k-1}}n_k^{m_k}}. \tag{62}$$

Note the slightly different structure of $(n_{l+1}-n_l)$ in the denominators of the subsums. Only in the innermost sum a factor n_k appears in the denominator. Changing the summation variables according to

$$n_1=j_1+j_2+\cdots+j_k,\qquad n_2=j_2+\cdots+j_k,\qquad\ldots,\qquad n_k=j_k, \tag{63}$$

this sum is equivalent to

$$\Gamma\left(1-\frac{p}{q}\right)\sum_{j_1=1}^{\infty}\cdots\sum_{j_k=1}^{\infty}\frac{\Gamma(j_1+\cdots+j_k+a)}{\Gamma\left(j_1+\cdots+j_k+b-\frac{p}{q}\right)}\frac{x_1^{j_1}}{j_1^{m_1}}\frac{(x_1x_2)^{j_2}}{j_2^{m_2}}\cdots\frac{(x_1\cdots x_k)^{j_k}}{j_k^{m_k}}. \tag{64}$$

A special case of this form are inverse binomial sums

$$\sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{z^n}{n^{m_1}}, \tag{65}$$

which are obtained by setting $p=1$, $q=2$, $a=b=1$, $k=1$ and $x_1=z/4$ in Eq. (64). Inverse binomial sums have been studied in Refs. 5, 7–9, 32, and 33 and have been related in the literature to log-sine integrals.[10,11] Here I follow a different path for the evaluation of inverse binomial sums. The method presented here is closely connected to the transformation

$$x' = \frac{-x}{1-x}, \tag{66}$$

whose inverse transformation is again given by

$$x = \frac{-x'}{1-x'}. \tag{67}$$

To start with the evaluation of sums of type (64) one replaces all factors $1/j$ by

$$\frac{1}{j} = \lim_{\lambda \to 0} \frac{\Gamma(j+\lambda)}{\Gamma(j+1+\lambda)}. \tag{68}$$

The original sum is recovered as the $\lambda \to 0$ limit of the regularized sum. The introduction of the regularization in λ allows us to extend the lower summation boundary of all sums from 1 to 0. This can be done recursively according to

$$\sum_{j=1}^{\infty} f(j) = -f(0) + \sum_{j=0}^{\infty} f(j). \tag{69}$$

$f(0)$ corresponds to a sum of lower depth. We therefore deal with sums of the type

$$\Gamma\left(1-\frac{p}{q}\right) \sum_{j_1=0}^{\infty} \cdots \sum_{j_k=0}^{\infty} \frac{\Gamma(j_1+\cdots+j_k+a)}{\Gamma\left(j_1+\cdots+j_k+b-\frac{p}{q}\right)} x_1^{j_1} (x_1 x_2)^{j_2} \cdots (x_1 \cdots x_k)^{j_k}$$

$$\times \left[\frac{\Gamma(j_1+\lambda)}{\Gamma(j_1+1+\lambda)}\right]^{m_1} \cdots \left[\frac{\Gamma(j_k+\lambda)}{\Gamma(j_k+1+\lambda)}\right]^{m_k}. \tag{70}$$

For these sums we have the following integral representation:

$$\frac{\Gamma\left(1-\frac{p}{q}\right)}{\Gamma\left(b-a-\frac{p}{q}\right)} \int_0^1 du u^{a-1} (1-u)^{b-a-(p/q)-1} \int_0^1 dt_1 t_1^{\lambda-1} \cdots \int_0^1 dt_{i_k} t_{i_k}^{\lambda-1} (1-u t_1 \cdots t_{i_1} x_1)^{-1}$$

$$\times (1-u t_{i_1+1} \cdots t_{i_2} x_1 x_2)^{-1} \cdots (1-u t_{i_{k-1}+1} \cdots t_{i_k} x_1 \cdots x_k)^{-1}, \tag{71}$$

where

$$i_1 = m_1, \qquad i_2 = m_1+m_2, \qquad \ldots, \qquad i_k = m_1+\cdots+m_k. \tag{72}$$

For the integration variable u we now perform the substitution

$$u \to 1-u, \tag{73}$$

and we obtain for Eq. (71),

$$\begin{aligned}
&\frac{\Gamma\left(1-\frac{p}{q}\right)\Gamma(a)}{\Gamma\left(b-a-\frac{p}{q}\right)} \sum_{j_1=0}^{\infty} \cdots \sum_{j_k=0}^{\infty} \frac{\Gamma\left(j_1+\cdots+j_k+b-a-\frac{p}{q}\right)}{\Gamma\left(j_1+\cdots+j_k+b-\frac{p}{q}\right)} \int_0^1 dt_1 t_1^{\lambda-1} \cdots \int_0^1 dt_{i_k} t_{i_k}^{\lambda-1} \\
&\quad \times (-t_1 \cdots t_{i_1} x_1)^{j_1} (1-t_1 \cdots t_{i_1} x_1)^{-j_1-1} \cdots (-t_{i_{k-1}+1} \cdots t_{i_k} x_1 \cdots x_k)^{j_k} \\
&\quad \times (1-t_{i_{k-1}+1} \cdots t_{i_k} x_1 \cdots x_k)^{-j_k-1} \\
&= \frac{\Gamma\left(1-\frac{p}{q}\right)\Gamma(a)}{\Gamma\left(b-a-\frac{p}{q}\right)} \sum_{n_1=0}^{\infty} \cdots \sum_{n_k=0}^{n_{k-1}} \frac{\Gamma\left(n_1+b-a-\frac{p}{q}\right)}{\Gamma\left(n_1+b-\frac{p}{q}\right)} \int_0^1 dt_1 t_1^{\lambda-1} \cdots \int_0^1 dt_{i_k} t_{i_k}^{\lambda-1} \\
&\quad \times (-t_1 \cdots t_{i_1} x_1)^{n_1-n_2} (1-t_1 \cdots t_{i_1} x_1)^{-n_1+n_2-1} \cdots (-t_{i_{k-2}+1} \cdots t_{i_{k-1}} x_1 \cdots x_{k-1})^{n_{k-1}-n_k} \\
&\quad \times (1-t_{i_{k-2}+1} \cdots t_{i_{k-1}} x_1 \cdots x_{k-1})^{-n_{k-1}+n_k-1} (-t_{i_{k-1}+1} \cdots t_{i_k} x_1 \cdots x_k)^{n_k} \\
&\quad \times (1-t_{i_{k-1}+1} \cdots t_{i_k} x_1 \cdots x_k)^{-n_k-1}.
\end{aligned} \tag{74}$$

Note that the substitution Eq. (73) induces the transformation $x \to -x/(1-x)$ as follows:

$$[1-(1-u)x]^{-c} = (1-x)^{-c}\left[1-\left(\frac{-x}{1-x}\right)u\right]^{-c}. \tag{75}$$

As a sideremark it is worth noting that as a special case one obtains by this procedure the transformation of the hypergeoemetric function

$${}_2F_1(a,b;c;x) = (1-x)^{-a}\,{}_2F_1\left(a,c-b;c;\frac{-x}{1-x}\right) = (1-x)^{-b}\,{}_2F_1\left(c-a,b;c;\frac{-x}{1-x}\right).$$

The purpose of the substitution in Eq. (73) is to change the ratio of gamma functions from

$$\frac{\Gamma(j_1+\cdots+j_k+a)}{\Gamma\left(j_1+\cdots+j_k+b-\frac{p}{q}\right)} \quad \text{to} \quad \frac{\Gamma\left(j_1+\cdots+j_k+b-a-\frac{p}{q}\right)}{\Gamma\left(j_1+\cdots+j_k+b-\frac{p}{q}\right)}. \tag{76}$$

In the last form, the rational number p/q appears both in the numerator and the denominator and can therefore be treated with the methods discussed in Sec. III. It remains to perform the integration over $t_1, \ldots, t_{i_k}$. These integration are recursively done according to the formula

$$\int_0^1 dt_1 t_1^{a-1} (-t_0 t_1 x)^n (1-t_0 t_1 x)^{-n-c} = \frac{\Gamma(n+a)}{\Gamma(n+c)} \sum_{k=n}^{\infty} \frac{\Gamma(k+c)}{\Gamma(k+1+a)} (-t_0 x)^k (1-t_0 x)^{-k-c}.$$

As a net result we obtain a rooted tree with side-branches, which can be expanded in λ and converted to nested sums with the help of the algorithms discussed in Ref. 3 and in Sec. III. In the final result all poles in λ cancel and one can extract the λ^0-term, which yields the evaluation of the inverse binomial sum Eq. (62). Some examples are

$$\Gamma\left(\frac{1}{2}\right)\sum_{n=1}^{\infty}\frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})}\frac{x^n}{n}=\chi\ln\frac{1-\chi}{1+\chi},$$

$$\Gamma\left(\frac{1}{2}\right)\sum_{n=1}^{\infty}\frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})}\frac{x^n}{n^2}=-\mathrm{Li}_{11}(\chi,1)+\mathrm{Li}_{11}(\chi,-1)-\mathrm{Li}_{11}(-\chi,1)+\mathrm{Li}_{11}(-\chi,-1),$$

$$\begin{aligned}\Gamma\left(\frac{1}{2}\right)\sum_{n=1}^{\infty}\sum_{j=1}^{n}\frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})}\frac{x^n}{n}\frac{y^j}{j}=&-\mathrm{Li}_{11}(v,1)-\mathrm{Li}_{11}(-v,1)+\mathrm{Li}_{11}(v,-1)+\mathrm{Li}_{11}(-v,-1)\\&-\chi\left[\mathrm{Li}_{11}\left(\chi,\frac{v}{\chi}\right)+\mathrm{Li}_{11}\left(\chi,-\frac{v}{\chi}\right)-\mathrm{Li}_{11}\left(-\chi,\frac{v}{\chi}\right)\right.\\&\left.-\mathrm{Li}_{11}\left(-\chi,-\frac{v}{\chi}\right)\right]-\chi\ln(1-xy)\ln\frac{1-\chi}{1+\chi},\end{aligned}\tag{77}$$

where $\chi=\sqrt{-x/(1-x)}$ and $v=\sqrt{-xy/(1-xy)}$.

VI. APPLICATIONS

In this section I give some applications of the techniques described in the previous sections relevant to the calculation of Feynman loop integrals with massive particles or to phase space integrals. The first example concerns a one-loop triangle with a uniform internal mass $m_1=m_2=m_3=m$ and two vanishing external momenta $p_1^2=p_2^2=0$. The third external momentum $p_3^2=p^2$ is kept arbitrary. Such diagrams are for example relevant to Higgs physics. Specific examples are Higgs production via $gg\to H$ or Higgs decay into two photons $H\to\gamma\gamma$. In both cases the interaction proceeds via an internal top quark loop. It is well known that the corresponding integral in dimensional regularization is proportional to[7,38]

$${}_3F_2\left(1,1,1+\varepsilon;\ \frac{3}{2},2;\ \frac{p^2}{4m_{top}^2}\right).\tag{78}$$

Here $\varepsilon=(4-D)/2$ denotes the deviation from four space–time dimensions. The expansion of the hypergeometric function to sufficient high order in ε is a nontrivial task.[7,9] The expansion can be accomplished systematically with the methods presented here. First one notices that there is one unbalanced half-integer number in the denominator. With the results of Sec. V one can show that

$$\begin{aligned}&{}_3F_2\left(1+a_1\varepsilon,1+a_2\varepsilon,1+a_3\varepsilon;\ \frac{3}{2}+b\varepsilon,C+c\varepsilon;\ z\right)\\&=(1-z)^{-1-a_1\varepsilon}\frac{\Gamma(\frac{3}{2}+b\varepsilon)\Gamma(C+c\varepsilon)}{\Gamma(1+a_1\varepsilon)\Gamma(1+a_3\varepsilon)\Gamma(\frac{1}{2}+(b-a_2)\varepsilon)\Gamma(C-1+(c-a_3)\varepsilon)}\\&\quad\times\sum_{n=0}^{\infty}\frac{\Gamma(n+1+a_1\varepsilon)}{\Gamma(n+C+c\varepsilon)}\left(\frac{-z}{1-z}\right)^n\sum_{j=0}^{n}\\&\quad\times\frac{\Gamma(j+1+a_3\varepsilon)}{\Gamma(j+1)}\frac{\Gamma(j+\frac{1}{2}+(b-a_2)\varepsilon)}{\Gamma(j+\frac{3}{2}+b\varepsilon)}\frac{\Gamma(n-j+C-1+(c-a_3)\varepsilon)}{\Gamma(n-j+1)}.\end{aligned}\tag{79}$$

This yields a nested sum where all half-integer numbers are balanced in the numerator and in the denominator. This expression can now be expanded systematically in ε with the algorithms described in Sec. III. For the example mentioned above one finds

$$
\begin{aligned}
{}_3F_2\left(1,1,1+\varepsilon;\ \frac{3}{2},2;\ z\right) = &-\frac{1}{2z}(1-z)^{-\varepsilon}\Bigg\{\mathrm{Li}_{11}\left(\sqrt{\frac{-z}{1-z}},1\right)+\mathrm{Li}_{11}\left(-\sqrt{\frac{-z}{1-z}},1\right)\\
&-\mathrm{Li}_{11}\left(\sqrt{\frac{-z}{1-z}},-1\right)-\mathrm{Li}_{11}\left(-\sqrt{\frac{-z}{1-z}},-1\right)\\
&+2\varepsilon\Bigg[\mathrm{Li}_{111}\left(\sqrt{\frac{-z}{1-z}},1,1\right)+\mathrm{Li}_{111}\left(-\sqrt{\frac{-z}{1-z}},1,1\right)\\
&-\mathrm{Li}_{111}\left(\sqrt{\frac{-z}{1-z}},-1,-1\right)-\mathrm{Li}_{111}\left(-\sqrt{\frac{-z}{1-z}},-1,-1\right)\Bigg]+O(\varepsilon^2)\Bigg\}.
\end{aligned}
\tag{80}
$$

As a second example I discuss briefly phase space integrals. Analytic results for phase space integrals are needed for example in the calculation of higher order corrections for jet observables as integrals over approximation terms within the subtraction method.[14,17,18,39] An example is the integral over a subtraction term, which approximates the emission of a soft gluon from a heavy quark pair. This integral is given by[14]

$$
\begin{aligned}
V_{QQ}(r_0,\varepsilon) = &\left(\frac{r_0}{2}\right)^{-2\varepsilon}\int_0^1 dr\, r^{-2\varepsilon-1}(1-r)^{-\varepsilon}(1-r_0 r)^{-1}\int_{-1}^1 ds(1-s^2)^{-\varepsilon}[(2(1-r_0 r)-(1-r_0))\\
&\times(1-s_0 s)^{-1}-(1-r_0)(1-s_0 s)^{-2}],
\end{aligned}
\tag{81}
$$

where

$$
s_0 = \sqrt{\frac{r_0(1-r)}{1-r_0 r}}. \tag{82}
$$

This integral corresponds to the following triple sum:

$$
\begin{aligned}
V_{QQ}(r_0,\varepsilon) = &\frac{\Gamma(1-\varepsilon)}{\Gamma(\varepsilon)}\left(\frac{r_0}{2}\right)^{-2\varepsilon}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}(-1)^i\\
&\times(1+(-1)^j)r_0^{k+j/2}\frac{\Gamma(i+j+1)}{\Gamma(i+j+2-\varepsilon)}\frac{\Gamma(i+\varepsilon)}{\Gamma(i+1)}\frac{\Gamma(k-2\varepsilon)\Gamma(j/2+1-\varepsilon)\Gamma(k+j/2)}{\Gamma(k+1)\Gamma(j/2)\Gamma(k+j/2+1-3\varepsilon)}\\
&\times\left[2-(1-r_0)(2+j)\frac{j+2k}{j}\right].
\end{aligned}
\tag{83}
$$

Using the methods of Sec. III this sum can be expanded systematically in ε. The result is

$$
\begin{aligned}
V_{QQ}(r_0,\varepsilon) = &\frac{1}{\varepsilon}\left(1-\frac{1}{2}\frac{1+r_0}{\sqrt{r_0}}\ln\frac{1+\sqrt{r_0}}{1-\sqrt{r_0}}\right)-2\ln r_0-\ln^2\left(\frac{1+\sqrt{r_0}}{1-\sqrt{r_0}}\right)+\frac{1}{\sqrt{r_0}}\ln\left(\frac{1+\sqrt{r_0}}{1-\sqrt{r_0}}\right)\\
&-\frac{1+r_0}{2\sqrt{r_0}}\Bigg[\mathrm{Li}_2(\sqrt{r_0})-\mathrm{Li}_2(-\sqrt{r_0})+2\ \mathrm{Li}_2\left(\frac{1+\sqrt{r_0}}{2}\right)-2\ \mathrm{Li}_2\left(\frac{1-\sqrt{r_0}}{2}\right)\\
&+\mathrm{Li}_2\left(\frac{\sqrt{r_0}-1}{2\sqrt{r_0}}\right)-\mathrm{Li}_2\left(\frac{\sqrt{r_0}-1}{\sqrt{r_0}}\right)+\mathrm{Li}_2\left(\frac{1}{1+\sqrt{r_0}}\right)-\mathrm{Li}_2\left(\frac{1-\sqrt{r_0}}{1+\sqrt{r_0}}\right)\\
&-2\ln r_0\ln\left(\frac{1+\sqrt{r_0}}{1-\sqrt{r_0}}\right)+\frac{1}{2}\ln^2 2+\ln 2\ln\frac{\sqrt{r_0}}{1+\sqrt{r_0}}+\ln(1-\sqrt{r_0})\ln\left(\frac{1+\sqrt{r_0}}{\sqrt{r_0}}\right)
\end{aligned}
$$

$$+\frac{1}{2}\ln^2(1+\sqrt{r_0})-\frac{1}{2}\ln^2(1-\sqrt{r_0})\Bigg]+O(\varepsilon). \tag{84}$$

VII. SUMMARY AND CONCLUSIONS

In this paper I reported on algorithms which allow the expansion of certain transcendental functions in a small parameter around rational values. These algorithms extend the ones for the expansion around integer values and are based on the manipulation of specific forms of nested sums. Of particular importance is the case of the expansion around half-integer values. This case occurs frequently in the calculation of radiative corrections in quantum field theories with massive particles. The methods presented in this paper allow a systematic approach for the calculation of these integrals.

APPENDIX A: LOG-SINE INTEGRALS

Inverse binomial sums are often expressed in terms of log-sine integrals. In this appendix I briefly summarize the results from the literature. The following inverse binomial sum can be evaluated with elementary functions as follows:

$$\Gamma\left(\frac{1}{2}\right)\sum_{n=1}^{\infty}\frac{\Gamma(n+1)}{\Gamma\left(n+\frac{1}{2}\right)}\frac{x^n}{n}=\frac{2\sqrt{x}\arcsin(\sqrt{x})}{\sqrt{1-x}}. \tag{A1}$$

This result agrees with the one given in Eq. (77). In the literature, evaluations of inverse binomial sums of higher weights are given in terms of log-sine functions:[5,7–11,32,33]

$$\Gamma\left(\frac{1}{2}\right)\sum_{n=1}^{\infty}\frac{\Gamma(n+1)}{\Gamma\left(n+\frac{1}{2}\right)}\frac{z^n}{n^m}=-\sum_{j=0}^{m-2}\frac{(-2)^j}{j!(m-2-j)!}(\ln 4z)^{m-2-j}\mathrm{Ls}_{j+2}^{(1)}(\theta), \tag{A2}$$

where $\theta=2\arcsin\sqrt{z}$ and the log-sine functions are defined by

$$\mathrm{Ls}_j^{(k)}(\theta)=-\int_0^{\theta}d\theta'(\theta')^k\ln^{j-k-1}\left|2\sin\frac{\theta'}{2}\right|. \tag{A3}$$

By analytic continuation the log-sine functions are then related to polylogarithms.[9] A simple example is given by

$$\mathrm{Ls}_2^{(0)}(\theta)=\mathrm{Cl}_2(\theta), \tag{A4}$$

involving the Clausen function Cl_2. The Clausen functions Cl_n are given in terms of polylogarithms by

$$\mathrm{Cl}_n(\theta)=\begin{cases}\dfrac{1}{2i}[\mathrm{Li}_n(e^{i\theta})-\mathrm{Li}_n(e^{-i\theta})], & n \text{ even},\\ \dfrac{1}{2}[\mathrm{Li}_n(e^{i\theta})+\mathrm{Li}_n(e^{-i\theta})], & n \text{ odd}.\end{cases} \tag{A5}$$

APPENDIX B: RELATIONS FOR POLYLOGARITHMS

Multiple polylogarithms of low weight can be expressed in terms of ordinary logarithms and polylogarithms. Relations relevant to the examples in this paper are

$$\mathrm{Li}_1(x) = -\ln(1-x),$$

$$\mathrm{Li}_{11}(x,1) = \tfrac{1}{2}\ln^2(1-x),$$

$$\mathrm{Li}_{11}(x,-1) = \frac{1}{2}\zeta_2 - \frac{1}{2}\ln^2 2 - \ln(1-x)\ln(1+x) + \ln 2\,\ln(1+x) - \mathrm{Li}_2\left(\frac{1+x}{2}\right),$$

$$\mathrm{Li}_{11}(x,y) = \ln(1-x)\ln(1-y) + \mathrm{Li}_2\left(\frac{-y}{1-y}\right) - \mathrm{Li}_2\left(\frac{-y(1-x)}{1-y}\right),$$

$$\mathrm{Li}_{111}(x,1,1) = -\tfrac{1}{6}\ln^3(1-x),$$

$$\mathrm{Li}_{111}(x,-1,-1) = \tfrac{1}{2}\zeta_2\ln 2 - \tfrac{7}{8}\zeta_3 - \tfrac{1}{6}\ln^3 2 - \tfrac{1}{2}\ln(1-x)\ln^2(1+x) + \tfrac{1}{2}\ln 2\,\ln^2(1+x) - \ln(1+x)\mathrm{Li}_2\left(\frac{1+x}{2}\right) + \mathrm{Li}_3\left(\frac{1+x}{2}\right). \tag{B1}$$

More relations can be found in Refs. 37 and 40.

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The use of so(2,1) algebra for the evaluation of atomic integrals: The study of two-electron atoms

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The use of the so(2,1) algebra for the study of the two-electron atoms is suggested. The radial part of the two-electron function is expanded into the products of the one-electron functions. These one-electron functions form complete, entirely discrete set and are identified as the eigenfunctions of one of the generators of the so(2,1) algebra. By applying this algebra we are able to express all the matrix elements in analytic and numericaly stable form. For matrix elements of the two-electron interaction this is done in three steps, all of them completely novel from the methodological point of view. First, repulsion integrals over four radial functions are written as a linear combination of the integrals over two radial functions and the coefficients of the linear combination are given in terms of hypergeometric functions. Second, combining algebraic technique with the integration by parts we derive recurrence relations for the repulsion integrals over two radial functions. Third, the derived recurrence relations are solved analytically in terms of the hypergeometric functions. Thus we succeed in expressing the repulsion integrals as rational functions of the hypergeometric functions. In this way we resolve the problem of the numerical stability of calculation of the repulsion integrals. Finally, as an illustration, the configuration interaction calculation of the lowest lying states of the He atom is discussed. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Two-electron atoms (like He, H^-, Li^+) are of great importance for their relative simplicity. There are primarily three interesting problems to be studied on the two-electron atoms. First, since the nonrelativistic Schrödinger equation can be solved very accurately for the ground as well as low excited states,[1–13] the relativistic and QED effects can be taken into account[13–18] and compared to the experiment.[19–22] This yields together with the study of the hydrogenlike atoms precise test of QED as a fundamental theory of the interaction of the electrically charged particles.[23–25] The second interesting point is the study of resonances.[26–28] This was stimulated by the experimental discovery of the strong correlation effects in the doubly excited states of helium[29] and led to new theoretical concepts, like approximate quantum numbers[30–32] and others. For an excellent review of these methods, see Ref. 33. Third, if the many-electron wave function is searched for in the form of expansion of a properly symmetrized product of the one-electron functions all the necessary matrix elements can be reduced either to one- or two-electron matrix elements whatever the number of the electrons involved. Therefore, if we find an effective method of calculating these matrix elements for the two-electron atoms, this method can be directly applied to *all* atoms and to the simplest molecules where it is physically reasonable to use orbitals localized at one center.

For low lying states of the two-electron atoms with low nuclear charge, the best approach is the one based on the use of the explicitly correlated functions.[1–11,13] This method consists of considering the interelectronic distance r_{12} as one of the coordinates. For example, for the S-states

of helium, the two electron wave function is considered as a function of three variables r_1, r_2, and r_{12}, $\psi=\psi(r_1,r_2,r_{12})$. However, the disadvantage of this method is that transition to the three-electron atoms is very difficult[34] and increasing the number of the electrons further the method quickly loses its attractivity. Therefore, the method is not generally considered as a suitable tool for solving the many-electron problem.

The most accurate available method applicable for many electron problems is the configuration interaction method (CI) (see e.g., Refs. 35, 36). This method has been applied on the two-electron atoms either for finding some general trends of behavior of correlation energy like its angular dependence, optimization of the screening constant, and so on[37–44] or in combination with the complex scaling method (see, e.g., Ref. 45) for a description of resonances.[26–28,31,32]

However, the problem is when one wants to perform very large scale CI calculation to get very accurate results. Then one encounters what is usually refered to as the effect of linear dependence of the basis set. Due to numerical errors, for large basis sets the linear independence of the basis functions is lost. Thus, from some point the inclusion of more basis functions does not improve the variational results. To avoid this, one should keep the basis functions orthogonal. However, this requirement causes the highly excited functions to have large number of nodes and to change their sign frequently. That leads to the numerical instability of the calculation of the repulsion integrals.

This effect is quite general and appears also in the case of the explicitely correlated functions. However, here the convergence of the method is so fast that very accurate results are obtained before the problem appears.

To ensure numerical stability for the large scale CI calculations nonanalytic types of the basis functions like B-splines[12] or piecewise polynomials[41] or analytic types with many parameters[28] were invoked.

The aim of this paper is to suggest an efficient analytic method for calculating the one- and two-electron matrix elements applicable to all atoms and with numerical stability under control.

In this paper, a great deal of attention is devoted to the calculation of the repulsion integrals and the numerical stability of such a procedure. We expand the two-electron wave function into the symmetrized product of the complete, entirely discrete one-electron basis set. This basis set is in literature often refered to as a Sturmian one and its use goes back to the classical paper of Hylleraas.[46] However, in contrast to the usual treatment we identify these basis functions as the eigenfunction of one of the generators of the so(2,1) algebra.[47–52] This algebra is used for the calculation of the radial integrals appearing in the multipole expansion. We first introduce an analog to the Wigner–Eckart theorem for the so(2,1) algebra, i.e., we write the product of two radial functions as a linear combination of the radial functions. The coefficients of the linear combination can be expressed in terms of the hypergeometric functions. In this way we reduce the two-dimensional integration over four radial functions to the two-dimensional integration over two radial functions. Combining commutations relations of the so(2,1) algebra and analytic integration by parts we derive the reccurence relations for the integrals over two radial functions. In this way we reduce all the integrals to the integrals over nodeless functions. These integrals are calculated analytically. Finally, the derived reccurence relations are solved analytically in terms of the hypergeometric functions. Thus, we are able to express all the repulsion integrals as rational functions of the hypergeometric functions. Succeeding in this, this paper represents the solution of the problem of the numerical instability for the large scale CI calculations.

The problem considered in this paper was already tackled in Ref. 53. For the following reasons we believe that our solution is better suited for the computational purposes than that given in Ref. 53. First, when writing the products of the Laguerre polynomials as a linear combination of the Laguerre polynomials we succeded in expressing the coefficients of the linear combination in terms of the hypergeometric functions. Second, our recurrence relations for the integrals are much more simpler than that derived in Ref. 53. Third, we were able to solve them in terms of the hypergeometric functions. In this way all possible numerical instabilities are localized into the calculation of the well-known hypergeometric functions. These functions were thoroughly investigated by mathematicians and are known for long time. Once the values of these functions are

calculated, the computation can be run in the double presicion arithmetics. In Ref. 53, the numerically unstable parts of the calculation had to be performed in integer arithmetics. On the other hand, at the present stage, the method described in this paper is less general than that given in Ref. 53. Possible generalizations of our method are indicated in the conclusions and will be described in detail in the forthcoming paper.

The paper is organized as follows: First, the algebraic solution of the hydrogen atom by means of the so(2,1) Lie algebra is described. Second, the problem of the helium atom is put into the form suitable for the use of so(2,1) algebra. Then we turn to the calculation of the repulsion integrals. Relying on the usual multipole expansion and integrating out the angular degrees of freedom in the usual manner, we concentrate on the calculation of the radial integrals. The two methods for calculation of the radial integrals are described. The first one consists of the expansion of the radial functions into the Slater-type orbitals, i.e., into the products of the exponential function and power of r. It is shown that this method is numerically unstable and reason of the instability is clarified. The second, ''quasialgebraic'' method is that described above. Finally, as an illustration, the CI calculation for the lowest lying states of helium atom is made and the optimization of the screening constant is discussed.

We would like to stress that we are not going to compete with the techniques using explicitly correlated functions. We apply the method for the states where CI is known to be converging very slowly to see numerical stability of our computation of the integrals. It is reasonable to expect that for other states the performance of the method will be better.

II. ALGEBRAIC TREATMENT OF THE HYDROGEN ATOM

In this section we introduce the so(2,1) algebra and show its use for the solution of the Schrödinger equation for hydrogen atom. For more detailed discussion see, e.g., Ref. 47. We adopt the same notation as that in Refs. 47 and 48.

Let us consider the Schrödinger equation for the hydrogen atom in atomic units

$$\left[-\frac{\nabla^2}{2}-\frac{1}{r}\right]\psi=E\psi. \tag{1}$$

The key idea for solving this equation algebraically is to transform this equation into the equation for the eigenvalues n of the operator T_3

$$T_3|l,n\rangle=n|l,n\rangle, \tag{2}$$

where the operator T_3 equals

$$T_3=\frac{1}{2}\left(rp_r^2+\frac{l(l+1)}{r}+r\right). \tag{3}$$

Here p_r is the conjugated radial momentum

$$p_r=-i\left(\frac{d}{dr}+\frac{1}{r}\right), \tag{4}$$

$l(l+1)$ is the eigenvalue of L^2, the square of the angular momentum and n is the principal quantum number (see below).

Equation (1) can be transformed to Eq. (2) as follows. Using the expression for the Laplace operator in the spherical coordinates

$$\nabla^2=p_r^2+\frac{L^2}{r^2}, \tag{5}$$

multiplying Eq. (1) by r and making the scaling transformation $r\rightarrow nr$ we get

$$\left[\frac{1}{2}r\left(p_r^2+\frac{L^2}{r^2}\right)-n^2Er\right]\psi=n\psi. \tag{6}$$

We separate the angular and radial degrees of freedom

$$\langle \mathbf{x}|\psi\rangle=\langle r|l,n\rangle\langle \mathbf{n}|l,m\rangle, \tag{7}$$

where $\mathbf{n}$ is a unit vector pointing in arbitrary direction and $\langle \mathbf{n}|l,m\rangle$ are spherical harmonics, the eigenfunctions of the square and the third component of the angular momentum, L^2 and L_3, respectively. Setting

$$E=-\frac{1}{2n^2}, \tag{8}$$

Eqs. (2) and (6) are the same.

The advantage of this reformulation of the problem of the hydrogen atom is that first, as we show below, the problem of the eigenvalues of the operator T_3 can be solved purely algebraically, second, the spectrum of the operator T_3 is purely discrete. Therefore, this operator is much more advantageous for description of bound atomic states than the usual operator in Eq. (1).

The eigenvalues of the operator T_3 can be obtained by observation that T_3 and the operators

$$T_1=\frac{1}{2}\left(rp_r^2+\frac{l(l+1)}{r}-r\right) \tag{9}$$

and

$$T_2=rp_r \tag{10}$$

are closed under the commutation and form the so-called so(2,1) Lie algebra

$$[T_1,T_2]=-iT_3, \tag{11}$$

$$[T_2,T_3]=iT_1, \tag{12}$$

and

$$[T_3,T_1]=iT_2. \tag{13}$$

Proceeding in analogy with the usual treatment of the so(3) algebra of the components of the angular momentum we introduce the ladder operators

$$T_\pm=T_1\pm iT_2. \tag{14}$$

From the commutation relations (12) and (13) we get

$$[T_3,T_\pm]=\pm T_\pm. \tag{15}$$

Applying the last equation to the eigenvectors $|l,n\rangle$ we get after some manipulation

$$T_3(T_\pm|l,n\rangle)=(n\pm1)(T_\pm|l,n\rangle). \tag{16}$$

It is clear from the last equation that the vectors $T_\pm|l,n\rangle$ are the eigenvectors of the operator T_3 with the eigenvalues corresponding to $n\pm1$. Therefore, we can write

$$T_\pm|l,n\rangle=\alpha^\pm(l,n)|l,n\pm1\rangle, \tag{17}$$

where $\alpha^{\pm}(l,n)$ are numbers specified as follows. From Eqs. (14), (11), (9), (10), and (3) we get successively

$$T_+T_-=T_1^2+T_2^2+i[T_2,T_1]=T_1^2+T_2^2-T_3=T_3^2-l(l+1)-T_3. \tag{18}$$

Applying the last equation to the eigenvectors $|l,n\rangle$ we get from Eqs. (2) and (17)

$$\alpha^+(l,n-1)\alpha^-(l,n)=n^2-n-l(l+1)=(n+l)(n-l-1). \tag{19}$$

Requiring that the spectrum of the operator T_3 is bounded from below, i.e., there exists some $n_{\min}$ such that

$$T_-|l,n_{\min}\rangle=0, \tag{20}$$

we get from Eq. (19) that $\alpha^-(l,n_{\min})=0$. This implies

$$n_{\min}=l+1. \tag{21}$$

Therefore, the eigenvalue spectrum of the operator T_3 starts at $n=l+1$ and then increases by 1 up to the infinity. Since the energy E is given by Eq. (8) we identify n with the usual principal quantum number.

To determine the numbers $\alpha^{\pm}(l,n)$ uniquely we require that the eigenvectors $|l,n\rangle$ are normalized ($\langle l,n|l,n\rangle=1$). It leads to the following solution of Eq. (19):[48]

$$\alpha^+(l,n-1)=\alpha^-(l,n)=\sqrt{(n+l)(n-l-1)}. \tag{22}$$

For further considerations, let us show how the matrix elements of the radial coordinate r can be obtained. The radial coordinate r can be expressed as the difference of the operators T_3 and T_1 [see Eq. (3) and (9)]. From Eqs. (14), (17), and (22) we get that the operator r acts on the states $|l,n\rangle$ as follows (see, e.g., Ref. 48)

$$r|l,n\rangle=-\tfrac{1}{2}\sqrt{(n+l)(n-l-1)}|l,n-1\rangle+n|l,n\rangle-\tfrac{1}{2}\sqrt{(n+l+1)(n-l)}|l,n+1\rangle. \tag{23}$$

III. ALGEBRAIC TREATMENT OF THE HELIUM ATOM

In this section we first transform the Schrödinger equation into the form suitable for the use of the so(2,1) algebra. Next we turn our attention to the symmetry adaptation of the wave function. Relying on the multipole expansion, we separate angular and radial degrees of freedom in the conventional manner. We note that one of the alternatives to such an approach was recently suggested in Ref. 57. Finally, we integrate out the angular part and derive the expression for the radial integrals.

A. Schrödinger equation

The Schrödinger equation for the two-electron atoms in atomic units takes the form

$$\left[-\frac{\nabla_{(1)}^2}{2}-\frac{\nabla_{(2)}^2}{2}-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}\right]\psi=E\psi, \tag{24}$$

where Z is the charge of the nucleus and r_{12} denotes the interelectronic distance.

By scaling the coordinates of the electrons $\mathbf{x}^{(i)}\to\eta Z^{-1}\mathbf{x}^{(i)}$, $i=1,2$, we get an equivalent equation

$$\left[-\frac{\nabla_{(1)}^2}{2}-\frac{\nabla_{(2)}^2}{2}-\frac{\eta}{r_1}-\frac{\eta}{r_2}+\frac{\eta}{Z}\frac{1}{r_{12}}\right]\psi=\frac{\eta^2}{Z^2}E\psi. \tag{25}$$

Here, η is an arbitrary scaling parameter that can be subject to further optimization. Multiplying Eq. (25) by $r_1 r_2$, writing the energy E as

$$E = -\frac{Z^2}{\eta^2} + \Delta E \tag{26}$$

and using Eqs. (3) and (5) we rewrite Eq. (25) into the form

$$\left[r_1 (T_3^{(2)} - \eta) + r_2 (T_3^{(1)} - \eta) + \frac{\eta}{Z} r_1 r_2 r_{12}^{-1} \right] \psi = \frac{\eta^2}{Z^2} \Delta E r_1 r_2 \psi. \tag{27}$$

Since the matrix elements of the one-electron operators r_i and $T_3^{(i)}$ can be calculated from Eqs. (23) and (2), respectively, the only remaining matrix elements to be calculated are the matrix elements of the operator $r_1 r_2 r_{12}^{-1}$, i.e., the repulsion integrals. Before doing so, we turn our attention to the construction of the wave function.

B. Construction of the wave function

The two electron wave function $|\psi\rangle$ has to be antisymmetric with respect to the interchange of the electrons. In this paper we restrict ourselves to the calculation of the ground state energy. Since the spin part of the ground state wave function of the helium atom is antisymmetric, the space part has to be symmetric. Further, because of the spherical symmetry of the problem, the components and the square of the total angular momentum $\mathbf{L} = \mathbf{L}^{(1)} + \mathbf{L}^{(2)}$ commute with the Hamiltonian. It means that the Hamiltonian has the block structure and the states with different eigenvalues of L_3 and L^2 do not mutually interact. The ground state is the singlet state with $L = 0$, where $L(L+1)$ is the eigenvalue of the operator L^2. Therefore, the angular part of the wave function equals

$$|(l,l)0\rangle = \sum_{m=-l}^{l} (l,m,l,-m|0,0)|l,m\rangle^{(1)}|l,-m\rangle^{(2)}. \tag{28}$$

Here, $(\,|\,)$ denotes the Clebsch–Gordan (CG) coefficients. It follows from the properties of CG coefficients that Eq. (28) is the only nonzero combination of the products of one-electron angular states yielding the state with $L = 0$. It means that to characterize the angular part of the total wave function we need just one quantum number l. It also follows from the properties of CG coefficients that the linear combination is symmetric with respect to the interchange of the electrons. Therefore, we expand the exact wave function into the unperturbed wave functions as follows:

$$|\psi\rangle = \sum_{i=0}^{\infty} f_i |i\rangle, \tag{29}$$

where

$$|i\rangle = 2^{-(1+\delta_{n_{i1},n_{i2}})/2} (|l_i, n_{i1}\rangle^{(1)}|l_i, n_{i2}\rangle^{(2)} + |l_i, n_{i2}\rangle^{(1)}|l_i, n_{i1}\rangle^{(2)})|(l_i, l_i)0\rangle. \tag{30}$$

Here, the states $|l,n\rangle$ are the eigenstates of the operator T_3 given by Eq. (2). The coefficients f_i will be determined from the diagonalization of Eq. (27).

C. Matrix elements

Now we describe how the matrix elements of the operator $r_1 r_2 r_{12}^{-1}$ among the functions (30) are calculated.

Projecting the states $|l,n\rangle$ onto the coordinate basis we get the radial functions $R_{n,l}(r) = \langle r|l,n\rangle$. Introducing the inner product

$$\langle l_1,n_1|l_2,n_2\rangle=\int_0^\infty dr\, r\, R_{n_1,l_1}(r)R_{n_2,l_2}(r) \tag{31}$$

the functions $R_{n,l}(r)$ are orthonormal for $l_1=l_2$, $\langle l_1,n_1|l_1,n_2\rangle=\delta_{n_1,n_2}$. We note that this inner product differs from the usual one by the factor r^{-1} in the integrand (see, e.g., Refs. 47, 48).

To separate the angular and radial degrees of freedom we expand r_{12}^{-1} in the multipole expansion

$$r_{12}^{-1}=\frac{1}{r_>}\sum_{l=0}^{\infty}\left(\frac{r_<}{r_>}\right)^l P_l(\mathbf{n}_1\cdot\mathbf{n}_2), \tag{32}$$

where $r_<=r_1$, $r_>=r_2$ if $r_1<r_2$ and $r_<=r_2$, $r_>=r_1$ if $r_1>r_2$. Here, the $P_l(x)$ denotes the Legendre polynomials. With the definition of the inner product (31) and multipole expansion (32) the matrix elements of $r_1r_2r_{12}^{-1}$ can be written as

$$\langle i|r_1r_2r_{12}^{-1}|j\rangle=2^{-(\delta_{n_{i1},n_{i2}}+\delta_{n_{j1},n_{j2}})/2}\sum_{l=|l_i-l_j|}^{l_i+l_j}\theta_{l_i,l_j,l}[X^{l_i,l_j,l}_{n_{i1},n_{i2},n_{j1},n_{j2}}+X^{l_i,l_j,l}_{n_{i1},n_{i2},n_{j2},n_{j1}}], \tag{33}$$

where l in the summation increases by 2.

Here, the angular part $\theta_{l_i,l_j,l}$ corresponds to the calculation of the matrix elements of the Legendre polynomials between the coupled states (28)

$$\theta_{l_i,l_j,l}=\langle(l_i,l_i)0|P_l(\mathbf{n}_1\cdot\mathbf{n}_2)|(l_j,l_j)0\rangle=(-1)^{l_i+l_j}\frac{[(2l_i+1)(2l_j+1)]^{1/2}}{2l+1}(l_i,0,l_j,0|l,0)^2. \tag{34}$$

This result is obtained with help of the algebraic angular-momentum methods (see e.g., Refs. 54–56). It follows from the properties of the CG coefficients that $\theta_{l_i,l_j,l}$ is zero unless $|l_i-l_j|\leqslant l\leqslant l_i+l_j$ and l_i+l_j+l is even. Therefore, the sum in Eq. (33) is not infinite and in fact contains only a few terms.

The radial part of the integration reads

$$\begin{aligned}X^{l_i,l_j,l}_{n_{i1},n_{i2},n_{j1},n_{j2}}&=\int_0^\infty dr_1\int_0^\infty dr_2 r_1^2r_2^2R_{n_{i1},l_i}(r_1)R_{n_{i2},l_i}(r_2)\frac{r_<^l}{r_>^{l+1}}R_{n_{j1},l_j}(r_1)R_{n_{j2},l_j}(r_2)\\&=\int_0^\infty dr_1R_{n_{i1},l_i}(r_1)R_{n_{j1},l_j}(r_1)r_1^{l+2}\int_{r_1}^\infty dr_2R_{n_{i2},l_i}(r_2)R_{n_{j2},l_j}(r_2)r_2^{-l+1}\\&\quad+\int_0^\infty dr_1R_{n_{i1},l_i}(r_1)R_{n_{j1},l_j}(r_1)r_1^{-l+1}\int_0^{r_1}dr_2R_{n_{i2},l_i}(r_2)R_{n_{j2},l_j}(r_2)r_2^{l+2}.\end{aligned} \tag{35}$$

The following section is devoted to the calculation of these integrals.

IV. CALCULATION OF THE RADIAL INTEGRALS

In this section that is the main part of the paper, two methods of the calculations of the radial integrals (35) are described. The first method is given in the Sec. IV A and is based on the reduction of the integrals to the integrals over the Slater-type orbitals. This method is essentially the same as that used in Ref. 37. This method is shown to be numerically unstable. The second method is described in the remaining three subsections. In the Sec. IV B the integrals over four radial functions are transformed to the integrals over two radial functions with help of the analog

of Wigner–Eckart theorem for so(2,1) algebra. In Sec. IV C the recurrence relations for the remaining integrals over two radial functions are derived. In Sec. IV D these recurrence relations are solved analytically.

A. Expansion into the Slater-type orbitals

The expansion of the integrals into the Slater-type orbitals is based on the explicit form of the radial functions

$$R_{n,l}(r)=2\sqrt{\frac{(n-l-1)!}{(n+l)!}}e^{-r}(2r)^l L_{n-l-1}^{2l+1}(2r), \tag{36}$$

where $L_{n-l-1}^{2l+1}(2r)$ are generalized Laguerre polynomials (see, e.g., Refs. 59–61).

Using the explicit form of the Laguerre polynomials we can rewrite the radial functions $R_{n,l}(r)$ as the linear combination of the Slater-type orbitals, i.e., as the products of the exponential function and power of r

$$R_{n,l}(r)=2\sum_{q=0}^{n-l-1} d_{n,l,q}e^{-r}r^{q+l}, \tag{37}$$

where the coefficients $d_{n,l,q}$ equal

$$d_{n,l,q}=\sqrt{\frac{(n-l-1)!}{(n+l)!}}\frac{(n+l)!}{(n-l-1-q)!q!(2l+1+q)!}(-1)^q 2^{q+l}. \tag{38}$$

Inserting this expansion into the integrals (35) we obtain after some manipulation

$$X_{n_{i1},n_{i2},n_{j1},n_{j2}}^{l_i,l_j,l}=\sum_{q_{i1}=0}^{n_{i1}-l_i-1} d_{n_{i1},l_i,q_{i1}}\sum_{q_{i2}=0}^{n_{i2}-l_i-1} d_{n_{i2},l_i,q_{i2}}\sum_{q_{j1}=0}^{n_{j1}-l_j-1} d_{n_{j1},l_j,q_{j1}}\sum_{q_{j2}=0}^{n_{j2}-l_j-1} d_{n_{j2},l_j,q_{j2}}$$
$$\times[I_{q_{i1}+q_{j1}+l_i+l_j+1,q_{i2}+q_{j2}+l_i+l_j+1}^{l}+I_{q_{i2}+q_{j2}+l_i+l_j+1,q_{i1}+q_{j1}+l_i+l_j+1}^{l}], \tag{39}$$

where

$$\begin{aligned}I_{a,b}^{l}&=2^4\int_0^\infty dr_1 e^{-2r_1}r_1^{a-l}\int_0^{r_1}dr_2 e^{-2r_2}r_2^{b+l+1}\\&=2^4\int_0^\infty dr_1 e^{-2r_1}r_1^{b+l+1}\int_{r_1}^\infty dr_2 e^{-2r_2}r_2^{a-l}\\&=(a-l)!2^{-1-2b-l-a}\sum_{q=0}^{a-l}\frac{(b+l+q+1)!}{q!}2^{-q}.\end{aligned} \tag{40}$$

This way of calculation of the integrals (35) suffers by numerical instability. For example, running the formula (39) between the states with $n_{i1}=21$, $n_{i2}=19$, $l_i=3$ and $n_{j1}=17$, $n_{j2}=23$, $l_j=1$ in the double precision arithmetics yields the totally meaningless result 10^{20} for both $l=2$ and $l=4$. The reason for the instability is the changing sign of the $d_{n,l,q}$ coefficients, Eq. (38), that causes cancellation errors (see also discussion in Ref. 53). These changes are related to the orthogonality of the Laguerre polynomials. There is, of course, possibility to relax the requirement of having the orthonormal system of the functions and to consider the radial wave functions in the form $\tilde{R}_{n,l}(r)=\tilde{U}_{n,l}e^{-r}r^{n-1}$. This system is complete as well as the system (36). The pertinent radial integrals (35) can then be calculated according to the formula (40) and the matrix elements of the operators in Eq. (27) are calculated easily as well. The problem of doing this is

that the numerical instability is just moved from the calculation of the integrals (35) to the generalized eigenvalue problem (27). In the case of the nonorthogonal basis the matrix $r_1 r_2$ on the right-hand side of Eq. (27) is not just quasitridiagonal, but full.

Therefore, we will solve the problem of the numerical stability on the level of calculation of the integrals (35).

B. "Wigner–Eckart theorem" for so(2,1) algebra

Looking at Eq. (35) we observe that there are always the products of the wave functions of the same variable (like $R_{n_{i1},l_i}(r_1)R_{n_{j1},l_j}(r_1)$) that enter into the integration. Therefore, in the first step we try to write the product of two radial functions as a linear combination of the radial functions. Here, we proceed analogously to the angular integration. This trick of writing the product of two spherical harmonics as a linear combination of the spherical harmonics is a special case of much more general theorem called Wigner–Eckart theorem (see e.g., Refs. 54–58). We found its analog for so(2,1) algebra to be

$$rR_{n_i,l_i}(r)R_{n_j,l_j}(r)=A^{l_i,l_j}_{n_i,n_j}\sum_{n=-1}^{n_i+n_j-l_i-l_j-2} c^{l_i,l_j}_{n_i,n_j,n}\sqrt{\frac{(n_i+n_j-n-1+l_i+l_j)!}{(n_i+n_j-n-l_i-l_j-2)!}}R_{n_i+n_j-n-1,l_i+l_j}(2r), \tag{41}$$

where the multiplicative factor $A^{l_i,l_j}_{n_i,n_j}$ equals

$$A^{l_i,l_j}_{n_i,n_j}=\frac{2^{1-n_i-n_j}(n_i+n_j-l_i-l_j-2)!(n_i+l_i+n_j+l_j)!}{(n_i-l_i-1)!(n_j-l_j-1)!}\sqrt{\frac{(n_i-l_i-1)!}{(n_i+l_i)!}}\sqrt{\frac{(n_j-l_j-1)!}{(n_j+l_j)!}}. \tag{42}$$

The coefficients $c^{l_i,l_j}_{n_i,n_j,n}$ of the linear combination read

$$c^{l_i,l_j}_{n_i,n_j,n}=C^{l_i,l_j}_{n_i,n_j,n}-(n_i+n_j-l_i-l_j-2-n)C^{l_i,l_j}_{n_i,n_j,n+1}, \tag{43}$$

where the coefficients $C^{l_i,l_j}_{n_i,n_j,n}$ are given as

$$C^{l_i,l_j}_{n_i,n_j,n}=\frac{F(-n_i+l_i+1,-n;-n_i-n_j+l_i+l_j+2;2)\,F(-n_i-l_i,-n;-n_i-n_j-l_i-l_j;2)}{(n_i+l_i+n_j+l_j-n-1)!n!} \tag{44}$$

for $n\geqslant 0$ and equal zero otherwise. Here, $F(\alpha,\beta;\gamma;z)$ denotes the hypergeometric function (see e.g., Refs. 59–61).

The formula (41) was derived from the identities for the Laguerre polynomials found in Ref. 59, namely Eq. (5) of Sec. 8.6.4 and Eq. (11) of Sec. 5.5.2.

It is evident from the orthonormality of the radial functions for $l_i=l_j$ that an expression like (41) has to exist. What is new here is the explicit form of the coefficients $c^{l_i,l_j}_{n_i,n_j,n}$.

Using Eq. (41) in the radial integrals (35) we rewrite them into the form

$$\begin{aligned}X^{l_i,l_j,l}_{n_{i1},n_{i2},n_{j1},n_{j2}}=&A^{l_i,l_j}_{n_{i1},n_{j1}}A^{l_i,l_j}_{n_{i2},n_{j2}}\sum_{n_1=-1}^{n_{i1}+n_{j1}-l_i-l_j-2} c^{l_i,l_j}_{n_{i1},n_{j1},n_1}\sum_{n_2=-1}^{n_{i2}+n_{j2}-l_i-l_j-2} c^{l_i,l_j}_{n_{i2},n_{j2},n_2}\\ &\times\sqrt{\frac{(n_{i1}+n_{j1}-n_1-1+l_i+l_j)!}{(n_{i1}+n_{j1}-n_1-l_i-l_j-2)!}}\sqrt{\frac{(n_{i2}+n_{j2}-n_2-1+l_i+l_j)!}{(n_{i2}+n_{j2}-n_2-l_i-l_j-2)!}}\\ &\times Q^{l_i+l_j,l}_{n_{i1}+n_{j1}-1-n_1,n_{i2}+n_{j2}-1-n_2},\end{aligned} \tag{45}$$

where $Q^{L,l}_{N_1,N_2}$ denotes the integrals over two radial functions

$$Q^{L,l}_{N_1,N_2}=Q^{+,L,l}_{N_1,N_2}+Q^{-,L,l}_{N_1,N_2}. \tag{46}$$

Here,

$$Q^{+,L,l}_{N_1,N_2}=\int_0^\infty dr_1 R_{N_1,L}(2r_1)r_1^{l+1}\int_{r_1}^\infty dr_2 R_{N_2,L}(2r_2)r_2^{-l} \tag{47}$$

and

$$Q^{-,L,l}_{N_1,N_2}=\int_0^\infty dr_1 R_{N_1,L}(2r_1)r_1^{-l}\int_0^{r_1} dr_2 R_{N_2,L}(2r_2)r_2^{l+1}. \tag{48}$$

Before proceeding further let us point out that once the values of the hypergeometric functions and factorials are calculated, Eq. (43) is numerically stable. Therefore, this step of the calculation, the reduction of the integrals over four radial functions to the integrals over two radial functions, is numerically stable. The next step is to find the stable way of calculation of the integrals (46)–(48).

C. Derivation of the reccurrence relations for the integrals

In this subsection, we derive the recurrence relations for the integrals (47) and (48).

To motivate our further considerations we note that when we expand the radial functions in the integrals (47) and (48) into the powers of r, Eq. (37), the numerical instabilities appear again. Obviously, to achieve numerical stabilization we have to treat the functions $R_{n,l}(2r)$ as one indivisible object. The functions $R_{n,l}(2r)$ are treated in this way, when applying algebraic approach. The ladder operators $T_\pm$ change the whole function $R_{n,l}(2r)$ into the other functions $R_{n\pm1,l}(2r)$. Therefore, in the following we try to apply these ladder operators to the radial functions. To do so, we have to combine this algebraic technique with the analytic integration by parts.

1. Elementary example

For the sake of transparency, let us first consider the integral

$$\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2). \tag{49}$$

After we show the numerically stable way how to calculate this integral, we extend it to the integrals (47) and (48).

First, let us show that

$$\int_0^{r_1} dr_2\, r_2\left(\frac{d}{dr_2}+\frac{1}{r_2}\right)[R_{N_2,L}(2r_2)]=r_1 R_{N_2,L}(2r_1). \tag{50}$$

The proof is elementary. Expanding the brackets on the left hand side we get

$$\int_0^{r_1} dr_2\, r_2\left(\frac{d}{dr_2}+\frac{1}{r_2}\right)[R_{N_2,L}(2r_2)]=\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2)+\int_0^{r_1} dr_2\, r_2\frac{d}{dr_2}[R_{N_2,L}(2r_2)]. \tag{51}$$

Integrating the second term by parts

$$\int_0^{r_1} dr_2\, r_2\frac{d}{dr_2}[R_{N_2,L}(2r_2)]=[r_2 R_{N_2,L}(2r_2)]_0^{r_1}-\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) \tag{52}$$

and inserting this term into Eq. (51) we get Eq. (50).

Second, we observe that the operator $r((d/dr)+(1/r))$ is up to the imaginary unit equal to the operator T_2, Eq. (10) and the operator T_2 can be expressed as the difference of the creation and annihilation operators T_+ and T_-, Eq. (14)

$$r\left(\frac{d}{dr}+\frac{1}{r}\right)=irp_r=iT_2=\frac{1}{2}(T_+-T_-). \tag{53}$$

Thus, from the algebraic side we see that the operator (53) acts on the radial functions as

$$r\left(\frac{d}{dr}+\frac{1}{r}\right)[R_{N_2,L}(2r)]=\frac{1}{2}\sqrt{(N_2+L+1)(N_2-L)}R_{N_2+1,L}(2r) - \frac{1}{2}\sqrt{(N_2+L)(N_2-L-1)}R_{N_2-1,L}(2r), \tag{54}$$

where Eq. (17) was used.

Finally, combining the analytic result (50) with the algebraic one (54) we get the recurrence relation for the integrals (49)

$$\frac{1}{2}\sqrt{(N_2+L+1)(N_2-L)}\int_0^{r_1}dr_2\,R_{N_2+1,L}(2r_2)-\frac{1}{2}\sqrt{(N_2+L)(N_2-L-1)}\int_0^{r_1}dr_2\,R_{N_2-1,L}(2r_2) =r_1R_{N_2,L}(2r_1). \tag{55}$$

With this reccurence relation we reduce the quantum number N_2 to $L+1$. The integral over nodeless function $R_{L+1,L}(2r_2)$ is calculated analytically according to Eq. (40). The advantage of the recurrence relation (55) is that calculating integral over $R_{N_2+1,L}(2r_2)$ from the integral over $R_{N_2-1,L}(2r_2)$ contains the sum of positive numbers and not the difference of two numbers. Therefore, it is numerically stable.

2. Recurrence relations for $Q^{-;L,l}_{N_1;N_2}$ connecting different values of N_2

Now, we extend the described procedure to the calculation of the integrals appearing in Eq. (48)

$$\int_0^{r_1}dr_2\,r_2^{l+1}R_{N_2,L}(2r_2). \tag{56}$$

The analytic aspect is the same. By the same calculation as for Eq. (50) we get

$$\int_0^{r_1}dr_2\,r_2\left(\frac{d}{dr_2}+\frac{1}{r_2}\right)[R_{N_2,L}(2r_2)r_2^{l+1}]=r_1^{l+2}R_{N_2,L}(2r_1). \tag{57}$$

From the algebraic side we can deal with the extra term r^{l+1} using the commutation relation[47]

$$[r^k,irp_r]=-kr^k \tag{58}$$

that holds for every integer $k>0$. Applying this operator identity for $k=l+1$ to the radial functions $R_{N_2,L}(2r)$ we get

$$\int_0^{r_1} dr_2\, ir_2 p_{r_2}[R_{N_2,L}(2r_2) r_2^{l+1}] = \int_0^{r_1} dr_2\, r_2^{l+1} ir_2 p_{r_2}[R_{N_2,L}(2r_2)] + (l+1)\int_0^{r_1} dr_2\, r_2^{l+1} R_{N_2,L}(2r_2). \tag{59}$$

Combining again the analytical result (57) with the algebraic results (54) and (59) we get

$$r_1^{l+2} R_{N_2,L}(2r_1) = \frac{1}{2}\sqrt{(N_2+L+1)(N_2-L)}\int_0^{r_1} R_{N_2+1,L}(2r_2) r_2^{l+1} dr_2 - \frac{1}{2}\sqrt{(N_2+L)(N_2-L-1)}\int_0^{r_1} R_{N_2-1,L}(2r_2) r_2^{l+1} dr_2 + (l+1)\int_0^{r_1} R_{N_2,L}(2r_2) r_2^{l+1}. \tag{60}$$

Finally, multiplying the last equation by $r_1^{-l} R_{N_1,L}(2r_1)$ and integrating from zero to infinity we obtain

$$\tfrac{1}{8}\langle L, N_1 | r | L, N_2\rangle = \tfrac{1}{2}\sqrt{(N_2+L+1)(N_2-L)}\, Q^{-,L,l}_{N_1,N_2+1} - \tfrac{1}{2}\sqrt{(N_2+L)(N_2-L-1)}\, Q^{-,L,l}_{N_1,N_2-1} + (l+1) Q^{-,L,l}_{N_1,N_2}, \tag{61}$$

where we used Eqs. (31) and (48). Matrix elements of r are calculated from Eq. (23).

3. Recurrence relations for $Q^{-,L,l}_{N_1,N_2}$ connecting different values of N_1

To derive recurrence relations for $Q^{-,L,l}_{N_1,N_2}$ connecting the different values of N_1 we will need a slight modification of Eq. (57)

$$\int_0^{\infty} dr_1\, r_1\left(\frac{d}{dr_1}+\frac{1}{r_1}\right)[r_1^{-l} R_{N_1,L}(2r_1)]\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1} = -\int_0^{\infty} dr_1\, r_1^2 R_{N_1,L}(2r_1) R_{N_2,L}(2r_1). \tag{62}$$

This equation can be derived as follows. We expand the bracket on the left-hand side

$$\int_0^{\infty} dr_1\, r_1\left(\frac{d}{dr_1}+\frac{1}{r_1}\right)[r_1^{-l} R_{N_1,L}(2r_1)]\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1} = \int_0^{\infty} dr_1\, r_1^{-l} R_{N_1,L}(2r_1)\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1} + \int_0^{\infty} dr_1\, r_1 \frac{d}{dr_1}[r_1^{-l} R_{N_1,L}(2r_1)]\int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1} \tag{63}$$

and integrate the second term by parts

$$\int_0^\infty dr_1\, r_1 \frac{d}{dr_1}[r_1^{-l} R_{N_1,L}(2r_1)] \int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1}$$
$$= \left[r_1^{-l+1} R_{N_1,L}(2r_1) \int_0^{r_1} dr_2\, R_{N_2,L}(2r_2) r_2^{l+1} \right]_0^\infty - \int_0^\infty dr_1\, r_1^{-l} R_{N_1,L}(2r_1) \int_0^{r_1} dr_2$$
$$\times R_{N_2,L}(2r_2) r_2^{l+1} - \int_0^\infty dr_1\, r_1^2 R_{N_1,L}(2r_1) R_{N_2,L}(2r_1), \tag{64}$$

where we used the Newton formula for differentiation of the integral with respect to the upper bound. Since the boundary term vanishes, by inserting Eq. (64) into Eq. (63) we get Eq. (62).

Also the algebraic side of the calculation requires only slight modification of the previous case. Instead of the commutation relation (58) we use the commutation relation

$$[r^{-k}, irp_r] = -kr^{-k} \tag{65}$$

that is obtained from Eq. (58) by multiplying both sides by r^{-k}. Applying this operator identity to the radial functions $R_{N_1,L}(2r_1)$ for $k=l$ leads to

$$ir_1 p_{r_1}[r_1^{-l} R_{N_1,L}(2r_1)] = r_1^{-l} ir_1 p_{r_1}[R_{N_1,L}(2r_1)] - lr_1^{-l} R_{N_1,L}(2r_1). \tag{66}$$

We use the last equation in the integrand on the left hand side of Eq. (62), then apply Eq. (54), where we just replace N_2 by N_1. After some manipulation we get the sought reccurence relation

$$-\tfrac{1}{8}\langle L, N_1|r|L, N_2\rangle = \tfrac{1}{2}\sqrt{(N_1+L+1)(N_1-L)}\, Q^{-,L,l}_{N_1+1,N_2}$$
$$- \tfrac{1}{2}\sqrt{(N_1+L)(N_1-L-1)}\, Q^{-,L,l}_{N_1-1,N_2} - l Q^{-,L,l}_{N_1,N_2}. \tag{67}$$

4. Recurrence relations for the integrals $Q^{+,L,l}_{N_1,N_2}$

No new ideas are required to derive the recurrence relations for the integrals $Q^{+,L,l}_{N_1,N_2}$. Proceeding in analogy with the previous cases we derive recurrence relations connecting the integrals with different values of N_2,

$$-\tfrac{1}{8}\langle L, N_1|r|L, N_2\rangle = \tfrac{1}{2}\sqrt{(N_2+L+1)(N_2-L)}\, Q^{+,L,l}_{N_1,N_2+1}$$
$$- \tfrac{1}{2}\sqrt{(N_2+L)(N_2-L-1)}\, Q^{+,L,l}_{N_1,N_2-1} - l Q^{+,L,l}_{N_1,N_2} \tag{68}$$

and the recurrence relations connecting the integrals with different values of N_1,

$$\tfrac{1}{8}\langle L, N_1|r|L, N_2\rangle = \tfrac{1}{2}\sqrt{(N_1+L+1)(N_1-L)}\, Q^{+,L,l}_{N_1+1,N_2}$$
$$- \tfrac{1}{2}\sqrt{(N_1+L)(N_1-L-1)}\, Q^{+,L,l}_{N_1-1,N_2} + (l+1) Q^{+,L,l}_{N_1,N_2}. \tag{69}$$

It is immediately seen from Eqs. (61), (67), (68), and (69) that

$$Q^{+,L,l}_{N_1,N_2} = Q^{-,L,l}_{N_2,N_1}. \tag{70}$$

Through the derived recurrence relations all the needed integrals are reduced to the calculation of the integrals $Q^{+,L,l}_{L+1,L+1}$. These integrals can be calculated from Eq. (40),

$$Q^{+,L,l}_{L+1,L+1}=\frac{2^{-2+4L}}{(2L+1)!}I^{l}_{L,L}=2^{-1}(2L+1)!\,F(1,-L+l;-2L-1;2). \tag{71}$$

D. Solution of recurrence relations

To solve recurrence relations derived in the previous section it is advantageous to eliminate the irrational factors by introducing the unnormalized integrals

$$\tilde{Q}^{\pm,L,l}_{N_1,N_2}=4\sqrt{\frac{(N_1+L)!}{(N_1-L-1)!}}\sqrt{\frac{(N_2+L)!}{(N_2-L-1)!}}\,Q^{\pm,L,l}_{N_1,N_2}. \tag{72}$$

Then the recurrence relations take the form

$$\begin{aligned}&-\sqrt{\frac{(N_1+L)!}{(N_1-L-1)!}}\sqrt{\frac{(N_2+L)!}{(N_2-L-1)!}}\langle L,N_1|r|L,N_2\rangle\\&\quad=(N_2-L)\tilde{Q}^{+,L,l}_{N_1,N_2+1}-(N_2+L)\tilde{Q}^{+,L,l}_{N_1,N_2-1}-2l\tilde{Q}^{+,L,l}_{N_1,N_2}\end{aligned} \tag{73}$$

and

$$\begin{aligned}&\sqrt{\frac{(N_1+L)!}{(N_1-L-1)!}}\sqrt{\frac{(N_2+L)!}{(N_2-L-1)!}}\langle L,N_1|r|L,N_2\rangle\\&\quad=(N_1-L)\tilde{Q}^{+,L,l}_{N_1+1,N_2}-(N_1+L)\tilde{Q}^{+,L,l}_{N_1-1,N_2}+2(l+1)\tilde{Q}^{+,L,l}_{N_1,N_2}.\end{aligned} \tag{74}$$

The recurrence relations for $\tilde{Q}^{-,L,l}_{N_1,N_2}$ are obtained using Eq. (70).

1. Solution in the variable N_1

Because of Eq. (70) we can restrict our attention to the case $N_1\geqslant N_2$. We note that the matrix elements $\langle L,N_1|r|L,N_2\rangle$ vanish whenever $|N_2-N_1|>1$, see Eq. (23). That means that for $N_1>N_2+1$ the recurrence relation (74) is homogenous. Since it is the three-term recursion relation we need two initial values of $\tilde{Q}^{+,L,l}_{N_1,N_2}$, namely $\tilde{Q}^{+,L,l}_{N_2+2,N_2}$ and $\tilde{Q}^{+,L,l}_{N_2+1,N_2}$ to determine the solution uniquely.

General solution of homogenous Eq. (74) is

$$\begin{aligned}\tilde{Q}^{+,L,l}_{N_1,N_2}&=g_1(N_2)F(N_1-L,-L+l+1;-2L;2)\\&\quad+g_2(N_2)(-1)^{N_1-L-1}F(N_1-L,-L-l-1;-2L;2).\end{aligned} \tag{75}$$

We found this solution by realizing that the recurrence relation (74) can be transformed to the one of the relations between contigous hypergeometric functions (see, e.g., Ref. 61). This solution holds for all $N_1>N_2$ including the cases $N_1=N_2+2$ and $N_1=N_2+1$, that can be viewed as the initial conditions. In principle we could determine the functions $g_1(N_2)$ and $g_2(N_2)$ by considering Eq. (75) for $N_1=N_2+1$ and $N_1=N_2+2$. However, it is more advantageous to proceed in different way; to insert directly solution (75) into Eq. (73). This is done in the following paragraph.

2. Solution in the variable N_2

If we consider Eq. (73) for $N_1=N_2+2$ we obtain

$$(N_2-L)\tilde{Q}^{+,L,l}_{N_2+2,N_2+1}-2l\tilde{Q}^{+,L,l}_{N_2+2,N_2}-(N_2+L)\tilde{Q}^{+,L,l}_{N_2+2,N_2-1}=0. \tag{76}$$

Further, considering Eq. (73) for $N_1=N_2+3$ we get

$$(N_2-L)\tilde{Q}^{+,L,l}_{N_2+3,N_2+1}-2l\tilde{Q}^{+,L,l}_{N_2+3,N_2}-(N_2+L)\tilde{Q}^{+,L,l}_{N_2+3,N_2-1}=0, \tag{77}$$

and so on. It seen from these equations that the values of $\tilde{Q}^{+,L,l}_{N_1,N_2}$ for $N_2=N_1+1$ can be calculated from Eq. (76), the values of $\tilde{Q}^{+,L,l}_{N_1,N_2}$ for $N_2=N_1+2$ can be calculated from Eq. (77), and so on. Therefore, all the values of $\tilde{Q}^{+,L,l}_{N_1,N_2}$ for $N_1>N_2$ including the values $N_1=N_2+1$ and $N_1=N_2+2$ can be calculated from *homogenous* Eq. (73).

By inserting solution (75) into the homogenous equation (73) we get

$$\begin{aligned}&F(N_1-L,-L+l+1;-2L;2)[(N_2-L)g_1(N_2+1)-(N_2+L)g_1(N_2-1)-2lg_1(N_2)]\\&\quad+(-1)^{N_1-L-1}F(N_1-L,-L-l-1;-2L;2)[(N_2-L)g_2(N_2+1)\\&\quad-(N_2+L)g_2(N_2-1)-2lg_2(N_2)]=0.\end{aligned} \tag{78}$$

Requiring that this equation is satisfied for $N_1=N_2+1$ and $N_1=N_2+2$ the expression in the brackets have to vanish. It is the three-term recursion relation having the solution

$$\begin{aligned}g_i(N_2)=&g_i^{(1)}(-1)^{N_2-L-1}F(N_2-L,-L+l;-2L;2)\\&+g_i^{(2)}F(N_2-L,-L-l;-2L;2),\quad i=1,2.\end{aligned} \tag{79}$$

Thus, Eqs. (75) and (79) represent a general solution for $\tilde{Q}^{+,L,l}_{N_1,N_2}$ for all $N_1>N_2$. Four constants $g_i^{(j)}$, $i,j=1,2$ are determined from four values $\tilde{Q}^{+,L,l}_{L+i+j,L+j}$, $i,j=1,2$.

The solution for $\tilde{Q}^{-,L,l}_{N_1,N_2}$ is obtained by reversing the role of N_1 and N_2 in Eqs. (75) and (79). The constants $g_i^{(j)}$, $i,j=1,2$ are determined as in the previous case.

3. Final result

Proceeding in the way described above we arrive to the explicit solution for the integrals $\tilde{Q}^{\pm,L,l}_{N_1,N_2}$,

$$\begin{aligned}\tilde{Q}^{+,L,l}_{N_1,N_2}=&K(L,l)F(N_1-L,-L+l+1;-2L;2)[(-1)^{N_2+1-L}\\&\times F(N_2-L,-L+l;-2L;2)+F(N_2-L,-L-l;-2L;2)]\end{aligned} \tag{80}$$

and

$$\begin{aligned}\tilde{Q}^{-,L,l}_{N_1,N_2}=&K(L,l)(-1)^{N_1-L-1}F(N_1-L,-L+l;-2L;2)\times[(-1)^{N_2+1-L}F(N_2-L,-L-l-1;\\&-2L;2)+F(N_2-L,-L+l+1;-2L;2)].\end{aligned} \tag{81}$$

The constant $K(L,l)$ is in both cases the same and equals

$$K(L,l)=\frac{(2L+1)!}{F(2,-L+l+1;-2L;2)}\,\frac{L+1-(l+1)F(1,-L+l;-2L-1;2)}{F(1,-L+l;-2L;2)+F(1,-L-l;-2L;2)}. \tag{82}$$

These solutions hold for all $N_1>N_2$ and for all $L>l$. The solution for $L=l$ has very simple form

$$\tilde{Q}^{+,L,L}_{N_1,N_2}=0 \tag{83}$$

and

$$\tilde{Q}^{-,L,L}_{N_1,N_2}=(-1)^{N_2-N_1}\frac{(N_2+L)!}{(N_2-L-1)!}. \tag{84}$$

TABLE I. Labeling of the basis sets. States are ordered in accordance with the increasing unperturbed energies, i.e., in accordance with the sum of principal quantum numbers $n_{12}(i)=n_{i1}+n_{i2}$.

i	n_{i1}	n_{i2}	l_i	n_{12}
1	1	1	0	2
2	1	2	0	3
3	1	3	0	4
4	2	2	0	4
5	2	2	1	4
6	1	4	0	5
7	2	3	0	5
8	2	3	1	5

The solutions for $N_1=N_2$ for $N_1>L+1$ are obtained by considering Eq. (73) for $N_2=N_1-1$.

The explicit solution of reccurence relations given in this subsection finishes our way to the stable calculation of the radial integrals. The final solution of numerical stable calculation of the radial integrals is the use of Eq. (45), where the integrals $Q^{L,l}_{N_1,N_2}$ are calculated from Eqs. (46), (72), (80), (81), (83), and (84). Running these equations in the double precision arithmetics for $n_{i1}=21$, $n_{i2}=19$, $n_{j1}=17$, and $n_{j2}=23$ for different values of l_i, l_j, and l yields the relative error in the worst cases of the order 10^{-14}.

Finally, we would like to emphasize that all the hypergeometric functions appearing in Eqs. (44), (80), (81), and (82) are in fact polynomials, so the question of convergence of the corresponding series in their computation does not arise.

V. CONFIGURATION INTERACTION

As an illustration, we solve Eq. (27) variationally for the helium atom, i.e., for $Z=2$. It is well-known that the ground state of helium is one of the most difficult cases of calculation of the electron–electron correlation (see below), so we give this example to see the performance of the method under unfavorable circumstances. We label the basis vectors $|i\rangle$ in the way indicated in Table I. The states are ordered in such a way that the unperturbed energies increase, i.e., according to the sum of the hydrogen principal quantum numbers $n_{i1}+n_{i2}$. The truncated basis sets are characterized by the number n_{12} that denotes the maximum of the sums $n_{i1}+n_{i2}$ of the states included in the truncated basis sets. For example, the basis set characterized by $n_{12}=2$ includes all the states with $2\geqslant n_{i1}+n_{i2}$. This basis set is one-dimensional $\{|0,1\rangle^{(1)}|0,1\rangle^{(2)}|(0,0)0\rangle\}$. The basis set characterized by $n_{12}=3$ is two-dimensional: $\{|0,1\rangle^{(1)}|0,1\rangle^{(2)}|(0,0)0\rangle, 2^{-1/2}(|0,1\rangle^{(1)}|0,2\rangle^{(2)}+|0,2\rangle^{(1)}|0,1\rangle^{(2)})|(0,0)0\rangle\}$. Similarly, the basis set characterized by $n_{12}=4$ is five-dimensional, by $n_{12}=5$ eight-dimensional, and so on.

We note that our variational calculation corresponds to what is usually called the full CI with the successivelly increasing basis set.

The parameter η in Eq. (27) was optimized numerically by calculating the values of the energy for some discrete values of η and looking for the minimum of these discrete values. Results are shown in Table II.

We found that the parameter η with increasing basis set decreases, see Table II. This can be intuitively understood as follows. We have to build the atomic orbitals in such a way to describe the motion of the electrons properly, i.e., to obtain high probability of their appearence in the places where they ''really'' are. As we enlarge the basis sets the maximum of this probability is moving to the places more distant from the nucleus. Therefore, to get it to the proper place, close to the nucleus, the screening constant η has to decrease. Numerical analysis shows that the optimal screening constant η goes to zero roughly like n_{12}^{-1}. However, this analysis is not very reliable since the optimal screening constant η is determined with lower accuracy than the variational

TABLE II. The variational energy levels $E(\eta)$ of the ground state of helium obtained by diagonalization of the generalized eigenvalue problem (27) with the optimized choices of the parameter η. *order* denotes the order of the truncated matrix. The relative error is calculated with respect to the value -2.903724377 given in Ref. 8. ∞ denotes the extrapolated value, the extrapolation was made with respect to n_{12}^{-3}, see text for details.

n_{12}	Order	η	$E(\eta)$	Error $E(\eta)$ [%]
2	1	1.18518	-2.847656250000	1.930
3	2	1.18518	-2.847656250000	1.930
4	5	0.97196	-2.895444678791	0.285
5	8	0.94051	-2.897109123114	0.227
6	14	0.79681	-2.900714155920	0.103
7	20	0.76085	-2.901452790421	0.0782
8	30	0.68217	-2.902341254761	0.0476
9	40	0.64803	-2.902654772148	0.0368
10	55	0.59598	-2.902975741200	0.0257
28	1015	0.28285	-2.903681963068	0.00146
29	1120	0.27532	-2.903685852234	0.00132
30	1240	0.26782	-2.903689437387	0.00120
31	1360	0.26104	-2.903692451003	0.00109
32	1496	0.25431	-2.903695236574	0.00100
33	1632	0.24821	-2.903697608901	0.000928
34	1785	0.24206	-2.903699807464	0.000846
35	1938	0.23660	-2.903701701251	0.000780
36	2109	0.23126	-2.903703460890	0.000720
37	2280	0.22601	-2.903704991252	0.000667
38	2470	0.22129	-2.903706417162	0.000618
39	2660	0.21684	-2.903707667974	0.000575
40	2870	0.21223	-2.903708835966	0.000535
∞	∞		-2.903724034618	0.0000117

energy $E(\eta)$. The reason is that with the increasing basis set the second derivative of the function $E(\eta)$ in minimum goes to zero, see Ref. 37. Therefore small variations of η around the minimum yield energies that differ negligibly.

It is seen from Table II that convergence of the variational energy levels towards the exact one is rapid at the beginning but rather slow afterwards. It is quite remarkable that we can get ''chemical accuracy'' -2.903, i.e., error about 1 kcal/mol just with 55 basis functions considering the simplicity of the wave function used. However, it is seen from Table II that to go beyond this ''chemical accuracy'' it is very difficult. This slow convergence can be partially removed by extrapolating the results for finite basis sets to the infinite one by using the Thiele–Padé extrapolation.[50,62] The result for $n_{12}=40$ is $E(40)=-2.903\,708\,8$ compared to the exact result obtained with the explicitely correlated functions $-2.903\,724\,377$.[8] Extrapolating the values given in the Table II from n_{12} equal to 30 to n_{12} equal to 40 with respect to n_{12}^{-3} we obtained $-2.903\,724\,0$. Extrapolating from the interval $n_{12}=28$ to $n_{12}=38$ we obtained $-2.903\,723\,98$, so reliable part of the extrapolated result is $E_{\mathrm{extr}}=-2.903\,724$. The dependence of $E(n_{12})$ on n_{12}^{-3} was guessed by analyzing the values from $n_{12}=20$ to $n_{12}=40$. It is seen that the extrapolation improves the variational result by two orders.

The slow convergence of the CI method for the ground state of helium is well known and was analyzed in detail in several papers.[38,39,41,42] This slow convergence is related to slow convergence of the multipole expansion for the ground state energy because of the cusp of the wave function for $r_1=r_2$. For this reason the multipole expansion of r_{12}^{-1} has been abandoned in the accurate calculations of two electron atoms and the explicitely correlated functions were introduced. Nevertheless, even for the two-electron atoms the standard CI is more advantegeous than the use of the explicitely correlated functions in the cases when the electron–electron correlation is not so strong. This appears first for the highly ionized two-electron atoms when the interaction between the electrons is supressed by the factor $1/Z$. For such systems, the relativistic and QED effects become very important and it is much easier to calculate the pertinent matrix elements of the

TABLE III. The variational energy levels $E(\eta)$ of the first excited S-state of helium obtained by diagonalization of the generalized eigenvalue problem (27) with the optimized choices of the parameter η. *Order* denotes the order of the truncated matrix. The relative error is calculated with respect to the value -2.1459740292 given in Ref. 64. ∞ denotes the extrapolated value, the extrapolation was made with respect to n_{12}^{-3}.

n_{12}	Order	η	$E(\eta)$	Error $E(\eta)$ [%]
28	1015	0.75446	−2.145962069450	0.000557
29	1120	0.73376	−2.145963231801	0.000503
30	1240	0.71477	−2.145964245885	0.000455
31	1360	0.69624	−2.145965134389	0.000414
32	1496	0.67907	−2.145965916881	0.000378
33	1632	0.66286	−2.145966608567	0.000345
34	1785	0.64685	−2.145967222783	0.000317
35	1938	0.63233	−2.145967769878	0.000291
36	2109	0.61763	−2.145968259173	0.000268
37	2280	0.60442	−2.145968697983	0.000248
38	2470	0.59219	−2.145969092719	0.000230
39	2660	0.57911	−2.145969449151	0.000213
40	2870	0.56765	−2.145969771531	0.000198
∞	∞		−2.145974038455	0.419×10^{-6}

relativistic and QED operators in the basis considered in this paper than in the basis of the explicitely correlated functions. Second, for the excited states, especially for the states with total angular momenta larger than zero, the electron–electron correlation is decreased due to the different angular distribution of the electron orbitals. Intuitively, the electron-electron correlation is the strongest in the case of the S-states and especially for the ground state where the electrons, roughly speaking, occupy the same orbital. From Table III it is seen that already for the first excited S-state the performance of the method is better. It is expected than in the combination with the complex scaling method the performance of the method for higher excited states will further improve.[27]

Finally, let us point out that to judge overall performance of the technique described we should have in mind the last sentences from the Introduction.

VI. CONCLUSIONS

In this paper the use of so(2,1) Lie algebra for calculation of the spectra of the two-electron atoms was suggested. It was shown that by applying this algebra we were able to express all the necessary matrix elements in the analytic form. Particularly, we succeeded in expressing the repulsion integrals in terms of the hypergeometric functions. This was done in three steps, all of them are completely novel from the methodological point of view.

First, we formulated analog of the Wigner–Eckart theorem for so(2,1) algebra. In this way we reduced the repulsion integrals over four radial functions to the repulsion integrals over two radial functions. Second, combining algebraic technique with the integration by parts we derived recurrence relations for the repulsion integrals over two radial functions. Third, we solved the recurrence relations, in form of the difference equations in two variables, in terms of the hypergeometric functions. These *analytic and numerical stable* formulas for the repulsion integrals are the main result of this paper. It solves the problem of the numerical stability and enables us to make the large scale CI calculation with analytic basis functions.

As an illustration, the full CI calculation with increasing basis set for the ground state of helium was made. It is well-known that the electron–electron correlation is in this case very strong. Nevertheless, we showed that by means of the Thiele–Padé extrapolation more accurate results can be obtained. This extrapolation technique is rather straightforward. With more sophisticated technique of extrapolation we can expect even better results. This will be published in the forthcoming paper in which also the methodical problems of extrapolation (including *ab initio* estimate of the error) will be discussed. Our calculation cannot, of course, compete with that

obtained by means of the explicitely correlated functions. However, since the numerical difficulties are encountered also within that approach, some of the ideas introduced in this paper could be usefull also in those calculations.

Also, one may expect that the ideas introduced in this paper can be applied to Gaussian functions used in most of quantum chemical calculations.

In this paper we restricted our attention to the calculation of the states with the total square of the angular momentum equal to zero and to the singlet spin states and we used just one screening constant to optimize the energy. However, only slight modifications are necessary to deal also with the states of different symmetry and with more screening constants. These modifications will be discussed in the forthcoming paper.

The method described in this paper can also be used for calculation of $1/Z$ expansion (see, e.g., Refs. 9, 63), the variational and perturbational calculation of atoms with more than two electrons, the inclusion of the relativistic and QED corrections for the two-electron atoms with large Z and the calculation of the dynamical problems on helium like one- and two-photon transitions.[64,65]

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Temporally stable coherent states for a free magnetic Schrödinger operator

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Eigenfunctions and eigenvalues of the free magnetic Schrödinger operator, describing a spinless particle confined to an infinite layer of fixed width, are discussed in detail. The eigenfunctions are realized as an orthonormal basis of a suitable Hilbert space. Four different classes of temporally stable coherent states associated with the operator are presented. The first two classes are derived as coherent states with one degree of freedom and the last two classes are derived with two degrees of freedom. The dynamical algebra of each class is found. Statistical quantities associated to each class of coherent states are calculated explicitly. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1760846]

I. INTRODUCTION

By generalizing the definition of canonical coherent states (CS), Gazeau and Klauder[9] proposed a method to construct temporally stable CS for a quantum system with one degree of freedom. Since then, the method has been successfully applied to different quantum systems.[2,8] As an extension of Ref. 9, a method was presented to build CS for systems with several degrees of freedom.[11,16] Motivated from the recent interest on temporally stable coherent states, we present in this article four different classes of CS using the spectrum of the free magnetic Schrödinger operator

$$H_0=\frac{1}{2M}\left(\mathbf{P}-\frac{e}{c}\mathbf{A}\right)^2, \tag{1.1}$$

where $\mathbf{A}$ is the magnetic vector potential, e is the charge of the particle, c is the speed of light, and $\mathbf{P}=-i\hbar\nabla$ with $\hbar$ being the Planck's constant divided by 2π. By constructing the CS for the operator H_0 we also demonstrate the method proposed in Ref. 16 and analyze the temporal stability and action identity conditions for the multidimensional case. These features were excluded from the discussion of Ref. 16.

The article is organized as follows: In Sec. II, we introduce the detailed description of the free magnetic Schrödinger operator (1.1), exploring its spectrum and the eigenvectors. In Sec. III we realize the eigenfunctions of Sec. II as an orthonormal basis of a Hilbert space. For the sake of completeness in Sec. IV we discuss the definition of the Gazeau–Klauder CS. In Sec. V, associated with the spectrum of (1.1), two classes of CS with one degree of freedom are constructed. In Sec.

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VI, two classes of CS with two degrees of freedom are constructed. In Sec. VII, a detailed classification of the dynamical algebra is provided. In Sec. VIII we explicitly calculate the quantum statistical quantities associated with the CS.

II. THE FREE MAGNETIC SCHRÖDINGER OPERATOR

Consider an infinite layer of fixed width d, that is, $\Sigma=\mathbb{R}^2\times[0,d]$. Suppose the layer is placed into a perpendicular homogeneous magnetic field of intensity $\mathbf{B}=(0,0,B)$, where B is a constant. The Hamiltonian of this system can be written using (1.1) as

$$H_0=\frac{1}{2M}\left(\mathbf{P}^2-\frac{e}{c}\mathbf{P}\cdot\mathbf{A}-\frac{e}{c}\mathbf{A}\cdot\mathbf{P}+\frac{e^2}{c^2}\mathbf{A}^2\right). \tag{2.1}$$

When the circular gauge $\mathbf{A}=-\frac{1}{2}\mathbf{r}\times\mathbf{B}=\frac{1}{2}|B|(-y,x,0)$ is chosen, we have for a state vector ψ

$$\mathbf{P}\cdot\mathbf{A}\psi=-i\hbar(\nabla\cdot\mathbf{A})\psi-i\hbar\mathbf{A}\cdot\nabla\psi=\mathbf{A}\cdot\mathbf{P}\psi.$$

Consequently, a spinless quantum particle confined to the layer is described by the free magnetic Schrödinger operator

$$H_0=\frac{1}{2M}\left(\mathbf{P}^2-\frac{2e}{c}\mathbf{A}\cdot\mathbf{P}+\frac{e^2}{c^2}\mathbf{A}^2\right) \tag{2.2}$$

acting in $L^2(\Sigma)$ with Dirichlet boundary conditions

$$\psi(\mathbf{x},0)=\psi(\mathbf{x},d)=0,\quad \mathbf{x}=(x,y)\in\mathbb{R}^2.$$

In the absence of an additional interaction, the operator H_0 can be written as

$$H_0=-\frac{\hbar^2}{2M}\nabla^2+\frac{ie\hbar|B|}{2Mc}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)+\frac{e^2|B|^2}{8Mc^2}(x^2+y^2). \tag{2.3}$$

The presence of the potential x^2+y^2 suggests the use of the cylindrical coordinates for the separation of the variables. Thus we have

$$H_0=-\frac{\hbar^2}{2M}\nabla^2+\frac{e^2|B|^2}{8Mc^2}r^2+\frac{ie\hbar|B|}{2Mc}\frac{\partial}{\partial\theta}, \tag{2.4}$$

where

$$\nabla^2=\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+\frac{\partial^2}{\partial z^2}.$$

If we define the cyclotron frequency $\omega_c=-(e|B|/Mc)$, then

$$H_0=-\frac{\hbar^2}{2M}\nabla^2+\frac{M\omega_c^2}{8}r^2+\frac{\omega_c}{2}L_z, \tag{2.5}$$

where

$$L_z=-i\hbar\frac{\partial}{\partial\theta}.$$

Let

$$\Psi(r,\theta,z)=\psi(r,\theta)\chi(z),$$

we can easily find that the differential equation satisfied by $\chi(z)$ and obeying boundary conditions $\chi(0)=\chi(d)=0$ yields

$$\chi_n(z)\equiv\sqrt{\frac{2}{d}}\sin\left(\frac{\pi nz}{d}\right),\quad n=1,2,\ldots, \tag{2.6}$$

which form an orthonormal basis in $L^2[0,d]$. Note that the case of $n=0$ correspondence to $\chi_0(z)=0$ is physically insignificant. The corresponding eigenvalues are

$$\epsilon_n=\frac{\hbar^2}{2M}\left(\frac{\pi(n+1)}{d}\right)^2,\quad n=0,1,2,\ldots\ . \tag{2.7}$$

This solution is usually ignored in most of the research on such problems[8,10,16] on account of the interest being confined to the motion of the particle in the plane at right angles to the magnetic field.

On the other hand, the differential equation satisfied by $\psi(r,\theta)$ describes a two-dimensional particle in the perpendicular homogeneous field in the circular gauge. Setting $\psi(r,\theta)=\phi(r)e^{il\theta}$ with l an integer, one can easily show after some algebraic calculations, that the differential equation satisfied by

$$\phi(r)=\left(\frac{e|B|}{2\hbar c}\right)^{|l|/2}r^{|l|}e^{-(e|B|/4\hbar c)r^2}G\left(\sqrt{\frac{e|B|}{2\hbar c}}r\right) \tag{2.8}$$

is

$$\frac{d^2G}{d\xi^2}+\left(\frac{|l|+1}{\xi}-1\right)\frac{dG}{d\xi}+\frac{\lambda-2-2|l|}{4\xi}G=0,$$

where $\xi=(e|B|/2\hbar c)r^2$ and $\lambda=(4Mc/e|B|\hbar)\epsilon_{ml}-2l$. This is known as Kummer's differential equation, which has a solution

$$G(\xi)={}_1F_1\left(\frac{-\lambda+2+2|l|}{4};|l|+1;\xi\right)$$

with the eigenvalue condition $(-\lambda+2+2|l|)/4=-m$, where $m=0,1,2,\ldots$ are the principal quantum numbers and $l=0,\pm1,\pm2,\ldots$ are the angular momentum quantum numbers. The eigenvalue condition yields the Landau levels

$$\epsilon_{ml}=\frac{e|B|\hbar}{2Mc}(2m+l+|l|+1),$$

and the eigenfunctions become

$$\psi_{m,l}(r,\theta)=N_{ml}r^{|l|}e^{-(e|B|/4\hbar c)r^2}{}_1F_1\left(-m;|l|+1;\frac{e|B|}{2\hbar c}r^2\right)e^{il\theta}, \tag{2.9}$$

where N_{ml} is a normalization constant and ${}_1F_1$ is the confluent hypergeometric function defined by

$${}_1F_1(-m;\gamma;z)=\sum_{k=0}^{m}\frac{(-m)_k}{(\gamma)_k\ k!}z^k.$$

The Pochhammer symbol $(a)_k$ is defined by $(a)_0=1$ and $(a)_k=a(a+1)(a+2)\cdots(a+k-1)$ for $k=1,2,3,\ldots$, and may be expressed in terms of the gamma function by $(a)_k=\Gamma(a+k)/\Gamma(a)$,

when a is not a negative integer $-m$. In the exceptional cases, $(-m)_k=0$ if $k>m$ and otherwise $(-m)_k=(-1)^k m!/(m-k)!$. The normalization constant N_{ml} follows out of the inner product relation

$$\langle \psi_{ml}|\psi_{m'l'}\rangle=\int_0^{2\pi}\int_0^{\infty}\psi_{ml}(r,\theta)\overline{\psi_{m'l'}(r,\theta)}rdrd\theta=\delta_{mm'}\delta_{ll'}. \tag{2.10}$$

This yields

$$N_{ml}^{-2}=\left(\frac{2\hbar c}{e|B|}\right)^{|l|+1}\frac{\pi\Gamma(|l|+1)}{(|l|+1)_m}m!,$$

and by means of the identities

$$\int_0^{\infty}r^{2\gamma-1}e^{-sr^2}{}_1F_1(-n;\gamma;sr^2){}_1F_1(-m;\gamma;sr^2)dr=\frac{1}{2}\frac{n!\Gamma(\gamma)}{s^{\gamma}(\gamma)_n}\delta_{mn} \tag{2.11}$$

and

$$\int_0^{2\pi}e^{i(l-l')\theta}d\theta=0 \text{ or } 2\pi \text{ according as } l\neq l' \text{ or } l=l'$$

we readily conclude that $\{\psi_{ml}(r,\theta)\}$ is indeed an orthonormal set with respect to the measure $rdrd\theta$, where $0\leqslant\theta<2\pi$. Finally, the spectrum of the free Hamiltonian H_0 is

$$E(m,l,n)=\frac{e|B|\hbar}{2Mc}(2m+l+|l|+1)+\frac{\hbar^2}{2M}\left(\frac{\pi(n+1)}{d}\right)^2,\quad n=0,1,2,\ldots. \tag{2.12}$$

We immediately observe that the energy levels ϵ_{ml} for positive l, yield

$$E(m,l,n)=\frac{e|B|\hbar}{2Mc}(2m+2l+1)+\frac{\hbar^2}{2M}\left(\frac{\pi(n+1)}{d}\right)^2,\quad n=0,1,2,\ldots. \tag{2.13}$$

For l negative or zero, we have $|l|+l=0$ which cause the infinite degeneracy of Landau levels ϵ_{ml}. Thereby the spectrum (2.12) becomes

$$E(m,n)=\frac{e|B|\hbar}{2Mc}(2m+1)+\frac{\hbar^2}{2M}\left(\frac{\pi(n+1)}{d}\right)^2,\quad n=0,1,2,\ldots. \tag{2.14}$$

This particular expression of the spectrum[13] was the starting point of the interesting study of Exner and Nemcova[6] concerning the spectral properties of a Hamiltonian describing the motion of a spinless quantum particle confined to an infinite planar layer with hard walls and interacting with a periodic lattice of point perturbations as well as in a homogeneous magnetic field perpendicular to the layer. They remark therein that the spectrum (2.14) is nondegenerate if the ratio of the coefficients $|B|$ and π^2/d^2 is irrational.[7] We shall claim this in the next section.

For simplicity we may assume hereafter that $e=\hbar=2M=c=1$, and hence we summarize the situation as follows. For each $n=0,1,2,\ldots$ there is an orthonormal set of wave functions $\Psi_{mln}(r,\theta,z)\equiv\psi_{ml}(r,\theta)\chi_n(z)$, eigensolutions for the Hamiltonian H_0, given by

$$\Psi_{mln}(r,\theta,z)=\sqrt{\left(\frac{|B|}{2}\right)^{|l|+1}\frac{2(|l|+1)_m}{\pi\, d\, m!\Gamma(|l|+1)}}\,r^{2|l|}e^{-(|B|/4)r^2}$$
$$\times{}_1F_1\left(-m;|l|+1;\frac{|B|r^2}{2}\right)e^{il\theta}\sin\left(\frac{(n+1)\pi z}{d}\right) \tag{2.15}$$

in the state Hilbert space $\mathfrak{L}^2(\Sigma)$, which actually is the direct product $\mathfrak{L}^2[0,\infty)\otimes L^2[0,2\pi)\otimes L^2[0,d])$.

III. DENSITY ARGUMENT

Making use of the tensor product concept immediately preceding, we lump the tensor product $\mathfrak{L}^2[0,\infty)\otimes L^2[0,2\pi)$ of the first two Hilbert spaces into the Hilbert space $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$, which consists of all complex-valued Lebesgue measurable functions h on $[0,\infty)\times[0,2\pi)$ with

$$\int_0^\infty \int_0^{2\pi} |h(r,\theta)|^2 r\,d\theta dr<\infty.$$

Let $\mathfrak{L}^2(\Sigma')\equiv\mathfrak{L}^2([0,\infty)\times[0,2\pi))\otimes L^2[0,d]$, where

$$\left\{\Psi_{ml}(r,\theta)=\sqrt{\left(\frac{|B|}{2}\right)^{|l|+1}\frac{(|l|+1)_m}{\pi\, m!\Gamma(|l|+1)}}\,r^{2|l|}e^{-(|B|/4)\,r^2}{}_1F_1\left(-m;|l|+1;\frac{|B|r^2}{2}\right)e^{il\theta}\right\}$$

with $m=0,1,2,\ldots$ and $l=0,\pm1,\pm2,\ldots$ is an orthonormal system of the Hilbert space $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$ and

$$\left\{\sqrt{\frac{2}{d}}\sin\left(\frac{\pi(n+1)z}{d}\right):n=0,1,2,\ldots\right\}$$

is an orthonormal basis of the Hilbert space $L^2[0,d]$. If we can show that $\{\Psi_{ml}:m=0,1,2,\ldots,l=0,\pm1,\pm2,\ldots\}$ is an orthonormal basis of the Hilbert space $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$, then $\{\Psi_{mln}:m=0,1,2,\ldots,l=0,\pm1,\pm2,\ldots,n=0,1,2,\ldots\}$ becomes an orthonormal basis (Ref. 22, p. 52, Theorem 3.12) of the Hilbert space $\mathfrak{L}^2(\Sigma')$.

Theorem 3.1: *The set* $\{\Psi_{ml}:m=0,1,2,\ldots,l=0,\pm1,\pm2,\ldots\}$ *is an orthonormal basis of the Hilbert space* $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$.

Proof: Let us assume that it is not. Thus there exist a nontrivial $\Psi\in\mathfrak{L}^2([0,\infty)\times[0,2\pi))$ satisfying

$$\int_0^\infty\int_0^{2\pi}\Psi_{ml}(r,\theta)\overline{\Psi(r,\theta)}r\,dr\,d\theta=0 \quad \text{for all } m=0,1,2,\ldots \text{ and } l=0,\pm1,\pm2,\ldots .$$

Since the linear hull[18]

$$(\text{L.H.})\left({}_1F_1\left(-k;|l|+1;\frac{|B|r^2}{2}\right)(0\leqslant k\leqslant m)\right)=(\text{L.H.})(r^{2k}(0\leqslant k\leqslant m)),$$

it follows after taking suitable linear combination of the orthonormal set $\{\Psi_{kl}:0\leqslant k\leqslant n\}$ with l fixed, that

$$\int_0^\infty\int_0^{2\pi}r^{2|l|+2m}e^{-(|B|r^2/4)}e^{il\theta}\overline{\Psi(r,\theta)}r\,dr\,d\theta=\int_0^\infty r^{2|l|+2m+1}e^{-(|B|r^2/4)}\int_0^{2\pi}e^{il\theta}\overline{\Psi(r,\theta)}\,d\theta\,dr=0$$

for all $m=0,1,2,\ldots$ and $l=0,\pm1,\pm2,\ldots$. By a further linear combination involving the complex parameter s, namely,

$$e_m(sr^2)=\sum_{k=0}^{m}\frac{(sr^2)^k}{k!}, \tag{3.1}$$

we obtain, by means of Lebesgue dominated convergence theorem[20] applied in terms of the following inequality:

$$|r^{2|l|+1}e_m(-sr^2)e^{-(|B|r^2/4)}e^{il\theta}| \leqslant r^{2|l|+1}e^{(|s|-(|B|/4))r^2}|\Psi(r,\theta)| \in L^1([0,\infty)\times[0,2\pi))$$

for all $m=0,1,2,\ldots$ and after taking limit $m\to\infty$, that the holomorphic function of variable s,

$$\int_0^\infty \int_0^{2\pi} r^{2|l|+1}e^{-(s+(|B|/4))r^2}e^{il\theta}\overline{\Psi(r,\theta)}dr = \int_0^\infty r^{2|l|+1}e^{-(s+(|B|/4))r^2}\int_0^{2\pi} e^{il\theta}\overline{\Psi(r,\theta)}d\theta dr = 0$$

for all s in the half-plane $\Re(s) > -(|B|/4)$. We arrive at this conclusion by means of analytic continuation of the fact that the immediately preceding holomorphic function takes on the value 0 if $|s|<|B|/4$. We make the substitution $r=\sqrt{t}$, and thus achieve

$$\int_0^\infty t^{|l|}e^{-(s+(|B|/4))t}\int_0^{2\pi} e^{il\theta}\overline{\Psi(\sqrt{t},\theta)}d\theta dt = 0 \quad \text{for all} \quad l=0,\pm 1,\pm 2,\ldots .$$

Utilizing the uniqueness of Laplace transform,[3] we conclude that

$$\int_0^{2\pi} e^{il\theta}\overline{\Psi(r,\theta)}d\theta = 0 \quad \text{a.e. in } r \text{ on } [0,\infty) \text{ for } l=0,\pm 1,\pm 2,\ldots .$$

In consequence hereof, there exist Lebesgue measurable subsets E_l of $[0,\infty)$, such that their complements in $[0,\infty)$ have one-dimensional Lebesgue measure zero, i.e., $\mu_1((0,\infty)\backslash E_l)=0$ for all $l=0,\pm 1,\pm 2,\ldots$. We define $E=\cap_{l=-\infty}^{\infty}E_l$ and note

$$\int_0^{2\pi} e^{il\theta}\overline{\Psi(r,\theta)}d\theta = 0 \quad \forall r\in E \quad \text{and} \quad \mu_1((0,\infty)\backslash E)=0,$$

which follows directly from

$$(0,\infty)\backslash\left(\bigcap_{l=-\infty}^{\infty} E_l\right) = \bigcup_{l=-\infty}^{\infty}((0,\infty)\backslash E_l) \quad \text{with} \quad \mu_1((0,\infty)\backslash E) \leqslant \sum_{l=-\infty}^{\infty}\mu_1((0,\infty)\backslash E_l)=0.$$

Thus it becomes clear that

$$\int_0^{2\pi} e^{il\theta}\overline{\Psi(r,\theta)}d\theta = 0 \quad \forall\ r\in E \ \text{ and } \ \forall\ l=0,\pm 1,\pm 2,\ldots .$$

Since $\Psi(r,\theta)\in\mathfrak{L}^2([0,\infty)\times[0,2\pi))$, namely,

$$\int_0^\infty\int_0^{2\pi}|\Psi(r,\theta)|^2 r d\theta dr = \int_0^{2\pi}\int_0^\infty |\Psi(r,\theta)|^2 r dr d\theta = \int\int_{[0,\infty)\times[0,2\pi)} |\Psi(r,\theta)|^2 d\mu(r,\theta) < \infty$$

with $d\mu(r,\theta)=rdrd\theta$, which follows from the Tonelli–Hobson theorem,[21] we may conclude without loss of generality that

$$\int_0^{2\pi} e^{il\theta}\overline{\Psi(r,\theta)}d\theta = 0 \quad \forall\ l=0,\pm 1,\pm 2,\ldots \ \text{ and } \ r\in E \ \text{ with } \ \Psi(r,\cdot)\in\mathfrak{L}^2[0,\infty).$$

We consequently have for $r\in E$ with $\Psi(r,\cdot)\in\mathfrak{L}^2[0,\infty)$ that

$$\int_0^{2\pi}|\Psi(r,\theta)|^2 d\theta = 0 \quad \text{for all } r \text{ satisfying } \int_0^{2\pi}|\Psi(r,\theta)|^2 d\theta < \infty.$$

Because this holds for almost all $r\in[0,\infty)$, it follows that

$$\int_0^\infty\int_0^{2\pi}|\Psi(r,\theta)|^2 r\,d\theta\,dr=0,$$

which in turn implies Ψ is a trivial $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$-function. Hence $\{\Psi_{ml}:m=0,1,2,\ldots,l=0,\pm1,\pm2,\ldots\}$ is an orthonormal basis of $\mathfrak{L}^2([0,\infty)\times[0,2\pi))$. □

Thus $\{\Psi_{mln}:m=0,1,2,\ldots,l=0,\pm1,\pm2,\ldots,n=0,1,2,\ldots\}$ is an orthonormal basis of $\mathfrak{L}^2(\Sigma')=\mathfrak{L}^2([0,\infty)\times[0,2\pi))\otimes L^2[0,d]$.

We shall also consider the case where $|l|+l=0$, where in this case the spectrum takes the form

$$E(m,n)=|B|(2m+1)+\left(\frac{\pi(n+1)}{d}\right)^2. \tag{3.2}$$

We fix $l=0$ for the wave function ψ_{mnl} of (2.15). In this case $\psi_{mnl}:=\psi_{mn}$ can be written as $\psi_{mn}=\phi_m\otimes\chi_n$ where

$$\phi_m(r)=\sqrt{|B|}e^{-(|B|/4)r^2}\,{}_1F_1\left(-m;1;\frac{|B|r^2}{2}\right)\quad\text{and}\quad\chi_n(z)=\sqrt{\frac{2}{d}}\sin\left(\frac{\pi(n+1)z}{d}\right).$$

From (2.11) we have

$$\int_0^\infty e^{-(|B|/2)r^2}\,{}_1F_1\left(-n;1;\frac{|B|r^2}{2}\right)\,{}_1F_1\left(-m;1;\frac{|B|r^2}{2}\right)r\,dr=\frac{1}{|B|}\,\delta_{mn}.$$

Thus $\{\phi_m:m=0,1,2,\ldots\}$ is an orthonormal system in the Hilbert space $\mathfrak{L}^2[0,\infty)$.

Corollary 3.1: When $|B|$ and π^2/d^2 are irrationally related, the spectrum $E(m,n)$ of (3.2) is nondegenerate and the set of vectors

$$\{\psi_{mn}=\phi_m\otimes\chi_n:m=0,1,2,\ldots;n=0,1,2,\ldots\}$$

forms an orthonormal basis of the Hilbert space $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$.

Proof: If we have two pairs (m,n) and (m',n') such that $E(m,n)=E(m',n')$, then

$$\frac{\pi^2}{|B|d^2}=\frac{2(m'-m)}{(n+1)^2-(n'+1)^2}$$

is a rational number. To prove $\mathfrak{B}_1=\{\psi_{mn}:m=0,1,2,\ldots;n=0,1,2,\ldots\}$ is an orthonormal basis of $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ it is enough to show that $\mathfrak{B}_2=\{\phi_m:\ m=0,1,2,\ldots\}$ is an orthonormal basis of $\mathfrak{L}^2[0,\infty)$. Suppose $\mathfrak{B}_2$ is not an orthonormal basis of $\mathfrak{L}^2[0,\infty)$, then there exists a nontrivial $\phi\in\mathfrak{L}^2[0,\infty)$ such that

$$\int_0^\infty\phi_m(r)\overline{\phi(r)}r\,dr=0$$

for all $m=0,1,2,\ldots$. Since

$$(\text{L.H.})\left({}_1F_1\left(-k;1;\frac{|B|r^2}{2}\right)(0\leqslant k\leqslant m)\right)=(\text{L.H.})(r^{2k}\ (0\leqslant k\leqslant m)),$$

we have after taking suitable linear combination of the orthonormal set $\{\phi_k:0\leqslant k\leqslant m\}$ that

$$\int_0^\infty r^{2m+1}e^{-(|B|r^2/2)}\overline{\phi(r)}\,dr=0\quad\text{for all}\quad m=0,1,2,\ldots\ .$$

By a further linear combination of (3.1) and by means of the Lebesgue dominated convergence theorem applied to

$$|e_m(-sr^2)e^{-(|B|r^2/4)}| \leqslant e^{|s|-(|B|r^2/4)}|\phi(r)| \in L^1[0,\infty); \quad m=0,1,2,\ldots$$

we obtain

$$\int_0^\infty e^{-(s+(|B|/4))r^2}\overline{\phi(r)}r\,dr=0$$

for all s such that $\Re e(s)>-(|B|/4)$. By letting $r=\sqrt{t}$ we have

$$\int_0^\infty e^{-st}e^{-(|B|t/4)}\overline{\phi(\sqrt{t})}\,dt=0$$

for all s such that $\Re e(s)>-(|B|/4)$. Uniqueness of the Laplace transform yields

$$e^{-(|B|t/4)}\overline{\phi(\sqrt{t})}=0 \text{ a.e. in } t \text{ on } [0,\infty) \quad \text{or} \quad \phi(r)=0 \text{ a.e. in } r \text{ on } [0,\infty)$$

and consequently

$$\int_0^\infty |\phi(r)|^2 r\,dr=0.$$

Hereby ϕ is trivial in $\mathfrak{L}^2([0,\infty))$, which contradict the assumption. Thus $\{\phi_m : m=0,1,2,\ldots\}$ is an orthonormal basis of $\mathfrak{L}^2[0,\infty)$. □

Remark 3.2: Since

$$\bigoplus_{l=-\infty}^{\infty} \mathfrak{L}^2[0,\infty)\otimes\{e^{il\theta}\}\otimes L^2[0,d]=\mathfrak{L}^2[0,\infty)\otimes L^2[0,2\pi)\otimes L^2[0,d],$$

one can prove for each fixed $l<0$ that the spectrum $E(m,n)$ is nondegenerate and the set of vectors $\{\psi_{mnl} : m=0,1,2,\ldots;\ n=0,1,2,\ldots;\ l \text{ fixed and } <0\}$ is an orthonormal basis of the subspace $\mathfrak{L}^2[0,\infty)\otimes\{e^{il\theta}\}\otimes L^2[0,d]$.

IV. GAZEAU–KLAUDER COHERENT STATES

In this section, we introduce the general features of Gazeau–Klauder CS. Let H be a Hamiltonian with a bounded below discrete spectrum $\{e_m\}_{m=0}^\infty$ and it has been adjusted so that $H\geqslant 0$. Further assume that the eigenvalues e_m are nondegenerate and arranged in increasing order $e_0<e_1<e_2<\cdots$. For such a Hamiltonian, a class of CS was suggested by Gazeau and Klauder,[9] the so-called *Gazeau–Klauder coherent states* (GKCS), as

$$|J,\alpha\rangle=\mathcal{N}(J)^{-1}\sum_{m=0}^{\infty}\frac{J^{m/2}e^{-ie_m\alpha}}{\sqrt{\rho(m)}}\eta_m, \tag{4.1}$$

where $J\geqslant 0$, $-\infty<\alpha<\infty$, $\{\eta_m\}_{m=0}^\infty$ is the set of eigenfunctions of the Hamiltonian and $\rho(m)=e_1e_2\cdots e_m=e_m!$. In order to be GKCS the states (4.1) need to satisfy the following:

(a) For each J,α the state is normalized, i.e., $1=\langle J,\alpha|J,\alpha\rangle=\mathcal{N}(J)^{-2}\Sigma_{m=0}^\infty J^m/\rho(m)$;
(b) the set of states $\{|J,\alpha\rangle : J\in[0,\infty),\alpha\in(-\infty,\infty)\}$ satisfies a resolution of the identity

$$\lim_{\delta\to\infty}\frac{1}{2\delta}\int_{-\delta}^{\delta}d\alpha\int_0^\infty \lambda(J)dJ|J,\alpha\rangle\langle J,\alpha|=I, \tag{4.2}$$

where $\lambda(J)$ is an appropriate weight function;

(c) the states are temporally stable, i.e., $e^{-iHt}|J,\alpha\rangle=|J,\alpha+t\rangle$;
(d) the states satisfy the action identity, i.e., $\langle J,\alpha|H|J,\alpha\rangle=J$.

Condition (d) requires $e_0=0$. In the case where only conditions (a)–(c) are satisfied we phrase the resulting CS as "temporally stable CS." In the case where $e_0\neq 0$ one can shift the spectrum backward by e_0 and work with the shifted spectrum.

The dynamical algebra of the system can be defined as follows: The generalized annihilation, creation, and number operators defined on the state Hilbert space $\mathfrak{H}$ with respect to the basis $\{\eta_m\}_{m=0}^{\infty}$ can be given by (see Refs. 1, 12, 17)

$$\begin{aligned}\mathfrak{a}\eta_m&=\sqrt{e_m}\,\eta_{m-1},\quad \text{with}\quad \mathfrak{a}\eta_0=0,\\ \mathfrak{a}^\dagger\eta_m&=\sqrt{e_{m+1}}\,\eta_{m+1},\\ \mathfrak{n}\eta_m&=e_m\eta_m\quad(\mathfrak{n}=\mathfrak{a}^\dagger\mathfrak{a}),\end{aligned}\tag{4.3}$$

and the commutators take the form

$$\begin{aligned}[\mathfrak{a},\mathfrak{a}^\dagger]\eta_m&=(e_{m+1}-e_m)\eta_m,\\ [\mathfrak{n},\mathfrak{a}^\dagger]\eta_m&=(e_{m+1}-e_m)\mathfrak{a}^\dagger\eta_m,\\ [\mathfrak{n},\mathfrak{a}]\eta_m&=(e_{m-1}-e_m)\mathfrak{a}\eta_m.\end{aligned}\tag{4.4}$$

The algebra generated by the operators $\{\mathfrak{a},\mathfrak{a}^\dagger,\mathfrak{n}\}$ and its deformations (up to isomorphisms) serve as a dynamical algebra of the Hamiltonian.

In Ref. 16 the definition (4.1) was generalized to multidimensions as

$$|\mathbf{J},\mathbf{b}\rangle=\mathcal{N}(\mathbf{J})^{-1}\sum_{\{n_1,\ldots,n_r\}}\frac{\mathbf{J}^{\mathbf{n}/2}}{\sqrt{\rho(\mathbf{n})}}e^{-i\mathbf{b}e(\mathbf{n})}|\mathbf{n}\rangle,\tag{4.5}$$

where the sum runs over all possible values of the variables n_j, $\mathcal{N}$ is a normalization factor, and $\rho(\mathbf{n})$ is an arbitrary positive function of all the indices. Further, $\mathbf{J}^{\mathbf{n}/2}=\Pi_{j=1}^{r}J_j^{n_j/2}$, $\mathbf{b}\cdot e(\mathbf{n})=\alpha_1e_1(\mathbf{n})+\cdots+\alpha_re_r(\mathbf{n})$ and $|\mathbf{n}\rangle=|n_1\rangle\otimes\cdots\otimes|n_r\rangle$, where $\{|n_j\rangle\}$ forms an orthonormal basis for an appropriate Hilbert space $\mathfrak{H}_j$. Using (4.5) GKCS for the rth degree of freedom is defined as

$$|n_1,\ldots,n_{r-1},J_r,\alpha_r\rangle=\mathcal{N}_r(J_r)^{-1}\sum_{n_r}\frac{J_r^{n_r/2}}{\sqrt{\rho_r}}e^{-i\alpha_re_r(\mathbf{n})}|\mathbf{n}\rangle,\tag{4.6}$$

where the normalization factor $\mathcal{N}_r$ and the function ρ_r may depend on the other indices. In addition to the normalization condition, when $n_1,\ldots,n_{r-1}$ are fixed, the states (4.6) should satisfy a resolution of the identity on the subspace obtained by fixing $n_1,n_2,\ldots,n_{r-1}$:

$$\int|n_1,\ldots,n_{r-1},J_r,\alpha_r\rangle\langle n_1,\ldots,n_{r-1},J_r,\alpha_r|\,d\mu(J_r,\alpha_r)=I_{n_1,n_2,\ldots,n_{r-1}}.\tag{4.7}$$

For the multidimensional case, if one takes $\rho_j(\mathbf{n})=\rho_j(n_1,n_2,\ldots,n_j)$ and $e_j(\mathbf{n})=e_j(n_1,n_2,\ldots,n_j)$,

$$|\mathbf{J},\mathbf{b}\rangle=\mathcal{N}_1^{-1}\sum_{n_1}\frac{J_1^{n_1/2}}{\sqrt{\rho_1}}e^{i\alpha_1e_1}\mathcal{N}_2^{-1}\sum_{n_2}\frac{J_2^{n_2/2}}{\sqrt{\rho_2}}e^{i\alpha_2e_2}\cdots\mathcal{N}_r^{-1}\sum_{n_r}\frac{J_r^{n_r/2}}{\sqrt{\rho_r}}e^{i\alpha_re_r}|\mathbf{n}\rangle,\tag{4.8}$$

where $\mathcal{N}_j=\mathcal{N}_j(J_j,\ldots,J_r;n_1,\ldots,n_{j-1})$. If ρ_j and e_j are independent of n_k, $k<j$ then the states (4.8) may give us simple tensor product of states. For the states (4.8) a resolution of the identity takes the following form:

$$\lim_{\delta\to\infty}\frac{1}{2\delta}\int_{-\delta}^{\delta}d\alpha_1\int_0^{\infty}\lambda_1(J_1)\lim_{\delta\to\infty}\frac{1}{2\delta}\int_{-\delta}^{\delta}d\alpha_2\int_0^{\infty}\lambda_1(J_1,J_2,n_1)\cdots\lim_{\delta\to\infty}\frac{1}{2\delta}\int_{-\delta}^{\delta}d\alpha_r$$
$$\times\int_0^{\infty}\lambda_r(J_1,\ldots,J_r,n_1,\ldots,n_{r-1})|n_1,\ldots,n_r,\mathbf{J},\mathbf{b}\rangle\langle n_1,\ldots,n_r,\mathbf{J},\mathbf{b}|dJ_1\cdots dJ_r$$
$$=I_{\mathfrak{H}_1}\otimes\cdots\otimes I_{\mathfrak{H}_r},$$

where λ_j, $j=1,2,\ldots,r$ are positive weight functions. For the multidimensional case, the temporal stability and the action identity can also be added. We will discuss these issues through the problem of this paper in Sec. VI.

In the following sections, when $l=0$ we derive temporally stable CS for the Hamiltonian H_0 with the spectrum $E(m,n)$ on the subspace $\mathfrak{L}^2[0,\infty)\otimes 1/\sqrt{2\pi}\otimes L^2[0,d]$, which is indeed a subspace of $\mathfrak{L}^2(\Sigma)$. However, $\mathfrak{L}^2[0,\infty)\otimes 1/\sqrt{2\pi}\otimes L^2[0,d]$ is isomorphic (in the Hilbert space sense) to $1/\sqrt{2\pi}\otimes\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ as subspaces of $\mathfrak{L}^2[0,\infty)\otimes L^2[0,2\pi]\otimes L^2[0,d]$ and $L^2[0,2\pi]\otimes\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$, respectively. Nevertheless, the subspace $1/\sqrt{2\pi}\otimes\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ is (Hilbert space) isomorphic to $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ and hence, we may consider the Hilbert space $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ instead of the subspace $\mathfrak{L}^2[0,\infty)\otimes 1/\sqrt{2\pi}\otimes L^2[0,d]$ to which it is isomorphic. Therefore, the action of the Hamiltonian H_0 on $\mathfrak{L}^2[0,\infty)\otimes 1/\sqrt{2\pi}\otimes L^2[0,d]$ carries to the Hilbert space $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$. Hereafter we refer the Hilbert space $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$ as the state Hilbert space of the Hamiltonian H_0 for $l=0$.

The GKCS studied in Ref. 8 for the Landau levels may be regarded as a set of GKCS constructed in the absence of n and l from the spectrum $E(m,l,n)$ of (2.12). The GK-like CS (in the terminology of Ref. 16) studied in Ref. 16 can be taken as a class of CS for the spectrum $E(m,l,n)$ in the absence of n.

V. CS WITH ONE DEGREE OF FREEDOM

We introduce two classes of temporally stable CS with the form (4.6) for the spectrum (3.2), by first fixing n followed by another class where m is fixed. In both cases the orthonormal basis is denoted by the same symbol $\psi_{m,n}$. However, it should be clear that in each case the other index is fixed and the vectors $\psi_{m,n}$ belong to the corresponding subspace of the state Hilbert space $\mathfrak{L}^2[0,\infty)\otimes L^2[0,d]$. For sake of simplicity $|B|:=B$.

A. When *n* is fixed

Here we discuss a class of temporally stable CS for the first degree of freedom (the freedom through m). Since the energy spectrum of the Landau problem is $E_m=B(2m+1)$, the following set of CS can also be considered as a set of CS with a forward shift of the Landau levels. Further, the construction also serves as a preparatory step of the formation of CS for two degrees of freedom. Let

$$\rho(m)=E(1,n)E(2,n)\cdots E(m,n),$$

where $E(m,n)$ is given by (3.2). We have

$$\rho(m)=\prod_{k=1}^{m}\left(B(2k+1)+\left(\frac{\pi(n+1)}{d}\right)^2\right)=(2B)^m(\gamma)_m,$$

where

$$\gamma = 1 + \frac{Bd^2 + \pi^2 (n+1)^2}{2Bd^2}.$$

Let us study the following class of vectors:

$$|J,\alpha,n\rangle = \mathcal{N}(J,n)^{-1} \sum_{m=0}^{\infty} \frac{J^{m/2} e^{-iE(m,n)\alpha}}{\sqrt{\rho(m)}} \psi_{m,n}. \tag{5.1}$$

The normalization condition $\langle J,\alpha,n|J,\alpha,n\rangle = 1$ yields

$$\mathcal{N}(J,n)^2 = \sum_{m=0}^{\infty} \frac{J^m}{2^m B^m (\gamma)_m} = {}_1F_1\left(1;\gamma;\frac{J}{2B}\right) > 0, \tag{5.2}$$

which converges for all $J>0$. For a resolution of the identity, let $-\infty<\alpha<\infty$ and set a measure

$$d\mu(J,\alpha) = d\nu(J)d\alpha = \frac{1}{2^\gamma B^\gamma \Gamma(\gamma)} {}_1F_1\left(1;\gamma;\frac{J}{2B}\right) e^{-(J/2B)} J^{\gamma-1} dJ d\alpha.$$

The knowledge of Eqs. (4.2) and (4.7) leads to

$$\begin{aligned}
\int_0^\infty \int |J,\alpha,n\rangle\langle J,\alpha,n| d\mu(J,\alpha) &= \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \frac{|\psi_{m,n}\rangle\langle\psi_{l,n}|}{\sqrt{\rho(m)\rho(l)}} \int_0^\infty \int \frac{J^{m/2+l/2}}{\mathcal{N}(J,n)^2} e^{i(E(m,n)-E(l,n))\alpha} d\nu(J) d\alpha \\
&= \sum_{m=0}^{\infty} \frac{|\psi_{m,n}\rangle\langle\psi_{m,n}|}{2^{m+\gamma} B^{m+\gamma} (\gamma)_m \Gamma(\gamma)} \int_0^\infty J^{m+\gamma-1} e^{-(J/2B)} dJ \\
&= \sum_{m=0}^{\infty} |\psi_{m,n}\rangle\langle\psi_{m,n}| = I_n,
\end{aligned}$$

where we employed the identity[5]

$$\int_0^\infty e^{-ax} x^{s-1} dx = a^{-s}\Gamma(s) \tag{5.3}$$

with $s = m+\gamma$ and $a = 1/2B$. For the temporal stability, since for fixed n

$$H_0 \psi_{m,n} = E(m,n)\psi_{m,n}, \qquad m = 0,1,2,\ldots$$

and

$$e^{-iE(m,n)\alpha} e^{-iH_0 t} \psi_{m,n} = e^{-iE(m,n)\alpha} e^{-iE(m,n)t} \psi_{m,n} = e^{-iE(m,n)(\alpha+t)} \psi_{m,n}$$

we have

$$e^{-iH_0 t} |J,\alpha,n\rangle = |J,\alpha+t,n\rangle. \tag{5.4}$$

Thus the states $|J,\alpha,n\rangle$ form a set of temporally stable CS. Since $E(0,n) \neq 0$ the action identity cannot be obtained. The overlap of two states takes the form

$$\langle J,\alpha,n|J',\alpha',n\rangle = \frac{e^{-i(\alpha-\alpha')(B+(\pi^2(n+1)^2/d^2))}}{\sqrt{{}_1F_1\left(1;\gamma;\frac{J}{2B}\right) {}_1F_1\left(1;\gamma;\frac{J'}{2B}\right)}} {}_1F_1\left(1;\gamma;\frac{JJ' e^{-2iB(\alpha-\alpha')}}{2B}\right).$$

If $\alpha=\alpha'$ we get

$$\langle J,\alpha,n|J',\alpha,n\rangle=\frac{{}_1F_1\left(1;\gamma;\frac{\sqrt{JJ'}}{2B}\right)}{\sqrt{{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)\ {}_1F_1\left(1;\gamma;\frac{J'}{2B}\right)}}.$$

Remark 5.1: (a) In (5.1) instead of taking $\rho(m)=E(1,n)\cdots E(m,n)$ if we take $\rho(m)=e(1,m)\cdots e(m,n)$ with $e(m,n)=E(m,n)-E(0,n)$, then we can have $0=e(0,n)<e(1,n)<\cdots$ and thereby we can have a set of GKCS. In this case, $\rho(m)=2^mB^m m!$, $\mathcal{N}(J)^2=e^{J/(2B)}$ and a resolution of the identity is obtained with the measure $d\mu(J,\alpha)=(1/2B\mathcal{N}^2(J))\,e^{-J/(2B)}d\alpha dJ$. The temporal stability and the action identity follow straightforwardly.

(b) The spectrum of the isotonic oscillator

$$H=-\frac{d^2}{dx^2}+x^2+\frac{A}{x^2}\qquad(A\geqslant 0)$$

is $\epsilon_m=2(2m+\gamma)$, where $\gamma=1+\frac{1}{2}\sqrt{1+4A}$. Since this spectrum is nondegenerate and the eigenfunctions form an orthonormal basis of the Hilbert space $L^2[0,\infty)$,[19] when $B=2$ and ψ_{mn} is replaced by the wave functions of H, the set of CS given in (5.1) can also be considered as a set of temporally stable CS for H with a forward shift of the spectrum.

B. When *m* is fixed

We discuss a class of temporally stable CS for the second degree of freedom obtained through n by fixing m. That is, the following class of CS can be considered as a class of CS constructed with the effective part of the spectrum due to the infinite layer. The other aim of this subsection is to facilitate the calculations of the following sections. For fixed m let

$$\rho(n)=E(m,1)E(m,2)\cdots E(m,n).$$

Thereby

$$\rho(n)=\prod_{k=1}^{n}\left(B(2m+1)+\left(\frac{\pi(k+1)}{d}\right)^2\right)=\left(\frac{\pi}{d}\right)^{2n}(\beta)_n(\overline{\beta})_n,$$

where

$$\beta=2+\frac{id}{\pi}\sqrt{B(2m+1)}$$

and $\overline{\beta}$ is the complex conjugate of β. Note that, the product $(\beta)_n(\overline{\beta})_n$ is a real positive number. Consider the set of vectors

$$|J,\alpha,m\rangle=\mathcal{N}(J,m)^{-1}\sum_{n=0}^{\infty}\frac{J^{n/2}}{\sqrt{\rho(n)}}e^{-iE(m,n)\alpha}\psi_{m,n}. \tag{5.5}$$

The normalization factor $\mathcal{N}(J,m)$ is obtained, by demanding $\langle J,\alpha,m|J,\alpha,m\rangle=1$, in the following form:

$$\mathcal{N}(J,m)^2=\sum_{n=0}^{\infty}\frac{J^n}{\rho(n)}=\sum_{n=0}^{\infty}\frac{\left(\frac{d^2J}{\pi^2}\right)^n}{(\beta)_n(\overline{\beta})_n}={}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right), \tag{5.6}$$

which is a real positive function and defined for all $J\geqslant 0$. For $J>0$ and $-\infty<\alpha<\infty$ set

$$d\mu(J,\alpha)=\mathcal{N}(J,m)^2\lambda(J)dJd\alpha.$$

For a resolution of the identity, we have

$$\int_0^{\infty}\int|J,\alpha,m\rangle\langle J,\alpha,m|d\mu(J,\alpha)=\sum_{n=0}^{\infty}\frac{|\psi_{m,n}\rangle\langle\psi_{m,n}|}{\rho(n)}\int_0^{\infty}J^n\lambda(J)dJ=\sum_{n=0}^{\infty}|\psi_{m,n}\rangle\langle\psi_{m,n}|=I_m$$

if there is a density $\lambda(J)$ to satisfy

$$\int_0^{\infty}J^n\lambda(J)dJ=\rho(n)=\left(\frac{\pi}{d}\right)^{2n}(\beta)_n(\overline{\beta})_n. \tag{5.7}$$

Since

$$\int_0^{\infty}2K_{2\eta}(2\sqrt{x})x^{s-1}dx=\Gamma(s-\eta)\Gamma(s+\eta) \tag{5.8}$$

the density

$$\lambda(J)=\frac{2d^2}{\pi^2\Gamma(\beta)\Gamma(\overline{\beta})}K_{\beta-\overline{\beta}}\left(\frac{2d}{\pi}\sqrt{J}\right) \tag{5.9}$$

satisfies (5.7), where K is the modified Bessel function of the third kind of imaginary order[4] and may be regarded as the kernel of the Kontorovich–Lebedev transform[15] in the light of (5.8). The temporal stability follows similar to the previous case. Thus we have a set of temporally stable CS without the action identity. As in the previous case, when $\alpha=\alpha'$ the overlap of two states takes the form

$$\langle J,\alpha,m|J',\alpha,m\rangle=\frac{{}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2\sqrt{JJ'}}{\pi^2}\right)}{\sqrt{{}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right)\ {}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J'}{\pi^2}\right)}}.$$

Remark 5.2: (a) Let $E_n=E(m,n)-E(m,0)$. In (5.5) if we replace the $\rho(n)=E(m,1)\cdots E(m,n)$ by $\rho(n)=E_1\cdots E_n=n!(n+2)!/2$ we can have the action identity and thereby a class of GKCS. In this case the normalization factor takes the form $\mathcal{N}(J)^2=J/[2I_2(2\sqrt{J})]$ and a resolution of the identity can be obtained with the measure $d\mu(J,\alpha)=\mathcal{N}(J)^2\lambda(J)d\alpha dJ$, where

$$\lambda(J)=\frac{1}{2}G_{0,2}^{2,0}\left(J\ \middle|\ \begin{matrix}-\\2,0\end{matrix}\right),$$

which is given in terms of the MeijerG-function (see Ref. 14, p. 303, formula (37)).

(b) A class of GKCS for the infinite well potential with the spectrum $\mathbf{e}_n = n(n+2)$ is given in Ref. 2. When $d=\pi$ the above class of CS can be considered as a class of temporally stable CS for the infinite well with a forward shift of the spectrum. In this case the state Hilbert space has to be replaced by the Hilbert space of the infinite well.

VI. CS WITH TWO DEGREES OF FREEDOM

In this section we present two different classes of CS with two degrees of freedom in the form (4.8). In the first case, we present a class of CS as a tensor product of two classes of states by setting ρ_1, ρ_2, e_1, and e_2 independent. In the second case, within the multiple sum, by letting one sum depends on the other through ρ_1, ρ_2, e_1, and e_2, we present a class of CS where the resulting CS cannot be considered as a tensor product of two states. Further, both classes are considered as temporally stable CS for the Hamiltonian H_0 with the spectrum $E(m,n)$.

A. When summations are independent

Let $e_m = B(2m+1)$, $\epsilon_n = [\pi(n+1)/d]^2$, $\rho_1(m) = e_1 e_2 \cdots e_m = e_m!$, and $\rho_2(n) = \epsilon_1 \epsilon_2 \cdots \epsilon_n = \epsilon_n!$. Thus

$$\rho_1(m) = \prod_{k=1}^{m} [B(2k+1)] = 2^m B^m \left(\frac{3}{2}\right)_m ,$$

$$\rho_2(n) = \prod_{j=1}^{n} \left(\frac{\pi(j+1)}{d}\right)^2 = \left(\frac{\pi}{d}\right)^{2n} (2)_n (2)_n .$$

The set of vectors under consideration is as follows:

$$|J_1, J_2, \alpha_1, \alpha_2\rangle = \mathcal{N}_1(J_1)^{-1} \mathcal{N}_2(J_2)^{-1} \left[\sum_{m=0}^{\infty} \frac{J_1^{m/2}}{\sqrt{\rho_1(m)}} e^{-i e_m \alpha_1} \sum_{n=0}^{\infty} \frac{J_2^{n/2}}{\sqrt{\rho_2(n)}} e^{-i \epsilon_n \alpha_2} \phi_m \otimes \chi_n \right]. \tag{6.1}$$

Since

$$\langle J_1, J_2, \alpha_1, \alpha_2 | J_1, J_2, \alpha_1, \alpha_2 \rangle = \mathcal{N}_1(J_1)^{-2} \sum_{m=0}^{\infty} \frac{J_1^m}{\rho_1(m)} \mathcal{N}_2(J_2)^{-2} \sum_{n=0}^{\infty} \frac{J_2^n}{\rho_2(n)},$$

the normalization requirement $\langle J_1, J_2, \alpha_1, \alpha_2 | J_1, J_2, \alpha_1, \alpha_2 \rangle = 1$ yields

$$\mathcal{N}_2(J_2)^2 = \sum_{n=0}^{\infty} \frac{J_2^n}{\rho_2(n)} = \sum_{n=0}^{\infty} \frac{1}{(2)_n \ (2)_n} \left(\frac{d^2 J_2}{\pi^2}\right)^n = {}_1F_2\left(1; 2, 2; \frac{d^2 J_2}{\pi^2}\right)$$

and

$$\mathcal{N}_1(J_1)^2 = \sum_{m=0}^{\infty} \frac{J_1^m}{2^m B^m \left(\frac{3}{2}\right)_m} = {}_1F_1\left(1; \frac{3}{2}; \frac{J_1}{2B}\right).$$

For $J_1, J_2 \in (0,\infty)$ and $-\infty < \alpha_1, \alpha_2 < \infty$, let us assume that the measure

$$d\mu(J_1, J_2, \alpha_1, \alpha_2) = \mathcal{N}_1(J_1)^2 \mathcal{N}_2(J_2)^2 \lambda_1(J_1) \lambda_2(J_2) dJ_1 dJ_2 d\alpha_1 d\alpha_2 . \tag{6.2}$$

The weight functions $\lambda_1(J_1)$ and $\lambda_2(J_2)$ will be chosen to satisfy a resolution of the identity. In this case, we have

$$\int_0^\infty \int_0^\infty \int \int |J_1,J_2,\alpha_1,\alpha_2\rangle\langle J_1,J_2,\alpha_1,\alpha_2| d\mu(J_1,J_2,\alpha_1,\alpha_2)$$

$$= \sum_{m=0}^{\infty} \frac{|\phi_m\rangle\langle\phi_m|}{\rho_1(m)} \int_0^\infty J_1^m \lambda_1(J_1) dJ_1 \otimes \sum_{n=0}^{\infty} \frac{|\chi_n\rangle\langle\chi_n|}{\rho_2(n)} \int_0^\infty J_2^n \lambda_2(J_2) dJ_2$$

$$= \sum_{m=0}^{\infty} |\phi_m\rangle\langle\phi_m| \otimes \sum_{n=0}^{\infty} |\chi_n\rangle\langle\chi_n| = I_{\mathfrak{L}^2[0,\infty)} \otimes I_{L^2[0,d]}$$

under the assumption that the densities $\lambda_1(J_1)$ and $\lambda_2(J_2)$ are such that

$$\int_0^\infty J_1^m \lambda_1(J_1) dJ_1 = \rho_1(m) = 2^m B^m \left(\frac{3}{2}\right)_m \tag{6.3}$$

and

$$\int_0^\infty J_2^n \lambda_2(J_2) dJ_2 = \rho_2(n) = \left(\frac{\pi}{d}\right)^{2n} (2)_n (2)_n . \tag{6.4}$$

The density

$$\lambda_1(J_1) = \sqrt{\frac{J}{2\pi B^3}} e^{-(J/2B)}$$

satisfies (6.3) and the density

$$\lambda_2(J_2) = \frac{2d^4}{\pi^4 J_2} K_0\left(\frac{2d\sqrt{J_2}}{\pi}\right),$$

where K_0 is the modified Bessel function of order 0, will prove (6.4). Since $\psi_{m,n} = \phi_m \otimes \chi_n$ and $H_0 \psi_{m,n} = E(m,n)\psi_{m,n}$ we have

$$H_0(\phi_m \otimes \chi_n) = (e_m + \epsilon_n)\phi_m \otimes \chi_n .$$

Therefore, we have

$$e^{-iH_0 t} \phi_m \otimes \chi_n = e^{-i(e_m+\epsilon_n)t} \phi_m \otimes \chi_n$$

and thereby

$$e^{-iH_0 t} |J_1,J_2,\alpha_1,\alpha_2\rangle = |J_1,J_2,\alpha_1+t,\alpha_2+t\rangle.$$

Thus the states $|J_1,J_2,\alpha_1,\alpha_2\rangle$ are temporally stable.

Remark 6.1: (a) Since $H_0\phi_m \otimes \chi_n = (e_m+\epsilon_n)\phi_m \otimes \chi_n$, even under the assumption $e_0 = \epsilon_0 = 0$ (i.e., even if we shift the spectrum backward), we cannot have the action identity. Therefore, we only have a set of temporally stable CS.

(b) If we shift e_m and ϵ_n backward by e_0 and ϵ_0 we get $\tilde{e}_m = e_m - e_0 = 2Bm$ and $\tilde{\epsilon}_n = \epsilon_n - \epsilon_0 = \pi^2 n(n+2)/d^2$ and thereby $\tilde{\rho}_1(m) = \tilde{e}_1 \cdots \tilde{e}_m = 2^m B^m m!$ and $\tilde{\rho}_2(n) = \tilde{\epsilon}_n \cdots \tilde{\epsilon}_n = \pi^{2n} n!(n+2)!/(2d^{2n})$. In (6.1) when we replace $\rho_1(m), \rho_2(n), e_m$ and ϵ_n by $\tilde{\rho}_1(m), \tilde{\rho}_2(n), \tilde{e}_m$ and $\tilde{\epsilon}_n$ we get

$$\tilde{\mathcal{N}}_2(J_2)^2 = {}_0F_1\left(-;3;\frac{J_2 d^2}{\pi^2}\right) = \frac{2\pi^2}{J_2 d^2} I_2\left(\frac{2d\sqrt{J_2}}{\pi}\right)$$

and

$$\tilde{\mathcal{N}}_1(J_1)^2 = e^{J_1/2B}.$$

In this case, a resolution of the identity is obtained with the measure

$$d\mu(J_1,J_2,\alpha_1,\alpha_2) = \tilde{\mathcal{N}}_1(J_1)^2 \tilde{\mathcal{N}}_2(J_2)^2 \tilde{\lambda}_1(J_1)\tilde{\lambda}_2(J_2) dJ_1 dJ_2 d\alpha_1 d\alpha_2,$$

where

$$\tilde{\lambda}_1(J_1) = \frac{1}{2B} e^{-J_1/(2B)}$$

and

$$\tilde{\lambda}_2(J_2) = \frac{\pi^2}{2d^2} G^{2,0}_{0,2}\left(\frac{J_2\pi^2}{d^2} \;\Big|^{-}_{2,0} \right).$$

The temporal stability follows easily.

B. When summations depend one on the other

For fixed m let

$$\rho_1(m,n) = E(m,1)E(m,2)\cdots E(m,n).$$

From Sec. V B we have

$$\rho_1(m,n) = \left(\frac{\pi}{d}\right)^{2n} (\beta)_n (\overline{\beta})_n,$$

where β and $\overline{\beta}$ are as in Sec. V B. Let

$$\rho_2(m) = e_1 \cdots e_m = 2^m B^m \left(\frac{3}{2}\right)_m.$$

Consider the following set of vectors:

$$|J_1,J_2,\alpha_1,\alpha_2\rangle = \mathcal{N}_1(J_1,J_2)^{-1} \sum_{m=0}^{\infty} \frac{J_1^{m/2}}{\sqrt{\rho_2(m)}} e^{-ie_m\alpha_1} \mathcal{N}_2(J_2,m)^{-1}$$

$$\times \sum_{n=0}^{\infty} \frac{J_2^{n/2}}{\sqrt{\rho_1(m,n)}} e^{-i\epsilon_n\alpha_2} \phi_m \otimes \chi_n. \tag{6.5}$$

In order to obtain the normalization factor let us compute the norm of the vector $|J_1,J_2,\alpha_1,\alpha_2\rangle$,

$$\langle J_1,J_2,\alpha_1,\alpha_2|J_1,J_2,\alpha_1,\alpha_2\rangle = \mathcal{N}_1(J_1,J_2)^{-2} \sum_{m=0}^{\infty} \frac{J_1^m}{\rho_2(m)} \mathcal{N}_2(J_2,m)^{-2} \sum_{n=0}^{\infty} \frac{J_2^n}{\rho_1(m,n)} = 1$$

if

$$\mathcal{N}_2(J_2,m)^2 = \sum_{n=0}^{\infty} \frac{J_2^n}{\rho_1(m,n)} \tag{6.6}$$

and

$$\mathcal{N}_1(J_1,J_2)^2=\sum_{m=0}^{\infty}\frac{J_1^m}{\rho_2(m)\mathcal{N}_2(J_2,m)^2}. \tag{6.7}$$

By (5.6) we have

$$\mathcal{N}_2(J_2,m)^2={}_1F_2\left(1;\beta,\overline{\beta};\frac{d^2J_2}{\pi^2}\right)\geqslant 1 \quad \forall \quad J_2\in(0,\infty).$$

Thus, we have

$$\mathcal{N}_1(J_1,J_2)^2=\sum_{m=0}^{\infty}\frac{J_1^m}{\rho_2(m)\,{}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J_2}{\pi^2}\right)}\leqslant\sum_{m=0}^{\infty}\frac{J_1^m}{\rho_2(m)}=\sum_{m=0}^{\infty}\frac{\left(\frac{J_1}{2B}\right)^m}{\left(\frac{3}{2}\right)_m}={}_1F_1\left(1;\frac{3}{2};\frac{J_1}{2B}\right),$$

which converges for all $J_1\geqslant 0$. For $J_1,J_2\in[0,\infty)$ and $-\infty<\alpha_1,\alpha_2<\infty$ we have

$$\begin{aligned}&\int_0^{\infty}\int_0^{\infty}\int\int|J_1,J_2,\alpha_1,\alpha_2\rangle\langle J_1,J_2,\alpha_1,\alpha_2|\lambda_1(J_1)\lambda_2(J_2,m)dJ_1dJ_2d\alpha_1d\alpha_2\\&=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{|\phi_m\rangle\langle\phi_m|\otimes|\chi_n\rangle\langle\chi_n|}{\rho_2(m)\rho_1(m,n)}\int_0^{\infty}\frac{J_1^m}{\mathcal{N}_1(J_1,J_2)^2}\lambda_1(J_1)dJ_1\int_0^{\infty}\frac{J_2^n}{\mathcal{N}_2(J_2,m)^2}\lambda_2(J_2,m)dJ_2\\&=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}|\phi_m\langle\phi_m|\otimes|\chi_n\rangle\langle\chi_n|=I_{\mathfrak{L}^2[0,\infty)}\otimes I_{L^2[0,d]}\end{aligned}$$

if there are densities $\lambda_1(J_1)$ and $\lambda_2(J_2,m)$ such that

$$\int_0^{\infty}\frac{J_1^m}{\mathcal{N}_1(J_1,J_2)^2}\lambda_1(J_1)dJ_1\int_0^{\infty}\frac{J_2^n}{\mathcal{N}_2(J_2,m)^2}\lambda_2(J_2,m)dJ_2=\rho_2(m)\rho_1(m,n). \tag{6.8}$$

Let

$$\lambda_2(J_2)=\mathcal{N}_2(J_2,m)^2\Lambda_2(J_2,m) \qquad \text{and} \qquad \lambda_1(J_1)=\mathcal{N}_1(J_1,J_2)^2\Lambda_1(J_1).$$

Then (6.8) reduces to

$$\int_0^{\infty}J_1^m\Lambda_1(J_1)dJ_1\int_0^{\infty}J_2^n\Lambda_2(J_2,m)dJ_2=\rho_2(m)\rho_1(m,n). \tag{6.9}$$

If we combine (6.3) and (6.4) we can have (6.9). Thus we have a resolution of the identity. By the same argument of Sec. VI A we have

$$e^{-iH_0t}|J_1,J_2,\alpha_1,\alpha_2\rangle=|J_1,J_2,\alpha_1+t,\alpha_2+t\rangle.$$

Thus the states $|J_1,J_2,\alpha_1,\alpha_2\rangle$ are temporally stable.

Remark 6.2: (a) Instead of defining the states as in (6.5), if we define them as (notice that the change will not affect the calculations preceding this remark; thereby the following class of vectors also forms a set of CS)

$$|J_1,J_2,\alpha_1,\alpha_2\rangle=\mathcal{N}_1(J_1,J_2)^{-1}\sum_{m=0}^{\infty}\frac{J_1^{m/2}}{\sqrt{\rho_2(m)}}e^{-ie_m\alpha_1}\mathcal{N}_2(J_2,m)^{-1}$$

$$\times\sum_{n=0}^{\infty}\frac{J_2^{n/2}}{\sqrt{\rho_1(m,n)}}e^{-iE(m,n)\alpha_2}\phi_m\otimes\chi_n, \tag{6.10}$$

we can have

$$e^{iH_0t}|J_1,J_2,\alpha_1,\alpha_2\rangle=|J_1,J_2,\alpha_1,\alpha_2+t\rangle.$$

Still we have the temporal stability, but only the second part of the states evolve with time. In this case, if we shift the spectrum so that $E(m,0)=0$ we can have an action identity in the following sense:

$$\langle J_1,J_2,\alpha_1,\alpha_2|H_0|J_1,J_2,\alpha_1,\alpha_2\rangle=\mathcal{N}_1(J_1,J_2)^{-2}\sum_{m=0}^{\infty}\frac{J_1^m}{\rho_2(m)}\mathcal{N}_2(J_2,m)^{-2}\sum_{n=1}^{\infty}\frac{J_2^mE(m,n)}{\rho_1(m,n)}=J_2.$$

(b) If we shift e_m and $E(m,n)$ backward by e_0 and $E(m,0)$ we get $\tilde{e}_m=e_m-e_0=2Bm$ and $\tilde{E}(m,n)=E(m,n)-E(m,0)=\pi^2n(n+2)/d^2$, which is the same case considered in Remark 6.1.

VII. DYNAMICAL ALGEBRA

In this section we discuss the dynamical algebra associated to each set of temporally stable states of the previous sections. Here we follow the operator structure developed in Sec. IV. That is, we follow the annihilation, creation and the number operators of (4.3).

A. For the states of Sec. V A

When n is fixed the spectrum $E(m,n)=B(2m+1)+(\pi(n+1)/d)^2$ can be written as

$$\overline{E}(m)=b_1m+c_1,$$

where $b_1=2B$ and $c_1=B+(\pi(n+1)/d)^2$ are constants. The corresponding generators take the form (4.3) with $x_m=\overline{E}(m)$. From (4.4) the commutators take the form

$$[\mathfrak{a},\mathfrak{a}^\dagger]=b_1I,\qquad[\mathfrak{n},\mathfrak{a}]=b_1\mathfrak{a}^\dagger,\qquad[\mathfrak{n},\mathfrak{a}]=-b_1\mathfrak{a}.$$

Thus the dynamical algebra is isomorphic to the Weyl–Heisenberg algebra, $\mathfrak{g}_{\mathrm{W-H}}$. To get the exact commutation relations of the Weyl–Heisenberg algebra one can define a new set of operators as follows:

$$\overline{\mathfrak{a}}=\frac{1}{\sqrt{b_1}}\mathfrak{a},\qquad\overline{\mathfrak{a}}^\dagger=\frac{1}{\sqrt{b_1}}\mathfrak{a}^\dagger,\qquad\overline{\mathfrak{n}}=\frac{1}{\sqrt{b_1}}\mathfrak{n}.$$

In terms of these new operators one gets

$$[\overline{\mathfrak{a}},\overline{\mathfrak{a}}^\dagger]=I,\qquad[\overline{\mathfrak{n}},\overline{\mathfrak{a}}^\dagger]=\overline{\mathfrak{a}}^\dagger,\qquad[\overline{\mathfrak{n}},\overline{\mathfrak{a}}]=-\overline{\mathfrak{a}}.$$

B. For the states of Sec. V B

When m is fixed the spectrum

$$E(m,n)=B(2m+1)+(\pi(n+1)/d)^2$$

can be written as

$$\tilde{E}(n)=b_2(n+1)^2+c_2,$$

where $b_2=\pi^2/d^2$ and $c_2=B(m+1)$ are constants. The corresponding generators take the form (4.3) with $e_n=\tilde{E}(n)$. Let us see the commutation relations. It can be easily seen that

$$[\mathfrak{a},\mathfrak{a}^\dagger]\psi_{m,n}=b_2(2n+3)\psi_{m,n}.$$

As it was done in Ref. 2, let us define a new set of operators

$$\bar{\mathfrak{a}}=\frac{1}{\sqrt{b_2}}\mathfrak{a},\qquad \bar{\mathfrak{a}}^\dagger=\frac{1}{\sqrt{b_2}}\mathfrak{a}^\dagger,\qquad \bar{\mathfrak{n}}\psi_{m,n}=\left(n+\frac{3}{2}\right)\psi_{m,n}. \tag{7.1}$$

With these new operators we obtain

$$[\bar{\mathfrak{a}},\bar{\mathfrak{a}}^\dagger]=2\bar{\mathfrak{n}},\qquad [\bar{\mathfrak{n}},\bar{\mathfrak{a}}]=-\bar{\mathfrak{a}},\qquad [\bar{\mathfrak{n}},\bar{\mathfrak{a}}^\dagger]=\bar{\mathfrak{a}}^\dagger. \tag{7.2}$$

The above commutation relations are the ones satisfied by the generators of the algebra $\mathfrak{su}(1,1)$ of the classical group SU(1,1). Thus in this case the dynamical algebra is isomorphic to $\mathfrak{su}(1,1)$.

C. For the states of Sec. VI A

Since $\rho_1(m)=e_m!$, $\rho_2(n)=\epsilon_n!$, $e_m=B(2m+1)$ and $\epsilon_n=\pi^2(n+1)^2/d^2$, let us define two sets of operators as follows:

$$\mathfrak{a}_1\phi_m=\sqrt{e_m}\phi_{m-1},\qquad \mathfrak{a}_1^\dagger\phi_m=\sqrt{e_{m+1}}\phi_{m+1},\qquad \mathfrak{n}_1\phi_m=e_m\phi_m, \tag{7.3}$$

$$\mathfrak{a}_2\chi_n=\sqrt{\epsilon_n}\chi_{n-1},\qquad \mathfrak{a}_2^\dagger\chi_n=\sqrt{\epsilon_{n+1}}\chi_{n+1},\qquad \mathfrak{n}_2\chi_n=\epsilon_n\chi_n. \tag{7.4}$$

For the operators $\mathfrak{a}_1,\mathfrak{a}_1^\dagger,\mathfrak{n}_1$, the commutators take the form,

$$[\mathfrak{a}_1,\mathfrak{a}_1^\dagger]=2BI,\qquad [\mathfrak{n}_1,\mathfrak{a}_1^\dagger]=2B\mathfrak{a}_1^\dagger,\qquad [\mathfrak{n}_1,\mathfrak{a}_1]=-2B\mathfrak{a}_1.$$

Thus the dynamical algebra is isomorphic to $\mathfrak{g}_{\mathrm{W-H}}$. To get the exact commutation relations of $\mathfrak{g}_{\mathrm{W-H}}$ one can define a new set of operators as follows:

$$\bar{\mathfrak{a}}_1=\frac{1}{\sqrt{2B}}\mathfrak{a}_1,\qquad \bar{\mathfrak{a}}_1^\dagger=\frac{1}{\sqrt{2B}}\mathfrak{a}_1^\dagger,\qquad \bar{\mathfrak{n}}_1=\frac{1}{\sqrt{2B}}\mathfrak{n}_1.$$

In terms of these new operators one gets

$$[\bar{\mathfrak{a}}_1,\bar{\mathfrak{a}}_1^\dagger]=I,\qquad [\bar{\mathfrak{n}}_1,\bar{\mathfrak{a}}_1^\dagger]=\bar{\mathfrak{a}}_1^\dagger,\qquad [\bar{\mathfrak{n}}_1,\bar{\mathfrak{a}}_1]=-\bar{\mathfrak{a}}_1.$$

For the operators $\mathfrak{a}_2,\mathfrak{a}_2^\dagger$ we get

$$[\mathfrak{a}_2,\mathfrak{a}_2^\dagger]\chi_n=\frac{2\pi^2}{d^2}\left(n+\frac{3}{2}\right)\chi_n.$$

By defining a new set of operators

$$\bar{\mathfrak{a}}_2=\frac{d}{\pi}\mathfrak{a}_2,\qquad \bar{\mathfrak{a}}_2^\dagger=\frac{d}{\pi}\mathfrak{a}_2^\dagger,\qquad \bar{\mathfrak{n}}_2\chi_n=\left(n+\frac{3}{2}\right)\chi_n, \tag{7.5}$$

it can readily be seen that the commutators take the following form:

$$[\bar{\mathfrak{a}}_2,\bar{\mathfrak{a}}_2^\dagger]=2\bar{\mathfrak{n}}_2,\qquad [\bar{\mathfrak{n}}_2,\bar{\mathfrak{a}}_2]=-\bar{\mathfrak{a}}_2,\qquad [\bar{\mathfrak{n}}_2,\bar{\mathfrak{a}}_2^\dagger]=\bar{\mathfrak{a}}_2^\dagger, \tag{7.6}$$

which are the commutation relations satisfied by the generators of the algebra $\mathfrak{su}(1,1)$. Now for the set of CS we define the following set of operators:

$$\mathfrak{a}=\mathfrak{a}_1\otimes\mathfrak{a}_2, \qquad \mathfrak{a}^\dagger=\mathfrak{a}_1^\dagger\otimes\mathfrak{a}_2^\dagger, \qquad \mathfrak{n}=\mathfrak{n}_1\otimes\bar{\mathfrak{n}}_2. \tag{7.7}$$

Thus the algebra associated to the CS is isomorphic to the tensor product of the two algebras, $\mathfrak{g}_{\mathrm{W-H}}$ and $\mathfrak{su}(1,1)$, that is, $\mathfrak{g}_{\mathrm{W-H}}\otimes\mathfrak{su}(1,1)$. If we take the operators as

$$\bar{\mathfrak{a}}=\bar{\mathfrak{a}}_1\otimes\bar{\mathfrak{a}}_2, \qquad \bar{\mathfrak{a}}^\dagger=\bar{\mathfrak{a}}_1^\dagger\otimes\bar{\mathfrak{a}}_2^\dagger, \qquad \bar{\mathfrak{n}}=\bar{\mathfrak{n}}_1\otimes\bar{\mathfrak{n}}_2, \tag{7.8}$$

we get the exact commutation relations of $\mathfrak{g}_{\mathrm{W-H}}\otimes\mathfrak{su}(1,1)$. One can also define another set of operators as follows:

$$\mathbf{a}\phi_m\otimes\chi_n=\sqrt{e_m\epsilon_n}\,\phi_{m-1}\otimes\chi_{n-1}, \qquad \mathbf{a}\phi_0\otimes\chi_0=0,$$

$$\mathbf{a}^\dagger\phi_m\otimes\chi_n=\sqrt{e_{m+1}\epsilon_{n+1}}\,\phi_{m+1}\otimes\chi_{n+1},$$

$$\mathbf{n}\phi_m\otimes\chi_n=e_m\epsilon_n\phi_m\otimes\chi_n. \tag{7.9}$$

Observe that here also the CS become the eigenstates of **a**. But it may be difficult to identify this algebra to a known type.

D. For the states of Sec. VI B

Since $\rho_1(m)=e_m!$, $\rho_2(n)=E(m,n)!$, let us define two sets of operators as follows:

$$\mathfrak{a}_1\phi_m=\sqrt{e_m}\,\phi_{m-1}, \quad \mathfrak{a}_1^\dagger\phi_m=\sqrt{e_{m+1}}\,\phi_{m+1}, \quad \mathfrak{n}_1\phi_m=e_m\phi_m,$$

$$\mathfrak{a}_2\chi_n=\sqrt{E(m,n)}\,\chi_{n-1}, \quad \mathfrak{a}_2^\dagger\chi_n=\sqrt{E(m,n+1)}\,\chi_{n+1}, \quad \mathfrak{a}_2\chi_n=E(m,n)\chi_n.$$

Again an analog of Sec. VII A can be worked out for the operators $\mathfrak{a}_1,\mathfrak{a}_1^\dagger,\mathfrak{n}_1$. Thus the operators generate the algebra $\mathfrak{g}_{\mathrm{W-H}}$. Since within the second sum of the CS m is considered as a constant we are in the exact situation of Sec. VII B. Thus the algebra generated by $\mathfrak{a}_2,\mathfrak{a}_2^\dagger,\mathfrak{n}_2$ is isomorphic to the algebra $\mathfrak{su}(1,1)$. The rest of the details follows from Sec. VII C.

VIII. STATISTICAL QUANTITIES

Quantum revivals are associated with wave functions. A revival of a wave function occurs when a wave function evolves in time to a state closely reproducing its initial form. Further the weighting distribution is crucial for understanding the temporal behavior of the wave function. In the case of the states (4.1), the probability of finding the state η_m in the state $|J,\alpha\rangle$ is given by

$$P(m,J)=|\langle\eta_m|J,\alpha\rangle|^2.$$

A quantitative estimate is given by the so-called Mandel parameter,

$$Q=\frac{\langle J,\alpha|\mathfrak{n}^2|J,\alpha\rangle-\langle J,\alpha|\mathfrak{n}|J,\alpha\rangle^2-\langle J,\alpha|\mathfrak{n}|J,\alpha\rangle}{\langle J,\alpha|\mathfrak{n}|J,\alpha\rangle},$$

where $\mathfrak{n}\eta_m=e_m\eta_m$. If the photon distribution is Poissonian, then $Q=0$. If $Q<0$ it is called sub-Poissonian and if $Q>0$ it is called super-Poissonian.[2] In this section we explicitly calculate the weighting distribution and the Mandel parameter for each of the CS discussed in the above sections.

A. For the states of Eq. (5.1)

For this class of states we obtain

$$P(m,J)=\frac{|J|^m}{\mathcal{N}(J,n)^2\rho(m)}=\frac{(J/2B)^m}{{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)(\gamma)_m}.$$

Since $\mathfrak{n}|\psi_{m,n}\rangle=E(m,n)|\psi_{m,n}\rangle$ and $E(0,n)\neq 0$ we have

$$\mathfrak{n}|J,\alpha,n\rangle=\mathcal{N}(J,n)^{-1}\sum_{m=0}^{\infty}\frac{J^{m/2}E(m,n)}{\sqrt{\rho(m)}}e^{-iE(m,n)\alpha}|\psi_{m,n}\rangle$$

and

$$\mathfrak{n}^2|J,\alpha,n\rangle=\mathcal{N}(J,n)^{-1}\sum_{m=0}^{\infty}\frac{J^{m/2}E(m,n)^2}{\sqrt{\rho(m)}}e^{-iE(m,n)\alpha}|\psi_{m,n}\rangle.$$

Thus

$$\langle J,\alpha,n|\mathfrak{n}|J,\alpha,n\rangle=\frac{J}{\gamma}\frac{{}_1F_1\left(2;1+\gamma;\frac{J}{2B}\right)}{{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)}+\omega,$$

where $\omega=B+(\pi(n+1)/d)^2$ and thereby $E(m,n)=2Bm+\omega$. Further

$$\langle J,\alpha,n|\mathfrak{n}^2|J,\alpha,n\rangle=\frac{1}{{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)}\left[\frac{2J(B+\omega)}{\gamma}{}_1F_1\left(2;\gamma+1;\frac{J}{2B}\right)+\frac{2J^2}{\gamma(\gamma+1)}{}_1F_1\left(3;\gamma+2;\frac{J}{2B}\right)\right]+\omega^2.$$

Therefore

$$Q=\frac{2J(B+\omega)(\gamma+1){}_1F_1\left(2;\gamma+1;\frac{J}{2B}\right)+2J^2{}_1F_1\left(3;\gamma+2;\frac{J}{2B}\right)+\gamma(\gamma+1)\omega^2{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)}{(\gamma+1)\left[J{}_1F_1\left(2;\gamma+1;\frac{J}{2B}\right)+\gamma\omega{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)\right]}$$
$$-\frac{J{}_1F_1\left(2;\gamma+1;\frac{J}{2B}\right)}{\gamma{}_1F_1\left(1;\gamma;\frac{J}{2B}\right)}-\omega-1.$$

For particular values of B,d, and n the sign of Q can be determined.

B. For the states of Eq. (5.5)

We have

$$P(n,J)=\frac{d^{2n}J^n}{\pi^{2n}(\beta)_n(\overline{\beta})_{n1}F_2\left(1;\beta,\overline{\beta};\frac{d^2J}{\pi^2}\right)}.$$

For fixed m, $E(m,n)=p+q(n+1)^2$, where $p=B(2m+1)$ and $q=\pi^2/d^2$. Since $E(m,0)\neq 0$ and $\mathfrak{n}|\psi_{mn}\rangle=E(m,n)|\psi_{mn}\rangle$ we have

$$\langle J,\alpha,m|\mathfrak{n}|J,\alpha,m\rangle=p+\frac{q}{\mathcal{N}(J,m)^2}\sum_{n=0}^{\infty}\frac{J^n(n+1)^2}{\rho(n)}=p+qQ_1,$$

where

$$Q_1=\frac{1}{{}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right)}\left[{}_1F_2\left(2;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right)+\frac{2Jd^2}{|\beta|^2\pi^2}{}_1F_2\left(3;\overline{\beta}+1,\beta+1;\frac{d^2J}{\pi^2}\right)\right]$$

and

$$\langle J,\alpha,m|\mathfrak{n}^2|J,\alpha,m\rangle=\mathcal{N}(J,m)^{-2}\sum_{n=0}^{\infty}\frac{J^nd^{2n}(p+q(n+1)^2)^2}{\pi^{2n}(\beta)_n(\overline{\beta})_n}=p^2+2pqQ_1+q^2Q_2,$$

where

$$Q_2=\frac{1}{{}_1F_2\left(1;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right)}\left[\frac{2Jd^2+\pi^2}{\pi^2}{}_1F_2\left(2;\overline{\beta},\beta;\frac{d^2J}{\pi^2}\right)-\frac{2Jd^2(\pi^2|\beta|^2-Jd^2-7\pi^2)}{|\beta|^2\pi^4}\right.$$

$$\left.\times{}_1F_2\left(3;\overline{\beta}+1,\beta+1;\frac{d^2J}{\pi^2}\right)-\frac{6J^2d^4(\beta+\overline{\beta}-5)}{|\beta|^2\pi^4(\beta+1)(\overline{\beta}+1)}{}_1F_2\left(4;\overline{\beta}+2,\beta+2;\frac{d^2J}{\pi^2}\right)\right].$$

Thus

$$Q=\frac{p^2+2pqQ_1+q^2Q_2}{p+qQ_1}-p-qQ_1-1.$$

Here again for specific values of B, d, and m the sign of Q can be determined.

C. For the states of Eq. (6.1)

The probability of finding the state $\phi_m\otimes\chi_n$ in the state $|J_1,J_2,\alpha_1,\alpha_2\rangle$ is given by

$$P(m,n,J_1,J_2)=\frac{J_1^mJ_2^n}{{}_1F_1\left(1;\frac{3}{2};\frac{J_1}{2B}\right){}_0F_1\left(-;1;\frac{J_2d^2}{\pi^2}\right)2^mB^m\left(\frac{\pi}{d}\right)^{2n}(2)_n(2)_n\left(\frac{3}{2}\right)_m}.$$

Since $\mathfrak{n}_1\phi_m=e_m\phi_m$, $\mathfrak{n}_2\chi_n=\epsilon_n\chi_n$, $\mathfrak{n}=\mathfrak{n}_1\otimes\mathfrak{n}_2$, and $e_0\neq 0,\epsilon_0\neq 0$ we have

$$\langle J_1,J_2,\alpha_1,\alpha_2|\mathfrak{n}|J_1,J_2,\alpha_1,\alpha_2\rangle=\frac{B\pi^2Q_4}{d^2}[2Q_3+1],$$

where

$$Q_3=\frac{1}{\mathcal{N}_1(J_1)^2}\sum_{m=0}^{\infty}\frac{J_1^m m}{2^m B^m\left(\frac{3}{2}\right)_m}=\frac{J}{3B\mathcal{N}_1(J_1)^2}{}_1F_1\left(2;\frac{5}{2};\frac{J}{2B}\right)$$

and

$$Q_4=\frac{1}{\mathcal{N}_2(J_2)^2}\sum_{m=0}^{\infty}\frac{d^{2m}J_2^m(m+1)^2}{\pi^{2m}(2)_m(2)_m}.$$

Further

$$\begin{aligned}\langle J_1,J_2,\alpha_1,\alpha_2|\mathfrak{n}^2|J_1,J_2,\alpha_1,\alpha_2\rangle&=\langle J_1,J_2,\alpha_1,\alpha_2|\mathfrak{n}_1^2\otimes\mathfrak{n}_2^2|J_1,J_2,\alpha_1,\alpha_2\rangle\\&=\mathcal{N}_1(J_1)^{-2}\sum_{m=0}^{\infty}\frac{J_1^m e_m^2}{e_m!}\mathcal{N}_2(J_2)^{-2}\sum_{n=0}^{\infty}\frac{J_2^n\epsilon_n^2}{\epsilon_n!}\\&=\frac{B^2\pi^4Q_6}{d^4}[4Q_5+4Q_3+1],\end{aligned}$$

where

$$Q_5=\frac{1}{\mathcal{N}_1(J_1)^2}\sum_{m=0}^{\infty}\frac{J_1^m m^2}{2^m B^m\left(\frac{3}{2}\right)_m}$$

and Q_6 can be obtained from Q_2 by substituting $J=J_2,\beta=\overline{\beta}=2$ and $\mathcal{N}(J,m)=\mathcal{N}_1(J_1)$ in the expression of Q_2. Q_4 can be obtained from Q_1 by the same substitution. Thereby we have

$$Q=\frac{B\pi^2Q_6(4Q_5+4Q_3+1)}{d^2Q_4(2Q_3+1)}-\frac{B\pi^2Q_4(2Q_3+1)}{d^2}-1.$$

For specific values of B and d the sign of Q can be determined.

D. For the states of Eq. (6.5)

The probability of finding the state $\phi_m\otimes\chi_n$ in the state $|J_1,J_2,\alpha_1,\alpha_2\rangle$ is given by

$$P(m,n,J_1,J_2)=\frac{J_1^m J_2^n}{{}_1F_2\left(1;\beta,\overline{\beta};\frac{d^2J_2}{\pi^2}\right)\mathcal{N}_1(J_1,J_2)^2 2^m B^m\left(\frac{3}{2}\right)_n\left(\frac{\pi}{d}\right)^{2n}(\beta)_n(\overline{\beta})_n}.$$

Further, by taking $\mathfrak{n}_1\phi_m=e_m\phi_m$, $\mathfrak{n}_2\chi_n=E(m,n)\chi_n$ and $\mathfrak{n}=\mathfrak{n}_1\otimes\mathfrak{n}_2$ one can find Q as in the previous section. Since we do not have a closed form for $\mathcal{N}_1(J_1,J_2)$ we avoid calculating it.

IX. CONCLUSION

Eigenfunctions and eigenvalues of the free magnetic Schrödinger operator $H_0=(1/2M)(\mathbf{P}-e/c\,\mathbf{A})^2$ were discussed. The eigenfunctions were realized as an orthonormal basis of a Hilbert space. Four classes of temporally stable CS associated to the eigenfunctions and eigenvalues of the

operator H_0 were demonstrated. The first two classes were constructed with one degree of freedom and the last two with two degrees of freedom. To each class of CS the corresponding dynamical algebra was specified. The dynamical algebras were identified to the Weyl–Heisenberg algebra, $\mathfrak{su}(1,1)$ algebra and their tensor products. For each class of CS, quantum statistical quantities were calculated explicitly.

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On limits to convective heat transport at infinite Prandtl number with or without rotation

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We prove rigorous upper bounds for the bulk heat transport in infinite Prandtl number Rayleigh–Bénard convection with or without rotation. For the rotation free case, our estimate shows that the Nusselt number is bounded by Rayleigh number according to $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{4/11}$ with constant $c<2$. In the presence of rotation, we prove $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{4/11}(\frac{1}{2}\sqrt{\mathrm{Ta}}+1)^{4/11}$ with constant $c<2$. Moreover, for weak rotating constraint ($\mathrm{Ta}\leqslant O(\mathrm{Ra}^{1/2})$), the Nusselt number is uniformly bounded above by $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{4/11}$. © *2004 American Institute of Physics.*
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I. INTRODUCTION

We derive upper bound for the bulk heat transport in infinite Prandtl number Rayleigh–Bénard convection with or without rotation. Rayleigh–Bénard convection describes motion of a fluid layer which is heated from below. Typically, the motion is modeled by Boussinesq equations. These are a system of equations consisting of the heat advection–diffusion equation for the local temperature coupled with the incompressible Navier–Stokes equation via a bouyancy force proportional to the local temperature.

One of the fundamental quantities of interest for Boussinesq equations is the total heat transport across the layer, which is expressed in terms of Nusselt number in standard nondimensional formulation. A major goal is to identify a functional relation in the form Nu(Ra,Ta), where Nu is the Nusselt number, Ra denotes the Rayleigh number, and Ta represents the Taylor number. In high Rayleigh number flows, this relation is expected to take the scaling form $\mathrm{Nu}\sim\mathrm{Ra}^{\alpha}$, and much effort has been put into determining the value of α (e.g., Refs. 6, 13, 15, 23, and 29). There is no unambigious experimental value of α though. Many experiments show that α varies between 2/7 and 1/3 (see, e.g., Refs. 1–4, 6, 7, 19–21, 26–31). On the other hand, the best known rigorous bounds uniform in Prandtl number is $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{1/2}$.[8,17]

In this paper, we focus our attention on the infinite Prandtl number limit of the Boussinesq equations. In this case, the vector field is linearly slaved to the temperature field, and one can prove global existence and uniqueness of smooth solutions.[14] In particular, in absence of rotation, the scaling law is expected to be $\mathrm{Nu}\sim\mathrm{Ra}^{1/3}$, based on arguments of marginally stable boundary layer analysis[18,22] or on the basis of sophisticated asymptotic approximations of an upper bound analysis utilizing mild statistical assumptions.[3] A 1/3 exponent with logarithmic corrections in the form $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{1/3}(\log\mathrm{Ra})^{2/3}$ was proved by Constantin and Doering,[9] the value of c is not explicitly evaluated though. An estimate in the form $\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{2/5}$ with explicit prefactor $c<1$ was obtained in Ref. 10.

Less results are known for the rotating convective heat transport. To date, the only known rigorous estimates are a uniform bound[10]

$$\mathrm{Nu}\leqslant c\,\mathrm{Ra}^{2/5}$$

with constant $c<1$ independent of rotation rate, and the rotation dependent bound[12]

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$$\mathrm{Nu} \leqslant 1 + c\,\mathrm{Ra}^2/\sqrt{\mathrm{Ta}}$$

with c independent of Ra, Ta. Moreover, when the rotation rate is fast enough, the purely conductive solution is the globally and nonlinearly attractive fixed point.

Our main results are rigorous upper bounds of the form $\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{4/11}$ in absence of rotation and $\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{4/11}(\frac{1}{2}\sqrt{\mathrm{Ta}}+1)^{4/11}$ when $\mathrm{Ta} \neq 0$. Both are for infinite Prandtl number system and prefactor c is calculated explicitly. Observe our estimate in the rotating case is particularly interesting for weakly rotating infinite Prandtl system. Moreover, we show that for weakly rotating constraint $\mathrm{Ta} \leqslant O(\mathrm{Ra}^{1/2})$, the Nusselt number is uniformly controlled by $O(\mathrm{Ra}^{4/11})$. This is in the same spirit as Ref. 11, where it is shown that for moderate rotation $\mathrm{Ta} \leqslant \mathrm{Ra}^{1/3}(\log \mathrm{Ra})^{5/3}$, the Nusselt number is controlled by $O(\mathrm{Ra}^{1/3}(\log \mathrm{Ra})^{5/3})$.

Our proof relies on a modified background field method. This method, based on an idea of Hopf in study of Navier–Stokes equations,[16] was revived and successful in handling rigorous bounds for bulk-flow quantities in several fundamental fluid flows. When applied to Rayleigh–Bénard convection with fixed temperature boundary conditions, the method has been successful in deriving many best known to date rigorous bounds. For example, a uniform bound for all Prandtl number $0 < \mathrm{Pr} \leqslant \infty$ in the form $\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{1/2}$;[8] a 1/3 bound with logarithm corrections $\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{1/3}(\log \mathrm{Ra})^{2/3}$ for infinite Prandtl number convection without rotation;[9] a uniform 2/5 bound independent of rotaion rate $\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{2/5}$ for infinite number convection with or without rotation.[10] Most recently, numerical techniques based on background method have been developed (see, e.g., Refs. 24 and 25). In particular, using an enlarged set of test functions, Plasting[25] derived numerical results in the form $\mathrm{Nu} \leqslant 0.139\,\mathrm{Ra}^{1/3}$ as $\mathrm{Ra} \to \infty$.

The starting point of this variational method is to decompose the temperature field into background and fluctuating components. The background profile is time independent and carry the boundary conditions of the temperature field. For each background, there is a quadratic form naturally associated. The main task is to estimate the quadratic form. Usually, there are two approaches to bound the heat flux. The first one is to adjust the background so that the quadratic form is positive semidefinite and the Nusselt number is bounded above by a quadratic form of the derivative of the background. The second is to esimtate the quadratic form in terms of the background, the upper bound on the Nusselt number is then estimated through minimizing a certain intergral of the background. Both approaches depend on estimates for higher derivatives of the vertical velocity. The only difference is the following: in the first approach, the quadratic form is decomposed into its Fourier modes in horizontal direction, and analysis depends on estimates for Fourier modes of the vertical velocity; while in the second approach, vertical velocity is estimated directly through the associated PDE. In this paper, we shall follow the same decomposition of the temperature field, while major modifications come at the point of estimating the quadratic form. We estimate the quadratic form in terms of the background, by estimating its Fourier modes. The main technical interest of this paper is some new estimates on higher derivatives for Fourier modes of the vertical velocity. Based on these estimates, we can estimate each Fourier mode of the quadratic form from below, which turns out to be sufficient for our purpose when summing up.

The rest of the paper is organized as follows. In Sec. II we recall the basic equations together with some necessary notations. Section III is devoted to the major estimates on the vertical velocity. The upper bound on the total heat flux for rotation free system is presented in Sec. IV and the bounds for rotating system are derived in the last two sections.

II. FORMULATION OF THE PROBLEM

Consider an incompressible Newtonian fluid confined to horizontal rigid isothermal plates separated by vertical distance h. The top plate is held at constant temperature T_2 and the bottom plate is held at constant temperature T_1. In the standard nondimensional units the fluid velocity field $\mathbf{u}(\mathbf{x},t)=(u,v,w)$ and temperature field $\mathbf{T}(\mathbf{x},t)$, pressure field $p(\mathbf{x},t)$ are governed by Boussinesq equations[5]

$$\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} + \mathrm{Pr}\sqrt{\mathrm{Ta}}\,\mathbf{k}\times\mathbf{u} + \mathrm{Pr}\,\nabla p = \mathrm{Pr}\,\Delta\mathbf{u} + \mathrm{Pr}\,\mathrm{Ra}\,\mathbf{k}T,$$

$$\nabla\cdot\mathbf{u} = 0,$$

$$T_t + \mathbf{u}\cdot\nabla T = \Delta T,$$

with boundary conditions

$$\mathbf{u}|_{z=0,1} = 0, \quad T|_{z=1} = 0, \quad T|_{z=0} = 1, \quad \left.\frac{\partial w}{\partial z}\right|_{z=0,1} = 0.$$

Here $\mathbf{k}$ is the z direction, $\mathrm{Pr} = \nu/\kappa$ is the Prandtl number (a ratio of the material parameters, ν is the kinematic viscosity, and κ is the thermal diffusivity), Rayleigh number $\mathrm{Ra} = g\alpha(T_1 - T_2)h^3/\nu\kappa$ is a ratio of the overall buoyancy force to the damping coefficients [g is the acceleration of gravity, α is the thermal expansion coefficient, $(T_1 - T_2)$ is the temperature drop across the gap, h is the gap width] and Taylor number $\mathrm{Ta} = (2\Omega h^2/\nu)^2$ measures the rotation (Ω is the rotation rate). Lengths are measured in units of h and $\mathbf{u}$, T, p are periodic in x and y directions with periods L_x/h and L_y/h, respectively.

In this paper, we are concerned with the infinite Prandtl number model where the equation for the velocity field is reduced to

$$\sqrt{\mathrm{Ta}}\,\mathbf{k}\times\mathbf{u} + \boldsymbol{\nabla} p = \boldsymbol{\Delta}\mathbf{u} + \mathrm{Ra}\,\mathbf{k}T.$$

Eliminating the pressure term from the equation above, we immediately obtain

$$\Delta^2 w - \sqrt{\mathrm{Ta}}\,\frac{\partial\zeta}{\partial z} = -\mathrm{Ra}\,\Delta_H T \tag{2.1}$$

and

$$-\Delta\zeta - \sqrt{\mathrm{Ta}}\,\frac{\partial w}{\partial z} = 0. \tag{2.2}$$

Here $\zeta = v_x - u_y$ is the vertical vorticity and $\Delta_H = \partial_x^2 + \partial_y^2$ denotes the horizontal Laplacian. The boundary conditions for (2.1), (2.2) are

$$w|_{z=0,1} = 0, \quad \zeta|_{z=0,1} = 0, \quad \left.\frac{\partial w}{\partial z}\right|_{z=0,1} = 0.$$

The ultimate goal is to find a functional relation of the form Nu(Ra,Ta). At current stage, only upper bounds on Nu have been obtained. Here Nu is the Nusselt number which is defined as the ratio of the total vertical heat flux to the conductive heat flux. Standard derivations give a variety of expressions for the Nusselt number in terms of solutions of (2.1) and (2.2),

$$\mathrm{Nu} = 1 + \frac{1}{\mathcal{A}}\left\langle \int_V wT\,\mathrm{d}V \right\rangle = \frac{1}{\mathcal{A}}\langle\|\nabla T\|^2\rangle = \frac{1}{\mathrm{Ra}}\,\frac{1}{\mathcal{A}}\langle\|\nabla\mathbf{u}\|^2\rangle.$$

Here and throughout the paper, we use the following notations:

$$\int_V \mathrm{d}V = \int_0^{L_x/h}\int_0^{L_y/h}\int_0^1 \mathrm{d}z\,\mathrm{d}y\,\mathrm{d}x$$

for the volume integration,

$$\mathcal{A}=\frac{L_x L_y}{h^2}$$

for the nondimensional area of the layer,

$$\|f\|=\left(\int_V |f|^2\,\mathrm{d}V\right)^{1/2}$$

for the L_2 norm on the domain, and

$$\langle f\rangle=\limsup_{t\to\infty}\frac{1}{t}\int_0^t f(s)\,\mathrm{d}s$$

for the long time average of f.

We also need the following notations for functions defined on [0,1]:

$$\|g\|_2=\left(\int_0^1 g^2(z)\,\mathrm{d}z\right)^{1/2}$$

denotes the L_2 norm on [0,1] and

$$\|g\|_\infty=\sup_{0\leqslant z\leqslant 1} g(z)$$

represents the L_∞ norm on [0,1].

A useful variational principle was introduced by Constantin and Doering[8–10] to prove rigorous upper bounds on Nu, building upon a method of analysis for the Navier–Stokes equations introduced by Hopf.[16] The starting point of this variational principle is to decompose the temperature field into a steady background profile and a time-dependent fluctuation field,

$$T(\mathbf{x},t)=\tau(z)+\theta(\mathbf{x},t),$$

where $\tau(z)$ inherits the boundary conditions of T and θ satisfies homogeneous boundary conditions in the z direction and periodic in horizontal directions. Under this decomposition, standard manipulation yields the following fundamental relation:

$$\mathrm{Nu}=\int_0^1 \tau'(z)^2\,\mathrm{d}z-\frac{1}{\mathcal{A}}\left\langle\int_V(|\nabla\theta|^2+2\tau'(z)w\theta)\mathrm{d}V\right\rangle=\int_0^1\tau'(z)^2\,\mathrm{d}z-\frac{1}{\mathcal{A}}\langle Q(\theta)\rangle,$$

where $Q(\theta)=\int_V(|\nabla\theta|^2+2\tau'(z)w\theta)\mathrm{d}V$ is a quadratic form. There are two ways to estimate upper bound of Nu based on this relation. The first approach is to choose background profile τ to ensure $Q(\theta)\geqslant 0$, then the Nusselt number is bounded above by $\int_0^1\tau'(z)^2\,\mathrm{d}z$; the second approach amounts to estimate the indefinite term in $Q(\theta)$ in terms of Ra and the functional form of τ, followed by an appropriate choice of τ to balance this estimate with $\int_0^1\tau'(z)^2\,\mathrm{d}z$. In both approaches, $\tau(z)$ is chosen so that the support of $\tau'(z)$ is concentrated near the boundaries where w,θ vanish. With such choice of background profile, both approaches rely on detailed growth estimates for θ and w in the boundary layer near $z=0$ and $z=1$. More precisely, in the first approach, one decomposes $Q(\theta)$ into Fourier modes $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ in horizontal direction, then adjusts τ to ensure $Q_{\mathbf{m}}(\theta_{\mathbf{m}})\geqslant 0$ for each $\mathbf{m}$. The argument relies on growth estimates for each Fourier mode $w_{\mathbf{m}}$ of the vertical velocity; in the second approach, w is estimated directly through the associated PDE.

Motivated by these two approaches, we estimate Q by estimating its Fourier modes $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$. Recall for each horizontal wave number $\mathbf{m}=[(2\pi h/L_x)\,m_x,(2\pi h/L_y)\,m_y]$ $[|\mathbf{m}|=m,\ (m_x,m_y)\in\mathbf{Z}^2]$,

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}})=\int_0^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{dz}}\right|^2+m^2|\theta_{\mathbf{m}}|^2+\tau'(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+w_{\mathbf{m}}\theta_{\mathbf{m}}^*)\mathrm{dz}.$$

Here $\theta_{\mathbf{m}}(z)$, $w_{\mathbf{m}}(z)$ are the Fourier coefficients for θ and w, respectively. We choose the following profile of τ:

$$\tau(z)=\begin{cases}1-\dfrac{z}{2\delta}, & 0\leqslant z\leqslant\delta,\\ \dfrac{1}{2}, & \delta\leqslant z\leqslant 1-\delta,\\ \dfrac{1-z}{2\delta}, & 1-\delta\leqslant z\leqslant 1.\end{cases}\tag{2.3}$$

We obtain some new estimates on higher derivatives of $w_{\mathbf{m}}$. Based on this, we can bound $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ in terms of Ra, Ta, δ and $\|\theta_{\mathbf{m}}\|_2$, and the Nusselt number is bounded above by

$$\int_0^1\tau'(z)^2\,\mathrm{dz}-\sum_{\mathbf{m}}Q_{\mathbf{m}}(\theta_{\mathbf{m}}).$$

It turns out that the second term can be bounded above in terms of Ra, Ta, and the functional form of τ. The estimates on Nu then follows. Our main results are the following Theorems.

Theorem 2.1: *For infinite Prandtl number convection without rotation, we have the following estimates on the Nusselt number*:

$$\mathrm{Nu}\leqslant 1.26\,\mathrm{Ra}^{4/11}.$$

Theorem 2.2: *For rotating system, we have*

$$\mathrm{Nu}\leqslant 1.3\,\mathrm{Ra}^{4/11}\,\mathrm{Ta}^{1/6}+0.13\,\mathrm{Ra}^{4/11}\,\mathrm{Ta}^{-5/3}+0.18\,\mathrm{Ra}^{2/11}\,\mathrm{Ta}^{1/6}$$

and

$$\mathrm{Nu}\leqslant 1.26\,\mathrm{Ra}^{4/11}\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^{4/11}.$$

We also have the following theorem for weakly rotating system.

Theorem 2.3: *There exist constants $B_1,B_2>0$ independent of Ra,Ta, such that when $Ta\leqslant B_1\,Ra^{1/2}$,*

$$Nu\leqslant B_2\,Ra^{4/11}.$$

III. ESTIMATES ON VERTICAL VELOCITY

In this section, we derive estimates for higher derivatives of $w_{\mathbf{m}}$ for Fourier modes $|\mathbf{m}|\geqslant 1$. Our main estimate is

Proposition 3.1: For $|\mathbf{m}|=m\geqslant 1$, if $w_{\mathbf{m}}$ satisfies

$$\left(-\frac{\mathrm{d}^2}{\mathrm{dz}^2}+m^2\right)^2 w_{\mathbf{m}}=f_{\mathbf{m}},$$

$$w_{\mathbf{m}}(0)=w_{\mathbf{m}}(1)=\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{dz}}(0)=\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{dz}}(1)=0,$$

then

$$\left\| \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2} \right\|_{\infty} \leqslant C_1 m^{-3/2} \|f_{\mathbf{m}}\|_2 .$$

Here

$$C_1 = \left[1 + \frac{e^2+1}{e^2-1} \cdot \frac{4\cosh 1 + 2\sinh 1}{\sinh 1 - 1} \right] \approx 64.8734.$$

We prove Proposition 3.1 in several steps. First we recall some basic facts. For $m>0$, the solution to

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2} - m^2 \right) u = f$$

with zero Dirichlet boundary conditions,

$$u(0) = u(1) = 0$$

is given using the Green's function $G^{(m)}(z,\zeta)$ by

$$u(z) = G^{(m)}(f)(z) = \int_0^1 G^{(m)}(z,\zeta) f(\zeta)\,\mathrm{d}\zeta.$$

Recall that the Green's function is calculated from two independent solutions to the homogeneous ODE with one point boundary conditions,

$$G^{(m)}(z,\zeta) = \frac{1}{U_m} \begin{cases} y_1(z) y_2(\zeta), & z < \zeta, \\ y_1(\zeta) y_2(z), & z \geqslant \zeta. \end{cases}$$

Here $U_m = y_1(z) y_2'(z) - y_1'(z) y_2(z)$ is the Wronskian.

We will take

$$y_1(z) = \frac{e^{mz} - e^{-mz}}{2m}, \quad y_2(z) = y_1(z-1),$$

and therefore the Wronskian $U_m = y_1 y_2' - y_1' y_2$ satisfies

$$U_m(z) = y_1(1) = \frac{e^m - e^{-m}}{2m}.$$

In particular, we can write the Green's function explicitly as

$$G^{(m)}(z,\zeta) = \frac{1}{2m^2 U_m} [\cosh(m(z+\zeta-1)) - \cosh(m(1-|z-\zeta|))]. \tag{3.1}$$

To prove Proposition 3.1, we decompose

$$w_{\mathbf{m}} = u_{\mathbf{m}} + h_{\mathbf{m}}$$

with

$$u_{\mathbf{m}}(z)=\int_0^1 G^{(m)}(z,\zeta)g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta,$$

$$g_{\mathbf{m}}(\zeta)=\int_0^1 G^{(m)}(\zeta,\zeta')f_{\mathbf{m}}(\zeta')\mathrm{d}\zeta', \tag{3.2}$$

$$h_{\mathbf{m}}(z)=A_{\mathbf{m}}(1-z)y_1(z)+B_{\mathbf{m}}zy_2(z) \tag{3.3}$$

with

$$A_{\mathbf{m}}=\frac{1}{U_m^2-1}(u'_{\mathbf{m}}(0)+U_m u'_{\mathbf{m}}(1)),$$

$$B_{\mathbf{m}}=\frac{1}{U_m^2-1}(U_m u'_{\mathbf{m}}(0)+u'_{\mathbf{m}}(1)).$$

One can check directly that $u_{\mathbf{m}},h_{\mathbf{m}}$ satisfies

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2}-m^2\right)^2 u_{\mathbf{m}}=f_{\mathbf{m}},$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2}-m^2\right)^2 h_{\mathbf{m}}=0,$$

with $u_{\mathbf{m}}=0$, $h_{\mathbf{m}}=0$, and $h'_{\mathbf{m}}=-u'_{\mathbf{m}}$ on the boundaries.

We claim the following estimates:

$$\left\|\frac{\mathrm{d}^2u_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty\leqslant\frac{c_1}{m^{3/2}}\|f_{\mathbf{m}}\|_2,\quad \left\|\frac{\mathrm{d}^2h_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty\leqslant\frac{c_2}{m^{3/2}}\|f_{\mathbf{m}}\|_2. \tag{3.4}$$

Here c_i are constants independent of m.

First we prove the following lemma.

Lemma 3.2: If

$$g(z)=\int_0^1 G^{(m)}(z,\zeta)f(\zeta)\mathrm{d}\zeta,$$

then

$$\|g\|_\infty\leqslant\frac{1}{m^2}\|f\|_\infty,\quad \left\|\frac{\mathrm{d}g}{\mathrm{d}z}\right\|_\infty\leqslant 2\,\frac{e^2+1}{e^2-1}\,\frac{1}{m}\|f\|_\infty,$$

$$\|g\|_\infty\leqslant\frac{1}{2}\,\frac{\|f\|_2}{m^{3/2}},\quad \left\|\frac{\mathrm{d}g}{\mathrm{d}z}\right\|_\infty\leqslant\frac{1}{\sqrt{2}}\sqrt{\frac{e^2+1}{e^2-1}}\frac{\|f\|_2}{\sqrt{m}}.$$

Proof: From explicit formula of $G^{(m)}(z,\zeta)$, we can write

$$
\begin{aligned}
g(z) &= \int_0^1 \frac{1}{2m^2U_m}[\cosh(m(z+\zeta-1))-\cosh(m(1-|z-\zeta|))]f(\zeta)\mathrm{d}\zeta \\
&= \int_0^1 \frac{1}{2m^2U_m}\cosh(m(z+\zeta-1))f(\zeta)\mathrm{d}\zeta - \int_0^z \frac{1}{2m^2U_m}\cosh(m(1-z+\zeta))f(\zeta)\mathrm{d}\zeta \\
&\quad - \int_z^1 \frac{1}{2m^2U_m}\cosh(m(1-\zeta+z))f(\zeta)\mathrm{d}\zeta \\
&= \int_0^z \frac{\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)}{2m\sinh m}f(\zeta)\mathrm{d}\zeta \\
&\quad + \int_z^1 \frac{\cosh m(z+\zeta-1)-\cosh m(1-\zeta+z)}{2m\sinh m}f(\zeta)\mathrm{d}\zeta. \qquad (3.5)
\end{aligned}
$$

Observe for $0\leqslant z,\ \zeta\leqslant 1$,

$$|z+\zeta-1|\leqslant 1-z+\zeta$$

and

$$|z+\zeta-1|\leqslant 1-\zeta+z.$$

Therefore the following inequality always holds when $0\leqslant z,\ \zeta\leqslant 1$:

$$
\begin{aligned}
&\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)\leqslant 0, \\
&\cosh m(z+\zeta-1)-\cosh m(1-\zeta+z)\leqslant 0, \\
&\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)\geqslant 0, \\
&\sinh m(z+\zeta-1)-\sinh m(1-\zeta+z)\leqslant 0.
\end{aligned} \qquad (3.6)
$$

In particular, (3.6) implies

$$
\begin{aligned}
\|g\|_\infty &\leqslant \frac{\|f\|_\infty}{2m\sinh m}\left(\int_0^z(\cosh m(1-z+\zeta)-\cosh m(z+\zeta-1))\mathrm{d}\zeta\right) \\
&\quad + \frac{\|f\|_\infty}{2m\sinh m}\left(\int_z^1(\cosh m(1-\zeta+z)-\cosh m(z+\zeta-1))\right) \\
&= \frac{\|f\|_\infty}{2m\sinh m}\left(\frac{\sinh m(1-z+\zeta)-\sinh m(z+\zeta-1)}{m}\Big|_0^z\right) \\
&\quad + \frac{\|f\|_\infty}{2m\sinh m}\left(\frac{-\sinh m(1-\zeta+z)-\sinh m(z+\zeta-1)}{m}\Big|_z^1\right) \\
&= \frac{\|f\|_\infty}{m^2\sinh m}(\sinh m-\sinh(mz)-\sinh(m(1-z)))\leqslant \frac{\|f\|_\infty}{m^2}. \qquad (3.7)
\end{aligned}
$$

Apply Cauchy–Shwartz inequality twice, we can estimate $\|g\|_\infty$ in terms of L_2 norm of f as follows:

$$\|g\|_\infty \leqslant \frac{1}{2m\sinh m}\left(\int_0^z [\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)]^2\,\mathrm{d}\zeta\right)^{1/2}\left(\int_0^z f^2\right)^{1/2}$$
$$+\frac{1}{2m\sinh m}\left(\int_z^1 [\cosh m(z+\zeta-1)-\cosh m(1-\zeta+z)]^2\mathrm{d}\zeta\right)^{1/2}\left(\int_z^1 f^2\right)^{1/2}$$
$$\leqslant \frac{\|f\|_2}{2m\sinh m}\left(\int_0^z [\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)]^2+\int_z^1 [\cosh m(z+\zeta-1)\right.$$
$$\left.-\cosh m(1-\zeta+z)]^2\right)^{1/2} \leqslant \frac{\|f\|_2}{2m\sinh m}\left(\int_0^z [\cosh^2 m(1-z+\zeta)-\cosh^2 m(z+\zeta-1)]\mathrm{d}\zeta\right.$$
$$\left.+\int_z^1 [\cosh^2 m(1-\zeta+z)-\cosh^2 m(z+\zeta-1)]\right)^{1/2}$$
$$\leqslant \frac{\|f\|_2}{2m\sinh m}\left(\int_0^z \frac{\cosh 2m(1-z+\zeta)-\cosh 2m(z+\zeta-1)}{2}\right.$$
$$\left.+\int_z^1 \frac{\cosh 2m(1-\zeta+z)-\cosh 2m(z+\zeta-1)}{2}\right)^{1/2}$$
$$\leqslant \frac{\|f\|_2}{2m\sinh m}\left(\frac{\sinh 2m-\sinh(2mz)-\sinh(2m(1-z))}{2m}\right)^{1/2}$$
$$\leqslant \frac{\|f\|_2}{2m\sinh m}\left(\frac{\sinh 2m-2\sinh m}{2m}\right)^{1/2}=\frac{\|f\|_2}{\sqrt{2}m^{3/2}}\frac{\sinh\frac{m}{2}}{\sqrt{\sinh m}}=\frac{\|f\|_2}{2m^{3/2}}\sqrt{\frac{e^m-1}{e^m+1}}\leqslant\frac{1}{2}\frac{\|f\|_2}{m^{3/2}}. \quad (3.8)$$

Here we used the fact that when $0\leqslant z\leqslant 1$,

$$\sinh 2m-\sinh(2mz)-\sinh(2m(1-z))\leqslant\sinh 2m-2\sinh m,$$

and when $m\geqslant 1$,

$$\frac{e^m-1}{e^m+1}\leqslant 1.$$

To estimate $\|\,\mathrm{d}g/\mathrm{d}z\,\|_\infty$, we differentiate the explicit expression $g(z)$, we get

$$\frac{\mathrm{d}g}{\mathrm{d}z}=\int_0^z \frac{\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)}{2\sinh m}f(\zeta)\mathrm{d}\zeta$$
$$+\int_z^1 \frac{\sinh m(z+\zeta-1)-\sinh m(1-\zeta+z)}{2\sinh m}f(\zeta)\mathrm{d}\zeta. \quad (3.9)$$

Observe that for $0\leqslant z,\ \zeta\leqslant 1$,

$$\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)\geqslant 0,$$

$$\sinh m(z+\zeta-1)-\sinh m(1-\zeta+z)\leqslant 0.$$

Apply this to (3.9), we get

$$\begin{aligned}\left\|\frac{dg}{dz}\right\|_\infty &\leqslant \frac{\|f\|_\infty}{2\sinh m}\int_0^z [\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)]d\zeta \\ &\quad + \frac{\|f\|_\infty}{2\sinh m}\int_z^1 [\sinh m(1-\zeta+z)-\sinh m(z+\zeta-1)]d\zeta \\ &= \frac{\|f\|_\infty}{2\sinh m}\left(\frac{\cosh m(z+\zeta-1)+\cosh m(1-z+\zeta)}{m}\Big|_0^z\right. \\ &\quad \left. + \frac{-\cosh m(1-\zeta+z)-\cosh m(z+\zeta-1)}{m}\Big|_z^1\right) \\ &= \frac{\|f\|_\infty}{m\sinh m}(\cosh m-\cosh m(1-z)-\cosh mz+\cosh m(2z-1)) \\ &\leqslant \frac{2\|f\|_\infty\cosh m}{m\sinh m} \leqslant \frac{2(e^2+1)}{m(e^2-1)}\|f\|_\infty . \end{aligned} \tag{3.10}$$

Here we used the fact that when $0\leqslant z\leqslant 1$,

$$\cosh mz \geqslant 0, \quad \cosh m(2z-1)\leqslant \cosh m,$$

and when $m\geqslant 1$

$$\frac{\cosh m}{\sinh m}\leqslant \frac{e^2+1}{e^2-1}.$$

We can also estimate $\|\,dg/dz\,\|_\infty$ in terms of $\|f\|_2$ as follows:

$$\begin{aligned}\left\|\frac{dg}{dz}\right\|_\infty &\leqslant \frac{1}{2\sinh m}\left[\int_0^z(\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta))^2\right]^{1/2}\left(\int_0^z f^2\right)^{1/2} \\ &\quad + \frac{1}{2\sinh m}\left[\int_z^1(\sinh m(1-\zeta+z)-\sinh m(z+\zeta-1))^2\right]^{1/2}\left(\int_z^1 f^2\right)^{1/2} \\ &\leqslant \frac{\|f\|_2}{2\sinh m}\left(\int_0^z[\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)]^2\,d\zeta\right. \\ &\quad \left. + \int_z^1[\sinh m(1-\zeta+z)-\sinh m(z+\zeta-1)]^2\,d\zeta\right)^{1/2} \\ &\leqslant \frac{\|f\|_2}{2\sinh m}\left(2\int_0^z[\sinh^2 m(z+\zeta-1)+\sinh^2 m(1-z+\zeta)]d\zeta\right. \\ &\quad \left. + 2\int_z^1[\sinh^2 m(1-\zeta+z)+\sinh^2 m(z+\zeta-1)]d\zeta\right)^{1/2} \\ &\leqslant \frac{\|f\|_2}{2\sinh m}\left(\int_0^z[\cosh 2m(z+\zeta-1)+\cosh 2m(1-z+\zeta)]d\zeta\right. \\ &\quad \left. + \int_z^1[\cosh 2m(1-\zeta+z)+\cosh 2m(z+\zeta-1)]d\zeta\right)^{1/2}\end{aligned}$$

$$=\frac{\|f\|_2}{2\sinh m}\left(\frac{\sinh 2m(z+\zeta-1)+\sinh 2m(1-z+\zeta)}{2m}\Big|_0^z\right.$$
$$\left.+\frac{-\sinh 2m(1-\zeta+z)+\sinh 2m(z+\zeta-1)}{2m}\Big|_z^1\right)^{1/2}$$
$$=\frac{\|f\|_2}{2\sinh m}\frac{(2\sinh 2m)^{1/2}}{\sqrt{2m}}=\frac{\|f\|_2}{\sqrt{2m}}\left(\frac{e^{2m}+1}{e^{2m}-1}\right)^{1/2}\leqslant\frac{\|f\|_2}{\sqrt{2m}}\left(\frac{e^2+1}{e^2-1}\right)^{1/2}. \tag{3.11}$$

□

For

$$u_{\mathbf{m}}(z)=\int_0^1 G^{(m)}(z,\zeta)g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta$$

and

$$g_{\mathbf{m}}(z)=\int_0^1 G^{(m)}(z,\zeta)f_{\mathbf{m}}(\zeta)\mathrm{d}\zeta,$$

Lemma 3.2 immediately implies the following estimates:

$$\|u_{\mathbf{m}}\|_\infty\leqslant\frac{1}{m^2}\|g_{\mathbf{m}}\|_\infty,\quad \|u_{\mathbf{m}}\|_\infty\leqslant\frac{1}{2}\frac{\|g_{\mathbf{m}}\|_2}{m^{3/2}},$$
$$\left\|\frac{\mathrm{d}u_{\mathbf{m}}}{\mathrm{d}z}\right\|_\infty\leqslant 2\frac{e^2+1}{e^2-1}\frac{\|g_{\mathbf{m}}\|_\infty}{m},\quad \left\|\frac{\mathrm{d}u_{\mathbf{m}}}{\mathrm{d}z}\right\|_\infty\leqslant\frac{1}{\sqrt{2}}\sqrt{\frac{e^2+1}{e^2-1}}\frac{\|g_{\mathbf{m}}\|_2}{m^{1/2}}, \tag{3.12}$$
$$\|g_{\mathbf{m}}\|_\infty\leqslant\frac{1}{2}\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2,$$
$$\left\|\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}\right\|_\infty\leqslant\frac{1}{\sqrt{2}}\sqrt{\frac{e^2+1}{e^2-1}}\frac{1}{\sqrt{m}}\|f_{\mathbf{m}}\|_2.$$

In particular, estimates in (3.12) are useful in the following lemma.

Lemma 3.3: Let

$$u_{\mathbf{m}}(z)=\int_0^1 G^{(m)}(z,\zeta)g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta,\quad g_{\mathbf{m}}(\zeta)=\int_0^1 G^{(m)}(\zeta,\zeta')f_{\mathbf{m}}(\zeta')\mathrm{d}\zeta',$$

then

$$\left\|\frac{\mathrm{d}^2u_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty\leqslant\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2.$$

Proof: From explicit expression of $G^{(m)}(z,\zeta)$, we have

$$u_{\mathbf{m}}(z)=\int_0^1\frac{\cosh m(z+\zeta-1)}{2m\sinh m}g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta-\int_0^z\frac{\cosh m(1-z+\zeta)}{2m\sinh m}g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta$$
$$-\int_z^1\frac{\cosh m(1-\zeta+z)}{2m\sinh m}g_{\mathbf{m}}(\zeta)\mathrm{d}\zeta.$$

Differentiate twice, we get

$$\begin{aligned}\frac{d^2u_{\mathbf{m}}}{dz^2}&=\int_0^1\frac{m\cosh m(z+\zeta-1)}{2\sinh m}g_{\mathbf{m}}(\zeta)d\zeta+g_{\mathbf{m}}(z)-\int_0^z\frac{m\cosh m(1-z+\zeta)}{2\sinh m}g_{\mathbf{m}}(\zeta)d\zeta\\&\quad-\int_z^1\frac{m\cosh m(1-\zeta+z)}{2\sinh m}g_{\mathbf{m}}(\zeta)d\zeta\\&=\int_0^z\frac{m[\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)]}{2\sinh m}g_{\mathbf{m}}(\zeta)d\zeta+g_{\mathbf{m}}(z)\\&\quad+\int_z^1\frac{m[\cosh m(z+\zeta-1)-\cosh m(1-\zeta+z)]}{2\sinh m}g_{\mathbf{m}}(\zeta)d\zeta.\end{aligned}$$

Recall for $0\leqslant z,\ \zeta\leqslant 1$,

$$\begin{aligned}&\cosh m(z+\zeta-1)-\cosh m(1-z+\zeta)\leqslant 0,\\&\cosh m(z+\zeta-1)-\cosh m(1-\zeta+z)\leqslant 0,\\&\sinh m(z+\zeta-1)+\sinh m(1-z+\zeta)\geqslant 0,\\&\sinh m(z+\zeta-1)-\sinh m(1-\zeta+z)\leqslant 0.\end{aligned}\tag{3.13}$$

Equation (3.13) implies the following estimates:

$$\begin{aligned}\left\|\frac{d^2u_{\mathbf{m}}}{dz^2}\right\|_\infty&\leqslant\|g_{\mathbf{m}}\|_\infty+\frac{m\|g_{\mathbf{m}}\|_\infty}{2\sinh m}\left(\int_0^z[\cosh m(1-z+\zeta)-\cosh m(z+\zeta-1)]d\zeta\right.\\&\qquad\left.+\int_z^1[\cosh m(1-\zeta+z)-\cosh m(z+\zeta-1)]d\zeta\right)\\&=\|g_{\mathbf{m}}\|_\infty+\frac{m\|g_{\mathbf{m}}\|_\infty}{2\sinh m}\left(\frac{\sinh m(1-z+\zeta)-\sinh m(z+\zeta-1)}{m}\Big|_0^z\right.\\&\qquad\left.-\frac{\sinh m(1-\zeta+z)+\sinh m(z+\zeta-1)}{m}\Big|_z^1\right)\\&=\|g_{\mathbf{m}}\|_\infty+\frac{\sinh m-\sinh mz-\sinh m(1-z)}{\sinh m}\|g_{\mathbf{m}}\|_\infty\\&\leqslant 2\|g_{\mathbf{m}}\|_\infty\leqslant 2\,\frac{1}{2}\,\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2=\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2.\end{aligned}\tag{3.14}$$

Next we shall prove estimates on derivatives of $h_{\mathbf{m}}$, first we state two simple lemmas.
Lemma 3.4: Let $a\geqslant 0$, $m\geqslant 1$, $u(z)=m(1-z)\sinh m(z+a)$, $0\leqslant z\leqslant 1$, *then*

$$\max_{0\leqslant z\leqslant 1}u(z)\leqslant\sinh m(1+a).$$

Proof: Differentiate u, we have

$$u'(z)=m^2(1-z)\cosh m(z+a)-m\sinh m(z+a)$$

$$=\frac{m}{2}[e^{m(z+a)}(m(1-z)-1)+e^{-m(z+a)}(m(1-z)+1)].$$

In particular,

$$u'(z)>0 \quad \text{when} \quad m(1-z)-1\geqslant 0.$$

On the other hand, $u'(1)<0$, therefore $\max_{0\leqslant z\leqslant 1} u(z)$ is achieved at some $0<z_0<1$ with

$$m(1-z_0)\leqslant 1.$$

Therefore

$$\max_{0\leqslant z\leqslant 1} u(z)=u(z_0)=m(1-z_0)\sinh m(z_0+a)\leqslant \sinh m(1+a).$$

□

Remark 3.5: Consider $v(z)=mz\sinh m(a-z)$, $a\geqslant 1$, $0\leqslant z\leqslant 1$, then a direct corollary of the previous lemma is $\max_{0\leqslant z\leqslant 1} v(z)\leqslant \sinh ma$.

Lemma 3.6: When $m\geqslant 1$, we have

$$\text{(a)} \quad \frac{\cosh m}{\sinh m-m}\leqslant \frac{\cosh 1}{\sinh 1-1},$$

$$\text{(b)} \quad \frac{\sinh m}{\sinh m-m}\leqslant \frac{\sinh 1}{\sinh 1-1},$$

$$\text{(c)} \quad \frac{m}{\sinh m-m}\leqslant \frac{1}{\sinh 1-1}.$$

Proof: Since

$$\frac{\sinh m}{\sinh m-m}=1+\frac{m}{\sinh m-m},$$

we only need to prove (a) and (c).

Let

$$f_1(x)=\frac{\cosh x}{\sinh x-x}, \quad f_2(x)=\frac{x}{\sinh x-x}.$$

Then

$$f_1'(x)=\frac{1}{(\sinh x-x)^2}[\sinh x(\sinh x-x)-\cosh x(\cosh x-1)]$$

$$=\frac{1}{2(\sinh x-x)^2}(-2-xe^x+xe^{-x}+e^x+e^{-x}).$$

Observe that when $x\geqslant 1$, $(x+1)e^{-x}\leqslant 2$, we have

$$f_1'(x)\leqslant 0 \quad \text{for} \quad x\geqslant 1.$$

Thus $\max_{m\geqslant 1} f_1(m)\leqslant f_1(1)$.

Similarly

$$f_2'(x)=\frac{1}{(\sinh x-x)^2}(\sinh x-x\cosh x)\leqslant 0 \quad \text{when } x\geqslant 1,$$

therefore $\max_{m\geqslant 1} f_2(m)\leqslant f_2(1)$.

Now we estimate derivatives of $h_{\mathbf{m}}$ for $|\mathbf{m}|=m\geqslant 1$.

Lemma 3.7: $h_{\mathbf{m}}=A_{\mathbf{m}}(1-z)y_1(z)+B_{\mathbf{m}}zy_2(z)$,

$$A_{\mathbf{m}}=\frac{u_{\mathbf{m}}'(0)+U_m u_{\mathbf{m}}'(1)}{U_m^2-1},\quad B_{\mathbf{m}}=\frac{u_{\mathbf{m}}'(0)U_m+u_{\mathbf{m}}'(1)}{U_m^2-1},\quad y_1(z)=\frac{e^{mz}-e^{-mz}}{2m},\quad y_2(z)=y_1(z-1).$$

Then there exists $c_1>0$ independent of m such that

$$\left\|\frac{\mathrm{d}^2 h_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty \leqslant c_1\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2.$$

Proof: Differentiate $h_{\mathbf{m}}$ directly, we have

$$\frac{\mathrm{d}^2 h_{\mathbf{m}}}{\mathrm{d}z^2}=-2A_{\mathbf{m}}y_1'(z)+A_{\mathbf{m}}y_1''(z)(1-z)+2B_{\mathbf{m}}y_2'(z)+B_{\mathbf{m}}y_2''(z)z.$$

Recall

$$\begin{aligned} y_1'(z)&=\frac{e^{mz}+e^{-mz}}{2},\quad y_2'(z)=\frac{e^{m(z-1)}+e^{-m(z-1)}}{2},\\ y_1''(z)&=\frac{m(e^{mz}-e^{-mz})}{2},\quad y_2''(z)=\frac{m(e^{m(z-1)}-e^{-m(z-1)})}{2}, \end{aligned} \tag{3.15}$$

and

$$\begin{aligned} |A_{\mathbf{m}}|&\leqslant\frac{U_m+1}{U_m^2-1}\|u_{\mathbf{m}}'\|_\infty=\frac{m}{\sinh m-m}\|u_{\mathbf{m}}'\|_\infty,\\ |B_{\mathbf{m}}|&\leqslant\frac{U_m+1}{U_m^2-1}\|u_{\mathbf{m}}'\|_\infty=\frac{m}{\sinh m-m}\|u_{\mathbf{m}}'\|_\infty. \end{aligned} \tag{3.16}$$

Equations (3.15) and (3.16) and Lemma 3.4, Lemma 3.6 imply

$$\begin{aligned} \|h_{\mathbf{m}}''\|_\infty &\leqslant 2|A_{\mathbf{m}}|\cosh m+2|B_{\mathbf{m}}|\cosh m+|A_{\mathbf{m}}|\max_{0\leqslant z\leqslant 1}(m(1-z)\sinh mz)\\ &\quad+|B_m|\max_{0\leqslant z\leqslant 1}(mz\sinh m(1-z))\\ &\leqslant\frac{4m\cosh m}{\sinh m-m}\|u_{\mathbf{m}}'\|_\infty+\frac{2m\sinh m}{\sinh m-m}\|u_{\mathbf{m}}'\|_\infty\leqslant\frac{4\cosh m+2\sinh m}{\sinh m-m}m\frac{1}{m}2\frac{e^2+1}{e^2-1}\|g_{\mathbf{m}}\|_\infty\\ &\leqslant 2\frac{e^2+1}{e^2-1}\frac{4\cosh m+2\sinh m}{\sinh m-m}\frac{1}{2m^{3/2}}\|f_{\mathbf{m}}\|_2\leqslant\frac{e^2+1}{e^2-1}\frac{4\cosh m+2\sinh m}{\sinh m-m}\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2\\ &\leqslant\frac{e^2+1}{e^2-1}\frac{4\cosh 1+2\sinh 1}{\sinh 1-1}\frac{1}{m^{3/2}}\|f_{\mathbf{m}}\|_2. \end{aligned}$$

Summarize the estimates on the higher derivatives of $u_{\mathbf{m}}$, $h_{\mathbf{m}}$, we have proved

$$\|w''_{\mathbf{m}}\|_\infty \leqslant C_1 \frac{1}{m^{3/2}} \|f_{\mathbf{m}}\|_2$$

with

$$C_1 = \left[1 + \frac{e^2+1}{e^2-1} \cdot \frac{4\cosh 1 + 2\sinh 1}{\sinh 1 - 1}\right] \approx 64.8734.$$

IV. HEAT FLUX COVECTION WITHOUT ROTATION

In this section, we prove upper bound on heat flux convection in absence of rotation. We first quote the following Lemma from Ref. 10.

Lemma 4.1 (Ref. 10): *If* $w_{\mathbf{m}}(z)$ *satisfies*

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2} + m^2\right)^2 w_{\mathbf{m}} = \mathrm{Ra}\, m^2 \theta_{\mathbf{m}},$$

$$w_{\mathbf{m}}(0) = w_{\mathbf{m}}(1) = \frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}(0) = \frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}(1) = 0,$$

then there is a constant C_2 *independent of* m *such that* $\|\mathrm{d}^2 w_{\mathbf{m}}/\mathrm{d}z^2\|_\infty \leqslant C_2\, \mathrm{Ra}\, m \|\theta_{\mathbf{m}}\|_2$. *In particular, one can choose* $C_2^2 = 2/(7-\sqrt{41})$.

Lemma 4.1 and Proposition 3.1 implies the growth of $w_{\mathbf{m}}$ near boundaries. By Proposition 3.1, when $|\mathbf{m}| \geqslant 1$, the growth of $w_{\mathbf{m}}$ near the boundary at $z=0$ is controlled by

$$|w_{\mathbf{m}}(z)| = \left|\int_0^z \int_0^\zeta \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}(\zeta')\mathrm{d}\zeta'\,\mathrm{d}\zeta\right| \leqslant \frac{1}{2} z^2 \left\|\frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty \leqslant \frac{1}{2} z^2 C_1\, \mathrm{Ra}\sqrt{m}\, \|\theta_{\mathbf{m}}\|_2. \tag{4.1}$$

For $|\mathbf{m}| \leqslant 1$, Lemma 4.1 implies the growth of $w_{\mathbf{m}}$ near $z=0$ is limited by

$$|w_{\mathbf{m}}(z)| = \left|\int_0^z \int_0^\zeta \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}(\zeta')\mathrm{d}\zeta'\,\mathrm{d}\zeta\right| \leqslant \frac{1}{2} z^2 \left\|\frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty \leqslant \frac{1}{2} z^2 C_2\, \mathrm{Ra}\, m \|\theta_{\mathbf{m}}\|_2 \leqslant \frac{1}{2} z^2 C_2\, \mathrm{Ra} \|\theta_{\mathbf{m}}\|_2. \tag{4.2}$$

An analogous pointwise bound holds near $z=1$ when $|\mathbf{m}| \geqslant 1$ and $|\mathbf{m}| \leqslant 1$.

On the other hand, the growth of $\theta_{\mathbf{m}}$ near the boundary is estimated by

$$|\theta_{\mathbf{m}}(z)| = \left|\int_0^z \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}(\zeta)\mathrm{d}\zeta\right| \leqslant \sqrt{z}\sqrt{\int_0^{1/2} \left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2} \tag{4.3}$$

for $0 \leqslant z \leqslant \frac{1}{2}$, a similar estimate holds for the growth of $\theta_{\mathbf{m}}$ near $z=1$.

When $|\mathbf{m}| \geqslant 1$, the indefinite term in $Q_{\mathbf{m}}$ now can be bounded according to (4.1) and (4.3) as

$$\begin{aligned}
\left|\int_0^1 \tau'(z)(w^*_{\mathbf{m}}\theta_{\mathbf{m}} + \theta^*_{\mathbf{m}} w_{\mathbf{m}})\mathrm{d}z\right| &\leqslant \frac{1}{\delta}\int_0^\delta |w_{\mathbf{m}}(z)||\theta_{\mathbf{m}}(z)|\mathrm{d}z + \frac{1}{\delta}\int_{1-\delta}^1 |w_{\mathbf{m}}(z)||\theta_{\mathbf{m}}(z)|\mathrm{d}z \\
&\leqslant \frac{1}{\delta}\int_0^\delta \frac{1}{2} z^2 C_1\, \mathrm{Ra}\sqrt{m}\, \|\theta_{\mathbf{m}}\|_2 \sqrt{z}\sqrt{\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\,\mathrm{d}z \\
&\quad + \frac{1}{\delta}\int_{1-\delta}^1 \frac{1}{2}(1-z)^2 C_1\, \mathrm{Ra}\sqrt{m}\, \|\theta_{\mathbf{m}}\|_2 \sqrt{1-z}\sqrt{\int_{1/2}^1 \left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\,\mathrm{d}z
\end{aligned}$$

$$\leqslant \frac{1}{7}\delta^{5/2}C_1\,\mathrm{Ra}\sqrt{m}\|\theta_{\mathbf{m}}\|_2\left(\sqrt{\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}+\sqrt{\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\right)$$

$$\leqslant \frac{\sqrt{2}}{7}\delta^{5/2}C_1\,\mathrm{Ra}\sqrt{m}\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2. \tag{4.4}$$

When $|\mathbf{m}|\leqslant 1$, the indefinite term in $Q_{\mathbf{m}}$ is estimated via (4.2) and (4.3),

$$\left|\int_0^1 \tau'(z)(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+\theta_{\mathbf{m}}^*w_{\mathbf{m}})\mathrm{d}z\right| \leqslant \frac{1}{\delta}\int_0^\delta |w_{\mathbf{m}}(z)||\theta_{\mathbf{m}}(z)|\mathrm{d}z+\frac{1}{\delta}\int_{1-\delta}^1 |w_{\mathbf{m}}(z)||\theta_{\mathbf{m}}(z)|\mathrm{d}z$$

$$\leqslant \frac{1}{\delta}\int_0^\delta \frac{1}{2}z^2C_2\,\mathrm{Ra}\,m\|\theta_{\mathbf{m}}\|_2\sqrt{z}\sqrt{\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\,\mathrm{d}z$$

$$+\frac{1}{\delta}\int_{1-\delta}^1 \frac{1}{2}(1-z)^2C_2\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\sqrt{1-z}\sqrt{\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\,\mathrm{d}z$$

$$\leqslant \frac{1}{7}C_2\delta^{5/2}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\left(\sqrt{\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}+\sqrt{\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2}\right)$$

$$\leqslant \frac{\sqrt{2}}{7}C_2\delta^{5/2}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2. \tag{4.5}$$

For $|\mathbf{m}|\geqslant 1$, (4.4) implies

$$\left|\int_0^1 \tau'(z)(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+\theta_{\mathbf{m}}^*w_{\mathbf{m}})\mathrm{d}z\right| \leqslant \frac{(\sqrt{2})^4}{64\times 7^4}C_1^4\delta^{10}\,\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2+m^2\|\theta_{\mathbf{m}}\|_2^2+\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2. \tag{4.6}$$

In particular, this implies when $|\mathbf{m}|\geqslant 1$, $Q_{\mathbf{m}}$ is bounded below by

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}})\geqslant -\frac{C_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2. \tag{4.7}$$

On the other hand, for $|\mathbf{m}|\leqslant 1$, (4.5) gives

$$\left|\int_0^1 \tau'(z)(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+\theta_{\mathbf{m}}^*w_{\mathbf{m}})\mathrm{d}z\right| \leqslant \frac{C_2\sqrt{2}}{7}\delta^{5/2}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2 \leqslant \frac{C_2^2}{98}\delta^5\,\mathrm{Ra}^2\|\theta_{\mathbf{m}}\|_2^2+\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2. \tag{4.8}$$

Hence for $|\mathbf{m}|\leqslant 1$, $Q_{\mathbf{m}}$ is bounded below by

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}})\geqslant -\frac{C_2^2}{98}\delta^5\,\mathrm{Ra}^2\|\theta_{\mathbf{m}}\|_2^2. \tag{4.9}$$

Therefore the convective heat flux

$$\begin{aligned}\mathrm{Nu} &\leqslant \frac{1}{2\delta} - \frac{1}{\mathcal{A}}\left\langle \int_0^{L_x/h}\int_0^{L_y/h} \sum_{\mathbf{m}} Q_{\mathbf{m}}(\theta_{\mathbf{m}})\,dx\,dy \right\rangle \\ &\leqslant \frac{1}{2\delta} + \frac{C_2^2}{98}\delta^5\,\mathrm{Ra}^2 \sum_{|\mathbf{m}|\leqslant 1} \|\theta_{\mathbf{m}}\|_2^2 + \frac{C_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4 \sum_{|\mathbf{m}|\geqslant 1} \|\theta_{\mathbf{m}}\|_2^2 \\ &\leqslant \frac{1}{2\delta} + \max\left(\frac{C_2^2}{98}\delta^5\,\mathrm{Ra}^2, \frac{C_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\right).\end{aligned}$$

The last inequality used the fact that $|\theta(\mathbf{x},t)|\leqslant 1$ and

$$\sum_{\mathbf{m}} \|\theta_{\mathbf{m}}\|_2^2 \leqslant \frac{1}{\mathcal{A}}\int_V \theta^2\,\mathrm{d}V \leqslant 1.$$

In fact, apply Maximum principle to T, we have $0\leqslant T(\mathbf{x},t)\leqslant 1$. Choice of τ implies $0\leqslant \tau(z)\leqslant 1$, therefore

$$|\theta(\mathbf{x},t)| = |T(\mathbf{x},t) - \tau(z)| \leqslant 1.$$

Choose $\delta = [(8\times 7^4/10C_1^4)\,\mathrm{Ra}^{-4}]^{1/11}$, we get

$$\mathrm{Nu} \leqslant c\,\mathrm{Ra}^{4/11}$$

with

$$c = \left(\frac{1}{2\delta} + \frac{C_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\right)\mathrm{Ra}^{-4/11} \approx 1.26.$$

□

V. UPPER BOUND FOR ROTATIONAL SYSTEM

In this section, we discuss the bound on Nusselt number for rotational system. We follow similar ideas as in Sec. IV. We first prove the following estimates.

Lemma 5.1: For $|\mathbf{m}|\geqslant 1$,

$$\left\|\frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty \leqslant c_1\,\mathrm{Ra}\sqrt{m}\,\|\theta_{\mathbf{m}}\|_2 + \frac{c_1}{2}\mathrm{Ra}\sqrt{\mathrm{Ta}}\,\|\theta_{\mathbf{m}}\|_2$$

with $c_1 \approx 64.87$.

Lemma 5.2: For $|\mathbf{m}|\leqslant 1$,

$$\left\|\frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_\infty \leqslant c_2\,\mathrm{Ra}\left(\frac{\mathrm{Ta}}{4}+1\right)^{1/4}\|\theta_{\mathbf{m}}\|_2 \tag{5.1}$$

with $c_2 = 6^{1/4}$.

To prove Lemma 5.1 and Lemma 5.2. We need the following Lemma.

Lemma 5.3:

$$\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2 \leqslant \frac{1}{2}\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2, \quad \left\|\frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_2 \leqslant \frac{1}{2}\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2,$$

$$\left\|\frac{\mathrm{d}^4 w_{\mathbf{m}}}{\mathrm{d}z^4}\right\|_2^2 \leqslant 6\left(\mathrm{Ta}\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2 + \mathrm{Ra}^2 m^4\|\theta_{\mathbf{m}}\|_2^2\right).$$

Proof: Recall $w_{\mathbf{m}}, \zeta_{\mathbf{m}}$ satisfies

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2}+m^2\right)\zeta_{\mathbf{m}}=\sqrt{\mathrm{Ta}}\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}, \tag{5.2}$$

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2}+m^2\right)^2 w_{\mathbf{m}}-\sqrt{\mathrm{Ta}}\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}=\mathrm{Ra}\,m^2\theta_{\mathbf{m}} \tag{5.3}$$

subject to boundary conditions

$$\zeta_{\mathbf{m}}(0)=\zeta_{\mathbf{m}}(1)=0,$$

$$w_{\mathbf{m}}(0)=w_{\mathbf{m}}(1)=\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}(0)=\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}(1)=0.$$

Equation (5.2) multiplied by $\zeta_{\mathbf{m}}$+(5.3) multiplied by $w_{\mathbf{m}}$, integrate by parts using boundary constraints, we obtain

$$\int_0^1\left(\left|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right|^2+m^2\zeta_{\mathbf{m}}^2+\left|\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}\right|^2+2m^2\left|\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}\right|^2+m^4w_{\mathbf{m}}^2\right)\mathrm{d}z$$
$$=\int_0^1\mathrm{Ra}\,m^2\theta_{\mathbf{m}}w_{\mathbf{m}}\leqslant\int_0^1\frac{\mathrm{Ra}^2\,\theta_{\mathbf{m}}^2(z)}{4}\mathrm{d}z+\int_0^1 m^4w_{\mathbf{m}}^2.$$

In particular, we have

$$\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\leqslant\frac{1}{2}\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2,\quad \left\|\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_2\leqslant\frac{1}{2}\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2. \tag{5.4}$$

On the other hand, move $\sqrt{\mathrm{Ta}}\,\mathrm{d}\zeta_{\mathbf{m}}/\mathrm{d}z$ to the right, squaring (5.3), integrate by parts, we get

$$\left\|\frac{\mathrm{d}^4w_{\mathbf{m}}}{\mathrm{d}z^4}\right\|_2^2-2m^2\int_0^1\left[\frac{\mathrm{d}^4w_{\mathbf{m}}^*}{\mathrm{d}z^4}\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}+\frac{\mathrm{d}^2w_{\mathbf{m}}^*}{\mathrm{d}z^2}\frac{\mathrm{d}^4w_{\mathbf{m}}}{\mathrm{d}z^4}\right]\mathrm{d}z+6m^4\left\|\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_2^2+4m^6\left\|\frac{\mathrm{d}w_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2+m^8\|w_{\mathbf{m}}\|_2^2$$
$$\leqslant 2\,\mathrm{Ta}\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2+2\,\mathrm{Ra}^2\,m^4\|\theta_{\mathbf{m}}\|_2^2.$$

The indefinite term above can be estimated by its neighboring terms. For $\epsilon>0$,

$$\left|2m^2\int_0^1\frac{\mathrm{d}^4w_{\mathbf{m}}^*}{\mathrm{d}z^4}\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}+\frac{\mathrm{d}^2w_{\mathbf{m}}^*}{\mathrm{d}z^2}\frac{\mathrm{d}^4w_{\mathbf{m}}}{\mathrm{d}z^4}\right|\leqslant\epsilon\left\|\frac{\mathrm{d}^4w_{\mathbf{m}}}{\mathrm{d}z^4}\right\|_2^2+\frac{4m^4}{\epsilon}\left\|\frac{\mathrm{d}^2w_{\mathbf{m}}}{\mathrm{d}z^2}\right\|_2^2.$$

Choose $\epsilon=\frac{2}{3}$, we have

$$\left\|\frac{\mathrm{d}^4w_{\mathbf{m}}}{\mathrm{d}z^4}\right\|_2^2\leqslant 6\left(\mathrm{Ta}\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2+\mathrm{Ra}^2\,m^4\|\theta_m\|_2^2\right).$$

□

Proof of Lemma 5.1: Since

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2}+m^2\right)^2 w_{\mathbf{m}}=\sqrt{\mathrm{Ta}}\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}+\mathrm{Ra}\,m^2\theta_{\mathbf{m}}.$$

By Lemma 5.3, $\| \mathrm{d}\zeta_{\mathbf{m}}/\mathrm{d}z \|_2 \leqslant \frac{1}{2}\mathrm{Ra}\| \theta_{\mathbf{m}}\|_2$, therefore for $|\mathbf{m}| \geqslant 1$, by Proposition 3.1,

$$\left\| \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2} \right\|_\infty \leqslant c_1 m^{-3/2}\left(\sqrt{\mathrm{Ta}}\frac{1}{2}\mathrm{Ra}\| \theta_{\mathbf{m}}\|_2 + \mathrm{Ra}\, m^2 \| \theta_{\mathbf{m}}\|_2 \right) \leqslant \frac{c_1}{2}\mathrm{Ra}\sqrt{\mathrm{Ta}}\| \theta_{\mathbf{m}}\|_2 + c_1\, \mathrm{Ra}\sqrt{m}\| \theta_{\mathbf{m}}\|_2 .$$

To prove Lemma 5.2, we need the following lemma from Ref. 10.

Lemma 5.4 (Ref. 10): *Let $f(z)$ be a smooth real valued function satisfying both homogeneous Dirichlet and Neumann boundary conditions on [0,1]. Then*

$$\left\| \frac{\mathrm{d}^2 f}{\mathrm{d}z^2} \right\|_\infty \leqslant \sqrt{2\left\| \frac{\mathrm{d}^4 f}{\mathrm{d}z^4} \right\|_2 \left\| \frac{\mathrm{d}^2 f}{\mathrm{d}z^2} \right\|_2}.$$

An immediate corollary of Lemma 5.4 is

Lemma 5.5: Let $w(z)$ be a smooth complex valued function satisfying both homogeneous Dirichlet and Neumann boundary conditions on [0,1]. Then

$$\left\| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2} \right\|_\infty \leqslant \sqrt{2\left\| \frac{\mathrm{d}^4 w}{\mathrm{d}z^4} \right\|_2 \left\| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2} \right\|_2}.$$

Proof: Write $w(z) = u(z) + iv(z)$, then $u(z), v(z)$ are real valued smooth functions satisfying both homogeneous Dirichlet and Neumann boundary conditions on [0,1]. Therefore

$$\begin{aligned} \left| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2}(z) \right|_2^2 &= \left| \frac{\mathrm{d}^2 u}{\mathrm{d}z^2}(z) \right|_2^2 + \left| \frac{\mathrm{d}^2 v}{\mathrm{d}z^2}(z) \right|_2^2 \leqslant 2\left\| \frac{\mathrm{d}^2 u}{\mathrm{d}z^2} \right\|_2 \left\| \frac{\mathrm{d}^4 u}{\mathrm{d}z^4} \right\|_2 + 2\left\| \frac{\mathrm{d}^2 v}{\mathrm{d}z^2} \right\|_2 \left\| \frac{\mathrm{d}^4 v}{\mathrm{d}z^4} \right\|_2 \\ &\leqslant \frac{1}{\epsilon}\left\| \frac{\mathrm{d}^2 u}{\mathrm{d}z^2} \right\|_2^2 + \epsilon\left\| \frac{\mathrm{d}^4 u}{\mathrm{d}z^4} \right\|_2^2 + \frac{1}{\epsilon}\left\| \frac{\mathrm{d}^2 v}{\mathrm{d}z^2} \right\|_2^2 + \epsilon\left\| \frac{\mathrm{d}^4 v}{\mathrm{d}z^4} \right\|_2^2 = \frac{1}{\epsilon}\left\| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2} \right\|_2^2 + \epsilon\left\| \frac{\mathrm{d}^4 w}{\mathrm{d}z^4} \right\|_2^2 \end{aligned}$$

for any $\epsilon > 0$. Minimize the right-hand side in ϵ, we obtain

$$\left| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2}(z) \right|_2^2 \leqslant 2\left\| \frac{\mathrm{d}^2 w}{\mathrm{d}z^2} \right\|_2 \left\| \frac{\mathrm{d}^4 w}{\mathrm{d}z^4} \right\|_2 .$$

□

Proof of Lemma 5.2: By Lemma 5.3, we have $\| \mathrm{d}^2 w_{\mathbf{m}}/\mathrm{d}z^2 \|_2 \leqslant \frac{1}{2}\mathrm{Ra}\| \theta_{\mathbf{m}}\|_2$ and

$$\begin{aligned} \left\| \frac{\mathrm{d}^4 w_{\mathbf{m}}}{\mathrm{d}z^4} \right\|_2^2 &\leqslant 6\left(\mathrm{Ta}\left\| \frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2^2 + \mathrm{Ra}^2 m^4 \| \theta_{\mathbf{m}}\|_2^2 \right) \\ &\leqslant 6\left(\frac{1}{4}\mathrm{Ta}\,\mathrm{Ra}^2 \| \theta_{\mathbf{m}}\|_2^2 + \mathrm{Ra}^2 \| \theta_{\mathbf{m}}\|_2^2 \right) = 6\,\mathrm{Ra}^2 \| \theta_m\|_2^2 \left(\frac{1}{4}\mathrm{Ta} + 1 \right). \end{aligned}$$

It then follows from Lemma 5.5 that

$$\left\| \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2} \right\|_\infty \leqslant \mathrm{Ra}\| \theta_{\mathbf{m}}\|_2 6^{1/4}\left(\frac{1}{4}\mathrm{Ta} + 1 \right)^{1/4} \leqslant \mathrm{Ra}\| \theta_{\mathbf{m}}\|_2 6^{1/4}\left(\frac{\sqrt{\mathrm{Ta}}}{2} + 1 \right).$$

In the last inequality, we used the fact that

$$\left(\frac{1}{4}\mathrm{Ta} + 1 \right)^{1/4} \leqslant \left(\frac{\sqrt{\mathrm{Ta}}}{2} + 1 \right).$$

Proof of Theorem 2.2: Theorem 2.2 now follows from the same line of proof as in Sec. IV. In fact, estimates in Lemma 5.1 imply for $|\mathbf{m}|\geqslant 1$, the growth of $w_{\mathbf{m}}$ near $z=0$ is controlled by (similar estimates near $z=1$)

$$|w_{\mathbf{m}}(z)|\leqslant \tfrac{1}{2}z^2\|w_{\mathbf{m}}''\|_\infty \leqslant \tfrac{1}{2}z^2 c_1\sqrt{m}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2+\tfrac{1}{4}z^2c_1\,\mathrm{Ra}\sqrt{\mathrm{Ta}}\|\theta_{\mathbf{m}}\|_2,$$

this together with growth estimate on $\theta_{\mathbf{m}}$,

$$|\theta_{\mathbf{m}}(z)|\leqslant\sqrt{z}\left(\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}$$

imply the following estimates for the indefinite term in $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$:

$$\begin{aligned}
\left|\int_0^1\tau'(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+w_{\mathbf{m}}\theta_{\mathbf{m}}^*)\right| &\leqslant \frac{1}{\delta}\left(\int_0^\delta\frac{1}{2}z^{5/2}\|w_{\mathbf{m}}''\|_\infty\left(\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}\right.\\
&\quad\left.+\int_{1-\delta}^1\frac{1}{2}z^{5/2}\|w_{\mathbf{m}}''\|_\infty\left(\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}\right)\\
&\leqslant \frac{c_1}{7}\delta^{5/2}\sqrt{m}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\left[\left(\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}+\left(\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}\right]\\
&\quad+\frac{c_1}{14}\delta^{5/2}\,\mathrm{Ra}\sqrt{\mathrm{Ta}}\|\theta_{\mathbf{m}}\|_2\left[\left(\int_0^{1/2}\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}+\left(\int_{1/2}^1\left|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right|^2\right)^{1/2}\right]\\
&\leqslant \frac{\sqrt{2}c_1}{7}\delta^{5/2}\sqrt{m}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2+\frac{\sqrt{2}c_1}{14}\delta^{5/2}\,\mathrm{Ra}\sqrt{\mathrm{Ta}}\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\\
&\leqslant \frac{(\sqrt{2})^4c_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2+m^2\|\theta_{\mathbf{m}}\|_2^2+\frac{1}{2}\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2+\frac{c_1^2}{4\times 49}\delta^5\,\mathrm{Ra}^2\,\mathrm{Ta}\|\theta_{\mathbf{m}}\|_2^2\\
&\quad+\frac{1}{2}\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2. \qquad (5.5)
\end{aligned}$$

Therefore when $|\mathbf{m}|\geqslant 1$, $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ is bounded below by

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}})\geqslant-\frac{(\sqrt{2})^4c_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2-\frac{c_1^2}{4\times 49}\delta^5\,\mathrm{Ra}^2\,\mathrm{Ta}\|\theta_{\mathbf{m}}\|_2^2.$$

On the other hand, for $|\mathbf{m}|\leqslant 1$, Lemma 3.3 gives

$$\begin{aligned}
\left|\int_0^1\tau'(w_{\mathbf{m}}^*\theta_{\mathbf{m}}+w_{\mathbf{m}}\theta_{\mathbf{m}}^*)\right| &\leqslant \frac{1}{\delta}\int_0^\delta|w_{\mathbf{m}}||\theta_{\mathbf{m}}|\mathrm{d}z+\frac{1}{\delta}\int_{1-\delta}^1|w_{\mathbf{m}}||\theta_{\mathbf{m}}|\mathrm{d}z\\
&\leqslant \frac{\sqrt{2}c_2}{7}\delta^{5/2}\,\mathrm{Ra}\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)\|\theta_{\mathbf{m}}\|_2\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\\
&\leqslant \frac{c_2^2}{98}\delta^5\,\mathrm{Ra}^2\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^2\|\theta_{\mathbf{m}}\|_2^2+\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2.
\end{aligned}$$

Therefore when $|\mathbf{m}|\leqslant 1$, $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ is bounded from below by

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}}) \geqslant -\frac{c_2^2}{98}\delta^5 \mathrm{Ra}^2\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^2 \|\theta_{\mathbf{m}}\|_2^2 \tag{5.6}$$

and

$$\begin{aligned}
\mathrm{Nu} &\leqslant \int_0^1 \tau'(z)^2\,\mathrm{d}z - \frac{1}{\mathcal{A}}\int_0^{L_x/h}\int_0^{L_y/h}\sum_{\mathbf{m}} Q_{\mathbf{m}}(\theta_{\mathbf{m}})\mathrm{d}x\,\mathrm{d}y \\
&\leqslant \frac{1}{2\delta} + \frac{c_2^2}{98}\delta^5 \mathrm{Ra}^2\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^2 \sum_{|\mathbf{m}|\leqslant 1}\|\theta_{\mathbf{m}}\|_2^2 + \frac{c_1^4}{4\times 7^4}\delta^{10}\mathrm{Ra}^4 \sum_{|\mathbf{m}|\geqslant 1}\|\theta_{\mathbf{m}}\|_2^2 \\
&\quad + \frac{c_1^2}{4\times 49}\delta^5 \mathrm{Ra}^2\,\mathrm{Ta}\sum_{|\mathbf{m}|\geqslant 1}\|\theta_{\mathbf{m}}\|_2^2 \\
&\leqslant \frac{1}{2\delta} + \max\left(\frac{c_2^2}{98}\delta^5 \mathrm{Ra}^2\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^2, \frac{c_1^4}{4\times 7^4}\delta^{10}\mathrm{Ra}^4 + \frac{c_1^2}{4\times 49}\delta^5 \mathrm{Ra}^2\,\mathrm{Ta}\right) \\
&= \frac{1}{2\delta} + \frac{c_1^4}{4\times 7^4}\delta^{10}\mathrm{Ra}^4 + \frac{c_1^2}{4\times 49}\delta^5 \mathrm{Ra}^2\,\mathrm{Ta}.
\end{aligned}$$

The last inequality uses the fact that $|\theta(\mathbf{x},t)|\leqslant 1$ and

$$\sum_{|\mathbf{m}|\leqslant 1}\|\theta_{\mathbf{m}}\|_2^2 \leqslant \frac{1}{\mathcal{A}}\int_V \theta^2\,\mathrm{d}V \leqslant 1.$$

Choose $\delta=(2\times 7^4/10\cdot c_1^4)^{1/11}\mathrm{Ra}^{-4/11}\mathrm{Ta}^{-1/6}$, we get

$$\begin{aligned}
\mathrm{Nu} &\leqslant \frac{1}{2}\left(\frac{10c_1^4}{2\times 7^4}\right)^{1/11}\mathrm{Ra}^{4/11}\mathrm{Ta}^{1/6} + \frac{c_1^4}{4\times 7^4}\left(\frac{2\times 7^4}{10\cdot c_1^4}\right)^{10/11}\mathrm{Ra}^{4/11}\mathrm{Ta}^{-5/3} \\
&\quad + \frac{c_1^2}{4\times 49}\left(\frac{2\times 7^4}{10\cdot c_1^4}\right)^{5/11}\mathrm{Ra}^{2/11}\mathrm{Ta}^{1/6} \\
&= 1.3\,\mathrm{Ra}^{4/11}\mathrm{Ta}^{1/6} + 0.13\,\mathrm{Ra}^{4/11}\mathrm{Ta}^{-5/3} + 0.18\,\mathrm{Ra}^{2/11}\mathrm{Ta}^{1/6}.
\end{aligned}$$

To prove the second bound, we observe that

$$|w_{\mathbf{m}}(z)| \leqslant \tfrac{1}{2}z^2\|w_{\mathbf{m}}''\|_\infty \leqslant \tfrac{1}{2}z^2 c_1\sqrt{m}\,\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2 + \tfrac{1}{4}z^2 c_1\,\mathrm{Ra}\sqrt{\mathrm{Ta}}\|\theta_{\mathbf{m}}\|_2 \leqslant \tfrac{1}{2}z^2 c_1\,\mathrm{Ra}(\tfrac{1}{2}\sqrt{\mathrm{Ta}}+1)\sqrt{m}\|\theta_{\mathbf{m}}\|_2, \tag{5.7}$$

therefore when $|\mathbf{m}|\geqslant 1$,

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}}) \geqslant -\frac{c_1^4}{16\times 7^4}\left[\mathrm{Ra}\left(\frac{1}{2}\sqrt{\mathrm{Ta}}+1\right)\right]^4 \delta^{10}\|\theta_{\mathbf{m}}\|_2^2$$

and

$$\begin{aligned}
\mathrm{Nu} &\leqslant \frac{1}{2\delta} + \frac{c_2^2}{98}\delta^5 \mathrm{Ra}^2\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^2 \sum_{|\mathbf{m}|\leqslant 1}\|\theta_{\mathbf{m}}\|_2^2 + \frac{c_1^4}{16\times 7^4}\left[\mathrm{Ra}\left(\frac{1}{2}\sqrt{\mathrm{Ta}}+1\right)\right]^4 \delta^{10}\sum_{|\mathbf{m}|\geqslant 1}\|\theta_{\mathbf{m}}\|_2^2 \\
&\leqslant \frac{1}{2\delta} + \frac{c_1^4}{16\times 7^4}\left[\mathrm{Ra}\left(\frac{1}{2}\sqrt{\mathrm{Ta}}+1\right)\right]^4 \delta^{10}.
\end{aligned}$$

Choose $\delta=(8\times 7^4/10c_1^4)^{1/11}[\mathrm{Ra}(\frac{1}{2}\sqrt{\mathrm{Ta}}+1)]^{-4/11}$, we get

$$\mathrm{Nu} \leqslant c[\mathrm{Ra}(\tfrac{1}{2}\sqrt{\mathrm{Ta}}+1)]^{4/11},$$

$$c=\left(\frac{1}{2\delta}+\frac{c_1^4}{16\times 7^4}\delta^{10}\,\mathrm{Ra}^4\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^4\right)\mathrm{Ra}^{-4/11}\left(\frac{\sqrt{\mathrm{Ta}}}{2}+1\right)^{-4/11}\approx 1.26.$$

□

VI. UNIFORM BOUND FOR WEAKLY ROTATING SYSTEM

In this section, we prove Theorem 2.3. We shall need the following expression for Nu in terms of the velocity field

$$\mathrm{Nu}=\frac{1}{\mathcal{A}}\frac{1}{\mathrm{Ra}}\langle\|\nabla\mathbf{u}\|^2\rangle.$$

In particular, for $\mathbf{u}=(u,v,w)$, this relation implies

$$\sum_{\mathbf{m}}\|w'_{\mathbf{m}}\|_2^2\leqslant\frac{1}{\mathcal{A}}\langle\|\nabla w\|^2\rangle\leqslant\mathrm{Ra}\,\mathrm{Nu}.$$

Here $w_{\mathbf{m}}(z)$ is the Fourier modes of w.

We start with the background field decomposition. As in Sec. V, we work with Fourier modes to estimate the quadratic form. We shall use slightly different versions of estimates on higher derivatives of $w_{\mathbf{m}}$. Corresponding versions of Lemma 5.1 and Lemma 5.2 are the following.

Lemma 6.1: For $|\mathbf{m}|\geqslant 1$,

$$\|w''_{\mathbf{m}}\|_\infty\leqslant\frac{C_1}{m^2}\sqrt{\mathrm{Ta}}\|w'_{\mathbf{m}}\|_2+c_1\,\mathrm{Ra}\sqrt{m}\|\theta_{\mathbf{m}}\|_2.$$

Here c_1 is the same constant as in Lemma 5.1, C_1 is a constant independent of m, Ra, Ta.

Lemma 6.2. For $|\mathbf{m}|\leqslant 1$,

$$\|w''_{\mathbf{m}}\|_\infty\leqslant 6^{1/4}\sqrt{\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2(\mathrm{Ta}\|w'_{\mathbf{m}}\|_2+\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2)}.$$

To prove Lemma 6.1 and 6.2, we first prove the following Lemma.

Lemma 6.3: If $g_{\mathbf{m}}$ *satisfies*

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2}-m^2\right)g_{\mathbf{m}}=h_{\mathbf{m}},$$

then

$$\left\|\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\leqslant\|h_{\mathbf{m}}\|_2,$$

and when $|\mathbf{m}|\geqslant 1$

$$\left\|\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\leqslant\frac{c_0}{\sqrt{m}}\|h_{\mathbf{m}}\|_2$$

with $c_0=1/\sqrt{2}\sqrt{(e^2+1)(e^2-1)}\approx 0.810\,258$.

Proof: From explicit expression of the Green's function, we have

$$g_{\mathbf{m}}(z)=\int_0^1 \frac{\cosh m(z+\zeta-1)}{2m\sinh m}h_{\mathbf{m}}(\zeta)\mathrm{d}\zeta-\int_0^1 \frac{\cosh m(1-|z-\zeta|)}{2m\sinh m}h_{\mathbf{m}}(\zeta)\mathrm{d}\zeta.$$

Differentiate, we get

$$\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}(z)=\int_0^1 \frac{\sinh m(z+\zeta-1)}{2\sinh m}h_{\mathbf{m}}(\zeta)\mathrm{d}\zeta-\int_0^z \frac{\sinh m(1-z+\zeta)}{2\sinh m}h_{\mathbf{m}}(\zeta)\mathrm{d}\zeta$$
$$-\int_z^1 \frac{\sinh m(1+z-\zeta)}{2\sinh m}h_{\mathbf{m}}(\zeta)\mathrm{d}\zeta.$$

In particular,

$$\left|\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}(z)\right|\leqslant\int_0^1\left|\frac{\sinh m(z+\zeta-1)}{2\sinh m}h_{\mathbf{m}}(\zeta)\right|\mathrm{d}\zeta+\int_0^z\left|\frac{\sinh m(1-z+\zeta)}{2\sinh m}h_{\mathbf{m}}(\zeta)\right|\mathrm{d}\zeta$$
$$+\int_z^1\left|\frac{\sinh m(1+z-\zeta)}{2\sinh m}h_{\mathbf{m}}(\zeta)\right|\mathrm{d}\zeta\leqslant\int_0^1|h_{\mathbf{m}}|\mathrm{d}\zeta\leqslant\|h_{\mathbf{m}}\|_2.$$

Here we use the fact that when $0\leqslant z,\ \zeta\leqslant 1$,

$$|\sinh m(z+\zeta-1)|\leqslant\sinh m,$$

$$|\sinh m(1-|z-\zeta|)|\leqslant\sinh m.$$

On the other hand, from Lemma 3.2, we have when $|\mathbf{m}|\geqslant 1$,

$$\left\|\frac{\mathrm{d}g_{\mathbf{m}}}{\mathrm{d}z}\right\|_\infty\leqslant\frac{1}{\sqrt{2}\sqrt{m}}\sqrt{\frac{e^2+1}{e^2-1}}\|h_{\mathbf{m}}\|_2.$$

The conclusion of the Lemma follows directly. □

A direct corollary of Lemma 6.3 is

$$\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\leqslant\frac{c_0}{\sqrt{m}}\sqrt{\mathrm{Ta}}\|w'_{\mathbf{m}}\|_2\quad\text{for }|\mathbf{m}|\geqslant 1 \tag{6.1}$$

and

$$\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2\leqslant\sqrt{\mathrm{Ta}}\|w'_{\mathbf{m}}\|_2\quad\text{for }|\mathbf{m}|\leqslant 1. \tag{6.2}$$

Proof of Lemma 6.1: When $|\mathbf{m}|\geqslant 1$, Proposition 3.1 and (6.1) derives

$$\|w''_{\mathbf{m}}\|_\infty\leqslant\frac{c_1}{m^{3/2}}\left(\sqrt{\mathrm{Ta}}\left\|\frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2+\mathrm{Ra}\,m^2\|\theta_{\mathbf{m}}\|_2\right)\leqslant\frac{c_1}{m^{3/2}}\mathrm{Ra}\,m^2\|\theta_{\mathbf{m}}\|_2+\frac{c_1}{m^{3/2}}\sqrt{\mathrm{Ta}}\frac{c_0}{\sqrt{m}}\sqrt{\mathrm{Ta}}\|w'_{\mathbf{m}}\|_2$$
$$=c_1\,\mathrm{Ra}\sqrt{m}\|\theta_{\mathbf{m}}\|_2+\frac{C_1}{m^2}\mathrm{Ta}\|w'_{\mathbf{m}}\|_2,$$

with $C_1=c_1c_0$.

Proof of Lemma 6.2: By Lemma 5.3 and (6.2),

$$\left\| \frac{\mathrm{d}^4 w_{\mathbf{m}}}{\mathrm{d}z^4} \right\|_2^2 \leqslant 6\left(\mathrm{Ta} \left\| \frac{\mathrm{d}\zeta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2^2 + \mathrm{Ra}^2 \| \theta_{\mathbf{m}} \|_2^2 \right) \leqslant 6(\mathrm{Ta}^2 \| w'_{\mathbf{m}} \|_2^2 + \mathrm{Ra}^2 \| \theta_{\mathbf{m}} \|_2^2)$$

and

$$\left\| \frac{\mathrm{d}^2 w_{\mathbf{m}}}{\mathrm{d}z^2} \right\|_2 \leqslant \frac{1}{2} \mathrm{Ra} \| \theta_{\mathbf{m}} \|_2 ,$$

conclusion follows from Lemma 5.5.

We are now ready to estimate $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$. The indefinite term in $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ can be estimated as follows. For $|\mathbf{m}| \geqslant 1$,

$$\begin{aligned}
\left| \int_0^1 \tau' (w_{\mathbf{m}} \theta_{\mathbf{m}}^* + w_{\mathbf{m}}^* \theta_{\mathbf{m}}) \mathrm{d}z \right| &\leqslant \frac{1}{\delta} \int_0^\delta \frac{1}{2} z^2 \left(c_1 \, \mathrm{Ra} \sqrt{m} \| \theta_{\mathbf{m}} \|_2 |\theta_{\mathbf{m}}(z)| + \frac{C_1}{m^2} \sqrt{\mathrm{Ta}} \| w'_{\mathbf{m}} \|_2 |\theta_{\mathbf{m}}(z)| \right) \mathrm{d}z \\
&\quad + \frac{1}{\delta} \int_{1-\delta}^1 \frac{1}{2} (1-z)^2 \left(c_1 \, \mathrm{Ra} \sqrt{m} \| \theta_{\mathbf{m}} \|_2 |\theta_{\mathbf{m}}(z)| \right. \\
&\quad \left. + \frac{C_1}{m^2} \sqrt{\mathrm{Ta}} \| w'_{\mathbf{m}} \|_2 |\theta_{\mathbf{m}}(z)| \right) \mathrm{d}z \\
&\leqslant \frac{1}{\delta} \int_0^\delta \frac{1}{2} z^{5/2} c_1 \, \mathrm{Ra} \sqrt{m} \| \theta_{\mathbf{m}} \|_2 \left(\int_0^{1/2} \left| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right|^2 \right)^{1/2} \mathrm{d}z \\
&\quad + \frac{1}{\delta} \int_{1-\delta}^1 \frac{1}{2} (1-z)^{5/2} c_1 \, \mathrm{Ra} \sqrt{m} \| \theta_{\mathbf{m}} \|_2 \left(\int_{1/2}^1 \left| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right|^2 \right)^{1/2} \mathrm{d}z \\
&\quad + \frac{1}{\delta} \int_0^\delta \frac{1}{2} z^{5/2} \frac{C_1}{m^2} \sqrt{\mathrm{Ta}} \| w'_{\mathbf{m}} \|_2 \left(\int_0^{1/2} \left| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right|^2 \right)^{1/2} \mathrm{d}z \\
&\quad + \frac{1}{\delta} \int_{1-\delta}^1 \frac{1}{2} (1-z)^{5/2} \frac{C_1}{m^2} \sqrt{\mathrm{Ta}} \| w'_{\mathbf{m}} \|_2 \left(\int_{1/2}^1 \left| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right|^2 \right)^{1/2} \mathrm{d}z \\
&\leqslant \frac{\sqrt{2}}{7} c_1 \delta_1^{5/2} \mathrm{Ra} \sqrt{m} \| \theta_{\mathbf{m}} \|_2 \left\| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2 + \frac{\sqrt{2}}{7} \delta^{5/2} \frac{C_1}{m^2} \sqrt{\mathrm{Ta}} \| w'_{\mathbf{m}} \|_2 \left\| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2 \\
&\leqslant \frac{c_1^4}{4 \times 7^4} \delta^{10} \mathrm{Ra}^4 \| \theta_{\mathbf{m}} \|_2^2 + m^2 \| \theta_{\mathbf{m}} \|_2^2 + \frac{1}{2} \left\| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2^2 + \frac{C_1^2}{49} \delta^5 \frac{\mathrm{Ta}}{m^4} \| w'_{\mathbf{m}} \|_2^2 \\
&\quad + \frac{1}{2} \left\| \frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z} \right\|_2^2 . \qquad (6.3)
\end{aligned}$$

Therefore for $|\mathbf{m}| \geqslant 1$, $Q_{\mathbf{m}}(\theta_{\mathbf{m}})$ is bounded from below by

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}}) \geqslant - \frac{c_1^4}{4 \times 7^4} \delta^{10} \mathrm{Ra}^4 \| \theta_{\mathbf{m}} \|_2^2 - \frac{C_1^2}{49} \delta^5 \frac{\mathrm{Ta}}{m^4} \| w'_{\mathbf{m}} \|_2^2 .$$

On the other hand, for $|\mathbf{m}| \leqslant 1$,

$$\left|\int_0^1 \tau'(w_{\mathbf{m}}\theta_{\mathbf{m}}^*+w_{\mathbf{m}}^*\theta_{\mathbf{m}})\mathrm{d}z\right| \leqslant \frac{6^{1/4}\sqrt{2}}{7}\delta^{5/2}\sqrt{\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2(\mathrm{Ta}\|w'_{\mathbf{m}}\|_2+\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2)}\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2$$
$$\leqslant \frac{\sqrt{6}}{98}\delta^5[\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2(\mathrm{Ta}\|w'_{\mathbf{m}}\|+\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2)]+\left\|\frac{\mathrm{d}\theta_{\mathbf{m}}}{\mathrm{d}z}\right\|_2^2,$$

therefore

$$Q_{\mathbf{m}}(\theta_{\mathbf{m}}) \geqslant -\frac{\sqrt{6}}{98}\delta^5[\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2(\mathrm{Ta}\|w'_{\mathbf{m}}\|+\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2)] \quad \text{for } |\mathbf{m}|\leqslant 1.$$

Hence

$$\begin{aligned}
\mathrm{Nu} &\leqslant \frac{1}{2\delta}-\frac{1}{\mathcal{A}}\int_0^{L_x/h}\int_0^{L_y/h}\sum_{\mathbf{m}} Q_{\mathbf{m}}(\theta_{\mathbf{m}})\mathrm{d}x\,\mathrm{d}y \\
&\leqslant \frac{1}{2\delta}+\sum_{|\mathbf{m}|\leqslant 1}\frac{\sqrt{6}}{98}\delta^5[\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2(\mathrm{Ta}\|w'_{\mathbf{m}}\|+\mathrm{Ra}\|\theta_{\mathbf{m}}\|_2)]+\sum_{1\leqslant|\mathbf{m}|}\frac{c_1^4}{4\times 7^4}\delta^{10}\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2 \\
&\quad +\sum_{|\mathbf{m}|\geqslant 1}\frac{C_1^2}{49}\delta^5\,\mathrm{Ta}\frac{1}{m^4}\|w'_{\mathbf{m}}\|_2^2 \\
&\leqslant \frac{1}{2\delta}+\sum_{|\mathbf{m}|\leqslant 1}\frac{\sqrt{6}}{98}\delta^5\,\mathrm{Ra}^2\|\theta_{\mathbf{m}}\|_2^2+\sum_{|\mathbf{m}|\geqslant 1}\frac{c_1^4}{4\times 7^4}\delta^{10}\,\mathrm{Ra}^4\|\theta_{\mathbf{m}}\|_2^2 \\
&\quad +\frac{\sqrt{6}}{98}\delta^5\,\mathrm{Ra}\,\mathrm{Ta}\left(\sum_{|\mathbf{m}|\leqslant 1}\|w'_{\mathbf{m}}\|_2^2\right)^{1/2}\left(\sum_{|\mathbf{m}|\leqslant 1}\|\theta_{\mathbf{m}}\|_2^2\right)^{1/2}+\frac{C_1^2}{49}\delta^5\,\mathrm{Ta}\sum_{|\mathbf{m}|\geqslant 1}\frac{1}{m^4}\|w'_{\mathbf{m}}\|_2^2 \\
&\leqslant \frac{1}{2\delta}+\max\left(\frac{\sqrt{6}}{98}\delta^5\,\mathrm{Ra}^2,\frac{c_1^4}{4\times 7^4}\delta^{10}\,\mathrm{Ra}^4\right)+\frac{\sqrt{6}}{98}\delta^5\,\mathrm{Ra}\,\mathrm{Ta}\sqrt{\mathrm{Ra}\,\mathrm{Nu}}+\frac{C_1^2}{49}\delta^5\,\mathrm{Ta}\,\mathrm{Ra}\,\mathrm{Nu}.
\end{aligned}$$

Choose

$$\delta=\left(\frac{2\times 7^4}{10\cdot c_1^4}\mathrm{Ra}^{-4}\right)^{1/11},$$

we have

$$\begin{aligned}
\mathrm{Nu} &\leqslant \left(\frac{1}{2}\left(\frac{10\cdot c_1^4}{2\times 7^4}\right)^{1/11}+\frac{c_1^4}{4\times 7^4}\left(\frac{2\times 7^4}{10\cdot c_1^4}\right)^{10/11}\right)\mathrm{Ra}^{4/11}+\frac{\sqrt{6}}{98}\left(\frac{10\cdot c_1^4}{2\times 7^4}\right)^{-5/11}\mathrm{Ra}^{-7/22}\,\mathrm{Ta}\sqrt{\mathrm{Nu}} \\
&\quad +\frac{C_1^2}{49}\left(\frac{10\cdot c_1^4}{2\times 7^4}\right)^{-5/11}\mathrm{Ra}^{-9/11}\,\mathrm{Ta}\,\mathrm{Nu} \\
&\approx 1.43\,\mathrm{Ra}^{4/11}+0.0002\,\mathrm{Ra}^{-7/22}\,\mathrm{Ta}\sqrt{\mathrm{Nu}}+0.47\,\mathrm{Ra}^{-9/11}\,\mathrm{Ta}\,\mathrm{Nu},
\end{aligned}$$

without loss of generality, we assume $\mathrm{Ra}\geqslant 1$ and choose $B_1=1/0.94$, it follows that there exist constants $B_2>0$ such that when $\mathrm{Ta}\leqslant B_1\,\mathrm{Ra}^{1/2}$, $\mathrm{Nu}\leqslant B_2\,\mathrm{Ra}^{4/11}$. □

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A diffusion process in curved space–time

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We construct a curved space–time generalization of the special relativistic Ornstein–Uhlenbeck Process. This is done by deriving a manifestly covariant Kolmogorov equation that describes diffusion in curved space–times. The simple case of diffusion in a spatially flat Friedmann–Robertson–Walker universe is then considered. It is proven that, at least in these space–times, Kolmogorov equation admits as possible solution a natural generalization of the flat space–time Jüttner equilibrium solution. The first correction to Jüttner's distribution in a slowly expanding universe is also obtained explicitly. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Relativistic irreversible phenomena are notoriously difficult to model.[1–3] In 1997, Debbasch, Mallick, and Rivet[4] introduced a new diffusion process, the Relativistic Ornstein–Uhlenbeck Process (ROUP). This process is not only the simplest possible model of relativistic diffusion, it is also the simplest toy–model of relativistic irreversible phenomena. Up to now, the ROUP has only been studied in the special relativistic realm; this has notably shed new light on the respective status of special relativistic hydrodynamics and special relativistic kinetic theory.[5] The aim of the present article is to lay down the basis for the study of the ROUP in curved space–time.

The matter is organized as follows. A first section reviews the principal results pertaining to the special relativistic case. An important point made in that section is that the ROUP can be defined in flat space–time by two different but completely equivalent approaches. The first one consists in specifying the stochastic equations of motion for the particle whose diffusion is modelled by the process. The other approach consists in writing down the transport or Kolmogorov equation verified by the phase-space density associated to the diffusing particle. Both routes have naturally been explored in the special relativistic case. It turns out that, to extend the definition of the ROUP to the general relativistic case, it is easier to write directly the transport equation associated to the process in curved space–time. This equation is obtained in Sec. II of this article, as a direct generalization of the manifestly covariant Kolmogorov equation associated to the ROUP in flat space–time. Section III is devoted to a simple but enlightening application of the formalism just developed. The spatially flat homogeneous and isotropic Friedmann–Robertson–Walker universes are surely among the simplest solutions to Einstein's equations and are also of particular physical relevance; it is, therefore, quite natural to investigate the properties of the ROUP in these space–times. In the study of Galilean and relativistic flat space–time diffusion processes, an important role is played by the invariant measure(s) of the process, i.e., the equilibrium solution(s) to the transport equation. In the absence of any force-field, the invariant measure of the special relativistic process is space and time independent in the rest-frame of the fluid in which the particle diffuses. In this frame, it is also isotropic in momentum space. In the case of diffusion occurring in a spatially flat Friedmann model, one should not expect to find a time-independent solution to the transport equation. The question is, therefore: Does Kolmogorov equation then admit a generalized equilibrium solution, i.e., a solution which is, in the so-called comoving coordinates, independent of spatial position and isotropic in momentum space? It is

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proven in Sec. III that such a solution can be obtained perturbatively as a series expansion where the small parameter is the ratio of the characteristic ''microscopic'' relaxation time of the diffusion process (in flat space–time) to the characteristic evolution-time of the expansion factor of the universe. Unicity of the expansion is also proven and the first correction to the special relativistic Jütnner equilibrium solution is explicitly derived. As a conclusion, Sec. IV reviews all the new results of the article and puts them into perspective by comparing them with similar results already obtained on the general relativistic Boltzmann equation. Finally, Sec. IV also mentions some of the many possible extensions to this work.

II. THE SPECIAL RELATIVISTIC ORNSTEIN–UHLENBECK PROCESS

A. Basics

To present the special relativistic Ornstein–Uhlenbeck process most succinctly, it is best to use the image of a Brownian special relativistic particle diffusing in a surrounding (special relativistic) fluid. The diffusion process has originally been defined[4] by a couple of covariant stochastic equations which determine, in an arbitrary Lorentz frame, the time-evolution of both the position and momentum of the diffusing particle.

Let us suppose now that the fluid which surrounds the particle is in a state of global equilibrium. Then, there exists a Lorentz frame $\mathcal{R}$ where this fluid is at rest; this frame is usually called the global rest-frame of the fluid; it constitutes a naturally preferred Lorentz frame for the diffusion process.[6] In this reference frame, the equations of motion for the diffusing particle take the simple form

$$\begin{cases} \dfrac{d}{dt}\mathbf{x} = \dfrac{\mathbf{p}}{m\gamma}, \\ \dfrac{d}{dt}\mathbf{p} = -\alpha\dfrac{\mathbf{p}}{\gamma} + \sqrt{2D}\dfrac{d\mathbf{W}}{dt}, \end{cases} \tag{1}$$

where $d\mathbf{W}/dt$ indicates that the stochastic part $\mathbf{F}_s$ of the force which acts on the diffusing particle is, up to the multiplicative constant $\sqrt{2D}$, the derivative of the Wiener process, i.e., a Gaussian white noise. The positive constant α enters the definition of the deterministic part $\mathbf{F}_d$ of the force acting on the particle and plays the role of a friction coefficient. And the Lorentz factor $\gamma(\mathbf{p})$ is defined by

$$\gamma(\mathbf{p}) = \left(1 + \frac{\mathbf{p}^2}{m^2c^2}\right)^{1/2}. \tag{2}$$

Let now $\Pi(t,\mathbf{x},\mathbf{p})$ be the phase-space distribution function of the diffusing particle in $\mathcal{R}$. More precisely, let $\Pi(t,\mathbf{r},\mathbf{p})d^3xd^3p$ be the probability to find in $\mathcal{R}$ the diffusing particle at time t in the volume d^3xd^3p centered on $(\mathbf{x},\mathbf{p})$. It is possible to derive from (1) a transport equation verified by Π. One obtains from (1) (see Ref. 4)

$$\partial_t\Pi + \nabla_{\mathbf{x}}.\left(\frac{\mathbf{p}}{m\gamma}\Pi\right) + \nabla_{\mathbf{p}}.\left(-\alpha\frac{\mathbf{p}}{\gamma}\Pi\right) = D\ \Delta_{\mathbf{p}}\Pi. \tag{3}$$

As just presented, (3) is merely a consequence of (1). A stronger result actually applies. Quite generally speaking, the correspondence between a sufficiently regular Itô process and its forward Kolmogorov equation is one-to-one.[7] Consequently, the transport equation (3) can also be considered as implying the stochastic equations of motion (1).

Equations (1) or (3) fully define the process in $\mathcal{R}$. By Lorentz transforming all quantities involved in these equations, it is then possible to obtain the stochastic equations which fix the motion of the particle in another arbitrary Lorentz frame; and one can also be led to the transport

equation associated to the process in this same Lorentz frame.[6] Either of these new equations entirely defines the process in this other Lorentz frame. Therefore, Eqs. (1) or (3) entirely define the process, in all Lorentz frames.

This formulation of the special relativistic Ornstein–Uhlenbeck process is perfectly covariant, but it is not manifestly covariant. It is impossible to obtain a simple manifestly covariant form of the stochastic equations of motion. One can, however, write down a manifestly covariant Kolmogorov equation for the process. This equation will be presented in the next section. It will serve as a starting point for the extension of the process to the general relativistic realm.

B. Manifestly covariant special relativistic Kolmogorov equation

The idea behind the manifestly covariant formulation[8] is to introduce a new, unphysical distribution function f, defined over the extended phase-space $\mathbb{R}^8=\{(x^\mu,p^\mu)\}$, and whose restriction to the mass-shell gives back, in any Lorentz-frame, the physical distribution function Π:

$$\Pi(t,\mathbf{x},\mathbf{p})=\int_{p\in\mathcal{P}} f(t,\mathbf{x},p^0,\mathbf{p})\ \delta(p^0-mc\,\gamma(\mathbf{p}))\ \ dp^0. \tag{4}$$

Naturally, given a distribution Π, it is always possible to find at least one f which verifies (4), but the solution is generally *not* unique. The domain $\mathcal{P}$ contains the mass-shell and is defined by

$$\mathcal{P}=\{p\in\mathbb{R}^4; p.U>0\}, \tag{5}$$

where U stands for the 4-velocity of the fluid in which the particle diffuses. This is the largest domain in which all coefficients of the manifestly covariant Kolmogorov equation are defined and regular.[8] One can choose the function f to be a Lorentz scalar and Kolmogorov equation (3) can be rewritten as

$$\int_{p\in\mathcal{P}} \frac{1}{p^0}\mathcal{L}(f)\ \ \delta(p^0-mc\,\gamma(\mathbf{p}))\,dp^0=0, \tag{6}$$

where the differential operator $\mathcal{L}$ is defined by[8]

$$\mathcal{L}(f)=\partial_{x^\mu}(p^\mu f)+\partial_{p^\mu}(mc\ \ F_d^\mu f)+DK^{\mu\rho\beta\nu}\partial_{p^\rho}\left(\ \frac{p_\mu p_\beta}{p.U}\partial_{p^\nu}f\right). \tag{7}$$

The manifestly covariant expression of the deterministic 4-force F_d^μ is

$$F_d^\mu=-\lambda_\nu^\mu p^\nu\frac{p^2}{m^2c^2}+\lambda_\beta^\alpha\frac{p_\alpha p^\beta}{m^2c^2}p^\mu, \tag{8}$$

with

$$\lambda_\nu^\mu=\frac{\alpha(mc)^2}{(p.U)^2}\Delta_\nu^\mu, \tag{9}$$

$$\Delta_{\mu\nu}=\eta_{\mu\nu}-U_\mu U_\nu. \tag{10}$$

Δ is evidently the projector unto the subspace of momentum 4-space orthogonal to U. The tensor K is itself defined by

$$K^{\mu\rho\beta\nu}=\ \ U^\mu U^\beta\Delta^{\rho\nu}-U^\mu U^\nu\Delta^{\rho\beta}+U^\rho U^\nu\Delta^{\mu\beta}-U^\rho U^\beta\Delta^{\mu\nu}. \tag{11}$$

The manifestly covariant special relativistic Kolmogorov equation is $\mathcal{L}(f) = 0$. It can serve as a manifestly covariant definition of the special relativistic Ornstein–Uhlenbeck process because its restriction to the mass-shell is, in $\mathcal{R}$, identical to Eq. (3), which itself fully defines the process in all Lorentz frames.

III. THE GENERAL RELATIVISTIC ORNSTEIN–UHLENBECK PROCESS

The general relativistic Ornstein–Uhlenbeck process will be defined by a general relativistic, manifestly covariant extension of the special relativistic transport equation $\mathcal{L}(f)=0$.

A. Choice of the extended phase-space

There are two natural candidates for the general relativistic extended phase-space. If one momentarily leaves aside the constraint $p.U$, the first candidate is the bundle tangent to the space–time manifold; its elements are most naturally represented, within a chart (coordinate system), by the four space–times coordinates x^μ and four contravariant momentum components p^μ. The second candidate is the bundle *co*tangent to space–time, whose elements can be represented by the four space–time coordinates x^μ and the four covariant momentum components p_μ.

The distinction between these two possibilities is rather academic in special relativity since, in flat space–time, the contravariant and covariant components of p differ at the most by a sign. This is generally not so in curved space–time and, although both possibilities naturally give back the same physics, experience in relativistic kinetic theory teaches that choosing the cotangent bundle as phase-space is usually the most technically convenient solution.[9] Remember also that momenta in Hamiltonian formalism naturally appear through their covariant components, i.e., as covector, and not as (tangent) vectors.[10]

To avoid any possible confusion and to simplify some notations in the next section, we will adopt the following nonstandard convention. p will always stand for a vector tangent to space–time and only its so-called contravariant components p^μ will appear in the text. Elements of the cotangent space will be denoted by q and only their covariant components q_μ will appear below.

The extended phase-space is thus chosen to be $\{(x^\mu,q_\mu)\in\mathbb{R}^8; q.U=q_\mu U^\mu>0\}$. Note that, in curved space–time, the components U^μ generally depend on x (since U is normed to unity). Thus, generally speaking, the condition $q.U>0$ also involves x.

B. Choice of measures on the extended phase-space

The curved space–time equivalent to the completely antisymmetric symbol $\epsilon_{\mu\nu\rho\alpha}$ is[11]

$$E_{\mu\nu\rho\alpha}=\sqrt{-\det g}\ \ \epsilon_{\mu\nu\rho\alpha}; \tag{12}$$

its purely contravariant components read

$$E^{\mu\nu\rho\alpha}=\frac{1}{\sqrt{-\det g}}\epsilon^{\mu\nu\rho\alpha}. \tag{13}$$

The natural four-dimensional volume measure in space–time is, therefore, simply $(1/4!)\ E_{\mu\nu\rho\alpha}dx^\mu\wedge dx^\nu\wedge dx^\rho\wedge dx^\alpha=\sqrt{-\det g}\,d^4x$ and the natural 4d-volume measure in momentum space is $(1/4!)\ E^{\mu\nu\rho\alpha}dq_\mu\wedge dq_\nu\wedge dq_\rho\wedge dq_\alpha=(\sqrt{-\det g})^{-1}d^4q$.

However, four-dimensional volume integrals in space–time or in momentum space do not appear in physics; indeed, only integrals over three-dimensional space-like submanifolds of space–time are needed and, as far as momentum space is concerned, only integrals over the three-dimensional mass-shell have physical relevance. Let us now recall what measures are to be used in both cases.[9]

The measure

$$dS_\mu=\frac{1}{3!}E_{\mu\nu\rho\alpha}dx^\nu\wedge dx^\rho\wedge dx^\alpha \tag{14}$$

will be used on space-like three-dimensional submanifolds of space–time. This measure behaves like a pseudo-cotangent vector to space–time. In particular, it can be integrated against tangent vector fields to yield pseudo-scalars.

As far as momentum space is concerned, it is customary to proceed differently; one usually does not introduce directly a measure defined on the mass-shell but one works rather with a measure which is defined over the whole momentum space but which enforces itself the mass-shell restriction. The simplest procedure is to define this measure $d\Sigma$ to be[9]

$$d\Sigma = \theta(q_0)\,\delta(g^{\mu\nu}(x)q_\mu q_\nu - m^2c^2)\,\frac{1}{4!}E^{\mu\nu\rho\alpha}dq_\mu\wedge dq_\nu\wedge dq_\rho\wedge dq_\alpha$$

$$= \theta(q_0)\,\delta(g^{\mu\nu}(x)q_\mu q_\nu - m^2c^2)\;\;(\sqrt{-\det g})^{-1}d^4q. \tag{15}$$

This measure is clearly a pseudo-scalar.

Given an arbitrary coordinate system, one can choose the three independent ''spatial'' components $(q_1,q_2,q_3)=\mathbf{q}$ as coordinates on the mass-shell. On the mass-shell, the component q_0 can then be considered to be a positive function of both x and $\mathbf{q}$, implicitly defined by $g^{\mu\nu}(x)q_\mu q_\nu = m^2c^2$. This function will be denoted by $mc\,\gamma(x,\mathbf{q})$. The zeroth *contravariant* component of q, $g^{0\mu}(x)q_\mu$, is then also a function of x and $\mathbf{q}$, which will be denoted by $mc\,\tilde{\gamma}(x,\mathbf{q})$. It is then straightforward to prove that, for any field ϕ (not necessarily scalar) defined over the extended phase-space, one has, for all t and $\mathbf{x}$,

$$\int_{q.U>0}\phi(t,\mathbf{x},q_0,\mathbf{q})\;\;d\Sigma = \int_{\mathbb{R}^3}\phi(t,\mathbf{x},mc\,\gamma(t,\mathbf{x},\mathbf{q}),\mathbf{q})\,\frac{1}{\sqrt{-\det g}}\,\frac{d^3q}{mc\,\tilde{\gamma}(t,\mathbf{x},\mathbf{q})}. \tag{16}$$

Similarly, the restrictions of dS_μ to the three-dimensional submanifolds of space–time defined by an equation of the form $t=a$, where a is an arbitrary real number, read

$$dS_\mu = (\sqrt{-\det g}\;\,d^3x,0,0,0). \tag{17}$$

It follows from (16) and (17) that, for an arbitrary field ϕ,

$$\int_{q.U>0}\phi(t,\mathbf{x},q_0,\mathbf{q})\;\;dS_\mu d\Sigma = \int_{\mathbb{R}^6}\phi(t,\mathbf{x},mc\,\gamma(t,\mathbf{x},\mathbf{q}),\mathbf{q})d^3x[d^3q/mc\,\tilde{\gamma}(t,\mathbf{x},\mathbf{q})]. \tag{18}$$

Equations (16) and (18) will be used in the next sections to transcribe manifestly covariant, off-shell relations into nonmanifestly covariant, on-shell results.

C. Manifestly covariant general relativistic Kolmogorov equation

The operator $\mathcal{L}$, as defined by (7), is manifestly invariant under Lorentz transformation, but not under arbitrary coordinate changes. Let us then examine each contribution to (7) separately and find a reasonable generalization of (7) to curved space–times. Let us start with the projector Δ. Its proper general relativistic expression is

$$\Delta_{\mu\nu} = g_{\mu\nu} - U_\mu U_\nu. \tag{19}$$

Definition (11) of the tensor K is then perfectly valid, as is expression (9) for the tensor λ, taking care of replacing p by q:

$$\lambda^{\mu\nu} = \frac{\alpha(mc)^2}{(q_\mu U^\mu)^2}\,\Delta^{\mu\nu}. \tag{20}$$

The same goes also for the definition (8) of the deterministic 4-force; thus, the general relativistic deterministic 4-force is defined as a function of q by

$$F_{d\mu} = -\lambda^{\nu}_{\mu} q_{\nu} \frac{g^{\mu\nu} q_{\mu} q_{\nu}}{m^2 c^2} + \lambda^{\alpha\beta} \frac{q_{\alpha} q_{\beta}}{m^2 c^2} q_{\mu}. \tag{21}$$

Let us now examine if the various partial derivatives appearing in (7) should be modified for the general relativistic realm.

Let ϕ be an arbitrary field defined over phase-space. To simplify the discussion, let us suppose ϕ behaves like a scalar under arbitrary coordinate changes in space–time. Let us consider such a change of coordinates. Then, with obvious notations,

$$\phi'(x^{\mu'}, q_{\nu'}) = \phi(x^{\mu}, q_{\nu}). \tag{22}$$

Since

$$q_{\nu} = \frac{\partial x^{\nu'}}{\partial x^{\nu}} q_{\nu'}, \tag{23}$$

one has

$$\frac{\partial}{\partial x^{\mu'}} \phi' = \frac{\partial x^{\mu}}{\partial x^{\mu'}} \frac{\partial \phi}{\partial x^{\mu}} + \frac{\partial^2 x^{\nu'}}{\partial x^{\mu} \partial x^{\nu}} \frac{\partial x^{\mu}}{\partial x^{\mu'}} q_{\nu'} \frac{\partial \phi}{\partial q_{\nu}} \tag{24}$$

and

$$\frac{\partial}{\partial q_{\nu'}} \phi' = \frac{\partial x^{\nu'}}{\partial x^{\nu}} \frac{\partial \phi}{\partial q_{\nu}}. \tag{25}$$

Equation (25) proves that the operator $\partial/\partial q_{\nu}$ transforms scalar fields into vector fields tangent to space–time. This can easily be generalized to fields of arbitrary tensor type. The notion of partial differentiation with respect to impulse components is thus a perfectly generally covariant notion and the operator $\partial/\partial q_{\nu}$ transforms arbitrary tensor fields of type (a,b) into tensor fields of type $(a+1,b)$. This can be easily understood without any calculation if one remembers that, at any point in space–time, momentum space is a *flat* four-dimensional manifold. The concept of partial differentiation with respect to one of the coordinates used on that manifold is therefore a perfectly covariant and natural geometrical concept.

On the other hand, Eq. (24) proves that, even for scalar fields, partial differentiation with respect to one of the space–time coordinates is *not* a covariant notion. This again is quite simple to understand.

In passing from x to $x+dx$, the usual partial differentiation maintains the *components* of q constant. In flat space–time, this amounts to maintaining the vector q itself constant. But in curved space–time, the basis covectors in q space are themselves x dependent. Maintaining the components of q constant is therefore not equivalent to maintaining the covector q itself constant. Of these two notions, the second (maintaining the covector itself constant) is an invariant one, while the other is not. The correct general relativistic concept is, therefore: Derivative with respect to the space–time degrees of freedom, maintaining the covector q constant, and not its components in the local coordinate basis.

Let now q be defined at x and let q_{ν} be its components in the local coordinate basis. The covector "equal" to q at point $x+dx$ is obtained by parallel transporting q from x to $x+dx$; let this covector at point $x+dx$ have components $q_{\nu}+dq_{\nu}$ in the coordinate basis (at point $x+dx$). By definition one has[11,12]

$$dq_{\nu} = +\Gamma^{\alpha}_{\nu\mu} q_{\alpha} dx^{\mu}, \tag{26}$$

where the Γ's are the Christoffel symbols.

One, therefore, defines[9] a new operator D_μ, acting on arbitrary fields defined over the eight-dimensional phase-space, by

$$D_\mu = \nabla_\mu + \Gamma^\alpha_{\mu\nu} q_\alpha \frac{\partial}{\partial q_\nu}, \tag{27}$$

where ∇ stands for the usual covariant derivative operator with respect to space–time degrees of freedom. Thus defined, D_μ is generally covariant and transforms arbitrary tensor fields of type (a,b) into tensor fields of type $(a,b+1)$.

Using D_μ, one can write the following relativistic generalization of definition (7):

$$\mathcal{L}(f) = D_\mu(g^{\mu\nu}(x) q_\nu f) + \frac{\partial}{\partial q_\mu}(mcF_{d\mu} f) + DK^\mu{}_\rho{}^\beta{}_\nu \; \partial_{q_\rho}\left(\frac{q_\mu q_\beta}{q_\mu U^\mu} \partial_{q_\nu} f \right), \tag{28}$$

with F_d and K given by Eqs. (19)–(21).

The general relativistic Ornstein–Uhlenbeck process is then defined by the manifestly covariant tranport equation $\mathcal{L}(f)=0$, where f represents the scalar probability distribution of the diffusing particle in its extended eight-dimensional phase-space.

Note that (28) is not the only possible generalization of (7) to curved space–time. It is merely the simplest and, therefore, the most natural one. No other generalization will be envisaged in this article.

Let me finally stress that the general relativistic Kolmogorov equation involves the fluid surrounding the diffusing particle (through U) as well as the Einstein gravitational field (through the metric g). Since U and g can be prescribed independently (the only constraint being $U^2=1$), one can consider that the general relativistic Ornstein–Uhlenbeck process describes the stochastic motion of a diffusing particle interacting with both a surrounding fluid in arbitrary motion and an arbitrary gravitationnal field.

D. Transition to an on-shell formulation

It is useful, in view of practical applications, to elaborate briefly about how this manifestly covariant ''off-shell'' formulation can be transcribed, in an arbitrary coordinate system, into a more standard, covariant but not manifestly covariant on-shell treatment, which involves a ''physical'' distribution function defined on the mass-shell only.

Let ϕ be an arbitrary field defined over the extended phase-space. Its mean-value $\overline{\phi}(x)$ at point x is, by definition,

$$\overline{\phi}(x) = \int_{q.U>0} \phi(x,q) f(x,q) d\Sigma. \tag{29}$$

The field $\overline{\phi}$ represents a spatial density. For example, if $\phi(x,q)=g^{\mu\nu}(x)q_\mu$, $\overline{\phi}$ is simply the usual particle 4-current j^μ. As any spatial density, $\overline{\phi}$ is ultimately to be integrated against dS_μ on an arbitrary space-like three-dimensional submanifold S of space–time. Let us choose a coordinate system in which this submanifold is a constant-time submanifold and let us consider the quantities $\overline{\phi}\, dS_\mu$ in greater detail. Because of equation (17), only $\overline{\phi}\, dS_0$ does not vanish. Using (16) and (18), one can write it under the form

$$\overline{\phi}(x) dS_0 = d^3x \int_{\mathbb{R}^3} \phi(t,\mathbf{x},mc\,\gamma(t,\mathbf{x},\mathbf{q}),\mathbf{q}) f(t,\mathbf{x},mc\,\gamma(t,\mathbf{x},\mathbf{q}),\mathbf{q}) \frac{d^3q}{mc\,\tilde{\gamma}(t,\mathbf{x},\mathbf{q})}. \tag{30}$$

This in turn can be rewritten as

$$\overline{\phi} dS_0 = d^3x \int_{\mathbb{R}^3} \frac{\phi(t,\mathbf{x},mc\gamma(t,\mathbf{x},\mathbf{q}),\mathbf{q})}{mc\tilde{\gamma}(t,\mathbf{x},\mathbf{q})} \Pi(t,\mathbf{x},\mathbf{q}) \quad d^3q, \tag{31}$$

with Π defined by

$$\Pi(t,\mathbf{x},\mathbf{q}) = \int_{\mathbb{R}} f(t,\mathbf{x},q_0,\mathbf{q}) \delta(q_0 - mc\gamma(t,\mathbf{x},\mathbf{q})) dq_0. \tag{32}$$

To understand the physical meaning of Π, let us elaborate further on the case where $\phi(x,q) = g^{\mu\nu}(x) q_\nu$; as mentioned earlier, $\overline{\phi}$ then coincides with the 4-current j^μ and the only non-vanishing components of $\overline{\phi} dS_\nu = j^\mu dS_\nu$ are $j^\mu dS_0$. The quantity $j^0 dS_0$ represents the probability dn of finding the diffusing particle at time t in the volume d^3x centered on $\mathbf{x}$. Equation (31) gives

$$j^0(t,\mathbf{x}) dS_0 = dn = d^3x \int_{\mathbb{R}^3} \Pi(t,\mathbf{x},\mathbf{q}) d^3q, \tag{33}$$

which proves that Π plays, in the considered coordinate system, the role of a standard probability distribution. Inspecting the other components $j^k dS_0$ trivially confirms this interpretation of Π.

Now, to the dynamics of Π. In each coordinate system, the manifestly covariant Kolmogorov equation can be transcribed into a transport equation for Π; this transport equation fully characterizes the general relativistic Ornstein–Uhlenbeck process in the chosen coordinate system. This transport equation is however not manifestly covariant and its general expression is neither simple nor particularly tractable. It was, therefore, not deemed useful to reproduce this expression here. In any practical application, the best is to obtain this equation directly from the covariant Kolmogorov equation, which is easier to write down. This will be done in the next section on a very simple space–time background.

IV. DIFFUSION IN A SPATIALLY FLAT FRIEDMANN–ROBERTSON–WALKER UNIVERSE

A. Kolmogorov equation for *f* in comoving coordinates

In comoving coordinates, the space–time metric of a spatially flat Friedmann–Robertson–Walker universe takes the well-known form[12]

$$\begin{aligned} ds^2 &= c^2 dt^2 - a^2(t) \quad (dx_1^2 + dx_2^2 + dx_3^2) \\ &= c^2 dt^2 - a^2(t) \quad d\mathbf{x}^2, \end{aligned} \tag{34}$$

where $a(t)$ is the so-called expansion factor of the universe. Its evolution is fixed via Einstein's equation by the equation of state of the matter present in the universe and by suitable initial conditions. Quite naturally, the fluid in which the particle diffuses will be taken to be the matter in the universe. This matter follows the expansion and is at rest in the comoving frame. Consequently, in the comoving coordinates,

$$(U^\mu) = (1,0,0,0). \tag{35}$$

And the components of the projector Δ are

$$\Delta_{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -a^2(t) & 0 & 0 \\ 0 & 0 & -a^2(t) & 0 \\ 0 & 0 & 0 & -a^2(t) \end{pmatrix}. \tag{36}$$

The only nonvanishing Christoffel symbols are[12]

$$\Gamma^0_{11}=\Gamma^0_{22}=\Gamma^0_{33}=a\dot{a} \tag{37}$$

and

$$\Gamma^1_{01}=\Gamma^2_{02}=\Gamma^3_{03}=\frac{\dot{a}}{a}. \tag{38}$$

Evaluating directly the various contributions to (28), one first obtains

$$\begin{cases} g^{0\nu}q_\nu=q_0, \\ g^{i\nu}q_\nu=-\dfrac{1}{a^2(t)}q_i \end{cases} \tag{39}$$

and

$$D_0=\frac{\partial}{\partial t}+\frac{\dot{a}}{a}\sum_{i=1}^{3} q_i\frac{\partial}{\partial q_i}, \tag{40}$$

$$D_i=\frac{\partial}{\partial x^i}+\frac{\dot{a}}{a}q_i\frac{\partial}{\partial q_0}+\dot{a}a\ q_0\frac{\partial}{\partial q_i}+\frac{\dot{a}}{a}q_0, \tag{41}$$

where $i=1,2,3$.

As for $F_{d\mu}$, one finds that, in comoving coordinates,

$$F_{d\mu}=\frac{\alpha}{q_0}(g^{\rho\nu}(x)q_\rho q_\nu U_\mu-q_0q_\mu), \tag{42}$$

so that

$$F_{d0}=-\frac{\alpha}{a^2(t)}\frac{1}{q_0}\sum_{i=1}^{3} q_i\ q_i \tag{43}$$

and

$$F_{di}=-\alpha\ q_i \tag{44}$$

for $i=1,2,3$.

It is then easy to check that, in comoving coordinates,

$$D_\mu(g^{\mu\nu}(x)q_\nu f)=q_0\frac{\partial f}{\partial t}-\frac{1}{a^2}\sum_{i=1}^{3} q_i\frac{\partial f}{\partial x^i}-\frac{\dot{a}}{a^3}\sum_{i=1}^{3} q_i\ q_i\frac{\partial f}{\partial q_0} \tag{45}$$

and

$$\frac{\partial}{\partial q_\mu}(mc\ F_{d\mu}f)=-\alpha mc\left[\sum_{i=1}^{3}\frac{\partial}{\partial q_i}(q_if)+\frac{\partial}{\partial q_0}\left(\frac{1}{a^2}\frac{1}{q_0}\sum_{i=1}^{3} q_i\ q_i\ f\right)\right]. \tag{46}$$

Finally, a direct evaluation of the components of K in comoving coordinates delivers

$$K^{\mu}{}_{\rho}{}^{\beta}{}_{\nu}\ \partial_{q_\rho}\left(\ \frac{q_\mu q_\beta}{q_\mu U^\mu}\partial_{q_\nu} f\right) = -\ \frac{\partial}{\partial q_0}\left[\sum_{i=1}^{3} q_i \frac{\partial f}{\partial q_i}\ +\ \frac{1}{a^2}\frac{1}{q_0}\sum_{i=1}^{3} q_i\ q_i \frac{\partial f}{\partial q_0}\right]$$
$$-\ \frac{a^2}{q_0}\sum_{i=1}^{3}\frac{\partial}{\partial q_i}\left[\ \frac{\partial f}{\partial q_i}\ +\ \frac{1}{a^2}\frac{1}{q_0} q_i \frac{\partial f}{\partial q_0}\right]. \tag{47}$$

Combining the last three equations leads to the Kolmogorov equation verified by f.

B. Kolmogorov equation for the physical distribution Π

Using (35), one easily finds that

$$\gamma(t,\mathbf{x},\mathbf{q}) = \left(1 + \ \frac{\mathbf{q}^2}{a^2(t)\ \ m^2c^2}\right)^{1/2}, \tag{48}$$

where the notation $\Sigma_{i=1}^{3} q_i\ q_i = \mathbf{q}^2$ has been used. Since in this case γ does not depend on $\mathbf{x}$, we will adopt the shorter notation $\gamma(t,\mathbf{q})$ for the remainder of this section.

Let us now define, for an arbitary field $h(t,\mathbf{x},q_0,\mathbf{q})$, the field $\tilde{h}(t,\mathbf{x},\mathbf{q})$ by

$$\tilde{h}(t,\mathbf{x},\mathbf{q}) = \int_{\mathbb{R}} h(t,\mathbf{x},q_0,\mathbf{q})\,\delta(q_0 - mc\,\gamma(t,\mathbf{q}))\,dq_0. \tag{49}$$

In particular, $\Pi = \tilde{f}$.

Taking into account expression (48) for γ, the standard properties of δ lead to

$$\frac{\partial}{\partial t}\tilde{h}(t,\mathbf{x},\mathbf{q}) = \int_{\mathbb{R}}\left[\ \frac{\partial}{\partial t}h(t,\mathbf{x},q_0,\mathbf{q}) - \ \frac{\dot{a}}{a^3}\frac{1}{q_0}\mathbf{q}^2\frac{\partial f}{\partial q_0}\right]\ \delta(q_0 - mc\,\gamma(t,\mathbf{q}))\ \ dq_0, \tag{50}$$

$$\frac{\partial}{\partial \mathbf{x}}\tilde{h}(t,\mathbf{x},\mathbf{q}) = \int_{\mathbb{R}}\frac{\partial}{\partial \mathbf{x}}h(t,\mathbf{x},q_0,\mathbf{q})\ \ \delta(q_0 - mc\,\gamma(t,\mathbf{q}))\ \ dq_0 \tag{51}$$

and

$$\frac{\partial}{\partial \mathbf{q}}\tilde{h}(t,\mathbf{x},\mathbf{q}) = \int_{\mathbb{R}}\left[\ \frac{\partial}{\partial \mathbf{q}}h(t,\mathbf{x},q_0,\mathbf{q}) + \ \frac{1}{a^2}\frac{1}{q_0}\mathbf{q}\frac{\partial f}{\partial q_0}\right]\ \delta(q_0 - mc\,\gamma(t,\mathbf{q}))\ \ dq_0. \tag{52}$$

Using these three relations, it is possible to deduce from the transport equation $\mathcal{L}(f) = 0$ a transport equation for the physical distribution $\Pi(t,\mathbf{x},\mathbf{q})$. More precisely, the equation

$$\int_{\mathbb{R}}\frac{1}{q_0}\mathcal{L}(f)\,\delta(q_0 - mc\,\gamma(t,\mathbf{q}))\,dq_0 = 0 \tag{53}$$

is equivalent to

$$\frac{\partial}{\partial t}\Pi - \ \frac{1}{a^2(t)}\ \frac{\partial}{\partial \mathbf{x}}.\left(\frac{\mathbf{q}}{m\,\gamma(t,\mathbf{q})}\Pi\right) + \ \frac{\partial}{\partial \mathbf{q}}.\ \left(-\alpha\frac{\mathbf{q}}{\gamma(t,\mathbf{q})}\Pi\right) - D\ \ a^2(t)\frac{\partial^2}{\partial \mathbf{q}^2}\Pi = 0. \tag{54}$$

The stochastic equations of motion which correspond to this transport equation are

$$\begin{cases} \dfrac{d}{dt}\mathbf{x} = -\ \dfrac{1}{a^2(t)}\ \dfrac{\mathbf{q}}{m\gamma(t,\mathbf{q})}, \\ \dfrac{d}{dt}\mathbf{q} = -\alpha\dfrac{\mathbf{q}}{\gamma(t,\mathbf{q})} + \sqrt{2D}\ \ a(t)\dfrac{d\mathbf{W}}{dt}. \end{cases} \tag{55}$$

These equations clearly show that the process is time-inhomogeneous.

C. Proof of the existence and unicity of a perturbative expression for the generalized equilibrium solution

One of the first questions to ask about a time-homogeneous diffusion process is whether or not the process admits an invariant measure.[7] The Galilean and the special relativistic Ornstein–Uhlenbeck process both admit invariant measures;[4,13] their densities Π are both time and space independent and coincide, respectively, with the Maxwell and Maxwell–Jüttner equilibrium distributions at temperature $T=D/k_B\alpha$.

Considering the process (55) is not time-homogeneous, it surely makes no sense to search for standard, time- and space-independent equilibrium solutions to (55). But, since the process describes diffusion in a universe which is spatially homogeneous and isotropic, it seems reasonable to search for solutions to (55) which depend only on the time and momentum variables, and which coincide with the Maxwell–Jüttner distribution at temperature T when the expansion factor $a(t)$ is set constant, equal to unity. These solutions will be said to describe generalized equilibriums.

They verify

$$\frac{\partial}{\partial t}\Pi = \ \frac{\partial}{\partial \mathbf{q}}\cdot\ \left(\alpha\frac{\mathbf{q}}{\gamma(t,\mathbf{q})}\Pi + D\ \ a^2(t)\frac{\partial}{\partial \mathbf{q}}\Pi\right). \tag{56}$$

Unfortunately, it does not seem possible to obtain exact solutions to (56) valid for an arbitrary $a(t)$. It is, however, possible to solve (56) perturbatively in situations where $a(t)$ varies slowly with respect to the natural "microscopic" time scale $\tau=1/\alpha$.

The best-known method for finding slowly varying solutions to transport equations has been introduced by Chapman and Enskog; it was originally developed in Galilean physics to solve approximately the Boltzmann equation in near-equilibrium situations.[14,15] The method has then been extended to the relativistic Boltzmann equation;[9] it has also been used to exhibit near-equilibrium solutions to other Galilean transport equations (including Kolmogorov equations),[13,16] and the Kolmogorov equation associated to the special relativistic Ornstein–Uhlenbeck process has been recently solved by a Chapman–Enskog expansion.[5]

As far as the general relativistic Ornstein–Uhlenbeck process is concerned, Chapman's and Enskog's method can be used for two different purposes. As in the special relativistic case, it can naturally be implemented to find solutions to Kolmogorov equation which are close to the generalized equilibrium solution. But it can also be used to find a perturbative expression for the generalized equilibrium solution itself, valid when the coefficients of (56) are, through the expansion factor $a(t)$, "slowly varying" functions of the time coordinate.

Let us make the discussion precise by introducing $a_0=a(t=0)$ and the "slow" dimensionless time-variable $\bar{t}$, defined by

$$\bar{t} = \epsilon\ \alpha\ t, \tag{57}$$

where ϵ is an arbitrary infinitesimal. We propose to solve the transport equation perturbatively in ϵ for cases where the expansion-factor $a(t)$ can be written

$$a(t) = a_0\ \ \bar{a}(\bar{t}) \tag{58}$$

with

$$\frac{\partial \overline{a}}{\partial \overline{t}} = O(1). \tag{59}$$

A convenient length-scale is

$$\lambda = a_0 \frac{1}{m\alpha} \sqrt{\frac{D}{\alpha}}, \tag{60}$$

which corresponds to the momentum-scale ζ:

$$\zeta = m\lambda\alpha. \tag{61}$$

We therefore define the dimensionless quantities

$$\overline{\mathbf{x}} = \frac{\mathbf{x}}{\lambda}, \tag{62}$$

$$\overline{\mathbf{q}} = \frac{\mathbf{q}}{\zeta} \tag{63}$$

and

$$\overline{\Pi}(\overline{t}, \overline{\mathbf{x}}, \overline{\mathbf{q}}) = \zeta^3 \Pi(t, \mathbf{x}, \mathbf{q}). \tag{64}$$

Solving Eq. (56) is equivalent to solving

$$\epsilon \frac{\partial}{\partial \overline{t}} \overline{\Pi} = \frac{\partial}{\partial \overline{\mathbf{q}}} \cdot \left(\frac{\overline{\mathbf{q}}}{\overline{\gamma}(\overline{t}, \overline{\mathbf{q}})} \overline{\Pi} + \overline{a}^2(\overline{t}) \frac{\partial}{\partial \overline{\mathbf{q}}} \overline{\Pi} \right) \tag{65}$$

with

$$\overline{\gamma}(\overline{t}, \overline{\mathbf{q}}) = \left(1 + \frac{Q^2}{\overline{a}^2(\overline{t})} \overline{\mathbf{q}}^2 \right)^{1/2}, \tag{66}$$

$$Q^2 = \frac{D}{\alpha m^2 c^2}. \tag{67}$$

We also impose the normalization condition

$$\int_{\mathbb{R}^3} \overline{\Pi}(\overline{t}, \overline{\mathbf{q}}) d^3\overline{q} = \int_{\mathbb{R}^3} \Pi(t, \mathbf{q}) d^3q = 1, \tag{68}$$

which is the direct equivalent of the normalization usually chosen for equilibrium distributions in flat space–time.[4]

As indicated earlier, we search a solution to (65) in the form of a perturbation series in ϵ:

$$\overline{\Pi}(\overline{t}, \overline{\mathbf{q}}) = \sum_{k=0}^{\infty} \epsilon^k \overline{\Pi}_k(\overline{t}, \overline{\mathbf{q}}), \tag{69}$$

where all the partial derivatives of the functions $\overline{\Pi}_k$ are supposed to be $O(1)$. We also assume, as is usually done in similar calculations, that all $\overline{\Pi}_k$ decrease at infinity more rapidly than any power of $\overline{\mathbf{q}}$.

The normalization condition (68) does not suffice to determine the $\overline{\Pi}_k$ unambiguously. Following the Chapman–Enskog method, we impose the subsidiary condition

$$\int_{\mathbb{R}^3} \overline{\Pi}_k(\overline{t},\overline{\mathbf{q}})\, d^3\overline{q} = \delta_{k0} \tag{70}$$

for all $k \geqslant 0$.

Inserting (69) into (65) leads, for all $k \geqslant 0$, to

$$\frac{\partial}{\partial \overline{\mathbf{q}}} \cdot \left(\frac{\overline{\mathbf{q}}}{\overline{\gamma}(\overline{t},\overline{\mathbf{q}})} \overline{\Pi}_k + \overline{a}^2(\overline{t}) \frac{\partial}{\partial \overline{\mathbf{q}}} \overline{\Pi}_k \right) = \frac{\partial}{\partial \overline{t}} \overline{\Pi}_{k-1}, \tag{71}$$

with the convention that $\overline{\Pi}_{-1} = 0$.

It is quite easy to find a solution to (70) and (71) at order $k=0$. It reads

$$\overline{\Pi}_0(\overline{t},\overline{\mathbf{q}}) = \frac{1}{4\pi} \frac{1}{\overline{a}^3(\overline{t})} \frac{1}{Q^2\, K_2(1/Q^2)} \exp\left(- \frac{\overline{\gamma}(\overline{t},\overline{\mathbf{q}})}{Q^2} \right). \tag{72}$$

This is indeed the only (normalized) solution to (71) which decreases at infinity more rapidly than any power of $\overline{\mathbf{q}}$.[4] $\overline{\Pi}_0$ thus turns out to be identical with the Jüttner distribution at time t.[9,17] This distribution would describe an actual, standard equilibrium if the expansion factor were time independent.

Let now $\overline{\Pi}_{k-1}$ be a function verifying (70). Let us prove that one can then find a function $\overline{\Pi}_k$ which satisfies both (70) and (71).

The solvability condition for (71), conceived as an equation for $\overline{\Pi}_k$, is simply that the integral of its right-hand side with respect to $d^3\overline{q}$ vanishes (see Refs. 15 and 18 for extensive discussions of the role of solvability conditions in the Chapman–Enskog method). The fact that $\overline{\Pi}_{k-1}$ verifies (70), therefore, ensures that (71) admits solutions. Let $\overline{\Pi}_k^*$ be one of these solutions and let

$$I^* = \int_{\mathbb{R}^3} \overline{\Pi}_k^*(\overline{t},\overline{\mathbf{q}})\, d^3\overline{q}. \tag{73}$$

It is then obvious that the function $\overline{\Pi}_k$ defined by

$$\overline{\Pi}_k = \overline{\Pi}_k^* - I^* \overline{\Pi}_0 \tag{74}$$

verifies both (70) and (71); this proves the statement.

Since we could exhibit a function $\overline{\Pi}_0$ which verifies both (70) and (71) at order 0, we conclude that a function $\overline{\Pi}_k$ verifying these two equations exists at all order. This proves that Eq. (65) admits a perturbative solution of the form (69) verifying (70).

Unicity can be proven by the following argument. We have already mentioned that $\overline{\Pi}_0$ given by (72) is the only solution to (70) and (71) at order 0 which decreases sufficiently rapidly at infinity. Suppose that $\overline{\Pi}_{k-1}$ is known and unique, and let $\overline{\Pi}_k^1$ and $\overline{\Pi}_k^2$ be two solutions to (70) and (71) at order k. Their difference $\Delta\overline{\Pi}_k$ then verifies

$$\frac{\partial}{\partial \overline{\mathbf{q}}} \cdot \left(\frac{\overline{\mathbf{q}}}{\overline{\gamma}(\overline{t},\overline{\mathbf{q}})} \Delta\overline{\Pi}_k + \overline{a}^2(\overline{t}) \frac{\partial}{\partial \overline{\mathbf{q}}} \Delta\overline{\Pi}_k \right) = 0, \tag{75}$$

which is identical to the equation verified by $\overline{\Pi}_0$. Moreover, $\Delta\overline{\Pi}_k$ decreases at least as rapidly as $\overline{\Pi}_k^1$ and $\overline{\Pi}_k^2$ at infinity. It therefore follows that $\Delta\overline{\Pi}_k$ is proportional to $\overline{\Pi}_0$. By (70), the integral of $\Delta\overline{\Pi}_k$ over momentum space vanishes. The proportionality constant between $\Delta\overline{\Pi}_k$ and $\overline{\Pi}_0$ therefore vanishes too, and so does $\Delta\overline{\Pi}_k$. This proves that (70) ensures the existence and unicity of a perturbative solution to (65).

A final remark concerning this solution. Equation (71) makes obvious that $\overline{\Pi}_k$ is even in $\overline{\mathbf{q}}$ if $\overline{\Pi}_{k-1}$ is. Since $\overline{\Pi}_0$ is an even function of $\overline{\mathbf{q}}$, so are all the $\overline{\Pi}_k$'s and, consequently, so is $\overline{\Pi}$ too. It is therefore isotropic, as expected. Let me mention two interesting consequences. By parity, the first moments of $\overline{\Pi}$ vanish. This means that the particle current density 3-vector associated to the generalized equilibrium solution vanishes in the comoving frame, as it should. On the contrary, some second moments of $\overline{\Pi}$ do not vanish. This means in particular that the energy k_BT, which can be interpreted as the mean-value of the energy of the diffusing particle when the distribution function coincides with Π_0,[19] is actually *not* the mean-value of the particle-energy for the real generalized equilibrium distribution. This point will be further elaborated upon in forthcoming publications fully dedicated to specific examples of physical interest.

D. Explicit expression for the first correction to Jütnner's distribution

It is perhaps useful to evaluate explicitly the function $\overline{\Pi}_1$, which represents the first correction to the special relativistic equilibrium solution.

Equation (72) leads to

$$\frac{\partial}{\partial\overline{t}}\overline{\Pi}_0=\frac{\dot{\overline{a}}}{\overline{a}}\left(-3+\frac{1}{\overline{a}^2}\frac{\overline{\mathbf{q}}^2}{\overline{\gamma}}\right). \tag{76}$$

It is best to introduce A_1 defined by

$$\overline{\Pi}_1(\overline{t},\overline{\mathbf{q}})=A_1(\overline{t},\overline{\mathbf{q}})\overline{\Pi}_0(\overline{t},\overline{\mathbf{q}}) \tag{77}$$

and Eq. (71) for $\overline{\Pi}_1$ is equivalent to

$$\overline{a}^2\left(\frac{\partial^2}{\partial\overline{\mathbf{q}}^2}A_1-\frac{1}{\overline{a}^2}\frac{\overline{\mathbf{q}}}{\overline{\gamma}}\cdot\frac{\partial}{\partial\overline{\mathbf{q}}}A_1\right)=\frac{\dot{\overline{a}}}{\overline{a}}\left(-3+\frac{1}{\overline{a}^2}\frac{\overline{\mathbf{q}}^2}{\overline{\gamma}}\right). \tag{78}$$

The general solution to this equation is

$$A_1(\overline{t},\overline{\mathbf{q}})=a_{12}\frac{\overline{\mathbf{q}}^2}{2}+a_{10} \tag{79}$$

with

$$a_{12}=-\frac{\dot{\overline{a}}}{\overline{a}}\frac{1}{\overline{a}^2}, \tag{80}$$

a_{10} being an arbitrary real integration constant.

This constant is fixed by the normalization condition (70). Since $\overline{\Pi}_0$ is normed to unity, one has

$$a_{10}=-a_{12}\int_{\mathbb{R}^3}\frac{\overline{\mathbf{q}}^2}{2}\overline{\Pi}_0 d^3\overline{q}. \tag{81}$$

Because of (72),

$$\int_{\mathbb{R}^3} \overline{\mathbf{q}}^2 \overline{\Pi}_0 \; d^3\overline{q} = \frac{1}{\overline{a}^3(\overline{t})} \frac{1}{Q^2 \; K_2(1/Q^2)} \int_{\mathbb{R}} \overline{q}^4 \exp\left(- \frac{\overline{\gamma}}{Q^2} \right) \; d\overline{q}. \tag{82}$$

Introducing $\theta = Q\overline{q}/\overline{a}$, one can write

$$\int_{\mathbb{R}} \overline{q}^4 \exp\left(- \frac{\overline{\gamma}}{Q^2} \right) d\overline{q} = \frac{\overline{a}^5}{Q^5} \int_{\mathbb{R}} ch\,\theta \; sh^4\theta \exp\left(- \frac{1}{Q^2} ch\,\theta \right) \; d\theta. \tag{83}$$

A simple integration by part shows that

$$\int_{\mathbb{R}} ch\,\theta \; sh^4\theta \exp\left(- \frac{1}{Q^2} ch\,\theta \right) \; d\theta = \frac{1}{5Q^2} \int_{\mathbb{R}} sh^6\theta \exp\left(- \frac{1}{Q^2} ch\,\theta \right) d\theta, \tag{84}$$

which leads to (see Ref. 20)

$$\int_{\mathbb{R}} ch\,\theta \; sh^4\theta \exp\left(- \frac{1}{Q^2} ch\,\theta \right) \; d\theta = \frac{1}{5Q^2} \Gamma(7/2) \frac{1}{\sqrt{\pi}} (2Q^2)^3 \; K_3(1/Q^2). \tag{85}$$

Using the fact that[20] $\Gamma(\frac{7}{2}) = 15\sqrt{\pi}/8$, one finds

$$\int_{\mathbb{R}} \overline{q}^4 \exp\left(- \frac{\overline{\gamma}}{Q^2} \right) d\overline{q} = \frac{3\overline{a}^5}{Q} K_3\left(\frac{1}{Q^2} \right) \tag{86}$$

and

$$a_{10} = - \frac{1}{2} \frac{\overline{a}^2}{Q^3} \frac{K_3(1/Q^2)}{K_2(1/Q^2)} a_{12}. \tag{87}$$

The function $\overline{\Pi}_1$ is, therefore, given by

$$\overline{\Pi}_1(\overline{t}, \overline{\mathbf{q}}) = - \frac{\dot{\overline{a}}}{\overline{a}} \frac{1}{2\overline{a}^2} \left(\overline{\mathbf{q}}^2 - \frac{\overline{a}^2}{Q^3} \frac{K_3(1/Q^2)}{K_2(1/Q^2)} \right) \overline{\Pi}_0(\overline{t}, \overline{\mathbf{q}}). \tag{88}$$

V. CONCLUSION

In this article, the construction of the relativistic Ornstein–Uhlenbeck process has been extended from flat to curved space–time. The general relativistic Ornstein–Uhlenbeck process has been defined through a manifestly covariant Kolmogorov equation. This transport equation fixes the space–time evolution of the scalar one-particle distribution function defined over the relativistic eight-dimensional extended phase-space. Given an arbitrary coordinate system in space–time, the manifestly covariant Kolmogorov equation can be transcribed into a more conventional transport equation which fixes the time-evolution of the usual one particle distribution function, defined at any instant over the standard six-dimensional phase-space.

As a simple application, both transport equations have been explicitly written down in a spatially flat Friedmann–Robertson–Walker universe and the corresponding stochastic equations of motion have also been derived. At least for a spatially flat Friedmann–Robertson–Walker model, there is a unique natural generalization of the flat space–time equilibrium Jüttner distribution. In comoving coordinates, this generalized equilibrium solution is independent of the space coordinates and isotropic in 3-momentum space. It has been proven that this solution can be obtained perturbatively as a series expansion where the small parameter is the ratio of the characteristic ''microscopic'' relaxation-time of the diffusion process (in flat space–time) to the characteristic evolution-time of the expansion factor of the universe. The first order correction to the Jüttner distribution has also been obtained explicitly.

Let me now put these results into perspective by comparing them with what is known about the solutions to the other transport equation which has been studied extensively in curved space–time, i.e., the general relativistic Boltzmann equation.

Quite expectedly, this equation has also been studied in spatially flat Friedmann–Robertson–Walker space–times.[19] There is naturally no time-independent equilibrium solution and, therefore, only generalized equilibriums similar to those discussed in the present article may exist. No exact calculation of such solutions is possible, just as no exact expression can be obtained for the solutions to (56).

As has been done in this article, approximate expressions for generalized equilibrium solutions (to Boltzmann equation) have been searched for in situations where the expansion factor $a(t)$ is a slowly varying function of time, i.e., when the expansion factor varies only on time scales much larger than the characteristic time associated to the collisions between particles.

But, for Boltzmann equation, only the first correction to Jüttner's distribution seems to have been considered and evaluated.[19] In particular, no general expansion like (69) has ever been proven to exist, nor has the unicity of the solution ever been examined, let alone been proven.

I would like now to end this article by mentioning some of its many possible extensions. On the technical side, the proof of the existence of a generalized equilibrium distribution for the general relativistic Ornstein–Uhlenbeck process should be extended to the other Friedmann–Robertson–Walker metrics and, possibly, to more general curved space–times. For example, are there generalized equilibrium distributions for particles diffusing in a fluid orbiting a black-hole?

At least in cases where a generalized equilibrium solution exists, one should be able to construct a conditional entropy 4-current for the process (the entropy 4-current for the process in flat space–time has already been obtained in Ref. 8). The exact physical interpretation of a conditional entropy (as opposed to the Boltzmann–Gibbes entropy) is still a matter of debate, even for Galilean stochastic processes (a good introductory dicussion can be found in Ref. 21); determining a reasonable interpretation of a conditional entropy 4-current in curved space–time will certainly not be straightforward either and may involve addressing the possibility of applying the very concept of entropy to the space–time itself (see Refs. 12 and 22 for a discussion of this issue in the context of nonquantum gravitation and Ref. 23 for a pedagogical presentation of the superstrings approach to black-holes thermodynamics).

In another direction, the Chapman–Enskog procedure will also permit the large-scale study of the diffusion process in situations close to the generalized equilibrium configurations and, thus, contribute to a better understanding of the relationship between hydrodynamics and statistical physics (kinetic theory) in the presence of a gravitational field.

Finally, it has already been mentioned that the curved space–time diffusion process presented in this article is only one of the possible extensions of the special relativistic Ornstein–Uhlenbeck process. It is certainly the simplest and most natural one, but this does not make other extensions uninteresting. In particular, one can wonder how a curvature-dependent form of the friction coefficient or of the amplitude of the noise would change the properties of the process. This will also be investigated in forthcoming articles.

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Spherical harmonics and basic coupling coefficients for the group SO(5) in an SO(3) basis

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An easily programmable algorithm is given for the computation of SO(5) spherical harmonics needed to complement the radial (beta) wave functions to form an orthonormal basis of wave functions for the five-dimensional harmonic oscillator. It is shown how these functions can be used to compute the (Clebsch–Gordan a.k.a. Wigner) coupling coefficients for combining pairs of irreps in this space to other irreps. This is of particular value for the construction of the matrices of Hamiltonians and transition operators that arise in applications of nuclear collective models. Tables of the most useful coupling coefficients are given in the Appendix. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763004]

I. INTRODUCTION

The group SO(5) is used as a dynamical group in several contexts in nuclear physics and elsewhere. For example, in an SO(3) basis, it plays a central role in the classification of states of the nuclear collective model[1–3] and the Interacting Boson Model;[4] in an $SO(4)\cong SU(2)\times SU(2)$ basis, it is also used in a neutron–proton pairing model[5] and in a model of high temperature superconductivity.[6,7] In application of such models, there is a need for SO(5) spherical harmonics as basis wave functions and SO(5) Clebsch–Gordan (CG) coefficients for the calculation of matrix elements of the various tensor operators that appear. Many SO(5) coupling coefficients have been given in an SO(4) basis[8] and in a U(2) basis.[9] In this paper, we construct them in an SO(3) (angular momentum) basis.

It will be recalled that standard SO(3) spherical harmonics are eigenfunctions of the Laplacian on a two-dimensional sphere S_2. The geometry of S_2 is inferred by regarding it as an SO(3) orbit in the real three-dimensional Euclidean space $\mathbb{R}^3$ generated by rotating a point in this space through all possible angles. Because a point on such a sphere is invariant under SO(2) rotations about the radial line through that point, it follows that a sphere is isomorphic to the factor space SO(3)/SO(2). SO(3) spherical harmonics are also an orthonormal basis of functions for the Hilbert space $\mathcal{L}^2(S_2)\simeq\mathcal{L}^2(\mathrm{SO}(3)/\mathrm{SO}(2))$ of square integrable functions on S_2 relative to the SO(3)-invariant measure; the invariant measure assigns a *volume* to an element on S_2 equal to its area on a sphere of unit radius. It is known from the Peter–Weyl theorem that a complete orthonormal basis of functions on the group SO(3), relative to its invariant measure, is given to within norm factors by Wigner functions $\{\mathcal{D}^l_{mn}\}$, i.e., matrix coefficient functions on SO(3) defined in terms of basis states $\{|lm\rangle, m=-l,\ldots,l\}$ for an SO(3) irrep $\hat{R}^l$ of highest weight l by

$$\mathcal{D}^l_{mn}(\Omega)=\langle lm|\hat{R}^l(\Omega)|ln\rangle\,,\quad \Omega\in\mathrm{SO}(3)\,. \tag{1}$$

It follows that an (unnormalized) basis of functions for $\mathcal{L}^2(\mathrm{SO}(3)/\mathrm{SO}(2))$ is given by reducing the set of functions $\{\mathcal{D}^l_{mn}\}$ to the subset $\{\mathcal{D}^l_{m0}\}$ of well-defined functions on the SO(3)/SO(2) coset space. Standard spherical harmonics are normalized and conventionally defined as the complex conjugates of these functions

$$Y_{lm}(\theta,\varphi)=\sqrt{\frac{2l+1}{4\pi}}(\mathcal{D}^{l}_{m0}(\Omega(\theta,\varphi)))^{*}=\sqrt{\frac{2l+1}{4\pi}}\mathcal{D}^{l}_{0m}(\Omega^{-1}(\theta,\varphi)), \tag{2}$$

where $\Omega(\theta,\varphi)$ denotes a group element, defined to within an SO(3)/SO(2) coset, by a pair of spherical coordinates (θ,φ) for the sphere. This identity shows that there is a set of spherical harmonics $\{Y_{lm}, m=-l,\ldots,l\}$ associated with every SO(3) irrep and that they are given by the matrix coefficient (Wigner) functions for these irreps.

SO(5) spherical harmonics are similarly defined. They are eigenfunctions of the Laplacian on the four-sphere and an orthonormal basis of functions for the Hilbert space $\mathcal{L}^2(S_4)$ relative to the SO(5)-invariant measure. A four-sphere is isomorophic to the surface generated by rotating a point about the origin in a real five-dimensional Euclidean space $\mathbb{R}^5$ with all elements of the SO(5) rotation group. Since any point in $\mathbb{R}^5$ remains unchanged under the subgroup $\mathrm{SO}(4)\subset\mathrm{SO}(5)$ of rotations about the radial line through the point, such a four-sphere is isomorphic to the factor space SO(5)/SO(4). Moreover, the SO(5)-invariant measure on such a four-sphere is given by the area of elements on a four-sphere of unit radius as defined by the Euclidean measure of volumes in $\mathbb{R}^5$.

The above observations imply that SO(5) spherical harmonics can be defined, in a generalization of Eq. (1) to SO(5), in terms of a subset of Wigner functions. However, there are two differences. First, only a subset of SO(5) irreps are needed to define SO(5) spherical harmonics, namely those carried by subspaces of the Hilbert space $\mathcal{L}^2(\mathbb{R}^5)$ of the five-dimensional harmonic oscillator. Second, the Wigner functions for these SO(5) irreps are not known in analytical form. Thus, we construct SO(5) spherical harmonics by a simple algorithm that could also be used for standard spherical harmonics if one did not already have analytical expressions for the SO(3) rotation matrices. The algorithm is based on the observation that the spherical harmonics of the fundamental five-dimensional irrep of SO(5) are simple and known. We then observe that any product of bounded functions in $\mathcal{L}^2(S_4)$ is another function in $\mathcal{L}^2(S_4)$. Thus they are readily used to generate a basis for $\mathcal{L}^2(S_4)$. Given the inner product, it is then straightforward to Gram–Schmidt orthonormalize this basis to obtain the spherical harmonics.

Spherical harmonics for SO(5) were computed by Bès,[10] for values of the angular momentum $L=0,\ldots,6$, by solving the Schrödinger equation

$$\hat{\Lambda}\Psi_{v\alpha LM}=v(v+3)\Psi_{v\alpha LM} \tag{3}$$

for $\hat{\Lambda}$, the SO(5) Casimir operator, as a system of coupled differential equations, where v labels a so-called one-row irrep of type $[v,0]$ of SO(5), L and M are angular momentum quantum numbers and α is a multiplicity label; v is referred to as a *seniority* quantum number (a terminology introduced by Racah in atomic physics). Unfortunately, this approach becomes prohibitively complicated for $L>6$ because of the number of coupled equations.[10]

An algorithm for constructing a basis for the five-dimensional harmonic oscillator as products of radial (beta) wave functions and SO(5) spherical harmonics, was given by Chacón, Moshinsky, and Sharp[11] and used in many nuclear collective model calculations.[12] The construction of SO(5) spherical harmonics presented herein has substantial overlap with the CMS approach. However, by restricting the calculations to $\mathcal{L}^2(S_4)$, as opposed to the five-dimensional harmonic oscillator Hilbert space, much of the complexity of the CMS approach is avoided. As a result, the construction becomes simple and more versatile. The methods used here were initiated in some recent collective model calculations.[3] As shown in the following, they provide an efficient algorithm for computing the CG coefficients needed for SO(5) tensor coupling in the space of the five-dimensional harmonic oscillator.

II. THE FOUR-SPHERE AS A SUBMANIFOLD OF $\mathbb{R}^5$

The five-dimensional vector space $\mathbb{R}^5$ can be given many physical interpretations. For present purposes, it is convenient to think of an element $Q\in\mathbb{R}^5$ as the quadrupole tensor of a distribution

of particles in $\mathbb{R}^3$. Q is then realized as a real 3×3 traceless symmetric matrix. The independent entries $\{Q_{ij}\}$ of Q can be considered its components relative to nonorthogonal axes and its length $\|Q\|$ conveniently defined by

$$\|Q\|^2=\mathrm{Tr}(Q^2)=\sum_{ij} Q_{ij}^2 . \tag{4}$$

Thus, the four-sphere S_4 is identified with the set of 3×3 real symmetric matrices that satisfy the constraints

$$\mathrm{Tr}(Q)=0 , \quad \mathrm{Tr}(Q^2)=1 . \tag{5}$$

Convenient coordinates for S_4 are constructed by use of various SO(5) subgroup actions. The group SO(5) is itself the subgroup of SL(5,$\mathbb{R}$) transformations of $\mathbb{R}^5$ that leave the lengths of vectors, i.e., $\mathrm{Tr}(Q^2)$, invariant. The group SO(3) also has a natural action on $\mathbb{R}^5$ in which an element $\Omega\in\mathrm{SO}(3)$ transforms a matrix Q into the matrix $\Omega Q\Omega^{-1}$. This SO(3) action is observed to leave both $\mathrm{Tr}(Q^2)$ and $\mathrm{Tr}(Q^3)$ invariant. Thus, SO(3) is identified with the subgroup of SO(5) that leaves $\mathrm{Tr}(Q^3)$ invariant. It is realized as a subset of SO(5) matrices by the $L=2$ irrep $\mathcal{D}^2$ [cf. Eq. (8)]. Note that this particular SO(3) subgroup is distinct from the $\mathrm{SO}(3)\subset\mathrm{SO}(4)\subset\mathrm{SO}(5)$ subgroup.

Any matrix $Q\in\mathbb{R}^5$ can be brought to diagonal form by some SO(3) transformation. Conversely, any $Q\in\mathbb{R}^5$ can be expressed in the form

$$Q=\Omega^{-1}\overline{Q}\Omega \tag{6}$$

for some diagonal matrix $\overline{Q}$ and some element $\Omega\in\mathrm{SO}(3)$. Thus, a set of coordinates for a point $Q\in S_4$ is given by a triple of coordinates (e.g., Euler angles) for the SO(3) rotation Ω and another coordinate γ that defines the diagonal matrix $\overline{Q}$ [subject to the two constraints of Eq. (5)].

A coordinate system for S_4 extends immediately to a system of spherical polar coordinates for $\mathbb{R}^5$ by the addition of the radial coordinate $\beta=\|Q\|\equiv\sqrt{\mathrm{Tr}(Q^2)}$. Such coordinates are related to the standard spherical components for a quadrupole tensor Q given in terms of the matrix entries $\{Q_{ij}\}$ by

$$q_0=\frac{1}{\sqrt{6}}(2Q_{33}-Q_{11}-Q_{22}) ,$$

$$q_{\pm 1}=\mp(Q_{31}\pm iQ_{32}) ,$$

$$q_{\pm 2}=\tfrac{1}{2}(Q_{11}-Q_{22}\pm 2iQ_{12}) . \tag{7}$$

These spherical functions of q transform under SO(3) in the same way as $L=2$ spherical harmonics, i.e.,

$$\hat{R}(\Omega)q_\nu=\sum_\mu q_\mu\mathcal{D}^2_{\mu\nu}(\Omega) . \tag{8}$$

Now, the spherical components of a diagonal matrix $\overline{Q}$ are given by

$$\overline{q}_0=\frac{1}{\sqrt{6}}(2\overline{Q}_{33}-\overline{Q}_{11}-\overline{Q}_{22}) , \quad \overline{q}_{\pm 1}=0 , \quad \overline{q}_{\pm 2}=\frac{1}{2}(\overline{Q}_{11}-\overline{Q}_{22}) , \tag{9}$$

with $\mathrm{Tr}(Q)=\overline{Q}_{11}+\overline{Q}_{22}+\overline{Q}_{33}=0$. Thus, if $\|q\|=\|Q\|=\beta$, then

$$\|q\|^2=\sum_{\nu}(-1)^{\nu}q_{\nu}q_{-\nu}\equiv \mathrm{Tr}(Q^2)=\overline{q_0^2}+2\overline{q_2^2}=\beta^2\,. \tag{10}$$

This means that $\overline{q_\nu}$ can be expressed

$$\overline{q_\nu}=\delta_{\nu,0}\beta\cos\gamma+\delta_{\nu,\pm 2}\frac{1}{\sqrt{2}}\beta\sin\gamma\,. \tag{11}$$

The functions $\{q_\nu\}$ are then given in terms of (β,γ,Ω) by

$$q_\nu(\beta,\gamma,\Omega)=\hat{R}(\Omega)\overline{q_\nu}=\beta\cos\gamma\,\mathcal{D}^2_{0\nu}(\Omega)+\frac{1}{\sqrt{2}}\beta\sin\gamma\,(\mathcal{D}^2_{2\nu}(\Omega)+\mathcal{D}^2_{-2\nu}(\Omega))\,. \tag{12}$$

This is a standard expression for the spherical components of a quadrupole tensor in the nuclear collective model.[1]

For present purposes, the restriction of these functions to S_4, i.e., fixing $\beta=1$, gives the set of functions

$$\mathcal{Q}_\nu(\gamma,\Omega)=\cos\gamma\,\mathcal{D}^2_{0\nu}(\Omega)+\frac{1}{\sqrt{2}}\sin\gamma\,(\mathcal{D}^2_{2\nu}(\Omega)+\mathcal{D}^2_{-2\nu}(\Omega))\,, \tag{13}$$

which are both a basis for the fundamental five-dimensional $v=1$ irrep of SO(5) and of the five-dimensional $L=2$ irrep of its SO(3) subgroup. Thus, to within a normalization factor, they are the fundamental SO(5) spherical harmonics in an SO(3) basis.

The Laplacian on $\mathbb{R}^5$ has a well-known expression[1] in terms of the above spherical polar coordinates

$$\nabla^2=\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}-\frac{1}{\beta^2}\hat{\Lambda}\,, \tag{14}$$

where

$$\hat{\Lambda}=-\frac{1}{\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma}+\sum_{k=1}^{3}\frac{\overline{L_k^2}}{4\sin^2(\gamma-2\pi k/3)} \tag{15}$$

is a realization of the (second order) SO(5) Casimir for the irreps carried by $\mathcal{L}^2(S_4)$ and $\{\overline{L_1},\overline{L_2},\overline{L_3}\}$ are three components of SO(3) angular momentum in the so-called *intrinsic frame*, i.e., the frame in which the quadrupole components have values

$$\overline{\mathcal{Q}_\nu}=\cos\gamma\,\delta_{\nu 0}+\frac{1}{\sqrt{2}}\sin\gamma\,(\delta_{\nu 2}+\delta_{\nu,-2})\,. \tag{16}$$

The volume element for $\mathbb{R}^5$ is given by

$$\mathrm{d}v(\beta,\gamma,\Omega)=\beta^4\,\mathrm{d}\beta\,\mathrm{d}v(\gamma,\Omega) \tag{17}$$

(Refs. 1, 2), where

$$\mathrm{d}v(\gamma,\Omega)=\sin 3\gamma\,\mathrm{d}\gamma\,\mathrm{d}\Omega \tag{18}$$

is the SO(5)-invariant measure on S_4 and $\mathrm{d}\Omega$ is the SO(3)-invariant measure. Note, however, that the range of γ is restricted to $0\leqslant\gamma\leqslant\pi/3$ because of the equivalence of the coordinates

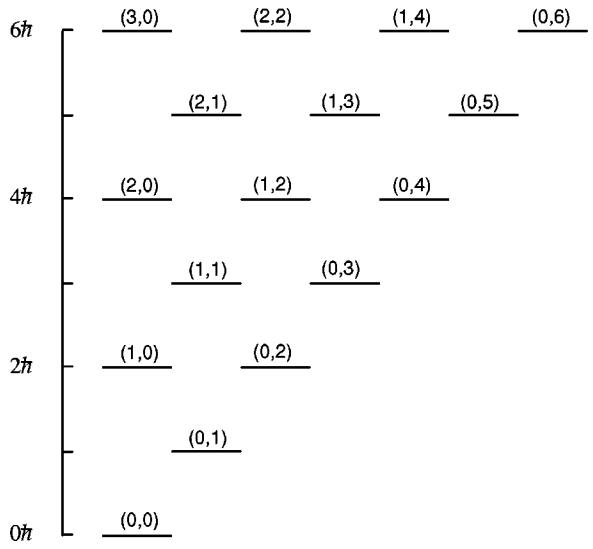

FIG. 1. The energy-level spectrum of the five-dimensional harmonic oscillator with levels labeled by (n,v), where n is the radial (beta) quantum number and v labels an SO(5) irrep of highest weight $[v,0]$. Each level shown represents a multiplet of states that span an SO(5) irrep. Each SO(5) $[v,0]$ irrep is reproduced an infinite number of times at energy intervals of $2\hbar\omega$. The states of a column of SO(5) irreps span an infinite-dimensional $\mathrm{SU}(1,1)\times\mathrm{SO}(5)$ irrep.

$$\pm\gamma, \quad \pm\gamma+2\pi/3, \quad \pm\gamma-2\pi/3, \tag{19}$$

as shown in Ref. 2 (p. 678).

III. THE HILBERT SPACE $\mathcal{L}^2(S_4)$

Observation: The Hilbert space $\mathcal{L}^2(S_4)$ is the carrier space for a direct sum of SO(5) irreps of highest weight $[v,0]$ with v running over the non-negative integers.

This observation is inferrred by a ''separation of variables'' technique, decomposing $\mathbb{R}^5$ into radial and spherical components.

The harmonic oscillator Hamiltonian spectrum comprises sets of energy levels of energy $n\hbar\omega$ with n taking all non-negative integer values. The states of each energy level span a U(5) irrep of highest weight $\{n\}\equiv\{n,0,0,0,0\}$ each of which restricts to a direct sum of $\mathrm{SO}(5)\subset\mathrm{U}(5)$ irreps given by the branching rule

$$\{n\}\downarrow[n,0]\oplus[n-2,0]\oplus[n-4,0]\oplus\cdots\oplus[1,0] \quad \text{or} \quad [0,0], \tag{20}$$

where $[v_1,v_2]$ labels an SO(5) irrep by its highest weight. The decomposition of the Hilbert space $\mathcal{L}^2(\mathbb{R}^5)$ into energy eigenspaces of the five-dimensional harmonic oscillator is illustrated schematically in Fig. 1. It is seen that only the so-called one-row SO(5) irreps of type $[v,0]$ occur in $\mathcal{L}^2(\mathbb{R}^5)$. However, each $[v,0]$ irrep occurs repeatedly at $2\hbar\omega$ intervals to form a column of such irreps. Because the volume element (17) is a product of a volume element $\beta^4\,\mathrm{d}\beta$ for $\mathbb{R}^+$ and a volume element $\mathrm{d}v(\gamma,\Omega)$ for S_4, it follows that $\mathcal{L}^2(\mathbb{R}^5)\simeq\mathcal{L}^2(\mathbb{R}^+\times S_4)$ is the tensor product space $\mathcal{L}^2(\mathbb{R}^+)\otimes\mathcal{L}^2(S_4)$. It also follows that the Hilbert space $\mathcal{L}^2(\mathbb{R}^5)$ is a direct sum of irreducible $\mathrm{SU}(1,1)\times\mathrm{SO}(5)$ subspaces. In fact, it is known from invariant theory[13,14] that the decomposition of $\mathcal{L}^2(\mathbb{R}^5)$ into $\mathrm{SU}(1,1)\times\mathrm{SO}(5)$ irreducible subspaces is multiplicity free. Complete sets of irreducible SO(5) subspaces are given by the eigenspaces of the energy levels shown in Fig. 1. They are shown with all states belonging to equivalent SO(5) irreps in the same column. Thus, the states of each column of SO(5) irreps span an irrep of the direct product group SU(1,1)

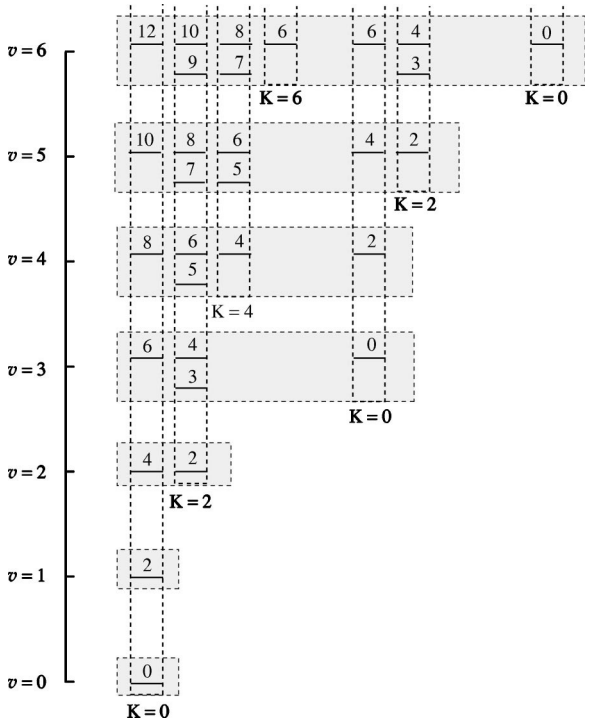

FIG. 2. The spectrum of SO(3) (angular momentum) irreps for $\mathcal{L}^2(S_4)$ put into sequences of K bands. The SO(3) irreps are labeled by their angular momenta L. Angular momentum irreps belonging to a common SO(5) irrep are put into a common shaded area.

$\times$SO(5). It is seen that every SO(5) irrep $[v,0]$ with v taking a non-negative integer value gives rise to a column. It follows that $\mathcal{L}^2(S_4)$ contains each SO(5) irrep $[v,0]$ just once, as claimed in the observation.

The decomposition of $\mathcal{L}^2(S_4)$ into SO(3) subspaces is inferred from the SO(5)$\downarrow$SO(3) branching rules, given for the one-row irreps by Kemmer *et al.*[15] who show that an irrep $[v,0]$ of SO(5) restricts to a direct sum of SO(3) irreps of angular momentum L given by

$$L = 2k, \quad 2k-2, \quad 2k-3, \quad 2k-4, \quad \ldots, \quad k$$

$$k = v, \quad v-3, \quad v-6, \quad \ldots, \quad k_{\min}, \tag{21}$$

where $k_{\min}=0$, 1, or 2.

The angular momentum states contained in the $v=0,\ldots,6$ irreps are shown in Fig. 2. It is seen that they fall into sequences of bands that can be characterized by the value K of the lowest angular momentum of each band. The band structure follows a recognizable pattern. A sequence of $K=0,2,4,6,\ldots$ bands appear with lowest states at intervals of $v=2$ with each band comprising a sequence of angular momentum states

$$L = 0,2,4,6,\ldots \quad \text{for } K=0,$$

$$L = K, K+1, K+2, K+3,\ldots \quad \text{for } K>0. \tag{22}$$

This sequence is then repeated at intervals of $v=3$. Such K bands are familiar in the context of rotor models. However, in the present context, K should simply be regarded as a convenient label for a set of basis wave functions.

We proceed to the construction of basis wave functions for $\mathcal{L}^2(S_4)$. First recall that the five quadrupole moments $\{\mathcal{Q}_\nu\}$ of Eq. (13), regarded as functions on S_4, provide a basis for a realization of the fundamental $v=1$ irrep of SO(5). From the observation that products of bounded square-integrable functions on S_4 are also square integrable functions on S_4 it follows that $\mathcal{L}^2(S_4)$ is spanned by polynomials in the $\{\mathcal{Q}_\nu\}$ coordinates with the understanding that $\|\mathcal{Q}\|^2 = \Sigma_\nu(-1)^\nu \mathcal{Q}_\nu \mathcal{Q}_{-\nu}=1$.

It can be seen, by inspection of Fig. 2, that the subspace of highest-weight SO(3) states in $\mathcal{L}^2(S_4)$; i.e., the space spanned by $M=L$ polynomials, is spanned by the polynomials

$$\Phi_{tKL}=\Phi(n)\equiv[\Phi_{002}]^{n_1}[\Phi_{022}]^{n_2}[\Phi_{100}]^{n_3}[\Phi_{023}]^{n_4}, \tag{23}$$

where $n=[n_1,n_2,n_3,n_4]$ is a quartet of non-negative integers,

$$\Phi_{002}\propto \mathcal{Q}_2\,, \tag{24}$$

$$\Phi_{022}\propto[\mathcal{Q}\otimes\mathcal{Q}]_{22}\,, \tag{25}$$

$$\Phi_{100}\propto[\mathcal{Q}\otimes\mathcal{Q}\otimes\mathcal{Q}]_{0}\,, \tag{26}$$

$$\Phi_{023}\propto[\mathcal{Q}\otimes\mathcal{Q}\otimes\mathcal{Q}]_{33}\,, \tag{27}$$

and

$$t=n_3,\quad K=2n_2+2n_4,\quad L=2n_1+2n_2+3n_4,\quad n_4=0 \text{ or } 1\,. \tag{28}$$

The square brackets in these equations indicate standard SO(3) angular-momentum coupling; i.e.,

$$[\mathcal{Q}\otimes\mathcal{Q}]_{LM}=\sum_{\mu\nu}(2,\nu,2,\mu|LM)\mathcal{Q}_\mu\mathcal{Q}_\nu\,, \tag{29}$$

where $(2,\nu,2,\mu|LM)$ is an SO(3) CG coefficient.

The polynomials $\{\Phi_{tKL}\}$ can be put into one-to-one correspondence with the SO(3) irreps depicted in Fig. 2. Note that each SO(3) irrep of angular momentum L corresponds to a single state in the subspace of highest-weight $M=L$ states. A moment's reflection on this correspondence and the shifts induced by each of the generator functions indicates what the indices n_i and the labels t and K mean. The lowest SO(3) irrep corresponds to the $(t=K=L=0)$ unit function for which $n_1=n_2=n_3=n_4=0$; at this point, we are not concerned with normalizations or even orthogonality of wave functions—merely with the construction of a basis. The function Φ_{002} is the basis function identified with the lowest $K=0$, $L=2$ irrep of Fig. 2. Thus, the set $\{[\Phi_{002}]^{n_1}\}$ corresponds to the sequence of $\{L=2n_1\}$ angular momenta irreps of the $K=0$ band and, in general, Φ_{002} is a $\Delta K=0$, $\Delta L=2$ shift operator on the Φ basis functions. Similarly, it is seen that Φ_{022} is a $\Delta K=2$, $\Delta L=2$ shift operator and Φ_{023} is a $\Delta K=2$, $\Delta L=3$ shift operator. Finally, Φ_{100} is a $\Delta t=1$, $\Delta K=\Delta L=0$ shift operator. A basis function Φ_{tKL} is assigned an index $t=i-1$ when it appears in the ith occurrence of the K band (e.g., $t=0$ for irreps of the lowest $K=0$ band and $t=1$ for irreps of the first excited $K=0$ band). Thus, t is the number of Φ_{100} zero-coupled triplets in parallel with a corresponding index in Ref. 11. It is stressed, however, that neither t nor K is a good quantum number because the Φ_{tKL} basis functions do not form an orthogonal set.

The generator functions and, hence, the complete set of basis functions $\{\Phi_{tKL}\}$ are conveniently expressed in the form

$$\Phi_{tKL}(\gamma,\Omega)=\sum_{\kappa\geqslant 0}^{\text{even}} F^n_\kappa(\gamma)\sqrt{\frac{2L+1}{16\pi^2(1+\delta_{\kappa 0})}}[\mathcal{D}^L_{\kappa L}(\Omega)+(-1)^L\mathcal{D}^L_{-\kappa L}(\Omega)]. \tag{30}$$

For the generator functions, the $\{F^n_\kappa\}$ functions are

$$F_0^{[1000]}(\gamma)=\cos\gamma\,,\quad F_2^{[1000]}(\gamma)=\sin\gamma\,, \tag{31}$$

$$F_0^{[0100]}(\gamma)=\cos 2\gamma\,,\quad F_2^{[0100]}(\gamma)=-\sin 2\gamma\,, \tag{32}$$

$$F_0^{[0010]}(\gamma)=\cos 3\gamma\,, \tag{33}$$

$$F_0^{[0001]}(\gamma)=0\,,\quad F_2^{[0001]}(\gamma)=\sin 3\gamma\,. \tag{34}$$

From the observation that

$$\mathcal{D}^{L_2}_{\kappa_2 L_2}(\Omega)\mathcal{D}^{L_1}_{\kappa_1 L_1}(\Omega)=\sum_{\kappa}\,(L_1\kappa_1,L_2\kappa_2|L\kappa)\,\mathcal{D}^{L}_{\kappa L}(\Omega)\,, \tag{35}$$

with $L=L_1+L_2$, it is now easy to build up the complete $\{\Phi_{tKL}\}$ basis, for the $M=L$ subspace, defined by F^n_κ functions in the form

$$F^n_\kappa(\gamma)=\sum_{i=0}^{n_1}\sum_{j=0}^{n_2} f^n_{ij\kappa}\,(\cos\gamma)^{n_1-i}\,(\sin\gamma)^i\,(\cos 2\gamma)^{n_2-j}\,(\sin 2\gamma)^j\,(\cos 3\gamma)^{n_3}\,(\sin 3\gamma)^{n_4}\,. \tag{36}$$

The overlaps and norms of basis wave functions, expressed in the form (30), are given by

$$\langle\Phi_{tKL}|\Phi_{t'K'L'}\rangle=\delta_{LL'}\sum_{\kappa\geqslant 0}^{\text{even}}\int_0^{\pi/3}F^n_\kappa(\gamma)F^{n'}_\kappa(\gamma)\sin 3\gamma\,\mathrm{d}\gamma\,. \tag{37}$$

These integrals can be carried out analytically, in the monomial basis given by Eq. (36), with the help of a computer to keep track of the coefficients. Thus, the overlaps of the basis wave functions can be computed in exact arithmetic using one of the several algebraic computer programs available; the present calculations were done with MAPLE.

IV. COMPUTATION OF SO(5) SPHERICAL HARMONICS

Having determined the overlaps of the above-defined basis functions $\{\Phi(n)\}$, it is is now a routine procedure to transform them to an orthonormal basis of SO(5) spherical harmonics.

The important observations are (i) that a polynomial $\Phi(n)$ is a linear combination of spherical harmonics of seniority $v\leqslant N$, where $N=n_1+2n_2+3n_3+3n_4$ and (ii) that q-parity is invariant under SO(5) transformations, where a polynomial is said to have even or odd q-parity if the polynomial is, respectively, of even or odd degree in $\{q_\nu\}$. As a consequence of these observations, the $\{\Phi(n)\}$ basis has a natural ordering and is readily transformed to an orthonormal (spherical harmonic) basis $\{\Psi_{v\alpha L}\}$ by a sequential Gram–Schmidt orthonormalization; α is a multiplicity index.

The first step is to identify which among the first of a specified number of states of a given angular momentum L have even q-parity (Π) and which odd. It is determined, for example, that for the first 12 states of $L=7$

$$\Pi(L_i)=\begin{cases}\text{even} & \text{for } i=2,4,6,8,10,12\\ \text{odd} & \text{for } i=1,3,5,7,9,11.\end{cases} \tag{38}$$

The next step is to identify the $n=[n_1,n_2,n_3,n_4]$ indices and the basis wave functions associated with these states. It is determined, for example, that $n=[2,0,0,1]$ for the state 7_1 (the first $L=7$ state) and $n=[0,2,0,1]$ for the next 7_3 odd-parity state and that the corresponding basis wave functions are given, in terms of their $[F^n_0,F^n_2,\ldots]$ functions, by

$$\Phi([2,0,0,1]) \sim \Big[0,\ 6\sqrt{\frac{3}{1001}}\sin 3\gamma\cos^2\gamma + \frac{1}{2}\sqrt{\frac{3}{1001}}\sin^2\gamma\sin 3\gamma,$$
$$3\sqrt{\frac{2}{91}}\cos\gamma\sin\gamma\sin 3\gamma, \frac{1}{2}\sqrt{\frac{3}{7}}\sin^2\gamma\sin 3\gamma\Big], \tag{39}$$

$$\Phi([0,2,0,1]) \sim \Big[0,\ 6\sqrt{\frac{3}{1001}}\sin 3\gamma\cos^2 2\gamma + \frac{1}{2}\sqrt{\frac{3}{1001}}\sin^2 2\gamma\sin 3\gamma,$$
$$-3\sqrt{\frac{2}{91}}\cos 2\gamma\sin 2\gamma\sin 3\gamma, \frac{1}{2}\sqrt{\frac{3}{7}}\sin^2 2\gamma\sin 3\gamma\Big].$$

The overlap matrix for these wave functions is next determined and from it the Gram–Schmidt transformation to an orthonormal basis of spherical harmonics. For the above two $L=7$ states one obtains the Gram–Schmidt transformation in the form

$$\left[\left[\frac{48}{1001}, \frac{304}{6825}\right], \quad \begin{bmatrix} 1 & 0 \\ -\frac{4}{15} & 1 \end{bmatrix}\right], \tag{40}$$

where the first vector gives the squared norms of the orthogonalized vectors, and the matrix that follows is the transformation from the Φ functions to an orthogonal set. Thus the first two $L=7$ spherical harmonics, $\Psi_{v\alpha L}$, which, from Fig. 2, are seen to have seniority $v=5$ and 7, respectively, are given by

$$\Psi_{5,1,7} = \sqrt{\frac{1001}{48}}\Phi([2,0,0,1]), \quad \Psi_{7,1,7} = \sqrt{\frac{6825}{304}}\left(\Phi([0,2,0,1]) - \frac{4}{15}\Phi([2,0,0,1])\right). \tag{41}$$

Note that the multiplicity index α is restricted to 1 for $L=7$ because all states of $L=7$ are multiplicity free.

V. SO(5) CLEBSCH–GORDAN COEFFICIENTS

Given SO(5) spherical harmonics $\{\Psi_{v\alpha L}\}$ in an SO(3) basis, the Clebsch–Gordan coefficients of type $(v_1\alpha_1 L_1, v_2\alpha_2 L_2 \| v_3\alpha_3 L_3)$ are obtained by simply evaluating the overlap integrals

$$\int \Psi^*_{v_3\alpha_3 L_3 M_3}(\gamma,\Omega)\,[\Psi_{v_2\alpha_2 L_2}(\gamma,\Omega)\otimes\Psi_{v_1\alpha_1 L_1}(\gamma,\Omega)]_{L_3 M_3}\sin 3\gamma\,\mathrm{d}\gamma\,\mathrm{d}\Omega$$
$$= \langle v_3\|\hat{\Psi}_{v_2}\|v_1\rangle\,(v_1\alpha_1 L_1, v_2\alpha_2 L_2\|v_3\alpha_3 L_3), \tag{42}$$

where $\hat{\Psi}_{v_2}$ is interpreted as a tensor operator whose components act on other wave functions by simple multiplication, i.e.,

$$[\hat{\Psi}_{v_2\alpha_2 L_2 M_2}\Psi_{v_1\alpha_1 L_1 M_1}](\gamma,\Omega) = \Psi_{v_2\alpha_2 L_2 M_2}(\gamma,\Omega)\Psi_{v_1\alpha_1 L_1 M_1}(\gamma,\Omega). \tag{43}$$

Thus, $\langle v_3\|\hat{\Psi}_{v_2}\|v_1\rangle$ is an SO(5)-reduced matrix element of this operator. The norms and phases of the CG coefficients are here defined by choosing the $\langle v_3\|\hat{\Psi}_{v_2}\|v_1\rangle$ factors to be positive and normalizing the coefficients such that

$$\sum_{\alpha_1 L_1 \alpha_2 L_2} (v_1\alpha_1 L_1, v_2\alpha_2 L_2\|v_3\alpha_3 L_3)^2 = 1. \tag{44}$$

TABLE I. The $(v_1\alpha_1L_1, v_2\alpha_2L_2\|v_3\alpha_3L_3)$ CG coefficients for $v_1=v_2=2$. Note, that the $v=2$ and $v=4$ irreps are multiplicity free so that $\alpha_1=\alpha_2=\alpha_3=1$ in all cases. Cf. the Appendix for an explanation of the notations.

$v_1\cdot L_1$	$v_2\cdot L_2$	4.2	4.4	4.5	4.6	4.8
2.2	2.2	$-\frac{2}{21}\sqrt{66}$	$\frac{1}{63}\sqrt{2145}$	0	0	0
2.4	2.2	$\frac{1}{42}\sqrt{330}$	$\frac{2}{63}\sqrt{78}$	$\frac{1}{2}\sqrt{2}$	$\frac{1}{14}\sqrt{70}$	0
2.2	2.4	$\frac{1}{42}\sqrt{330}$	$\frac{2}{63}\sqrt{78}$	$-\frac{1}{2}\sqrt{2}$	$\frac{1}{14}\sqrt{70}$	0
2.4	2.4	$\frac{2}{21}\sqrt{3}$	$\frac{20}{63}\sqrt{3}$	0	$-\frac{1}{7}\sqrt{14}$	1

Thus, tables of SO(5) CG coefficients are computed by evaluating the integrals of Eq. (42) and multiplying by normalization factors such that Eq. (44) is satisfied. An example of a table of CG coefficients obtained in this way is shown in Table I.

Tables of CG coefficients for $v_1\leqslant 9$ and $v_2=1$ are given in the Appendix. Other coefficients can be obtained from them by use of the following symmetry relations.

VI. PHASES AND SYMMETRY RELATIONS

It follows from the definition given in the first paragraph of Sec. V, that the CG coefficients satisfy the symmetry relation

$$(v_2\alpha_2L_2, v_1\alpha_1L_1\|v_3\alpha_3L_3)=(-1)^{L_1+L_2-L_3}(v_1\alpha_1L_1, v_2\alpha_2L_2\|v_3\alpha_3L_3)\,. \tag{45}$$

They also satisfy the symmetry relation

$$(v_3\alpha_3L_3, v_2\alpha_2L_2\|v_1\alpha_1L_1)=(-1)^{L_1+L_2-L_3}\sqrt{\frac{\dim(v_1)}{\dim(v_3)}\frac{(2L_3+1)}{(2L_1+1)}}(v_1\alpha_1L_1, v_2\alpha_2L_2\|v_3\alpha_3L_3)\,, \tag{46}$$

where $\dim(v)$ is the dimension of the SO(5) irrep of seniority v.

The latter relationship is derived by first using the identity

$$\Psi^*_{v_3\alpha_3L_3M_3}=(-1)^{L_3+M_3}\Psi_{v_3\alpha_3L_3,-M_3}=\sqrt{2L_3+1}\;(L_3M_3,L_3,-M_3|00)\,\Psi_{v_3\alpha_3L_3,-M_3} \tag{47}$$

to rewrite Eq. (42) in the coupled form

$$\frac{1}{\sqrt{2L_3+1}}\int[\Psi_{v_3\alpha_3L_3}(\gamma,\Omega)\otimes\Psi_{v_2\alpha_2L_2}(\gamma,\Omega)\otimes\Psi_{v_1\alpha_1L_1}(\gamma,\Omega)]_0\sin 3\gamma\,d\gamma\,d\Omega$$
$$=\langle v_3\|\|\hat{\Psi}_{v_2}\|\|v_1\rangle\,(v_1\alpha_1L_1, v_2\alpha_2L_2\|v_3\alpha_3L_3)\,. \tag{48}$$

The integrand on the left of this equation can then be reordered to give

$$\langle v_3\|\|\hat{\Psi}_{v_2}\|\|v_1\rangle\,(v_1\alpha_1L_1, v_2\alpha_2L_2\|v_3\alpha_3L_3)$$
$$=(-1)^{L_1+L_2-L_3}\sqrt{\frac{2L_1+1}{2L_3+1}}\langle v_1\|\|\hat{\Psi}_{v_2}\|\|v_3\rangle\,(v_3\alpha_3L_3, v_2\alpha_2L_2\|v_1\alpha_1L_1)\,. \tag{49}$$

Next observe that, if $\{|v\,\nu\rangle\}$ is any complete orthonormal basis for an SO(5) irrep of seniority v, then the unitarity of the CG coefficients implies that

$$\sum_{\nu_1\nu_2\nu_3} (\upsilon_1\nu_1,\upsilon_2\nu_2|\upsilon_3\nu_3)^2 = \dim(\upsilon_3)\,, \tag{50}$$

and, hence, that

$$\sum_{\alpha_1 L_1,\alpha_2 L_2,\alpha_3 L_3} (2L_3+1)(\upsilon_1\alpha_1 L_1,\upsilon_2\alpha_2 L_2\|\upsilon_3\alpha_3 L_3)^2 = \dim(\upsilon_3)\,. \tag{51}$$

Squaring both sides of Eq. (49), and applying this identity, then gives

$$\frac{\langle \upsilon_1\|\|\hat{\Psi}_{\upsilon_2}\|\|\upsilon_3\rangle}{\langle \upsilon_3\|\|\hat{\Psi}_{\upsilon_2}\|\|\upsilon_1\rangle} = \sqrt{\frac{\dim(\upsilon_3)}{\dim(\upsilon_1)}} \tag{52}$$

and the desired result (46).

VII. CONCLUDING REMARKS

Basis wave functions for the irreps of SO(5) can be defined and constructed in many ways. If one is concerned with a particular irrep, then vector coherent state (VCS) methods provide a construction both of an orthonormal basis and the matrix elements of the SO(5) Lie algebra; e.g., Rowe and Hecht[21] gave an algorithm for deriving the so-called one-row irreps and, recently, a construction for the generic SO(5) irreps has been developed by Turner, Rowe, Repka, and Bahri.[22] However, if one needs basis wave functions for many one-row irreps [i.e., SO(5) spherical harmonics], e.g., for nuclear collective model calculations, the more direct method presented above is simpler. This method simplifies that of Chacón *et al.*[11] by restricting the active space to $\mathcal{L}^2(S_4)$ rather than the Hilbert space

$$\mathcal{L}^2(\mathbb{R}^+)\otimes\mathcal{L}^2(S_4) \simeq \mathcal{L}^2(\mathbb{R}^5)\,, \tag{53}$$

where $\mathcal{L}^2(\mathbb{R}^+)$ is the Hilbert space of radial (beta) wave functions; many complications and subtle concepts (like traceless bosons) are thereby avoided.

Clebsch–Gordan coefficients can also be computed in many ways. For complex situations, sophisticated algebraic methods have been developed (cf. Refs. 9, 17–19, and references therein). However, it is possible to compute the coefficients relating one-row irreps of many groups directly from their spherical harmonics in parallel with Wigner's method[20] for SU(2); this is demonstrated above for SO(5). It is generally most useful to generate CG coefficients as they are needed with a program rather than a set of tables. A simple MAPLE code based on the above algorithm has been developed and was used to give the results reported in this paper. A faster routine (using floating point arithmetic) is being prepared[16] and will be made generally available in the near future. Some of the most useful coefficients, from which many others can be derived, are given (in exact arithmetical form) in the Appendix.

Given such CG coefficients, and knowledge of a complete basis of beta wave functions (cf. Ref. 3), it is possible to do many model calculations, e.g., in the Hilbert space $\mathcal{L}^2(\mathbb{R}^5)$ of the five-dimensional harmonic oscillator or in the space of a U(5) or U(6) irrep spanned by wave functions classified by SO(5) quantum numbers. For example, the matrix elements of the infinitesimal generators of SO(5) are easily computed by expressing them as coupled products

$$L_k = -\sqrt{10}\ (d^\dagger\otimes d)_{1k}, \quad O_\nu = -\sqrt{10}\ (d^\dagger\otimes d)_{3\nu}, \tag{54}$$

of the raising and lowering operators $\{d^\dagger_\nu, d_\nu\}$ of the five-dimensional harmonic oscillator. For example, the reduced matrix elements of the octupole tensor O are given by

$$\langle v j L_3 \| O \| v i L_1 \rangle = -\sqrt{70}\ \upsilon \sum_{kL_2} (-1)^{L_1 - L_2} \sqrt{(2L_1+1)(2L_3+1)}\ W(L_1 2 L_3 2; L_2 3)$$
$$\times (\upsilon - 1, k L_2, 12 \| v j L_3)\, (\upsilon - 1, k L_2, 12 \| v i L_1)\,. \tag{55}$$

We have ascertained that this expression gives precisely the same matrix elements, albeit to within a unitary transformation between subsets of states of an irrep having the same angular momentum, as those quoted by Rowe and Hecht.[21] Matrix elements of other bilinear combinations of the d-boson operators within the space of the five-dimensional harmonic oscillator are also easily computed. Morever, because the matrix elements of $L=0$ s-boson operators are well-known, the SO(5) CG coefficients are all that are needed to compute the matrix elements of any bilinear combination of boson operators in the space of the six-dimensional harmonic oscillator.

APPENDIX: TABLES OF BASIC SO(5) CLEBSCH–GORDAN COEFFICIENTS

The following tables give the CG coefficients $(v_1, \alpha_1, L_1; 1,1,2 \| v_3, \alpha_3, L+3)$. The tables are shown in the form in which they are computed. The first two columns give the values of $v_1 \cdot L_1$ and $v_2 \cdot L_2 = 1 \cdot 2$. The subsequent columns are headed by the value of $v_3 \cdot L_3$. The multiplicity indices are not given explicitly. Instead, if a given value of $v \cdot L$ has a multiplicity, it is simply repeated as, for example, for $v \cdot L = 6.6$.

$$\begin{bmatrix} v_1 \cdot L_1 & v_2 \cdot L_2 & 2.2 & 2.4 \\ 1.2 & 1.2 & -1 & 1 \end{bmatrix}$$

$$\begin{bmatrix} v_1 \cdot L_1 & v_2 \cdot L_2 & 3.0 & 3.3 & 3.4 & 3.6 \\ 2.2 & 1.2 & 1 & -\frac{\sqrt{35}}{7} & \frac{\sqrt{231}}{21} & 0 \\ 2.4 & 1.2 & 0 & -\frac{\sqrt{14}}{7} & -\frac{\sqrt{210}}{21} & 1 \end{bmatrix}$$

$$\begin{bmatrix} v_1 \cdot L_1 & v_2 \cdot L_2 & 4.2 & 4.4 & 4.5 & 4.6 & 4.8 \\ 3.0 & 1.2 & \frac{\sqrt{330}}{30} & 0 & 0 & 0 & 0 \\ 3.3 & 1.2 & -\frac{\sqrt{66}}{12} & -\frac{\sqrt{4290}}{90} & \frac{\sqrt{210}}{20} & 0 & 0 \\ 3.4 & 1.2 & \frac{\sqrt{70}}{20} & -\frac{\sqrt{2002}}{66} & -\frac{\sqrt{462}}{44} & \frac{\sqrt{330}}{22} & 0 \\ 3.6 & 1.2 & 0 & -\frac{4\sqrt{165}}{495} & -\frac{\sqrt{715}}{55} & -\frac{\sqrt{154}}{22} & 1 \end{bmatrix}$$

$v_1\cdot L_1$	$v_2\cdot L_2$	5.2	5.4	5.5	5.6	5.7	5.8	5.10
4.2	1.2	$-\frac{\sqrt{910}}{35}$	$\frac{\sqrt{3003}}{77}$	0	0	0	0	0
4.4	1.2	$\frac{3\sqrt{35}}{35}$	$\frac{24\sqrt{21}}{385}$	$-\frac{3\sqrt{231}}{55}$	$\frac{3\sqrt{23205}}{715}$	0	0	0
4.5	1.2	0	$-\frac{\sqrt{1001}}{55}$	$-\frac{\sqrt{6}}{5}$	$-\frac{2\sqrt{6545}}{385}$	$\frac{2\sqrt{210}}{35}$	0	0
4.6	1.2	0	$\frac{7\sqrt{5}}{55}$	$-\frac{2\sqrt{55}}{55}$	$-\frac{6\sqrt{34}}{55}$	$-\frac{\sqrt{3}}{5}$	$\frac{\sqrt{19}}{5}$	0
4.8	1.2	0	0	0	$-\frac{16\sqrt{1001}}{5005}$	$-\frac{\sqrt{238}}{35}$	$-\frac{\sqrt{6}}{5}$	1

$v_1\cdot L_1$	$v_2\cdot L_2$	6.0	6.3	6.4	6.6	6.6
5.2	1.2	1	$-\frac{\sqrt{105}}{14}$	$\frac{\sqrt{221}}{26}$	0	0
5.4	1.2	0	$-\frac{\sqrt{385}}{35}$	$-\frac{\sqrt{663}}{39}$	$\frac{\sqrt{2510}}{65}$	0
5.5	1.2	0	$\frac{\sqrt{15}}{10}$	$-\frac{\sqrt{663}}{78}$	$-\frac{28\sqrt{2510}}{16315}$	$-\frac{5\sqrt{14755286}}{22841}$
5.6	1.2	0	0	$\frac{\sqrt{195}}{39}$	$\frac{4\sqrt{55471}}{3263}$	$-\frac{11\sqrt{166915}}{8785}$
5.7	1.2	0	0	0	$-\frac{135\sqrt{2510}}{13052}$	$-\frac{\sqrt{14755286}}{22841}$
5.8	1.2	0	0	0	$\frac{7\sqrt{162146}}{13052}$	$-\frac{\sqrt{228410}}{8785}$

$v_1\cdot L_1$	$v_2\cdot L_2$	6.7	6.8	6.9	6.10	6.12
5.5	1.2	$\frac{\sqrt{3094}}{91}$	0	0	0	0
5.6	1.2	$-\frac{\sqrt{385}}{35}$	$\frac{\sqrt{692835}}{1105}$	0	0	0
5.7	1.2	$-\frac{11\sqrt{546}}{546}$	$-\frac{\sqrt{494}}{78}$	$\frac{\sqrt{110}}{12}$	0	0
5.8	1.2	$-\frac{\sqrt{3990}}{210}$	$-\frac{11\sqrt{17290}}{2470}$	$-\frac{\sqrt{418}}{76}$	$\frac{\sqrt{2622}}{57}$	0
5.10	1.2	0	$-\frac{8\sqrt{20995}}{12597}$	$-\frac{2\sqrt{133}}{57}$	$-\frac{\sqrt{627}}{57}$	1

$v_1\cdot L_1$	$v_2\cdot L_2$	7.2	7.4	7.5	7.6	7.7	7.8
6.0	1.2	$\frac{\sqrt{357}}{35}$	0	0	0	0	0
6.3	1.2	$-\frac{\sqrt{595}}{35}$	$-\frac{\sqrt{4522}}{105}$	$\frac{\sqrt{1122}}{55}$	0	0	0
6.4	1.2	$\frac{\sqrt{273}}{35}$	$-\frac{\sqrt{570570}}{1155}$	$-\frac{\sqrt{30030}}{385}$	$\frac{2\sqrt{114114}}{1001}$	0	0
6.6	1.2	0	$-\frac{4\sqrt{81154073}}{289905}$	$-\frac{26\sqrt{4271267}}{96635}$	$-\frac{\sqrt{62426210}}{13805}$	0	$\frac{\sqrt{50592815}}{8785}$
6.6	1.2	0	$\frac{9\sqrt{13805}}{2761}$	$-\frac{8\sqrt{262295}}{19327}$	$\frac{52\sqrt{71786}}{96635}$	$-\frac{\sqrt{8283}}{105}$	$\frac{164\sqrt{35915339}}{66159835}$
6.7	1.2	0	0	$\frac{\sqrt{429}}{77}$	$-\frac{\sqrt{570}}{70}$	$-\frac{\sqrt{692835}}{1785}$	$-\frac{8\sqrt{37655}}{15505}$
6.8	1.2	0	0	0	$\frac{11\sqrt{546}}{910}$	$-\frac{\sqrt{3003}}{315}$	$\frac{8\sqrt{5759}}{2215}$
6.9	1.2	0	0	0	0	$-\frac{4\sqrt{1785}}{5355}$	$-\frac{\sqrt{55089265}}{15505}$
6.10	1.2	0	0	0	0	0	$\frac{7\sqrt{866065}}{37655}$

$v_1\cdot L_1$	$v_2\cdot L_2$	7.8	7.9	7.10	7.11	7.12	7.14
6.6	1.2	$\frac{\sqrt{913005723}}{52717}$	0	0	0	0	0
6.7	1.2	$-\frac{5\sqrt{345559935}}{158151}$	$\frac{\sqrt{5610}}{102}$	0	0	0	0
6.8	1.2	$-\frac{13\sqrt{52850343}}{176757}$	$-\frac{\sqrt{114114}}{798}$	$\frac{\sqrt{937365}}{1197}$	0	0	0
6.9	1.2	$-\frac{4\sqrt{28580145}}{112965}$	$-\frac{13\sqrt{3570}}{1785}$	$-\frac{2\sqrt{5313}}{693}$	$\frac{2\sqrt{30030}}{385}$	0	0
6.10	1.2	$-\frac{256\sqrt{15024345}}{15024345}$	$-\frac{2\sqrt{91770}}{1995}$	$-\frac{52\sqrt{9177}}{9177}$	$-\frac{\sqrt{31395}}{805}$	$\frac{3\sqrt{2415}}{161}$	0
6.12	1.2	0	0	$-\frac{16\sqrt{759}}{5313}$	$-\frac{5\sqrt{17710}}{1771}$	$-\frac{\sqrt{4186}}{161}$	1

$v_1 \cdot L_1$	$v_2 \cdot L_2$	8.2	8.4	8.5	8.6	8.7	8.8	8.8
7.2	1.2	$-\frac{\sqrt{133}}{14}$	$\frac{\sqrt{22610}}{238}$	0	0	0	0	0
7.4	1.2	$\frac{3\sqrt{7}}{14}$	$\frac{24\sqrt{6545}}{6545}$	$-\frac{3\sqrt{770}}{110}$	$\frac{3\sqrt{782782}}{4862}$	0	0	0
7.5	1.2	0	$-\frac{\sqrt{11305}}{170}$	$-\frac{\sqrt{3705}}{130}$	$-\frac{\sqrt{1352078}}{3094}$	$\frac{\sqrt{4849845}}{3094}$	0	0
7.6	1.2	0	$\frac{\sqrt{17017}}{374}$	$-\frac{\sqrt{2002}}{154}$	$-\frac{3\sqrt{1956955}}{6545}$	$-\frac{\sqrt{102102}}{952}$	$\frac{\sqrt{12133030}}{4760}$	0
7.7	1.2	0	0	$\frac{3\sqrt{455}}{182}$	$-\frac{3\sqrt{782782}}{12376}$	$\frac{6\sqrt{455}}{1547}$	$-\frac{38\sqrt{3079923}}{1586627}$	$-\frac{175\sqrt{5213203}}{453322}$
7.8	1.2	0	0	0	$-\frac{8\sqrt{2994852770}}{3426605}$	$-\frac{\sqrt{11017853}}{6202}$	$-\frac{\sqrt{1506162345}}{75310}$	0
7.8	1.2	0	0	0	$\frac{135\sqrt{2937090}}{783224}$	$-\frac{2\sqrt{5716029}}{22593}$	$\frac{270\sqrt{1535783537785}}{1907805637}$	$-\frac{5\sqrt{18516937065}}{1519962}$
7.9	1.2	0	0	0	0	$\frac{13\sqrt{42}}{408}$	$-\frac{189\sqrt{10266410}}{1813288}$	$-\frac{8\sqrt{156396090}}{679983}$
7.10	1.2	0	0	0	0	0	$\frac{55\sqrt{1345926351}}{8613118}$	$-\frac{4\sqrt{4306559}}{253327}$

$v_1 \cdot L_1$	$v_2 \cdot L_2$	8.9	8.10	8.10	8.11	8.12	8.13	8.14	8.16
7.7	1.2	$\frac{5\sqrt{79534}}{2584}$	0	0	0	0	0	0	0
7.8	1.2	0	$\frac{65\sqrt{37655}}{15062}$	0	0	0	0	0	0
7.8	1.2	$-\frac{\sqrt{613851810}}{38760}$	$\frac{28\sqrt{345559935}}{27902355}$	$\frac{3\sqrt{648109}}{3458}$	0	0	0	0	0
7.9	1.2	$-\frac{\sqrt{31395}}{357}$	$-\frac{8\sqrt{3570}}{4641}$	$-\frac{15\sqrt{3542}}{2002}$	$\frac{\sqrt{15015}}{154}$	0	0	0	0
7.10	1.2	$-\frac{5\sqrt{92378}}{7106}$	$\frac{60\sqrt{323}}{4199}$	$-\frac{243\sqrt{72105}}{124982}$	$-\frac{3\sqrt{3289}}{506}$	$\frac{9\sqrt{16214770}}{43010}$	0	0	0
7.11	1.2	$-\frac{8\sqrt{373065}}{124355}$	$-\frac{19\sqrt{533715}}{30940}$	$-\frac{6\sqrt{1001}}{1001}$	$-\frac{5\sqrt{154}}{154}$	$-\frac{3\sqrt{70499}}{4862}$	$\frac{5\sqrt{91}}{52}$	0	0
7.12	1.2	0	$\frac{3\sqrt{1785}}{884}$	$-\frac{38\sqrt{1771}}{23023}$	$-\frac{3\sqrt{2530}}{506}$	$-\frac{5\sqrt{56695}}{2346}$	$-\frac{\sqrt{5}}{12}$	$\frac{\sqrt{31}}{6}$	0
7.14	1.2	0	0	0	0	$-\frac{2\sqrt{15470}}{3315}$	$-\frac{\sqrt{754}}{78}$	$-\frac{\sqrt{5}}{6}$	1

$v_1 \cdot L_1$	$v_2 \cdot L_2$	9.0	9.3	9.4	9.6	9.6	9.7	9.8
8.2	1.2	1	$-\frac{\sqrt{210}}{21}$	$\frac{\sqrt{874}}{57}$	0	0	0	0
8.4	1.2	0	$-\frac{\sqrt{3570}}{105}$	$-\frac{\sqrt{163438}}{627}$	$\frac{\sqrt{4649205}}{3135}$	0	0	0
8.5	1.2	0	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{437}}{57}$	$-\frac{136\sqrt{14370270}}{5494515}$	$-\frac{50\sqrt{39395895}}{404859}$	$\frac{\sqrt{45885}}{399}$	0
8.6	1.2	0	0	$\frac{2\sqrt{17765}}{627}$	$\frac{224\sqrt{278022459}}{12087933}$	$-\frac{55\sqrt{13765206}}{404859}$	$-\frac{\sqrt{176358}}{798}$	$\frac{5\sqrt{7106}}{646}$
8.7	1.2	0	0	0	$-\frac{315\sqrt{1859682}}{732602}$	$-\frac{20\sqrt{12176913}}{404859}$	$-\frac{\sqrt{33649}}{399}$	$-\frac{5\sqrt{22287}}{2907}$
8.8	1.2	0	0	0	$\frac{\sqrt{2254103646}}{169062}$	$-\frac{20\sqrt{1785902591319}}{415229619}$	$-\frac{\sqrt{9013627987}}{279993}$	$-\frac{55\sqrt{70838229}}{759981}$
8.8	1.2	0	0	0	0	$\frac{\sqrt{19772839}}{13333}$	$-\frac{40\sqrt{108677283}}{2279943}$	$\frac{136\sqrt{226661}}{759981}$
8.9	1.2	0	0	0	0	0	$\frac{\sqrt{8778}}{342}$	$-\frac{5\sqrt{8398}}{1938}$
8.10	1.2	0	0	0	0	0	0	$-\frac{40\sqrt{12903}}{37791}$
8.10	1.2	0	0	0	0	0	0	$\frac{27\sqrt{5}}{247}$

$v_1 \cdot L_1$	$v_2 \cdot L_2$	9.9	9.9	9.10	9.10	9.11
8.7	1.2	$\frac{\sqrt{68430}}{342}$	0	0	0	0
8.8	1.2	$-\frac{\sqrt{170614534530}}{1519962}$	0	$\frac{2\sqrt{85609993030}}{759981}$	0	0
8.8	1.2	$-\frac{172\sqrt{48964242530}}{1733516661}$	$-\frac{\sqrt{37559527655}}{216695}$	$\frac{848\sqrt{14616975766470}}{445544181117}$	$\frac{\sqrt{93316753489505}}{18564805}$	0
8.9	1.2	$\frac{8\sqrt{64791805}}{650085}$	$-\frac{17\sqrt{159670}}{15967}$	$-\frac{352\sqrt{724027395}}{167083245}$	$-\frac{2\sqrt{10597572370}}{307087}$	$\frac{30\sqrt{572033}}{33649}$
8.10	1.2	$-\frac{2\sqrt{8143170}}{11115}$	0	$-\frac{\sqrt{3070870}}{3705}$	0	0
8.10	1.2	$-\frac{432\sqrt{8079302}}{6197477}$	$-\frac{26\sqrt{6197477}}{476729}$	$\frac{3672\sqrt{65493282}}{158596477}$	$-\frac{884\sqrt{50592276163}}{402591057}$	$\frac{13\sqrt{312455}}{14421}$
8.11	1.2	$\frac{13\sqrt{37511045}}{476729}$	$-\frac{4\sqrt{33371030}}{878185}$	$-\frac{23\sqrt{24616931430}}{11138883}$	$-\frac{16}{1535435}\sqrt{311693305}$	$-\frac{17}{7315}\sqrt{43890}$
8.12	1.2	0	0	$\frac{55\sqrt{96585254493}}{85398103}$	$-\frac{160\sqrt{1680994238}}{148323021}$	$-\frac{2\sqrt{462120945}}{187473}$
8.13	1.2	0	0	0	0	$-\frac{8\sqrt{198835}}{85215}$

$v_1 \cdot L_1$	$v_2 \cdot L_2$	9.12	9.12	9.13	9.14	9.15	9.16	9.18
8.10	1.2	$\frac{\sqrt{10111515}}{3705}$	0	0	0	0	0	0
8.10	1.2	$\frac{216\sqrt{10032209}}{34320715}$	$\frac{13\sqrt{215980259495}}{7920165}$	0	0	0	0	0
8.11	1.2	$-\frac{184\sqrt{13085490}}{6542745}$	$-\frac{\sqrt{11268535278}}{298441}$	$\frac{\sqrt{26390}}{195}$	0	0	0	0
8.12	1.2	$\frac{8\sqrt{6744380505}}{2736057}$	$-\frac{34\sqrt{6905951871}}{5616117}$	$-\frac{\sqrt{1105}}{117}$	$\frac{5\sqrt{124571733}}{64467}$	0	0	0
8.13	1.2	$-\frac{189\sqrt{198265}}{198265}$	$-\frac{8\sqrt{170735383}}{569751}$	$-\frac{17\sqrt{910}}{1365}$	$-\frac{2\sqrt{2947945}}{25935}$	$\frac{4\sqrt{595}}{105}$	0	0
8.14	1.2	$\frac{7\sqrt{106944141}}{594795}$	$-\frac{352\sqrt{2848755}}{8546265}$	$-\frac{2\sqrt{14105}}{819}$	$-\frac{34\sqrt{272118}}{37107}$	$-\frac{\sqrt{11067}}{651}$	$\frac{7\sqrt{155}}{93}$	0
8.16	1.2	0	0	0	$-\frac{16\sqrt{1195670}}{256215}$	$-\frac{\sqrt{23870}}{465}$	$-\frac{\sqrt{1054}}{93}$	1

$v_1 \cdot L_1$	$v_2 \cdot L_2$	10.2	10.4	10.5	10.6	10.7	10.8
9.0	1.2	$\frac{\sqrt{322}}{35}$	0	0	0	0	0
9.3	1.2	$-\frac{\sqrt{2415}}{70}$	$-\frac{\sqrt{161}}{21}$	$\frac{\sqrt{3795}}{110}$	0	0	0
9.4	1.2	$\frac{3\sqrt{133}}{70}$	$-\frac{\sqrt{21945}}{231}$	$-\frac{\sqrt{4389}}{154}$	$\frac{5\sqrt{15015}}{1001}$	0	0
9.6	1.2	0	$-\frac{4\sqrt{22056448414}}{4453449}$	$-\frac{\sqrt{110282242070}}{570955}$	$-\frac{5\sqrt{580432853}}{212069}$	0	$\frac{\sqrt{2789507524895}}{2294201}$
9.6	1.2	0	$\frac{63\sqrt{19279}}{19279}$	$-\frac{8\sqrt{96395}}{10381}$	$\frac{128\sqrt{732602}}{674765}$	$-\frac{\sqrt{115674}}{420}$	$\frac{188\sqrt{426019052030}}{7134290345}$
9.7	1.2	0	0	$\frac{\sqrt{627}}{77}$	$-\frac{\sqrt{30}}{14}$	$-\frac{\sqrt{106590}}{714}$	$-\frac{16\sqrt{274898}}{74011}$
9.8	1.2	0	0	0	$\frac{\sqrt{102102}}{910}$	$-\frac{\sqrt{13566}}{630}$	$\frac{64\sqrt{22097570}}{1004435}$
9.9	1.2	0	0	0	0	$-\frac{2\sqrt{1779282645}}{2442951}$	$-\frac{\sqrt{42711230023}}{370055}$
9.9	1.2	0	0	0	0	$\frac{63\sqrt{15123030}}{775540}$	0
9.10	1.2	0	0	0	0	0	$\frac{13\sqrt{95338760443}}{17075395}$

$v_1 \cdot L_1$	$v_2 \cdot L_2$	10.8	10.9	10.10	10.10
9.6	1.2	$\frac{39\sqrt{108221696618}}{25163740}$	0	0	0
9.7	1.2	$-\frac{5\sqrt{76258714070}}{2516374}$	$\frac{5\sqrt{7106}}{646}$	0	0
9.8	1.2	$-\frac{13\sqrt{948672998}}{740110}$	$-\frac{\sqrt{293930}}{1330}$	$\frac{61\sqrt{4845}}{5985}$	0
9.9	1.2	$-\frac{22\sqrt{337726570852645}}{2049946105}$	$-\frac{13\sqrt{81160261}}{271439}$	$-\frac{61\sqrt{24237906}}{1580733}$	0
9.9	1.2	$-\frac{\sqrt{832278118630}}{5428780}$	$\frac{76\sqrt{1473526}}{1357195}$	$-\frac{288\sqrt{18592431}}{53569285}$	$-\frac{2\sqrt{112784045}}{23485}$
9.10	1.2	$-\frac{128\sqrt{42841933078945}}{10330825435}$	$-\frac{46\sqrt{820564381}}{3712961}$	$-\frac{1586\sqrt{8710606506}}{256194309}$	0
9.10	1.2	$\frac{\sqrt{20021139693030}}{16610615}$	$-\frac{16\sqrt{374031966}}{1535435}$	$\frac{12312\sqrt{18639259639}}{15079507135}$	$-\frac{\sqrt{436811296845}}{1620465}$
9.11	1.2	0	$\frac{51\sqrt{1045}}{7315}$	$-\frac{243\sqrt{2145}}{46970}$	$-\frac{4\sqrt{187891}}{14091}$
9.12	1.2	0	0	$-\frac{976\sqrt{1584033}}{11088231}$	0
9.12	1.2	0	0	$\frac{27\sqrt{12310874791215}}{450921394}$	$-\frac{4\sqrt{3696077}}{324093}$
9.13	1.2	0	0	0	0

$v_1 \cdot L_1$	$v_2 \cdot L_2$	10.11	10.11	10.12	10.12
9.9	1.2	$\frac{3\sqrt{54748511818}}{878185}$	0	0	0
9.9	1.2	$\frac{472\sqrt{364145683}}{2549019781}$	$\frac{\sqrt{158403372105}}{798215}$	0	0
9.10	1.2	$-\frac{3\sqrt{11908850861453}}{44946370}$	0	$\frac{9\sqrt{635492230793}}{8989274}$	0
9.10	1.2	$-\frac{56\sqrt{5428325922558}}{4456753631}$	$-\frac{\sqrt{311972754170}}{798215}$	$\frac{488\sqrt{17672590355602182}}{6168012828285}$	$\frac{\sqrt{3476516321397}}{2869365}$
9.11	1.2	$\frac{8\sqrt{395637}}{48587}$	$-\frac{19\sqrt{19122455}}{173525}$	$-\frac{40\sqrt{9606135}}{1921227}$	$-\frac{7\sqrt{387831108210}}{8109075}$
9.12	1.2	$-\frac{5\sqrt{132936801459}}{3696077}$	0	$-\frac{\sqrt{544941192705}}{1680035}$	0
9.12	1.2	$-\frac{8\sqrt{58407233032005}}{333174941}$	$-\frac{\sqrt{134269501223}}{2075359}$	$\frac{152\sqrt{20457451676031}}{3593018853}$	$-\frac{19\sqrt{342534463986}}{22381047}$
9.13	1.2	$\frac{\sqrt{16414203}}{29026}$	$-\frac{176\sqrt{943345}}{4716725}$	$-\frac{5\sqrt{481180035}}{349314}$	$-\frac{128\sqrt{7742544810}}{56763525}$
9.14	1.2	0	0	$\frac{11\sqrt{1727183073}}{2619855}$	$-\frac{184\sqrt{86280558}}{34058115}$
9.15	1.2	0	0	0	0

$v_1 \cdot L_1$	$v_2 \cdot L_2$	10.13	10.14	10.14	10.15	10.16	10.17	10.18	10.20
9.11	1.2	$\frac{\sqrt{18874505}}{5850}$	0	0	0	0	0	0	0
9.12	1.2	0	$\frac{2\sqrt{832713}}{2087}$	0	0	0	0	0	0
9.12	1.2	$-\frac{\sqrt{461227}}{1638}$	$\frac{4\sqrt{365861535}}{3812949}$	$\frac{\sqrt{363501138}}{23751}$	0	0	0	0	0
9.13	1.2	$-\frac{38\sqrt{5960370}}{197925}$	$-\frac{4\sqrt{5655}}{3045}$	$-\frac{\sqrt{5399394}}{7917}$	$\frac{2\sqrt{189805}}{1015}$	0	0	0	0
9.14	1.2	$-\frac{2\sqrt{230945}}{4095}$	$\frac{2\sqrt{1254}}{315}$	$-\frac{19\sqrt{61845}}{9765}$	$-\frac{\sqrt{70091}}{1085}$	$\frac{\sqrt{20376455}}{5115}$	0	0	0
9.15	1.2	$-\frac{32\sqrt{145}}{9135}$	$-\frac{23\sqrt{45849}}{12180}$	$-\frac{\sqrt{1138830}}{6090}$	$-\frac{19\sqrt{29}}{290}$	$-\frac{\sqrt{3145}}{510}$	$\frac{3\sqrt{11305}}{340}$	0	0
9.16	1.2	0	$\frac{\sqrt{33495}}{1740}$	$-\frac{5\sqrt{5394}}{5394}$	$-\frac{7\sqrt{155}}{310}$	$-\frac{19\sqrt{24087}}{6510}$	$-\frac{\sqrt{399}}{140}$	$\frac{2\sqrt{273}}{35}$	0
9.18	1.2	0	0	0	0	$-\frac{8\sqrt{2618}}{6545}$	$-\frac{2\sqrt{8806}}{595}$	$-\frac{\sqrt{133}}{35}$	1

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A generalization of Chetaev's principle for a class of higher order nonholonomic constraints

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The constraint distribution in nonholonomic mechanics has a double role. On the one hand, it is a kinematic constraint, that is, it is a restriction on the motion itself. On the other hand, it is also a restriction on the allowed variations when using D'Alembert's principle to derive the equations of motion. We will show that many systems of physical interest where D'Alembert's principle does not apply can be conveniently modeled within the general idea of the principle of virtual work by the introduction of both kinematic constraints and variational constraints as being independent entities. This includes, for example, elastic rolling bodies and pneumatic tires. Also, D'Alembert's principle and Chetaev's principle fall into this scheme. We emphasize the geometric point of view, avoiding the use of local coordinates, which is the appropriate setting for dealing with questions of global nature, like reduction. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763245]

I. INTRODUCTION

Nonholonomic mechanics: The universal formalism created by Lagrange is not appropriate to derive the equations of motion for systems with rolling constraints, that is, this motion is not described by classical variational principles. Several systems with rolling constraints, like the idealized rigid ball rolling on a plane with only one point of contact and many others, are successfully described geometrically by distributions on configuration space and the corresponding equations of motion are derived by D'Alembert's principle, which has been the purpose of extensive research[3,5,14,17,18,22,30] for more than a century (see also, for instance, Refs. 24, 2, 7, and 8 for a list of references and historical remarks). However, as we will see in the examples studied in the present work the dynamics of elastic rolling bodies is not generally described by D'Alembert's principle, even in those cases where the restriction on the motion is given by linear constraints. On the other hand, *second order constraints*, that is, subsets of the second order tangent bundle rather than the tangent bundle of the configuration space, naturally appear in several examples. The purpose of the present work is to establish the basic geometric definitions and procedures within the general idea of the principle of virtual work, generalizing D'Alembert's principle to deal with nonlinear and higher order constraints. One of our main examples will be elastic rolling bodies, like pneumatic tires, where some second order constraints appear naturally.

In D'Alembert's principle the constraint distribution has a double role. On one hand, it is a *kinematic constraint*, that is, it is a restriction on the motion itself. On the other hand, it is, *in*

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addition, a *variational constraint*. This perspective was already adopted in Ref. 13 where a general approach to nonholonomic constrained systems considered as implicit differential equations was considered. There it was discussed that the kinematical constraints defining a submanifold on the tangent space of the configuration space of the system and the reaction or control forces described by a subbundle of the cotangent bundle of the configuration space, where independent entities and a condition for the compatibility of both ingredients was obtained. In this paper we will push forward this point of view by considering nonlinear higher order nonholonomic constraints, not only constraints on the velocities but on higher order derivatives.

We will show that many systems of physical interest where D'Alembert's principle does not apply, can be conveniently modeled by a principle based in the introduction of both higher order *kinematic constraints* and higher order *variational constraints* as being independent entities. This includes, for example, elastic rolling bodies and pneumatic tires. Also, D'Alembert's principle and Chetaev's principle fall into this scheme.

Our point of view is geometric, avoiding the use of local coordinates, which is appropriate for dealing global problems, like reduction. We also write equations of motion for systems with higher order constraints in an intrinsic fashion, using the natural structures of the tangent bundle and higher order bundles.

Basic notation: As usual we will consider that the configuration space of a Lagrangian system is a smooth manifold Q of dimension n with local coordinates q^i. We shall introduce higher order tangent bundles in order to deal with higher order constraints. Thus, by definition, two given curves in Q, say, $q_1(t)$ and $q_2(t)$, $t\in(-a,a)$, have a contact of order k at $q_0=q_1(0)=q_2(0)$ if there is a local chart (φ,U) such that $q_i(0)\in U$, for $i=1,2$, and $D_t^s(\varphi\circ q_1)(0)=D_t^s(\varphi\circ q_2)(0)$, for $s=0,\ldots,k$. This is a well-defined equivalence relation, and the equivalence class of a given curve $q(t)$ is denoted $[q]^{(k)}$. For each $q_0\in Q$, let $T^{(k)}_{q_0}Q$ be the set of all $[q]^{(k)}$ such that $q(0)=q_0$, and let $T^{(k)}Q$ be the collection of all $T^{(k)}_{q_0}Q$, for $q_0\in Q$. It is well known (see, for instance, Refs. 19 and 9 and references therein) that $\tau^k:T^{(k)}Q\to Q$, where $\tau^k([q]^{(k)})=q(0)$, is a fiber bundle, called the tangent bundle of order k of Q. There are natural maps $\tau^{(l,k)}:T^{(k)}Q\to T^{(l)}Q$, for $k,l=1,2,\ldots$, given by $\tau^{(l,k)}([q]^{(k)})=[q]^{(l)}$. It is easy to see that $T^{(1)}Q\equiv TQ$. Also, we can identify $T^{(0)}Q\equiv Q$, via $[q]^{(0)}\equiv q(0)$.

In local coordinates, we have $q=(q^1,\ldots,q^n)$, and, for $s=1,2,\ldots$, we denote $q^{(s)}=(q^{1,(s)},\ldots,q^{n,(s)})$, where

$$q^{i,(s)}=\frac{\mathrm{d}^s q^i}{\mathrm{d}t^s}(0),$$

where $i=1,\ldots,n$. Then we have, $[q]^{(k)}=(q^{(0)},\ldots,q^{(k)})$.

Denote by $j_k:T^{(k)}Q\to T(T^{(k-1)}Q)$ the canonical immersion defined by $j_k([q]^{(k)})=[q^{(k-1)}]^{(1)}$ where $q^{(k-1)}$ is the lift to $T^{(k-1)}Q$ of the curve q, that is, the curve $q^{(k-1)}:(-a,a)\to T^{(k-1)}Q$ is defined as $q^{(k-1)}(t)=[q_t]^{(k-1)}$ where $q_t(s)=q(t+s)$.

In this paper, it will be useful to introduce, geometrically, the concept of implicit differential equations. This concept has often received less attention than the notion of an explicit differential equation in the differential geometry literature (see Refs. 21, 23, and 13). Geometrically, a system of implicit kth-order differential equations is a submanifold M of $T^{(k)}Q$ and a curve $\gamma:I\to Q$ is a solution to the differential equation M, if its k-lift $\gamma^{(k)}(s)\in M$ for all $s\in I$. The implicit differential equation will be said to be integrable at a point if there exists a solution γ such that its k-lift passes through it. The integrable part of M is the subset of all integrable points of M. The system is said to be integrable if its integrable part coincides with M. A notorious algorithm has been developed to extract the integrable part of an arbitrary implicit differential equation,[23] but it will not be the objective of this paper to discuss this issue for systems with higher order nonholonomic constraints and we will restrict ourselves to the description of the corresponding implicit differential equation, leaving the questions of the existence and uniqueness of its solutions for future discussion.

In Sec. II we describe a first example of the elastic rolling ball, where some of the features of the general procedure already appear. In Secs. III and IV we show how to study Rocard's theory and also Greidanus's theory of a pneumatic tire (see Refs. 11, 26, and 27 and also Ref. 24) as a nonholonomic system with higher order constraints and, motivated by the previous examples, in Sec. IV we establish a general principle for dealing with systems involving higher order constraints. The distinction between kinematic constraints and variational constraints as being independent entities is a key point to this discussion. In Sec. V intrinsic equations of motion for systems with higher order constraints are derived. In Sec. VI further examples are provided and some basic results about reduction and the equations for Lagrangian systems with symmetries with higher-order nonholonomic constraints are discussed.

II. A SIMPLE EXAMPLE: THE ELASTIC HOMOGENEOUS ROLLING BALL

The main purpose of this section is to show an example that can be treated using D'Alembert's principle and also using some other procedures involving different types of constraints, including second order nonlinear constraints. All those procedures are equivalent in the sense that they give equivalent systems of equations.

Let us consider an elastic ball subjected to gravity and rolling on a plane. Without loss of generality we will assume that the radius of the ball is 1, for simplicity. For a static ball the contact between the ball and the plane is a circle, whose diameter was calculated by Hertz,[12] see also Ref. 16, p. 27. The effect of internal viscosity, adhesion and other dissipative forces is important in some cases,[4] however, in the present section we shall assume that heat dissipation is small, in other words, we will consider only the idealized model of a perfect elastic ball. Also, we shall consider only the important case where the circle of contact is small and the motion is quasistatic, which, in particular, implies that the zone of contact is approximately a circle of the same size as the contact circle in the static case (see Ref. 16). This also implies that the size and inertia of the flattened part of the sphere is negligible. Now we shall define the *nonsliding condition*. It is given by the condition that the points of the sphere belonging to the circle of contact cannot slide against the plane. It is clear that this has to be understood in an approximate sense since the exact solution of elasticity equations is not known in general, not even under the quasistatic assumption. More precisely, we accept the following approximate model. We assume that for all kinematic and dynamical purposes the ball is rigid, it has only one point of contact a with the plane, representing the center of the circle of contact, which does not slides, and the spatial angular velocity and the translation velocity combine in such a way that the velocity of points z of the surface of the ball near a have a velocity which is of order $|a-z|^2$. This is a rigorous way of defining the constraint given by the nonsliding condition, in the case where there is a circle rather than a point of contact. It is easy to prove that, in fact, the nonsliding condition is satisfied if and only if the vertical component of the spatial angular velocity is 0, that is, $\omega_3 = 0$. We emphasize that this model is realistic only for slow motion and small deformation. In agreement with all these physical assumptions we have the following geometric model.

Kinematics of the elastic rolling ball. The manifold $Q=\mathrm{SO}(3)\times\mathbb{R}^2$ is the configuration space for the model. A position of the system is given by a point $(A,a)\in Q$, where a is the point of contact of the sphere with the plane representing in the approximation described above the center of the circle of contact. Let $V=\dot{a}$ be the translation velocity of the ball and let $\omega=\dot{A}A^{-1}$ be the spatial angular velocity $\omega=(\omega_1,\omega_2,\omega_3)$, after the identification of $\mathfrak{so}(3)$ with $\mathbb{R}^3$. We have $\dot{V}=\ddot{a}$ and $\dot{\omega}=\ddot{A}A^{-1}-\dot{A}A^{-1}\dot{A}A^{-1}$. The following two equations describe the nonsliding constraint:

$$V=(\omega_2,-\omega_1), \tag{1}$$

$$\omega_3=0. \tag{2}$$

The first equation represents the usual nonsliding condition for a rigid rolling ball while the second expresses the fact that there is really a circle of contact rather than a point, and that the points of that circle belonging to the sphere have zero velocity with respect to the plane, at least to first

order approximation. The previous equations define a distribution, which is the *kinematic constraint* for the system of the elastic rolling ball. We will show that, provided that we accept higher order constraints, there are other equivalent ways of choosing the constraints all of them giving equivalent equations of motion. For instance, let the curve $a(t)$ in the plane have curvature radius $r(t)$. Then we define the constraint

$$r^2\omega_3^2=\omega_1^2+\omega_2^2, \tag{3}$$

whose physical meaning is that the instantaneous motion of the sphere is a superposition of a rotation about some vertical axis, with angular velocity ω_3, and the motion of rolling on the plane with speed

$$|V|=\sqrt{\omega_1^2+\omega_2^2}, \tag{4}$$

and the point of contact is located at a distance r from the vertical axis. This is an example of a *second order constraint*, it is a *kinematic constraint* in the terminology introduced in Sec. IV and it is equivalent to the constraint (2), in the sense that it gives equivalent equations of motion, as we will explain later. However, as we have said before the nonsliding condition is satisfied only if $r=\infty$, which of course implies $\omega_3=0$. Equation (1) has the following consequence:

$$\dot{V}=(\dot{\omega}_2,-\dot{\omega}_1).$$

Let $\mathbf{t}$ and $\mathbf{n}$ be the tangent and normal vectors to the curve $a(t)$. We have

$$|V|\mathbf{n}=\pm(\omega_1,\omega_2),$$

and also

$$\dot{V}=\frac{\mathrm{d}|V|}{\mathrm{d}t}\mathbf{t}+\frac{|V|^2}{r}\mathbf{n}.$$

Then we can deduce

$$\langle|V|\mathbf{n},\dot{V}\rangle=\pm(\omega_1\dot{\omega}_2-\omega_2\dot{\omega}_1) \tag{5}$$

$$=\frac{|V|^3}{r}, \tag{6}$$

from which we obtain the constraint (3) in the form

$$\omega_1\dot{\omega}_2-\omega_2\dot{\omega}_1=\omega_3(\omega_1^2+\omega_2^2), \tag{7}$$

where the choice of the sign $\pm$ is the only one consistent with the standard choice for the direction of the normal $\mathbf{n}$ and the sign of ω_3 for the given physical description. We have a subset $C\subseteq T^{(2)}Q$, given by (1) and (7), rewritten in terms of $\dot{a}$, A, $\dot{A}$, and $\ddot{A}$. This is a *second order kinematic constraint*. Observe that, in this example, the projection $\tau_Q^{(1,2)}:T^{(2)}Q\to TQ$ defines a distribution $D\subseteq TQ$, by $D=\tau_Q^{(1,2)}(C)$, which is given by (1), and that rewritten in terms of A, $\dot{A}$, a, and $\dot{a}$, gives an expression linear in $\dot{A}$ and $\dot{a}$.

Dynamics of the elastic rolling ball: The Lagrangian is given by the kinetic energy

$$L(A,a,\dot{A},\dot{a})=\tfrac{1}{2}I(\dot{A}A^{-1})^2+\tfrac{1}{2}M(\dot{a})^2,$$

where I is the moment of inertia of the ball with respect to any of its symmetry axis, and M is the mass of the ball. The dynamics of the elastic rolling ball is given by the following variational description, as we will see later,

$$\delta\int_{t_0}^{t_1}\left(\frac{1}{2}I(\dot{A}A^{-1})^2+\frac{1}{2}M(\dot{a})^2\right)\mathrm{d}t=0, \tag{8}$$

$$(\delta A(t_i),\delta a(t_i))=0 \quad \text{for } i=0,1, \tag{9}$$

$$(\delta A(t),\delta a(t))\in D_{(A(t),a(t))} \quad \text{for all} \quad t, \tag{10}$$

$$(\dot{A}(t),\dot{a}(t))\in D_{(A(t),a(t))} \quad \text{for all} \quad t, \tag{11}$$

$$\omega_3=0. \tag{12}$$

We will show that we can replace the last equation by Eq. (7) and we will obtain an equivalent system. We note that in this formulation the *constraints on the variations* are the same as in the case of the rigid rolling ball (see, for instance, Refs. 24 and 2). However, the *kinematic constraints* are not, in other words, the motion is effectively constrained by our choice of the last equation, namely, either Eq. (2) or Eq. (7). For any of those choices, we derive from the previous principle a *differential-algebraic system* of equations and we will have existence and uniqueness of solution for those initial conditions compatible with the constraints.

By applying the usual integration by parts argument, we obtain the equations of motion. However, as it already happens in the case of the rigid body, this is not completely trivial unless one is willing to use reduction arguments, (see, for instance, Refs. 6 and 7). We will postpone the details of the computation until Sec. VI. We obtain,

$$(I+M)\dot{\omega}_1=0, \tag{13}$$

$$(I+M)\dot{\omega}_2=0, \tag{14}$$

$$(I+M)\dot{\omega}_3=0, \tag{15}$$

$$(\omega_2,-\omega_1)=V, \tag{16}$$

$$\omega_3=0. \tag{17}$$

Of course this system is over determined, but it is correct. The fifth equation, which coincides with Eq. (2), may be replaced by Eq. (7) and we obtain a system which is clearly equivalent. The first four equations are exactly the equations for the rigid rolling ball and they imply that $\dot{\omega}=0$ and also that the translation velocity V is constant. We can show that there is solution provided that the initial condition (ω_0,V_0) satisfies the constraints given by the last two equations and that this solution is unique.

We must remark at this point that the only guiding idea to establish the previous procedure is the principle of virtual work, and one should check that the final equations are consistent with the basic laws of mechanics, essentially Newton's law, so the force should be equal to the rate of change of linear momentum and the torque should be equal to the rate of change of angular momentum. In the case of the elastic rolling ball the forces of the constraint must satisfy the following conditions: the resultant force exerted by the plane on the ball has a positive component in the vertical upwards direction while the torque has a zero horizontal component. All this is obviously compatible with the previous system of equations. Moreover, the same equations can be derived by an elementary exercise in rational mechanics. We observe that preservation of energy is satisfied in this example. As a final remark to this example we observe that even if the constraints (1), (2) are linear, we have not applied D'Alembert's principle. However, it will become clear at the end in Sec. VI that D'Alembert's principle gives correct equations of motion in this example, and it is perhaps the best procedure in this case since it produces a nonoverdetermined system. Showing that it is not always the case that D'Alembert's principle can be applied is part of the purpose of the present work. It is also clear from what we have explained so far that, for a

given system, there is in principle the possibility of introducing several classes of higher order constraints which are equivalent in the sense that they lead to equivalent equations of motion.

The case of the nonhomogeneous elastic ball and also the case of the nonhomogeneous viscoelastic ball could be interesting, for instance because of possible applications to spherical robots, and can be treated with the methods of the present work. In particular, the nonsliding condition (2) will be part of the kinematic constraints. The case of the symmetric elastic or viscoelastic rolling ball, in which two of the three moments of inertia of the ball are equal, presents an extra symmetry and we can expect that some kind of reduction by this symmetry will help to understand the behavior of the reduced variables such as the angular momentum. The case of the rigid symmetric rolling ball has been studied in Ref. 6.

III. AN EXAMPLE OF NONLINEAR HIGHER ORDER NONHOLONOMIC CONSTRAINTS

In the example of the elastic rolling ball described in the preceding section the second order constraint gives rise to a distribution D defined by (1) which provides a restriction for the variations to obtain some of the equations of motion. The rest of the equations of motion are the ones given by the same distribution, plus an extra equation provided by the nonlinear second order constraint (7) or, equivalently, by the linear constraint (2). This gives a procedure whose correctness in the example under consideration is established by the fundamental principles of mechanics.

Rocard's theory of a pneumatic tire: Before we try to establish any general procedure we will describe another example where the restrictions, both kinematic restrictions and restrictions on the variations, are of an entirely different nature. This is the simplified model of a pneumatic tire rolling on a plane according to Rocard's theory, as described, for instance, in Refs. 27, 26, 24. For simplicity we shall study the case of a single elastic pneumatic tire whose plane is constrained to remain vertical while it rolls without sliding. The zone of contact of the pneumatic tire with the plane is a small surface with a central point of contact $x=(x_1,x_2)$, which for simplicity we will assume that it coincides with the projection of the center of the wheel on the plane. The nonsliding condition means that the velocity of the points of the tire belonging to the zone of contact with respect to the plane is zero. In an approximate sense this nonsliding condition implies that the vertical component of the angular velocity of the small piece of surface of the pneumatic in contact with the floor is zero. However, contrary to what we have assumed for the homogeneous elastic rolling ball, the fact that the vertical component of the angular velocity of the zone of contact is zero does not mean that the vertical component of the angular velocity of the plane of the tire is zero. This is because according to Rocard's theory the elasticity of the material allows for a small angle ϵ between the axis of the zone of contact (an oblong-like symmetric zone), which is assumed to have the direction of $\dot{x}$, and the plane of the wheel. We will call K the corresponding constant of elasticity. It turns out that the nonsliding condition for the small zone of contact is not the relevant constraint. Instead, there will appear another second order constraint of a different nature. Finally, we must remark that the previous description of Rocard's theory gives only an approximation, and for more accurate results one must have into account some other observed effects. For instance, the projection x of the center of the wheel onto the plane is not exactly the center of the zone of contact, which produce a small torque not taken into account in the simplified model described above. Part, but only part, of this problem is taken into account in the simplified version of Greidanu's theory described later in the present work.

Taking into account all the physical considerations explained above we will describe Rocard's theory by the following geometric model. For all kinematic and dynamical purposes the wheel is simply an undeformable disk kept vertical and rolling on a plane, where the point of contact is $x=(x_1,x_2)$. We choose once for all a normal vector $N=(-\sin\theta,\cos\theta)$ rigidly fixed to the wheel. Then the angle between the plane of the wheel and the x_1 axis is θ. The angle between the velocity vector $\dot{x}$ and the plane of the wheel is called ϵ, with the physical meaning that we have explained before. Therefore, the angle between the axis x_1 and $\dot{x}$ is $\theta-\epsilon$, and the vector $\mathbf{n}$, normal to the trajectory of the point x and pointing in the direction of the concavity of the curve, is $\mathbf{n}=(-\sin(\theta-\epsilon),\cos(\theta-\epsilon))$. The angle of rotation of the wheel about its own axis is called ψ. In order to obtain precise formulas one should be careful about the sign conventions. Positive angles

in the x_1x_2 plane satisfy the usual convention. Thus the angle between the x_1 axis and the x_2 axis is, by definition, $(1/2)\pi$ while the angle between the x_2 axis and the x_1 axis is $-(1/2)\pi$. The sign for the angle ψ is established by the convention that the vector angular velocity is of the form $\dot{\psi}N$. The configuration space of the system is $Q=\mathbb{T}^3\times\mathbb{R}^2$, and a generic point is $q=(q_1,q_2,q_3,q_4,q_5)\equiv(\psi,\theta,\epsilon,x_1,x_2)$. The Lagrangian is given by

$$L(q,\dot{q})=\tfrac{1}{2}I\dot{\psi}^2+\tfrac{1}{2}J\dot{\theta}^2+\tfrac{1}{2}M\dot{x}^2-\tfrac{1}{2}K\epsilon^2,$$

where I is the moment of inertia of the wheel with respect to its axis, J is the moment of inertia of the wheel with respect to any one of its diameters, M is the mass of the wheel, and K is the constant of elasticity introduced before, which by definition satisfies $T=-K\epsilon$, where T is the vertical torque. The kinetic energy due to the velocity of rotation $\dot{\epsilon}$ of the small flattened piece of material about the zone of contact is small and we will assume that it is 0 for simplicity, which is also in agreement with general standard assumptions for this kind of approximate models.[24]

Next we shall describe the kinematic constraints and the variational constraints. The kinematic constraint C_K, is given by the equations

$$\dot{x}_1=\dot{\psi}\cos(\theta-\epsilon), \tag{18}$$

$$\dot{x}_2=\dot{\psi}\sin(\theta-\epsilon), \tag{19}$$

$$-\ddot{\psi}\,\mathrm{tg}\,\epsilon+\dot{\psi}(\dot{\theta}-\dot{\epsilon})=(\mathrm{sign}\,\dot{\psi})\frac{a}{M}\mathrm{tg}\,\epsilon. \tag{20}$$

The first two equations represent the nonsliding condition for the center of the zone of contact, and they are the same as the ones that appear in the case of a rigid rolling disk, or wheel, except for the small angle ϵ. We should emphasize that here we are working to first order approximation only, which means that powers of ϵ greater than 1 may be neglected. The last equation comes from Rocard's condition,

$$|F|=a\sin|\epsilon|,$$

where a is a positive physical constant and F is the force normal to the wheel exerted by the floor, while the wheel is rolling with nonzero velocity. More precisely, F is the N component of the centripetal force, that is we have $F=\langle M\ddot{x},N\rangle$. The sign conventions are encoded in the following more precise version of Rocard's formula

$$F=(\mathrm{sign}\,\dot{\psi})a\sin\epsilon,$$

where ϵ must be interpreted as being the angle between the normal $\mathbf{n}$ to the curve and N if $F>0$ while it must be interpreted as being the angle between $\mathbf{n}$ and $-N$ if $F<0$. Recall that Rocards's formula is valid for ϵ close to 0 only. A couple of remarks are in order for future use. First, as we have said before, Rocard's theory is valid modulo infinitesimals of order $(\sin\epsilon)^2$. Second, with the previous sign conventions and according to Rocard's formula it is not difficult to show that $\epsilon(\dot{\theta}-\dot{\epsilon})\geqslant 0$. It also follows from the expression of Rocard's formula given by (20) that for $\epsilon=0$ the curve $x(t)$ must have a point of inflection, that is $\dot{\theta}-\dot{\epsilon}=0$.

It is clear that (20) involves the first and second derivatives of some of the variables with respect to time, moreover, the dependence on the first derivatives is nonlinear, therefore it is far from the typical constraints of D'Alembert type. To obtain equation (20) we may assume, without loss of generality, that $\dot{\psi}>0$. We simply differentiate (18) and (19) with respect to time, and replace in the equation $(\mathrm{sign}\,\dot{\psi})a\sin\epsilon=\langle M\ddot{x},N\rangle$. Now let us consider the following variational constraints C_V, to be imposed on variations δq:

$$\delta\psi\cos\theta-\delta x_1=0, \tag{21}$$

$$\delta\psi\sin\theta-\delta x_2=0, \tag{22}$$

$$\delta\theta-\delta\epsilon=0. \tag{23}$$

Consider the curves $q(t)$ satisfying

$$\delta\int_{t_0}^{t_1}L(q,\dot{q})\mathrm{d}t=0,$$

for variations δq satisfying $\delta q(t_i)=0$, for $i=1,2$, and also the variational constraints C_V. Those curves are the ones satisfying the following *dynamic equations*:

$$I\ddot{\psi}+M\ddot{x}_1\cos\theta+M\ddot{x}_2\sin\theta=0, \tag{24}$$

$$J\ddot{\theta}+K\epsilon=0, \tag{25}$$

obtained by the usual integration by parts arguments. These dynamic equations give balance between forces of the constraint and rate of change of momentum. The resultant of the forces exerted by the plane of contact on the wheel has positive upwards vertical component which is compensated by gravity, while the horizontal component, which is given by $M\ddot{x}$, is decomposed in the directions $(\cos\theta,\sin\theta)$ and $(-\sin\theta,\cos\theta)$. The first one is compensated by the rate of change of the angular momentum $I\ddot{\psi}$ and the second is compensated by the nonsliding constraint force. The vertical component of the torque of the forces exerted by the plane on the wheel is $K\epsilon$ which is compensated by $J\ddot{\theta}$. The other components of the torque are automatically compensated because we are assuming that the wheel is forced to remain vertical. The system of dynamic equations together with the kinematic constraints equations C_K completely describe the motion of the wheel.

In the previous example, we should emphasize, again, the distinction between *kinematic constraints* and *variational constraints*. They are conceptually different, and this difference is implicit in the usual statement of the principle of virtual work. However, in the literature this distinction is usually not emphasized, and for good reason, since in those cases where D'Alembert's principle can be applied the variational constraints and the kinematic constraints coincide. Nonholonomic systems that cannot be treated using D'Alembert method have been considered for instance by Chetaev[10] where a procedure to deal with general first order nonlinear constraints is devised (see also Refs. 1 and 25). In Marle[22] it is clearly stated that constraint forces cannot be derived in general from the kinematic constraints and have to be added as part of the physical description of the system. Furthermore in Ref. 13 it was explicitly stated a formulation for first order Lagrangian and Poisson nonholonomic systems where kinematic constraints and constraint forces are given as independent entities.

In the case of the elastic rolling ball the forces of the constraint are normal to the direction of the motion of the ball and there is no dissipation of energy. However, for a viscoelastic rolling ball there is certainly dissipation of energy and the component of the force of the constraint in the direction of the motion can be calculated using results from Ref. 4. This kind of system can also be approached using the kind of generalization of D'Alembert's principle described in Sec. IV. The rate of dissipation of energy for a pneumatic tire rolling according to Rocard's theory can be easily calculated. Since the energy is given by $E=(1/2)I\dot{\psi}^2+(1/2)J\dot{\theta}^2+(1/2)M\dot{x}^2+(1/2)K\epsilon^2$, using the kinematic constraints (18), (19) and the dynamic equations derived before we can show after some easy calculations that $\dot{E}=-(M\dot{\psi}^2+K)\epsilon(\dot{\theta}-\dot{\epsilon})$, modulo infinitesimals of order ϵ^2. Since $\epsilon(\dot{\theta}-\dot{\epsilon})\geqslant 0$ as we have explained before we have $\dot{E}\leqq 0$, which means that in general there is dissipation of energy. The limit case $\epsilon=0$ gives $\dot{E}=0$, which reveals that Rocard's theory does

not take into account the relatively small dissipation of energy that occurs when the tire rolls in a straight line. To prove the previous formula we proceed as follows. We can easily see that $\dot{E}=I\dot{\psi}\ddot{\psi}+J\dot{\theta}\ddot{\theta}+M\dot{x}\cdot\ddot{x}+K\epsilon\dot{\epsilon}$. By differentiating (18) and (19) we can easily see that $\dot{x}\cdot\ddot{x}=\dot{\psi}\ddot{\psi}$ and from this and the dynamic equation (25) we obtain $(I+M)\dot{\psi}\ddot{\psi}-K\epsilon(\dot{\theta}-\dot{\epsilon})=0$. Using (18), (19), and (24) we obtain, modulo higher order infinitesimals, that $(I+M)\ddot{\psi}=-M\dot{\psi}\epsilon(\dot{\theta}-\dot{\epsilon})$ therefore $(I+M)\ddot{\psi}\dot{\psi}=-M\dot{\psi}^2\epsilon(\dot{\theta}-\dot{\epsilon})$, from which we finally obtain $\dot{E}=-(M\dot{\psi}^2+K)\epsilon(\dot{\theta}-\dot{\epsilon})$. From a general point of view we may say that the distinction between variational and kinematic constraints implies that the infinitesimal work of the constraint forces in general does not vanish for some admissible infinitesimal displacements, which is the reason why the forces of the constraint may produce work.

In the next section we define a class of nonholonomic systems with higher order nonlinear constraints based on the introduction of both kinematic and variational constraints. We will also show that procedures like D'Alembert's principle or Chetaev's procedure fall into this scheme. We propose that questions of a general nature on nonholonomic systems, like reduction by the symmetry, Legendre transformation, and many others should be approached for the general case of higher order constraints using the scheme based on the introduction of both kinematic and variational constraints.

IV. A PRINCIPLE OF VIRTUAL WORK FOR LAGRANGIAN SYSTEMS WITH NONLINEAR HIGHER ORDER NONHOLONOMIC CONSTRAINTS

Let Q be a configuration space of dimension n and let $L:TQ\to\mathbb{R}$ be a given Lagrangian. Then we have the Euler–Lagrange operator $\mathcal{EL}:T^{(2)}Q\to T^*Q$ which is given in coordinates by

$$\mathcal{EL}_i([q]^{(2)})\,\delta q^i=\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{q}^i}([q]^{(2)})-\frac{\partial L}{\partial q}([q]^{(2)})\right)\delta q^i.$$

A *kinematic constraint of order k* is, by definition, a subset $C_K\subseteq T^{(k)}Q$, for some $k=0,1,2,\ldots$. The subset C_K is often defined by equations $R_K([q]^{(k)})=0$, where $R_K:T^{(k)}Q\to\mathbb{R}^r$, for some $r=1,2,\ldots$. For example, if $k=0$ and R_K is a submersion then C_K is a nonsingular holonomic constraint. If $k=1$ and $R_K(q,\dot{q})=R_{Ki}(q)\dot{q}^i$ defines a distribution of constant rank, we have the typical situation of D'Alembert's principle. If $R_K(q,\dot{q})$ is a general function we have the situation considered by Chetaev.[10] In the case of the elastic rolling ball we have, if we choose the constraint given by Eq. (2) as we have explained before, $n=5$, $k=1$, $r=3$, and

$$R_K(A,a,\dot{A},\dot{a})=(\omega_2-\dot{a}_1,-\omega_1-\dot{a}_2,\omega_3).$$

Alternatively, as we have explained before, if we choose the constraint given by Eq. (7), we have, $n=5$, $k=2$, $r=3$,

$$R_K(A,a,\dot{A},\dot{a},\ddot{A},\ddot{a})=(\omega_2-\dot{a}_1,-\omega_1-\dot{a}_2,\omega_1\dot{\omega}_2-\omega_2\dot{\omega}_1-\omega_3(\omega_1^2+\omega_2^2)). \tag{26}$$

In the case of the Rocard's theory of a pneumatic tire, we have $n=5$, $k=2$, $r=3$, and

$$R_K(\psi,\theta,\epsilon,x_1,x_2,\dot{\psi},\dot{\theta},\dot{\epsilon},\dot{x}_1,\dot{x}_2)=\Big(\dot{x}_1-\dot{\psi}\cos(\theta-\epsilon),\dot{x}_2-\dot{\psi}\sin(\theta-\epsilon),-\ddot{\psi}\,\mathrm{tg}\,\epsilon+\dot{\psi}(\dot{\theta}-\dot{\epsilon})$$
$$-(\mathrm{sign}\,\dot{\psi})\frac{a}{M}\mathrm{tg}\,\epsilon\Big). \tag{27}$$

A *constraint on the variations of order l* is a subset $C_V\subseteq T^{(l)}Q\times_Q TQ$ defined by equations $R_V([q]^{(l)},\delta q)=0$ where R_V is linear in the variable δq, so we shall write as usual $R_V([q]^{(l)},\delta q)=R_V([q]^{(l)})\,\delta q$ or, in coordinates, $R_V([q]^{(l)},\delta q)=R_{Vi}([q]^{(l)})\,\delta q^i$. For each $[q]^{(l)}\in T^{(l)}Q$, we let $C_V([q]^{(l)})=\{\delta q\in TQ:([q]^{(l)},\delta q)\in C_V\}$.

Statement of the principle: The main object defined in this paper is the class of Lagrangian nonholonomic systems defined by data (L, C_K, C_V) whose *dynamical equations* are derived by using the variational principle

$$\delta \int_{t_0}^{t_1} L(q,\dot{q})\mathrm{d}t = 0,$$

where variations δq are restricted by $\delta q \in C_V([q]^{(l)})$, or, equivalently, $R_V([q]^{(l)}) \cdot \delta q = 0$. Then the *equations of motion* are given by the *dynamical equations*

$$\mathcal{EL}_i([q]^{(2)}) \in R_V([q]^{(l)})^o$$

and the *kinematic constraint* equations $[q]^{(l)} \in C_K$ or, equivalently,

$$R_K([q]^{(k)}) = 0.$$

Equations of motion will be derived in the next section.

The previous principle, which is contained in the general idea of the principle of virtual work, imposes, through the dynamical equations, restrictions on the forces of the constraints. But, contrary to what happens with D'Alembert's principle, the forces of the constraints derived from the principle stated above will in general produce work.

The class of higher order nonholonomic systems just defined contains several important classes of nonholonomic systems. For example, for the class of nonholonomic systems that are tractable using D'Alembert's principle we have, by definition, $k=1$, $l=0$ and C_K is the distribution where for each $q \in Q$ the space of the distribution is $C_V(q) \subseteq TQ$. Thus, the kinematic constraint and the constraint on the variations essentially coincide in this case. In the case of nonlinear kinematic constraints considered by Chetaev given by $R_K(q,\dot{q}) = 0$ we have $l=1$ and the variational constraints are defined, according to Chetaev, by

$$R_V(q,\dot{q}) \cdot \delta q = \frac{\partial R_K(q,\dot{q})}{\partial \dot{q}} \cdot \delta q.$$

Remark 4.1: In the mathematical literature one finds some examples of higher order constraints in nonholonomic problems (for instance, see Refs. 28, 25, 15, and 29). In the previous references an extension of the Chetaev principle for kinematic second order constraints is applied, namely,

$$(R_K)_i(q,\ \dot{q},\ \ddot{q}) = 0, \quad 1 \leqslant i \leqslant m$$

and variational constraints R_V are derived from the kinematic constraints by

$$R_V(q,\dot{q},\ddot{q}) \cdot \delta q = \frac{\partial R_K}{\partial \ddot{q}} \cdot \delta q = 0.$$

In the case of the elastic rolling ball the variational constraints are given by (10). In the case of the pneumatic tire according to Rocard's theory the kinematic constraints are given by (18), (19), (20) and the variational constraints are given by (21), (22), (23).

We emphasize once again that the notions of kinematic constraints and variational constraints are independent and one should not attempt, for instance, to derive variational constraints from kinematic constraints by a universal procedure. In order to illustrate further the necessity of such a point of view we will describe next the example of Greidanus's theory of a pneumatic tire, where the kinematic constraint defines a distribution like in D'Alembert's principle but the variational constraints are not given by the same distribution, therefore they are not the ones prescribed by D'Alembert's principle.

Pneumatic tires according to Greidanus: Several approaches to the dynamics of a pneumatic tire like those of Rocard, Greidanus, Keldys, and others can be found in Refs. 11, 27, 26, 24. To describe Greidanu's approach we shall consider the simpler setting of Rocard's approach described before, but this time we allow, in addition, for a lateral deformation ξ. The absolute value of the quantity ξ is the distance between the projection of the center of the wheel on the plane (x_1,x_2) and the center of the zone of contact. In the Rocard's approach described above the value of ξ is 0. We must remark that we are considering in this paper only the case of Greidanus's theory in which the wheel is kept vertical. The physical reason for the appearance of the displacement ξ is of course the lateral deformation due to the centrifugal force given the elasticity of the material.

The kinematic constraints are

$$\dot{x}_1=\dot{\psi}\cos(\theta-\epsilon), \tag{28}$$

$$\dot{x}_2=\dot{\psi}\sin(\theta-\epsilon), \tag{29}$$

$$\dot{\theta}-\dot{\epsilon}=\dot{\psi}(\alpha\xi+\beta\epsilon). \tag{30}$$

The first two equations are the same as in Rocard's approach. The last one expresses the fact that the curvature of the trajectory of the center of the contact zone is, for a given speed of rotation of the wheel, proportional to a linear combination of the deformation parameters ξ and ϵ, where $\alpha>0$ and $\beta>0$. This replaces Rocard's constraint. We see that the kinematic constraints define a distribution. The variational constraints are

$$\delta x_1=\delta\psi\cos\theta, \tag{31}$$

$$\delta x_2=\delta\psi\sin\theta, \tag{32}$$

$$\delta\theta-\delta\epsilon=0. \tag{33}$$

These variational constraints are different from the kinematic constraints, therefore we are not using here D'Alembert's principle. The projection of the center of the wheel on the plane is the point (y_1,y_2) given by

$$y_1=x_1+\xi\sin\theta, \tag{34}$$

$$y_2=x_2-\xi\cos\theta. \tag{35}$$

It is more convenient to calculate the kinematic constraints and the variational constraints in terms of y_1 and y_2 instead of x_1 and x_2. The kinematic constraints are

$$\dot{y}_1=\dot{\psi}\cos(\theta-\epsilon)+\dot{\xi}\sin\theta+\xi(\cos\theta)\dot{\theta}, \tag{36}$$

$$\dot{y}_2=\dot{\psi}\sin(\theta-\epsilon)-\dot{\xi}\cos\theta+\xi(\sin\theta)\dot{\theta}, \tag{37}$$

$$\dot{\theta}-\dot{\epsilon}=\dot{\psi}(\alpha\xi+\beta\epsilon). \tag{38}$$

The variational constraints are

$$\delta y_1=\delta\psi\cos\theta+\delta\xi\sin\theta+\xi(\cos\theta)\delta\theta, \tag{39}$$

$$\delta y_2=\delta\psi\sin\theta-\delta\xi\cos\theta+\xi(\sin\theta)\delta\theta, \tag{40}$$

$$\delta\theta-\delta\epsilon=0. \tag{41}$$

The Lagrangian is

$$L(\psi,\theta,\epsilon,y_1,y_2,\xi,\dot{\psi},\dot{\theta},\dot{\epsilon},\dot{y}_1,\dot{y}_2,\dot{\xi})=\tfrac{1}{2}I\dot{\psi}^2+\tfrac{1}{2}J\dot{\theta}^2+\tfrac{1}{2}M((\dot{y}_1)^2+(\dot{y}_2)^2)-\tfrac{1}{2}\alpha\xi^2-\tfrac{1}{2}\beta\epsilon^2.$$

Then, equations of motion are given by kinematic constraints (36), (37), (38) and dynamic equations

$$I\ddot{\psi}+M\ddot{y}_1\cos\theta+M\ddot{y}_2\sin\theta=0, \tag{42}$$

$$J\ddot{\theta}+M\xi\ddot{y}_1\cos\theta+M\xi\ddot{y}_2\sin\theta+\beta\epsilon=0, \tag{43}$$

$$-M\ddot{y}_1\sin\theta+M\ddot{y}_2\cos\theta-\alpha\xi=0. \tag{44}$$

We can easily check that the previous equations represent the balance between rate of change of momentum and forces of the constraints.

For high values of α the deformation ξ remains small. Moreover, for $\alpha\to\infty$ we have $\xi\to 0$ and the dynamic equations (42), (43) of Greidanu's theory become the equations (24), (25) of Rocard's theory, provided that $K=\beta$. Using this and the fact that the two first kinematic constraints (18), (19) of Rocard's theory coincide with the first two kinematic constraints (28), (29) of Greidanu's theory and also the fact that for $\alpha\to\infty$ the mechanical energy E for both theories tend to the same value, one can prove, proceeding as in the case of Rocard's theory, that at least for high values of α a pneumatic tire moving according to Greidanus theory is a dissipative system. This shows that D'Alembert's principle does not provides a good model for this kind of system, even though the kinematic constraints are linear.

V. EQUATIONS OF MOTION

Let us recall some basic facts of the geometry of the tangent bundle. The *vertical endomorphism S* is defined in local natural coordinates $(q^A,\dot{q}^A)$ on TQ by

$$S=\frac{\partial}{\partial\dot{q}^A}\otimes \mathrm{d}\,q^A \quad .$$

The Liouville vector field Δ on TQ is locally defined by

$$\Delta=\dot{q}^A\frac{\partial}{\partial\dot{q}^A} \quad .$$

A second order differential equation is a vector field Γ on TQ such that $S(\Gamma)=\Delta$. We have the following local expression for Γ:

$$\Gamma=\dot{q}^A\frac{\partial}{\partial q^A}+F^A(q,\dot{q})\frac{\partial}{\partial\dot{q}^A} \quad .$$

An integral curve of Γ is always the tangent prolongation of its projection $q(t)$ on Q, called a *solution* of Γ. It satisfies the following explicit system of second order differential equations:

$$\frac{\mathrm{d}^2q^A}{\mathrm{d}t^2}=F^A(q,\dot{q}) \quad .$$

We also note that the kernel and image of S consist of vertical vector fields. Moreover, S acts by duality on forms and the kernel and image of S^* consists of horizontal one-forms.

Given a Lagrangian function $L:TQ\to\mathbb{R}$, we construct the two-form $\omega_L=-\mathrm{d}(S^*(\mathrm{d}L))$ on TQ, and the energy function $E_L=\Delta L-L$ (see Ref. 20). A remarkable property of S and ω_L is the following $i_S\omega_L=0$, or, in other words,

$$S^*\circ\hat{\omega}_L=-\hat{\omega}_L\circ S, \tag{45}$$

where $\hat{\omega}_L$ denotes the map $T(TQ)\to T^*(TQ)$ defined by contraction with ω_L.

Observe that if L is regular, then ω_L is a symplectic form, and there is a unique vector field Γ_L satisfying

$$i_{\Gamma_L}\omega_L = \mathrm{d}E_L,$$

or, in other words, Γ_L is the Hamiltonian vector field with Hamiltonian energy E_L. It is well known that Γ_L is a second order differential equation on TQ, namely, the Euler–Lagrange equations for L.

Without the regularity condition, the Euler–Lagrange equations form a system of second order differential equations in Q, in implicit form, that is, a submanifold D_2 of $T^{(2)}Q$, determined by

$$D_2=\{w\in T^{(2)}Q \;\mid\; i_{j_2(w)}\omega_L(\tau^{(1,2)}(w))=\mathrm{d}E_L(\tau^{(1,2)}(w))\} \tag{46}$$

or, in other words,

$$D_2=\{w\in T^{(2)}Q \;\mid\; \mathcal{EL}(w)=0\}\quad .$$

The class of higher order nonholonomic systems studied in this paper, are determined by data (L,C_K,C_V). Next we will show that the equations of motion of this kind of systems is a system of implicit kth-order differential equations. In what follows, and without loss of generality, we will always suppose that $k\geqslant l$ and $k\geqslant 2$.

In our case the constraint on the variations are determined by a subset $C_V\subseteq T^{(l)}Q\times_Q TQ$. Therefore for each point $[q]^{(l)}$ we obtain the annihilator $C_V^0([q]^{(l)})\subseteq T_q^*Q$ of $C_V([q]^{(l)})$. Denote by $F_V([q]^{(l)})$ the subspace of $T^*(TQ)$ determined by $F_V([q]^{(l)})=(\tau_Q)^*(C_V^0([q]^{(l)}))$. Now, we shall define the subset of $T^{(k)}Q$:

$$M_V=\{[q]^{(k)}\in T^kQ \;\mid\; i_{j_2([q]^{(2)})}\omega_L([q]^{(1)})-\mathrm{d}E_L([q]^{(1)})\in F_V([q]^{(l)})\}\quad .$$

Therefore, the nonholonomic system associated to (L,C_K,C_V), determines a kth-order implicit system given by the submanifold $M_{KV}=C_K\cap M_V$. The solutions of the problem (L,C_K,C_V) are the curves $\gamma: I\to Q$ such that $\gamma^{(k)}\subset M_{KV}$.

VI. FURTHER RESULTS AND EXAMPLES

The scheme generalizing D'Alembert principle, for the case of higher order constraints described in Sec. IV is not of course the most general case. It is not the purpose of the present work to expose the most general possible formalism, but on the contrary, to provide a scheme which is useful in a variety of problems in mechanics. This scheme is also useful to deal with important questions of a general character in mechanics, like reduction, Legendre transformation and others. Some of these questions will be the purpose of future work and in this section we will consider some partial results only.

Reduction of invariant systems with higher order constraints on a group: In this paragraph we explain how to reduce invariant Lagrangian systems with higher order nonholonomic constraints on a group. The more general case of systems on a principal bundle will be the purpose of a future work. However, in the present section we will show how to proceed in an example where the bundle is trivial, which illustrates some of the features of the general theory. Assume that the configuration space is a group G and that the Lagrangian L, the kinematic constraint C_K and the constraint on the variations C_V are left invariant. For right invariant systems we can proceed in a similar way. For each $r=1,2,\ldots$ we have an identification

$$\alpha_r: T^{(r)}G/G\to r\mathfrak{g},$$

where $r\mathfrak{g}=\mathfrak{g}\oplus\cdots\oplus\mathfrak{g}$, is the direct sum of r copies of $\mathfrak{g}$. This identification is uniquely defined by the map $[g]^{(r)}\to[v]^{(r)}$, where $v=g^{-1}\dot{g}$, and $[v]^{(r)}=(v^{(0)},v^{(1)},\ldots,v^{(r-1)})$, where, by definition, we have

$$v^{(i)}=\frac{\mathrm{d}^i}{\mathrm{d}t^i}v,$$

for $r=0,1,\ldots,r-1$. Under the identification α_k, the quotient of the kinematic constraint C_K/G, becomes a subset, called *reduced kinematic constraint*, $\mathfrak{C}_K\subseteq k\mathfrak{g}$. Similarly, for each $r=1,2,\ldots$ we have an identification

$$\beta_r:(T^{(r)}G\times_G TG)/G\to r\mathfrak{g}\oplus\mathfrak{g}.$$

This identification is uniquely defined by the map $([g]^{(r)},\delta g)\to([v]^{(r)},\eta)$ with $[v]^{(r)}=(v^{(0)},v^{(1)},\ldots,v^{(r-1)})$, as before, and $\eta=g^{-1}\delta g$. Under the identification β_l, the quotient of the constraint on the variations C_V/G, becomes a subset, called *reduced variational constraints*, $\mathfrak{C}_D\subseteq l\mathfrak{g}\oplus\mathfrak{g}$. Since the equations $R_K([g]^{(k)})=0$ and $R_V([g]^{(l)},\delta g)=0$ are invariant, we have reduced equations $\mathfrak{R}_K([v]^{(k)})=0$ and $\mathfrak{R}_V([v]^{(l)},\eta)=0$. Since $R_V([g]^{(l)},\delta g)=R_V([g]^{(l)})\cdot\delta g$ is linear in δg, we have that $\mathfrak{R}_V([g]^{(l)})\cdot\eta$ is also linear in η. The Lagrangian L gives rise to a reduced Lagrangian $l:\mathfrak{g}\to\mathbb{R}$. We have the following theorem.

Theorem 6.1: *The following conditions are equivalent*:

(i) *The curve $g(t)$ satisfies*

$$\delta\int_{t_0}^{t_1}L(g,\dot{g})\mathrm{d}t=0,$$

for all δg such that $\delta g(t)\in C_V([g]^{(l)}(t))$, for all $t\in[t_0,t_1]$ [equivalently $R_V([g]^{(l)}(t),\delta g(t))=0$ for all $t\in[t_0,t_1]$] and $\delta g(t_i)=0$ for $i=0,1$; $[g]^{(k)}(t)\in C_K$ [equivalently $R_K([g]^{(k)}(t))=0$ for all $t\in[t_0,t_1]$].

(ii) *The curve $g(t)$ satisfies the equation*

$$\left(\frac{\partial L}{\partial g}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{g}}\right)([g]^{(2)}(t))\cdot\delta g=0,$$

for all δg such that $\delta g(t)\in C_V([g]^{(l)}(t))$, for all $t\in[t_0,t_1]$ [equivalently $R_V([g]^{(l)}(t),\delta g(t))=0$ for all $t\in[t_0,t_1]$] and $\delta g(t_i)=0$ for $i=0,1$; $[g]^{(k)}(t)\in C_K$ [equivalently $R_K([g]^{(k)}(t))=0$ for all $t\in[t_0,t_1]$].

(iii) *The curve $v(t)=g^{-1}(t)\dot{g}(t)$ satisfies*

$$\delta\int_{t_0}^{t_1}l(v)\mathrm{d}t=0$$

for all $\delta v=\dot{\eta}+[v,\eta]$ where $\eta(t)\in\mathfrak{C}_V([v]^{(l)}(t))$ for all $t\in[t_0,t_1]$ [equivalently $\mathfrak{R}_V([v]^{(l)}(t),\eta(t))=0$ for all $t\in[t_0,t_1]$] and $\eta(t_i)=0$, for $i=0,1$; $[v]^{(k)}(t)\in\mathfrak{C}_K$ [equivalently $\mathfrak{R}_K([v]^{(k)}(t))=0$ for all $t\in[t_0,t_1]$].

(iv) *The curve $v(t)=g^{-1}(t)\dot{g}(t)$ satisfies the equation*

$$\left(-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial l}{\partial v}+\mathrm{ad}^*\frac{\partial l}{\partial v}\right)([v]^{(2)}(t))\cdot\eta$$

for all η such that $\eta(t)\in\mathfrak{C}_V([v]^{(l)}(t))$ for all $t\in[t_0,t_1]$ [equivalently $\mathfrak{R}_V([v]^{(l)}(t),\eta(t))=0$ for all $t\in[t_0,t_1]$] and $\eta(t_i)=0$, for $i=0,1$; $[v]^{(k)}(t)\in\mathfrak{C}_K$ [equivalently $\mathfrak{R}_K([v]^{(k)}(t))=0$ for all $t\in[t_0,t_1]$].

The proof of this theorem can be performed proceeding as in Ref. 7. The idea of the proof is simple. Given a curve $g(t)$ such that $[g]^{(k)}(t)\in C_K$ for all $t\in[t_0,t_1]$ we take variations $\delta g(t)=g(t)\eta(t)$ for all $t\in[t_0,t_1]$ such that $\delta g(t)\in C_V([g]^{(l)}(t))$ for all $t\in[t_0,t_1]$. Since $v(t)=g^{-1}(t)\dot{g}(t)$ we can easily check that $\delta v(t)=\eta(t)+[v(t),\eta(t)]$. The rest of the proof follows by keeping track of the reduction of both the kinematic constraints and the variational constraints.

Symmetry of the elastic rolling ball: An interesting case occurs when, for each $[g]^{(l)}$, $C_V([g]^{(l)})$ depends only on g giving rise to a distribution D on G. This happens in the case of the rolling ball studied in Sec. II. Let us see how the previous theorem applies to this case. First of all we observe that the configuration space is the direct product group $\mathrm{SO}(3)\times\mathbb{R}^2$. Since we are assuming an homogeneous ball the kinetic energy Lagrangian is not only left invariant but also right invariant. This is important because the constraints are also right invariant. We can thus reduce by the right action of the group on itself. For $\eta=(\alpha,w)$ and taking into account that the Lie bracket in $\mathfrak{so}(3)$ is *minus* the standard one because we are reducing by *right* actions, we have

$$\delta\int_{t_0}^{t_1}\left(\frac{1}{2}I\omega^2+\frac{1}{2}MV^2\right)\mathrm{d}t=0, \tag{47}$$

$$\delta\omega=\dot{\alpha}-[\omega,\alpha], \tag{48}$$

$$\alpha(t_i)=0 \quad \text{for } i=0,1, \tag{49}$$

$$\delta V=\dot{w}, \tag{50}$$

$$w(t_i)=0 \quad \text{for } i=0,1, \tag{51}$$

$$w=(\alpha_2,-\alpha_1), \tag{52}$$

$$V=(\omega_2,-\omega_1), \tag{53}$$

$$\omega_3=0. \tag{54}$$

Equations (48), (50), (51) represent the reduced variational constraints while Eqs. (52), (53), (54) represent the reduced kinematic constraints [as we have explained before, Eq. (54) can be replaced by $\omega_2\dot{\omega}_1-\omega_1\dot{\omega}_2=\omega_3(\omega_1^2+\omega_2^2)$]. We obtain the equations of motions written in Sec. II, that is Eqs. (13), (14), (15), (16), (17). The reduced version of D'Alembert's principle consists of all the previous conditions plus the condition $\alpha_3=0$, which of course corresponds to the kinematic constraint $\omega_3=0$. The D'Alembert equations are (13), (14), (16), (17).

Rigid ball rolling on a moving plane: For dealing with examples where the configuration space is a principal bundle rather than a group and the constraints and also the Lagrangian are invariant we need to generalize the previous theory, which we plan to do as part of future works. However, some simple examples can be worked out directly as we will see next. Let us consider a rigid ball rolling on a plane while this plane is being continuously deformed according to the law $\varphi_t:\mathbb{R}^2\to\mathbb{R}^2$. The Eulerian velocity is $v_t(x)=\dot{\varphi}_t\circ\varphi_t^{-1}(x)$ and we will assume that $v_t(x)=v(x)$ is independent of t. For a rigid ball rolling on a fixed plane, that is when $v(x)=0$, the system is governed by the D'Alembert principle which in this case is like the principle of virtual work described in Sec. II for an elastic ball except that one should eliminate the kinematic constraint $\omega_3=0$. When $v(x)\neq 0$ there is an extra force since the point a of the ball which is in contact with the plane, is moving with velocity $v(a)$, that is, the kinematic constraint becomes $(\omega_2,-\omega_1)=\dot{a}-v(a)$. By differentiating with respect to t we obtain $(\dot{\omega}_2,-\dot{\omega}_1)=\ddot{a}-Dv(a)\dot{a}$. Using this it can be easily seen that the force exerted by the floor on the ball is $M((\dot{\omega}_2,-\dot{\omega}_1)+Dv(a)\cdot(\omega_2,-\omega_1)+Dv(a)\cdot v(a))$. Equations of motion can be easily derived by direct application of the basic rules of mechanics and we obtain

$$(I+M)(\dot{\omega}_2,-\dot{\omega}_1)=-MDv(a)\cdot[(\omega_2,-\omega_1)+v(a)], \tag{55}$$

$$\dot{\omega}_3=0. \tag{56}$$

Now we want to obtain the same equations using the formalism of the principle stated in Sec. IV. As in the case of the elastic rolling ball this is not straightforward, which emphasizes the advan-

tages of having a way of reducing by the symmetry as we will show next. The example under consideration is invariant with respect to the right action of SO(3) only because in this case the kinematic constraint is not necessarily invariant under translations. As we have said before in this simple example a general theory of reduction for systems on a principal bundle is not needed. Moreover, it is not difficult to prove directly that the following reduced principle of virtual work gives the correct equations of motion,

$$\delta \int_{t_0}^{t_1} \left(\frac{1}{2} I \omega^2 + \frac{1}{2} M \dot{a}^2 \right) \mathrm{d}t = 0, \tag{57}$$

$$\delta \omega = \dot{\alpha} - [\omega, \alpha], \tag{58}$$

$$\alpha(t_i) = 0 \quad \text{for } i = 0,1, \tag{59}$$

$$\delta a = (\alpha_2, -\alpha_1), \tag{60}$$

$$(\omega_2, -\omega_1) = \dot{a} - v(a). \tag{61}$$

Equations (58), (59), and (60) represent the variational constraints while Eq. (61) is the kinematic constraint.

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Separable Hilbert space in loop quantum gravity

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We study the separability of the state space of loop quantum gravity. In the standard construction, the kinematical Hilbert space of the diffeomorphism-invariant states is nonseparable. This is a consequence of the fact that the knot space of the equivalence classes of graphs under diffeomorphisms is noncountable. However, the continuous moduli labeling these classes do not appear to affect the physics of the theory. We investigate the possibility that these moduli could be only the consequence of a poor choice in the fine-tuning of the mathematical setting. We show that by simply choosing a minor extension of the functional class of the classical fields and coordinates, the moduli disappear, the knot classes become countable, and the kinematical Hilbert space of loop quantum gravity becomes separable. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763247]

I. INTRODUCTION

Loop quantum gravity (LQG) is a background-independent quantization of classical general relativity which yields a discrete, combinatorial picture of Planck-scale quantum geometry. (For an introduction and references, see, for instance, Ref. 9.) Quantum space turns out to be described in terms of a basis of abstract spin-network states, or s-knot states, labeled by discrete quantum numbers. However, the picture is not truly entirely discrete. If the nodes of the s-knots have sufficiently high valence (that is, when a sufficiently high number of links meet), s-knots are labeled also by certain *continuous* moduli parameters. The existence of these moduli was pointed out in Ref. 11 and their structure studied in Ref. 6. Below we give an example of one of these moduli explicitly. These moduli are puzzling. They are virtually undetectable by the operators that represent physical measurements, as well as by the hamiltonian operator that governs the dynamics, and therefore they do not appear to play any significant role in the theory. Still, they spoil the discreetness of the picture and they change the structure of the space of the diffeomorphism-invariant states, $\mathcal{H}_{\text{diff}}$, rather drastically, making it nonseparable. (The space $\mathcal{H}_{\text{diff}}$ is denoted $\mathcal{K}_{\text{diff}}$ in Ref. 9.)

Nonseparability (absence of a countable basis) is generally regarded as pathological in quantum field theory (QFT). A classic discussion on this issue is in Ref. 13. As pointed out in Ref. 14, the nonseparability of $\mathcal{H}_{\text{diff}}$ is not necessarily unacceptable, because $\mathcal{H}_{\text{diff}}$ is a kinematical space that must still be reduced by the hamiltonian constraint equation. But it is nevertheless disturbing. Do we have to interpret it as an indication of a difficulty of the background-independent loop quantization?

In this paper, motivated by the fact that the moduli do not appear to have any physical significance, we consider the possibility that they are indeed spurious. We study the possibility that they are the consequence of a poor choice in setting up the details of the mathematical framework of the theory. It is not unusual that a naive way of setting up a QFT produces a nonseparable

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Hilbert space, which is later cured, making it separable. Indeed, recall that Fock space itself, the prototypical QFT state space, was born precisely to cure nonseparability. A free scalar field can be decomposed into an infinite set of oscillators φ_i, $i=1,\ldots,\infty$. If we quantize each degree of freedom φ_i as a standard quantum harmonic oscillator, we are immediately led to a state space which is the tensor product of an infinite number of separable Hilbert spaces

$$\mathcal{H}=\bigotimes_{i=1,\ldots,\infty} H_i. \tag{1}$$

A basis in $\mathcal{H}$ is given by an infinite sequence of nonnegative integers $|n_1,n_2,\ldots,n_i,\ldots\rangle$, and such infinite sequences are noncountable (for instance, the states with $n_i<10$ are put into one-to-one correspondence with the real numbers $0\leqslant x<1$ by the decimal representation of x); hence $\mathcal{H}$ is nonseparable. Fock found a way to circumvent the problem by simply selecting the subspace $\mathcal{F}$ of $\mathcal{H}$ spanned by basis vectors where an arbitrary but finite number of n_i differ from zero. It is $\mathcal{F}$, called today Fock space, which is the appropriate state space for free QFT. Unlikely $\mathcal{H}$, the Fock space $\mathcal{F}$ provides an *irreducible* representation of the field algebra of the creation and annihilation operators. Thus, a straightforward and simple minded quantization strategy leading to a nonseparable state space has been later corrected to get rid of the nonseparability. Can we do the same in quantum gravity? Are there physical reasons for doing the same in quantum gravity?

In classical field theory, the choice of the functional class of fields and coordinates is to a large extent just a matter of convenience. We can work with solutions of the field equations that are smooth (C^∞), or just twice differentiable (C^2), sometimes distributional, or piecewise constant as in the lattice approximation, or else, according to what is more convenient. The relation between the formal apparatus of field theory and reality is only via the smearing of fields on finite regions of space, and therefore we never empirically test the functional class of a physical field. In quantum gravity, the smooth category is generally chosen, because it appears to be a natural and convenient setting. In the background-independent loop construction, the gauge invariance of general relativity washes away virtually any remnant of the functional class we started from, because the entire short-scale structure is canceled by the gauge transformations. Virtually, but not entirely. Indeed, as we show below, the nodes of sufficiently high valence have a surprising ''rigidity'' under smooth transformation, and this rigidity turns out to be the one responsible for the moduli. Therefore the nonseparability of $\mathcal{H}_{\text{diff}}$ is a bizarre remnant of the initial choice of the smooth category. It is therefore natural to explore the possibility of using a slightly different functional class of fields to start with.

Here we explore a minimal extension of this kind, where fields are allowed isolated points of nondifferentiability. The gauge invariance group of the theory becomes then a ''small'' extension of the diffeomorphism group, which we call *extended diffeomorphism* and denote $Diff^*$. As far as we can see, none of the physical results, physical predictions or physical consequences of LQG studied so far, are affected. However, the knot classes, now formed by graphs under $Diff^*$, turn out to be countable. The continuous moduli disappear and $\mathcal{H}_{\text{diff}}$ becomes separable. The theory describes a quantum structure of space–time that is genuinely combinatorial at the Planck scale.

These results can be taken as evidence that the moduli associated to high-valence nodes are indeed spurious. If we build LQG using the setting described here, or a variant of the same, the moduli are not anymore present, and the kinematical Hilbert space of the diffeomorphism invariant states of LQG is separable.

In Sec. II we review the basic mathematical setting of LQG and the origin of the nonseparability. This paper is mathematically self-contained but for physical motivations and details see Ref. 9. In Sec. III we introduce our main tool, $Diff^*$, and show that the equivalence classes of graphs under $Diff^*$ are countable and the resulting space $\mathcal{H}_{\text{diff}}$ is separable. In Sec. IV, we show that the modification introduced has no effect on the geometrical operators of LQG. We discuss in particular the area operator. In Sec. V we summarize and conclude.

II. NONSEPARABILITY

A. $\mathcal{H}_{\text{diff}}$, the space of the quantum states of physical space

We begin by briefly reviewing the basic mathematical setting of the kinematics of LQG. Classical general relativity can be defined on a four-dimensional differentiable manifold M with topology $\Sigma \times R$, where Σ is a three-dimensional differentiable manifold with a fixed arbitrary topology. The gravitational field can be taken to be a smooth (that is, infinitely differentiable) pseudo-Riemannian metric tensor g on M, satisfying the Einstein equations. Call $\mathcal{E}$ the space of such fields. The corresponding Hamiltonian theory can be defined on Σ. The configuration variable of general relativity can be defined as a smooth local connection one-form A on a SU(2)-principal bundle $\mathcal{P}$ over Σ. Call $\mathcal{A}$ the space of such connections.

We shall use extensively the notion of graph, whose relevance for quantum gravity was first realized by Lewandowski. Here a graph Γ is a finite collection of $L(\Gamma)$ smooth oriented one-dimensional submanifolds of Σ, called links and noted l, overlapping (if they do) only at endpoints, called nodes and denoted n. We say that the link l ends at the node n if n is a boundary point of l. The valence of a node n is the number of links ending at n. We call $\mathcal{G}$ the space of such graphs.

Quantum states are limit of sequences of cylindrical functions, converging in the norm defined below. A cylindrical function $\Psi_{\Gamma,f}: \mathcal{A} \to \mathbb{C}$ is defined as follows. Let $\mathrm{U}_l(A) \in \mathrm{SU}(2)$ be the holonomy of the connection A along l

$$\mathrm{U}_l(A) \equiv \mathcal{P} \exp \int_l A, \tag{2}$$

$\mathcal{P}$ denotes path ordering. A graph Γ defines a map $p_\Gamma: \mathcal{A} \to [\mathrm{SU}(2)]^{\times L(\Gamma)}$; $A \to (\mathrm{U}_l(A))$. By composing this map with a complex valued function f on $[\mathrm{SU}(2)]^{\times L(\Gamma)}$, we obtain the cylindrical function $\Psi_{\Gamma,f} = f \circ p_\Gamma$, given by

$$\Psi_{\Gamma,f}(A) \equiv f(\mathrm{U}_{l_1}(A), \ldots, \mathrm{U}_{l_{L(\Gamma)}}(A)). \tag{3}$$

Since it is always possible to write any two cylindrical functions in terms of the same graph (a cylindrical function on a graph Γ can be re-expressed on another graph Γ' that contains Γ), we can define a scalar product on the space of states using the Haar measure on SU(2)

$$\langle \Psi_{(\Gamma,f)} | \Psi_{(\Gamma,f')} \rangle \equiv \int \mathrm{dU}_1 \cdots \mathrm{dU}_{L(\Gamma)}\, \overline{f(\mathrm{U}_1, \ldots, \mathrm{U}_{L(\Gamma)})} f'(\mathrm{U}_1, \ldots, \mathrm{U}_{L(\Gamma)}). \tag{4}$$

The kinematical Hilbert space $\mathcal{K}$ of LQG is defined as the completion in the Hilbert norm (4) of the space of the cylindrical functions.

Local SU(2) gauge transformations act naturally on this space and the invariant states form a proper subspace $\mathcal{K}_0$. An orthonormal basis in $\mathcal{K}_0$ can be obtained using the spin-network states.[11,3] Consider a graph Γ and color each link l with a unitary irreducible representations j_l of SU(2). At each node n, fix a basis in the space of the invariant elements (the "intertwiners") in the tensor product of the representation spaces associated to the links that end at n, and color the node with an intertwiner i_n of this basis (see Ref. 9 for details). The triple $S = (\Gamma, j_l, i_n)$ is called a spin network. Let the function f_S be defined by the representation matrices for each link l in the representation j_l, contracted with the invariant tensors at each node. The state $\Psi_S[A] \equiv \Psi_{\Gamma,f_S}[A] \equiv \langle A|S \rangle$ is a spin network state. Varying the graph Γ in $\mathcal{G}$, the irreducible representations j_l and the intertwiners i_n in the chosen bases, we obtain an orthonormal basis in $\mathcal{K}_0$.

Finite linear combinations of spin-network states form a dense subspace $\mathcal{S}$ in $\mathcal{K}_0$. Sequences of states that converge weakly on $\mathcal{S}$, form the dual $\mathcal{S}'$. The Gelfand triple $(\mathcal{S} \subset \mathcal{K}_0 \subset \mathcal{S}')$ describes the space of the SU(2) invariant states of the theory. Now, $\mathcal{K}_0$ carries a natural unitary representation $\Psi[A] \to \mathrm{U}_\phi \Psi[A] = \Psi[\phi^{-1} A]$ of the group $Diff_\Sigma$ of the diffeomorphisms of Σ

$$\phi:\Sigma\to\Sigma, \tag{5}$$

which extends naturally to $\mathcal{S}'$ by duality (we have indicated with ϕ also the pull back action generated by the diffeomorphism ϕ on forms). The diffeomorphism invariant states form a linear subspace $\mathcal{H}_{\text{diff}}$ of $\mathcal{S}'$. This space describes the diff-invariant quantum states of the gravitational field; that is, the quantum states of physical space.

A map $P_{\text{diff}}:\mathcal{S}\to\mathcal{S}'$ is naturally defined by

$$(P_{\text{diff}}\Psi)(\Psi')=\sum_{\Psi''=\mathrm{U}_\phi\Psi}\langle\Psi'',\Psi'\rangle, \tag{6}$$

where the sum is over all distinct states Ψ'' that are equal to $\mathrm{U}_\phi\Psi$ for some $\phi\in Diff$. This sum converges and is well defined. The state $P_{\text{diff}}\Psi\in\mathcal{S}'$ is diff-invariant because clearly states related by diffeomorphisms are projected by P_{diff} on the same element of $\mathcal{H}_{\text{diff}}$,

$$P_{\text{diff}}\Psi_S=P_{\text{diff}}(\mathrm{U}_\phi\Psi_S). \tag{7}$$

Furthermore, the states of this form span $\mathcal{H}_{\text{diff}}$. The linear space $\mathcal{H}_{\text{diff}}$ is naturally equipped with a Hilbert space structure by the scalar product

$$\langle P_{\text{diff}}\Psi_S,P_{\text{diff}}\Psi_{S'}\rangle_{\mathcal{H}_{\text{diff}}}\equiv(P_{\text{diff}}\Psi_S)(\Psi_{S'}). \tag{8}$$

Equivalently, the Hilbert space $\mathcal{H}_{\text{diff}}$ can be defined by the bilinear form

$$\langle\Psi,\Psi'\rangle_{\mathcal{H}_{\text{diff}}}\equiv\langle\Psi|P_{\text{diff}}|\Psi'\rangle\equiv\sum_{\Psi''=\mathrm{U}_\phi\Psi}\langle\Psi'',\Psi'\rangle. \tag{9}$$

We can unravel the structure of $\mathcal{H}_{\text{diff}}$ by studying the action of a diffeomorphism on a spin-network state. Since the holonomy transforms as

$$\mathrm{U}_l(\phi^{-1}A)=\mathrm{U}_{\phi\circ l}(A), \tag{10}$$

shifting A with $\phi\in Diff(\Sigma)$ is equivalent to shifting the curve l. Consequently, the (representation of the) spatial diffeomorphism group acts directly on the spin network of a spin-network state,

$$\mathrm{U}_\phi|S\rangle=|\phi\circ S\rangle. \tag{11}$$

Since $|\phi\circ S\rangle$ may be formed by invariant tensors that are not in the intertwiner basis chosen at the nodes, $|\phi\circ S\rangle$ may fail to be a basis state even if $|S\rangle$ is; but as the spaces of intertwiners are finite dimensional, it will be a finite linear combination of basis states, all having the same graph $\Gamma'=\phi\circ\Gamma$. In particular, given a spin-network state, there is a finite group of transformations g_k, $k=1,\ldots,K$, in the (tensor over the nodes of the) spaces of the intertwiners, that can be obtained by a diffeomorphism mapping the graph into itself. We can therefore write

$$\langle S|P_{\text{diff}}|S'\rangle=\begin{cases}0 & \text{if } \Gamma'\neq\phi\circ\Gamma,\\ \displaystyle\sum_k\langle S|g_k|S'\rangle & \text{if } \Gamma'=\phi\circ\Gamma.\end{cases} \tag{12}$$

From the first line, we see that two spin networks S and S' define orthogonal states in $\mathcal{H}_{\text{diff}}$ if the corresponding graphs Γ and Γ' belong to different equivalence classes under diffeomorphism transformations. We call these equivalence classes "diff-knot classes" and indicate them as K_d, where "d" is for diffeomorphism. The basis states in $\mathcal{H}_{\text{diff}}$ are therefore firstly labeled by a diff-knot class K_d. Call $\mathcal{H}_{K_d}$ the subspace of $\mathcal{H}_{\text{diff}}$ spanned by the basis states labeled by the knot class K_d. The states in $\mathcal{H}_{K_d}$ are then only distinguished by the coloring of links and nodes. Hence

$\mathcal{H}_{K_d}$ is separable. These colorings are however not necessarily orthogonal because of the nontrivial action of the discrete group. A diagonalization of the matrix of the bilinear form in the second line of expression (12) yields states $|s\rangle = |K_d, c\rangle$, where the discrete label c depends only on colorings. The states $|s\rangle = |K_d, c\rangle$ are called s-knot states.

If $|s\rangle = P_{\text{diff}}|S\rangle$, the state $|s\rangle$ represents the diffeomorphism equivalence class to which the spin network S belongs. In going from the spin-network state $|S\rangle$ to the s-knot state $|s\rangle$, we preserve the information in $|S\rangle$ except for it's location in Σ. This is the quantum analog to the fact that physically distinguishable solutions of the classical Einstein equations are not fields, but equivalence classes of fields under diffeomorphisms. It reflects the core of the conceptual revolution of general relativity: spatial localization concerns only the *relative* location of the dynamical fields, and not their location in a background space. Accordingly, the s-knot states are not quantum excitations *in* space, they are quantum excitation *of* space. An s-knot does not reside ''somewhere'': the s-knot itself defines the ''where.''

However, a remnant of the background structure oddly remains, when a node has sufficiently high valence, as we show in the next section.

B. Moduli space structure

We have seen above that quantum states of the gravitational field are labeled by diff-knot classes. Following Ref. 6, we now study the structure of these classes and the way this affects the structure of $\mathcal{H}_{\text{diff}}$. The key point that we underline below is the fact that diff-knots are not countable, hence $\mathcal{H}_{\text{diff}}$ is nonseparable.

To begin with, consider usual knots, namely ones without intersections. These can be defined in two equivalent manners. Let $\mathcal{L}$ be the space of loops without intersections, namely the space of smooth embeddings of S_1 into Σ. We denote loops in $\mathcal{L}$ as $\alpha,\beta,\ldots$. Consider *two* equivalence relations on this space. First (see, for instance, Ref. 5) we say that α and β are iso-equivalent, and write $\alpha \sim_i \beta$, if there is a *continuous* ambient isotopy relating the two; that is, a one parameter family of *homeomorphisms* $h_t : \Sigma \to \Sigma$, $t \in [0,1]$, such that h_0 is the identity map on Σ while h_1 maps α to β. We call the equivalence classes of loops in $\mathcal{L}$ under this equivalence relation ''iso-knots.'' Next, (see, for instance, Ref. 2) we say that α and β are diff-equivalent, and write $\alpha \sim_d \beta$ if there exists a *diffeomorphism* ϕ of Σ in the connected component of the identity, such that $\alpha = \phi \circ \beta$ (or, equivalently, if there exists a *smooth* ambient isotopy relating the two). We denote the corresponding equivalence classes in $\mathcal{L}$ as ''diff-knots.'' A classic result of knot theory states that two loops are diff-equivalent if and only if they are iso-equivalent. Hence diffeomorphism equivalence is the same as isotopy, as far as loops without intersections are concerned, and a diff-knot is also an iso-knot. (This is also equivalent to the existence of a *smooth homotopy* between α and β, that is, a smooth one-parameter family of embeddings α_t, $t \in [0,1]$, such that $\alpha_0 = \alpha$ and $\alpha_1 = \beta$. However, this is *not* equivalent to the existence of a *continuous homotopy* between α and β, since, perhaps surprisingly, any two knots can be related by continuous homotopy. See, for instance, Ref. 8, p. 14 or Ref. 5, exercise 3.5.4, p. 53.)

However, this result does not extend to the case in which intersections, or nodes, are present; something peculiar happens at the intersection points. Let $\mathcal{G}$ be the space of the graphs defined in the preceding section, of which $\mathcal{L}$ is a subset. Define isotopy equivalence and diff-equivalence between graphs precisely as we did for loops. Let us indicate iso-knots by K_i and the space of the iso-knots as $\mathcal{K}_i$. Similarly, let us indicate diff-knots by K_d and the space of the diff-knots as $\mathcal{K}_d$. Thus

$$\mathcal{K}_i = \frac{\mathcal{G}}{\sim_i}, \quad \mathcal{K}_d = \frac{\mathcal{G}}{\sim_d}. \tag{13}$$

It is still easy to see that diff-equivalence implies iso-equivalence, because a diffeomorphism in the connected component of the identity is indeed connected to the identity by a smooth one parameter family of diffeomorphisms which generates the isotopy. But now the converse is not

true: there are iso-equivalent graphs that are not diff-equivalent. Furthermore, while iso-knots are countable, diff-knots are not: they are distinguished by moduli. (In general, a "modulus" is a continuous parameter labeling equivalence classes.)

The roots of this fact, which at first might seem surprising, can be illustrated using a simple example presented by Arnold in his book on catastrophe theory.[1] Let L_n be the set of all n-tuples of lines in the plane, passing through the origin. Say that two n-tuples are equivalent if they can be mapped into each other by a linear transformation of the plane, and let T_n be the space of the equivalence classes of n-tuples under this equivalence relation. The spaces T_1, T_2, and T_3 are discrete, but T_4 is a one-dimensional space. Indeed the group of linear transformation of the plane, GL(2), is four dimensional, but it does not act effectively on T_n because the dilatations do not affect lines through the origin, hence we can consider just its SL(2) subgroup, which is three dimensional. But L_4 is four dimensional, and the dimension of $T_4 = L_4/\mathrm{SL}(2)$ is $4-3=1$. More explicitly, if $\phi_1,\ldots,\phi_4$ are the angles formed by the lines with a given axis, then it is easy to see that

$$\lambda(\phi_1,\ldots,\phi_4) = \frac{\sin(\phi_1-\phi_3)\sin(\phi_2-\phi_4)}{\sin(\phi_1-\phi_4)\sin(\phi_2-\phi_3)} \tag{14}$$

is invariant under linear transformations. Indeed, let $\vec{v}_1,\ldots,\vec{v}_4$ be four vectors of arbitrary length parallel to the four lines. The ratio

$$\lambda(\vec{v}_1,\ldots,\vec{v}_4) = \frac{(\vec{v}_1\times\vec{v}_3)\ \ (\vec{v}_2\times\vec{v}_4)}{(\vec{v}_1\times\vec{v}_4)\ \ (\vec{v}_2\times\vec{v}_3)}, \tag{15}$$

where $\vec{v}_1\times\vec{v}_2 = \det(\vec{v}_1,\vec{v}_2)$ is the two-dimensional (2D) vector product, is invariant under linear transformations because the vector product transforms with the determinant of the linear transformation. On the other hand, the ratio does not depend on the length of the vectors, and is equal to (14). Therefore λ is a continuous modulus that distinguishes GL(2) equivalence classes in L_4, and T_4 is a continuous space.

The same happens in three dimensions. Here GL(3) has nine dimensions, of which only eight affect the n-tuplets of lines through the origin; five lines through the origin are determined by 10 angles; hence in three-dimensions (3D) $T_n = L_n/\mathrm{GL}(3)$ is only discrete for $n<5$. If $\vec{v}_1,\ldots,\vec{v}_5$ are five vectors of arbitrary length parallel to the five lines, the ratio

$$\lambda(\vec{v}_1,\ldots,\vec{v}_5) = \frac{\vec{v}_1\cdot(\vec{v}_2\times\vec{v}_3)\ \ \vec{v}_1\cdot(\vec{v}_4\times\vec{v}_5)}{\vec{v}_1\cdot(\vec{v}_2\times\vec{v}_5)\ \ \vec{v}_1\cdot(\vec{v}_4\times\vec{v}_3)}, \tag{16}$$

where $\vec{v}_1\cdot(\vec{v}_2\times\vec{v}_3) = \det(\vec{v}_1,\vec{v}_2,\vec{v}_3)$ is the triple product, is invariant under linear transformation. It classifies quintuplets of straight lines into equivalence classes. The invariant (15) is well known in projective geometry since the 19th century, as the *cross ratio*. It distinguishes orbits of quadruplets of points generated by the action of the projective group on the real projective line. The generalization of the cross-ratio projective invariant to higher dimensions has been studied by Hilbert.

Let us return to nodes. Consider for simplicity a graph Γ with a single node n. Say that the node is five valent. Let Γ' be a node iso-equivalent to Γ. The graph Γ' will have a single five-valent node n' as well. Say, for simplicity, that n' is located at the same point p as n. Can we always find a diffeomorphism ϕ that sends Γ' into Γ? A condition on ϕ is that $\phi(p)=p$. The tangent map $\phi_*: T_p \to T_p$ defines a linear action on the tangent space T_p of Σ at p. The tangents to the five links of Γ at p determine a quintuplet of straight lines in T_p. Similarly, the tangents to the links of Γ' determine another quintuplet of straight lines in T_p. A condition on ϕ is then that the linear transformation ϕ_* maps the first quintuplet of lines into the second. As observed above, in general such a linear transformation does not exist. Equivalence classes under linear transformations of quintuplets of lines are distinguished by continuous moduli. If $\vec{v}_i(\Gamma,n)$, $i=1,\ldots,5$ are the tangents to the five links of Γ at the node n, in an arbitrary parametrization and an arbitrary coordinate system, the quantity

$$\lambda(\Gamma,n)=\lambda(\vec{v}_1(\Gamma,n),\ldots,\vec{v}_5(\Gamma,n)), \tag{17}$$

where the function on the right-hand side is defined in (16), does not depend either on the parametrization or on the coordinates chosen, and is invariant under diffeomorphisms. Hence if $\lambda(\Gamma,n)\neq\lambda(\Gamma',n')$, the two iso-equivalent graphs Γ and Γ' are not diff-equivalent. The function (17) is an example of the continuous moduli that distinguish diff-knots.

In general, a single iso-knot K_i is therefore formed by a continuous set of diff-knots K_d; diff-knots are labeled by moduli at the intersections. These moduli have a structure far richer than Hilbert's projective invariants. Indeed, it is not only the tangent structure that may distinguish iso-equivalent nodes, but also, for sufficiently high valence, the higher derivatives of the links at the intersection. For instance, assume that the tangents of the links at the node of two graphs are the same, but their curvatures differ. Under a diffeomorphism ϕ, the transformation of these curvatures is determined by the second derivatives of ϕ at the node, but these are finite in number as well (they are 18) and therefore for a sufficiently high valence they are not sufficient, in general, to map all curvatures of one graph into the curvatures of the second. We refer to Ref. 6 for a detailed analysis of the structure of the moduli.

We have seen in the preceding section that the diff-knots K_d label a basis in $\mathcal{H}_{\text{diff}}$. Since they are not countable, the kinematical state space $\mathcal{H}_{\text{diff}}$ space admits a continuous basis and therefore is nonseparable. Thus the root of the nonseparability of the state space of LQG is the ''rigidity'' of the diffeomorphisms at isolated points: the differential structure of the underlying manifold is rigid in the sense that it produces the linear structure of the tangent spaces T_p, which leaves quantities such as the cross-ratio (14) invariant.

C. Discussion

The nonseparability of the kinematical Hilbert space $\mathcal{H}_{\text{diff}}$ is disturbing for several reasons.

First, the background independence of general relativity implies that the localization of the dynamical fields on the coordinate manifold has no physical meaning: only relative localization of dynamical objects with respect to one another is physically significant. In the classical theory, background independence is implemented by the fact that diffeomorphisms turn out to be gauges. When implementing gauge invariance in the quantum theory, the localization of the spin network in the manifold is washed away by the gauge transformation, and only the discrete combinatorial relations remain—but not completely so. The moduli distinguishing diff-knots are a remnant of the localization of the spin network in the coordinate manifold. It is difficult to reconcile the presence of this remnant with the physical principle, underlying general relativity, that wants the localization on the coordinate manifold to be physically irrelevant.

Second, recall that loop states and spin-network states form a good basis in lattice Yang–Mills theory, but in continuous Yang–Mills theory they are ''too singular'' and ''too many,'' because of their continuous dependence on position. In gravity, the continuous dependence of position is gauged away by diffeomorphism invariance, dramatically reducing the size of the resulting state space.[10,12] This is the reason for which the loop basis becomes viable thanks to background independence, and therefore the rationale underlying the background-independent loop quantization. It is quite puzzling that this dramatic reduction of the state space fails to be complete because of the moduli.

Third, if we accept the formalization of generally covariant quantum theory described in Ref. 9, the Hilbert space $\mathcal{H}_{\text{diff}}$ describes distinguishable quantum states. A realistic space of distinguishable quantum states should be described by a separable Hilbert space.[13]

Now, if the continuous moduli had a physical meaning, they should affect measurements, or affect the dynamics. Two states that differ only by different values of their moduli should in principle be distinguishable by means of physical measurements. However, as mentioned in the introduction, this does not appear to be the case. The only effect of the moduli appears to be to vastly enlarging the kinematical Hilbert space, with no visible effect on the physics of the theory. One is therefore naturally led to the idea that these moduli may be spurious.

Above we have observed that the moduli are a consequence of the incapacity of diffeomorphisms to act at vertices in a way sufficiently general to map iso-equivalent graphs into each other. Diffeomorphisms are ''rigid'' at vertices. If gauge transformations included maps $\phi:\Sigma\to\Sigma$ less rigid at nodes (homeomorphisms, for instance), the continuous moduli would disappear: states distinguished by different moduli would become gauge equivalent. So, it is natural to ask: what is it that forces gauge transformations $\phi:\Sigma\to\Sigma$ implementing background independence, to be diffeomorphisms? Namely to be smooth?

To a large extent, the answer is just the conventional way we set up the theory. It is simple and convenient to use smooth fields on a smooth manifold, and stay in the smooth category. The moduli are a consequence of this choice, which might have little to do with physics. It is therefore natural to investigate the possibility of a different mathematical starting point, that would not affect classical physics, but would free the quantum theory from the moduli.

A very natural setting one may consider is the piecewise smooth category. Another possibility, investigated by Zapata[15] is to start from a piecewise linear manifold. With these choices, the moduli disappear and $\mathcal{H}_{\text{diff}}$ becomes separable. In this paper we investigate a minimal choice: we consider fields that are *everywhere continuous and smooth everywhere except possibly at a finite number of points*. We call these fields ''almost smooth.'' This minor enlargement of the space of the fields has practically no effect on the classical theory, nor on the physical results of LQG. But it gets rid of moduli and nonseparability.

III. EXTENDED DIFFEOMORPHISM GROUP

We now define a modified theory, where the gauge group is an extension of the diffeomorphism group. We show that the knot classes defined by the equivalence relation determined by this extended gauge group are countable, and lead to a separable $\mathcal{H}_{\text{diff}}$.

A. Almost smooth physical fields

Consider a four-dimensional differentiable manifold M with topology $\Sigma\times R$, as before. However, we now allow the gravitational field g to be almost smooth, as defined in the preceding section, that is, g is a continuous field which is smooth everywhere except possibly at a finite number of points, which we call the singular points of g. Any such g can be seen as a (pointwise) limit of a sequence of smooth fields. We say that g is a solution of the Einstein equations if it is the limit of a sequence of smooth solutions of the Einstein equations. Call $\mathcal{E}^*$ the space of such fields.

Let now ϕ be an invertible map from M to M such that ϕ and ϕ^{-1} are continuous and are infinitely differentiable everywhere except possibly at a finite number of points. The space of these maps form a group under composition, because the composition of two homeomorphisms that are smooth except at a finite number of singular points is clearly an homeomorphisms which is smooth except at a finite number of singular points. We call this group the *extended diffeomorphism group* and we denote it as $Diff^*_M$. It is clear that if $g\in\mathcal{E}^*$ then $(\phi g)\in\mathcal{E}^*$ for any $\phi\in Diff^*_M$. Hence $Diff^*_M$ is a gauge group for the theory.

In the Hamiltonian theory, we can now take almost smooth connections A on Σ. Notice that the holonomy of an almost smooth connection on a link l is well defined, because it is the product of the holonomies on the portions in which l is partitioned by the eventual singular points of A. We can thus define cylindrical functions, $\mathcal{K}$ and $\mathcal{K}_0$ as before. However, the gauge group *Diff* is now replaced by the gauge group *Diff**, formed by the homeomorphisms of Σ that are almost smooth (with their inverse). The group *Diff* considered above is a dense subgroup of *Diff**. (*Diff** can be given a topological group structure as a subgroup of the homeomorphism group of Σ. The question of whether it can be given a Lie group structure is more difficult.) Notice that *Diff** has a well-defined action on the space of the graphs $\mathcal{G}$. Unlike *Diff*, *Diff** does not preserve the number of nodes of a graph, because a singular point of ϕ may break a link into two links and create a bivalent node.

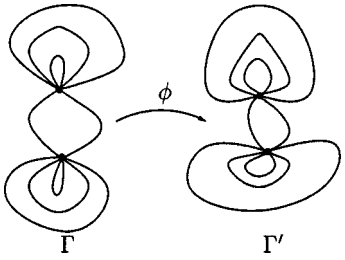

FIG. 1. Two graphs living in the same iso-knot but not in the same diff-knot.

The construction $\mathcal{H}_{\text{diff}}$ is the same as before, with the only difference that ϕ in (12) is now in $Diff^*$. Hence $\mathcal{H}_{\text{diff}}$ is now spanned by a basis of states $|s\rangle = |K_{d^*}, c\rangle$ where c is a discrete quantum number as before, but K_{d^*} is an element of $\mathcal{K}_{d^*}$, namely an equivalence class of graphs under *extended* diffeomorphisms

$$\mathcal{K}_{d^*} = \frac{\mathcal{G}}{\sim_{d^*}}, \tag{18}$$

where $\Gamma \sim_{d^*} \Gamma'$ if there is a $\phi \in Diff^*$ such that $\Gamma' = \phi \circ \Gamma$. We denote the elements K_{d^*} of $\mathcal{K}_{d^*}$ as diff*-knots.

B. *Diff**-knots are countable

We now prove that diff*-knots are countable. Two diff-equivalent graphs are also diff*-equivalent, because *Diff* is a subgroup of $Diff^*$. Therefore diff*-knots are equivalence classes of diff-knots. To prove that diff*-knots are countable it is sufficient to prove that any two diff-knots distinguished by a continuous parameter are diff*-equivalent. For this, it is sufficient to consider two iso-equivalent but diff-inequivalent graphs Γ and Γ'. Our strategy will be to explicitly build an extended diffeomorphism mapping Γ into Γ' (see Fig. 1). Since iso-knots are countable, this will be sufficient to show that $\mathcal{K}_{d^*}$ is countable.

Choose an arbitrary smooth metric g on Σ. Consider a node n of Γ, say with valence v. Consider the open ball B_n of fixed radius $\epsilon(n)$ about n. Let S_r be the spheres of radius $r(n)$, $0 < r(n) < \epsilon(n)$, centered at the same point n. Introduce (nonmetrical) angular coordinates $(\theta, \phi)_r$ on each sphere S_r of radius r, smooth in r. By choosing ϵ sufficiently small, each link l ending at n will intersect each sphere only once, say in the point with coordinates $(\theta_l, \phi_l)_r$. (No fold-backs, see Fig. 2.) Now, we can always choose the coordinates $(\theta, \phi)_r$ in such a way that the coordinates $(\theta_l, \phi_l)_r$ of the link l are independent from r, and are equal to v arbitrarily chosen values (θ_l, ϕ_l). This construction can be repeated for the node n' of Γ' which is isotopically associated to the

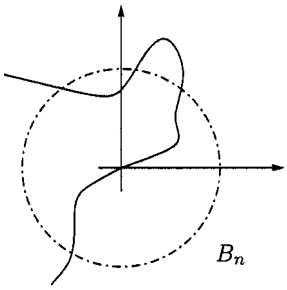

FIG. 2. A link presenting fold-backs.

node n. For the coordinates on the ball $B_{n'}$ around the node n' we use the notation (r',θ',ϕ') and we choose $(\theta'_{l'}=\theta_l,\phi'_{l'}=\phi_l)$, namely equal angular coordinates for corresponding links. We call Γ_n the restriction of Γ to B_n and Γ'_n the restriction of Γ' to $B_{n'}$.

Consider now the space $\Sigma\backslash B_n$ obtained by removing all balls B_n, for all nodes n, from Σ, and the space $\Sigma\backslash B'_n$ obtained removing all balls $B_{n'}$. Let $\tilde{\Gamma}$ be the restriction of Γ to $\Sigma\backslash B_n$ and $\tilde{\Gamma}'$ be the restriction of Γ' to $\Sigma\backslash B_{n'}$. Under the hypothesis we made that Γ and Γ' are iso-equivalent, a smooth invertible map

$$\tilde{\phi}:\Sigma\backslash B_n\to\Sigma\backslash B'_n,$$
$$\tilde{\Gamma}\mapsto\tilde{\Gamma}' \tag{19}$$

exists, because we are here in the simpler case of loops without intersections (on a space with boundaries), where standard knot-theory results apply. The failure of iso-equivalence to yield diffeo-equivalence regards *only* the neighborhoods of the nodes.

To prove that Γ and Γ' are diff*-equivalent, we have therefore just to construct maps

$$\phi_n:B_n\to B'_n,$$
$$\Gamma_n\mapsto\Gamma'_n \tag{20}$$

such that $\tilde{\phi}$ and ϕ_n, taken together, give an almost smooth map $\phi:\Sigma\to\Sigma$. Let ϕ_n be given simply by

$$\phi_n:B_n\to B'_n,$$
$$(r,\theta,\phi)\mapsto(r'=r,\theta'=\theta,\phi'=\phi). \tag{21}$$

$\tilde{\phi}$ can be chosen so that at the boundaries of the balls ϕ is smooth. Hence ϕ is smooth for all $r>0$. The map ϕ_n can immediately be continued to $r=0$, yielding by continuity $\phi_n(n)=n'$. But there is no reason for this continuation to be smooth, and in fact, in general it will not be. Hence ϕ is not in *Diff*. But it is in *Diff**, because it is continuous, invertible, and smooth everywhere except at the nodes, which are finite in number. Therefore iso-equivalent graphs Γ and Γ' are diff*-equivalent. Therefore we have the following.

Proposition 1: The space of the diff-knots $\mathcal{K}_{d*}$ is countable.*

It follows immediately that we have Proposition 2.

Proposition 2: If $\phi\in Diff^*$, the space $\mathcal{H}_{\text{diff}}$ defined by the bilinear form (12) is separable.

Therefore we have shown that a minor extension of the functional space of the fields considered eliminates the continuous moduli and the nonseparability of the kinematical state space of LQG.

IV. OPERATORS

In this section we discuss some consequences of the extension of *Diff* to *Diff** and clarify some apparent difficulties that this extension raises.

A. Conical singularities and area operator

If the gauge group is *Diff**, a smooth two-dimensional surface is gauge equivalent to a "singular" surface, that is a surface with conical singularities. The area operator $A(\mathcal{S})$ of LQG has been defined for smooth surfaces $\mathcal{S}$. Is it well defined also for a singular surface $\mathcal{S}$? Naively, one may think that $A(\mathcal{S})$ is ill defined for a singular $\mathcal{S}$, for the following reason. Consider a two-dimensional surface $\mathcal{S}$ embedded in Σ. Let $x=(x^a)$, $a=1,2,3$ be coordinates on Σ and $u=(u^m)$, $m=1,2$ coordinates on $\mathcal{S}$; the embedding is given by the functions $x^a(u)$. Let $g_{ab}(x)$ be the 3D metric, namely the gravitational field. The classical expression for the area of $\mathcal{S}$ is

$$A(\mathcal{S})=\int_{\mathcal{S}} \mathrm{d}^2u \quad \sqrt{\det g_{mn}(u)}, \tag{22}$$

where

$$g_{mn}(u)=\frac{\partial x^a(u)}{\partial u^m}\frac{\partial x^b(u)}{\partial u^n}g_{ab}(x(u)) \tag{23}$$

is the two-dimensional metric induced on the surface. The area operator is constructed by expressing the area in terms of the variable canonically conjugated to A, which is the inverse densitized triad $E^a_i(x), i=1,2,3$, related to the metric by $\det q\, q^{ab}=E^a_i(x)E^b_j(x)\delta^{ij}$. This gives

$$A(\mathcal{S})=\int_A \mathrm{d}^2u \ \sqrt{n_a\ n_b\ E^a_i\ E^b_j\ \delta^{ij}}, \tag{24}$$

where

$$n_a(u)=\epsilon_{abc}\frac{\partial x^b(u)}{\partial u^1}\frac{\partial x^c(u)}{\partial u^2} \tag{25}$$

is the one-form normal to the surface $\mathcal{S}$. If $\mathcal{S}$ is singular at a point p, the normal $n_a(u)$ is not defined at p. This has no effect on the expression of the classical area (24) because the singular point is a set of measure zero. Obviously, indeed, the area of a cone is defined in the same manner as the area of a smooth surface. However, what happens at single points becomes important for the LQG quantum operator $A(\mathcal{S})$ that corresponds to the classical quantity (24). A spin-network state determined by a spin-network S that crosses the surface at a single point p contributes to the area of the surface. In the derivation of this contribution, the tangent to the link of S at p gets contracted with the normal $n_a(p)$. If this is ill defined, we might expect a problem.

The proper way of addressing this issue is in the context of a quantization of the area operator based on a well-defined regularization. Several equivalent regularization schemes to define area operator are discussed in the literature. Not all of these schemes can be immediately adapted to a surface with conical singularities, but the regularization discussed in Ref. 4, which uses a smearing transversal to the surface, remains well defined for singular surfaces. This regularization is based on a continuous family of surfaces $\mathcal{S}_\lambda$, with $\lambda\in[-\delta/2,\delta/2]$, where δ is a positive real number, such that $\mathcal{S}_0=\mathcal{S}$. To extend the technique to singular surfaces, we demand that $\mathcal{S}_\lambda$ is a smooth surface for $\lambda\neq 0$ and that $\mathcal{S}_0=\mathcal{S}$ is singular. The area of $\mathcal{S}$ is then written as the limit

$$A(\mathcal{S})=\lim_{\delta\to 0}\frac{1}{\delta}\int_{-\delta/2}^{\delta/2}\mathrm{d}\lambda\, A(\mathcal{S}_\lambda)=\lim_{\delta\to 0}\frac{1}{\delta}\int_{\mathcal{D}}\mathrm{d}^3\sigma\sqrt{n_a n_b E^{aj}E^b_j}, \tag{26}$$

where $\mathcal{D}=\mathcal{S}\times[-\delta/2,\delta/2]$. The nonvanishing contribution of the last integral comes now from the entire one-dimensional intersection between the spin network and the three-dimensional region $\mathcal{D}$. In this, the contribution of the singular points of the $\lambda=0$ surface have measure zero. The fact that $\mathcal{S}$ has singular points is therefore irrelevant, and the operator $A(\mathcal{S})$ is well defined also for singular surfaces.

Recall that the LQG operator $A(\mathcal{S})$ is *Diff*-covariant in the sense that

$$A(\phi(\mathcal{S}))=\mathrm{U}_\phi A(\mathcal{S})\mathrm{U}_{\phi^{-1}} \tag{27}$$

for all $\phi\in Diff$. The above construction implies immediately that (27) remains true also if $\phi\in Diff^*$, because the differentiable structure at the intersection point plays no role in the definition of $A(\mathcal{S})$. The action of the area operator of a singular surface $\mathcal{S}$ is therefore immediately

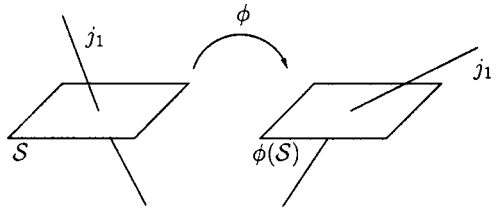

FIG. 3. An extended diffeomorphism may generate a conical singularity but does not change the topological relation between a surface $\mathcal{S}$ and the link of a spin network.

obtained by (27) by choosing ϕ such that $\phi(\mathcal{S})$ is smooth. We see that what matters is not the linear structure at the intersection point, but just the topological relation between the surface and the spin networks defining the quantum states. (See Fig. 3.)

From this, it follows immediately that we have Proposition 3.

Proposition 3: The spectrum of the operator $A(\mathcal{S})$ where $\mathcal{S}$ is singular (has a finite number of conical singularities) is the same as the spectrum of the operator $A(\mathcal{S})$ where $\mathcal{S}$ is smooth.

In conclusion, extended diffeomorphisms are indistinguishable from ordinary diffeomorphisms as far as the area operator is concerned. An extended diffeomorphism may generate singular points in the surface or in the spin network, but does not affect the topological relation between a surface and the spin network, and the area depends only on this relation.

B. Volume and Hamiltonian

Call $V(\mathcal{R})$ the volume of a 3D region $\mathcal{R}$ in Σ. There exist two versions of the volume operator $V(\mathcal{R})$ in LQG.[7] The first [let us call it $V_1(\mathcal{R})$ here], used for instance in Ref. 9, depends only on the intertwiners of the nodes inside $\mathcal{R}$. The second [let us call it $V_2(\mathcal{R})$ here], used for instance in Ref. 14, depends also on whether or not the links at the nodes are linearly dependent. The operator $V_1(\mathcal{R})$ is *Diff**-covariant, that is

$$V_1(\phi(\mathcal{R})) = \mathrm{U}_\phi V_1(\mathcal{R}) \mathrm{U}_{\phi^{-1}} \tag{28}$$

for all $\phi \in Diff^*$. The operator $V_2(\mathcal{R})$, on the other hand, does not transform well under $\phi \in Diff^*$, because an extended diffeomorphism can modify the linear dependence of the links at the node. Therefore the formulation of LQG considered here requires the use of the version $V_1(\mathcal{R})$ of the volume operator.

Finally, the Hamiltonian can be defined entirely in terms of the volume operator and holonomy operators, and is not affected by the modification of the theory considered here.

V. CONCLUSION

We have studied the problem of the separability of the background-independent space of the quantum states of the gravitational field, $\mathcal{H}_{\mathrm{diff}}$, in loop quantum gravity. We have shown that a small extension of the functional class of the classical fields leads to an enlargement of the gauge group of the theory. In particular *Diff* is enlarged to *Diff**, the group of homeomorphisms that are smooth (with their inverse) except possibly at a finite number of points. The space of the knot classes become countable and the kinematical Hilbert space $\mathcal{H}_{\mathrm{diff}}$ is separable. The area, volume, and Hamiltonian operator are naturally covariant under this extended gauge invariance, provided that the appropriate regularization and the appropriate version of the volume operator are chosen. The spectra of area and volume, in particular, are unaffected. We expect that analogous results could be obtained also using other mathematical settings, in particular the piecewise smooth category.

We take these results as indications that the continuous moduli that made $\mathcal{H}_{\mathrm{diff}}$ nonseparable might be physically spurious. Using the setting described in this paper, the theory appears to be cleaner and to realize more completely its purely combinatorial character as well as background

independence. If we adopt this point of view, background independent quantum microphysics is entirely discrete and smoothness can be seen, *a posteriori*, just as a property arising from averaging over regions much larger than the Planck scale.

Note added: After the posting of this work in the Archives, J. Lewandowski has informed us that related ideas have been developed by him and A. Ashtekar in work which is still unpublished.

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The loss of stability of surface superconductivity

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The Ginzburg–Landau equations in a half-plane are considered in the large κ limit. We look at the reduced set of equations obtained in that limit. It is proved that the one-dimensional solution presented by Pan [Commun. Math. Phys. **228**, 327 (2002)] undergoes a bifurcation for an infinite number of applied magnetic field values which are lower than H_{C_2}. We also prove that each bifurcating mode is energetically preferable to the one-dimensional surface superconductivity solution, and thus, prove that the surface superconductivity becomes unstable for applied fields which are lower than H_{C_2} © *2004 American Institute of Physics.*
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I. INTRODUCTION

Consider a planar superconducting body which is placed at a sufficiently low temperature (below the critical one) under the action of an applied magnetic field. Its energy is given by the Ginzburg–Landau energy functional which can be represented in the following dimensionless form:[1]

$$E=\int_{\Omega}\left(-|\Psi|^2+\frac{|\Psi|^4}{2}+|h-h_{\mathrm{ex}}|^2+\left|\frac{i}{\kappa}\nabla\Psi+A\Psi\right|^2\right)dx_1dx_2\,, \tag{1.1}$$

in which Ψ is the (complex) superconducting order parameter, such that $|\Psi|$ varies from $|\Psi|=0$ (when the material is at a normal state) to $|\Psi|=1$ (for the purely superconducting state). The magnetic vector potential is denoted by A (the magnetic field is, then, given by $h=\nabla\times A$), h_{ex} is the constant applied magnetic field, and κ is the Ginzburg–Landau parameter which is a material property. Superconductors for which $\kappa<1/\sqrt{2}$ are called type I superconductors, and those for which $\kappa>1/\sqrt{2}$ are called type II. Ω is a connected domain of superconductor, whose Gibbs free energy is given by E. Note that E is invariant to the gauge transformation

$$\Psi\to e^{i\kappa\eta}\Psi;\quad A\to A+\nabla\eta, \tag{1.2}$$

where η is any smooth function.

For sufficiently large magnetic fields it is well known, both from experimental observations[2] and both from theoretical predictions,[3] that superconductivity is destroyed and the material must be in the normal state. If the applied magnetic field is then decreased there is a critical field where the material enters the superconducting phase once again. This field is called ''the onset field'' and is denoted by H_{C_3}.

It is well-known that at the bifurcation from the normal state, superconductivity remains concentrated near the boundary. Alternatively we can say that Ψ decays exponentially fast away from the boundaries as either κ or the size of Ω tend to infinity, which is the reason why the phenomenon has been termed surface superconductivity. This result has first been obtained for a half-plane,[4] then also for disks,[5] and for general smooth domains in $\mathbb{R}^2$.[6–9] It was extended later to weakly nonlinear cases in the large κ limit.[10]

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In the absence of boundaries the critical field at which superconductivity nucleates is denoted by H_{C_2} and is smaller than H_{C_3} ($H_{C_3}\approx 1.7\kappa$ whereas $H_{C_2}=\kappa$). Furthermore, the bifurcating modes are periodic lattices, named after Abrikosov[11–13] which have been observed experimentally.[14] It has been conjectured, therefore, by Rubinstein[15] that superconductivity remains concentrated near the boundary for $H_{C_2}<h_{\text{ex}}<H_{C_3}$. When $h_{\text{ex}}\approx H_{C_2}$ (either for κ large or for large domains) a bifurcation of Abrikosov's lattices far away from the wall was conjectured.[15]

Recently, it has been proved both in the large κ limit,[16,17] and in the large domain limit[18] that as long as $H_{C_2}<h_{\text{ex}}<H_{C_3}$ superconductivity remains concentrated near the boundaries. From a different direction, Sandier and Serfaty[19] showed for the global minimizer of (1.1) that as $h_{\text{ex}}\to H_{C_2}$ from below and $\kappa\to\infty$, superconductivity vanishes in the domain's interior, away from the boundaries.

Despite the above-mentioned progress the transition from the surface superconductivity solution to the mixed state, where Abrikosov's lattices appear in the bulk of the material, has not been clarified yet. In particular, if the applied magnetic field is decreased below H_{C_2} it has not been proved yet that:

(1) The surface superconductivity solution becomes unstable, i.e., it is not a local minimizer of E for $h_{\text{ex}}<H_{C_2}$.
(2) The bifurcating mode is indeed the global minimizer and has to be periodic.

In the present contribution we prove, in the large κ limit, for a domain wall, that the surface superconductivity solution in a half-plane is not a local minimizer of E for $h_{\text{ex}}<H_{C_2}$, and hence cannot be stable. To this end we assume, just like Pan[16] did, that the global minimizer is essentially one-dimensional in the boundary layer. In addition to the instability proof, we find the bifurcating modes and show, by an heuristic argument, that when properly superposed, Abrikosov's lattices can be formed. However, since linear superposition of modes is impossible, in view of the equation's nonlinearity, further research is necessary in that direction.

The Euler–Lagrange equations associated with (1.1), known as the steady state Ginzburg–Landau equations, are given in the form

$$\left(\frac{i}{\kappa}\nabla+A\right)^2\Psi=\Psi(1-|\Psi|^2), \tag{1.3a}$$

$$-\nabla\times\nabla\times A=\frac{i}{2\kappa}(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*)+|\Psi|^2A, \tag{1.3b}$$

and the natural boundary conditions by

$$\left(\frac{i}{\kappa}\nabla+A\right)\Psi\cdot\hat{n}=0, \tag{1.4a}$$

$$h=h_{\text{ex}}. \tag{1.4b}$$

In Refs. 16 and 17 it is proved that as $\kappa\to\infty$, $h_{\text{ex}}-\kappa\gg 1/\kappa$ we have, near the boundary

$$\Psi(x_0+\xi/\kappa)\xrightarrow[\kappa\to\infty]{}\psi(\xi)\quad\text{pointwise},$$

where $x_0\in\partial\Omega$, $\xi\in\mathbb{R}^2_+$,

$$\mathbb{R}^2_+=\{(x_1,x_2);\ \ x_1>0\}$$

and ψ must satisfy

$$(i\nabla + x_1 \hat{i}_2)^2 \psi = \lambda \psi (1 - |\psi|^2) \quad \text{in } \mathbb{R}^2_+, \tag{1.5a}$$

$$\frac{\partial \psi}{\partial x_1} = 0 \quad \text{on } \partial \mathbb{R}^2_+, \tag{1.5b}$$

where

$$\lambda = \frac{\kappa}{h_{\text{ex}}}.$$

Let

$$\mathcal{H} = \{u \in H^1(z,\infty) | xu \in L^2(z,\infty)\}, \tag{1.6}$$

where z is a real number, and let

$$\beta(z) = \inf_{\phi \in \mathcal{H}} \frac{\int_z^\infty |\phi'|^2 + x^2 |\phi|^2}{\int_z^\infty |\phi|^2}. \tag{1.7}$$

The dependence of β on z has been studied in Refs. 20 and 21 afterward. In particular, it has been proved that there exist $z_1(\lambda)$ and $z_2(\lambda)$ such that $\lambda > \beta(z)$ if and only if $z_1 < z < z_2$, and that $z_2(1) = 0$ and $z_1(1) = -\infty$. It is also proved in Ref. 7 that

$$\beta_0 = \inf_{z \in \mathbb{R}} \beta(z) = \lim_{\kappa \to \infty} \frac{\kappa}{H_{C_3}} \approx 0.59.$$

The same result was also proved in Ref. 8.

Pan[16] conjectured that any bounded solution of (1.5a) for $\beta_0 < \lambda \leqslant 1$ must be in the form

$$\psi = e^{i(\omega_0 x_2 + c)} f(x_1), \tag{1.8}$$

where ω_0 is a real number and $f(x_1, \lambda)$ satisfies in $\mathbb{R}_+$

$$-f'' + (x - \omega_0)^2 f = \lambda f (1 - f^2); \quad f'(0) = 0. \tag{1.9}$$

In Ref. 16 it is proved that if $\beta(-\omega_0) < \lambda \leqslant 1$ and

$$-z_2 < \omega_0 < -z_1$$

then there exists a solution for (1.9). Furthermore, it is proved in Ref. 16 the

$$f(x) \sim x^{-1-\lambda/2} e^{-1/2 x^2} \quad \text{as } x \to \infty. \tag{1.10}$$

The discussion in Ref. 16 was limited to the case $\lambda \leqslant 1$, since this is the regime where the surface superconductivity solution is expected to be the global minimizer of E. Nevertheless, it is not difficult to show that the above existence result and (1.10) still hold when $\lambda > 1$ for any $\omega_0 \geqslant 0$. We bring the proof in Appendix A.

Weaker conjectures can be made instead of assuming that (1.8) is the unique class of bounded solutions of (1.5a). Consider the energy functional

$$\mathcal{E}(\psi) = \int_{\mathbb{R}^2_+} |(i\nabla + x_1 \hat{i}_2)\psi|^2 + \lambda(\tfrac{1}{2}|\psi|^4 - |\psi|^2), \tag{1.11}$$

where $\hat{i}_2$ is a unit vector in the x_2 direction, and let

$$H^1_{\mathrm{mag}}(\Omega)=\{\phi\in L^2(\Omega)\,|\,\partial_{x_1}\phi\in L^2,\quad \partial_{x_2}\phi+ix_1\phi\in L^2\}. \tag{1.12}$$

It is well known[16] that when $\lambda>\beta_0$ we have

$$\inf_{\phi\in H^1_{\mathrm{mag}}(R^2_+)}\mathcal{E}(\phi)=-\infty.$$

We therefore modify the definition of H^1_{mag} so it would guarantee the existence of a global minimizer to $\mathcal{E}$ in the modified space. We thus apply the transformation

$$x_1\to x_1-\omega_0;\quad \psi\to e^{-i\omega_0 x_2}\psi$$

to obtain

$$\mathcal{E}(\psi)=\int_{-\omega_0}^{\infty}dx_1\int_{\mathbb{R}}dx_2\left\{|(i\nabla+x_1\hat{i}_2)\psi|^2+\lambda\left(\frac{1}{2}|\psi|^4-|\psi|^2\right)\right\}, \tag{1.13}$$

and define the space

$$\mathcal{P}_L^{\omega_0}=\{\phi\in H^1_{\mathrm{mag}}([-\omega_0,\infty)\times\mathbb{R})\,|\,\phi(x_1,x_2+L)=\phi(x_1,x_2)\}. \tag{1.14}$$

We can now conjecture, just like Pan[16] did, that

$$\psi=f(x_1,\lambda)$$

is the global minimizer of $\mathcal{E}$ in $\mathcal{P}_L^{\omega_0}$, for every $L>0$ and $\omega_0\geqslant 0$.

We note that Pan[16] studied the same problem for $\lambda>1$ and found that the global minimizer of (1.11) in $\mathcal{P}_L^{\omega_0}$ decays exponentially fast away from the wall. Moreover, it is proved in Ref. 16 that the global minimizer of (1.1) in a smooth bounded domain must tend, as $\kappa\to\infty$, to a periodic solution whose period is of $O(\kappa)$.

Periodic solutions have already been studied in the absence of boundaries.[11–13] Periodicity was imposed in those works in both the x_1 and the x_2 directions. In this work we add the effect of a planar wall: We impose periodicity only in the direction which is parallel to the wall, whereas away from the wall we expect the solution to decay. This problem, which is still much simpler than the determination of the global minimizer of (1.1), is much closer to real situations than the problem in $\mathbb{R}^2$.[11–13]

The present contribution can be summarized by the following theorem.

Theorem 1.1: *There exists $n_0\in\mathbb{N}$, which may depend on $\omega=2\pi/L$ and ω_0, and a sequence $\{\lambda_n\}_{n=n_0}^{\infty}$, such that*

(1) There exists a solution to (1.5a) in $\mathcal{P}_L^{\omega_0}$ which bifurcates from $\psi=f(x_1,\lambda)$, in some right semi-neighborhood of λ_n for every $n\geqslant n_0$.

(2) For every $n\geqslant n_0$

$$1+C_1\exp\left\{\frac{-(n\omega+\omega_0)^2}{2}\right\}<\lambda_n<1+C_2\exp\left\{\frac{-(n\omega+\omega_0)^2}{2}\right\}, \tag{1.15}$$

where C_1 and C_2 are positive and independent of n.

(3) Denote the bifurcating solution in $\mathcal{P}_L^{\omega_0}$ by $\psi_n(x_1,\lambda)$. Then

$$\mathcal{E}(\psi_n,\lambda)<\mathcal{E}(f,\lambda)$$

in some right semi-neighborhood of λ_n for every $n\geqslant n_0$.

In the next section we discuss the linearized equation and prove (1.15). Statements 1 and 3 are proved in Sec. III. Finally, in Sec. IV we briefly summarized the results obtained in Secs. II and III and list some related open problems.

II. LINEAR ANALYSIS

Consider the problem

$$(i\nabla + x_1\hat{i}_2)^2\psi = \lambda\psi(1-|\psi|^2) \quad (x_1,x_2)\in(-\omega_0,\infty)\times\mathbb{R}, \tag{2.1a}$$

$$\psi_{x_1}(-\omega_0,x_2)=0; \quad \psi(x_1,x_2+L)=\psi(x_1,x_2). \tag{2.1b}$$

Let

$$u=\psi(x_1,x_2)-f(x_1,\lambda), \tag{2.2}$$

wherein f satisfies (1.9). Denote by $\mathbb{X}$ the space

$$\mathbb{X}=\{u\in C^2\{[-\omega_0,\infty)\times\mathbb{R}\}\cap\mathcal{P}_L^{\omega_0}|u_{x_1}(-\omega_0,x_2)=0\}$$

with the C^2 norm. Let $F:\mathbb{R}^+\times\mathbb{X}\to C\{[-\omega_0,\infty)\times\mathbb{R}\}$ be the operator

$$F(\lambda,u)=(i\nabla+x_1\hat{i}_2)^2u-\lambda[u-f^2(2u+\overline{u})-f(2|u|^2+u^2)-|u|^2u]. \tag{2.3}$$

Clearly, if $u\in\mathbb{X}$ satisfies $F(u,\lambda)=0$ for some $\lambda>\beta_0$, then $\psi=u+f$ is a solution of (2.1). Furthermore, since $F(\lambda,0)\equiv 0$ for all $\lambda>\beta_0$ we can consider the linear bifurcation of nontrivial solutions of $F(u,\lambda)=0$ from $u\equiv 0$. Let F_u denote the Fréchet derivative of F. Then, the linearized form of $F(u,\lambda)=0$ near $u\equiv 0$ is

$$F_u(0,\lambda)\phi=0$$

or

$$(i\nabla+x_1\hat{i}_2)^2\phi-\lambda[\phi-f^2(2\phi+\overline{\phi})]=0. \tag{2.4}$$

Our first result proves the existence of nontrivial solutions in $\mathbb{X}$ for (2.4) and gives the corresponding critical values of λ.

Theorem 2.1: *There exists $n_0(\omega_0,\omega)\in\mathbb{N}$ and a sequence $\{\lambda_n\}_{n=n_0}^{\infty}$, such that when $\lambda=\lambda_n$ non trivial solutions of (2.4) exist. Furthermore, for all $n\geqslant n_0$ λ_n satisfies (1.15).*

Proof: Since we look for periodic solutions we multiply (2.4) by $e^{-in\omega x_2}$ where $n\in\mathbb{N}$ and integrate with respect to x_2 over $[-\pi/\omega,\pi/\omega]$ to obtain

$$-\hat{\phi}_n''+[(x-n\omega)^2-\lambda]\hat{\phi}_n+\lambda f^2(2\hat{\phi}_n+\overline{\hat{\phi}_{-n}})=0, \tag{2.5a}$$

$$-\hat{\phi}_{-n}''+[(x+n\omega)^2-\lambda]\hat{\phi}_{-n}+\lambda f^2(2\hat{\phi}_{-n}+\overline{\hat{\phi}_n})=0, \tag{2.5b}$$

$$\hat{\phi}_n'(-\omega_0)=\hat{\phi}_{-n}'(-\omega_0)=0, \tag{2.5c}$$

where

$$\hat{\phi}_n(x_1)=\int_{-\pi/\omega}^{\pi/\omega}\phi(x_1,x_2)e^{-in\omega x_2}dx_2. \tag{2.6}$$

To prove the lower bound in (1.15) we need the following perturbation lemma.

Lemma 2.2: Let $\mathcal{H}(\xi)$ be defined by (1.6), and let

$$\alpha(\xi,g)=\inf_{\substack{\phi\in\mathcal{H}\\ \|\phi\|_{L^2(-\xi,\infty)}=1}}\int_{-\xi}^{\infty}|\phi'|^2+(x^2+g(x+\xi))|\phi|^2dx,$$

where $g:[0,\infty)\to\mathbb{R}$ *is continuous and decays as* $x\to\infty$. *Then,*

$$\alpha=1+\int_{-\xi}^{\infty}gv^2+\delta(\xi). \tag{2.7a}$$

In which v *is the quasi-mode*

$$v=c_\xi\chi(x+\xi)e^{-x^2/2} \tag{2.7b}$$

whose $L^2(-\xi,\infty)$ *norm is unity,* χ *is a* C^∞ *cutoff function satisfying*

$$\chi=\begin{cases}0, & 0\leqslant x<\frac{1}{2}\\ 1, & 1<x\end{cases} \tag{2.7c}$$

and, for sufficiently large ξ,

$$\delta(\xi)\leqslant 2\int_{-\xi}^{\infty}g^2v^2+Ce^{-\xi^2}, \tag{2.7d}$$

where C *is independent of* ξ.

Proof: Denote by $\mathcal{P}$ the operator

$$\mathcal{P}=:-\frac{d^2}{dx^2}+x^2+g,$$

and let

$$\nu=1+\int_{-\xi}^{\infty}gv^2.$$

Then,

$$(\mathcal{P}-\nu)v=c_\xi[-\chi''+2x\chi'+g\chi]e^{-x^2/2}-(\nu-1)v,$$

and hence,

$$\left|\int_{-\xi}^{\infty}v(\mathcal{P}-\nu)v\right|\leqslant\int_{-\xi}^{\infty}\left|-\frac{\chi''}{\chi}+2x\frac{\chi'}{\chi}\right|v^2\leqslant Ce^{-\xi^2}. \tag{2.8}$$

Let $\{\mu_j\}_{j=0}^{\infty}$ denote the eigenvalues and $\{u_j\}_{j=0}^{\infty}$ the corresponding eigenmodes, whose L^2 norm is unity, of the following problem:

$$\mathcal{P}u_j=\mu_ju_j,\quad x>\xi,$$

$$u_j'(-\xi)=0.$$

It is well known,[22] that $\mu_j\uparrow\infty$ and that $\{u_j\}_{j=0}^{\infty}$ are square integrable and orthogonal. Let

$$\tilde{v}=v-a_0u_0, \tag{2.9a}$$

where

$$a_0=\int_{-\xi}^{\infty}vu_0. \tag{2.9b}$$

Substituting (2.9) in (2.8) we obtain (note that $\mu_0=\alpha$)

$$a_0^2|\alpha-\nu|\leqslant\int_{-\xi}^{\infty}|\tilde{v}(\mathcal{P}-\nu)\tilde{v}|+Ce^{-\xi^2}. \tag{2.10}$$

To estimate the first term on the right-hand side of (2.10) we make use of the following inequality:

$$\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)\tilde{v}|^2\leqslant\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)v|^2=\int_{-\xi}^{\infty}\left|-\frac{\chi''}{\chi}+2x\frac{\chi'}{\chi}+g-(\nu-1)\right|^2v^2\leqslant\int_{-\xi}^{\infty}g^2v^2+Ce^{-\xi^2}. \tag{2.11}$$

Since the distance of ν from the spectrum of $\mathcal{P}$ in $\mathcal{H}\backslash\mathrm{Span}(u_0)$ is $|\mu_1-\nu|$ we have

$$(\mu_1-\nu)^2\int_{-\xi}^{\infty}|\tilde{v}|^2\leqslant\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)\tilde{v}|^2\leqslant\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)v|^2. \tag{2.12}$$

It is not difficult to show, using standard arguments from semi-classical analysis (cf. for instance theorem 3.4.1 in Ref. 23), that

$$\mu_1\xrightarrow[\xi\to\infty]{}3. \tag{2.13}$$

Hence, for sufficiently large ξ,

$$\int_{-\xi}^{\infty}|\tilde{v}(\mathcal{P}-\nu)\tilde{v}|\leqslant\left[\int_{-\xi}^{\infty}|\tilde{v}|^2\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)\tilde{v}|^2\right]^{1/2}\leqslant\int_{-\xi}^{\infty}|(\mathcal{P}-\nu)v|^2.$$

Substituting (2.10) in the above inequality yields

$$a_0^2|\alpha-\nu|\leqslant\int_{-\xi}^{\infty}g^2v^2+Ce^{-\xi^2}. \tag{2.14}$$

By (2.12) and (2.13) we have

$$a_0^2=1-\int_{-\xi}^{\infty}|\tilde{v}|^2\geqslant1-\int_{-\xi}^{\infty}g^2v^2-Ce^{-\xi^2}$$

from which (2.7) can be easily obtained. □

We now continue the proof of Theorem 2.1. Let

$$\alpha_n(\lambda)=:\alpha(-n\omega-\omega_0,\lambda f^2). \tag{2.15}$$

Since, by (1.10)

$$\int_{-n\omega-\omega_0}^{\infty}f^2(x+n\omega+\omega_0)e^{-x^2}\geqslant C(n\omega+\omega_0)^{\lambda-1}\exp\{-\tfrac{1}{2}(n\omega+\omega_0)^2\},$$

we have, by (2.7),

$$\alpha_n\geqslant1+C(n\omega+\omega_0)^{\lambda-1}\exp\{-\tfrac{1}{2}(n\omega+\omega_0)^2\}. \tag{2.16}$$

We now define the functional

$$\mathcal{J}(\chi_n,\chi_{-n})=:\int_{-\omega_0}^{\infty}|\chi_n'|^2+(x-n\omega)^2|\chi_n|^2+|\chi_{-n}'|^2+(x+n\omega)^2|\chi_{-n}|^2-\lambda[|\chi_n|^2+|\chi_{-n}|^2 - f^2(|\chi_n|^2+|\chi_n+\overline{\chi}_{-n}|^2+|\chi_{-n}|^2)]. \tag{2.17}$$

Let $(\phi_n,\phi_{-n})\in\mathcal{H}\times\mathcal{H}$ satisfy (2.5a) and (2.5b) and

$$\int_{-\omega_0}^{\infty}(|\phi_n|^2+|\phi_{-n}|^2)=1.$$

Multiplying (2.5a) by $\overline{\phi}_n$ and the complex conjugate of (2.5b) by ϕ_{-n} and integrating their sum over $[-\omega_0,\infty)$ we obtain

$$\mathcal{J}(\phi_n,\phi_{-n})=0.$$

However, from the definition of α_n it follows that

$$\int_{-\omega_0}^{\infty}|\phi_n'|^2+(x-n\omega)^2|\phi_n|^2-\lambda(1-f^2)|\phi_n|^2\geqslant(\alpha_n-\lambda)\int_{-\omega_0}^{\infty}|\phi_n|^2.$$

Furthermore, for sufficiently large n, we have $(x+n\omega)^2>(x-n\omega)^2$ for every $x\in[-\omega_0,\infty)$, and hence

$$\mathcal{J}(\phi_n,\phi_{-n})\geqslant(\alpha_n-\lambda). \tag{2.18}$$

Consequently, the value of λ for which the minimal value of $\mathcal{J}$ vanishes, must be greater than α_n. Therefore, by (2.16) the lower bound in (1.15) is proved.

To prove the upper bound we need, once again, to prove an auxiliary result:

Lemma 2.3: Let

$$\gamma_n(\lambda)=\inf_{\substack{(\chi_n,\chi_{-n})\in\mathcal{H}\times\mathcal{H}\\ \|\chi_n\|_{L^2}^2+\|\chi_{-n}\|_{L^2}^2=1}}\mathcal{J}(\chi_n,\chi_{-n}).$$

Then,

(1) For every $\lambda\geqslant 1$, *there exists a minimizer in* $\mathcal{H}\times\mathcal{H}$.
(2) γ_n *is a continuous function of* λ.

Proof: Since the proof is rather standard, we bring here only the main details and very briefly. Let $\{\phi_n^m,\phi_{-n}^m\}_{m=1}^{\infty}$ denote a minimizing sequence satisfying $\|\phi_n^m\|^2+\|\phi_{-n}^m\|^2=1$ for all m. Obviously,

$$\int_a^{\infty}|\phi_n^m|^2+|\phi_{-n}^m|^2\leqslant\frac{C}{a^2},$$

otherwise $\limsup_{m\to\infty}\mathcal{J}(\phi_n^m,\phi_{-n}^m)=\infty$. It is easy to show that the minimizing sequence is bounded in $H^1\times H^1$, and hence, there exists a subsequence which converges weakly to (ϕ_n,ϕ_{-n}). Clearly,

$$1\geqslant\int_{-\omega_0}^{a}|\phi_n|^2+|\phi_{-n}|^2\geqslant 1-\frac{C}{a^2},$$

and hence $\|\phi_n\|^2+\|\phi_{-n}\|^2=1$. To complete the proof of existence we need yet to show that E is weakly lower semicontinuous. This, however, is a very simple task. For instance,

$$\int_{-\omega_0}^{\infty} (\phi_n^m)' \overline{\phi_n'} \to \int_{-\omega_0}^{\infty} |\phi_n'|^2$$

in view of the weak convergence. Applying the Cauchy–Schwarz inequality we obtain

$$\liminf_{m\to\infty} \|(\phi_n^m)'\| \geqslant \|\phi_n'\|.$$

Similar treatment can be given to the rest of the terms in (2.17).

The proof that $\gamma_n(\lambda)$ is continuous is completely straightforward. □

We now calculate $\mathcal{J}(w_n,0)$ where $w_n = \exp\{-(x-n\omega)^2/2\}$. It is not difficult to show that

$$\mathcal{J}(w_n,0) \leqslant (1-\lambda)\sqrt{\pi} + \int_{-\omega_0}^{\infty} f^2 w_n^2 + Ce^{-(\omega_0+n\omega)^2} \leqslant (1-\lambda)\sqrt{\pi} + Ce^{-(\omega_0+n\omega)^2/2}.$$

Hence, there exists $C>0$ such that when

$$\lambda > 1 + Ce^{-(\omega_0+n\omega)^2/2},$$

we have $\mathcal{J}(w_n,0)<0$, and therefore, $\gamma_n(\lambda)<0$. Since, in view of (2.18), for sufficiently large n, $\gamma_n(\lambda)>0$ whenever $\lambda<\alpha_n$, and since $\gamma_n(\lambda)$ must be continuous, there exists λ_n satisfying (1.15) and $\gamma_n(\lambda_n)=0$. By lemma 2.3 there exists a minimizer which must satisfy (2.5), which completes the proof of the theorem. □

We note that the above theorem proves, only for sufficiently large n, that bifurcating modes can exist and that $\lambda_n>1$. Nevertheless, it seems plausible to conjecture that the bifurcation may take place only for $\lambda>1$. Furthermore, it appears reasonable to believe that λ_n is monotone decreasing, from which the previous conjecture readily follows.

It still remains necessary to find the dimension of the space of solutions of (2.4) for $\lambda=\lambda_n$. Consider then, (2.5), once again. Let $\phi_n^r = \Re\phi_n$, and $\phi_n^i = \Im\phi_n$. Then, the real part satisfies

$$-(\phi_n^r)'' + [(x-n\omega)^2 - \lambda]\phi_n^r + \lambda f^2(2\phi_n^r + \phi_{-n}^r) = 0, \tag{2.19a}$$

$$-(\phi_{-n}^r)'' + [(x+n\omega)^2 - \lambda]\phi_{-n}^r + \lambda f^2(2\phi_{-n}^r + \phi_n^r) = 0, \tag{2.19b}$$

$$(\phi_n^r)'(-\omega_0) = (\phi_{-n}^r)'(-\omega_0) = 0, \tag{2.19c}$$

whereas the imaginary part satisfies

$$-(\phi_n^i)'' + [(x-n\omega)^2 - \lambda]\phi_n^i + \lambda f^2(2\phi_n^i - \phi_{-n}^i) = 0, \tag{2.20a}$$

$$-(\phi_{-n}^i)'' + [(x+n\omega)^2 - \lambda]\phi_{-n}^i + \lambda f^2(2\phi_{-n}^i - \phi_n^i) = 0, \tag{2.20b}$$

$$(\phi_n^i)'(-\omega_0) = (\phi_{-n}^i)'(-\omega_0) = 0. \tag{2.20c}$$

Consequently, if (ϕ_n^r, ϕ_{-n}^r) is a solution of (2.19), then $(\phi_n^r, -\phi_{-n}^r)$ is a solution of (2.20). By (2.6) we have

$$\phi = \phi_n e^{in\omega x_2} + \phi_{-n} e^{-in\omega x_2}.$$

Substituting in the above a linear combination of the two independent modes (ϕ_n^r, ϕ_{-n}^r) and $(i\phi_n^r, -i\phi_{-n}^r)$ we obtain

$$\phi = C\phi_n^r e^{in\omega x_2} + \overline{C}\phi_{-n}^r e^{-in\omega x_2},$$

where $C\in\mathbb{C}$ is an arbitrary constant. We can now represent ϕ, upon substituting $C=|C|e^{-ix_2^0}$, in the following form:

$$\phi=|C|[\phi_n^r e^{in\omega(x_2-x_2^0)}+\phi_{-n}^r e^{-in\omega(x_2-x_2^0)}].$$

Consequently, the additional mode stands for translations in the x_2 direction and is, therefore, of very limited interest. Furthermore, since λ_n must be of even multiplicity in $\mathbb{X}$, it is not possible to apply the Crandall–Rabinowitz theorem.[24] Thus, it is desirable to confine the discussion to an appropriate *real* subspace of $\mathbb{X}$. We thus define

$$\mathbb{X}^*=\{u\in\mathbb{X}|\overline{u}(x_1,x_2)=u(x_1,L-x_2)\}.$$

In this space, we have $\phi_n=\phi_n^r$ for all n, and hence we need only to show that the solution space of (2.19) is one-dimensional.

Lemma 2.4: λ_n *is a simple eigenvalue of (2.19).*

Proof: Let (ϕ_n,ϕ_{-n}) and $(\tilde{\phi}_n,\tilde{\phi}_{-n})$ be two different solutions of (2.19). We show that they must be linearly dependent. To this end we first multiply (2.19a) by $\tilde{\phi}_n$ to obtain

$$\int_{-\omega_0}^{\infty} f^2(\phi_n\tilde{\phi}_{-n}-\tilde{\phi}_n\phi_{-n})=0.$$

Hence,

$$\exists x_0\in(-\omega_0,\infty)\quad [\phi_n\tilde{\phi}_{-n}-\tilde{\phi}_n\phi_{-n}]_{x=x_0}=0.$$

Consequently,

$$\exists C\in\mathbb{R}\ \text{ such that }\ \begin{bmatrix}\chi_n\\ \chi_{-n}\end{bmatrix}=\begin{bmatrix}\phi_n\\ \phi_{-n}\end{bmatrix}+C\begin{bmatrix}\tilde{\phi}_n\\ \tilde{\phi}_{-n}\end{bmatrix} \tag{2.21}$$

vanishes at $x=x_0$. Since (χ_n,χ_{-n}) is a solution of (2.19) we must have $\mathcal{J}(\chi_n,\chi_{-n})=0$. Let then,

$$\tilde{\chi}_n=\begin{cases}\chi_n & x_0\leqslant x\\ -\chi_n & -\omega_0\leqslant x<x_0\end{cases}.$$

Clearly, $\mathcal{J}(\tilde{\chi}_n,\tilde{\chi}_{-n})=0$, and hence, $(\tilde{\chi}_n,\tilde{\chi}_{-n})$ is a minimizer, which must have a continuous derivative at x_0. Consequently, $\chi_n'(x_0)=\chi_{-n}'(x_0)=0$ from which we conclude that $\chi_n\equiv\chi_{-n}\equiv 0$. □

III. WEAKLY NONLINEAR ANALYSIS

In the previous section, we showed that the linearized equation (2.4) has nontrivial solutions for a sequence of eigenvalues satisfying (1.15). However, our goal is to prove that each of these eigenvalues is a bifurcation point for the nonlinear equation

$$F(\lambda,u)=0, \tag{3.1}$$

where F is defined in (2.3).

In this section we prove the existence of a bifurcating branch at $(0,\lambda_n)$, for sufficiently large n. Furthermore, we prove that the bifurcation is supercritical and prove that the bifurcating branch is energetically lower than $u\equiv 0$, representing the one-dimensional solution (1.8).

A. Existence of the bifurcation

Theorem 3.1: *Equation (3.1) has a bifurcation point at* $(0,\lambda_n)$ *in* $\overset{*}{\mathbb{W}}$.

Proof: We use Theorem 1.7 in Ref. 24 to prove the existence of bifurcation. In view of the results of the previous section it remains to show that

$$F_{\lambda u}\phi \notin R(F_u(0,\lambda_n)),$$

where ϕ spans the solution space of (2.4) in $\mathbb{X}*$ at $\lambda=\lambda_n$. Alternatively, we can write

$$\Re\left\{\int_{-\omega_0}^{\infty}\overline{\phi}F_{\lambda u}\phi\right\}\neq 0. \tag{3.2}$$

The above condition may be applied also by applying to (3.1) the Taylor expansion

$$u=\epsilon u^{(0)}+\epsilon^2\tilde{u}, \tag{3.3a}$$

$$\lambda=\lambda^{(0)}+\epsilon\tilde{\lambda}. \tag{3.3b}$$

In the above $\lambda^{(0)}=\lambda_n$ satisfies (1.15), and $u^{(0)}$ is a solution of (2.4). Theorem 1.18 in Ref. 24 guarantees that

$$\tilde{u}=u^{(1)}+\epsilon u^{(2)}+O(\epsilon^2), \tag{3.4a}$$

$$\tilde{\lambda}=\lambda^{(1)}+\epsilon\lambda^{(2)}+O(\epsilon^2). \tag{3.4b}$$

This Taylor expansion, in powers of ϵ, would be useful while investigating whether the bifurcation is subcritical or supercritical and while estimating the energy of the bifurcating branch near the bifurcation point.

The $O(\epsilon^2)$ equation is given by

$$\begin{aligned}(i\nabla+x_1\hat{i}_2)^2u^{(1)}-\lambda^{(0)}[u^{(1)}-(f(x,\lambda^{(0)}))^2(2u^{(1)}+\overline{u}^{(1)})]\\ =\lambda^{(1)}g_\lambda+\lambda^{(0)}f(x,\lambda^{(0)})[2|u^{(0)}|^2+(u^{(0)})^2],\end{aligned} \tag{3.5a}$$

where

$$g_\lambda=\frac{\partial}{\partial\lambda}\{\lambda[u^{(0)}-(f(x,\lambda))^2(2u^{(0)}+\overline{u}^{(0)})]\}|_{\lambda=\lambda^{(0)}}, \tag{3.5b}$$

which is exactly equation 1.20 in Ref. 24 applied to our particular case. Multiplying (3.5a) by $\overline{u}^{(0)}$ we obtain after some manipulation that

$$\lambda^{(1)}I_\lambda=\lambda^{(0)}\Re\left\{\int f|u^{(0)}|^2(u^{(0)}+2\overline{u}^{(0)})\right\}, \tag{3.6a}$$

where

$$I_\lambda=\frac{\partial}{\partial\lambda}\left\{\lambda\int|u^{(0)}|^2-\frac{1}{2}f^2(x,\lambda^{(0)})|u^{(0)}+\overline{u}^{(0)}|^2-f^2|u^{(0)}|^2\right\}\Bigg|_{\lambda=\lambda^{(0)}}. \tag{3.6b}$$

Condition (3.2) is a solvability condition of (3.5). By (3.6) it can be expressed in the form $I_\lambda\neq 0$.

In the previous section we showed that when $\lambda^{(0)}=\lambda_n$ we have

$$u^{(0)}=\phi_n e^{i\omega n x_2}+\phi_{-n}e^{-i\omega n x_2}, \tag{3.7}$$

where (ϕ_n,ϕ_{-n}) is a solution of (3.6). Hence,

$$I_\lambda=\frac{2\pi}{\omega}\int_{-\omega_0}^{\infty}|\phi_n'|^2+(x-n\omega)^2|\phi_n|^2+|\phi_{-n}'|^2+(x+n\omega)^2|\phi_{-n}|^2$$
$$-2\lambda_n^2 f\frac{\partial f}{\partial\lambda}(|\phi_n|^2+|\phi_n+\overline{\phi}_{-n}|^2+|\phi_{-n}|^2). \tag{3.8}$$

In the following, we prove that $I_\lambda>0$. To this end we need first the following lemma.

Lemma 3.2: Let

$$\tilde{\beta}_n=\inf_{\phi\in\mathcal{H}}\frac{\int_{-\omega_0}^{\infty}|\phi'|^2+(x-n\omega)^2|\phi|^2-2\lambda_n^2 f\frac{\partial f}{\partial\lambda}|\phi|^2}{\int_{-\omega_0}^{\infty}|\phi|^2}. \tag{3.9}$$

Then, $\lim\tilde{\beta}_n=1$.

Proof: We first prove that

$$\left\|\frac{\partial f}{\partial\lambda}\right\|_\infty\leqslant C.$$

The equation satisfied by $\partial f/\partial\lambda=f_\lambda$ is

$$-f_\lambda''+[x^2-\lambda+3\lambda f^2]f_\lambda=f(1-f^2);\quad f_\lambda'(0)=0.$$

Clearly, there exists x_0 such that

$$x>x_0\Rightarrow x^2-\lambda+3\lambda f^2>1.$$

Suppose now, for a contradiction, that at some $x_1>x_0$, for some $\lambda=\lambda_0$ we have $f_\lambda(x_1,\lambda_0)>1$ and $f_\lambda'(x_1,\lambda_0)>0$. Then, since for $x>x_0$ f_λ cannot have a maximum greater than 1 we must have $f_\lambda(x,\lambda_0)>1$ for all $x>x_1$. Since both f_λ and f_λ' are continuous in λ there must be a neighborhood $(\lambda_0-\epsilon,\lambda_0+\epsilon)$ where $f_\lambda(x_1,\lambda)>1$ and $f_\lambda'(x_1,\lambda)>0$. Consequently,

$$x\geqslant x_1;\quad\lambda\in(\lambda_0-\epsilon,\lambda_0+\epsilon)\Rightarrow f_\lambda(x,\lambda)>1,$$

and hence,

$$f(x,\lambda_0+\epsilon)-f(x,\lambda_0-\epsilon)\geqslant 2\epsilon$$

for all $x\geqslant x_1$, contradicting (1.10). Thus, for $x>x_0$ we have

$$f_\lambda(x,\lambda)>1\Rightarrow f_\lambda'(x,\lambda)\leqslant 0$$

from which we can conclude that, for $x>x_0$,

$$f_\lambda(x,\lambda)\leqslant\max(f_\lambda(x_0,\lambda),1)\leqslant C(\lambda),$$

where C is independent of x. In a similar manner we can obtain a lower bound for f_λ, and hence,

$$\left|f\frac{\partial f}{\partial\lambda}\right|\leqslant Cx^{(\lambda-1)/2}\exp\{-x^2/2\}. \tag{3.10}$$

The lemma now follows from (2.7) with $g=-2\lambda_n^2 f\partial f/\partial\lambda$ and $\xi=-n\omega-\omega_0$. □

We now return to the proof of Theorem 3.1. From (3.8) it easily follows that

$$I_\lambda \geqslant \frac{4\pi}{\omega}\tilde{\beta}_n,$$

and hence, for sufficiently large n, I_λ must be positive, which proves our theorem.

B. Nature of the bifurcation

In the following we show that in some neighborhood of $(0,\lambda_n)$ in $X^*\times\mathbb{R}$ we must have $\lambda>\lambda_n$ along the bifurcating branch. Alternatively, we can state that the bifurcation is supercritical. From a physical point of view we can say that if we decrease the applied magnetic field (and consequently increase λ) below the critical field which corresponds to λ_n then the bifurcating branch continues to develop, i.e., $\|u\|$ increases.

Consider then, once again, (3.6). Using (3.7) it is not difficult to show that $\lambda^{(1)}=0$, which is a natural result in as much as we do not expect the sign of $\lambda-\lambda^{(0)}$ to depend on the sign of ϵ. Hence,

$$(i\nabla+x_1\hat{i}_2)^2u^{(1)}-\lambda^{(0)}[u^{(1)}-f^2(2u^{(1)}+\overline{u^{(1)}})]=\lambda^{(0)}f[2|u^{(0)}|^2+(u^{(0)})^2]. \tag{3.11}$$

The next order equation is given by

$$\begin{aligned}(i\nabla+x_1\hat{i}_2)^2u^{(2)}-\lambda^{(0)}&[u^{(2)}-f^2(2u^{(2)}+\overline{u^{(2)}})]\\ &=\lambda^{(2)}g_\lambda-\lambda^{(0)}\{|u^{(0)}|^2u^{(0)}+2f[u^{(0)}\overline{u^{(1)}}+u^{(1)}\overline{u^{(0)}}+u^{(1)}u^{(0)}]\}.\end{aligned} \tag{3.12}$$

The above equation no longer follows directly from Theorem 1.18 in Ref. 24. Nevertheless, it can be easily obtained, using the implicit function Theorem, in the same way it is used in the proof of equation 1.20 in Ref. 24.

Multiplying (3.12) by $\overline{u^{(0)}}$ and integrating by parts we obtain

$$\lambda^{(2)}I_\lambda=\lambda^{(0)}\int |u^{(0)}|^4+2f|u^{(0)}|^2(u^{(1)}+\overline{u^{(1)}})+2f\overline{u^{(0)}})^2u^{(1)}. \tag{3.13}$$

We now multiply (3.11) by $u^{(1)}$ to obtain

$$\begin{aligned}\int |(i\nabla+x_1\hat{i}_2)u^{(1)}|^2-\lambda^{(0)}&[|u^{(1)})|^2-2f^2|u^{(1)})|^2-\tfrac{1}{2}f^2(\overline{u^{(1)}}^2+(u^{(1)})^2)]\\ &=\lambda^{(0)}\int 2f|u^{(0)}|^2(u^{(1)}+\overline{u^{(1)}})+\tfrac{1}{2}f[\overline{u^{(0)}}^2u^{(1)}+\overline{u^{(1)}}(u^{(0)})^2].\end{aligned} \tag{3.14}$$

Hence,

$$\lambda^{(2)}I_\lambda=\lambda^{(0)}\int |u^{(0)}|^4+2\int |(i\nabla+x_1\hat{i}_2)u^{(1)}|^2-\lambda^{(0)}[|u^{(1)}|^2-f^2|u^{(1)})|^2-\tfrac{1}{2}f^2|\overline{u^{(1)}}+u^{(1)}|^2]. \tag{3.15}$$

By (2.17) and (3.7) we obtain, that if we substitute $u^{(0)}$ instead of $u^{(1)}$ in the second integral on the right hand side of (3.15) it must vanish identically. Furthermore, except for a finite number of n values, (3.7) must span the solution space of (2.4) in $\mathbb{X}^*$ when $\lambda^{(0)}=\lambda_n$. Hence, $u^{(0)}$ must serve as the nontrivial global minimizer of the second integral on the right hand side of (3.15). Consequently,

$$\int |(i\nabla + x_1\hat{i}_2)u^{(1)}|^2 - \lambda^{(0)}[|u^{(1)}|^2 - f^2|u^{(1)})|^2 - \tfrac{1}{2}f^2|\overline{u^{(1)}} + u^{(1)}|^2] \geqslant 0 \tag{3.16}$$

and hence,

$$\lambda^{(2)} \geqslant \frac{\lambda^{(0)}}{I_\lambda} \int |u^{(0)}|^4 > 0. \tag{3.17}$$

This proves our assertion, namely, that $\lambda > \lambda^{(0)}$ along the bifurcating branch, or, that the bifurcation is supercritical.

C. Energy

In this subsection we prove that (1.8) is not a local minimizer of (1.13) for $\lambda > 1$. To this end we show that for every $n \geqslant n_0$, there exist a right neighborhood of λ_n in $\mathbb{R}$ such that $\mathcal{E}(f+u,\lambda) < \mathcal{E}(f,\lambda)$. Let

$$\mathcal{E}_0(\lambda) = \mathcal{E}(f,\lambda) = \frac{2\pi}{\omega}\int_{-\omega_0}^{\infty} |f'| + x^2 f^2 + \lambda\left[\frac{1}{2}f^4 - f^2\right].$$

Let further

$$\begin{aligned}\Delta\mathcal{E}(u,\lambda) &= \mathcal{E}(f+u) - \mathcal{E}_0(\lambda) \\ &= 2\Re\left\{\int (i\nabla + x_1\hat{i}_2)f\cdot(-i\nabla + x_1\hat{i}_2)\overline{u}\right\} + \int |(i\nabla + x_1\hat{i}_2)u|^2 + 2\lambda\Re\left\{\int |f|^2[f\overline{u} + |u|^2]\right. \\ &\quad \left. + \tfrac{1}{2}f^2\overline{u}^2 + |u|^2[f\overline{u} + \tfrac{1}{4}|u|^2] - f\overline{u} - \tfrac{1}{2}|u|^2\right\}.\end{aligned}$$

Using (1.9) and integration by parts yields

$$\Delta\mathcal{E}(u,\lambda) = \int |(i\nabla + x_1\hat{i}_2)u|^2 + \lambda\int 2|f|^2|u|^2 + 2|u|^2\Re(f\overline{u}) + \lambda\int \frac{1}{2}|u|^4 - |u|^2 + \tfrac{1}{2}|f\overline{u} + \overline{\psi}_0 u|^2. \tag{3.18}$$

We now multiply the (3.1) by $\overline{u}$ and integrate to obtain

$$\int |(i\nabla + x_1\hat{i}_2)u|^2 = -\lambda\int 2|f|^2|u|^2 + |u|^2(2f\overline{u} + u\overline{\psi}_0) + f^2\overline{u}^2 + |u|^4 - |u|^2.$$

Combining the above with (3.18) we obtain

$$\Delta\mathcal{E}(u,\lambda) = -\frac{1}{2}\lambda\int [|f+u|^2 - |f|^2]|u|^2. \tag{3.19}$$

We now expand $\Delta\mathcal{E}$ in powers of ϵ. By (3.4) we have

$$\Delta\mathcal{E} = \epsilon^3\Delta\mathcal{E}^{(0)} + \epsilon^4\Delta\mathcal{E}^{(1)} + O(\epsilon^5).$$

Substituting (3.4) into (3.19) yields

$$\Delta\mathcal{E}^{(0)} = -\lambda^{(0)}\int |u^{(0)}|^2\Re(f\overline{u^{(0)}}) = 0.$$

Once again, this result corresponds to the natural expectation that the sign of ΔE does not depend on the sign of ϵ. The next order term is expressible in the form

$$\Delta\mathcal{E}^{(1)}=-\lambda^{(0)}\int\frac{1}{2}|u^{(0)}|^4+|u^{(0)}|^2\Re(f\overline{u^{(1)}})+2\Re(f\overline{u^{(0)}})\Re(u^{(0)}\overline{u^{(1)}}). \tag{3.20}$$

Using (3.14) we obtain

$$\Delta\mathcal{E}^{(1)}=-\lambda^{(0)}\int\frac{1}{2}|u^{(0)}|^4-\left\{\int|(i\nabla+x_1\hat{i}_2)u^{(1)}|^2-\lambda^{(0)}[|u^{(1)}|^2-f^2|u^{(1)})|^2-\frac{1}{2}f^2|\overline{u^{(1)}}+u^{(1)}|^2\right]$$

and by (3.16) we have

$$\Delta\mathcal{E}^{(1)}\leqslant-\frac{1}{2}\lambda^{(0)}\int|u^{(0)}|^4<0,$$

which proves our assertion, and hence completes the proof of theorem 1.1.

IV. CONCLUDING REMARKS

In Sec. II we proved the existence of a set of critical values $\{\lambda_n\}_{n=n_0}^{\infty}$ for which nontrivial solutions of (2.4) exist. We also show that $\lambda_n\downarrow 1$ exponentially fast according to (1.15). However, there might exist, finitely many, additional values of λ for which nontrivial solutions of (2.4) can exist. It would be reasonable to conjecture that $\{\lambda_n\}_{n=1}^{\infty}$ is monotone decreasing, yet, this hypothesis is proved only for large n. In fact, it is not proved yet that $\lambda_n>1$ for all n.

One can formulate the above conjecture in the following alternative manner: Let $\omega=1$ and

$$\gamma(\lambda,\alpha)=\inf_{\substack{(\phi_\alpha,\phi_{-\alpha})\in\mathcal{H}\times\mathcal{H}\\ \|\phi_\alpha\|_{L^2}^2+\|\phi_{-\alpha}\|_{L^2}^2=1}}\mathcal{J}(\phi_\alpha,\phi_{-\alpha}),$$

where $\mathcal{J}$ is defined in (2.17). We look for values of λ and α for which $\gamma=0$. For sufficiently large α it is proved in Sec. II that there exists $\alpha_0>0$ and a function $\lambda(\alpha):[\alpha_0,\infty)\to\mathbb{R}$ such that $\gamma(\lambda(\alpha),\alpha)=0$, and such that $\lambda(\alpha)\downarrow 1$ as $\alpha\to\infty$. If one can show that $\lambda(\alpha)$ can be continued into $\mathbb{R}_+$ such that $\lambda(\alpha)$ is monotone decreasing, the the above conjecture is proved.

In Sec. III we proved:

(1) Existence of the bifurcation points;
(2) super-criticality of the bifurcation;
(3) that the bifurcating solution is energetically preferable to the one-dimensional surface superconductivity solution.

Statements 1 and 2 were proved only for sufficiently large n. For n which is not large, the existence of nontrivial solutions of (2.4) does not guarantee $I_\lambda>0$, and hence the bifurcation points do not necessarily exist. In fact, even if the bifurcation from $(\lambda_n,0)$ exists, it is not clear that it must be supercritical (if $I_\lambda<0$ then a subcritical bifurcation exists).

In contrast, statement 3 is correct whenever a bifurcating solution exists. It is correct even for n which is not necessarily large, and even in the unlikely situation that the bifurcation takes place at $\lambda<1$. The surface superconductivity one-dimensional solution becomes therefore locally unstable at each bifurcation point.

Finally, we note that if it was possible to linearly superpose the bifurcating modes then the resulting combination would have the form

$$\psi=f+\sum_{n=-\infty}^{\infty}C_n\phi_n e^{i\omega n x_2},$$

and since

$$\phi_n \sim e^{-1/2(x_1 - n\omega)^2}$$

as $n \to \infty$ for $x_1 \sim O(n)$ we have

$$\psi \sim e^{i\omega P x_2} \sum_{n=-\infty}^{\infty} C_{n+P} e^{i\omega n x_2} e^{-1/2[x_1 - (n+P)\omega]^2} \tag{4.1}$$

for $P \gg 1$ and $x \sim O(P)$. The above formula thus approximates ψ far away from the wall at $x_1 = 0$. If

$$\exists N: \quad C_{n+N} = C_n \ \forall n.$$

Then the right-hand-side of (4.1) is periodic, or an Abrikosov lattice.[11–13]

Clearly, it is impossible to linearly superpose modes since the equations are nonlinear and since the bifurcations take place at different values of λ. Nevertheless, if $0 < \lambda - 1 \ll 1$ then $0 < \lambda - \lambda_n < \lambda - 1$ for almost every n. Hence, one might expect that the effect of nonlinearity tends to 0 as $\lambda \to 1$, and thus, that the solution far away from the wall can be approximated by an Abrikosov lattice.

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APPENDIX A: THE ONE-DIMENSIONAL SOLUTION

Theorem A.1: *Let $\mathcal{H}$ and $\beta(z)$ be, respectively, defined by (1.6) and (1.7). Let $\lambda > \beta(z)$. Then, there exists a positive solution in $\mathcal{H}$ to the equation*

$$-f'' + x^2 f = \lambda f(1 - f^2); \quad f'(z) = 0. \tag{A1}$$

Moreover,

$$f(x) \sim x^{-1-\lambda/2} e^{-1/2 x^2} \quad as \quad x \to \infty. \tag{A2}$$

Proof: Let

$$\epsilon_z(\phi) = \int_z^{\infty} (\phi')^2 + x^2 \phi^2 - \lambda \left[\phi^2 - \frac{1}{2} \phi^4 \right] dx.$$

We first prove the existence of a minimizer $\mathcal{H}$. Clearly, there exists $x_0 > z$ such that for $x \geqslant x_0$ we have $x^2 \geqslant \lambda + 1$. Then, since

$$\phi^2 - \tfrac{1}{2}\phi^4 \leqslant \tfrac{1}{2}$$

we have for all $\phi \in \mathcal{H}$

$$\epsilon_z(\phi) \geqslant -\frac{\lambda}{2}(x_0 - z).$$

Since ϵ_z is semibounded there is a minimizing sequence $\{\phi_n\}_{n=1}^{\infty}$ in $\mathcal{H}$. As

$$\frac{1}{x_0 - z} \left(\int_z^{x_0} \phi_n^2 \right)^2 \leqslant \int_z^{x_0} \phi_n^4 \leqslant 2 \int_z^{x_0} \phi_n^2 + C,$$

where C is independent of n, we obtain that $\|\phi_n\|_{L^2[z,x_0]} \leqslant C$. Recalling that $x^2-\lambda \geqslant 1$ in $[x_0,\infty)$ yields $\|\phi_n\|_{L^2(z,\infty)} \leqslant C$ and hence $\|\phi_n\|_{H^1(z,\infty)} \leqslant C$. Thus, there is a subsequence which converges weakly in $H^1(z,\infty)$ to a limit, which we denote by f. We skip the proof of lower semicontinuity–some of the details can be found in the proof of lemma 2.4.

Since f is a minimizer of ϵ_z in $\mathcal{H}$ it must satisfy (A1). Suppose for a contradiction that it changes sign at $x=x_1$. Then let

$$g=\begin{cases} f(x) & x \leqslant x_1 \\ -f(x) & x>x_1 \end{cases}.$$

Clearly, $\epsilon_z(f)=\epsilon_z(g)$, and thus, g must be a minimizer and, therefore, a solution of (A1). Thus, either $f \equiv 0$, or f does not change its sign (both f and $-f$ are minimizers).

We now prove that f is nontrivial. Let u_z be the minimizer of the fraction on the right-hand-side of (1.7) such that $\|u_z\|_2=1$. Then

$$\epsilon_z(cu_z)=-c^2[\lambda-\beta(z)]+c^4\int_z^\infty |u_z|^4.$$

Therefore, for sufficiently small c the minimizer must be nontrivial.

It remains necessary, yet, to prove (A2). We first prove that $f \to 0$ as $x \to \infty$. Suppose first, for a contradiction, that for some $x_2>x_0$ we have $f'(x_2)>0$. Then, since f cannot have a maximum for $x>x_0$, f must be greater than $f(x_2)$, contradicting $f \in \mathcal{H}$. Thus, $f' \leqslant 0$ for all $x>x_0$ from which we easily conclude that $f \to 0$ at infinity.

Let $w(x,t)$, where $t>x_0$, denote the decaying solution of

$$-w''+[x^2-\lambda]w=0; \quad x>t \quad w(t,t)=1.$$

By the maximum principle we must have that $f<f(t)w$ for all $x>x_0$. Let $f(x)=f(t)v(x,t)w(x,t)$. Substituting in (A1) we obtain

$$v'=-\frac{\lambda}{f(t)w^2}\int_x^\infty f^3(s)w(s,t)ds \geqslant -\lambda f^2(t)\int_x^\infty w^2(s,t)ds.$$

The properties of w have been obtain in Ref. 21 but can be also found in chapter 19 of Ref. 25. From both references we find that as $t \to \infty$, $x \to \infty$

$$w \sim \left(\frac{x}{t}\right)^{\lambda-1/2} e^{-1/2(x^2-t^2)} \quad \forall x \geqslant t$$

and hence, for all $x>t$

$$-2\lambda f^2(t)\frac{x^{\lambda-2}}{t^{\lambda-1}}e^{t^2-x^2} \leqslant v' < 0.$$

Since v is decreasing it must converge to a limit as $x \to \infty$. Integrating the above inequality by parts we obtain

$$v_\infty(t)=\lim_{x\to\infty} v(x,t) \geqslant 1-\lambda\frac{f^2(t)}{t}.$$

For sufficiently large t we, therefore, have $v_\infty(t)>0$, proving (A2).

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Existence and construction of the transmutation operator

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We prove the existence of a transmutation operator between two weighted Sturm–Liouville operators. We also provide an explicit formula for the transmutation operator and a construction algorithm. An example and an application to an inverse spectral problem are also considered. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Let L_1 and L_2, where

$$\begin{cases} L_1(\varphi) := -\dfrac{1}{w(x)}\varphi''(x,\lambda) + q(x)\varphi(x,\lambda) = \lambda\varphi(x,\lambda) & x \geqslant 0 \\ \varphi(0,\lambda) = 0, \end{cases} \tag{1.1}$$

$$\begin{cases} L_2(y) := -\dfrac{1}{w(x)}y''(x,\lambda) = \lambda y(x,\lambda) & x \geqslant 0 \\ y(0,\lambda) = 0, \end{cases} \tag{1.2}$$

and $w(x) \geqslant 0$, $qw, w \in L^{\mathrm{loc}}[0,\infty)$, be singular differential operators acting in the Hilbert space $L^2_w(0,\infty) := \{f$ measurable: $\int_0^\infty |f(x)|^2 w(x)dx < \infty\}$. The operator L_1 can be viewed as a perturbation of the more simple operator L_2, in which w is known as the density of the string and is allowed to vanish inside $[0,\infty)$. The string is well known to have numerous applications in prediction theory, Gaussian processes, function theory, moment problems and inverse problems, see Refs. 5–9.

Recall that the operator L_2 is in the limit-point case at infinity when $\int_0^\infty x^2 w(x)dx = \infty$ and (1.2) then defines a self-adjoint operator acting in $L^2_w(0,\infty)$. In case $\int_0^\infty x^2 w(x)dx < \infty$, then L_2 is in the limit circle at $x = \infty$ and we need to add a boundary condition at $x = \infty$. Thus without loss of generality, in all that follows, we can assume that both operators L_1 and L_2 are self-adjoint operators, adding a boundary condition at $x = \infty$, in the limit circle case. Denote, respectively, by σ_1 and σ_2 their spectra and by $\varphi(x,\lambda)$ and $y(x,\lambda)$ their eigensolutions which we normalize by $\varphi'(0,\lambda) = y'(0,\lambda) = 1$. It is known that the spectra are simple and the pair of transforms associated with L_1 is given by

$$\begin{aligned} &\mathbb{F}_1(f)(\lambda) = \int_0^\infty f(x)\varphi(x,\lambda)w(x)dx \quad \text{for } f \in L^2_w(0,\infty), \\ &f(x) = \int_{\sigma_1} \mathbb{F}_1(f)(\lambda)\overline{\varphi(x,\lambda)}d\Gamma_1(\lambda) \quad \text{for } \mathbb{F}_1(f) \in L^2_{\Gamma_1}(\sigma_1). \end{aligned} \tag{1.3}$$

Similarly for L_2 we have

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$$\mathbb{F}_2(f)(\lambda)=\int_0^\infty f(x)y(x,\lambda)w(x)dx \quad \text{for } f\in L^2_w(0,\infty),$$
$$f(x)=\int_{\sigma_2}\mathbb{F}_2(f)(\lambda)\overline{y(x,\lambda)}d\Gamma_2(\lambda) \quad \text{for } \mathbb{F}_2(f)\in L^2_{\Gamma_2}(\sigma_2). \tag{1.4}$$

We recall that λ belongs to the discrete spectrum, only in the case when the solution $y(x,\lambda)\in L^2_w(0,\infty)$. Thus if λ is in the continuous spectrum, then the eigensolutions are outside $L^2_w(0,\infty)$, i.e., $\int_0^\infty|y(x,\lambda)|^2w(x)dx=\infty$. An operator which transforms solutions $\varphi(x,\lambda)$ into $y(x,\lambda)$, i.e., $y(x,\lambda)=V\varphi(x,\lambda)$ for all values $\lambda\in\mathbb{C}$, is called a transmutation operator and plays a crucial role in the inverse spectral problem. For example if V exists then it is easy to see that

$$L_2V\varphi=L_2y=\lambda y=\lambda V\varphi=VL_1\varphi.$$

Since the set of eigenfunctionals φ is complete in $L^2_w(0,\infty)$, see Ref. 1, then $L_2V=VL_1$ and if we also assume that V^{-1} exists then

$$L_1=V^{-1}L_2V,$$

which means that we can reconstruct L_1 from the knowledge of V and L_2. In other words given w and V we can reconstruct the potential q. More details about the theory of transmutation operators and their applications can be found in Refs. 2–4 and 11.

The existence and construction of the operator V is at the heart of the theory of inverse problems. Note that the only well understood case of the transmutation operator is when $w(x)=1$. In this case V is a Volterra-type integral operator of the second kind, whose kernel satisfies a second order hyperbolic differential equation, see Ref. 10. In this paper we are concerned with the existence and construction of the transmutation operator V between L_1 and L_2 for a general nonnegative w. We will show that V is again a Volterra type integral operator of the second kind. Its construction, under some extra smoothness conditions on w and q, does not require any partial differential equation. Since a Volterra integral operator of the second kind has an inverse, the result of this paper can be used in the inverse problem of reconstructing the potential q.

II. EXISTENCE OF THE TRANSMUTATION OPERATOR

Our starting point is to use the variation of parameters to solve

$$\varphi''(x,\lambda)+\lambda w(x)\varphi(x,\lambda)=q(x)w(x)\varphi(x,\lambda),$$

which leads to the obvious relation between φ and y,

$$\varphi(x,\lambda)=y(x,\lambda)+\int_0^x G(x,t,\lambda)q(t)\varphi(t,\lambda)w(t)dt, \tag{2.1}$$

that can be rewritten in the form

$$y(x,\lambda)=\varphi(x,\lambda)-\int_0^x G(x,t,\lambda)q(t)\varphi(t,\lambda)w(t)dt, \tag{2.2}$$

where

$$G(x,t,\lambda)=y_1(x,\lambda)y_2(t,\lambda)-y_2(x,\lambda)y_1(t,\lambda), \tag{2.3}$$

and y_1 and y_2 are the fundamental solutions of the equation

$$y''(x,\lambda)+\lambda w(x)y(x,\lambda)=0$$

satisfying the initial conditions

$$y_1(0,\lambda)=1,\ \ y_1'(0,\lambda)=0,\quad y_2(0,\lambda)=0,\ \ y_2'(0,\lambda)=1.$$

At this point observe that although (2.2) is a mapping between y and φ, it does not define an operator, because the kernel $G(x,t,\lambda)$ depends on λ.

Since the solutions y_1 and y_2 are entire functions of λ, it follows that

$$G(x,t,\lambda)=\sum_{n\geqslant 0}\xi_n(x,t)\lambda^n$$

and (2.2) reduces to

$$\begin{aligned} y(x,\lambda)&=\varphi(x,\lambda)-\int_0^x\sum_{n\geqslant 0}\xi_n(x,t)q(t)\lambda^n\varphi(t,\lambda)w(t)dt\\ &=\varphi(x,\lambda)-\int_0^x\sum_{n\geqslant 0}\xi_n(x,t)q(t)L_1^n\varphi(t,\lambda)w(t)dt. \end{aligned}$$

Having replaced λ^n by operator L_1^n we arrive at the operator

$$Vf(x)=f(x)-\int_0^x\sum_{n\geqslant 0}\xi_n(x,t)q(t)L_1^nf(t)w(t)dt, \tag{2.4}$$

that is defined at least over the set $\{\varphi(t,\lambda)\}_{\lambda\in R}$. To find the domain of definition of V, observe first that

Proposition 1: For any $x>0$, there exists a sequence $\lambda_n\nearrow\infty$ such that $\{\varphi(t,\lambda_n)\}_{n\geqslant 0}$ is an orthogonal basis in $L_w^2(0,x)$.

Proof: First consider the regular self-adjoint differential operator on the interval $[0,x]$ with a Dirichlet boundary condition at the right end point

$$\begin{cases} L_x(\varphi_x)=-\dfrac{1}{w(t)}\varphi_x''(t,\lambda)+q(t)\varphi_x(t,\lambda)=\lambda\varphi_x(t,\lambda), & 0\leqslant t\leqslant x\\ \varphi_x(0,\lambda)=0, \quad \varphi_x(x,\lambda)=0. \end{cases} \tag{2.5}$$

This new regular self-adjoint problem on $[0,x]$ has a discrete spectrum, $\sigma_x:=\{\lambda_n\}\subset\mathbb{R}$ and obviously its eigenfunctions $\{\varphi_x(t,\lambda_n)\}_{n\geqslant 0}$ are orthogonal and form a basis in $L_w^2(0,x)$. But the solutions $\varphi_x(t,\lambda_n)$ and $\varphi(t,\lambda_n)$ differ by a constant multiplier only, so the set $\{\varphi(t,\lambda_n)\}_{n\geqslant 0}$ is also an orthogonal basis in $L_w^2(0,x)$. Thus the functional $V(f)(x)$ is defined on an orthogonal basis of $L_w^2(0,x)$.

Proposition 2: For any $x>0$ and $\lambda>0$ we have $\sup_{0\leqslant t\leqslant x}|G(x,t,\lambda)|\leqslant|x-t|$.

Proof: From Lemma 1 of Sec. III it is not difficult to see that the sequence $\xi_n(x,t)$ changes signs, and therefore $G(x,t,\lambda)=\Sigma_{n\geqslant 0}\xi_n(x,t)\lambda^n$ is an alternating series. The remainder theorem for alternating series yields

$$|G(x,t,\lambda)|\leqslant\xi_0(x,t)=(x-t)\quad \text{when}\ \ 0\leqslant t\leqslant x\quad \text{and}\ \ \lambda>0.$$

$G(x,t,\lambda)$ is uniformly bounded on $\lambda>0$, and since there is possibly only a finite number of nonpositive eigenvalues, $G(x,t,\lambda)$ is then bounded over the whole set σ_x of eigenvalues. From (2.1) it follows

$$|V\varphi(x,\lambda_n)-\varphi(x,\lambda_n)|\leqslant\sqrt{\int_0^x|G(x,t,\lambda_n)q(t)|^2w(t)dt}\ \ \|\varphi(t,\lambda_n)\|\leqslant C(x)\|\varphi(t,\lambda_n)\|.$$

Since $V-1$ is a bounded functional on the orthogonal basis $\{\varphi(t,\lambda)\}_{\lambda\in[0,1]}$ it can be extended uniquely to a linear bounded functional on $L^2_w(0,x)$. By the Riesz representation theorem, there exists $H(x,.)\in L^2_w(0,x)$ such that

$$Vf(x)-f(x)=\int_0^x H(x,t)f(t)w(t)dt$$

for all $f\in L^2_w(0,x)$. In particular

$$V\varphi(x,\lambda)-\varphi(x,\lambda)=\int_0^x H(x,t)\varphi(t,\lambda)w(t)dt$$

which leads to

Proposition 3: Assume that $w,qw\in L^{\mathrm{loc}}[0,\infty)$ and L_1 is self-adjoint then there exists a transmutation operator V such that

$$y(x,\lambda)=V\varphi(x,\lambda)=\varphi(x,\lambda)+\int_0^x H(x,t)\varphi(t,\lambda)w(t)dt, \tag{2.6}$$

where $H(x,.)\in L^2_w(0,x)$.

Remark: The completeness of $\varphi(x,\lambda)$ is a result of the self-adjointness of L_1. We could have used the operator L_2, whose classification is simpler, instead of L_1 to obtain a similar result. Recall that end-point classification for L_2 depends on the convergence of $\int_0^\infty x^2w(x)dx$ only.

Proposition 4: Assume that $w,\ qw\in L^{\mathrm{loc}}[0,\infty)$ and L_2 is self-adjoint then there exists a transmutation operator V^{-1} such that

$$\varphi(x,\lambda)=V^{-1}y(x,\lambda)=y(x,\lambda)+\int_0^x K(x,t)y(t,\lambda)w(t)dt,$$

where $K(x,.)\in L^2_w(0,x)$.

III. CONSTRUCTION OF THE TRANSMUTATION OPERATOR

Although the Riesz representation theorem guarantees the existence of the transmutation operator V, see Proposition 3, it does not help us construct its kernel $H(x,t)$. In this section we show how Green's function $G(x,t,\lambda)$ can be used to construct the transmutation operator.

We would like now to remove the λ appearing in the integral term in (3.7). From the uniform convergence of the $G(x,t,\lambda)=\Sigma_{n\geqslant 0}\xi_n(x,t)\lambda^n$ over $t\in(0,x),\ \lambda\in(0,1)$ we deduce that

$$\int_0^x G(x,\ t,\ \lambda)q(t)\varphi(t,\lambda)\,w(t)\,dt=\sum_{n\geqslant 0}\ \int_0^x q(t)\xi_n(x,t)\ \ L_1^n\varphi(t,\lambda)\,w(t)\,dt.$$

Since $G(x,x,\lambda)=0$, then $\xi_n(x,x)=0$ for any n. To simplify the integration by part, we assume $q\in C_0^\infty(0,\infty)$ and $w\in C^\infty(0,\infty)$, thus $q^{(n)}(0)=0$ for all $n\geqslant 0$ and

$$\int_0^x q(t)\xi_n(x,t)\ \ L_1\varphi(t,\lambda)\,w(t)\,dt$$

$$= -\int_0^x q(t)\xi_n(x,t)\ \ \varphi''(t,\lambda)dt + \int_0^x q^2(t)\xi_n(x,t)\ \ \varphi(t,\lambda)\,w(t)\,dt$$

$$= [-q(t)\xi_n(x,t)\ \ \varphi'(t,\lambda) + \partial_t[q(t)\xi_n(x,t)]\ \ \varphi(t,\lambda)]\big|_{t=0}^{t=x}$$

$$+ \int_0^x L_1[q(t)\xi_n(x,t)]\ \ \varphi(t,\lambda)\,w(t)\,dt$$

$$= q(x)[\partial_t\xi_n(x,t)]_{t=x}\ \ \varphi(x,\lambda) + \int_0^x L_1[q(t)\xi_n(x,t)]\ \ \varphi(t,\lambda)\,w(t)\,dt.$$

We will show that the term outside the integral vanishes. For that purpose we now prove few Lemmas that are also needed in the sequel.

Lemma 1: For each fixed x, $L_2\xi_n(x,.) = \xi_{n-1}(x,.)$ *and* $L_2\xi_0(x,.) = 0$

Proof: From the fact that $L_2G(x,t,\lambda) = \lambda G(x,t,\lambda)$, where L_2 acts on the t variable and the uniform convergence we have

$$\sum_{n\geqslant 0} L_2\xi_n(x,t)\lambda^n = \sum_{n\geqslant 1} \xi_{n-1}(x,t)\lambda^n$$

and so the Lemma follows.

Lemma 2: For each fixed x, we have

$$L_1^{n+1}\xi_n(x,t) = \sum_{k=0}^{n} L_1^k(q(t)\xi_k(x,t)).$$

Proof: From

$$L_1^{k+1}\xi_k(x,t) = L_1^k(L_2 + q(t))\ \ \xi_k(x,t) = L_1^k L_2\ \ \xi_k(x,t) + L_1^k(q(t)\ \ \xi_k(x,t)),$$

$$L_1^{k+1}\xi_k(x,t) = L_1^k\ \ \xi_{k-1}(x,t) + L_1^k(q(t)\xi_k(x,t)),$$

it follows that

$$L_1\ \ \xi_0(x,t) = L_2\ \ \xi_0(x,t) + q(t)\ \ \xi_0(x,t) = q(t)\ \ \xi_0(x,t)$$

and

$$\sum_{k=1}^{n} L_1^{k+1}\xi_k(x,t) = \sum_{k=1}^{n} L_1^k\xi_{k-1}(x,t) + \sum_{k=1}^{n} L_1^k(q(t)\ \ \xi_k(x,t)),$$

$$L_1^{n+1}\xi_n(x,t) = L_1\xi_0(x,t) + \sum_{k=1}^{n} L_1^k(q(t)\xi_k(x,t)) = \sum_{k=0}^{n} L_1^k(q(t)\xi_k(x,t)).$$

Lemma 3: $\xi_n(x,t) = \Sigma_{k\geqslant 2n} a_{nk}(x)\,(x-t)^k/k!$.

Proof: From (2.3) we have

$$\frac{\partial^2}{\partial t^2}G(x,t,\lambda) = -\lambda w(t)G(x,t,\lambda)$$

and Leibnitz's formula then yields

$$\frac{\partial^k}{\partial t^k}G(x,t,\lambda)=-\lambda\frac{\partial^{k-2}}{\partial t^{k-2}}[w(t)G(x,t,\lambda)]=-\lambda\sum_{j=0}^{k-2}\binom{k-2}{j}(w(t))^{(k-2-j)}\frac{\partial^j}{\partial t^j}G(x,t,\lambda). \tag{3.1}$$

For each fixed x we can also write

$$G(x,t,\lambda)=\sum_{k\geqslant 0} f_k(x,\lambda)\frac{(t-x)^k}{k!}, \tag{3.2}$$

where $f_k(x,\lambda)=(\partial^k/\partial t^k)\,G(x,t,\lambda)_{|t=x}$. Thus it follows from (3.1) that the sequence f_k satisfies a recurrence relation

$$f_k(x,\lambda)=-\lambda\sum_{j=0}^{k-2}\binom{k-2}{j}(w(x))^{(k-2-j)}f_j(x,\lambda). \tag{3.3}$$

The first two terms are (3.2)

$$f_0(x,\lambda)=0, \qquad f_1(x,\lambda)=W(y_1,y_2)=1.$$

From (3.3) it follows that f_k is a polynomial in λ of degree at most $[k/2]$

$$f_k(x,\lambda)=\sum_{j=1}^{[k/2]} a_{jk}(x)\lambda^j,$$

which leads to

$$G(x,t,\lambda)=\sum_{k\geqslant 1} f_k(x,\lambda)\frac{(t-x)^k}{k!}=\sum_{k\geqslant 1}\sum_{j=1}^{[k/2]} a_{jk}(x)\lambda^j\frac{(t-x)^k}{k!}=\sum_{j\geqslant 1}\left(\sum_{[k/2]\geqslant j} a_{jk}(x)\frac{(t-x)^k}{k!}\right)\lambda^j$$

and so

$$\xi_n(x,t)=\sum_{[k/2]\geqslant n} a_{nk}(x)\frac{(t-x)^k}{k!}=\sum_{k\geqslant 2n} a_{nk}(x)\frac{(t-x)^k}{k!}.$$

Thus using the above Lemma we have proven that

Proposition 5: If $n\geqslant 1$, *then* $\partial^k\xi_n(x,t)/\partial t^k{}_{|t=x}=0$ *for* $k=0,\ldots,2n-1$.

Using the above result we have

$$\begin{aligned}\int_0^x & q(t)\xi_n(x,t)\;\; L_1\varphi(t,\lambda)\,w(t)\,dt\\ &=q(x)[\partial_t\xi_n(x,t)]_{t=x}\;\;\varphi(x,\lambda)+\int_0^x L_1[q(t)\xi_n(x,t)]\;\;\varphi(t,\lambda)\,w(t)\,dt\\ &=\int_0^x L_1[q(t)\xi_n(x,t)]\;\;\varphi(t,\lambda)\,w(t)\,dt\end{aligned}$$

and in general for $k<n$,

$$\int_0^x L_1^k[q(t)\xi_n(x,t)]\ \ L_1\varphi(t,\lambda)\,w(t)\,dt$$
$$= -L_1^k[q(t)\xi_n(x,t)]_{|t=x}\varphi'(x,\lambda)+\partial_t L_1^k[q(t)\xi_n(x,t)]_{|t=x}\quad \varphi(x,\lambda)$$
$$+\int_0^x L_1^{k+1}[q(t)\xi_n(x,t)]\ \ \varphi(t,\lambda)\,w(t)\,dt.$$

Consider the first boundary term. We have

$$L_1^k[q(t)\xi_n(x,t)]_{|t=x}=\sum_{j=0}^{2k} A_j(t)\frac{\partial^j \xi_n(x,t)}{\partial t^j}_{|t=x} \tag{3.4}$$

which vanishes as long as $k<n$ (3.4). Similarly $(\partial/\partial t)\,L_1^k[q(t)\xi_n(x,t)]_{|t=x}=0$ and thus all boundary terms vanish if $k<n$.

Thus we have proven

Proposition 6: Assume that $w\geqslant 0$, and $w,\ q\in C^\infty(0,\infty)$. Then for any $n\geqslant 0$, we have

$$\int_0^x q(t)\xi_n(x,t)\ L_1^n\varphi(t,\lambda)\,w(t)\,dt=\int_0^x L_1^n[q(t)\xi_n(x,t)]\ \varphi(t,\lambda)\,w(t)\,dt.$$

The next step is to start from (2.6) and (2.2) to deduce that

$$-\int_0^x H(x,t)\varphi(t,\lambda)\,w(t)\,dt=\lim_{m\to\infty}\sum_{n=0}^{m}\ \int_0^x q(t)\xi_n(x,t)\ \ \lambda^n\varphi(t,\lambda)\,w(t)\,dt$$
$$=\lim_{m\to\infty}\sum_{n=0}^{m}\ \int_0^x q(t)\xi_n(x,t)L_1^n\varphi(t,\lambda)\,w(t)\,dt$$
$$=\lim_{m\to\infty}\sum_{n=0}^{m}\ \int_0^x L_1^n(q(t)\xi_n(x,t))\ \ \varphi(t,\lambda)\,w(t)\,dt$$
$$=\lim_{m\to\infty}\int_0^x\sum_{n=0}^{m}\ L_1^n(q(t)\xi_n(x,t))\ \ \varphi(t,\lambda)\,w(t)\,dt$$
$$=\lim_{m\to\infty}\int_0^x\sum_{n=0}^{m}\ L_1^n(q(t)\xi_n(x,t))\ \ \varphi(t,\lambda)\,w(t)\,dt$$
$$=\lim_{m\to\infty}\int_0^x L_1^{m+1}\xi_m(x,t)\ \ \varphi(t,\lambda)\,w(t)\,dt. \tag{3.5}$$

Since $\{\varphi(t,\lambda)\}_{0<\lambda<1}$ is dense in $L_w^2(0,x)$, the sequence $L_1^{m+1}\xi_m(x,.)$ converges weakly to $-H(x,.)$ in $L_w^2(0,x)$. We now show that $L_1^{m+1}\xi_m(x,.)$ is a bounded sequence in $L_w^2(0,x)$. As done previously, from (3.5) we have

$$\int_0^x L_1^{m+1}\xi_m(x,t)\ \ \varphi(t,\lambda)\,w(t)\,dt=\int_0^x G_m(x,t,\lambda)\varphi(t,\lambda)\,w(t)\,dt,$$

where

$$G_m(x,t,\lambda)=\sum_{n=0}^{m}\ \xi_n(x,t)\,\lambda^n$$

is the partial sum of the MacLaurin series of the Green function $G(x,t,\lambda)$. Since $G_m(x,t,\lambda)$ converges uniformly to $G(x,t,\lambda)$ for $t\in(0,x)$ and $\lambda\in(0,1)$, and $G(x,t,\lambda)$ is bounded there, then $G_m(x,t,\lambda)$ is uniformly bounded for $t\in(0,x)$ and $\lambda\in(0,1)$. Now

$$\left|\int_0^x L_1^{m+1}\xi_m(x,t)\ \varphi(t,\lambda)\,w(t)\,dt\right| = \left|\int_0^x G_m(x,t,\lambda)\varphi(t,\lambda)\,w(t)\,dt\right| \leqslant \sqrt{\int_0^x |G_m(x,t,\lambda)|^2 w(t)\,dt}\ \|\varphi(.,\lambda)\|,$$

which means

$$\|L_1^{m+1}\xi_m(x,.)\| \leqslant \sup_{m\geqslant 0}\ \sup_{\lambda\in(0,1)} \sqrt{\int_0^x |G_m(x,t,\lambda)|^2 w(t)\,dt} = C<\infty.$$

Thus the sequence $L_1^{m+1}\xi_m(x,.)$ is bounded in $L_w^2(0,\ x)$. But a bounded and weakly convergent sequence in a Hilbert space converges strongly to the same limit. Hence we have proven

Proposition 7: For each fixed $x>0$, $L_1^{m+1}\xi_m(x,t)\to -H(x,t)$, *strongly in* $L_w^2(0,\ x)$ *as* $m\to\infty$.

This proposition allows us to construct the kernel $H(x,t)$ of the transmutation operator V from the Green function $G(x,t,\lambda)$. To illustrate the above theory, we now present a very simple example which corresponds to the case $w(x)=x^\alpha$ where $\alpha>-1$. Clearly L_2 is in the limit point at $x=\infty$. Consider the Bessel operators defined by

$$S_1\begin{cases} L_1(\varphi) := -\dfrac{1}{x^\alpha}\dfrac{d^2}{dx^2}\varphi(x,\lambda)+q(x)\varphi(x,\lambda)=\lambda\varphi(x,\lambda), \quad x\geqslant 0 \\ \varphi(0,\lambda)=0, \quad \varphi'(0,\lambda)=1, \end{cases}$$

$$S_2\begin{cases} L_2(y) := -\dfrac{1}{x^\alpha}\dfrac{d^2}{dx^2}y(x,\lambda)=\lambda y(x,\lambda), \quad x\geqslant 0 \\ y(0,\lambda)=0 \quad y'(0,\lambda)=1. \end{cases}$$

Here $q\in L_{x^\alpha}^{\mathrm{loc}}[0,\infty)$.

Denote the normalized eigensolutions of the operator L_2

$$y''(x,\lambda)+\lambda x^\alpha y(x,\lambda)=0 \tag{3.6}$$

by

$$\mathcal{J}_1(x,\lambda)=a(\lambda)\sqrt{x}\mathbf{J}_{1/(\alpha+2)}\left(\frac{2\sqrt{\lambda}}{\alpha+2}x^{(\alpha+2)/2}\right),$$

$$\text{where}\quad a(\lambda)=\Gamma\left(\frac{\alpha+3}{\alpha+2}\right)(\alpha+2)^{1/(\alpha+2)}\lambda^{-\{1/[2(\alpha+2)]\}},$$

$$\mathcal{J}_2(x,\lambda)=b(\lambda)\sqrt{x}\mathbf{J}_{-1/(\alpha+2)}\left(\frac{2\sqrt{\lambda}}{\alpha+2}x^{\alpha+2/2}\right),$$

$$\text{where}\quad b(\lambda)=\Gamma\left(\frac{\alpha+1}{\alpha+2}\right)(\alpha+2)^{-[1/(\alpha+2)]}\lambda^{1/[2(\alpha+2)]}.$$

Here $\mathbf{J}_\nu(x)$ is the Bessel function. It is readily seen from $\mathbf{J}_\nu(x)\approx[1/\Gamma(1+\nu)](x/2)^\nu$ as $x\to 0$ that

$$\mathcal{J}_1(0,\lambda)=0 \quad \mathcal{J}_1'(0,\lambda)=1 \quad \text{and} \quad \mathcal{J}_2(0,\lambda)=1 \quad \mathcal{J}_2'(0,\lambda)=0,$$
$$\varphi(x,\lambda)=\mathcal{J}_1(x,\lambda)+\int_0^x G(x,\ t,\ \lambda)q(t)\varphi(t,\lambda)t^{\alpha}dt, \tag{3.7}$$

where Green's function is

$$\begin{aligned}G(x,\ t,\ \lambda)&=\mathcal{J}_1(x,\lambda)\mathcal{J}_2(t,\lambda)-\mathcal{J}_2(x,\lambda)\mathcal{J}_1(t,\lambda)\\&=\Gamma\left(\frac{\alpha+3}{\alpha+2}\right)\Gamma\left(\frac{\alpha+1}{\alpha+2}\right)\sqrt{xt}\\&\quad\times\left[\mathbf{J}_{1/(\alpha+2)}\left(\frac{2\sqrt{\lambda}}{\alpha+2}x^{(\alpha+2)/2}\right)\mathbf{J}_{-[1/(\alpha+2)]}\left(\frac{2\sqrt{\lambda}}{\alpha+2}t^{(\alpha+2)/2}\right)-\mathbf{J}_{1/(\alpha+2)}\right.\\&\quad\left.\times\left(\frac{2\sqrt{\lambda}}{\alpha+2}t^{(\alpha+2)/2}\right)\mathbf{J}_{-[1/(\alpha+2)]}\left(\frac{2\sqrt{\lambda}}{\alpha+2}x^{(\alpha+2)/2}\right)\right].\end{aligned}$$

A direct calculation with $\nu=1/(\alpha+2)$, reduces

$$\begin{aligned}\mathbf{J}_{\nu}(2\sqrt{\lambda}\nu x^{1/2\nu})\mathbf{J}_{-\nu}(2\sqrt{\lambda}\nu t^{1/2\nu})&=\sum_{n,k\geqslant 0}\frac{(-1)^n(2\sqrt{\lambda}\nu x^{1/2\nu})^{\nu+2n}}{n!\Gamma(\nu+n+1)}\frac{(-1)^k(2\sqrt{\lambda}\nu t^{1/2\nu})^{-\nu+2k}}{k!\Gamma(-\nu+k+1)}\\&=\sqrt{\frac{x}{t}}\sum_{n,k\geqslant 0}\frac{(-1)^{n+k}}{n!k!\Gamma(\nu+n+1)\Gamma(-\nu+k+1)}(2\nu)^{2n+2k}\\&\quad\times x^{n/\nu}t^{k/\nu}\lambda^{n+k},\end{aligned}$$

$$\begin{aligned}&\mathbf{J}_{\nu}(2\sqrt{\lambda}\nu t^{1/2\nu})\mathbf{J}_{-\nu}(2\sqrt{\lambda}\nu x^{1/2\nu})\\&\quad=\sqrt{\frac{t}{x}}\sum_{n,k\geqslant 0}\frac{(-1)^{n+k}}{n!k!\Gamma(\nu+k+1)\Gamma(-\nu+n+1)}(2\nu)^{2n+2k}t^{k/\nu}x^{n/\nu}\lambda^{n+k}.\end{aligned}$$

Therefore we arrive at an explicit formula for $G(x,t,\lambda)$,

$$\begin{aligned}G(x,\ t,\ \lambda)&=\Gamma(1+\nu)\Gamma(1-\nu)\sum_{n,k\geqslant 0}\frac{(-4\nu^2)^{n+k}(x-t)x^{n/\nu}t^{k/\nu}}{n!k!\Gamma(\nu+n+1)\Gamma(-\nu+k+1)}\lambda^{n+k}\\&=\sum_{n,k\geqslant 0}g_{nk}(x,t)\lambda^{n+k}\\&=\sum_{j\geqslant 0}\xi_j(x,t)\lambda^j,\end{aligned}$$

where

$$\xi_j(x,\ t)=(x-t)\sum_{k=0}^{j}\frac{1}{(1+\nu)_{j-k}}\frac{1}{(1-\nu)_k}(-4\nu^2)^j\frac{x^{(j-k)/\nu}}{(j-k)!}\frac{t^{k/\nu}}{k!} \tag{3.8}$$

and $(a)_n=a(a+1)\cdots(a+n-1)$. We arrive at

Proposition 8: If $w(x)=x^{\alpha}$ *where* $\alpha>-1$ *and* $q\in C_0^{\infty}(0,\infty)$, *then*

$$H(x,t)=-\lim_{m\to\infty}(-t^{-\alpha}D^2+q(t))^{m+1}\xi_m(x,\ t)$$

in $L^2_w(0,x)$, *with* $\xi_m(x,\ t)$ *being given by (3.8).*

IV. APPLICATIONS

We now briefly outline an interesting application of the transmutation operator $V^{-1}=1+K$. Using the above notation the Gelfand–Levitan theory would read as follows: Recover the potential q from the given spectral function Γ_1. To do so, we assume that we know $y(x,\lambda)$, Γ_2 and w such that the following function:

$$F(x,t)=\int y(x,\lambda)y(t,\lambda)d\sigma(\lambda),$$

where $\sigma(\lambda)=\Gamma_1(\lambda)-\Gamma_2(\lambda)$, is at least C^2 in x,t. Then we would form the linear integral equation

$$K(x,t)+F(x,t)+\int_0^x K(x,s)F(s,t)w(s)ds=0 \quad \text{for } 0<t<x,$$

which we solve for $K(x,t)$. Then define the function φ from the relation

$$\varphi(x,\lambda)=y(x,\lambda)+\int_0^x K(x,t)y(t,\lambda)w(t)dt.$$

It is then easy to show that there exists a function q such that

$$q(x)=\frac{1}{w(x)}\frac{d}{dx}[K(x,x)w(x)]+\frac{d}{dx}K(x,x)$$

and the newly constructed φ is a solution of Eq. (1.1).

The above analysis of constructing transmutation operators can be extended to the more general Sturm–Liouville operators

$$L_3(y)(x):=-\frac{1}{w(x)}(p(x)y'(x))'+q(x)y(x),$$

where $1/p,w,qw\in L^{\text{loc}}[0,\infty)$ and $p>0, w\geqslant 0$. To get the transmutation operator between L_2 and L_3 we can relate L_3 to L_1 in a very simple way. Denote by

$$\phi(t(x))=y(x),$$

where $t(x)=\int_0^x[1/p(t)]\,dt$. Then it follows that $\phi(t)$ satisfies $\phi'(t(x))=p(x)y'(x)$ and from

$$-\frac{1}{w(x)p(x)}p(x)(p(x)y'(x,\lambda))'+q(x)y(x,\lambda)=\lambda y(x,\lambda)$$

we deduce that

$$-\frac{1}{W(t)}\phi''(t,\lambda)+Q(t)\phi(t,\lambda)=\lambda\phi(t,\lambda),$$

which is similar to L_1 with $W(t(x))=w(x)p(x)$ and $Q(t(x))=q(x)$.

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Covariant Poisson equation with compact Lie algebras

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The covariant Poisson equation for Lie algebra-valued mappings defined on $\mathbb{R}^3$ is studied using functional analytic methods. Weighted covariant Sobolev spaces are defined and used to derive sufficient conditions for the existence and smoothness of solutions to the covariant Poisson equation. These conditions require, apart from suitable continuity, appropriate local L^p integrability of the gauge potential and global weighted L^p integrability of the curvature form and the source. The possibility of nontrivial asymptotic behavior of a solution is also considered. As a by-product, weighted covariant generalizations of Sobolev embeddings are established. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763001]

I. INTRODUCTION

Let us consider two mappings Z and F taking values in some compact Lie algebra $\mathcal{G}$. The covariant generalization of Poisson's equation on $\mathbb{R}^3$ is then

$$\Delta(A)Z=F, \tag{1}$$

where

$$\Delta(A)=\sum_{k=1}^{3}\nabla_k^2,$$

$$\nabla_k=\partial_k+[A_k,\cdot\,],$$

and A_k stands for a $\mathcal{G}$-valued gauge potential. This equation arises frequently in gauge theories and it is mostly connected with Gauss's law. In the Lagrangian formulation of Yang–Mills theory this connection is explicit, since Gauss's law reads

$$\Delta(A)A_0=\sum_{k=1}^{3}\nabla_k\dot{A}_k-J_0,\quad \dot{A}_k=\frac{\partial A_k}{\partial t},$$

J_0 denoting the matter density. In the Hamiltonian formalism the Gauss law becomes a divergence equation

$$\sum_{k=1}^{3}\nabla_k E_k=J_0,$$

but if we split the color-electric field E_k into longitudinal and transverse components by

$$E_k=E_k^L+E_k^T,$$

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$$\sum_{k=1}^{3} \nabla_k E_k^L = J_0, \quad \sum_{k=1}^{3} \nabla_k E_k^T = 0,$$

then a solution for the longitudinal component is given by

$$E_k^L = \nabla_k \Phi,$$

where Φ satisfies the covariant Poisson equation

$$\Delta(A)\Phi = J_0.$$

In addition to these cases the Poisson equation also arises if one tries to transform an arbitrary gauge potential $\mathcal{A}_\mu$ into an equivalent potential

$$A_\mu = \omega^{-1}\mathcal{A}_\mu\omega + \omega^{-1}\partial_\mu\omega,$$

where A_μ satisfies the generalized Coulomb gauge condition

$$\sum_{k=1}^{3} \nabla_k \dot{A}_k = 0,$$

which was proposed by Cronström in Ref. 1. It turns out that the gauge transformation matrix ω takes the form of a time-ordered exponential

$$\omega(x^0,\mathbf{x}) = \left[T\exp\left(-\int_0^{x^0} Z(\tau,\mathbf{x})\, d\tau \right) \right] \omega(0,\mathbf{x}),$$

where Z satisfies the Poisson equation

$$\Delta(\mathcal{A})Z = \sum_{k=1}^{3} \nabla_k(\mathcal{A})\dot{\mathcal{A}}_k.$$

These are the most important physical reasons for studying this equation. From a purely mathematical point of view the covariant Poisson equation is also interesting, because it is a special case of an elliptic system of partial differential equations which probably has not been considered before in the literature. Research has been done regarding solutions of the whole set of classical Yang–Mills equations,[2–5] but these approaches lead to hyperbolic evolution equations where Gauss's law becomes a constraint which must hold at all times. The Cauchy data of the problem is assumed to satisfy the constraint and the evolution equations are used to show that the constraint then persists. The starting point of this paper is quite different, because time evolution is not present in the covariant Poisson equation. Time serves only as a parameter of the mappings in question, but no specific evolution equations are required to hold.

The line of thought and the most important results of this paper are included in the next three sections. Section II deals with the existence of a distributional solution to the covariant Poisson equation. Conditions for making this solution smoother are derived in Sec. III, and the possibility of constructing a solution formula is touched upon in Sec. IV. Proofs are gathered in the last section, but the preceding sections are meant to be comprehensible even without reference to the proofs. The notations and conventions used in this paper are summarized below. Gauge potentials are written as

$$A_k(x) = A_k^a(x)T_a,$$

where the Lie algebra generators T_a satisfy

$$[T_a, T_b] = f_{ab}{}^c T_c .$$

Summation over repeated indices is implied. The components A_k^q and the structure constants $f_{ab}{}^c$ are real, because all compact Lie algebras are real. The curvature form of the gauge potential is defined as

$$G_{kl} = \partial_l A_k - \partial_k A_l - [A_k, A_l],$$

and the covariant divergence of G_{kl} is

$$(\nabla \cdot G)_k = \sum_{j=1}^{3} \nabla_j G_{jk} .$$

The definition of a compact Lie algebra implies that there exists a positive definite inner product

$$(X, Y) = h_{ab} X^a Y^b,$$

which is invariant under the adjoint action of the gauge group. The infinitesimal form of this property states that

$$(X, [Y, Z]) = -([Y, X], Z) \quad \text{for all } X, Y, Z \in \mathcal{G}. \tag{2}$$

If $\mathcal{G}$ is semisimple, this inner product can be chosen to be the negative of the Killing form (i.e., $h_{ab} = -f_{ac}{}^d f_{bd}{}^c$). The norm induced by this inner product will be denoted by $|\cdot|$. More generally, for $\mathcal{G}$-valued tensors $X_{i_1 \cdots i_r}$ the norm with nth covariant derivatives reads

$$|\nabla^n X| = \left(\sum_{k_1} \cdots \sum_{k_n} \sum_{i_1} \cdots \sum_{i_r} |\nabla_{k_1} \cdots \nabla_{k_n} X_{i_1 \cdots i_r}|^2 \right)^{1/2},$$

and the norm $|\partial^n X|$ with ordinary derivatives is defined analogously. Within the context of L^p norms it is always understood that the notation $\|X\|_p$ stands for $\| |X| \|_p$. We will also need multi-index notations for the covariant derivatives. Due to the noncommuting nature of these derivatives it is appropriate to deviate here from the usual definition and instead let a multi-index α denote an n-tuple of ordered coordinate indices

$$\alpha = (k_1, \ldots, k_n)$$

with the notation for covariant derivatives

$$\nabla^\alpha X = \nabla_{k_1} \cdots \nabla_{k_n} X.$$

The partial derivatives ∂^α are defined similarly. The order of a multi-index is simply $|\alpha| = n$, and the symbol ∇^n stands for the collection of all covariant derivatives ∇^α of order n. At this point the reader should take care so as not to confuse the collection of second order covariant derivatives ∇^2 with the covariant Laplacian $\Delta(A)$, and the same warning also applies to the norms $|\nabla^2 X|$ and $|\Delta(A) X|$, which have different meanings. Throughout the paper positive constants will be denoted by C, but the values of the constants may change from line to line as they are inessential for the proofs.

II. EXISTENCE OF A WEAK SOLUTION

A weak solution of the covariant Poisson equation (1) satisfies

$$-\int \sum_{k=1}^{3} (\nabla_k \tilde{\Phi}, \nabla_k Z)\, d^3x = \int (\tilde{\Phi}, F)\, d^3x \quad \text{for all } \tilde{\Phi} \in C_c^\infty(\mathbb{R}^3, \mathcal{G}),$$

when the weak covariant derivatives $\nabla_k Z$ and their commutators with A_k are locally integrable. The subscript c above refers to compact support. In order to control the asymptotic behavior of Z in subsequent calculations, introduce weights by writing

$$\tilde{\Phi}(x)=\frac{1}{w(x)^{1-\sigma}}\Phi(x), \quad w(x)=(1+|x|^2)^{1/2}, \quad 0<\sigma\leqslant 1.$$

This leads to an equivalent definition

$$\int \sum_{k=1}^{3} \frac{1}{w^{1-\sigma}}(\nabla_k\Phi,\nabla_k Z)\, d^3x - (1-\sigma)\int \sum_{k=1}^{3} \frac{x_k}{w^{3-\sigma}}(\Phi,\nabla_k Z)\, d^3x$$

$$= -\int \frac{1}{w^{1-\sigma}}(\Phi,F)\, d^3x \quad \text{for all } \Phi\in C_c^{\infty}(\mathbb{R}^3,\mathcal{G}). \tag{3}$$

The proof that there exists a solution to this equation is based on the well-known theorem by Lax and Milgram.[6,7] In order to apply this theorem we identify the left-hand side of the definition (3) as a bilinear mapping $B(\Phi,Z)$ and the right-hand side as a linear functional $f(\Phi)$. A suitably defined Sobolev space will play the role of a Hilbert space. We start by defining an inner product on the space $C_c^1(\mathbb{R}^3,\mathcal{G})$ by

$$\langle\Phi,\Psi\rangle_1=\int \frac{1}{w^{1-\sigma}}\sum_{k=1}^{3}(\nabla_k\Phi,\nabla_k\Psi)\, d^3x, \tag{4}$$

where it is assumed that $A_k\in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$. The norm associated with this inner product will be denoted by $\|\cdot\|_{1,2}$. In order to check that this formula really defines an inner product we need the following two results:

Lemma 1: Let $\mathcal{G}$ be a compact Lie algebra. Then there exists a constant $C>0$ such that

$$|[X,Y]|\leqslant C|X|\,|Y|$$

for all elements $X,Y\in\mathcal{G}$.

Proof: See Sec. V A.

Proposition 1: Let $A_k\in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$. Then the inequality

$$\left(\int \frac{1}{w^{3-\sigma}}|\Phi|^2\, d^3x\right)^{1/2}\leqslant C\left(\int \frac{1}{w^{1-\sigma}}\sum_{k=1}^{3}|\nabla_k\Phi|^2\, d^3x\right)^{1/2} \tag{5}$$

holds for all mappings $\Phi\in C_c^1(\mathbb{R}^3,\mathcal{G})$. The constant C does not depend on Φ.

Proof: See Sec. V B.

Lemma 1 together with Hölder's inequality ensures that the expression (4) is defined, and Proposition 1 guarantees that the norm $\|\Phi\|_{1,2}$ vanishes only when $\Phi\equiv 0$. The first order Sobolev space is now defined as the completion of $C_c^1(\mathbb{R}^3,\mathcal{G})$ in the norm $\|\cdot\|_{1,2}$, i.e.,

$$H_1(\mathbb{R}^3,\mathcal{G})=\overline{C_c^1(\mathbb{R}^3,\mathcal{G})}.$$

It goes without saying that this Sobolev space depends on σ, which is kept fixed in forthcoming calculations. Considering Cauchy sequences in $H_1(\mathbb{R}^3,\mathcal{G})$ with elements of class $C_c^1(\mathbb{R}^3,\mathcal{G})$ we can extend the inner product (4) and Proposition 1 to $H_1(\mathbb{R}^3,\mathcal{G})$. As a result, we see that the norm $\|\cdot\|_{1,2}$ can be extended to $H_1(\mathbb{R}^3,\mathcal{G})$ as it only vanishes for mappings equivalent to zero. Let us now apply the Lax–Milgram theorem to the bilinear mapping B of Eq. (3). Employing Schwarz's inequality and Proposition 1 yields

$$|B(Y,Z)|\leqslant[1+C(1-\sigma)]\|Y\|_{1,2}\|Z\|_{1,2} \quad \text{for all } Y,Z\in H_1(\mathbb{R}^3,\mathcal{G}),$$

which establishes the boundedness of B. Coercivity is proved by examining the second term of B with mappings of class $C_c^1(\mathbb{R}^3,\mathcal{G})$ first. Equation (2) shows that almost everywhere

$$(\Phi,\nabla_k\Phi)=(\Phi,\partial_k\Phi)=\tfrac{1}{2}\partial_k|\Phi|^2,$$

and this leads to the identity

$$-(1-\sigma)\int\sum_{k=1}^{3}\frac{x_k}{w^{3-\sigma}}(\Phi,\nabla_k\Phi)\,d^3x=-\frac{1}{2}(1-\sigma)\int\sum_{k=1}^{3}\partial_k\left(\frac{x_k}{w^{3-\sigma}}|\Phi|^2\right)d^3x+\frac{1}{2}(1-\sigma)\int\frac{3+\sigma|x|^2}{w^{5-\sigma}}|\Phi|^2\,d^3x.$$

The first integral on the right-hand side can be converted into a surface integral which vanishes due to the compact support of Φ. The second integral is non-negative and hence

$$-(1-\sigma)\int\sum_{k=1}^{3}\frac{x_k}{w^{3-\sigma}}(\Phi,\nabla_k\Phi)\,d^3x\geqslant 0.$$

Taking a Cauchy sequence (Φ_m) of mappings belonging to $C_c^1(\mathbb{R}^3,\mathcal{G})$ and converging to an arbitrary element Z in $H_1(\mathbb{R}^3,\mathcal{G})$ we see that the inequality above holds for Z also. Indeed, the integrals with Φ_m converge to the integral with Z by virtue of Proposition 1 and Schwarz's inequality. As a result,

$$B(Z,Z)\geqslant\|Z\|_{1,2}^2\quad\text{for all}\quad Z\in H_1(\mathbb{R}^3,\mathcal{G})$$

and the coercivity condition is satisfied. Now the Lax–Milgram theorem yields a solution to Eq. (3) whenever the right-hand side defines a bounded linear functional on $H_1(\mathbb{R}^3,\mathcal{G})$. By Schwarz's inequality the condition

$$\|w^{(1/2)(1+\sigma)}F\|_2<\infty \tag{6}$$

suffices for that purpose. We can summarize the result as follows:

Theorem 1: *Suppose that $A_k\in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$ and the condition (6) is satisfied. Then there exists in $H_1(\mathbb{R}^3,\mathcal{G})$ a weak solution of the covariant Poisson equation (1).*

Some words about the asymptotic behavior of the solution are appropriate at this stage. Roughly speaking, the mappings of $H_1(\mathbb{R}^3,\mathcal{G})$ tend to zero at infinity like some negative power of the radius $|x|$. In fact, there is a more general theorem by Cronström[8] stating that two classical solutions of the covariant Poisson equation are equal if their difference vanishes at infinity. Thus in order to obtain more solutions we must consider mappings with nontrivial behavior at infinity. Let us assume that a mapping Z_0 solves the Poisson equation asymptotically in the sense that

$$\|w^{(1/2)(1+\sigma)}(F-\Delta(A)Z_0)\|_2<\infty. \tag{7}$$

Then by Theorem 1 there exists a solution $Y\in H_1(\mathbb{R}^3,\mathcal{G})$ to the equation

$$\Delta(A)Y=F-\Delta(A)Z_0$$

and accordingly, a mapping defined by

$$Z=Y+Z_0 \tag{8}$$

solves the original equation (1). Since the mapping Y tends to zero at infinity in a generalized sense, the asymptotic behavior of Z is now determined by Z_0. Solutions with nontrivial behavior

can thus be obtained by constructing such a mapping Z_0 that the condition (7) is in force. To a great extent the details of the construction depend on the asymptotic behavior of the source F.

III. SMOOTHNESS OF SOLUTIONS

Now that we have proved the existence of a distributional solution to the Poisson equation, it is time to consider the smoothness properties of this solution. The standard technique is to define higher order Sobolev spaces and then apply the fact that these spaces are continuously embedded in the spaces of mappings with continuous and bounded derivatives. Then it remains to derive a suitable *a priori* estimate which enables us to conclude that a solution under certain assumptions belongs to a higher order Sobolev space. Let us begin with the definitions of nth order Sobolev spaces. Throughout this section the following local assumptions are supposed to hold:

Assumption: If $n=2$, we assume that

$$A_k \in C(\mathbb{R}^3,\mathcal{G}), \quad \partial^1 A_k \in L^3_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}), \quad \partial^2 A_k \in L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}), \quad G_{kl} \in C(\mathbb{R}^3,\mathcal{G}), \tag{9a}$$

while in the case $n \geqslant 3$ these assumptions are replaced by

$$A_k \in C^{n-3}(\mathbb{R}^3,\mathcal{G}), \quad \partial^{n-2} A_k \in L^q_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}) \quad \textit{for some } q>3, \quad \partial^{n-1} A_k \in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}),$$

$$G_{kl} \in C^{n-3}(\mathbb{R}^3,\mathcal{G}). \tag{9b}$$

These conditions enable us to define a higher order inner product on the space $C^n_c(\mathbb{R}^3,\mathcal{G})$ by

$$\langle \Phi,\Psi\rangle_n = \sum_{p=1}^{n} \int w^{(2p-3)(1-\sigma)} \sum_{k_1=1}^{3} \cdots \sum_{k_p=1}^{3} (\nabla_{k_1}\cdots\nabla_{k_p}\Phi, \nabla_{k_1}\cdots\nabla_{k_p}\Psi)\, d^3x.$$

The corresponding norm will be denoted by $\|\cdot\|_{n,2}$. Now the nth order Sobolev space is defined as

$$H_n(\mathbb{R}^3,\mathcal{G}) = \overline{C^n_c(\mathbb{R}^3,\mathcal{G})},$$

where the closure is taken in the norm $\|\cdot\|_{n,2}$. These spaces are going to be embedded in the spaces $C^{n-2}_B(\mathbb{R}^3,\mathcal{G})$ consisting of $C^{n-2}(\mathbb{R}^3,\mathcal{G})$ mappings for which the norm

$$\|\Phi\|_{n-2,\infty} = \max_{0 \leqslant p \leqslant n-2} \sup_{x\in\mathbb{R}^3} \{w(x)^{p(1-\sigma)} |\nabla^p \Phi(x)|\}$$

is finite. Note that $A_k \in C^{n-3}(\mathbb{R}^3,\mathcal{G})$ at this stage and the covariant derivatives in this definition thus yield continuous mappings. We can now formulate the embedding property exactly:

Theorem 2 (Sobolev embeddings): *Suppose that the assumptions (9) hold. Then the spaces $H_n(\mathbb{R}^3,\mathcal{G})$ are continuously embedded in the spaces $C^{n-2}_B(\mathbb{R}^3,\mathcal{G})$, i.e.,*

$$H_n(\mathbb{R}^3,\mathcal{G}) \subset C^{n-2}_B(\mathbb{R}^3,\mathcal{G}). \tag{10}$$

Proof: See Sec. V C.

The following *a priori* estimate establishes the inductive chain that allows us to include the distributional solution into higher order Sobolev spaces:

Proposition 2: Suppose that the conditions (9) are in force. Then the inequality

$$\|\Phi\|_{n,2} \leqslant C(\|\Phi\|_{n-1,2} + \|w^{(n-3/2)(1-\sigma)} \nabla^{n-2} \Delta(A)\Phi\|_2) \tag{11}$$

holds for all $\Phi \in C^{n+1}_c(\mathbb{R}^3,\mathcal{G})$. The constant C is independent of Φ, but it depends on weighted L^p norms of the curvature form as follows:

$$C = C(\|w^{2(1-\sigma)} G\|_\infty, \|w^{2(1-\sigma)} (\nabla \cdot G)\|_3),$$

when $n=2$, *whereas*

$$C=C(\|w^{(p+2)(1-\sigma)}\nabla^p G\|_\infty,\|w^{(p+2)(1-\sigma)}\nabla^p(\nabla\cdot G)\|_3),\quad p=0,\ldots,n-3,$$

when $n\geqslant 3$. *The constant is finite when the norms in question are finite.*

Proof: See Sec. V D.

It should be mentioned that the form of this estimate is not unique as there is some freedom in choosing the curvature norms which are to be bounded. The guideline here has been to keep the asymptotic requirements on the curvature as mild as possible and to make the transition to the unweighted case $\sigma=1$ easy. It is possible to relax the local assumptions, but that might happen at the cost of asymptotic conditions. The reason for worrying about the asymptotic behavior of the curvature form is a paper by Coleman[9] in which he shows that the only nonsingular solution satisfying the source-free Yang–Mills equations is the vacuum solution provided that the condition

$$\lim_{|x|\to\infty}|x|^{3/2+\epsilon}G^a_{\mu\nu}(x,t)=0,\quad 0<\epsilon<\tfrac{1}{2}$$

holds uniformly in time in the region $t>0$. It is easy to check that the norms of Proposition 2 escape this condition since $\sigma=1$ in the source-free case. When sources are present, the solution will always be nontrivial. Now in order to extend Proposition 2 to mappings in $H_n(\mathbb{R}^3,\mathcal{G})$ we employ the following density result:

Lemma 2: Suppose that the conditions (9) are in force. If

$$Z\in H_{n-1}(\mathbb{R}^3,\mathcal{G})\ \ and\ \ w^{(n-3/2)(1-\sigma)}\nabla^{n-2}\Delta(A)Z\in L^2(\mathbb{R}^3,\mathcal{G}),\tag{12}$$

then there exists a sequence (Φ_m) *of mappings belonging to* $C_c^\infty(\mathbb{R}^3,\mathcal{G})$ *such that* $\Phi_m\to Z$ *in* $H_{n-1}(\mathbb{R}^3,\mathcal{G})$ *and also*

$$\|w^{(n-3/2)(1-\sigma)}\nabla^{n-2}\Delta(A)(Z-\Phi_m)\|_2\to 0.$$

Proof: See Sec. V E.

Taking a Cauchy sequence (Φ_m) of $C_c^\infty(\mathbb{R}^3,\mathcal{G})$ mappings converging to Z in both norms of Lemma 2 and inserting it into the estimate (11) shows that the sequence also converges in $H_n(\mathbb{R}^3,\mathcal{G})$ towards Z. As a result,

$$Z\in H_n(\mathbb{R}^3,\mathcal{G})\subset C_B^{n-2}(\mathbb{R}^3,\mathcal{G}).$$

If the derivatives of Z satisfy the Poisson equation (1) in a distributional sense, the covariant Laplacian norms of Z can then be replaced by the corresponding norms of F. In short:

Theorem 3: *Suppose that the assumptions (9) hold and the curvature norms of Proposition 2 are finite. If in addition*

$$\|w^{(p+1/2)(1-\sigma)}\nabla^p F\|_2<\infty,\quad p=0,\ldots,n-2,\tag{13}$$

then the solution of the covariant Poisson equation given by Theorem 1 belongs to $C_B^{n-2}(\mathbb{R}^3,\mathcal{G})$.

When solutions with nontrivial asymptotic behavior are constructed by writing Z in the form (8), this theorem can be used to deduce the smoothess properties of Y, replacing only F with $F-\Delta(A)Z_0$ in the condition (13). The ultimate smoothness of Z then depends on the properties of Z_0.

IV. CONCLUSIONS

Theorems 1 and 3 are the main results regarding solutions of the covariant Poisson equation. All the assumptions of these theorems are only sufficient, and it remains an open question to determine the necessary conditions. However, it is likely that some bounds should be imposed on the curvature form. In fact, similar studies by Aubin,[10] Cantor,[11] and Eichhorn[12] on Riemannian

manifolds and vector bundles indicate that bounds are also needed for the curvature tensor and its derivatives in these approaches. As regards the smoothness assumptions (9), the fact that they are all local is consistent with the principles of fibre bundle theory in the sense that gauge potentials are considered as local objects. Global integrability conditions can be imposed on the curvature form without problems because the Lie algebra norms $|\nabla^p G|$ and $|\nabla^p(\nabla\cdot G)|$ are gauge invariant.

A slight shortcoming of the Lax–Milgram theorem is the fact that it does not give an explicit formula for the solution whose existence it proves. A formal procedure exists for separable Hilbert spaces, though. Following the proof of separability for ordinary Sobolev spaces (see, e.g., Ref. 7, Sec. 6.3) it is straightforward to check that the weighted covariant Sobolev space $H_1(\mathbb{R}^3,\mathcal{G})$ is indeed separable. Then it is possible, at least in principle, to construct a countable orthonormal basis $\{\Psi_n\}$ for $H_1(\mathbb{R}^3,\mathcal{G})$. Expressing Z and Φ in Eq. (3) as generalized Fourier series,

$$Z=\sum_{n=1}^{\infty} a_n\Psi_n, \quad \Phi=\sum_{n=1}^{\infty} b_n\Psi_n,$$

we see that the coefficients a_n are to be determined from the equation

$$a_n-\sum_{m=1}^{\infty} a_m(1-\sigma)\int \sum_{k=1}^{3}\frac{x_k}{w^{3-\sigma}}(\Psi_n,\nabla_k\Psi_m)\,d^3x=-\int \frac{1}{w^{1-\sigma}}(F,\Psi_n)\,d^3x.$$

The superficial simplicity of this solution formula hides the practical difficulties in constructing an orthonormal basis for $H_1(\mathbb{R}^3,\mathcal{G})$. Also in traditional approaches to the covariant Poisson equation the solution formulas tend to be too complicated. Employing suitable asymptotic conditions and inverting the ordinary Laplacian it is possible to convert the equation into an integral equation. No matter whether one iterates the resulting equation or applies Fredholm's formulas, the solution will always be rather complicated. Maybe we should not even expect the covariant Poisson equation to have simple and elegant solutions.

V. PROOFS

A. Lemma 1

This result is almost self-evident because the structure constants are bounded. Anyway, let us be explicit and consider the norm of the commutator

$$|[X,Y]|^2=X^aM_{ae}X^e,$$

$$M_{ae}=h_{cd}f_{ab}{}^{c}f_{ef}{}^{d}Y^bY^f.$$

Using Cauchy's inequality

$$X^aX^e\leqslant \tfrac{1}{2}[(X^a)^2+(X^e)^2]$$

we can derive the bound

$$|[X,Y]|^2\leqslant C(Y)\sum_{a=1}^{d}(X^a)^2, \tag{14}$$

where

$$C(Y)=\max_{1\leqslant a\leqslant d}\left\{\sum_{e=1}^{d}|M_{ae}|\right\}$$

and d denotes the dimension of the algebra. Applying similar techniques to the matrix M_{ae} we can also bound its elements by

$$|M_{ae}| \leqslant \tilde{C}_{ae} \sum_{b=1}^{d} (Y^b)^2,$$

where the matrix $\tilde{C}_{ae}$ is independent of Y. Hence we obtain an identical bound for the constant $C(Y)$ above. The proof is completed by noting that the metric tensor h_{ab} has strictly positive eigenvalues and the norm $|\cdot|$ is thus equivalent with the d-dimensional Euclidean norm appearing in inequality (14). □

B. Proposition 1

Let us begin with a more general theorem due to Gurka and Opic[13] regarding real functions on $\mathbb{R}^3$.

Theorem 4 (Gurka–Opic): *Let $1 \leqslant p < \infty$ and let $\overline{v_0}$, $\overline{v_1}$ be real, measurable, almost everywhere positive and finite functions of one real variable. Suppose further that they are bounded below and above by positive constants on every compact interval of the positive real axis and that there exists a constant $k > 0$ and a number $t_0 \in]0,\infty[$ such that*

$$\overline{v_0}(t) \geqslant k\, \overline{v_1}(t) t^{-p} \quad for\ all \quad t \geqslant t_0.$$

Finally, if

$$\sup_{0<\tau<\infty} \left(\int_0^\tau \overline{v_0}(t) t^2\, dt \right)^{1/p} \left(\int_\tau^\infty [\overline{v_1}(t) t^2]^{-1/(p-1)} dt \right)^{1-1/p} < \infty, \tag{15}$$

then there exists a constant $C > 0$ such that

$$\left(\int |u(x)|^p\, \overline{v_0}(|x|)\, d^3x \right)^{1/p} \leqslant C \left(\sum_{i=1}^{3} \int |\partial_i u(x)|^p\, \overline{v_1}(|x|)\, d^3x \right)^{1/p} \tag{16}$$

for all integrable functions u such that the norms of the inequality are finite. The constant C is independent of u.

Proof: This is a special case of Theorem 14.5. in Ref. 13. In their remarks Gurka and Opic state without proof that the conditions (15) and (16) are actually equivalent. □

We can now make use of this theorem and choose

$$p = 2, \quad \overline{v_0}(t) = (1+t^2)^{-[(3-\sigma)/2]}, \quad \overline{v_1}(t) = (1+t^2)^{-[(1-\sigma)/2]}, \quad 0 < \sigma \leqslant 1.$$

This leads to the inequality

$$\left(\int \frac{1}{w^{3-\sigma}} |u|^2\, d^3x \right)^{1/2} \leqslant C \left(\int \frac{1}{w^{1-\sigma}} \sum_{k=1}^{3} |\partial_k u|^2\, d^3x \right)^{1/2}, \tag{17}$$

which holds in particular for all $u \in C_c^1(\mathbb{R}^3)$. Condition (15) fails for $\sigma = 0$, indicating that the inequality (17) cannot be improved by setting σ to zero. In order to derive the inequality (5) we make use of a trick employed by Ginibre and Velo in Ref. 3. Namely, for a mapping $\Phi \in C_c^1(\mathbb{R}^3, \mathcal{G})$ we define a family of functions

$$u_\delta(x) = (|\Phi(x)|^2 + \delta^2)^{1/2} - \delta, \quad \delta > 0. \tag{18}$$

Clearly $u_\delta \in C_c^1(\mathbb{R}^3)$ and

$$\partial_k u_\delta = (|\Phi|^2 + \delta^2)^{-1/2} (\partial_k \Phi, \Phi). \tag{19}$$

As before, we note that

$$(\partial_k\Phi,\Phi)=(\nabla_k\Phi,\Phi) \tag{20}$$

whenever A_k is finite. Since $A_k\in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$, it follows that $\nabla_k\Phi\in L^2(\mathbb{R}^3,\mathcal{G})$ and Eq. (20) holds almost everywhere. Combining Eqs. (19) and (20) we see that

$$|\partial_k u_\delta|\leqslant|\nabla_k\Phi| \tag{21}$$

almost everywhere. Inequalities (17) and (21) finally yield inequality (5) in the limit $\delta\to 0$. □

C. Sobolev embeddings (10)

These embeddings constitute an obvious generalization of well-known results for real functions. Sobolev embeddings for Riemannian vector bundles have previously been derived by Cantor[11] and Eichhorn,[12] but the results are not directly applicable here, because they deal with unweighted inequalities only. For this reason it may be appropriate to present a derivation of the embeddings (10) here. The most essential part of the proof consists of deriving weighted generalizations of the ordinary embeddings, and the rest follows by employing the trick (18). Although there are very general weighted inequalities in Refs. 13 and 14 already, they are of little use here, because inequalities involving L^∞ norms are not included in them. For that reason we are going to proceed using a method presented in Chap. VI.6 of Ref. 15. Yet there is a small improvement in the calculations below compared with those of Ref. 15. Namely, it proved to be possible to lower the Sobolev space weight factors of the nth partial derivatives from $w^{n-[(3-\sigma)/2]}$ to $w^{(n-3/2)(1-\sigma)}$, which in turn leads to milder asymptotic conditions in Theorem 3. Let us begin with the familiar interpolation inequalities for real functions:[16]

Theorem 5 (Gagliardo–Nirenberg–Sobolev): *Let* $1\leqslant q\leqslant\infty$, $1\leqslant r\leqslant\infty$, $1\leqslant p\leqslant\infty$, $0\leqslant a\leqslant 1$ *and assume that the following relation holds true*:

$$\frac{1}{p}=\frac{1-a}{r}+a\left(\frac{1}{q}-\frac{1}{3}\right).$$

In the case $p=\infty$ *assume further that* $r<\infty$ *and* $a<1$. *Now if* $r<\infty$ *or* $q\geqslant 3$, *then there exists a constant* C, *depending only on* p, q, *and* r, *such that the inequality*

$$\|v\|_p\leqslant C\,\|v\|_r^{1-a}\,\|\partial v\|_q^a \tag{22}$$

holds for all functions $v\in L^r$ *whose derivatives lie in* L^q. *In the case* $r=\infty$, $q<3$ *the inequality holds for functions which in addition tend to zero at infinity or which lie in* L^{r_0} *for some finite* $r_0>0$.

The next step is to perform a change of variables by

$$y_k=\frac{x_k}{w(x)^{1-\sigma}},\quad 0<\sigma\leqslant 1.$$

This mapping is one-to-one and smooth in the range of σ and we can define a new function u by

$$u(y)=v(x(y)).$$

It is easily seen that

$$\int |u(y)|^r\,d^3y=\int |v(x)|^r(\det M)\,w(x)^{-3(1-\sigma)}\,d^3x,$$

where

$$M_{kl}=\delta_{kl}-(1-\sigma)\frac{x_k x_l}{1+|x|^2},\quad \det M=\frac{1+\sigma|x|^2}{1+|x|^2},\quad \sigma\leqslant\det M\leqslant 1.$$

As a result, we obtain the inequalities

$$\sigma^{1/r}\|w^{-(3/r)(1-\sigma)}v\|_r\leqslant\|u\|_r\leqslant\|w^{-(3/r)(1-\sigma)}v\|_r. \tag{23}$$

This is also valid if $r=\infty$, because the norms of u and v are equal then. For the derivative norm we need to know in addition that

$$|\partial u|^2=\sum_{k,l=1}^{3}\frac{\partial v}{\partial x_k}[M^{-1}(M^{-1})^T]_{kl}\frac{\partial v}{\partial x_l}w(x)^{2(1-\sigma)},$$

$$|\xi|^2\leqslant\sum_{k,l=1}^{3}\xi_k[M^{-1}(M^{-1})^T]_{kl}\xi_l\leqslant\frac{1}{\sigma^2}|\xi|^2\quad\text{for all}\quad\xi\in\mathbb{R}^3.$$

These properties together with the previous ones enable us to establish the inequality

$$\sigma^{1/q}\|w^{(1-(3/q))(1-\sigma)}\partial v\|_q\leqslant\|\partial u\|_q\leqslant\frac{1}{\sigma}\|w^{(1-(3/q))(1-\sigma)}\partial v\|_q. \tag{24}$$

Combining the inequalities (22)–(24) we are finally led to

$$\|w^{-(3/p)(1-\sigma)}v\|_p\leqslant C\sigma^{-a-1/p}\|w^{-(3/r)(1-\sigma)}v\|_r^{1-a}\|w^{(1-(3/q))(1-\sigma)}\partial v\|_q^a.$$

It is still possible to go a step further by defining a new function u through

$$v(x)=w(x)^\beta u(x),\quad \beta\in\mathbb{R},$$

and a fairly straightforward application of Minkowski's inequality then yields

$$\|w^{\beta-(3/p)(1-\sigma)}u\|_p\leqslant C\|w^{\beta-(3/r)(1-\sigma)}u\|_r^{1-a}(\|w^{\beta+(1-(3/q))(1-\sigma)}\partial u\|_q + |\beta|\,\|w^{\beta-1+(1-(3/q))(1-\sigma)}u\|_q)^a.$$

Now the trick (18) allows us to pass over to Lie algebra-valued mappings and to replace $|u|$ by $|\Phi|$ and $|\partial u|$ by $|\nabla\Phi|$ in the inequality above. In addition to that, it is only required that the weak derivatives of u_δ are given by the formula

$$\partial_k u_\delta=(|\Phi|^2+\delta^2)^{-1/2}(\nabla_k\Phi,\Phi).$$

Following the proof by Ginibre and Velo[3] it suffices to assume that there exists a sequence $(\Phi)_m$ of continuously differentiable mappings satisfying

$$\Phi_m\to\Phi\quad\text{in}\ L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})\ \text{and almost everywhere},$$

$$\nabla_k\Phi_m\to\nabla_k\Phi\quad\text{in}\ L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$$

in order to guarantee the validity of the derivative formula. In particular, Φ does not have to be continuous—local integrability of Φ and its covariant derivatives suffices. Using standard smoothing techniques (see Sec. V E) it is possible to prove that a sequence $(\Phi)_m$ with the desired properties can be constructed if A_k is continuous. Thus

$$\|w^{\beta-(3/p)(1-\sigma)}\Phi\|_p\leqslant C\|w^{\beta-(3/r)(1-\sigma)}\Phi\|_r^{1-a}(\|w^{\beta+(1-(3/q))(1-\sigma)}\nabla\Phi\|_q + |\beta|\,\|w^{\beta-(3/q)(1-\sigma)}\Phi\|_q)^a,$$

where we have also made use of the fact that $w^{-1}\leqslant w^{-(1-\sigma)}$. More generally, we can now apply the above inequality to mth covariant derivatives of Φ provided that the norms on the right-hand side are finite and the assumptions of Theorem 5 are in force. For the Sobolev embeddings we need the following three applications of this inequality:
(1)

$$\|w^{(n-2)(1-\sigma)}\nabla^{n-2}\Phi\|_\infty\leqslant C\,\|w^{(n-5/2)(1-\sigma)}\nabla^{n-2}\Phi\|_6^{1-a}(\|w^{(n-1-3/q)(1-\sigma)}\nabla^{n-1}\Phi\|_q + (n-2)\,\|w^{(n-2-3/q)(1-\sigma)}\nabla^{n-2}\Phi\|_q)^a, \tag{25a}$$

$$q>3,\quad a=\frac{q}{3(q-2)},$$

(2)

$$\|w^{(n-5/2)(1-\sigma)}\nabla^{n-2}\Phi\|_6\leqslant C\,(\|w^{(n-5/2)(1-\sigma)}\nabla^{n-1}\Phi\|_2+(n-2)\,\|w^{(n-7/2)(1-\sigma)}\nabla^{n-2}\Phi\|_2), \tag{25b}$$

(3)

$$\|w^{(n-1-3/q)(1-\sigma)}\nabla^{n-1}\Phi\|_q\leqslant C\,\|w^{(n-5/2)(1-\sigma)}\nabla^{n-1}\Phi\|_2^{1-b}(\|w^{(n-3/2)(1-\sigma)}\nabla^{n}\Phi\|_2 + (n-1)\,\|w^{(n-5/2)(1-\sigma)}\nabla^{n-1}\Phi\|_2)^b, \tag{25c}$$

$$q\leqslant 6,\quad b=3\left(\frac{1}{2}-\frac{1}{q}\right).$$

Here it is assumed that $\Phi\in C_c^n(\mathbb{R}^3,\mathcal{G})$ and the conditions (9) are satisfied. Combining these inequalities and recalling the definitions of the norms $\|\cdot\|_{n,2}$ and $\|\cdot\|_{n-2,\infty}$ we get

$$\|w^{(n-2)(1-\sigma)}\nabla^{n-2}\Phi\|_\infty\leqslant C\,\|\Phi\|_{n,2},$$

and hence

$$\|\Phi\|_{n-2,\infty}\leqslant C\,\|\Phi\|_{n,2}\quad\text{for all}\quad\Phi\in C_c^n(\mathbb{R}^3,\mathcal{G}).$$

Taking a Cauchy sequence $(\Phi)_m\in C_c^n(\mathbb{R}^3,\mathcal{G})$ converging to an element $Z\in H_n(\mathbb{R}^3,\mathcal{G})$ proves the embedding (10) in the limit $m\to\infty$. □

D. Proposition 2

The proof is elementary in principle but tedious in practice. It consists of two parts, the first being straightforward calculus with smooth enough gauge potentials, while in the second part the smoothness assumptions are relaxed by examining the convergence properties of the curvature norms. We begin by assuming that $A_k\in C^n(\mathbb{R}^3,\mathcal{G})$ and then consider a mapping $\Psi\in C_c^3(\mathbb{R}^3,\mathcal{G})$. Making use of the fact that

$$[\nabla_k,\nabla_l]_{\mathrm{op}}\Psi=-[G_{kl},\Psi],$$

where $[\cdot,\cdot]_{\mathrm{op}}$ stands for the operator commutator of two covariant derivatives, we deduce the identity

$$\begin{aligned}w^\beta|\nabla_k\nabla_l\Psi|^2=&\,\partial_l[w^\beta(\nabla_k\Psi,\nabla_k\nabla_l\Psi)]-\partial_k[w^\beta(\nabla_k\Psi,\nabla_l\nabla_l\Psi)]-\partial_k[w^\beta([G_{kl},\Psi],\nabla_l\Psi)]\\&-\partial_k[(\partial_l w^\beta)(\nabla_k\Psi,\nabla_l\Psi)]+(\partial_k\partial_l w^\beta)(\nabla_k\Psi,\nabla_l\Psi)+(\partial_l w^\beta)(\nabla_k\nabla_k\Psi,\nabla_l\Psi)\\&+(\partial_k w^\beta)(\nabla_l\nabla_l\Psi,\nabla_k\Psi)+(\partial_k w^\beta)([G_{kl},\Psi],\nabla_l\Psi)+w^\beta([\nabla_k G_{kl},\Psi],\nabla_l\Psi)\\&-2w^\beta(\nabla_k\Psi,[G_{kl},\nabla_l\Psi])+w^\beta(\nabla_k\nabla_k\Psi,\nabla_l\nabla_l\Psi).\end{aligned}$$

Integrating this equation with the help of the Gauss–Green theorem, the surface terms vanish due to the compact support of Ψ. Let us denote this support by K. Using now Lemma 1 and the inequality

$$|\partial^k w^\beta| \leqslant C w^{\beta-k}$$

together with Hölder's inequality we find the estimate

$$\begin{aligned}\|w^{\beta/2}\nabla^2\Psi\|_2^2 \leqslant C(&\|w^{\beta/2-1}\nabla\Psi\|_2^2 + \|w^{\beta/2}\Delta(A)\Psi\|_2 \|w^{\beta/2-1}\nabla\Psi\|_2 \\ &+ \|w^{2(1-\sigma)}G\|_{\infty,K} \|w^{\beta/2-(2-\sigma)}\Psi\|_2 \|w^{\beta/2-(1-\sigma)}\nabla\Psi\|_2 \\ &+ \|w^{2(1-\sigma)}(\nabla\cdot G)\|_{3,K} \|w^{\beta/2-(1-\sigma)}\Psi\|_6 \|w^{\beta/2-(1-\sigma)}\nabla\Psi\|_2 \\ &+ \|w^{2(1-\sigma)}G\|_{\infty,K} \|w^{\beta/2-(1-\sigma)}\nabla\Psi\|_2^2 + \|w^{\beta/2}\Delta(A)\Psi\|_2^2).\end{aligned}$$

Let us apply this inequality by choosing

$$\Psi = \nabla_{l_1}\cdots\nabla_{l_{n-2}}\Phi, \quad \beta = (2n-3)(1-\sigma).$$

If $n=2$, we employ Proposition 1, inequality (25b), the property $w^{-1} \leqslant w^{-(1-\sigma)}$ and finally Cauchy's inequality to get

$$\begin{aligned}\|w^{(1-\sigma)/2}\nabla^2\Phi\|_2^2 \leqslant C\{&\|w^{(1-\sigma)/2}\Delta(A)\Phi\|_2^2 + (1 + \|w^{2(1-\sigma)}G\|_{\infty,K} \\ &+ \|w^{2(1-\sigma)}(\nabla\cdot G)\|_{3,K}) \|w^{-[(1-\sigma)/2]}\nabla\Phi\|_2^2\}. \end{aligned} \tag{26}$$

This establishes a prestage of inequality (11), where the curvature norms are local, i.e., they are taken over the support of Φ. The constant C depends on Φ only through these curvature norms. For higher order derivatives with $n \geqslant 3$ we use inequality (25b) to bound the derivative norms up to the $(n-1)$th order. The highest order term with the covariant Laplacian is handled by writing

$$\nabla_k\nabla_k\nabla_{l_1}\cdots\nabla_{l_{n-2}}\Phi = \nabla_{l_1}\cdots\nabla_{l_{n-2}}\nabla_k\nabla_k\Phi + [\nabla_k\nabla_k, \nabla_{l_1}\cdots\nabla_{l_{n-2}}]_{\mathrm{op}}\Phi$$

and employing the decomposition

$$\begin{aligned}[\nabla_k\nabla_k, \nabla_{l_1}\cdots\nabla_{l_{n-2}}]_{\mathrm{op}}\Phi = -\sum_{p=0}^{n-3}\sum_{s_1=0}^{1}\cdots\sum_{s_p=0}^{1}(&[\nabla_{l_1}^{s_1}\cdots\nabla_{l_p}^{s_p}\nabla_k G_{kl_{p+1}}, \nabla_{l_1}^{1-s_1}\cdots\nabla_{l_p}^{1-s_p}\nabla_{l_{p+2}}\cdots\nabla_{l_{n-2}}\Phi] \\ &+ 2[\nabla_{l_1}^{s_1}\cdots\nabla_{l_p}^{s_p}G_{kl_{p+1}}, \nabla_{l_1}^{1-s_1}\cdots\nabla_{l_p}^{1-s_p}\nabla_k\nabla_{l_{p+2}}\cdots\nabla_{l_{n-2}}\Phi]),\end{aligned}$$

which can be proved by induction. If $p=0$ or $p=n-3$ this formula requires some interpretation, suppressing those sums and derivatives that become ill-defined. The important thing is to notice that the terms of this decomposition, when summed over k, are bounded in the Lie algebra norm by the norms

$$|\nabla^p(\nabla\cdot G)|\,|\nabla^{n-3-p}\Phi|, \quad |\nabla^p G|\,|\nabla^{n-2-p}\Phi|, \quad 0 \leqslant p \leqslant n-3.$$

Therefore, upon using Hölder's and Cauchy's inequalities together with the estimate (25b), we deduce the bound

$$\begin{aligned}\|w^{(n-3/2)(1-\sigma)}\nabla^n\Phi\|_2^2 \leqslant C\Bigg\{ & \|w^{(n-3/2)(1-\sigma)}\nabla^{n-2}\Delta(A)\Phi\|_2^2 \\ & + \sum_{p=0}^{n-3} (\|w^{(p+2)(1-\sigma)}\nabla^p(\nabla\cdot G)\|_{3,K}^2 \|\Phi\|_{n-2-p,2}^2 \\ & + \|w^{(p+2)(1-\sigma)}\nabla^p G\|_{\infty,K}^2 \|\Phi\|_{n-2-p,2}^2) \\ & + (1+\|w^{2(1-\sigma)}G\|_{\infty,K} + \|w^{2(1-\sigma)}(\nabla\cdot G)\|_{3,K}) \|\Phi\|_{n-1,2}^2 \Bigg\}, \end{aligned} \tag{27}$$

which in turn leads to an inequality like (11) with local curvature norms.

We are now done with the first part of the proof. The requirement $A_k \in C^n(\mathbb{R}^3,\mathcal{G})$ was dictated by the Gauss–Green theorem, but we can relax this condition by a few orders of smoothness. In fact, the assumptions (9) will prove to be sufficient for Proposition 2 to hold. The technique is to apply the estimates (26) and (27) to mollified gauge potentials. If the norms appearing in these inequalities converge to the original norms in the limit when the mollification is removed, we have succeeded in proving the inequalities with relaxed smoothness assumptions. Mollification is defined by the usual formula

$$A_k^{(\delta)}(x) = (\eta_\delta * A_k)(x) = \int \eta_\delta(x-y)A_k(y)\, d^3y$$

with

$$\eta_\delta(x) = \frac{1}{\delta^3}\eta\left(\frac{x}{\delta}\right), \quad \eta(x) = \begin{cases} C\exp\left(-\dfrac{1}{1-|x|^2}\right), & |x|<1 \\ 0, & |x|\geqslant 1, \end{cases} \quad \int \eta(x)\, d^3x = 1.$$

It is also assumed that all derivatives of the gauge potential A_k up to the highest order implied by the curvature norms are at least locally integrable. This assumption ensures that the order of differentiation and mollification can be reversed. The covariant derivative related to the mollified potential will be denoted by

$$\nabla_k^{(\delta)} = \partial_k + [A_k^{(\delta)}, \cdot\,],$$

and the corresponding curvature form is

$$\hat{G}_{kl}^{(\delta)} = \partial_l A_k^{(\delta)} - \partial_k A_l^{(\delta)} - [A_k^{(\delta)}, A_l^{(\delta)}].$$

Also define a mollified norm $|\nabla^p G|^{(\delta)}$ by

$$|\nabla^p G|^{(\delta)} = \left(\sum_{k_1} \cdots \sum_{k_p} \sum_l \sum_m \left| \int \eta_\delta(x-y)\nabla_{k_1}\cdots\nabla_{k_p} G_{lm}(y)\, d^3y \right|^2 \right)^{1/2}.$$

It is well-known that in the limit $\delta \to 0$

$$\|w^{(p+2)(1-\sigma)}|\nabla^p G|^{(\delta)}\|_{\infty,K} \to \|w^{(p+2)(1-\sigma)}|\nabla^p G|\,\|_{\infty,K}, \tag{28}$$

when $\nabla^p G_{lm} \in C(\mathbb{R}^3,\mathcal{G})$. However, we eventually need the result

$$\|w^{(p+2)(1-\sigma)}|(\nabla^{(\delta)})^p \hat{G}^{(\delta)}|\,\|_{\infty,K} \to \|w^{(p+2)(1-\sigma)}|\nabla^p G|\,\|_{\infty,K}, \tag{29}$$

and this can be proved using the limit (28) combined with the estimate

$$\| w^{(p+2)(1-\sigma)}(|\nabla^p G|^{(\delta)} - |(\nabla^{(\delta)})^p \hat{G}^{(\delta)}|)\|_{\infty,K}$$
$$\leqslant \sum_{k_1} \cdots \sum_{k_p} \sum_{l} \sum_{m} \| w^{(p+2)(1-\sigma)} |\, \eta_\delta * (\nabla_{k_1} \cdots \nabla_{k_p} G_{lm}) - \nabla^{(\delta)}_{k_1} \cdots \nabla^{(\delta)}_{k_p} \hat{G}^{(\delta)}_{lm}| \,\|_{\infty,K}. \tag{30}$$

Using the decomposition

$$\nabla_{k_1} \cdots \nabla_{k_p} G_{lm} = \sum_{j=0}^{p} \sum_{i_1=1}^{i_2-1} \cdots \sum_{i_j=j}^{p} \partial_{k_1} \cdots \partial_{k_{i_1-1}} (\mathrm{ad} A_{k_{i_1}}) \partial_{k_{i_1+1}} \cdots \partial_{k_{i_j-1}} (\mathrm{ad}\, A_{k_{i_j}}) \partial_{k_{i_j+1}} \cdots \partial_{k_p} G_{lm} \tag{31}$$

with the notation $\mathrm{ad}\, A_k = [A_k, \cdot\,]$ and recalling the definition of the curvature form we see that each term of this decomposition takes the form

$$\mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A_{k_{i_j}}) \partial^{\alpha_{i_{j+1}}} A_{k_{p+2}}, \tag{32a}$$

where the multi-indices α_{i_j} satisfy

$$\sum_{s=1}^{j+1} |\alpha_{i_s}| = p+1-j, \quad 0 \leqslant j \leqslant p+1. \tag{32b}$$

Since there are a finite number of terms in the formulas (30) and (31) altogether, it suffices to consider each term separately. In inequality (30) the contribution from each term of the form (32a) is

$$\begin{aligned}
&\| w^{(p+2)(1-\sigma)} |\, \eta_\delta * (\mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A_{k_{i_j}}) \partial^{\alpha_{i_{j+1}}} A_{k_{p+2}}) \\
&\quad - \mathrm{ad}(\partial^{\alpha_{i_1}} A^{(\delta)}_{k_{i_1}}) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A^{(\delta)}_{k_{i_j}}) \partial^{\alpha_{i_{j+1}}} A^{(\delta)}_{k_{p+2}} | \,\|_{\infty,K} \\
&\leqslant \operatorname*{ess\,sup}_{x \in K} C \left| \int d^3y_1 \cdots d^3y_{j+1}\, \eta_\delta(x-y_1) \cdots \eta_\delta(x-y_{j+1}) \right. \\
&\qquad \times \{ \mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}(y_{j+1})) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A_{k_{i_j}}(y_{j+1})) \partial^{\alpha_{i_{j+1}}} A_{k_{p+2}}(y_{j+1}) \\
&\qquad \left. - \mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}(y_1)) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A_{k_{i_j}}(y_j)) \partial^{\alpha_{i_{j+1}}} A_{k_{p+2}}(y_{j+1}) \} \right| \qquad (33a) \\
&\leqslant C \sum_{s=1}^{j} \operatorname*{ess\,sup}_{x \in K} \left| \int d^3y_1 \cdots d^3y_{j+1}\, \eta_\delta(x-y_1) \cdots \eta_\delta(x-y_{j+1}) \right. \\
&\qquad \times \mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}(y_{j+1})) \cdots \mathrm{ad}(\partial^{\alpha_{i_s}} A_{k_{i_s}}(y_{j+1}) - \partial^{\alpha_{i_s}} A_{k_{i_s}}(y_s)) \\
&\qquad \left. \times \mathrm{ad}(\partial^{\alpha_{i_{s+1}}} A_{k_{i_{s+1}}}(y_{s+1})) \cdots \partial^{\alpha_{i_{j+1}}} A_{k_{p+2}}(y_{j+1}) \right|, \quad j \geqslant 1, \qquad (33b)
\end{aligned}$$

and in the case $j=0$ expression (33a) vanishes. The constant C corresponds to the upper bound of the weight factor on K, and in deriving the last inequality the formula

$$\mathrm{ad}\, B_1 \cdots \mathrm{ad}\, B_m - \mathrm{ad}\, C_1 \cdots \mathrm{ad}\, C_m = \sum_{s=1}^{m} \mathrm{ad}\, B_1 \cdots \mathrm{ad}(B_s - C_s) \mathrm{ad}\, C_{s+1} \cdots \mathrm{ad}\, C_m$$

was used. Applying now Hölder's inequality and Lemma 1 to the expression (33b) we see that each term in the sum is bounded by

$$\operatorname*{ess\,sup}_{\substack{y_s,y_{j+1}\in K_\delta\\ |y_s-y_{j+1}|\leqslant 2\delta}}\left|\partial^{\alpha_{i_s}}A_{k_{i_s}}(y_{j+1})-\partial^{\alpha_{i_s}}A_{k_{i_s}}(y_s)\right|\prod_{\substack{r=1\\ r\neq s}}^{j+1}\operatorname*{ess\,sup}_{y\in K_\delta}\left|\partial^{\alpha_{i_r}}A_{k_{i_r}}(y)\right|,$$

$$K_\delta=\{x\in\mathbb{R}^3\,|\,\mathrm{dist}(x,K)\leqslant\delta\}.$$

Since now

$$|\alpha_{i_s}|\leqslant p\leqslant p_{\max}=\begin{cases}0, & n=2,\\ n-3, & n\geqslant 3,\end{cases}$$

the bound above tends to zero in the limit $\delta\to 0$ for gauge potentials of class $C^{p_{\max}}(\mathbb{R}^3,\mathcal{G})$. As a result,

$$\|\,w^{(p+2)(1-\sigma)}(|\nabla^p G|^{(\delta)}-|(\nabla^{(\delta)})^p\hat{G}^{(\delta)}|)\|_{\infty,K}\to 0,$$

and together with the limit (28) this establishes the desired convergence property (29). The L^3 curvature norm is treated similarly. We define a mollified norm

$$|\nabla^p(\nabla\cdot G)|^{(\delta)}=\left(\sum_{k_1}\cdots\sum_{k_p}\sum_m\left|\int\eta_\delta(x-y)\nabla_{k_1}\cdots\nabla_{k_p}\sum_l\nabla_l G_{lm}(y)\,d^3y\right|^2\right)^{1/2},$$

which satisfies

$$\|w^{(p+2)(1-\sigma)}|\nabla^p(\nabla\cdot G)|^{(\delta)}\|_{3,K}\xrightarrow[\delta\to 0]{}\|w^{(p+2)(1-\sigma)}|\nabla^p(\nabla\cdot G)|\,\|_{3,K}\tag{34}$$

when $|\nabla^p(\nabla\cdot G)|\in L^3_{\mathrm{loc}}$. An estimate for the norm

$$\|\,w^{(p+2)(1-\sigma)}(|\nabla^p(\nabla\cdot G)|^{(\delta)}-|(\nabla^{(\delta)})^p(\nabla^{(\delta)}\cdot\hat{G}^{(\delta)})|)\|_{\,3,K}\tag{35}$$

is obtained by decomposing the expression

$$\nabla_{k_1}\cdots\nabla_{k_p}\sum_l\nabla_l G_{lm}$$

into terms of the form (32) with p replaced by $p+1$ as there is one additional derivative now. As before, only terms with $j\geqslant 1$ contribute to the norm (35), these contributions being bounded by the integrals

$$\begin{aligned}&\int_K d^3x\left|\int d^3y_1\cdots d^3y_{j+1}\,\eta_\delta(y_1)\cdots\eta_\delta(y_{j+1})\,\mathrm{ad}(\partial^{\alpha_{i_1}}A_{k_{i_1}}(x-y_{j+1}))\cdots\right.\\ &\left.\times\,\mathrm{ad}(\partial^{\alpha_{i_s}}A_{k_{i_s}}(x-y_{j+1})-\partial^{\alpha_{i_s}}A_{k_{i_s}}(x-y_s))\,\mathrm{ad}(\partial^{\alpha_{i_{s+1}}}A_{k_{i_{s+1}}}(x-y_{s+1}))\cdots\partial^{\alpha_{i_{j+1}}}A_{k_{p+3}}(x-y_{j+1})\right|^3\\ &\leqslant C\operatorname*{ess\,sup}_{|y_1|\leqslant\delta}\cdots\operatorname*{ess\,sup}_{|y_{j+1}|\leqslant\delta}\int_K d^3x\,(|\,\partial^{\alpha_{i_1}}A_{k_{i_1}}(x-y_{j+1})|\cdots|\,\partial^{\alpha_{i_s}}A_{k_{i_s}}(x-y_{j+1})-\partial^{\alpha_{i_s}}A_{k_{i_s}}(x-y_s)|\\ &\quad\times|\,\partial^{\alpha_{i_{s+1}}}A_{k_{i_{s+1}}}(x-y_{s+1})|\cdots|\,\partial^{\alpha_{i_{j+1}}}A_{k_{p+3}}(x-y_{j+1})|)^3.\end{aligned}\tag{36}$$

The last inequality was derived by employing Lemma 1 and Hölder's inequality repeatedly. Now if $j \geqslant 2$, we have $|\alpha_{i_s}| \leqslant p_{\max}$ and the integrand of the estimate (36) is continuous, meaning that the whole expression vanishes in the limit $\delta \to 0$. In the case $j=1$ there are two multi-indices satisfying

$$|\alpha_{i_1}| + |\alpha_{i_2}| \leqslant p_{\max} + 1.$$

If one of them takes the maximal value, the other vanishes and accordingly, we can make use of the fact that $\partial^{p_{\max}+1} A_k \in L^3_{\mathrm{loc}}(\mathbb{R}^3, \mathcal{G})$ and employ Hölder's inequality to get such a bound for the integral (36) that it vanishes when δ is sent to zero. As a result, the norm (35) also has a vanishing limit, and combined with the limit (34) we get

$$\| w^{(p+2)(1-\sigma)} | (\nabla^{(\delta)})^p (\nabla^{(\delta)} \cdot \hat{G}^{(\delta)}) | \|_{3,K} \to \| w^{(p+2)(1-\sigma)} | \nabla^p (\nabla \cdot G) | \|_{3,K}. \tag{37}$$

It still remains to consider the convergence of the Sobolev norms. Let us denote by $\|\Phi\|^{(\delta)}_{n,2}$ the norm evaluated with the mollified gauge potential. From the estimate

$$| \|\Phi\|_{n,2} - \|\Phi\|^{(\delta)}_{n,2} | \leqslant \sum_{p=1}^{n} \sum_{k_1} \cdots \sum_{k_p} \| w^{(p-3/2)(1-\sigma)} | \nabla_{k_1} \cdots \nabla_{k_p} \Phi - \nabla^{(\delta)}_{k_1} \cdots \nabla^{(\delta)}_{k_p} \Phi | \|_2 \tag{38}$$

and the decomposition of the derivatives $\nabla_{k_1} \cdots \nabla_{k_p} \Phi$ into terms of the form

$$\mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}) \cdots \mathrm{ad}(\partial^{\alpha_{i_j}} A_{k_{i_j}}) \partial^{\alpha_{i_{j+1}}} \Phi,$$

$$\sum_{s=1}^{j+1} |\alpha_{i_s}| = p - j, \quad 0 \leqslant j \leqslant p$$

it is evident that each term in inequality (38) is bounded by integrals of the form

$$\begin{aligned}
&\int_K d^3x \left| \int d^3y_1 \cdots d^3y_j \, \eta_\delta(y_1) \cdots \eta_\delta(y_j) \mathrm{ad}(\partial^{\alpha_{i_1}} A_{k_{i_1}}(x)) \cdots \mathrm{ad}(\partial^{\alpha_{i_s}} A_{k_{i_s}}(x) - \partial^{\alpha_{i_s}} A_{k_{i_s}}(x - y_s)) \right. \\
&\left. \times \mathrm{ad}(\partial^{\alpha_{i_{s+1}}} A_{k_{i_{s+1}}}(x - y_{s+1})) \cdots \partial^{\alpha_{i_{j+1}}} \Phi(x) \right|^2 \\
&\leqslant C \operatorname*{ess\,sup}_{|y_1| \leqslant \delta} \cdots \operatorname*{ess\,sup}_{|y_j| \leqslant \delta} \int_K d^3x \, (|\partial^{\alpha_{i_1}} A_{k_{i_1}}(x)| \cdots |\partial^{\alpha_{i_s}} A_{k_{i_s}}(x) - \partial^{\alpha_{i_s}} A_{k_{i_s}}(x - y_s)| \\
&\quad \times |\partial^{\alpha_{i_{s+1}}} A_{k_{i_{s+1}}}(x - y_{s+1})| \cdots |\partial^{\alpha_{i_{j+1}}} \Phi(x)|)^2
\end{aligned} \tag{39}$$

with $j \geqslant 1$. Inspection of all possible values of the multi-indices $|\alpha_{i_s}|$ indicates that the previous smoothness assumptions, complemented by $\partial^{n-1} A_k \in L^2_{\mathrm{loc}}(\mathbb{R}^3, \mathcal{G})$, are sufficient to make the bound (39) vanish in the limit $\delta \to 0$. What this means is that

$$\|\Phi\|^{(\delta)}_{n,2} \to \|\Phi\|_{n,2},$$

and together with the limits (29) and (37) this completes the proof of inequalities (26) and (27) under the relaxed assumptions (9). Replacing the local curvature norms by global ones we finally find ourselves at the end of this long proof. □

E. Lemma 2

Intuitively this lemma is rather obvious, but strictly speaking we do not yet know that a smooth enough sequence converging in $H_{n-1}(\mathbb{R}^3, \mathcal{G})$ also converges in the norm involving the

covariant Laplacian. The proof follows the usual steps, beginning with approximations with truncated mappings and ending with density results for mollified mappings. A sequence of truncated mappings is defined by

$$Z_m(x)=\tau_m(x)Z(x)$$

with

$$\tau_m(x)=\tau\left(\frac{x}{m}\right),\quad \tau(x)=\begin{cases}1, & 0\leqslant|x|\leqslant 1,\\ 0, & |x|\geqslant 2.\end{cases}$$

When $1\leqslant|x|\leqslant 2$, it is assumed that τ is infinitely smooth and $0\leqslant\tau(x)\leqslant 1$. In order to approximate the Sobolev norm we notice that

$$\|Z_m-Z\|_{n-1,2}\leqslant\sum_{p=1}^{n-1}\sum_{k_1}\cdots\sum_{k_p}\|w^{(p-3/2)(1-\sigma)}\nabla_{k_1}\cdots\nabla_{k_p}(Z_m-Z)\|_2 \tag{40}$$

and then estimate each term in the sum separately. The covariant derivatives are decomposed as

$$\nabla_{k_1}\cdots\nabla_{k_p}(Z_m-Z)=(\tau_m-1)\nabla_{k_1}\cdots\nabla_{k_p}Z+\sum_{|\alpha|\leqslant p-1}{}'\ (\partial^{\alpha_c}\tau_m)\,\nabla^{\alpha}Z, \tag{41}$$

where the prime indicates that the indices of α are assumed to be in ascending order,

$$\alpha=(k_{i_1},\ldots,k_{i_q}),\quad 1\leqslant i_1<\cdots<i_q\leqslant p,$$

and where α_c stands for the complement of α, i.e.,

$$\alpha_c=(k_1,\ldots,k_p)\backslash\alpha.$$

The norm of the first term in the decomposition (41) can be made small by using the result that

$$\int_{|x|\geqslant m}w^{(2p-3)(1-\sigma)}|\nabla^p Z|^2\,d^3x\xrightarrow[m\to\infty]{}0, \tag{42}$$

when $Z\in H_{n-1}(\mathbb{R}^3,\mathcal{G})$. For the remaining terms with $|\alpha|\geqslant 1$ we deduce the bound

$$\int w^{(2p-3)(1-\sigma)}|\partial^{\alpha_c}\tau_m|^2\,|\nabla^{\alpha}Z|^2\,d^3x\leqslant\left(\sup_{1\leqslant|x|/m\leqslant 2}w^{2(p-|\alpha|)(1-\sigma)}|\partial^{\alpha_c}\tau_m|^2\right)\times\int_{1\leqslant|x|/m\leqslant 2}w^{(2|\alpha|-3)(1-\sigma)}|\nabla^{\alpha}Z|^2\,d^3x. \tag{43}$$

The factor on the right-hand side is bounded, because

$$\sup_{1\leqslant|x|/m\leqslant 2}w(x)^{2(p-|\alpha|)(1-\sigma)}|\partial^{\alpha_c}\tau_m(x)|^2\leqslant m^{-2(p-|\alpha|)\sigma}\sup_{1\leqslant\xi\leqslant 2}w(\xi)^{2(p-|\alpha|)(1-\sigma)}|\partial^{\alpha_c}\tau(\xi)|^2,$$

$$\xi=\frac{x}{m},$$

and the integral in the formula (43) tends to zero by virtue of the limit (42). Similarly, the term with $|\alpha|=0$, $\alpha_c=(k_1,\ldots,k_p)$ is seen to converge to zero by the estimates

$$\int w^{(2p-3)(1-\sigma)}\left|\partial^{\alpha_c}\tau_m\right|^2|Z|^2\,d^3x \leqslant \left(\sup_{1\leqslant|x|/m\leqslant 2} w^{2p-2(p-1)\sigma}\left|\partial^{\alpha_c}\tau_m\right|^2\right) \times \int_{1\leqslant|x|/m\leqslant 2} w^{-(3-\sigma)}|Z|^2\,d^3x$$

and

$$\sup_{1\leqslant|x|/m\leqslant 2} w(x)^{2p-2(p-1)\sigma}\left|\partial^{\alpha_c}\tau_m(x)\right|^2 \leqslant m^{-2(p-1)\sigma}\sup_{1\leqslant\xi\leqslant 2} w(\xi)^{2p-2(p-1)\sigma}\left|\partial^{\alpha_c}\tau(\xi)\right|^2.$$

The norm with the covariant Laplacian is handled similarly, employing the decomposition

$$\nabla_{k_1}\cdots\nabla_{k_{n-2}}\Delta(A)(Z_m-Z)=(\tau_m-1)\nabla_{k_1}\cdots\nabla_{k_{n-2}}\Delta(A)Z+\sum_l{\sum_{|\alpha|\leqslant n-1}}'\ (\partial^{\hat{\alpha}_c}\tau_m)\,\nabla^{\alpha}Z$$

with

$$\hat{\alpha}_c=(k_1,\ldots,k_{n-2},l,l)\backslash\alpha.$$

The first term yields a norm tending to zero due to the assumption (12), and the other terms are made small by the limit (42). Since there are a finite number of terms in both decompositions, we see that it is possible to choose a truncated mapping Z_m arbitrarily close to Z in both norms.

The mapping Z_m above vanishes (modulo sets of measure zero) outside some compact set K. Therefore we can define a mapping of class $C_c^{\infty}(\mathbb{R}^3,\mathcal{G})$ by

$$\Phi^{(\delta)}(x)=\int \eta_\delta(y)Z_m(x-y)\,d^3y.$$

Let us now estimate the distance of this mapping from Z_m in the two norms in question. Making use of formula (40) with Z replaced by $\Phi^{(\delta)}$ we are led to consider weighted L^2 norms of the derivatives $\left|\nabla^p(\Phi^{(\delta)}-Z_m)\right|$. For this purpose we write

$$\nabla_k^{(x)}Z_m(x-y)=(\nabla_k^{(x-y)}+\mathrm{ad}\mathcal{A}_k(x,y))Z_m(x-y),$$

$$\mathcal{A}_k(x,y)=A_k(x)-A_k(x-y),$$

and derive a decomposition similar to Eq. (31),

$$\begin{aligned}\nabla_{k_1}^{(x)}\cdots\nabla_{k_p}^{(x)}Z_m(x-y)&=\sum_{j=0}^{p}\sum_{i_1=1}^{i_2-1}\cdots\sum_{i_j=j}^{p}\nabla_{k_1}^{(x-y)}\cdots\nabla_{k_{i_1-1}}^{(x-y)}\\&\quad\times(\mathrm{ad}\mathcal{A}_{k_{i_1}})\nabla_{k_{i_1+1}}^{(x-y)}\cdots\nabla_{k_{i_j-1}}^{(x-y)}(\mathrm{ad}\mathcal{A}_{k_{i_j}})\nabla_{k_{i_j+1}}^{(x-y)}\cdots\nabla_{k_p}^{(x-y)}Z_m(x-y)\\&=\nabla_{k_1}^{(x-y)}\cdots\nabla_{k_p}^{(x-y)}Z_m(x-y)+\cdots,\end{aligned}\tag{44}$$

where the remaining terms take the form

$$\mathrm{ad}(\nabla_{(x-y)}^{\alpha_{i_1}}\mathcal{A}_{k_{i_1}})\cdots\mathrm{ad}(\nabla_{(x-y)}^{\alpha_{i_j}}\mathcal{A}_{k_{i_j}})\nabla_{(x-y)}^{\alpha_{i_{j+1}}}Z_m(x-y)\tag{45a}$$

with

$$\sum_{s=1}^{j+1}|\alpha_{i_s}|=p-j\,,\quad 1\leqslant j\leqslant p\,.\tag{45b}$$

The first term of the decomposition (44) is combined with the pth covariant derivative of $Z_m(x)$ to get a bound

$$\int_{K_\delta} d^3x\, w(x)^{(2p-3)(1-\sigma)} \left| \int d^3y\ \eta_\delta(y)(\nabla_{k_1}^{(x-y)}\cdots\nabla_{k_p}^{(x-y)} Z_m(x-y) - \nabla_{k_1}^{(x)}\cdots\nabla_{k_p}^{(x)} Z_m(x)) \right|^2$$

$$\leqslant C \operatorname*{ess\,sup}_{|y|\leqslant\delta} \int_{K_\delta} d^3x \,|\, \nabla_{k_1}^{(x-y)}\cdots\nabla_{k_p}^{(x-y)} Z_m(x-y) - \nabla_{k_1}^{(x)}\cdots\nabla_{k_p}^{(x)} Z_m(x) \,|^{\,2},$$

which tends to zero in the limit $\delta\to 0$, because now $\nabla^p Z_m \in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$. For terms of the form (45) we get bounds of the form

$$\operatorname*{ess\,sup}_{|y|\leqslant\delta} \int_{K_\delta} d^3x\, (|\nabla_{(x-y)}^{\alpha_{i_1}} \mathcal{A}_{k_{i_1}}| \cdots |\nabla_{(x-y)}^{\alpha_{i_j}} \mathcal{A}_{k_{i_j}}|\, |\nabla_{(x-y)}^{\alpha_{i_{j+1}}} Z_m(x-y)|)^2.$$

Making use of Hölder's inequality and the fact that Z_m is continuous for $n\geqslant 3$ we can check that conditions (9) are sufficient to make this integral converge to zero as $\delta\to 0$. The Laplacian norm is treated identically, writing

$$\nabla_{k_1}^{(x)}\cdots\nabla_{k_{n-2}}^{(x)} \Delta^{(x)}(A) Z_m(x-y) = \nabla_{k_1}^{(x-y)}\cdots\nabla_{k_{n-2}}^{(x-y)} \Delta^{(x-y)}(A) Z_m(x-y) + \cdots,$$

where the remaining terms take the form (45) with p replaced by n. For the first term we use the property that $\nabla^{n-2}\Delta(A) Z_m \in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G})$ and for the others the properties

$$Z_m \in L^6_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}), \quad n\geqslant 2,$$

$$Z_m \in C(\mathbb{R}^3,\mathcal{G}), \quad \nabla^1 Z_m \in L^6_{\mathrm{loc}}(\mathbb{R}^3,\mathcal{G}), \quad n\geqslant 3.$$

There being only a finite number of terms, we can thus always find a mapping $\Phi^{(\delta)}$ arbitrarily close to Z_m in both norms. Accordingly, we can construct a sequence (Φ_m) converging to Z in these norms. □

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AKS hierarchy and bi-Hamiltonian geometry of Gelfand–Zakharevich type

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A bi-Hamiltonian system is a system of differential equations which can be written in Hamiltonian form in two distinct ways. The applications of Gelfand–Zakharevich bi-Hamiltonian structure, which is an extension of a Poisson–Nijenhuis structure on phase space, has been extensively explored by Falqui, Magri, and Pedroni in the context of separation of variables. It is well known that the integrable Hamiltonian systems defined by the Adler–Kostant–Symes (AKS) scheme contains bi-Hamiltonian structure. In this paper we unveil the connection between Adler–Kostant–Symes formalism applied to loop algebra and the Gelfand–Zakharevich bi-Hamiltonian structure by superposition the results of Fordy and Kulish in the AKS scheme. We also study the commuting flows of the AKS hierachy and its connection to the Zakharov–Shabat hierarchy. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1756698]

I. INTRODUCTION

One of the many important aspects of soliton theory is the interpretation of soliton equations as completely integrable Hamiltonian systems.[13] A particularly important notion to have arisen in this theory is that of bi-Hamiltonian systems (cf. Ref. 5), i.e., they are Hamiltonian with respect to two different compatible Hamiltonian operators.

In 1978 Magri[29] proved a remarkable theorem that, subject to some technical hypothesis, any such bi-Hamiltonian system is completely integrable in the sense that it possesses an infinite number of conservation laws in involution. Bi-Hamiltonian systems appear to be very special situation, yet, they occur in numerous situations as model equations for more complicated physical systems. Examples include the Korteweg–de Vries (KdV) equation, the Boussinesq equation, and most of the other soliton equations. Later Magri's result has been further refined by Gelfand and Dorfman,[17,18] and Fuchssteiner and Fokas.[16]

From the Poisson geometry's point of view, a bi-Hamiltonian manifold is a Poisson manifold endowed with a pair of compatible Poisson brackets.[10,11] A direct consequence of compatibility is the existence of an infinite [in the case of partial differential equations (PDEs)] sequence of Hamiltonians which commute with respect to all the compatible Poisson brackets.

In the late 1970s, Adler[3] proposed a scheme for deriving such Hamiltonian operators starting from a given Lax operator. Gelfand and Dikii[19] proved that Adler's scheme indeed produces Hamiltonian operators. Adler's approach was based on Lie algebraic structure on the space of pseudodifferential operators. This paper represents a beautiful extension of work of Kostant.[27] The crucial observation is that in both cases the corresponding symplectic structure is the orbit symplectic structure of Kostant and Kirillov.

Later, Symes[38,39] has ellucided the extension of the classical Toda system results to Hamiltonian systems on so-called Toda orbits, a wider class than the Jacobi sets of split semisimple Lie algebras considered by Kostant.[27]

Following the above scheme, we are now able to construct in a systematic way completely integrable systems. This scheme is popularly called Adler–Kostant–Symes (AKS) scheme. The AKS scheme applying to some Lie algebra $\mathfrak{g}$ equipped with an ad-invariant nondegenerate bilin-

ear form yields various integrable systems. In other words, this construction associates Hamiltonian systems that are in many cases integrable with certain Lie algebraic data. It was shown by Reyman and Semenov-Tian-Shansky[33–36] that these systems may be viewed as symmetry reductions of corresponding Hamiltonian systems on cotangent bundles of Lie groups generated by Hamiltonians invariant under left and right translations.

We assume the Lie algebra $\mathfrak{g}$ be a vector space, presented as the linear sum of two subalgebras $\mathfrak{g}=k+l$. The bilinear form $\langle .,. \rangle$ induces an isomorphism $\mathfrak{g}\simeq\mathfrak{g}^*$. Hence, with the help of bilinear form we can identify $k^*\simeq l^\perp$ and $l^*\simeq k^\perp$ where

$$\langle k^\perp, k\rangle = \langle l^\perp, l\rangle = 0.$$

So $k^\perp$ acquires a Poisson structure from that of l^*. The co-adjoint action of L on $k^\perp\simeq l^*$ is given by

$$g\circ p = \pi_{k^\perp}(gpg^{-1})$$

for $g\in L$ and $p\in k^\perp$. Then the infinitesimal action is $\eta(p)=\pi_k^\perp[\eta,p]$ for $\eta\in l$.

The symplectic manifold here is some co-adjoint L-orbit $\mathcal{M}\subset k^\perp\simeq l^*$. We associate to it a Hamiltonian equation of suitable ad-invariant function $f:\mathfrak{g}^*\to R$ for all $f|_{\mathcal{M}}$.

We know many important equations can be derived from this approach, for example, Adler and van Moerbeke[4] obtained Euler–Arnold–Poincaré equation as a geodesic flow on ellipsoid, Ratiu[32] obtained the Neumann equation, and so on. These are all finite-dimensional systems. To apply this formalism to partial differential equation we must work with the infinite-dimensional Lie algebras. This was demonstrated on loop algebras by Reyman, Semenov-Tian-Shansky, and Frenkel.[33–36]

Using a pencil of R-matrices on the Lie algebra, Burrough[6] proved that the KdV hierarchies have an Adler–Kostant–Symes construction on the underlying current algebra. The co-adjoint orbits are reduced by Hamiltonian symmetries (cf. Ref. 30). The reduction process reproduces the gauge group and the bi-Hamiltonian structure.

Thus, this entices one to apply AKS method to construct hierarchy of commuting Hamiltonians of various integrable systems related to infinite-dimensional Lie algebras. At this stage of integrable systems, all of us are looking for a unified theory of various integrable systems. Naturally, AKS scheme is considered to be very appealing. Recently, people turn their attention to the self-dual Yang–Mills (SDYM) equations. The SDYM equations are an important example of a multidimensional integrable system, with all the properties one would expect from an integrable system. An additional property is that this system contains many lower-dimensional systems (such as the KdV and NLS equations) via a process of dimensional reduction. Naturally, almost all integrable equations on $(1+1)$ can be derived from the four-dimensional SDYM equation by reductions. Thus, various reductions of the SDYM equation become a primary source to construct large classes of integrable systems. We have seen that the AKS scheme also yields various 1 $+1$ dimensional integrable equations.

This idea has been generalized to hierarchy level by Ablowitz, Chakravarty, and Takhtajan.[1] They developed the notion of a self-dual Yang–Mills hierarchy (with first member the original self-dual Yang–Mills equations) by introducing an infinite number of higher-order times in such a way that all the flows commute, together with a recursion operator which takes one between adjacent members of the hierarchy. In our earlier work[23,24] we have shown that the PDE version of the AKS hierarchy is the reduction of $1+1$ dimensional SDYM hierarchy.

We have already said that a differential equation is called bi-Hamiltonian if it can be written in Hamiltonian form in two distinct ways with respect to two different Poisson structures $\{.,.\}_0$ and $\{.,.\}_1$:

$$\dot{f}=\{f,H_0\}_0=\{f,H_1\}_1$$

for some functions $H_0, H_1\in C^\infty(M)$.

Suppose one of the Poisson structures is nondegenerate, then this allows us to define a recursion operator $R=P_1P_0^{-1}$, where P_0 and P_1 are the Poisson tensors associated with the brackets $\{.,.\}_0$ and $\{.,.\}_1$, respectively. This recursion operator R can be used to construct a family of functions which are first integrals to the Hamiltonian system and these functions turn out to be in involution with respect to both Poisson brackets. This suffices to show the integrability in the sense Liouville of the Hamiltonian system.[2]

Thus an important class of bi-Hamiltonian manifold occurs when one element of the Poisson pencil is everywhere invertible. As a remarkable consequence of the compatibility of P_0 and P_1 the Nijenhuis torsion of N (or recursion operator), defined by its action on a pair of vector fields X and Y as

$$T(N)(X,Y)=[NX.NY]-N([NX,Y]+[X,NY]-N[X,Y]),$$

vanishes identically.

The recursion operator is interpreted as Nijenhuis operators, and possessses the Nijenhuis property, for finite-dimensional systems was introduced in 1951, and for infinite-dimensional systems by Fuchssteiner.[15] In the infinite-dimensional case Nijenhuis operators are nonlocal, and this problem has been overcomed by Gelfand and Dorfman[18] in by working with Nijenhuis relations instead of Nijenhuis operators. The connection between bi-Hamiltonian structures and AKS scheme and the Lie pencil of R-matrices has been studied in Refs. 25, 31, and 34.

Recently, the famous Italian School of integrable systems[9–12] has considered a more general case of a Poisson manifold together with a pencil of Poisson tensors. The assumption of polynomial Casimirs allows one to use the theory of Gelfand–Zakharevich (GZ) manifolds.[20–22] The Gelfand–Zakharevich bi-Hamiltonian structure is an extension of a Poisson–Nijenhuis structure[28,41] on phase space. The polynomial Casimirs are computed in the spirit of the GZ scheme. Under some technical assumptions the resulting system is separable in Darboux–Nijenhuis coordinates. Thus, they found a new test of separability for a special class of Hamiltonian integrable systems defined on bi-Hamiltonian manifolds. This defines the notion of Stäckel-separable systems,[26] criteria for separability and outline the construction of these separating coordinates. An interesting fact is that the eigenvalues of the Nijenhuis tensor account for one-half of the separating variables. Actually, this is the main issue studied by both the classical Eisenhart–Benenti theory of separability of natural systems defined on cotangent bundles to Riemannian manifolds, as well as the present theory of separation of variables for systems admitting a Lax representation (see Ref. 37, and references therein).

In fact, Italian school unveiled the deep links connecting the classical theory of separation of variables (of the Hamilton–Jacobi equations) and the geometry of Gelfand–Zakharevich bi-Hamiltonian manifolds.

In this paper we address the Gelfand–Zakharevich geometry from the point of view that the Adler–Kostant–Symes scheme superposed with the Fordy–Kulish decomposition.[14] We show how the integrable systems appearing in the AKS program yield the Gelfand–Zakharevich bi-Hamiltonian structure. We also study the commuting flows of nonextended AKS hierarchy (hierarchy of AKS equation without cocycle) and its connection to the Zakharov–Shabat hierarchy.

This paper is organized as follows: In Sec. II we discuss the Kostant–Kirillov structure on co-adjoint orbits and the Adler–Kostant–Symes scheme. A self-contained review of this subject is given. We apply this scheme in Sec. III to obtain several standard integrable systems, such as nonlinear Schrödinger, coupled KdV, Chen–Liu–Lee[40] or derivative nonlinear Schrödinger equations, related to Hermitian symmetric spaces. This type of construction has an important geometrical significance from the point of harmonic maps. In an important paper Burstall *et al.* showed how to construct a large class of harmonic and pluriharmonic maps called ''(pluri)harmonic maps of finite type'' from tori to symmetric spaces G/H, where G is a compact Lie group. Section IV is devoted to the AKS hierarchy and Zakharov–Shabat hierarchy (or the hierarchy of ''zero curvature'' equation). We formulate the Zakharov–Shabat hierarchy from the AKS hierarchy. In Sec. V we establish how the Gelfand–Zakharevich bi-Hamiltonian geometry can be carried out

from the Adler–Kostant–Symes formalism. Here the polynomial Casimirs will be interpreted as ad-invariant functions. We conclude this paper with some modest remarks.

II. ADLER–KOSTANT–SYMES SCHEME

Let G be a connected compact semisimple Lie group with the Lie algebra $\mathfrak{g}$, endowed with a nondegenerate ad-invariant and symmetric inner product $\langle .,. \rangle : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, that is,

$$\langle X,[Y,Z]\rangle = \langle [X,Y],Z\rangle \quad \forall X,Y,Z \in \mathfrak{g}.$$

Its dual space $\mathfrak{g}^*$ has a natural Poisson structure

$$\{g_1,g_2\}(\alpha) = \left\langle \alpha, \left[\frac{\delta g_1}{\delta \mu}, \frac{\delta g_2}{\delta \mu} \right] \right\rangle,$$

of two smooth functions g_1 and g_2 on $\mathfrak{g}^*$. The functional derivative of g (or gradient of g) at μ is the unique element $\delta f/\delta \mu$ of $\mathfrak{g}$ defined by

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}[f(\mu + \epsilon \delta \mu) - f(\mu)] = \left\langle \delta \mu, \frac{\delta f}{\delta \mu} \right\rangle.$$

Here the gradient of g_i are interpreted as elements of $\mathfrak{g}$ due to the identification of $\mathfrak{g} \simeq \mathfrak{g}^{**}$.

Let us introduce an additional structure from which, in addition to the ordinary bracket, a modified bracket can be defined as follows.

Let

$$R : \mathfrak{g} \to \mathfrak{g}$$

be an R-matrix, and this defines another Lie bracket on $\mathfrak{g}$,

$$[X,Y]_R = \tfrac{1}{2}([RX,Y] + [X,RY]), \tag{1}$$

such a pair $(\mathfrak{g},R)$ is called a double Lie algebra. It is known that $(\mathfrak{g},R)$ is a double Lie algebra if and only if the following bilinear map:

$$B_R : (\mathfrak{g},R) \times (\mathfrak{g},R) \to (\mathfrak{g},R)$$

is given by

$$B_R(X,Y) = [RX,RY] - R([X,Y]_R) \tag{2}$$

is ad-invariant, that is, the equation

$$[X,B_R(Y,Z)] + [Y,B_R(Z,X)] + [Z,B_R(X,Y)] = 0 \tag{3}$$

holds for all $X,Y,Z \in \mathfrak{g}$.

It is clear that the trivial solution $B_R(X,Y) = 0$ yields the Yang–Baxter equation. The second solution satisfies the so-called modified Yang–Baxter equation

$$B_R(X,Y) = -[X,Y]. \tag{4}$$

The best known class of R-matrices arise when the Lie algebra $\mathfrak{g}$ split into a direct sum of two subalgebras $\mathfrak{g} = \mathfrak{g}_+ \oplus \mathfrak{g}_-$. Since there is a vector space decomposition of $\mathfrak{g}$ into a direct sum of two Lie subalgebras, hence, we set

$$R = P_+ - P_-, \tag{5}$$

where $P_{\pm}$ be the corresponding projection onto $\mathfrak{g}_{\pm}$. Under this identification, the bracket is

$$[X,Y]_R=[X_+,Y_+]-[X_-,Y_-],$$

where $X_{\pm}=P_{\pm}X$.

By $\mathfrak{g}^*$ and $\mathfrak{g}_R^*$ we denote the dual of $\mathfrak{g}$ endowed with the Lie–Poisson structures arising from $[.,.]$ and $[.,.]_R^*$, respectively. The Poisson bi-vectors arising from the Lie brackets $[.,.]$ and $[.,.]_R$ are related by $P_R=R^*P+PR$, where R is considered to be a pointwise lift of the map R on $\mathfrak{g}$ to the vector fields over $\mathfrak{g}$ and R^* is the transpose of this map.

The R-matrix construction on $\mathfrak{g}$ allows us to define an additional Lie–Poisson bracket of the following form:

$$\{f,g\}(\mu)=\langle\mu,[R(\nabla f),(\nabla g)]+[\nabla f,R(\nabla g)]\rangle, \quad f,g\in C^{\infty}(\mathfrak{g}^*). \tag{6}$$

We wish to take a look at the special case of an R-structure (6) given by a splitting into two subalgebras. With $\mathfrak{g}=\mathfrak{g}_-\oplus\mathfrak{g}_+$, $R=P_+-P_-$, $\mu\in\mathfrak{g}^*$ one computes the Lie–Poisson bracket arising from $[.,.]_R$,

$$\{f,g\}(\mu)=2\langle\mu,[(\nabla f)_+,(\nabla g)_+]\rangle-2\langle\mu,[(\nabla f)_-,(\nabla g)_-]\rangle. \tag{7}$$

Definition 1: We say a smooth function $H:\mathfrak{g}^*\to\mathbf{R}$ is Ad^* invariant if

$$H(Ad_g^*\alpha)=H(\alpha)$$

for all $\alpha\in\mathfrak{g}^*$ and $g\in G$.

Theorem 2 (AKS): *Let $\mathfrak{g}$ be Lie algebra with R-matrix $R:\mathfrak{g}\to\mathfrak{g}$, then the ad^* invariant functions on $\mathfrak{g}^*$ are in involution with respect to*

$$\{f,g\}(\mu)=\langle\mu,[R(\nabla f),(\nabla g)]+[\nabla f,R(\nabla g)]\rangle.$$

Then the Hamiltonian flow on the co-adjoint orbits in $L\subset\in\mathfrak{g}^*$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}L=ad^*_{R(\nabla H)}L+R^*ad^*_{\nabla H}L, \tag{8}$$

where R^* is the transpose of R.

A. Loop algebra and AKS scheme

In this section we apply the AKS construction on loop algebra.

Let $\Omega\mathfrak{g}=\mathrm{gl}(n,\mathbf{C})\otimes\mathbf{C}[\lambda,\lambda^{-1}]$ be a loop algebra of semi-infinite formal Laurent series in λ with coefficients in $\mathrm{gl}(n,\mathbf{C})$. An element $X(\lambda)\in\Omega g$ can be expressed as a formal series of the form

$$X(\lambda)=\sum_{i=\infty}^{m}x_i\lambda^i \quad \text{for all} \quad x_i\in\mathrm{gl}(n,\mathbf{C}),$$

the Lie bracket with $Y(\lambda)=\Sigma_{j=-\infty}^{l}y_j\lambda^j$ is given by

$$[X(\lambda),Y(\lambda)]=\sum_{k=-\infty}^{m+l}\sum_{i+j=k}[x_i,y_j]\lambda^k.$$

We will now consider the extended loop algebra $\widetilde{\Omega g}$, the one-dimensional central extension of Ωg defined by two cocycle

$$\omega(X,Y) := \langle \partial X(\lambda), Y(\lambda) \rangle \equiv \int_{S^1} X'(\lambda) Y(\lambda) \mathrm{d}x,$$

where $\partial: \mathfrak{g} \to \mathfrak{g}^*$.

We define extended loop group ΩG to be

$$0 \to R \to \widetilde{\Omega G} \to \Omega G \to 1.$$

The corresponding loop algebra $\widetilde{\Omega \mathfrak{g}} = \Omega \mathfrak{g} \oplus \mathbf{R}$. The Lie bracket of the extended loop algebra $\widetilde{\Omega \mathfrak{g}}$ satisfies

$$[(X(\lambda),a),(Y(\lambda),b)] = \left([X,Y], \int_{S^1} \mathrm{tr}(XY') \right),$$

where $X \in \Omega \mathfrak{g}$ and $a \in \mathbf{R}$.

We define a nondegenerate ad-invariant bilinear form on $\Omega \mathfrak{g}$,

$$\langle X(\lambda), Y(\lambda) \rangle = \mathrm{res}_{\lambda=0} \, \mathrm{tr}(\lambda^{-1} X(\lambda) Y(\lambda)) = \mathrm{tr}(X(\lambda) Y(\lambda))_0,$$

and this bilinear form can be extended to define the bilinear form on $\widetilde{\Omega \mathfrak{g}}$ by

$$\langle (X,a),(Y,b) \rangle = ab + \int_{S^1} \mathrm{tr}(XY).$$

We assume that the algebra $\widetilde{\Omega \mathfrak{g}}$ as a vector space, and it is presented as the linear sum of two subalgebras

$$\widetilde{\Omega \mathfrak{g}} = \widetilde{\Omega \mathfrak{g}}^+ \oplus \widetilde{\Omega \mathfrak{g}}^-,$$

where $\widetilde{\Omega \mathfrak{g}}^+$ denote the subalgebra of $\widetilde{\Omega \mathfrak{g}}$ given by the polynomial in λ and $\widetilde{\Omega \mathfrak{g}}^-$ is the subalgebra of strictly negative series.

By means of ad-invariant bilinear form $\langle , \rangle$ we identify

$$(\widetilde{\Omega \mathfrak{g}}^+)^* \simeq (\widetilde{\Omega \mathfrak{g}}^-)^\perp \quad \text{and} \quad (\widetilde{\Omega \mathfrak{g}}^-)^* \simeq (\widetilde{\Omega \mathfrak{g}}^-)^\perp.$$

This induces another decomposition $\widetilde{\Omega \mathfrak{g}} = \Omega \mathfrak{g}^{+\perp} \oplus \Omega \mathfrak{g}^{-\perp}$.

Definition 3: Let $(\Omega \mathfrak{g}, R)$ be a double Lie algebra on which we define a modified Lie algebraic structure and suppose ω be a two cocycle on $\Omega \mathfrak{g}$. Then

$$\omega_R(X,Y) = \omega(RX,Y) + \omega(X,RY)$$

is a two cocycle on $\Omega \mathfrak{g}_R$.

We want to find the co-adjoint representation of $\widehat{\Omega g}_R$ on the dual space $\widehat{\Omega g}_R^*$. We use the following identity:

$$\langle ad_R^*(X,a)(U,c),(Y,b) \rangle + \langle (U,c), ad_R(X,a)(Y,b) \rangle = 0.$$

Proposition 4: The co-adjoint representation of the loop algebra $\hat{g}_R$ on its dual is given by the following expresion:

$$ad_R^*(X,a)(\alpha,c) = ((ad^* RX)(\alpha) - cRX', 0) + R^*(ad^* X(\alpha) - cX', 0).$$

Note that the symbols ad^* and ad_R^* stand, respectively, for the co-adjoint representations of the algebras $\Omega \mathfrak{g}$ and $\Omega \mathfrak{g}_R$. The proof of this proposition is fairly easy, so we omit it.

The dual space $\widetilde{\Omega g}^{\perp}$ stratifies into Poisson submanifolds corresponding to different values of the parameter; each of them is endowed with a Poisson bracket. Let us fix $c=1$, so we confine us to a hyperplane in $\widetilde{\Omega g}^*$. By abuse of notation we shall continue to call it $\widetilde{\Omega g}^*$.

Let $\hat{f}_1$ and $\hat{f}_2$ be the ad-invariant function and when they are restricted to $\Omega g^{-}{}^* \sim \Omega g^{+\perp}$ these satisfy $\{\hat{f}_1,\hat{f}_2\}_{\Omega g^{-}{}^*}=0$.

Lemma 5: Suppose H is Ad^* invariant function on g^* then

$$ad_R^*(\mathrm{d}H(\alpha),a)(\alpha,1)=((ad^*R(\mathrm{d}H(\alpha))(\alpha)+R(\mathrm{d}H)',0).$$

It should be again be noted that the gradient of a function is the vector field $\nabla H : \mathfrak{g}^* \to \mathfrak{g}$, such that $\langle \nabla H(\mu), X(\mu)\rangle = \mathrm{d}H(X(\mu))$ for all $\mu \in \mathfrak{g}^*$.

The co-adjoint representation leaves invariant the hyperplanes $e=$constant. Thus we conclude: (1) The center of the $\hat{g}$ acts trivially on $\hat{g}^*$, the space of $\hat{g}^*$ is a natural G-module.

(2) $\hat{G}$ acts on $\hat{g}^*$ by gauge transformation.

The Poisson bracket is

$$\begin{aligned}\{f,g\}(\mu+cI)&=\langle \hat{\mu},[\hat{R}(\nabla \hat{f}),\nabla \hat{g}]+[\nabla f,\hat{R}(\nabla \hat{g})]\rangle\\ &=\langle \hat{\mu},[\hat{R}(\nabla f),\nabla g]+\omega(R(\nabla f),\nabla g)I+[\nabla f,R(\nabla g)]+\omega(\nabla f,R(\nabla g))I\rangle\\ &=\langle \hat{\mu},[\hat{R}(\nabla f),\nabla g]+[\nabla f,R(\nabla g)]+c\langle R\partial(\nabla f),\nabla g\rangle+c\langle \partial\nabla f,R(\nabla g)\rangle,\end{aligned}$$

where $\hat{R}$ is the R-matrix on $\hat{\mathfrak{g}}$, it satisfies

$$\hat{R}:\widetilde{\Omega \mathfrak{g}}\to\widetilde{\Omega \mathfrak{g}},\quad \hat{R}(k+\alpha I):=R(k).$$

Proposition 6: The Poisson bracket in the space of $\widetilde{\Omega \mathfrak{g}}^*$ for the two smooth functions has the form

$$\{f_1,f_2\}(Y)=\langle[\hat{R}(\nabla f_1),\nabla f_2],Y\rangle+[\nabla f,R(\nabla g)]+\int_{S^1}R\nabla f_1\frac{\mathrm{d}\nabla f_2}{\mathrm{d}x}+\int_{S^1}\nabla f_1 R\frac{\mathrm{d}\nabla f_2}{\mathrm{d}x},$$

where $Y \in \Omega g$.

In presence of cocycle, that is, when an ad-invariant function satisfies

$$[X,\nabla H]=\frac{\partial \nabla H}{\partial x},$$

∇H is obtained recursively,

$$\nabla H=\lambda^2 h_2+\lambda h_1+h_0+\lambda^{-1}h_{-1}+\cdots.$$

Theorem 7: *Let $\widetilde{\Omega g}^{+}=\widetilde{\Omega \mathfrak{g}}^{+}\oplus\widetilde{\Omega \mathfrak{g}}^{-}$ and $M\subset\widetilde{\Omega \mathfrak{g}}^{+}$ a co-adjoint orbit equipped with a natural weak orbit symplectic structure ω. Let $H_i:\widetilde{\Omega \mathfrak{g}}\to\mathbf{R}$ be the set ad-invariant functions in $I(\mathfrak{g}^*)$ restricted to $(\widetilde{\Omega \mathfrak{g}}^{+})^{\perp}$ is an involutive system on the co-adjoint orbit. The Hamiltonian equations of motion on $\widetilde{\Omega \mathfrak{g}}^*$ generated by the Hamiltonian (ad-invariant function) have the form*

$$\frac{\partial L}{\partial t}=ad^*_{R(\nabla H)}L+\frac{\partial}{\partial x}(R(\nabla H)). \tag{9}$$

So this defines a flat connection $L\,\mathrm{d}x+P\,\mathrm{d}t$ on a cylinder $S^1\times\mathbf{R}$ associated with the above zero curvature equation. In order to apply the Adler–Kostant–Symes scheme we require the knowledge of the ad-invariant function.

When we deal with the AKS scheme for the group without cocycles we obtain a dynamical equation instead of a partial differential equation.

Corollary 8: Let H be the ad-invariant function on $\Omega\mathfrak{g}^*$. The associated Hamiltonian vector fields have orbits L in the symplectic leaves of $\Omega\mathfrak{g}^*$, foliated by co-adjoint action. Then the Hamiltonian flow corresponding to the function $H \in C^\infty(\mathfrak{g}^*)$ is

$$\frac{dL}{dt} = [R\nabla H, L]. \tag{10}$$

Using $R = P_+ - P_-$ in (10) we obtain

$$\frac{dL}{dt} = 2[P_+ \nabla H, L].$$

B. Bi-Hamiltonian chain

In this section we construct the bi-Hamiltonian chain from the AKS method.

Let us consider again

$$[L, \nabla F] + \partial_x(\nabla F) = 0,$$

where

$$L = \lambda^2 A + \lambda Q + W^{\text{off}} + WA,$$

where $A = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ and $Q = \left(\begin{smallmatrix} 0 & q \\ r & 0 \end{smallmatrix}\right)$.

Let us make an ansatz,

$$\nabla F = F_0 + \lambda^{-1} F_1 + \lambda^{-2} F_2 + \cdots,$$

where

$$F_i = F_i^{\text{off}} + f_i A = \begin{pmatrix} f_0 & F_0^+ \\ F_0^- & -f_0 \end{pmatrix}.$$

Here F_i^{off} is the off-diagonal elements, that is, $F_i^{\text{off}} \in m$, and $A \in k$. Equating all the powers of λ we obtain

$$\begin{aligned} [A, F_n] &= [Q, F_{n-1}] + [W^{\text{off}}, F_{n-2}] + W[A, F_{n-2}] + F_{(n-2)x} \\ &= [Q, F_{n-1}^{\text{off}}] + [W^{\text{off}}, F_{n-2}] + W[A, F_{n-2}^{\text{off}}] + F_{(n-2)x}^{\text{off}} + f_{(n-2)x} A \\ &\quad + [Q, f_{n-1} A] + [W^{\text{off}}, f_{n-2} A], \end{aligned}$$

where we tacitly assume

$$F_0 = A, \quad F_1 = Q + f_1 A.$$

So we have two recursive relations

$$F_n^{\text{off}} = -f_{n-1} Q - f_{n-2} W^{\text{off}} + W F_{n-2}^{\text{off}} + ad_A^{-1} F_{(n-2)x}^{\text{off}}, \tag{11}$$

$$[Q, F_{n-1}^{\text{off}}] + [W^{\text{off}}, F_{n-2}^{\text{off}}] + f_{(n-2)x} = 0. \tag{12}$$

Let us study the chain. Suppose $F_0^{\text{off}} = 0$ and $f_0 = 1$. We also assume $F_1^{\text{off}} = Q$. Thus F_2^{off} is given by (11) and f_1 by (12).

Thus we obtain

(1) F_2^{off} is given by f_1, f_0, F_0^{off},
(2) F_3^{off} is given by f_2, f_1, F_1^{off},
(3) F_4^{off} is given by f_3, f_2, F_2^{off},
(4) f_{1x} is given by F_1^{off}, F_0^{off},
(5) f_{2x} is given by F_3^{off}, F_1^{off},

etc. Hence the chain is completed.

III. AKS HIERARCHY AND ZAKHAROV–SHABAT HIERARCHY

In this section we focus on the construction and properties of AKS hierachy. We consider the Adler–Kostant–Symes equation without cocycle. Since it is always possible to construct the zero curvature form of the AKS equation from this version.

A. AKS hierarchy

Let $\mathfrak{g}$ be a Lie algebra with standard splitting. Let the Hamiltonians be

$$H_i(\Gamma)=\tfrac{1}{2}\operatorname{tr}_0\lambda^{-(n-i)}L^2, \qquad 0\leqslant i\leqslant n.$$

Thus we obtain

$$\langle \nabla H_i, X\rangle = \mathrm{d}H_i(X)=\operatorname{tr}_0(\lambda^{-(n-i)}LX),$$

and from the degeneracy of tr_0 this implies

$$\nabla H_i=\lambda^{-(n-i)}L.$$

Let us consider an invariant submanifold to be

$$\Lambda=\left\{ L(\lambda)\ \ L(\lambda)=\sum_{i=0}^{n} Q_{n-i}\lambda^i,\ \ Q_{n-i}\in\mathfrak{g}\right\}.$$

Let $L:\mathbf{R}^{n+1}\to\Lambda$ be a function of $t_0,\ldots,t_n$ taking values in Λ, that is

$$L(t_0,\ldots,t_n,\lambda)=\sum_{i=0}^{n} Q_{n-i}\lambda^i\in\Lambda\subset\mathfrak{g}^{-}*.$$

Thus the Hamiltonian equations of motion for H_i is given by

$$\frac{\mathrm{d}}{\mathrm{d}t_i}L=[(\lambda^{-(n-i)}L)_+,L]. \tag{13}$$

Proposition 9: All the equations of the AKS hierarchy commute each other.
Proof: Let us rewrite (∇H_i) as B_i and $\partial/\partial t_i$ as ∂_i. Let $i>j$ and

$$B_i=\lambda^{i-j}B_j+Q_i+Q_{i-1}\lambda+\cdots+Q_{j+1}\lambda^{i-j-1}.$$

Hence,

$$\partial_i B_j=\partial_i(\lambda^{-(n-j)}L)_+=(\lambda^{-(n-j)}\partial_i L)_+=(\lambda^{-(n-j)}[B_i,L])_+=[B_i,\lambda^{-(n-j)}L]_+.$$

Thus we obtain

$$\begin{aligned}\partial_i B_j - \partial_j B_i &= [B_i, \lambda^{-(n-j)}L]_+ - [B_j, \lambda^{-(n-i)}L]_+ \\ &= [B_i - \lambda^{i-j}B_j, \lambda^{-(n-j)}L]_+ \\ &= [B_i - \lambda^{i-j}B_j, (\lambda^{-(n-j)}L)_+]_+ + [B_i - \lambda^{i-j}B_j, \lambda^{-(n-j)}L)_-]_+ \\ &= [B_i, B_j] + [B_i - \lambda^{i-j}B_j, \lambda^{-(n-j)}L)_-]_+ .\end{aligned}$$

The last expression can be further reduced to

$$\begin{aligned}&[B_i - \lambda^{i-j}B_j, (\lambda^{-(n-j)}L)_-]_+ \\ &\quad = [Q_i + Q_{i-1}\lambda + \cdots + Q_{j+1}\lambda^{i-j-1}, Q_n\lambda^{-(n-j)}Q)_+ \cdots + Q_{j+1}\lambda^{-(i+j+1)}]_+ \\ &\quad = [Q_i + \cdots + Q_{j+1}\lambda^{i-j-1}, Q_n\lambda^{-(n-j)} + \cdots + Q_{i-1}\lambda^{-(i-j-1)}]_+ = 0,\end{aligned}$$

since the greatest degree in λ in the expression above is $i-j-1+(-(i-j+1))=-2$. □

B. Higher flows

In this section we will consider the higher flows of the Hamiltonians of the form

$$H_{i,j} := \frac{1}{j+1}\mathrm{tr}_0(\lambda^{-(jn-i)}L^{j+1}),$$

where $1 \leqslant j,\ l \leqslant m = \mathrm{rank}\, g,\ 0 \leqslant i \leqslant jn$, and $0 \leqslant k \leqslant ln$.

The gradient of $H_{i,j}$ is

$$\nabla H_{i,j} = \lambda^{(jn-i)}L^j - \mathrm{tr}(\lambda^{-(jn-i)}L^j)I.$$

Thus we obtain

$$B_{i,j} := (\nabla H_{i,j})_+ = (\lambda^{-(jn-i)}L^j)_+ - \mathrm{tr}(\lambda^{-(jn-i)}L^j)_+ I.$$

Theorem 10: *Let the Hamiltonians be* $H = \nabla_{i,j} = \lambda^{(jn-i)}L^j - \mathrm{tr}(\lambda^{-(jn-i)}L^j)I$ *for all* $0 \leqslant i \leqslant jn$. *Let us assume the invariant submanifold to be* $\gamma = \{L(\lambda): L(\lambda) = \Sigma_0^n Q_{n-i}\lambda^i\}$. *Let* $L: \mathbf{R}^{n+1} \to \gamma$ *be a function of* $t_0, \ldots, t_n$ *taking values in* γ, *given by*

$$L(t_0, \ldots t_n, \lambda) = \sum_{i=0}^{n} Q_{n-i}\lambda^i \in \gamma \subset \mathfrak{g}^- * = \mathfrak{g}^{+\perp}.$$

This generates a Hamiltonian flow for $H_{i,j}$,

$$\partial_{i,j}L = [B_{i,j}, L] \quad \text{with} \quad \partial_{i,j} = \frac{\partial}{\partial t_{i,j}}. \tag{14}$$

Lemma 11: Let $0 \leqslant i \leqslant jn$ *and* $0 \leqslant k \leqslant ln$. Then

$$\partial_{i,j}L^q = [B_{i,j}, L^q]. \tag{15}$$

Proof: It is to show

$$\partial_{i,j}L^n = \sum L \cdots \partial_{i,j}L \cdots L = \sum L \cdots [B_{i,j}, L] \cdots L = [B_{i,j}, L^q].$$

□

Lemma 12:

$$\partial_{i,j}B_{k,l}-\partial_{k,l}B_{i,j}=[B_{i,j},B_{k,l}]. \tag{16}$$

Proof: It is given by

$$\begin{aligned}
&\partial_{i,j}B_{k,l}-\partial_{k,l}B_{i,j}\\
&\quad=\partial_{i,j}(\lambda^{-(ln-k)}L^l)_+-\partial_{i,j}\,\mathrm{tr}(\lambda^{-(ln-k)}L^l)_+I-\partial_{k,l}(\lambda^{-(jn-i)}L^j)_++\partial_{k,l}\,\mathrm{tr}(\lambda^{-(jn-i)}L^j)_+I\\
&\quad=[B_{i,j},\lambda^{-(ln-k)}L^l]_+-[B_{k,l},\lambda^{-(jn-i)}L^j]_+\\
&\quad=[B_{i,j},B_{k,l}]+[B_{i,j},(\lambda^{-(ln-k)}L^l)_-]_+-[B_{k,l},\lambda^{-(jn-i)}L^j]_+\\
&\quad=[B_{i,j},B_{k,l}]+[\lambda^{-(jn-i)}L^j,(\lambda^{-(ln-k)}L^l)_-])_++[\lambda^{-(jn-i)}L^j,(\lambda^{-(ln-k)}L)_+]_+\\
&\quad=[B_{i,j},B_{k,l}]+[\lambda^{-(jn-i)}L^j,\lambda^{-(ln-k)}L^l]\\
&\quad=[B_{i,j},B_{k,l}].
\end{aligned}$$

□

Theorem 13: *All operators ∂_{ij} commute.*
Proof: We obtain

$$\begin{aligned}
\partial_{k,l}\partial_{i,j}L^q&=[\partial_{k,l}B_{i,j},L^q]+[B_{i,j},\partial_{k,l}L^q]\\
&=[\partial_{i,j}B_{k,l}-[B_{i,j},B_{k,l}],L^q]+[B_{i,j},[B_{k,l},L^q]]\\
&=[\partial_{i,j}B_{k,l},L^q]+[B_{k,l},[B_{i,j},L^q]\\
&=\partial_{i,j}\partial_{k,l}L^q,
\end{aligned}$$

where we have used Eq. (16) and the Jacobi identity. □

Thus, we have given an alternative proof of Dickey's result.[8]

Remark: We get an equivalent form of the zero curvature equations of the hierarchy

$$\partial_{ij}w=B_{ij}w. \tag{17}$$

The expression w is called a formal Baker function. The same equation can also be expressed as

$$w\partial_{ij}w^{-1}=\partial_{ij}-B_{ij}.$$

Thus, w acts like a dressing operator. It can be shown that the operators ∂_{ij} commute. This fact and the commutativity of operator (17) imply the zero curvature equation.

IV. HERMITIAN SYMMETRIC SPACES AND INTEGRABLE SYSTEMS

Let G be a semisimple Lie group and $\mathfrak{g}$ be the corresponding Lie algebra. Let M be a homogeneous space of $\mathcal{G}$, so, M is a differentiable manifold on which G acts transitively. There is a homeomorphism of the coset space G/K onto M for some isotropy subgroup K of G at a point of M. Let k be the Lie algebra of K and $\mathfrak{g}$ satisfies

$$\mathfrak{g}=k\oplus m \quad \text{and } [k,k]\subset k,$$

where m is the vector space complement of k. The Lie algebra $\mathfrak{g}$ splits in such a way that M is equipped with two kinds of extra structure, these are

(1) left translation of m around G gives rise to a canonical connection on the principle K bundle: $G\to G/K$.
(2) When $x\in M$, the map $\mathfrak{g}\to T_xM$ given by

$$\eta \mapsto \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \exp(t\,\eta.x),$$

restricts to give an isomorphism $[m]_x \to T_xM$.

The inverse map

$$\omega_x : T_xM \to [m]_x$$

defines a $\mathfrak{g}$-valued one form on M, known as Maurer Cartan form.

If k and m satisfy

$$[k,m] \subset m$$

then G/K is called reductive homogeneous space. We can associate to these spaces a canonical connection with curvature and torsion. Curvature and torsion at a fixed point p are given purely in terms of the Lie bracket operation,

$$(R(X,Y)Z)_p = -[[X,Y]_k, Z], \quad X,Y,Z \in m,$$

$$T(X,Y)_p = -[X,Y]_m, \quad X,Y \in m.$$

If k and m satisfy above two conditions and also satisfy

$$[m,m] \subset k,$$

then G/K is a symmetric space. Here the curvature satisfies

$$(R(X,Y)Z)_p = -[[X,Y],Z], \quad X,Y,Z \in m.$$

Here $[X,Y] \in k$ happens automatically due to $[m,m] \in k$.

Let h be the Cartan subalgebra of $\mathfrak{g}$ which is the maximal Abelian subalgebra of diagonalizable elements of $\mathfrak{g}$. In terms of the Weyl basis

$$[H_i, H_j] = 0, \quad [H_i, X_\alpha] = \alpha(H_i) X_\alpha,$$

$$[X_\alpha, X_\beta] = N_{\alpha,\beta} X_{\alpha+\beta} (\alpha+\beta \in \Delta) = \sum_{i=1}^{mh} C_{\alpha,i} H_i (\alpha+\beta = 0),$$

for any $H_i \in h$ and $X_\alpha \in \mathfrak{g}\ h$, and $N_{\alpha,\beta}$ and $C_{\alpha,i}$ are structure constants and Δ is a set of all roots.

The components R^i_{jkl} and T^i_{jk} of the curvature and torsion with respect to a basis X_i of T_pM are defined by

$$R(X_k, X_l) X_j = R^i_{jkl} X_i, \quad T(X_j, X_k) = T^i_{jk} X_i,$$

and the component of the metric $g(X,Y) = \mathrm{tr}(ad(X)ad(Y))$ is $g_{ij} = g(X_i, X_j)$.

Let ϱ be an element of h we select the isotropy group K such that its Lie algebra is k. This is given by the centralizer

$$C_g(\varrho) = \{X \in g | [X, \varrho] = 0\}.$$

If ϱ is regular, i.e., the eigenvalues $\alpha(\varrho)$ of $ad\,\varrho$ are mutually distinct then $C_g(\varrho) = h$ and here $[h,m] \subset m$.

In this case since $k = h$ hence the corresponding coset space G/K decomposition is essentially Cartan decomposition.

When $k=C_g(\varrho)\supset h$, then the eigenvalues $\alpha(\varrho)$ coalesce, and thus $C_g(\varrho)$ becomes larger than h. Hence in this case the homogeneous space G/K becomes smaller.

In the case of Hermitian symmetric spaces $\alpha(\varrho)$ have eigenvalues $\{0,\pm\alpha\}$. Thus g splits up into

$$g=k\oplus m^+\oplus m^-.$$

If we set $X^0\in k$, $X^\pm\in m^\pm$ for any $X\in g$,

$$[\varrho,X^0]=0,\quad [\varrho,X^\pm]=\pm\alpha X^\pm,$$

here eigenvalues $\alpha(\varrho)$ take the same eigenvalue for all $X^\pm\in m^\pm$. From the second commutation relation we can assert that Hermitian symmetric space has almost complex structure.

A. Computation of ad-invariant functions through example

Let us compute the ad^* invariant functions.

Suppose L be an arbitrary element of the orbit, then the gradient of the ad-invariant function F, in presence of the cocycle must satisfy

$$[L,\nabla H]+\frac{\partial\nabla H}{\partial x}=0.$$

In the absence of any central extension, H would have satisfied $ad^*_{\nabla H}L=0$ whose immediate solution is $H=\mathrm{tr}(L^p)$, where $p\in\mathbf{Z}_+$.

Let us discuss the method of obtaining ad-invariant function in presence of cocycle through an example. We expand ∇H in the powers of λ and set

$$\nabla H=\lambda^4h_4+\lambda^3h_3+\lambda^2h_2+\lambda h_1+h_0+\lambda^{-1}h_{-1}+\lambda^{-2}h_{-2}+\cdots$$

in the above equation for

$$L=\lambda^2A+\lambda Q+W,$$

where

$$A=\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix},$$

$$Q=\begin{pmatrix}0 & q\\ r & 0\end{pmatrix},$$

$$W=\begin{pmatrix}0 & 0\\ 0 & \frac{i}{2}rq\end{pmatrix}.$$

Thus equating various powers of λ we obtain the following recursive relations:

$$\lambda^6:\quad [A,h_4]=0,$$

$$\lambda^5:\quad [A,h_3]+[Q,h_4]=0,$$

$$\lambda^4:\quad [A,h_2]+[Q,h_3]+[W,h_4]=\frac{\partial h_4}{\partial x},$$

$$\lambda^3: \quad [W,h_3]+[Q,h_2]+[A,h_1]=\frac{\partial h_3}{\partial x},$$

$$\lambda^2: \quad [A,h_0]+[Q,h_1]+[W,h_2]=\frac{\partial h_2}{\partial x},$$

$$\lambda^1: \quad [Q,h_0]+[W,h_1]=\frac{\partial h_1}{\partial x},$$

$$\lambda^0: \quad [W,h_0]=\frac{\partial h_0}{\partial x}.$$

It is easy to see that h_4 and h_3 follows from the first two expressions:

$$h_4=2A, \quad h_3=2Q.$$

h_2 follows from the λ^4 term. Let us choose

$$h_2=2W+2w, \quad \text{s.t.}[A,w]=0,$$

where

$$w=\begin{pmatrix} -\frac{i}{2}rq & 0 \\ 0 & 0 \end{pmatrix}.$$

Thus we write $h_2=-iqr\sigma_3$.

Equating the λ^3 term we obtain

$$[A,h_1]=h_{3x}-2[Q,w],$$

or

$$h_1=\frac{i}{2}h_{3x}^{+}-\frac{i}{2}h_{3x}^{-}-i[Q,w]^{+}+i[Q,w]^{-}.$$

Thus

$$h_1=\begin{pmatrix} 0 & iq_x+\frac{1}{2}q^2r \\ -ir_x+\frac{1}{2}qr^2 & 0 \end{pmatrix}.$$

It is easy to see that the λ^2 term,

$$[A,h_0]+[Q,h_1]=\frac{\partial h_2}{\partial x}, \quad \text{since } [W,h_2]=0,$$

boils down to $[A,h_0]=0$. Hence, we say h_0 is a diagonal matrix. This should be evaluated from the λ^1 relation. Thus equating the λ^1 term we obtain

$$h_0=\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}(r_xq-q_xr)+\frac{i}{4}r^2q^2 \end{pmatrix}.$$

Equating λ^0 we obtain a set of stationary equations,

$$q_{xx}-iqq_xr=0, \quad r_{xx}+irr_xq=0. \tag{18}$$

Thus, we obtain the ∇H function.

Lemma 14:

$$\nabla H=\lambda^4\begin{pmatrix}-2i & 0\\ 0 & 2i\end{pmatrix}+\lambda^3\begin{pmatrix}0 & 2q\\ 2r & 0\end{pmatrix}+\lambda^2\begin{pmatrix}-iqr & 0\\ 0 & iqr\end{pmatrix}$$
$$+\lambda\begin{pmatrix}0 & iq_x+\frac{1}{2}q^2r\\ -ir_x+\frac{1}{2}qr^2 & 0\end{pmatrix}+\begin{pmatrix}0 & 0\\ 0 & \frac{1}{2}(r_xq-q_xr)+\frac{i}{4}r^2q^2\end{pmatrix}.$$

Thus plucking it into the extended Adler–Kostant–Symes (AKS) equation we obtain the Chen–Lee–Liu type derivative Schrödinger equation,

$$iq_t=q_{xx}-iqrq_x,$$

$$ir_t=-r_{xx}-ir_xqr.$$

B. Nonlinear Schrödinger equation

In this case we assume

$$L=\lambda A+Q, \tag{19}$$

and our ansatz is

$$\nabla H=h_2\lambda^2+h_1\lambda+h_0.$$

Thus equating λ^3 and λ^2 terms we obtain $h_2=A$ and $h_1=Q$. Then equating λ^1 we obtain

$$[A,h_0]=Q_x.$$

This gives rise to

$$h_0=\frac{i}{2}Q_x^+-\frac{i}{2}Q_x^--\frac{i}{2}[Q^-,Q^+].$$

The λ^0 term gives rise to the stationary nonlinear Schrödinger equation.

Lemma 15:

$$\nabla H=A\lambda^2+Q\lambda+\frac{i}{2}Q_x^+-\frac{i}{2}Q_x^--\frac{i}{2}[Q^-,Q^+].$$

Thus substituting the value of ∇H in the extended AKS equation we obtain the nonlinear Schrödinger equation for

$$Q=\begin{pmatrix}0 & q\\ q^* & 0\end{pmatrix}.$$

C. Lie–Poisson structure on orbit and the Falqui–Magri–Pedroni construction

Let us consider a manifold $M=\mathfrak{g}^*$ equipped with two Poisson tensors P_0 and P_1, such that the Poisson pencil on $\mathfrak{g}^*$,

$$\{f,g\}_\lambda=\left\langle Q+\lambda A,\left[\frac{\delta f}{\delta Q},\frac{\delta g}{\delta Q}\right]\right\rangle, \tag{20}$$

where A is any fixed element in $\mathfrak{g}^*$ and f and g are defined on the dual space of $\mathfrak{g}^*$.

Let us study a dynamical flow of $f\in C^*(\mathfrak{g})$. The following equation

$$\frac{\mathrm{d}f}{\mathrm{d}t}=\left\langle \frac{\delta f}{\delta Q},\dot{Q}\right\rangle$$

defines a flow passing through the point Q.

Let G denote a semisimple Lie group and $\mathfrak{g}$ its Lie algebra. Then any smooth function f on $\mathfrak{g}^*$ gives rise to a Hamiltonian flow on T_e^*G, the cotangent space of G at the identity, by extending f to a Hamiltonian H which is left invariant. The Lie–Poisson equations are the Hamiltonian equations on the dual of a Lie algebra and represent an abstraction of the Euler equations for a rigid dynamics and ideal incompressible fluid.

The Lie–Poisson equation is

$$\dot{Q}=-ad^*_{\delta H/\delta Q}Q,$$

where $ad_\xi:\mathfrak{g}\to\mathfrak{g}$ is the adjoint map and $ad^*_\xi:\mathfrak{g}^*\to\mathfrak{g}^*$ is its dual.

Thus the Euler–Poincaré flow

$$\dot{Q}=\left[\lambda A+Q,\frac{\delta f}{\delta Q}\right] \tag{21}$$

coincides with the Adler–Kostant–Symes equation.

FMP Construction: The polynomial extension of the above scheme was given by the Italian school. Consider two copies of the algebra $\mathfrak{g}$. Let us denote (Q_0,Q_1) be a point in $\mathfrak{g}^*\times\mathfrak{g}^*\in M$. Let us consider the flow

$$\frac{\mathrm{d}f}{\mathrm{d}t}=\left\langle \frac{\delta f}{\delta Q_0},\dot{Q}_0\right\rangle+\left\langle \frac{\delta f}{\delta Q_1},\dot{Q}_1\right\rangle.$$

The copies of the algebras are intertwined by the Poisson brackets. Magri *et al.* have chosen the following Poisson brackets:

$$\{f,g\}_0=\left\langle A,\left[\frac{\delta f}{\delta Q_0},\frac{\delta g}{\delta Q_1}\right]+\left[\frac{\delta f}{\delta Q_1},\frac{\delta g}{\delta Q_0}\right]\right\rangle,$$

$$\{f,g\}_1=\left\langle A,\left[\frac{\delta f}{\delta Q_1},\frac{\delta g}{\delta Q_1}\right]+\left[\frac{\delta f}{\delta Q_0},\frac{\delta g}{\delta Q_0}\right]\right\rangle.$$

Definition 16: Let us define two sets of equations

$$\dot{Q}_0=\left[A,\frac{\delta f}{\delta Q_1}\right]+\left[Q_1,\frac{\delta f}{\delta Q_0}\right],\quad \dot{Q}_1=\left[A,\frac{\delta f}{\delta Q_0}\right]$$

and

$$\dot{Q}_0 = -\left[Q_0, \frac{\delta f}{\delta Q_0}\right], \quad \dot{Q}_1 = \left[A, \frac{\delta f}{\delta Q_1}\right].$$

It must be noted that the definitions of Q_0 and Q_1 are compatible with the Poisson structures. Combining these two sets,

$$\dot{Q}_0 = -\left[Q_0 + \lambda Q_1, \frac{\delta f}{\delta Q_0}\right] - \left[\lambda A, \frac{\delta f}{\delta Q_1}\right], \tag{22}$$

$$\dot{Q}_1 = -\left[\lambda A, \frac{\delta f}{\delta Q_0}\right] + \left[A, \frac{\delta f}{\delta Q_1}\right]. \tag{23}$$

Hence we obtain

$$(\lambda^2 A + \lambda Q_1 + Q_0)_t = -\left[\lambda^2 A + \lambda Q_1 + Q_0, \frac{\delta f}{\delta Q_0}\right]. \tag{24}$$

Thus we assert the following.

Claim 17: The AKS equation (without cocycle) superposed with the Fordy–Kulish decomposition yields the Falqui–Magri–Pedroni scheme.

Generalization of FMP construction: The FMP construction can be easily extended to more general frame work. In this case one can identify the FMP scheme with the extended AKS equation or AKS equation with cocycle.

Definition 18: Let us define two sets of equations

$$\dot{Q}_0 = \left[A, \frac{\delta f}{\delta Q_1}\right] + \left[Q_1, \frac{\delta f}{\delta Q_0}\right] - \left(\frac{\delta f}{\delta Q_1}\right)_x, \quad \dot{Q}_1 = \left[A, \frac{\delta f}{\delta Q_0}\right]$$

and

$$\dot{Q}_0 = -\left[Q_0, \frac{\delta f}{\delta Q_0}\right] + \left(\frac{\delta f}{\delta Q_0}\right)_x, \quad \dot{Q}_1 = \left[A, \frac{\delta f}{\delta Q_1}\right] + \left(\frac{\delta f}{\delta Q_1}\right)_x,$$

all these extra derivative terms are generated from the cocycle terms.

Combining these two sets,

$$\dot{Q}_0 = -\left[Q_0 + \lambda Q_1, \frac{\delta f}{\delta Q_0}\right] - \left[\lambda A, \frac{\delta f}{\delta Q_1}\right] + \left(\frac{\delta f}{\delta Q_0}\right)_x - \lambda\left(\frac{\delta f}{\delta Q_1}\right)_x, \tag{25}$$

$$\dot{Q}_1 = -\left[\lambda A, \frac{\delta f}{\delta Q_0}\right] + \left[A, \frac{\delta f}{\delta Q_1}\right] + \left(\frac{\delta f}{\delta Q_1}\right)_x. \tag{26}$$

Again combining these two expressions we obtain

$$(\lambda^2 A + \lambda Q_1 + Q_0)_t = -\left[\lambda^2 A + \lambda Q_1 + Q_0, \frac{\delta f}{\delta Q_0}\right] + \left(\frac{\delta f}{\delta Q_0}\right)_x. \tag{27}$$

Thus we obtain the extended AKS equation from the FMP construction.

V. CONNECTION TO GELFAND–ZAKHAREVICH CONSTRUCTION

Suppose L be an arbitrary element of the orbit, then the gradient of the ad-invariant function F, in presence of the cocycle must satisfy

$$[L,\nabla F]+\frac{\partial \nabla F}{\partial x}=0.$$

The gradient of F is obtained from the power series expansion of gl,

$$\nabla F=\lambda^2 h_2+\lambda h_1+h_0+\lambda^{-1}h_{-1}+\lambda^{-2}h_{-2}+\cdots.$$

Actually the dual space of loop algebra is endowed with two Poisson tensors P_0 and P_1, given by

$$P_0=[A,\cdot],\quad P_1=\frac{\mathrm{d}}{\mathrm{d}x}+[Q,\cdot]. \tag{28}$$

Hence the Poisson pencil is $P_\lambda=P_0+\lambda P_1$. The associated Poisson bracket is given by

$$\{f,g\}_\lambda=\langle \mathrm{d}f,P_\lambda\,\mathrm{d}g\rangle, \tag{29}$$

and it is well known that $\{f,g\}_\lambda$ satisfies the Jacobi identity.

Let $\{,\}_1$ and $\{,\}_2$ be two compatible Poisson brackets on M. Then every vector field which is Hamiltonian with respect to both brackets is called bi-Hamiltonian vector field and a sequence of functions $\{f_i|i\in\mathbf{Z}\}$ is called bi-Hamiltonian hierarchy if

$$\{\cdot,f_i\}_2=\{\cdot,f_{i+1}\}_1.$$

It is known that all functions f_i of a bi-Hamiltonian hierachy $\{f_i|i\in\mathbf{Z}\}$ are in involution with respect to both Poisson brackets. This follows straight from the Lenard scheme:

$$\{f_i,f_j\}_1=\{f_i,f_{j-1}\}_2=\{f_{i+1},f_{j-1}\}_1=\cdots=\{f_j,f_i\}_1,$$

so $\{f_i,f_j\}_1=0$ by skew symmetry.

The parameter λ plays an interesting role in this construction. It is known that this parameter λ influences all the major geometrical objects on the Poisson manifold. This is cited in the work of Gelfand and Zakharevich.

The same thing can be repeated from the Poisson bi-vectors point of view, and this view point is closer to the Gelfand–Zakharevich formalism.

Proposition 19: Let f and g be two functions on a bi-Hamiltonian manifold M which satisfy $P_0\mathrm{d}f=P_1\mathrm{d}g$. Then the Poisson brackets $\{f,g\}_i$, $i=0,1$ vanish.

Proof: It follows straight from

$$\{f,g\}_0=\langle \mathrm{d}f,\ P_0\,\mathrm{d}g\rangle=-\langle \mathrm{d}g,\ P_0\,\mathrm{d}f\rangle=\langle \mathrm{d}g,\ P_1\,\mathrm{d}g\rangle=0.$$

Similarly for $\{f,g\}_1$. □

A Hamiltonian vector field is called bi-Hamiltonian vector field if it satisfies

$$\mathcal{X}_H=P_0^\sharp\,\mathrm{d}H=P_1^\sharp\,\mathrm{d}H, \tag{30}$$

where $P_i^\sharp: T^*M\to TM$ is the bundle homomorphism associated to P_i-Poisson bi-vectors.

The Gelfand–Zakharevich construction relies on Weinstein's work of local Poisson structure.[42] It states that under a suitable assumptions on the regularity of the Poisson brackets, the Poisson bi-vector P on an open dense set of M is rank $2n$. M is foliated there in regular Poisson submanifolds, called generic symplectic leaves, generically these are common level sets of k functions $C_1,\ldots,C_k$ called Casimir functions of P. The key property of the Casimirs of P is that their differentials lie in the kernel of P. The dimension of M is related with the integers n and k by $\dim M=2n+k$.

Now we state the theorem of Gelfand and Zakharevich.[20,21]

Theorem 20: *On a* $(2n+1)$*-dimensional bi-Hamiltonian manifold, whose Poisson pencil has maximal rank, the leaves of the suppost are generically Lagrangian submanifolds of dimension n contained on each symplectic leaf of dimension* $2n$.

This theorem is difficult to digest. To better understand the essence of the Gelfand–Zakharevich theorem, we tacitly assume the approach of the Falqui, Magri, and Pedroni viewpoint. There first amplification is to reformulate the Lenard scheme in terms

$$(P_1+\lambda P_0)\mathrm{d}C(\lambda)=0. \tag{31}$$

One must note that the Casimirs of a single Poisson bracket are uninteresting functions, Casimirs of pencil of Poisson bracket compactly encode nontrivial dynamics and constants of motion.

The main concent of the Gelfand–Zakharevich theorem is that there exists a Casimir function depending polynomially on the parameter λ, and that the degree of the polynomial is exactly n if dim $= 2n+1$. Thus we can write the Casimir function in the form

$$C(\lambda)=C_0\lambda^n+C_1\lambda^{n-1}+\cdots+C_n. \tag{32}$$

Thus the Poisson pencil selects $n+1$ distinguished functions $(C_0,C_1,C_2,\ldots,C_n)$. Their common level sets are the leaves of the support of the pencil.

This can be expressed as

$$P_\lambda\,\mathrm{d}C_\lambda=0.$$

This yields a chain

$$P_0\,\mathrm{d}C_0=0,$$

$$P_0\,\mathrm{d}C_1=\mathcal{X}_1=P_1\,\mathrm{d}C_0,$$

$$\cdots,$$

$$P_0\,\mathrm{d}C_n=\mathcal{X}_n=P_1\,\mathrm{d}C_{n-1},$$

$$0=P_1\,\mathrm{d}C_n,$$

where $\mathcal{X}_1,\ldots,\mathcal{X}_n$ are bi-Hamiltonian vector fields.

A bi-Hamiltonian manifold endowed with a Poisson pencil with at least one of the elements of the Poisson pencil is invertible then such a manifold is called *regular bi-Hamiltonian manifolds*. On a regular bi-Hamiltonian manifold we can define a class of canonical coordinates, called the Darboux–Nijenhuis coordinates. It is known that *one-half* of the Darboux–Nijenhuis coordinates are algebraically provided by the Nijenhuis tensor itself, and the remaining *one-half* can always be found by quadratures. This would take us to separation of variables.

VI. CONCLUSION AND OUTLOOK

In this paper we have studied a special class of bi-Hamiltonian geometry—the torsionless Gelfand–Zakharevich bi-Hamiltonian hierarchy and its connection to the Adler–Kostant–Symes hierarchy. This AKS hierarchy is the reduction of $1+1$ dimensional SDYM hierarchy. We have extracted many interesting properties of the Gelfand–Zakharevich geometry from the AKS construction. We present a dictionary below.

AKS scheme	GZ–FMP scheme
AKS construction applied to loop algebra superposed with Fordy–Kulish decomposition	FMP equation
Ad-invariant functions	Casimirs of pencil of Poisson operators
Poisson structures related to dressed and undressed orbits	Pencil of compatible Poisson structures

This fact once again suggests that the classical separation of variables admitting a Lax representation can be studied via AKS construction, which is of course known to mathematicians.

Recently in an interesting paper Burstall *et al.*[7] have shown how to reformulate the (pluri)harmonic map equations for maps of a surface into a Lie group G as zero-curvature equations so that the (pluri)harmonic maps correspond to loops of flat connections. It would be rather fascinating if one tried to unevil the connection between the (pluri)harmonic maps of a surface into a Lie group G in light of Gelfand–Zakharevich bi-Hamiltonian geometry. Certainly the proximity between the two subjects will entice harmonic maps specialists to study bi-Hamiltonian geometry.

The method we have discussed in this paper can be seen as a kind of bridge between bi-Hamiltonian and the Lie algebraic nature of integrable system. The author believes that this paper would further support the program of Italian school.

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Construction and uniqueness of the C*-Weyl algebra over a general pre-symplectic space

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A systematic approach to the C*-Weyl algebra $\mathcal{W}(E,\sigma)$ over a possibly degenerate pre-symplectic form σ on a real vector space E of possibly infinite dimension is elaborated in an almost self-contained manner. The construction is based on the theory of Kolmogorov decompositions for σ-positive-definite functions on involutive semigroups and their associated projective unitary group representations. The σ-positive-definite functions provide also the C*-norm of $\mathcal{W}(E,\sigma)$, the latter being shown to be *-isomorphic to the twisted group C*-algebra of the discrete vector group E. The connections to related constructions are indicated. The treatment of the fundamental symmetries is outlined for arbitrary pre-symplectic σ. The construction method is especially applied to the trivial symplectic form $\sigma=0$, leading to the commutative Weyl algebra over E, which is shown to be isomorphic to the C*-algebra of the almost periodic continuous function on the topological dual E'_τ of E with respect to an arbitrary locally convex Hausdorff topology τ on E. It is demonstrated that the almost periodic compactification aE'_τ of E'_τ is independent of the chosen locally convex τ on E, and that aE'_τ is continuously group isomorphic to the character group $\hat{E}$ of E. Applications of the results to the procedures of strict and continuous deformation quantizations are mentioned in the outlook. [DOI: 10.1063/1.1757036]

I. INTRODUCTION

In the present investigation we analyze mathematically the canonical commutation relations (CCR) in Weyl form[1,2] for a general type of physical system, in which the degrees of freedom are to be described partially in classical and partially in quantum mechanical terms. For the quantized degrees of freedom the incompatibility of position and momentum is significant, for the classical degrees of freedom it is not, resp., may be neglected. In a coordinate-independent manner we express the existing degrees of freedom for the considered system in terms of a pre-symplectic space (E,σ) of arbitrary dimension. By definition, E is a real vector space, which is equipped with a possibly degenerate pre-symplectic form σ, a real-bilinear, antisymmetric mapping $\sigma: E\times E \to \mathbb{R}$. [The more general set up, in which (E,σ) is replaced by a pre-symplectic manifold, is not treated under the headline ''Weyl algebra'' in the literature.]

A combination of the ansatz of Weyl with the abstract set up of Dirac[3] leads to the notion of *algebraic* Weyl relations, resp., of an algebraic Weyl system, connected with the pre-symplectic space (E,σ). In Ref. 4 Dirac developed formal strategies to define functions, which map

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q-numbers onto q-numbers, and generalize the operations of differentiation and integration. Such a formalism would then allow for functions of the q-number Weyl elements and their derivatives. The mathematically much more refined Hilbert space formalism of von Neumann[5,6] has pushed aside Dirac's q-number analysis. In algebraic quantum theory (cf. Refs. 7–9 and references therein) one seeks, however, for a synthesis of the abstract and the Hilbert space approach: One starts with a rather universal *-algebraic formalism, but restricts oneself to bounded elements with a finite norm. The ultimate model calculations are then performed by means of a representation of the algebraic structure in terms of Hilbert space operators. There, the limits to unbounded (self-adjoint) operators may also be carried through. (An early discussion, which relates Hilbert space Weyl systems with C*-algebras, may be found, in the case of nondegenerate, infinite dimensional, symplectic forms, in Ref. 10.)

In the spirit of algebraic quantum theory we assume now for a general physical system, with the degrees of freedom (E,σ), that there exists a family $\{W(f)|f\in E\}$ of elements in a complex *-algebra, which are linearly independent and which satisfy the Weyl relations (we set, henceforth, $\hbar$ equal to unity),

$$W(f)W(g)=\exp\left\{-\frac{i}{2}\sigma(f,g)\right\}W(f+g),\quad \forall f,g\in E. \qquad (1.1)$$
$$W(f)^*=W(-f),$$

We call the family of all $W(f)$, $f\in E$, which satisfies the preceding requirements, an *abstract Weyl system* and refer to E as its *test function space*.

A Weyl system is considered as a concise minimal structure, which is necessary to characterize the set of observables. It is, of course, natural to form its linear hull, which is a sub-*-algebra (cf. Sec. III B), but the properties of the latter are already implied by those of the Weyl system. Because of the assumed linear independence of the abstract Weyl elements, all abstract Weyl systems are algebraically *-isomorphic and we speak of *the* abstract Weyl system associated with a given pre-symplectic space (E,σ).

If E has the finite dimension $2n$ and σ is a nondegenerate symplectic form, then we are back with the original Weyl relations, considered by Weyl and von Neumann, but now in abstract q-number form. There exists an ordered symplectic basis, which, written as a $2n$-tupel, has the structure $(\mathbf{e},\eta\mathbf{e})=(e_1,\ldots,e_n,\eta e_1,\ldots,\eta e_n)$ such that $\sigma(e_i,\eta e_j)=\delta_{ij}$ and $\sigma(e_i,e_j)=0$ for all $1\leqslant i,j\leqslant n$. Here η is an imaginary unit in the real vector space E.[11] It holds by definition: $\eta^{-1}=-\eta$, $\sigma(\eta f,\eta g)=\sigma(f,g)$, and $\sigma(f,\eta f)\geqslant 0$ for all $f,g\in E$. Each $f\in E$ has the expansion $f=\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\eta\mathbf{e}=\sum_{i=1}^{n}[r_ie_i+s_i\eta e_i]$, where $\mathbf{r},\mathbf{s}\in\mathbb{R}^n$. By means of the symplectic basis, we obtain σ in normal form and find for the Weyl multiplication law,

$$W(f)W(f')=\exp\left\{-\frac{i}{2}(\mathbf{r}\cdot\mathbf{s}'-\mathbf{s}\cdot\mathbf{r}')\right\}W(f+f'). \qquad (1.2)$$

A *realization* of an abstract Weyl system in a complex Hilbert space $\mathcal{H}_R$ is a family of possibly not linearly independent, but unitary operators $W_R(f)$, $f\in E$, in $\mathcal{H}_R$, which satisfy Eq. (1.1). Especially, for an infinite dimensional test function space E there are essentially different realizations of an abstract Weyl system over a given (E,σ). The physical meaning of a Weyl system depends on its realization. A realization of an abstract Weyl system is called *regular*, if the function $\mathbb{R}\ni t\mapsto W_R(tf)\in\mathcal{U}(\mathcal{H}_R)$ is continuous in the weak, resp. strong, operator topology [$\mathcal{U}(\mathcal{H}_R)$ denotes the group of unitaries acting on $\mathcal{H}_R$]. Stone's theorem implies, in a regular realization, the exponential form of the Weyl operators, that is

$$W_R(f)=\exp\{i\Phi_R(f)\}, \qquad (1.3)$$

where the so-called field operators $\Phi_R(f)$, $f\in E$, are self-adjoint, depending real-linearly on f. They satisfy on a common dense domain in $\mathcal{H}_R$ the commutation relations

$$[\Phi_R(f),\Phi_R(g)]=i\sigma(f,g),\quad f,g\in E. \tag{1.4}$$

For finitely many degrees of freedom and nondegenerate σ this reduces to the original CCR (Refs. 12, 13, 3),

$$\begin{matrix} p_iq_j-q_jp_i=:[p_i,q_j]=-i\delta_{i,j}\mathbb{1}, \\ [q_i,q_j]=0=[p_i,p_j], \end{matrix}\quad 1\leqslant i,j\leqslant n, \tag{1.5}$$

if one employs a symplectic basis $(\mathbf{e},\eta\,\mathbf{e})$ and writes

$$\Phi_R(f)=\mathbf{r}\cdot\mathbf{q}^R+\mathbf{s}\cdot\mathbf{p}^R,\quad \text{again denoting}\quad f=\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\eta\mathbf{e}, \tag{1.6}$$

where $\mathbf{q}^R=(q_j^R):=(\Phi_R(e_j))$ and $\mathbf{p}^R=(p_j^R):=(\Phi_R(\eta e_j))$ for $1\leqslant j\leqslant n$.

In the finite dimensional case with *nondegenerate* σ there holds the well-known von Neumann–Stone uniqueness theorem:[2,14,15–17] Each regular, unitary realization of an abstract Weyl system is unitarily equivalent to a direct sum of Schrödinger representations. [In the Schrödinger representation $R\equiv S$, we have $\mathcal{H}_S=L^2(\mathbb{R}^n)$, and $q_j^S=x_j$ and $p_j^S=-i(\partial/\partial x_j)$ for $1\leqslant j\leqslant n$.]

A direct sum of Schrödinger representations is employed, if one deals with different systems in an alternative manner, e.g., with a microscopic particle, which is either an electron or a positron. The operators which commute with the represented Weyl elements—and typically arise in direct sum representations—define so-called superselection rules as, e.g., the electric charge (cf., e.g., Refs. 18–21). They express, thus, also physically important quantities, which are compatible with all other observables. Let us denote them by the more general term *classical observables*, since—as is indicated below—in many body physics also dynamical effects may lead to central observables. The (bounded) classical observables may be incorporated into the abstract Weyl system, if one extends the orginally nondegenerate symplectic form to a degenerate one, denoted again by σ, which then displays a nontrivial null space,

$$\ker_\sigma:=\{h\in E\,|\,\sigma(h,f)=0,\forall f\in E\}. \tag{1.7}$$

Clearly, for $h\in\ker_\sigma$ the associated Weyl element $W(h)$ commutes with all other Weyl elements and signifies a classical observable—if we call the non-Hermitian functions of Weyl elements also observables—in the sense of abstract q-numbers.

For infinitely many degrees of freedom the algebraic approach is especially useful. (For an account of the early papers on this topic, cf., e.g., Refs. 22, 23, 8.) In the physical applications the infinite dimensional test function space E is often a complex-linear dense subspace of a one-Boson Hilbert space, and the nondegenerate symplectic form is the imaginary part of the pertinent scalar product. The degrees of freedom of the quantized field are, so to speak, tested by means of (smooth) functions taken from the one-Boson Hilbert space. This smearing of the quantized fields in terms of test functions had been already requested by physical arguments.[24,25]

It is well known, that for a nondegenerate symplectic form σ there exists, up to *-isomorphisms, a unique C*-algebra $\mathcal{W}(E,\sigma)$, which is the norm-closure of the linear span of the abstract Weyl system (cf. Refs. 26–30). For nondegenerate σ the simple C*-algebra $\mathcal{W}(E,\sigma)$ is in quantum field theory and in many body physics used as the primary observable algebra of a Boson system.[31,32] It contains the universal observables the system always displays, irrespective of the external influences it may experience. All of these primary observables are present in each nontrivial Hilbert space representation.

A field theoretic example, where the primary observable algebra is a Weyl algebra with a degenerate symplectic form, exhibiting genuine superselection rules, is elaborated in Ref. 33. Another example, which we shall investigate more closely in future work, is the nonrelativistic photon algebra, where only the transversal components of the canonical fields give rise to nonvanishing values of σ. In these cases one encounters nontrivial Hilbert space realizations of the Weyl relations, in which the classical observables are not faithfully represented. As is emphasized in Ref. 34, apparently the first systematic investigation of the C*-Weyl algebra over a pre-symplectic

test function space, this feature reflects the nonuniqueness of the corresponding abstract C*-Weyl algebra: The CCR (in Weyl form) alone do not determine the primary observable algebra.

Let us recall that the choice of a special Hilbert space representation, where the Weyl elements are given by unitary operators in $\mathcal{L}(\mathcal{H}_\Pi)$, the bounded operators in the representation Hilbert space $\mathcal{H}_\Pi$, is usually induced by the selection of a distinguished state, as, e.g., a coherent state, or a ground, resp. equilibrium, state. In the GNS-representation $\Pi:\mathcal{W}(E,\sigma)\to\mathcal{L}(\mathcal{H}_\Pi)$ over a regular state with a special ordered structure (e.g., optical coherence, or thermodynamic phase ordering; cf. Ref. 9, Section 3.3) the field operators $\Phi_\Pi(f)=(d/dt)\Pi(W(tf))|_{t=0}$ may exhibit a classical part in addition to the quantum mechanical part. This peculiar feature is a manifestation of the underlying ordered structure the system attains under a special influence (e.g., optical pumping, resp. low temperature) and clearly transcends the purely algebraic regime of the theory. This most interesting effect leads in a natural manner to a continuous extension of (E,σ) to a larger pre-symplectic space and to its associated Weyl algebra (cf. Refs. 35–38). These extended Weyl algebras deserve special attention, also in the context of modern quantization and dequantization strategies. They add to the motivation to study Weyl algebras with a pre-symplectic test function space.

Before outlining our method and describing its implications, let us mention various mathematical approaches, which bear a certain technical relationship to our construction. Common to almost all of these ansatzes is that the test function space E is considered merely as a topological, Abelian group. The physical terminology of a Weyl system realized in a Hilbert space is then a projective representation of this group in the mathematical language. The theory of projective group representations begins already with Schur (cf. Ref. 39) and has especially been advocated by Mackey.[40] Further investigations are contained in Refs. 41 and 42. The connection to representations of generalized (nowadays called ''twisted'') L^1-algebras has been developed in Ref. 43 and further pursued in Refs. 44–48.

In Ref. 34 the Weyl algebra $\mathcal{W}(E,\sigma)$ over the pre-symplectic space (E,σ) is defined as the twisted group C*-algebra corresponding to the multiplier

$$E\times E\ni(f,g)\mapsto\exp\left\{-\frac{i}{2}\sigma(f,g)\right\}. \tag{1.8}$$

Hereby the test function space E is taken as a real vector group (and not only as a group) and is equipped with the discrete topology. (See Sec. III E for special implications of a vector group.)

In Ref. 49 Kolmogorov decompositions are used in the form of algebraic inducing, and thus there is a certain similarity to our method.

The ''Weyl algebra'' over compact manifolds, especially over the torus group,[50] provides prominent examples for a noncommutative geometry (cf. Refs. 51–53, and references therein).

The problem of nonregular states and discontinuous quasi-free dynamical systems is treated already in Refs. 54 and 55, and more recently in Ref. 56. In our context, related developments were undertaken in Refs. 37 and 38.

Let us also mention the work[58] of Weaver, in which for (infinite dimensional) Hilbert spaces E, with the imaginary part of the scalar product taken as the symplectic form σ, deformed von Neumann and C*-algebras are constructed in special realizations.

In our present exposition we do not rely on earlier results but we start anew from an arbitrary pre-symplectic test function space (E,σ) (where the inifinite dimensional case is, of couse, the interesting one). We give a straight-forward and almost self-contained construction method for a natural C*-Weyl algebra $\mathcal{W}(E,\sigma)$, associated with (E,σ), which does not use a special realization or Hilbert space representation. That means that we work directly with the linear hull $\Delta(E,\sigma)$ of the abstract Weyl elements and with the states on this abstract *-algebra, where the latter are given in terms of the σ-positive definite functions $\mathcal{C}(E,\sigma)$ on E. These data are shown to determine a distinguished C*-norm on $\Delta(E,\sigma)$, and the subsequent norm-completion of $\Delta(E,\sigma)$ leads already to $\mathcal{W}(E,\sigma)$. The clear-cut strategy appears useful for quantum field theoretic applications.

More specifically, we collect in Sec. II the basic notions and prove some necessary results concerning projective representations of J-involutive groups, in the case that an antisymmetric bicharacter Σ is given, employing Kolmogorov decompositions.[57] These techniques are then applied to the GNS-representations of so-called U*-algebras (where a ''representation'' is here always realized in terms of *bounded* operators). We prove especially an original extension theorem for Σ-positive definite functions (Prop. 2-2). In this manner we adapt the even more general results of Ref. 29 to our requirements and refine some of their arguments.

In Sec. III the formalism is specialized to Weyl systems connected with the pre-symplectic space (E,σ), now considered a J-involutive group. According to the previously derived results, each σ-positive definite function in $C(E,\sigma)$ defines a Hilbert space representation of the abstract Weyl system, resp., of $\Delta(E,\sigma)$ (whereas, in general, GNS-constructions for *-algebras would lead to unbounded operators.)

As indicated above, the C*-norm is introduced on $\Delta(E,\sigma)$ by means of $C(E,\sigma)$ without considering, at first, the Hilbert space realizations. In contradistinction to Ref. 34 and to Ref. 58 our approach is completely algebraic and emphasizes the uniqueness of $\mathcal{W}(E,\sigma)$, if all of the σ-positive definite functions $C(E,\sigma)$ are taken into account for defining the C*-norm.

Of course, it is valuable to acquire information on the connection between the abstract Weyl algebra $\mathcal{W}(E,\sigma)$ and the represented Weyl systems. In Prop. 3-4 it is demonstrated that the abstract C*-norm is also obtainable as the supremum of all operator norms of the representations. In Theorem 3-7 it is shown that $\mathcal{W}(E,\sigma)$ is the unique C*-algebra, whose represention give all Weyl systems in Hilbert spaces.

The homeorphism between $C(E,\sigma)$ and the total state space of $\mathcal{W}(E,\sigma)$, which we found in the literature only for *nondegenerate* σ as a map of the *continuous* functions in $C(E,\sigma)$ onto the *regular* states on $\mathcal{W}(E,\sigma)$, is proven in Theorem 3-5. A fundamental role in the analysis of $\mathcal{W}(E,\sigma)$ plays the tracial state, which we show to be faithful in Corollary 3-6 (a fact already stated, but not completely proven, in Ref. 34 and also mentioned within a more special context in Ref. 58).

In Sec. III D the gauge transformations of the second kind and the symplectic transformations, that are the fundamental structural symmetries, are introduced in a more general manner than in the previous literature.

The norm estimates in Sec. III E, concerning beside the C*-norm two other Banach norms, refine and supplement essentially the considerations regarding this topic in Ref. 34. It is demonstrated, besides other things, that the chosen C*-norm is the only C*-norm, which majorizes the $\|\cdot\|_2$-norm.

In Sec. IV we treat, as a special case of the general formalism, the commutative Weyl algebra $\mathcal{W}(E,0)$ with the totally degenerate pre-symplectic form—the zero form $\sigma=0$—on an arbitrary real vector space E. We derive several *-isomorphic C*-algebras of functions, which illuminate the structure of this commutative C*-algebra. More precisely, it follows that

$$\mathcal{W}(E,0)\cong \mathrm{AP}(E'_\tau)=C(aE'_\tau)\cong C(\hat{E}). \tag{1.9}$$

Observe that in group theoretical language the commutative Weyl algebra is just the group C*-algebra of the discrete vector group E (with a trivial multiplier). Here $\mathrm{AP}(E'_\tau)$ is the commutative C*-algebra of the continuous almost periodic functions on the topological dual E'_τ of E, where E is equipped with a locally convex Hausdorff topology τ. The symbols $\mathrm{C}(aE'_\tau)$, resp. $\mathrm{C}(\hat{E})$, denote the C*-algebras of the continuous, $\mathbb{C}$-valued functions over the indicated compact spaces. The first compact space is the almost periodic compactification aE'_τ of the dual E'_τ[59] (cf. also Ref. 60 for connecting almost periodic functions and compactifications). The second is the topological character group $\hat{E}$ of E, the latter being regarded as a discrete additive group. [As the classical pendent of Weyl algebras, $\mathrm{AP}(E'_\tau)$ appears already in Ref. 58, but only in the special case of E'_τ being a Hilbert space.]

The *-isomorphism $\mathcal{W}(E,0)\cong\mathrm{C}(\hat{E})$ is identified as the Gelfand representation of the commutative C*-Weyl algebra $\mathcal{W}(E,0)$. As a consequence the state space of $\mathcal{W}(E,0)$ is affine homeo-

morphic to the Bauer simplex of probability measures on the compact character group $\hat{E}$; cf. Ref. 61.

By use of the *-isomorphism $C(aE'_\tau)\cong C(\hat{E})$ in Eq. (1.9), we deduce that the embedding $F\mapsto\exp\{iF(\cdot)\}$ of E'_τ into the character group $\hat{E}$ extends continuously to a continuous group isomorphism between the topological compact groups aE'_τ and $\hat{E}$. As a consequence of this, the almost periodic compactification aE'_τ of the topological dual E'_τ is independent from the chosen locally convex Hausdorff topology τ on E, that is,

$$aE'_{\tau_1}\cong aE'_{\tau_2}\cong\hat{E},$$

for two given locally convex topologies τ_1, resp., τ_2 on E.

These apparently still unpublished results on the classical Weyl algebra enable the free choice of a topology in the field theoretic phase space E'_τ without losing the uniqueness of the observable algebra.

In order to emphasize again that our mathematical developments are motivated by physical intentions, namely to clarify the structure of systems which exhibit quantum and classical features simultaneously and to relate also the extreme cases with each other in terms of the deformation concepts, we draw some conclusions in Sec. V and give an outlook on related works under preparation.

II. POSITIVE-DEFINITENESS AND KOLMOGOROV DECOMPOSITION

A. Projective representations of J-involutive groups

Let first X be an arbitrary (nonempty) set. A mapping $K:X\times X\to\mathbb{C}$, $(x,y)\mapsto K(x,y)$ is called a *kernel* on X, whereas a mapping $C:X\to\mathbb{C}$, $x\mapsto C(x)$ is named a *function*.

A kernel K on X is called *positive-definite*, if for every number $n\in\mathbb{N}$ and all $z_1,\ldots,z_n\in\mathbb{C}$ and all $x_1,\ldots,x_n\in X$ we have $\Sigma_{i,j=1}^{n}\overline{z_i}z_jK(x_i,x_j)\geqslant 0$. Every positive-definite kernel K on X admits a *Kolmogorov decomposition*,[57,29] that is a mapping $v:X\to\mathcal{H}_v$ from X into a complex Hilbert space $\mathcal{H}_v$, which satisfies

$$K(x,y)=(v(x)|v(y)),\quad \forall x,y\in X, \tag{2.1}$$

where $(\cdot|\cdot)$ is the right-linear complex scalar product on $\mathcal{H}_v$. Conversely, a kernel is positive-definite, if it possesses a Kolmogorov decomposition. The Kolmogorov decomposition $v:X\mapsto\mathcal{H}_v$ of K is called minimal, if the set $\{v(x)|x\in X\}$ is total in $\mathcal{H}_v$. If the Kolmogorov decomposition $v:X\to\mathcal{H}_v$ is not minimal, then one constructs a minimal Kolmogorov decomposition by restricting $\mathcal{H}_v$ to the closure of the linear hull of $\{v(x)|x\in X\}$. It is immediately checked that the minimal Kolmogorov decomposition is unique up to unitary equivalence.[29]

We assume from now on that X is a semigroup, i.e., X is equipped with an associative (possibly noncommutative) operation $\circ:X\times X\to X$ and a neutral element $e\in X$, which is defined to satisfy $e\circ x=x\circ e=x$ for all $x\in X$. There may exist some elements in X which are invertible, possessing an element $x^{-1}\in X$ such that $x^{-1}\circ x=x\circ x^{-1}=e$. At least the neutral element e is invertible with $e^{-1}=e$. The inverse x^{-1} is unique and invertible with $(x^{-1})^{-1}=x$. If $x,y\in X$ are invertible, then $x\circ y$ is invertible with $(x\circ y)^{-1}=y^{-1}\circ x^{-1}$.

In addition, suppose to be given an involution J on the semigroup X, that is a mapping $J:X\to X$ satisfying $J^2(x)=x$ and $J(x\circ y)=J(y)\circ J(x)$ for all $x,y\in X$, defining the involutive semigroup (X,J). It follows that

$$X_J:=\{x\in X|J(x)\circ x=x\circ J(x)=e\} \tag{2.2}$$

is a group with the group operation $\circ$, called the *J-involutive group corresponding to* (X,J). Its neutral element just is e, and the inversion is given by $J(x)=x^{-1}$, $x\in X_J$. It holds $J(X_J)=X_J$. Examples are found below.

A kernel Σ on the semigroup X is called an *antisymmetric bicharacter*, if, for all $x, y, z \in X$, one has

$$|\Sigma(x,y)|=1, \quad \Sigma(x,x)=1, \quad \Sigma(x,y\circ z)=\Sigma(x,y)\Sigma(x,z), \quad \Sigma(x\circ y,z)=\Sigma(x,z)\Sigma(y,z).$$

It follows that $\Sigma(x,y)=\overline{\Sigma(y,x)}$ and $\Sigma(x,e)=1$ for all $x, y \in X$. Furthermore, it is $\Sigma(x,y^{-1})=\overline{\Sigma(x,y)}$ for every $x \in X$ and each invertible element $y \in X$. The antisymmetric bicharacter Σ is called *nondegenerate*, if $\Sigma(x,y)=\Sigma(x,z)\ \forall x \in X$ implies $y=z$. Note that a nondegenerate Σ yields the semigroup X to be commutative, since $\Sigma(x,y\circ z)=\Sigma(x,y)\Sigma(x,z)=\Sigma(x,z)\Sigma(x,y)=\Sigma(x,z\circ y)$. We consider here, however, possibly degenerate Σs.

The triplet (X,J,Σ) of the quantities just described is denoted a *projective involutive semigroup*.

A function $C:X\to\mathbb{C}$ on (X,J,Σ) is called Σ*-positive-definite*, if the associated kernel K_C is positive definite, where

$$K_C:X\times X\to\mathbb{C}, \quad (x,y)\mapsto K_C(x,y):=\overline{\Sigma(x,y)}C(J(x)\circ y). \tag{2.3}$$

Explicitly, C is Σ-positive-definite, if

$$\sum_{i,j=1}^{n} \overline{z_i} z_j \overline{\Sigma(x_i,x_j)} C(J(x_i)\circ x_j) \geqslant 0,$$

for every number $n \in \mathbb{N}$, all $z_1,\ldots,z_n \in \mathbb{C}$, and all $x_1,\ldots,x_n \in X$. A Kolmogorov decomposition of C is defined as a Kolmogorov decomposition for the kernel K_C.

A *unitary* Σ*-representation* $(U,\mathcal{H}_U)$ of the group X_J is a mapping $U:X_J \ni x\mapsto U(x)$ from X_J into the unitary operators acting on the complex Hilbert space $\mathcal{H}_U$ such that the relations [cf. also Eq. (1.1)],

$$U(x)U(y)=\Sigma(x,y)U(x\circ y), \quad U(x)^*=U(x)^{-1}=U(x^{-1}), \quad \forall x,y \in X_J, \tag{2.4}$$

are fulfilled. In other words, $(U,\mathcal{H}_U)$ is a projective group representation with respect to the multiplier Σ.

Theorem 2-1 (Σ-representation): *Let C be a Σ-positive-definite function on the projective involutive semigroup (X,J,Σ), and let $v:X\to\mathcal{H}_v$ be the minimal Kolmogorov decomposition of C. Then there exists a unique mapping $V:X_J \ni x\mapsto V(x)$ from the group X_J into the unitary operators on the Hilbert space $\mathcal{H}_v$, such that*

$$V(x)v(y)=\Sigma(x,y)v(x\circ y), \quad \forall y \in X, \quad \forall x \in X_J.$$

Furthermore, the mapping V is a unitary Σ-representation of the J-involutive group X_J.

Proof: For a fixed $x \in X_J$ let us consider the mapping $v^x:X\to\mathcal{H}_v$ defined by $v^x(z):=\Sigma(x,z)v(x\circ z)$ for all $z \in X$. With $J(x\circ y)=J(y)\circ J(x)=J(y)\circ x^{-1}$, the properties of Σ, and Eq. (2.3) we conclude that $(v^x(y)|v^x(z))=K_C(y,z)$ for all $y, z \in X$. Thus the map $v^x:X\to\mathcal{H}_v$ is a Kolmogorov decomposition of C, too, which is minimal since x is invertible. But two minimal Kolmogorov decompositions are unitarily equivalent. Consequently, there exists a unique unitary $V(x)$ on $\mathcal{H}_v$, such that $v^x(z)=V(x)v(z)$ for all $z \in X$. It is straightforward to verify that in application to the total elements $\{v(z)|z \in X\}$ the mapping $V:X_J \ni x\mapsto V(x)$ is a unitary Σ-representation. ■

B. Extension of Σ-positive-definite functions

In this subsection let X be a group with the group operation $\circ$. We define the involution J by $J(x):=x^{-1}$ for all $x \in X$, and thus we have $X=X_J$.

We have $C(e)\geqslant 0$ for every Σ-positive-definite function C on the projective group (X,Σ) by Eq. (2.1). So let us define $\mathcal{C}(X,\Sigma)$ to be the convex set of all normalized, Σ-positive-definite functions $C:X\to\mathbb{C}$, where normalization means $C(e)=1$. The restriction of the antisymmetric bicharacter Σ from X to a subgroup $G\subseteq X$ is also denoted by Σ.

Proposition 2-2: Let G be a subgroup of X. If $C_G\in\mathcal{C}(G,\Sigma)$ is extended trivially to X by putting $C(x):=C_G(x)$ for $x\in G$ and $C(x):=0$ elsewhere, then $C\in\mathcal{C}(X,\Sigma)$. Moreover, the restriction $C\mapsto C|_G$ from X to G is a surjective affine map from $\mathcal{C}(X,\Sigma)$ onto $\mathcal{C}(G,\Sigma)$.

Proof: Let $u:G\to\mathcal{H}$ be a Kolmogorov decomposition of C_G. There exists a subset $I\subset X$ such that X decomposes into the disjoint union $X=\cup_{w\in I}w\circ G$. For each $w\in I$ let $\mathcal{H}_w$ be a copy of $\mathcal{H}$, and perform the direct sum $\mathcal{K}:=\oplus_{w\in I}\mathcal{H}_w$; κ_w be the component of $\kappa\in\mathcal{K}$ in $\mathcal{H}_w$. For $z\in I$ put $u^z:G\to\mathcal{K}$ with $(u^z(y))_w=u(y)\in\mathcal{H}_w$ for $z=w$ but $(u^z(y))_w=0$ for $z\neq w$. Define the map $v:X\to\mathcal{K}$ by $v(x):=\Sigma(x,z)u^z(z^{-1}\circ x)$ for $x\in z\circ G$. With the properties of Σ and Eq. (2.3) we derive that $(v(x)|v(y))=K_C(x,y)$ for all $x, y\in X$. Thus v is a Kolmogorov decomposition of C implying $C\in\mathcal{C}(X,\Sigma)$. ■

Let us present a simple example. Consider the trivial subgroup $G:=\{e\}$. Then $\mathcal{C}(\{e\},\Sigma)$ consists of a single element, which extends trivially to $C_{\mathrm{tr}}\in\mathcal{C}(X,\Sigma)$ satisfying $C_{\mathrm{tr}}(e)=1$ and $C_{\mathrm{tr}}(x)=0$ for $e\neq x\in X$. In Subsection 3.2 we construct from the function C_{tr} a tracial state ω_{tr} on the twisted group C*-algebra, which explains the index "tr."

C. The GNS representation of U*-algebras

Let $\mathcal{A}$ be a complex *-algebra. A linear functional ω on $\mathcal{A}$ is called *positive*, if $\langle\omega;A^*A\rangle\geqslant 0$ for all $A\in\mathcal{A}$, where $\langle\cdot;\cdot\rangle$ means the algebraic duality relation. A representation $(\Pi,\mathcal{H}_\Pi)$ of the *-algebra $\mathcal{A}$ is a *-homomorphism Π from $\mathcal{A}$ into the C*-algebra $\mathcal{L}(\mathcal{H}_\Pi)$ of all *bounded* operators on the complex Hilbert space $\mathcal{H}_\Pi$; it is called nondegenerate, if $\Pi(\mathcal{A})\mathcal{H}_\Pi$ is dense in $\mathcal{H}_\Pi$ [equivalently, $\Pi(\mathbb{1})=\mathbb{1}_\Pi$, whenever $\mathcal{A}$ contains an identity $\mathbb{1}$]. Because of the absence of a norm, there exist *-algebras, which do not admit any nontrivial representation. Especially, certain *-algebras of unbounded operators as, e.g., the *-algebra of the polynomials of the position and momentum operators, $Q=x$, resp., $P=-i(d/dx)$ in $\mathrm{L}^2(\mathbb{R})$, do not possess any nontrivial representation (by bounded operators).

A Gelfand-Naimark-Segal construction $(\Pi_\omega,\mathcal{H}_\omega,\Omega_\omega)$ of a positive linear functional ω on the *-algebra $\mathcal{A}$ is defined as for C*-algebras: $(\Pi_\omega,\mathcal{H}_\omega)$ is a representation of $\mathcal{A}$ and $\Omega_\omega\in\mathcal{H}_\omega$ a cyclic vector [i.e., $\Pi_\omega(\mathcal{A})\Omega_\omega$ is dense in $\mathcal{H}_\omega$], such that $\langle\omega;A\rangle=(\Omega_\omega|\Pi_\omega(A)\Omega_\omega)\forall A\in\mathcal{A}$. Two different GNS representations of a positive linear functional ω are unitarily equivalent.

In the operator algebraic textbooks, e.g. Refs. 62–64; also Ref. 65, the existence of the GNS construction is derived in a way, which requires the norm-completeness of the *-algebra $\mathcal{A}$ (as is the case for Banach *—resp. C*—algebras) to demonstrate the boundedness of the representing operators. Our derivation is based on Ref. 29. It demands $\mathcal{A}$ to be a U*-algebra instead of requiring the mentioned norm-completeness. A U*-algebra $\mathcal{A}$ is a*-algebra with identity $\mathbb{1}$, such that every element of $\mathcal{A}$ is a (finite) linear combination of unitary elements from $\mathcal{A}$ ($U\in\mathcal{A}$ is called unitary, if $UU^*=U^*U=\mathbb{1}$). Especially every Banach *—resp. C*—algebra with an identity is a U*-algebra, and so is the pre-Weyl algebra in Eq. (3.2) below.

Let our *-algebra $\mathcal{A}$ possess an identity $\mathbb{1}$. We obtain an involutive semigroup $(\mathcal{A},J)$ by defining the operation $\circ$ as the algebraic product—implying $\mathbb{1}$ to be the neutral element—and by introducing the involution J as the algebraic *-operation $J(A):=A^*$, $\forall A\in\mathcal{A}$. So the J-involutive group $\mathcal{A}_J$ consists of all unitary elements of $\mathcal{A}$. Put $\Sigma:=1$. Then each positive linear functional $\omega:\mathcal{A}\ni A\mapsto\langle\omega;A\rangle$ is a 1-positive-definite function with associated positive-definite kernel $K_\omega(A,B)=\langle\omega;A^*B\rangle$ for $A, B\in\mathcal{A}$. Whereas the minimal Kolmogorov decomposition exists for every positive linear functional ω on an arbitrary *-algebra (also on those without an identity), a GNS representation of ω may not exist.

Theorem 2-3: *The GNS representation exists for every positive linear functional on a U*-algebra $\mathcal{A}$.*

Proof: ω being a linear form implies the minimal Kolmogorov decomposition $v_\omega:\mathcal{A}\to\mathcal{H}_\omega$ of ω, resp. of the kernel K_ω, to be linear, too. By Theorem 2-1 there exists a unitary representation

Π_ω of the unitary group $\mathcal{A}_J$, which we extend linearly to a representation of the whole U*-algebra $\mathcal{A}$. v being linear yields $\Pi_\omega(A)v_\omega(B)=v_\omega(AB)$ for all $A, B\in\mathcal{A}$, which implies the independence of $\Pi_\omega(A)$ from the linear decomposition of A into unitaries. Finally, set $\Omega_\omega := v_\omega(\mathbb{1})$. ■

The extension from the unitaries to the whole U*-algebra in the above proof fits well to the construction of the Weyl algebra in the next section; see especially Observation 3-2.

III. THE C*-WEYL ALGEBRA

Throughout the present section let (E,σ) be a fixed *pre-symplectic space*, namely a real vector space equipped with an $\mathbb{R}$-bilinear mapping $\sigma: E\times E\to\mathbb{R}$, $(f,g)\mapsto\sigma(f,g)$, which is antisymmetric, i.e., $\sigma(f,f)=0$, $\forall f\in E$ or equivalently, $\sigma(f,g)=-\sigma(g,f)$, $\forall f, g\in E$.

In order to conform with Sec. II A we consider E as a commutative group with the addition $\circ := +$ as the group operation. The involution J is defined as forming the additive inverses $J(f) := -f$, and thus we have $E_J=E$ for the J-involutive group. The antisymmetric bicharacter Σ is chosen as in Eq. (1.8), i.e., as $\Sigma(f,g) := \exp\{-(i/2)\sigma(f,g)\}$. Instead of $\mathcal{C}(E,\Sigma)$ we write $\mathcal{C}(E,\sigma)$ for the set of normalized, σ-positive-definite functions $C: E\to\mathbb{C}$. The nondegeneracy of Σ is equivalent to the nondegeneracy of σ, i.e., $(\sigma(f,g)=0\,\forall f\in E)\Rightarrow g=0$. In our investigation, however, σ may be degenerate, and in Sec. IV we even treat the trivial case of a vanishing pre-symplectic form.

In the Introduction we associated with a pre-symplectic space (E,σ) an abstract Weyl system, which consists of linearly independent Weyl elements $W(f)$, $f\in E$, in a *-algebra, fulfilling the Weyl relations

$$W(f)W(g)=\exp\left\{-\frac{i}{2}\sigma(f,g)\right\}W(f+g),\quad W(f)^*=W(-f),\quad \forall f,g\in E', \tag{3.1}$$

cf. Eq. (1.1). In the present section we search for an appropriate C*-Weyl algebra, which be naturally given, resp. generated, by the abstract Weyl system.

A. Weyl systems as projective group representations

In the Introduction we discriminated conceptually between the abstract Weyl system and its Hilbert space realizations $(W_R,\mathcal{H}_R)$ in terms of unitary operators, the latter simply called *Weyl systems*. Up to now, we did not deal with the existence either of the abstract or of the (Hilbert space) Weyl systems.

In mathematical investigations Weyl systems over (E,σ) are viewed as unitary σ-representations $W_R: E\ni f\mapsto W_R(f)$ of the additive group E on the complex Hilbert space $\mathcal{H}_R$. That means that the operator product of the unitary Weyl operators $W_R(f)\in\mathcal{L}(\mathcal{H}_R)$, $f\in E$, represents, by satisfying the Weyl relations (3.1), the addition of E homomorphically up to a phase factor, given by the bicharacter $\Sigma(f,g)$.

There is the following connection between Weyl systems and σ-positive-definite functions on (E,σ).

Theorem 3-1: *The following assertions are valid.*

(a) *Let $C\in\mathcal{C}(E,\sigma)$ be a σ-positive-definite function. Then there exists a Weyl system $(W_C,\mathcal{H}_C)$ over (E,σ) and a normalized vector $\Omega_C\in\mathcal{H}_C$, such that $\{W_C(f)\Omega_C|f\in E\}$ is total in $\mathcal{H}_C$ and the function C is given by the expectations $C(f)=(\Omega_C|W_C(f)\Omega_C)$ for all $f\in E$.*

(b) *Let $(W_R,\mathcal{H}_R)$ be a Weyl system over (E,σ). Then for every density operator ρ on $\mathcal{H}_R$ (a positive trace class operator with $\mathrm{tr}[\rho]=1$) the mapping $E\ni f\mapsto C_\rho(f) := \mathrm{tr}[\rho W_R(f)]$ is an element of $\mathcal{C}(E,\sigma)$.*

Proof: Part (a) is an application of Theorem 2-1 to the present case with $E_J=E$, where $\Omega_C := v_C(0)$ for the minimal Kolmogorov decomposition $v_C: E\to\mathcal{H}_C$ of C. Part (b): The relation

$C_\rho(0)=1$ is immediate, since $W_R(0)=\mathbb{1}_R$ is the identity on $\mathcal{H}_R$. If $A=\Sigma_{j=1}^n z_j W_R(f_j)$ is an arbitrary linear combination of Weyl operators with different f_j's, then we obtain by the positivity of ρ and by the Weyl relations that

$$0\leqslant \mathrm{tr}[\rho A^*A]=\sum_{i,j=1}^n \overline{z}_i z_j \exp\left\{\frac{i}{2}\sigma(f_i,f_j)\right\}\mathrm{tr}[\rho W_R(f_j-f_i)]$$

$$=\sum_{i,j=1}^n \overline{z}_i z_j \exp\left\{\frac{i}{2}\sigma(f_i,f_j)\right\}C_\rho(f_j-f_i),$$

which is the σ-positive-definiteness of C_ρ. Hence $C_\rho\in\mathcal{C}(E,\sigma)$. ■

Observe, that for a given $C\in\mathcal{C}(E,\sigma)$ the elements of $W_C(E)$, need not be linearly independent.

B. Construction of the Weyl algebra

In order to construct the desired *-algebra for the Weyl relations, we have a need for a mapping W from E into a subset of linearly independent elements of a vector space $\mathcal{F}$. The latter means, of course, that the image $W(E)\subset\mathcal{F}$ consists of linearly independent elements $W(f)\in\mathcal{F}$, $f\in E$.

As a main example one may choose $\mathcal{F}$ as the linear space of all $\mathbb{C}$-valued functions on E and define for every $f\in E$ the element $W(f)$ as the Kronecker delta function $W(f):E\to\mathbb{C}$ satisfying $W(f)[g]=1$ for $g=f$ and $W(f)[g]=0$ for $g\neq f$. The set of these $W(f)$ is clearly linearly independent.

For any linearly independent family $W(E)\subset\mathcal{F}$ we denote by $\Delta(E,\sigma)$ the vector space of all (finite) complex linear combinations of the $W(f)$, $f\in E$,

$$\Delta(E,\sigma):=\mathrm{LH}\{W(f)|f\in E\}. \tag{3.2}$$

Here LH means the complex linear hull, so an arbitrary element of $\Delta(E,\sigma)$ is given by $A=\Sigma_{j=1}^n z_j W(f_j)$ with some $n\in\mathbb{N}$ and $z_j\in\mathbb{C}$ and $f_j\in E$. In the above example $A=\Sigma_{j=1}^n z_j W(f_j)$ is a $\mathbb{C}$-valued function on E with $A[g]=0$ for $g\in\{f_1,\ldots,f_n\}$ and $A[g]=z_j\in\mathbb{C}$ for $g=f_j$, whenever the f_j's are mutually different.

Defining the product and the *-operation as in the Weyl relations in Eq. (3.1) every polynomial of the $W(f)$, now rightly called *Weyl elements*, reduces to a linear combination, which implies that $\Delta(E,\sigma)$ becomes a *-algebra. Obviously, all of the $\Delta(E,\sigma)$ are *-isomorphic to each other and we speak of *the* *-algebra $\Delta(E,\sigma)$ associated with (E,σ). It contains the abstract Weyl system as a sub-family. (Our main example proves now the existence of the abstract Weyl system.)

Moreover, $\Delta(E,\sigma)$ is a U*-algebra, where its identity is given by $\mathbb{1}:=W(0)$ (and not by the unit function in the main example), and every Weyl element $W(f)$ is unitary.

Observation 3-2: Since the Weyl elements $W(f)\in\Delta(E,\sigma)$, $f\in E$, are linearly independent we may identify each $f\in E$ with the associated Weyl element $W(f)$. Thus every function $\Gamma:E\to\mathcal{V}$ from E into a vector space $\mathcal{V}$ extends uniquely to a linear mapping $\Gamma_{ext}:\Delta(E,\sigma)\to\mathcal{V}$ by setting

$$\Gamma_{ext}\left(\sum_{j=1}^n z_j W(f_j)\right):=\sum_{j=1}^n z_j\Gamma(f_j), \tag{3.3}$$

where $n\in\mathbb{N}$ and $z_j\in\mathbb{C}$ and the different $f_j\in E$ are arbitrary. (Note that this extension coincides with the extension from the unitaries $\mathcal{A}_J$ onto the whole U-algebra $\mathcal{A}$ given in the proof of the GNS representation in Theorem 2-3.)*

We use the Observation to extend normalized σ-positive-definite functions and Weyl systems from E to states and representations of the *-algebra $\Delta(E,\sigma)$.

Lemma 3-3: The following assertions are valid.

(a) *For each $C\in\mathcal{C}(E,\sigma)$ let ω_C be the linear functional on $\Delta(E,\sigma)$, which is obtained by the linear extension of the prescription $\langle\omega_C;W(f)\rangle:=C(f)$ to all of $\Delta(E,\sigma)$ in terms of Eq. (3.3). Then the mapping $C\mapsto\omega_C$ constitutes an affine bijection from $\mathcal{C}(E,\sigma)$ onto the convex set of all states on the *-algebra $\Delta(E,\sigma)$. (A state ω is a positive linear functional satisfying the normalization condition $\langle\omega;\mathbb{1}\rangle=1$.)*

(b) *Let $(W_R,\mathcal{H}_R)$ be a Weyl system over (E,σ). Then there exists a unique representation $(\Pi_R,\mathcal{H}_R)$ of the *-algebra $\Delta(E,\sigma)$ such that $\Pi_R(W(f))=W_R(f)$ for all $f\in E$. Conversely, every nondegenerate representation $(\Pi,\mathcal{H}_\Pi)$ of $\Delta(E,\sigma)$ induces a Weyl system $(W_\Pi,\mathcal{H}_\Pi)$ via $W_\Pi(f):=\Pi(W(f))$ for all $f\in E$.*

(c) *Let $C\in\mathcal{C}(E,\sigma)$ with associated Weyl system $(W_C,\mathcal{H}_C)$ over (E,σ) and normalized vector $\Omega_C\in\mathcal{H}_C$ according to Theorem 3-1(a). Furthermore, let ω_C and the representation $(\Pi_C,\mathcal{H}_C)$ of $\Delta(E,\sigma)$ be determined as described in the parts (a) and (b). Then $(\Pi_C,\mathcal{H}_C,\Omega_C)$ is the GNS representation of the state ω_C on $\Delta(E,\sigma)$.* [*Note that $\Delta(E,\sigma)$ is a U*-algebra, and thus every state admits a GNS representation by Theorem 2-3.*]

Proof: (a) The positivity of the so defined linear form ω_C follows from the σ-positive-definiteness of $C\in\mathcal{C}(E,\sigma)$ and the Weyl relations with

$$\langle\omega_C;A^*A\rangle=\sum_{i,j=1}^{n}\bar{z}_i z_j\exp\left\{\frac{i}{2}\sigma(f_i,f_j)\right\}C(f_j-f_i)\geqslant 0,\quad A:=\sum_{j=1}^{n}z_j W(f_j). \tag{3.4}$$

And the normalization is given by $\langle\omega_C;\mathbb{1}\rangle=\langle\omega_C;W(0)\rangle=C(0)=1$. Conversely, if ω is a state on $\Delta(E,\sigma)$, then as in (3.4) the σ-positive-definiteness of $E\ni f\mapsto\langle\omega;W(f)\rangle$ is derived.

With the extension (3.3) the parts (b) and (c) are immediate. ■

A simple example $C_{\mathrm{tr}}\in\mathcal{C}(E,\sigma)$ is given by $C_{\mathrm{tr}}(0):=1$ and $C_{\mathrm{tr}}(f):=0$ for $0\neq f\in E$, defined at the end of Sec. II B. It is immediately checked that the minimal Kolmogorov decomposition of C_{tr} is determined to be $v_{\mathrm{tr}}:E\to 1^2(E)$ with $v_{\mathrm{tr}}(f)[g]=1$ for $f=g$ and $v_{\mathrm{tr}}(f)[g]=0$ for $f\neq g$. Here $1^2(E)$ is the Hilbert space of square summable sequences over E, i.e., its elements are functions $\phi:E\to\mathbb{C}$, $g\mapsto\phi[g]$ satisfying $\|\phi\|_2^2=\Sigma_{g\in E}|\phi[g]|^2<\infty$. According to Theorem 2-1 the associated Weyl system W_{tr} acts on $1^2(E)$ as the projective shifts,

$$(W_{\mathrm{tr}}(f)\phi)[g]=\exp\left\{-\frac{i}{2}\sigma(f,g)\right\}\phi[g-f],\quad \forall g\in E,\quad \phi\in 1^2(E).$$

The state ω_{tr} associated to C_{tr} satisfies

$$\langle\omega_{\mathrm{tr}};AB\rangle=\langle\omega_{\mathrm{tr}};BA\rangle,\quad \forall A,B\in\Delta(E,\sigma), \tag{3.5}$$

hence it is a tracial state on $\Delta(E,\sigma)$. Note, in case of a nondegenerate σ it follows from the Weyl relations that ω_{tr} is the only tracial state. If $A:=\Sigma_{j=1}^{n}z_j W(f_j)$ is an arbitrary element of $\Delta(E,\sigma)$ with different f_j's, then

$$\langle\omega_{\mathrm{tr}};A^*A\rangle=\sum_{j=1}^{n}|z_j|^2. \tag{3.6}$$

The tracial state ω_{tr} is the only state which is invariant under all gauge transformations γ_χ defined in Sec. III D below. By the proof of Theorem 3-1(a) its GNS representation $(\Pi_{\mathrm{tr}},1^2(E),\Omega_{\mathrm{tr}})$ has the cyclic vector $\Omega_{\mathrm{tr}}=v_{\mathrm{tr}}(0)$, where $\Pi_{\mathrm{tr}}(W(f))=W_{\mathrm{tr}}(f)$, $\forall f\in E$.

For an arbitrary representation $(\Pi,\mathcal{H}_\Pi)$ of $\Delta(E,\sigma)$ define the representation $(\tilde{\Pi},\tilde{\mathcal{H}}_\Pi)$ by

$$(\tilde{\Pi}(W(f))\psi)[g]=W_\Pi(f)\psi[g-f],\quad \forall g\in E,\quad \psi\in\tilde{\mathcal{H}}_\Pi, \tag{3.7}$$

on the Hilbert space $\tilde{\mathcal{H}}_\Pi := 1^2(E,\mathcal{H}_\Pi) = \mathcal{H}_\Pi \otimes 1^2(E)$. Here the representation $\Pi_{\rm tr}$ is interesting in so far as the fact that the representation $\tilde{\Pi}$ is quasi-equivalent to $\Pi_{\rm tr}$. Exactly, by direct computation one immediately verifies that

$$U_\Pi \tilde{\Pi}(A) U_\Pi^* = \mathbb{1}_\Pi \otimes \Pi_{\rm tr}(A), \quad \forall A \in \Delta(E,\sigma),$$

with the unitary U_Π on $\mathcal{H}_{\tilde{\Pi}}$ defined by $(U_\Pi \psi)[g] = W_\Pi(-g)\psi[g] \forall g \in E$. Consequently,

$$\|\Pi(A)\| \leqslant \|\tilde{\Pi}(A)\| = \|\Pi_{\rm tr}(A)\|, \quad \forall A \in \Delta(E,\sigma), \tag{3.8}$$

where the inequality sign is a direct consequence of the definition of $\tilde{\Pi}$ in (3.7).

A (vector space) norm $\|\cdot\|$ is called a *-algebra norm, if the product and the *-operation are norm-continuous, i.e., $\|AB\| \leqslant \|A\|\|B\|$ and $\|A^*\| = \|A\|$. If in addition the *-algebra norm $\|\cdot\|$ satisfies the C*-norm property $\|A^*A\| = \|A\|^2$ for all $A \in \Delta(E,\sigma)$, then it is called a *C*-norm*.

We now introduce a C*-norm on $\Delta(E,\sigma)$. Two further norms on $\Delta(E,\sigma)$ are given in Sec. III E.

Proposition 3-4 (C*-norm)*: The mapping,*

$$\Delta(E,\sigma) \ni A \mapsto \|A\| := \sup\{\sqrt{\langle \omega_C ; A^*A\rangle} \,|\, C \in \mathcal{C}(E,\sigma)\}, \tag{3.9}$$

defines a C-norm on the *-algebra $\Delta(E,\sigma)$. It may also be expressed as*

$$\|A\| = \sup\{\|\Pi_R(A)\| \,|\, \textit{all Weyl systems } (W_R,\mathcal{H}_R) \textit{ over } (E,\sigma)\}, \quad \forall A \in \Delta(E,\sigma). \tag{3.10}$$

Moreover, $\|\cdot\|$ is the unique C-norm on $\Delta(E,\sigma)$, such that every representation Π of $\Delta(E,\sigma)$ is $\|\cdot\|$-continuous, i.e., $\|\Pi(A)\| \leqslant \|A\|$, $\forall A \in \Delta(E,\sigma)$.*

Proof: Let $(W_R,\mathcal{H}_R)$ be a Weyl system over (E,σ). Theorem 3-1(b) yields that for every normalized $\psi \in \mathcal{H}_R$ the mapping $E \ni f \mapsto (\psi|W_R(f)\psi) =: C_R^\psi(f)$ is an element of $\mathcal{C}(E,\sigma)$. Hence,

$$\begin{aligned}\|\Pi_R(A)\| &= \sup\{\|\Pi_R(A)\psi\| \,|\, \psi \in \mathcal{H}_R, \|\psi\| = 1\} \\ &= \sup\{\sqrt{(\psi|\Pi_R(A^*A)\psi)} \,|\, \psi \in \mathcal{H}_R, \|\psi\| = 1\} = \sup\{\sqrt{\langle \omega_{C_R^\psi}; A^*A\rangle} \,|\, \psi \in \mathcal{H}_R, \|\psi\| = 1\}.\end{aligned}$$

Consequently, Eq. (3.10) follows from Theorem 3-1(a), ensuring that $A \mapsto \|A\|$ is a semi-norm. Since $\|A\|^2 \geqslant \langle \omega_{\rm tr}; A^*A\rangle$ it follows from Eq. (3.6) that $\|A\| = 0$, if and only if $A = 0$, i.e., the strict positivity of $\|\cdot\|$. So, $\|\cdot\|$ being indeed a C*-norm is a consequence of the C*-norm property of the norms on the bounded operators on Hilbert spaces. It follows from Eq. (3.10) and Lemma 3-3(b) that every representation Π of $\Delta(E,\sigma)$ satisfies $\|\Pi(A)\| \leqslant \|A\|$ for all $A \in \Delta(E,\sigma)$.

Suppose a further C*-norm $\|\cdot\|'$ on $\Delta(E,\sigma)$ exists, such that every representation Π of $\Delta(E,\sigma)$ is $\|\cdot\|'$-continuous. Π extends continuously to the $\|\cdot\|'$-completion, and thus $\|\Pi(A)\| \leqslant \|A\|'$ by a standard result, e.g., Ref. 62, Lemma 2.3.1. Let Π be a faithful representation of the $\|\cdot\|'$-completion (the existence of faithful representations of a C*-algebra is also a standard result, e.g., Ref. 62, Theorem 2.1.10), then $\|\Pi(A)\| = \|A\|'$ for all $A \in \Delta(E,\sigma)$. By our above construction we in have in addition $\|\Pi(A)\| \leqslant \|A\|$. Hence $\|A\|' \leqslant \|A\|$ for all $A \in \Delta(E,\sigma)$. Interchanging the roles of $\|\cdot\|$ and $\|\cdot\|'$ yields $\|\cdot\| = \|\cdot\|'$. ■

A further uniqueness characterization of the C*-norm on $\Delta(E,\sigma)$ is given in Corollary 3-11 below.

By the above result every representation of the *-algebra $\Delta(E,\sigma)$ extends continuously to its $\|\cdot\|$-completion,

$$\mathcal{W}(E,\sigma) := \overline{\Delta(E,\sigma)} \tag{3.11}$$

(the overbar indicates the $\|\cdot\|$-completion). The C*-algebra $\mathcal{W}(E,\sigma)$ is called the *Weyl algebra* over the pre-symplectic space (E,σ). In the literature also the notion of CCR algebra is found.

By a $\|\cdot\|$-continuous extension, especially of the GNS representations and thus of the states, we obtain immediately the following characterization of the state space of the Weyl algebra.

Theorem 3-5 (state space): *The map $C\mapsto\omega_C$ is an affine homeomorphism from $\mathcal{C}(E,\sigma)$ onto the state space $\mathcal{S}(\mathcal{W}(E,\sigma))$ of $\mathcal{W}(E,\sigma)$, where on $\mathcal{C}(E,\sigma)$ it is considered the topology of pointwise convergence and on $\mathcal{S}(\mathcal{W}(E,\sigma))$ the weak *-topology.*

If E_0 is a subspace of E—the restriction of σ from E to E_0 is also denoted by σ—then the question arises as to how the associated Weyl algebras $\mathcal{W}(E_0,\sigma)$ and $\mathcal{W}(E,\sigma)$ are related to each other. We may do the same construction for $\Delta(E_0,\sigma)$ as above. $\Delta(E_0,\sigma)$ may be regarded as a sub-*-algebra of $\Delta(E,\sigma)$, when identifying the Weyl elements $W(f)\in\Delta(E_0,\sigma)$ with the associated Weyl elements $W(f)\in\Delta(E,\sigma)$ for each $f\in E_0$ [in our main example, where the Weyl elements are Kronecker functions, every $A\in\Delta(E_0,\sigma)$ is a $\mathbb{C}$-valued function on E_0, which extends trivially to a function on E by putting $A[g]=0$ for $g\in E\backslash E_0$]. Because of Proposition 2-2 the definition (3.9) leads to the same C*-norm on the *-algebra $\Delta(E_0,\sigma)$ as the C*-norm arising by a restriction of the C*-norm on $\Delta(E,\sigma)$,

$$\|A\|=\sup\{\sqrt{\langle\omega_{C'};A^*A\rangle}\,|\,C'\in\mathcal{C}(E_0,\sigma)\}=\sup\{\sqrt{\langle\omega_C;A^*A\rangle}\,|\,C\in\mathcal{C}(E,\sigma)\},\quad A\in\Delta(E_0,\sigma).$$

Consequently, $\mathcal{W}(E_0,\sigma)=\overline{\Delta(E_0,\sigma)}$ is a sub-C*-algebra of $\overline{\Delta(E,\sigma)}=\mathcal{W}(E,\sigma)$. If the inclusion $E_0\subset E$ is proper, then Eq. (3.6) yields that $\|A-W(f)\|\geqslant 1$ for all $A\in\mathcal{W}(E_0,\sigma)$ and $f\in E\backslash E_0$. Thus, $\mathcal{W}(E_0,\sigma)=\mathcal{W}(E,\sigma)$, if and only if $E_0=E$.

Corollary 3-6: The tracial state $\omega_{tr}\in\mathcal{S}(\mathcal{W}(E,\sigma))$ is faithful, i.e., $\langle\omega_{tr};A^*A\rangle\neq 0$ for all $A\in\mathcal{W}(E,\sigma)\backslash\{0\}$.

Proof: Because of (3.5) we have that $\{A\,|\,\langle\omega_{\rm tr};A^*A\rangle=0\}$ is a closed *-ideal of $\mathcal{W}(E,\sigma)$ (e.g., Ref. 63, Lemma I.9.6]), which is easily identified to coincide with the kernel of the GNS representation $\Pi_{\rm tr}$. But Eq. (3.8) yields that $\|\Pi(A)\|\leqslant\|\Pi_{\rm tr}(A)\|\forall A\in\mathcal{W}(E,\sigma)$ for every representation Π. Hence $\Pi_{\rm tr}$ is a faithful representation of $\mathcal{W}(E,\sigma)$, or equivalently, $\ker(\Pi_{\rm tr})=\{0\}$. ■

C. Uniqueness of the Weyl algebra

The previous construction demonstrates the existence of the C*-Weyl algebra $\mathcal{W}(E,\sigma)$. The next result characterizes its uniqueness in the desired sense, namely, that every Weyl system arises from one of its representations. Observe that in the assumptions the linear independence of the Weyl elements is replaced by the weaker condition that the elements $W(f)$ all be nonzero.

Theorem 3-7 (uniqueness): *$\mathcal{W}(E,\sigma)$ is the unique C*-algebra (up to *-isomorphy) generated by nonzero elements $W(f)$, $f\in E$, satisfying the following two assumptions:*

(U1) The elements $W(f)$, $f\in E$, fulfill the Weyl relations, Eq. (3.1).

(U2) Every Weyl system $(W_R,\mathcal{H}_R)$ over (E,σ) arises from a representation $(\Pi_R,\mathcal{H}_R)$ of $\mathcal{W}(E,\sigma)$ with $W_R(f)=\Pi_R(W(f))$ for all $f\in E$ (a relation which characterizes the representation Π_R uniquely).

Proof: The fact the Weyl algebra $\mathcal{W}(E,\sigma)$ from Eq. (3.11) satisfies the relations (U1) and (U2) has already been established. So let us demonstrate its uniqueness.

Suppose there exists a further C*-algebra $\mathcal{W}'(E,\sigma)$ with norm $\|\cdot\|'$ generated by nonzero elements $W'(f)$, $f\in E$, satisfying the assumptions (U1) and (U2). We show the linear independence of the $W'(f)$, $f\in E$. Consider the Weyl system $(W_{\rm tr},\mathcal{H}_{\rm tr})$ with normalized vector $\Omega_{\rm tr}\in\mathcal{H}_{\rm tr}$, such that $C_{\rm tr}(f)=(\Omega_{\rm tr}|W_{\rm tr}(f)\Omega_{\rm tr})$, $\forall f\in E$, which corresponds to the tracial $C_{\rm tr}\in\mathcal{C}(E,\sigma)$ according to Theorem 3-1(a). Then by assumption (U2) there exists a representation $(\Pi_{\rm tr},\mathcal{H}_{\rm tr})$ of $\mathcal{W}'(E,\sigma)$ with $W_{\rm tr}(f)=\Pi_{\rm tr}(W'(f))$. But we then have for $B:=\sum_{j=1}^n z_jW'(f_j)$ with different f_j's that

$$\|B\|'^2\geqslant\|\Pi_{\rm tr}(B)\|^2\geqslant(\Omega_{\rm tr}|\Pi_{\rm tr}(B^*B)\Omega_{\rm tr})=\sum_{i,j=1}^n\overline{z}_iz_j\exp\left\{\frac{i}{2}\sigma(f_i,f_j)\right\}C_{\rm tr}(f_j-f_i)=\sum_{j=1}^n|z_j|^2.$$

Hence $B=0$, if and only if $z_j=0$ for all $j=1,...,n$, expressing the linear independence.

The linear independence of the $W'(f)$, $f\in E$, implies the linear extensibility of the mapping $W(f)\mapsto W'(f)$, $\forall f\in E$ to a *-isomorphism from $\Delta(E,\sigma)$ onto the *-algebra $\mathrm{LH}\{W'(f)|f\in E\}$, so we may incorporate the norm $\|\cdot\|'$ also into $\Delta(E,\sigma)$ by setting $\|\Sigma_j z_j W(f_j)\|' := \|\Sigma_j z_j W'(f_j)\|'$. The $\|\cdot\|$-completion of $\Delta(E,\sigma)$ gives $\mathcal{W}(E,\sigma)$, and its $\|\cdot\|'$-completion gives $\mathcal{W}'(E,\sigma)$ up to an *-isomorphism. By assumption (U2) we now have two norms on $\Delta(E,\sigma)$, such that for both of which every Weyl system arises from a *continuous* representation of the *-algebra $\Delta(E,\sigma)$. The one-to-one correspondence between Weyl systems and nondegenerate representations from Lemma 3-3(b) implies that every representation of $\Delta(E,\sigma)$ is continuous with respect to both of the norms. By Proposition 3-4 the two norms must then coincide. ■

Let us communicate some additional results from the literature.

(a) The Weyl algebra $\mathcal{W}(E,\sigma)$ is simple, if and only if σ is nondegenerate. (It is shown in Ref. 28, resp., in the proof of Ref. 23, Theorem 5.2.8 that one has equality in Eq. (3.8), i.e., $\|\Pi(A)\|=\|\tilde{\Pi}(A)\|=\|\Pi_{\mathrm{tr}}(A)\|$, $\forall A\in\Delta(E,\sigma)$ for every representation Π of $\Delta(E,\sigma)$, if and only if σ is nondegenerate. The essential point is that the characters $f\mapsto\exp\{i\sigma(g,f)\}$, $g\in E$, are dense in the character group $\hat{E}$ of E for nondegenerate σ, only, by Lemma 4-2 [then the locally convex topology on E arising from the semi-norms $f\mapsto|\sigma(g,f)|$, $g\in E$, is Hausdorff].) Consequently, in case of a nondegenerate σ for the uniqueness of $\mathcal{W}(E,\sigma)$ in Theorem 3-7 it suffices that assumption (U1) is valid, and so the second uniqueness condition (U2) is necessary for the degenerate case, only.
(b) The C*-Weyl algebra $\mathcal{W}(E,\sigma)$ is not separable for $E\neq\{0\}$.
(c) A detailed analysis of the closed *-ideals of $\mathcal{W}(E,\sigma)$ (the kernels of representations), resp., of C*-norms on $\Delta(E,\sigma)$ is given in Ref. 34.

We finally present an easy example, which illustrates that for degenerate σ the Weyl algebra $\mathcal{W}(E,\sigma)$ cannot be simple. The degeneracy of σ is equivalent to a nontrivial null space $\ker_\sigma$, the latter being defined in Eq. (1.7). Then the symplectic form $\tilde{\sigma}$ on the quotient $\tilde{E}:=E/\ker_\sigma$ defined by $\tilde{\sigma}(\tilde{f},\tilde{g}):=\sigma(f,g)$ is nondegenerate ($\tilde{f}$ denotes the equivalence class containing f). Since $\mathcal{W}(\tilde{E},\tilde{\sigma})$ is simple, every nondegenerate representation $(\tilde{\Pi},\mathcal{H}_\Pi)$ is faithful. But $W_\Pi(f):=\tilde{\Pi}(\tilde{W}(\tilde{f}))$, $f\in E$, defines a Weyl system $(W_\Pi,\mathcal{H}_\Pi)$ over the original degenerate pre-symplectic space (E,σ) [the Weyl elements of $\mathcal{W}(\tilde{E},\tilde{\sigma})$ are denoted by $\tilde{W}(\tilde{f})$]. Hence by the above Theorem there exists a unique representation $(\Pi,\mathcal{H}_\Pi)$ of $\mathcal{W}(E,\sigma)$ with $W_\Pi(f)=\Pi(W(f))$ for each $f\in E$. It follows that

$$\Pi(W(f))=\Pi(W(g)),\ \text{but}\ \|W(f)-W(g)\|=2,\quad \text{for}\ 0\neq f-g\in\ker_\sigma$$

(the latter follows from Proposition 3-10 below). It holds $\Pi(\mathcal{W}(\ker_\sigma,0))=\mathbb{C}\mathbb{1}_\Pi$ for the commutative (σ vanishes on $\ker_\sigma$) sub-C*-Weyl algebra $\mathcal{W}(\ker_\sigma,0)$ of $\mathcal{W}(E,\sigma)$. Whereas the abstract Weyl elements $W(f)$, $f\in E$, are linearly independent, the represented Weyl operators $\Pi(W(f))=W_\Pi(f)$, $f\in E$, become linearly dependent.

D. Gauge and Bogoliubov *-automorphisms

For states and representations the continuous extension from $\Delta(E,\sigma)$ to its completion $\mathcal{W}(E,\sigma)$ has been already discussed. Here we consider *-isomorphisms, resp. *-anti-isomorphisms, in terms of such an extension.

*Proposition 3-8: Let $(\tilde{E},\tilde{\sigma})$ be a further pre-symplectic space, and suppose β to be an *-(anti-)-isomorphism from $\Delta(E,\sigma)$ onto $\Delta(\tilde{E},\tilde{\sigma})$. Then β is an isometry and extends continuously to a unique *-(anti-)isomorphism from $\mathcal{W}(E,\sigma)$ onto $\mathcal{W}(\tilde{E},\tilde{\sigma})$.*

Proof: Let Π be a faithful representation of the C*-Weyl algebra $\mathcal{W}(\tilde{E},\tilde{\sigma})$. Then $\Pi\circ\beta$ is a representation of $\Delta(E,\sigma)$, and thus we have $\|\beta(A)\|=\|(\Pi\circ\beta)(A)\|\leq\|A\|$, $\forall A\in\Delta(E,\sigma)$. The same argumentation for β^{-1} yields $\|\beta^{-1}(B)\|\leq\|B\|$, $\forall B\in\Delta(\tilde{E},\tilde{\sigma})$. Thus $\|\beta(A)\|=\|A\|$, $\forall A\in\Delta(E,\sigma)$. The extension may now be performed, since the algebraic operations are norm-continuous. ■

We specialize the above result to the case $(\tilde{E},\tilde{\sigma})=(E,\sigma)$, that is, to *-automorphisms on $\Delta(E,\sigma)$. The most basic *-automorphisms are the gauge transformations of the second kind and the Bogoliubov transformations, which are going to be treated according to the scheme described above.

Regarding E as an additive group, we denote by $\hat{E}$ the commutative group of all characters on E. For $\chi\in\hat{E}$ the associated gauge transformation of the second kind is the *-automorphism γ_χ on the *-algebra $\Delta(E,\sigma)$ satisfying

$$\gamma_\chi(W(f))=\chi(f)W(f),\quad \forall f\in E, \tag{3.12}$$

which extends continuously to $\mathcal{W}(E,\sigma)$ by Proposition 3-8. It follows that the mapping

$$\hat{E}\ni\chi\mapsto\gamma_\chi\in *\text{-aut}(\mathcal{W}(E,\sigma)) \tag{3.13}$$

is a representation of the commutative group $\hat{E}$ in terms of the group *-aut$(\mathcal{W}(E,\sigma))$ of all *-automorphisms on the Weyl algebra $\mathcal{W}(E,\sigma)$.

A symplectic transformation T on (E,σ) is a bijective $\mathbb{R}$-linear mapping $T:E\to E$ which respects the pre-symplectic form σ, that is,

$$\sigma(f,g)=\sigma(Tf,Tg),\quad \forall f,g\in E. \tag{3.14}$$

The set symp(E,σ) of all symplectic transformations on (E,σ) consitutes a group, where the group operation is given by the usual multiplication for operators. If $\dim_{\mathbb{R}}(E)>1$, then the group symp(E,σ) is noncommutative. The Bogoliubov transformation corresponding to $T\in\text{symp}(E,\sigma)$ is the unique *-automorphism α_T on $\Delta(E,\sigma)$, resp. on $\mathcal{W}(E,\sigma)$, satisfying

$$\alpha_T(W(f))=W(Tf),\quad \forall f\in E. \tag{3.15}$$

We get the following representation of the group symp(E,σ) by *-automorphisms on $\mathcal{W}(E,\sigma)$,

$$\text{symp}(E,\sigma)\ni T\mapsto\alpha_T\in *\text{-aut}(\mathcal{W}(E,\sigma)). \tag{3.16}$$

E. Norm estimates

In addition to the C*-norm $\|\cdot\|$ from Proposition 3-4 we introduce two further norms $\|\cdot\|_1$ and $\|\cdot\|_2$ on the *-algebra $\Delta(E,\sigma)$.

Proposition 3-9 (additional norms)*: Let us define two additional norms on* $\Delta(E,\sigma)$ *by*

$$\|A\|_1:=\sum_{j=1}^{n}|z_j|,\quad \|A\|_2:=\sqrt{\langle\omega_{\text{tr}};A^*A\rangle}=\sqrt{\sum_{j=1}^{n}|z_j|^2},$$

for arbitrary elements $A:=\Sigma_{j=1}^{n}z_jW(f_j)$ *of* $\Delta(E,\sigma)$ *with different* f_j*'s [cf. Eq.* (3.6)*]. Then there hold the inequalities*

$$\|A\|_2\leq\|A\|\leq\|A\|_1,\quad \forall A\in\Delta(E,\sigma). \tag{3.17}$$

$\|\cdot\|_1$ *is an *-algebra norm on the *-algebra* $\Delta(E,\sigma)$*, whereas the product is not* $\|\cdot\|_2$*-continuous.*

Proof: The first inequality sign in (3.17) follows from $\|A\|^2\geq\langle\omega_{\text{tr}};A^*A\rangle$ by the construction in Eq. (3.9). The second inequality sign in Eq. (3.17) follows from $\|W(f)\|=1$. The rest is immediate. ■

Generally the norms $\|\cdot\|_1$, $\|\cdot\|_2$, and the C*-norm $\|\cdot\|$ are different, which we are going to show. Especially, inequality (3.17) implies for $u,v\in\mathbb{C}$ and $f\neq g$ that

$$\sqrt{|u|^2+|v|^2}=\|uW(f)+vW(g)\|_2\leq\|uW(f)+vW(g)\|\leq\|uW(f)+vW(g)\|_1=|u|+|v|.$$

In the literature it is well known that $\|W(f)-W(g)\|=2$, where for its demonstration it suffices that E is an Abelian group. The following Proposition strengthens these results, making use from E being really a vector group.

Proposition 3-10: We have $\|uW(f)+vW(g)\|=\|uW(f)+vW(g)\|_1=|u|+|v|$ *for all* $u, v \in \mathbb{C}$ *and* $f\neq g$. *Further on, for* $B:=\mathbb{1}+W(f)-W(-f)$ *with* $f\neq 0$ *it holds that*

$$\|B\|_2^2=3<\|B\|^2=\|B^*B\|=\|B^*B\|_1=5<\|B\|_1^2=9.$$

Proof: Let $0\neq f\in E$ and put $E_0:=\mathbb{R}f$. Observe that $\sigma|_{\mathbb{R}f}=0$ acts trivially on the one-dimensional subspace $\mathbb{R}f$ of E. Let $z\in\mathbb{C}$. We have $W(f)+z\mathbb{1}\in\Delta(\mathbb{R}f,0)$. For every $x\in\mathbb{R}$ the continuous character $C_x(tf):=\exp\{itx\}$, $\forall t\in\mathbb{R}$ is an element of $\mathcal{C}(\mathbb{R}f,0)$. For all $x\in\mathbb{R}$ we get

$$\begin{aligned}\|W(f)+z\mathbb{1}\|^2 &\geqslant \langle \omega_{C_x};(W(f)+z\mathbb{1})^*(W(f)+z\mathbb{1})\rangle \\ &= 1+|z|^2+2\,\mathrm{Re}(zC_x(-f))=1+|z|^2+2\,\mathrm{Re}(z\exp\{-ix\}).\end{aligned}$$

Now choose $x\in\mathbb{R}$ such that $z\exp\{-ix\}=|z|$. Then we obtain $\|W(f)+z\mathbb{1}\|\geqslant 1+|z|$. Consequently the estimation (3.17) implies $\|W(f)+z\mathbb{1}\|=1+|z|$. For $f\neq g$ the Weyl relations now imply

$$\|W(f)+zW(g)\|=\|W(-g)(W(f)+zW(g))\|=\left\|W(f-g)+z\exp\left\{-\frac{i}{2}\sigma(g,f)\right\}\mathbb{1}\right\|=1+|z|.$$

Moreover, by Corollary 4-4 below we actually have $\|A\|=\sup_{x\in\mathbb{R}}|\langle\omega_{C_x};A\rangle|=\sup_{x\in\mathbb{R}}\sqrt{\langle\omega_{C_x};A^*A\rangle}$ for all $A\in\Delta(\mathbb{R}f,0)$, which finally implies $\|\mathbb{1}+W(f)-W(-f)\|^2=5$. ■

For $j=1,2$ the completion $\overline{\Delta(E,\sigma)}^j$ of $\Delta(E,\sigma)$ with respect to the norm $\|\cdot\|_j$ coincides with the sequence space $\overline{\Delta(E,\sigma)}^j\cong 1^j(E)$, where here the Weyl elements are considered as Kronecker delta functions on E. Because the tracial state ω_{tr} is faithful by Corollary 3-6, it follows from Eq. (3.17) that $\|\cdot\|_2$ extends $\|\cdot\|_1$-, resp. $\|\cdot\|$-continuously, to a norm on the completions $\overline{\Delta(E,\sigma)}^1$ and $\mathcal{W}(E,\sigma)=\overline{\Delta(E,\sigma)}$, respectively (and not only to a semi-norm). Consequently we get the inclusions

$$\Delta(E,\sigma)\subseteq\overline{\Delta(E,\sigma)}^1\subseteq\mathcal{W}(E,\sigma)\subseteq\overline{\Delta(E,\sigma)}^2, \tag{3.18}$$

which, by the above reasoning, are realized in terms of injective, continuous, *-algebraic homomorphisms, with the exception of the last one, which is not product homomorphic. The inclusions are proper for nontrivial E, since the occurring three norms are not equivalent. Observe that the inner product $(\cdot|\cdot)_2$ on the Hilbert space $\overline{\Delta(E,\sigma)}^2$ satisfies $(A|B)_2=\langle\omega_{\mathrm{tr}};A^*B\rangle$ for all $A, B\in\mathcal{W}(E,\sigma)$.

Corollary 3-11: If there exists a further C-norm* $\|\cdot\|'$ *on* $\Delta(E,\sigma)$ *with* $\|A\|_2\leqslant\|A\|'$ *for all* $A\in\Delta(E,\sigma)$, *then* $\|\cdot\|'=\|\cdot\|$.

Proof: Take a faithful representation Π of $\Delta(E,\sigma)$ with respect to the norm $\|\cdot\|'$. Then Π is $\|\cdot\|$-continuous by Proposition 3-4, i.e., $\|A\|_2\leqslant\|A\|'=\|\Pi(A)\|\leqslant\|A\|$. Especially, Π extends $\|\cdot\|$-continuously to all of $\mathcal{W}(E,\sigma)$. So $\|A\|_2\leqslant\|\Pi(A)\|$, $\forall A\in\mathcal{W}(E,\sigma)$ yields $\Pi(A)=0$, if and only if $A=0$. This is the faithfulness of Π, which is equivalent to $\|\Pi(A)\|=\|A\|$. ■

$\overline{\Delta(E,\sigma)}^1$ together with the product and *-operation as in the Weyl relations (3.1) constitutes a Banach-*-algebra, however, its norm $\|\cdot\|_1$ does not satisfy the C*-norm property in virtue of Proposition 3-10.

F. Connection to the twisted group C*-algebra

In order to establish the connection to harmonic analysis of locally compact groups, we regard E as an Abelian group with respect to the addition equipped with the discrete topology. The corresponding Borel sets are all subsets of E. The set of all regular complex Borel measures equipped with a twisted convolution product is a standard Banach-*-algebra, which we denote by

$M(E,\sigma)$ in our case. More precisely, every element B of $M(E,\sigma)$ is of the form $B=\Sigma_k z_k \delta_{f_k}$ with the point measures δ_{f_k} and some $z_k \in \mathbb{C}$. The norm $\|B\|_1=\Sigma_k|z_k|<\infty$ is the total variation norm. Thus $M(E,\sigma)$ coincides with $1^1(E)$, which may also be viewed as the space $L^1(E)$ with respect to the Haar measure, i.e., the counting measure. We introduce in $M(E,\sigma)$ the *-operation $B\mapsto B^*$, given by $B^*(\Lambda)=\overline{B(-\Lambda)}$ for all $B\in M(E,\sigma)$ and for all subsets $\Lambda\subseteq E$, and define an associative product: For B, $C\in M(E,\sigma)$ the twisted convolution is given as

$$BC(\Lambda) := \int_E dB(f) \int_E dC(g) \exp\left\{ -\frac{i}{2}\sigma(f,g)\right\} \Lambda(f+g), \quad \forall \Lambda \subseteq E, \tag{3.19}$$

where $E \ni f \mapsto \Lambda(f)$ means the characteristic function of the set Λ, [i.e., $\Lambda(f)=1$ for $f\in\Lambda$ and $\Lambda(f)=0$ elsewhere]. The Banach-*-algebra $M(E,\sigma)$, which possesses the identity δ_0 is called the *twisted algebra* of the discrete additive group E with respect to the multiplier from Eq. (1.8).[64] For the point measures one obtains a projective realization of the Abelian group E (Weyl relations),

$$\delta_f \delta_g = \exp\left\{ -\frac{i}{2}\sigma(f,g)\right\} \delta_{f+g}, \quad \delta_f^* = \delta_{-f}, \quad \forall f,g \in E. \tag{3.20}$$

The twisted group C*-algebra is defined as the enveloping C*-algebra of the twisted group Banach-*-algebra $M(E,\sigma)$, that is the completion of $M(E,\sigma)$ with respect to the C*-norm,

$$\|B\| := \sup\{\|\Pi(B)\| | \Pi \text{ representation of } M(E,\sigma)\}, \quad B\in M(E,\sigma), \tag{3.21}$$

which resembles the construction in Eq. (3.10). That this definition provides indeed a norm follows from the fact that there exists a faithful representation. Hence the representations of $M(E,\sigma)$ and those of its enveloping C*-algebra are in one-to-one correspondence given by continuous extension, resp., restriction (see, e.g., Ref. 63, Sect. I.9; Ref. 66, Sect. 7.1).

Collecting our notions we get the following connection with the previous subsections.

Corollary 3-12: The mapping $W(f)\leftrightarrow \delta_f$, $\forall f\in E$ *defines a unique isometric *-isomorphism between the Banach-*-algebras* $\Delta(E,\sigma)^1$ *and* $M(E,\sigma)$, *which extends continuously to an *-isomorphism between the C*-Weyl algebra* $\mathcal{W}(E,\sigma)$ *and the enveloping C*-algebra of* $M(E,\sigma)$.

IV. THE COMMUTATIVE WEYL ALGEBRA AND ALMOST PERIODIC COMPACTIFICATIONS

Throughout the present section suppose E to be a fixed, arbitrary, real vector space.

A. Spectrum of the commutative C*-Weyl algebra

Let us specialize the construction of the C*-Weyl algebra from Sect. III to the case of the trivial pre-symplectic form $\sigma=0$ on E. Then we obtain the commutative C*-Weyl algebra $\mathcal{W}(E,0)$, which is uniquely (in the sense of Theorem 3-7) generated by nonzero Weyl elements $W(f)$, $f\in E$, satisfying the commutative Weyl relations [cf. Eq. (3.1)]

$$W(f)W(g)=W(f+g), \quad W(f)^*=W(-f), \quad \forall f,g\in E. \tag{4.1}$$

Note, that $\mathcal{C}(E,0)$ is just the convex set of all normalized, positive-definite functions $C:E\to\mathbb{C}$ (e.g., Ref. 67, Eq. 32.1), and $\mathcal{W}(E,0)$ is the group C*-algebra of the discrete vector group E.

For later purposes we determine the spectrum $\Sigma(\mathcal{W}(E,0))$ of the commutative C*-Weyl algebra $\mathcal{W}(E,0)$, which consists of the pure states on $\mathcal{W}(E,0)$ (Ref. 62, Proposition 2.3.27). Since $\mathcal{W}(E,0)$ contains an identity, the spectrum $\Sigma(\mathcal{W}(E,0))$ is a compact subset of the compact state space $\mathcal{S}(\mathcal{W}(E,0))$ (Ref. 63, Sect. 1.3). Since the group $\hat{E}$ of all characters on E is a subset of $\mathcal{C}(E,0)$, it follows from Theorem 3-5 that for each character $\chi\in\hat{E}$ there exists a unique state ω_χ on $\mathcal{W}(E,0)$.

Proposition 4-1: It holds that $\Sigma(\mathcal{W}(E,0))=\{\omega_\chi|\chi\in\hat{E}\}$.

Proof: Since $\Sigma(\mathcal{W}(E,0))\subset\mathcal{S}(\mathcal{W}(E,0))$ every element of the spectrum $\Sigma(\mathcal{W}(E,0))$ is of the type ω_C with some $C\in\mathcal{C}(E,0)$ by Theorem 3-5. By definition of the spectrum (Ref. 62, Definition 2.3.25) we have $\langle\omega_C;AB\rangle=\langle\omega_C;A\rangle\langle\omega_C;B\rangle$ for all A, $B\in\mathcal{W}(E,0)$. Especially, with the Weyl relations (4.1) we conclude that

$$C(f+g)=\langle\omega_C;W(f+g)\rangle=\langle\omega_C;W(f)W(g)\rangle=\langle\omega_C;W(f)\rangle\langle\omega_C;W(g)\rangle=C(f)C(g),$$

for all f, $g\in E$, which implies that C is a character on E. Conversely, if $\chi\in\hat{E}\subseteq\mathcal{C}(E,0)$ is a character on E, then the corresponding state ω_χ satisfies

$$\langle\omega_\chi;W(f)W(g)\rangle=\langle\omega_\chi;W(f+g)\rangle=\chi(f+g)=\chi(f)\chi(g)=\langle\omega_\chi;W(f)\rangle\langle\omega_\chi;W(g)\rangle,$$

for all f, $g\in E$. Taking linear combinations of the Weyl elements we arrive at $\langle\omega_\chi;AB\rangle=\langle\omega_\chi;A\rangle\langle\omega_\chi;B\rangle$ for all A, $B\in\Delta(E,0)$, which by continuity extends to all A, $B\in\mathcal{W}(E,0)$. Hence $\omega_\chi\in\Sigma(\mathcal{W}(E,0))$. ■

B. Commutative C*-algebra of almost periodic functions

The subsequent commutative *-resp. C*-algebras are algebras of $\mathbb{C}$-valued functions on certain sets Λ (specified below), where the *-algebraic operations are defined pointwise in the usual way:

$$(\psi+z\phi)[\lambda]:=\psi[\lambda]+z\phi[\lambda],\quad(\psi\phi)[\lambda]:=\psi[\lambda]\phi[\lambda],\quad\psi^*[\lambda]:=\overline{\psi[\lambda]},\tag{4.2}$$

for all points $\lambda\in\Lambda$. The identity $\mathbb{1}$ is the constant function $\mathbb{1}[\lambda]=1$, $\forall\lambda\in\Lambda$, and the C*-norm is the sup-norm,

$$\|\psi\|:=\sup\{|\psi[\lambda]||\lambda\in\Lambda\}.\tag{4.3}$$

Let be given a locally convex Hausdorff vector space topology τ on E. On the topological dual of E with respect to τ, denoted by E'_τ, we define for each $f\in E$ the periodic function $\xi(f)$ as the bounded $\sigma(E'_\tau,E)$-continuous mapping,

$$\xi(f):E'_\tau\to\mathbb{C},\quad F\mapsto\exp\{iF(f)\}=:\xi(f)[F],\quad F\in E'_\tau.\tag{4.4}$$

The $\xi(f)$, $f\in E$, are linearly independent (by Hahn-Banach arguments, cf., e.g., Ref. 65, Sec. IV.3). The linear hull $\mathrm{LH}\{\xi(f)|f\in E\}$ is actually a commutative *-algebra, where the product and the *-operation from Eq. (4.2) give a realization of the commutative Weyl relations (4.1),

$$\xi(f)\xi(g)=\xi(f+g),\quad\xi(f)^*=\xi(-f),\quad\forall f,g\in E.$$

Its completion with respect to the sup-norm (4.3) coincides with the commutative C*-algebra $\mathrm{AP}(E'_\tau)$ of the almost periodic, $\sigma(E'_\tau,E)$-continuous, $\mathbb{C}$-valued functions on E'_τ, (Ref. 67, Eqs. 18.2 and 33.26).

In Ref. 59 the Gelfand representation of $\mathrm{AP}(E'_\tau)$ is constructed in terms of the so-called almost periodic compactification aE'_τ of E'_τ: For every $F\in E'_\tau$ the translation T_F is a bounded operator acting on the Banach space $\mathrm{AP}(E'_\tau)$ by $(T_F\psi)[G]:=\psi[G-F]$, $\forall G\in E'_\tau$ for each $\psi\in\mathrm{AP}(E'_\tau)$. (For the Gelfand representation, cf., e.g., Ref. 62, Sect. 2.3.5; Ref. 63, Sect. I.3.) The mapping $F\mapsto T_F$ constitutes a group representation of the additive group E. The closure of the group $\{T_F|F\in E'_\tau\}$ with respect to the strong operator topology leads to a compact commutative group, which is called the almost periodic compactification aE'_τ, and into which the additive group E'_τ is injectively, densely, and continuously embedded via $F\mapsto T_F$. In this sense we consider E'_τ as a dense subgroup of aE'_τ.

Each $\psi \in \mathrm{AP}(E'_\tau)$ extends uniquely to a continuous function on aE'_τ, in which sense $\mathrm{AP}(E'_\tau)$ is *-isomorphic to the C*-algebra $\mathrm{C}(aE'_\tau)$ of the continuous, $\mathbb{C}$-valued functions on the compact group aE'_τ. In the following we identify these two C*-algebras. Note that for finite dimensional E the almost periodic compactification of E'_τ coincides with its Bohr compactification.

C. Continuous functions algebra on the character group

The character group $\hat{E}$ is compact in the so-called Δ-resp. P-topology arising from the discrete topology on E, cf., e.g., Ref. 67, Eqs. 23.13 and 23.15. This topology on $\hat{E}$ coincides with the topology of pointwise convergence.

Similarly to (4.4) we define for each $f \in E$ the bounded continuous evaluation map,

$$\eta(f): \hat{E} \to \mathbb{C}, \quad \chi \mapsto \chi(f) =: \eta(f)[\chi]. \tag{4.5}$$

It suffices to evaluate the $\eta(f)$, $f \in E$, on the τ-continuous characters to prove their linear independence similarly to that of the $\xi(f)$, $f \in E$, [cf. also Lemma 4-2(a)]. Also here the linear hull is actually a commutative *-algebra, where the product and the *-operation from Eq. (4.2) provide the following realization of the commutative Weyl relations (4.1),

$$\eta(f)\,\eta(g) = \eta(f+g), \quad \eta(f)^* = \eta(-f), \quad \forall f,g \in E.$$

The Stone-Weierstrass theorem implies that the completion of the *-algebra $\mathrm{LH}\{\eta(f) | f \in E\}$ with respect to the sup-norm (4.3) coincides with the commutative C*-algebra $\mathrm{C}(\hat{E})$ of all continuous, $\mathbb{C}$-valued functions on the compact set $\hat{E}$.

D. *-Isomorphic commutative algebras

Let us first point out connections between the topological dual E'_τ and the character group $\hat{E}$.

Lemma 4-2: Let our real vector space E be equipped with a locally convex Hausdorff topology τ. The following two assertions are valid:

(a) The mapping $F \mapsto \exp\{iF(\cdot)\}$ is a bijection from E'_τ onto the group $\hat{E}_\tau$ of all τ-continuous characters on the additive group E.

(b) $\hat{E}_\tau$ is dense in $\hat{E}$ with respect to the topology of pointwise convergence.

Proof: Part (a) is well known, e.g., Ref. 68, Sec. IV-1.2, resp., Ref. 67, Eq. 23.32(a). Part (b). $\hat{E}_\tau$ is a subgroup of $\hat{E}$ with the annihilator

$$A(\hat{E}_\tau) = \{f \in E | \chi(f) = 1, \forall \chi \in \hat{E}_\tau\} = \{f \in E | \exp\{iF(f)\} = 1, \forall F \in E'_\tau\}.$$

But by the assumptions on τ and E the Hahn-Banach theorem is valid, and thus there exists for every $0 \neq g \in E$ a $G \in E'_\tau$ with $G(g) = 1$ (cf., e.g., Ref. 65, Corollary IV.3.15). Consequently, $A(\hat{E}_\tau) = \{0\}$. A vanishing annihilator implies $\hat{E}_\tau$ to be dense in $\hat{E}$ with respect to the Δ-topology on $\hat{E}$, Ref. 67, Eq. 23.24. ■

In Theorem 4-5 below the bijection $E'_\tau \ni F \mapsto \exp\{iF(\cdot)\} \in \hat{E}_\tau$ from part (a) of the above lemma is shown to extend continuously to a group isomorphism between the compact groups aE'_τ and $\hat{E}$. For the proof of this result we need, however, the *-isomophic structure of the considered commutative algebras, which is of interest for its own.

Theorem 4-3: *Let the real vector space E be equipped with a locally convex Hausdorff topology τ. There exist unique *-isomorphisms,*

$$\mathcal{W}(E,0) \cong \mathrm{AP}(E'_\tau) \cong \mathrm{C}(\hat{E}),$$

which satisfy $W(f) \leftrightarrow \xi(f) \leftrightarrow \eta(f)$ for all $f \in E$.

Consequently, the C-algebra $\mathrm{AP}(E'_\tau) = \mathrm{C}(aE'_\tau)$ is independent from the chosen locally convex Hausdorff topology τ on E.*

Proof: The elements $\xi(f)$ are linearly independent, as well as the $\eta(f)$, and as the Weyl elements $W(f)$, $f\in E$. Hence the linear extensions of the bijections $W(f)\leftrightarrow\xi(f)\leftrightarrow\eta(f)\forall f\in E$ lead to *-isomorphisms between the commutative *-algebras $\Delta(E,0)$, $\mathrm{LH}\{\xi(f)|f\in E\}$, and $\mathrm{LH}\{\eta(f)|f\in E\}$ (using the fact that every polynomial of the generating elements reduces to a linear combination).

Let us first prove the *-isomorphism $\mathrm{AP}(E'_\tau)\cong\mathrm{C}(\hat{E})$! Since $\hat{E}_\tau\cong E'_\tau$ is dense in $\hat{E}$ by the above lemma, we have for arbitrary linear combinations,

$$\left\|\sum_{j=1}^{n} z_j\eta(f_j)\right\| = \sup_{\chi\in\hat{E}}\left|\sum_{j=1}^{n} z_j\chi(f_j)\right| = \sup_{F\in E'_\tau}\left|\sum_{j=1}^{n} z_j\exp\{iF(f_j)\}\right| = \left\|\sum_{j=1}^{n} z_j\xi(f_j)\right\|,$$

which leads to the *-isomorphism $\mathrm{C}(\hat{E})\cong\mathrm{AP}(E'_\tau)$.

We turn to the *-isomorphism $\mathcal{W}(E,0)\cong\mathrm{C}(\hat{E})$! Denote by β the *-isomorphism from $\Delta(E,0)$ onto $\mathrm{LH}\{\eta(f)|f\in E\}$, given by $\beta(\Sigma_{j=1}^{n}z_jW(f_j))=\Sigma_{j=1}^{n}z_j\eta(f_j)$ for arbitrary $z_j\in\mathbb{C}$, $f_j\in E$, and $n\in\mathbb{N}$. If Π is a faithful representation of $\mathrm{C}(\hat{E})$, then $\Pi\circ\beta$ is a representation of $\Delta(E,0)$. From the last assertion in Proposition 3-4 it follows that $\|\beta(A)\|=\|(\Pi\circ\beta)(A)\|\leqslant\|A\|$ for all $A\in\Delta(E,0)$.

We now show the converse relation $\|\beta(A)\|\geqslant\|A\|$. $\hat{E}$ being compact, the states on the commutative C*-algebra $\mathrm{C}(\hat{E})$ are the probability measures $M_p(\hat{E})$ on $\hat{E}$, i.e., for the state $\mu\in M_p(\hat{E})$ we have the expectations $\langle\mu;B\rangle=\int_{\hat{E}}B\,d\mu$ for all $B\in\mathrm{C}(\hat{E})$ (see, e.g., Ref. 69, Theorem 7.3.5; Ref. 65, Proposition IV.4.1). With Bochner's theorem (Ref. 67, Eq. 33.3) it follows that the Fourier transformation $C_\mu(f):=\int_{\hat{E}}\eta(f)\,d\mu=\langle\mu;\eta(f)\rangle$, $\forall f\in E$ is an affine bijection from $M_p(\hat{E})$ onto $\mathcal{C}(E,0)$. Thus with the construction of the states on $\Delta(E,0)$ from the elements of $\mathcal{C}(E,0)$ given in Lemma 3-3(a) we conclude that $\langle\omega_{C_\mu};A\rangle=\langle\mu;\beta(A)\rangle$ for every $A\in\Delta(E,0)$. Finally with Eq. (3.9) it follows that

$$\|A\|^2=\sup\{\langle\omega_{C_\mu};A^*A\rangle|\mu\in M_p(\hat{E})\}=\sup\{\langle\mu;\beta(A^*A)\rangle|\mu\in M_p(\hat{E})\}\leqslant\|\beta(A)\|^2,$$

for all $A\in\Delta(E,0)$, where we have used $\|\mu\|=1$ in the estimation $\langle\mu;B^*B\rangle\leqslant\|B^*B\|=\|B\|^2$. Hence $\|A\|=\|\beta(A)\|$ for all $A\in\Delta(E,0)$.

The existence of the *-isomorphism $\mathcal{W}(E,0)\cong\mathrm{C}(\hat{E})$ may also be proved without the use of Bochner's theorem, as we are going to show. Restricting the affine homeomorphism $\mathcal{C}(E,0)\ni C\mapsto\omega_C\in\mathcal{S}(\mathcal{W}(E,0))$ in Theorem 3-5 to the subset $\hat{E}\subseteq\mathcal{C}(E,0)$, it follows with Proposition 4.1 that the mapping $\chi\mapsto\omega_\chi$ is a homeomorphism from $\hat{E}$ onto the spectrum $\Sigma(\mathcal{W}(E,0))$ [on $\hat{E}$ we consider the topology of pointwise convergence and on $\Sigma(\mathcal{W}(E,0)]$ the weak *-topology inherited from the dual $\mathcal{W}(E,0)^*$, resp. from the state space $\mathcal{S}(\mathcal{W}(E,0))$. Thus we may identify the commutative C*-algebras $\mathrm{C}(\Sigma(\mathcal{W}(E,0))$ and $\mathrm{C}(\hat{E})$. Consequently the *-isomorphism β from $\mathcal{W}(E,0)$ onto $\mathrm{C}(\hat{E})$ with $\beta(W(f))=\eta(f)$ for all $f\in E$ is nothing other than the Gelfand representation of the commutative C*-algebra $\mathcal{W}(E,0)$. It fulfills $\beta(A)(\chi)=\langle\omega_\chi;A\rangle$ for all $A\in\mathcal{W}(E,0)$ and each $\chi\in\hat{E}$. ■

The above Theorem simplifies the construction of the norm on $\Delta(E,0)$ given in Eq. (3.9).

Corollary 4-4: For the C-norm $\|\cdot\|$ on $\Delta(E,0)$ from Eq.* (3.9) *we have for all $A\in\mathcal{W}(E,0)$ that*

$$\|A\|=\sup\{|\langle\omega_\chi;A\rangle||\chi\in\hat{E}_\tau\cong E'_\tau\}=\sup\{\sqrt{\langle\omega_\chi;A^*A\rangle}|\chi\in\hat{E}_\tau\cong E'_\tau\}. \tag{4.6}$$

E. Universality of almost periodic compactifications

Let Λ be a compact set and $\mathrm{C}(\Lambda)$ the commutative C*-algebra of the continuous, $\mathbb{C}$-valued functions on Λ. It is well known (e.g., Ref. 63, Proposition 1.4.5), that the mapping $\Lambda\ni\lambda\mapsto\delta_\lambda$ defined by the point evaluation $\langle\delta_\lambda;B\rangle:=B[\lambda]$, $\forall B\in\mathrm{C}(\Lambda)$ [$\delta_\lambda\in M_p(\Lambda)$ is the point measure at

$\lambda \in \Lambda]$ is a homeomorphism from Λ onto the spectrum $\Sigma(\mathrm{C}(\Lambda))$ (pure states) of the C*-algebra $\mathrm{C}(\Lambda)$, where on $\Sigma(\mathrm{C}(\Lambda))$ we consider the weak *-topology. Hence the *-isomorphism $\mathrm{AP}(E'_\tau) = \mathrm{C}(aE'_\tau) \cong \mathrm{C}(\hat{E})$ from Theorem 4-3 leads to the following conclusion.

Theorem 4-5: *Let our real vector space E be equipped with a locally convex Hausdorff topology τ. The embedding $E'_\tau \ni F \mapsto \exp\{iF(\cdot)\} \in \hat{E}$ extends continuously to a continuous group isomorphism between the compact groups aE'_τ and $\hat{E}$.*

Consequently, the almost periodic compactification aE'_τ of the dual E'_τ is independent from the chosen locally convex Hausdorff topology τ on E.

Proof: Denote by γ the *-isomorphism from $\mathrm{AP}(E'_\tau) = \mathrm{C}(aE'_\tau)$ onto $\mathrm{C}(\hat{E})$ satisfying $\gamma(\xi(f)) = \eta(f)$ for all $f \in E$ from Theorem 4-3. The (restriction of the) dual mapping γ^* is a homeomorphism from $\Sigma(\mathrm{C}(\hat{E}))$ onto $\Sigma(\mathrm{C}(aE'_\tau))$. Using the homeomorphisms $\Sigma(\mathrm{C}(\hat{E})) \cong \hat{E}$ and $\Sigma(\mathrm{C}(aE'_\tau)) \cong aE'_\tau$, we conclude that the mapping γ^* gives rise to a homeomorphism $\tilde{\gamma}$ from $\hat{E}$ onto aE'_τ.

Now we specify $\tilde{\gamma}$. From Eqs. (4.4) and (4.5) it follows that we have $\xi(f)[F] = \exp\{iF(f)\} = \eta(f)[\exp\{iF(\cdot)\}]$ for all $F \in E'_\tau$, which implies

$$\langle \delta_F ; B \rangle = B[F] = \gamma(B)[\exp\{iF(\cdot)\}] = \langle \delta_{\exp\{iF(\cdot)\}} ; \gamma(B) \rangle = \langle \gamma^*(\delta_{\exp\{iF(\cdot)\}}); B \rangle, \quad \forall F \in E'_\tau,$$

for every $B \in \mathrm{AP}(E'_\tau) = \mathrm{C}(aE'_\tau)$. Equivalently we have $\delta_F = \gamma^*(\delta_{\exp\{iF(\cdot)\}})$ for all $F \in E'_\tau$. Consequently, $\tilde{\gamma}(\exp\{iF(\cdot)\}) = F$ for all $F \in E'_\tau$. Now observe that $\hat{E}_\tau$ is dense in $\hat{E}$ by Lemma 4-2, and that E'_τ is dense in aE'_τ. ■

V. CONCLUSIONS AND OUTLOOK

The preceding treatment of a distinguished C*-Weyl algebra over a general pre-symplectic space (E,σ) decisively takes advantage of the Kolmogorov decomposition for Σ-positive-definite functions on projective involutive semigroups (cf. Sect. II A). In our case, the projective involutive semigroup is the additive group E with the antisymmetric bicharacter $\Sigma(f,g) = \exp\{-i/2\hbar\sigma(f,g)\}$, $f, g \in E$, where we now make explicit Planck's constant $\hbar$, for discussing some physical conclusions.

Each Σ-positive-definite function $C \in \mathcal{C}(E,\hbar\sigma)$, including the nonregular ones, determines a Weyl system $(\mathcal{W}_C, \mathcal{H}_C)$ in the Hilbert space $\mathcal{H}_C$, as well as a norm for each element A in the U*-algebra $\Delta(E,\hbar\sigma)$, given by the linear hull of the abstract Weyl system. The supremum of these norms is the natural C*-norm in $\Delta(E,\hbar\sigma)$. The C*-norm-completion of $\Delta(E,\hbar\sigma)$ leads to the C*-Weyl algebra $\mathcal{W}(E,\hbar\sigma)$, with Weyl elements $W^\hbar(f)$, $f \in E$.

The fundamental symmetries may be treated in complete analogy to Bogoliubov and gauge automorphisms in the case of a nondegenerate symplectic form; cf. Sec. III D. For $\sigma = 0$ our treatment produces a smeared classical field theory over the flat Poisson manifold E'_τ, which in general decomposes into several symplectic leaves. It has a surprising analogy to the procedure of second quantization, especially for the symmetry generators, as will be shown in the forthcoming work.

In $\mathcal{W}(E,\hbar\sigma)$ there are also natural generalizations of L^1- and L^2-norms, which we have analyzed in more detail than in the mentioned literature. Completing $\Delta(E,\hbar\sigma)$ with respect to the L^1-norm leads to a Banach-*-algebra, which is *-isomorphic to the twisted convolution algebra of the discrete finite measures on (E,σ). Let us stress in view of future applications that the presented method, based on Kolmogorov decompositions, is quite generally applicable to discrete Abelian groups with only the exception of Proposition 3-10.

As will be substantiated by subsequent work, it is a powerful technical instrument to have a unique C*-Weyl algebra over $(E,\hbar\sigma)$, for every pre-symplectic space E and for every $\hbar \in \mathbb{R}$. For the classical case $\hbar = 0$, discussed in Sec. IV, the C*-algebraic set up leads in many respects to a fresh point of view. In Ref. 70 we treat the commutative Weyl algebra as the C*-algebra of observables for a classical Hamiltonian field theory, which—similarly to the more familiar quantum case—is formulated in terms of the smeared field formalism. This provides not only a smooth

transition between the quantized and the classical theory but offers also new mathematical and calculational possibilities for dealing with classical fields. This applies especially to Hamiltonian electrodynamics in suitable flat gauges. The Poisson bracket $\{\cdot,\cdot\}$ of the classical field theory is commonly formulated as

$$\{A,B\}[F] := -\sigma(d_F A, d_F B), \quad \forall F \in E'_\tau, \quad A,B \in \mathcal{P},$$

where the constant Poisson tensor field on the flat phase space E'_τ arises from a nontrivial pre-symplectic form σ on the test function space E (cf. also Refs. 71, 72). The Poisson algebra $\mathcal{P}$ consists of suitable differentiable functions $A: E'_\tau \to \mathbb{C}$ on phase space, which constitute a dense set in $\mathrm{AP}(E'_\tau)$.

In this context let us emphasize that the introduction of the quantized observable algebras for a given pre-symplectic space (E,σ) does not, for itself, constitute a quantization of the classical theory. A family of canonical quantizations may be introduced within the frame of the C*-Weyl algebras, however, by associating with the classical algebraic Weyl elements $W^0(f) \in \mathcal{W}(E,0)$, $f \in E$, certain elements $Q_\hbar(W^0(f)) \in \mathcal{W}(E,\hbar\sigma)$. It is a natural—but by no means the only—choice to set $Q_\hbar(W^0(f)) := W^\hbar(f)$, that is, to relate the Weyl elements in $\mathcal{W}(E,\hbar\sigma)$ with the classical Weyl elements, and to extend this mapping in a linear and *-preserving manner. In Ref. 73 this quantization is elaborated in the case of degenerate σ, so that one employs the general C*-Weyl algebras $\mathcal{W}(E,\hbar\sigma)$, $\hbar \in \mathbb{R}$, described in the main text. This form of a Weyl quantization is identified in Ref. 73 as a *strict deformation quantization* in the sense of Refs. 74 and 75 of certain Poisson algebras $(\mathcal{P},\{\cdot,\cdot\})$, which are sub-*-algebras of the commutative Weyl algebra $\mathcal{W}(E,0) \cong \mathrm{AP}(E'_\tau)$. These constructions, conforming with the strategy of algebraic quantum field theory, generalize then the set up of Weaver,[76] who erects over an infinite-dimensional Hilbert space as test function space E, with the nondegenerate $\sigma(\cdot,\cdot) = \mathrm{Im}(\cdot|\cdot)$, a strict deformation quantization by using a special von Neumann algebra.

Considering the set of all Planck parameters $\mathbb{R} \ni \hbar$ simultaneously, one obtains in Ref. 73 a family of the general C*-Weyl algebras $(\mathcal{W}(E,\hbar\sigma))_{\hbar\in\mathbb{R}}$, which can be turned into a certain *continuous field of C*-algebras* in the sense of Ref. 77. In this manner one arrives at a continuous quantization,[75] which exhibits especially strong continuity properties for the classical limit $\hbar \to 0$.

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Algebraic and Dirac–Hestenes spinors and spinor fields

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Almost all presentations of Dirac theory in first or second quantization in physics (and mathematics) textbooks make use of covariant Dirac spinor fields. An exception is the presentation of that theory (first quantization) offered originally by Hestenes and now used by many authors. There, a new concept of spinor field (as a sum of nonhomogeneous even multivectors fields) is used. However, a careful analysis (detailed below) shows that the original Hestenes definition cannot be correct since it conflicts with the meaning of the Fierz identities. In this paper we start a program dedicated to the examination of the mathematical and physical basis for a comprehensive definition of the objects used by Hestenes. In order to do that we give a *preliminary* definition of algebraic spinor fields (ASF) and Dirac–Hestenes spinor fields (DHSF) on Minkowski space–time as some equivalence classes of pairs (Ξ_u, ψ_{Ξ_u}), where Ξ_u is a spinorial frame field and ψ_{Ξ_u} is an appropriate sum of multivectors fields (to be specified below). The necessity of our definitions are shown by a careful analysis of possible formulations of Dirac theory and the meaning of the set of Fierz identities associated with the bilinear covariants (on Minkowski space–time) made with ASF or DHSF. We believe that the present paper clarifies some misunderstandings (past and recent) appearing on the literature of the subject. It will be followed by a sequel paper where definitive definitions of ASF and DHSF are given as appropriate sections of a vector bundle called the *left* spin-Clifford bundle. The bundle formulation is essential in order to be possible to produce a coherent theory for the covariant derivatives of these fields on arbitrary Riemann–Cartan space–times. The present paper contains also Appendixes A–E which exhibits a truly useful collection of results concerning the theory of Clifford algebras (including many tricks of the trade) necessary for the intelligibility of the text. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1757037]

I. INTRODUCTION

Physicists usually make first contact with Dirac spinors and Dirac spinor fields when they study relativistic quantum theory. At that stage they are supposed to have had contact with a good introduction to relativity theory and know the importance of the Lorentz and Poincaré groups. So, they are told that Dirac spinors are elements of a complex four-dimensional space $\mathbb{C}^4$, which are the carrier space of a particular representation of the Lorentz group. They are told that when you do Lorentz transformations Dirac spinors behave in a certain way, which is different from the way vectors and tensors behave under the same transformation. Dirac matrices are introduced as certain matrices on $\mathbb{C}(4)$ satisfying certain anticommutation rules and it is said that they close a particular Clifford algebra, known as Dirac algebra. The next step is to introduce Dirac wave functions. These are mappings, $\Psi: \mathcal{M} \to \mathbb{C}^4$, from Minkowski space–time $\mathcal{M}$ (at that stage often introduced as an affine space) to the space $\mathbb{C}^4$, which must have the structure of a Hilbert space. After that, Dirac equation, which is a first order partial differential equation is introduced for $\Psi(x)$. Physics come into play by interpreting $\Psi(x)$ as the quantum wave function of the electron. Problems with

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this theory are discussed and it is pointed out that the difficulties can only be solved in relativistic quantum theory, where the Dirac spinor field, gains a new status. It is no more simply a mapping $\Psi:\mathcal{M}\rightarrow\mathbb{C}^4$, but a more complicated object [it becomes an operator valued distribution in a given Hilbert space (see, e.g., Ref. 162 for a correct characterization of these objects)] whose expectation values on certain one particle states can be represented by objects like Ψ. From a pragmatic point of view, only this knowledge is more than satisfactory. However, that approach, we believe, is not a satisfactory one to any scientist with an enquiring mind, in particular to one that is worried with the foundations of quantum theory. For such person the first questions which certainly occur are what is the geometrical meaning of the Dirac spinor wave function? From where did this concept come from?

Pure mathematicians, who study the theory of Clifford algebras, e.g., using Chevalley's classical books,[38,39] learn that spinors are elements of certain minimal *ideals* (do not worry if you did not know the meaning of this concept, it is not a difficult one and is introduced in Appendix B) in Clifford algebras. In particular Dirac spinors are the elements of a minimal ideal in a particular Clifford algebra, the Dirac algebra. Of course, the relation of that approach (*algebraic spinors*), with the one learned by physicists (covariant spinors) is known (see, e.g., Refs. 14, 67, and 68), but is not well known by the great majority of physicists, even for many which specialize in general relativity and more advanced theories, like string and *M*-theory.

Now, the fact is that the algebraic spinor concept (algebraic spinor fields on Minkowski space–time will be studied in details in what follows, and in Ref. 126 where the concept is introduced using fiber bundle theory on general Lorentzian manifolds) (as it is the case of the covariant spinor concept) fail to reveal the true geometrical meaning of spinor in general and Dirac spinors in particular.

In 1966, Hestenes[81] introduced a new definition of spinor field, that he called later *operator* spinor field. Objects in this class which in this paper, will be called Dirac–Hestenes spinor fields, have been introduced by Hestenes as mappings $\psi:\mathcal{M}\rightarrow\mathbb{R}^0_{1,3}$, where $\mathbb{R}^0_{1,3}$ is the even subalgebra of $\mathbb{R}_{1,3}$, a particular Clifford algebra, technically known as the *space–time* algebra. [$\mathbb{R}_{1,3}$ is not the original Dirac algebra, which is the Clifford algebra $\mathbb{R}_{4,1}$, but is closely related to it, indeed $\mathbb{R}_{1,3}$ is the even subalgebra of the Dirac algebra (see the Appendix B for details).] Hestenes in a series of remarkable papers[80,82–85,75] applied his new concept of spinor to the study of Dirac theory. He introduced an equation, now known as the Dirac–Hestenes equation, which does *not* contain (explicitly) imaginary numbers and obtained a very clever interpretation of that theory through the study of the geometrical meaning of the so-called bilinear covariants, which are the observables of the theory. He further developed an interpretation of quantum theory from his formalism,[88,89] that he called the *Zitterbewegung* interpretation. Also, he showed how his approach suggests a geometrical link between electromagnetism and the weak interactions, different from the original one of the standard model.[87]

Hestenes papers and his book with Sobczyk[86] have been the inspiration for a series of international conferences on *"Clifford Algebras and their Applications in Mathematical Physics"* which in 2002 has had its sixth edition. A consultation of the table of contents of the last two conferences[1,145,2] certainly will show that Clifford algebras and their applications generated a wider interest among many physicists, mathematicians, and even in engineering and computer sciences. (In what follows we quote some of the principal papers that we have had opportunity to study. We apologize to any author who thinks that his work is a worthy one concerning the subject and is not quoted in the present paper.) Physicists used Clifford algebras concepts and Hestenes methods, in many different applications. As some examples, we quote some developments in relativistic quantum theory as, e.g., Refs. 36, 37, 45, 46, 48–52, 56, 58, 74, and 70. The papers by De Leo and collaborators exhibit a close relationship between Hestenes methods and quaternionic quantum mechanics, as developed, e.g., by Adler,[4] a subject that is finding a renewed interest. Also, Clifford algebra methods have been used[102,135,149,151,152,165–168] to give an intuitive and geometrical clear picture of the dynamics of superparticles.[3,11,12,140,143,153,160,163] Also, that papers clarify the meaning of Grassmann variables and their calculus.[17] The relation with the *Zitterbewegung* model of Barut and collaborators[8–10] appears in a novel and less speculative way. Even

more, in Ref. 151 it is shown that the concept of Dirac–Hestenes spinor field is closely related to the concepts of superfields as introduced by Witten.[169] Clifford algebras methods have also been used in disclosing a surprising connection between the Dirac and Maxwell and Seiberg–Witten[159] equations, as studied, e.g., in Refs. 155, 164, and 168, which suggest several physical developments. Applications of Clifford algebras methods in general relativity appeared also, e.g., in Refs. 35, 90, 54, 55, 57, 58, 62, 103–105, 119, 134, and 154, and suggest new ways for looking to the gravitational field. Clifford algebras methods, have been applied successfully also in quantum field theory, as, e.g., in Refs. 60 and 138 and more recently in string and p-brane theories, with noticeable results[25–34,136,137] which are worth being more carefully investigated.

Of course, Clifford algebras and Dirac operators are standard topics of research in Mathematics (see, e.g., Ref. 20), but we must say that Hestenes ideas have been an inspiring idea for mathematicians also. In particular, the concept of Clifford valued functions with domain in a manifold (the operator spinor fields are particular functions of this type) developed in a new, beautiful and powerful branch of mathematics.[47] Hestenes ideas, as we said, have found also their use in engineering and computer sciences, as in the study of neural circuits[91,92] and robotics and perception action systems.[18,19,99,100,42,59,101,125,161]

Having made all this propaganda, which we hope have awakened the reader's interest in studying Clifford algebras, we must remark, that (as often happens for every pioneer work) the concept of Dirac–Hestenes spinor field, as originally introduced by Hestenes, and used by many other researchers, is not a concept free of criticisms and objections from the mathematical point of view.

However, it is an important concept and one of the objectives of this paper and also of Ref. 126 is to give a presentation of the subject free of all previous criticisms, which are discussed in the next sections. The reader may ask if the enterprising for learning the theory presented below is worth the time. We think that the answer is yes, whether it be a physicist or mathematician. To encourage physicists, which may eventually become interested in the subject after reading the above propaganda, we say that the mathematical tools used, even if they may look complex at first sight, are indeed nothing more than easy additions to the contents of a linear algebra course. The main reward to someone that studies what follows is that they will start seeing some subjects that they thought were well known, under a new and (we believe) illuminating point of view. This hopefully may help anyone who is searching for new physical theories. For mathematicians, we say that the point of view developed here is somewhat new in relation to the original Chevalley's one and we believe, it is more satisfactory. In particular, the present paper serves as a preliminary step towards a rigorous theory of algebraic and Dirac–Hestenes spinor fields as sections of some well-defined fiber bundles, and the theory of the covariant derivatives of these fields. Having said all that, what is the present paper about?

We give definitions of algebraic spinor fields (ASF) and Dirac–Hestenes spinor fields (DHSF) living on Minkowski space–time and show how Dirac theory can be formulated in terms of these objects. [Minkowski space–time is parallelizable and as such admits a spin structure. In general, a spin structure does not exist for an arbitrary manifold equipped with a metric of signature (p,q). The conditions for existence of a spin structure in a general manifold are discussed in Refs. 93, 131, and 133. For the case of Lorentzian manifolds, see Ref. 72.] We start our presentation in Sec. II by studying a not-well-known subject, namely, the geometrical equivalence of representation modules of simple Clifford algebras $\mathcal{C}\ell(V,\mathbf{g})$. This concept, together with the concept of *spinorial frames* play a crucial role in our definition of algebraic spinors (AS) and of ASF. Once we grasp the definition of AS and particularly of Dirac AS we define Dirac–Hestenes spinors (DHS) in Sec. IV. Whereas AS may be associated to any real vector space of arbitrary dimension $n=p+q$ equipped with a nondegenerated metric of arbitrary signature (p,q), this is not the case for DHS. (ASF can be defined on more general manifolds called spin manifolds. This will be studied in Ref. 126. There, we show that the concept of Dirac–Hestenes spinor fields which exists for four-dimensional Lorentzian spin manifolds modeling a relativistic space–time, can be generalized for the case of general *spin* manifold of dimension $n=p+q$ [equipped with a metric of signature (p,q), only if the spinor bundle structure $P_{\mathrm{Spin}^e_{p,q}}M$ is trivial].) However, these objects exist for a

four-dimensional vector space V equipped with a metric of Lorentzian signature and this fact makes them very much important mathematical objects for physical theories. Indeed, as we shall show in Sec. V it is possible to express Dirac equation in a consistent way using DHSF living on Minkowski space–time. Such equation is called the Dirac–Hestenes equation (DHE). In Sec. VII we express the Dirac equation using ASF. In Sec. IV we define Clifford fields and then ASF and DHSF. We observe here that our definitions of ASF and DHSF as some equivalence classes of pairs (Ξ_u, ψ_{Ξ_u}), where Ξ_u is a *spinorial coframe* field and ψ_{Ξ_u} is an appropriated Clifford field, i.e., a sum of multivector (or multiform) fields are not the usual ones that can be found in the literature. [Take notice that in this paper the term spinorial (co)frame field (defined below) is related, but distinct from the concept of a spin (co)frame, which is a section of a particular principal bundle called the spin (co)frame bundle (see Sec. IV and Ref. 126 for more details).] These definitions that, of course, come after the definitions of AS and DHS are essentially different from the definition of spinors given originally by Chevalley.[38,39] There, spinors are simply defined as elements of a minimal ideal carrying a modular representation of the Clifford algebra $\mathcal{C}\ell(V,\mathbf{g})$ associated to a structure $(V,\mathbf{g})$, where V is a real vector space of dimension $n=p+q$ and $\mathbf{g}$ is a metric of signature (p,q). And, of course, in that book there is no definition of DHS. Concerning DHS we mention that our definition of these objects is different also from the originally given in Refs. 79–81. [The definitions of AS, DHS, ASF, and DHSF given below are an improvement over preliminary tentative definitions of these objects given in Ref. 150. Unfortunately, that paper contains some equivocated results and errors (besides many misprints), which we correct here and in Ref. 126. We take the opportunity to apologize for any incovenience and misunderstandings that Ref. 150 may have caused. Some other papers where related (but not equivalent) material to the one presented in the present paper and in Ref. 126 can be found in Refs. 14–41, 44–69, 73–78, 93–109, 121–133, 144, and 146.] In view of these statements a justification for our definitions must be given and part of Sec. V and Sec. VI are devoted to such an enterprise. There it is shown that our definitions are the only ones compatible with the DHE and the meaning of the Fierz identities.[43,66] We discuss in Sec. VIII some misunderstandings resulting from the presentations of the standard Dirac equation when written with covariant Dirac spinors and also some misunderstandings concerning the DHE. It is important to emphasize here that the definitions of ASF, DHSF on Minkowski space–time and of the spin–Dirac operator given in Sec. V although correct are to be considered only as preliminaries. Indeed, these objects can be defined in a truly satisfactory way on a general Riemann–Cartan space–time only after the introduction of the concepts of the Clifford and the left (and right) spin–Clifford bundles. Moreover, a comprehensive formulation of Dirac equation on these manifolds requires a theory of connections acting on sections of these bundles. This nontrivial subject is studied in a forthcoming paper.[126] Section IX presents our conclusions. Finally we recall that our notations and some necessary results for the intelligibility of the paper are presented in Appendixes A–E. Although the appendixes contain known results, we decided to write them for the benefit of the reader, since the material cannot be found in a single reference. In particular Appendix A contains some of the ''tricks of the trade'' necessary to perform quickly calculations with Clifford algebras. If the reader needs more details concerning the theory of Clifford algebras and their applications than the ones provided by the Appendixes, the Refs. 14, 63, 64, 78, 86, 109, 141, 142 will certainly help. A final remark is necessary before we start our enterprise: the theory of the Dirac–Hestenes spinor fields of this (and the sequel paper[126]) does not contradict the standard theory of covariant Dirac spinor fields that is used by physicists and indeed it will be shown that the standard theory is no more than a matrix representation of theory described below.

Some acronyms are used in the present paper (to avoid long sentences) and they are summarized below for the reader's convenience:

AS, Algebraic spinor;

ASF, Algebraic spinor field;

CDS, Covariant Dirac spinor;

DHE, Dirac–Hestenes equation;

DHSF, Dirac–Hestenes spinor field.

II. ALGEBRAIC SPINORS

This section introduces the algebraic ideas that motivated the theory of ASF (which will be developed with full rigor in Ref. 126), i.e., we give a precise definition of AS. The algebraic side of the theory of DHSF, namely the concept of DHS is given in Sec. III. The justification for that definition will become clear in Secs. V and VI.

A. Geometrical equivalence of representation modules of simple Clifford algebras $\mathcal{C}\ell(V,\mathbf{g})$

We start with the introduction of some notations and clarification of some subtleties.

(i) In what follows V is a n-dimensional vector space over the real field $\mathbb{R}$. The dual space of V is denoted V^*. Let

$$\mathbf{g}: V\times V\to\mathbb{R} \tag{1}$$

be a metric of signature (p,q).

(ii) Let $\mathrm{SO}(V,\mathbf{g})$ be the group of endomorphisms of V that preserves $\mathbf{g}$ and the space orientation. This group is isomorphic to $\mathrm{SO}_{p,q}$ (see Appendix C), but there is no natural isomorphism. We write $\mathrm{SO}(V,\mathbf{g})\simeq\mathrm{SO}_{p,q}$. Also, the connected component to the identity is denoted by $\mathrm{SO}^e(V,\mathbf{g})$ and $\mathrm{SO}^e(V,\mathbf{g})\simeq\mathrm{SO}^e_{p,q}$. In the case $p=1$, $q=3$, $\mathrm{SO}^e(V,\mathbf{g})$ preserves besides orientation also the time orientation. In this paper we are mainly interested in $\mathrm{SO}^e(V,\mathbf{g})$.

(iii) We denote by $\mathcal{C}\ell(V,\mathbf{g})$ the Clifford algebra of V associated to $(V,\mathbf{g})$ and by $\mathrm{Spin}^e(V,\mathbf{g})$ $(\simeq\mathrm{Spin}^e_{p,q})$ the connected component of the spin group $\mathrm{Spin}(V,\mathbf{g})\simeq\mathrm{Spin}_{p,q}$ (see Appendix C for the definitions). [We reserve the notation $\mathbb{R}_{p,q}$ for the Clifford algebra of the vector space $\mathbb{R}^n$ equipped with a metric of signature (p,q), $p+q=n$. $\mathcal{C}\ell(V,\mathbf{g})$ and $\mathbb{R}_{p,q}$ are isomorphic, but there is no canonical isomorphism. Indeed, an isomorphism can be exhibited only after we fix an orthonormal basis of V.] Let $\mathbf{L}$ denote 2:1 homomorphism $\mathbf{L}:\mathrm{Spin}^e(V,\mathbf{g})\to\mathrm{SO}^e(V,\mathbf{g})$, $u\mapsto\mathbf{L}(u)\equiv\mathbf{L}_u$. $\mathrm{Spin}^e(V,\mathbf{g})$ acts on V identified as the space of 1-vectors of $\mathcal{C}\ell(V,\mathbf{g})\simeq\mathbb{R}_{p,q}$ through its adjoint representation in the Clifford algebra $\mathcal{C}\ell(V,\mathbf{g})$ which is related with the vector representation of $\mathrm{SO}^e(V,\mathbf{g})$ as follows [$\mathrm{Aut}(\mathcal{C}\ell(V,\mathbf{g}))$ denotes the (inner) automorphisms of $\mathcal{C}\ell(V,\mathbf{g})$]:

$$\mathrm{Spin}^e(V,g)\ni u\mapsto \mathrm{Ad}_u\in\mathrm{Aut}(\mathcal{C}\ell(V,\mathbf{g}))$$

$$\mathrm{Ad}_u|_V: V\to V, \mathbf{v}\mapsto u\mathbf{v}u^{-1}=\mathbf{L}_u\cdot\mathbf{v}. \tag{2}$$

In Eq. (2) $\mathbf{L}_u\cdot\mathbf{v}$ denotes the standard action $\mathbf{L}_u$ on $\mathbf{v}$ [see Eq. (5)] and where identified (without much ado) $\mathbf{L}_u\in\mathrm{SO}^e(V,\mathbf{g})$ with $\mathbf{L}_u\in\mathbf{V}\otimes\mathbf{V}^*$, $\mathbf{g}(\mathbf{L}_u\cdot\mathbf{v},\mathbf{L}_u\cdot\mathbf{v})=\mathbf{g}(\mathbf{v},\mathbf{v})$.

(iv) We denote by $\mathcal{C}\ell(V,\mathbf{g})$ the Clifford algebra of V associated to $(V,\mathbf{g})$ and by $\mathrm{Spin}^e(V,\mathbf{g})$ $(\simeq\mathrm{Spin}^e_{p,q})$ the connected component of the spin group $\mathrm{Spin}(V,\mathbf{g})\simeq\mathrm{Spin}_{p,q}$ (see Appendix C for the definitions).

(v) Let $\mathcal{B}$ be the set of all oriented and time oriented orthonormal basis [we will call the elements of $\mathcal{B}$ (in what follows) simply by orthonormal basis] of V. Choose among the elements of $\mathcal{B}$ a basis $b_0=\{\mathbf{E}_1,\ldots,\mathbf{E}_p,\mathbf{E}_{p+1},\ldots,\mathbf{E}_{p+q}\}$, hereafter called the fiducial frame of V. With this choice, we define a 1–1 mapping

$$\Sigma:\mathrm{SO}^e(V,\mathbf{g})\to\mathcal{B}, \tag{3}$$

given by

$$\mathbf{L}_u \mapsto \Sigma(\mathbf{L}_u) \equiv \Sigma_{\mathbf{L}_u} = \mathbf{L}_u b_0, \tag{4}$$

where $\Sigma_{\mathbf{L}_u} = \mathbf{L}_u b_0$ is a short for $\{\mathbf{e}_1, \ldots, \mathbf{e}_p, \mathbf{e}_{p+1}, \ldots, \mathbf{e}_{p+q}\} \in \mathcal{B}$, such that denoting the action of $\mathbf{L}_u$ on $\mathbf{E}_i \in b_0$ by $\mathbf{L}_u \cdot \mathbf{E}_i$ we have

$$\mathbf{e}_i = \mathbf{L}_u \cdot \mathbf{E}_i \equiv L_i^j \mathbf{E}_j, \quad i,j = 1,2,\ldots,n. \tag{5}$$

In this way, we can identify a given vector basis b of V with the isometry $\mathbf{L}_u$ that takes the fiducial basis b_0 to b. The fiducial basis b_0 will be also denoted by $\Sigma_{\mathbf{L}_0}$, where $\mathbf{L}_0 = e$, is the identity element of $\mathrm{SO}^e(V,\mathbf{g})$.

Since the group $\mathrm{SO}^e(V,\mathbf{g})$ is not simple connected their elements cannot distinguish between frames whose spatial axes are rotated in relation to the fiducial vector frame $\Sigma_{\mathbf{L}_0}$ by multiples of 2π or by multiples of 4π. For what follows it is crucial to make such a distinction. This is done by introduction of the concept of spinorial frames.

Definition 1: Let $b_0 \in \mathcal{B}$ be a fiducial frame and choose an arbitrary $u_0 \in \mathrm{Spin}^e(V,\mathbf{g})$. Fix once and for all the pair (u_0, b_0) with $u_0 = 1$ and call it the fiducial spinorial frame.

Definition 2: The space $\mathrm{Spin}^e(V,\mathbf{g}) \times \mathcal{B} = \{(u,b), ubu^{-1} = u_0 b_0 u_0^{-1}\}$ will be called the space of spinorial frames and denoted by Θ.

Remark 3: It is crucial for what follows to observe here that the definition 2 implies that a given $b \in \mathcal{B}$ determines two and only two spinorial frames, namely (u,b) and $(-u,b)$, since $\pm ub(\pm u^{-1}) = u_0 b_0 u_0^{-1}$.

(vi) We now parallel the construction in (v) but replacing $\mathrm{SO}^e(V,\mathbf{g})$ by its universal covering group $\mathrm{Spin}^e(V,\mathbf{g})$ and $\mathcal{B}$ by Θ. Thus, we define the 1–1 mapping

$$\Xi : \mathrm{Spin}^e(V,\mathbf{g}) \to \Theta,$$

$$u \mapsto \Xi(u) \equiv \Xi_u = (u,b), \tag{6}$$

where $ubu^{-1} = b_0$.

The fiducial spinorial frame will be denoted in what follows by Ξ_0. It is obvious from Eq. (6) that $\Xi(-u) = \Xi_{(-u)} = (-u,b) \neq \Xi_u$.

Definition 4: The natural right action of $a \in \mathrm{Spin}^e(V,\mathbf{g})$ denoted by $\cdot$ on Θ is given by

$$a \cdot \Xi_u = a \cdot (u,b) = (ua, \mathrm{Ad}_{a^{-1}} b) = (ua, a^{-1} b a). \tag{7}$$

Observe that if $\Xi_{u'} = (u',b') = u' \cdot \Xi_0$ and $\Xi_u = (u,b) = u \cdot \Xi_0$ then,

$$\Xi_{u'} = (u^{-1}u') \cdot \Xi_u = (u', u^{-1} u b u^{-1} u').$$

Note that there is a natural 2–1 mapping

$$\mathbf{s} : \Theta \to \mathcal{B}, \quad \Xi_{\pm u} \mapsto b = (\pm u^{-1}) b_0 (\pm u), \tag{8}$$

such that

$$\mathbf{s}((u^{-1}u') \cdot \Xi_u)) = \mathrm{Ad}_{(u^{-1}u')^{-1}}(\mathbf{s}(\Xi_u)). \tag{9}$$

Indeed, $\mathbf{s}((u^{-1}u') \cdot \Xi_u)) = \mathbf{s}((u^{-1}u') \cdot (u,b)) = u'^{-1} u b (u'^{-1} u)^{-1} = b' = \mathrm{Ad}_{(u^{-1}u')^{-1}} b = \mathrm{Ad}_{(u^{-1}u')^{-1}}(\mathbf{s}(\Xi_u))$. This means that the natural right actions of $\mathrm{Spin}^e(V,\mathbf{g})$, respectively, on Θ and $\mathcal{B}$, commute. In particular, this implies that the spinorial frames $\Xi_u, \Xi_{-u} \in \Theta$, which are, of course distinct, determine the same vector frame $\Sigma_{\mathbf{L}_u} = \mathbf{s}(\Xi_u) = \mathbf{s}(\Xi_{-u}) = \Sigma_{\mathbf{L}_{-u}}$. We have

$$\Sigma_{\mathbf{L}_u} = \Sigma_{\mathbf{L}_{-u}} = \mathbf{L}_{u^{-1}u_0} \Sigma_{\mathbf{L}_{u_0}}, \quad \mathbf{L}_{u^{-1}u_0} \in \mathrm{SO}^e_{p,q}. \tag{10}$$

Also, from Eq. (9), we can write explicitly

$$u_0\Sigma_{\mathbf{L}_{u_0}}u_0^{-1}=u\Sigma_{\mathbf{L}_u}u^{-1},\quad u_0\Sigma_{\mathbf{L}_{u_0}}u_0^{-1}=(-u)\Sigma_{\mathbf{L}_{-u}}(-u)^{-1},\quad u\in \mathrm{Spin}^e(V,\mathbf{g}), \tag{11}$$

where the meaning of Eq. (11) of course, is that if $\Sigma_{\mathbf{L}_u}=\Sigma_{\mathbf{L}_{-u}}=b=\{\mathbf{e}_1,\ldots,\mathbf{e}_p,\mathbf{e}_{p+1},\ldots,\mathbf{e}_q\}\in\mathcal{B}$ and $\Sigma_{\mathbf{L}_{u_0}}=b_0\in\mathcal{B}$ is the fiducial frame, then

$$u_0\mathbf{E}_ju_0^{-1}=(\pm u)\mathbf{e}_j(\pm u^{-1}). \tag{12}$$

In resume we can say that the space Θ of spinorial frames can be thought of as an extension of the space $\mathcal{B}$ of vector frames, where even if two vector frames have the same ordered vectors, they are considered distinct if the spatial axes of one vector frame is rotated by a odd number of 2π rotations relative to the other vector frame and are considered the same if the spatial axes of one vector frame is rotated by an even number of 2π rotations relative to the other frame. Even if this construction seems to be impossible at first sight, Aharonov and Susskind[6] warrants that it can be implemented physically.

(vii) Before we proceed an important digression on our notation used below is necessary. We recalled in Appendix B how to construct a minimum left (or right) ideal for a given real Clifford algebra once a vector basis $b\in\mathcal{B}$ for $V\hookrightarrow\mathcal{C}\ell(V,\mathbf{g})$ is given. That construction suggests to label a given primitive idempotent and its corresponding ideal with the subindex b. However, taking into account the above discussion of vector and spinorial frames and their relationship we find useful for what follows [especially in view of the definition 5 and the definitions of algebraic and Dirac–Hestenes spinors (see definitions 6 and 8 below)] to label a given primitive idempotent and its corresponding ideal with the subindex Ξ_u. Recall after all, that a given idempotent is according to definition 6 representative of a particular spinor in a given spinorial frame Ξ_u.

(viii) Next we recall Theorem 49 of Appendix B which says that a minimal left ideal of $\mathcal{C}\ell(V,\mathbf{g})$ is of the type

$$I_{\Xi_u}=\mathcal{C}\ell(V,\mathbf{g})e_{\Xi_u}, \tag{13}$$

where e_{Ξ_u} is a primitive idempotent of $\mathcal{C}\ell(V,\mathbf{g})$.

It is easy to see that all ideals $I_{\Xi_u}=\mathcal{C}\ell(V,\mathbf{g})e_{\Xi_u}$ and $I_{\Xi_{u'}}=\mathcal{C}\ell(V,\mathbf{g})e_{\Xi_{u'}}$ such that

$$e_{\Xi_{u'}}=(u'^{-1}u)e_{\Xi_u}(u'^{-1}u)^{-1}, \tag{14}$$

$u,u'\in\mathrm{Spin}^e(V,g)$ are isomorphic. We have the following.

Definition 5: Any two ideals $I_{\Xi_u}=\mathcal{C}\ell(V,\mathbf{g})e_{\Xi_u}$ and $I_{\Xi_{u'}}=\mathcal{C}\ell(V,\mathbf{g})e_{\Xi_{u'}}$ such that their generator idempotents are related by Eq. (14) are said geometrically equivalent.

But take care, no *equivalence relation* has been defined until now. We observe moreover that we can write

$$I_{\Xi_{u'}}=I_{\Xi_u}(u'^{-1}u)^{-1}, \tag{15}$$

a equation that will play a key role in what follows.

B. Algebraic spinors of type I_{Ξ_u}

Let $\{I_{\Xi_u}\}$ be the set of all ideals geometrically equivalent to a given minimal $I_{\Xi_{u_0}}$ as defined by Eq. (15). Let

$$\mathfrak{T}=\{(\Xi_u,\Psi_{\Xi_u})|u\in\mathrm{Spin}^e(V,\mathbf{g}),\Xi_u\in\Theta,\Psi_{\Xi_u}\in I_{\Xi_u}\}. \tag{16}$$

Let $\Xi_u,\Xi_u\in\Theta$, $\Psi_{\Xi_u}\in I_{\Xi_u}$, $\Psi_{\Xi_{u'}}\in I_{\Xi_{u'}}$. We define an equivalence relation $\mathcal{R}$ on $\mathfrak{T}$ by setting

$$(\Xi_u,\Psi_{\Xi_u})\sim(\Xi_{u'},\Psi_{\Xi_{u'}}) \tag{17}$$

if and only if $u\mathbf{s}(\Xi_u)u^{-1}=u'\mathbf{s}(\Xi_{u'})u'^{-1}$ and

$$\Psi_{\Xi_{u'}}u'^{-1}=\Psi_{\Xi_u}u^{-1}. \tag{18}$$

Definition 6: An equivalence class

$$\Psi_{\Xi_u}=[(\Xi_u,\Psi_{\Xi_u})]\in\mathfrak{T}/\mathcal{R} \tag{19}$$

is called an algebraic spinor of type I_{Ξ_u} for $\mathcal{C}\ell(V,\mathbf{g})$. $\psi_{\Xi_u}\in I_{\Xi_u}$ is said to be a representative of the algebraic spinor Ψ_{Ξ_u} in the spinorial frame Ξ_u.

We observe that the pairs (Ξ_u,Ψ_{Ξ_u}) and $(\Xi_{-u},-\Psi_{\Xi_{-u}})$ are equivalent, but the pairs (Ξ_u,Ψ_{Ξ_u}) and $(\Xi_{-u},-\Psi_{\Xi_{-u}})$ are not. This distinction is *essential* in order to give a structure of linear space (over the real field) to the set $\mathfrak{T}$. Indeed, a natural linear structure on $\mathfrak{T}$ is given by

$$a[(\Xi_u,\Psi_{\Xi_u})]+b[(\Xi_u,\Psi'_{\Xi_u})]=[(\Xi_u,a\Psi_{\Xi_u})]+[(\Xi_{u'},b\Psi'_{\Xi_u})],$$

$$(a+b)[(\Xi_u,\Psi_{\Xi_u})]=a[(\Xi_u,\Psi_{\Xi_u})]+b[(\Xi_u,\Psi_{\Xi_u})]. \tag{20}$$

The definition that we just gave is not a standard one in the literature.[38,39] However, the fact is that the standard definition (licit as it is from the mathematical point of view) is *not* adequate for a comprehensive formulation of the Dirac equation using algebraic spinor fields or Dirac–Hestenes spinor fields as we show in a preliminary way in Sec. V and in a rigorous and definitive way in a sequel paper.[126]

As observed on Appendix D a given Clifford algebra $\mathbb{R}_{p,q}$ may have minimal ideals that are not geometrically equivalent since they may be generated by primitive idempotents that are related by elements of the group $\mathbb{R}^{\star}_{p,q}$ which are not elements of $\mathrm{Spin}^e(V,\mathbf{g})$ (see Appendix C where different, nongeometrically equivalent primitive ideals for $\mathbb{R}_{1,3}$ are shown). These ideals may be said to be of different types. However, from the point of view of the representation theory of the real Clifford algebras (Appendix B) all these primitive ideals carry equivalent (i.e., isomorphic) modular representations of the Clifford algebra and no preference may be given to any one. (The fact that there are ideals that are algebraically, but not geometrically equivalent seems to contain the seed for new physics, see Refs. 123, and 124.) In what follows, when no confusion arises and the ideal I_{Ξ_u} is clear from the context, we use the wording algebraic spinor for any one of the possible types of ideals.

Remark 7: We observe here that the idea of definition of algebraic spinor fields as equivalent classes has it seed in a paper by Riez.[147] *However, Riez used in his definition simply orthonormal frames instead of the spinorial frames of our approach. As such, Riez defintion generates contradictions, as it is obvious from our discussion above.*

C. Algebraic Dirac spinors

These are the algebraic spinors associated with the Clifford algebra $\mathcal{C}\ell(\mathcal{M})\simeq\mathbb{R}_{1,3}$ (the space–time algebra) of Minkowski space–time $\mathcal{M}=(V,\boldsymbol{\eta})$, where V is a four-dimensional vector space over $\mathbb{R}$ and η is a metric of signature (1,3).

Some special features of this important case are as follows.

(a) The group $\mathrm{Spin}^e(\mathcal{M})$ is the universal covering of $\mathcal{L}^{\uparrow}_{+}$, the special and orthochronous Lorentz group that is isomorphic to the group $\mathrm{SO}^e(\mathcal{M})$ which preserves space–time orientation and also the time orientation[120] (see also Appendix B).

(b) $\mathrm{Spin}^e(\mathcal{M})\subset\mathcal{C}\ell^0(\mathcal{M})$, where $\mathcal{C}\ell^0(\mathcal{M})\simeq\mathbb{R}_{1,3}$ is the even subalgebra of $\mathcal{C}\ell(\mathcal{M})$ and is called the Pauli algebra (see Appendix C).

The most important property is a coincidence given by Eq. (21) below. It permits us to define a new kind of spinors.

III. DIRAC–HESTENES SPINORS (DHS)

Let $\Xi_u \in \Theta$ be a spinorial frame for $\mathcal{M}$ such that $\mathbf{s}(\Xi_u)=\{e_0,e_1,e_2,e_3\}\in\mathcal{B}$. Then, it follows from Eq. (D18) of Appendix D that

$$I_{\Xi_u}=\mathcal{C}\ell(\mathcal{M})e_{\Xi_u}=\mathcal{C}\ell^0(\mathcal{M})e_{\Xi_u}, \tag{21}$$

if

$$e_{\Xi_u}=\tfrac{1}{2}(1+e_0). \tag{22}$$

Then, each $\Psi_{\Xi_u}\in I_{\Xi_u}$ can be written as

$$\Psi_{\Xi_u}=\psi_{\Xi_u}e_{\Xi_u}, \quad \psi_{\Xi_u}\in\mathcal{C}\ell^0(\mathcal{M}). \tag{23}$$

From Eq. (18) we get

$$\psi_{\Xi_{u'}}u'^{-1}ue_{\Xi_u}=\psi_{\Xi_u}e_{\Xi_u}, \quad \psi_{\Xi_u},\psi_{\Xi_{u'}}\in\mathcal{C}\ell^0(\mathcal{M}). \tag{24}$$

A possible solution for Eq. (24) is

$$\psi_{\Xi_{u'}}u'^{-1}=\psi_{\Xi_u}u^{-1}. \tag{25}$$

Let $\Theta\times\mathcal{C}\ell(\mathcal{M})$ and consider an equivalence relation $\mathcal{E}$ such that

$$(\Xi_u,\phi_{\Xi_u})\sim(\Xi_{u'},\phi_{\Xi_{u'}}) \pmod{\mathcal{E}} \tag{26}$$

if and only if $\psi_{\Xi_{u'}}$ and ψ_{Ξ_u} are related by

$$\phi_{\Xi_{u'}}u'^{-1}=\phi_{\Xi_u}u^{-1}. \tag{27}$$

This suggests the following.

Definition 8: The equivalence classes $[(\Xi_u,\phi_{\Xi_u})]\in(\Theta\times\mathcal{C}\ell(\mathcal{M}))/\mathcal{E}$ *are the Hestenes spinors. Among the Hestenes spinors, an important subset is the one consisted of Dirac–Hestenes spinors where* $[(\Xi_u,\psi_{\Xi_u})]\in(\Theta\times\mathcal{C}\ell^0(\mathcal{M}))/\mathcal{E}$. *We say that* $\phi_{\Xi_u}(\psi_{\Xi_u})$ *is a representative of a Hestenes (Dirac–Hestenes) spinor in the spinorial frame* Ξ_u.

How to justify the above definitions of algebraic and Dirac–Hestenes spinors? The question is answered in the next section.

IV. CLIFFORD FIELDS, ASF AND DHSF

The objective of this section is to introduce the concepts of Dirac–Hestenes spinor fields (DHSF) and algebraic spinor fields (ASF) living on Minkowski space–time. A definitive theory of these objects that can be applied for arbitrary Riemann–Cartan space–times can be given only after the introduction of the Clifford and left (and right) spin–Clifford bundles and the theory of connections acting on these bundles. This theory will be presented in Ref. 126 and the presentation given below (which can be followed by readers that have only a rudimentary knowledge of the theory of fiber bundles) must be considered as a preliminary one.

Let $(M,\eta,\tau,\uparrow,\nabla)$ be Minkowski space–time, where M is diffeomorphic to $\mathbb{R}^4$, η is a constant metric field, ∇ is the Levi–Civita connection of η. M is oriented by $\tau\in\sec\Lambda^4M$ and is also time oriented by $\uparrow$ (Refs. 156–158).

Let ($P_{\mathrm{SO}^e_{1,3}}M$ is the orthonormal frame bundle, $\sec P_{\mathrm{SO}^e_{1,3}}M$ means a section of the frame bundle) $\{e_a\}\in\sec P_{\mathrm{SO}^e_{1,3}}M$ be an orthonormal (moving) frame, not necessarily a coordinate frame

and let $\gamma^a \in \sec T^*M$ $(a=0,1,2,3)$ be such that the set $\{\gamma^a\}$ is dual to the set $\{e_a\}$, i.e., $\gamma^a(e_b) = \delta^a_b$. (Orthonormal moving frames are not to be confused with the concept of reference frames. The concepts are related, but distinct.[156–158])

The set $\{\gamma^a\}$ will be called also a (moving) frame. Let $\gamma_a = \eta_{ab}\gamma^b$, $a,b=0,1,2,3$. The set $\{\gamma_a\}$ will be called the reciprocal frame to the frame $\{\gamma^a\}$. Recall that [$\check{\eta}$ is the metric of the contangent space and $\check{\eta}(\gamma^a,\gamma^b) = \eta^{ab} = \eta_{ab} = \mathrm{diag}(1,-1,-1,-1)$] $(T^*_xM,\check{\eta}) \simeq \mathcal{M}$. We will denote $(T^*_xM,\check{\eta})$ by $\mathcal{M}^*$. Now, due to the affine structure of Minkowski space–time we can identify all the cotangent spaces as usual. Consider then the Clifford algebra $\mathcal{C}\ell(\mathcal{M}^*)$ generated by the coframe $\{\gamma^a\}$, where now we can take $\gamma^a: x \mapsto \Lambda^1(\mathcal{M}^*) \subset \mathcal{C}\ell(\mathcal{M}^*)$. We have

$$\gamma^a(x)\,\gamma^b(x) + \gamma^b(x)\,\gamma^a(x) = 2\,\eta^{ab}, \quad \forall x \in M. \tag{28}$$

Definition 9 (preliminary): A Clifford field is a mapping

$$C: M \ni x \mapsto C(x) \in \mathcal{C}\ell(\mathcal{M}^*). \tag{29}$$

In a coframe $\{\gamma^a\}$ the expression of a Clifford field is

$$\mathcal{C} = S + A_a\gamma^a + \frac{1}{2!}B_{ab}\gamma^a\gamma^b + \frac{1}{3!}T_{abc}\gamma^a\gamma^b\gamma^c + P\gamma^5, \tag{30}$$

where $S, A_a, B_{ab}, T_{abc}, P$ are scalar functions (the ones with two or more indices antisymmetric on that indices) and $\gamma^5 = \gamma^0\gamma^1\gamma^2\gamma^3$ is the volume element. Saying with other words, a Clifford field is a sum of nonhomogeneous differential forms. [This result follows once we recall that as a vector space the Clifford algebra $\mathcal{C}\ell(\mathcal{M}^*)$ is isomorphic to the the Grassmann algebra $\Lambda(V^*) = \Sigma_{p=0}^4 \Lambda^p(V^*)$, where $\Lambda^p(V^*)$ is the space of p-forms. This is clear from the definition of Clifford algebra given in the Appendix A. Recall that $\mathcal{M}^* = (V^* \simeq T^*M, \check{\eta})$.]

Here is the point where a minimum knowledge of the theory of fiber bundles is required. Minkowski space–time is parallelizable and admits a spin structure. See, e.g., Refs. 72, 131–139, and 126. This means that Minkowski space–time has a spin strucutre, i.e., there exists a principal bundle called the spin frame bundle and denoted by $P_{\mathrm{Spin}^e_{1,3}M}$ that is the double covering of $P_{\mathrm{SO}^e_{1,3}M}$, i.e., there is a 2:1 mapping $\rho: P_{\mathrm{Spin}^e_{1,3}M} \to P_{\mathrm{SO}^e_{1,3}M}$. The elements of $P_{\mathrm{Spin}^e_{1,3}M}$ are called the spin frame fields (when there is no possibility of confusion we abreviate spin frame field simply as spin frame), and if $F_u \in P_{\mathrm{Spin}^e_{1,3}M}$ then $\rho(F_u) = \{e_a\} \in P_{\mathrm{SO}^e_{1,3}M}$ (once we fix a spin frame and associate it to an arbitrary but fixed element of $u \in P_{\mathrm{Spin}^e_{1,3}M}$). This means, that as in Sec. I, we distinguish frames that differ from a 2π rotation. Besides $P_{\mathrm{SO}^e_{1,3}M}$, we introduce also $P'_{\mathrm{SO}^e_{1,3}M}$, the coframe orthonormal bundle, such that for $\{\gamma^a\} \in P'_{\mathrm{SO}^e_{1,3}M}$ there exists $\{e_a\} \in P_{\mathrm{SO}^e_{1,3}M}$, such that $\gamma^a(e_b) = \delta^a_b$. Note that $\{\gamma^a\} \in P'_{\mathrm{SO}^e_{1,3}M}$, but, as already observed, keep in mind that each $\gamma^a: x \mapsto \Lambda^1(\mathcal{M}^*) \subset \mathcal{C}\ell(\mathcal{M}^*)$. To proceed choose a fiducial coframe $\{\Gamma^a\} \in P'_{\mathrm{SO}^e_{1,3}M}$, dual to a fiducial frame $\rho(F_{u_0}) \equiv \{E_a\} \in \sec P_{\mathrm{SO}^e_{1,3}M}$.

Now, let

$$u: x \mapsto u(x) \in \mathrm{Spin}^e(\mathcal{M}^*) \subset \mathcal{C}\ell^0(\mathcal{M}^*). \tag{31}$$

In complete analogy with Sec. I let $\Theta'_{\mathcal{M}} = \mathrm{Spin}^e(\mathcal{M}^*) \times P'_{\mathrm{SO}^e_{1,3}M}$ be the space of spinorial coframe fields. We define also the 1–1 mapping

$$\begin{gathered} \Xi: \mathrm{Spin}^e(\mathcal{M}^*) \to \Theta'_{\mathcal{M}}, \\ u \mapsto \Xi(u) \equiv \Xi_u = (u, \{u^{-1}\Gamma_a u\}). \end{gathered} \tag{32}$$

Note that there is a 2–1 natural mapping

$$\mathbf{s}':\Theta'_{\mathcal{M}}\ni\Xi_u\mapsto\{\gamma^a\}\in P'_{\mathrm{SO}^e_{1,3}}M,$$
$$\gamma^a=u^{-1}\Gamma^a u. \tag{33}$$

Also, denoting the action of $a(x)\in\mathrm{Spin}^e(\mathcal{M}^*)$ on $\Theta'_{\mathcal{M}}$ by $a\cdot\Xi_u=(ua,\{\gamma^a\})$ we have

$$\Xi_{u'}=(u^{-1}u')\cdot\Xi_u, \tag{34}$$

$$\mathbf{s}'((u^{-1}u')\cdot\Xi_u))=\mathrm{Ad}_{(u^{-1}u')^{-1}}(\mathbf{s}'(\Xi_u)). \tag{35}$$

As in the preceding section we have associated $1\in\mathrm{Spin}^e(\mathcal{M}^*)$ to the fiducial spinorial coframe field, but of course we could associate any other element $u_0;x\mapsto u_0(x)\in\mathrm{Spin}^e(\mathcal{M}^*)$ to the fiducial spinorial coframe. In this general case, writing Ξ_{u_0} for the fiducial spinorial coframe, we have $\mathbf{s}'(\Xi_{u_0})=\{\Gamma^a\}$.

Note that $\mathbf{s}'(\Xi_u)=\mathbf{s}'(\Xi_{(-u)})$ and that any other coframe field $\mathbf{s}'(\Xi_u)$ is then related to $\mathbf{s}'(\Xi_{u_0})$ by

$$u_0\mathbf{s}'(\Xi_{u_0})u_0^{-1}=\pm u\mathbf{s}'(\Xi_u)(\pm u^{-1})=\pm u\mathbf{s}'(\Xi_{(-u)})(\pm u^{-1}), \tag{36}$$

where the meaning of this equation is analogous to the one given to Eq. (11), through Eq. (12).

Taking into account the results of the preceding sections and of the Appendixes A and B we are lead to the following definitions.

Let $\{I_{\Xi_u}\}$ be the set of all ideals geometrically equivalent to a given minimal $I_{\Xi_{u_0}}$ as defined by Eq. (15) where now u, u' are Clifford fields defined by mappings like the one defined in Eq. (31).

Let

$$\mathfrak{T}_{\mathcal{M}}=\{(x,(\Xi_u,\Psi_{\Xi_u}))|x\in M,u(x)\in\mathrm{Spin}^e(\mathcal{M}^*),\Xi_u\in\Theta'_{\mathcal{M}},$$
$$\Psi_{\Xi_u}:x\mapsto\Psi_{\Xi_u}(x)\in I_{\Xi_u},\Psi_{\Xi_{u'}}:x\mapsto\in\Psi_{\Xi_u}(x)\in I_{\Xi_{u'}}\}. \tag{37}$$

Consider an equivalence relation $\mathcal{R}_{\mathcal{M}}$ on $\mathfrak{T}_{\mathcal{M}}$ such that

$$(x,(\Xi_u,\Psi_{\Xi_u}))\sim(y,(\Xi_{u'},\Psi_{\Xi_{u'}})) \tag{38}$$

if and only if $x=y$,

$$u(x)\mathbf{s}'(\Xi_{u(x)})u^{-1}(x)=u'(x)\mathbf{s}'(\Xi_{u'(x)})u'^{-1}(x) \tag{39}$$

and

$$\Psi_{\Xi_{u'}}u'^{-1}=\Psi_{\Xi_u}u^{-1}. \tag{40}$$

Definition 10 (preliminary): An algebraic spinor field (ASF) of type I_{Ξ_u} for $\mathcal{M}^*$ is an equivalence class $\Psi_{\Xi_u}=[(x,(\Xi_u,\Psi_{\Xi_u}))]\in\mathfrak{T}_{\mathcal{M}}/\mathcal{R}_{\mathcal{M}}$. We say that $\Psi_{\Xi_u}\in I_{\Xi_u}$ is a representative of the ASF Ψ_{Ξ_u} in the spinorial coframe field Ξ_u.

Consider an equivalence relation $\mathcal{E}_{\mathcal{M}}$ on the set $M\times\Xi_{\mathcal{M}}\times\mathcal{C}\ell(\mathcal{M}^*)$ such that [given $\psi_{\Xi_u}:x\mapsto\psi_{\Xi_u}(x)\in\mathcal{C}\ell(\mathcal{M}^*)$, $\psi_{\Xi_{u'}}:x\mapsto\in\psi_{\Xi_u}(x)\in\mathcal{C}\ell(\mathcal{M}^*)$] $((x,(\Xi_u,\psi_{\Xi_u})))$ and $((y,(\Xi_{u'},\psi_{\Xi_{u'}})))$ are equivalent if and only if $x=y$,

$$u(x)\mathbf{s}'(\Xi_{u(x)})u^{-1}(x)=u'(x)\mathbf{s}'(\Xi_{u'(x)})u'^{-1}(x) \tag{41}$$

and

$$\psi_{\Xi_u}, u'^{-1} = \psi_{\Xi_u} u^{-1}. \tag{42}$$

Definition 11 (preliminary): An equivalence class $\psi = [(x, (\Xi_u, \psi_{\Xi_u}))] \in M \times \Xi_{\mathcal{M}} \times \mathcal{C}\ell(\mathcal{M}^*)/\mathcal{E}_{\mathcal{M}}$ *is called a Hestenes spinor field for* $\mathcal{M}^*$. $\psi_{\Xi_u} \in \mathcal{C}\ell(\mathcal{M}^*)$ *is said to be a representative of the Hestenes spinor field* ϕ_{Ξ_u} *in the spinorial coframe field* Ξ_u. *When* $\psi_{\Xi_u}: x \mapsto \psi_{\Xi_u}(x) \in \mathcal{C}\ell^0(\mathcal{M}^*)$, $\psi_{\Xi_u}: x \mapsto \in \psi_{\Xi_u}(x) \in \mathcal{C}\ell^0(\mathcal{M}^*)$ *we call the equivalence class a Dirac–Hestenes spinor field (DHSF).*

V. THE DIRAC–HESTENES EQUATION (DHE)

In our preliminary presentation of the Dirac equation (on Minkowski space–time) that follows we shall restrict our exposition to the case where any spinorial coframe field appearing in the equations that follows, e.g., $\mathbf{s}'(\Xi_u) = \{\gamma^a\}$ is teleparallel and constant. By this we mean that $\forall x, y \in M$ and $a = 0,1,2,3$,

$$\gamma^a(x) \equiv \gamma^a(y), \tag{43}$$

$$\nabla_{e_a} \gamma^b = 0. \tag{44}$$

Equation (43) has meaning due to the affine structure of Minkowski space–time which permits the usual identification of all tangent spaces (and of all cotangent spaces) of the manifold and Eq. (44), is the definition of a teleparallel frame. Of course, the unique solution for Eq. (44) is $\gamma^\mu = \mathrm{d}x^\mu$, where $\{x^\mu\}$ are the coordinate functions of a global Lorentz chart of Minkowski space–time. Such a restriction is a necessary one in our elementary presentation, because otherwise we would need first to study the theory of the covariant derivative of spinor fields, a subject that simply cannot be appropriately introduced with the present formalism, thus clearly showing its limitation. Thus, to continue our elementary presentation we need some results of the general theory of the covariant derivatives of spinor fields studied in details in Ref. 126.

Using the results of the preceding sections and of the Appendixes we can show[80,148] that the usual Dirac equation[5,53] (which, as well known is written in terms of covariant Dirac spinor fields) for a representative of a DHSF in interaction with an electromagnetic potential $A: x \mapsto A(x) \in \Lambda^1(\mathcal{M}^*) \subset \mathcal{C}\ell(\mathcal{M}^*)$ is

$$\mathbf{D}^s \psi_{\Xi_u} \gamma_2 \gamma_1 - m \psi_{\Xi_u} \gamma_0 + qA \psi_{\Xi_u} = 0. \tag{45}$$

[Covariant Dirac spinor fields are defined in an obvious way once we take into account the definition of covariant Dirac spinors given by Eq. (E6) and Eq. (E7) of the Appendix E. See also Refs. 41, 131–133.]

Remark 12: It is important for what follows to have in mind that although each representative $\psi_{\Xi_u}: x \mapsto \psi_{\Xi_u}(x) \in \mathcal{C}\ell^0(\mathcal{M}^*)$ *of a* DHSF *is a sum of nonhomogeneous differential forms, spinor fields are not a sum of nonhomogeneous differential forms. Thus, they are mathematical objects of a nature different from that of Clifford fields*. (*Not* taking this difference into account can lead to misconceptions, as, e.g., some appearing in Ref. 71. See our comments in Ref. 155 on that paper.) *The crucial difference between a Clifford field, e.g., an electromagnetic potential A and a* DHSF *is that A is frame independent whereas a* DHSF *is frame dependent.*

In the DHE the spinor covariant derivative $\mathbf{D}^s$ is a first order differential operator, often called the spin–Dirac operator. [If we use more general frames, that are not Lorentzian coordinate frames, e.g., $\Xi_u = \{\gamma^a\}$ then $\mathbf{D}^s \psi_{\Xi_u}(x) = \gamma^a \nabla^s_{e_a} \psi_{\Xi_u}(x) = \gamma^a (e_a + \frac{1}{2}\omega_a) \psi_{\Xi_u}(x)$, where ω_a is a two form field associated with the spinorial connection, which is zero only for teleparallel frame fields,

if they exist. Details in Ref. 126.] Let $\nabla^s_{f_a}$ be the spinor covariant derivative. We have the following representation for $\mathbf{D}^s$ in an arbitrary orthonormal frame $\{t^a\}$ dual of the frame $\{f_a\} \in P_{\mathrm{SO}^e_{1,3}}$,

$$\mathbf{D}^s = t^a \nabla^s_{f_a}. \tag{46}$$

In a teleparallel spin (co)frame $\mathbf{s}'(\Xi_u) = \{\gamma^\mu\}$ the above equation reduces to

$$\mathbf{D}^s = \mathrm{d}x^\mu \frac{\partial}{\partial x^\mu}. \tag{47}$$

The spin–Dirac operator in an arbitrary orthonormal frame acts on a product $(C\psi_{\Xi_u})$ where C is a Clifford field and ψ_{Ξ_u} a representative of a DHSF (or a Hestenes field) as a modular derivation,[20,126] i.e.,

$$\mathbf{D}^s(C\psi_{\Xi_u}) = t^a \nabla^s_{f_a}(C\psi_{\Xi_u}) = t^a[(\nabla_{f_a} C)\psi_{\Xi_u} + C(\nabla^s_{f_a}\psi_{\Xi_u})].$$

Also in Eq. (45) m and q are real parameters (mass and charge) identifying the elementary fermion described by that equation. (Note that we used natural unities in which the value of the velocity of light is $c=1$ and the value of Planck's constant is $\hbar = 1$.)

Now, from Eq. (42) we have

$$\psi_{\Xi_{u'}} = \psi_{\Xi_u} s^{-1}, \quad \Xi_{u'} = s \cdot \Xi_u, \tag{48}$$

$$A \mapsto A, \tag{49}$$

where $s: x \mapsto s(x) \in \mathrm{Spin}^e(\mathcal{M}^*) \subset \mathcal{C}\ell^0(\mathcal{M}^*)$ is to be considered a Clifford field. Consider the case where $s(x) = s(y) = s$, $\forall x, y \in M$. Such equation has a precise meaning due to our restriction to teleparallel frames. We see that the DHE is trivially covariant under this kind of transformation, which can be called a right gauge transformation.

Returning to the DHE we see also that the equation is covariant under active Lorentz gauge transformations, or left gauge transformations. Indeed, under an active left Lorentz gauge transformation (without changing the spinorial coframe field), we have

$$\begin{gathered} \psi_{\Xi_u} \mapsto \psi'_{\Xi_u} = s\psi_{\Xi_u}, \quad A \mapsto sAs^{-1}, \\ \mathbf{D}^s \psi_{\Xi_u} \mapsto \mathbf{D}'^s \psi'_{\Xi_u} = s\mathbf{D}^s \psi_{\Xi_u}. \end{gathered} \tag{50}$$

The justification for the active left Lorentz gauge transformation law $\mathbf{D}^s \psi_{\Xi_u} \mapsto \mathbf{D}'^s \psi'_{\Xi_u} = s\mathbf{D}^s \psi_{\Xi_u}$ is the following. (A study of active local left Lorentz gauge transformations will be presented elsewhere, for it needs the concept of gauge covariant derivatives.) The Dirac operator is a 1-form valued derivative operator $\mathbf{D}^s = \mathrm{d}x^\mu (\partial/\partial x^\mu)$. Then, under an active Lorentz gauge transformation s it must transform like a vector, i.e., $\mathbf{D}^s \mapsto \mathbf{D}'^s = s\, \mathrm{d}x^\mu\, s^{-1} (\partial/\partial x^\mu)$.

Note that ψ'_{Ξ_u} is a representative (in the spinorial coframe field Ξ_u) of a new spinor. Then, it follows, of course, that the representative of the new spinor in the spinorial coframe field $\Xi_{u'}$ is

$$\psi'_{\Xi_{u'}} = s\psi_{\Xi_u} s^{-1}. \tag{51}$$

We also recall that the DHE is invariant under simultaneous left and right (constants) gauge Lorentz transformations. In this case the relevant transformations are

$$\psi_{\Xi_u} \mapsto \psi'_{\Xi_u} = s\psi_{\Xi_u} s^{-1},$$
$$A \mapsto sAs^{-1}, \quad \mathbf{D}'^{s}\psi'_{\Xi_{u'}} = s\mathbf{D}^{s}\psi_{\Xi_u} s^{-1}. \tag{52}$$

VI. JUSTIFICATION OF THE TRANSFORMATION LAWS OF DHSF BASED ON THE FIERSZ IDENTITIES

We now give another justification for the definition of Dirac spinors and DHSF presented in the preceding sections. We start by recalling that a usual covariant Dirac spinor field determines a set of p-form fields, called bilinear covariants, which describe the physical contents of a particular solution of the Dirac equation described by that field. The same is true also for a DHSF.

In order to present the bilinear covariants using that fields, we introduce first the notion of the Hodge dual operator of a Clifford field $\mathcal{C}: M \ni x \mapsto \mathcal{C}(x) \in \mathcal{C}\ell(\mathcal{M}^*)$. We have the following.

Definition 13: The Hodge dual operator is the mapping

$$\star : \mathcal{C} \to \star\mathcal{C} = \widetilde{\mathcal{C}}\gamma_5, \tag{53}$$

where $\widetilde{\mathcal{C}}$ is the reverse of C [Eq. (A5), Appendix A].

Then, in terms of a representative of a DHSF in the spinorial frame field Ξ_u the bilinear covariants of Dirac theory reads (with $J = J_\mu\gamma^\mu$, $S = \frac{1}{2}S_{\mu\nu}\gamma^\mu\gamma^\nu$, $K = K_\mu\gamma^\mu$)

$$\psi_{\Xi_u}\widetilde{\psi}_{\Xi_u} = \sigma + \star\omega, \quad \psi_{\Xi_u}\gamma^0\widetilde{\psi}_{\Xi_u} = J,$$
$$\psi_{\Xi_u}\gamma^1\gamma^2\widetilde{\psi}_{\Xi_u} = S, \quad \psi_{\Xi_u}\gamma^0\gamma^3\widetilde{\psi}_{\Xi_u} = \star S, \tag{54}$$
$$\psi_{\Xi_u}\gamma^3\widetilde{\psi}_{\Xi_u} = K, \quad \psi_{\Xi_u}\gamma^0\gamma^1\gamma^2\widetilde{\psi}_{\Xi_u} = \star K.$$

The so-called *Fierz identities* are

$$J^2 = \sigma^2 + \omega^2, \quad J\cdot K = 0, \quad J^2 = -K^2, \quad J\wedge K = -(\omega + \star K)S, \tag{55}$$

$$S \llcorner J = \omega K, \quad S \llcorner K = \omega J,$$
$$(\star S) \llcorner J = -\sigma K, \quad (\star S) \llcorner K = -\sigma J, \tag{56}$$
$$S\cdot S = \omega^2 - \sigma^2, \quad (\star S)\cdot S = -2\sigma\omega,$$

$$JS = -(\omega + \star\sigma)K,$$
$$SJ = -(\omega - \star\sigma)K,$$
$$KS = -(\omega + \star\sigma)J,$$
$$SK = -(\omega - \star\sigma)J, \tag{57}$$
$$S^2 = \omega^2 - \sigma^2 - 2\sigma(\star\omega),$$
$$S^{-1} = -S(\sigma - \star\omega)^2/J^2 = KSK/J^4.$$

The proof of these identities using the DHSF is almost a triviality and can be done in a few lines. This is not the case if you use covariant Dirac spinor fields (columns matrix fields). In this case you will need to perform several pages of matrix algebra calculations.

The importance of the bilinear covariants is due to the fact that we can recover from them the associate covariant Dirac spinor field (and thus the DHSF) except for a phase. This can be done with an algorithm due to Crawford[43] and presented in a very pedagogical way in Ref. 109.

Let us consider, e.g., the equation $\psi_{\Xi_u}\gamma_0\tilde{\psi}_{\Xi_u}=J$ in (54). Now, $J(x)\in\Lambda^1(\mathcal{M}^*)\subset\mathcal{C}\ell(\mathcal{M}^*)$ is an intrinsic object on Minkowski space–time and according to the accepted first quantization interpretation theory of the Dirac equation it is proportional to the electromagnetic current generated by an elementary fermion. The expression of J in terms of the representative of a DHSF in the spinorial coframe $\Xi_{u'}$ is (of course)

$$\psi_{\Xi_{u'}}\gamma_0'\tilde{\psi}_{\Xi_{u'}}=J. \tag{58}$$

Now, since

$$\gamma_0'=(u'^{-1}u)\,\gamma_0(u'^{-1}u)^{-1}, \tag{59}$$

we see that we must have

$$\psi_{\Xi_{u'}}=\psi_{\Xi_u}(u'^{-1}u)^{-1}, \tag{60}$$

which justifies the definition of DHSF given above [see Eq. (40)].

We observe also that if $\psi_{\Xi_u}\tilde{\psi}_{\Xi_u}=\sigma+\star\omega\neq 0$, then we can write

$$\psi_{\Xi_u}=\rho^{1/2}e^{1/2\,\beta\gamma^5}R, \tag{61}$$

where $\forall x\in M$,

$$\begin{aligned}&\rho(x)\in\Lambda^0(\mathcal{M}^*)\subset\mathcal{C}\ell(\mathcal{M}^*),\\ &\beta(x)\in\Lambda^0(\mathcal{M}^*)\subset\mathcal{C}\ell(\mathcal{M}^*),\\ &R\in\mathrm{Spin}^e_{1,3}(\mathcal{M}^*)\subset\mathcal{C}\ell(\mathcal{M}^*).\end{aligned} \tag{62}$$

With this result the current J can be written

$$J=\rho v \tag{63}$$

with $v=R\gamma^0R^{-1}$. Equation (63) discloses the secret geometrical meaning of DHSF. These objects rotate and dilate vector fields, this being the reason why they are sometimes called operator spinors.[80–86,109]

VII. DIRAC EQUATION IN TERMS OF ASF

We recall from Eq. (D2) of Appendix D that

$$e'_{\Xi_u}=\tfrac{1}{2}(1+\gamma_3\gamma_0) \tag{64}$$

is also a primitive idempotent field (here understood as a Hestenes spinor field) that is algebraically, but not geometrically equivalent to the idempotent field $e_{\Xi_u}=\frac{1}{2}(1+\gamma_0)$. Let $I'_{\Xi_u}=\mathcal{C}\ell(\mathcal{M}^*)e'_{\Xi_u}$ be a minimal left ideal generated by e'_{Ξ_u}. Now, multiply the DHE [Eq. (45)] on the left, first by the primitive idempotent e_{Ξ_u} and then by the primitive idempotent e'_{Ξ_u}. We get after some algebra

$$\mathbf{D}^s\Phi_{\Xi_u}-m\Phi_{\Xi_u}(\star 1)+qA\Phi_{\Xi_u}=0, \tag{65}$$

where $\star 1=\gamma_5$ is the oriented volume element of Minkowski space–time and

$$\Phi_{\Xi_u}=\psi_{\Xi_u}e_{\Xi_u}e'_{\Xi_u}\in I'_{\Xi_u}=\mathcal{C}\ell(\mathcal{M}^*)e'_{\Xi_u}. \tag{66}$$

Equation (65) is one of the many faces of the original equation found by Dirac in terms of ASF and using teleparallel orthonormal frames.

Of course, Eq. (65), as it is the case of the DHE [Eq. (45)] is compatible with the transformation law of ASF that follows directly from the transformation law of AS given in Sec. II. In contrast to the DHE, in Eq. (65) there seems to be no explicit reference to elements of a spinorial coframe field (except for the indices Ξ_u) since $\star 1$, the volume element is invariant under (Lorentz) gauge transformations. We emphasize also that the transformation law for ASF is compatible with the presentation of Fierz identities using these objects, as the interested reader can verify without difficulty.

VIII. MISUNDERSTANDINGS CONCERNING COORDINATE REPRESENTATIONS OF THE DIRAC AND DIRAC–HESTENES EQUATIONS

We investigate now some subtleties of the Dirac and Dirac–Hestenes equations. We start by pointing out and clarifying some misunderstandings that often appears in the literature of the subject of the DHE when that equation is presented in terms of a representative of a DHSF in a global coordinate chart (M,φ) of the maximal atlas of M with Lorentz coordinate functions $\langle x^\mu\rangle$ associated to it (see, e.g., Ref. 156). In that case, $\mathbf{s}'(\Xi_u)=\{\gamma^\mu=\mathrm{d}x^\mu\}$. After that we study the (usual) matrix representation of Dirac equation and show how it hides many features that are only visible in the DHE.

Let $\{e_\mu=\partial/\partial x^\mu\}$ and $\{e'_\mu=\partial/\partial x'^\mu\}$. The spinorial coframe fields Ξ_u and $\Xi_{u'}$ (as defined in the preceding section) are associated to the coordinate bases (dual basis) $\mathbf{s}'(\Xi_u)=\{\gamma^\mu=\mathrm{d}x^\mu\}$ and $\mathbf{s}'(\Xi_{u'})=\{\gamma'^\mu=dx'^\mu\}$, corresponding to the global Lorentz charts (M,φ) and (M,φ'). The DHE is written in the charts $\langle x^\mu\rangle$ and $\langle x'^\mu\rangle$ as

$$\begin{aligned}
&\gamma^\mu\left(\frac{\partial}{\partial x^\mu}\Psi_{\Xi_u}+qA_\mu\Psi_{\Xi_u}\gamma_1\gamma_2\right)\gamma_2\gamma_1-m\Psi_{\Xi_u}\gamma_0=0,\\
&\gamma'^\mu\left(\frac{\partial}{\partial x'^\mu}\Psi'_{\Xi_{u'}}+qA'_\mu\Psi_{\Xi_{u'}}\gamma'_1\gamma'_2\right)\gamma'_2\gamma'_1-m\Psi_{\Xi_{u'}}\gamma'_0=0,
\end{aligned} \tag{67}$$

where $\mathbf{D}^s=\gamma^\mu(\partial/\partial x^\mu)=\gamma'^\mu(\partial/\partial x'^\mu)$ and where (Ψ_{Ξ_u},A_μ) and $(\Psi_{\Xi_{u'}},A'_\mu)$ are the coordinate representations of (ψ_{Ξ_u},A) and $(\psi_{\Xi_{u'}},A)$, i.e., for any $x\in M$, we have

$$\begin{aligned}
&A=A'_\mu(x'^\mu)\mathrm{d}x'^\mu=A_\mu(x^\mu)\mathrm{d}x^\mu,\\
&A'_\mu(x'^0,x'^1,x'^2,x'^3)=\mathbf{L}^\nu_\mu A_\nu(x^0,x^1,x^2,x^3),\\
&(\Psi_{\Xi_{u'}}U'^{-1})|_{(x'^0(x),x'^1(x),x'^2(x),x'^3(x))}=(\Psi_{\Xi_u}U^{-1})|_{(x^0(x),x^1(x),x^2(x),x^3(x))},
\end{aligned} \tag{68}$$

with U and U' the coordinate representations of u and u' [see Eq. (42)] and L^ν_μ is an appropriate Lorentz transformation.

Now, taking into account that the complexification of the algebra $\mathcal{C}\ell(\mathcal{M}^*)$, i.e., $\mathbb{C}\otimes\mathcal{C}\ell(\mathcal{M}^*)$ is isomorphic to the Dirac algebra $\mathbb{R}_{4,1}$ (Appendix C), we can think of all the objects appearing in Eqs. (67) as having values also in $\mathbb{C}\otimes\mathcal{C}\ell(\mathcal{M}^*)$. Multiply then, both sides of each one of the Eqs. (67) by the following primitive idempotents fields [considered as complexified Hestenes spinor fields (see Definition 8)] of $\mathbb{C}\otimes\mathcal{C}\ell(\mathcal{M}^*)$ [see Eq. (D14) of Appendix D]

$$f_{\Xi_u} = \tfrac{1}{2}(1+\gamma^0)\tfrac{1}{2}(1+i\gamma^1\gamma^2),$$
$$f_{\Xi_{u'}} = \tfrac{1}{2}(1+\gamma'^0)\tfrac{1}{2}(1+i\gamma'^1\gamma'^2). \tag{69}$$

Next, look for a matrix representation in $\mathbb{C}(4)$ of the resulting equations. We get (using the notation of Appendix D)

$$\overline{\gamma}^\mu\left(i\frac{\partial}{\partial x^\mu}\right) + qA_\mu(x^\mu)\Psi(x^\mu) - m\Psi(x^\mu) = 0, \tag{70}$$

$$\underline{\gamma}^\mu\left(i\frac{\partial}{\partial x'^\mu}\right) + qA'_\mu(x'^\mu)\Psi'(x'^\mu) - m\Psi'(x'^\mu) = 0, \tag{71}$$

where $\Psi(x^\mu), \Psi'(x'^\mu)$ are the matrix representations [Eq. (D15), Appendix D] of Ψ_{Ξ_u} and $\Psi_{\Xi_{u'}}$. The matrix representations of the spinors are related by an equation analogous to Eq. (E2) of Appendix E, except that now, these equations refer to fields. The $\{\underline{\gamma}^\mu\}$, $\mu = 0,1,2,3$ is the set of Dirac matrices given by Eq. (D13) of Appendix D. Of course, we arrived at the usual form of the Dirac equation, except for the irrelevant fact that in general the Dirac spinor is usually represented by a column spinor field, and here we end with a 4×4 matrix field, which however has non-null elements only in the first column. [The reader can verify without great difficulty that Eq. (65) also has a matrix representation analogous to Eq. (71) but with a set of gamma matrices differing from the set $\{\underline{\gamma}^\mu\}$ by a similarity transformation.]

Equation (70), that is the usual presentation of Dirac equation in Physics textbooks, hides several important facts. First, it hides the basic dependence of the spinor fields on the spinorial frame field, since the spinorial frames Ξ_u, $\Xi_{u'}$ are such that $\mathbf{s}'(\Xi_u) = \{\gamma^\mu\}$ and $\mathbf{s}'(\Xi_{u'}) = \{\gamma'^\mu\}$ are mapped on the same set of matrices, namely $\{\underline{\gamma}^\mu\}$. Second, it hides an obvious geometrical meaning of the theory, as first disclosed by Hestenes.[80,81] Third, taking into account the discussion in a preceding section, we see that the usual presentation of the Dirac equation does not leave clear at all if we are talking about passive or active Lorentz gauge transformations. Finally, since diffeomorphisms on the world manifold are in general erroneous associated with coordinate transformations in many Physics textbooks, Eq. (70) suggests that spinors must change under diffeomorphisms in a way different from the true one, for indeed Dirac spinor fields (and also, DHSF) are scalars under diffeomorphisms, an issue that we will discuss in another publication.

IX. CONCLUSIONS

In this paper we investigated how to define algebraic and Dirac–Hestenes spinor fields on *Minkowski* space–time. We showed first, that in general, algebraic spinors can be defined for any real vector space of any dimension and equipped with a nondegenerated metric of arbitrary signature, but that is not the case for *Dirac–Hestenes spinors*. These objects exist for a four-dimensional real vector space equipped with a metric of Lorentzian signature. It is this fact that makes them very important objects (and gave us the desire to present a rigorous mathematical theory for them), since as shown in Secs. V and VII the Dirac equation can be written in terms of *Dirac–Hestenes spinor fields* or *algebraic spinor fields*. We observe that our definitions of algebraic and Dirac–Hestenes spinor fields as some equivalence classes in appropriate sets are not the standard ones and the core of the paper was to give genuine motivations for them. We observe moreover that the definitions of Dirac–Hestenes spinor fields and of the spin–Dirac operator given in Sec. V although correct are to be considered only as preliminaries. The reason is that any rigorous presentation of the theory of the spin–Dirac operator (an in particular, on a general Riemann–Cartan space–time) can only be given after the introduction of the concepts of Clifford and spin–Clifford bundles over these space–times. This is studied in a sequel paper.[126] In Ref. 155

we show some nontrivial applications of the concept of Dirac–Hestenes spinor fields by proving (mathematical) Maxwell–Dirac equivalences of the first and second kinds and showing how these equivalences can eventually put some light on a possible physical interpretation of the famous Seiberg–Witten equations for Minkowski space–time.

Noted added: After we finished the writing of the present paper and of Ref. 126, we learned about the very interesting papers by Marchuck.[110–118] There, a different point of view concerning the writing of the Dirac equation using tensor fields is developed. (Reference 110, indeed, uses a particular case of objects that we called extensors in a recent series of papers.[63–65,127–130]) We will discuss Marchuck papers elsewhere.

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APPENDIX A: SOME FEATURES ABOUT REAL AND COMPLEX CLIFFORD ALGEBRAS

In this appendix we fix the notations that we used and introduce the main ideas concerning the theory of Clifford algebras necessary for the intelligibility of the paper.

1. Definition of the Clifford algebra $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$

In this paper we are interested only in Clifford algebras of a vector space (we reserve the notation V for real vector spaces) $\mathbf{V}$ of finite dimension n over a field $\mathbb{F}=\mathbb{R}$ or $\mathbb{C}$. Let $\mathbf{q}:\mathbf{V}\to\mathbb{F}$ be a nondegenerate quadratic form over $\mathbf{V}$ with values in $\mathbb{F}$ and $\mathbf{b}:\mathbf{V}\times\mathbf{V}\to\mathbb{F}$ the associated bilinear form (which we call a metric in the case $\mathbb{F}=\mathbb{R}$). We use the notation

$$x\cdot y=\mathbf{b}(x,y)=\tfrac{1}{2}(\mathbf{q}(x+y)-\mathbf{q}(x)-\mathbf{q}(y). \tag{A1}$$

Let $\Lambda\mathbf{V}=\Sigma_{i=0}^{n}\Lambda^{i}\mathbf{V}$ be the exterior algebra of $\mathbf{V}$ where $\Lambda^{i}\mathbf{V}$ is the $\binom{n}{i}$ dimensional space of the i-vectors. $\Lambda^{0}\mathbf{V}$ is identified with $\mathbb{F}$ and $\Lambda^{1}\mathbf{V}$ is identified with $\mathbf{V}$. The dimension of $\Lambda\mathbf{V}$ is 2^{n}. A general element $X\in\Lambda\mathbf{V}$ is called a multivector and can be written as

$$X=\sum_{i=0}^{n}\langle X\rangle_{i},\quad \langle X\rangle_{i}\in\Lambda^{i}\mathbf{V}, \tag{A2}$$

where

$$\langle\ \rangle_{i}:\Lambda\mathbf{V}\to\Lambda^{i}\mathbf{V} \tag{A3}$$

is the projector in $\Lambda^{i}\mathbf{V}$, also called the i-part of X.

Definition 14: The main involution or grade involution is an automorphism

$$\hat{}:\Lambda\mathbf{V}\ni\mathbf{X}\mapsto\hat{\mathbf{X}}\in\Lambda\mathbf{V} \tag{A4}$$

such that

$$\hat{X}=\sum_{k=0}^{n}(-1)^{k}\langle X\rangle_{k}. \tag{A5}$$

$\hat{X}$ is called the grade involution of X or simply the involuted of X.

Definition 15: The reversion operator is the anti-automorphism

$$\tilde{}:\Lambda\mathbf{V}\ni\mathbf{X}\mapsto\tilde{\mathbf{X}}\in\Lambda\mathbf{V} \tag{A6}$$

such that

$$\tilde{X}=\sum_{k=0}^{n}(-1)^{1/2\,k(k-1)}\langle X\rangle_k, \tag{A7}$$

$\tilde{X}$ is called the reverse of X.

The composition of the grade evolution with the reversion operator, denote by $-$ is called by some authors (e.g., Refs. 109, 141, 142) the conjugation and, $\overline{X}$ is called the conjugate of X. We have $\overline{X}=(\tilde{X})=(\hat{X})$.

Since the grade and reversion operators are involutions on the vector space of multivectors, we have that $\hat{\hat{X}}=X$ and $\tilde{\tilde{X}}=X$. both involutions commute with the k-part operator, i.e., $\widehat{\langle X\rangle_k}=\langle\hat{X}\rangle_k$ and $\widetilde{\langle X\rangle_k}=\langle\tilde{X}\rangle_k$, for each $k=0,1,\ldots,n$.

Definition 16: The exterior product of multivectors X and Y is defined by

$$\langle X\wedge Y\rangle_k=\sum_{j=0}^{k}\langle X\rangle_j\wedge\langle Y\rangle_{k-j}, \tag{A8}$$

for each $k=0,1,\ldots,n$. Note that on the right-hand side there appears the exterior product of j-vectors and $(k-j)$-vectors with $0\leqslant j\leqslant n$. (We assume that the reader is familiar with the exterior algebra. We only caution that there are some different definitions of the exterior product in terms of the tensor product differing by numerical factors. This may lead to some confusions, if care is not taken. Details can be found in Refs. 63 and 64.)

This exterior product is an internal composition law on $\Lambda\mathbf{V}$. It is associative and satisfies the distributives laws (on the left and on the right).

Definition 17: The vector space $\Lambda\mathbf{V}$ endowed with this exterior product Λ is an associative algebra called the exterior algebra of multivectors.

We recall now some of the most important properties of the exterior algebra of multivectors.

For any $\alpha,\beta\in\mathbb{F}$, $X\in\Lambda\mathbf{V}$,

$$\begin{aligned}&\alpha\wedge\beta=\beta\wedge\alpha=\alpha\beta\ \ (\text{product of }\mathbb{F}\text{ numbers}),\\&\alpha\wedge X=X\wedge\alpha=\alpha X\ \ (\text{multiplication by scalars}).\end{aligned} \tag{A9}$$

For any $X_j\in\Lambda^j\mathbf{V}$ and $Y_k\in\Lambda^k\mathbf{V}$

$$X_j\wedge Y_k=(-1)^{jk}Y_k\wedge X_j. \tag{A10}$$

For any $X,Y\in\Lambda\mathbf{V}$

$$\begin{aligned}&\widehat{X\wedge Y}=\hat{X}\wedge\hat{Y},\\&\widetilde{X\wedge Y}=\tilde{X}\wedge\tilde{Y}.\end{aligned} \tag{A11}$$

2. Scalar product of multivectors

Definition 18: A scalar product between the multivectors $X,Y\in\Lambda\mathbf{V}$ is given by

$$X\cdot Y=\sum_{i=0}^{n}\langle X\rangle_i\cdot\langle Y\rangle_i, \tag{A12}$$

where $\langle X\rangle_0\cdot\langle Y\rangle_0=\langle X\rangle_0\langle Y\rangle_0$ is the multiplication in the field $\mathbb{F}$ and $\langle X\rangle_i\cdot\langle Y\rangle_i$ is given by Eq. (A2), and writing

$$\begin{aligned}\langle X\rangle_k&=\frac{1}{k!}X^{i_1i_2\cdots i_k}b_{i_1}\wedge b_{i_2}\cdots b_{i_k},\\ \langle Y\rangle_k&=\frac{1}{k!}Y^{i_1i_2\cdots i_k}b_{i_1}\wedge b_{i_2}\cdots b_{i_k}\end{aligned} \tag{A13}$$

where $\{b_k\},k=1,2,\ldots,n$ is an arbitrary basis of $\mathbf{V}$ we have

$$\langle X\rangle_k\cdot\langle Y\rangle_k=\frac{1}{(k!)^2}X^{i_1i_2\cdots i_k}Y^{j_1j_2\cdots j_k}(b_{i_1}\wedge b_{i_2}\cdots b_{i_k})\cdot(b_{j_1}\wedge b_{j_2}\cdots b_{j_k}), \tag{A14}$$

with

$$(b_{i_1}\wedge b_{i_2}\cdots b_{i_k})\cdot(b_{j_1}\wedge b_{j_2}\cdots b_{j_k})=\begin{vmatrix} b_{i_1}\cdot b_{j_1} & \cdots & \cdots & b_{i_1}\cdot b_{j_k}\\ \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots\\ b_{i_k}\cdot b_{j_1} & \cdots & \cdots & b_{i_k}\cdot b_{j_k}\end{vmatrix}. \tag{A15}$$

It is easy to see that for any $X,Y\in\Lambda\mathbf{V}$,

$$\begin{aligned}\hat{X}\cdot Y&=X\cdot\hat{Y},\\ \tilde{X}\cdot Y&=X\cdot\tilde{Y}.\end{aligned} \tag{A16}$$

Remark 19: Observe that the definition of the scalar product given in this paper by Eq. (A12) differs by a signal from the scalar product of multivectors defined, e.g., in Ref. 79. Our definition is a natural one if we start the theory with the euclidean Clifford algebra of multivectors of a real vector space $\mathbf{V}$. The euclidean Clifford algebra is fundamental for the construction of the theory of extensors and extensor fields.[63–65,127–130]

3. Interior algebras

Definition 20: We define two different contracted products *for arbitrary multivectors $X,Y\in\Lambda\mathbf{V}$ by*

$$\begin{aligned}(X\lrcorner Y)\cdot Z&=Y(\tilde{X}\wedge Z),\\ (X\llcorner Y)&=X\cdot(Z\wedge\tilde{Y}),\end{aligned} \tag{A17}$$

where $Z\in\Lambda\mathbf{V}$. The internal composition rules $\lrcorner$ *and* $\llcorner$ *will be called, respectively, the left and the right contracted product.*

These contracted products $\lrcorner$ and $\llcorner$ are internal laws on $\Lambda\mathbf{V}$. Both contract products satisfy the distributive laws (on the left and on the right) but they are *not* associative.

Definition 21: The vector space $\Lambda\mathbf{V}$ *endowed with each one of these contracted products (either* $\lrcorner$ *or* $\llcorner$*) is a nonassociative algebra. They are called the interior algebras of multivectors*.

We present now some of the most important properties of the interior products:

(a) For any $\alpha,\beta\in\mathbb{F}$, and $X\in\Lambda\mathbf{V}$,

$$\alpha\lrcorner\beta=\alpha\llcorner\beta=\alpha\beta \text{ (product in } \mathbb{F}),$$
$$\alpha\lrcorner X=X\llcorner\alpha=\alpha X \text{ (multiplication by scalars)}. \tag{A18}$$

(b) For any $X_j\in\Lambda^j\mathbf{V}$ and $Y_k\in\Lambda^k\mathbf{V}$ with $j\leqslant k$,

$$X_j\lrcorner Y_k=(-1)^{j(k-j)}Y_k\llcorner X_j. \tag{A19}$$

(c) For any $X_j\in\Lambda^j\mathbf{V}$ and $Y_k\in\Lambda^k\mathbf{V}$,

$$X_j\lrcorner Y_k=0, \text{ if } j>k,$$
$$X_j\llcorner Y_k=0, \text{ if } j<k. \tag{A20}$$

(d) For any $X_k,Y_k\in\Lambda^k\mathbf{V}$

$$X_j\lrcorner Y_k=X_j\llcorner Y_k=\tilde{X}_k\cdot Y_k=X_k\cdot\tilde{Y}_k. \tag{A21}$$

(e) For any $v\in\mathbf{V}$ and $X,Y\in\Lambda\mathbf{V}$

$$v\lrcorner(X\wedge Y)=(v\lrcorner X)\wedge Y+\hat{X}\wedge(v\lrcorner Y). \tag{A22}$$

4. Clifford algebra $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$

Definition 22: The Clifford product of multivectors X *and* Y (*denoted by juxtaposition) is given by the following axiomatic:*

(i) For all $\alpha\in\mathbb{F}$ and $X\in\Lambda\mathbf{V}$: $\alpha X=X\alpha$ equals multiplication of multivector X by scalar α.
(ii) For all $v\in\mathbf{V}$ and $X\in\Lambda\mathbf{V}$: $vX=v\lrcorner X+v\wedge X$ and $Xv=X\llcorner v+X\wedge v$.
(iii) For all $X,Y,Z\in\Lambda\mathbf{V}$: $X(YZ)=(XY)Z$.

The Clifford product is an internal law on $\Lambda\mathbf{V}$. It is associative [by the axiom (iii)] and satisfies the distributives laws (on the left and on the right). The distributive laws follow from the corresponding distributive laws of the contracted and exterior products.

Definition 23: The vector space of multivectors over $\mathbf{V}$ *endowed with the Clifford product is an associative algebra with unity called* $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$.

5. Relation between the exterior and the Clifford algebras and the tensor algebra

Modern algebra books give the

Definition 24: The exterior algebra of $\mathbf{V}$ *is the quotient algebra* $\Lambda\mathbf{V}=T(\mathbf{V})/I$, *where* $T(\mathbf{V})$ *is the tensor algebra of* $\mathbf{V}$ *and* $I\subset T(\mathbf{V})$ *is the bilateral ideal generated by the elements of the form* $\mathbf{x}\otimes\mathbf{x}$, $\mathbf{x}\in\mathbf{V}$.

Definition 25: The Clifford algebra of $(\mathbf{V},\mathbf{b})$ *is the quotient algebra* $\mathcal{C}\ell(\mathbf{V},\mathbf{b})=T(\mathbf{V})/I_b$, *where* I_b *is the bilateral ideal generated by the elements of the form* $\mathbf{x}\otimes\mathbf{x}-\mathbf{2b}(\mathbf{x},\mathbf{x})$, $\mathbf{x}\in\mathbf{V}$.

We can show that this definition is equivalent to the one given above. [When the exterior algebra is defined as $\Lambda\mathbf{V}=T(\mathbf{V})/I$ and the Clifford algebra as $\mathcal{C}\ell(\mathbf{V},\mathbf{b})=T(\mathbf{V})/I_{\mathbf{b}}$, the (associative) exterior product of the multivectors in the terms of the tensor product of these multivectors is fixed once and for all. We have, e.g., that for $x,y\in\mathbf{V}$, $x\wedge y=\frac{1}{2}(x\otimes y-y\otimes x)$. However, keep in mind that it is possible to define an (associative) exterior product in $\Lambda\mathbf{V}$ differing from the above one by numerical factors, and indeed in Refs. 63–65, 127–130 we used another choice. When reading a text on the subject it is a good idea to have in mind the definition used by the author, for otherwise confusion may result.] The space $\mathbf{V}$ is naturally *embedded* on $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$, i.e.,

$$\mathbf{V}\overset{i}{\hookrightarrow}T(\mathbf{V})\overset{j}{\rightarrow}T(\mathbf{V})/I_{\mathbf{b}}=\mathcal{C}\ell(\mathbf{V},\mathbf{b}),$$
$$\text{and}\quad \mathbf{V}\equiv j\circ i(\mathbf{V})\subset\mathcal{C}\ell(\mathbf{V},\mathbf{b}). \tag{A23}$$

Let $\mathcal{C}\ell^0(\mathbf{V},\mathbf{b})$ and $\mathcal{C}\ell^1(\mathbf{V},\mathbf{b})$ be, respectively, the j-images of $\oplus_{i=0}^{\infty}T^{2i}(\mathbf{V})$ and $\oplus_{i=0}^{\infty}T^{2i+1}(\mathbf{V})$ in $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$. The elements of $\mathcal{C}\ell^0(\mathbf{V},\mathbf{b})$ form a subalgebra of $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$ called the even subalgebra of $\mathcal{C}\ell(\mathbf{V},\mathbf{b})$. Also, there is a canonical vector isomorphism $\Lambda\mathbf{V}\rightarrow\mathcal{C}\ell(\mathbf{V},\mathbf{b})$, which permits to speak of the embeddings $\Lambda^p\mathbf{V}\subset\mathcal{C}\ell(\mathbf{V},\mathbf{b})$, $0\leqslant p\leqslant n$, where n is the dimension of $\mathbf{V}$ (Ref. 20). [The isomorphism is compatible with the filtrations of the filtered algebra $\Lambda\mathbb{V}$, i.e., $(\Lambda^r\mathbb{V})\wedge(\Lambda^s\mathbb{V})\subseteq\Lambda^{r+s}\mathbb{V}$.]

6. Some useful properties of the real Clifford algebras $\mathcal{C}\ell(V,\mathbf{g})$

We now collect some useful formulas which hold for a real Clifford algebra $\mathcal{C}\ell(V,\mathbf{g})$ and which has been used in calculations in the text and Appendixes. (As the reader can verify, many of these properties are also valid for the complex Clifford algebras.)

For any $v\in V$ and $X\in\Lambda V$,

$$\begin{aligned} v\lrcorner X&=\tfrac{1}{2}(vX-\overline{X}v)\quad\text{and}\quad X\lrcorner v=\tfrac{1}{2}(Xv-v\overline{X}),\\ v\wedge X&=\tfrac{1}{2}(vX+\overline{X}v)\quad\text{and}\quad X\wedge v=\tfrac{1}{2}(Xv+v\overline{X}). \end{aligned}\tag{A24}$$

For any $X,Y\in V$,

$$X\cdot Y=\langle\tilde{X}Y\rangle_0=\langle X\tilde{Y}\rangle_0.\tag{A25}$$

For any $X,Y,Z\in V$,

$$\begin{aligned} (XY)\cdot Z&=Y\cdot(\tilde{X}Z)=X\cdot(Z\tilde{Y}),\\ X\cdot(YZ)&=(\tilde{Y}X)\cdot Z=(X\tilde{Z})\cdot Y. \end{aligned}\tag{A26}$$

For any $X,Y\in V$,

$$\begin{aligned} \overline{XY}&=\overline{X}\,\overline{Y},\\ \widetilde{XY}&=\tilde{Y}\tilde{X}. \end{aligned}\tag{A27}$$

Let $I\in\Lambda^nV$ then for any $v\in V$ and $X\in\Lambda V$,

$$I(v\wedge X)=(-1)^{n-1}v\lrcorner(IX).\tag{A28}$$

Equation (A22) is sometimes called the duality identity and plays an important role in the applications involving the Hodge dual operator [see Eq. (53)].

For any $X,Y,Z\in V$,

$$\begin{aligned} X\lrcorner(Y\wedge Z)&=(X\wedge Y)\lrcorner Z,\\ (X\llcorner Y)\llcorner Z&=X\llcorner(Y\wedge Z). \end{aligned}\tag{A29}$$

For any $X,Y\in V$,

$$X\cdot Y=\langle\tilde{X}Y\rangle_0.\tag{A30}$$

For $X_r\in\Lambda^rV$, $Y_s\in\Lambda^sV$ we have

$$X_rY_s=\langle X_rY_s\rangle_{|r-s|}+\langle X_rY_s\rangle_{|r-s|+2}+\cdots+\langle X_rY_s\rangle_{r+s}.\tag{A31}$$

(We observe also that when $K=\mathbb{R}$ and the quadratic form is Euclidean then $X\cdot Y$ is positive definite.)

APPENDIX B: REPRESENTATION THEORY OF THE REAL CLIFFORD ALGEBRAS $\mathbb{R}_{p,q}$

The real Clifford algebras $\mathbb{R}_{p,q}$ are associative algebras and they are simple or semisimple algebras. For the intelligibility of the present paper, it is then necessary to have in mind some results concerning the presentation theory of associative algebras, which we collect in what follows, without presenting proofs.

1. Some results from the representation theory of associative algebras

Let $\mathbf{V}$ be a set and $\mathbb{K}$ a division ring. Give to the set $\mathbf{V}$ a structure of finite-dimensional linear space over $\mathbb{K}$. Suppose that $\dim_{\mathbb{K}}\mathbf{V}=n$, where $n\in\mathbb{Z}$. We are interested in what follows in the cases where $\mathbb{K}=\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. When $\mathbb{K}=\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$, we call $\mathbf{V}$ a vector space over $\mathbb{K}$. When $\mathbb{K}=\mathbb{H}$ it is necessary to distinguish between right or left $\mathbb{H}$-linear spaces and in this case $\mathbf{V}$ will be called a right or left $\mathbb{H}$-module. Recall that $\mathbb{H}$ is a division ring (sometimes called a noncommutative field or a skew field) and since $\mathbb{H}$ has a natural vector space structure over the real field, then $\mathbb{H}$ is also a division algebra.

Let $\dim_{\mathbb{R}}\mathbf{V}=2m=n$. In this case it is possible to give the following.

Definition 26: A linear mapping

$$\mathbf{J}:\mathbf{V}\to\mathbf{V}, \tag{B1}$$

such that

$$\mathbf{J}^2=-\mathrm{Id}_{\mathbf{V}}, \tag{B2}$$

is called a complex structure mapping.

*Definition 27: The pair (***V**,**J***) will be called a complex vector space structure and denote by* $\mathbf{V}_{\mathbb{C}}$ *if the following product holds. Let* $\mathbb{C}\ni z=a+ib$ *and let* $\mathbf{v}\in\mathbf{V}$. *Then*

$$z\mathbf{v}=(a+ib)\mathbf{v}=a\mathbf{v}+b\mathbf{J}\mathbf{v}. \tag{B3}$$

It is obvious that $\dim_{\mathbb{C}}=m/2$.

Definition 28: Let $\mathbf{V}$ *be a vector space over* $\mathbb{R}$. *A* complexification *of* $\mathbf{V}$ *is a complex structure associated with the real vector space* $\mathbf{V}\oplus\mathbf{V}$. *The resulting complex vector space is denoted by* $\mathbf{V}^{\mathbb{C}}$. *Let* $\mathbf{v},\mathbf{w}\in\mathbf{V}$. *Elements of* $\mathbf{V}^{\mathbb{C}}$ *are usually denoted by* $\mathbf{c}=\mathbf{v}+i\mathbf{w}$, *and if* $\mathbb{C}\ni z=a+ib$ *we have*

$$z\mathbf{c}=a\mathbf{v}-b\mathbf{w}+i(a\mathbf{w}+b\mathbf{v}). \tag{B4}$$

Of course, we have that $\dim_{\mathbb{C}}\mathbf{V}^{\mathbb{C}}=\dim_{\mathbb{R}}\mathbf{V}$.

Definition 29: A $\mathbb{H}$*-module is a real vector space* $\mathbf{V}$ *carrying three linear transformation,* **I**, **J**, *and* **K** *each one of them satisfying*

$$\begin{gathered}\mathbf{I}^2=\mathbf{J}^2=-\mathbf{I}\mathrm{d}_{\mathbf{S}},\\ \mathbf{IJ}=-\mathbf{JI}=\mathbf{K},\quad \mathbf{JK}=-\mathbf{KJ}=\mathbf{I},\quad \mathbf{KI}=-\mathbf{IK}=\mathbf{J}.\end{gathered} \tag{B5}$$

Definition 30: Any subset $I\subseteq\mathcal{A}$ *such that*

$$\begin{gathered}a\psi\in I,\forall a\in\mathcal{A},\forall\psi\in I,\\ \psi+\phi\in I,\forall\psi,\phi\in I\end{gathered} \tag{B6}$$

is called a left ideal of $\mathcal{A}$.

Remark 31: An analogous definition holds for right ideals where Eq. (B6) reads $\psi a \in I, \forall a \in \mathcal{A}, \forall \psi \in I$, *for* bilateral *ideals where in this case Eq. (B6) reads* $a\psi b \in I, \forall a, b \in \mathcal{A}, \forall \psi \in I$.

Definition 32: An associative $\mathcal{A}$ *algebra on the* field $\mathbb{F}$ ($\mathbb{R}$ or $\mathbb{C}$) *is* simple *if the only bilateral ideals are the zero ideal and* $\mathcal{A}$ *itself.*

We give without proofs the following theorems.

Theorem 33: *All minimal left (respectively, right) ideals of* $\mathcal{A}$ *are of the form* $J = \mathcal{A}e$ (*respectively,* $e\mathcal{A}$), *where* e *is a primitive idempotent of* $\mathcal{A}$.

Theorem 34: *Two minimal left ideals of* $\mathcal{A}$, $J = \mathcal{A}e$ *and* $J = \mathcal{A}e'$ *are* isomorphic *if and only if there exist a non-null* $X' \in J'$ *such that* $J' = JX'$.

We recall that $e \in \mathcal{A}$ *is an* idempotent *element if* $e^2 = e$. *An idempotent is said to be* primitive *if it cannot be written as the sum of two nonzero annihilating (or orthogonal) idempotent,* i.e., $e \neq e_1 + e_2$, *with* $e_1 e_2 = e_2 e_1 = 0$ *and* $e_1^2 = e_1$, $e_2^2 = e_2$.

Not all algebras are simple and in particular semisimple algebras are important for our considerations. A definition of semisimple algebras requires the introduction of the concepts of nilpotent ideals and radicals. To define these concepts adequately would lead us to a long incursion on the theory of associative algebras, so we avoid to do that here. We only quote that semisimple algebras are the direct sum of simple algebras. Then, the study of semisimple algebras is reduced to the study of simple algebras.

Now, let $\mathcal{A}$ be an associative and simple algebra on the field $\mathbb{F}$ ($\mathbb{R}$ or $\mathbb{C}$), and let $\mathbf{S}$ be a finite-dimensional linear space over a division ring $\mathbb{K} \subseteq \mathbb{F}$.

Definition 35: *A* representation *of* $\mathcal{A}$ *in* $\mathbf{S}$ *is a* $\mathbb{K}$ *algebra homomorphism* [we recall that a $\mathbb{K}$-algebra homomorphism is a $\mathbb{K}$-linear map ρ such that $\forall X, Y \in \mathcal{A}$, $\rho(XY) = \rho(X)\rho(Y)$] $\rho: \mathcal{A} \to \mathbf{E} = \mathrm{End}_{\mathbb{K}}\mathbf{S}$ ($\mathbf{E} = \mathrm{End}_{\mathbb{K}}\mathbf{S} = \mathrm{Hom}_{\mathbb{K}}(\mathbf{S}, \mathbf{S})$ *is the endomorphism algebra of* $\mathbf{S}$) *which maps the unit element of* $\mathcal{A}$ *to* $\mathbf{Id}_{\mathbf{E}}$. *The dimension* $\mathbb{K}$ *of* $\mathbf{S}$ *is called the* degree *of the representation.*

The addition in $\mathbf{S}$ together with the mapping $\mathcal{A} \times \mathbf{S} \to \mathbf{S}$, $(a, x) \mapsto \rho(a)x$ turns $\mathbf{S}$ in a left $\mathcal{A}$-module, called the left *representation module*. [We recall that there are left and right modules, so we can also define right modular representations of $\mathcal{A}$ by defining the mapping $\mathbf{S} \times \mathcal{A} \to \mathbf{S}$, $(x, a) \mapsto x\rho(a)$. This turns $\mathbf{S}$ in a right $\mathcal{A}$-module, called the right *representation module*.]

Remark 36: It is important to recall that when $\mathbb{K} = \mathbb{H}$ *the usual recipe for* $\mathrm{Hom}_{\mathbb{H}}(\mathbf{S}, \mathbf{S})$ *to be a linear space over* $\mathbb{H}$ *fails and in general* $\mathrm{Hom}_{\mathbb{H}}(\mathbf{S}, \mathbf{S})$ *is considered as a linear space over* $\mathbb{R}$, *which is the center of* $\mathbb{H}$.

Remark 37: We also have that if $\mathcal{A}$ *is an algebra over* $\mathbb{F}$ *and* $\mathbf{S}$ *is an* $\mathcal{A}$*-module, then* $\mathbf{S}$ *can always be considered as a vector space over* $\mathbb{F}$ *and if* $e \in \mathcal{A}$, *the mapping* $\chi: a \to \chi_a$ *with* $\chi_a(\mathbf{s}) = a\mathbf{s}$, $\mathbf{s} \in \mathbf{S}$, *is a homomorphism* $\mathcal{A} \to \mathbf{E} = \mathrm{End}_{\mathbb{F}}\mathbf{S}$, *and so it is a representation of* $\mathcal{A}$ *in* $\mathbf{S}$. *The study of* $\mathcal{A}$ *modules is then equivalent to the study of the* $\mathbb{F}$ *representations of* $\mathcal{A}$.

Definition 38: A representation ρ *is faithful if its kernel is zero, i.e.,* $\rho(a)x = 0, \forall x \in \mathbf{S} \Rightarrow a = 0$. *The kernel of* ρ *is also known as the* annihilator *of its module.*

Definition 39: ρ *is said to be* simple *or irreducible if the only invariant subspaces of* $\rho(a)$, $\forall a \in \mathcal{A}$, *are* $\mathbf{S}$ *and* $\{0\}$.

Then, the representation module is also simple. That means that it has no proper submodules.

Definition 40: ρ *is said to be semisimple, if it is the direct sum of simple modules, and in this case* $\mathbf{S}$ *is the direct sum of subspaces which are globally invariant under* $\rho(a)$, $\forall a \in \mathcal{A}$.

When no confusion arises $\rho(a)x$ may be denoted by $a \cdot x$, $a * x$ or ax.

Definition 41: Two $\mathcal{A}$*-modules* $\mathbf{S}$ *and* $\mathbf{S}'$ *(with the exterior multiplication being denoted, respectively, by* $\cdot$ *and* $*$*) are* isomorphic *if there exists a bijection* $\varphi: \mathbf{S} \to \mathbf{S}'$ *such that*

$$\varphi(x + y) = \varphi(x) + \varphi(y), \quad \forall x, y \in \mathbf{S},$$

$$\varphi(a \cdot x) = a * \varphi(x), \quad \forall a \in \mathcal{A},$$

and we say that representation ρ *and* ρ' *of* $\mathcal{A}$ *are equivalent if their modules are isomorphic.*

This implies the existence of a $\mathbb{K}$-linear isomorphism $\varphi: \mathbf{S} \to \mathbf{S}'$ such that $\varphi \circ \rho(a) = \rho'(a) \circ \varphi$, $\forall a \in \mathcal{A}$ or $\rho'(a) = \varphi \circ \rho(a) \circ \varphi^{-1}$. If $\dim \mathbf{S} = n$, then $\dim \mathbf{S}' = n$.

TABLE I. Representation of the Clifford algebras $\mathbb{R}_{p,q}$ as matrix algebras.

$p-q$ mod 8	0	1	2	3	4	5	6	7
$\mathbb{R}_{p,q}$	$\mathbb{R}(2^{[n/2]})$	$\mathbb{R}(2^{[n/2]})$ $\oplus$ $\mathbb{R}(2^{[n/2]})$	$\mathbb{R}(2^{[n/2]})$	$\mathbb{C}(2^{[n/2]})$	$\mathbb{H}(2^{[n/2]-1})$	$\mathbb{H}(2^{[n/2]-1})$ $\oplus$ $\mathbb{H}(2^{[n/2]-1})$	$\mathbb{H}(2^{[n/2]-1})$	$\mathbb{C}(2^{[n/2]})$

Definition 42: A complex representation *of $\mathcal{A}$ is simply a real representation $\rho:\mathcal{A}\to\mathrm{Hom}_{\mathbb{R}}(\mathbf{S},\mathbf{S})$ for which*

$$\rho(X)\circ\mathbf{J}=\mathbf{J}\circ\rho(X),\quad \forall X\in\mathcal{A}. \tag{B7}$$

This means that the image of ρ commutes with the subalgebra generated by $\{\mathbf{Id}_{\mathbf{S}}\}\sim\mathbb{C}$.

Definition 43: A quaternionic representation of $\mathcal{A}$ is a representation $\rho:\mathcal{A}\to\mathrm{Hom}_{\mathbb{R}}(\mathbf{S},\mathbf{S})$ such that

$$\rho(X)\circ\mathbf{I}=\mathbf{I}\circ\rho(X),\quad \rho(X)\circ\mathbf{J}=\mathbf{J}\circ\rho(X),\quad \rho(X)\circ\mathbf{K}=\mathbf{K}\circ\rho(X),\quad \forall X\in\mathcal{A}. \tag{B8}$$

This means that the representation ρ has a commuting subalgebra isomorphic to the quaternion ring.

The following theorem[61,109] is crucial.

Theorem 44 (Wedderburn): *If $\mathcal{A}$ is simple algebra over $\mathbb{F}$ then $\mathcal{A}$ is isomorphic to $\mathbb{D}(m)$, where $\mathbb{D}(m)$ is a matrix algebra with entries in $\mathbb{D}$ (a division algebra), and m and $\mathbb{D}$ are unique (modulo isomorphisms).*

Now, it is time to specialize our results to the Clifford algebras over the field $\mathbb{F}=\mathbb{R}$ or $\mathbb{C}$. We are particularly interested in the case of real Clifford algebras. In what follows we take $(\mathbf{V},\mathbf{b})=(\mathbb{R}^n,\mathbf{g})$. We denote by $\mathbb{R}^{p,q}$ a real vector space of dimension $n=p+q$ endowed with a nondegenerate metric $\mathbf{g}:\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}$. Let $\{E_i\}$, $(i=1,2,\ldots,n)$ be an orthonormal basis of $\mathbb{R}^{p,q}$,

$$\mathbf{g}(E_i,E_j)=g_{ij}=g_{ji}=\begin{cases}+1, & i=j=1,2,\ldots,p\\ -1, & i=j=p+1,\ldots,p+q=n\\ 0, & i\neq j.\end{cases} \tag{B9}$$

Definition 45: The Clifford algebra $\mathbb{R}_{p,q}=\mathcal{C}\ell(\mathbb{R}^{p,q})$ is the Clifford algebra over $\mathbb{R}$, generated by 1 and the $\{E_i\}$ $(i=1,2,\ldots,n)$, such that $E_i^2=\mathbf{q}(E_i)=\mathbf{g}(E_i,E_i)$, $E_iE_j=-E_jE_i$ $(i\neq j)$, and $E_1E_2\ldots E_n\neq\pm 1$.

$\mathbb{R}_{p,q}$ is obviously of dimension 2^n and as a vector space it is the direct sum of vector spaces $\Lambda^k\mathbb{R}^n$ of dimensions $\binom{n}{k}$, $0\leqslant k\leqslant n$. The canonical basis of $\Lambda^k\mathbb{R}^n$ is given by the elements $e_A=E_{\alpha_1}\cdots E_{\alpha_k}$, $1\leqslant\alpha_1<\cdots<\alpha_k\leqslant n$. The element $e_J=E_1\cdots E_n\in\Lambda^k\mathbb{R}^n\subset\mathbb{R}_{p,q}$ commutes (n odd) or anticommutes (n even) with all vectors $E_1\cdots E_n\in\Lambda^1\mathbb{R}^n\equiv\mathbb{R}^n$. The center $\mathcal{C}\ell_{p,q}$ is $\Lambda^0\mathbb{R}^n\equiv\mathbb{R}$ if n is even and it is the direct sum $\Lambda^0\mathbb{R}^n\oplus\Lambda^0\mathbb{R}^n$ if n is odd.

All Clifford algebras are semisimple. If $p+q=n$ is even, $\mathbb{R}_{p,q}$ is simple and if $p+q=n$ is odd we have the following possibilities.

(a) $\mathbb{R}_{p,q}$ is simple $\leftrightarrow c_J^2=-1\leftrightarrow p-q\neq 1\pmod 4\leftrightarrow$ center of $\mathbb{R}_{p,q}$ is isomorphic to $\mathbb{C}$;

(b) $\mathbb{R}_{p,q}$ is not simple (but is a direct sum of two simple algebras)$\leftrightarrow c_J^2=+1\leftrightarrow p-q=1\pmod 4\leftrightarrow$ center of $\mathbb{R}_{p,q}$ is isomorphic to $\mathbb{R}\oplus\mathbb{R}$.

Now, for $\mathbb{R}_{p,q}$ the division algebras $\mathbb{D}$ are the division rings $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. The explicit isomorphism can be discovered with some hard but not difficult work. It is possible to give a general classification off all real (and also the complex) Clifford algebras and a classification table can be found, e.g., in Refs. 141 and 142. Table I is reproduced and $[n/2]$ means the integer part of $n/2$.

Now, to complete the classification we need the following theorem.[141]

Theorem 46 (Periodicity):

$$\mathbb{R}_{n+8}=\mathbb{R}_{n,0}\otimes\mathbb{R}_{8,0},\quad \mathbb{R}_{0,n+8}=\mathbb{R}_{0,n}\otimes\mathbb{R}_{0,8},$$
$$\mathbb{R}_{p+8,q}=\mathbb{R}_{p,q}\otimes\mathbb{R}_{8,0},\quad \mathbb{R}_{p,q+8}=\mathbb{R}_{p,q}\otimes\mathbb{R}_{0,8}. \tag{B10}$$

Remark 47: We emphasize here that since the general results concerning the representations of simple algebras over a field $\mathbb{F}$ applies to the Clifford algebras $\mathbb{R}_{p,q}$ we can talk about real, complex or quaternionic representation of a given Clifford algebra, even if the natural matrix identification is not a matrix algebra over one of these fields. A case that we shall need is that $\mathbb{R}_{1,3}\simeq\mathbb{H}(2)$. But it is clear that $\mathbb{R}_{1,3}$ has a complex representation, for any quaternionic representation of $\mathbb{R}_{p,q}$ is automatically complex, *once we restrict $\mathbb{C}\subset\mathbb{H}$ and of course, the complex dimension of any $\mathbb{H}$-module must be even. Also, any complex representation of $\mathbb{R}_{p,q}$ extends automatically to a representation of $\mathbb{C}\otimes\mathbb{R}_{p,q}$.*

Remark 48: *Now, $\mathbb{C}\otimes\mathbb{R}_{p,q}$ is an abbreviation for the* complex *Clifford algebra $\mathcal{C}\ell_{p+q}=\mathbb{C}\otimes\mathbb{R}_{p,q}$, i.e., it is the tensor product of the algebras $\mathbb{C}$ and $\mathbb{R}_{p,q}$, which are subalgebras of the finite-dimensional algebra $\mathcal{C}\ell_{p+q}$ over $\mathbb{C}$.*

For the purposes of the present paper we must keep in mind that

$$\mathbb{R}_{0,1}\simeq\mathbb{C},$$
$$\mathbb{R}_{0,2}\simeq\mathbb{H},$$
$$\mathbb{R}_{3,0}\simeq\mathbb{C}(2),$$
$$\mathbb{R}_{1,3}\simeq\mathbb{H}(2), \tag{B11}$$
$$\mathbb{R}_{3,1}\simeq\mathbb{R}(4),$$
$$\mathbb{R}_{4,1}\simeq\mathbb{C}(4).$$

$\mathbb{R}_{3,0}$ is called the Pauli algebra, $\mathbb{R}_{1,3}$ is called the *space–time* algebra, $\mathbb{R}_{3,1}$ is called *Majorana* algebra and $\mathbb{R}_{4,1}$ is called the *Dirac* algebra. Also the following particular results have been used in the text and below:

$$\mathbb{R}^0_{1,3}\simeq\mathbb{R}^0_{3,1}=\mathbb{R}_{3,0},\quad \mathbb{R}^0_{4,1}\simeq\mathbb{R}_{1,3},$$
$$\mathbb{R}_{4,1}\simeq\mathbb{C}\otimes\mathbb{R}_{3,1},\quad \mathbb{R}_{4,1}\simeq\mathbb{C}\otimes\mathbb{R}_{3,1}, \tag{B12}$$

which means that the Dirac algebra is the complexification of both the space–time or the Majorana algebras.

Equation (B11) show moreover, in view of Remark 7 that the space–time algebra has a complexification matrix representation in $\mathbb{C}(4)$. Obtaining such a representation is fundamental for the present work and it is given in Appendix D.

2. Minimal lateral ideals of $\mathbb{R}_{p,q}$

It is important for the objectives of this paper to know some results concerning the minimal lateral ideals of $\mathbb{R}_{p,q}$. The identification table of these algebras as matrix algebras helps a lot. Indeed, we have[61] the following theorem.

Theorem 49: *The maximum number of pairwise orthogonal idempotents in $\mathbb{K}(m)$ (where $\mathbb{K}=\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$) is m.*

The decomposition of $\mathbb{R}_{p,q}$ into minimal ideals is then characterized by a spectral set $\{e_{pq,j}\}$ of idempotents elements of $\mathbb{R}_{p,q}$ such that

(a) $\Sigma_{i=1}^{n} e_{pq,i}=1$,
(b) $e_{pq,j}e_{pq,k}=\delta_{jk}e_{pq,j}$,

(c) the rank of $e_{pq,j}$ is minimal and nonzero, i.e., is primitive.

By rank of $e_{pq,j}$ we mean the rank of the $\Lambda\mathbb{R}^{p,q}$ morphism, $e_{pq,j}:\phi\mapsto\phi e_{pq,j}$. Conversely, any $\phi\in\mathbf{I}_{pq,j}$ can be characterized by an idempotent $e_{pq,j}$ of minimal rank$\neq 0$, with $\phi=\phi e_{pq,j}$.

We now need to know the following theorem.[109]

Theorem 50: *A minimal left ideal of* $\mathbb{R}_{p,q}$ *is of the type*

$$\mathbf{I}_{pq}=\mathbb{R}_{p,q}e_{pq},$$

where

$$e_{pq}=\tfrac{1}{2}(1+e_{\alpha_1})\cdots\tfrac{1}{2}(1+e_{\alpha_k}) \tag{B13}$$

is a primitive idempotent of $\mathbb{R}_{p,q}$ *and were* $e_{\alpha_1},\cdots,e_{\alpha_k}$ *are commuting elements in the canonical basis of* $\mathbb{R}_{p,q}$ *generated in the standard way through the elements of the basis* Σ *such that* $(e_{\alpha_i})^2=1$, $(i=1,2,\ldots,k)$ *generate a group of order* 2^k, $k=q-r_{q-p}$ *and* r_i *are the Radon–Hurwitz numbers, defined by the recurrence formula* $r_{i+8}=r_i+4$ *and*

i	0	1	2	3	4	5	6	7
r_i	0	1	2	2	3	3	3	3

(B14)

Recall that $\mathbb{R}_{p,q}$ is a ring and the minimal lateral ideals are modules over the ring $\mathbb{R}_{p,q}$. They are *representation modules* of $\mathbb{R}_{p,q}$, and indeed we have (recall the table above) the following theorem.[141]

Theorem 51: *If* $p+q$ *is even or odd with* $p-q\neq 1$ *(mod 4), then*

$$\mathbb{R}_{p,q}=\mathrm{Hom}_{\mathbb{K}}(I_{pq})\simeq\mathbb{K}(m), \tag{B15}$$

where (as we already know) $\mathbb{K}=\mathbb{R}$, $\mathbb{C}$ *or* $\mathbb{H}$. *Also,*

$$\dim_{\mathbb{K}}(I_{pq})=m \tag{B16}$$

and

$$\mathbb{K}\simeq e\mathbb{K}(m)e, \tag{B17}$$

where e *is the representation of* $\mathbf{e}_{pq}$ *in* $\mathbb{K}(m)$.

If $p+q=n$ *is odd, with* $p-q=1$ *(mod 4), then*

$$\mathbb{R}_{p,q}=\mathrm{Hom}_{\mathbb{K}}(I_{pq})\simeq\mathbb{K}(m)\oplus\mathbb{K}(m), \tag{B18}$$

with

$$\dim_{\mathbb{K}}(I_{pq})=m \tag{B19}$$

and

$$e\mathbb{K}(m)e\simeq\mathbb{R}\oplus\mathbb{R}$$

or (B20)

$$e\mathbb{K}(m)e\simeq\mathbb{H}\oplus\mathbb{H}.$$

With the above isomorphisms we can immediately identify the minimal left ideals of $\mathbb{R}_{p,q}$ with the column matrices of $\mathbb{K}(m)$.

Algorithm for finding primitive idempotents of $\mathbb{R}_{p,q}$: With the ideas introduced above it is now a simple exercise to find primitive idempotents of $\mathbb{R}_{p,q}$. First we look at Table I and find the matrix algebra to which our particular Clifford algebra $\mathbb{R}_{p,q}$ is isomorphic. Suppose $\mathbb{R}_{p,q}$ is simple. (Once we know the algorithm for a simple Clifford algebra it is straightfoward to devise an algorithm for the semisimple Clifford algebras.) Let $\mathbb{R}_{p,q}\simeq\mathbb{K}(m)$ for a particular $\mathbb{K}$ and m. Next we take an element $e_{\alpha_1}\in\{e_A\}$ from the canonical basis $\{e_A\}$ of $\mathbb{R}_{p,q}$ such that

$$e_{\alpha_1}^2=1, \tag{B21}$$

then construct the idempotent $e_{pq}=(1+e_{\alpha_1})/2$ and the ideal $\mathbf{I}_{pq}=\mathbb{R}_{p,q}e_{pq}$ and calculate $\dim_{\mathbb{K}}(I_{pq})$. If $\dim_{\mathbb{K}}(I_{pq})=m$, then e_{pq} is primitive. If $\dim_{\mathbb{K}}(I_{pq})\neq m$, we choose $e_{\alpha 2}\in\{e_A\}$ such that $e_{\alpha 2}$ commutes with e_{α_1} and $e_{\alpha_2}^2=1$ [see Theorem 39 and construct the idempotent $e'_{pq}=(1+e_{\alpha_1})(1+e_{\alpha_1})/4$]. If $\dim_{\mathbb{K}}(I'_{pq})=m$, then e'_{pq} is primitive. Otherwise we repeat the procedure. According to the Theorem 39 the procedure is finite.

These results will be used in Appendix D in order to obtain necessary results for our presentation of the theory of algebraic and Dirac–Hestenes spinors (and spinors fields).

APPENDIX C: $\mathbb{R}^{\star}_{p,q}$, CLIFFORD, PINOR AND SPINOR GROUPS

The set of the invertible elements of $\mathbb{R}_{p,q}$ constitutes a non-Abelian group which we denote by $\mathbb{R}^{\star}_{p,q}$. It acts naturally on $\mathbb{R}_{p,q}$ as an algebra homomorphism through its adjoint representation

$$\mathrm{Ad}:\mathbb{R}^{\star}_{p,q}\rightarrow\mathrm{Aut}(\mathbb{R}_{p,q});u\mapsto\mathrm{Ad}_u,\ \text{with}\ \mathrm{Ad}_u(x)=uxu^{-1}. \tag{C1}$$

Definition 52: The Clifford–Lipschitz *group is the set*

$$\Gamma_{p,q}=\{u\in\mathbb{R}^{\star}_{p,q}|\forall x\in\mathbb{R}^{p,q},uxu^{-1}\in\mathbb{R}^{p,q}\}. \tag{C2}$$

Definition 53: The set $\Gamma^{+}_{p,q}=\Gamma_{p,q}\cap\mathbb{R}_{p,q}$ *is called* special *Clifford–Lipshitz group.*

Definition 54: The Pinor group $\mathrm{Pin}_{p.q}$ *is the subgroup of* $\Gamma_{p,q}$ *such that*

$$\begin{gathered}\mathrm{Pin}_{p,q}=\{u\in\Gamma_{p,q}|N(u)=\pm 1\},\\ N:\mathbb{R}_{p,q}\rightarrow\mathbb{R}_{p,q},N(x)=\langle\overline{x}x\rangle_0.\end{gathered} \tag{C3}$$

Definition 55: The Spin group $\mathrm{Spin}_{p,q}$ *is the set*

$$\mathrm{Spin}_{p,q}=\{u\in\Gamma_{p,q}|N(u)=\pm 1\}. \tag{C4}$$

It is easy to see that $\mathrm{Spin}_{p,q}$ is not connected.

Definition 56: The group $\mathrm{Spin}^{e}_{p,q}$ *is the set*

$$\mathrm{Spin}^{e}_{p,q}=\{u\in\Gamma_{p,q}|N(u)=+1\}. \tag{C5}$$

The superscript e, means that $\mathrm{Spin}^{e}_{p,q}$ is the connected component to the identity. We can prove that $\mathrm{Spin}^{e}_{p,q}$ is connected for all pairs (p,q) with the exception of $\mathrm{Spin}^{e}(1,0)\simeq\mathrm{Spin}^{e}(0,1)$.

We recall now some classical results[120] associated with the pseudo-orthogonal groups $\mathrm{O}_{p,q}$ of a vector space $\mathbb{R}^{p,q}$ $(n=p+q)$ and its subgroups.

Let $\mathbf{G}$ be a diagonal $n\times n$ matrix whose elements are

$$G_{ij}=\mathrm{diag}(1,1,\ldots,-1,-1,\ldots-1), \tag{C6}$$

with p positive and q negative numbers.

Definition 57: $O_{p,q}$ is the set of $n\times n$ real matrices $\mathbf{L}$ *such that*

$$\mathbf{L}\mathbf{G}\mathbf{L}^T=\mathbf{G},\quad \det\mathbf{L}^2=1. \tag{C7}$$

Equation (C7) shows that $\mathrm{O}_{p,q}$ is not connected.

Definition 58: $SO_{p,q}$, the special (proper) pseudo-orthogonal group is the set of $n\times n$ real matrices $\mathbf{L}$ *such that*

$$\mathbf{L}\mathbf{G}\mathbf{L}^T=\mathbf{G},\quad \det\mathbf{L}=1. \tag{C8}$$

When $p=0$ $(q=0)$ $\mathrm{SO}_{p,q}$ is connected. However, $\mathrm{SO}_{p,q}$ is not connected and has two connected components for $p,q\geqslant 1$. The group $\mathrm{SO}^e_{p,q}$, the connected component to the identity of $\mathrm{SO}_{p,q}$ will be called the special *orthocronous* pseudo-orthogonal group. [This nomenclature comes from the fact that $\mathrm{SO}^e(1,3)=\mathcal{L}^{\uparrow}_{+}$ is the special (proper) orthochronous Lorentz group. In this case the set is easily defined by the condition $L^0_0\geqslant +1$. For the general case see Ref. 120.]

Theorem 59: *$Ad_{|\mathrm{Pin}_{p,q}}:\mathrm{Pin}_{p,q}\to \mathrm{O}_{p,q}$ is onto with kernel $\mathbb{Z}_2$. $Ad_{|\mathrm{Spin}_{p,q}}:\mathrm{Spin}_{p,q}\to\mathrm{SO}_{p,q}$ is onto with kernel $\mathbf{Z}_2$. $Ad_{|\mathrm{Spin}^e_{p,q}}:\mathrm{Spin}^e_{p,q}\to\mathrm{SO}^e_{p,q}$ is onto with kernel $\mathbf{Z}_2$. We have*

$$\mathrm{O}_{p,q}=\frac{\mathrm{Pin}_{p,q}}{\mathbb{Z}_2},\quad \mathrm{SO}_{p,q}=\frac{\mathrm{Spin}_{p,q}}{\mathbb{Z}_2},\quad \mathrm{SO}^e_{p,q}=\frac{\mathrm{Spin}^e_{p,q}}{\mathbb{Z}_2}. \tag{C9}$$

The group homomorphism between $\mathrm{Spin}^e_{p,q}$ and $\mathrm{SO}^e(p,q)$ will be denoted by

$$\mathbf{L}:\mathrm{Spin}^e_{p,q}\to\mathrm{SO}^e_{p,q}. \tag{C10}$$

The following theorem that first appears in Porteous book[141] is very important. (In particular, when Theorem 49 is taken into account together with some of the coincidence between the complexifications of some low dimensions Clifford algebras it becomes clear that the construction of Dirac–Hestenes spinors [and its representation as in Eq. (D20)] for Minkowski vector space has no generalization for vector spaces of arbitrary dimensions and signatures.[109])

Theorem 60 (Porteous): *For $p+q\leqslant 5$, $\mathrm{Spin}^e(p,q)=\{u\in\mathbb{R}_{p,q}|u\tilde{u}=1\}$.*

Lie algebra of $\mathrm{Spin}^e_{1,3}$: It can be shown[109] that for each $u\in\mathrm{Spin}^e_{1,3}$ it holds $u=\pm e^F$, $F\in\Lambda^2\mathbb{R}^{1,3}\subset\mathbb{R}_{1,3}$ and F can be chosen in such a way to have a positive sign in Eq. (C8), except in the particular case $F^2=0$ when $u=-e^F$. From Eq. (C8) it follows immediately that the Lie algebra of $\mathrm{Spin}^e_{1,3}$ is generated by the bivectors $F\in\Lambda^2\mathbb{R}^{1,3}\subset\mathbb{R}_{1,3}$ through the commutator product. More details on the relations of Clifford algebras and the rotation groups may be found, e.g., in Refs. 7 and 170.

APPENDIX D: SPINOR REPRESENTATIONS OF $\mathbb{R}_{4,1}$, $\mathbb{R}^{+}_{4,1}$, AND $\mathbb{R}_{1,3}$

Let $b_0=\{E_0,E_1,E_2,E_3\}$ be an orthogonal basis of $\mathbb{R}^{1,3}\subset\mathbb{R}_{1,3}$, such that $E_\mu E_\nu+E_\nu E_\mu=2\eta_{\mu\nu}$, with $\eta_{\nu\mu}=\mathrm{diag}(+1,-1,-1,-1)$. Now, with the results of Appendix B we can verify without difficulties that the elements e, e', $e''\in\mathbb{R}_{1,3}$,

$$e=\tfrac{1}{2}(1+E_0), \tag{D1}$$

$$e'=\tfrac{1}{2}(1+E_3E_0), \tag{D2}$$

$$e''=\tfrac{1}{2}(1+E_1E_2E_3), \tag{D3}$$

are primitive idempotents of $\mathbb{R}_{1,3}$ The minimal left ideals, $I=\mathbb{R}_{1,3}e$, $I'=\mathbb{R}_{1,3}e'$, $I''=\mathbb{R}_{1,3}e''$ are *right* two dimension linear spaces over the quaternion field (e.g., $\mathbb{H}e=e\mathbb{H}=e\mathbb{R}_{1,3}e$). According to a definition given originally in Ref. 150 these ideals are algebraically equivalent. For example, $e'=ueu^{-1}$, with $u=(1+E_3)\notin\Gamma_{1,3}$.

Definition 61: The elements $\Phi\in\mathbb{R}_{1,3}\frac{1}{2}(1+E_0)$ *are called* mother *spinors*.

The above denomination has been given (with justice) by Lounesto.[109] It can be shown[67,68] that each Φ can be written

$$\Phi=\psi_1 e+\psi_2 E_3E_1e+\psi_3E_3E_0e+\psi_4E_1E_0e=\sum_i\ \psi_i s_i\,, \tag{D4}$$

$$s_1=e,\quad s_2=E_3E_1e,\quad s_3=E_3E_0e,\quad s_4=E_1E_0e \tag{D5}$$

and where the ψ_i are *formally* complex numbers, i.e., each $\psi_i=(a_i+b_iE_2E_1)$ with a_i, $b_i\in\mathbb{R}$ and the set $\{s_i,i=1,2,3,4\}$ is a basis in the mother spinors space.

We recall from the general result of Appendix C that $\mathrm{Pin}_{1,3}/\mathbb{Z}_2\simeq\mathrm{O}_{1,3}$, $\mathrm{Spin}_{1,3}/\mathbb{Z}_2\simeq\mathrm{SO}_{1,3}$, $\mathrm{Spin}^e_{1,3}/\mathbb{Z}_2\simeq\mathrm{SO}^e_{1,3}$, and $\mathrm{Spin}^e_{1,3}\simeq\mathrm{Sl}(2,\mathbb{C})$ is the universal covering group of $\mathcal{L}^{\uparrow}_{+}\equiv\mathrm{SO}^e_{1,3}$, the *special* (proper) *orthocronous* Lorentz group.

In order to determine the relation between $\mathbb{R}_{4,1}$ and $\mathbb{R}_{3,1}$ we proceed as follows: let $\{F_0,F_1,F_2,F_3,F_4\}$ be an orthonormal basis of $\mathbb{R}_{4,1}$ with

$$-F_0^2=F_1^2=F_2^2=F_3^2=F_4^2=1,F_AF_B=-F_BF_A(A\neq B;A,B=0,1,2,3,4).$$

Define the pseudoscalar

$$\mathbf{i}=F_0F_1F_2F_3F_4,\quad \mathbf{i}^2=-1,\quad \mathbf{i}F_A=F_A\mathbf{i},\quad A=0,1,2,3,4. \tag{D6}$$

Define

$$\mathcal{E}_\mu=F_\mu F_4\,. \tag{D7}$$

We can immediately verify that $\mathcal{E}_\mu\mathcal{E}_\nu+\mathcal{E}_\nu\mathcal{E}_\mu=2\,\eta_{\mu\nu}$. Taking into account that $\mathbb{R}_{1,3}\simeq\mathbb{R}^0_{4,1}$ we can explicitly exhibit here this isomorphism by considering the map $\mathrm{j}:\mathbb{R}_{1,3}\to\mathbb{R}_{4,1}$ generated by the linear extension of the map $\mathrm{j}^{\#}:\mathbb{R}^{1,3}\to\mathbb{R}_{4,1}$, $\mathrm{j}^{\#}(F_\mu)=\mathcal{E}_\mu=F_\mu F_4$, where $\mathcal{E}_\mu$ $(\mu=0,1,2,3)$ is an orthogonal basis of $\mathbb{R}^{1,3}$. Also $\mathrm{j}(1_{\mathbb{R}_{1,3}})=1_{\mathbb{R}^+_{4,1}}$, where $1_{\mathbb{R}_{1,3}}$ and $1_{\mathbb{R}^+_{4,1}}$ are the identity elements in $\mathbb{R}_{1,3}$ and $\mathbb{R}^+_{4,1}$. Now consider the primitive idempotent of $\mathbb{R}_{1,3}\simeq\mathbb{R}^0_{4,1}$,

$$e_{41}=\mathrm{j}(e)=\tfrac{1}{2}(1+\mathcal{E}_0) \tag{D8}$$

and the minimal left ideal $I_{4,1}=\mathbb{R}_{4,1}e_{41}$.

In what follows we use (when convenient) for minimal idempotents and the minimal ideals generated by them, the labels involving the notion of spinorial frames discussed in Sec. II. Let then, Ξ_0 be a fiducial spinorial frame. The elements [in what follows we use (when convenient) for minimal idempotents and the minimal ideals generated by them, the labels involving the notion of spin frames discussed in Sec. II] $Z_{\Xi_0}\in I_{4,1}$ can be written analogously to $\Phi\in\mathbb{R}_{1,3}\frac{1}{2}(1+E_0)$ as

$$Z_{\Xi_0}=\sum\ z_i\overline{s_i}\,, \tag{D9}$$

where

$$\overline{s_1}=e_{41},\quad \overline{s_2}=\mathcal{E}_1\mathcal{E}_3e_{41},\quad \overline{s_3}=\mathcal{E}_3\mathcal{E}_0e_{41},\quad \overline{s_4}=\mathcal{E}_1\mathcal{E}_0e_{41} \tag{D10}$$

and where

$$z_i = a_i + \mathcal{E}_2\mathcal{E}_1 b_i$$

are formally complex numbers, a_i, $b_i \in \mathbb{R}$.

Consider now the element $f_{\Xi_0} \in \mathbb{R}_{4,1}$,

$$f_{\Xi_0} = e_{41}\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2) = \tfrac{1}{2}(1+\mathcal{E}_0)\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2), \tag{D11}$$

with **i** defined as in Eq. (D6).

Since $f_{\Xi_0}\mathbb{R}_{4,1}f_{\Xi_0} = \mathbb{C}f_{\Xi_0} = f_{\Xi_0}\mathbb{C}$ it follows that f_{Ξ_0} is a primitive idempotent of $\mathbb{R}_{4,1}$. We can easily show that each $\Phi_{\Xi_0} \in I_{\Xi_0} = \mathbb{R}_{4,1}f_{\Xi_0}$ can be written

$$\Psi_{\Xi_0} = \sum_i \psi_i f_i, \quad \psi_i \in \mathbb{C},$$
$$f_1 = f_{\Xi_0}, \quad f_2 = -\mathcal{E}_1\mathcal{E}_3 f_{\Xi_0}, \quad f_3 = \mathcal{E}_3\mathcal{E}_0 f_{\Xi_0}, \quad f_4 = \mathcal{E}_1\mathcal{E}_0 f_{\Xi_0} \tag{D12}$$

with the methods described in Refs. 67 and 68 we find the following representation in $\mathbb{C}(4)$ for the generators $\mathcal{E}_\mu$ of $\mathbb{R}_{4,1} \simeq \mathbb{R}_{1,3}$:

$$\mathcal{E}_0 \mapsto \underline{\gamma}_0 = \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix} \leftrightarrow \mathcal{E}_i \mapsto \underline{\gamma}_i = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}, \tag{D13}$$

where $\mathbf{1}_2$ is the unit 2×2 matrix and σ_i $(i=1,2,3)$ are the standard Pauli matrices. We immediately recognize the $\underline{\gamma}$-matrices in Eq. (D13) as the standard ones appearing, e.g., in Ref. 13.

The matrix representation of $\Psi_{\Xi_0} \in I_{\Xi_0}$ will be denoted by the same letter without the index, i.e., $\Psi_{\Xi_0} \mapsto \boldsymbol{\Psi} \in \mathbb{C}(4)f$, where

$$f = \tfrac{1}{2}(1 + i\,\underline{\gamma}_1\underline{\gamma}_2) \quad i = \sqrt{-1}. \tag{D14}$$

We have

$$\boldsymbol{\Psi} = \begin{pmatrix} \psi_1 & 0 & 0 & 0 \\ \psi_2 & 0 & 0 & 0 \\ \psi_3 & 0 & 0 & 0 \\ \psi_4 & 0 & 0 & 0 \end{pmatrix}, \quad \psi_i \in \mathbb{C}. \tag{D15}$$

Equations (D13), (D14), and (D15) are sufficient to prove that there are bijections between the elements of the ideals $\mathbb{R}_{1,3}\frac{1}{2}(1+E_0)$, $\mathbb{R}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)$, and $\mathbb{R}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)\frac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2)$.

We can easily find that the following relation exist between $\Psi_{\Xi_0} \in \mathbb{R}_{4,1}f_{\Xi_0}$ and $Z_{\Xi_0} \in \mathbb{R}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)$, $\Xi_0 = (u_0, \Sigma_0)$ being a spinorial frame (see Sec. I)

$$\Psi_{\Xi_0} = Z_{\Xi_0}\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2). \tag{D16}$$

Decomposing Z_{Ξ_0} into even and odd parts relative to the $\mathbf{Z}_2$-graduation of $\mathbb{R}^0_{4,1} \simeq \mathbb{R}_{1,3}$, $Z_{\Xi_0} = Z^0_{\Xi_0} + Z^1_{\Xi_0}$ we obtain $Z^0_{\Xi_0} = Z^1_{\Xi_0}\mathcal{E}_0$ which clearly shows that all information of Z_{Ξ_0} is contained in $Z^0_{\Xi_0}$. Then,

$$\Psi_{\Xi_0} = Z^0_{\Xi_0}\tfrac{1}{2}(1+\mathcal{E}_0)\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2). \tag{D17}$$

Now, if we take into account[150] that $\mathbb{R}^{0}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)=\mathbb{R}^{00}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)$ where the symbol $\mathbb{R}^{00}_{4,1}$ means $\mathbb{R}^{00}_{4,1}\simeq\mathbb{R}^{0}_{1,3}\simeq\mathbb{R}_{3,0}$ we see that each $Z_{\Xi_0}\in\mathbb{R}_{4,1}\frac{1}{2}(1+\mathcal{E}_0)$ can be written

$$Z_{\Xi_0}=\psi_{\Xi_0}\tfrac{1}{2}(1+\mathcal{E}_0),\quad \psi_{\Xi_0}\in\mathbb{R}^{00}_{4,1}\simeq\mathbb{R}^{0}_{1,3}. \tag{D18}$$

Then setting $Z^{0}_{\Xi_0}=\psi_{\Xi_0}/2$, Eq. (D18) can be written

$$\Psi_{\Xi_0}=\psi_{\Xi_0}\tfrac{1}{2}(1+\mathcal{E}_0)\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2)=Z^{0}_{\Xi_0}\tfrac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2). \tag{D19}$$

The matrix representation of Z_{Ξ_0} and ψ_{Ξ_0} in $\mathbb{C}(4)$ (denoted by the same letter in boldface without index) in the spin basis given by Eq. (D12) are

$$\Psi=\begin{pmatrix}\psi_1 & -\psi_2^* & \psi_3 & \psi_4^*\\ \psi_2 & \psi_1^* & \psi_4 & -\psi_3^*\\ \psi_3 & \psi_4^* & \psi_1 & -\psi_2^*\\ \psi_4 & -\psi_3^* & \psi_2 & \psi_1^*\end{pmatrix},\quad \mathbf{Z}=\begin{pmatrix}\psi_1 & -\psi_2^* & 0 & 0\\ \psi_2 & \psi_1^* & 0 & 0\\ \psi_3 & \psi_4^* & 0 & 0\\ \psi_4 & -\psi_3^* & 0 & 0\end{pmatrix}. \tag{D20}$$

APPENDIX E: WHAT IS A COVARIANT DIRAC SPINOR (CDS)

As we already know $f_{\Xi_0}=\frac{1}{2}(1+\mathcal{E}_0)\frac{1}{2}(1+\mathbf{i}\mathcal{E}_1\mathcal{E}_2)$ [Eq. (D12)] is a primitive idempotent of $\mathbb{R}_{4,1}\simeq\mathbb{C}(4)$. If $u\in\mathrm{Spin}(1,3)\subset\mathrm{Spin}(4,1)$ then all ideals $I_{\Xi_u}=I_{\Xi_0}u^{-1}$ are geometrically equivalent to I_{Ξ_0}. Now, let $\mathbf{s}(\Xi_u)=\{\mathfrak{E}_0,\mathfrak{E}_1,\mathfrak{E}_2,\mathfrak{E}_3\}$ and $\mathbf{s}(\Xi_{u'})=\{\mathfrak{E}'_0,\mathfrak{E}'_1,\mathfrak{E}'_2,\mathfrak{E}'_3\}$ with $\mathbf{s}(\Xi_u)=u^{-1}\mathbf{s}(\Xi_0)u$, $\mathbf{s}(\Xi_{u'})=u'^{-1}\mathbf{s}(\Xi_0)u'$ be two arbitrary basis for $\mathbb{R}^{1,3}\subset\mathbb{R}_{4,1}$. From Eq. (D13) we can write

$$I_{\Xi_u}\ni\Psi_{\Xi_u}=\sum\ \psi_i f_i,\quad \text{and } I_{\Xi'_u}\ni\Psi_{\Xi_{u'}}=\sum\ \psi'_i f'_i, \tag{E1}$$

where

$$f_1=f_{\Xi_u},\quad f_2=-\mathfrak{E}_1\mathfrak{E}_3 f_{\Xi_u},\quad f_3=\mathfrak{E}_3\mathfrak{E}_0 f_{\Xi_u},\quad f_4=\mathfrak{E}_1\mathfrak{E}_0 f_{\Xi_u}$$

and

$$f'_1=f_{\Xi_{u'}},\quad f'_2=-\mathfrak{E}'_1\mathfrak{E}'_3 f_{\Xi_{u'}},\quad f'_3=\mathfrak{E}'_3\mathfrak{E}'_0 f_{\Xi_{u'}},\quad f_4=\mathfrak{E}'_1\mathfrak{E}'_0 f_{\Xi_{u'}}.$$

Since $\Psi_{\Xi_{u'}}=\Psi_{\Xi_u}(u'^{-1}u)^{-1}$, we get

$$\Psi_{\Xi_{u'}}=\sum_i\ \psi_i(u'^{-1}u)^{-1}f'_i=\sum_{i,k}\ S_{ik}[(u^{-1}u')]\psi_i f_k=\sum_k\ \psi'_k f_k.$$

Then

$$\psi'_k=\sum_i\ S_{ik}(u^{-1}u')\psi_i, \tag{E2}$$

where $S_{ik}(u^{-1}u')$ are the matrix components of the representation in $\mathbb{C}(4)$ of $(u^{-1}u')\in\mathrm{Spin}^{e}_{1,3}$. As proved in Refs. 67 and 68 the matrices $S(u)$ correspond to the representation $D^{(1/2,0)}\oplus D^{(0,1/2)}$ of $\mathrm{SL}(2,\mathbb{C})\simeq\mathrm{Spin}^{e}_{1,3}$.

We remark that all the elements of the set $\{I_{\Xi_u}\}$ of the ideals geometrically equivalent to I_{Ξ_0} under the action of $u \in \mathrm{Spin}^e_{1,3} \subset \mathrm{Spin}^e_{4,1}$ have the same image $I = \mathbb{C}(4)f$ where f is given by Eq. (D11), i.e.,

$$f = \tfrac{1}{2}(1+\underline{\gamma}_0)(1+i\underline{\gamma}_1\underline{\gamma}_2), \quad i = \sqrt{-1}, \tag{E3}$$

where $\underline{\gamma}_\mu$, $\mu = 0,1,2,3$ are the Dirac matrices given by Eq. (D14).

Then, if

$$\begin{gathered}\gamma: \mathbb{R}_{4,1} \to \mathbb{C}(4) \equiv \mathrm{End}(\mathbb{C}(4)f), \\ x \mapsto \gamma(x): \mathbb{C}(4)f \to \mathbb{C}(4)f\end{gathered} \tag{E4}$$

it follows that

$$\gamma(\mathfrak{E}_\mu) = \gamma(\mathfrak{E}'_\mu), \quad \gamma(f_\mu) = \gamma(f'_\mu) \tag{E5}$$

for all $\{\mathfrak{E}_\mu\}$, $\{\mathfrak{E}'_\mu\}$ such that $\mathfrak{E}'_\mu = (u'^{-1}u)\mathfrak{E}_\mu(u'^{-1}u)^{-1}$. Observe that *all information* concerning the geometrical images of the spinorial frames Ξ_u, $\Xi_{u'}, \ldots,$ under **s** disappear in the matrix representation of the ideals I_{Ξ_u}, $I_{\Xi_{u'}}, \ldots,$ in $\mathbb{C}(4)$ since all these ideals are mapped in the same ideal $I = \mathbb{C}(4)f$.

With the above remark and taking into account the definition of algebraic spinors given in Sec. II C and Eq. (E2) we are lead to the following.

Definition 62: A covariant Dirac spinor (CDS) for $\mathbb{R}^{1,3}$ *is an equivalence class of pairs* $(\Xi^m_u, \boldsymbol{\Psi})$, *where* Ξ^m_u *is a matrix spinorial frame associated to the spinorial frame* Ξ_u *through the* $S(u^{-1}) \in D^{(1/2,0)} \oplus D^{(0,1/2)}$ *representation of* $\mathrm{Spin}^e_{1,3}$, $u \in \mathrm{Spin}^e_{1,3}$. *We say that* $\Psi, \Psi' \in \mathbb{C}(4)f$ *are equivalent and write*

$$(\Xi^m_u, \Psi) \sim (\Xi^m_{u'}, \Psi') \tag{E6}$$

if and only if

$$\Psi' = S(u'^{-1}u)\Psi, \quad u\mathbf{s}\Xi_u u^{-1} = u'\mathbf{s}(\Xi_{u'})u'^{-1}. \tag{E7}$$

Remark 63: The definition of CDS just given agrees with that given in Ref. 40 except for the irrelevant fact that there, as well as in the majority of Physics textbook's, authors use as the space of representatives of a CDS a complex four-dimensional space $\mathbb{C}^4$ *instead of* $I = \mathbb{C}(4)f$.

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The bundles of algebraic and Dirac–Hestenes spinor fields

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Our main objective in this paper is to clarify the *ontology* of Dirac–Hestenes spinor fields (DHSF) and its relationship with even multivector fields, on a Riemann–Cartan spacetime (RCST) $\mathfrak{M}=(M,g,\nabla,\tau_g,\uparrow)$ admitting a spin structure, and to give a mathematically rigorous derivation of the so-called Dirac–Hestenes equation (DHE) in the case where $\mathfrak{M}$ is a Lorentzian spacetime (the general case when $\mathfrak{M}$ is a RCST will be discussed in another publication). To this aim we introduce the Clifford bundle of multivector fields $(\mathcal{C}\ell(M,g))$ and the *left* $(C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M))$ and *right* $(\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M))$ spin-Clifford bundles on the spin manifold (M,g). The relation between *left ideal algebraic spinor fields* (LIASF) and Dirac–Hestenes *spinor* fields (both fields are sections of $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$) is clarified. We study in detail the theory of covariant derivatives of Clifford fields as well as that of left and right spin-Clifford fields. A consistent Dirac equation for a DHSF $\Psi\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ (denoted DE$\mathcal{C}\ell^{l}$) on a Lorentzian spacetime is found. We also obtain a *representation* of the DE$\mathcal{C}\ell^{l}$ in the Clifford bundle $\mathcal{C}\ell(M,g)$. It is such equation that we call the DHE and it is satisfied by Clifford fields $\psi_{\Xi}\in\sec\mathcal{C}\ell(M,g)$. This means that to each DHSF $\Psi\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ and spin frame $\Xi\in\sec P_{\mathrm{Spin}^{e}_{1,3}}(M)$, there is a well-defined sum of even multivector fields $\psi_{\Xi}\in\sec\mathcal{C}\ell(M,g)$ (EMFS) associated with Ψ. Such an EMFS is called a *representative* of the DHSF on the given spin frame. And, of course, such a EMFS (the representative of the DHSF) is *not* a spinor field. With this crucial distinction between a DHSF and its *representatives* on the Clifford bundle, we provide a consistent theory for the covariant derivatives of Clifford and spinor fields of all kinds. We emphasize that the DE$\mathcal{C}\ell^{l}$ and the DHE, although related, are equations of different mathematical natures. We study also the local Lorentz invariance and the electromagnetic gauge invariance and show that only for the DHE such transformations are of the same mathematical nature, thus suggesting a possible link between them. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1757038]

I. INTRODUCTION

The main objective of this paper is to clarify the *ontology* of Dirac–Hestenes spinor fields (DHSF) (for the genesis of these objects we quote Ref. 19) on general Riemann–Cartan spacetimes (RCST) and to give a mathematically justified account of the Dirac–Hestenes equation

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(DHE) on Lorentzian spacetimes, subjects that have been a matter of many misunderstandings and controversies (as discussed in Ref. 34). Recall that the flat spacetime DHE represents the state of an electron by a map Ψ with values in the even part of the Clifford algebra $\mathbb{R}_{1,3}$. However, a covariant formulation of the DHE on a (possibly curved) Lorentzian spacetime cannot promote Ψ, in a canonical way, to a section of the Clifford bundle $\mathcal{C}\ell(M,g)$ (whose objects transform as tensors and therefore cannot describe spin-1/2 particles). In Ref. 34, DHSF on a Minkowski spacetime were defined as equivalence classes of Clifford fields. Here we follow a different approach, and define DHSF as even sections of an appropriate spinorial Clifford bundle. The objects satisfying the Dirac–Hestenes equation are then even multivector fields which are *representatives* of DHSF on the tensorial Clifford bundle. Moreover, such a representative is manifestly spin-frame dependent, so that no contradiction arises in representing spinors by Clifford fields.

To achieve our goals, we introduce in Sec. II the Clifford bundle of multivector fields $(\mathcal{C}\ell(M,g))$, and the *left* $(\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M))$ and *right* $(\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M))$ spin-Clifford bundles on the spin manifold (M,g), and study in detail how these bundles are related. [Of course, all the results of the present paper could also be obtained in the case where $\mathcal{C}\ell(M,g)$ is a Clifford bundle of nonhomogeneous differential forms.] Left algebraic spinor fields and Dirac–Hestenes spinor fields [both fields are sections of $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$] are defined and the relation between them is established. In Sec. IV, a consistent Dirac equation for a DHSF $\Psi \in \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ (denoted DE$\mathcal{C}\ell^{l}$) on a Lorentzian manifold is found. In Sec. V, we obtain a *representation* of the DE$\mathcal{C}\ell^{l}$ in the Clifford bundle, an equation we call the Dirac–Hestenes equation (DHE), which is satisfied by Clifford fields $\psi_{\Xi} \in \sec \mathcal{C}\ell(M,g)$. This means that to each DHSF $\Psi \in \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ and to each *spin frame* $\Xi \in \sec P_{\mathrm{Spin}^{e}_{1,3}}(M)$ there is a well-defined sum of even multivector fields $\psi_{\Xi} \in \sec \mathcal{C}\ell(M,g)$ (EMFS) associated with Ψ. Such an EMFS is called a *representative* of the DHSF on the given spin frame. And, of course, such an EMFS (the representative of the DHSF) is *not* a spinor field. With this crucial distinction between a DHSF and their EMFS representatives, we present in Sec. V an *effective* spinorial connection for the representatives of a DHSF on $\mathcal{C}\ell(M,g)$, thus providing a consistent theory for the covariant derivatives of Clifford and spinor fields of all kinds.

We emphasize that the DE$\mathcal{C}\ell^{l}$ and the DHE, although related, are of different mathematical natures. This issue has been particularly scrutinized in Secs. IV and V. We study also the local Lorentz invariance and the electromagnetic gauge invariance and show that only for the DHE such transformations are of the same mathematical nature, thus suggesting a possible link between them. In a sequel paper we are going to investigate this issue and also (a) the formulation of the DE$\mathcal{C}\ell$ and DHE in an arbitrary Riemann–Cartan spacetime through the use of a variational principle (we shall use in our approach to the subject the techniques of the multivector and extensor calculus developed in Refs. 12–14, 25–28); (b) the theory of the Lie derivative of the LIASF and DHSF; and (c) the claim in Ref. 17 that the existence of spinor fields in a Lorentzian manifold requires a minimum amount of curvature. This problem is important in view of the proposed teleparallel theories of the gravitational field.

Finally, in the Appendix we derive some formulas employed in the main text for the covariant derivative of Clifford and spinor fields, using the general theory of covariant derivatives on associated vector bundles. In general, our notation corresponds to that in Ref. 34.

A few acronyms are used in the present paper (to avoid long sentences) and they are summarized below for the reader's convenience:

DHE—Dirac–Hestenes Equation

DHSF—Dirac–Hestenes Spinor Field

DE$\mathcal{C}\ell^{l}$—Dirac equation for a DHSF $\Psi \in \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$

EMFS—Even Multivector Fields

LIASF—Left Ideal Algebraic Spinor Field

PFB—Principal Fiber Bundle

RIASF—Right Ideal Algebraic Spinor Field
RCST—Riemann–Cartan Spacetime

II. THE CLIFFORD BUNDLE OF SPACETIME AND THEIR IRREDUCIBLE MODULE REPRESENTATIONS

A. The Clifford bundle of spacetime

Let M be a four dimensional, real, connected, paracompact and noncompact manifold. Let TM $[T^*M]$ be the tangent [cotangent] bundle of M.

Definition 1: A Lorentzian manifold is a pair (M,g), *where* $g \in \sec T^{2,0}M$ *is a Lorentzian metric of signature* (1,3), *i.e., for all* $x \in M$, $T_xM \simeq T_x^*M \simeq \mathbb{R}^{1,3}$, *where* $\mathbb{R}^{1,3}$ *is the vector Minkowski space.*

Definition 2: A spacetime $\mathfrak{M}$ *is a pentuple* $(M,g,\nabla,\tau_g,\uparrow)$ *where* $(M,g,\tau_g,\uparrow)$ *is an oriented Lorentzian manifold (oriented by* τ_g*) and time oriented by an appropriated equivalence relation (denoted* $\uparrow$*) for the timelike vectors at the tangent space* T_xM, $\forall x \in M$. *(See Ref. 35 for details.)* ∇ *is a linear connection for* M *such that* $\nabla g = 0$.

Definition 3: Let $\mathbf{T}$ *and* $\mathbf{R}$ *be respectively, the torsion and curvature tensors of* ∇. *If in addition to the requirements of the previous definitions,* $\mathbf{T}(\nabla)=0$, *then* $\mathfrak{M}$ *is said to be a Lorentzian spacetime. The particular Lorentzian spacetime where* $M \simeq \mathbb{R}^4$ *and such that* $\mathbf{R}(\nabla)=0$ *is called Minkowski spacetime and will be denoted by* $\mathcal{M}$. *When* $\mathbf{T}(\nabla)$ is possibly nonzero, $\mathfrak{M}$ *is said to be a Riemann–Cartan spacetime (RCST). A particular RCST such that* $\mathbf{R}(\nabla)=0$ *is called a teleparallel spacetime.*

In what follows $P_{\mathrm{SO}^e_{1,3}}(M)$ denotes the principal bundle of oriented *Lorentz tetrads*. [We assume that the reader is acquainted with the structure of $P_{\mathrm{SO}^e_{1,3}}(M)$, whose sections are the time oriented and oriented orthonormal frames, each one associated by a local trivialization to a *unique* element of $SO^e_{1,3}(M)$. See, e.g., Refs. 16, 22, 29, 30.]

It is well known[32] that the natural operations on metric vector spaces, such as direct sum, tensor product, exterior power, etc., carry over canonically to vector bundles with metrics. We have the following definition.

Definition 4: The Clifford bundle of the Lorentzian manifold (M,g) *is the bundle of algebras,*

$$\mathcal{C}\ell(M,g) = \bigcup_{x \in M} \mathcal{C}\ell(T_xM,g_x), \tag{1}$$

where $\mathcal{C}\ell(T_xM,g_x)$ *is the Clifford algebra associated with* (T_xM,g_x) *(see, e.g. Ref. 34).*

As is well known,[4,5,10] $\mathcal{C}\ell(M,g)$ is a *quotient* (or *factor*) bundle, namely

$$\mathcal{C}\ell(M,g) = \frac{\tau M}{\mathcal{J}(M,g)}, \tag{2}$$

where $\tau M = \oplus_{r=0}^{\infty} T^{0,r}M$ and $T^{(0,r)}M$ is the space of r-contravariant tensor fields, and $\mathcal{J}(M,g)$ is the bundle of ideals whose fibers are the two-sided ideals in τM generated by the elements of the form $a\otimes b + b\otimes a - 2g(a,b)$, with $a,b \in TM$. In what follows, we denote the real Clifford algebra associated to $\mathbb{R}^{p,q}$ by $\mathbb{R}_{p,q}$. The even subalgebra of $\mathbb{R}_{p,q}$ will be denoted by $\mathbb{R}^0_{p,q}$ (see, e.g., Ref. 34).

Let $\pi_c : \mathcal{C}\ell(M,g) \to M$ be the canonical projection of $\mathcal{C}\ell(M,g)$ and let $\{U_\alpha\}$ be an open covering of M. There are trivialization mappings $\psi_i : \pi_c^{-1}(U_i) \to U_i \times \mathbb{R}_{1,3}$ of the form $\psi_i(p) = (\pi_c(p), \psi_{i,x}(p)) = (x, \psi_{i,x}(p))$. If $x \in U_i \cap U_j$ and $p \in \pi_c^{-1}(x)$, then

$$\psi_{i,x}(p) = h_{ij}(x)\psi_{j,x}(p), \tag{3}$$

for $h_{ij}(x) \in \mathrm{Aut}(\mathbb{R}_{1,3})$, where $h_{ij} : U_i \cap U_j \to \mathrm{Aut}(\mathbb{R}_{1,3})$ are the transition mappings of $\mathcal{C}\ell(M,g)$. We know that every automorphism of $\mathbb{R}_{1,3}$ is *inner* and it follows that

$$h_{ij}(x)\psi_{j,x}(p)=g_{ij}(x)\psi_{i,x}(p)g_{ij}(x)^{-1}, \tag{4}$$

for some $g_{ij}(x)\in\mathbb{R}^{\star}_{1,3}$, the group of invertible elements of $\mathbb{R}_{1,3}$.

Now, the group $\mathrm{SO}^{e}_{1,3}$ has as it is well known (see, e.g., Refs. 2, 3, 5, 21, 34) a natural extension in the Clifford algebra $\mathbb{R}_{1,3}$. Indeed we know that $\mathbb{R}^{\star}_{1,3}$ acts naturally on $\mathbb{R}_{1,3}$ as an algebra automorphism through its adjoint representation. A set of *lifts* of the transition functions of $\mathcal{C}\ell(M,g)$ is a set of $\mathbb{R}^{\star}_{1,3}$-valued functions $\{g_{ij}\}$ such that if

$$\begin{gathered}\mathrm{Ad}:g\mapsto \mathrm{Ad}_g,\\ \mathrm{Ad}_g(a)=gag^{-1},\forall a\in\mathbb{R}_{1,3},\end{gathered} \tag{5}$$

then $\mathrm{Ad}_{g_{ij}}=h_{ij}$ in all intersections.

Also $\sigma=\mathrm{Ad}|_{\mathrm{Spin}^{e}_{1,3}}$ defines a group homeomorphism $\sigma:\mathrm{Spin}^{e}_{1,3}\to\mathrm{SO}^{e}_{1,3}$ which is onto with kernel $\mathbb{Z}_2$. [Recall that $\mathrm{Spin}^{e}_{1,3}=\{a\in\mathbb{R}^{0}_{1,3}:a\tilde{a}=1\}\simeq\mathrm{SL}(2,\mathbb{C})$ is the universal covering group of the restricted Lorentz group $\mathrm{SO}^{e}_{1,3}$. See, e.g., Ref. 34.] We have that $\mathrm{Ad}_{-1}=$identity, and so $\mathrm{Ad}:\mathrm{Spin}^{e}_{1,3}\to\mathrm{Aut}(\mathbb{R}_{1,3})$ descends to a representation of $\mathrm{SO}^{e}_{1,3}$. Let us call Ad' this representation, i.e., $\mathrm{Ad}':\mathrm{SO}^{e}_{1,3}\to\mathrm{Aut}(\mathbb{R}_{1,3})$. Then we can write $\mathrm{Ad}'_{\sigma(g)}a=\mathrm{Ad}_g a=gag^{-1}$.

From this it is clear that the structure group of the Clifford bundle $\mathcal{C}\ell(M,g)$ is reducible from $\mathrm{Aut}(\mathbb{R}_{1,3})$ to $\mathrm{SO}^{e}_{1,3}$. This follows immediately from the Lorentzian structure of (M,g) and the fact that $\mathcal{C}\ell(M,g)$ is the exterior bundle where the fibers are equipped with the Clifford product. Thus the transition maps of the principal bundle of oriented Lorentz tetrads $P_{\mathrm{SO}^{e}_{1,3}}(M)$ can be (through Ad') taken as transition maps for the Clifford bundle. We then have[5]

$$\mathcal{C}\ell(M,g)=P_{\mathrm{SO}^{e}_{1,3}}(M)\times_{\mathrm{Ad}'}\mathbb{R}_{1,3}, \tag{6}$$

i.e., the Clifford bundle is an associated vector bundle to the principal bundle $P_{\mathrm{SO}^{e}_{1,3}}(M)$ of orthonormal Lorentz frames.

Definition 5: Sections of $\mathcal{C}\ell(M,g)$ are called Clifford fields. (We note that the term Clifford fields was used in Ref. 34 for mappings from Minkowski spacetime to the Clifford algebra $\mathbb{R}_{1,3}$.)

B. Spinor bundles

Definition 6: A spin structure on M consists of a principal fiber bundle $\pi_s:P_{\mathrm{Spin}^{e}_{1,3}}(M)\to M$ (called the Spin Frame Bundle) with group $\mathrm{Spin}^{e}_{1,3}$ and a map

$$s:P_{\mathrm{Spin}^{e}_{1,3}}(M)\to P_{\mathrm{SO}^{e}_{1,3}}(M), \tag{7}$$

satisfying the following conditions.

(i) $\pi(s(p))=\pi_s(p)\forall p\in P_{\mathrm{Spin}^{e}_{1,3}}(M)$; π is the projection map of the bundle $P_{\mathrm{SO}^{e}_{1,3}}(M)$.

(ii) $s(pu)=s(p)Ad_u$, $\forall p\in P_{\mathrm{Spin}^{e}_{1,3}}(M)$ and $Ad:\mathrm{Spin}^{e}_{1,3}\to\mathrm{Aut}(\mathbb{R}_{1,3})$, $Ad_u:\mathbb{R}_{1,3}\ni x\mapsto uxu^{-1}\in\mathbb{R}_{1,3}$.

Recall that minimal left (right) ideals of $\mathbb{R}_{p,q}$ are left (right) modules for $\mathbb{R}_{p,q}$.[34] In Ref. 34, covariant, algebraic and Dirac–Hestenes spinors [when $(p,q)=(1,3)$] were defined as certain equivalence classes in appropriate sets, and a *preliminary* definition for fields of these objects living on *Minkowski* spacetime was given. We are now interested in defining algebraic Dirac spinor fields and also Dirac–Hestenes spinor fields, on a general Riemann–Cartan spacetime (Definition 3), as sections of appropriate vector bundles (spinor bundles) associated to $P_{\mathrm{Spin}^{e}_{1,3}}(M)$. The compatibility between $P_{\mathrm{Spin}^{e}_{1,3}}(M)$ and $P_{\mathrm{SO}^{e}_{1,3}}(M)$, as captured in Definition 6, is essential for that matter.

It is therefore natural to ask the following: When does a spin strucute exist on an oriented manifold M? The answer, which is a classical result (Refs. 1, 4, 5, 10, 15, 22, 29–31, 33, 32) is that the necessary and sufficient conditions for the existence of a spin structure on M is that the second Stiefel–Whitney class $w_2(M)$ of M is trivial. Moreover, when a spin structure exists, one can show that it is unique (modulo isomorfisms) if and only if $H^1(M,\mathbb{Z}_2)$ is trivial.

Remark 7: For a spacetime $\mathfrak{M}$ (Definition 2), a spin structure exists if and only if $P_{\mathrm{SO}^e_{1,3}}(M)$ is a trivial *bundle. This was originally shown by Geroch.*[16]

Definition 8: We call global sections $\xi \in \sec P_{\mathrm{SO}^e_{1,3}}(M)$ Lorentz frames *and global sections $\Xi \in \sec P_{\mathrm{Spin}^e_{1,3}}(M)$* spin frames.

Remark 9: Recall that a principal bundle is trivial if and only if it admits a global section. Therefore, Geroch's result says that a (noncompact) spacetime admits a spin structure if and only if it admits a (globally defined) Lorentz frame. In fact, it is possible to replace $P_{\mathrm{SO}^e_{1,3}}(M)$ by $P_{\mathrm{Spin}^e_{1,3}}(M)$ in Remark 7 (see Ref. 16, Footnote 25). In this way, when a (noncompact) spacetime admits a spin structure, the bundle $P_{\mathrm{Spin}^e_{1,3}}(M)$ is trivial and, therefore, every bundle associated to it is also trivial.

Definition 10: An oriented manifold endowed with a spin structure will be called a spin manifold.

We now present the most usual definitions of spinor bundles appearing in the literature and next we find appropriate vector bundles such that particular sections are LIASF or DHSF. [We recall that there are some other (equivalent) definitions of spinor bundles that we are not going to introduce in this paper as, e.g., the one given in Ref. 6 in terms of mappings from $P_{\mathrm{Spin}^e_{1,3}}$ to some appropriate vector space.]

Definition 11: A real spinor bundle for M is a vector bundle,

$$S(M) = P_{\mathrm{Spin}^e_{1,3}}(M) \times_{\mu_l} \mathbf{M}, \tag{8}$$

where $\mathbf{M}$ is a left module for $\mathbb{R}_{1,3}$ and μ_l is a representation of $\mathrm{Spin}^e_{1,3}$ *on $End(\mathbf{M})$ given by left multiplication by elements of* $\mathrm{Spin}^e_{1,3}$.

Definition 12: The dual bundle $S^\star(M)$ is a real spinor bundle,

$$S^\star(M) = P_{\mathrm{Spin}^e_{1,3}}(M) \times_{\mu_r} \mathbf{M}^\star, \tag{9}$$

where $\mathbf{M}^\star$ is a right module for $\mathbb{R}_{1,3}$ and μ_r is a representation of $\mathrm{Spin}^e_{1,3}$ *in $End(\mathbf{M})$ given by right multiplication by (inverse) elements of* $\mathrm{Spin}^e_{1,3}$. *[More precisely, this means that given $u \in \mathrm{Spin}^e_{1,3}$, $a \in \mathbf{M}^*$, $\mu_r(u)a = au^{-1}$, so that $\mu_r(uu')a = a(uu')^{-1} = au'^{-1}u^{-1} = \mu_r(u)\mu_r(u')a$.]*

Definition 13: A complex spinor bundle for M is a vector bundle,

$$S_c(M) = P_{\mathrm{Spin}^e_{1,3}}(M) \times_{\mu_c} \mathbf{M}_c, \tag{10}$$

where $\mathbf{M}_c$ is a complex left module for $\mathbb{C}\otimes\mathbb{R}_{1,3} \simeq \mathbb{R}_{4,1} \simeq \mathbb{C}(4)$, and where μ_c is a representation of $\mathrm{Spin}^e_{1,3}$ *in* $\mathrm{End}(\mathbf{M}_c)$ *given by left multiplication by elements of* $\mathrm{Spin}^e_{1,3}$.

Definition 14: The dual complex spinor bundle for M is a vector bundle,

$$S_c^\star(M) = P_{\mathrm{Spin}^e_{1,3}}(M) \times_{\mu_c} \mathbf{M}_c^\star, \tag{11}$$

where $\mathbf{M}_c^\star$ is a complex right module for $\mathbb{C}\otimes\mathbb{R}_{1,3} \simeq \mathbb{R}_{4,1} \simeq \mathbb{C}(4)$, and where μ_c is a representation of $\mathrm{Spin}^e_{1,3}$ *in $End(\mathbf{M}_c)$ given by right multiplication by (inverse) elements of* $\mathrm{Spin}^e_{1,3}$. *[More precisely, this means that given $u \in \mathrm{Spin}^e_{1,3}$, $a \in \mathbf{M}^*$, $\mu_r(u)a = au^{-1}$.]*

Taking, e.g., $\mathbf{M}_c = \mathbb{C}^4$ and μ_c the $D^{(1/2,0)} \oplus D^{(0,1/2)}$ representation of $\mathrm{Spin}^e_{1,3} \cong \mathrm{SL}(2,\mathbb{C})$ in $\mathrm{End}(\mathbb{C}^4)$, we immediately recognize the usual definition of the covariant spinor bundle of M as given, e.g., in (Refs. 7, 8, 9, 15, 29, 30).

C. Left spin-Clifford bundle

As shown in Ref. 34, besides the ideal $I=\mathbb{R}_{1,3}\frac{1}{2}(1+E_0)$, other ideals exist in $\mathbb{R}_{1,3}$ that are only *algebraically* equivalent to this one. (This fact gives rise to a large class of multivector Dirac equations in flat spacetime, generalizing the Dirac–Hestenes equation.[23,24]) In order to capture all possibilities we recall that $\mathbb{R}_{1,3}$ can be considered as a module over itself by left (or right) multiplication. We are thus led to the following definition.

Definition 15: The left real spin-Clifford bundle of M is the vector bundle,

$$\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)=P_{\mathrm{Spin}^e_{1,3}}(M)\times_l\mathbb{R}_{1,3}, \tag{12}$$

where l is the representation of $\mathrm{Spin}^e_{1,3}$ *on* $\mathbb{R}_{1,3}$ *given by $l(a)x=ax$. Sections of $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ are called left spin-Clifford fields.*

Remark 16: $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ is a "principal $\mathbb{R}_{1,3}$-bundle," i.e., it admits a free action of $\mathbb{R}_{1,3}$ on the right,[5] which is denoted by R_g, $g\in\mathbb{R}_{1,3}$. This will be considered in Sec. V.

Remark 17: There is a natural *embedding $P_{\mathrm{Spin}^e_{1,3}}(M)\hookrightarrow\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ which comes from the embedding* $\mathrm{Spin}^e_{1,3}\hookrightarrow\mathbb{R}^0_{1,3}$. *(The symbol $A\hookrightarrow B$ means that A is embedded in B and $A\subseteq B$.) Hence (as we shall see in more details below), every real left spinor bundle (see Definition 15) for M can be captured from $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$, which is a vector bundle very different from $\mathcal{C}\ell(M,g)$. Their relation is presented below, but before that we give the following definition.*

Definition 18: Let $I(M)$ be a subbundle of $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ such that there exists a primitive idempotent **e** *of* $\mathbb{R}_{1,3}$ *(see, e.g., Ref. 34) with*

$$R_{\mathbf{e}}\Psi=\Psi\mathbf{e}=\Psi, \tag{13}$$

for all $\Psi\in\sec I(M)\subset\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$. *Then, $I(M)$ is called a subbundle of left ideal algebraic spinor fields. Any $\Psi\in\sec I(M)\subset\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ is called a left ideal algebraic spinor field (LIASF). $I(M)$ can be thought of as a real spinor bundle for M such that* **M** *in Eq. (8) is a minimal left ideal of* $\mathbb{R}_{1,3}$.

Definition 19: Two subbundles $I(M)$ and $I'(M)$ of LIASF are said to be geometrically equivalent if the idempotents e, $e'\in\mathbb{R}_{1,3}$ (appearing in the previous definition) are related by an element $u\in\mathrm{Spin}^e_{1,3}$, i.e., $e'=ueu^{-1}$.

Definition 20: The right *real spin-Clifford bundle of M is the vector bundle*

$$\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)=P_{\mathrm{Spin}^e_{1,3}}(M)\times_r\mathbb{R}_{1,3}. \tag{14}$$

Sections of $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ are called right spin-Clifford fields.

In Eq. (14) r refers to the representation of $\mathrm{Spin}^e_{1,3}$ on $\mathbb{R}_{1,3}$ given by $r(a)x=xa^{-1}$. As in the case for the left real spin-Clifford bundle, there is a natural embedding $P_{\mathrm{Spin}^e_{1,3}}(M)\hookrightarrow\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ which comes from the embedding $\mathrm{Spin}^e_{1,3}\hookrightarrow\mathbb{R}^0_{1,3}$. There exists also a natural left action L_a of $a\in\mathbb{R}_{1,3}$ on $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$. This will be proved in Sec. V.

Definition 21: Let $I^{\star}(M)$ be a subbundle of $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ such that there exists a primitive idempotent element **e** *of* $\mathbb{R}_{1,3}$ *with*

$$L_{\mathbf{e}}\Psi=e\Psi=\Psi, \tag{15}$$

for any $\Psi \in \sec I^{\star}(M) \subset \sec \mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M)$. *Then,* $I^{\star}(M)$ *is called a subundle of right ideal algebraic spinor fields. Any* $\Psi \in \sec I^{\star}(M) \subset \sec \mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M)$ *is called a right ideal algebraic spinor field (RIASF).* $I^{\star}(M)$ *can be thought of as a real spinor bundle for M such that* $\mathbf{M}^{\star}$ *in Eq. (9) is a minimal right ideal of* $\mathbb{R}_{1,3}$.

Definition 22: Two subbundles $I^{*}(M)$ *and* $I^{*\prime}(M)$ *of RIASF are said to be geometrically equivalent if the idempotents* e, $e' \in \mathbb{R}_{1,3}$ *(appearing in the previous definition) are related by an element* $u \in \mathrm{Spin}^{e}_{1,3}$, *i.e.,* $e' = ueu^{-1}$.

Proposition 23: In a spin manifold, we have

$$\mathcal{C}\ell(M,g) = P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{\mathrm{Ad}} \mathbb{R}_{1,3}.$$

Proof: Remember once again that the representation,

$$\mathrm{Ad}: \mathrm{Spin}^{e}_{1,3} \to \mathrm{Aut}(\mathbb{R}_{1,3}), \quad \mathrm{Ad}_{u} a = uau^{-1}, \quad u \in \mathrm{Spin}^{e}_{1,3},$$

is such that $\mathrm{Ad}_{-1} =$ identity and so Ad descends to a representation Ad′ of $\mathrm{SO}^{e}_{1,3}$ which we considered above. It follows that when $P_{\mathrm{Spin}^{e}_{1,3}}(M)$ exists $\mathcal{C}\ell(M,g) = P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{\mathrm{Ad}} \mathbb{R}_{1,3}$. ■

D. Bundle of modules over a bundle of algebras

Proposition 24: $S(M)$ [*or* $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$] *is a bundle of (left)* modules *over the bundle of algebras* $\mathcal{C}\ell(M,g)$. *In particular, the sections of the spinor bundle S(M) [or* $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$*] constitute a module over the sections of the Clifford bundle.*

For the proof, see Ref. 5, p. 97.

Corollary 25: Let Φ, $\Psi \in \sec C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ *and* $\Psi \neq 0$. *Then there exists* $\psi \in \sec \mathcal{C}\ell(M,g)$ *such that*

$$\Psi = \psi\Phi. \tag{16}$$

Proof: It is an immediate consequence of Proposition 24. ■

So, the corollary allows us to identify a *correspondence* between some sections of $\mathcal{C}\ell(M,g)$ and some sections of $I(M)$ or $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ once we fix a section on $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$. This and other correspondences will be essential for the theory of Sec. V. Once we clarified the meaning of a bundle of modules $S(M)$ over a bundle of algebras $\mathcal{C}\ell(M,g)$, we can give the following.

Definition 26: Two real left spinor bundles (see Definition 15) are equivalent if and only if they are equivalent as bundles of $\mathcal{C}\ell(M,g)$ *modules.*

Remark 27: Of course, geometrically equivalenty real left spinor bundles are equivalent.

Remark 28: In what follows we denote the complexified left spin Clifford bundle by $\mathbb{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M) = P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{l} \mathbb{C}\otimes\mathbb{R}_{1,3} \equiv P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{r} \mathbb{R}_{4,1}$ *and the complexified right spin Clifford bundle by* $\mathbb{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M) = P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{r} \mathbb{C}\otimes\mathbb{R}_{1,3} \equiv P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{r} \mathbb{R}_{4,1}$.

III. DIRAC–HESTENES SPINOR FIELDS

Let $\mathbf{E}^{\mu}$, $\mu = 0,1,2,3$ be the canonical basis of $\mathbb{R}^{1,3} \hookrightarrow \mathbb{R}_{1,3}$ which generates the algebra $\mathbb{R}_{1,3}$. They satisfy the basic relation $\mathbf{E}^{\mu}\mathbf{E}^{\nu} + \mathbf{E}^{\nu}\mathbf{E}^{\mu} = 2\eta^{\mu\nu}$. As shown, e.g., in Ref. 34,

$$\mathbf{e} = \frac{1}{2}(1 + \mathbf{E}^{0}) \in \mathbb{R}_{1,3}, \tag{17}$$

is a primitive idempotent of $\mathbb{R}_{1,3}$ and

$$\mathbf{f}=\frac{1}{2}(1+\mathbf{E}^0)\frac{1}{2}(1+i\mathbf{E}^2\mathbf{E}^1)\in\mathbb{C}\otimes\mathbb{R}_{1,3} \tag{18}$$

is a primitive idempotent of $\mathbb{C}\otimes\mathbb{R}_{1,3}$. Now, let $\mathbf{I}=\mathbb{R}_{1,3}\mathbf{e}$ and $\mathbf{I}_{\mathbb{C}}=\mathbb{C}\otimes\mathbb{R}_{1,3}\mathbf{f}$ be, respectively, the minimal left ideals of $\mathbb{R}_{1,3}$ and $\mathbb{C}\otimes\mathbb{R}_{1,3}$ generated by $\mathbf{e}$ and $\mathbf{f}$. Let $\phi=\phi\mathbf{e}\in\mathbf{I}$ and $\Psi=\Psi\mathbf{f}\in\mathbf{I}_{\mathbb{C}}$. Then, any $\phi\in\mathbf{I}$ can be written as

$$\phi=\psi\mathbf{e}, \tag{19}$$

with $\psi\in\mathbb{R}^0_{1,3}$. Analogously, any $\Psi\in\mathbf{I}_{\mathbb{C}}$ can be written as

$$\Psi=\psi\mathbf{e}\frac{1}{2}(1+i\mathbf{E}^2\mathbf{E}^1), \tag{20}$$

with $\psi\in\mathbb{R}^0_{1,3}$.

Now, $\mathbb{C}\otimes\mathbb{R}_{1,3}\simeq\mathbb{R}_{4,1}\simeq\mathbb{C}(4)$, where $\mathbb{C}(4)$ is the algebra of the 4×4 complex matrices. We can verify that

$$\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix} \tag{21}$$

is a primitive idempotent of $\mathbb{C}(4)$ which is a matrix representation of $\mathbf{f}$. In this way we can prove (as shown, e.g., in Ref. 34) that there is a bijection between column spinors, i.e., elements of $\mathbb{C}^4$ (the complex 4-dimensional vector space) and the elements of $\mathbf{I}_{\mathbb{C}}$. All that, plus the definitions of the left real and complex spin bundles and the subbundle $I(M)$, suggests the following.

Definition 29: Let $\Phi\in\sec I(M)\subset\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ *be as in Definition 18, i.e.,*

$$R_{\mathbf{e}}\Phi=\Phi\mathbf{e}=\Phi,\quad \mathbf{e}^2=\mathbf{e}=\frac{\mathbf{1}}{\mathbf{2}}(\mathbf{1}+\mathbf{E^0})\in\mathbb{R}_{1,3}. \tag{22}$$

A Dirac–Hestenes Spinor field (DHSF) associated with Φ *is an even section* ψ *of* $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ *such that*

$$\Phi=\psi\mathbf{e}. \tag{23}$$

[Note that it is meaningful to speak about even (or odd) elements in $C\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ since $\mathrm{Spin}^e_{1,3}\subseteq\mathbb{R}^0_{1,3}$.]

Remark 30: An equivalent definition of a DHSF is the following. Let $\Psi\in\sec\mathbb{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ *be such that*

$$R_{\mathbf{f}}\Psi=\Psi\mathbf{f}=\Psi,\quad \mathbf{f}^2=\mathbf{f}=\frac{\mathbf{1}}{\mathbf{2}}(\mathbf{1}+\mathbf{E^0})\frac{\mathbf{1}}{\mathbf{2}}(\mathbf{1}+\mathbf{iE^2E^1})\in\mathbb{C}\otimes\mathbb{R}_{1,3}. \tag{24}$$

Then, a DHSF associated to Ψ *is an even section* ψ *of* $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)\subset\mathbb{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ *such that*

$$\Psi=\psi\mathbf{f}. \tag{25}$$

Remark 31: In what follows, when we refer to a Dirac–Hestenes spinor field ψ *we omit for simplicity the wording associated with* Φ *(or* Ψ*). It is very important to observe that DHSF are not sums of even multivector (tensor) fields although, under a local trivialization,* ψ

$\in \sec C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ *is mapped on an even element of* $\mathbb{R}_{1,3}$. *We emphasize that DHSF are particular sections of a spinor bundle, not of the Clifford bundle. However, we show in Sec. V how these objects have representatives in the Clifford bundle.*

IV. THE MANY FACES OF THE DIRAC EQUATION

A. Dirac equation for covariant Dirac fields

As is well known,[8] a *covariant* Dirac spinor field is a section $\Psi \in \sec S_c(M) = P_{\mathrm{Spin}^{e}_{1,3}}(M) \times_{\mu_l} \mathbb{C}^4$. Let $(U=M,\Phi), \Phi(\boldsymbol{\Psi}) = (x, |\Psi(x)\rangle)$ be a global trivialization corresponding to a spin frame Ξ (Definition 8), such that

$$s(\Xi) = \{e_a\} \in P_{\mathrm{SO}^{e}_{1,3}}(M), \quad e^a \in \sec C\ell(M,g),$$
$$e^a e^b + e^b e^a = 2\eta^{ab}, a,b = 0,1,2,3 \tag{26}$$

(see Definition 6). The usual Dirac equation in a Lorentzian spacetime for the spinor field Ψ—in interaction with an electromagnetic field $A \in \sec\Lambda^1(M) \subset \sec \mathcal{C}\ell(M,g)$—is then[11]

$$i\gamma^a(\boldsymbol{\nabla}^{s}_{e_a} + iqA_a)|\Psi(x)\rangle - m|\Psi(x)\rangle = 0, \tag{27}$$

where $\gamma^a \in \mathbb{C}(4)$, $a = 0,1,2,3$ is a set of *constant* Dirac *matrices* satisfying

$$\gamma^a\gamma^b + \gamma^b\gamma^a = 2\eta^{ab}. \tag{28}$$

[We denote the space of sections of p-vectors by $\sec\Lambda^p(M)$.]

B. Dirac equation in $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M,g)$

Due to the one-to-one correspondence between *ideal* sections of $\mathbb{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$, $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ and of $S_c(M)$ as explained in Sec. III, we can *translate* the Dirac equation (27) for a covariant spinor field into an equation for a spinor field, which is a section of $\mathbb{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$, and finally write an equivalent equation for a DHSF $\psi \in \sec C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$. In order to do that we introduce the spin-Dirac operator.

Definition 32: The (spin) Dirac operator acting on sections of $C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ *is the first order differential operator*,[5]

$$D^s = e^a\boldsymbol{\nabla}^{s}_{e_a}, \tag{29}$$

where $\{e^a\}$ *is as in Eq. (26) and* ∇^s *is the spinor covariant derivative (see the Appendix).*

Now we give the details of the inverse translation. We start with the following equation which we call Dirac equation in $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$, denoted DE$\mathcal{C}\ell^{l}$:

$$D^s\psi\mathbf{E}^{21} - m\psi\mathbf{E}^0 - qA\boldsymbol{\psi} = 0, \tag{30}$$

where $\psi \in \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$ is a DHSF and the $\mathbf{E}^a \in \mathbb{R}_{1,3}$ are such that $\mathbf{E}^a\mathbf{E}^b + \mathbf{E}^b\mathbf{E}^a = 2\eta^{ab}$. Multiplying Eq. (30) on the right by the idempotent $\mathbf{f} = \frac{1}{2}(1+\mathbf{E}^0)\frac{1}{2}(1+i\mathbf{E}^2\mathbf{E}^1) \in \mathbb{C}\otimes\mathbb{R}_{1,3}$ we get after some simple algebraic manipulations the following equation for the (complex) left ideal spin-Clifford field $\Psi = \psi\mathbf{f} \in \sec \mathbb{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$:

$$iD^s\Psi - m\Psi - qA\Psi = 0. \tag{31}$$

Now we can easily show, using the methods of Ref. 34, that given any global trivializations $(U=M,\Theta)$ and $(U=M,\Phi)$, of $\mathcal{C}\ell(M,g)$ and $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$, there exists matrix representations of the $\{e^a\}$ that are equal to the Dirac matrices $\boldsymbol{\gamma}^a$ [appearing in Eq. (27)]. In that way the correspondence between Eqs. (27), (30) and (31) is proved.

Remark 33: We emphasize at this point that we call Eq. (30) the DE$\mathcal{C}\ell^{l}$. *It looks similar to the Dirac–Hestenes equation (on Minkowski spacetime) discussed in Ref. 34, but it is indeed very different regarding its mathematical nature. It is an intrinsic equation satisfied by a legitimate spinor field, namely a DHSF* $\psi\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$. *The question naturally arises: May we write an equation with the same mathematical information of Eq. (30) but satisfied by objects living on the Clifford bundle* $\mathcal{C}\ell(M,g)$ *of an arbitrary Lorentzian spacetime, admitting a spin structure? In the next section we show that the answer to that question is yes.*

C. Electromagnetic gauge invariance of the DE$\mathcal{C}\ell^{l}$

Proposition 34: The DE$\mathcal{C}\ell^{l}$ *is invariant under electromagnetic gauge transformations,*

$$\psi\mapsto\psi'=\psi e^{q\mathbf{E}^{21}\chi}, \tag{32}$$

$$A\mapsto A+\partial\chi, \tag{33}$$

$$\omega_{e_a}\mapsto\omega_{e_a}, \tag{34}$$

$$\psi,\psi'\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M), \tag{35}$$

$$A\in\sec\Lambda^{1}(M)\subset\sec\mathcal{C}\ell(M,g), \tag{36}$$

with ψ,ψ' *distinct DHSF, and where* $\chi:M\to\mathbb{R}\subset\mathbb{R}_{1,3}$ *is a gauge function.*

Proof: The proof is obtained by direct verification. ■

Remark 35: We note that, for the DE$\mathcal{C}\ell^{l}$, *local rotations and electromagnetic gauge transformations are very different mathematical transformations, without any obvious geometrical link between them, differently of what seems to be the case for the Dirac–Hestenes equation, which is studied in the next section.*

V. THE DIRAC–HESTENES EQUATION (DHE)

We obtained above a Dirac equation, which we called DE$C\ell^{l}$, describing the motion of spinor fields represented by sections Ψ of $C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M,g)$ in interaction with an electromagnetic field $A\in\sec C\ell(M,g)$,

$$D^{s}\Psi\mathbf{E}^{21}-qA\Psi=m\Psi\mathbf{E}^{0}, \tag{37}$$

where $D^{s}=e^{a}\boldsymbol{\nabla}^{s}_{e_a}$, $\{e^a\}$ is given by Eq. (26), $\boldsymbol{\nabla}^{s}_{e_a}$ is the natural spinor covariant derivative acting on $\sec C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M,g)$ (see the Appendix), and $\{\mathbf{E}^a\}\in\mathbb{R}^{1,3}\subseteq\mathbb{R}_{1,3}$ is such that $\mathbf{E}^a\mathbf{E}^b+\mathbf{E}^b\mathbf{E}^a=2\eta^{ab}$. As we already mentioned, although Eq. (37) is written in a kind of Clifford bundle [i.e. $C\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M,g)$], it does not suffer from the inconsistency of representing spinors as pure differential forms and, in fact, the object Ψ behaves as it should under Lorentz transformations.

As a matter of fact, Eq. (37) can be thought of as a mere *rewriting* of the usual Dirac equation, where the role of the constant gamma matrices is undertaken by the constant elements $\{\mathbf{E}^a\}$ in $\mathbb{R}_{1,3}$ and by the set $\{e^a\}$. In this way, Eq. (37) is *not* a kind of Dirac–Hestenes equation as discussed, e.g., in Ref. 34. It suffices to say that (i) the state of the electron, represented by Ψ, is not a *Clifford field* and (ii) the $\mathbf{E}^a$'s are just *constant* elements of $\mathbb{R}_{1,3}$ and not sections of vectors in $\mathcal{C}\ell(M,g)$. Nevertheless, as we show in the following, Eq. (37) does lead to a multivector Dirac

equation once we carefully employ the theory of right and left actions on the various Clifford bundles introduced earlier. It is the multivector equation to be derived below that we call the DHE (of course, we can write an equivalent multiform equation). We shall need several preliminary results that we collect in the next two subsections.

A. The various natural actions on the vector bundles associated to $P_{\mathrm{Spin}^e_{1,3}}(M)$

Recall that, when M is a spin manifold the following occurs.

(i) The elements of $\mathcal{C}\ell(M,g)=P_{\mathrm{Spin}^e_{1,3}}(M)\times_{\mathrm{Ad}}\mathbb{R}_{1,3}$ are equivalence classes $[(p,a)]$ of pairs (p,a), where $p\in P_{\mathrm{Spin}^e_{1,3}}(M)$, $a\in\mathbb{R}_{1,3}$ and $(p,a)\sim(p',a')\Leftrightarrow p'=pu^{-1}$, $a'=uau^{-1}$, for some $u\in\mathrm{Spin}^e_{1,3}$.

(ii) The elements of $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ are equivalence classes of pairs (p,a), where $p\in P_{\mathrm{Spin}^e_{1,3}}(M)$, $a\in\mathbb{R}_{1,3}$ and $(p,a)\sim(p',a')\Leftrightarrow p'=pu^{-1}$, $a'=ua$, for some $u\in\mathrm{Spin}^e_{1,3}$.

(iii) The elements of $\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$ are equivalence classes of pairs (p,a), where $p\in P_{\mathrm{Spin}^e_{1,3}}(M)$, $a\in\mathbb{R}_{1,3}$ and $(p,a)\sim(p',a')\Leftrightarrow p'=pu^{-1}$, $a'=au^{-1}$, for some $u\in\mathrm{Spin}^e_{1,3}$.

In this way, it is possible to define the following natural actions on these associated bundles.

Proposition 36: There is a natural right action of $\mathbb{R}_{1,3}$ *on* $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ *and a natural left action of* $\mathbb{R}_{1,3}$ *on* $\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M,g)$.

Proof: Given $b\in\mathbb{R}_{1,3}$ and $\alpha\in\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M,g)$, select a representative (p,a) for α and define $\alpha b:=[(p,ab)]$. If another representative (pu^{-1},ua) is chosen for α, we have $(pu^{-1},uab)\sim(p,ab)$ and thus αb is a well-defined element of $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$. ■

Let us denote the space of $\mathbb{R}_{1,3}$-valued smooth functions on M by $\mathcal{F}(M,\mathbb{R}_{1,3})$. Then, the above proposition immediately yields the following.

Corollary 37: There is a natural right action of $\mathcal{F}(M,\mathbb{R}_{1,3})$ *on* $\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ *and a natural left action of* $\mathcal{F}(M,\mathbb{R}_{1,3})$ *on* $\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M,g)$.

Proposition 38: There is a natural left action of $\sec\mathcal{C}\ell(M,g)$ *on* $\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ *and a natural right action of* $\sec\mathcal{C}\ell(M,g)$ *on* $\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$.

Proof: Given $\alpha\in\sec\mathcal{C}\ell(M,g)$ and $\beta\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M,g)$, select representatives (p,a) for $\alpha(x)$ and (p,b) for $\beta(x)$ [with $p\in\pi^{-1}(x)$] and define $(\alpha\beta)(x):=[(p,ab)]\in\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M,g)$. If alternative representatives (pu^{-1},uau^{-1}) and (pu^{-1},ub) are chosen for $\alpha(x)$ and $\beta(x)$, we have

$$(pu^{-1},uau^{-1}ub)=(pu^{-1},uab)\sim(p,ab),$$

and thus $(\alpha\beta)(x)$ is a well-defined element of $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M,g)$. ■

Proposition 39: There is a natural pairing,

$$\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)\times\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)\to\sec\mathcal{C}\ell(M,g).$$

Proof: Given $\alpha\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $\beta\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$, select representatives (p,a) for $\alpha(x)$ and (p,b) for $\beta(x)$ [with $p\in\pi^{-1}(x)$] and define $(\alpha\beta)(x):=[(p,ab)]\in\mathcal{C}\ell(M,g)$. If alternative representatives (pu^{-1},ua) and (pu^{-1},bu^{-1}) are chosen for $\alpha(x)$ and $\beta(x)$, we have $(pu^{-1},uabu^{-1})\sim(p,ab)$ and thus $(\alpha\beta)(x)$ is a well-defined element of $C\ell(M,g)$. ■

Proposition 40: There is a natural pairing,

$$\sec \mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M)\times \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)\to \mathcal{F}(M,\mathbb{R}_{1,3}).$$

Proof: Given $\alpha\in \sec \mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M)$ and $\beta\in \sec \mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{1,3}}(M)$, select representatives (p,a) for $\alpha(x)$ and (p,b) for $\beta(x)$ [with $p\in\pi^{-1}(x)$] and define $(\alpha\beta)(x):=ab\in\mathbb{R}_{1,3}$. If alternative representatives (pu^{-1},au^{-1}) and (pu^{-1},ub) are chosen for $\alpha(x)$ and $\beta(x)$, we have $au^{-1}ub=ab$ and thus $(\alpha\beta)(x)$ is a well-defined element of $\mathbb{R}_{1,3}$. ■

B. Fiducial sections associated with a spin frame

We start by exploring the possibility of defining ''unit sections'' on the various vector bundles associated with the principal bundle $P_{\mathrm{Spin}^{e}_{1,3}}(M)$. It immediately follows from the definition given by Eq. (1) that the unit section $\mathbf{1}\in\sec\mathcal{C}\ell(M,g)$, given by $x\mapsto 1\in\mathcal{C}\ell(T_xM,g_x)$, is certainly well defined. For future reference, let us consider how this can also be seen from the associated bundle structure of $P_{\mathrm{Spin}^{e}_{1,3}}(M)\times_{ad}\mathbb{R}_{1,3}$.

Let

$$\Phi_i:\pi^{-1}(U_i)\to U_i\times \mathrm{Spin}^{e}_{1,3},\quad \Phi_j:\pi^{-1}(U_j)\to U_j\times \mathrm{Spin}^{e}_{1,3}$$

be two local trivializations for $P_{\mathrm{Spin}^{e}_{1,3}}(M)$, with

$$\Phi_i(u)=(\pi(u)=x,\phi_{i,x}(u)),\quad \Phi_j(u)=(\pi(u)=x,\phi_{j,x}(u)).$$

Recall that the transition function on $g_{ij}:U_i\cap U_j\to\mathrm{Spin}^{e}_{1,3}$ is then given by

$$g_{ij}(x)=\phi_{i,x}(u)\circ\phi_{j,x}(u)^{-1},$$

which does not depend on u.

Proposition 41: $\mathcal{C}\ell(M,g)$ has a naturally defined global unit section.

Proof: For the associated bundle $\mathcal{C}\ell(M,g)=P_{\mathrm{Spin}^{e}_{1,3}}(M)\times_{\mathrm{Ad}}\mathbb{R}_{1,3}$, the transition functions corresponding to local trivializations,

$$\Psi_i:\pi_c^{-1}(U_i)\to U_i\times\mathbb{R}_{1,3},\quad \Psi_j:\pi_c^{-1}(U_j)\to U_j\times\mathbb{R}_{1,3},\tag{38}$$

are given by $h_{ij}(x)=Ad_{g_{ij}(x)}$. Define the local sections

$$\mathbf{1}_i(x)=\Psi_i^{-1}(x,1),\quad \mathbf{1}_j(x)=\Psi_j^{-1}(x,1),\tag{39}$$

where 1 is the unit element of $\mathbb{R}_{1,3}$. Since $h_{ij}(x)\cdot 1=\mathrm{Ad}_{g_{ij}(x)}(1)=g_{ij}(x)1g_{ij}(x)^{-1}=1$, we see that the expressions above uniquely define a global section $\mathbf{1}\in\mathcal{C}\ell(M,g)$ with $\mathbf{1}|_{U_i}=\mathbf{1}_i$. ■

It is clear that such a result can be immediately generalized for the Clifford bundle $\mathcal{C}\ell_{p,q}(M,g)$, of any n-dimensional manifold endowed with a metric of arbitrary signature (p,q) (where $n=p+q$). Now, we observe also that the left (and also the right) spin-Clifford bundle can be generalized in an obvious way for any spin manifold of arbitrary finite dimension $n=p+q$, with a metric of arbitrary signature (p,q). However, another important difference between $\mathcal{C}\ell(M,g)$ and $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{p,q}}(M)$ or $\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{1,3}}(M,g)$ is that these latter bundles only admit a global unit section if they are *trivial*.

Proposition 42: There exists an unit section on $\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{p,q}}(M)$ [and also on $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{p,q}}(M)$] if and only if $P_{\mathrm{Spin}^{e}_{p,q}}(M)$ is trivial.

Proof: We show the necessity for the case of $\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{p,q}}(M)$, the sufficiency is trivial. [The proof for the case of $\mathcal{C}\ell^{l}_{\mathrm{Spin}^{e}_{p,q}}(M)$ is analogous.] For $\mathcal{C}\ell^{r}_{\mathrm{Spin}^{e}_{p,q}}(M)$, the transition functions corresponding to local trivializations,

$$\Omega_i:\pi_{sc}^{-1}(U_i)\to U_i\times\mathbb{R}_{p,q},\quad \Omega_j:\pi_{sc}^{-1}(U_j)\to U_j\times\mathbb{R}_{p,q},\tag{40}$$

are given by $k_{ij}(x)=R_{g_{ij}(x)}$, with $R_a:\mathbb{R}_{p,q}\to\mathbb{R}_{p,q}, x\mapsto xa^{-1}$. Let 1 be the unit element of $\mathbb{R}_{1,3}$. A unit section in $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{p,q}}(M)$—if it exists—is written in terms of these two local trivializations as

$$\mathbf{1}^r_i(x)=\Omega_i^{-1}(x,1),\quad \mathbf{1}^r_j(x)=\Omega_j^{-1}(x,1),\tag{41}$$

and we must have $\mathbf{1}^r_i(x)=\mathbf{1}^r_j(x)$, $\forall x\in U_i\cap U_j$. As $\Omega_i(\mathbf{1}^r_i(x))=(x,1)=\Omega_j(\mathbf{1}^r_j(x))$, we have $\mathbf{1}^r_i(x)=\mathbf{1}^r_j(x)\Leftrightarrow 1=k_{ij}(x)\cdot 1\Leftrightarrow 1=1g_{ij}(x)^{-1}\Leftrightarrow g_{ij}(x)=1$. This proves the proposition. ■

Remark 43: For general spin manifolds, the bundle $P_{\mathrm{Spin}^e_{p,q}}(M)$ is not necessarily trivial for arbitrary (p,q), but Geroch's theorem (Remark 9) warrants that, for the special case $(p,q)=(1,3)$ with M noncompact, $P_{\mathrm{Spin}^e_{1,3}}(M)$ is trivial. By the above proposition, we then see that $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ and also $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ have global "unit sections." It is most important to note, however, that each different choice of a (global) trivialization Ω_i on $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ [respectively, $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{p,q}}(M)$] induces a different global unit section $\mathbf{1}^r_i$ (respectively, $\mathbf{1}^l_i$). Therefore, even in this case there is no canonical unit section on $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M,g)$ [respectively, on $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M,g)$].

By Remark 9, when the (noncompact) spacetime M is a spin manifold, the bundle $P_{\mathrm{Spin}^e_{1,3}}(M)$ admits global sections. With this in mind, let us fix a spin frame Ξ for M. This induces a global trivialization for $P_{\mathrm{Spin}^e_{1,3}}(M)$, which we denote by $\Phi_\Xi:P_{\mathrm{Spin}^e_{1,3}}(M)\to M\times\mathrm{Spin}^e_{1,3}$, with $\Phi_\Xi^{-1}(x,1)=\Xi(x)$. As we show in the following, the spin frame Ξ can also be used to induce certain fiducial global sections on the various vector bundles associated with $P_{\mathrm{Spin}^e_{1,3}}(M)$.

(i) $\mathcal{C}\ell(M,g)$ Let $\{\mathbf{E}^a\}$ be a fixed orthonormal basis of $\mathbb{R}^{1,3}\subseteq\mathbb{R}_{1,3}$ (which can be thought of as the *canonical* basis of $\mathbb{R}^{1,3}$). We define basis sections in $\mathcal{C}\ell(M,g)=P_{\mathrm{Spin}^e_{1,3}}(M)\times_{\mathrm{Ad}}\mathbb{R}_{1,3}$ by $e_a(x)=[(\Xi(x),\mathbf{E}_a)]$. Of course, this induces a multivector basis $\{e_I(x)\}$ for each $x\in M$. Note that a more precise notation for e_a would be, for instance, $e_a^{(\Xi)}$.

(ii) $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ Let $\mathbf{1}^l_\Xi\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ be defined by $\mathbf{1}^l_\Xi(x)=[(\Xi(x),1)]$. Then the natural right action of $\mathbb{R}_{1,3}$ on $\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ leads to $\mathbf{1}^l_\Xi(x)a=[(\Xi(x),a)]$ for all $a\in\mathbb{R}_{1,3}$. It follows from Corollary 37 that an arbitrary section $\alpha\in\sec\mathcal{C}\ell^{l}_{\mathrm{Spin}^e_{1,3}}(M)$ can be written as $\alpha=\mathbf{1}^l_\Xi f$, with $f\in\mathcal{F}(M,\mathbb{R}_{1,3})$.

(iii) $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M,g)$ Let $\mathbf{1}^r_\Xi\in\sec\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M,g)$ be defined by $\mathbf{1}^r_\Xi(x)=[(\Xi(x),1)]$. Then the natural left action of $\mathbb{R}_{1,3}$ on $\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ leads to $a\mathbf{1}^r_\Xi(x)=[(\Xi(x),a)]$ for all $a\in\mathbb{R}_{1,3}$. It follows from Corollary 37 that an arbitrary section $\alpha\in\sec\mathcal{C}\ell^{r}_{\mathrm{Spin}^e_{1,3}}(M)$ can be written as $\alpha=f\mathbf{1}^r_\Xi$, with $f\in\mathcal{F}(M,\mathbb{R}_{1,3})$.

Now recall (Definition 6) that a spin structure on M is a 2-1 bundle map $s:P_{\mathrm{Spin}^e_{1,3}}(M)\to P_{\mathrm{SO}^e_{1,3}}(M)$ such that $s(pu)=s(p)\mathrm{Ad}_u$, $\forall p\in P_{\mathrm{Spin}^e_{1,3}}(M)$, $u\in\mathrm{Spin}^e_{1,3}$, where $\mathrm{Ad}:\mathrm{Spin}^e_{1,3}\to\mathrm{SO}^e_{1,3}$, $\mathrm{Ad}_u:x\mapsto uxu^{-1}$. We see that the specification of the global section in the case (i) above is compatible with the Lorentz frame $\{e_a\}=s(\Xi)$ assigned by s. More precisely, for each $x\in M$, the element $s(\Xi(x))\in P_{\mathrm{SO}^e_{1,3}}(M)$ is to be regarded as a proper isometry $s(\Xi(x)):\mathbb{R}^{1,3}\to T_xM$, so that $e_a(x):=s(p)\cdot\mathbf{E}_a$ yields a Lorentz frame $\{e_a\}$ on M, which we denoted by $s(\Xi)$. On the other hand, $\mathcal{C}\ell(M,g)$ is isomorphic to $P_{\mathrm{Spin}^e_{1,3}}(M)\times_{\mathrm{Ad}}\mathbb{R}_{1,3}$, and we can always arrange things so that $e_a(x)$ is represented in this bundle as $e_a(x)=[(\Xi(x),\mathbf{E}_a)]$. In fact, all we have to do is to verify that this identification is covariant under a change of frames. To see that, let $\Xi'\in\sec(P_{\mathrm{Spin}^e_{1,3}}(M))$ be another spin frame on M. From the principal bundle structure of $P_{\mathrm{Spin}^e_{1,3}}(M)$, we know that, for each $x\in M$, there exists (a unique) $u(x)\in\mathrm{Spin}^e_{1,3}$ such that

$\Xi'(x)=\Xi(x)u(x)$. If we define, as above, $e'_a(x)=s(\Xi'(x))\cdot\mathbf{E}_a$, then $e'_a(x)=s(\Xi(x)u(x))\cdot\mathbf{E}_a$ $=s(\Xi(x))\mathrm{Ad}_{u(x)}\cdot\mathbf{E}_a=[(\Xi(x),\mathrm{Ad}_{u(x)}\cdot\mathbf{E}_a)]=[(\Xi(x)u(x),\mathbf{E}_a)]=[(\Xi'(x),\mathbf{E}_a)]$, which proves our claim.

Proposition 44:

$$(i)\ \mathbf{E}_a=\mathbf{1}^r_\Xi(x)e_a(x)\mathbf{1}^l_\Xi(x),\ \forall x\in M,$$

$$(ii)\ \mathbf{1}^l_\Xi\mathbf{1}^r_\Xi=1\in\mathcal{C}\ell(M,g),$$

$$(iii)\ \mathbf{1}^r_\Xi\mathbf{1}^l_\Xi=1\in\mathbb{R}_{1,3}.$$

Proof: This follows from the form of the various actions defined in Propositions 36–40. For example, for each $x\in M$, we have $\mathbf{1}^r_\Xi(x)e_a(x)=[(\Xi(x),1\mathbf{E}_a)]=[(\Xi(x),\mathbf{E}_a)]\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$ (from Proposition 38). Then, it follows from Proposition 40 that $\mathbf{1}^r_\Xi(x)e_a(x)\mathbf{1}^l_\Xi(x)=\mathbf{E}_a1=\mathbf{E}_a$, $\forall x\in M$. ■

Let us now consider how the various global sections defined above transform when the spin frame Ξ is changed. Let $\Xi'\in\sec P_{\mathrm{Spin}^e_{1,3}}(M)$ be another spin frame with $\Xi'(x)=\Xi(x)u(x)$, where $u(x)\in\mathrm{Spin}^e_{1,3}$. Let e_a, $\mathbf{1}^r_\Xi$, $\mathbf{1}^l_\Xi$ and e'_a, $\mathbf{1}^r_{\Xi'}$, $\mathbf{1}^l_{\Xi'}$ be the global sections, respectively, defined by Ξ and Ξ' (as above). We then have the following.

Proposition 45: Let Ξ,Ξ' be two spin frames related by $\Xi'=\Xi u$, where $u:M\to\mathrm{Spin}^e_{1,3}$. Then

$$(i)\ e'_a=Ue_aU^{-1},$$

$$(ii)\ \mathbf{1}^l_{\Xi'}=\mathbf{1}^l_\Xi u=U\mathbf{1}^l_\Xi, \tag{42}$$

$$(iii)\ \mathbf{1}^r_{\Xi'}=u^{-1}\mathbf{1}^r_\Xi=\mathbf{1}^r_\Xi U^{-1},$$

where $U\in\sec\mathcal{C}\ell(M,g)$ is the Clifford field associated to u by $U(x)=[(\Xi(x),u(x))]$. Also, in (ii) and (iii), u and u^{-1}, respectively, act on $\mathbf{1}^l_\Xi\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $\mathbf{1}^r_\Xi\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$ according to Proposition 37.

Proof: (i) We have

$$e'_a(x)=[(\Xi'(x),\mathbf{E}_a)]=[(\Xi(x)u(x),\mathbf{E}_a)]=[(\Xi(x),u(x)\mathbf{E}_au(x)^{-1})]=[(\Xi(x),u(x))]$$
$$\times[(\Xi(x),\mathbf{E}_a)][(\Xi(x),u(x)^{-1})]=U(x)e_a(x)U(x)^{-1}. \tag{43}$$

(iii) It follows from Proposition 38 that

$$\mathbf{1}^r_{\Xi'}(x)=[(\Xi'(x),1)]=[(\Xi(x)u(x),1)]=[(\Xi(x),1u(x)^{-1})]=[(\Xi(x),u(x)^{-1})]=u(x)^{-1}\mathbf{1}^r_\Xi(x), \tag{44}$$

where in the last step we used Proposition 37 and the fact that $\mathbf{1}^r_\Xi(x)=[(\Xi(x),1)]$. To demonstrate the second part, note that

$$u^{-1}(x)\mathbf{1}^r_\Xi(x)=[(\Xi(x),u(x)^{-1})]=[(\Xi(x),1u(x)^{-1})]=[(\Xi(x),1)][(\Xi(x),u(x)^{-1})]$$
$$=\mathbf{1}^r_\Xi(x)U^{-1}(x), \tag{45}$$

for all $x\in M$. It is important to note that in the last step we have a product between an element of $\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$ [i.e., $[(\Xi(x),1)]$] and an element of $\mathcal{C}\ell(M,g)$ [i.e., $[(\Xi(x),u(x)^{-1})]$]. ■

We emphasize that the right unit sections associated with spin frames are *not* constant in any covariant way. In fact, we have the following.

Proposition 46: Let $\mathbf{1}^r_\Xi \in \sec \mathcal{C}\ell^{\,r}_{\mathrm{Spin}^e_{1,3}}(M)$ *be the right unit section associated to the spin frame* Ξ. *Then*

$$\boldsymbol{\nabla}^s_{e_a}\mathbf{1}^r_\Xi = -\frac{1}{2}\mathbf{1}^r_\Xi \omega_{e_a}, \tag{46}$$

where ω_{e_a} *is the connection 1-form (Proposition 54) written in the basis* $\{e_a\}$.

Proof: It follows from Eq. (A9) of the Appendix. ■

C. Representatives of DHSF on the Clifford bundle

Let $\{\mathbf{E}^a\}$ be, as before, a fixed orthonormal basis of $\mathbb{R}^{1,3}\subseteq\mathbb{R}_{1,3}$. Remember that these objects are fundamental to the Dirac equation (37) in terms of sections Ψ of $\mathcal{C}\ell^{\,l}_{\mathrm{Spin}^e_{1,3}}(M,g)$:

$$D^s\Psi\mathbf{E}^{21} - qA\Psi = m\Psi\mathbf{E}^0.$$

Let $\Xi \in \sec P_{\mathrm{Spin}^e_{1,3}}(M)$ be a spin frame on M and define the sections $\mathbf{1}^l_\Xi$, $\mathbf{1}^r_\Xi$ and e_a, respectively, on $\mathcal{C}\ell^{\,l}_{\mathrm{Spin}^e_{1,3}}(M)$, $\mathcal{C}\ell^{\,r}_{\mathrm{Spin}^e_{1,3}}(M)$ and $\mathcal{C}\ell(M,g)$, as above. Now we can use Proposition 44 to write the above equation in terms of sections of $\mathcal{C}\ell(M,g)$:

$$(D^s\Psi)\mathbf{1}^r_\Xi e^{21}\mathbf{1}^l_\Xi - qA\Psi = m\Psi\mathbf{1}^r_\Xi e^0\mathbf{1}^l_\Xi. \tag{47}$$

Right-multiplying by $\mathbf{1}^r_\Xi$ yields, using Proposition 44,

$$e^a(\boldsymbol{\nabla}^s_{e_a}\Psi)\mathbf{1}^r_\Xi e^{21} - qA\Psi\mathbf{1}^r_\Xi = m\Psi\mathbf{1}^r_\Xi e^0. \tag{48}$$

It follows from Proposition 59 that

$$(\boldsymbol{\nabla}^s_{e_a}\Psi)\mathbf{1}^r_\Xi = \boldsymbol{\nabla}_{e_a}(\Psi\mathbf{1}^r_\Xi) - \Psi\boldsymbol{\nabla}^s_{e_a}(\mathbf{1}^r_\Xi) = \boldsymbol{\nabla}_{e_a}(\Psi\mathbf{1}^r_\Xi) + \frac{1}{2}\Psi\mathbf{1}^r_\Xi\omega_a, \tag{49}$$

where Proposition 46 was employed in the last step. Therefore

$$e^a\left[\boldsymbol{\nabla}_{e_a}(\Psi\mathbf{1}^r_\Xi) + \frac{1}{2}\Psi\mathbf{1}^r_\Xi\omega_a\right]e^{21} - qA(\Psi\mathbf{1}^r_\Xi) = m(\Psi\mathbf{1}^r_\Xi)e^0. \tag{50}$$

Thus it is natural to define, for each spin frame Ξ, the Clifford field $\psi_\Xi \in \sec C\ell(M,g)$ (see Proposition 39) by

$$\psi_\Xi := \Psi\mathbf{1}^r_\Xi. \tag{51}$$

We then have

$$e^a\left[\boldsymbol{\nabla}_{e_a}\psi_\Xi + \frac{1}{2}\psi_\Xi\omega_a\right]e^{21} - qA\psi_\Xi = m\psi_\Xi e^0. \tag{52}$$

A comment about the nature of spinors is in order. As we repeatedly said in the previous sections, spinor fields should not be ultimately regarded as fields of multivectors (or multiforms), for their behavior under Lorentz transformations is not tensorial (they are able to distinguish between 2π and 4π rotations). So, how can the identification above be correct? The answer is that the definition in Eq. (51) is intrinsically spin-frame dependent. Clearly, this is the price one ought to pay if one wants to make sense of the procedure of representing spinors by differential forms.

Note also that the covariant derivative acting on ψ_Ξ in Eq. (52) is the tensorial covariant derivative ∇_V on $C\ell(M,g)$, as it should be. However, we see from the expression above that ∇_V always acts on ψ_Ξ together with the term $\frac{1}{2}\psi_\Xi\omega_a$. Therefore, it is natural to define an "effective covariant derivative" $\nabla_V^{(s)}$ acting on ψ_Ξ by

$$\nabla_{e_a}^{(s)}\psi_\Xi := \nabla_a\psi_\Xi + \frac{1}{2}\psi_\Xi\omega_a . \tag{53}$$

Then, Proposition 54 yields

$$\nabla_{e_a}^{(s)}\psi_\Xi = \partial_{e_a}(\psi_\Xi) + \frac{1}{2}\omega_a\psi_\Xi , \tag{54}$$

which emulates the spinorial covariant derivative, as it should. We observe moreover that if $U \in \sec C\ell(M,g)$ and if $\psi_\Xi \in \sec C\ell(M,g)$ is a representative of a Dirac-Hestenes spinor field then

$$\nabla_{e_a}^{(s)}(U\psi_\Xi) = (\nabla_{e_a}U)\psi_\Xi + U\nabla_{e_a}^{(s)}\psi_\Xi . \tag{55}$$

(This is the derivative used in Ref. 34, there introduced in an *ad hoc* way.)

With this notation, we finally have the Dirac–Hestenes equation for the *representative* Clifford field $\psi_\Xi \in \sec C\ell(M,g)$, on a Lorentzian spacetime:

$$e^a\nabla_{e_a}^{(s)}\psi_\Xi e^{21} - qA\psi_\Xi = m\psi_\Xi e^0, \tag{56}$$

where ψ_Ξ is the representative of a DHSF Ψ of $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M,g)$, relative to the spin frame Ξ. (The DHE on a Riemann–Cartan spacetime will be discussed in another publication.)

Let us finally show that this formulation recovers the usual transformation properties characteristic of the Hestenes's formalism as described, e.g., in Ref. 34. For that matter, consider two spin frames $\Xi, \Xi' \in \sec P_{\mathrm{Spin}^e_{1,3}}(M)$, with $\Xi'(x) = \Xi(x)u(x)$, where $u(x) \in \mathrm{Spin}^e_{1,3}$. It follows from Proposition 45 that $\psi_{\Xi'} = \Psi\mathbf{1}^r_{\Xi'} = \Psi u^{-1}\mathbf{1}^r_\Xi = \Psi\mathbf{1}^r_\Xi U^{-1} = \psi_\Xi U^{-1}$. Therefore, the various spin frame dependent Clifford fields from Eq. (56) transform as

$$\begin{aligned} e'_a &= Ue_aU^{-1}, \\ \psi_{\Xi'} &= \psi_\Xi U^{-1}. \end{aligned} \tag{57}$$

These are exactly the transformation rules one expects from fields satisfying the Dirac–Hestenes equation (see, e.g., Ref. 34).

D. Bilinear covariants

1. Bilinear covariants associated to a DHSF

We are now in position to give a precise definition of the bilinear covariants of the Dirac theory, associated with a given DHSF.

Definition 47: Recalling that $\Lambda^p(M) \hookrightarrow \mathcal{C}\ell(M,g)$, $p = 0,1,2,3,4$, *and recalling Propositions 39 and 40, the bilinear covariants associated to a DHSF* $\Psi \in \sec C\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ *[and* $\tilde{\Psi} \in \sec \mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$*] are the following sections of* $\mathcal{C}\ell(M,g)$:

$$\begin{aligned} S &= \Psi\tilde{\Psi} = \sigma + e_5\,\omega \in \sec(\Lambda^0(M) + \Lambda^4(M)), \\ J &= \Psi\mathbf{E}_0\tilde{\Psi} \in \sec\Lambda^1(M), \quad K = \Psi\mathbf{E}_3\tilde{\Psi} \in \sec\Lambda^1(M), \end{aligned} \tag{58}$$

$$M = \Psi \mathbf{E}_{12} \tilde{\Psi} \in \sec \Lambda^2(M),$$

where $\Psi = \Psi \frac{1}{2}(1 + \mathbf{E}_0)$, *and* $e_5 = e_0 e_1 e_2 e_3$.

Remark 48: Of course, since all bilinear covariants in Eq. (58) are sections of $\mathcal{C}\ell(M,g)$, *they have the right transformation properties under arbitrary local Lorentz transformations, as required. As shown, e.g., in Ref. 21 these bilinear covariants and their Hodge duals satisfy a set of identities, called the Fierz identities (see, e.g., Ref. 34) that are crucial for the physical interpretation of the Dirac equation (in first and second quantizations).*

Remark 49: Crumeyrolle[10] *gives the name of* amorphous *spinor fields to ideal sections of the Clifford bundle* $\mathcal{C}\ell(M,g)$. *Thus an amorphous spinor field* ϕ *is a section of* $\mathcal{C}\ell(M,g)$ *such that* $\phi P = \phi$, *where* $P = P^2$ *is an idempotent section of* $\mathcal{C}\ell(M,g)$. *However, these fields and also the so-called Dirac–Kähler (Refs. 18, 20) fields, which are also sections of* $\mathcal{C}\ell(M,g)$, *cannot be used in a physical theory of fermion fields since they do not have the correct transformation law under a Lorentz rotation of the local spin frame.*

2. Bilinear covariants associated to a representative of a DHSF

We note that the bilinear covariants, when written in terms of $\psi_\Xi := \Psi \mathbf{1}^r_\Xi$, read (from Proposition 44) as

$$S = \psi_\Xi \tilde{\psi}_\Xi = \sigma + e_5\, \omega \in \sec(\Lambda^0(M) + \Lambda^4(M)),$$

$$J = \psi_\Xi e_0 \tilde{\psi}_\Xi \in \sec \Lambda^1(M), \quad K = \psi_\Xi e_3 \tilde{\psi}_\Xi \in \sec \Lambda^1(M),$$

$$M = \psi_\Xi e_1 e_2 \tilde{\psi}_\Xi \in \sec \Lambda^2(M),$$

where $e_5 = e_0 e_1 e_2 e_3$. These are all intrinsic quantities, as they should be.

E. Electromagnetic gauge invariance of the DHE

Proposition 50: The DHE is invariant under electromagnetic gauge transformations,

$$\psi_\Xi \mapsto \psi'_\Xi = \psi_\Xi e^{q e_{21} \chi}, \tag{59}$$

$$A \mapsto A + \partial\chi, \tag{60}$$

$$\omega_{e_a} \mapsto \omega_{e_a}, \tag{61}$$

where $\psi_\Xi, \psi'_\Xi \in \sec C\ell^0(M,g)$, $A \in \sec \Lambda^1(M) \subset \sec C\ell(M,g)$ *and where* $\chi \in \sec \Lambda^0(M) \subset \sec C\ell(M,g)$ *is a gauge function.*

Proof: It is a direct calculation. ■

But, what are the meanings of these transformations? Equation (59) looks similar to Eq. (57) defining the change of a representative of a DHSF once we change the spin frame, but here we have an active transformation, since we did *not* change the spin frame. On the other hand, Eq. (60) does not correspond either to a passive (no transformation at all) or active local Lorentz transformation for A. Nevertheless, writing $\chi = \theta/2$ yields

$$\begin{aligned}
e^{-qe^{21}\theta/2} e^0 e^{qe^{21}\theta/2} &= e'^0 = e^0, \\
e^{-qe^{21}\theta/2} e^1 e^{qe^{21}\theta/2} &= e'^1 = \cos q\theta \;\; e^1 + \sin q\theta \;\; e^2, \\
e^{-qe^{21}\theta/2} e^2 e^{qe^{21}\theta/2} &= e'^2 = -\sin q\theta \;\; e^1 + \cos q\theta \;\; e^2, \\
e^{-qe^{21}\theta/2} e^3 e^{qe^{21}\theta/2} &= e'^3 = e^3.
\end{aligned} \tag{62}$$

We see that Eqs. (62) define a spin frame Ξ' to which corresponds, as we already know, a basis $\{e'^0, e'^1, e'^2, e'^3\}$ for $\Lambda^1(M) \hookrightarrow C\ell(M,g)$. We can then think of the electromagnetic gauge transformation as a rotation in the spin plane e^{21} by identifying ψ'_Ξ in Eq. (59) with $\psi_{\Xi'}$, the representative of the DHSF in the spin frame Ξ' and by supposing that instead of transforming the spin connection ω_{e_a} as in Eq. (A7) it is taken as fixed and instead of maintaining the electromagnetic potential A fixed it is transformed as in Eq. (60). We observe that, since in the theory of the gravitational field ω_{e_a} is associated with some aspects of that field, our interpretation for the electromagnetic gauge transformation suggests a possible nontrivial coupling between electromagnetism and gravitation, *if* the Dirac–Hestenes equation is taken as a fundamental representation of fermionic matter. We will explore this possibility in another publication.

VI. CONCLUSIONS

In this paper, we hope to have clarified the ontology of Dirac–Hestenes spinor fields [on a general spacetime $\mathfrak{M}=(M,g,\nabla,\tau_g,\uparrow)$ of the Riemann–Cartan type admitting a spin structure] and its relationship with sums of even multivector fields (or differential forms). This has been achieved through the introduction of the Clifford bundle of multivector fields $(\mathcal{C}\ell(M,g))$ and the *left* $(\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M))$ and *right* $(\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M))$ spin-Clifford bundles on a spin manifold (M,g), as well as a study of the relations among these bundles. Left algebraic spinor fields and Dirac–Hestenes spinor fields [both fields are sections of $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$] have been defined and the relation between them has been established. Moreover, a consistent Dirac equation for a DHSF $\Psi \in \sec \mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ (denoted DE$\mathcal{C}\ell^l$) on a Lorentzian spacetime was found. We succeeded also in obtaining in a consistent way a *representation* of the DE$\mathcal{C}\ell^l$ in the Clifford bundle. It is such equation satisfied by Clifford fields $\psi_\Xi \in \sec \mathcal{C}\ell(M,g)$ that we called the Dirac–Hestenes equation (DHE). This means that to each DHSF $\Psi \in \sec \mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $\Xi \in \sec P_{\mathrm{Spin}^e_{1,3}}(M)$ there is a well-defined even nonhomogeneous multivector field $\psi_\Xi \in \sec \mathcal{C}\ell(M,g)$ (EMFS) associated with Ψ. Such a EMFS is called a *representative* of the DHSF on the given spin frame. And, of course, such a EMFS (the representative of the DHSF) is *not* a spinor field. With this crucial distinction between a DHSF and their EMFS representatives we presented a consistent theory for Clifford and spinor fields of all kinds.

We emphasize that the DE$\mathcal{C}\ell^l$ and the DHE, although related, are of different mathematical natures. This issue has been particularly scrutinized in Secs. IV and V. We studied also the local Lorentz invariance and the electromagnetic gauge invariance and showed that only for the DHE such transformations are of the same mathematical nature, something that suggests by itself a possible link between them.

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APPENDIX: COVARIANT DERIVATIVES OF CLIFFORD AND SPINOR FIELDS

1. Covariant derivative of Clifford fields

In this appendix, $(M,g,\nabla,\tau_g,\uparrow)$ denotes a general *Riemann–Cartan* spacetime (see Definition 3). Since $\mathcal{C}\ell(M,g)=\tau M/J(M,g)$, it is clear that any metric compatible $(\nabla g=0)$ connection

defined in τM passes to the quotient $\tau M/J(M,g)$, and thus define an algebra bundle connection.[10] In this way, the covariant derivative of a Clifford field $A \in \sec \mathcal{C}\ell(M,g)$ is completely determined.

We will find formulas for the covariant derivative of Clifford fields and of DHSF using the general theory of connections in principal bundles and covariant derivatives in associate vector bundles, as described in many excellent textbooks, e.g., Refs. 8, 15, 29, 30.

Let (E,M,π_1,G,F) denoted by $E=P\times_\rho F$ be a vector bundle associated to a PFB (P,M,π,G) by the linear representation ρ of G in $F=\mathbf{V}$.

Definition 51: Let $\sigma:\mathbb{R}\supset I\to M$, $t\mapsto\sigma(t)$ *be a curve in* M *with* $x_0=\sigma(0)\in M$, *and let* $p_0 \in \pi^{-1}(x_0)$. *The parallel transport of* p_0 *along* σ *is given by the curve* $\hat{\sigma}:\mathbb{R}\supset I\to P, t\mapsto\hat{\sigma}(t)$ *defined by*

$$\frac{d}{dt}\hat{\sigma}(t)=\Gamma_p\left(\frac{d}{dt}\sigma(t)\right), \tag{A1}$$

with $p_0=\hat{\sigma}(0)$ *and* $\pi(\hat{\sigma}(t))=\sigma(t)$. *We also denote* $p_{\|t}=\hat{\sigma}(t)$.

In Eq. (A1), $\Gamma_p: T_xM\to T_pP$ is a connection on (P,M,π,G) (see, e.g., definition (a) on p. 358 of Ref. 8).

Consider the trivializations of P,

$$\Phi_i:\pi^{-1}(U_i)\to U_i\times G,\quad \Phi_i(p)=(\pi(p),\phi_{i,x}(p)),$$

and E,

$$\Xi_i:\pi_1^{-1}(U_i)\to U_i\times F,\quad \Xi_i(q)=(\pi_1(q),\chi_i(q))=(x,\chi_i(q)).$$

Then, we have the following.

Definition 52: The parallel transport *of* $\Psi_0\in E$, $\pi_1(\Psi_0)=x_0$, *along the curve* $\sigma:\mathbb{R}\supset I\to M$, $t\mapsto\sigma(t)$ *from* $x_0=\sigma(0)\in M$ *to* $x=\sigma(t)$ *is the element* $\Psi_{\|t}\in E$ *such that the following occurs*:

(i) $\pi_1(\Psi_{\|t})=x$,
(ii) $\chi_i(\Psi_{\|t})=\rho(\phi_i(p_{\|t})\circ\phi_i(p_0)^{-1})\chi_i(\Psi_0)$.
(iii) $p_{\|t}\in P$ is the parallel transport of $p_0\in P$ along σ from x_0 to x.

Definition 53: Let v *be a vector at* x_0 *tangent to the curve* σ *(as defined above). The covariant derivative of* $\Psi\in\sec E$ *along* v *is denoted* $(D_v^E\Psi)_{x_0}\in\sec E$ *and*

$$(D_v^E\Psi)(x_0)\equiv(D_v^E\Psi)_{x_0}=\lim_{t\to 0}\frac{1}{t}(\Psi_{\|t}^0-\Psi_0), \tag{A2}$$

where $\Psi_{\|t}^0$ *is the parallel transport of the vector* $\Psi_t\equiv\Psi(\sigma(t))$ *of the given section* $\Psi\in\sec E$ *along* σ *from* $\sigma(t)$ *to* x_0. *The only requirements on* σ *are that* $\sigma(0)=x_0$ *and*

$$\left.\frac{d}{dt}\sigma(t)\right|_{t=0}=v. \tag{A3}$$

Proposition 54: Let $V\in\sec TM$. *The covariant derivative of a Clifford field* $A \in\sec\mathcal{C}\ell(M,g)$ *is given by*

$$\nabla_V A=V(A)+\frac{1}{2}[\omega_V,A], \tag{A4}$$

where $V(A):=V(A^I)e_I$ *and* ω_V *is the connection 1-form* $V\mapsto\omega_V=-\frac{1}{2}V^a\Gamma_{abc}e^b\wedge e^c$, *written in the basis* $\{e_a\}$, *with* Γ_{abc} *given by* $\nabla_{e_a}e_b=\Gamma_{ab}{}^c e_c=\Gamma_{abc}e^c$.

Proof: Writing $A(t)=A(\sigma(t))$ in terms of the multivector basis $\{e_I\}$ of sections associated to a given spin frame, as in Sec. V B, we have $A(t)=A^I(t)e_I(t)=A^I(t)[(\Xi(t),E_I)]=[(\Xi(t),A^I(t)E_I)]=[(\Xi(t),a(t))]$, with $a(t):=A^I(t)E_I\in\mathbb{R}_{1,3}$. If follows from item (ii) of Definition 52 that

$$A^0_{\|t}=[(\Xi(0),g(t)a(t)g(t)^{-1})], \tag{A5}$$

for some $g(t)\in \mathrm{Spin}^e_{1,3}$, with $g(0)=1$. Thus

$$\lim_{t\to 0}\frac{1}{t}(g(t)a(t)g(t)^{-1}-a(0))=\left[\frac{dg}{dt}ag^{-1}+g\frac{da}{dt}g^{-1}+ga\frac{dg^{-1}}{dt}\right]_{t=0}$$
$$=\dot a(0)+\dot g(0)a(0)-a(0)\dot g(0)=V(A^I)E_I+[\dot g(0),a(0)],$$

where $\dot g(0)\in \mathrm{Lie}(\mathrm{Spin}^e_{1,3})=\Lambda^2(\mathbb{R}^{1,3})$. Therefore

$$\boldsymbol{\nabla}_V A=V(A^I)e_I+\frac{1}{2}[\omega_V,A],$$

for some $\omega_V\in \sec\Lambda^2(M)$. In particular, calculating the covariant derivative of the basis 1-vector fields e_b yields $V^a\Gamma_{ab}{}^c e_c=\boldsymbol{\nabla}_V e_b=\frac{1}{2}[\omega_V,e_b]$, so that $\omega_V=-\frac{1}{2}V^a\Gamma_{abc}e^b\wedge e^c$. ■

Remark 55: Equation (A4) shows that the covariant derivative preserves the degree of a homogeneous Clifford field, as can be easily verified.

The general formula Eq. (A4) and the associative law in the Clifford algebra immediately yields the following.

Corollary 56: The covariant derivative $\boldsymbol{\nabla}_V$ on $\mathcal{C}\ell(M,g)$ acts as a derivation on the algebra of sections, i.e., for $A,B\in\sec\mathcal{C}\ell(M,g)$ and $V\in\sec TM$, it holds that

$$\boldsymbol{\nabla}_V(AB)=(\boldsymbol{\nabla}_V A)B+A(\boldsymbol{\nabla}_V B). \tag{A6}$$

Under a change of gauge (local Lorentz transformation) $e^a\mapsto e'^a=Ue^aU^{-1}$, with $U\in\sec\mathcal{C}\ell(M,g), U\tilde U=\tilde U U=1$, the corresponding transformation law for ω_V is as follows.

Corollary 57: Under a change of gauge (local Lorentz transformation), ω_V transforms as

$$\frac{1}{2}\omega_V\mapsto U\frac{1}{2}\omega_V U^{-1}+(\boldsymbol{\nabla}_V U)U^{-1}. \tag{A7}$$

Proof: It is a simple calculation using Eq. (A4). ■

2. Covariant derivatives of spinor fields

The spinor bundles introduced in Sec. II, like $I(M)=P_{\mathrm{Spin}^e_{1,3}}(M)\times_\ell I$, $I=\mathbb{R}_{1,3}\frac{1}{2}(1+E_0)$, and $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$, $\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$ (and subbundles) are examples of vector bundles. Thus, the general theory of covariant derivative operators on associate vector bundles can be used (as in the previous section) to obtain formulas for the covariant derivatives of sections of these bundles. Given $\Psi\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $\Phi\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$, we denote the corresponding covariant derivatives by $\boldsymbol{\nabla}^s_V\Psi$ and $\boldsymbol{\nabla}^s_V\Phi$. [Recall that $I^l(M)\hookrightarrow C\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $I^r(M)\hookrightarrow C\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$.]

Proposition 58: Given $\Psi\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ and $\Phi\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$,

$$\boldsymbol{\nabla}^s_V\Psi=V(\Psi)+\frac{1}{2}\omega_V\Psi, \tag{A8}$$

$$\nabla^s_V \Phi = V(\Psi) - \frac{1}{2}\Psi\,\omega_V. \tag{A9}$$

Proof: It is analogous to that of Proposition 54, with the difference that Eq. (A5) should be substituted by $\Psi^0_{\|t}=[(\Xi(0),g(t)a(t))]$ and $\Phi^0_{\|t}=[(\Xi(0),a(t)g(t)^{-1})]$. ■

Proposition 59: Let ∇ be the connection on $\mathcal{C}\ell(M,g)$ to which ∇^s is related. Then, for any $V\in\sec TM$, $A\in\sec\mathcal{C}\ell(M,g)$, $\Psi\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$) and $\Phi\in\sec\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)$,

$$\nabla^s_V(A\Psi) = A\nabla^s_V\Psi + (\nabla_V A)\Psi, \tag{A10}$$

$$\nabla^s_V(\Phi A) = \Phi\nabla_V A + (\nabla^s_V\Phi)A. \tag{A11}$$

Proof: Recalling that $\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ $[\mathcal{C}\ell^r_{\mathrm{Spin}^e_{1,3}}(M)]$ is a module over $\mathcal{C}\ell(M,g)$, the result follows from a simple computation. ■

Finally, let $\Psi\in\sec\mathcal{C}\ell^l_{\mathrm{Spin}^e_{1,3}}(M)$ be such that $\Psi\mathbf{e}=\Psi$ where $\mathbf{e}^2=\mathbf{e}\in\mathbb{R}_{1,3}$ is a primitive idempotent. Then, since $\Psi\mathbf{e}=\Psi$,

$$\nabla^s_V\Psi = \nabla^s_V(\Psi\mathbf{e}) = V(\Psi\mathbf{e}) + \frac{1}{2}\omega_V\Psi\mathbf{e} = \left[V(\Psi)+\frac{1}{2}\omega_V\Psi\right]\mathbf{e} = (\nabla^s_V\Psi)\mathbf{e}, \tag{A12}$$

from where we verify that the covariant derivative of a LIASF is indeed a LIASF.

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Bounds on convection driven by internal heating

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Bounds are derived for the space–time averaged temperature $\langle T \rangle$ of a fluid layer in the Boussinesq approximation between fixed-temperature horizontal boundaries subject to uniform heating H throughout the volume. The analysis is carried out for both finite and infinite Prandtl number fluids. While the average temperature $\langle T \rangle \sim H$ in the purely conductive state, convection enhances the heat transport beyond static conduction reducing the temperature. Lower bounds to the average temperature of the layer scale with the magnitude of the imposed heat flux, with one scaling exponent for the arbitrary Prandtl number case and another for the infinite Prandtl number model. Specifically, it is proven here that at large heating rates where convection is important, $\langle T \rangle \geqslant c_1 H^{2/3}$ for finite Prandtl number fluids and $\langle T \rangle \geqslant c_2 H^{5/7}$ for infinite Prandtl number fluids. Explicit prefactors c_1 and c_2 for the scaling bounds are computed as well. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Turbulent transport of mass, momentum, and heat remains one of the most important problems for modern theoretical physics and applied mathematics. For incompressible fluid flows, fundamental models such as the Navier–Stokes and related equations are believed to quantitatively describe these phenomena. However the complexity of the dynamics in these systems of nonlinear partial differential equations prohibits exact solutions, and the wide range of length and time scales in turbulent solutions makes direct numerical simulation extremely challenging and expensive. One mathematical approach to the analysis of these systems is to derive rigorous bounds on physically relevant quantities.[12,3,8] This approach is of more than just mathematical interest because it turns out that in some cases the bounds tend to capture aspects of the turbulent scaling of the quantities with respect to the control parameters (e.g., the Reynolds or Rayleigh number). In the case of Rayleigh–Bénard convection, for example, where a fluid layer between horizontal plates is heated from below, the enhancement of the heat flux due to convection, usually measured by a Nusselt number, can be bounded from above in terms of the temperature drop across the layer[11,1,9,6,10,14] expressed in terms of the Rayleigh number.

In this paper we consider the problem of convective heat transport in a fluid layer between fixed-temperature horizontal boundaries with uniform heating throughout the volume. This problem is motivated by geophysical applications;[7,17] the Earth's plate tectonics is a result of convection in the mantle which is predominantly driven by uniform heating due to radioactive decay of elements distributed throughout the mantle. Mantle dynamics is generally modeled as the flow of a high (infinite) Prandtl number fluid with strongly temperature dependent viscosity. The models we focus on here are simpler, with constant material parameters. The boundary conditions for mantle convection are complicated—especially on ''top''—but we restrict the investigation here to rigid no-slip isothermal boundaries in order to make progress. In principle, if all the relevant

materical and boundary effects could be included, the kinds of bounds derived here could be used to put limits on the thermal history of the Earth. A distinct engineering application of this kind of analysis is to the problem of nuclear reactor meltdown.[4]

The rest of this paper is organized as follows: in the next section we present the details of the models we will analyze. In a brief Sec. III we apply the "background" method[9] to the arbitrary Prandtl number problem to derive a scaling lower bound on the space–time averaged temperature of the layer along with an explicit prefactor. In the following Sec. IV we apply a multiple boundary layer asymptotic theory[1] to sharpen the estimate, increasing the prefactor in the lower bound by a factor of 4. Section V is concerned with the infinite Prandtl number problem, and the background method utilizing a recently derived inequality[10] results in a scaling lower bound with a smaller exponent. In the concluding Sec. VI we summarize our results in the context of direct numerical simulations, and discuss some possible areas for further development of this approach.

II. GOVERNING EQUATIONS

The fluid layer is confined between two parallel plates of horizontal extent L_x and L_y separated by vertical (z) distance d. The no-slip upper and lower plates are held at fixed temperatures T_0 and T_1, respectively; the temperature difference $\Delta T = T_0 - T_1$ which will eventually be taken to be zero for the work presented here. A uniform volumetric heat flux H (with units power/volume) is pumped into the layer. The governing equations for the velocity field $\mathbf{u}$, the pressure p and the temperature T in the standard Boussinesq approximation are

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\nabla^2\mathbf{u} + \hat{\mathbf{k}} g\alpha T, \tag{1a}$$

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T = \kappa\nabla^2 T + \gamma, \tag{1b}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{1c}$$

with the boundary conditions

$$\mathbf{u}|_{z=0,d} = 0, \quad T|_{z=0} = T_0, \quad T|_{z=d} = T_1, \tag{1d}$$

where ν is the viscosity, g is the acceleration of gravity along the z axis (in the $-\hat{\mathbf{k}}$ direction), α is the thermal expansion coefficient, κ is the thermal diffusion coefficient and $\gamma = H/\rho c$, where ρ is the density and c is the specific heat capacity of the fluid. We impose periodic boundary conditions in the horizontal directions with periods L_x and L_y.

Using d^2/κ as the unit of time, d as the unit of length, and $\gamma d^2/\kappa$ as the unit of temperature, the governing equations are put into the nondimensional form

$$\mathrm{Pr}^{-1}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) + \nabla p = \nabla^2\mathbf{u} + RT\hat{\mathbf{k}}, \tag{2a}$$

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T = \nabla^2 T + 1, \tag{2b}$$

where $\mathrm{Pr} = \nu/\kappa$ is the Prandtl number and $R = g\alpha d^5\gamma/\kappa^2\nu$ is the heat Rayleigh number.[16] We consider R, proportional to the internal heating rate, to be the control parameter. The boundary conditions in nondimensional form are

$$\mathbf{u}|_{z=0,1} = 0, \quad T|_{z=0} = \tilde{T}, \quad T|_{z=1} = 0, \tag{2c}$$

where $\tilde{T}=(\kappa/\gamma d^2)\Delta T$; this shows that $R\tilde{T}$ is the usual Rayleigh number $\mathrm{Ra}=g\alpha\Delta T d^3/\nu\kappa$ for bottom heating.

In the following discussion, we only consider the special case where both boundaries are held at the same temperature, i.e., $\Delta T=0$ or $\tilde{T}=0$. With this boundary condition, the static conduction solution has a quadratic profile:

$$T=\tfrac{1}{2}z(1-z), \tag{3}$$

which becomes unstable for sufficiently large R.[19] Once convection sets in, the flow tends to lower the average temperature of the fluid, so the estimate of interest is the minimum possible bulk average temperature for a given value R. We define the space–time average of a function $f(\mathbf{x},t)$ as

$$\langle f\rangle=\lim_{t\to\infty}\frac{1}{t}\int_0^t ds\,\frac{d^2}{L_xL_y}\int dxdydz f(\mathbf{x},s). \tag{4}$$

In the following discussion, we apply the background and multiple boundary layer methods to derive lower bounds for the bulk average (nondimensional) temperature with respect to R in the form $\langle T\rangle\geqslant cR^{\alpha}$ as $R\to\infty$.

III. BACKGROUND METHOD FOR FINITE Pr

To apply the background method, first we decompose the temperature field $T(x,y,z,t)$ into a time-independent background profile $\tau(z)$ and a fluctuating part $\theta(x,y,z,t)$:

$$T(x,y,z,t)=\tau(z)+\theta(x,y,z,t). \tag{5}$$

The boundary conditions of $T(x,y,z,t)$ are contained in $\tau(z)$:

$$\tau(0)=\tau(1)=0 \tag{6}$$

and the fluctuating part $\theta(x,y,z,t)$ satisfies homogeneous boundary conditions

$$\theta(x,y,0,t)=\theta(x,y,1,t)=0. \tag{7}$$

The velocity field $\mathbf{u}$ is divergence-free with no-slip boundary conditions:

$$\nabla\cdot\mathbf{u}=0,\quad \mathbf{u}|_{z=0,1}=0. \tag{8}$$

With this decomposition the governing Eqs. (2) become

$$\mathrm{Pr}^{-1}\left(\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)+\nabla p=\nabla^2\mathbf{u}+\tau\hat{\mathbf{k}}+R\theta\hat{\mathbf{k}}, \tag{9a}$$

$$\frac{\partial\theta}{\partial t}+\mathbf{u}\cdot\nabla\theta=\nabla^2\theta+\tau''+1-w\tau'. \tag{9b}$$

Then taking the space–time average of $\mathbf{u}\cdot(9\mathrm{a})$ yields

$$\langle|\nabla\mathbf{u}|^2\rangle=R\langle w\theta\rangle, \tag{10}$$

and averaging $\theta\cdot(9\mathrm{b})$ and $\tau\cdot(9\mathrm{b})$ yield, respectively,

$$\langle w\theta\tau'\rangle=-\langle|\nabla\theta|^2\rangle-\langle\theta_z\tau'\rangle+\langle\theta\rangle, \tag{11}$$

$$-\langle w\theta\tau'\rangle=-\langle\theta_z\tau'\rangle+\langle\tau\rangle-\langle\tau'^2\rangle. \tag{12}$$

The difference of the above two identities is

$$(\langle\theta\rangle-\langle\tau\rangle)=\langle|\nabla\theta|^2\rangle+2\langle w\theta\tau'\rangle-\langle\tau'^2\rangle. \tag{13}$$

Since $\langle T\rangle=\langle\tau\rangle+\langle\theta\rangle$, we have

$$\langle T\rangle=\langle|\nabla\theta|^2\rangle+2\langle w\theta\tau'\rangle+2\langle\tau\rangle-\langle\tau'^2\rangle. \tag{14}$$

The identity (10) can also be written as

$$0=\frac{a}{R}\langle|\nabla\mathbf{u}|^2\rangle-a\langle w\theta\rangle, \tag{15}$$

where a is a positive number (a ''balance parameter'') to be adjusted to yield the best prefactor.[13] Adding Eq. (15) to Eq. (14) enables us to express the average temperature as follows:

$$\langle T\rangle=2\langle\tau\rangle-\langle\tau'^2\rangle+H, \tag{16}$$

where

$$H=\langle|\nabla\theta|^2\rangle+\langle(2\tau'-a)w\theta\rangle+\frac{a}{R}\langle|\nabla\mathbf{u}|^2\rangle. \tag{17}$$

If the functional H is positive semidefinite among the fields $\mathbf{u}$ and θ satisfying

$$\nabla\cdot\mathbf{u}=0,\quad \mathbf{u}|_{z=0,1}=0,\quad \theta|_{z=0,1}=0,$$

then we have a lower bound for $\langle T\rangle$:

$$\langle T\rangle\geqslant 2\langle\tau\rangle-\langle\tau'^2\rangle. \tag{18}$$

So the goal is to choose a background profile τ satisfying the boundary conditions (6) guaranteeing that H is positive semidefinite while making the lower bound in (18) as large as possible.

If we could take a linear background profile with the slope $a/2>0$, then $2\tau'-a$ would vanish and thus the functional H would clearly be non-negative, but this choice can not allow both $\tau(0)$ and $\tau(1)$ to vanish simultaneously. However, the indefinite term in H is proportional to $w\theta$ that vanishes at the boundaries. This suggests that we can take $2\tau'=a$ in the middle while introducing two boundary layers to enforce τ's boundary conditions. These considerations lead us to focus on the family of piecewise linear background profiles

$$\tau(z)=\begin{cases}\left(\dfrac{a}{2}+\dfrac{b}{\delta_1}\right)z, & 0\leqslant z<\delta_1,\\ \dfrac{a}{2}z+b, & 1-\delta_1\leqslant z\leqslant 1-\delta_2,\\ -\left[\dfrac{a}{2}\left(\dfrac{a}{\delta_2}-1\right)+\dfrac{b}{\delta_2}\right](z-1), & 1-\delta_2\leqslant z\leqslant 1,\end{cases} \tag{19}$$

where δ_1 (δ_2) is the thickness of the boundary layer at $z=0$ ($z=1$) introduced to satisfy the boundary conditions (see Fig. 1). Then

$$\langle T\rangle\geqslant 2\langle\tau\rangle-\langle\tau'^2\rangle=\frac{a}{2}(1-\delta_2)+b(1-\delta_1-\delta_2)-\left\{\frac{a^2}{4}\left(\frac{1}{\delta_2}-1\right)+b^2\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}\right)+\frac{ab}{\delta_2}\right\}, \tag{20}$$

provided the quadratic functional H in (17) is positive definite. Before estimating the size of H, we can maximize $2\langle\tau\rangle-\langle\tau'^2\rangle$ over a and b, and this procedure yields

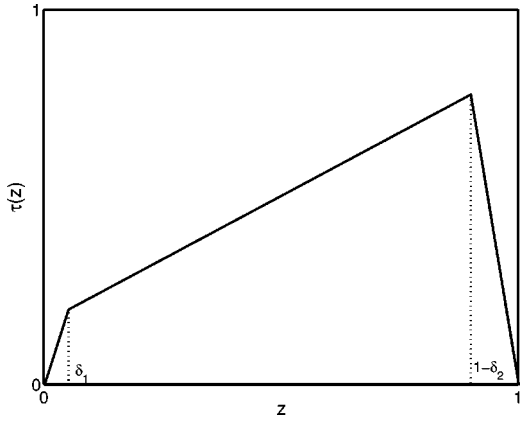

FIG. 1. The background profile for finite Prandtl number.

$$\langle T\rangle \geqslant \tfrac{1}{4}(1-\delta_1)(1-\delta_2)(\delta_1+\delta_2) \tag{21}$$

with

$$\begin{cases} a=\delta_2-\delta_1 \\ b=\dfrac{\delta_1}{2}(1-\delta_2). \end{cases} \tag{22}$$

Then using the inequality[9]

$$\left|\int_0^1 w\theta\right| \leqslant \left(\frac{c}{4}\|\mathbf{u}\|_2^2+\frac{1}{c}\|\theta\|_2^2\right) \tag{23}$$

for any $c>0$, the term $\langle(2\tau'-a)w\theta\rangle$ can be estimated by

$$\begin{aligned}|\langle(2\tau'-a)w\theta\rangle| &\leqslant \frac{b\delta_1}{2}\left[\frac{c_1}{4}\langle|\nabla\mathbf{u}|^2\rangle+\frac{1}{c_1}\langle|\nabla\theta|^2\rangle\right]+\frac{(a+2b)\delta_2}{4}\left[\frac{c_2}{4}\langle|\nabla\mathbf{u}|^2\rangle+\frac{1}{c_2}\langle|\nabla\theta|^2\rangle\right] \\ &= \frac{\delta_1^2(1-\delta_2)}{4}\left[\frac{c_1}{4}\langle|\nabla\mathbf{u}|^2\rangle+\frac{1}{c_1}\langle|\nabla\theta|^2\rangle\right]+\frac{\delta_2^2(1-\delta_1)}{4}\left[\frac{c_2}{4}\langle|\nabla\mathbf{u}|^2\rangle+\frac{1}{c_2}\langle|\nabla\theta|^2\rangle\right].\end{aligned}$$

Then

$$H\geqslant\left[1-\frac{\delta_1^2(1-\delta_2)}{4c_1}-\frac{\delta_2^2(1-\delta_1)}{4c_2}\right]\langle|\nabla\theta|^2\rangle+\left[\frac{a}{R}-\frac{\delta_1^2(1-\delta_2)c_1}{16}-\frac{\delta_2^2(1-\delta_1)c_2}{16}\right]\langle|\nabla\mathbf{u}|^2\rangle.$$

Thus H is positive semidefinite if

$$1-\frac{\delta_1^2(1-\delta_2)}{4c_1}-\frac{\delta_2^2(1-\delta_1)}{4c_2}\geqslant 0 \tag{24}$$

and

$$\frac{a}{R}-\frac{\delta_1^2(1-\delta_2)c_1}{16}-\frac{\delta_2^2(1-\delta_1)c_2}{16}\geqslant 0. \tag{25}$$

We can choose $c_1=c_2=c$ and then it is sufficient to require

$$[\delta_1^2(1-\delta_2)+\delta_2^2(1-\delta_1)]^2=\frac{64(\delta_2-\delta_1)}{R}, \tag{26}$$

and

$$c=\frac{a}{4}. \tag{27}$$

Now the lower bound of $\langle T\rangle$ in (21) can be maximized over δ_1 and δ_2 subject to condition (26). But before fully optimizing the bound in (21) we consider the special case where there is only one boundary layer in the background field at $z=1$, i.e., the choice $\delta_1=0$. Although this will not give us the optimal bound, it is still a rigorous lower bound which is easier to compute and which can be compared with the optimal bound later.

For $\delta_1=0$ we should set $b=0$ in the general background profile (19). Thus (21) becomes

$$\langle T\rangle \geqslant \tfrac{1}{4}(1-\delta_2)\delta_2, \tag{28}$$

and the constraint (26) is simplified to be

$$\delta_2^3=\frac{64}{R}. \tag{29}$$

We can now write down the estimate

$$\langle T\rangle \geqslant R^{-1/3}(1-4R^{-1/3}). \tag{30}$$

So as $R\to\infty$, $\langle T\rangle \geqslant R^{-1/3}$ with prefactor 1.

To fully optimize the bound, we need to maximize the right-hand side of the inequality (21) subject to the constraint (26):

$$\langle T\rangle \geqslant \max_{\delta_1,\delta_2}\left\{\frac{1}{4}(1-\delta_1)(1-\delta_2)(\delta_1+\delta_2)\right\}, \tag{31}$$

with δ_1 and δ_2 satisfying

$$[\delta_1^2(1-\delta_2)+\delta_2^2(1-\delta_1)]^2=\frac{64(\delta_2-\delta_1)}{R}. \tag{32}$$

This is easily done numerically and the result is shown in Fig. 2. It is seen from the graph that this better bound follows the same scaling as in (30), i.e., $\sim R^{-1/3}$ as $R\to\infty$. The prefactor can be measured from the graph, showing that the asymptotic prefactor is improved slightly:

$$\langle T\rangle \geqslant 1.09R^{-1/3} \quad \text{as} \quad R\to\infty. \tag{33}$$

IV. MULTIPLE BOUNDARY LAYER METHOD FOR FINITE Pr

In this section, we will derive the lower bound of the bulk average temperature using the homogeneous ratio approach introduced by Howard[11] and the multiple boundary layer method due to Busse.[1] First we decompose the temperature and velocity fields into their horizontal average and fluctuating parts:

$$T=\overline{T}+\theta, \quad \text{with} \quad \overline{\theta}=0 \quad \text{and} \quad \overline{\mathbf{u}}=0, \tag{34}$$

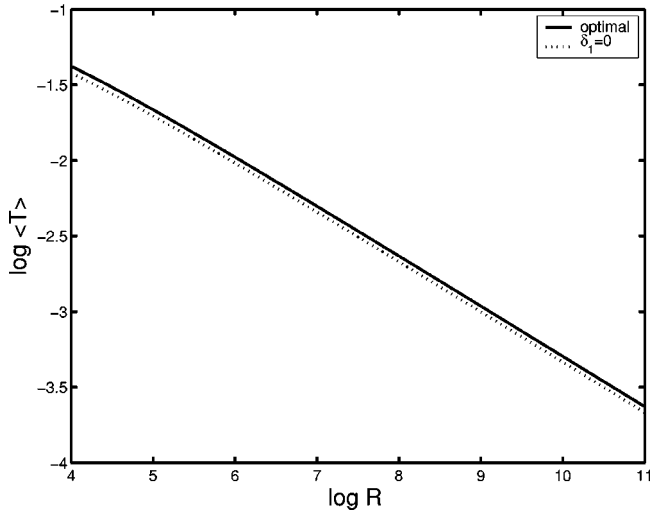

FIG. 2. The solid line is the fully optimized lower bound of the bulk average temperature compared to the estimate (30) (the dotted line).

where overline denotes the horizontal average. We will assume that the flow is statistically stationary so that the horizontal average is time-independent and the fluctuating part has vanishing horizontal mean. This is most easily justified in the limit of a horizontally infinite layer, so we take

$$\overline{f}(z)=\lim_{L_x,L_y\to\infty}\frac{1}{L_xL_y}\int f(x,y,z,t)\;\;dxdy. \tag{35}$$

The horizontal average of the temperature Eq. (2b) is

$$\frac{d\overline{w\theta}}{dz}=\frac{d^2\overline{T}}{d^2z}+1. \tag{36}$$

Integrate once to obtain

$$\overline{w\theta}=\frac{d\overline{T}}{dz}+z+c. \tag{37}$$

The integration constant c here is determined by integrating above equation over $[0,1]$, yielding

$$\frac{d\overline{T}}{dz}=\overline{w\theta}-\langle w\theta\rangle-\left(z-\frac{1}{2}\right). \tag{38}$$

Using the decomposition (34) along with (36), Eq. (2b) can be written

$$\frac{\partial\theta}{\partial t}+w\frac{d\overline{T}}{dz}+\mathbf{u}\cdot\nabla\theta=\nabla^2\theta+\frac{d^2\overline{T}}{d^2z}+1=\nabla^2\theta+\frac{d\overline{w\theta}}{dz}. \tag{39}$$

Multiplying both sides by θ and integrate over the bulk, we deduce

$$\left\langle w\theta\frac{d\overline{T}}{dz}\right\rangle=-\langle|\nabla\theta|^2\rangle. \tag{40}$$

Together with Eq. (38), we find the ''power integral''

$$\left\langle \left(z-\frac{1}{2} \right) w\theta \right\rangle = \langle |\nabla \theta|^2 \rangle + \langle (\overline{w\theta} - \langle w\theta \rangle)^2 \rangle. \tag{41}$$

Another power integral is derived by multiplying Eq. (2a) by **u** and integrating over the bulk:

$$\langle |\nabla \mathbf{u}|^2 \rangle = R \langle w\theta \rangle. \tag{42}$$

Finally, we derive an expression for the average temperature by multiplying Eq. (38) by z and integrating over $[0,1]$:

$$\langle T \rangle = -\left\langle \left(z-\frac{1}{2} \right) w\theta \right\rangle + \frac{1}{12}. \tag{43}$$

In summary we have the following balances:

$$\langle |\nabla \mathbf{u}|^2 \rangle = R \langle w\theta \rangle, \tag{44}$$

$$\langle (z-\tfrac{1}{2}) w\theta \rangle = \langle |\nabla \theta|^2 \rangle + \langle (\overline{w\theta} - \langle w\theta \rangle)^2 \rangle, \tag{45}$$

$$\langle T \rangle = -\langle (z-\tfrac{1}{2}) w\theta \rangle + \tfrac{1}{12}. \tag{46}$$

Now rewrite (45) as

$$1 = \frac{\langle |\nabla \theta|^2 \rangle + \langle (\overline{w\theta} - \langle w\theta \rangle)^2 \rangle}{\left\langle \left(z-\frac{1}{2} \right) w\theta \right\rangle} \tag{47}$$

and multiply the $\frac{1}{12}$ in (46) so disguised to find

$$\langle T \rangle = \frac{\langle |\nabla \theta|^2 \rangle + \langle (\overline{w\theta} - \langle w\theta \rangle)^2 \rangle - 12\left\langle \left(z-\frac{1}{2} \right) w\theta \right\rangle^2}{12\left\langle \left(z-\frac{1}{2} \right) w\theta \right\rangle}. \tag{48}$$

Let

$$h(z) = \sqrt{12}(z-\tfrac{1}{12}). \tag{49}$$

Notice that

$$\langle h \rangle = 0, \quad \langle h^2 \rangle = 1. \tag{50}$$

Then

$$\langle (\overline{w\theta} - h\langle hw\theta \rangle - \langle w\theta \rangle)^2 \rangle = \langle \overline{w\theta}^2 \rangle - \langle w\theta \rangle^2 - \langle hw\theta \rangle^2. \tag{51}$$

Thus together with (44), the average temperature can be expressed as

$$\begin{aligned} \langle \sqrt{12} RT \rangle &= R \frac{\langle |\nabla \theta|^2 \rangle + \langle (\overline{w\theta} - \langle w\theta \rangle)^2 \rangle - \langle hw\theta \rangle^2}{\langle hw\theta \rangle} \\ &= \frac{\langle |\nabla \theta|^2 \rangle \langle |\nabla \mathbf{u}|^2 \rangle}{\langle w\theta \rangle \langle hw\theta \rangle} + R \frac{\langle (\overline{w\theta} - h\langle hw\theta \rangle - \langle w\theta \rangle)^2 \rangle}{\langle hw\theta \rangle}. \end{aligned} \tag{52}$$

The variational problem can be formulated as follows:
Given $\mu = R\langle hw\theta\rangle$, *find the minimum of the functional*

$$\mathcal{F} = \frac{\langle|\nabla\theta|^2\rangle\langle|\nabla\mathbf{u}|^2\rangle}{\langle hw\theta\rangle\langle w\theta\rangle} + \mu\frac{\langle(\overline{w\theta} - h\langle hw\theta\rangle - \langle w\theta\rangle)^2\rangle}{\langle hw\theta\rangle^2} \tag{53}$$

among the $\mathbf{u}$, θ *fields with*

$$\nabla\cdot\mathbf{u} = 0, \quad \mathbf{u}|_{z=0,1} = 0, \quad \theta|_{z=0,1} = 0, \tag{54}$$

where

$$w = \mathbf{u}\cdot\hat{\mathbf{k}}, \quad h(z) = \sqrt{12}(z - \tfrac{1}{2}). \tag{55}$$

Since the functional $\mathcal{F}$ is homogeneous in both w and θ, we can impose two normalization conditions

$$\langle hw\theta\rangle = 1, \quad \langle w^2\rangle = \langle\theta^2\rangle. \tag{56}$$

We are seeking the minimum of the functional $\mathcal{F}$ as $\mu\to\infty$. This implies that $\overline{w\theta} = h + \langle w\theta\rangle$ [here and in the following discussion the normalization conditions (56) have been assumed] throughout most of the interval $0<z<1$, which makes the second term in the functional vanish in this interval. Only near the boundary $z=0,1$ the boundary conditions prevent a close appoach of $\overline{w\theta}$ to $h+\langle w\theta\rangle$. And the contribution to the functional is thus from possible boundary layers at $z=0,1$. (Note: the boundary layers are distinct in this problem, as is the case for a similar analysis of circular Couette flow where the inner and outer cylinders must be handled seperately.[2]) Since $h(1)+\langle w\theta\rangle = \sqrt{3} + \langle|\nabla\mathbf{u}|^2\rangle > 0$ [from Eq. (44) and definition (49)] there must be a boundary layer at $z=1$. At $z=0$, $h(0)+\langle w\theta\rangle = -\sqrt{3}+\langle w\theta\rangle$ is indefinite. Thus the existence of a boundary layer at $z=0$ depends on whether $h(0)+\langle w\theta\rangle$ is zero. Without loss of generality we assume there are two boundary layers at $z=0,1$ respectively, and make the ansatz

$$w = \sum\ w_n\phi_n + w_n^*\phi_n^*, \quad \theta = \sum\ \theta_n\phi_n + \theta_n^*\phi_n^*, \tag{57}$$

where ϕ_n and ϕ_n^* satisfy

$$\Delta_2\phi_n = -\alpha_n^2\phi_n, \quad \Delta_2\phi_n^* = -\alpha_n^{*2}\phi_n^*. \tag{58}$$

We introduce the following boundary layer variables:

$$w = \begin{cases} \mu^{-p_n}\hat{w}(\zeta_n) & \text{for } 1-z = O(\mu^{-r_n}), \\ \mu^{-s_n}\tilde{w}(\zeta_{n-1}) & \text{for } 1-z = O(\mu^{-r_{n-1}}), \end{cases} \tag{59}$$

$$\theta = \begin{cases} \mu^{p_n}\hat{\theta}(\zeta_n) & \text{for } 1-z = O(\mu^{-r_n}), \\ \mu^{s_n}\tilde{\theta}(\zeta_{n-1}) & \text{for } 1-z = O(\mu^{-r_{n-1}}), \end{cases} \tag{60}$$

$$w^* = \begin{cases} \mu^{-p_n}\hat{w}^*(\zeta_n^*) & \text{for } z = O(\mu^{-r_n}), \\ \mu^{-s_n}\tilde{w}^*(\zeta_{n-1}^*) & \text{for } z = O(\mu^{-r_{n-1}}), \end{cases} \tag{61}$$

$$\theta^* = \begin{cases} \mu^{p_n}\hat{\theta}^*(\zeta_n^*) & \text{for } z = O(\mu^{-r_n}), \\ \mu^{s_n}\tilde{\theta}^*(\zeta_{n-1}^*) & \text{for } z = O(\mu^{-r_{n-1}}), \end{cases} \tag{62}$$

where

$$\zeta_n=(1-z)\mu^{r_n},\quad \zeta_n^*=z\mu^{r_n}. \tag{63}$$

The boundary layer structure is such that in the interior

$$\tilde{w}_1\tilde{\theta}_1+\tilde{w}_1^*\tilde{\theta}_1^*\approx h+\langle w\theta\rangle, \tag{64}$$

and in the boundary layers

$$\tilde{w}_n\tilde{\theta}_n+\hat{w}_{n-1}\hat{\theta}_{n-1}\approx h_1+\langle w\theta\rangle,\quad \tilde{w}_n^*\tilde{\theta}_n^*+\hat{w}_{n-1}^*\hat{\theta}_{n-1}^*\approx h_0+\langle w\theta\rangle \tag{65}$$

for $n=1,\ldots,N-1$, where

$$h_0=h(0)=-\sqrt{3},\quad h_1=h(1)=\sqrt{3}.$$

With the boundary layer approximations, the functional becomes

$$\begin{aligned}\hat{\mathcal{F}}_N=\frac{1}{\langle w\theta\rangle}\Bigg\{&\sum_1^N \mu^{2p_n+r_n}\Bigg(\int_0^\infty \hat{\theta}_n'^2 d\zeta_n+\int_0^\infty \hat{\theta}_n^{*\prime 2} d\zeta_n^*\Bigg)+\sum_2^N \mu^{q_n-r_n+2s_n}\Bigg(b_n^2\int_0^\infty \tilde{\theta}_n^2 d\zeta_{n-1}\\&+b_n^{*2}\int_0^\infty \tilde{\theta}_n^{*2} d\zeta_{n-1}^*\Bigg)+\mu^{q_1}(b_1^2\langle\tilde{\theta}_1^2\rangle+b_1^{*2}\langle\tilde{\theta}_1^{*2}\rangle)\Bigg\}\Bigg\{\sum_1^N \mu^{3r_n-2p_n-q_n}\Bigg(\frac{1}{b_n^2}\int_0^\infty \hat{w}_n''^2 d\zeta_n\\&+\frac{1}{b_n^{*2}}\int_0^\infty \hat{w}_n^{*\prime\prime 2} d\zeta_n^*\Bigg)+\sum_2^N \mu^{q_n-r_{n-1}-2s_n}\Bigg(b_n^2\int_0^\infty \tilde{w}_n^2 d\zeta_{n-1}+b_n^{*2}\int_0^\infty \tilde{w}_n^{*2} d\zeta_{n-1}^*\Bigg)\mu^{q_1}(b_1^2\langle\tilde{w}_1^2\rangle\\&+b_1^{*2}\langle\tilde{w}_1^{*2}\rangle)\Bigg\}+\Bigg\{\mu^{1-r_N}\Bigg(\int_0^\infty(\hat{w}_N\hat{\theta}_N-h_1-\langle w\theta\rangle)^2 d\zeta_N+\int_0^\infty(\hat{w}_N^*\hat{\theta}_N^*-h_0-\langle w\theta\rangle)^2 d\zeta_N^*\Bigg)\Bigg\}.\end{aligned} \tag{66}$$

Balancing the exponents in the above expression yields

$$r_n=\frac{1-4^{-n}}{3-4^{-n}},\quad q_n=\frac{2-4^{-n}}{3-4^{-n}},\quad s_n=0,\quad 2p_n=\frac{4^{-n}}{3-4^{-n}}. \tag{67}$$

Then we have

$$\hat{\mathcal{F}}_N=\mu^{2/3-4^{-N}}F_N, \tag{68}$$

where

$$\begin{aligned}F_N=\frac{1}{\langle w\theta\rangle}\Bigg\{&\sum_1^N\Bigg(\int_0^\infty \hat{\theta}_n'^2 d\zeta_n+\int_0^\infty \hat{\theta}_n^{*\prime 2} d\zeta_n^*\Bigg)\sum_2^N\Bigg(b_n^2\int_0^\infty \tilde{\theta}_n^2 d\zeta_{n-1}+b_n^{*2}\int_0^\infty \tilde{\theta}_n^{*2} d\zeta_{n-1}^*\Bigg)+(b_1^2\langle\tilde{\theta}_1^2\rangle\\&+b_1^{*2}\langle\tilde{\theta}_1^{*2}\rangle)\Bigg\}\Bigg\{\sum_1^N\Bigg(\frac{1}{b_n^2}\int_0^\infty \hat{w}_n''^2 d\zeta_n+\frac{1}{b_n^{*2}}\int_0^\infty \hat{w}_n^{*\prime\prime 2} d\zeta_n^*\Bigg)\sum_2^N\Bigg(b_n^2\int_0^\infty \tilde{w}_n^2 d\zeta_{n-1}\\&+b_n^{*2}\int_0^\infty \tilde{w}_n^{*2} d\zeta_{n-1}^*\Bigg)+(b_1^2\langle\tilde{w}_1^2\rangle+b_1^{*2}\langle\tilde{w}_1^{*2}\rangle)\Bigg\}+\Bigg\{\int_0^\infty(\hat{w}_N\hat{\theta}_N-h_1-\langle w\theta\rangle)^2 d\zeta_N\\&+\int_0^\infty(\hat{w}_N^*\hat{\theta}_N^*-h_0-\langle w\theta\rangle)^2 d\zeta_N^*\Bigg\}.\end{aligned} \tag{69}$$

Now the Euler–Lagrange equations for the functional F_N can be written down:

$$\frac{1}{\langle w\theta\rangle}\frac{D_\theta}{b_n^2}\hat{w}_n^{(4)}-\mu^{r_N-r_n}\hat{\theta}_n(h_1+\langle w\theta\rangle-\hat{w}_n\hat{\theta}_n-\tilde{w}_{n+1}\tilde{\theta}_{n+1})=0, \tag{70}$$

$$\frac{1}{\langle w\theta\rangle}D_w\hat{\theta}_n''+\mu^{r_N-r_n}\hat{w}_n(h_1+\langle w\theta\rangle-\hat{w}_n\hat{\theta}_n-\tilde{w}_{n+1}\tilde{\theta}_{n+1})=0, \tag{71}$$

$$n=1,\ldots,N, \tag{72}$$

$$\frac{b_{n+1}^2}{\langle w\theta\rangle}D_\theta\tilde{w}_{n+1}-\mu^{r_N-r_n}\tilde{\theta}_{n+1}(h_1+\langle w\theta\rangle-\hat{w}_n\hat{\theta}_n-\tilde{w}_{n+1}\tilde{\theta}_{n+1})=0, \tag{73}$$

$$\frac{b_{n+1}^2}{\langle w\theta\rangle}D_w\tilde{\theta}_{n+1}-\mu^{r_N-r_n}\tilde{w}_{n+1}(h_1+\langle w\theta\rangle-\hat{w}_n\hat{\theta}_n-\tilde{w}_{n+1}\tilde{\theta}_{n+1})=0, \tag{74}$$

$$n=1,\ldots,N-1. \tag{75}$$

And for $\tilde{w}_1$, $\tilde{\theta}_1$,

$$\frac{D_\theta}{\langle w\theta\rangle}b_1^2\tilde{w}_1-\tilde{\theta}_1\left\{\frac{D_\theta D_w}{2\langle w\theta\rangle^2}(h\langle w\theta\rangle+1)+\mu^{r_N}(h+\langle w\theta\rangle-\tilde{w}_1\tilde{\theta}_1-\tilde{w}_1^*\tilde{\theta}_1^*)+h\left(\int_0^\infty(\hat{w}_N\hat{\theta}_N-h_1\right.\right.$$
$$\left.\left.-\langle w\theta\rangle)^2d\zeta_N+\int_0^\infty(\hat{w}_N^*\hat{\theta}_N^*-h_0-\langle w\theta\rangle)^2d\zeta_N^*\right)\right\}=0, \tag{76}$$

and

$$\frac{D_w}{\langle w\theta\rangle}b_1^2\tilde{\theta}_1-\tilde{w}_1\left\{\frac{D_\theta D_w}{2\langle w\theta\rangle^2}(h\langle w\theta\rangle+1)+\mu^{r_N}(h+\langle w\theta\rangle-\tilde{w}_1\tilde{\theta}_1-\tilde{w}_1^*\tilde{\theta}_1^*)+h\left(\int_0^\infty(\hat{w}_N\hat{\theta}_N-h_1\right.\right.$$
$$\left.\left.-\langle w\theta\rangle)^2d\zeta_N+\int_0^\infty(\hat{w}_N^*\hat{\theta}_N^*-h_0-\langle w\theta\rangle)^2d\zeta_N^*\right)\right\}=0. \tag{77}$$

The same set of equations are also satisfied by the starred quantities $\tilde{w}_n^*,\tilde{\theta}_n^*,\hat{w}_n^*,\hat{\theta}_n^*$.

From Eqs. (76) and (77), we have

$$D_\theta\tilde{w}_1^2=D_w\tilde{\theta}_1^2, \tag{78}$$

$$D_\theta\tilde{w}_1^{*2}=D_w\tilde{\theta}_1^{*2}. \tag{79}$$

Adding these two identities yields

$$D_\theta\langle\tilde{w}_1^2+\tilde{w}_1^{*2}\rangle=D_w\langle\tilde{\theta}_1^2+\tilde{\theta}_1^{*2}\rangle. \tag{80}$$

Hence the normalization condition $\langle w^2\rangle=\langle\theta^2\rangle$ implies

$$D_\theta=D_w=D. \tag{81}$$

This identity together with Eqs. (76) and (77) yields

$$\tilde{w}_1^2=\tilde{\theta}_1^2,\quad b_1=b_1^*. \tag{82}$$

Equation (73) together with Eq. (75) gives

$$D_\theta \tilde{w}_{n+1}^2 = D_w \tilde{\theta}_{n+1}^2 .$$

The same identity holds for $\tilde{w}_{n+1}^*$ and $\tilde{\theta}_{n+1}^*$. Therefore

$$\tilde{w}_{n+1}^2 = \tilde{\theta}_{n+1}^2, \quad \tilde{w}_{n+1}^{*2} = \tilde{\theta}_{n+1}^{*2} \quad \text{for } n = 1, \ldots, N-1. \tag{83}$$

Substituting the above identity back into Eq. (73), we have

$$h_1 + \langle w\theta \rangle - \hat{w}_n \hat{\theta}_n - \tilde{w}_{n+1}\tilde{\theta}_{n+1} = \mu^{r_n - r_N} b_{n+1}^2 \frac{D}{\langle w\theta \rangle}, \tag{84}$$

$$h_0 + \langle w\theta \rangle - \hat{w}_n^* \hat{\theta}_n^* - \tilde{w}_{n+1}^* \tilde{\theta}_{n+1}^* = \mu^{r_n - r_N} b_{n+1}^{*2} \frac{D}{\langle w\theta \rangle} \tag{85}$$

for $n = 1, \ldots, N-1$. Then Eqs. (70) and (72) become

$$\frac{1}{b_n^2} \hat{w}_n^{(4)} - b_{n+1}^2 \hat{\theta}_n = 0, \tag{86}$$

$$\hat{\theta}_n'' + b_{n+1}^2 \hat{w}_n = 0, \quad n = 1, \ldots, N-1. \tag{87}$$

The above equations hold in the region where $\hat{w}_n \hat{\theta}_n \neq h_1 + \langle w\theta \rangle$. When the equality holds, then from Eq. (70) and Eq. (72) we can derive

$$\frac{\hat{w}_n^{(4)}}{b_n^2} = -\frac{\hat{\theta}_n \hat{\theta}_n''}{w_n} = (h_1 + \langle w\theta \rangle)^2 \frac{\hat{w}_n'' \hat{w}_n - 2\hat{w}_n'^2}{\hat{w}_n^5}. \tag{88}$$

With the following change of variables,

$$\begin{cases} \zeta = b_n^{1/3} b_{n+1}^{2/3} \zeta_n, \\ \hat{\Omega} = b_n^{-1/3} b_{n+1}^{1/3} (h_1 + \langle hw\theta \rangle)^{-1/2} \hat{w}_n, \\ \hat{\Theta} = b_n^{1/3} b_{n+1}^{-1/3} (h_1 + \langle hw\theta \rangle)^{-1/2} \hat{\theta}_n, \end{cases} \tag{89}$$

Eqs. (86), (87), and (88) become

$$\begin{cases} \hat{\Omega}^{(4)} - \hat{\Theta} = 0, \\ \hat{\Theta}'' + \hat{\Omega} = 0, \\ \hat{\Omega}^{(4)} = \dfrac{\hat{\Omega}''\hat{\Omega} - 2\hat{\Omega}'^2}{\hat{\Omega}^5}. \end{cases} \tag{90}$$

Starred quantities satisfy the same equations with h_1 replaced by h_0. This set of differential equations has been studied in Ref. 1, where the constant β is defined

$$3\beta = \int_0^\infty \hat{\Omega}''^2 d\zeta + \int_0^\infty (1 - \hat{\Omega}\hat{\Theta}) d\zeta = 1.847 \tag{91}$$

and the following integrals are evaluated:

$$\int_0^\infty \frac{w_n''^2}{b_n^2} d\zeta_n + \int_0^\infty b_{n+1}^2 \tilde{w}_{n+1}^2 d\zeta_n = 3\beta(h_1 + \langle w\theta\rangle) b_n^{-1/3} b_{n+1}^{4/3}, \quad n = 1, \ldots, N-1. \tag{92}$$

When $n = N$, the differential equations for $\hat{w}_N$ and $\hat{\theta}_N$ are

$$\frac{D}{\langle w\theta\rangle b_N^2} \hat{w}_N^{(4)} - (h_1 + \langle w\theta\rangle - \hat{w}_N \hat{\theta}_N) \hat{\theta}_N = 0, \tag{93}$$

$$\frac{D}{\langle w\theta\rangle b_N^2} \hat{\theta}_N'' + (h_1 + \langle w\theta\rangle - \hat{w}_N \hat{\theta}_N) \hat{w}_N = 0. \tag{94}$$

Then with the following change of variables,

$$\begin{cases} \zeta = b_N^{1/3} (h_1 + \langle w\theta\rangle)^{1/3} \left(\dfrac{D}{\langle w\theta\rangle} \right)^{-1/3} \zeta_N, \\ \Omega = b_N^{-1/3} (h_1 + \langle hw\theta\rangle)^{-1/3} \left(\dfrac{D}{\langle w\theta\rangle} \right)^{-1/6} \hat{w}_N, \\ \Theta = b_N^{1/3} (h_1 + \langle hw\theta\rangle)^{-2/3} \left(\dfrac{D}{\langle w\theta\rangle} \right)^{1/6} \hat{\theta}_N, \end{cases} \tag{95}$$

Eqs. (93) and (94) become

$$\Omega^{(4)} - (1 - \Omega\Theta)\Theta = 0, \tag{96}$$

$$\Theta'' + (1 - \Omega\Theta)\Omega = 0. \tag{97}$$

In Howard's paper[11] the following result is given:

$$\sigma = \int_0^\infty \Omega''^2 d\zeta = \int_0^\infty \Theta'^2 d\zeta = \tfrac{1}{4} \int_0^\infty (1 - \Omega\Theta)^2 d\zeta = 0.337. \tag{98}$$

Thus the following integrals can be expressed in σ:

$$\int_0^\infty \frac{(\hat{w}^{(4)})^2}{b_N^2} d\zeta_N = \sigma (h_1 + \langle w\theta\rangle)^{5/3} \left(\frac{D}{\langle w\theta\rangle} \right)^{-2/3} b_N^{-1/3}, \tag{99}$$

$$\int_0^\infty \hat{\theta}_N'^2 d\zeta_N = \sigma (h_1 + \langle w\theta\rangle)^{5/3} \left(\frac{D}{\langle w\theta\rangle} \right)^{-2/3} b_N^{-1/3}, \tag{100}$$

$$\int_0^\infty (h_1 + \langle hw\theta\rangle - \hat{w}_N \hat{\theta}_N)^2 d\zeta_N = 4\sigma (h_1 + \langle w\theta\rangle)^{5/3} \left(\frac{D}{\langle w\theta\rangle} \right)^{1/3} b_N^{-1/3}. \tag{101}$$

Putting the above integrals together, the functional F_N can then be expressed as

$$F_N = \frac{D^2}{\langle w\theta\rangle} \tag{102}$$

$$+ 4\sigma (h_1 + \langle w\theta\rangle)^{5/3} \left(\frac{D}{\langle w\theta\rangle} \right)^{1/3} b_N^{-1/3} + 4\sigma (h_0 + \langle w\theta\rangle)^{5/3} \left(\frac{D}{\langle w\theta\rangle} \right)^{1/3} b_N^{*-1/3}, \tag{103}$$

and

$$D=\sum_{n=1}^{N-1} 3\beta\left\{\left[\frac{b_{n+1}^4}{b_n}\right]^{1/3}(h_1+\langle w\theta\rangle)+\left[\frac{b_{n+1}^{*4}}{b_n^*}\right]^{1/3}(h_0+\langle w\theta\rangle)\right\}+\sigma\left(\frac{D}{\langle w\theta\rangle}\right)^{-2/3}\{(h_1+\langle w\theta\rangle)^{5/3}b_N^{-1/3}$$
$$+(h_0+\langle w\theta\rangle)^{5/3}b_N^{*-1/3}\}+b_1^2\langle w\theta\rangle. \tag{104}$$

Minimizing F_N with respect to b_n and b_n^* yields

$$\frac{\partial D}{\partial b_1}=0\Rightarrow 2b_1\langle w\theta\rangle=\beta\left[(h_1+\langle w\theta\rangle)\left(\frac{b_2}{b_1}\right)^{4/3}+(h_0+\langle w\theta\rangle)\left(\frac{b_2^*}{b_1}\right)^{4/3}\right], \tag{105}$$

$$\frac{\partial D}{\partial b_n}=0\Rightarrow\left[\frac{b_{n+1}}{b_n}\right]^{4/3}=4\left[\frac{b_n}{b_{n-1}}\right]^{1/3}, \tag{106}$$

$$\frac{\partial D}{\partial b_n^*}=0\Rightarrow\left[\frac{b_{n+1}^*}{b_n^*}\right]^{4/3}=4\left[\frac{b_n^*}{b_{n-1}^*}\right]^{1/3}, \tag{107}$$

$$\frac{\partial F_N}{\partial b_N}=0\Rightarrow\left[\frac{b_{N+1}}{b_N}\right]^{4/3}=4\left[\frac{b_N}{b_{N-1}}\right]^{1/3}, \tag{108}$$

$$\frac{\partial D}{\partial b_N^*}=0\Rightarrow\left[\frac{b_{N+1}^*}{b_N^*}\right]^{4/3}=4\left[\frac{b_N^*}{b_{N-1}^*}\right]^{1/3}, \tag{109}$$

where

$$b_{N+1}=\left(\frac{\sigma}{\beta}\right)^{4/3}\left(\frac{(h_1+\langle w\theta\rangle)\langle w\theta\rangle}{D}\right)^{1/2}, \tag{110}$$

$$b_{N+1}^*=\left(\frac{\sigma}{\beta}\right)^{4/3}\left(\frac{(h_0+\langle w\theta\rangle)\langle w\theta\rangle}{D}\right)^{1/2}. \tag{111}$$

From the above relations, the b_n can be determined:

$$b_{n+1}=4^{n-1}\left[\left(\frac{b_{N+1}}{4^{N-1}}\right)^{1-4^{-n}}\cdot(4b_1)^{4^{-n}-4^{-N}}\right]^{1/1-4^{-N}}. \tag{112}$$

And b_{n+1}^* has a similar form:

$$b_{n+1}^*=4^{n-1}\left[\left(\frac{b_{N+1}^*}{4^{N-1}}\right)^{1-4^{-n}}\cdot(4b_1)^{4^{-n}-4^{-N}}\right]^{1/1-4^{-N}}. \tag{113}$$

It is clear from the above expressions that $b_n\neq b_n^*$ for $n\neq 1$ since b_N [Eq. (110)] is different from b_N^* [Eq. (111)]. Finally, b_1 can be solved from (106) and the recursion relation

$$b_1=\left\{\frac{\beta}{2^{5/3}\langle w\theta\rangle}\left(\frac{\sigma}{\beta}\right)^{3/4(1-4^{-N})}[(h_1+\langle w\theta\rangle)^{4/(1-4^{-N})/3-4^{-N}}\right.$$
$$\left.+(h_0+\langle w\theta\rangle)^{4/(1-4^{-N})/3-4^{-N}}]\right\}^{1-4^{-N}/3-4^{-N}}. \tag{114}$$

Putting all these together, the prefactor F_N is a function of $\langle w\theta\rangle$ only:

$$F_N=\frac{D^2}{\langle w\theta\rangle}\frac{3-4^{-N}}{1-4^{-N}}$$

$$=(3-4^{-N})(1-4^{-N})2^{-4N4^{-N}/3-4^{-N}}\cdot\left(2^{5/3}\beta\times\left(\frac{\sigma}{\beta}\right)^{3/4(1-4^{-N})}\right)^{4(1-4^{-N})/3-4^{-N}}$$

$$\times\left[\frac{(h_1+\langle w\theta\rangle)^{3-2\cdot4^{-N}/2(1-4^{-N})}+(h_0+\langle w\theta\rangle)^{3-2\cdot4^{-N}/2(1-4^{-N})}}{\langle w\theta\rangle^{1-3\cdot4^{-N}/4(1-4^{-N})}}\right]^{4(1-4^{-N})/3-4^{-N}}. \tag{115}$$

Now the value of $\langle w\theta\rangle$ can be determined by setting $dF_N/d\langle w\theta\rangle$ to zero. The resulting equation for $\langle w\theta\rangle$ is

$$(\alpha-1)x^{(3-2c)/2(1-c)}-\alpha x-\alpha x^{1/(1-c)}+(\alpha-1)=0, \tag{116a}$$

where

$$x=\frac{\sqrt{3}+\langle w\theta\rangle}{\sqrt{3}-\langle w\theta\rangle},\quad \alpha=\frac{3-2c}{1-3c},\quad c=4^{-N}. \tag{116b}$$

For general values of N, the above equation has to be solved numerically:

$$N=1,\quad \langle w\theta\rangle=0.4831,$$

$$N=2,\quad \langle w\theta\rangle=0.9259,$$

$$N=3,\quad \langle w\theta\rangle=1.0120,$$

$$\vdots$$

When $N\to\infty$, the above equation can be solved exactly:

$$\langle w\theta\rangle_\infty=\frac{3\sqrt{3}}{5}=1.039. \tag{117}$$

This shows that there indeed is a boundary layer at $z=0$ since all $\langle w\theta\rangle$'s are less than $h_0=\sqrt{3}$.

Now we can write down the scaling of $\langle T\rangle$ as $N\to\infty$:

$$\langle T\rangle=\frac{1}{\sqrt{12}R}F_\infty\mu^{2/3}=10.285\mu^{2/3}R^{-1}. \tag{118}$$

Recalling the identity (46):

$$\langle T\rangle=-\langle(z-\tfrac{1}{2})w\theta\rangle+\tfrac{1}{12},$$

we know that as $\mu\to\infty$

$$\mu\sim\frac{1}{\sqrt{12}}R. \tag{119}$$

This leads to the scaling bound on $\langle T\rangle$ with respect to R:

$$\langle T\rangle\geqslant 4.421R^{-1/3}. \tag{120}$$

The profiles of $\tilde{w}_1$ and $\tilde{\theta}_1$ can be determined from the fact that in the interior of the interval $0<z<1$,

$$\tilde{w}_1\tilde{\theta}_1 \approx h+\langle w\theta\rangle, \quad \text{and} \quad \tilde{w}_1=\tilde{\theta}_1. \tag{121}$$

In the case $N\to\infty$, $h=2\sqrt{3}z-(2\sqrt{3}/5)$. And then

$$\tilde{w}_1=\sqrt{\left|2\sqrt{3}z-\frac{2\sqrt{3}}{5}\right|}, \quad \tilde{\theta}_1=\pm\sqrt{\left|2\sqrt{3}z-\frac{2\sqrt{3}}{5}\right|}. \tag{122}$$

However, whether θ changes sign in $0<z<1$ can not be inferred from the variational problem since only the product of w and θ appears in the functional $\mathcal{F}$. Thus the possibility of w changing its sign cannot be excluded.

V. BACKGROUND METHOD FOR INFINITE Pr

As can be seen from the momentum equation (2a), the velocity field is instantaneously slaved to the temperature field in the limit $\mathrm{Pr}\to\infty$. Then it is straightforward to extract the equation satisfied by the vertical velocity w for a given fluctuation field θ:

$$\Delta^2 w=-R\Delta_H\theta. \tag{123}$$

The incompressibility condition on the velocity field combined with the no-slip boundary conditions at $z=0$ and $z=1$ imply that both w and $\partial w/\partial z$ vanish at the rigid boundaries. To implement the background analysis we decompose the temperature field as we did for the finite Pr case and notice that identies (10) and (14) still hold. This observation leads to the bound (18):

$$\langle T\rangle \geqslant 2\langle\tau\rangle-\langle\tau'^2\rangle, \tag{124}$$

provided the functional (17)

$$H=\langle|\nabla\theta|^2\rangle+\langle(2\tau'-a)w\theta\rangle+\frac{a}{R}\langle|\nabla\mathbf{u}|^2\rangle \tag{125}$$

is positive semidefinite among divergence free velocity fields satisfying Eq. (123) and no-slip boundary conditions at $z=0,1$, and temperature fields $\theta(x,y,z,t)$ vanishing at $z=0,1$. The constraint on the background field $\tau(z)$ is the same: $\tau(0)=\tau(1)=0$.

It is convenient to find the sufficient conditions for the non-negativity of H in its Fourier series representation $H=\Sigma_{\mathbf{k}}H_{\mathbf{k}}$, where

$$H_{\mathbf{k}}\{\theta_{\mathbf{k}}\}=\int_0^1\left[|D\theta_{\mathbf{k}}|^2+k^2|\theta_{\mathbf{k}}|^2+\left(\tau'-\frac{a}{2}\right)(w_{\mathbf{k}}^*\theta_{\mathbf{k}}+w_{\mathbf{k}}\theta_{\mathbf{k}}^*)+\frac{a}{R}\left(\frac{1}{k^2}|D^2w_{\mathbf{k}}|^2+2|Dw_{\mathbf{k}}|^2\right.\right.$$
$$\left.\left.+k^2|w_{\mathbf{k}}|^2\right)\right]dz, \tag{126}$$

where $w_{\mathbf{k}}(z)$ and $\theta_{\mathbf{k}}(z)$ are the Fourier components of w and θ corresponding to wave number $\mathbf{k}$, satisfying

$$(-D^2+k^2)^2w_{\mathbf{k}}=Rk^2\theta_{\mathbf{k}}. \tag{127}$$

Then $H\geqslant 0$ iff each $H_{\mathbf{k}}$ is positive semidefinite for complex valued functions $\theta_{\mathbf{k}}$ of a single (real) variable z where $w_{\mathbf{k}}$ solves the fourth-order linear boundary value problem above with both homogeneous Dirichlet and Neumann boundary conditions on $[0,1]$.

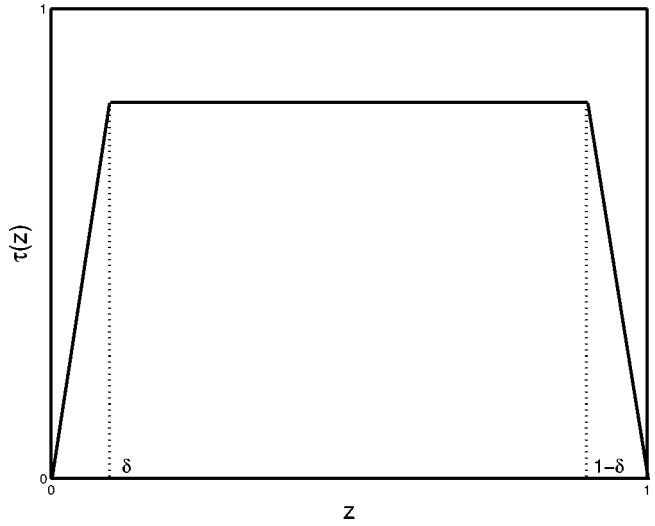

FIG. 3. The background profile for infinite Prandtl number.

We need to choose the background field $\tau(z)$ before we can estimate the magnitude of $H_{\mathbf{k}}$. Since the expressions for the lower bound (18) and the functional H (17) have the same forms as in the finite Pr case, we can choose the same background profile (19). And consequently, after maximizing the bound over a and b, we arrive at the same expression (21):

$$\langle T\rangle \geqslant \tfrac{1}{4}(1-\delta_1)(1-\delta_2)(\delta_1+\delta_2). \tag{128}$$

This expression is invariant if we exchange δ_1 and δ_2, and the estimate (132) is pointwise. This suggests that the maximum of the right-hand side of (21) occurs when $\delta_1=\delta_2=\delta$. And then

$$\begin{cases} a=0\,, \\ b=\dfrac{\delta(1-\delta)}{2} \end{cases} \tag{129}$$

by Eq. (22). The background profile becomes

$$\tau(z)=\begin{cases} \dfrac{1-\delta}{2}z\,, & 0\leqslant z<\delta, \\ \dfrac{\delta(1-\delta)}{2}, & 1-\delta\leqslant z\leqslant 1-\delta, \\ \dfrac{1-\delta}{2}(1-z)\,, & 1-\delta\leqslant z\leqslant 1, \end{cases} \tag{130}$$

and the bound is

$$\langle T\rangle \geqslant \frac{\delta(1-\delta)^2}{2} \tag{131}$$

as long as δ is chosen to ensure H is semipositive definite (see Fig. 3).

In the following we will use the inequality, proved in Ref. 10, for solutions of (127):

$$|w_{\mathbf{k}}| \leqslant \frac{1}{2} z^2 \frac{R}{\sqrt{C}} k \|\theta_{\mathbf{k}}\| \tag{132}$$

for $z \in [0, \frac{1}{2}]$, where $C = \frac{1}{2}(7 - \sqrt{41})$. (A similar estimate holds on the other end of the unit interval.) Applying this estimate, we have

$$\begin{aligned}
&\left| \int_0^1 \left(\tau' - \frac{a}{2} \right) (w_{\mathbf{k}}^* \theta_{\mathbf{k}} + w_{\mathbf{k}} \theta_{\mathbf{k}}^*) dz \right| \\
&= \left| \int_0^1 \tau' (w_{\mathbf{k}}^* \theta_{\mathbf{k}} + w_{\mathbf{k}} \theta_{\mathbf{k}}^*) dz \right| \\
&\leqslant 2 \frac{1-\delta}{2} \int_0^{\delta} |w_{\mathbf{k}}| |\theta_{\mathbf{k}}| dz + 2 \frac{1-\delta}{2} \int_{1-\delta}^1 |w_{\mathbf{k}}| |\theta_{\mathbf{k}}| dz \\
&\leqslant (1-\delta) \int_0^{\delta} \frac{1}{2} z^2 \left(\frac{R}{\sqrt{C}} k \|\theta_{\mathbf{k}}\| \right) \sqrt{z \int_0^{1/2} |D\theta_{\mathbf{k}}(z')|^2 dz'} dz + (1-\delta) \int_{1-\delta}^1 \frac{1}{2} (1-z)^2 \\
&\quad \times \left(\frac{R}{\sqrt{C}} k \|\theta_{\mathbf{k}}\| \right) \times \sqrt{(1-z) \int_{1/2}^1 |D\theta_{\mathbf{k}}(z')|^2 dz'} dz \\
&\leqslant (1-\delta) \frac{R}{\sqrt{C}} k \|\theta_{\mathbf{k}}\| \frac{1}{7} \delta_1^{7/2} \sqrt{\int_0^{1/2} |D\theta_{\mathbf{k}}(z')|^2 dz'} \\
&\quad + (1-\delta) \frac{R}{\sqrt{C}} k \|\theta_{\mathbf{k}}\| \frac{1}{7} \delta_1^{7/2} \sqrt{\int_{1/2}^1 |D\theta_{\mathbf{k}}(z')|^2 dz'} \\
&\leqslant (1-\delta) \frac{R}{\sqrt{C}} \frac{\delta^{7/2}}{7} \frac{k}{2} \left(\frac{k \|\theta_{\mathbf{k}}\|^2}{\sqrt{2}} + \frac{\sqrt{2}}{k} \int_0^{1/2} |D\theta_{\mathbf{k}}(z')|^2 dz' \right) \\
&\quad + (1-\delta) \frac{R}{\sqrt{C}} \frac{\delta^{7/2}}{7} \frac{k}{2} \left(\frac{k \|\theta_{\mathbf{k}}\|^2}{\sqrt{2}} + \frac{\sqrt{2}}{k} \int_0^{1/2} |D\theta_{\mathbf{k}}(z')|^2 dz' \right) \\
&= (1-\delta) \frac{R}{\sqrt{C}} \frac{1}{7} \delta^{7/2} \frac{1}{\sqrt{2}} (k^2 \|\theta_{\mathbf{k}}\|^2 + \|D\theta_{\mathbf{k}}\|^2).
\end{aligned} \tag{133}$$

Then

$$H \geqslant k^2 \left(1 - \frac{(1-\delta)\delta^{7/2}}{7\sqrt{2}} \frac{R}{\sqrt{C}} \right) (k^2 \|\theta_{\mathbf{k}}\|^2 + \|D\theta_{\mathbf{k}}\|^2). \tag{134}$$

Choosing δ such that

$$\frac{(1-\delta)\delta^{7/2}}{14} \frac{R}{\sqrt{C}} = 1, \tag{135}$$

the non-negativity of H is ensured. Then as $R \to \infty$, $\delta \sim (7\sqrt{2C}/R)^{2/7}$ and thus

$$\langle T \rangle \geqslant \frac{1}{2} \delta = \frac{1}{2} \left(\frac{7\sqrt{2C}}{R} \right)^{2/7}. \tag{136}$$

VI. SUMMARY AND DISCUSSION

The preceeding sections we have proven that for the finite (or arbitrary) Prandtl number case, in nondimensional units,

$$\langle T\rangle \geqslant c_1 R^{-1/3}, \tag{137}$$

and for the infinite Prandtl number model,

$$\langle T\rangle \geqslant c_2 R^{-2/7}. \tag{138}$$

In dimensional units of temperature and heat flux these results are

$$\langle T\rangle \geqslant \tilde{c}_1 H^{2/3} \tag{139}$$

for arbitrary Pr (see Ref. 4 for a similar estimate in that case of an internally heated self-gravitating sphere), and

$$\langle T\rangle \geqslant \tilde{c}_2 H^{5/7} \tag{140}$$

for the infinite Pr.

Recent numerical experiments[18] on thermal convection with internal heating in a fluid layer with infinite Prandtl number suggest that

$$\langle T\rangle \propto R^{-0.234}. \tag{141}$$

The observed exponent 0.234 is smaller than the rigorous estimate derived here, $2/7 \approx 0.286$, but consistent with the bound. In the case of Rayleigh–Bénard convection, the methods employed here produce scaling (upper) bounds on the heat transport[1,9,10] that are also consistent—but not in total agreement—with observed high Rayleigh number scalings.

It is worthwhile to note that the ''optimal'' background profile that the analysis suggests (Fig. 1) is suggestive of the mean temperature profile one expects for the internal heating problem. That is, the buoyancy force driving the convection will concentrate the warmer fluid near the top of the layer. Interestingly, this is not the case for the infinite Pr problem where the ''optimal'' temperature background maintains the symmetry of the conduction solution. It remains an open problem to apply the multiple boundary layer analysis to the case of infinite Pr, as it has previously been applied for the case of Rayleigh–Bénard convection.[5] A full (numerical) solution of the optimal background variational problem, as has recently been accomplished for Rayleigh–Bénard convection with finite Prandtl number,[15] could improve the estimates further.

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ERRATUM

Erratum: A sufficient condition for the existence of bound states in a potential [J. Math. Phys. 38, 4900 (1997)]

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In the above paper, formulas (22) and (23), while correct for the S-wave, $\ell=0$, are not correct for higher waves. The correct formulas are as follows. In order to secure a bound state, we must match continuously the interior wave function for $r<R_0$, formula (21), to the exterior solution which vanishes at infinity, namely, $ar^{-\ell}$.[1] It follows that, in the right-hand side of our formula (22), $j'_{\ell,1}$, the first maximum of the radial Bessel function, must be replaced by the first solution x of

$$\frac{J'_{\ell+1/2}(x)}{J_{\ell+1/2}(x)}=-\frac{\ell+\frac{1}{2}}{x}. \tag{1}$$

As a consequence, the same modification must be made in the right-hand side of (23). As explained in Ref. 1, the solution x of formula (1) above is larger than $j'_{\ell,1}$, and is located between this value and the first zero, $j_{\ell,1}$, of $J_{\ell+1/2}(x)$. We would like to thank Dr. Fabian Brau, who brought the mistake to our attention.

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Erratum: Three-quark exchange operators, crossing matrices and Fierz transformations in SU(2) and SU(3) [J. Math. Phys. 42, 991 (2001)]

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Errors have propagated into several related/equivalent formulas in Ref. 1 as a consequence of one fundamental minus sign error:

(1) The right-hand sides of Eqs. (15a) and (15b) have been erroneously shown as copies of Eqs. (14a) and (14b). The correct form is

$$\mathrm{P}_{123}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j=\frac{16}{9}+\frac{2}{3}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j-\frac{1}{2}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c-\frac{i}{2}f^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c,$$

$$\mathrm{P}_{132}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j=\frac{16}{9}+\frac{2}{3}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j-\frac{1}{2}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c+\frac{1}{2}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c.$$

(2) The second row, fourth column entries in the SU(3) crossing matrices C, Eq. (17) and C^2, Eq. (18) should switch signs, i.e., $\pm 1/2\rightarrow\mp 1/2$, or explicitly

$$\mathbf{C}=\begin{pmatrix}\frac{1}{9} & \frac{1}{6} & \frac{1}{4} & \frac{1}{4}\\ \frac{16}{9} & \frac{2}{3} & -\frac{1}{2} & -\frac{1}{2}\\ \frac{80}{81} & -\frac{5}{27} & \frac{13}{18} & -\frac{5}{18}\\ -\frac{16}{9} & \frac{1}{3} & \frac{1}{2} & -\frac{1}{2}\end{pmatrix},$$

$$\mathbf{C}^2=\begin{pmatrix}\frac{1}{9} & \frac{1}{6} & \frac{1}{4} & -\frac{1}{4}\\ \frac{16}{9} & \frac{2}{3} & -\frac{1}{2} & \frac{1}{2}\\ \frac{80}{81} & -\frac{5}{27} & \frac{13}{18} & \frac{5}{18}\\ \frac{16}{9} & -\frac{1}{3} & -\frac{1}{2} & -\frac{1}{2}\end{pmatrix}.$$

(3) Moreover, Eqs. (20a), (20b) need to have the signs in their last terms changed, as follows:

$$\delta_{\alpha\delta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\sigma\beta}+\delta_{\gamma\rho}\boldsymbol{\lambda}_{\alpha\delta}\cdot\boldsymbol{\lambda}_{\sigma\beta}+\delta_{\sigma\beta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\alpha\delta}$$
$$=\frac{2}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta})+\frac{16}{9}\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}$$
$$-\frac{1}{2}d^{abc}\boldsymbol{\lambda}^{a}_{\alpha\beta}\boldsymbol{\lambda}^{b}_{\gamma\delta}\boldsymbol{\lambda}^{c}_{\sigma\rho}-\frac{1}{2}if^{abc}\boldsymbol{\lambda}^{a}_{\alpha\beta}\boldsymbol{\lambda}^{b}_{\gamma\delta}\boldsymbol{\lambda}^{c}_{\sigma\rho},$$

$$\delta_{\alpha\rho}\boldsymbol{\lambda}_{\gamma\beta}\cdot\boldsymbol{\lambda}_{\sigma\delta}+\delta_{\gamma\beta}\boldsymbol{\lambda}_{\alpha\rho}\cdot\boldsymbol{\lambda}_{\sigma\delta}+\delta_{\sigma\beta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\alpha\delta}$$
$$=\frac{2}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta})+\frac{16}{9}\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}$$
$$-\frac{1}{2}d^{abc}\boldsymbol{\lambda}^{a}_{\alpha\beta}\boldsymbol{\lambda}^{b}_{\gamma\delta}\boldsymbol{\lambda}^{c}_{\sigma\rho}+\frac{1}{2}if^{abc}\boldsymbol{\lambda}^{a}_{\alpha\beta}\boldsymbol{\lambda}^{b}_{\gamma\delta}\boldsymbol{\lambda}^{c}_{\sigma\rho}.$$

All other results, as well as the conclusions of the paper remain unchanged.

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Symmetry operators for Riemann's method

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Riemann's method is one of the definitive ways of solving Cauchy's problem for a second order linear hyperbolic partial differential equation in 2 variables. Chaundy's equation, with 4 parameters, is the most general self-adjoint equation for which the Riemann function is known. Here we show that Chaundy's equation possesses a two-dimensional vector space of second-order symmetry operators. Hence a new equivalence class of Riemann functions, admitting no first-order symmetries and obtainable only via a higher order symmetry, is found. A new 5 parameter Riemann function is then subsequently derived. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763003]

I. INTRODUCTION

The most general self-adjoint partial differential equation (PDE) for which the Riemann function is known is that derived by Chaundy,[1]

$$U_{rs}+\left[\frac{m_1(1-m_1)}{(r+s)^2}-\frac{m_2(1-m_2)}{(r-s)^2}+\frac{m_3(1-m_3)}{(1-rs)^2}-\frac{m_4(1-m_4)}{(1+rs)^2}\right]U=0, \tag{1}$$

where $m_1,\ldots,m_4$ are real valued constants. For this equation the Riemann function, $R(r,s,r_0,s_0)$, is given by

$$R(r,s,r_0,s_0)=F_B(m_1,m_2,m_3,m_4,1-m_1,1-m_2,1-m_3,1-m_4,1,z_1,z_2,z_3,z_4), \tag{2}$$

where

$$z_1=-\frac{(r-r_0)(s-s_0)}{(r+s)(r_0+s_0)}, \quad z_2=\frac{(r-r_0)(s-s_0)}{(r-s)(r_0-s_0)}, \tag{3}$$

$$z_3=-\frac{(r-r_0)(s-s_0)}{(1-rs)(1-r_0s_0)}, \quad z_4=\frac{(r-r_0)(s-s_0)}{(1+rs)(1+r_0s_0)}, \tag{4}$$

and F_B is a Lauricella hypergeometric function of four variables.[2] Recall that for a self-adjoint equation such as (1), the Riemann function must satisfy[3]

$$\begin{gathered} L[R]=0, \\ \frac{\partial R}{\partial r}=0 \quad \text{on} \quad s=s_0, \\ \frac{\partial R}{\partial s}=0 \quad \text{on} \quad r=r_0, \\ R(r_0,s_0,r_0,s_0)=1. \end{gathered} \tag{5}$$

When $m_1(1-m_1)=m_3(1-m_3)=m_4(1-m_4)=0$, Chaundy's PDE simplifies to the Euler–Poisson–Darboux (EPD) equation which is the original problem solved by Riemann. For the EPD equation, the Riemann function F_B reduces to the standard hypergeometric function

$$R(r,s,r_0,s_0)={}_2F_1(m_2,1-m_2,1,z_2). \tag{6}$$

It is well known[4,5] that the EPD equation possesses a three-dimensional Lie algebra of first-order symmetry operators isomorphic to sl(2,R). From standard results in Lie theory,[5] the group SL(2,R) acts locally on the solution space of the EPD equation by

$$U(r,s)\to U\left(\frac{\alpha r+\beta}{\gamma r+\delta},\frac{\alpha s+\beta}{\gamma s+\delta}\right),\quad \begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}\in \mathrm{SL}(2,R). \tag{7}$$

Using (7), it is straightforward to show that the Riemann function for the EPD equation can be represented in terms of the hypergeoemtric function (6). This was first shown by Bluman.[7] Subsequently Daggit[8] and Ibragimov[9] extended this concept to more general problems. They considered a generic PDE, to which they could impose restrictions on the coefficients, so that a symmetry algebra isomorphic to sl(2,R) was obtained for the reduced equations. This led to invertible mappings from the candidate equations to the EPD equation, likewise for the solutions. In this way an extensive equivalence class of Riemann functions was derived. Apart from confluent contractions such as the Telegrapher's equation,[10] the EPD equation is the only PDE for which this approach has been shown to work.

A few calculations reveal that (1) possesses no nontrivial first-order symmetry operators whatsoever. Hence the theory developed for sl(2,R) is not applicable to Chaundy's equation. However in this paper we show that if the symmetry operators are extended to second-order,[6] then Chaundy's full PDE in fact admits a two-dimensional vector space that leads to 4 inequivalent orbits. For each of these orbits there exists a separable coordinate system for (1). They constitute a new equivalence class of Riemann functions, admitting no first-order symmetries and obtainable only via higher order symmetries. Two of the separable forms of (1) are completely new while the other two generalize several Riemann functions already found in the literature.

In Sec. II, the symmetries for (1) are calculated. In Sec. III the corresponding separable coordinate systems and separable forms of Chaundy's equation are found. In Sec. IV a new 5 parameter Riemann function is derived by combining two of the separable forms of Chaundy's equation in an addition formula due to Olevskiĭ.[11] The five parameter Riemann function is important as it incorporates one more essential parameter than Chaundy's equation.

II. SYMMETRY CALCULATIONS

Standard techniques[6] exist in the literature for seeking separable forms of (1). Following Ref. 6 we define the second-order operator

$$S=f_1\partial_{rr}+f_2\partial_{ss}+f_3\partial_r+f_4\partial_s+f_5. \tag{8}$$

We say that (8) is a symmetry operator for (1) provided

$$[S,L]=QL, \tag{9}$$

where

$$L=\partial_{rs}+\left[\frac{m_1(1-m_1)}{(r+s)^2}-\frac{m_2(1-m_2)}{(r-s)^2}+\frac{m_3(1-m_3)}{(1-rs)^2}-\frac{m_4(1-m_4)}{(1+rs)^2}\right] \tag{10}$$

and

$$Q=h_1\partial_r+h_2\partial_s+h_3 \tag{11}$$

is a first-order differential operator (here Q may vary with S) and $f_1,\ldots,h_3$ are arbitrary functions of r and s. Evaluating (9) produces 10 equations for the unknown functions $f_1,\ldots,h_3$. The solution of these equations is long and involved.

When $m_1(1-m_1),\ldots,m_4(1-m_4)$ are all nonzero, solving (9) yields a two-dimensional vector space of operators. The symmetries, S_1 and S_2, form a basis and have differential part

$$S_1=(r^4+1)\partial_{rr}+(s^4+1)\partial_{ss}+2r^3\partial_r+2s^3\partial_s, \tag{12}$$

$$S_2=r^2\partial_{rr}+s^2\partial_{ss}+r\partial_r+s\partial_s. \tag{13}$$

Importantly, there are no first-order symmetries, which means that Chaundy's equation is Class II in the sense of Miller.[6]

The dimension of the vector space now varies depending on the pivots for the constants $m_1,\ldots,m_4$. However the only new case is that stated above, where $m_1(1-m_1),\ldots,m_4(1-m_4)$ are all nonzero. All other cases reduce to equations for which the symmetries are well documented. The pivots found during the calculation of (9) fall into two types

$$m_i(1-m_i)=0, \quad i=1,\ldots,4$$

and

$$m_i(1-m_i)=m_j(1-m_j), \quad i,j=1,\ldots,4; \quad i\neq j$$

or a combination of both. Letting any one of $m_1(1-m_1),\ldots,m_4(1-m_4)$ equal to zero does not increase the dimension of the vector space from two. The next possibility is when any two of $m_1(1-m_1),\ldots,m_4(1-m_4)$ equal zero. This leads to 6 possible equations. However as Chaundy pointed out,[1] if we apply the discrete group

$$(r,s)=(-R,S),$$

$$(r,s)=\left(\frac{1}{R},S\right), \tag{14}$$

$$(r,s)=\left(\frac{1-R}{1+R},\frac{1-S}{1+S}\right),$$

to (1), then the suffixes, (1,2,3,4) on the constants m, become (2,1,4,3), (4,3,2,1) or (3,2,1,4), respectively. Hence the 6 PDEs can all be mapped to the harmonic equation

$$U_{rs}+\left[\frac{m_1(1-m_1)}{(r+s)^2}-\frac{m_2(1-m_2)}{(r-s)^2}\right]U=0. \tag{15}$$

The Riemann function for (15) has been documented by Henrici.[12] More recently Iwasaki[10] solved (15) in terms of a system of F_4 functions.[2] The symmetries for (15) have been studied by Kalnins and Miller.[13] In effect the vector space is four-dimensional with 3 second order symmetries and 1 first order symmetry. For more detail, see Ref. 13.

The next pivot occurs when we let $m_1(1-m_1)=m_2(1-m_2)$ and $m_3(1-m_3)=m_4(1-m_4)$ (or any combination of two constants) in (1) to obtain

$$U_{rs}-4rs\left[\frac{m_1(1-m_1)}{(r^2-s^2)^2}-\frac{m_3(1-m_3)}{(1-r^2s^2)^2}\right]U=0.$$

As Chaundy pointed out, now make the change of variables $r=R^{1/2}$, $s=S^{1/2}$ which gives

$$U_{RS}-\left[\frac{m_1(1-m_1)}{(R-S)^2}-\frac{m_3(1-m_3)}{(1-RS)^2}\right]U=0.$$

Then applying the discrete group (14), we arrive at the Harmonic equation (15). Setting three constants equal to zero leads to the EPD equation in all cases under the action of the discrete group (14). As shown in Ref. 4 this leads to an eight-dimensional vector space, and nine inequivalent separable coordinate systems.

Hence we continue by focusing our attention on the new case when all constants are arbitrary: the two-dimensional vector space with symmetry operators (12) and (13).

III. THE SEPARABLE COORDINATE SYSTEMS

Taking a linear combination of the operators (12) and (13), there are then four inequivalent orbits namely,

- $S_1+2qS_2, \quad q>1,$
- $S_1+2S_2,$
- $S_1-2S_2,$
- $S_1+2qS_2, \quad q<-1,$

where q is a real valued constant. Alternatively consider S_2 by itself. In this case the discrete symmetry (14) maps S_2 to

$$S_2'=\frac{(R^2-1)^2}{4}\partial_{RR}+\frac{(S^2-1)^2}{4}\partial_{SS}+\frac{R(R^2-1)}{2}\partial_R+\frac{S(S^2-1)}{2}\partial_S,$$

which is equivalent to S_1-2S_2. Also this discrete symmetry maps the case when $-1<q<1$ to the case when $q>1$ above. Hence we may ignore these possibilities and conclude that, in total, there are 4 inequivalent orbits for the two symmetries S_1 and S_2. We are now in a position to calculate the separable coordinate systems and to analyze their effect on (1).

System 1: S_1+2qS_2, where $q>1$.

The separable coordinates are

$$r=b\frac{\mathrm{sn}[a(\xi+\eta)]}{\mathrm{cn}[a(\xi+\eta)]}, \quad s=b\frac{\mathrm{sn}[a(\xi-\eta)]}{\mathrm{cn}[a(\xi-\eta)]}, \tag{16}$$

where $2q=(1+b^4)/b^2$, $k^2=1-b^4$, $0<b<1$ and k is the modulus of the Jacobian elliptic functions.[14]

When (16) is substituted into (1) the following separable equation is found:

$$\begin{aligned}U_{\xi\xi}-U_{\eta\eta}+\Bigg\{a^2\Bigg[&m_1(1-m_1)\left(\frac{\mathrm{dn}^2 a\xi}{\mathrm{sn}^2 a\xi\,\mathrm{cn}^2 a\xi}-k^4\frac{\mathrm{sn}^2 a\eta\,\mathrm{cn}^2 a\eta}{\mathrm{dn}^2 a\eta}\right)\\&-m_2(1-m_2)\left(\frac{\mathrm{dn}^2 a\eta}{\mathrm{sn}^2 a\eta\,\mathrm{cn}^2 a\eta}-k^4\frac{\mathrm{sn}^2 a\xi\,\mathrm{cn}^2 a\xi}{\mathrm{dn}^2 a\xi}\right)\Bigg]\\&+4a^2b^2\Bigg[m_3(1-m_3)\left(\frac{\mathrm{dn}^2 a\xi}{(\mathrm{cn}^2 a\xi-b^2\mathrm{sn}^2 a\xi)^2}+\frac{\mathrm{dn}^2(a\eta)}{(\mathrm{cn}^2 a\eta+b^2\mathrm{sn}^2 a\eta)^2}-1\right)\\&-m_4(1-m_4)\left(\frac{\mathrm{dn}^2 a\xi}{(\mathrm{cn}^2 a\xi+b^2\mathrm{sn}^2 a\xi)^2}+\frac{\mathrm{dn}^2 a\eta}{(\mathrm{cn}^2 a\eta-b^2\mathrm{sn}^2 a\eta)^2}-1\right)\Bigg]\Bigg\}U=0.\end{aligned} \tag{17}$$

The Riemann function for (17) is obtained by substituting (16) into (3), (4) and (2). Hence

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(m_1,m_2,m_3,m_4,1-m_1,1-m_2,1-m_3,1-m_4,1,z_{11},z_{12},z_{13},z_{14}), \quad (18)$$

where

$$z_5=\frac{(\mathrm{sn}\,a\,\eta\mathrm{cn}\,a\,\eta_0\mathrm{dn}\,a\,\xi_0-\mathrm{sn}\,a\,\eta_0\mathrm{cn}\,a\,\eta\mathrm{dn}\,a\,\xi)^2-(\mathrm{sn}\,a\,\xi\mathrm{cn}\,a\,\xi_0\mathrm{dn}\,a\,\eta_0-\mathrm{sn}\,a\,\xi_0\mathrm{cn}\,a\,\xi\mathrm{dn}\,a\,\eta)^2}{4\mathrm{sn}\,a\,\xi\,\mathrm{sn}\,a\,\xi_0\,\mathrm{cn}\,a\,\xi\,\mathrm{cn}\,a\,\xi_0\,\mathrm{dn}\,a\,\eta\,\mathrm{dn}\,a\,\eta_0},$$

$$z_6=\frac{(\mathrm{sn}\,a\,\xi\mathrm{cn}\,a\,\xi_0\mathrm{dn}\,a\,\eta_0-\mathrm{sn}\,a\,\xi_0\mathrm{cn}\,a\,\xi\mathrm{dn}\,a\,\eta)^2-(\mathrm{sn}\,a\,\eta\mathrm{cn}\,a\,\eta_0\mathrm{dn}\,a\,\xi_0-\mathrm{sn}\,a\,\eta_0\mathrm{cn}\,a\,\eta\mathrm{dn}\,a\,\xi)^2}{4\mathrm{sn}\,a\,\eta\,\mathrm{sn}\,a\,\eta_0\,\mathrm{cn}\,a\,\eta\,\mathrm{cn}\,a\,\eta_0\,\mathrm{dn}\,a\,\xi\,\mathrm{dn}\,a\,\xi_0},$$

$$z_7=b^2\frac{(\mathrm{sn}\,a\,\eta\mathrm{cn}\,a\,\eta_0\mathrm{dn}\,a\,\xi_0-\mathrm{sn}\,a\,\eta_0\mathrm{cn}\,a\,\eta\mathrm{dn}\,a\,\xi)^2-(\mathrm{sn}\,a\,\xi\mathrm{cn}\,a\,\xi_0\mathrm{dn}\,a\,\eta_0-\mathrm{sn}\,a\,\xi_0\mathrm{cn}\,a\,\xi\mathrm{dn}\,a\,\eta)^2}{(\mathrm{cn}^2a\,\xi-b^2\mathrm{sn}^2a\,\xi)(\mathrm{cn}^2\,a\,\eta+b^2\mathrm{sn}^2\,a\,\eta)(\mathrm{cn}^2a\,\xi_0-b^2\mathrm{sn}^2a\,\xi_0)(\mathrm{cn}^2\,a\,\eta_0+b^2\mathrm{sn}^2\,a\,\eta_0)},$$

$$z_8=b^2\frac{(\mathrm{sn}\,a\,\xi\mathrm{cn}\,a\,\xi_0\mathrm{dn}\,a\,\eta_0-\mathrm{sn}\,a\,\xi_0\mathrm{cn}\,a\,\xi\mathrm{dn}\,a\,\eta)^2-(\mathrm{sn}\,a\,\eta\mathrm{cn}\,a\,\eta_0\mathrm{dn}\,a\,\xi_0-\mathrm{sn}\,a\,\eta_0\mathrm{cn}\,a\,\eta\mathrm{dn}\,a\,\xi)^2}{(\mathrm{cn}^2a\,\xi+b^2\mathrm{sn}^2a\,\xi)(\mathrm{cn}^2\,a\,\eta-b^2\mathrm{sn}^2\,a\,\eta)(\mathrm{cn}^2a\,\xi_0+b^2\mathrm{sn}^2a\,\xi_0)(\mathrm{cn}^2\,a\,\eta_0-b^2\mathrm{sn}^2\,a\,\eta_0)}.$$

To the best of the author's knowledge, Chaundy's equation written as (17) and the associated Riemann function (18) have not previously been published, including subcases. They are completely new.

System 2: For the symmetry S_1+2S_2 we find the separable coordinate system

$$r=\tan\left[a\,\frac{(\xi+\eta)}{2}\right], \quad s=\tan\left[a\,\frac{(\xi-\eta)}{2}\right]. \quad (19)$$

Substituting (19) into (1) yields

$$U_{\xi\xi}-U_{\eta\eta}+a^2\left[\frac{m_1(1-m_1)}{\sin^2 a\,\xi}-\frac{m_2(1-m_2)}{\sin^2 a\,\eta}+\frac{m_3(1-m_3)}{\cos^2 a\,\xi}-\frac{m_4(1-m_4)}{\cos^2 a\,\eta}\right]U=0. \quad (20)$$

The Riemann function for (20) is then

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(m_1,m_2,m_3,m_4,1-m_1,1-m_2,1-m_3,1-m_4,1,z_9,z_{10},z_{11},z_{12}), \quad (21)$$

where

$$z_9=\frac{\cos a(\xi-\xi_0)-\cos a(\eta-\eta_0)}{2\sin a\,\xi\sin a\,\xi_0}, \quad z_{10}=\frac{\cos a(\eta-\eta_0)-\cos a(\xi-\xi_0)}{2\sin a\,\eta\sin a\,\eta_0}, \quad (22)$$

$$z_{11}=\frac{\cos a(\xi-\xi_0)-\cos a(\eta-\eta_0)}{2\cos a\,\xi\cos a\,\xi_0}, \quad z_{12}=\frac{\cos a(\eta-\eta_0)-\cos a(\xi-\xi_0)}{2\cos a\,\eta\cos a\,\eta_0}. \quad (23)$$

System 3: For the symmetry S_1-2S_2 we find the separable coordinate system

$$r=\tanh\left[a\,\frac{(\xi+\eta)}{2}\right], \quad s=\tanh\left[a\,\frac{(\xi-\eta)}{2}\right]. \quad (24)$$

Substituting (24) into (1) yields

$$U_{\xi\xi}-U_{\eta\eta}+a^2\left[\frac{m_1(1-m_1)}{\sinh^2 a\,\xi}-\frac{m_2(1-m_2)}{\sinh^2 a\,\eta}+\frac{m_3(1-m_3)}{\cosh^2 a\,\eta}-\frac{m_4(1-m_4)}{\cosh^2 a\,\xi}\right]U=0. \quad (25)$$

The Riemann function for (25) is now

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(m_1,m_2,m_3,m_4,1-m_1,1-m_2,1-m_3,1-m_4,1,z_{13},z_{14},z_{15},z_{16}), \quad (26)$$

where

$$z_{13}=\frac{\cosh a(\eta-\eta_0)-\cosh a(\xi-\xi_0)}{2\sinh a\xi\sinh a\xi_0},\quad z_{14}=\frac{\cosh a(\xi-\xi_0)-\cosh a(\eta-\eta_0)}{2\sinh a\eta\sinh a\eta_0},\tag{27}$$

$$z_{15}=\frac{\cosh a(\eta-\eta_0)-\cosh a(\xi-\xi_0)}{2\cosh a\eta\cosh a\eta_0},\quad z_{16}=\frac{\cosh a(\xi-\xi_0)-\cosh a(\eta-\eta_0)}{2\cosh a\xi\cosh a\xi_0}.\tag{28}$$

For (25) the Riemann function when $m_2(1-m_2)=m_3(1-m_3)=m_4(1-m_4)=0$ was first published by Cohn[15] but no connection to Chaundy or the EPD equation was made. The two parameter equation that results when $m_3(1-m_3)=m_4(1-m_4)=0$ was derived by Kalnins[13] although the focus was not on Riemann functions but rather separation of variables. The full equation (25) was first derived by Papadakis and Wood[16] but no connection to symmetry operators was made.

System 4: For the symmetry $S=S_1+2qS_2$, where $q<-1$ we find the separable coordinate system

$$r=b\,\mathrm{sn}\,a(\xi+\eta),\quad s=b\,\mathrm{sn}\,a(\xi-\eta),\tag{29}$$

where $k=b^2$, $2q=-(1+b^4)/b^2$, and $0<b<1$. As in system 1, a is arbitrary and k is the modulus of the elliptic functions. Substituting (29) into (1) yields

$$\begin{aligned}U_{\xi\xi}-U_{\eta\eta}+\Bigg\{a^2\Bigg[m_1(1-m_1)\Bigg(\frac{\mathrm{cn}^2a\xi\,\mathrm{dn}^2a\xi}{\mathrm{sn}^2a\xi}-(1-k^2)^2\frac{\mathrm{sn}^2a\eta}{\mathrm{cn}^2a\eta\,\mathrm{dn}^2a\eta}\Bigg)-m_2(1-m_2)\\ \times\Bigg(\frac{\mathrm{cn}^2a\eta\,\mathrm{dn}^2a\eta}{\mathrm{sn}^2a\eta}-(1-k^2)^2\frac{\mathrm{sn}^2a\xi}{\mathrm{cn}^2a\xi\mathrm{dn}^2a\xi}\Bigg)\Bigg]+4a^2b^2\Bigg[m_3(1-m_3)\Bigg(\frac{\mathrm{cn}^2a\xi\,\mathrm{dn}^2a\xi}{(1-b^2\mathrm{sn}^2a\xi)^2}\\ +\frac{\mathrm{cn}^2a\eta\,\mathrm{dn}^2a\eta}{(1+b^2\mathrm{sn}^2a\eta)^2}-1\Bigg)-m_4(1-m_4)\Bigg(\frac{\mathrm{cn}^2a\xi\,\mathrm{dn}^2a\xi}{(1+b^2\mathrm{sn}^2a\xi)^2}+\frac{\mathrm{cn}^2a\eta\,\mathrm{dn}^2a\eta}{(1-b^2\mathrm{sn}^2a\eta)^2}-1\Bigg)\Bigg]\Bigg\}U=0.\end{aligned}\tag{30}$$

The Riemann function for (30) is then

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(m_1,m_2,m_3,m_4,1-m_1,1-m_2,1-m_3,1-m_4,1,z_{17},z_{18},z_{19},z_{20}),\tag{31}$$

where

$$z_{17}=\frac{(\mathrm{sn}\,a\eta\,\mathrm{cn}\,a\xi\,\mathrm{dn}\,a\xi_0-\mathrm{sn}\,a\eta_0\,\mathrm{cn}\,a\xi_0\,\mathrm{dn}\,a\xi)^2-(\mathrm{sn}\,a\xi\,\mathrm{cn}\,a\eta\,\mathrm{dn}\,a\eta_0-\mathrm{sn}\,a\xi_0\,\mathrm{cn}\,a\eta_0\,\mathrm{dn}\,a\eta)^2}{4\mathrm{sn}\,a\xi\,\mathrm{sn}\,a\xi_0\,\mathrm{cn}\,a\eta\,\mathrm{cn}\,a\eta_0\,\mathrm{dn}\,a\eta\,\mathrm{dn}\,a\eta_0},$$

$$z_{18}=\frac{(\mathrm{sn}\,a\xi\,\mathrm{cn}\,a\eta\,\mathrm{dn}\,a\eta_0-\mathrm{sn}\,a\xi_0\,\mathrm{cn}\,a\eta_0\,\mathrm{dn}\,a\eta)^2-(\mathrm{sn}\,a\eta\,\mathrm{cn}\,a\xi\,\mathrm{dn}\,a\xi_0-\mathrm{sn}\,a\eta_0\,\mathrm{cn}\,a\xi_0\,\mathrm{dn}\,a\xi)^2}{4\mathrm{sn}\,a\eta\,\mathrm{sn}\,a\eta_0\,\mathrm{cn}\,a\xi\,\mathrm{cn}\,a\xi_0\,\mathrm{dn}\,a\xi\,\mathrm{dn}\,a\xi_0},$$

$$z_{19}=b^2\frac{(\mathrm{sn}\,a\eta\,\mathrm{cn}\,a\xi\,\mathrm{dn}\,a\xi_0-\mathrm{sn}\,a\eta_0\,\mathrm{cn}\,a\xi_0\,\mathrm{dn}\,a\xi)^2-(\mathrm{sn}\,a\xi\,\mathrm{cn}\,a\eta\,\mathrm{dn}\,a\eta_0-\mathrm{sn}\,a\xi_0\,\mathrm{cn}\,a\eta_0\,\mathrm{dn}\,a\eta)^2}{(1-b^2\mathrm{sn}^2\,a\xi)(1+b^2\mathrm{sn}^2\,a\eta)(1-b^2\mathrm{sn}^2\,a\xi_0)(1+b^2\mathrm{sn}^2\,a\eta_0)},$$

$$z_{20}=b^2\frac{(\mathrm{sn}\,a\xi\,\mathrm{cn}\,a\eta\,\mathrm{dn}\,a\eta_0-\mathrm{sn}\,a\xi_0\,\mathrm{cn}\,a\eta_0\,\mathrm{dn}\,a\eta)^2-(\mathrm{sn}\,a\eta\,\mathrm{cn}\,a\xi\,\mathrm{dn}\,a\xi_0-\mathrm{sn}\,a\eta_0\,\mathrm{cn}\,a\xi_0\,\mathrm{dn}\,a\xi)^2}{(1+b^2\mathrm{sn}^2\,a\xi)(1-b^2\mathrm{sn}^2\,a\eta)(1+b^2\mathrm{sn}^2\,a\xi_0)(1-b^2\mathrm{sn}^2\,a\eta_0)}.$$

As for system 1, Chaundy's equation written as (30) is completely new. We have now established all possible separable coordinate systems for Chaundy's full equation.

IV. A FIVE PARAMETER RIEMANN FUNCTION

In Ref. 11 Olevskiĭ showed that the Riemann function $R_{\rho_1-\rho_2}$, for the equation

$$U_{yy}-U_{xx}+(\rho_1(y)-\rho_2(x))U=0, \tag{32}$$

can be given by

$$R_{\rho_1-\rho_2}(x,y,x_0,y_0)=R_{\rho_1}(x,y,x_0,y_0)+\int_{x-x_0}^{y-y_0}R_{\rho_1}(t,y,0,y_0)\frac{\partial}{\partial t}R_{\rho_2}(x,t,x_0,0)dt, \tag{33}$$

where R_{ρ_1} and R_{ρ_2} are the Riemann functions for

$$U_{yy}-U_{xx}+\rho_1(y)U=0$$

and

$$U_{yy}-U_{xx}-\rho_2(x)U=0.$$

Looking through the results from the previous section, (20) and (25) can both be applied to (33). First let $m_1(1-m_1)=m_3(1-m_3)=0$ and $a\to\lambda_1$ in (20) to obtain

$$U_{\xi\xi}-U_{\eta\eta}-\lambda_1^2\left[\frac{m_2(1-m_2)}{\sin^2\lambda_1\eta}+\frac{m_4(1-m_4)}{\cos^2\lambda_1\eta}\right]U=0, \tag{34}$$

which has the Riemann function

$$R_4(\xi,\eta,\xi_0,\eta_0)=F_3(m_2,m_4,1-m_2,1-m_4,1,z_{10},z_{12}), \tag{35}$$

where z_{10} and z_{12} are defined in (22) and (23). Analogously we can obtain

$$U_{\xi\xi}-U_{\eta\eta}+\lambda_2^2\left[\frac{m_1(1-m_1)}{\sinh^2\lambda_2\xi}-\frac{m_3(1-m_3)}{\cosh^2\lambda_2\xi}\right]U=0 \tag{36}$$

from the PDE (25). The Riemann function for (36) is

$$R_5(\xi,\eta,\xi_0,\eta_0)=F_3(m_1,m_3,1-m_1,1-m_3,1,z_{13},z_{16}), \tag{37}$$

where z_{13} and z_{16} were defined in (27) and (28).

Combining (34) and (36) in (33) we find that the Riemann function for the equation

$$U_{\xi\xi}-U_{\eta\eta}+\left[\lambda_2^2\left(\frac{m_1(1-m_1)}{\sinh^2\lambda_2\xi}-\frac{m_3(1-m_3)}{\cosh^2\lambda_2\xi}\right)-\lambda_1^2\left(\frac{m_2(1-m_2)}{\sin^2\lambda_1\eta}+\frac{m_4(1-m_4)}{\cos^2\lambda_1\eta}\right)\right]U=0 \tag{38}$$

is given by

$$\begin{aligned}R(\xi,\eta,\xi_0,\eta_0)=&F_3(m_2,m_4,1-m_2,1-m_4,1,z_{33},z_{34})\\&+\int_{\xi-\xi_0}^{\eta-\eta_0}F_3(m_2,m_4,1-m_2,1-m_4,1,u_1(t),u_2(t))\\&\times\frac{\partial}{\partial t}F_3(m_1,m_3,1-m_1,1-m_3,1,v_1(t),v_2(t))dt,\end{aligned} \tag{39}$$

where

$$u_1(t)=\frac{\cos\lambda_1(\eta-\eta_0)-\cos\lambda_1 t}{2\sin\lambda_1\eta\sin\lambda_1\eta_0},\quad u_2(t)=\frac{\cos\lambda_1(\eta-\eta_0)-\cos\lambda_1 t}{2\cos\lambda_1\eta\cos\lambda_1\eta_0}$$

$$v_1(t)=\frac{\cosh\lambda_2 t-\cosh\lambda_2(\xi-\xi_0)}{2\sinh\lambda_2\xi\sinh\lambda_2\xi_0},\quad v_2(t)=\frac{\cosh\lambda_2(\xi-\xi_0)-\cosh\lambda_2 t}{2\cosh\lambda_2\xi\cosh\lambda_2\xi_0}.$$

The ratio λ_1/λ_2 is essential in (38). It is possible to transform away either λ_1 or λ_2 via a change of variables, but not both. It is useful to write the equation as (38) though, which at first glance incorporates six parameters, as the equation is then symmetric. Effectively a five parameter Riemann function has been obtained. Equation (38) contains one more essential parameter than Chaundy's equation (1). There is strong evidence to suggest that (38) is not isomorphic to Chaundy's equation (1). There are several reasons for this. First (38) possesses no nontrivial first-order symmetries and repeating the calculations of Sec. II shows that it has no second-order symmetry operators either. So combining (34) and (36) in the addition formula destroys the symmetries found in Sec. II. Of course this does not rule out the possibility of a contact, or other type of transformation, between (1) and (38) but the author believes that this is unlikely. Secondly, during the course of analyzing Chaundy's equation the unusual fact that the independent variables $z_1,\ldots,z_4$ of (1) are linearly dependent was discovered. In fact a few calculations will show that

$$\frac{1}{z_1}+\frac{1}{z_2}+\frac{1}{z_3}+\frac{1}{z_4}=2,$$

where $z_1,\ldots,z_4$ are given by (3) and (4). If a parallel calculation is performed with the independent variables of (38), then this linear relationship is lost. Effectively

$$\frac{1}{z_9}+\frac{1}{z_{11}}+\frac{1}{z_{13}}+\frac{1}{z_{16}}\neq 2.$$

The loss of such a property adds further weight to the conjecture that the two equations are not isomorphic.

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Riemann functions and the group $E(1,1)$

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Historically Lie algebras of first-order symmetry operators have proven to be a useful method for finding equivalence classes of Riemann functions. Here this idea is extended to higher order symmetries. The approach is to seek self-adjoint linear hyperbolic partial differential equations that separate variables in more than one coordinate system under the action of the group $E(1,1)$. The equations derived admit no nontrivial first-order operators and can only be obtained from second-order symmetry operators. Using this symmetry structure, a new equivalence class of Riemann functions can then be found. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1763002]

I. INTRODUCTION

The idea of applying first-order symmetry operators to Riemann's method has been well investigated.[1–6] The hyperbolic partial differential equation in two variables (PDE),

$$L[U]=U_{yy}-U_{xx}+a(x,y)U_y-b(x,y)U_x+c(x,y)U=0, \tag{1}$$

will admit a four-dimensional Lie algebra of first order symmetries if and only if the invariants

$$p=\frac{k}{h}, \quad q=\frac{\ln|h|_{yy-xx}}{h}, \tag{2}$$

are constants (if $h=0$ then swap k and h). When p or q (or both of them) is not constant then the symmetry algebra is two-dimensional or less. Here h and k are Laplace invariants of (1),

$$h=\left(\frac{\partial}{\partial y}+\frac{\partial}{\partial x}\right)(a+b)+\frac{1}{2}(a^2-b^2)-c, \quad k=\left(\frac{\partial}{\partial y}-\frac{\partial}{\partial x}\right)(a-b)+\frac{1}{2}(a^2-b^2)-c.$$

When p and q are constant with $q\neq 0$, removing the trivial symmetry of scaling solutions by a constant yields a symmetry algebra isomorphic to sl(2,R). Using this fact, it is straightforward to show that an invertible transformation exists between (1) and the Euler–Poisson–Darboux equation (EPD),

$$U_{yy}-U_{xx}-\frac{m(1-m)}{x^2}U=0. \tag{3}$$

This is Riemann's original example.[7] Bluman[1] was the first to show how to explicitly calculate the Riemann function from the symmetry operators as

$$R(x,y,x_0,y_0)={}_2F_1(m,1-m;1;z_0), \tag{4}$$

where

$$z_0=\frac{(y-y_0)^2-(x-x_0)^2}{4xx_0}, \tag{5}$$

and ${}_2F_1$ is the hypergeometric function. The case when $q=0$ corresponds to confluent forms of the EPD equation. Recall that the Riemann function must satisfy (1) and

$$R_x+R_y=\tfrac{1}{2}(a+b)R \quad \text{on} \quad y-y_0=x-x_0, \tag{6}$$

$$R_x-R_y=-\tfrac{1}{2}(a-b)R \quad \text{on} \quad y-y_0=-(x-x_0), \tag{7}$$

$$R(x_0,y_0,x_0,y_0)=1. \tag{8}$$

In this paper we consider the self-adjoint form of (1),

$$U_{yy}-U_{xx}+V(x,y)U=0. \tag{9}$$

In direct analogy to the results for Lie algebras of first-order operators isomorphic to sl(2,R), the aim here is to derive Riemann functions for (9) by applying second-order linear symmetry operators. Effectively we shall seek restrictions on the coefficient $V(x,y)$ in (9) so that the Riemann function can be determined. In Ref. 8 a link between second-order symmetry operators and Riemann's method was established where it was shown that Chaundy's equation[9] admitted a two-dimensional vector space of second-order operators that lead to 4 inequivalent orbits. Chaundy's PDE is the most general self-adjoint equation for which the Riemann function is known. Each orbit corresponded to a separable coordinate system. In this way a new equivalence class of Riemann functions was found. So by carefully choosing the form of $V(x,y)$ in (9) a rich symmetry structure can be built. The goal is then to connect these resulting PDEs to their Riemann functions by using the properties of the symmetries.

Here we shall derive the separable forms of (9) under the action of the group $E(1,1)$. The group $E(1,1)$ is chosen as it is the symmetry group for the Laplace equation ($V(x,y)\equiv$const in (9)).[10] By seeking those equations that separate variables in more than one coordinate system, suitable restrictions on $V(x,y)$ can be determined so that vector spaces of second-order symmetry operators are obtained. Equation (9) will not admit $E(1,1)$ as a symmetry group but the pure differential parts of the second-order symmetry operators belong to the enveloping algebra of the Lie algebra $e(1,1)$ of first-order differential operators that commute with $L'=\partial_{yy}-\partial_{xx}$. The PDEs found are then candidate equations for which the Riemann function is sought. The trick is to identify the Riemann function in one of the candidate equations. In many cases this is possible by linking the proposed PDE to the separable forms of Chaundy's equation found in Ref. 8 and to other known results. In fact one case will prove to be a new confluent form of Chaundy's equation.[9]

Unlike earlier symmetry studies, the equations derived here admit no nontrivial first-order symmetry operators. They are obtainable only via second-order symmetries. In this way, we shall construct a new equivalence class of Riemann functions. The study is then a natural extension of the results already derived for first-order operators.

In Sec. II, the separable forms of (9) are found. Section III details the calculation of those equations that separate variables in more than 1 coordinate system. In Sec. IV the Riemann functions are found where possible. Section V summarizes the results.

II. DERIVATION OF THE SEPARABLE POTENTIALS

For the group $E(1,1)$, the inequivalent second-order symmetric operators and the associated separable coordinate systems were established by Kalnins.[10] Define $P_1=\partial_y$, $P_2=\partial_x$, and $M=x\partial_y+y\partial_x$, then the second-order symmetry operators have differential part

$$M^2, \quad P_1P_2, \quad \{M,P_1\}, \quad \{M,P_2\}, \quad \{M,P_1+P_2\}+(P_1-P_2)^2,$$

$$P_2^2, \quad M^2-P_1P_2, \quad M^2\pm(P_1+P_2)^2, \quad M^2\pm P_2^2,$$

$$(P_1+P_2)^2, \quad \{M,P_1-P_2\},$$

where $\{\alpha,\beta\}=\alpha\beta+\beta\alpha$. Standard techniques exist in the literature for calculating the separable forms of (9). Taking the first operator and following Winternitz[11] and Miller,[12] define

$$L=\partial_{yy}-\partial_{xx}+V(x,y), \tag{10}$$

$$S=M^2+f(x,y), \tag{11}$$

where $f(x,y)$ is an arbitrary function. S is a symmetry operator of (9) provided that

$$[L,S]=0. \tag{12}$$

In Ref. 11 the function $V(x,y)$ is called the potential function. So for historical reasons, we shall also use this nomenclature. The search for multiseparable potentials has been an active area of investigation now for nearly 40 years. Multiseparable systems, such as the ones sought here, are called superintegrable in the literature.[11,13–17]

For the symmetry M^2, solving (12) yields three equations

$$xy\frac{\partial V}{\partial y}+y^2\frac{\partial V}{\partial x}-\frac{\partial f}{\partial x}=0, \tag{13}$$

$$xy\frac{\partial V}{\partial x}+x^2\frac{\partial V}{\partial y}+\frac{\partial f}{\partial y}=0, \tag{14}$$

$$x^2\frac{\partial^2 V}{\partial y^2}+2xy\frac{\partial^2 V}{\partial x\partial y}+y^2\frac{\partial^2 V}{\partial x^2}+x\frac{\partial V}{\partial x}+y\frac{\partial V}{\partial y}+\frac{\partial^2 f}{\partial y^2}-\frac{\partial^2 f}{\partial x^2}=0. \tag{15}$$

Eliminating f from (13) and (14) produces a special case of the well-known Bertrand–Darboux equation

$$xy\left(\frac{\partial^2 V}{\partial y^2}+\frac{\partial^2 V}{\partial x^2}\right)+(y^2+x^2)\frac{\partial^2 V}{\partial y\partial x}+3y\frac{\partial V}{\partial x}+3x\frac{\partial V}{\partial x}=0. \tag{16}$$

Now make the change of variables

$$x=e^{\xi}\cosh\eta,$$

$$y=e^{\xi}\sinh\eta$$

in (16) which is in fact the separable coordinate system for the Laplace equation corresponding to the symmetry M^2.[10] Thus we obtain

$$V_{\xi\eta}+2V_{\eta}=0$$

which has the solution

$$V=\frac{V_1(\xi)+V_2(\eta)}{e^{2\xi}}$$

and

TABLE I. Separable potentials.

Symmetry	Separable coordinates	Potential
(A) P_1P_2, P_2^2, $(P_1+P_2)^2$	$x\ y$	$V_1(x)+V_2(y)$
(B) M^2	$x=e^{\xi}\cosh\eta$ $y=e^{\xi}\sinh\eta$	$\frac{V_1(\xi)+V_2(\eta)}{e^{2\xi}}$
(C) $\{M,P_1\}$, $\{M,P_2\}$	$x=\frac{1}{2}(\xi^2+\eta^2)$ $y=\xi\eta$	$\frac{V_1(\xi)+V_2(\eta)}{\eta^2-\xi^2}$
(D) $\{M,P_1+P_2\}+(P_1-P_2)^2$	$x=\frac{1}{2}(\xi-\eta)^2-(\xi+\eta)$ $y=\frac{1}{2}(\xi-\eta)^2+(\xi+\eta)$	$\frac{V_1(\xi)+V_2(\eta)}{\eta-\xi}$
(E) $M^2-P_1P_2$	$x=\frac{1}{2}\cosh\left(\frac{\xi-\eta}{2}\right)+\frac{1}{2}\sinh\left(\frac{\xi+\eta}{2}\right)$ $y=\frac{1}{2}\cosh\left(\frac{\xi-\eta}{2}\right)-\frac{1}{2}\sinh\left(\frac{\xi+\eta}{2}\right)$	$\frac{V_1(\xi)+V_2(\eta)}{\sinh\xi-\sinh\eta}$
(F) $M^2-(P_1+P_2)^2$	$x=\cosh(\xi-\eta)-e^{\xi+\eta}$ $y=\cosh(\xi-\eta)+e^{\xi+\eta}$	$\frac{V_1(\xi)+V_2(\eta)}{e^{2\xi}-e^{2\eta}}$
(G) $M^2+(P_1+P_2)^2$	$x=\sinh(\xi-\eta)-e^{\xi+\eta}$ $y=\sinh(\xi-\eta)+e^{\xi+\eta}$	$\frac{V_1(\xi)+V_2(\eta)}{e^{2\xi}+e^{2\eta}}$
(H) $M^2+P_2^2$	$x=\sinh\xi\cosh\eta$ $y=\cosh\xi\sinh\eta$	$\frac{V_1(\xi)+V_2(\eta)}{\sinh^2\xi+\cosh^2\eta}$
(I) $M^2-P_2^2$	$x=\sin\xi\sin\eta$ $y=\cos\xi\cos\eta$	$\frac{V_1(\xi)+V_2(\eta)}{\cos^2\eta-\cos^2\xi}$
	$x=\sinh\xi\sinh\eta$ $y=\cosh\xi\cosh\eta$	$\frac{V_1(\xi)+V_2(\eta)}{\cosh^2\xi-\cosh^2\eta}$
(J) $\{M,P_1-P_2\}$	No separable coordinates	No separable potential

$$S=M^2-V_2(\eta).$$

This is then the form of the separable potential for the symmetry M^2. The other cases are analogous and the results are summarized in Table I.

III. POTENTIALS WITH TWO OR MORE INVARIANTS

In order to obtain a separable potential with a corresponding known Riemann function, we seek separability in more than one coordinate system. The idea is then to identify the Riemann function for the equation in one of its different coordinate systems. First we shall consider those cases which separate variables in Cartesian and one other coordinate system. Hence start with the systems A and B.

A. Invariants A and B

We must find a potential which can be written in the form

$$V(x,y)=V_1(x)+V_2(y)=f(\xi)+\frac{g(\eta)}{e^{2\xi}}, \tag{17}$$

where $x=e^{\xi}\cosh\eta$, $y=e^{\xi}\sinh\eta$. From (17) it follows that

$$\frac{\partial^2}{\partial\xi\partial\eta}e^{2\xi}[V_1(e^{\xi}\cosh\eta)+V_2(e^{\xi}\sinh\eta)]=0,$$

which can be solved by separation of variables to obtain

$$V(x,y)=\alpha(y^2-x^2)+\frac{\beta_1}{y^2}+\frac{\beta_2}{x^2}, \tag{18}$$

where α is the separation constant and β_1 and β_2 are constants of integration. This leads to the following pair of equations:

$$U_{yy}-U_{xx}+\left[\alpha(y^2-x^2)+\frac{\beta_1}{y^2}+\frac{\beta_2}{x^2}\right]U=\lambda U, \tag{19}$$

$$U_{\xi\xi}-U_{\eta\eta}+\left[\alpha e^{4\xi}-\lambda e^{2\xi}+\frac{\beta_1}{\sinh^2\eta}+\frac{\beta_2}{\cosh^2\eta}\right]U=0. \tag{20}$$

Note that an extra constant λ has been introduced. This is because the group $E(1,1)$ guarantees Liouville-type potentials.[11]

The potential (18) also arises for other invariants as a similar calculation on systems A and H as well as A and I produces the same potential (18). Hence using the corresponding coordinate systems for each of these invariants, we find the following separable equations:

$$U_{\xi\xi}-U_{\eta\eta}+\left[\alpha(\cos^4\eta-\cos^4\xi-\cos^2\eta+\cos^2\xi)+\lambda(\cos^2\xi-\cos^2\eta)\right.$$
$$\left.+\beta_1\left(\frac{1}{\cos^2\xi}-\frac{1}{\cos^2\eta}\right)+\beta_2\left(\frac{1}{\sin^2\eta}-\frac{1}{\sin^2\xi}\right)\right]U=0, \tag{21}$$

$$U_{\xi\xi}-U_{\eta\eta}+\left[\alpha(\cosh^4\eta-\cosh^4\xi-\cosh^2\eta+\cosh^2\xi)\mp\lambda(\cosh^2\eta\pm\cosh^2\xi)\right.$$
$$\left.+\beta_1\left(\frac{1}{\cosh^2\xi}\pm\frac{1}{\cosh^2\eta}\right)+\beta_2\left(\frac{1}{\sinh^2\eta}\pm\frac{1}{\sinh^2\xi}\right)\right]U=0. \tag{22}$$

B. Invariants A and E

For the invariants A and E, we find the potential

$$V(x,y)=\alpha(y^2-x^2)+\beta.$$

Subsequent searches also produce this potential for the invariants A and F as well as G. This results in the equations

$$U_{yy}-U_{xx}+\alpha(y^2-x^2)U=\lambda U, \tag{23}$$

$$U_{\xi\xi}-U_{\eta\eta}+[\alpha(e^{4\xi}-e^{4\eta})-\lambda(e^{2\xi}\pm e^{2\eta})]U=0, \tag{24}$$

$$U_{\xi\xi}-U_{\eta\eta}+[\alpha(\sinh^2\xi-\sinh^2\eta)-\lambda(\sinh\xi-\sinh\eta)]U=0. \tag{25}$$

Equation (23) is clearly a subcase of (19). Thus any results obtained for the Riemann function of (19) will consequently encompass (23)–(25).

C. Invariants A and C

Here take

$$x = \tfrac{1}{2}(\xi^2 + \eta^2),$$

$$y = \xi\eta.$$

In this case a few calculations show that

$$V(x,y) = \alpha(4x^2 - y^2) + \beta x + \frac{\gamma}{y^2}. \tag{26}$$

So one obtains the two equations

$$U_{yy} - U_{xx} + \left[\alpha(4x^2 - y^2) + \beta x + \frac{\gamma}{y^2}\right]U = \lambda U, \tag{27}$$

$$U_{\xi\xi} - U_{\eta\eta} + \left[\alpha(\eta^6 - \xi^6) + \frac{\beta}{2}(\eta^4 - \xi^4) + \lambda(\eta^2 - \xi^2) + \gamma\left(\frac{1}{\xi^2} - \frac{1}{\eta^2}\right)\right]U = 0. \tag{28}$$

D. Invariants A and D

Here we try

$$x = \tfrac{1}{2}(\xi - \eta)^2 - (\xi + \eta),$$

$$y = \tfrac{1}{2}(\xi - \eta)^2 + (\xi + \eta).$$

This choice of coordinates results in the potential

$$V(x,y) = \alpha(y - x) + \beta.$$

Hence we obtain the two equations

$$U_{yy} - U_{xx} + \alpha(y - x)U = \lambda U, \tag{29}$$

$$U_{\xi\xi} - U_{\eta\eta} + [8\alpha(\xi^2 - \eta^2) - 4\lambda(\xi - \eta)]U = 0, \tag{30}$$

where the constant λ incorporates β.

E. Other combinations of invariants

The study of those potentials which separate variables in Cartesian and one other coordinate system is now complete. However direct calculation shows that other combinations of invariants do not yield new nontrivial potentials. To qualify this, consider the invariants B and C. They give

$$V(x,y) \equiv \frac{1}{\xi^2 - \eta^2}\left(\alpha + \frac{\beta_1}{\xi^2} + \frac{\beta_2}{\eta^2}\right),$$

or in other words, the two equations

$$U_{\phi\phi} - U_{rr} + \left[\frac{\alpha}{2}e^r + \frac{1}{4}\left(\frac{\beta_1}{\cosh^2(\phi/2)} + \frac{\beta_2}{\sinh^2(\phi/2)}\right)\right]U = \lambda e^{2r}U,$$

$$U_{\xi\xi}-U_{\eta\eta}+\left(\alpha+\lambda(\eta^2-\xi^2)+\frac{\beta_1}{\xi^2}+\frac{\beta_2}{\eta^2}\right)U=0.$$

Both of these equations have already been seen in this paper. This then exhausts the possibilities for the group $E(1,1)$.

IV. THE CORRESPONDING RIEMANN FUNCTIONS

In order to make the reference potentials of Sec. III useful, we must find the accompanying Riemann functions for each case. The key is that the nine coordinate systems of Table I are contained within the set of transformations, T, consisting of

$$x=\phi(\xi+\eta)+\psi(\xi-\eta),$$

$$y=\phi(\xi+\eta)-\psi(\xi-\eta),$$

where $\phi,\psi\in C^2$ are arbitrary functions, and ϕ',ψ' do not vanish. This is the general solution of the vibrating string equations

$$\frac{\partial\xi}{\partial y}=\frac{\partial\eta}{\partial x},\quad \frac{\partial\xi}{\partial x}=\frac{\partial\eta}{\partial y}.$$

Importantly the Riemann function $R(x,y,x_0,y_0)$ is conformally invariant under T.[18] This means that the conditions (6)–(8), which essentially define Riemann's method, remain consistent with respect to functional structures if the variables x,y are replaced by ξ, η. Hence if the Riemann function can be found for one of the equations corresponding to a given set of invariants, then the Riemann function for the remaining equations can simply be obtained by a transformation of variables.

All the equations found in Sec. III are of the form

$$U_{yy}-U_{xx}+[\rho_1(y)-\rho_2(x)]U=0. \tag{31}$$

Olevskiĭ[19] showed that the Riemann function, $R_{\rho_1-\rho_2}$ of (31) can be given by

$$R_{\rho_1-\rho_2}(x,y,x_0,y_0)=R_{\rho_1}(x,y,x_0,y_0)+\int_{y-y_0}^{x-x_0}R_{\rho_1}(x,t;x_0,0)\frac{\partial}{\partial t}R_{\rho_2}(t,y,0,y_0)dt, \tag{32}$$

where for instance R_{ρ_1} is the Riemann function for (31) with $\rho_2=0$. This addition formula greatly simplifies the task of finding the Riemann solution. Among the families of equations that we have generated it is simply a question of picking the right equation for which the Riemann function can most easily be identified in the literature.

A. Riemann function for the invariants A, B, H, and I

Of the equations (19)–(22) found in Sec. III A, the keys to finding the Riemann function are (19) and (20). Unfortunately though, the author must impose the restriction that either $\alpha=0$ or $\lambda=0$ in order to satisfy Riemann's method. To illustrate why this is the case take (20). For this equation, Olevskiĭ's addition formula means that instead of treating the whole equation it is only necessary to find the Riemann functions for

$$U_{\xi\xi}-U_{\eta\eta}+(\alpha e^{4\xi}-\lambda e^{2\xi})U=0 \tag{33}$$

and

$$U_{\xi\xi}-U_{\eta\eta}+\left[\frac{\beta_1}{\sinh^2\eta}+\frac{\beta_2}{\cosh^2\eta}\right]U=0. \tag{34}$$

The Riemann function for (34) is straightforward. In Ref. 8 the hyperbolic form of Chaundy's equation

$$U_{\xi\xi}-U_{\eta\eta}+\left[\frac{m_1(1-m_1)}{\sinh^2\xi}-\frac{m_2(1-m_2)}{\sinh^2\eta}+\frac{m_3(1-m_3)}{\cosh^2\eta}-\frac{m_4(1-m_4)}{\cosh^2\xi}\right]=0, \tag{35}$$

has the Riemann function

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(m_1,m_2,m_3,m_4;1-m_1,1-m_2,1-m_3,1-m_4;1;z_1,z_2,z_3,z_4),$$

where

$$z_1=\frac{\cosh(\eta-\eta_0)-\cosh(\xi-\xi_0)}{2\sinh\xi\sinh\xi_0},\quad z_2=\frac{\cosh(\xi-\xi_0)-\cosh(\eta-\eta_0)}{2\sinh\eta\sinh\eta_0}, \tag{36}$$

$$z_3=\frac{\cosh(\eta-\eta_0)-\cosh(\xi-\xi_0)}{2\cosh\eta\cosh\eta_0},\quad z_4=\frac{\cosh(\xi-\xi_0)-\cosh(\eta-\eta_0)}{2\cosh\xi\cosh\xi_0}. \tag{37}$$

Setting $m_1=m_4=0$ and $\beta_1=-m_2(1-m_2)$, $\beta_2=m_3(1-m_3)$ reduces the solution to

$$R(\xi,\eta,\xi_0,\eta_0)=F_3(m_2,m_3;1-m_2,1-m_3;1,z_2,z_3),$$

which satisfies (34). Equation (33) is harder to deal with. Cohn[2] has shown how to find the Riemann function for (33) when either $\alpha=0$ or $\lambda=0$. However if both α and λ are nonzero the problem is much more difficult. The differing coefficients in the exponentials prevent the equation from being a confluent form of (35). Olevskiĭ's addition formula could be applicable here as Zhdanov, Revenko and Fushchych[20] have shown that (33) itself is separable. Unfortunately the other separable forms of the equation do not eliminate the differing coefficients. Furthermore Zhdanov *et al.* list (33) as one of the inequivalent separable forms of the equation $U_{yy}-U_{xx}+V(x)U=0$. Hence it is not easily transformable to any other PDE for which the Riemann solution is known. So in order to satisfy Riemann's method one must choose either α or λ to be zero.

If $\alpha=0$ the Riemann function for the whole equation (19) is then[21]

$$R(x,y,x_0,y_0)=F_B(m_1,1-m_1,m_2,1-m_2,1,z_5,z_6,z_7),$$

where $\beta_1=m_1(1-m_1)$, $\beta_2=-m_2(1-m_2)$ with

$$z_5=\frac{(x-x_0)^2-(y-y_0)^2}{4yy_0},\quad z_6=\frac{(y-y_0)^2-(x-x_0)^2}{4xx_0}, \tag{38}$$

and

$$z_7=\frac{\lambda}{4}[(x-x_0)^2-(y-y_0)^2]. \tag{39}$$

To further our analysis, consider the new option of taking $\lambda=0$. From Cohn,[2] the Riemann function for (33) with $\lambda=0$ is

$$R(\xi,\eta,\xi_0,\eta_0)=J_0(z_8),$$

where

$$z_8=\tfrac{1}{2}\sqrt{\alpha(e^{2(\xi+\eta)}-e^{2(\xi_0+\eta_0)})(e^{2(\xi-\eta)}-e^{2(\xi_0-\eta_0)})}.$$

Putting this all together, and using (32), the Riemann function for

$$U_{\xi\xi}-U_{\eta\eta}+\left[\alpha e^{4\xi}-\frac{m_1(1-m_1)}{\sinh^2\eta}+\frac{m_2(1-m_2)}{\cosh^2\eta}\right]U=0 \tag{40}$$

is given by

$$R(\xi,\eta,\xi_0,\eta_0)=J_0(z_8)+\int_{\eta-\eta_0}^{\xi-\xi_0}J_0[u_1(t)]dF_3[m_1,m_2,1-m_1,1-m_2,1,v_1(t),v_2(t)], \tag{41}$$

where

$$v_1(t)=\frac{\cosh(t)-\cosh(\eta-\eta_0)}{2\sinh\eta\sinh\eta_0},\quad v_2(t)=\frac{\cosh(\eta-\eta_0)-\cosh(t)}{2\cosh\eta\cosh\eta_0}, \tag{42}$$

$$u_1(t)=\tfrac{1}{2}\sqrt{\alpha(e^{2(\xi+t)}-e^{2(\xi_0)})(e^{2(\xi-t)}-e^{2(\xi_0)})}. \tag{43}$$

Rewriting the PDE (9) as

$$U_{\xi\xi}-U_{\eta\eta}+[V(\xi)-V(\eta)]U=0$$

we gain the following new potentials for which the Riemann function is now known:

$$V(\xi)=c_1\xi^2+\frac{c_2(1-c_2)}{\xi^2},$$

$$V(\xi)=c_1(\cos^4\xi-\cos^2\xi)+\frac{c_2(1-c_2)}{\cos^2\xi}-\frac{c_3(1-c_3)}{\sin^2\xi},$$

$$V(\xi)=c_1(\cosh^4\xi-\cosh^2\xi)+\frac{c_2(1-c_2)}{\cosh^2\xi}-\frac{c_3(1-c_3)}{\sinh^2\xi}.$$

A link to Chaundy's equation: A closer inspection of (40) shows that it is in fact a confluent form of Chaundy's equation[9]

$$U_{rs}+\left[\frac{m_1(1-m_1)}{(r+s)^2}-\frac{m_2(1-m_2)}{(r-s)^2}+\frac{m_3(1-m_3)}{(1-rs)^2}-\frac{m_4(1-m_4)}{(1+rs)^2}\right]U=0. \tag{44}$$

The Riemann function for this equation is

$$R(r,s,r_0,s_0)=F_B(m_1,m_2,m_3,m_4;1-m_1,1-m_2,1-m_3,1-m_4;1;z_9,z_{10},z_{11},z_{12}), \tag{45}$$

where

$$z_9=-\frac{(r-r_0)(s-s_0)}{(r+s)(r_0+s_0)},\quad z_{10}=\frac{(r-r_0)(s-s_0)}{(r-s)(r_0-s_0)}, \tag{46}$$

$$z_{11}=-\frac{(r-r_0)(s-s_0)}{(1-rs)(1-r_0s_0)},\quad z_{12}=\frac{(r-r_0)(s-s_0)}{(1+rs)(1+r_0s_0)}. \tag{47}$$

In Ref. 8 it was shown that there exists a second-order symmetry operator that maps (44) to (35), and likewise the Riemann solutions via the separable coordinate system $r=\exp(\xi+\eta)$, $s=\exp(\xi-\eta)$. So now choose the hyperbolic form (35) of Chaundy's equation and let $m_1(1-m_1)=m_4(1-m_4)=\alpha/2$ which may then be rewritten as

$$U_{\xi\xi}-U_{\eta\eta}+\left[\frac{\alpha}{\sinh^2 2\xi}-\frac{m_2(1-m_2)}{\sinh^2\eta}+\frac{m_3(1-m_3)}{\cosh^2\eta}\right]=0. \tag{48}$$

Translate the origin by setting

$$\xi\mapsto\xi-\nu,\quad \xi_0\mapsto\xi_0-\nu,\quad \alpha\mapsto\frac{\alpha}{4}e^{4\nu} \tag{49}$$

and take the limit as $\nu\to\infty$. This reduces (48) to (40).

In Ref. 8, Chaundy's equation was shown to possess a two-dimensional vector space of second-order symmetry operators. Hence the increased dimension of the vector space admitted by the confluent form (40) of Chaundy's equation is new.

B. Comments on the Riemann function for the invariants A, E, F, and G

As previously mentioned, the Riemann function (40) derived in Sec. IV A also includes the equations of Sec. III D. Unfortunately though, the restrictions placed on the coefficients α and λ imply that (23)–(25) are reduced to readily obtainable confluent forms of Chaundy's equation (44). To see this take (24), with $\alpha=0$, say. This produces the reference potential

$$V(\xi)=e^{4\xi}.$$

But the transformation (49) applied to both ξ and η in (35) yields (24) with either α or λ equal to zero depending on the scaling used. This potential has therefore already been discussed.

Similarly for (25), if $\lambda=0$, then no new potential is found. Letting $\alpha=0$ results in the potential

$$V(\xi)=\sinh\xi,$$

which is not among the potentials from Sec. IV A. However such an option is easily obtained from the Klein–Gordon or Telegrapher's equation, which is itself a confluent form of Chaundy's equation.[21] So the results for these invariants are included only for completeness. In order to obtain significant results from Sec. III D the Riemann function for the full equation (24) would need to be found. Unfortunately this remains an open problem.

C. Riemann function for the invariants A and C

For the two equations found in Sec. III C, the problem of finding the Riemann function when α, β, γ, and λ are all nonzero is quite difficult. The author has not had any success in this regard. However if we let $\alpha=0$, then the Riemann function can easily be obtained. So consider (27) with $\alpha=0$,

$$U_{yy}-U_{xx}+\left[\beta x+\frac{\gamma}{y^2}\right]U=\lambda U. \tag{50}$$

There are then two ways to separate variables in (50) as the constant λ may be grouped with either of the independent variables. Of the two options, take the equations

$$U_{yy}-U_{xx}+\left[\frac{\gamma(1-\gamma)}{y^2}-\lambda\right]U=0 \tag{51}$$

and

$$U_{yy}-U_{xx}+\beta xU=0. \tag{52}$$

Note that γ has been rescaled. From Ref. 21 the Riemann function for (51) is

$$R_1(x,y,x_0,y_0)=\Xi_2(\gamma,1-\gamma,1,z_5,z_7), \tag{53}$$

where z_5 is given by (38) and z_7 by (39).

On the other hand, in order to solve (52), the results of Wahlberg[22] are required who found that the Riemann function for

$$U_{yy}-U_{xx}+(1+\delta x)U=0 \tag{54}$$

can be represented by the contour integral

$$R(x,y,x_0,y_0)=\frac{1}{2\pi i}\int_\Gamma \exp\left\{\left[1+\frac{\delta}{2}(x+x_0)\right]z-\frac{(y-y_0)^2-(x-x_0)^2}{4z}-\frac{\delta^2}{12}z^3\right\}\frac{dz}{z},$$

where Γ is defined by $|z|=\rho$, encircling the origin in the positive direction (since the integrand is analytic everywhere except at $z=0$, Γ can be taken to be any closed contour encircling the origin in the positive direction).

Alternatively, as Wahlberg showed, expanding $\exp(-\delta^2z^3/12)$ of the integrand as a power series then applying the formula

$$J_n(\alpha)=\frac{1}{2\pi i}\int_\Gamma z^{-n-1}\exp\left[\frac{1}{2}\alpha\left(z-\frac{1}{z}\right)\right]dz$$

for the Bessel function of order n, gives

$$R(x,y,x_0,y_0)=\sum_{n=0}^{\infty}\frac{\Omega^n}{n!}J_{3n}(\Delta), \tag{55}$$

where

$$\Omega=\frac{\delta^2}{96}\left(\frac{(y-y_0)^2-(x-x_0)^2}{1+\frac{\delta}{2}(x+x_0)}\right)^{3/2}, \tag{56}$$

$$\Delta=\left\{\left[1+\frac{\delta}{2}(x+x_0)\right][(y-y_0)^2-(x-x_0)^2]\right\}^{1/2}. \tag{57}$$

By inspection, (52) is just (54) up to translation in x. Specifically if we let

$$x\mapsto x-\frac{1}{\delta},\quad x_0\mapsto x_0-\frac{1}{\delta},\quad \delta\mapsto\beta,$$

then (54) yields (52) as required. For the Riemann function, applying this same change of variables to (55) gives

$$R_2(x,y,x_0,y_0)=\sum_{n=0}^{\infty}\frac{\Omega_2^n}{n!}J_{3n}(\Delta_2), \tag{58}$$

where now

$$\Omega_2=\frac{\beta^2}{96}\left[\frac{(y-y_0)^2-(x-x_0)^2}{\frac{\beta}{2}(x+x_0)}\right]^{3/2}, \tag{59}$$

$$\Delta_2=\left\{\frac{\beta}{2}(x+x_0)[(y-y_0)^2-(x-x_0)^2]\right\}^{1/2}. \tag{60}$$

Applying Olevskiĭ's addition formula (32), the Riemann function for (50) is

$$R(x,y,x_0,y_0)=R_2(x,y,x_0,y_0)+\int_{y-y_0}^{x-x_0}R_2(x,t;x_0,0)\frac{\partial}{\partial t}R_1(t,y,0,y_0)dt, \tag{61}$$

where R_1 and R_2 are defined by (53)–(60). From (28) another new reference potential for (9) is then

$$V(\xi)=\frac{c_1}{2}\xi^4+c_2\xi^2+\frac{c_3(1-c_3)}{\xi^2}.$$

A quick calculation shows that (50) has a trivial first-order symmetry algebra. Hence (50) and (28) with $\alpha=0$ are not isomorphic to any other equations via a point transformation. Furthermore the second-order symmetries used here are inequivalent as are the equations they generate so we may also state that (50) and (28) are not transformable to any other equation via a second-order operator. Hence precluding the possibility of contact transformations we may conclude that the Riemann functions for these two equations are new.

D. Riemann function for the invariants A and D

For the two equations found in Sec. III D, the Riemann function is most easily found for (29). Applying Olevskiĭ's addition formula to (29) requires the Riemann functions for

$$U_{yy}-U_{xx}+\alpha xU=0 \tag{62}$$

and

$$U_{yy}-U_{xx}+(\alpha y-\lambda)U=0. \tag{63}$$

Equation (62) is just (52) with $\alpha=\beta$. Hence the Riemann function for (62) is (58)–(60) with $\alpha=\beta$. Similarly interchanging the roles of x and y and translating the origin by

$$y\mapsto y-\frac{1}{\delta}+\frac{\lambda}{\delta},\quad y_0\mapsto y_0-\frac{1}{\delta}+\frac{\lambda}{\delta},\quad \delta\mapsto-\alpha$$

transforms (54) into (63). Hence the Riemann function for this equation is

$$R_3(x,y,x_0,y_0)=\sum_{n=0}^{\infty}\frac{\Omega_3^n}{n!}J_{3n}(\Delta_3), \tag{64}$$

where

$$\Omega_3=\frac{\alpha^2}{96}\left[\frac{(y-y_0)^2-(x-x_0)^2}{\lambda+\frac{\alpha}{2}(y+y_0)}\right]^{3/2}, \tag{65}$$

$$\Delta_3=\left\{\left[\frac{\alpha}{2}(y+y_0)+\lambda\right][(y-y_0)^2-(x-x_0)^2]\right\}^{1/2}. \tag{66}$$

Now applying Olevskiĭ's addition formula (32), the Riemann function for (29) is

$$R(x,y,x_0,y_0)=R_2(x,y,x_0,y_0)+\int_{y-y_0}^{x-x_0}R_2(x,t;x_0,0)\frac{\partial}{\partial t}R_3(t,y,0,y_0)dt, \tag{67}$$

where R_2 and R_3 are given, respectively, by (58)–(60) with $\beta=\alpha$ and (64)–(66).

From (30) we obtain the potential

$$V(\xi)=c_1\xi^2+c_2\xi.$$

Applying similar arguments to the previous section, both (29) and (30) also represent new equations for which the Riemann function is now known.

V. SUMMARY

The aim of this paper was to develop a methodology for deriving equivalence classes of Riemann functions from second-order symmetry operators in an analogous way to the theory already in place for first-order symmetries. So let us collect together the results. For the PDE

$$U_{\xi\xi}-U_{\eta\eta}+[V(\xi)-V(\eta)]U=0$$

the following is a list of all potentials, $V(\xi)$, for which the Riemann function was found under the action of the group $E(1,1)$.

Case 1: $V(\xi)=c_1\xi^4/2+c_2\xi^2+c_3(1-c_3)/\xi^2$.

$$R(\xi,\eta,\xi_0,\eta_0)=R_2(\xi,\eta,\xi_0,\eta_0)+\int_{L_l}^{L_u}R_2\left[\frac{1}{2}(\xi^2+\eta^2),t,\frac{1}{2}(\xi_0^2+\eta_0^2),0\right]\frac{\partial}{\partial t}R_1(t,\xi\eta,0,\xi_0\eta_0)dt,$$

such that $L_l=\xi\eta-\xi_0\eta_0$, $L_u=\frac{1}{2}(\xi^2-\xi_0^2+\eta^2-\eta_0^2)$ and

$$R_1(t,\xi\eta,0,\xi_0\eta_0)=\Xi_2(c_3,1-c_3,1,u_1(t),u_2(t)),$$

where

$$u_1(t)=\frac{(t^2-\xi\eta-\xi_0\eta_0)^2}{4\xi\xi_0\eta\eta_0},\quad u_2(t)=\frac{c_2}{4}[t^2-(\xi\eta-\xi_0\eta_0)^2],$$

and

$$R_2(\xi,\eta,\xi_0,\eta_0)=\sum_{n=0}^{\infty}\frac{\Omega_2^n}{n!}J_{3n}(\Delta_2),$$

where

$$\Omega_2=\frac{\beta^2}{96}\left\{\frac{[(\eta+\eta_0)^2-(\xi+\xi_0)^2][(\xi-\xi_0)^2-(\eta-\eta_0)^2]}{\beta(\xi^2+\eta^2+\xi_0^2+\eta_0^2)}\right\}^{3/2},$$

$$\Delta_2=\left\{\frac{\beta}{8}(\xi^2+\eta^2+\xi_0^2+\eta_0^2)[(\eta+\eta_0)^2-(\xi+\xi_0)^2][(\xi-\xi_0)^2-(\eta-\eta_0)^2]\right\}^{1/2},$$

with

$$R_2\left[\frac{1}{2}(\xi^2+\eta^2),t,\frac{1}{2}(\xi_0^2+\eta_0^2),0\right]=\sum_{n=0}^{\infty}\frac{\Omega_2'^n(t)}{n!}J_{3n}(\Delta_2'(t)),$$

where

$$\Omega_2'=\frac{\beta^2}{96}\left\{\frac{4t^2-[(\xi^2-\xi_0^2)+(\eta^2-\eta_0^2)]^2}{\beta(\xi^2+\xi_0^2+\eta^2+\eta_0^2)}\right\}^{3/2},$$

$$\Delta_2'=\left\{\frac{\beta}{16}(\xi^2+\xi_0^2+\eta^2+\eta_0^2)[4t^2-[(\xi^2-\xi_0^2)+(\eta^2-\eta_0^2)]^2]\right\}^{1/2}.$$

Case 2: $V(\xi)=c_1\xi^2+c_2\xi$.

$$R(\xi,\eta,\xi_0,\eta_0)=R_2(\xi,\eta,\xi_0,\eta_0)+\int_{L_l}^{L_u}R_2\left[\frac{1}{2}(\xi-\eta)^2-(\xi+\eta),t,\frac{1}{2}(\xi_0-\eta_0)^2-(\xi_0+\eta_0),0\right]$$
$$\times\frac{\partial}{\partial t}R_3\left[t,\frac{1}{2}(\xi-\eta)^2+(\xi+\eta),0,\frac{1}{2}(\xi_0-\eta_0)^2+(\xi_0+\eta_0)\right]dt$$

such that $L_l=\frac{1}{2}[(\xi-\eta)^2-(\xi_0-\eta_0)^2]+(\xi-\xi_0)+(\eta-\eta_0)$, $L_u=\frac{1}{2}[(\xi-\eta)^2-(\xi_0-\eta_0)^2]-(\xi-\xi_0)-(\eta-\eta_0)$ and

$$R_2(\xi,\eta,\xi_0,\eta_0)=\sum_{n=0}^{\infty}\frac{\Omega_2^n}{n!}J_{3n}(\Delta_2),$$

where

$$\Omega_2=\frac{\beta^2}{96}\left\{\frac{4[(\xi+\xi_0)-(\eta+\eta_0)][(\xi-\xi_0)^2-(\eta-\eta_0)^2]}{\beta[[(\xi-\eta)^2+(\xi_0-\eta_0)^2]-2(\xi+\xi_0+\eta+\eta_0)]}\right\}^{3/2},$$

$$\Delta_2=\left\{\frac{\beta}{4}[(\xi-\eta)^2+(\xi_0-\eta_0)^2-2(\xi+\xi_0+\eta+\eta_0)]\right.$$
$$\left.\times[[(\xi+\xi_0)-(\eta+\eta_0)][(\xi-\xi_0)^2-(\eta-\eta_0)^2]]\right\}^{1/2},$$

as well as

$$R_2\left[\frac{1}{2}(\xi-\eta)^2-(\xi+\eta),t,\frac{1}{2}(\xi_0-\eta_0)^2-(\xi_0+\eta_0),0\right]=\sum_{n=0}^{\infty}\frac{\Omega_2'^n}{n!}J_{3n}(\Delta_2'),$$

where

$$\Omega_2'=\frac{\beta^2}{96}\left\{\frac{4t^2-[(\xi-\eta)^2-(\xi_0-\eta_0)^2-2(\xi-\xi_0+\eta-\eta_0)]^2}{\beta[(\xi-\eta)^2+(\xi_0-\eta_0)^2-2(\xi+\xi_0+\eta+\eta_0)]}\right\}^{3/2},$$

$$\Delta_2'=\left\{\frac{\beta}{16}[(\xi-\eta)^2+(\xi_0-\eta_0)^2-2(\xi+\xi_0+\eta+\eta_0)]\right.$$
$$\left.\times[4t^2-[(\xi-\eta)^2-(\xi_0-\eta_0)^2-2(\xi-\xi_0+\eta-\eta_0)]^2]\right\}^{1/2},$$

and

$$R_3\left[t,\frac{1}{2}(\xi-\eta)^2+(\xi+\eta),0,\frac{1}{2}(\xi_0-\eta_0)^2+(\xi_0+\eta_0)\right]=\sum_{n=0}^{\infty}\frac{\Omega_3'^n}{n!}J_{3n}(\Delta_3'),$$

where

$$\Omega_3'=\frac{\alpha^2}{96}\left\{\frac{[(\xi-\eta)^2-(\xi_0-\eta_0)^2+2(\xi-\xi_0+\eta-\eta_0)]^2-4t^2}{4\lambda+\alpha[(\xi-\eta)^2+(\xi_0-\eta_0)^2+2(\xi+\xi_0+\eta+\eta_0)]}\right\}^{3/2},$$

$$\Delta_3'=\frac{1}{16}\{[\alpha[(\xi-\eta)^2+(\xi_0-\eta_0)^2+2(\xi+\xi_0+\eta+\eta_0)]+4\lambda]$$
$$\times[[(\xi-\eta)^2-(\xi_0-\eta_0)^2-2(\xi-\xi_0+\eta-\eta_0)]^2-4t^2]\}^{1/2}.$$

Case 3: $V(\xi)=-c_1\cos^2\xi+c_2(1-c_2)/\cos^2\xi-c_3(1-c_3)/\sin^2\xi.$

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(c_2,c_3,1-c_2,1-c_3;1;z_{13},z_{14},z_{15}),$$

where

$$z_{13}=\frac{[\cos(\eta+\eta_0)-\cos(\xi+\xi_0)][\cos(\xi-\xi_0)-\cos(\eta-\eta_0)]}{4\cos\xi\cos\eta\cos\xi_0\cos\eta_0},$$

$$z_{14}=\frac{[\cos(\eta+\eta_0)-\cos(\xi+\xi_0)][\cos(\eta-\eta_0)-\cos(\xi-\xi_0)]}{4\sin\xi\sin\eta\sin\xi_0\sin\eta_0},$$

$$z_{15}=\frac{c_1}{4}[\cos(\eta+\eta_0)-\cos(\xi+\xi_0)][\cos(\xi-\xi_0)-\cos(\eta-\eta_0)].$$

Case 4: $V(\xi)=-c_1\cosh^2\xi+c_2(1-c_2)/\cosh^2\xi-c_3(1-c_3)/\sinh^2\xi.$

$$R(\xi,\eta,\xi_0,\eta_0)=F_B(c_2,c_3,1-c_2,1-c_3;1;z_{16},z_{17},z_{18}),$$

where

$$z_{16}=\frac{[\cosh(\eta+\eta_0)-\cosh(\xi+\xi_0)][\cosh(\xi-\xi_0)-\cosh(\eta-\eta_0)]}{4\cosh\xi\cosh\eta\cosh\xi_0\cosh\eta_0},$$

$$z_{17}=\frac{[\cosh(\eta+\eta_0)-\cosh(\xi+\xi_0)][\cosh(\eta-\eta_0)-\cosh(\xi-\xi_0)]}{4\sinh\xi\sinh\eta\sinh\xi_0\sinh\eta_0},$$

$$z_{18}=\frac{c_1}{4}[\cosh(\eta+\eta_0)-\cosh(\xi+\xi_0)][\cosh(\xi-\xi_0)-\cosh(\eta-\eta_0)].$$

Case 5: $V(\xi)=c_1(\cos^4\xi-\cos^2\xi)+c_2(1-c_2)/\sin^2\xi-c_3(1-c_3)/\cos^2\xi.$

$$R(\xi,\eta,\xi_0,\eta_0)=R_4(\xi,\eta,\xi_0,\eta_0)+\int_{L_l}^{L_u}R_4\left[\frac{1}{2}\ln(\sin^2\eta-\cos^2\xi),t,\frac{1}{2}\ln(\sin^2\eta_0-\cos^2\xi_0),0\right]$$
$$\times\frac{\partial}{\partial t}R_5\left[t,\frac{1}{2}\ln\left(\frac{\tan\eta\tan\xi+1}{\tan\eta\tan\xi-1}\right),0,\frac{1}{2}\ln\left(\frac{\tan\eta_0\tan\xi_0+1}{\tan\eta_0\tan\xi_0-1}\right)\right]dt$$

with

$$L_l=\frac{1}{2}\ln\left[\frac{(\tan\eta\tan\xi+1)(\tan\eta_0\tan\xi_0-1)}{(\tan\eta\tan\xi-1)(\tan\eta_0\tan\xi_0+1)}\right],$$

$$L_u=\frac{1}{2}\ln\left(\frac{\sin^2\eta-\cos^2\xi}{\sin^2\eta_0-\cos^2\xi_0}\right)$$

and

$$R_4(\xi,\eta,\xi_0,\eta_0)=J_0(z_{19}),$$

$$R_4\left[\frac{1}{2}\ln(\sin^2\eta-\cos^2\xi),t,\frac{1}{2}\ln(\sin^2\eta_0-\cos^2\xi_0),0\right]=J_0(u_3(t)),$$

$$R_5\left[t,\frac{1}{2}\ln\left(\frac{\tan\eta\tan\xi+1}{\tan\eta\tan\xi-1}\right),0,\frac{1}{2}\ln\left(\frac{\tan\eta_0\tan\xi_0+1}{\tan\eta_0\tan\xi_0-1}\right)\right]=F_3(c_2,c_3,1-c_2,1-c_3,1,v_3(t),v_4(t)),$$

where

$$z_{19}=\frac{1}{2}\sqrt{c_1\left[(\sin^2\eta-\cos^2\xi)\left(\frac{\tan\eta\tan\xi+1}{\tan\eta\tan\xi-1}\right)-(\sin^2\eta_0-\cos^2\xi_0)\left(\frac{\tan\eta_0\tan\xi_0+1}{\tan\eta_0\tan\xi_0-1}\right)\right]}$$
$$\times\sqrt{\left[(\sin^2\eta-\cos^2\xi)\left(\frac{\tan\eta\tan\xi-1}{\tan\eta\tan\xi+1}\right)-(\sin^2\eta_0-\cos^2\xi_0)\left(\frac{\tan\eta_0\tan\xi_0-1}{\tan\eta_0\tan\xi_0+1}\right)\right]},$$

$$u_3(t)=\tfrac{1}{2}\sqrt{c_1[e^{2t}(\sin^2\eta-\cos^2\xi)-(\sin^2\eta_0-\cos^2\xi_0)]}$$
$$\times\sqrt{[e^{-2t}(\sin^2\eta-\cos^2\xi)-(\sin^2\eta_0-\cos^2\xi_0)]},$$

$$v_3(t)=(\sqrt{(\sin^2\xi-\cos^2\eta)(\sin^2\xi_0-\cos^2\eta_0)}\cosh t-\sin\xi\sin\xi_0\sin\eta\sin\eta_0$$
$$+\cos\xi\cos\xi_0\cos\eta\cos\eta_0)/2\cos\xi\cos\xi_0\cos\eta\cos\eta_0,$$

$$v_4(t)=(\sin\xi\sin\xi_0\sin\eta\sin\eta_0+\cos\xi\cos\xi_0\cos\eta\cos\eta_0$$
$$-\sqrt{(\sin^2\xi-\cos^2\eta)(\sin^2\xi_0-\cos^2\eta_0)}\cosh t)/2\sin\xi\sin\xi_0\sin\eta\sin\eta_0.$$

Case 6: $V(\xi)=c_1(\cosh^4\xi-\cosh^2\xi)+c_2(1-c_2)/\sinh^2\xi-c_3(1-c_3)/\cosh^2\xi.$

$$R(\xi,\eta,\xi_0,\eta_0)=R_6(\xi,\eta,\xi_0,\eta_0)+\int_{L_l}^{L_u}R_6\left[\frac{1}{2}\ln(\cosh^2\xi-\cosh^2\eta),t,\frac{1}{2}\ln(\cosh^2\xi_0-\cosh^2\eta_0),0\right]$$
$$\times\frac{\partial}{\partial t}R_7\left[t,\frac{1}{2}\ln\left(\frac{\tanh\xi+\tanh\eta}{\tanh\xi-\tanh\eta}\right),0,\frac{1}{2}\ln\left(\frac{\tanh\xi_0+\tanh\eta_0}{\tanh\xi_0-\tanh\eta_0}\right)\right]dt$$

with

$$L_l=\frac{1}{2}\ln\left[\frac{(\tanh\xi+\tanh\eta)(\tanh\xi_0-\tanh\eta_0)}{(\tanh\xi-\tanh\eta)(\tanh\xi_0+\tanh\eta_0)}\right],$$

$$L_u=\frac{1}{2}\ln\left(\frac{\cosh^2\xi-\cosh^2\eta}{\cosh^2\xi_0-\cosh^2\eta_0}\right)$$

and

$$R_6(\xi,\eta,\xi_0,\eta_0)=J_0(z_{20}),$$

$$R_6\left[\frac{1}{2}\ln(\cosh^2\xi-\cosh^2\eta),t,\frac{1}{2}\ln(\cosh^2\xi_0-\cosh^2\eta_0),0\right]=J_0(u_4(t)),$$

$$R_7\left[t,\frac{1}{2}\ln\left(\frac{\tanh\xi+\tanh\eta}{\tanh\xi-\tanh\eta}\right),0,\frac{1}{2}\ln\left(\frac{\tanh\xi_0+\tanh\eta_0}{\tanh\xi_0-\tanh\eta_0}\right)\right]=F_3(c_2,c_3,1-c_2,1-c_3,1,v_5(t),v_6(t)),$$

where

$$z_{20}=\frac{1}{2}\sqrt{c_1\left[(\cosh^2\xi-\cosh^2\eta)\left(\frac{\tanh\xi+\tanh\eta}{\tanh\xi-\tanh\eta}\right)-(\cosh^2\xi_0-\cosh^2\eta_0)\left(\frac{\tanh\xi_0+\tanh\eta_0}{\tanh\xi_0-\tanh\eta_0}\right)\right]}$$
$$\times\sqrt{\left[(\cosh^2\xi-\cosh^2\eta)\left(\frac{\tanh\xi-\tanh\eta}{\tanh\xi+\tanh\eta}\right)-(\cosh^2\xi_0-\cosh^2\eta_0)\left(\frac{\tanh\xi_0-\tanh\eta_0}{\tanh\xi_0+\tanh\eta_0}\right)\right]},$$

$$u_4(t)=\tfrac{1}{2}\sqrt{c_1[e^{2t}(\cosh^2\xi-\cosh^2\eta)-(\cosh^2\xi_0-\cosh^2\eta_0)]}$$
$$\times\sqrt{[e^{-2t}(\cosh^2\xi-\cosh^2\eta)-(\cosh^2\xi_0-\cosh^2\eta_0)]}$$

$$v_5(t)=(\sqrt{(\cosh^2\xi-\cosh^2\eta)(\cosh^2\xi_0-\cosh^2\eta_0)}\cosh t-\sinh\xi\sinh\xi_0\cosh\eta\cosh\eta_0$$
$$+\cosh\xi\cosh\xi_0\sinh\eta\sinh\eta_0)/2\cosh\xi\cosh\xi_0\sinh\eta\sinh\eta_0,$$

$$v_6(t)=(\sinh\xi\sinh\xi_0\cosh\eta\cosh\eta_0-\cosh\xi\cosh\xi_0\sinh\eta\sinh\eta_0$$
$$-\sqrt{(\cosh^2\xi-\cosh^2\eta)(\cosh^2\xi_0-\cosh^2\eta_0)}\cosh t)/2\sinh\xi\sinh\xi_0\cosh\eta\cosh\eta_0.$$

Case 7: $V(\xi)=(c_1\sinh\xi)/2$,

$$R(\xi,\eta,\xi_0,\eta_0)=J_0(z_{21}),$$

where

$$z_{21}=2\sqrt{c_1\left[\cosh\frac{(\xi-\xi_0)}{2}-\cosh\frac{(\eta-\eta_0)}{2}\right]\left[\cosh\frac{(\xi+\xi_0)}{2}-\cosh\frac{(\eta+\eta_0)}{2}\right]}.$$

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Invariant and group theoretical integrations over the U(n) group

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In a previous article, an ''invariant method'' to calculate monomial integrals over the U(n) group was introduced. In this paper, we study the more traditional group-theoretical method, and compare its strengths and weaknesses with those of the invariant method. As a result, we are able to introduce a ''hybrid method'' which combines the respective strengths of the other two methods. There are many examples in the paper illustrating how each of these methods works. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765214]

I. INTRODUCTION

This article deals with the calculation of integrals of the form

$$\int (dU)\, U^*_{i_1 j_1} \cdots U^*_{i_p j_p} U_{k_1 l_1} \cdots U_{k_q l_q} \tag{1}$$

over the U(n) group, where (dU) is the invariant Haar measure normalized to $\int (dU) = 1$, and U_{ij} is a U(n) matrix element, with U^*_{ij} being its complex conjugate.

These integrals and their generating functions are useful in many areas of physics, including two-dimensional quantum gravity,[1] QCD, matrix models, and statistical and condensed-matter problems of various sorts.[2] They are also needed in the parton saturation problem at small Feynman-x.[3]

The integral (1) depends on the indices $I=\{i_1 \cdots i_p\}, J=\{j_1 \cdots j_p\}, K=\{k_1 \cdots k_q\}$, and $L=\{l_1 \cdots l_q\}$, so it will be denoted as $\langle IJ|KL\rangle$:

$$\langle IJ|KL\rangle = \int (dU)\, U^*_{IJ} U_{KL}\,, \tag{2}$$

where $U^*_{IJ} = \Pi_{a=1}^{p} U^*_{i_a j_a}$, and similarly for U_{KL}. Since the matrix elements commute, $U^*_{IJ} = U^*_{I_P J_P}$, where $I_P = \{i_{P(1)} \cdots i_{P(p)}\}$ is obtained from I by a permutation $P \in S_p$ of its p indices. Hence

$$\langle IJ|KL\rangle = \langle I_P J_P | K_T L_T\rangle \tag{3}$$

for any $P \in S_p$ and $T \in S_q$.

The integral is nonzero only when $p=q$, a number which will be referred to as the *degree* of the integral. Without loss of generality, it turns out that we may assume $K=I$ and L to be a permutation of J, namely, $L=J_Q$ for some $Q \in S_p$. The value of the integral depends on what the index sets I,J, and what the element Q are, so even for a given p, there are many distinct cases. The best way to distinguish them is to represent each integral by a diagram in a way to be explained in the next section.

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Integral (1) has been computed using a graphical technique.[4] It can also be obtained using the Itzykson–Zuber formula[5] as a generating function, or directly from group theory[6] using the Frobenius formula.[7] We shall refer to this last method as the *group-theoretical method* (GTM). In the GTM, a general formula is available to compute (1). It involves a triple sum over an expression containing characters of the symmetric group S_p, as well as the dimensions of irreducible representations of S_p and of the unitary group $\mathrm{U}(n)$. One of the sums is taken over all the relevant irreducible representations, and the others are taken over the symmetry groups of the index sets I and J. These sums could be long and tedious for a large p, and for most symmetry groups.

A different way to calculate (1) was introduced in a recent paper.[8] This method relies only on the unitary nature of the matrix elements, and the invariance of the Haar measure. In particular, no knowledge of group theory is necessary. The invariance of the Haar measure, as well as the off-diagonal unitarity relation, are used to derive relations between integrals of the same degree. The diagonal unitarity relation connects integrals of degree p with ones of degree $p-1$. Through a chain of these relations, the desired integral is finally related to the basic integral of degree 0, which is $\int dU=1$. The desired integral is then solved from this chain of relations. We have called this method the *invariant method* (IM).

The purpose of this paper is to compare the pros and cons of the GTM with the IM. In order to do so we must first study and understand better the nature of the GTM. Armed with this comparison, we will be able to design a new *hybrid method* which combines the strengths of these two other methods.

The IM is reviewed in Sec. II. It is used to derive a new ''double-fan'' relation needed in the example for the hybrid method.

The GTM is reviewed and studied in Sec. III. It can be used to derive simple relations, but the relations derived in this way are nowhere as powerful as those derived with the IM. The group-theoretical formula can be used to calculate any integral, but generally that is tedious and has to be done integral by integral. However, for integrals whose two symmetry groups are disjoint, or one is contained in the other, systematics emerge to make the calculation simpler. Several of these ''orderly'' integrals are studied in Sec. III.

A comparison of the strengths and weaknesses of the two methods is to be found in Sec. IV. Armed with an understanding of their relative merits, we design a ''hybrid method'' in Sec. V to take advantage of their respective strengths. This method is illustrated by the calculation of a class of ''double-fan'' integrals. There are also four Appendixes showing details of various calculations.

II. THE INVARIANT METHOD (IM)

A. A brief review

The invariant method presented in a previous paper[8] can be used to calculate the integral (1). The method exploits the unitarity of the $\mathrm{U}(n)$ group elements,

$$\sum_{j=1}^{n} U_{ij}^{*}U_{lj}=\sum_{j=1}^{n} U_{ji}^{*}U_{jl}=\delta_{il}, \tag{4}$$

and the invariance of the Haar measure, in the form

$$\int (dU)\, f(U,U^{*})=\int (dU)\, f(U^{*},U)=\int (dU)\, f(U^{T},U^{*\,T})=\int (dU)\, f(VU,V^{*}U^{*})$$
$$=\int (dU)\, f(UV,U^{*}V^{*}), \tag{5}$$

for any function f and any $V\in \mathrm{U}(n)$.

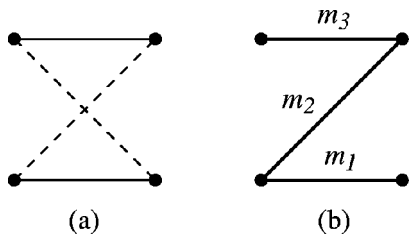

FIG. 1. Examples of U(n) integral diagrams. (a) The unique exchange integral for $p=2$; (b) a Z-integral with arbitrary multiplicities m_1, m_2, and m_3.

The unitarity relation (4) relates integrals of the same degree if $i \neq l$, and it relates integrals of degree p to integrals of degree $p-1$ if $i=l$. Other relations between integrals of the same degree can be obtained from (5), by suitable choices of V. Here are some of them discussed in the previous paper.[8]

(1) Using $V_{ij}=e^{i\phi}\delta_{ij}$, it follows that p must be equal to q in order to avoid the vanishing of integral (2). The number p will be called the *degree* of the integral.

(2) Using $V_{ij}=e^{i\phi_i}\delta_{ij}$, it follows that (2) is nonzero only when $K=I_M$ and $L=J_R$ for some $M,R\in S_p$. Using (3), and denoting RM^{-1} by Q, only integrals of the type

$$\langle IJ|IJ_Q\rangle=\int (dU)\, U^*_{IJ}\, U_{IJ_Q} \tag{6}$$

are nonzero, so from now on we need to consider only integrals of this type.

An integral with $J_Q=J$ will be called a *direct integral*. For such integrals we may always choose $Q=e$, the identity permutation. Otherwise, the integral is an *exchange integral*.

Integrals are represented diagrammatically as follows. Each distinct value in the index set I is represented by a dot on the left (L-dot), and each distinct value of the index set J or J_Q is represented by a dot on the right (R-dot). The factor U^*_{ij} is shown as a thin solid line between the L-dot i and the R-dot j, and the factor U_{ij} is shown as a dotted line between these two dots. The factor $U^*_{ij}U_{ij}$ is represented by a thick line, or more generally, the factor $U^{*m}_{ij}U^n_{ij}$ is represented by a thick line with a pair of numbers (m,n) written beside it. If $m=n$, then only a single number m is written. The numbers (m,n) or m will be known as the *multiplicities* of the line. See Fig. 1 for an illustration.

(3) With V chosen to be a permutation matrix of n objects, it follows that

$$\langle IJ|KL\rangle=\langle I'J|K'L\rangle=\langle IJ'|KL'\rangle,$$

where I' is obtained from I by a reassignment of the values of its indices, e.g., if $I=(334)$, then I' may be (558). K' is obtained from K by the *same* reassignment, and similarly for J' and L'. As a result, there is no need to know the values of the indices of the L-dots, nor the R-dots. This is why the dots in Fig. 1 are not labeled.

(4) As a consequence of the first two equalities in (5), an integral remains the same under the interchange of the solid lines with the dotted lines, or the L-dots with the R-dots.

(5) Using $V=R(ab)$, the rotation matrix in the (a,b) plane, a "spin-off relation" is obtained. Consider an R-dot imbedded in an arbitrary integral $M_0=\langle IJ|IJ_Q\rangle$, with d pairs of solid-dotted lines attached to the dot. Now spin off e pairs of these lines to create a new R-dot and a new integral. There are many ways to choose the e pair of lines, each possibly corresponds to a different integral. Let M_e be the sum of all these integrals. Then the quantities M_0 and M_e are related by the spin-off relation

$$M_e=M_0\binom{d}{e}, \tag{7}$$

where $\binom{e}{d}$ is the binomial coefficient. The relation is local in that it is independent of the structure of the rest of the diagram. The same relation can also be used to spin off an L-dot.

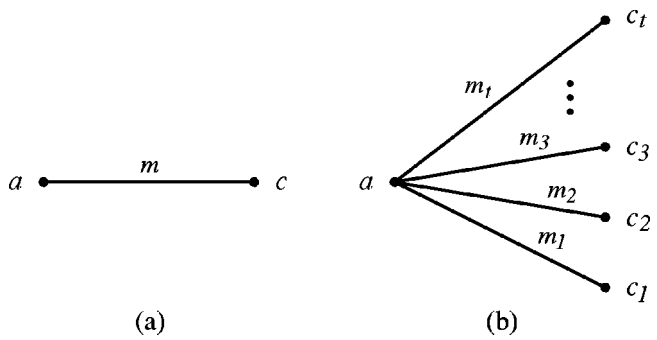

FIG. 2. The fan diagrams shown here can be a part of a larger diagram. In that case, there may be many more dots and many more lines in the complete diagram, provided none of the additional lines land on the R-dots shown. (a) A closed fan; (b) a partially opened fan. If all $m_i=1$, then it is said to be a fully opened fan, or just an opened fan.

In what follows, we summarize two general results obtained in the previous paper[8] using the IM.

1. The fan relation

The *fan relation*

$$\int (dU)\, A\, |U_{ac_1}|^{2m_1}\cdots|U_{ac_t}|^{2m_t} = \frac{\left(\prod_{j=1}^{t} m_j!\right)}{\left(\sum_{j=1}^{t} m_j\right)!} \int (dU)\, A\, |U_{ac}|^{2m} \tag{8}$$

relates integrals of the same $m=\Sigma_{j=1}^{t} m_j$, where A is an arbitrary product of matrix elements of U and U^* whose column indices are different from $c_1, c_2, \ldots, c_t$. The column index c on the right could be taken to be one of the c_i's.

Diagrammatically, the integral on the right of (8) is shown in Fig. 2(a), and the integral on the left is shown in Fig. 2(b). The additional lines and dots corresponding to the factor A are not shown, because they do not affect the spin-off relation. We shall refer to Fig. 2(a) as a *closed fan*, and Fig. 2(b) as a *partially opened fan*. If every $m_i=1$, then it will be said to be a *fully opened fan*, or simply an *opened fan*.

In particular, a closed fan integral is $m!$ times an opened fan integral. In fact, this relation between the two types of fans immediately gives rise to the relation (8) between a closed fan and a partially opened fan. To see it, note that each branch of a partially opened fan is itself a closed fan. By opening up all of them, we get the fully opened fan integral, multiplied by a multiplicity factor $\Pi_j m_j!$ from all the branches. Thus a closed fan is $m!/\Pi_j m_j!$ times a partially opened fan, as given by (8).

2. The Z-integral and the fan integral

In Ref. 8, we also obtained a general formula for integrals of the type shown in Fig. 1(b), for arbitrary non-negative integers m_1, m_2, and m_3. We call that the "Z-formula" because of the shape of the graph. It is

$$\begin{aligned} Z(m_1,m_2,m_3) &\equiv \int (dU)\, |U_{ij}|^{2m_1} |U_{il}|^{2m_2} |U_{kl}|^{2m_3} \\ &= \frac{m_1!\, m_2!\, m_3!\, (n-2)!(n-1)!\, (n+m_1+m_3-2)!}{(n+m_1-2)!\, (n+m_3-2)!\, (n+m_1+m_2+m_3-1)!}. \end{aligned} \tag{9}$$

In the special case where $m_2=m_3=0$, this becomes

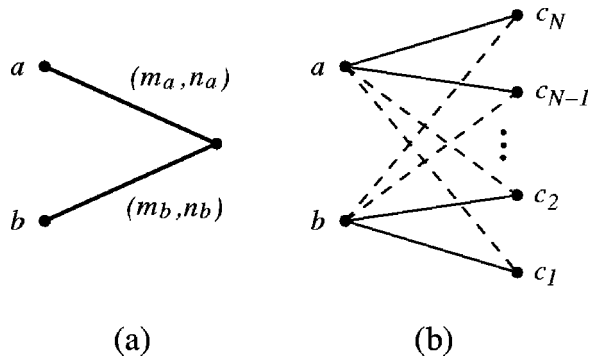

FIG. 3. Double-fan diagrams. (a) A closed diagram; (b) a fully opened diagram.

$$F(m) \equiv Z(m,0,0) = \frac{m!(n-1)!}{(n+m-1)!}, \tag{10}$$

which is the integral for Fig. 2(a) when there are no additional dots or lines around.

B. Double-fan relation

The fan relation can be generalized to a double-fan relation, connecting the closed ''double-fan'' diagram of Fig. 3(a) with a (fully) opened double-fan diagram such as Fig. 3(b). As in Fig. 2, there may be additional dots and lines in the integral, but none of them may end up on the R-dots shown. From that relation, we can also deduce relations between a closed double-fan and a partially opened double-fan, as done in the single-fan case.

The double-fan relation is considerably more complicated than the single-fan relation (8), because there are many more double-fan graphs. Each R-dot of a (fully) opened (double-fan) graph such as Fig. 3(b) falls into one of four *basic patterns*: $[A_a]$,$[A_b]$,$[B_a]$, and $[B_b]$, shown in Fig. 4. If the solid and dotted lines end up on the same L-dot, the pattern is a $[B]$; otherwise it is an $[A]$. The subscripts a and b tell us which L-dot the *solid* line emerges from.

Suppose there are α_i number of $[A_i]$ and β_i number of $[B_i]$ patterns in a (fully) opened (double-fan) graph. Then there are m_a solid and n_a dotted lines emerging from the L-dot a, and m_b solid and n_b dotted lines emerging from the L-dot b, where

$$\begin{aligned} m_a &= \alpha_a + \beta_a, \quad n_a = \alpha_b + \beta_a, \\ m_b &= \alpha_b + \beta_b, \quad n_b = \alpha_a + \beta_b. \end{aligned} \tag{11}$$

The total number of R-dots in the opened graph is $N = m_a + m_b = n_a + n_b$.

When these N R-dots are merged together, we get the closed (double-fan) graph depicted in Fig. 3(a), which will be denoted by $[(m_a n_a)(m_b n_b)]$. If $N=1$, this is just one of the four basic patterns discussed before. If $N>1$, we will call it a *compound pattern*.

From (11), we see that if we replace α_i and β_i by $\alpha_i' = \alpha_i + \xi$ and $\beta_i' = \beta_i - \xi$, with any integral ξ which keeps α_i' and β_i' non-negative, then we get the same closed graph by collapsing

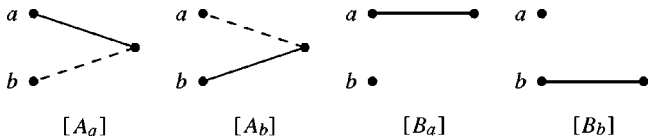

FIG. 4. The four basic patterns for the R-dots of a fully opened double-fan graph.

this new opened graph. Conversely, it will be shown in Appendix A that the closed graph $[(m_a n_a)(m_b n_b)]$ can be spinned off into a sum of several opened graphs, one for each (α_i', β_i'). The double-fan relation expressing that quantitatively is

$$[(m_a n_a)(m_b n_b)] = \sum v(\alpha_a' \alpha_b' \beta_a' \beta_b')\, [A_a]^{\alpha_a'} [A_b]^{\alpha_b'} [B_a]^{\beta_a'} [B_b]^{\beta_b'}$$

$$\equiv \sum [\alpha_a' A_a + \alpha_b' A_b + \beta_a' B_a + \beta_b' B_b], \tag{12}$$

where

$$v(\alpha_a' \alpha_b' \beta_a' \beta_b') = \frac{m_a!\, n_a!\, m_b!\, n_b!}{\alpha_a'!\, \alpha_b'!\, \beta_a'!\, \beta_b'!}, \tag{13}$$

and the sum is over all solutions $(\alpha_a', \alpha_b', \beta_a', \beta_b')$ of (11).

The double fan becomes a single fan if the L-dot b is not connected, namely, if $m_b = n_b = 0$ and $m_a = n_a \equiv m$. In that case (12) becomes

$$[m\, B_a] = m!\, [B_a]^m,$$

which is just (8) (when all $m_i = 1$) in another notation.

III. GROUP-THEORETICAL METHOD (GTM)

A. A brief review

Using group theory, the integral (6) can be turned into a multiple sum.[5,6] In the notation used in Appendix A of Ref. 8, the formula is

$$\langle IJ | IJ_Q \rangle = \sum_{R \in \mathcal{G}_I} \sum_{S \in \mathcal{G}_J} \sum_f \frac{d_f^2}{(p!)^2 \tilde{d}_f} \chi_f(SQR), \tag{14}$$

where p is the degree of the integral. The symbols $\mathcal{G}_I$ and $\mathcal{G}_J$ represent the symmetry groups of the row and column index sets. More precisely, $\mathcal{G}_X = \{P \in S_p | P(X) = X\}$, with X being either I or J. The irreducible representations of the symmetric and unitary groups are both labeled by a sequence $f = (f_1, f_2, \ldots, f_p)$, with $f_1 \geqslant f_2 \geqslant \cdots \geqslant f_p \geqslant 0$. $\chi_f(P)$ is the character of $P \in S_p$ in the irreducible representation with signature f. The dimension of the irreducible representation f is given by $d_f = \chi_f(e)$ for S_p, and by $\tilde{d}_f$ for U(n). A formula for $\tilde{d}_f$ is

$$\tilde{d}(f_1, \ldots, f_n) = \frac{D(f_1 + (n-1), f_2 + (n-2), \ldots, f_n)}{D(n-1, n-2, \ldots, 0)}, \tag{15}$$

where $D(x_1, \ldots, x_n)$ is the Vandermonde determinant given by $\Pi_{i<k}(x_i - x_k)$.

Since $\chi_f(g)$ depends only on the class c_g that g belongs to, we may write it as $\chi_f(c_g)$. With this notation, Eq. (14) can be rewritten as

$$\langle IJ | IJ_Q \rangle = \sum_c N[c]\, \xi[c], \tag{16}$$

where the sum is taken over all classes c of S_p,

$$N[c] = \sum_{R \in \mathcal{G}_I} \sum_{S \in \mathcal{G}_J} \delta(SQR \in c) \tag{17}$$

is the number of elements of the type SQR in the class c, and

$$\xi[c]=\sum_f \frac{d_f^2}{(p!)^2\tilde{d}_f}\chi_f(c). \tag{18}$$

It is not difficult to see that Q is not unique, because $Q'=SQ=QT$ for any $S\in\mathcal{G}_J$ and any $T\in\mathcal{G}_{J_Q}$ is another possible Q. It does not matter which Q we pick in (17). That equation can also be written as

$$N[c]=\sum_{R\in\mathcal{G}_I}\sum_{T\in\mathcal{G}_{J_Q}}\delta(QTR\in c). \tag{19}$$

It is straightforward but generally very tedious to compute $N[c]$, because we need to calculate the product QTR for every $T\in\mathcal{G}_{J_Q}$, every $R\in\mathcal{G}_I$, and determine what class c the product belongs to. Then we have to count up all the products that are in a given class c to get $N[c]$. However, the task becomes considerably more manageable if either $\mathcal{G}_I$ and $\mathcal{G}_{J_Q}$ are disjoint, or if one is contained in the other. We shall refer to integrals with those properties as *orderly*. Further simplification occurs for direct integrals, because in that case Q can always be chosen to be the identity e, so the triple product is reduced to a double product TR.

The calculation of $\xi[c]$ in (18) is simpler than the calculation of $N[c]$, but still we know of no closed form of it valid for every class c and every symmetric group S_p. The best we can do is to compute them case by case. Results are given in Sec. III C. Each $\xi[c]$ is actually an orderly integral with $\mathcal{G}_I=\mathcal{G}_J=e$, to be referred to as a *primitive integral*.

Other integrals can be computed in terms of the primitive integrals, if $N[c]$ is known. We shall discuss two orderly integrals for which $N[c]$ can easily be obtained. In Sec. III D, we discuss the *stack integrals*, which are direct integrals with $\mathcal{G}_I=\mathcal{G}_J$. In Sec. III E, we discuss the fully opened double-fan integrals of the type $[A_a]^\alpha[A_b]^\alpha$.

Relations between orderly integrals may be obtained without knowing the explicit values of $\xi[c]$, if their $N[c]$'s are related in a simple way. This is the case for the single-fan relation, and the double-fan relation with $n_a=m_b=0$ and $m_a=n_b=m$. They will be discussed in Sec. III B. However, general double-fan integrals are not orderly, so we cannot obtain the general double-fan relation by the group-theoretical method, at least not in the present way. We will also show that the closed (single-)fan *integral* can also be computed without explicitly knowing what $\xi[c]$ are. This is one of the very few cases where integrals can be obtained group-theoretically without explicitly knowing $\xi[c]$.

That leaves the nonorderly integrals, for which each term of the summand in (19) has to be calculated separately to get $N[c]$. The first nonorderly integral occurs in degree $p=3$. In Sec. III F, we shall show how to calculate some of the $p=3$ and $p=4$ nonorderly integrals.

B. Single-fan and simple double-fan relations

The single-fan integrals are orderly. The index sets for the closed fan Fig. 2(a) are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix}=\begin{pmatrix} 1 & \cdots & m & \cdots \\ a & \cdots & a & \cdots \\ c & \cdots & c & \\ c & \cdots & c & \end{pmatrix}. \tag{20}$$

The first row gives the index labels, and the next three rows give the values of the indices in the sets I,J, and J_Q, respectively. Different letters are understood to correspond to different values. Additional dots and lines may be present in the graph, as long as none of the lines end up in the R-dots shown. These additional lines and dots are not drawn because they do not affect the fan

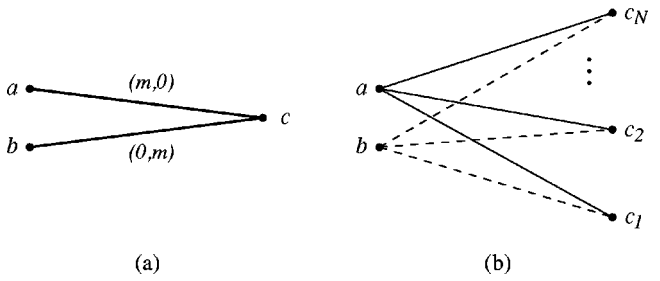

FIG. 5. Double-fan diagrams with $n_a=m_b=0$, and $m_a=n_b=m$. (a) A closed fan; (b) a fully opened fan.

relation in any way. Similarly, they are not shown in the index sets in (20) other than the ellipses in the first two rows, which remind us that there may be more lines connected to the L-dots. Such ellipses are absent in the last two rows because no additional lines are allowed to be connected to the R-dots shown.

Similarly, the index sets for the fully opened fan, Fig. 2(b) with all $m_i=1$, are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & \cdots & m & \cdots \\ a & \cdots & a & \cdots \\ c_1 & \cdots & c_m & \\ c_1 & \cdots & c_m & \end{pmatrix}. \tag{21}$$

Using S_m to denote the symmetric group for the permutation of the first m labels, the symmetric groups for Fig. 2(a) can be read off from (20) to be $\mathcal{G}_I \supset S_m$ and $\mathcal{G}_J=\mathcal{G}_{J_Q}=S_m$. Similarly, the symmetric groups for Fig. 2(b) can be read off from (21) to be $\mathcal{G}_I \supset S_m$ and $\mathcal{G}_J=\mathcal{G}_{J_Q}=e$. We may choose $Q=e$ in both cases. Then for Fig. 2(a), $T\mathcal{G}_I=\mathcal{G}_I$ for every $T\in\mathcal{G}_{J_Q}$, hence $N[c]=m!\Sigma_{R\in\mathcal{G}_I}\delta(R\in c)$. But the last sum is simply the $N[c]$ for Fig. 2(b) and (21). Hence it follows from (16) that the fan relation (with all $m_i=1$) is true.

Next, let us derive the double-fan relation (12) and (13) for the case $n_a=m_b=0$ and $m_a=n_b$. The solution of (11) is now unique. It gives $\alpha_a=m_a=n_b\equiv m$, and $\alpha_b=\beta_a=\beta_b=0$. The double-fan relation (12) then becomes

$$[m\,A_a]=m!\,[A_a]^m. \tag{22}$$

The closed double-fan is shown in Fig. 5(a). Its index sets are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & \cdots & m & \cdots & n & \ldots & n+m & \cdots \\ a & \cdots & a & \cdots & b & \cdots & b & \cdots \\ c & \cdots & c & & & & & \\ & & & & c & \cdots & c & \end{pmatrix}. \tag{23}$$

The opened double-fan is shown in Fig. 5(b). Its index sets are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & \cdots & m & \cdots & n & \ldots & n+m & \cdots \\ a & \cdots & a & \cdots & b & \cdots & b & \cdots \\ c_1 & \cdots & c_m & & & & & \\ & & & & c_1 & \cdots & c_m & \end{pmatrix}. \tag{24}$$

We may choose $Q=(1,n)(2,n+1)\cdots(m,n+m)$ in both cases. For (23), $\mathcal{G}_I \supset S_m \otimes S'_m$, $\mathcal{G}_J = S_m$, and $\mathcal{G}_{J_Q} = S'_m$, where S_m is the permutation group of the first m labels, and S'_m is the permutation group for the labels $(n,n+1,\ldots,n+m)$. For (24), $\mathcal{G}_I \supset S_m \otimes S'_m$, but $\mathcal{G}_J = \mathcal{G}_{J_Q} = e$.

For Fig. 5(a), $T\mathcal{G}_I = \mathcal{G}_I$ for every $T \in \mathcal{G}_{J_Q}$. Hence $N[c] = m! \Sigma_{T \in \mathcal{G}_I} \delta(QR \in c)$. But the last sum is simply the $N[c]$ of Fig. 5(b). In this way (22) is proven by the GTM.

The fan *integral* (10) can also be obtained from the GTM. It is given by Fig. 2(a) without extra dots and lines, or (20) without the ellipses at the end. Then $\mathcal{G}_I = S_m$, and $N[c] = m! \Sigma_R \delta(R \in c)$. From (16) and (18), we get

$$\langle IJ|IJ_Q\rangle \equiv F(m) = m! \sum_{R \in \mathcal{G}_I} \sum_f \frac{d_f^2}{(m!)^2 \tilde{d}_f} \chi_f(R) \tag{25}$$

$$= \frac{1}{m!} \sum_f \frac{d_f^2}{\tilde{d}_f} \sum_{R \in S_m} \chi_f(R)\ \chi^*_{(m)}(R) = \frac{d^2_{(m)}}{\tilde{d}_{(m)}} \tag{26}$$

$$= \frac{m!(n-1)!}{(m+n-1)!}. \tag{27}$$

In getting from (25) to (26), the character $\chi^*_{(m)}(R) = 1$ of the totally symmetric representation (m) of the permutation group has been inserted, and the orthogonality relation of the characters has been used. To get to (27), $d_{(m)} = \chi_{(m)}(e) = 1$ as well as $\tilde{d}_{(m)} = (m+n-1)!/(n-1)!m!$ (see (15)) have been used.

The result in (27) agrees with the result (10). It is one of the very few cases where the value of the integrals can be obtained group-theoretically without knowing the values of the individual $\xi[c]$'s.

C. Primitive integrals

Integrals in which both symmetry groups $\mathcal{G}_I$ and $\mathcal{G}_J$ consist only of the identity e will be called *primitive*. This happens when all the indices i_a in the set I assume distinct values, and all the indices j_b in the set J are also different. The corresponding diagrams have p dots each on both columns, and precisely one solid and one dotted lines connecting to each of the dots. The primitive diagrams for $p \leqslant 3$ are shown in Fig. 6, and the ones for $p = 4,5$ are contained in Appendix C.

Since $\mathcal{G}_I = \mathcal{G}_J = e$, it follows from (17) that $N[c] = \delta(Q \in c)$, where Q can be any element of S_p. The primitive integrals (16) are simply $\xi[c]$, one for each class c of S_p. We may therefore use an element of each cycle structure to label the primitive integrals, as is done in Fig. 6. Diagrammatically, the cycle structure is translated into the loop structure of its diagram, as can be seen in Fig. 6. Using (18) along with (15) and the character tables found in Appendix B (note that $d_f = \chi_f(e)$), the primitive integrals for $p \leqslant 3$ can be easily computed, and the results are displayed in Table I. The results for $p = 4,5$ can also be found in Table IV of Appendix C.

D. Stack integrals

The stack diagrams (see Fig. 7) are direct integrals made up of disconnected lines of arbitrary multiplicities. As such, $Q = e$, and J differs from I only by relabeling. Using item 3 of Sec. II B, we may assume $J = I$. Hence stack integrals are integrals of the form $\langle II|II\rangle$.

Let $p_1, p_2, \ldots, p_t$ be the multiplicities of the disconnected lines in a stack diagram. Then $\mathcal{G}_I = \mathcal{G}_J \equiv \mathcal{G} = S_{p_1} \otimes S_{p_2} \otimes \cdots \otimes S_{p_t}$, and $N[c]$ is nonzero only when the class c is a direct product of the classes c_i of the groups S_{p_i}. In that case,

$$N[c] = \prod_{i=1}^{t} p_i!\, n_i(c_i), \tag{28}$$

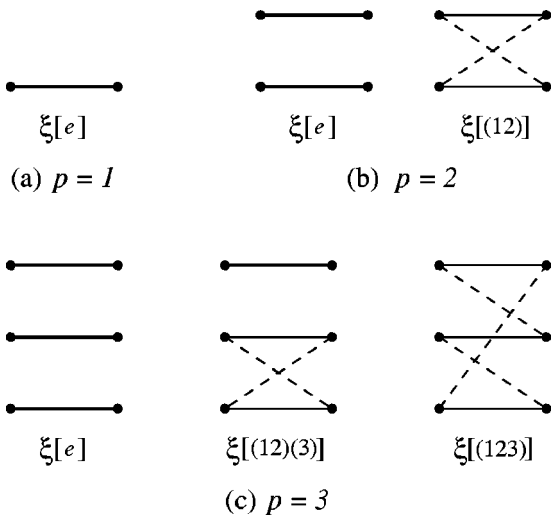

FIG. 6. Primitive diagrams for (a) $p=1$, (b) $p=2$, and (c) $p=3$. The identity element is everywhere denoted by e.

where $n_i(c_i)$ is the number of elements of S_{p_i} in the class c_i. In other words,

$$n_i(c_i)=\frac{p_i!}{\prod_{j=1}^{p_i} j^{\alpha_j}\alpha_j!}\ , \tag{29}$$

where the class c_i consists of α_j cycles of length j. Denoting the stack integral $\langle II|II\rangle$ by $\Xi(p_1,p_2,\ldots,p_t)$, we get

$$\Xi(p_1,p_2,\ldots,p_t)=\sum_{c_1,c_2,\ldots}\left(\prod_{i=1}^{t} p_i!\, n_i(c_i)\right)\xi(c_1\otimes c_2\otimes\cdots\otimes c_t). \tag{30}$$

All stack diagrams can be obtained by making the assignment $f_i\to p_i$ from each representation. In this way, we expect a same number of stack digrams as of primitive diagrams, or classes. Using the ξ expressions obtained in the preceding subsection, the stack integrals for $p\leqslant 3$ can be computed to yield the expressions in Table II.

E. Special double-fan integrals

The index sets for the fully opened double-fan integrals $[A_a]^\alpha[A_b]^\alpha$ (Fig. 3(b) with $N=2\alpha$) are

TABLE I. Algebraic expressions for the primitive diagrams of $p=1,2,3$.

		$\xi[c]$	
c	$p=1$	$p=2$	$p=3$
e	$\frac{1}{n}$	$\frac{1}{n^2-1}$	$\frac{n^2-2}{n(n^2-1)(n^2-4)}$
(12)		$\frac{-1}{n(n^2-1)}$	$\frac{-1}{(n^2-1)(n^2-4)}$
(123)			$\frac{2}{n(n^2-1)(n^2-4)}$

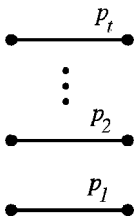

FIG. 7. Arbitrary stack diagram, $\Xi(p_1,p_2,\ldots,p_t)$, of degree $p=\Sigma_{i=1}^{t}p_i$.

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & \cdots & \alpha & \alpha+1 & \ldots & 2\alpha \\ b & \cdots & b & a & \cdots & a \\ c_1 & \cdots & c_\alpha & c_{\alpha+1} & \cdots & c_{2\alpha} \\ c_{\alpha+1} & \cdots & c_{2\alpha} & c_1 & \cdots & c_\alpha \end{pmatrix}. \tag{31}$$

Hence both $\mathcal{G}_J$ and $\mathcal{G}_{J_Q}$ consist only of the identity e. As for $\mathcal{G}_I$, it is given by $S_\alpha \otimes S_\alpha$, where the permutation groups S_α act respectively on the b and a indices in I. The element Q maps J_Q to J, i.e., $Q=(1,\alpha+1)(2,\alpha+2)\cdots(\alpha,2\alpha)$.

The fully opened integral can be computed using (16), with $N[c]$ given by (17) or (19). Thus,

$$N[c]=\sum_{R\in\mathcal{G}_I}\sum_{T\in\mathcal{G}_{J_Q}}\delta(QTR\in c)=\sum_{R\in\mathcal{G}_I}\delta(QR\in c) \quad = \quad \sum_{Q'}\delta(Q'\in c), \tag{32}$$

where the last sum is over *every* permutation Q' that sends *all* b indices in (31) to the positions labeled from $\alpha+1$ to 2α, and similarly *all* a indices to the positions labeled from 1 to α. As a consequence, the allowed cycles of Q' must be of even length, and they can be specified by a sequence of non-negative integers $(k)\equiv(k_1k_2\cdots k_\alpha)$, k_i being the number of cycles of length $2i$. The number of Q' with the class structure (k) that is related to c is given by

$$N[c]=\frac{(\alpha!)^2}{\prod_{i=1}^{\alpha} i^{k_i}\cdot k_i!}. \tag{33}$$

In order to see how this is arrived at, consider an example where $k_1=2$, $k_2=2$, and all other k_i values are zero. Then Q' is of the form $(ba)(ba)(baba)(baba)$, where the b and a letters should take the distinct index labels in $(1,\ldots,\alpha)$ and $(\alpha+1,\ldots,2\alpha)$, respectively. Another Q' with the same cycle structure can thus be obtained by permuting individually all the a and b labels. This accounts for the numerator in (33). However, such permutations do not necessarily give distinct Q' elements. The cyclic nature of a cycle tells us that each cycle of length $2i$ will appear i times; this accouts for the i^{k_i} factor in the denominator. Moreover, no new Q' is obtained if we permute cycles of the same length; that accounts for the other factor $k_i!$ in the denominator.

TABLE II. Algebraic expressions for the stack diagrams of $p=1$, 2, and 3.

$\Xi(p_1,\ldots,p_p)$	
$\Xi(1)=\frac{1}{n}$	$\Xi(3)=\frac{3!}{n(n+1)(n+2)}$
$\Xi(2)=\frac{2}{n(n+1)}$	$\Xi(2,1)=\frac{2}{(n-1)n(n+2)}$
$\Xi(1,1)=\frac{1}{n^2-1}$	$\Xi(1,1,1)=\frac{n^2-2}{n(n^2-1)(n^2-4)}$

TABLE III. Values of the monomial integrals $[A_a]^\alpha[A_b]^\alpha$ for $\alpha=1,2,3$.

α	$[A_a]^\alpha[A_b]^\alpha$
1	$\frac{-1}{n(n^2-1)}$
2	$\frac{2}{(n^2-1)n^2(n+2)(n+3)}$
3	$\frac{-6}{(n-1)n^2(n+1)^2(n+2)(n+3)(n+4)(n+5)}$

We may now return to (16) to calculate the integral $[A_a]^\alpha[A_b]^\alpha$ in terms of the primitive integrals $\xi[c]$. The results for the first few α values are listed in Table III.

F. Nonorderly integrals

All integrals with degree $p<3$ are orderly. The nonorderly integrals of $p=3$ are shown in Fig. 8, and those related to them by the fan relation (8). The calculation of $N[c]$ and the integral for each of them is discussed below. The integrals will be labeled by their figure, e.g., integral $I(8a)$.

The index sets for Fig. 8(a) are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ b & b & a \\ d & c & c \\ d & c & c \end{pmatrix}. \tag{34}$$

They give rise to the symmetry groups $\mathcal{G}_I=\{e,(12)\}$ and $\mathcal{G}_J=\mathcal{G}_{J_Q}=\{e,(23)\}$. Moreover, the element Q can be taken to be the identity element. In order to obtain the coefficients $N[c]$ of Eq. (16), we need to compute QTR for all $T\in\mathcal{G}_{J_Q}$ and $R\in\mathcal{G}_I$. That triple product is $Q\mathcal{G}_{J_Q}\mathcal{G}_I=\{e,(12),(23),(132)\}$. As a result,

$$I(8a)=Z(1,1,1)=\xi[e]+2\xi[(12)(3)]+\xi[(123)]=\frac{1}{(n^2-1)(n+2)}. \tag{35}$$

In the same way, the index sets of Fig. 8(b) are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ b & a & a \\ e & d & c \\ d & e & c \end{pmatrix}, \tag{36}$$

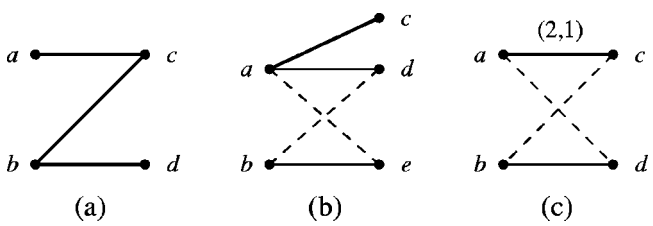

FIG. 8. Nonorderly integrals of $p=3$.

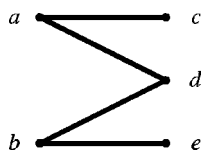

FIG. 9. Sigma integral with all lines being of multiplicity one.

and hence the symmetry groups are $\mathcal{G}_{J_Q}=\{e\}$ and $\mathcal{G}_I=\{e,(23)\}$, and the exchange element is $Q=(12)$. We thus obtain $Q\mathcal{G}_{J_Q}\mathcal{G}_I=\{(12),(123)\}$, from which

$$I(8b)=\xi[(12)(3)]+\xi[(123)]=\frac{-1}{(n^2-1)n(n+2)} \tag{37}$$

follows.

Finally, for Fig. 8(c), the index sets are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix}=\begin{pmatrix} 1 & 2 & 3 \\ b & a & a \\ d & c & c \\ c & d & c \end{pmatrix}. \tag{38}$$

The relevant symmetry groups are $\mathcal{G}_{J_Q}=\{e,(13)\}$ and $\mathcal{G}_I=\{e,(23)\}$. With $Q=(12)$, the set $Q\mathcal{G}_{J_Q}\mathcal{G}_I$ is {(12), (13), (123), (132)}, and formula (16) gives

$$I(8c)=2(\xi[(12)(3)]+\xi[(123)])=\frac{-2}{(n^2-1)n(n+2)}. \tag{39}$$

The calculation of $Q\mathcal{G}_{J_Q}\mathcal{G}_I$ is not that cumbersome for $p=3$, but it gets worse pretty quickly as p increases. For example, let us look at some examples of $p=4$.

Let us first calculate $Z(2,1,1)$ of Fig. 1(b), whose index sets are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix}=\begin{pmatrix} 1 & 2 & 3 & 4 \\ b & b & b & a \\ d & d & c & c \\ d & d & c & c \end{pmatrix}. \tag{40}$$

Then $Q=e$, $\mathcal{G}_{J_Q}=\{e,(12),(34),(12)(34)\}$ and $\mathcal{G}_I=\{e,(12),(13),(23),(123),(132)\}$. Thus $Q\mathcal{G}_{J_Q}\mathcal{G}_I=\{e,(12),(13),(23),(123),(132),(12),e,(132),(123),(23),(13),(34),(12)(34),(143),(243),(1243),(1432),(12)(34),(34),(1432),(1243),(243),(143)\}$, hence

$$\begin{aligned} Z(2,1,1)&=2\xi[e]+8\xi[(12)(3)(4)]+8\xi[(123)(4)]+2\xi[(12)(34)]+4\xi[(1234)] \\ &=\frac{2}{(n-1)n(n+2)(n+3)}. \end{aligned} \tag{41}$$

Our last example is the Σ-integral, shown in Fig. 9. Its index sets are

$$\begin{pmatrix} label \\ I \\ J \\ J_Q \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ b & b & a & a \\ e & d & d & c \\ e & d & d & c \end{pmatrix}. \tag{42}$$

Hence $Q=e$, $\mathcal{G}_{J_Q}=\{e,(23)\}$ and $\mathcal{G}_I=\{e,(12),(34),(12)(34)\}$. Multiplying such elements accordingly, the set $\{e,(12),(34),(12)(34),(23),(132),(234),(1342)\}$ is obtained for $Q\mathcal{G}_{J_Q}\mathcal{G}_I$. Hence

$$\begin{aligned} \Sigma &= \xi[e]+3\xi[(12)(3)(4)]+2\xi[(123)(4)]+\xi[(12)(34)]+\xi[(1234)] \\ &= \frac{n+1}{(n-1)n^2(n+2)(n+3)}. \end{aligned} \tag{43}$$

IV. COMPARISON OF THE IM AND THE GTM

We have discussed the computation of U(n) integrals (2) in two ways: the IM in Sec. II, and the GTM in Sec. III. Each of these two methods has its own merits, and drawbacks, and in a way they complement each other. The purpose of this section is to compare their relative stong and weak points.

The IM is based solely on the unitarity condition (4) and the invariance of the Haar Measure (5). The method is simple because there is no need to know group theory. The conditions relate integrals of the same degree, and also integrals of degree p to integrals of degree $p-1$. Through these relations, specific integrals such as the fan integrals (10) and the Z-integrals (9) can be obtained, and the general relation such as the single-fan relation (8) and the double-fan relation (12) can be worked out.

The GTM has the advantage of being general, in the sense that all integrals can be computed using the formula (14) or (16). The price to pay is that we have to know the characters of the irreducible representations of the appropriate symmetric group, and a triple sum has to be carried out, which can prove to be very tedious for integrals of high degrees. Furthermore, unlike the IM, relations between integrals are hard to come by, so one must calculate the integrals one by one. There are however certain classes of integrals, the orderly integrals, for which relations can be developed, and the quantity $N[c]$ in (16) can be relatively easily computed. Then we merely have to know the primitive integrals $\xi[c]$ in (16) to get the value of the orderly integral on hand. The stack integrals (30) and the special opened double-fan integrals (33) are examples of this kind. The primitive integrals $\xi[c]$ themselves must be calculated using (18).

To summarize, the IM gives a huge number of relations but it is not easy to obtain the value of any specific integral. The GTM allows us to calculate any specific integral, albeit rather tedious at times, but it is difficult to obtain relations between integrals. In the next section, we shall discuss a *hybrid method* which makes use of the advantages of both methods. We shall use the general GTM formula to calculate a specific set of integrals, and then use the IM relations to obtain all the other integrals.

In the rest of this section, we shall enlarge these general remarks about the IM and GTM, by using specific examples presented in the last two sections as concrete illustrations.

The single-fan relation (8) can be obtained by both the IM and the GTM. However the double-fan relation (12) in its general form can be obtained only by the IM, because most of the integrals involved are not orderly, making it hard to derive relations using the GTM. Nevertheless, in special cases involving only orderly integrals, (22), the GTM can also be used to derive the relation.

The Z-formula (9) is obtained using the IM, by a series of relations connecting it down to $\int dU=1$. Since the Z-integrals are not orderly, it is hard to compute them using the GTM except at low degrees. The calculation of those by the GTM is shown in Eqs. (35) and (41).

However, since the values of the integrals in the IM are obtained only through relations, it may be relatively complicated to calculate just one specific integral. This is where the GTM is

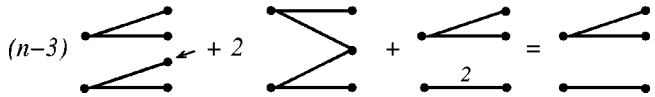

FIG. 10. Unitarity sum relation involving the Σ diagram (second from the left). The sum is performed on the index indicated by an arrow. Using the fan relation (8), the unitary sum can be written as $([(n-3)/4]+\frac{1}{2})Z(2,0,2)+2\Sigma=\frac{1}{2}Z(2,0,1)$.

superior, because of the general formula (14) valid for any one integral. For example, it is easy to obtain the Σ integral (43), assuming of course the $\xi[c]$'s to be already known. We can also obtain it using the IM, as we shall show below, but that involves a few steps because we must get it from relations. To see how that is done, look at Fig. 10, which is the unitarity relation applied to the dot of the first diagram indicated by an arrow. The first and third diagrams can be related to $Z(2,0,2)$ by using the fan relation (8), and similarly the diagram on the right can be related to $Z(2,0,1)$. Using the Z-formula (9), we then obtain

$$\Sigma=\frac{1}{4}\left[Z(2,0,1)-\left(\frac{n-3}{2}+1\right)Z(2,0,2)\right]=\frac{n+1}{(n-1)n^2(n+2)(n+3)}, \tag{44}$$

the same as the result (43) obtained by the GTM.

V. HYBRID METHOD

Having understood the relative merits of the GTM and the IM, it is possible to combine their strengths into a more efficient hybrid calculational scheme.

The strategy is to start with one or more integrals that can be computed by the GTM with relative ease. Generally speaking, such integrals are ordered. Once they are obtained, the many relations of the IM can be used to calculate other integrals from them.

To illustrate this strategy, we will consider how the hybrid method can be used to calculate all double-fan integrals.

By a double-fan integral, we mean any integral with two L-dots and any number of R-dots. Figure 3(a) shows a closed (double-fan) integral (with the understanding that there are no extra dots or lines than those shown), and Fig. 3(b) shows a fully opened (double-fan) integral. We may also have partially opened (double-fan) integrals, in which every branch, namely, every R-dot with its connecting lines, can be regarded as a closed integral. See Fig. 11 for an example of a partially opened integral.

As in Sec. II B, a fully opened integral is denoted by $[A_a]^{\alpha_a}[A_b]^{\alpha_b}[B_a]^{\beta_a}[B_b]^{\beta_b}$, and its corresponding closed integral is denoted by $[\alpha_a A_a+\alpha_b A_b+\beta_a B_a+\beta_b B_b]$. For a partially opened integral, we will denote it as a product of the closed integrals of each branch. See Fig. 11 for examples.

Using (12) and (13), all double-fan integrals can be expressed as sums of fully opened integrals. Integrals of the form $[A_a]^{\alpha}[A_b]^{\alpha}$ are given by (33) and Table III, but we still have to

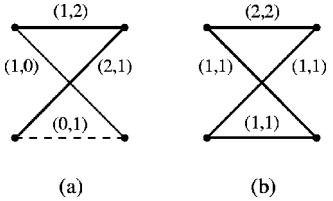

FIG. 11. Partially opened double-fan integrals. (a) There are two equivalent forms for this graph: $[A_a+2A_b][A_a]$ and $[A_b+B_a+B_b][A_a]$. (b) There are four equivalent forms for this graph: $[A_a+A_b+B_a][A_a+A_b]$, $[2B_a+B_b][A_a+A_b]$, $[A_a+A_b+B_a][B_a+B_b]$, $[2B_a+B_b][B_a+B_b]$.

know how to calculate a fully opened integral when $\beta_i \neq 0$. As shown in Appendix D, the IM allows us to relate them to those with $\beta_i = 0$, by using the following formula:

$$[A_a]^\alpha [A_b]^\alpha [B_a]^{\beta_a} [B_b]^{\beta_b} = \sum_{e=0}^{\min(\beta_a,\beta_b)} \left\{ (-1)^e e! \binom{\beta_a}{e} \binom{\beta_b}{e} (n+2\alpha-1+2e) \cdot \frac{(n+2\alpha-2+e)!\,(n+2\alpha-1+2e)!}{(n+2\alpha+\beta_a-1+e)!\,(n+2\alpha+\beta_b-1+e)!} [A_a]^{\alpha+e} [A_b]^{\alpha+e} \right\}. \tag{45}$$

We close this section by showing how to use (12) and (13) to calculate the integrals in Fig. 11.

A. Figure 11(a)

There are two equivalent forms for this diagram. One is

$$[A_a + 2A_b][A_a] = (2[A_a][A_b]^2)[A_a] = 2[A_a]^2[A_b]^2 \tag{46}$$

and the other is

$$[A_b + B_a + B_b][A_a] = 4([A_b][B_a][B_b])[A_a] = 4[A_a][A_b][B_a][B_b], \tag{47}$$

where Eqs. (12) and (13) have been used. The integral $I(11a)$ is obtained by adding up (46) and (47).

Using (45), we can express all fully opened integrals in the form $[A_a]^\alpha [A_b]^\alpha$. Applying this to the present case, we get

$$[A_a][A_b][B_a][B_b] = \frac{1}{(n+2)^2}[A_a][A_b] - \frac{1}{(n+2)}[A_a]^2[A_b]^2. \tag{48}$$

Using Table III, we finally obtain

$$I(11a) = 2[A_a]^2[A_b]^2 + 4[A_a][A_b][B_a][B_b] = \frac{2n}{(n+2)}[A_a]^2[A_b]^2 + \frac{4}{(n+2)^2}[A_a][A_b] = \frac{-4}{(n^2-1)n(n+2)(n+3)}.$$

B. Figure 11(b)

As shown in Fig. 11(b), $I(11b)$ has four equivalent forms. For one branch, the factors are

$$[A_a + A_b + B_a] = 4\,[A_a][A_b][B_a],$$
$$[2B_a + B_b] = 2\,[B_a]^2[B_b], \tag{49}$$

and for the other branch, they are

$$[A_a + A_b] = [A_a][A_b],$$
$$[B_a + B_b] = [B_a][B_b]. \tag{50}$$

Hence

$$I(11b) = 4\,[A_a]^2[A_b]^2[B_a] + 6\,[A_a][A_b][B_a]^2[B_b] + 2\,[B_a]^3[B_b]^2. \tag{51}$$

We will now express each of the three monomial integrals in (51) in terms of $[A_a]^\alpha[A_b]^\alpha$. First, with respect to (45), $[A_a]^2[A_b]^2[B_a]$ is characterized by $\alpha=2$, $\beta_a=1$, and $\beta_b=0$. The vanishing of β_b causes (45) to consist of the single term

$$[A_a]^2[A_b]^2[B_a]=\frac{1}{(n+4)}[A_a]^2[A_b]^2. \tag{52}$$

Second, $[A_a][A_b][B_a]^2[B_b]$ has $\alpha=1$, $\beta_a=2$, $\beta_b=1$, and the sum in (45) gives

$$[A_a][A_b][B_a]^2[B_b]=\frac{1}{(n+2)^2(n+3)}[A_a][A_b]-\frac{2}{(n+2)(n+4)}[A_a]^2[A_b]^2. \tag{53}$$

Finally, $[B_a]^3[B_b]^2$, having $\alpha=0$, $\beta_a=3$, $\beta_b=2$, can be expressed as

$$[B_a]^3[B_b]^2=\frac{1}{n^2(n+1)^2(n+2)}-\frac{6}{n(n+2)^2(n+3)}[A_a][A_b]+\frac{6}{(n+1)(n+2)(n+4)}[A_a]^2[A_b]^2 \tag{54}$$

from Eq. (45). Using the fan relation, notice that $[B_a]^3[B_b]^2$ can also be reduced to $(1/3!)\times(1/2!)\,Z(3,0,2)$.

The expressions of $[A_a][A_b]$ and $[A_a]^2[A_b]^2$ in terms of n have already been determined in Example 1. The final answer is obtained by inserting (52)–(54) into (51). The result is

$$\begin{aligned}[A_a+A_b+B_a][A_a+A_b]&=\frac{2}{n^2(n+1)^2(n+2)}+\frac{6(n-2)}{n(n+2)^2(n+3)}[A_a][A_b]\\&\quad+\frac{4(n^2+2)}{(n+1)(n+2)(n+4)}[A_a]^2[A_b]^2\\&=\frac{2(n^2+2n+4)}{(n^2-1)n^2(n+2)(n+3)(n+4)},\end{aligned}$$

which can be verified using the plain group theoretical formula (14).

VI. CONCLUSION

In this article, we have pursued the goal of finding an efficient method to calculate the monomial integral (1) or (2). We find that the IM discussed in Sec. II is superior for deriving relations between integrals, but the GTM is able to give a formula to calculate any integral. The GTM formula involves a triple sum whose computation is often tedious and prone to mistakes. The sums simplify for orderly integrals, in which the invariant groups $\mathcal{G}_I$ and $\mathcal{G}_{J_Q}$ are either disjoint, or one is contained in the other. For nonorderly integrals, the hybrid method is probably the most efficient. It uses the IM to relate them to some orderly integrals that can be calculated by the GTM with relative ease.

ACKNOWLEDGMENTS

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APPENDIX A: DERIVATION OF EQUATIONS (12) AND (13)

To prove (12) and (13), we use the rotation technique discussed in item 5 of Sec. II A, and Eq. (7), to spin off from the R-dot of Fig. 3(a) a new R-dot attached to a pair of solid-dotted lines. Depending on whether the basic pattern of this new R-dot is $[A_a]$, $[A_b]$, $[B_a]$, or $[B_b]$, we get the graphs shown in Figs. 12(a), 12(b), 12(c), and 12(d), respectively.

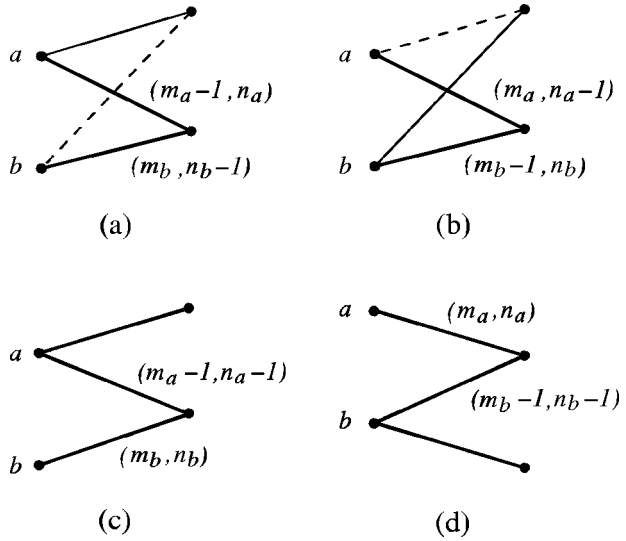

FIG. 12. Diagrams that result from rotating away the pairs of lines (a) $[A_a]$, (b) $[A_b]$, (c) $[B_a]$, and (d) $[B_b]$, from the compound pattern of Fig. 3.

Repeating this spin-off operation over and over again on the R-dot still containing a compound pattern, eventually we come to a graph where every R-dot is given by a basic pattern. The resulting integrals are given in (12), corresponding to the decompositions of the compound pattern into a sum of all possible fully opened integrals obtained by spinning off.

The coefficient $v(\alpha'_a\alpha'_b\beta'_a\beta'_b)$ of these basic integrals is derived from a combination of three factors:

(1) Each time that we spin off a basic pattern from a compound pattern with d pairs of solid-dotted lines, there is a factor $1/d$ arising from Eq. (7), by taking $e=1$. Since we start from a compound pattern with N pairs of lines, by the time we come to a fully-opened pattern we have accumulated a factor $1/N!$.
(2) The N R-dots in the final pattern that is fully opened can be spinned off in a different sequential order. According to (7), they must be summed over. This gives rise to a factor $N!/\alpha'_a!\alpha'_b!\beta'_a!\beta'_b!$.
(3) At any time when we spin off a basic pattern, we can choose its single pair of solid-dotted lines in all possible ways. Equation (7) says that we must sum over all these possibilities. The mulitipliciy factor is given by the number of permutations of these lines that lead back to the same basic integral. It is a factor of $m_a!\, m_b!\, n_a!\, n_b!$.

Assembling these three factors, we get

$$v(\alpha'_a\alpha'_b\beta'_a\beta'_b)=\frac{m_a!\, m_b!\, n_a!\, n_b!}{\alpha'_a!\alpha'_b!\beta'_a!\beta'_b!}, \tag{A1}$$

which is identical to (13).

APPENDIX B: CHARACTER TABLES

The character tables for $p=2,3$ are given here in the form used by Hamermesh in Ref. 9. The rows are labeled by the partitions that define the representations, and the columns are labeled by the cycle structures that define the classes. The number of elements in each class, $n(c)$, is written above the classes. The table for $p=1$ is trivial, and it consists of the sole value 1.

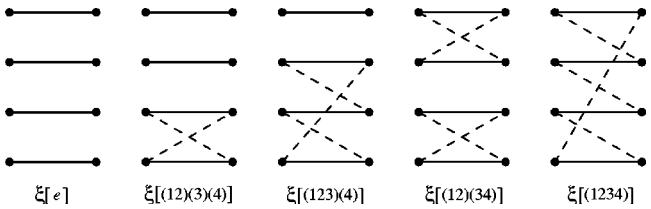

FIG. 13. The $p=4$ primitive diagrams.

1. $p=2$

Part.\Class	1 (1^2)	1 (2)
(2)	1	1
(1^2)	1	-1

2. $p=3$

Part.\Class	1 (1^3)	3 (1,2)	2 (3)
(3)	1	1	1
(2,1)	2	0	-1
(1^3)	1	-1	1

APPENDIX C: PRIMITIVE DIAGRAMS FOR $p=4$ AND $p=5$

Using (14) and the character tables for S_4 and S_5,[9] the algebraic expressions for the primitive diagrams of Fig. 13 and Fig. 14 can be obtained, and they are given in Table IV.

APPENDIX D: DERIVATION OF EQUATION (45)

We would like to express the general fully-opened integral $[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b}$ in terms of the special ones of the form $[A_a]^{\alpha'}[A_b]^{\alpha'}$. The idea is to apply a unitarity sum on the $[B_a]$ or $[B_b]$ basic patterns to get rid of them. To get the final result we also need to apply the fan relation (8) or the double-fan relations (12) and (13). Our approach is to first determine how can

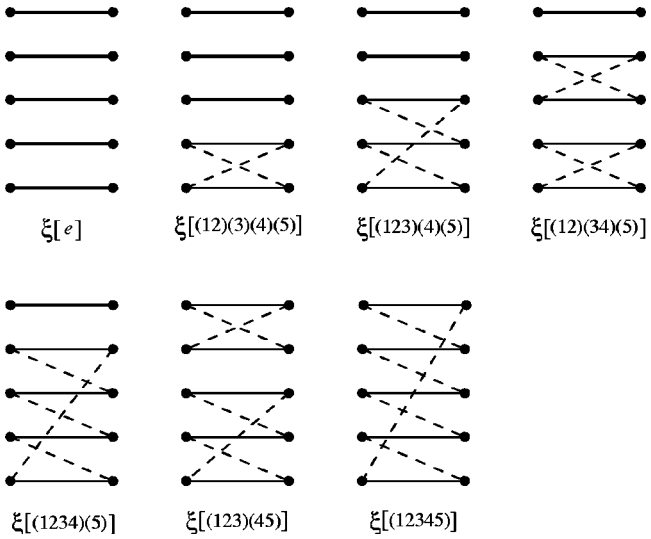

FIG. 14. The $p=5$ primitive diagrams.

TABLE IV. Algebraic expressions for the primitive diagrams of fourth and fifth degrees. In the $p=5$ case, the elements from row two to row five should be written with the additional (5) one-cycle.

	$\xi(c_Q)$	
Q	$p=4$	$p=5$
e	$\frac{n^4-8n^2+6}{n^2(n^2-1)(n^2-4)(n^2-9)}$	$\frac{n^4-20n^2+78}{n(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$
(12)(3)(4)	$\frac{-1}{n(n^2-1)(n^2-9)}$	$\frac{-(n^2-2)(n^2-12)}{n^2(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$
(123)(4)	$\frac{2n^2-3}{n^2(n^2-1)(n^2-4)(n^2-9)}$	$\frac{2}{n(n^2-1)(n^2-4)(n^2-16)}$
(12)(34)	$\frac{n^2+6}{n^2(n^2-1)(n^2-4)(n^2-9)}$	$\frac{n^2-2}{n(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$
(1234)	$\frac{-5}{n(n^2-1)(n^2-4)(n^2-9)}$	$\frac{-5n^2+24}{n^2(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$
(123)(45)		$\frac{-2(n^2+12)}{n^2(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$
(12345)		$\frac{14}{n(n^2-1)(n^2-4)(n^2-9)(n^2-16)}$

$[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}$ be reduced to fully opened integrals involving only the $[A_a]$ and $[A_b]$ patterns. With such an information at hand, we will then try to reduce the more general $[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}[B_b]^{\beta_b}$ integrals into the $[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}$ integrals.

Let us apply a unitarity sum on one of the $[B_a]$ patterns in $[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}$:

$$\begin{aligned}(n-(2\alpha+\beta_a-1))\,[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}+(\beta_a-1)\,[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a-2}[2B_a]\\ +\ \alpha([A_a]^\alpha[A_b]^{\alpha-1}[A_b+B_a][B_a]^{\beta_a-1}+[A_a]^{\alpha-1}[A_a+B_a][A_b]^\alpha[B_a]^{\beta_a-1})\\ =[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a-1}.\end{aligned} \tag{D1}$$

Using (8), $[2B_a]$, in the second term above, can be rewritten as $2[B_a]^2$. Furthermore, Eq. (13) tells us that $[A_b+B_a]$ and $[A_a+B_a]$ can, respectively, be rewritten as $2[A_b][B_a]$ and $2[A_a]\times[B_a]$, and the term in parentheses above simplifies to $4[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}$. As a result, relation (D1) reduces to

$$[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}=\frac{1}{n+2\alpha+\beta_a-1}[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a-1}. \tag{D2}$$

Using the relation (D2) recursively on its right-side, until no $[B_a]$ remains, we obtain

$$\begin{aligned}[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}&=\frac{1}{(n+2\alpha+\beta_a-1)}\,\frac{1}{(n+2\alpha+\beta_a-2)}\cdots\frac{1}{(n+2\alpha)}[A_a]^\alpha[A_b]^\alpha\\ &=\frac{(n+2\alpha-1)!}{(n+2\alpha+\beta_a-1)!}[A_a]^\alpha[A_b]^\alpha,\end{aligned} \tag{D3}$$

and the first step of the work is completed.

Assuming that $\beta_b\leqslant\beta_a$, let us perform a unitarity sum on a $[B_b]$ pattern in $[A_a]^\alpha[A_b]^\alpha[B_a]^{\beta_a}[B_b]^{\beta_b}$:

$$(n-(2\alpha+\beta_a+\beta_b-1))\,[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b}+(\beta_b-1)\,[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b-2}[2B_b]$$
$$+\beta_a\,[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a-1}[B_a+B_b][B_b]^{\beta_b-1}+\alpha([A_a]^{\alpha}[A_b]^{\alpha-1}[A_b+B_b][B_a]^{\beta_a}[B_b]^{\beta_b-1}$$
$$+\;[A_a]^{\alpha-1}[A_a+B_b][A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b-1})=[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b-1}. \tag{D4}$$

Relation (8), or formula (13), again permits us to make some simplifications, i.e., $[2B_b]=2[B_b]^2$, $[B_a+B_b]=[A_a][A_b]+[B_a][B_b]$, $[A_b+B_b]=2[A_b][B_b]$, $[A_a+B_b]=2[A_a][B_b]$. By making the proper substitutions in (D4), the recursion equation,

$$[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b}=\frac{1}{(n+2\alpha+\beta_b-1)}\{[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b-1}$$
$$-\;\beta_a[A_a]^{\alpha+1}[A_b]^{\alpha+1}[B_a]^{\beta_a-1}[B_b]^{\beta_b-1}\},$$

results. The above can be solved to give

$$[A_a]^{\alpha}[A_b]^{\alpha}[B_a]^{\beta_a}[B_b]^{\beta_b}=\sum_{e=0}^{\beta_b}\left\{(-1)^e e!\binom{\beta_a}{e}\binom{\beta_b}{e}(n+2\alpha-1+2e)\right.$$
$$\left.\cdot\,\frac{(n+2\alpha-2+e)!}{(n+2\alpha+\beta_b-1+e)!}[A_a]^{\alpha+e}[A_b]^{\alpha+e}[B_a]^{\beta_a-e}\right\},$$

which upon substitution of (D3) yields the desired Eq. (45).

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SLE-type growth processes and the Yang–Lee singularity

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The recently introduced SLE growth processes are based on conformal maps from an open and simply connected subset of the upper half-plane to the half-plane itself. We generalize this by considering a hierarchy of stochastic evolutions mapping open and simply connected subsets of smaller and smaller fractions of the upper half-plane to these fractions themselves. The evolutions are all driven by one-dimensional Brownian motion. Ordinary chordal SLE appears at grade one in the hierarchy. At grade two we find a direct correspondence to conformal field theory through the explicit construction of a level-four null vector in a highest-weight module of the Virasoro algebra. This conformal field theory has central charge $c=-22/5$ and is associated with the Yang–Lee singularity. Our construction may thus offer a novel description of this statistical model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765747]

I. INTRODUCTION

A new approach to the description of conformal field theories (CFTs) in two dimensions has recently appeared where instead of discussing objects in terms of local fields and their fusions, one is rather interested in a description based on spatially extended quantities defined through geometry. The differential equations of the stochastic Löwner evolution (SLE) have emerged as a mathematically precise way of describing certain CFTs directly in the continuum, without reference to an underlying lattice.

The chordal SLE processes are constructed through conformal maps from a subset of the upper half-plane onto the half-plane itself. The processes are driven by the random one-dimensional Brownian motion. Properties thereby described have an intrinsic geometrical nature.

The study of these stochastic evolutions or growth processes was initiated by Schramm[1] and has been pursued further in Refs. 2–10, for example. A review for physicists may be found in Ref. 11, while Ref. 12 contains a mathematical introduction.

An explicit relationship between SLE and CFT has been elucidated recently[13,14] by considering random walks on the Virasoro group. The link is found through a singular vector at level two in highest-weight modules. The kernel of the vector corresponds to conserved quantities under the random process.

Although the correspondence exists, the number of CFTs having geometrical properties described by SLE is still very limited. Furthermore, there is no apparent pattern assisting in the identification of these new descriptions of field theories.

The aim of the present work is to show that there might be conformal systems described by generalizations of SLE. The approach of Bauer and Bernard[13,14] may be extended to more general walks than the one generating SLE. A particular class of extensions corresponds to a hierarchy of stochastic evolutions in which SLE appears at grade one. These growth processes are associated to conformal maps of open and simply connected subsets of smaller and smaller fractions of the upper half-plane onto the fractions themselves, and are all driven by one-dimensional Brownian motion. Using two-sided Brownian motion the stochastic processes may be extended to also

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describing flows from fractions of the upper half-plane to subsets thereof. At grade two in the hierarchy we find a link to the Yang–Lee singularity through the construction of a level-four null vector. This in turn potentially offers a new geometrical description of that statistical model.

II. STOCHASTIC EVOLUTIONS

A. Stochastic Löwner evolution

Let Y_t be a real-valued continuous function, $t \geqslant 0$. For each element in the upper half-plane, $z \in \mathbb{H}$, we consider the solution $g_t(z)$ to Löwner's differential equation

$$\partial_t g_t(z) = \frac{2}{g_t(z) - Y_t}, \quad g_0(z) = z. \tag{1}$$

The factor 2 is conventional but could be changed by renormalization. Let $\tau = \tau(z)$ denote the time such that the solution $g_t(z)$ exists for all $t \in [0,\tau]$, while for increasing time $\lim_{t\to\tau} g_t(z) = Y_\tau$. Following Refs. 1, 8, and 12, one may define the evolving hull K_t as the closure of $\{z \in \mathbb{H}: \tau(z) \leqslant t\}$. In time, it is an increasing sequence of compact sets. As a conformal map from the simply connected domain $\mathbb{H}\backslash K_t$ onto the open half-plane $\mathbb{H}$, g_t is uniquely determined by the so-called hydrodynamic normalization at infinity:

$$\lim_{z\to\infty} (g_t(z) - z) = 0. \tag{2}$$

Stochastic Löwner evolutions are growth processes defined by choosing standard one-dimensional (and one-sided) Brownian motion, B_t, as the driving function: $Y_t = \sqrt{\kappa} B_t$, with $B_0 = 0$. The parameter κ characterizes the process which is denoted SLE_κ. For $t,s \geqslant 0$, the expectation value is normalized as $\mathbf{E}[(\sqrt{\kappa}B_t)(\sqrt{\kappa}B_s)] = \kappa \min(t,s)$.

One defines the function

$$f_t(z) := g_t(z) - Y_t. \tag{3}$$

It follows that it satisfies the differential equation

$$\partial_t f_t(z) = \frac{2}{f_t(z)} - \partial_t Y_t, \quad f_0(z) = z. \tag{4}$$

When Y_t denotes Brownian motion its time derivative is thought of as white noise: $dB_t/dt \sim W_t$. The inverse of the function f_t is related to the inverse of the SLE map: $f_t^{-1}(z) = g_t^{-1}(z + Y_t)$. The trace γ of SLE is then defined by

$$\gamma(t) := \lim_{z\to 0} f_t^{-1}(z). \tag{5}$$

By construction, z is an element of $\mathbb{H}$, so the limit is taken from the upper half-plane only. The nature of the trace is known to depend radically on κ (Ref. 8): for $0 \leqslant \kappa \leqslant 4$ it is a simple curve, for $4 < \kappa < 8$ a self-intersecting curve, whereas for $8 < \kappa$ it is space filling. The Hausdorff dimension of the SLE_κ trace is discussed in Refs. 8, 15, 16.

B. Hierarchy of stochastic evolutions

For positive integer n, we define the open subset of $\mathbb{H}$,

$$\mathbb{H}_n = \{z \in \mathbb{H}: z = re^{i\theta};\ r \in \mathbb{R}_>;\ 0 < \theta < \pi/n\}. \tag{6}$$

Note that $\mathbb{H}_1$ is the upper half-plane itself. We now introduce a hierarchy of Löwner-type differential equations whose solutions have properties similar to the SLE maps. For positive integer n we define the differential equation

$$\partial_t g_t(z) = \frac{2}{g_t^{n-1}(z)(g_t^n(z) - Y_t)}, \quad g_0(z) = z \tag{7}$$

with $Y_0 = 0$. For each $z \in \mathbb{H}_n$ the solution is well-defined up to a time $\tau_n(z)$. Similarly to the ordinary SLE case, the differential equation (7) describes the evolution of the hull $K_t^{(n)}$ defined as the closure of $\{z \in \mathbb{H}_n : \tau_n(z) \leqslant t\}$.

The solution to (7) is a conformal map from $\mathbb{H}_n \backslash K_t^{(n)}$ onto $\mathbb{H}_n$. To see this, one may generalize the proof of Proposition 2.2 in Ref. 12. One first verifies that $\partial_z g_t(z)$ is well-defined by analyzing $\partial_t \partial_z g_t(z)$. From the evaluation of $\partial_t(g_t(z) - g_t(z'))$ (which is shown to have $(g_t(z) - g_t(z'))$ as a factor), one deduces that $g_t(z) \neq g_t(z')$ when $z \neq z'$. It has thereby been established that g_t is a conformal transformation of $\mathbb{H}_n \backslash K_t^{(n)}$. To show that $g_t(\mathbb{H}_n \backslash K_t^{(n)}) = \mathbb{H}_n$, one studies the inverse flow $h_t(w)$, $w \in \mathbb{H}_n$, which is a solution to

$$\partial_t h_t(w) = -\frac{2}{h_t^{n-1}(w)(h_t^n(w) - Y_{t_0 - t})}, \quad h_0(w) = w \tag{8}$$

for some $t_0 \geqslant 0$. The solution $h_t(w)$ is well-defined for $0 \leqslant t \leqslant t_0$ since $\partial_t \operatorname{Im}(h_t^n(w)) > 0$ and $|h_t^{n-1}| \geqslant \min\{|h_t^n(w)|, 1\}$. This ensures that the solution cannot hit the singularities. With $z = h_{t_0}(w)$, $g_t(z) = h_{t_0 - t}(w)$ is seen to be a solution to (7) (implying that $h_t(w)$ is indeed the inverse flow), and $g_{t_0}(z) = w$ showing that $w \in g_{t_0}(\mathbb{H}_n \backslash K_t^{(n)})$.

The solution to (7) is determined uniquely by the hydrodynamic normalization at infinity (2). It has the power series expansion

$$g_t(z) = z + \frac{2t}{z^{2n-1}} + \mathcal{O}(1/|z|^{(2n)}), \quad z \to \infty. \tag{9}$$

We refer to the process as being of grade n.

When $n = 1$ (and $Y_t = \sqrt{\kappa} B_t$) we recover the ordinary SLE equation (1). In a subsequent section we shall focus on grade $n = 2$ as it is in this case we find a new relation to CFT and the Yang–Lee singularity.

Two important properties of ordinary SLE are scale invariance and a sort of stationarity. These apply to solutions to (7) as well. In the spirit of Proposition 2.1 in Ref. 8 (see also Ref. 3), we have that the growth process defined by (7) is scale invariant in the following sense. For $\alpha > 0$ the process $t \mapsto \alpha^{-1/(2n)} K_{\alpha t}^{(n)}$ has the same law as $t \mapsto K_t^{(n)}$, while the process $(z,t) \mapsto \alpha^{-1/(2n)} g_{\alpha t}(\alpha^{1/(2n)} z)$ has the same law as $(z,t) \mapsto g_t(z)$. Also, the map $\tilde{g}(z) := (g_{t_1} \circ g_{t_0}^{-1}) \times (z + Y_{t_0}) - Y_{t_0}$ has the same law as $g_{t_1 - t_0}$ when $t_1 > t_0 > 0$. Moreover, $\tilde{g}$ is independent of g_{t_0}. These assertions can be proved by a simple adaptation of the proof for ordinary SLE.

We define f_t through

$$f_t^n(z) = g_t^n(z) - Y_t. \tag{10}$$

It follows that $f_t(z)$ satisfies the differential equation

$$\partial_t f_t(z) = \frac{2}{f_t^{2n-1}(z)} - \frac{1/n}{f_t^{n-1}(z)} \partial_t Y_t, \quad f_0(z) = z \tag{11}$$

with a canonical choice of boundary condition. The solution respects the hydrodynamic normalization at infinity (2), and it corresponds to choosing the "principal root" in the relation (10). As in ordinary SLE, we use f_t to define an SLE-type trace for the hierarchy of evolutions:

$$\gamma_n(t) := \lim_{z\to 0} f_t^{-1}(z). \tag{12}$$

To illustrate our construction, we now consider the situation where the driving function vanishes for all t: $Y_t \equiv 0$ (corresponding to $\kappa \equiv 0$). The differential equation becomes

$$\partial_t g_t(z) = \frac{2}{g_t^{2n-1}(z)}, \quad g_0(z) = z \tag{13}$$

with solution

$$g_t(z) = (z^{2n} + 4nt)^{1/(2n)}. \tag{14}$$

The trace reads

$$\gamma_n(t) = |(4nt)^{1/(2n)}| e^{i\pi/(2n)} \tag{15}$$

while the hull is

$$K_t^{(n)} = \{re^{i\pi/(2n)} : r \in [0, |(4nt)^{1/(2n)}|]\}. \tag{16}$$

Following Ref. 8 on ordinary SLE, we may take B to be two-sided Brownian motion (or more generally, Y to be defined for negative t as well). Equation (7) can then also be solved for negative t, in which case g_t is a conformal map from $\mathbb{H}_n$ into a subset of $\mathbb{H}_n$. Indeed, Lemma 3.1 in Ref. 8 extends to our case. In the extended version it states that the map $z \mapsto g_{-t}(z)$ has the same distribution as the mapping of z into the principal nth root of $((g_t^{-1}((z^n + Y_t)^{1/n}))^n - Y_t)$. To see this we first observe that for $z \in \mathbb{H}_n$ the principal nth root of $(z^n + x)$ for x real also lies in $\mathbb{H}_n$. For $t_1 \in \mathbb{R}$ we then define the function $\hat{g}_t^{(t_1)}$ as the principal root in the functional relation

$$(\hat{g}_t^{(t_1)}(z))^n = (g_{t_1+t} \circ g_{t_1}^{-1}((z^n + Y_{t_1})^{1/n}))^n - Y_{t_1}. \tag{17}$$

It follows that $\hat{g}_t^{(t_1)}(z)$ is a solution to

$$\partial_t \hat{g}_t^{(t_1)}(z) = \frac{2}{(\hat{g}_t^{(t_1)}(z))^{n-1}((\hat{g}_t^{(t_1)}(z))^n - (Y_{t_1+t} - Y_{t_1}))}, \quad \hat{g}_0^{(t_1)}(z) = z. \tag{18}$$

We note that $\hat{Y}_t^{(t_1)} := Y_{t_1+t} - Y_{t_1}$ has the same law as Y_t as maps from $\mathbb{R}$ to $\mathbb{R}$, and since

$$(\hat{g}_{-t_1}^{(t_1)}(z))^n = (g_{t_1}^{-1}((z^n + Y_{t_1})^{1/n}))^n - Y_{t_1}, \tag{19}$$

the assertion of the extended lemma follows.

With two-sided Brownian motion at hand, we may define alternatively to (10)

$$f_t^n(z) = g_{-t}^n(z) - Y_{-t} \tag{20}$$

satisfying

$$\partial_t f_t(z) = \frac{-2}{f_t^{2n-1}(z)} - \frac{1/n}{f_t^{n-1}(z)} \partial_t Y_{-t}, \quad f_0(z) = z. \tag{21}$$

Choosing the driving function as $Y_t = \sqrt{\kappa} B_{-t}$ we have

$$df_t(z) = \frac{-2}{f_t^{2n-1}(z)} dt - \frac{\sqrt{\kappa}/n}{f_t^{n-1}(z)} dB_t, \quad f_0(z) = z. \tag{22}$$

This will appear in the link to the Yang–Lee singularity addressed below.

It is remarked that our construction may be interpreted as chordal SLE in $\mathbb{H}_n$. To appreciate this, we introduce $\phi_n(z)=z^n$ and let $G_t^{(n)}(z)$ denote the map in (7) when $Y_t=\sqrt{\kappa}B_t$. $G_t^{(1)}(z)$ thus corresponds to chordal SLE in the upper half-plane $\mathbb{H}_1=\mathbb{H}$. We then have that

$$\hat{G}_t^{(n)}(z)=\phi_n^{-1}\circ G_{nt}^{(1)}\circ\phi_n(z) \tag{23}$$

(where ϕ_n^{-1} singles out the principal root) satisfies (7) albeit with $\hat{\kappa}=n\kappa$. As a consequence, $K_t^{(n)}$ is seen to correspond to $\phi_n^{-1}(K_{nt}^{(1)})$.

III. RELATION TO CONFORMAL FIELD THEORY

A. Ordinary SLE

Bauer and Bernard[13,14] have recently discussed a direct relationship between SLE_κ and CFT. Their construction starts from a random walk on the (somewhat formal) Virasoro group:

$$G_t^{-1}dG_t=-2L_{-2}dt+\sqrt{\kappa}L_{-1}\circ dB_t,\quad G_0=1, \tag{24}$$

here written in the Stratonovich interpretation. We shall rather discuss it in the Ito form where it reads

$$G_t^{-1}dG_t=\left(-2L_{-2}+\frac{\kappa}{2}L_{-1}^2\right)dt+\sqrt{\kappa}L_{-1}dB_t,\quad G_0=1. \tag{25}$$

G_t is an element of Vir_- obtained by exponentiating the negative modes, L_n, $n<0$, of the Virasoro algebra. We write a generic element $G\in\mathrm{Vir}_-$ as

$$G=\cdots e^{x_2L_{-2}}e^{x_1L_{-1}} \tag{26}$$

and recall the definition of the Virasoro algebra:

$$[L_n,L_m]=(n-m)L_{n+m}+\frac{c}{12}n(n^2-1)\,\delta_{n+m,0}. \tag{27}$$

The central charge c plays a prominent role in CFT. As we shall discuss, it is through the construction of singular vectors in highest-weight modules of the Virasoro algebra that the connection to SLE_κ is established.[13,14]

The conformal transformation generated by (25) acts on a primary field of weight Δ as

$$G_t^{-1}\phi_\Delta(z)G_t=(\partial_z f_t(z))^\Delta\phi_\Delta(f_t(z)) \tag{28}$$

for some conformal map f_t to be determined. (For simplicity, we do not distinguish explicitly between boundary and bulk primary fields, nor do we write the antiholomorphic part.) Using that the Virasoro generators act as

$$[L_n,\phi_\Delta(z)]=(z^{n+1}\partial_z+\Delta(n+1)z^n)\phi_\Delta(z), \tag{29}$$

one finds that the conformal map associated to the random process (25) must be a solution to the stochastic differential equation

$$df_t(z)=\frac{2}{f_t(z)}dt-\sqrt{\kappa}dB_t,\quad f_0(z)=z \tag{30}$$

corresponding to (4). This follows from computing the Ito differential of (28) and is discussed in more details in Refs. 13, 14.

Observables of the random process (25) are thought of as functions on the Virasoro group, $F(G_t)$, and a goal is to find the evolution for the expectation values of these observables. With the left-invariant vector fields, ∇_ℓ, defined by

$$\nabla_\ell F(G_t)=\frac{d}{du}F(G_t e^{uL_\ell})|_{u=0} \tag{31}$$

one has[13] that the expectation value $\mathbf{E}[F(G_t)]$ satisfies

$$\partial_t \mathbf{E}[F(G_t)]=\mathbf{E}\left[\left(-2\nabla_{-2}+\frac{\kappa}{2}\nabla_{-1}^2\right)F(G_t)\right]. \tag{32}$$

We shall be interested in observables of the form $F_\Delta(G_t)=G_t|\Delta\rangle$ where $|\Delta\rangle$ is the highest-weight vector of weight Δ in the Verma module $\mathcal{V}_\Delta=\mathrm{Vir}_-|\Delta\rangle$ (see Refs. 13, 14 and below). In this case the expectation value reads

$$\partial_t \mathbf{E}[G_t|\Delta\rangle]=\mathbf{E}\left[G_t\left(-2L_{-2}+\frac{\kappa}{2}L_{-1}^2\right)|\Delta\rangle\right]. \tag{33}$$

For some values of κ (in relation to the central charge c), the linear combination $-2L_{-2}+(\kappa/2)L_{-1}^2$ will produce a singular vector when acting on the highest-weight vector in a highest-weight module. This is an important point as it enables one, through the representation theory of the algebra, to find quantities conserved in mean under the random process.

The Verma module $\mathcal{V}_\Delta$ contains the singular vector at level two

$$|\Delta;2\rangle=\left(L_{-2}-\frac{\kappa}{4}L_{-1}^2\right)|\Delta\rangle \tag{34}$$

provided $L_1|\Delta;2\rangle=L_2|\Delta;2\rangle=0$. It is straightforward to show that this implies the parametrizations

$$c_\kappa=1-\frac{3(4-\kappa)^2}{2\kappa},\quad \Delta_\kappa=\frac{6-\kappa}{2\kappa}. \tag{35}$$

The expectation value of the observable $F_\Delta(G_t)=G_t|\Delta\rangle$ thus vanishes (33):

$$\partial_t \mathbf{E}[G_t|\Delta\rangle]=0. \tag{36}$$

We see that this direct relationship between SLE_κ evolutions and CFT is through the existence of a level-two singular vector in a highest-weight module. As discussed in Ref. 14, this relationship provides links between conformal correlation functions and probabilities in SLE_κ.

B. Extended SLE

Since Brownian motion played a significant role in the derivation of (32) and (33), and hence in the correspondence between SLE and CFT, it remains unclear how to treat more general random processes than (25). An extension invites itself, though. Namely, consider the random walk

$$G_t^{-1}dG_t=v_{-n}L_{-2n}dt+\sqrt{\kappa}u_{-n}L_{-n}\circ dB_t,\quad G_0=1 \tag{37}$$

or in the Ito interpretation

$$G_t^{-1}dG_t=\left(v_{-n}L_{-2n}+\frac{\kappa u_{-n}^2}{2}L_{-n}^2\right)dt+\sqrt{\kappa}u_{-n}L_{-n}dB_t,\quad G_0=1. \tag{38}$$

In this case we have

$$\partial_t \mathbf{E}[F(G_t)] = \mathbf{E}\left[\left(v_{-n}\nabla_{-2n} + \frac{\kappa u_{-n}^2}{2}\nabla_{-n}^2\right)F(G_t)\right] \tag{39}$$

and in particular

$$\partial_t \mathbf{E}[G_t|\Delta\rangle] = \mathbf{E}\left[G_t\left(v_{-n}L_{-2n} + \frac{\kappa u_{-n}^2}{2}L_{-n}^2\right)|\Delta\rangle\right]. \tag{40}$$

To relate this to the SLE-type differential equations discussed above, we write (11) and (22) uniformly as

$$df_t(z) = \frac{2(-1)^{s+1}}{(f_t(z))^{2n-1}}dt - \frac{\sqrt{\kappa}/n}{(f_t(z))^{n-1}}dB_t, \tag{41}$$

where $s=1$ or $s=2$ depending on the choice of relation (10) or (20), respectively. Taking the Ito differential of the right-hand side of (28) results in

$$d\{(\partial_z f_t(z))^{\Delta}\phi_{\Delta}(f_t(z))\} = \left[\left(2(-1)^{s+1} + \frac{\kappa(n-1)}{2n^2}\right)L_{-2n}dt - \frac{\sqrt{\kappa}}{n}L_{-n}dB_t, (\partial_z f_t(z))^{\Delta}\phi_{\Delta}(f_t(z))\right]$$
$$+ \frac{\kappa}{2n^2}[L_{-n},[L_{-n},(\partial_z f_t(z))^{\Delta}\phi_{\Delta}(f_t(z))]]dt \tag{42}$$

while the Ito differential of the left-hand side of (28) generated by the random walk (38) reads

$$d\{G_t^{-1}\phi_{\Delta}(f_t(z))G_t\} = [-v_{-n}L_{-2n}dt - \sqrt{\kappa}u_{-n}L_{-n}dB_t, G_t^{-1}\phi_{\Delta}(f_t(z))G_t]$$
$$+ \frac{\kappa u_{-n}^2}{2}[L_{-n},[L_{-n},G_t^{-1}\phi_{\Delta}(f_t(z))G_t]]dt. \tag{43}$$

A comparison of the two Ito differentials suggests considering the walk

$$G_t^{-1}dG_t = \left(\left(2(-1)^s - \frac{\kappa(n-1)}{2n^2}\right)L_{-2n} + \frac{\kappa}{2n^2}L_{-n}^2\right)dt + \frac{\sqrt{\kappa}}{n}L_{-n}dB_t. \tag{44}$$

According to this, we should be looking for singular vectors of the form

$$|\Delta;2n\rangle = \left(\left(2(-1)^s - \frac{\kappa(n-1)}{2n^2}\right)L_{-2n} + \frac{\kappa}{2n^2}L_{-n}^2\right)|\Delta\rangle. \tag{45}$$

The upset, however, is that for $n>1$

$$L_1|\Delta;2n\rangle = \left(\left((2n+1)\left(2(-1)^s - \frac{\kappa(n-1)}{2n^2}\right) + \frac{(n+1)\kappa}{2n^2}\right)L_{-(2n-1)} + \frac{(n+1)\kappa}{n^2}L_{-n}L_{-(n-1)}\right)|\Delta\rangle$$
$$\neq 0 \tag{46}$$

for all κ. This means that (45) can be a singular vector only when $n=1$, and is then given by (34) (when $s=1$). One should not be completely discouraged by this. The pivotal property of the state $(L_{-2} - \kappa/4L_{-1}^2)|\Delta\rangle$ appearing in (33) and applications thereof,[14] is that it vanishes in the quotient space of $\mathcal{V}_{\Delta}$ where all singular vectors have been factored out. In other words, it is a null vector.

This means that we do not have to insist that the vector (45) is a (primitive) singular vector itself, but only require that it is a linear combination of descendants of (primitive) singular vectors. An example is provided below.

IV. YANG–LEE SINGULARITY

Generically, the Verma module $\mathcal{V}_\Delta$ is irreducible. Minimal models[17,18] are examples of CFTs for which it is reducible. They are labeled by a pair of positive and co-prime integers $p>p'$, and are denoted $\mathcal{M}(p,p')$. The central charge is

$$c=1-6\frac{(p-p')^2}{pp'} \tag{47}$$

while the spectrum of primary fields or highest-weight representations have conformal weights

$$\Delta_{r,s}=\frac{(rp-sp')^2-(p-p')^2}{4pp'},\quad 1\leqslant r<p',\quad 1\leqslant s<p, \tag{48}$$

with $\Delta_{p'-r,p-s}=\Delta_{r,s}$. There are two singular vectors not being descendants of singular vectors themselves, and they appear at levels rs and $(p'-r)(p-s)$.

For $p'=2$, there is only one primary field admitting a singular vector at level two, in which case $(r,s)=(1,2)$. For $p'>2$, on the other hand, there are two such fields, labeled by (1,2) and (2,1), respectively. It is easily verified that

$$\Delta_{1,2}=\Delta_{\kappa=4p/p'},\quad \Delta_{2,1}=\Delta_{\kappa=4p'/p}. \tag{49}$$

It follows that SLE_κ and $\mathrm{SLE}_{16/\kappa}$, with $\kappa=4p/p'$, may be linked to the same minimal model, albeit via two different primary fields in the model.

The simplest example of a null vector of the form (45) for $n>1$ that we have found is a level-four vector in the minimal model $\mathcal{M}(5,2)$ with $c=-22/5$, cf. (47). This model offers a CFT description of the statistical Yang–Lee singularity. Unlike ordinary SLE (except $\mathrm{SLE}_{\kappa=6}$ which is known to correspond to percolation, and has central charge $c=0$), the null vector appears in the *identity module* having singular vectors

$$|0\rangle_1=L_{-1}|0\rangle,$$

$$|0\rangle_4=\left(L_{-4}+\frac{5}{27}L_{-3}L_{-1}-\frac{5}{3}L_{-2}^2+\frac{125}{27}L_{-2}L_{-1}^2-\frac{125}{108}L_{-1}^4\right)|0\rangle. \tag{50}$$

The null vector of our interest reads

$$|0;4\rangle=|0\rangle_4+\left(-\frac{5}{27}L_{-3}-\frac{125}{27}L_{-2}L_{-1}+\frac{125}{108}L_{-1}^3\right)|0\rangle_1=\left(L_{-4}-\frac{5}{3}L_{-2}^2\right)|0\rangle. \tag{51}$$

Comparing this to (45), we find that the Yang–Lee singularity is related to a grade-two SLE-type evolution with

$$\kappa=40 \tag{52}$$

and $s=2$. There is no non-negative solution for κ when $s=1$. In summary, this SLE-type evolution reads

$$\partial_t g_t(z)=\frac{2}{g_t(z)(g_t^2(z)-\sqrt{40}B_t)},\quad g_0(z)=z \tag{53}$$

or in terms of $f_t(z)$, cf. (22) and (41):

$$df_t(z)=\frac{-2}{f_t^3(z)}dt-\frac{\sqrt{10}}{f_t(z)}dB_t, \quad f_0(z)=z. \tag{54}$$

This provides a novel approach to the Yang–Lee model, and may eventually lead to an explicit geometric realization.

V. CONCLUSION

As observed by Bauer and Bernard,[13,14] SLE may be linked to CFT through the construction of a singular vector in a Virasoro highest-weight module. We have extended their approach, and found that the Yang–Lee singularity may be described by a generalization of the SLE differential equation. This new stochastic evolution appears at grade two in a hierarchy of SLE-type growth processes in which ordinary SLE appears at grade one. Their approach has recently been extended also to stochastic evolutions in superspace and superconformal field theory.[19] Another extension will appear elsewhere where it is discussed how SLE-type growth processes may be linked to CFT via (nonprimary) descendant fields. A possible classification of these links will also be addressed.

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Group classification of (1+1)-dimensional Schrödinger equations with potentials and power nonlinearities

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We perform the complete group classification in the class of nonlinear Schrödinger equations of the form $i\psi_t+\psi_{xx}+|\psi|^\gamma\psi+V(t,x)\psi=0$, where V is an arbitrary complex-valued potential depending on t and x, γ is a real nonzero constant. We construct all the possible inequivalent potentials for which these equations have nontrivial Lie symmetries using a combination of algebraic and compatibility methods. The proposed approach can be applied to solving group classification problems for a number of important classes of differential equations arising in mathematical physics. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765748]

I. INTRODUCTION

Nonlinear Schrödinger equations (NSchEs) are important objects for investigation in different fields of physics and mathematics. They are used in geometric optics,[6] nonlinear quantum mechanics,[4] and the theory of Bose–Einstein condensation. NSchEs also have a number of applications in wave propagation in inhomogeneous medium and arise as a model of plasma phenomena. The cubic Schrödinger equation is one of the most known integrable models of mathematical physics. At the same time the physical interpretation of some known types of nonlinear Schrödinger equations is not completely clear and is an interesting problem to solve.

Schrödinger equations have been investigated by means of symmetry methods by a number of authors. (See, e.g., Refs. 7–13,15,17,18, and references therein for classical Lie symmetries.) In fact, group classification for Schrödinger equations was first performed by Lie. More precisely, his classification[14] of all the linear equations with two independent complex variables contains, in an implicit form, solving the classification problem for the linear $(1+1)$-dimensional Schrödinger equations with an arbitrary potential. And it is follows from Lie's proof that the equations for the harmonic and repulsive oscillators and free fall are locally equivalent to the free Schrödinger equation.

To the best of our knowledge, actual investigations of Lie symmetries for Schrödinger equations were started in 1970s with the linear case.[15,17,18] The next considered class covered $(1+n)$-dimensional NSchEs with nonlinearities of the form $f(|\psi|)\psi$, which are notable for their symmetry properties because any such equation is invariant with respect to the Galilean group. It turned out that extensions of this invariance group are possible only for the logarithm and power functions, and there exists the power value $\gamma=4/n$ which is special with respect to the symmetry

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point of view.[7] Namely, the free Schrödinger equation and the NSchE with the nonlinearity $|\psi|^{4/n}\psi$ are distinctive ones from a lot of similar equations, since they admit the complete Galilei group extended with both the scale and conformal transformations. (Here n is the number of spatial variables, and for $n=1$ and $n=2$ they are the quintic and cubic equations, respectively, that stand out against the other NSchEs.) This NSchE has also other special properties, and the value $\gamma=4/n$ is called now the critical power.

The results mentioned above formed a basis for symmetry studying more extended classes of NSchEs. So, finishing the series of papers[8–12] on group analysis and exact solutions of NSchEs, Gagnon and Winternitz[12] investigated a general class of $(1+1)$-dimensional variable coefficient cubic SchEs. It is the symmetry approach that was applied by Doebner and Goldin to obtain new equations which generalize the Schrödinger equation and can be used in nonlinear quantum mechanics.[4] These equations were investigated in more detail with the symmetry point of view by a number of authors.[5,16,26] The complete group classification of constant coefficient NSchEs with nonlinearities of the general form $F=F(\psi,\psi^*)$ was performed by Nikitin and Popovych.[19]

Group classification is one of symmetry methods used to choose physically relevant models from parametric classes of systems of (partial or ordinary) differential equations. The parameters can be constants or functions of independent variables, unknown functions and their derivatives. Exhaustive consideration of the problem of group classification for a parametric class $\mathcal{L}$ of systems of differential equations includes the following steps:

(1) Finding the group $G^{\rm ker}$ (the kernel of maximal invariance groups) of local transformations that are symmetries for all systems from $\mathcal{L}$.
(2) Construction of the group $G^{\rm equiv}$ (the equivalence group) of local transformations which transform $\mathcal{L}$ into itself.
(3) Description of all possible $G^{\rm equiv}$-inequivalent values of parameters that admit maximal invariance groups wider than $G^{\rm ker}$.

Following Lie, one usually considers infinitesimal transformations instead of finite ones. This approach essentially simplifies the problem of group classification, reducing it to problems for Lie algebras of vector fields. See Refs. 1,2,19,21,22,24–26 for precise formulation of group classification problems and more details on the used methods.

In this paper we study a class of NSchEs of the form

$$i\psi_t+\psi_{xx}+|\psi|^{\gamma}\psi+V\psi=0, \tag{1}$$

where the potential $V=V(t,x)$ is an arbitrary complex-valued smooth function of the variables t and x, γ is a real nonzero constant. (Here and below subscripts of functions denote differentiation with respect to the respective variables.) To find a complete set of inequivalent cases of V admitting extensions of the maximal Lie invariance algebra, we combine the classical Lie approach, studying the algebra generated by all the possible Lie symmetry operators for equations from class (1) (the adjoint representation, the inequivalent one-dimensional subalgebras, etc.) and investigation of compatibility of classifying equations. The subclass of (1) where $\gamma=2$ (the cubic SchEs with potentials) has been investigated in Ref. 23 in a similar way.

In fact, here we solve three classification problems for different classes of equations having the form (1): with the potentials depending only on t (Sec. III), with the stationary potentials (Sec. IV) and the general case with arbitrary potentials (Sec. II). Moreover, it is proved in Sec. II the constant γ can be assumed as *fixed* under our consideration. And there exists a special constant $\hat{\gamma}$ depending on the power γ ($\hat{\gamma}=\gamma^{-1}(4-\gamma)$), which arises at the beginning of the classification procedure when classification condition (3) is constructed and explicitly appears in the final results of classification. The value $\gamma=4$ (quintic nonlinearity, it is the same that $\hat{\gamma}=0$) is special with respect to group classification in class (1).

The classification approach used in this paper allows us to formulate a necessary and sufficient condition of mutual equivalence for the cases of extensions of maximal invariance algebras in algebraic terms (Corollary 2). The classical stationary potentials (free particle, the harmonic and

repulsive oscillators, free fall, radial free particle, the radial harmonic and repulsive oscillators[15]) naturally arise under the group classification with respect to the (smaller) equivalence group in the class of stationary potentials. Using Corollary 2 and the complete equivalence group of class (1) we easily construct transformations of these x-dependent potentials to x-free ones in explicit form (see Remark 8).

II. GENERAL CASE $V=V(t,x)$

Consider an operator $Q=\xi^t\partial_t+\xi^x\partial_x+\eta\partial_\psi+\eta^*\partial_{\psi^*}$ from the maximal Lie invariance algebra $A^{\max}(\gamma,V)$ of Eq. (1) with a power γ and a potential V. Here ξ^t, ξ^x, and η are smooth functions of t, x, ψ, and ψ^*. The infinitesimal invariance condition[21,20] of Eq. (1) with respect to the operator Q implies the linear overdetermined system on the coefficients of Q:

$$\xi^t_\psi=\xi^t_{\psi^*}=\xi^t_x=0,\quad \xi^x_\psi=\xi^x_{\psi^*}=0,\quad \xi^t_t=2\xi^x_x,\quad \eta_{\psi^*}=\eta_{\psi\psi}=0,\quad \psi\eta_\psi=\eta,$$

$$2\eta_{\psi x}=i\xi^x_t,\quad \gamma(\eta_\psi+\eta^*_\psi)=-2\xi^t_t,\quad i\eta_{\psi t}+\eta_{\psi xx}+\xi^tV_t+\xi^xV_x+\xi^t_tV=0.$$

Therefore, the following theorem holds:

Theorem 1: *Any operator Q from $A^{\max}(\gamma,V)$ of Eq. (1) with arbitrary potential V lies in the linear span of operators of the form*

$$D(\xi)=\xi\partial_t+\frac{1}{2}\xi_t x\partial_x+\frac{1}{8}\xi_{tt}x^2M-\frac{1}{\gamma}\xi_tI,\quad G(\chi)=\chi\partial_x+\frac{1}{2}\chi_t xM,\quad \lambda M. \tag{2}$$

Here $\chi=\chi(t)$, $\xi=\xi(t)$ and $\lambda=\lambda(t)$ are arbitrary smooth functions of t, $M=i(\psi\partial_\psi-\psi^*\partial_{\psi^*})$, $I=\psi\partial_\psi+\psi^*\partial_{\psi^*}$. Moreover, the coefficients of $Q=D(\xi)+G(\chi)+\lambda M\in A^{\max}(\gamma,V)$ should satisfy the classifying condition

$$\xi V_t+\left(\frac{1}{2}\xi_t x+\chi\right)V_x+\xi_tV=\frac{1}{8}\xi_{ttt}x^2+\frac{1}{2}\chi_{tt}x+\lambda_t+i\frac{\hat\gamma}{4}\xi_{tt}. \tag{3}$$

Here and below $\hat\gamma=\gamma^{-1}(4-\gamma)$.

Theorem 2: *The Lie algebra of the kernel of maximal Lie invariance groups of equations from class* (1) *is $A^{\ker}=\langle M\rangle$.*

Remark 1: Sometimes (e.g., for reduction and construction of solutions) it is convenient to use the amplitude ρ and the phase φ instead of the wave function $\psi=\rho e^{i\varphi}$. Then Eq. (1) is replaced by the system for two real-valued functions ρ and φ:

$$\rho_t+2\rho_x\varphi_x+\rho\varphi_{xx}+\rho\,\mathrm{Im}\,V=0,\quad -\rho\varphi_t-\rho(\varphi_x)^2+\rho_{xx}+\rho^{\gamma+1}+\rho\,\mathrm{Re}\,V=0.$$

Operators (2) have the same form with $M=\partial_\varphi$, $I=\rho\partial_\rho$.

To study equivalence transformations for class (1), both the infinitesimal and direct methods are used. In the framework of the infinitesimal method we consider a first-order differential operator of the most general form in the space of the variables t, x, ψ, ψ^*, V, V^*, and γ, i.e.,

$$Q=\xi^t\partial_t+\xi^x\partial_x+\eta\partial_\psi+\eta^*\partial_{\psi^*}+\theta\partial_V+\theta^*\partial_{V^*}+\Gamma\partial_\gamma,$$

where ξ^t, ξ^x, η, θ, and Γ may depend on all the variables, and assume it being an infinitesimal symmetry operator for the system

$$i\psi_t+\psi_{xx}+|\psi|^\gamma\psi+V\psi=0,\quad \gamma_t=\gamma_x=\gamma_\psi=\gamma_{\psi^*}=0,\quad V_\psi=V_{\psi^*}=0. \tag{4}$$

(Under the prolongation procedure for equivalence transformations we suppose ψ is a function of t and x as well as V and γ are functions of t, x, ψ, and ψ^*.)

Theorem 3: *The Lie algebra A^{equiv} of the equivalence group G^{equiv} of class (1) is generated by the operators*

$$D'(\xi)=D(\xi)+\frac{1}{8}\xi_{ttt}x^2(\partial_V+\partial_{V*})+\frac{i}{\gamma}\xi_{tt}(\partial_V-\partial_{V*})-\xi_t(V\partial_V+V^*\partial_{V*}),$$

$$G'(\chi)=G(\chi)+\tfrac{1}{2}\chi_{tt}x(\partial_V+\partial_{V*}),\quad M'(\lambda)=\lambda M+\lambda_t(\partial_V+\partial_{V*}).$$

In the framework of the direct method we look for all local transformations in the space of the variables t, x, ψ, ψ^*, V, V^*, and γ, which preserve system (4).

Theorem 4: *The equivalence group G^{equiv} of the class (1) is generated by the family of continuous transformations*

$$\tilde t=T,\quad \tilde x=x\sqrt{T_t}+X,\quad \tilde\psi=\psi\frac{1}{(T_t)^{1/\gamma}}\exp\left(\frac{i}{8}\frac{T_{tt}}{T_t}x^2+\frac{i}{2}\frac{X_t}{\sqrt{T_t}}x+i\Psi\right),\quad \tilde\gamma=\gamma,$$

$$\tilde V=\frac{1}{T_t}\left(V+\frac{1}{8}\left(\frac{T_{tt}}{T_t}\right)_t x^2+\frac{1}{2}\left(\frac{X_t}{\sqrt{T_t}}\right)_t x+i\frac{\hat\gamma}{4}\frac{T_{tt}}{T_t}-\left(\frac{1}{4}\frac{T_{tt}}{T_t}x+\frac{1}{2}\frac{X_t}{\sqrt{T_t}}\right)^2+\Psi_t\right) \tag{5}$$

and two discrete transformations: the space reflection I_x ($\tilde t=t$, $\tilde x=-x$, $\tilde\psi=\psi$, $\tilde\gamma=\gamma$, $\tilde V=V$) and the Wigner time reflection I_t ($\tilde t=-t$, $\tilde x=x$, $\tilde\psi=\psi^*$, $\tilde\gamma=\gamma$, $\tilde V=V^*$). Here T, X, and Ψ are arbitrary smooth functions of t, $T_t>0$.

We also prove the stronger statement than Theorem 4.

Theorem 5: *If two equations from class (1) with the parameter values (γ,V) and $(\tilde\gamma,\tilde V)$ are transformed each to other by local transformations, then $\tilde\gamma=\gamma$. Moreover, since $\gamma\neq0$ any transformation of such type belongs to G^{equiv}.*

Remark 2: It follows from Theorems 4 and 5 that there exist no equivalence and, moreover, local transformations changing γ. Therefore, we can assume that γ *is fixed* in our consideration below and omit it from notations of the maximal Lie invariance algebras of an equation of form (1), etc.

Remark 3: The linear span of operators of the form (2) (γ is fixed!) is an (infinite-dimensional) Lie algebra $A^{\cup}$ under the usual Lie bracket of vector fields. Since for any $Q\in A^{\cup}$, where $(\xi^t,\xi^x)\neq(0,0)$ we can find V satisfying condition (3), then $A^{\cup}=\langle\cup_V A^{\max}(V)\rangle$. The nonzero commutation relations between the basis elements of $A^{\cup}$ are the following ones:

$$[D(\xi^1),D(\xi^2)]=D(\xi^1\xi^2_t-\xi^2\xi^1_t),\quad [D(\xi),G(\chi)]=G(\xi\chi_t-\tfrac{1}{2}\xi_t\chi),\quad [D(\xi),\lambda M]=\xi\lambda_t M,$$

$$[G(\chi^1),G(\chi^2)]=\tfrac{1}{2}(\chi^1\chi^2_t-\chi^2\chi^1_t)M.$$

We use the notation $\mathrm{Aut}(A^{\cup})$ for the automorphism group acting on $A^{\cup}$, which is generated by all the one-parameter groups corresponding to the adjoint representations of operators of $A^{\cup}$ into $A^{\cup}$ and two discrete transformations $\mathrm{Ad}\,I_x$ and $\mathrm{Ad}\,I_t$ included additionally. The actions of $\mathrm{Ad}\,I_x$ and $\mathrm{Ad}\,I_t$ on the basis elements of $A^{\cup}$ are defined by the formulas $\mathrm{Ad}\,I_x\,G(\chi)=G(-\chi)$ (the other basis operators do not change) and $\mathrm{Ad}\,I_t\,D(\xi)=D(\tilde\xi)$, $\mathrm{Ad}\,I_t\,G(\chi)=G(\tilde\chi)$, $\mathrm{Ad}\,I_t\,\lambda M=\tilde\lambda M$, where $\tilde\xi(t)=-\xi(-t)$, $\tilde\chi(t)=\chi(-t)$, and $\tilde\lambda(t)=-\lambda(-t)$.

Corollary 1: $A^{\mathrm{equiv}}\simeq A^{\cup}$, $G^{\mathrm{equiv}}\simeq\mathrm{Aut}(A^{\cup})$, *and the isomorphism is determined by means of prolongation of operators from $A^{\cup}$ to the space (V,V^*).*

Corollary 2: Let A^1 and A^2 be the maximal Lie invariance algebras of equations from class (1) for some potentials, and $\mathcal{V}^i=\{V|A^{\max}(V)=A^i\}$, $i=1,2$. Then $\mathcal{V}^1\sim\mathcal{V}^2 \mathrm{mod} G^{\mathrm{equiv}}$ iff $A^1\sim A^2 \bmod \mathrm{Aut}(A^{\cup})$.

TABLE I. Results of classification. Here $W(t),\nu,\alpha,\beta\in\mathbb{R}$, $(\alpha,\beta)\neq(0,0)$.

N	V	Basis of $A^{\max}$
0	$V(t,x)$	M
1	$iW(t)$	$M,\ \partial_x,\ G(t)$
2	$\frac{i}{2}\frac{\hat\gamma t+\nu}{t^2+1}$	$M,\ \partial_x,\ G(t),\ D(t^2+1)$
3	$i\nu t^{-1},\ \nu\neq0,\ \frac{\hat\gamma}{2}$	$M,\ \partial_x,\ G(t),\ D(t)$
4	i	$M,\ \partial_x,\ G(t),\ \partial_t$
5	$0,\ \gamma\neq4$	$M,\ \partial_x,\ G(t),\ \partial_t,\ D(t)$
	$\gamma=4$	$M,\ \partial_x,\ G(t),\ \partial_t,\ D(t),\ D(t^2)$
6	$V(x)$	$M,\ \partial_t$
7	$(\alpha+i\beta)x^{-2},\ \gamma\neq4$	$M,\ \partial_t,\ D(t)$
	$\gamma=4$	$M,\ \partial_t,\ D(t),\ D(t^2)$

Lemma 1: A complete list of $\mathrm{Aut}\,A^{\cup}$*-inequivalent one-dimensional subalgebras of* $A^{\cup}$ *is exhausted by the algebras* $\langle\partial_t\rangle$, $\langle\partial_x\rangle$, $\langle tM\rangle$, $\langle M\rangle$.

Proof: Consider any operator $Q\in A^{\cup}$, i.e., $Q=D(\xi)+G(\chi)+\lambda M$. Depending on the values of ξ, χ and λ it is equivalent under $\mathrm{Aut}(A^{\cup})$ and multiplication by a number to one from the following operators: $D(1)$ if $\xi\neq0$; $G(1)$ if $\xi=0$ and $\chi\neq0$; tM if $\xi=\chi=0$, $\lambda_t\neq0$; M if $\xi=\chi=\lambda_t=0$.

Corollary 3: If $A^{\max}(V)\neq A^{\ker}$, *then* $V_tV_x=0 \bmod G^{\mathrm{equiv}}$.

Proof: Under the corollary assumption there exists an operator $Q=D(\xi)+G(\chi)+\lambda M\in A^{\max}(V)$ which do not belong to $\langle M\rangle$. Condition (3) implies $(\xi,\chi)\neq(0,0)$. Therefore, in force of Lemma 1 $\langle Q\rangle\sim\langle\partial_t\rangle$ or $\langle\partial_x\rangle \bmod \mathrm{Aut}\,A^{\cup}$, i.e., $V_tV_x=0 \bmod G^{\mathrm{equiv}}$.

Theorem 6: *A complete set of inequivalent cases of V admitting extensions of the maximal Lie invariance algebra of Eq. (1) is exhausted by the potentials given in Table I.*

For convenience we use below the double numeration T. N. of classification cases where T is a table number and N is a row number.

Remark 4: We mean that the invariance algebras for Cases 1.0, 1.1, 1.6 and analogous ones from Tables II and III are maximal if these cases are inequivalent under the corresponding equivalence group to the other, more specialized, cases from the same table.

Remark 5: There exists a discrete equivalence transformation τ for the set of potentials $i\nu t^{-1}$, $\nu\in\mathbb{R}$, which has form (5) with $T=-t^{-1}$, $X=0$, $\Psi=0$. It transforms ν in the following way: $\nu\to\hat\gamma/2-\nu$. For the cases under consideration to be completely inequivalent, we have to assume additionally that $\nu\geqslant\hat\gamma/4$ (or $\nu\leqslant\hat\gamma/4$) in Case 1.3. Since $I_t\in G^{\mathrm{equiv}}$ we can assume analogously

TABLE II. Classification of the subclass $V=V(x)$ if $\gamma\neq4$. Here $\nu,\alpha,\beta\in\mathbb{R}$, $(\alpha,\beta)\neq(0,0)$.

N	N_1	V	Basis of $A^{\max}$
0	6	$V(x)$	$M,\ \partial_t$
1	7	$(\alpha+i\beta)x^{-2}$	$M,\ \partial_t,\ D(t)$
2	7	$x^2+i\hat\gamma+(\alpha+i\beta)x^{-2}$	$M,\ \partial_t,\ D(e^{4t})$
3	4	i	$M,\ \partial_t,\ \partial_x,\ G(t)$
4	4	$x+i\nu,\quad\nu\neq0$	$M,\ \partial_t,\ \partial_x+tM,\ G(2t)+t^2M$
5	2	$-x^2+i\nu$	$M,\ \partial_t,\ G(\sin2t),\ G(\cos2t)$
6	3	$x^2+i\nu,\quad\nu\neq\pm\hat\gamma$	$M,\ \partial_t,\ G(e^{2t}),\ G(e^{-2t})$
7	5	0	$M,\ \partial_t,\ \partial_x,\ G(t),\ D(t)$
8	5	x	$M,\ \partial_t,\ \partial_x+tM,\ G(2t)+t^2M,\ D(2t)+G(3t^2)+t^3M$
9	5	$x^2+i\hat\gamma$	$M,\ \partial_t,\ G(e^{2t}),\ G(e^{-2t}),\ D(e^{4t})$

TABLE III. Classification of the subclass $V=V(x)$ if $\gamma=4$. Here $\nu,\alpha,\beta\in\mathbb{R}$, $\nu\neq 0$, $(\alpha,\beta)\neq(0,0)$.

N	N_1	V	Basis of $A^{\max}$
0	6	$V(x)$	$M,\ \partial_t$
1	7	$(\alpha+i\beta)x^{-2}$	$M,\ \partial_t,\ D(t),\ D(t^2)$
2	7	$x^2+(\alpha+i\beta)x^{-2}$	$M,\ \partial_t,\ D(e^{4t}),\ D(e^{-4t})$
3	7	$-x^2+(\alpha+i\beta)x^{-2}$	$M,\ \partial_t,\ D(\cos 4t),\ D(\sin 4t)$
4	4	i	$M,\ \partial_t,\ \partial_x,\ G(t)$
5	4	$x+i\nu$	$M,\ \partial_t,\ \partial_x+tM,\ G(2t)+t^2M$
6	2	$-x^2+i\nu$	$M,\ \partial_t,\ G(\sin 2t),\ G(\cos 2t)$
7	3	$x^2+i\nu$	$M,\ \partial_t,\ G(e^{2t}),\ G(e^{-2t})$
8	5	0	$M,\ \partial_t,\ \partial_x,\ G(t),\ D(t),\ D(t^2)$
9	5	x	$M,\ \partial_t,\ \partial_x+tM,\ G(2t)+t^2M,$ $D(2t)+G(3t^2)+t^3M,\ D(4t^2)+G(4t^3)+t^4M$
10	5	x^2	$M,\ \partial_t,\ G(e^{2t}),\ G(e^{-2t}),\ D(e^{4t}),\ D(e^{-4t})$
11	5	$-x^2$	$M,\ \partial_t,\ G(\cos 2t),\ G(\sin 2t),\ D(\cos 4t),\ D(\sin 4t)$

$\nu\geqslant 0$ in Case 1.2 and $\beta\geqslant 0$ in Case 1.7. Moreover, τ is a discrete symmetry transformation for Case 1.3 ($\nu=\hat{\gamma}/4$) and, as a limit of the continuous transformations generated by the operator $D(t^2+1)$, for Case 1.2.

If we use Corollary 3 then to prove Theorem 6 it is sufficient to study two cases: $V_x=0$ and $V_t=0$. In fact, below we obtain the complete results of group classifications for both special cases and then unite them for the general case under consideration.

III. CASE $V=V(t)$

Consider the equations from class (1) with potentials satisfying the additional assumption $V_x=0$, i.e., $V=V(t)$. The following chain of lemmas gives complete solving of classification problem in this subclass.

Lemma 2: $A^{\ker}_{V_x=0}=\langle M,G(1),G(t)\rangle$.

Lemma 3: $A^{\rm equiv}_{V_x=0}=\langle M'(\lambda)\ \forall\lambda=\lambda(t),G'(1),G'(t),D'(1),D'(t),D'(t^2)\rangle$. $G^{\rm equiv}_{V_x=0}$ *is generated by* I_t, I_x *and the transformations of form* (5), *where* $T=(a_1t+a_0)/(b_1t+b_0)$, $X=c_1t+c_0$, Ψ *is an arbitrary smooth function of* t. a_i, b_i *and* c_i *are arbitrary constants such that* $a_1b_0-b_1a_0>0$.

Lemma 4: For any $V=V(t)$: $V\sim iW \bmod G^{\rm equiv}_{V_x=0}$, *where* $W=\operatorname{Im}V$, i.e., $W=W(t)\in\mathbb{R}$.

Lemma 5: $A^{\ker}_{\{iW\}}=A^{\ker}_{V_x=0}$. $A^{\max}(iW)\subset A^{\cup}_{\{iW\}}=A^{\ker}_{\{iW\}}\supset S$, *where* $S=\langle D(1),D(t),D(t^2)\rangle$. $A^{\cup}_{\{iW\}}=\cup_W A^{\max}(iW)$.

$A^{\rm equiv}_{\{iW\}}=\langle M,G'(1),G'(t),D'(1),D'(t),D'(t^2)\rangle$. $\quad G^{\rm equiv}_{\{iW\}}=G^{\rm equiv}_{V_x=0}\big|_{\Psi=\rm const}$. $\quad A^{\cup}_{\{iW\}}\simeq A^{\rm equiv}_{\{iW\}}=\mathrm{pr}_{(V,V*)}A^{\cup}_{\{iW\}}$.

Lemma 6: $S\simeq sl(2,\mathbb{R})$. *The complete list of* $A^{\cup}_{\{iW\}}$*-inequivalent proper subalgebras of* S *is exhausted by the algebras* $\langle D(1)\rangle$, $\langle D(t)\rangle$, $\langle D(t^2+1)\rangle$, $\langle D(1),D(t)\rangle$.

Lemma 7: Let A^1 *and* A^2 *be the maximal Lie invariance algebras of equations from class (1) for some potentials from* $\{iW(t)\}$, *and* $\mathcal{W}^i=\{W(t)\,|\,A^{\max}(iW)=A^i\}$, $i=1,2$. *Then* $\mathcal{W}^1\sim\mathcal{W}^2 \bmod G^{\rm equiv}_{\{iW\}}$ *iff* $A^1\cap S\sim A^2\cap S \bmod \mathrm{Aut}(S)$.

Lemma 8: If $A^{\max}_{\{iW\}}\neq A^{\ker}_{V_x=0}$ *the potential* $iW(t)$ *is* $G^{\rm equiv}_{\{iW\}}$*-equivalent to one from Cases* 1.2–1.5.

Remark 6: If $\gamma\neq 4$ or $W\neq$ const $A^{\max}(iW)\not\supset S$ (otherwise, condition (3) would imply an incompatible system for W). If $W=$ const $W\in\{0,1\} \bmod G^{\rm equiv}_{\{iW\}}$ (Cases 1.5 and 1.4 correspondingly). Cases 1.2ν and 1.2$\tilde{\nu}$ (1.3ν and 1.3$\tilde{\nu}$ where $\nu,\tilde{\nu}\geqslant\gamma/4$) are $G^{\rm equiv}$-inequivalent if $\nu\neq\tilde{\nu}$. Since $D(t^2+1)$ cannot be contained in any two-dimensional subalgebra of S it is not possible to extend $A^{\max}$ in Case 1.2. There are two possibilities for extension of $A^{\max}(i\nu t^{-1})$, namely with either $D(1)$ (for $\nu=0$, Case 1.5) or $D(t^2)$ (for $\nu=(4-\gamma)/(2\gamma)$ that is equivalent to Case 1.5 with respect to $G^{\rm equiv}_{\{iW\}}$). That is why for $\nu=0$, $\gamma=4$ dimension of $A^{\max}$ is greatest.

IV. CASE $V=V(x)$

Consider class (1) with the additional assumption $V_t=0$, i.e., $V=V(x)$.

Lemma 9: $A^{\ker}_{V_t=0}=\langle M,D(1)\rangle$.

Lemma 10: $A^{\text{equiv}}_{V_t=0}=\langle M'(1),M'(t),G'(1),D'(1),D'(t)\rangle$. $G^{\text{equiv}}_{V_t=0}$ *is generated by* I_t, I_x *and the transformations of form* (5), *where* $T_{tt}=X_t=\Psi_{tt}=0$.

Lemma 11: If $A^{\max}(V)\neq A^{\ker}_{V_t=0}$ *the potential* $V(x)$ *is* $G^{\text{equiv}}_{V_t=0}$*-equivalent to one from cases of either Table II if* $\gamma\neq 4$ *or Table III if* $\gamma=4$. (*Since* $I_t\in G^{\text{equiv}}$ *we can assume* $\nu\geqslant 0$ *in Cases 2.5, 2.6, 3.5–3.7,* $\nu>0$ *in Case 2.4 and* $\beta\geqslant 0$ *in Cases 2.1, 3.1–3.3.*)

Proof: Let $V=V(x)$ and $A^{\max}(V)\neq A^{\ker}_{V_t=0}$. Consider an arbitrary operator $Q=D(\xi)+G(\chi)+\lambda M\in A^{\max}(V)$. Under Lemma's assumption, condition (3) implies a set of equations on V of the general form

$$(ax+b)V_x+2aV=c_2x^2+c_1x+\tilde{c}_0+ic_0,\quad \text{where}\quad a,b,c_2,c_1,\tilde{c}_0,c_0=\text{const}\in\mathbb{R}.$$

The exact number k of such equations with the linear independent sets of coefficients can be equal to either 1 or 2. (The value $k=0$ corresponds to the general case $V_t=0$ without any extensions of $A^{\max}$.)

For $k=1$ $(a,b)\neq(0,0)$ and there exist two possibilities $a=0$ and $a\neq 0$. If $a=0$ without loss of generality we can put $b=1$. Then condition (3) results in $\xi_t=0$, $c_2=c_0=0$, i.e., $V_x=c_1x+\tilde{c}_0$, and then $k=2$ that it is impossible.

Therefore, $a\neq 0$ and we can put $a=1$. $\tilde{c}_0,b=0 \bmod G^{\text{equiv}}_{V_t=0}$. Condition (3) results in $\chi=0$ (then $c_1=0$), $\lambda_t=0$, $\hat{\gamma}\xi_{tt}=2c_0\xi_t$, and $\hat{\gamma}c_2=c_0^2$. For $\gamma=4$, $c_0=0$, and $c_2\in\{-4,0,4\} \bmod G^{\text{equiv}}_{V_t=0}$ and these possibilities in the value of c_2 give Cases 3.1–3.3. If $\gamma\neq 4$ we obtain Cases 2.1 ($c_0=0$) and 2.2 ($c_0\neq 0$).

The condition $k=2$ results in $V=d_2x^2+d_1x+\tilde{d}_0+id_0$. $\tilde{d}_0=0 \bmod G^{\text{equiv}}_{V_t=0}$. Considering different possibilities for values of the constants d_2, d_1, and d_0 and taking into account the value of γ (either $\gamma\neq 4$ or $\gamma=4$), we obtain all the other classification cases:

$$d_2=d_1=d_0=0\ \rightarrow\ 2.7,3.8;\quad d_2=d_1=0,\ d_0\neq 0\ \rightarrow\ 2.3,3.4;$$

$$d_2=d_0=0,\ d_1\neq 0\ \rightarrow\ 2.8,3.9;\quad d_2=0,\ d_0,d_1\neq 0\ \rightarrow\ 2.4,3.5;$$

$$d_2<0,\ (d_0,\hat{\gamma})\neq(0,0)\ \rightarrow\ 2.5,3.6;\quad d_2<0,\ d_0=\hat{\gamma}=0\ \rightarrow\ 3.11;$$

$$d_2>0,\ \hat{\gamma}^2d_2\neq d_0^2\ \rightarrow\ 2.6,3.7;\quad d_2>0,\ \hat{\gamma}^2d_2=d_0^2\ \rightarrow\ 2.9,3.10.$$

Remark 7: To prove Theorem 6, it is sufficient to consider only the case $k=1$, $a\neq 0$ in Lemma 11 since other cases of extensions of $A^{\max}(V)$ with $V=V(x)$ admit operators of the form $G(\chi)+\lambda M$ ($\chi\neq 0$) and, therefore (by Corollary 2), are equivalent to Cases 1.1–1.5.

Remark 8: The number N_1 for each line of Tables II and III is equal to the number of the same or equivalent case in Table I. The corresponding equivalence transformations have the form (5) where the functions T, X, and Ψ are as follows:

$$2.2,\ 3.2\rightarrow 1.7,\quad 2.6,\ 3.7\rightarrow 1.3\left(\tilde{\nu}=\frac{\hat{\gamma}-\nu}{4}\right),\quad 2.9,\ 3.10\rightarrow 1.5:\quad T=-e^{-4t},\ X=\Psi=0;$$

$$3.3\rightarrow 1.7,\quad 2.5,\ 3.6\rightarrow 1.2(\tilde{\nu}=\nu),\quad 3.11\rightarrow 1.5:\quad T=\tan 2t,\ X=\Psi=0;$$

$$2.4,\ 3.5\rightarrow 1.4:\quad T=|\nu|t,\ X=-\sqrt{|\nu|}\,t^2,\ \Psi=\frac{t^3}{3};$$

$$2.8,\ \ 3.9\to 1.5:\quad T=t,\ \ X=-t^2,\ \ \Psi=\frac{t^3}{3}.$$

Remark 8 completes the proof of Theorem 6.

V. CONCLUSION

The results of group classification obtained in this paper can be extended to a more general class of $(1+n)$-dimensional NSchEs with potentials

$$i\psi_t+\Delta\psi+F(\psi,\psi^*)+V(t,\vec{x})\psi=0, \tag{6}$$

where $F=F(\psi,\psi^*)$ is an arbitrary complex-valued smooth function of the variables ψ and ψ^*. We have already described all possible inequivalent forms of the parameter-function F (without any restriction on the dimension n) for which an equation of the form (6) with a some potential V has an extension of the maximal Lie invariance algebra. We believe that the classification method suggested in this paper can be effectively applied to complete the group classification in (6) for the small values of n. This method can be also a tool to investigate symmetries of other classes of PDEs, and we will attempt to prove general statements on its applicability.

Another direction for us to develop the above results is construction of both invariant and partially invariant exact solutions of equations having the form (1) by means of using found Lie symmetries, and knowledge of explicit forms for equivalence transformations (see Theorem 4 and Remark 8) allows us to reduced consideration of known stationary potentials to simpler x-free ones. We also plan to study conditional and generalized symmetries of (1) to find non-Lie exact solutions.

As it was shown by Carles,[3] the equivalence transformations (5) also give an easy and effective way to produce new results on existence, uniqueness, estimations, etc., of solutions for some equations (1) by means of using known results on other potentials.

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Symmetry of matrix-valued stochastic processes and noncolliding diffusion particle systems

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As an extension of the theory of Dyson's Brownian motion models for the standard Gaussian random-matrix ensembles, we report a systematic study of Hermitian matrix-valued processes and their eigenvalue processes associated with the chiral and nonstandard random-matrix ensembles. In addition to the noncolliding Brownian motions, we introduce a one-parameter family of temporally homogeneous noncolliding systems of the Bessel processes and a two-parameter family of temporally inhomogeneous noncolliding systems of Yor's generalized meanders and show that all of the ten classes of eigenvalue statistics in the Altland–Zirnbauer classification are realized as particle distributions in the special cases of these diffusion particle systems. As a corollary of each equivalence in distribution of a temporally inhomogeneous eigenvalue process and a noncolliding diffusion process, a stochastic-calculus proof of a version of the Harish–Chandra (Itzykson–Zuber) formula of integral over unitary group is established. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765215]

I. INTRODUCTION

It is interesting to consider today mathematical-physical sequences of the two classic papers[10,11] by Dyson of random matrix theory, which appeared sequentially in the same volume of the journal in 1962. In one of them,[11] following the early work of Wigner, he gave a logical foundation for his classification scheme of random-matrix ensembles based on the group representation theory of Weyl and established the standard (Wigner–Dyson) random matrix theory for the three ensembles called the Gaussian unitary, orthogonal, and symplectic ensembles (GUE, GOE, and GSE). He introduced in the other paper[10] the Hermitian matrix-valued Brownian motions, which are associated with these Gaussian random-matrix ensembles, and studied the stochastic processes of eigenvalues of the matrix-valued processes. Combining the standard perturbation theory of the quantum mechanics and a simple but essential consideration of the scaling of Brownian motions, he generally proved that the obtained eigenvalue processes are identified with the one-dimensional systems of Brownian particles with the repulsive two-body forces proportional to the inverse of distances between particles. These processes are now called Dyson's Brownian motion models $\mathbf{Y}(t)=(Y_1(t),Y_2(t),\ldots,Y_N(t))$ described by the stochastic differential equations

$$dY_i(t)=dB_i(t)+\frac{\beta}{2}\sum_{1\leqslant j\leqslant N,j\neq i}\frac{1}{Y_i(t)-Y_j(t)}dt,\quad t\in[0,\infty),1\leqslant i\leqslant N, \tag{1}$$

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with $\beta=1,2,4$ for GOE, GUE, and GSE, respectively, where $B_i(t), 1\leqslant i\leqslant N$ are independent one-dimensional standard Brownian motions. Dyson's classification scheme has been extended. In addition to the standard three random-matrix ensembles, their *chiral versions* (chGUE, chGOE, and chGSE) were studied in the particle physics of QCD associated with consideration of the gauge groups and quantum numbers called flavors.[54,53,27,51] After that extension, Altland and Zirnbauer introduced more four ensembles called the classes C, CI, D, and DIII for the solid-state physics of mesoscopic systems considering the particle-hole symmetry, which plays an important role in the Bogoliubov–de Gennes framework of the BCS mean-field theory of superconductivity.[1,2] These totally ten Gaussian ensembles are systematically argued by Zirnbauer[56] based on Cartan's classification scheme of symmetric spaces[23] and Efetov's supersymmetry theory.[13]

One consequence of a combination of the two papers by Dyson may be to give a systematic study of matrix-valued diffusion processes (i.e., diffusion processes in groups or algebraic spaces) and perform the classification of eigenvalue processes as generalization of Dyson's Brownian motion models. This line has been taken by Bru,[6,7] Grabiner,[21] König and O'Connell,[36] and others, and one purpose of the present paper is to clarify the relationship between statistics of (nonstandard) random matrix theory and stochastic processes of interacting diffusion particles in the type of Dyson's Brownian motion models studied in the probability theory. We will claim in Sec. II that the matrix-valued processes called the Wishart process by Bru[7] and the Laguerre process by König and O'Connell[36] are the stochastic versions of chGOE and chGUE, respectively, in the sense of Dyson,[10] and derive in Sec. III the diffusion processes describing the eigenvalue statistics of the classes C and D of Altland and Zirnbauer, following Bru's matrix-version of the stochastic calculus based on the Ito rule for differentials.

Due to the strong repulsive forces in the processes of the types of Dyson's Brownian motion models, particle collisions are suppressed. Impossibility of collision may be generally proved by the same argument as Bru, who showed that the collision time between two eigenvalues of the Wishart process is infinite ($\tau=+\infty$ a.s.).[6] For the $\beta=2$ (GUE) case of Dyson's Brownian motion model (1), if $\mathbf{Y}(0)\in\mathbb{W}_N^{\mathrm{A}}$, then $\mathbf{Y}(t)\in\mathbb{W}_N^{\mathrm{A}}$ for all $t>0$ with probability 1, where $\mathbb{W}_N^{\mathrm{A}}$ denotes the Weyl chamber of type A_{N-1}; $\mathbb{W}_N^{\mathrm{A}}=\{\mathbf{x}\in\mathbb{R}^N; x_1<x_2<\cdots<x_N\}$. Using the Karlin–McGregor formula[28,29] the transition density of the absorbing Brownian motion in $\mathbb{W}_N^{\mathrm{A}}$ from the state $\mathbf{x}$ at time s to the state $\mathbf{y}$ at time $t(>s)$ is given by the determinant

$$f^{\mathrm{A}}(t-s,\mathbf{y}|\mathbf{x})=\det_{1\leqslant i,j\leqslant N}[G^{\mathrm{A}}(t-s,y_j|x_i)],\quad \mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{A}}, \tag{2}$$

where each element is the Gaussian heat-kernel $G^{\mathrm{A}}(t,y|x)=e^{-(x-y)^2/2t}/\sqrt{2\pi t}$. Grabiner[21] pointed out that the transition probability density of process (1) with $\beta=2$ is given by

$$p^{\mathrm{A}}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{h^{\mathrm{A}}(\mathbf{x})}f^{\mathrm{A}}(t-s,\mathbf{y}|\mathbf{x})h^{\mathrm{A}}(\mathbf{y}),$$

where $h^{\mathrm{A}}(\mathbf{x})=\Pi_{1\leqslant i<j\leqslant N}(x_j-x_i)$. Since $h^{\mathrm{A}}(\mathbf{x})$ is a strictly positive harmonic function in $\mathbb{W}_N^{\mathrm{A}}$, this is regarded as the h-transform in the sense of Doob,[9] and it implies that the eigenvalue process of GUE is realized as the noncolliding Brownian motions (i.e., the h-transform of an absorbing Brownian motion in the Weyl chamber of type A_{N-1}). König and O'Connell also showed that the eigenvalue process of the Laguerre process, which corresponds to chGUE, is realized as the noncolliding system of the squared Bessel processes.[36] In Sec. IV, we show that the eigenvalue processes of random matrices in the symmetry classes C and D of Altland and Zirnbauer are realized as the noncolliding system of the *Brownian motions with an absorbing wall at the origin*[35] (i.e., the h-transform of an absorbing Brownian motion in the Weyl chamber of type C_N) and as the noncolliding system of the *reflecting Brownian motions* (i.e., the h-transform of an absorbing Brownian motion in the Weyl chamber of type D_N), respectively. These three kinds of systems are

discussed as special cases of a family of noncolliding systems of diffusion particles with one parameter $\nu > -1$, in which each particle is following the $d=2(\nu+1)$-dimensional Bessel process defined by the transition probability density[5,48]

$$G^{(\nu)}(t,y|x)=\frac{y^{\nu+1}}{x^{\nu}}\frac{1}{t}e^{-(x^2+y^2)/2t}I_{\nu}\left(\frac{xy}{t}\right) \quad \text{for} \quad x>0,y\geqslant 0,$$

$$G^{(\nu)}(t,y|0)=\frac{y^{2\nu+1}}{2^{\nu}\Gamma(\nu+1)t^{\nu+1}}e^{-y^2/2t} \quad \text{for} \quad y\geqslant 0, \tag{3}$$

where Γ denotes the Gamma function and I_{ν} is the modified Bessel function; $I_{\nu}(z)=\Sigma_{n=0}^{\infty}(z/2)^{2n+\nu}/\{\Gamma(n+1)\Gamma(\nu+n+1)\}$.

How can we realize other six eigenvalue processes in Altland–Zirnbauer's ten classes of random-matrix ensembles as well by noncolliding systems of diffusion processes? In our previous papers[31,32] we considered the situation that the noncolliding condition is imposed not forever but for a finite time-interval $(0,T]$ to define the temporally inhomogeneous noncolliding Brownian motions $\mathbf{X}(t)=(X_1(t),X_2(t),\ldots,X_N(t))$. Of course, we can see that $\mathbf{X}(t)\to\mathbf{Y}(t)$ in distribution as $T\to\infty$. We observed for the finite time-interval $t\in[0,T]$ that, if we set $\mathbf{X}(0)=\mathbf{Y}(0)=\mathbf{0}$ with $\mathbf{0}=(0,0,\ldots,0)\in\mathbb{R}^N$, then

$$P(\mathbf{X}(\cdot)\in d\mathbf{w})=\frac{C[\mathrm{A}]T^{\psi[\mathrm{A}]}}{C[\mathrm{A}']h^{\mathrm{A}}(\mathbf{w}(T))}P(\mathbf{Y}(\cdot)\in d\mathbf{w}), \tag{4}$$

where $C[\mathrm{A}]=(2\pi)^{N/2}\Pi_{i=1}^{N}\Gamma(i)$, $C[\mathrm{A}']=2^{N/2}\Pi_{i=1}^{N}\Gamma(i/2)$, and $\psi[\mathrm{A}]=N(N-1)/4$. This is regarded as a multivariate version of the Imhof relation in the probability theory,[25] since it implies the absolute continuity in distribution of the temporally homogeneous process $\mathbf{Y}(t)$ and the inhomogeneous process $\mathbf{X}(t)$ in $[0,T]$, but from the viewpoint of random matrix theory the important consequence of this equality is the fact that the process $\mathbf{X}(t)$ exhibits a transition in distribution from the eigenvalue statistics of GUE to that of GOE and thus the GOE distribution is realized at the final time $t=T$. In Sec. V, we develop this argument by replacing the Brownian motions $X_i(t),1\leqslant i\leqslant N$ by the *generalized meanders* with two parameters $(\nu,\kappa),\nu>-1,\kappa\in[0,2(\nu+1))$, introduced as the temporally inhomogeneous diffusions associated with the Bessel process by Yor,[55] whose transition probability density is given by

$$G_T^{(\nu,\kappa)}(s,x;t,y)=\frac{1}{h_T^{(\nu,\kappa)}(s,x)}G^{(\nu)}(t-s,y|x)h_T^{(\nu,\kappa)}(t,y) \tag{5}$$

for $0\leqslant s<t\leqslant T,x,y\geqslant 0$ with $h_T^{(\nu,\kappa)}(t,x)=\int_0^{\infty}dz\ G^{(\nu)}(T-t,z|x)z^{-\kappa}$. By choosing the two parameters (ν,κ) appropriately, this family of noncolliding systems of generalized meanders provides such diffusion processes that exhibit the transitions from chGUE to chGOE and from class C to class CI. We will also consider the processes, in which the noncolliding condition collapses at the final time $t=T$ in the ways that all particles collide simultaneously or only pairwise collisions occur. In the special cases in the latter situation, we have the processes showing the transitions from GUE to GSE, from chGUE to chGSE, and from class D to class DIII.

The present study of the temporally inhomogeneous noncolliding diffusion processes gives two kinds of by-products. (i) Topology of path-configurations of our processes on the spatio-temporal plane $\mathbb{R}\times[0,T]$ is determined by the conditions at $t=0$ and $t=T$. We will be able to discuss the topology of random directed polymer networks[8,14] using the random matrix theory. Such correspondence between the topology of path-configurations and random-matrix ensembles is recently used by Sasamoto and Imamura to analyze one-dimensional polynuclear growth models.[49] (ii) A variety of versions of Harish–Chandra (Itzykson–Zuber) formulas of integrals

over unitary groups[22,26] are derived as corollaries of the equivalence in distribution of the eigenvalue processes of matrix-valued processes and noncolliding diffusion processes. Other remarks are given in Sec. VI.

II. BRU'S THEOREM

A. Hermitian matrix-valued stochastic processes

We denote the space of $N\times N$ Hermitian matrices by $\mathcal{H}(N)$, the group of $N\times N$ unitary matrices by $\mathrm{U}(N)$, and the group of $N\times N$ real orthogonal matrices by $\mathrm{O}(N)$. We also use the notations $\mathcal{S}(N)$ and $\mathcal{A}(N)$ for the spaces of $N\times N$ real symmetric and real antisymmetric matrices, respectively. We consider complex-valued processes $\xi_{ij}(t)\in\mathbb{C}, 1\leqslant i,j\leqslant N, t\in[0,\infty)$, with the condition $\xi_{ji}(t)^*=\xi_{ij}(t)$, and define the matrix-valued processes by $\Xi(t)=(\xi_{ij}(t))_{1\leqslant i,j\leqslant N}\in\mathcal{H}(N)$. We denote by $U(t)=(u_{ij}(t))_{1\leqslant i,j\leqslant N}$ the family of unitary matrices which diagonalize $\Xi(t)$ so that

$$U(t)^\dagger\Xi(t)U(t)=\Lambda(t)=\mathrm{diag}\{\lambda_1(t),\lambda_2(t),\ldots,\lambda_N(t)\},$$

where $\{\lambda_i(t)\}_{i=1}^N$ are eigenvalues of $\Xi(t)$ and we assume their increasing order

$$\lambda_1(t)\leqslant\lambda_2(t)\leqslant\cdots\leqslant\lambda_N(t). \tag{6}$$

Define $\Gamma_{ij}(t), 1\leqslant i,j\leqslant N$, by $\Gamma_{ij}(t)dt=(U(t)^\dagger d\Xi(t)U(t))_{ij}(U(t)^\dagger d\Xi(t)U(t))_{ji}$, where $d\Xi(t)=(d\xi_{ij})_{1\leqslant i,j\leqslant N}$. We denote by $\mathbf{1}(\omega)$ the indicator function: $\mathbf{1}(\omega)=1$ if the condition ω is satisfied, and $\mathbf{1}(\omega)=0$ otherwise. The following theorem is proved for the stochastic process of eigenvalues $\boldsymbol{\lambda}(t)=(\lambda_1(t),\lambda_2(t),\ldots,\lambda_N(t))$.

Theorem 1: *Assume that $\xi_{ij}(t), 1\leqslant i<j\leqslant N$ are continuous semimartingales. The process $\boldsymbol{\lambda}(t)=(\lambda_1(t),\lambda_2(t),\ldots,\lambda_N(t))$ satisfies the stochastic differential equations*

$$d\lambda_i(t)=dM_i(t)+dJ_i(t),\quad 1\leqslant i\leqslant N,$$

where $M_i(t)$ is the martingale with quadratic variation $\langle M_i\rangle_t=\int_0^t\Gamma_{ii}(s)ds$ and $J_i(t)$ is the process with finite variation given by

$$dJ_i(t)=\sum_{j=1}^N\frac{1}{\lambda_i(t)-\lambda_j(t)}\mathbf{1}(\lambda_i(t)\neq\lambda_j(t))\Gamma_{ij}(t)dt+d\Upsilon_i(t),$$

where $d\Upsilon_i(t)$ is the finite-variation part of $(U(t)^\dagger d\Xi(t)U(t))_{ii}$.

Since this theorem is obtained by simple generalization of Theorem 1 in Bru,[6] we call it Bru's theorem here. A key point to derive the theorem is applying the Ito rule for differentiating the product of matrix-valued semimartingales: If X and Y are $N\times N$ matrices with semimartingale elements, then

$$d(X^\dagger Y)=(dX)^\dagger Y+X^\dagger(dY)+(dX)^\dagger(dY).$$

B. Four basic examples

Let $\mathbb{N}=\{0,1,2,..\}$ and assume $\nu\in\mathbb{N}$. Let $B_{ij}(t)$, $\tilde{B}_{ij}(t)$, $1\leqslant i\leqslant N+\nu$, $1\leqslant j\leqslant N$ be independent one-dimensional standard Brownian motions. For $1\leqslant i,j\leqslant N$ we set

$$s_{ij}(t)=\begin{cases}\frac{1}{\sqrt{2}}B_{ij}(t), & \text{if } i<j,\\ B_{ii}(t), & \text{if } i=j,\\ \frac{1}{\sqrt{2}}B_{ji}(t), & \text{if } i>j,\end{cases}\quad\text{and}\quad a_{ij}(t)=\begin{cases}\frac{1}{\sqrt{2}}\widetilde{B}_{ij}(t), & \text{if } i<j,\\ 0, & \text{if } i=j,\\ -\frac{1}{\sqrt{2}}\widetilde{B}_{ji}(t), & \text{if } i>j.\end{cases}$$

Here we show four basic examples of Hermitian matrix-valued processes and applications of Theorem 1.

(i) The first example of the Hermitian matrix-valued process is defined by

$$\Xi(t)=(\xi_{ij}(t))_{1\leqslant i,j\leqslant N}=(s_{ij}(t)+\sqrt{-1}a_{ij}(t))_{1\leqslant i,j\leqslant N},\quad t\in[0,\infty).$$

By definition $d\xi_{ij}(t)d\xi_{k\ell}(t)=\delta_{i\ell}\delta_{jk}dt$, $1\leqslant i,j,k,\ell\leqslant N$, and thus $\Gamma_{ij}(t)=1$. Therefore $\boldsymbol{\lambda}(t)$ solves the equations of Dyson's Brownian motion model (1) with $\beta=2$.

(ii) The second example is given by

$$\Xi(t)=(s_{ij}(t))_{1\leqslant i,j\leqslant N}\in\mathcal{S}(N),\quad t\in[0,\infty).$$

In this case $d\xi_{ij}(t)d\xi_{k\ell}(t)=(\delta_{i\ell}\delta_{jk}+\delta_{ik}\delta_{j\ell})dt/2$, $1\leqslant i,j,k,\ell\leqslant N$, and thus $\Gamma_{ij}(t)dt=(1+\delta_{ij})dt/2$, $1\leqslant i,j\leqslant N$. Then $\boldsymbol{\lambda}(t)$ solves (1) with $\beta=1$.

(iii) We consider an $(N+\nu)\times N$ matrix-valued process by $M(t)=(B_{ij}(t)+\sqrt{-1}\widetilde{B}_{ij})_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$ and define the $N\times N$ Hermitian matrix-valued process by

$$\Xi(t)=M(t)^{\dagger}M(t),\quad t\in[0,\infty).\tag{7}$$

Since the matrix $\Xi(t)$ is positive definite, the eigenvalues are non-negative. By definition we see that the finite-variation part of $d\xi_{ij}(t)$ is $2(N+\nu)\delta_{ij}dt$ and $d\xi_{ij}(t)d\xi_{k\ell}(t)=2(\xi_{i\ell}(t)\delta_{jk}+\xi_{kj}(t)\delta_{i\ell})dt$, $1\leqslant i,j,k,\ell\leqslant N$, which imply that $d\Upsilon_i(t)=2(N+\nu)dt$ and $\Gamma_{ij}(t)=2(\lambda_i(t)+\lambda_j(t))$, $1\leqslant i,j\leqslant N$. Since $\langle M_i\rangle_t=\int_0^t 4\lambda_i(s)ds$, the stochastic differential equations for $\boldsymbol{\lambda}(t)$ are given by

$$d\lambda_i(t)=2\sqrt{\lambda_i(t)}dB_i(t)+\beta\left\{(N+\nu)+\sum_{1\leqslant j\leqslant N:j\neq i}\frac{\lambda_i(t)+\lambda_j(t)}{\lambda_i(t)-\lambda_j(t)}\right\}dt,\quad 1\leqslant i\leqslant N,\tag{8}$$

with $\beta=2$.

(iv) Set $B(t)=(B_{ij}(t))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$ and define

$$\Xi(t)=B(t)^{T}B(t)\in\mathcal{S}(N),\quad t\in[0,\infty).\tag{9}$$

We see that the finite-variation part of $d\xi_{ij}(t)$ is $(N+\nu)\delta_{ij}dt$ and $d\xi_{ij}(t)d\xi_{k\ell}(t)=(\xi_{ik}(t)\delta_{j\ell}+\xi_{i\ell}(t)\delta_{jk}+\xi_{jk}(t)\delta_{i\ell}+\xi_{j\ell}(t)\delta_{ik})dt$, $1\leqslant i,j,k,\ell\leqslant N$. Then $d\Upsilon_i(t)=(N+\nu)dt$ and $\Gamma_{ij}(t)=(\lambda_i(t)+\lambda_j(t))(1+\delta_{ij})$, $1\leqslant i,j\leqslant N$. The equations for $\boldsymbol{\lambda}(t)$ are given by (8) with $\beta=1$.

The process (9) was called the Wishart process and studied as matrix generalization of squared Bessel process by Bru.[7] König and O'Connell[36] called the process (7) the Laguerre process and studied its eigenvalue process (8) with $\beta=2$.

C. Relation with the standard and chiral random matrix theories

Here we assume that $B_{ij}(0)=\widetilde{B}_{ij}(0)=0$ for all $1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N$, and thus the initial distribution of $\Xi(t)$ is the pointmass on an $N\times N$ zero matrix O; $\mu(\Xi\in\cdot;0)=\delta_O$. In this case the distributions of $\Xi(t)$'s are related with those studies in the standard (Wigner–Dyson) random matrix theory[40] and the chiral random matrix theory.[54,53,27,51]

(i) *Example (i) and GUE:* For GUE with variance $\sigma^2=t$ of random matrices in the space $\mathcal{H}(N)\cong\mathbb{R}^{d[\mathrm{A}]}$ with $d[\mathrm{A}]=N^2$, the probability density of eigenvalues $\boldsymbol{\lambda}$ in the condition (6) is given as[40]

$$q^{\mathrm{GUE}}(\boldsymbol{\lambda};t)=\frac{t^{-d[\mathrm{A}]/2}}{C[\mathrm{A}]}\exp\left\{-\frac{|\boldsymbol{\lambda}|^2}{2t}\right\}h^{\mathrm{A}}(\boldsymbol{\lambda})^2,$$

where $|\boldsymbol{\lambda}|^2=\Sigma_{i=1}^N\lambda_i^2$. For (1) with $\beta=2$, $p^{\mathrm{A}}(0,\mathbf{0};t,\boldsymbol{\lambda})=q^{\mathrm{GUE}}(\boldsymbol{\lambda};t)$, $t>0$.

(ii) *Example (ii) and GOE:* The probability density of eigenvalues $\boldsymbol{\lambda}$ with the condition (6) is given as[40]

$$q^{\mathrm{GOE}}(\boldsymbol{\lambda};t)=\frac{t^{-d[\mathrm{A}']/2}}{C[\mathrm{A}']}\exp\left\{-\frac{|\boldsymbol{\lambda}|^2}{2t}\right\}h^{\mathrm{A}}(\boldsymbol{\lambda})$$

for GOE with variance $\sigma^2=t$ in $\mathcal{S}(N)\cong\mathbb{R}^{d[\mathrm{A}']}$, $d[\mathrm{A}']=N(N+1)/2$. If we denote by $p^{\mathrm{A}'}(s,\boldsymbol{\lambda};t,\boldsymbol{\lambda}')$ the transition probability density of the process (1) with $\beta=1$ from $\boldsymbol{\lambda}$ at time s to $\boldsymbol{\lambda}'$ at time $t(>s)$, then $p^{\mathrm{A}'}(0,\mathbf{0};t,\boldsymbol{\lambda})=q^{\mathrm{GOE}}(\boldsymbol{\lambda};t)$, $t>0$.

(iii) *Example (iii) and chiral GUE:* We denote by $\mathcal{M}(N+\nu,N;\mathbb{C})$ and $\mathcal{M}(N+\nu,N;\mathbb{R})$ the spaces of $(N+\nu)\times N$ complex and real matrices, respectively. We see that $\mathcal{M}(N+\nu,N;\mathbb{C})\cong\mathbb{R}^{2N(N+\nu)}$ and write its volume element as $\mathcal{V}(dM),M\in\mathcal{M}(N+\nu,N;\mathbb{C})$. The chiral Gaussian unitary ensemble (chGUE) with variance t is the ensemble of matrices $M\in\mathcal{M}(N+\nu,N;\mathbb{C})$ with the probability density

$$\mu_\nu^{\mathrm{chGUE}}(M;t)=\frac{t^{-N(N+\nu)/2}}{(2\pi)^{N(N+\nu)}}\exp\left\{-\frac{1}{2t}\mathrm{Tr}\,M^\dagger M\right\} \tag{10}$$

with respect to $\mathcal{V}(dM)$. It is known[24] that any matrix $M\in\mathcal{M}(N+\nu,N;\mathbb{C})$ has a family of pairs $(U,V),U\in\mathrm{U}(N+\nu),V\in\mathrm{U}(N)$, which transform M as $M=U^\dagger KV$, where $K\in\mathcal{M}(N+\nu,N;\mathbb{R})$ is in the form

$$K=\begin{pmatrix}\hat{K}\\ O\end{pmatrix}\quad\text{with}\quad\hat{K}=\mathrm{diag}\{\kappa_1,\kappa_2,...,\kappa_N\},\quad\kappa_i\geqslant 0,1\leqslant i\leqslant N,$$

and the $\nu\times N$ zero matrix O. We assume that U and V are chosen so that

$$0\leqslant\kappa_1\leqslant\kappa_2\leqslant\cdots\leqslant\kappa_N. \tag{11}$$

The matrices (U,K,V) can be regarded as "polar coordinates" in the space $\mathcal{M}(N+\nu,N;\mathbb{C})$. We have $M^\dagger M=V^\dagger\Lambda V$, where $\Lambda=\mathrm{diag}\{\lambda_1,\lambda_2,...,\lambda_N\}$ with the relations $\lambda_i=\kappa_i^2$, $1\leqslant i\leqslant N$. Then $\boldsymbol{\kappa}=(\kappa_1,\kappa_2,\ldots,\kappa_N)$ is a set of nonnegative square roots of the eigenvalues of $M^\dagger M$. Let $d\mu(U,V)$ be the Haar measure of the space $\mathrm{U}(N+\nu)\times\mathrm{U}(N)$ normalized as $\int_{\mathrm{U}(N+\nu)\times\mathrm{U}(N)}d\mu(U,V)=1$ and $d\boldsymbol{\kappa}=\Pi_{i=1}^N d\kappa_i$. Then we can show that

$$\mathcal{V}(dM)=\frac{(2\pi)^{N(N+\nu)}}{C_\nu}h^{((2\nu+1)/2)}(\boldsymbol{\kappa})^2 d\boldsymbol{\kappa}d\mu(U,V), \tag{12}$$

where $C_\nu=2^{N(N+\nu-1)}\Pi_{i=1}^N\{\Gamma(i)\Gamma(i+\nu)\}$ and

$$h^{(\alpha)}(\boldsymbol{\kappa})=\prod_{1\leqslant i<j\leqslant N}(\kappa_j^2-\kappa_i^2)\prod_{k=1}^N\kappa_k^\alpha.$$

For any pair of unitary matrices $U\in\mathrm{U}(N+\nu)$ and $V\in\mathrm{U}(N)$, the probability $\mu_\nu^{\mathrm{chGUE}}(M;t)\mathcal{V}(dM)$ is invariant under the automorphism $M\to U^\dagger MV$. By integrating over $d\mu(U,V)$, we obtain the probability density of $\boldsymbol{\kappa}$ with the condition (11) as[54,53,27,51]

$$q_\nu^{\mathrm{chGUE}}(\boldsymbol{\kappa};t)=\frac{t^{-N(N+\nu)}}{C_\nu}\exp\left\{-\frac{|\boldsymbol{\kappa}|^2}{2t}\right\}h^{((2\nu+1)/2)}(\boldsymbol{\kappa})^2.$$

König and O'Connell[36] studied the process (8) with $\beta=2$ as a multivariate version of squared Bessel process. Here we consider the multivariate version of Bessel process by extracting the square roots of eigenvalues $\lambda_i(t)\geqslant 0$ of $\Xi(t)=M(t)^\dagger M(t)$. Setting $\kappa_i(t)=\sqrt{\lambda_i(t)}\geqslant 0, 1\leqslant i\leqslant N$ in (8) with $\beta=2$ and applying the Ito rule for differentials, we find that $\boldsymbol{\kappa}(t)$ solves the stochastic differential equations

$$dZ_i(t)=dB_i(t)+\frac{\beta}{2}\left[\frac{\gamma}{Z_i(t)}+\sum_{j:j\neq i}\left\{\frac{1}{Z_i(t)-Z_j(t)}+\frac{1}{Z_i(t)+Z_j(t)}\right\}\right]dt,\quad 1\leqslant i\leqslant N, \tag{13}$$

with $(\beta,\gamma)=(2,(2\nu+1)/2)$. If we denote the transition probability density of this process by $p^{(\nu)}(s,\cdot\,;t,\cdot\,)$ for $0\leqslant s<t<\infty$, then

$$p^{(\nu)}(0,\mathbf{0};t,\boldsymbol{\kappa})=q_\nu^{\mathrm{chGUE}}(\boldsymbol{\kappa};t),\quad t>0. \tag{14}$$

(iv) *Example (iv) and chiral GOE:* We can see $\mathcal{M}(N+\nu,N;\mathbb{R})\cong\mathbb{R}^{N(N+\nu)}$. The chiral Gaussian orthogonal ensemble (chGOE) with variance t is the ensemble of matrices $B\in\mathcal{M}(N+\nu,N;\mathbb{R})\subset\mathcal{M}(N+\nu,N;\mathbb{C})$ with the probability density

$$\mu_\nu^{\mathrm{chGOE}}(B;t)=\frac{t^{-N(N+\nu)/2}}{(2\pi)^{N(N+\nu)/2}}\exp\left\{-\frac{1}{2t}\mathrm{Tr}\,B^TB\right\} \tag{15}$$

with respect to the volume element $\mathcal{V}'(dB)$ of $\mathcal{M}(N+\nu,N;\mathbb{R})$. We can show that

$$\mathcal{V}'(dB)=\frac{(2\pi)^{N(N+\nu)/2}}{C_{\nu,\nu+1}}h^{(\nu)}(\boldsymbol{\kappa})d\boldsymbol{\kappa}d\mu(U,V), \tag{16}$$

where $d\mu(U,V)$ is the normalized Haar measure of the space $\mathrm{O}(N+\nu)\times\mathrm{O}(N)$ and we have used the notation $C_{\nu,\kappa}=2^{N(N+2\nu-\kappa-1)/2}\pi^{-N/2}\Pi_{i=1}^N\{\Gamma(i/2)\Gamma((i+2\nu+1-\kappa)/2)\}$ and thus $C_{\nu,\nu+1}=2^{N(N+\nu-2)/2}\pi^{-N/2}\Pi_{i=1}^N\{\Gamma(i/2)\Gamma((i+\nu)/2)\}$. The probability density of $\boldsymbol{\kappa}$ with (11) is given as[54,53,27,51]

$$q_\nu^{\mathrm{chGOE}}(\boldsymbol{\kappa};t)=\frac{t^{-N(N+\nu)/2}}{C_{\nu,\nu+1}}\exp\left\{-\frac{|\boldsymbol{\kappa}|^2}{2t}\right\}h^{(\nu)}(\boldsymbol{\kappa}).$$

By setting $\kappa_i(t)=\sqrt{\lambda_i(t)}, 1\leqslant i\leqslant N$ in (8) with $\beta=1$, we can show that $\boldsymbol{\kappa}(t)=(\kappa_1(t),\kappa_2(t),\ldots,\kappa_N(t))$ solves (13) with $(\beta,\gamma)=(1,\nu)$. If we denote the transition probability density of this process $\boldsymbol{\kappa}(t)$ by $p^{(\nu)'}(s,\cdot\,;t,\cdot\,)$ for $0\leqslant s<t<\infty$, then $p^{(\nu)'}(0,\mathbf{0};t,\boldsymbol{\kappa})=q_\nu^{\mathrm{chGOE}}(\boldsymbol{\kappa};t)$, $t>0$.

III. HERMITIAN MATRIX-VALUED PROCESSES WITH ADDITIONAL SYMMETRIES

A. Subspaces of unitary and Hermitian matrices

The Pauli spin matrices are defined as

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-\sqrt{-1}\\\sqrt{-1}&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

which satisfy the algebra $\sigma_\mu^2=I_2$, $\mu=1,2,3$, and $\sigma_\mu\sigma_\rho=\sqrt{-1}\Sigma_{\omega=1}^3\varepsilon_{\mu\rho\omega}\sigma_\omega$ for $1\leqslant\mu\neq\rho\leqslant 3$, where I_N denotes the $N\times N$ unit matrix and $\varepsilon_{\mu\rho\omega}$ the totally antisymmetric unit tensor. They give the infinitesimal generators $\{X_\mu\}$ of SU(2) by $X_\mu=\sqrt{-1}\sigma_\mu/2$. For $N\geqslant 2$, define the $2N\times 2N$ matrices $\Sigma_\mu=I_N\otimes\sigma_\mu$, $\mu=1,2,3$. The matrices $\{\Sigma_\mu\}$ satisfy the same algebra as $\{\sigma_\mu\}$. We will use σ_0 to represent I_2.

We introduce six spaces of matrices as subspaces of $\mathcal{H}(2N)$,

$$\mathcal{H}_{\mu\pm}(2N)=\{H\in\mathcal{H}(2N):H^T\Sigma_\mu=\pm\Sigma_\mu H\},\quad \mu=1,2,3.$$

It is easy to see that $\mathcal{H}_{3+}(2N)=\mathcal{S}(2N)$ and $\mathcal{H}_{3-}(2N)=\sqrt{-1}\mathcal{A}(2N)$. Since we have already studied the matrix-valued process in $\mathcal{S}(N)$ as the example (ii) in Sec. II B, we will consider here the five subspaces of $\mathcal{H}(2N)$; $\sqrt{-1}\mathcal{A}(2N)$ and $\{\mathcal{H}_{\mu\sigma}(2N)\}$ with $\mu=1,2,\sigma=\pm$. We also introduce the three subspaces of $\mathrm{U}(2N)$:

$$\mathrm{U}_0(2N)=\{U\in\mathrm{U}(2N):U^TU=\Sigma_1\},$$

$$\mathrm{U}_\mu(2N)=\{U\in\mathrm{U}(2N):U^T\Sigma_\mu U=\Sigma_\mu^T\},\quad \mu=1,2.$$

The conditions imply that these subspaces, $\mathcal{H}_{\mu\sigma}(2N)$ and $\mathrm{U}_\mu(2N)$, have additional symmetries compared to $\mathcal{H}(2N)$ and $\mathrm{U}(2N)$. Concerning the eigenvalues and eigenvectors of the Hermitian matrices, the following lemma may be easily proved.

Lemma 2: Assume that Ω *denotes a diagonal matrix in the form* $\mathrm{diag}\{\omega_1,\omega_2,\ldots,\omega_N\}$ *with* $\omega_1\leqslant\omega_2\leqslant\cdots\leqslant\omega_N$.

(i) *Any* $H\in\sqrt{-1}\mathcal{A}(2N)$ *can be diagonalized by* $U\in\mathrm{U}_0(2N)$ *as* $U^\dagger HU=\Omega\otimes\sigma_3$.
(ii) *For* $\mu=1,2$ *any* $H\in\mathcal{H}_{\mu+}(2N)$ *can be diagonalized by* $U\in\mathrm{U}_\mu(2N)$ as $U^\dagger HU=\Omega\otimes\sigma_0$.
(iii) *For* $\mu=1,2$ *any* $H\in\mathcal{H}_{\mu-}(2N)$ *can be diagonalized by* $U\in\mathrm{U}_\mu(2N)$ as $U^\dagger HU=\Omega\otimes\sigma_3$.

Remark:

(a) Observing the pairing of eigenvalues in a way, $(\omega_i,-\omega_i),1\leqslant i\leqslant N$, for $\sqrt{-1}\mathcal{A}(2N)$ stated in Lemma 2 (i), the Gaussian random-matrix ensemble of antisymmetric Hermitian matrices was discussed by Mehta in Sec. 3.4 of Ref. 40.

(b) The condition for $\mathrm{U}_2(2N)$ addition to the unitarity is equivalent with $J=UJU^T$, where

$$J=I_N\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix}.$$

Then $\mathrm{U}_2(2N)$ forms the N-dimensional symplectic group. That is, $\mathrm{U}_2(2N)=\mathrm{Sp}(N,\mathbb{C})\cap\mathrm{U}(2N)$. (It is called the unitary-symplectic group $\mathrm{USp}(2N)$ in Ref. 19.) The matrices $H\in\mathcal{H}_{2+}(2N)$ are said to be *self-dual Hermitian matrices* in the random matrix theory.[40] The pairwise degeneracy stated in Lemma 2 (ii) for $\mathcal{H}_{2+}(2N)$ is known as the *Kramers doublet* in the quantum mechanics.

(c) The condition for $\mathcal{H}_{2-}(2N)$ addition to Hermiticity is rewritten as $H^TJ+JH=0$, which means that $H\in\mathcal{H}_{2-}(2N)$ satisfies the symplectic Lie algebra (see, for example, Ref. 18), that is, $\mathcal{H}_{2-}(2N)=\mathfrak{sp}(2N,\mathbb{C})\cap\mathcal{H}(2N)$. Similarly, we can see $\mathcal{H}_{1-}(2N)=\mathfrak{so}(2N,\mathbb{C})\cap\mathcal{H}(2N)$, where $\mathfrak{so}(2N,\mathbb{C})$ denotes the orthogonal Lie algebra. We can also see that $\mathrm{U}_1(2N)=\mathrm{SO}(2N,\mathbb{C})\cap\mathrm{U}(2N)$, where $\mathrm{SO}(2N,\mathbb{C})$ denotes the orthogonal Lie group.

(d) We can see that $\mathcal{H}_{\mu-}(2N)\cong\hat{\mathcal{H}}_{\mu-}(2N)$, $\mu=1,2$, where

$$\hat{\mathcal{H}}_{1-}(2N)=\left\{H=\begin{pmatrix}H_1&A_2\\A_2^\dagger&-H_1^T\end{pmatrix}:H_1\in\mathcal{H}(N),A_2\in\mathcal{A}(N;\mathbb{C})\right\},$$

$$\hat{\mathcal{H}}_{2-}(2N)=\left\{H=\begin{pmatrix}H_1&A_2\\A_2^\dagger&-H_1^T\end{pmatrix}:H_1\in\mathcal{H}(N),A_2\in\mathcal{S}(N;\mathbb{C})\right\},$$

where $\mathcal{S}(N;\mathbb{C})$ and $\mathcal{A}(N;\mathbb{C})$ denote the spaces of the $N\times N$ complex symmetric and complex antisymmetric matrices, respectively. Altland and Zirnbauer studied $\hat{\mathcal{H}}_{2-}(2N)$ and $\hat{\mathcal{H}}_{1-}(2N)$ as the sets of the Hamiltonians in the Bogoliubov–de Gennes formalism for the BCS mean-field theory of superconductivity, where the pairing of positive and negative eigenvalues $(\omega_i,-\omega_i)$, $1\leqslant i\leqslant N$, stated in Lemma 2 (iii) for $\mu=1$ and 2 represents the particle-hole symmetry in the Bogoliubov–de Gennes theory. They called $\hat{\mathcal{H}}_{2-}(2N)$ and

$\hat{\mathcal{H}}_{1-}(2N)$ the sets of Hermitian matrices in the symmetry classes C and D,[56,1,2] since $\mathfrak{sp}(2N,\mathbb{C})=\mathrm{C}_N$ and $\mathfrak{so}(2N,\mathbb{C})=\mathrm{D}_N$ in Cartan's notations (see Ref. 23).

B. Representation using Pauli matrices and application of Bru's theorem

Let $B_{ij}^{\rho}(t)$, $\tilde{B}_{ij}^{\rho}(t)$, $0\leqslant\rho\leqslant 3$, $1\leqslant i\leqslant j\leqslant N$ be independent one-dimensional standard Brownian motions starting from the origin. Put

$$s_{ij}^{\rho}(t)=\begin{cases}\dfrac{1}{\sqrt{2}}B_{ij}^{\rho}(t), & \text{if } i<j,\\ B_{ii}^{\rho}(t), & \text{if } i=j,\end{cases}\quad\text{and}\quad a_{ij}^{\rho}(t)=\begin{cases}\dfrac{1}{\sqrt{2}}\tilde{B}_{ij}^{\rho}(t), & \text{if } i<j,\\ 0, & \text{if } i=j,\end{cases}\tag{17}$$

with $s_{ij}^{\rho}(t)=s_{ji}^{\rho}(t)$ and $a_{ij}^{\rho}(t)=-a_{ji}^{\rho}(t)$ for $i>j$ and define $s^{\rho}(t)=(s_{ij}^{\rho}(t))_{1\leqslant i,j\leqslant N}\in\mathcal{S}(N)$, $t\in[0,\infty)$ and $a^{\rho}(t)=(a_{ij}^{\rho}(t))_{1\leqslant i,j\leqslant N}\in\mathcal{A}(N)$, $t\in[0,\infty)$, for $0\leqslant\rho\leqslant 3$.

We can see that the Hermitian matrix-valued process given as the first example (i) in Sec. II B can be represented, if we double the size of matrix to $2N$, as $\Xi(t)=\Sigma_{\rho=0}^{3}\{(s^{\rho}(t)\otimes\sigma_{\rho})+\sqrt{-1}(a^{\rho}(t)\otimes\sigma_{\rho})\}$. By choosing four terms in the eight terms, we define the following four different types of $2N\times 2N$ Hermitian matrix-valued processes:

$$\Xi_{\mu\sigma}(t)=\sum_{\rho=0}^{3}(\xi_{\mu\sigma}^{\rho}(t)\otimes\sigma_{\rho})\in\mathcal{H}_{\mu\sigma}(2N)\quad\text{for}\quad\mu=1,2,\quad\sigma=\pm,$$

where

$$\xi_{\mu+}^{\rho}(t)=\begin{cases}s^{\rho}(t) & \text{if } \mu=1,\ \rho\neq 3 \text{ or } \mu=2,\ \rho=0,\\ \sqrt{-1}a^{\rho}(t) & \text{if } \mu=1,\ \rho=3 \text{ or } \mu=2,\ \rho\neq 0,\end{cases}$$

$$\xi_{\mu-}^{\rho}(t)=\begin{cases}\sqrt{-1}a^{\rho}(t) & \text{if } \mu=1,\ \rho\neq 3 \text{ or } \mu=2,\ \rho=0,\\ s^{\rho}(t) & \text{if } \mu=1,\ \rho=3 \text{ or } \mu=2,\ \rho\neq 0.\end{cases}$$

We apply Theorem 1 to the five processes, $\sqrt{-1}\mathcal{A}(2N)$ and $\{\Xi_{\mu\sigma}(t)\}$ with $\mu=1,2,\sigma=\pm$. The results are listed below.

(a) $\sqrt{-1}\mathcal{A}(2N)$: Since $\Gamma_{ij}(t)=\{1-((\Sigma_1)_{ij})^2\}/2$, $1\leqslant i,j\leqslant 2N$, the equations of non-negative eigenvalues are

$$d\omega_i(t)=\frac{1}{\sqrt{2}}dB_i(t)+\frac{1}{2}\sum_{j:1\leqslant j\leqslant N,j\neq i}\left\{\frac{1}{\omega_i(t)-\omega_j(t)}+\frac{1}{\omega_i(t)+\omega_j(t)}\right\}dt,\quad 1\leqslant i\leqslant N.$$

By changing the time unit as $t\to 2t$, this equation can be identified with (13) with $(\beta,\gamma)=(2,0)$.

(b) $\mathcal{H}_{1+}(2N)$: Since $\Gamma_{ij}(t)=\{1+((\Sigma_1)_{ij})^2\}$, $1\leqslant i,j\leqslant 2N$, the distinct eigenvalues solve Dyson's Brownian motion model (1) with $\beta=4$.

(c) $\mathcal{H}_{1-}(2N)$: We see $\Gamma_{ij}(t)=\{1-((\Sigma_1)_{ij})^2\}$, $1\leqslant i,j\leqslant 2N$. Then the non-negative eigenvalues solve Eq. (13) with $(\beta,\gamma)=(2,0)$.

(d) $\mathcal{H}_{2+}(2N)$: Since $\Gamma_{ij}(t)=\{1+((\Sigma_2)_{ij})^2\}$, $1\leqslant i,j\leqslant 2N$, the distinct eigenvalues solve the Eq. (1) with $\beta=4$.

(e) $\mathcal{H}_{2-}(2N)$: We can see $\Gamma_{ij}(t)=\{1-((\Sigma_2)_{ij})^2\}$, $1\leqslant i,j\leqslant 2N$. Then the non-negative eigenvalues solve Eq. (13) with $(\beta,\gamma)=(2,1)$.

C. Relation with standard and nonstandard random matrix theories

(i) The eigenvalues of any matrix in the space $\mathcal{H}_{2+}(2N)\cong\mathbb{R}^{d[\mathrm{A}'']}$ with $d[\mathrm{A}'']=N(2N-1)$ are pairwise degenerated (the Kramers doublets) as $\boldsymbol{\lambda}=(\omega_1,\omega_1,\omega_2,\omega_2,\ldots,\omega_N,\omega_N)$. We assume that the N distinct eigenvalues are always arranged in the increasing order $\omega_1\leqslant\omega_2\cdots\leqslant\omega_N$. For GSE with variance t, the probability density of the N distinct eigenvalues in this ordering is given by[40]

$$q^{\mathrm{GSE}}(\boldsymbol{\omega};t)=\frac{t^{-d[\mathrm{A}'']/2}}{C[\mathrm{A}'']}\exp\left\{-\frac{|\boldsymbol{\omega}|^2}{2t}\right\}h^{\mathrm{A}}(\boldsymbol{\omega})^4,$$

where $C[\mathrm{A}'']=(2\pi)^{N/2}\Pi_{i=1}^{N}\Gamma(2i)$. If we denote the transition probability density of the process (1) with $\beta=4$ by $p^{\mathrm{A}''}(s,\cdot\,;t,\cdot\,)$ for $0\leqslant s<t<\infty$, then $p^{\mathrm{A}''}(0,\mathbf{0};t,\boldsymbol{\omega})=q^{\mathrm{GSE}}(\boldsymbol{\omega};t)$, $t>0$.

(ii) We can see that $\mathcal{H}_{2-}(2N)\cong\mathbb{R}^{d[\mathrm{C}]}$ and $\mathcal{H}_{1-}(2N)\cong\mathbb{R}^{d[\mathrm{D}]}$ with $d[\mathrm{C}]=N(2N+1)$ and $d[\mathrm{D}]=N(2N-1)$. The probability densities of the processes $\Xi_{2-}(t)$ and $\Xi_{1-}(t)$ with respect to the volume elements $\mathcal{V}(dH)$ of $\mathcal{H}_{2-}(2N)$ and $\mathcal{V}'(dH)$ of $\mathcal{H}_{1-}(2N)$ are given by

$$\mu^{\mathrm{C}}(H;t)=\frac{t^{-d[\mathrm{C}]/2}}{c[\mathrm{C}]}\exp\left\{-\frac{1}{4t}\mathrm{Tr}\,H^2\right\},\quad \mu^{\mathrm{D}}(H;t)=\frac{t^{-d[\mathrm{D}]/2}}{c[\mathrm{D}]}\exp\left\{-\frac{1}{4t}\mathrm{Tr}\,H^2\right\},$$

where $c[\mathrm{C}]=2^{3N/2}\pi^{N(2N+1)/2}$ and $c[\mathrm{D}]=2^{N/2}\pi^{N(2N-1)/2}$, respectively. As stated in Lemma 2 (iii), the eigenvalues are in the form $\boldsymbol{\lambda}(t)=(\omega_1(t),-\omega_1(t),\omega_2(t),-\omega_2(t),\ldots,\omega_N(t),-\omega_N(t))$. We will assume that

$$0\leqslant\omega_1\leqslant\omega_2\leqslant\cdots\leqslant\omega_N. \tag{18}$$

Then we have the expressions for volume elements

$$\mathcal{V}(dH)=\frac{c[\mathrm{C}]}{C[\mathrm{C}]}h^{\mathrm{C}}(\boldsymbol{\omega})^2d\boldsymbol{\omega}dU,\quad \mathcal{V}'(dH)=\frac{c[\mathrm{D}]}{C[\mathrm{D}]}h^{\mathrm{D}}(\boldsymbol{\omega})^2d\boldsymbol{\omega}dU', \tag{19}$$

where dU and dU' denote the Haar measures of $\mathrm{U}_2(2N)$ and $\mathrm{U}_1(2N)$, respectively, normalized as $\int_{\mathrm{U}_2(2N)}dU=1$ and $\int_{\mathrm{U}_1(2N)}dU'=1$. Here $C[\mathrm{C}]=C_{1/2}=(\pi/2)^{N/2}\Pi_{i=1}^{N}\Gamma(2i)$ and $C[\mathrm{D}]=C_{-1/2}=(\pi/2)^{N/2}\Pi_{i=1}^{N}\Gamma(2i-1)$, and $h^{\mathrm{C}}(\boldsymbol{\omega})\equiv h^{(1)}(\boldsymbol{\omega}),h^{\mathrm{D}}(\boldsymbol{\omega})\equiv h^{(0)}(\boldsymbol{\omega})$. At each time $t>0$, for any $U\in\mathrm{U}_2(2N)$, the probability $\mu^{\mathrm{C}}(H;t)\mathcal{V}(dH)$ is invariant under the automorphism $H\to U^{\dagger}HU$ for $H\in\mathcal{H}_{2-}(2N)$, and for any $U'\in\mathrm{U}_1(2N)$, $\mu^{\mathrm{D}}(H;t)\mathcal{V}'(dH)$ is invariant under the automorphism $H\to U'^{\dagger}HU'$ for $H\in\mathcal{H}_{1-}(2N)$. Altland and Zirnbauer named these two Gaussian random-matrix ensembles the classes C and D, respectively (see Remark (d) in Sec. III A).[1,2,56] The probability densities of the N non-negative eigenvalues with condition (18) are then obtained as

$$q^{\sharp}(\boldsymbol{\omega};t)=\frac{t^{-d[\sharp]/2}}{C[\sharp]}\exp\left\{-\frac{|\boldsymbol{\omega}|^2}{2t}\right\}h^{\sharp}(\boldsymbol{\omega})^2\quad\text{for}\quad\sharp=\mathrm{C},\mathrm{D}.$$

If we denote the transition probability densities of the processes (13) with $(\beta,\gamma)=(2,1)$ and with $(\beta,\gamma)=(2,0)$ by $p^{\mathrm{C}}(s,\cdot\,;t,\cdot\,)$ and $p^{\mathrm{D}}(s,\cdot\,;t,\cdot\,)$ for $0\leqslant s<t<\infty$, respectively, then

$$p^{\sharp}(0,\mathbf{0};t,\boldsymbol{\omega})=q^{\sharp}(\boldsymbol{\omega};t),\quad t>0\quad\text{for}\quad\sharp=\mathrm{C},\mathrm{D}. \tag{20}$$

D. Real symmetric matrix-valued processes

Here after, we denote the Hermitian matrix-valued processes $\Xi_{2-}(t)$ and $\Xi_{1-}(t)$ by $\Xi^{\mathrm{C}}(t)$ and $\Xi^{\mathrm{D}}(t)$, respectively. They are given by

$$\Xi^{\mathrm{C}}(t)=\sqrt{-1}a^0(t)\otimes\sigma_0+s^1(t)\otimes\sigma_1+s^2(t)\otimes\sigma_2+s^3(t)\otimes\sigma_3,$$

$$\Xi^{\mathrm{D}}(t)=\sqrt{-1}a^0(t)\otimes\sigma_0+\sqrt{-1}a^1(t)\otimes\sigma_1+\sqrt{-1}a^2(t)\otimes\sigma_2+s^3(t)\otimes\sigma_3. \tag{21}$$

Since $\sigma_\rho, \rho=0,1,3$, are real matrices and σ_2 is a pure imaginary matrix, if we define the processes as

$$\Xi^{\mathrm{C}'}(t)=s^1(t)\otimes\sigma_1+s^3(t)\otimes\sigma_3, \quad \Xi^{\mathrm{D}'}(t)=\sqrt{-1}a^2(t)\otimes\sigma_2+s^3(t)\otimes\sigma_3, \tag{22}$$

then $\Xi^{\mathrm{C}'}(t)\in\mathcal{S}_{2-}(2N)$ and $\Xi^{\mathrm{D}'}(t)\in\mathcal{S}_{1-}(2N)$, where $\mathcal{S}_{2-}(2N)\equiv\{S\in\mathcal{S}(2N):S^T\Sigma_2=-\Sigma_2S\}\cong\mathbb{R}^{d[\mathrm{C}']}$ and $\mathcal{S}_{1-}(2N)\equiv\{S\in\mathcal{S}(2N):S^T\Sigma_1=-\Sigma_1S\}\cong\mathbb{R}^{d[\mathrm{D}']}$ with $d[\mathrm{C}']=N(N+1)$ and $d[\mathrm{D}']=N^2$. The probability densities of $\Xi^{\mathrm{C}'}(t)$ and $\Xi^{\mathrm{D}'}(t)$ are given by

$$\mu^{\mathrm{C}'}(S;t)=\frac{t^{-d[\mathrm{C}']/2}}{c[\mathrm{C}']}\exp\left\{-\frac{1}{4t}\mathrm{Tr}\,S^2\right\}, \quad \mu^{\mathrm{D}'}(S;t)=\frac{t^{-d[\mathrm{D}']/2}}{c[\mathrm{D}']}\exp\left\{-\frac{1}{4t}\mathrm{Tr}\,S^2\right\}$$

with $c[\mathrm{C}']=2^N\pi^{N(N+1)/2}$ and $c[\mathrm{D}']=2^{N/2}\pi^{N^2/2}$, respectively. Set $\mathrm{O}_2(2N)=\mathrm{O}(2N)\cap\mathrm{Sp}(2N;\mathbb{R})$ and $\mathrm{O}_1(2N)=\mathrm{O}(2N)\cap\mathrm{SO}(2N;\mathbb{R})$ and denote their normalized Haar measures by dV and dV', respectively The eigenvalues are in the form $\boldsymbol{\lambda}(t)=(\omega_1(t),-\omega_1(t),\omega_2(t),-\omega_2(t),\ldots,\omega_N(t),-\omega_N(t))$. Under condition (18), we have the expressions for volume elements

$$\mathcal{V}(dS)=\frac{c[\mathrm{C}']}{C[\mathrm{C}']}h^{\mathrm{C}}(\boldsymbol{\omega})d\boldsymbol{\omega}dV, \quad \mathcal{V}'(dS)=\frac{c[\mathrm{D}']}{C[\mathrm{D}']}h^{\mathrm{D}}(\boldsymbol{\omega})d\boldsymbol{\omega}dV', \tag{23}$$

where $C[\mathrm{C}']=C_{1/2,1}=\Pi_{i=1}^N\Gamma(i)$ and $C[\mathrm{D}']=C_{-1/2,0}=2^{(N-2)/2}\Gamma(N/2)\Pi_{i=1}^{N-1}\Gamma(i)$. The probability densities of the N nonnegative eigenvalues with (18) are given as

$$q^{\sharp'}(\boldsymbol{\omega};t)=\frac{t^{-d[\sharp']/2}}{C[\sharp']}\exp\left\{-\frac{|\boldsymbol{\omega}|^2}{2t}\right\}h^{\sharp}(\boldsymbol{\omega}) \quad \text{for} \quad \sharp=\mathrm{C},\mathrm{D}.$$

It is remarked that the random-matrix ensemble with the distributions $\mu^{\mathrm{C}'}(S;t)$, whose nonnegative eigenvalue-distribution is given by $q^{\mathrm{C}'}(\boldsymbol{\omega};t)$, is the random-matrix ensemble in the symmetry class CI studied by Altland and Zirnbauer.[1,2,56]

By applying Theorem 1, we can show that the non-negative eigenvalues of $\Xi^{\mathrm{C}'}(t)$ solve Eq. (13) with $(\beta,\gamma)=(1,1)$ and those of $\Xi^{\mathrm{D}'}(t)$, Eq. (13) with $(\beta,\gamma)=(1,0)$. If we denote the transition probability densities of these processes by $p^{\mathrm{C}'}(s,\cdot;t,\cdot)$ and $p^{\mathrm{D}'}(s,\cdot;t,\cdot)$ for $0\leqslant s<t<\infty$, respectively, then $p^{\sharp'}(0,\mathbf{0};t,\boldsymbol{\omega})=q^{\sharp'}(\boldsymbol{\omega};t)$, $t>0$ for $\sharp=\mathrm{C},\mathrm{D}$.

IV. TEMPORALLY HOMOGENEOUS PROCESSES

Assume that $\nu>-1$, and we consider the process $\mathbf{Y}^{(\nu)}(t)=(Y_1^{(\nu)}(t),Y_2^{(\nu)}(t),\ldots,Y_N^{(\nu)}(t))$, $t\in[0,\infty)$, which solves the stochastic differential Eq. (13) with $(\beta,\gamma)=(2,(2\nu+1)/2)$, that is,

$$dY_i^{(\nu)}(t)=dB_i(t)+\left[\frac{2\nu+1}{2Y_i^{(\nu)}(t)}+\sum_{j:j\neq i}\left\{\frac{1}{Y_i^{(\nu)}(t)-Y_j^{(\nu)}(t)}+\frac{1}{Y_i^{(\nu)}(t)+Y_j^{(\nu)}(t)}\right\}\right]dt, \tag{24}$$

$1\leqslant i\leqslant N$. Remark that if $\nu=1/2$ and $-1/2$, the equation is reduced to (13) with $(\beta,\gamma)=(2,1)$ and $(\beta,\gamma)=(2,0)$, respectively. The Kolmogorov backward equation (the Fokker–Planck equation) for (24) is

$$\frac{\partial}{\partial t}p^{(\nu)}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{2}\Delta_{\mathbf{x}}p^{(\nu)}(s,\mathbf{x};t,\mathbf{y})+\mathbf{b}(\mathbf{x})\cdot\nabla_{\mathbf{x}}p^{(\nu)}(s,\mathbf{x};t,\mathbf{y}),$$

where $\mathbf{b}(\mathbf{x})=(b_1(\mathbf{x}),\ldots,b_N(\mathbf{x}))$ with $b_i(\mathbf{x})=(\partial/\partial x_i)\ln h^{((2\nu+1)/2)}(\mathbf{x})$. By simple calculation, we can confirm the following:

Lemma 3: Set

$$f^{(\nu)}(t,\mathbf{y}|\mathbf{x})=\det_{1\leqslant i,j\leqslant N}[G^{(\nu)}(t,y_j|x_i)]. \tag{25}$$

Then the transition probability density $p^{(\nu)}(s,\mathbf{x};t,\mathbf{y})$ *from the state* $\mathbf{x}$ *at time* s *to the state* $\mathbf{y}$ *at time* $t(>s)$ *of the process (24) is given by*

$$p^{(\nu)}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{h^{(0)}(\mathbf{x})}f^{(\nu)}(t-s,\mathbf{y}|\mathbf{x})h^{(0)}(\mathbf{y}),\quad \mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}. \tag{26}$$

Since $I_{1/2}(x)=(e^x-e^{-x})/\sqrt{2\pi x}$, $I_{-1/2}(x)=(e^x+e^{-x})/\sqrt{2\pi x}$, if we set

$$G^{\mathrm{C}}(t,y|x)=\frac{e^{-(y-x)^2/2t}-e^{-(y+x)^2/2t}}{\sqrt{2\pi t}},\quad G^{\mathrm{D}}(t,y|x)=\frac{e^{-(y-x)^2/2t}+e^{-(y+x)^2/2t}}{\sqrt{2\pi t}}, \tag{27}$$

and $f^{\sharp}(t,\mathbf{y}|\mathbf{x})=\det_{1\leqslant i,j\leqslant N}[G^{\sharp}(t,y_j|x_i)]$, $\sharp=\mathrm{C},\mathrm{D}$, then

$$p^{(1/2)}(s,\mathbf{x};t,\mathbf{y})=\frac{f^{\mathrm{C}}(t-s,\mathbf{y}|\mathbf{x})h^{\mathrm{C}}(\mathbf{y})}{h^{\mathrm{C}}(\mathbf{x})},\quad p^{(-1/2)}(s,\mathbf{x};t,\mathbf{y})=\frac{f^{\mathrm{D}}(t-s,\mathbf{y}|\mathbf{x})h^{\mathrm{D}}(\mathbf{y})}{h^{\mathrm{D}}(\mathbf{x})}. \tag{28}$$

The above implies the following. Let $\mathbb{W}_N^{\mathrm{C}}=\{\mathbf{x}\in\mathbb{R}^N:0<x_1<x_2<\cdots<x_N\}$ and $\mathbb{W}_N^{\mathrm{D}}=\{\mathbf{x}\in\mathbb{R}^N:|x_1|<x_2<\cdots<x_N\}$. The former is the Weyl chamber of type C_N and the latter of type D_N.[18] Since h^{C} and h^{D} vanish at the boundaries of the Weyl chambers $\mathbb{W}_N^{\mathrm{C}}$ and $\mathbb{W}_N^{\mathrm{D}}$, respectively, (28) implies that the processes $\mathbf{Y}^{(1/2)}(t)$ and $\mathbf{Y}^{(-1/2)}(t)$ can be regarded as the N-dimensional absorbing Brownian motions in $\mathbb{W}_N^{\mathrm{C}}$ and in $\mathbb{W}_N^{\mathrm{D}}$, respectively. That is, if $\mathbf{Y}^{(1/2)}(0)\in\mathbb{W}_N^{\mathrm{C}}$ and $\mathbf{Y}^{(-1/2)}(0)\in\mathbb{W}_N^{\mathrm{D}}$, then $\mathbf{Y}^{(1/2)}(t)\in\mathbb{W}_N^{\mathrm{C}}$ and $\mathbf{Y}^{(-1/2)}(t)\in\mathbb{W}_N^{\mathrm{D}}$ for all $t>0$ with probability 1. Moreover, we notice that (27) are the heat-kernels of the one-dimensional Brownian motion with an absorbing wall at the origin, and of the one-dimensional reflecting Brownian motion, respectively.[48] Then, we can also interpret the process $\mathbf{Y}^{(1/2)}(t)$ as the N-particle system of Brownian motions conditioned never to collide with each other nor with the wall at the origin in one-dimension,[35] and the process $\mathbf{Y}^{(-1/2)}(t)$ as the N-particle system of reflecting Brownian motions conditioned never to collide with each other. For $\sharp=\mathrm{C}$ and D, define

$$\mathcal{N}^{\sharp}(t,\mathbf{x})=\int_{\mathbb{W}_N^{\sharp}}d\mathbf{y}\,f^{\sharp}(t,\mathbf{y}|\mathbf{x}),\quad \mathbf{x}\in\mathbb{W}_N^{\sharp}. \tag{29}$$

$\mathcal{N}^{\mathrm{C}}(t,\mathbf{x})$ is the probability that N Brownian motions starting from $\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}$ does not collide with each other nor with the wall at the origin up to time t, and $\mathcal{N}^{\mathrm{D}}(t,\mathbf{x})$ is equal to the probability that N reflecting Brownian motions starting from $\mathbf{x}\in\mathbb{W}_N^{\mathrm{D}}$ does not collide with each other up to time t, respectively. We will show their long-time asymptotics in the next section. We can prove the following, which are consistent with (14) and (20).

Lemma 4: For $\nu>-1$ *with fixed* $t\in(0,\infty)$, *assume* $\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$. *Then*

$$\lim_{|\mathbf{x}|\to 0}p^{(\nu)}(0,\mathbf{x};t,\mathbf{y})=\frac{t^{-N(N+\nu)}}{C_\nu}\exp\left\{-\frac{|\mathbf{y}|^2}{2t}\right\}h^{((2\nu+1)/2)}(\mathbf{y})^2. \tag{30}$$

In particular, if $\nu\in\mathbb{N}$,

$$\lim_{|\mathbf{x}|\to 0}p^{(\nu)}(0,\mathbf{x};t,\mathbf{y})=q_\nu^{\mathrm{chGUE}}(\mathbf{y};t), \tag{31}$$

and

$$\lim_{|\mathbf{x}|\to 0} p^{(1/2)}(0,\mathbf{x};t,\mathbf{y}) = q^{\mathrm{C}}(\mathbf{y};t), \quad \lim_{|\mathbf{x}|\to 0} p^{(-1/2)}(0,\mathbf{x};t,\mathbf{y}) = q^{\mathrm{D}}(\mathbf{y};t). \tag{32}$$

Proof: By definition (25) with (3), if $x_i>0, 1\leqslant \forall i \leqslant N$, $f^{(\nu)}(t,\mathbf{y}|\mathbf{x}) = (1/t^N)\Pi_{k=1}^N (y_k^{\nu+1}/x_k^{\nu}) \times e^{-(|\mathbf{x}|^2+|\mathbf{y}|^2)/2t}\det_{1\leqslant i,j\leqslant N}[I_\nu(x_i y_j/t)]$. We can use (A2) in Appendix A by changing the variables $x_i \to x_i^2/2t$ and $y_j \to y_j^2/2t$ to evaluate $\det_{1\leqslant i,j\leqslant N}[I_\nu(x_i y_j/t)]$ and obtain the asymptotic form of $f^{(\nu)}(t,\mathbf{y}|\mathbf{x})$,

$$f^{(\nu)}(t,\mathbf{y}|\mathbf{x}) = \frac{t^{-N(N+2\nu+1)/2}}{C_\nu} \prod_{1\leqslant i<j\leqslant N} \left\{ \left(\frac{x_j}{\sqrt{t}}\right)^2 - \left(\frac{x_i}{\sqrt{t}}\right)^2 \right\} \prod_{1\leqslant k<\ell\leqslant N} (y_\ell^2 - y_k^2) \prod_{m=1}^N y_m^{2\nu+1} \times \exp\left\{ -\frac{|\mathbf{y}|^2}{2t} \right\} \times \left(1 + \mathcal{O}\left(\frac{|\mathbf{x}|}{\sqrt{t}} \right) \right) \tag{33}$$

in $|\mathbf{x}|/\sqrt{t}\to 0$. Using this form in (26), the limit (30) is proved. ■

V. TEMPORALLY INHOMOGENEOUS PROCESSES

A. Star topology

Using (2) the probability that the Brownian motion started at $\mathbf{x}\in \mathbb{W}_N^{\mathrm{A}}$ does not hit the boundary of $\mathbb{W}_N^{\mathrm{A}}$ up to time $t>0$ is given by $\mathcal{N}^{\mathrm{A}}(t,\mathbf{x}) = \int_{\mathbb{W}_N^{\mathrm{A}}} d\mathbf{y}\, f^{\mathrm{A}}(t,\mathbf{y}|\mathbf{x})$. In the previous papers,[31,32] we gave the asymptotic form

$$f^{\mathrm{A}}(t,\mathbf{y}|\mathbf{x}) = \frac{t^{-N(N+1)/4}}{C[\mathrm{A}]} h^{\mathrm{A}}\left(\frac{\mathbf{x}}{\sqrt{t}}\right) h^{\mathrm{A}}(\mathbf{y}) \exp\left\{ -\frac{|\mathbf{y}|^2}{2t} \right\} \times \left(1 + \mathcal{O}\left(\frac{|\mathbf{x}|}{\sqrt{t}} \right) \right) \tag{34}$$

in $|\mathbf{x}|/\sqrt{t}\to 0$ and showed that $\mathcal{N}^{\mathrm{A}}(t,\mathbf{x}) = (C[\mathrm{A}']/C[\mathrm{A}]) h^{\mathrm{A}}(\mathbf{x}/\sqrt{t}) \times (1+\mathcal{O}(|\mathbf{x}|/\sqrt{t}))$ as $|\mathbf{x}|/\sqrt{t} \to 0$. This estimate gives that for $\mathbf{x}\in \mathbb{W}_N^{\mathrm{A}}$ the noncolliding probability decays in the power-law as $t\to\infty$;[15,21,37] $\mathcal{N}^{\mathrm{A}}(t,\mathbf{x}) \sim t^{-\psi[\mathrm{A}]}$ with the exponent $\psi[\mathrm{A}] = N(N-1)/4$. (Note that (34) is derived readily by using (A1) in Appendix A.) For a given $T>0$, we defined

$$g_T^{\mathrm{A}}(s,\mathbf{x};t,\mathbf{y}) = \frac{f^{\mathrm{A}}(t-s,\mathbf{y}|\mathbf{x})\mathcal{N}^{\mathrm{A}}(T-t,\mathbf{y})}{\mathcal{N}^{\mathrm{A}}(T-s,\mathbf{x})}$$

for $0\leqslant s<t\leqslant T$, $\mathbf{x},\mathbf{y}\in \mathbb{W}_N^{\mathrm{A}}$. Using (34) we showed that as $|\mathbf{x}|\to 0$ it converges to $g_T^{\mathrm{A}}(0,\mathbf{0};t,\mathbf{y}) = (T^{\psi[\mathrm{A}]} t^{-d[\mathrm{A}]/2}/C[\mathrm{A}'])e^{-|\mathbf{y}|^2/2t} h^{\mathrm{A}}(\mathbf{y})\mathcal{N}^{\mathrm{A}}(T-t,\mathbf{y})$. This function $g_T^{\mathrm{A}}(s,\mathbf{x};t,\mathbf{y})$ can be regarded as the transition probability density from the state $\mathbf{x}\in \mathbb{W}_N^{\mathrm{A}}$ at time s to the state $\mathbf{y}\in \mathbb{W}_N^{\mathrm{A}}$ at time $t(>s)$ conditioned to stay inside $\mathbb{W}_N^{\mathrm{A}}$ up to time T and defines a temporally inhomogeneous diffusion process, which we denoted by $\mathbf{X}(t) = (X_1(t), X_2(t), \ldots, X_N(t))$, $t\in[0,T]$ in Sec. I. This represents the N-particle system of Brownian motions conditioned not to collide with each other in a finite time-interval $(0,T]$. The process $\mathbf{X}(t), t\in[0,T]$, starting from $\mathbf{X}(0)=\mathbf{0}$ is illustrated by Fig. 1, whose spatio-temporal path-configuration is said to be in *star topology* in the theory of directed polymer networks.[14] As mentioned in Sec. I, this process exhibits a transition of the eigenvalue statistics from GUE to GOE.[31,32]

In the present section, we consider the temporally inhomogeneous diffusion process associated with $\mathbf{Y}^{(\nu)}(t)$ studied in the previous section. We consider the N-particle system of generalized meanders (5) conditioned that they never collide with each other for a time interval $[0,T]$. The transition probability density is given by

$$g_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y}) = \frac{f_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y})\mathcal{N}_T^{(\nu,\kappa)}(t,\mathbf{y})}{\mathcal{N}_T^{(\nu,\kappa)}(s,\mathbf{x})} \tag{35}$$

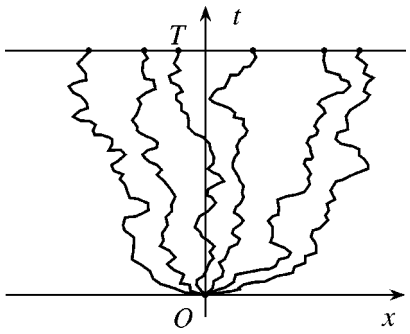

FIG. 1. Process $\mathbf{X}(t), t\in[0,T]$, with $\mathbf{X}(0)=\mathbf{0}$ showing star topology.

for $0\leqslant s<t\leqslant T, \mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$, where $f_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y})=\det_{1\leqslant i,j\leqslant N}[G_T^{(\nu,\kappa)}(s,x_i;t,y_j)]$ with (5) and $\mathcal{N}_T^{(\nu,\kappa)}(t,\mathbf{x})=\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{y}f_T^{(\nu,\kappa)}(t,\mathbf{x};T,\mathbf{y})$. Note that $f_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y})=f^{(\nu)}(t-s,\mathbf{y}|\mathbf{x})h_T^{(\nu,\kappa)}(t,\mathbf{y})/h_T^{(\nu,\kappa)}(s,\mathbf{x})$, where $h_T^{(\nu,\kappa)}(t,\mathbf{x})=\Pi_{i=1}^N h_T^{(\nu,\kappa)}(t,x_i)$. Since $\lim_{t\to 0}G^{(\nu)}(t,z|w)=\delta(z-w)\mathbf{1}(z\geqslant 0)$, $h_T^{(\nu,\kappa)}(T,\mathbf{x})=\Pi_{j=1}^N x_j^{-\kappa}$ for $\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}$, and then (35) can be written as

$$g_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{\tilde{\mathcal{N}}^{(\nu,\kappa)}(T-s,\mathbf{x})}f^{(\nu)}(t-s,\mathbf{y}|\mathbf{x})\tilde{\mathcal{N}}^{(\nu,\kappa)}(T-t,\mathbf{y}) \tag{36}$$

with

$$\tilde{\mathcal{N}}^{(\nu,\kappa)}(t,\mathbf{x})=\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{y}f^{(\nu)}(t,\mathbf{y}|\mathbf{x})\prod_{i=1}^N y_i^{-\kappa}. \tag{37}$$

Lemma 5: Assume that $\nu>-1$ *and* $\kappa\in[0,2(\nu+1))$. *Let* $\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$.

(i) *For* $0\leqslant s<t\leqslant T$, $\lim_{T\to\infty}g_T^{(\nu,\kappa)}(s,\mathbf{x};t,\mathbf{y})=p^{(\nu)}(s,\mathbf{x};t,\mathbf{y})$.

(ii) *For* $0<t<T$,

$$g_T^{(\nu,\kappa)}(0,\mathbf{0};t,\mathbf{y})\equiv\lim_{|\mathbf{x}|\to 0}g_T^{(\nu,\kappa)}(0,\mathbf{x};t,\mathbf{y})$$
$$=\frac{T^{N(N+\kappa-1)/2}t^{-N(N+\nu)}}{C_{\nu,\kappa}}\exp\left\{-\frac{|\mathbf{y}|^2}{2t}\right\}h^{(2\nu+1)}(\mathbf{y})\tilde{\mathcal{N}}^{(\nu,\kappa)}(T-t,\mathbf{y}). \tag{38}$$

(iii) *For* $T>0$, $\lim_{t\nearrow T}g_T^{(\nu,\kappa)}(0,\mathbf{0};t,\mathbf{y})=T^{-N(N+2\nu+1-\kappa)/2}/C_{\nu,\kappa}\exp\{-|\mathbf{y}|^2/2T\}h^{(2\nu+1-\kappa)}(\mathbf{y})$.

Proof: Using (33) for (37), we have the estimate of $\tilde{\mathcal{N}}^{(\nu,\kappa)}(t,\mathbf{x})$ in $|\mathbf{x}|/\sqrt{t}\to 0$ as

$$\tilde{\mathcal{N}}^{(\nu,\kappa)}(t,\mathbf{x})=\frac{t^{-N(N+2\nu+1)/2}}{C_\nu}\prod_{1\leqslant i<j\leqslant N}\left\{\left(\frac{x_j}{\sqrt{t}}\right)^2-\left(\frac{x_i}{\sqrt{t}}\right)^2\right\}$$
$$\times\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{y}\prod_{1\leqslant k\leqslant\ell\leqslant N}(y_\ell^2-y_k^2)\prod_{m=1}^N y_m^{2\nu+1-\kappa}\exp\left\{-\frac{|\mathbf{y}|^2}{2t}\right\}\times\left(1+\mathcal{O}\left(\frac{|\mathbf{x}|}{\sqrt{t}}\right)\right)$$
$$=\frac{t^{-N\kappa/2}C_{\nu,\kappa}}{C_\nu}\prod_{1\leqslant i<j\leqslant N}\left\{\left(\frac{x_j}{\sqrt{t}}\right)^2-\left(\frac{x_i}{\sqrt{t}}\right)^2\right\}\times\left(1+\mathcal{O}\left(\frac{|\mathbf{x}|}{\sqrt{t}}\right)\right), \tag{39}$$

where we have used a version of Selberg's integral formula[50,38]

$$\int_{\mathbb{R}^N} d\mathbf{u} \prod_{1\leqslant i<j\leqslant N} |u_j^2-u_i^2|^{2\gamma} \prod_{k=1}^{N} |u_k|^{2\alpha-1} e^{-|\mathbf{u}|^2/2} = 2^{\alpha N+\gamma N(N-1)} \prod_{i=1}^{N} \frac{\Gamma(1+i\gamma)\Gamma(\alpha+\gamma(i-1))}{\Gamma(1+\gamma)}$$

by setting $\alpha=\nu+1-\kappa/2$ and $\gamma=1/2$ (see Eq. (17.6.6) in Ref. 40). By (33) and (39), (i) and (ii) are obtained. Since $\lim_{t\to 0} G^{(\nu)}(t,y|x)=\delta(y-x)\mathbf{1}(y\geqslant 0)$, we have $\lim_{t\to 0} f^{(\nu)}(t,\mathbf{y}|\mathbf{x}) = \Pi_{i=1}^N \delta(y_i-x_i)$ for $\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$. Then $\lim_{t\to 0}\tilde{\mathcal{N}}^{(\nu,\kappa)}(t,\mathbf{x})=\Pi_{i=1}^N x_i^{-\kappa}\mathbf{1}(\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}})$ and (iii) is obtained. ■

Now we define the process $\mathbf{X}^{(\nu,\kappa)}(t)=(X_1^{(\nu,\kappa)}(t),X_2^{(\nu,\kappa)}(t),\ldots,X_N^{(\nu,\kappa)}(t)), t\in[0,T]$, as the temporally inhomogeneous diffusion process, whose transition probability density is given by (35) for $0\leqslant s<t\leqslant T,\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$ and (38) for $0<t\leqslant T,\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$. This process solves the stochastic differential equations

$$dX_i^{(\nu,\kappa)}(t)=dB_i(t)+\left[\frac{2\nu+1}{2X_i^{(\nu,\kappa)}(t)}+b_i^{(\nu,\kappa)}(T-t,\mathbf{X}^{(\nu,\kappa)}(t))\right]dt, \quad t\in[0,T],1\leqslant i\leqslant N,$$

where $b_i^{(\nu,\kappa)}(t,\mathbf{x})=(\partial/\partial x_i)\ln\tilde{\mathcal{N}}^{(\nu,\kappa)}(t,\mathbf{x})$, $1\leqslant i\leqslant N$.

Here we consider the special cases $(\nu,\kappa)=(1/2,1)$ and $(\nu,\kappa)=(-1/2,0)$. By the definitions (29) and (37), $\tilde{\mathcal{N}}^{(1/2,1)}(t,\mathbf{x})=\mathcal{N}^{\mathrm{C}}(t,x)/\Pi_{i=1}^N x_i$ and $\tilde{\mathcal{N}}^{(-1/2,0)}(t,\mathbf{x})=\mathcal{N}^{\mathrm{D}}(t,x)$, and then (36) gives

$$g_T^{(1/2,1)}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{\mathcal{N}^{\mathrm{C}}(T-s,\mathbf{x})} f^{\mathrm{C}}(t-s,\mathbf{y}|\mathbf{x})\mathcal{N}^{\mathrm{C}}(T-t,\mathbf{y}),$$

$$g_T^{(-1/2,0)}(s,\mathbf{x};t,\mathbf{y})=\frac{1}{\mathcal{N}^{\mathrm{D}}(T-s,\mathbf{x})} f^{\mathrm{D}}(t-s,\mathbf{y}|\mathbf{x})\mathcal{N}^{\mathrm{D}}(T-t,\mathbf{y}),$$

for $0\leqslant s<t\leqslant T,\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$. That is, we can interpret the process $\mathbf{X}^{(1/2,1)}(t)$ as the N-particle system of Brownian motions conditioned never to collide with each other nor with the wall at the origin in one-dimension during the time-interval $[0,T]$, and the process $\mathbf{X}^{(-1/2,0)}(t)$ as the N-particle system of reflecting Brownian motions conditioned never to collide with each other during the time-interval $[0,T]$, respectively. The asymptotic forms $\mathcal{N}^{\sharp}(t,\mathbf{x})=(C[\sharp']/C[\sharp])h^{\sharp}(\mathbf{x}/\sqrt{t})\times(1+\mathcal{O}(|\mathbf{x}|/\sqrt{t}))$ in $|\mathbf{x}|/\sqrt{t}\to 0$ for $\sharp=\mathrm{C}$ and D are obtained by (39), and thus we can see the power-laws of the noncolliding probabilities, $\mathcal{N}^{\sharp}(t,\mathbf{x})\sim t^{-\psi[\sharp]}$ as $t\to\infty$ for $\mathbf{x}\in\mathbb{W}_N^{\sharp}$, $\sharp=\mathrm{C}$ and D with the exponents $\psi[\mathrm{C}]=N^2/2,\psi[\mathrm{D}]=N(N-1)/2$. As a corollary of Lemma 5, we have the following:

Corollary 6:

(i) For $0<t<T$, *if* $\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}$,

$$g_T^{(1/2,1)}(0,\mathbf{0};t,\mathbf{x})=\frac{T^{\psi[\mathrm{C}]}t^{-d[\mathrm{C}]/2}}{C[\mathrm{C}']}\exp\left\{-\frac{|\mathbf{x}|^2}{2t}\right\}h^{\mathrm{C}}(\mathbf{x})\mathcal{N}^{\mathrm{C}}(T-t,\mathbf{x}),$$

$$g_T^{(-1/2,0)}(0,\mathbf{0};t,\mathbf{x})=\frac{T^{\psi[\mathrm{D}]}t^{-d[\mathrm{D}]/2}}{C[\mathrm{D}']}\exp\left\{-\frac{|\mathbf{x}|^2}{2t}\right\}h^{\mathrm{D}}(\mathbf{x})\mathcal{N}^{\mathrm{D}}(T-t,\mathbf{x}).$$

(ii) *For* $T>0$, *if* $\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}$,

$$\lim_{t\nearrow T} g_T^{(1/2,1)}(0,\mathbf{0};t,\mathbf{x})=q^{\mathrm{C}'}(\mathbf{x};T), \quad \lim_{t\nearrow T} g_T^{(-1/2,0)}(0,\mathbf{0};t,\mathbf{x})=q^{\mathrm{D}'}(\mathbf{x};T).$$

Figure 2 illustrates the processes $\mathbf{X}^{(1/2,1)}(t)$ and $\mathbf{X}^{(-1/2,0)}(t)$ both starting from $\mathbf{0}$. The path-configurations are in star topology. In the former any particle can not collide with the wall at the origin, while in the latter the leftmost particle is reflected at the wall. Another corollary of Lemma 5 is the following:

Corollary 7: If $\nu\in\mathbb{N},\mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}$, $\lim_{t\nearrow T} g_T^{(\nu,\nu+1)}(0,\mathbf{0};t,\mathbf{x})=q_\nu^{\mathrm{chGOE}}(\mathbf{x};T)$.

The combination of Lemma 5 (i) with (31) and (32) of Lemma 4, Corollaries 6 and 7 implies that $\mathbf{X}^{(1/2,1)}(t)$, $\mathbf{X}^{(-1/2,0)}(t)$ and $\mathbf{X}^{(\nu,\nu+1)}(t)$ with $\nu\in\mathbb{N}$, all starting from $\mathbf{0}$, exhibit the transitions

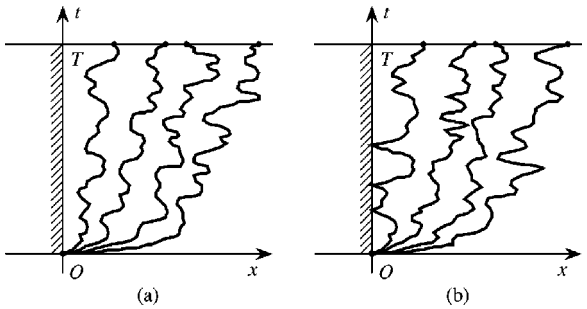

FIG. 2. (a) Process $\mathbf{X}^{(1/2,1)}(t), t \in [0,T]$ with the initial state $\mathbf{0}$ showing star topology. (b) Process $\mathbf{X}^{(-1/2,0)}(t), t \in [0,T]$ with the initial state $\mathbf{0}$ showing star topology.

from the eigenvalue statistics of the class C to the class CI, from the class D to the class associated with $q^{\mathrm{D}'}$ studied in Sec. III D, and from chGUE to chGOE, respectively, as time t goes on from 0 to T. (See Theorem 9 below.)

At the end of this subsection, we discuss the relation between the temporally homogeneous diffusion process $\mathbf{Y}^{(\nu)}(t)$ and the temporally inhomogeneous diffusion process $\mathbf{X}^{(\nu,\kappa)}(t)$ for $t \in [0,T]$. For a time sequence $t_0 \equiv 0 < t_1 < \cdots < t_{\ell-1} < t_\ell \equiv T < \infty$ with $\ell \in \{1,2,\ldots\}$, we consider the multitime probabilities with the initial state $\mathbf{Y}^{(\nu)}(0) = \mathbf{X}^{(\nu,\kappa)}(0) = \mathbf{x}^{(0)}$

$$P^{\mathbf{x}(0)}(\mathbf{Y}^{(\nu)}(t_1) \in d\mathbf{x}^{(1)}, \ldots, \mathbf{Y}^{(\nu)}(t_\ell) \in d\mathbf{x}^{(\ell)}) = \prod_{i=1}^{\ell} p^{(\nu)}(t_{i-1}, \mathbf{x}^{(i-1)}; t_i, \mathbf{x}^{(i)}) d\mathbf{x}^{(i)},$$

and

$$P^{\mathbf{x}(0)}(\mathbf{X}^{(\nu,\kappa)}(t_1) \in d\mathbf{x}^{(1)}, \ldots, \mathbf{X}^{(\nu,\kappa)}(t_\ell) \in d\mathbf{x}^{(\ell)}) = \prod_{i=1}^{\ell} g_T^{(\nu,\kappa)}(t_{i-1}, \mathbf{x}^{(i-1)}; t_i, \mathbf{x}^{(i)}) d\mathbf{x}^{(i)},$$

where we have used the Markov property of the processes. Assume that $\mathbf{x}^{(0)} = \mathbf{0}$ and $\mathbf{x}^{(i)} \in \mathbb{W}_N^{\mathrm{C}}$, $1 \leqslant i \leqslant \ell$. We use formulas (26) and (36) and apply Lemmas 4 and 5. Then we have the equality

$$\prod_{i=1}^{\ell} g_T^{(\nu,\kappa)}(t_{i-1}, \mathbf{x}^{(i-1)}; t_i, \mathbf{x}^{(i)}) = T^{N(N+\kappa-1)/2} \frac{C_\nu}{C_{\nu,\kappa}} \prod_{i=1}^{\ell} p^{(\nu)}(t_{i-1}, \mathbf{x}^{(i-1)}; t_i, \mathbf{x}^{(i)}) \frac{1}{h^{(\kappa)}(\mathbf{x}^{(\ell)})}.$$

Since this equality holds for arbitrary time sequence $t_0 = 0 < t_1 < \cdots < t_{\ell-1} < t_\ell = T < \infty$ with $\ell \in \{1,2,\ldots\}$, we can conclude the following:

Proposition 8: Assume that $\nu > -1, \kappa \in [0, 2(\nu+1))$. If $\mathbf{X}^{(\nu,\kappa)}(0) = \mathbf{Y}^{(\nu)}(0) = \mathbf{0}$, then the distribution of the process $\mathbf{X}^{(\nu,\kappa)}(t)$ is absolutely continuous with that of the process $\mathbf{Y}^{(\nu)}(t)$ for $t \in [0,T]$ and the Radon–Nikodým density is given by

$$\frac{P(\mathbf{X}^{(\nu,\kappa)}(\cdot) \in d\mathbf{w})}{P(\mathbf{Y}^{(\nu)}(\cdot) \in d\mathbf{w})} = \frac{C_\nu T^{N(N+\kappa-1)/2}}{C_{\nu,\kappa} h^{(\kappa)}(\mathbf{w}(T))}.$$

When $N = 1$ and $(\nu,\kappa) = (1/2,1)$, this proposition gives the Imhof relation between the Brownian meander and the three-dimensional Bessel process.[25] The relation stated by (4),[31,32] and the above proposition are regarded as the multivariate generalizations of the Imhof relation.

B. Brownian bridges and temporally inhomogeneous matrix-valued processes

Assume that $\nu \in \mathbb{N}, 0 < T < \infty$. Let $B_{ij}^{\rho}(t), \tilde{B}_{ij}^{\rho}(t), 1 \leqslant i \leqslant N+\nu, 1 \leqslant j \leqslant N, 0 \leqslant \rho \leqslant 3$ be independent one-dimensional standard Brownian motions. For a given matrix $m = (m_{ij}$

$+\sqrt{-1}\tilde{m}_{ij})_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$ with $m_{ij},\tilde{m}_{ij}\in\mathbb{R}$, let $(\beta_T^\rho)_{ij}(t:m_{ij}),(\tilde{\beta}_T^\rho)_{ij}(t:\tilde{m}_{ij}),1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N,0\leqslant\rho\leqslant 3$ be the diffusion processes, which are the solutions of the following stochastic differential equations:

$$(\beta_T^\rho)_{ij}(t:m_{ij})=B_{ij}^\rho(t)-\int_0^t\frac{(\beta_T^\rho)_{ij}(s:m_{ij})-m_{ij}}{T-s}ds,$$

$$(\tilde{\beta}_T^\rho)_{ij}(t:\tilde{m}_{ij})=\tilde{B}_{ij}^\rho(t)-\int_0^t\frac{(\tilde{\beta}_T^\rho)_{ij}(s:\tilde{m}_{ij})-\tilde{m}_{ij}}{T-s}ds,\quad t\in[0,T]. \tag{40}$$

The processes $(\beta_T^\rho)_{ij}(t:m_{ij})$ and $(\tilde{\beta}_T^\rho)_{ij}(t:\tilde{m}_{ij})$ are one-dimensional Brownian bridges of duration T both starting from 0 and ending at m_{ij} and $\tilde{m}_{ij}$, respectively.[55] Next for $z^\rho=(z_{ij}^\rho)_{1\leqslant i,j\leqslant N}\in\mathcal{S}(N)$ and $\tilde{z}^\rho=(\tilde{z}^\rho_{ij})_{1\leqslant i,j\leqslant N}\in\mathcal{A}(N)$, $0\leqslant\rho\leqslant 3$, we set

$$(s_T^\rho)_{ij}(t:z_{ij}^\rho)=\begin{cases}\dfrac{1}{\sqrt{2}}(\beta_T^\rho)_{ij}(t:\sqrt{2}z_{ij}^\rho), & \text{if } i<j,\\ (\beta_T^\rho)_{ii}(t:z_{ii}^\rho), & \text{if } i=j,\end{cases}$$

and

$$(a_T^\rho)_{ij}(t:\tilde{z}^\rho_{ij})=\begin{cases}\dfrac{1}{\sqrt{2}}(\tilde{\beta}_T^\rho)_{ij}(t:\sqrt{2}\tilde{z}^\rho_{ij}), & \text{if } i<j,\\ 0, & \text{if } i=j,\end{cases} \tag{41}$$

with $(s_T^\rho)_{ij}(t:z_{ij}^\rho)=(s_T^\rho)_{ji}(t:z_{ji}^\rho)$ and $(a_T^\rho)_{ij}(t:\tilde{z}^\rho_{ij})=-(a_T^\rho)_{ji}(t:\tilde{z}^\rho_{ji})$ for $i>j$, where $1\leqslant i,j\leqslant N$, $0\leqslant\rho\leqslant 3$ and $t\in[0,T]$. We define the matrix-valued processes $s_T^\rho(t:z^\rho)=((s_T^\rho)_{ij}(t:z_{ij}^\rho))_{1\leqslant i,j\leqslant N}\in\mathcal{S}(N)$ and $a_T^\rho(t:\tilde{z}^\rho)=((a_T^\rho)_{ij}(t:\tilde{z}^\rho_{ij}))_{1\leqslant i,j\leqslant N}\in\mathcal{A}(N)$.

In an earlier paper,[33] we considered the $N\times N$ Hermitian matrix-valued process $\Xi_T(t)=s^0(t)+\sqrt{-1}a_T^0(t:O),t\in[0,T]$, where O denotes the $N\times N$ zero matrix and $s^0(t)$ was defined below (17). This process is the temporally inhomogeneous matrix-valued process realized as an interpolation in duration T of the first and second processes given in Sec. II B. Using the invariance in distribution of the process $\Xi_T(t)$ under unitary transformations and our generalized version of the Imhof relation (4), we proved the equivalence in distribution of its eigenvalue process and $\mathbf{X}(t)$ with $\mathbf{X}(0)=\mathbf{0}$. As a corollary of this equivalence, we derived the formula for any $\sigma\in\mathbb{R}$,

$$\int_{\mathrm{U}(N)}dU\exp\left\{-\frac{1}{2\sigma^2}\mathrm{Tr}(\Lambda_{\mathbf{x}}-U^\dagger\Lambda_{\mathbf{y}}U)^2\right\}=\frac{C[\mathrm{A}]\sigma^{d[\mathrm{A}]}}{h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})}\det_{1\leqslant i,j\leqslant N}[G^{\mathrm{A}}(t,y_j|x_i)], \tag{42}$$

where dU denotes the Haar measure of $\mathrm{U}(N)$ normalized as $\int_{\mathrm{U}(N)}dU=1$, $\Lambda_{\mathbf{x}}=\mathrm{diag}\{x_1,...,x_N\}$ and $\Lambda_{\mathbf{y}}=\mathrm{diag}\{y_1,...,y_N\}$ with $\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{A}}$. This is a stochastic-calculus derivation of the Harish–Chandra (Itzykson–Zuber) integral formula.[22,26] In this subsection, we give extensions of this argument.

As an interpolation of the Laguerre process (7) and the Wishart process (9), we define the matrix-valued process

$$\Xi_T^{\mathrm{LW}}(t)=M_T(t)^\dagger M_T(t),\quad t\in[0,T],$$

where $M_T(t)=(B_{ij}^0(t)+\sqrt{-1}(\tilde{\beta}_T^0)_{ij}(t:O))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}\in\mathcal{M}(N+\nu,N;\mathbb{C}),t\in[0,T]$, where O denotes the $(N+\nu)\times N$ zero matrix. Similarly, the interpolations between the processes (21) and (22) are defined by

$$\Xi_T^{\mathrm{C}}(t)=\sqrt{-1}a_T^0(t{:}O)\otimes\sigma_0+s^1(t)\otimes\sigma_1+s_T^2(t{:}O)\otimes\sigma_2+s^3(t)\otimes\sigma_3,$$

$$\Xi_T^{\mathrm{D}}(t)=\sqrt{-1}a_T^0(t{:}O)\otimes\sigma_0+\sqrt{-1}a_T^1(t{:}O)\otimes\sigma_1+\sqrt{-1}a^2(t)\otimes\sigma_2+s^3(t)\otimes\sigma_3,$$

in which O denotes the $N\times N$ zero matrix. Let $\boldsymbol{\kappa}^{\mathrm{LW}}(t)=(\kappa_1^{\mathrm{LW}}(t),\ldots,\kappa_N^{\mathrm{LW}}(t)),t\in[0,T]$ be the square roots of the eigenvalues of $\Xi_T^{\mathrm{LW}}(t)$ with $0\leqslant\kappa_1^{\mathrm{LW}}(t)\leqslant\cdots\leqslant\kappa_N^{\mathrm{LW}}(t)$ and $\boldsymbol{\lambda}^{\sharp}(t)=(\lambda_1^{\sharp}(t),\lambda_2^{\sharp}(t),\ldots,\lambda_N^{\sharp}(t))$ be the non-negative eigenvalues of $\Xi_T^{\sharp}(t)$ with $0\leqslant\lambda_1^{\sharp}(t)\leqslant\cdots\leqslant\lambda_N^{\sharp}(t)$ for $\sharp=\mathrm{C}$ and D. We prove the following equivalence in distribution among the temporally inhomogeneous diffusion processes:

Theorem 9:

(i) *If* $\nu\in\mathbb{N}$ *and* $\mathbf{X}^{(\nu,\nu+1)}(0)=\mathbf{0}$, *then* $\boldsymbol{\kappa}^{\mathrm{LW}}(t)=\mathbf{X}^{(\nu,\nu+1)}(t)$, $t\in[0,T]$ *in distribution.*

(ii) *If* $\mathbf{X}^{(1/2,1)}(0)=\mathbf{X}^{(-1/2,0)}(0)=\mathbf{0}$, *then* $\boldsymbol{\lambda}^{\mathrm{C}}(t)=\mathbf{X}^{(1/2,1)}(t)$ *and* $\boldsymbol{\lambda}^{\mathrm{D}}(t)=\mathbf{X}^{(-1/2,0)}(t)$, $t\in[0,T]$ *in distribution.*

Proof: (i) For a given matrix $m=(m_{ij}+\sqrt{-1}\tilde{m}_{ij})_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$, $m_{ij},\tilde{m}_{ij}\in\mathbb{R}$, we consider $\mathcal{M}(N+\nu,N;\mathbb{C})$-valued process $M_T(t{:}m)=((\beta_T^0)_{ij}(t{:}m_{ij})+\sqrt{-1}(\tilde{\beta}_T^0)_{ij}(t{:}\tilde{m}_{ij}))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$, $t\in[0,T]$. From Eqs. (40), we have the equation

$$M_T(t{:}m)=M(t)-\int_0^t\frac{M_T(s{:}m)-m}{T-s}ds,\quad t\in[0,T],\tag{43}$$

where $M(t)=(B_{ij}^0(t)+\sqrt{-1}\tilde{B}_{ij}^0(t))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$. Let m_U and m_O be random matrices with distribution $\mu_\nu^{\mathrm{chGUE}}(\,\cdot\,;T)$ and $\mu_\nu^{\mathrm{chGOE}}(\,\cdot\,;T)$, respectively. Since $(\beta_T^0)_{ij}(t{:}\zeta)$ and $(\tilde{\beta}_T^0)_{ij}(t{:}\zeta)$, $t\in[0,T]$ are Brownian motions when ζ is a Gaussian random variable with variance T independent of $B_{ij}^0(t)$ and $\tilde{B}_{ij}^0(t)$, if m_U and m_O are independent of $M(t),t\in[0,T]$,

$$M_T(t{:}m_U)=M(t),\quad M_T(t{:}m_O)=M_T(t),\quad t\in[0,T]\tag{44}$$

in distribution. Moreover, since the distribution of the process $M(t)$ is invariant under any transformation $M(t)\to U^\dagger M(t)V$, $U\in\mathrm{U}(N+\nu)$, $V\in\mathrm{U}(N)$, the following lemma is obtained by Eq. (43).

Lemma 10: For any $U\in\mathrm{U}(N+\nu)$, $V\in\mathrm{U}(N)$, $U^\dagger M_T(t{:}m)V=M_T(t{:}U^\dagger mV)$, $t\in[0,T]$ *in distribution.*

By this lemma, if m and m' in $\mathcal{M}(N+\nu,N;\mathbb{C})$ have the same radial coordinates, the processes of radial coordinates of $M_T(t{:}m)$ and $M_T(t{:}m'),t\in[0,T]$, are identical in distribution. Let $\Xi_T^{\mathrm{LW}}(t{:}m)=M_T^\dagger(t{:}m)M_T(t{:}m)$. Then the above gives the identification in distribution of the processes of square roots of eigenvalues of $\Xi_T^{\mathrm{LW}}(t{:}m)$ and $\Xi_T^{\mathrm{LW}}(t{:}m'),t\in[0,T]$. Now we denote by $P_T^{\boldsymbol{\kappa}}(\,\cdot\,)$ the probability distribution of the process of square roots of eigenvalues of $\Xi_T^{\mathrm{LW}}(t{:}m)$ conditioned that the square roots of eigenvalues of m is $\boldsymbol{\kappa}=(\kappa_1,\ldots,\kappa_N)$ with condition (11). We also denote by $P(\,\cdot\,)$ and $P_T(\,\cdot\,)$ the distributions of the processes of square roots of eigenvalues of $\Xi(t)=M(t)^\dagger M(t)$ and $\Xi_T(t)=M_T^\dagger(t)M_T(t),t\in[0,T]$, respectively. The equalities (44) give

$$P(\,\cdot\,)=\int_{\mathbb{W}_N^{\mathrm{C}}}d\boldsymbol{\kappa}\,P_T^{\boldsymbol{\kappa}}(\,\cdot\,)q_\nu^{\mathrm{chGUE}}(\boldsymbol{\kappa};T),\quad P_T(\,\cdot\,)=\int_{\mathbb{W}_N^{\mathrm{C}}}d\boldsymbol{\kappa}\,P_T^{\boldsymbol{\kappa}}(\,\cdot\,)q_\nu^{\mathrm{chGOE}}(\boldsymbol{\kappa};T).$$

Then $P_T(\,\cdot\,)$ and $P(\,\cdot\,)$ satisfy the same relation as the generalized Imhof relation between $\mathbf{X}^{(\nu,\nu+1)}(t)$ and $\mathbf{Y}^{(\nu)}(t)$ obtained from Proposition 8 by setting $\nu\in\mathbb{N}$, $\kappa=\nu+1$. Since $P(\,\cdot\,)$ is equal to the distribution of the temporally homogeneous diffusion process $\mathbf{Y}^{(\nu)}(t)$ (see (31) of Lemma 4), we can conclude that $P_T(\,\cdot\,)$ is identical to the distribution of the process $\mathbf{X}^{(\nu,\nu+1)}(t)$.

The second part can be proved by the same argument as the first part. For given $y^\rho, z^\rho \in \mathcal{S}(N), \tilde{y}^\rho, \tilde{z}^\rho \in \mathcal{A}(N), 0 \leqslant \rho \leqslant 3$, put $Y = \sqrt{-1}\tilde{y}^0 \otimes \sigma_0 + y^1 \otimes \sigma_1 + y^2 \otimes \sigma_2 + y^3 \otimes \sigma_3 \in \mathcal{H}_{2-}(2N)$ and $Z = \sqrt{-1}\tilde{z}^0 \otimes \sigma_0 + \sqrt{-1}\tilde{z}^1 \otimes \sigma_1 + \sqrt{-1}\tilde{z}^2 \otimes \sigma_2 + z^3 \otimes \sigma_3 \in \mathcal{H}_{1-}(2N)$. For these Y and Z, we introduce the temporally inhomogeneous matrix-valued processes

$$\Xi_T^{\mathrm{C}}(t:Y) = \sqrt{-1}a_T^0(t:\tilde{y}^0) \otimes \sigma_0 + s_T^1(t:y^1) \otimes \sigma_1 + s_T^2(t:y^2) \otimes \sigma_2 + s_T^3(t:y^3) \otimes \sigma_3,$$

$$\Xi_T^{\mathrm{D}}(t:Z) = \sqrt{-1}a_T^0(t:\tilde{z}^0) \otimes \sigma_0 + \sqrt{-1}a_T^1(t:\tilde{z}^1) \otimes \sigma_1 + \sqrt{-1}a_T^2(t:\tilde{z}^2) \otimes \sigma_2 + s_T^3(t:z^3) \otimes \sigma_3.$$

The key lemma 10 of the proof is replaced by the following:

Lemma 11: For any $U \in \mathrm{U}_2(2N), V \in \mathrm{U}_1(2N)$, $U^\dagger \Xi_T^{\mathrm{C}}(t:Y)U = \Xi_T^{\mathrm{C}}(t:U^\dagger Y U)$, *and* $V^\dagger \Xi_T^{\mathrm{D}}(t:Z)V = \Xi_T^{\mathrm{D}}(t:V^\dagger Z V)$, $t \in [0,T]$ *in distribution.*

For $\sharp = \mathrm{C}$ and D we denote by $P_T^{\sharp,\boldsymbol{\omega}}(\cdot)$ the probability distributions of the processes of nonnegative eigenvalues of $\Xi_T^\sharp(t:Z)$ conditioned that the nonnegative eigenvalues of Z is $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_N)$ with (18). We also denote by $P^\sharp(\cdot)$ and $P_T^\sharp(\cdot)$ the distributions of the processes of nonnegative eigenvalues of $\Xi^\sharp(t)$ and $\Xi_T^\sharp(t), t \in [0,T]$, respectively. Then we have the expressions

$$P^\sharp(\cdot) = \int_{\mathbb{W}_N^{\mathrm{C}}} d\boldsymbol{\omega}\, P_T^{\sharp,\boldsymbol{\omega}}(\cdot) q^\sharp(\boldsymbol{\omega};T), \quad P_T^\sharp(\cdot) = \int_{\mathbb{W}_N^{\mathrm{C}}} d\boldsymbol{\omega}\, P_T^{\sharp,\boldsymbol{\omega}}(\cdot) q^{\sharp\prime}(\boldsymbol{\omega};T) \quad \text{for} \quad \sharp = \mathrm{C}, \mathrm{D}.$$

Comparing them with the $(\nu,\kappa) = (1/2,1)$ and $(\nu,\kappa) = (-1/2,0)$ cases of the generalized Imhof relations obtained from Proposition 8, we have the theorem. ■

As a corollary of Theorem 9, the following integral formulas are derived as proved in Appendix B.

Corollary 12:

(i) *Assume* $\nu \in \mathbb{N}$ *and* $\mathbf{x}, \mathbf{y} \in \mathbb{W}_N^{\mathrm{C}}$. *For any* $\sigma \in \mathbb{R}$,

$$\int_{\mathrm{U}(N+\nu)\times\mathrm{U}(N)} d\mu(U,V) \exp\left\{ -\frac{1}{2\sigma^2} \mathrm{Tr}(K_{\mathbf{x}} - U^\dagger K_{\mathbf{y}} V)^\dagger (K_{\mathbf{x}} - U^\dagger K_{\mathbf{y}} V) \right\}$$
$$= \frac{C_\nu \sigma^{N(N+\nu-2)}}{h^{(\nu)}(\mathbf{x}) h^{(\nu)}(\mathbf{y})} \det_{1 \leqslant i,j \leqslant N} \left[e^{-(x_i^2+y_j^2)/2\sigma^2} I_\nu\left(\frac{x_i y_j}{\sigma^2} \right) \right],$$

where

$$K_{\mathbf{x}} = \begin{pmatrix} \hat{K}_{\mathbf{x}} \\ O \end{pmatrix}, \quad K_{\mathbf{y}} = \begin{pmatrix} \hat{K}_{\mathbf{y}} \\ O \end{pmatrix},$$

with $\hat{K}_{\mathbf{x}} = \mathrm{diag}\{x_1, x_2, \ldots, x_N\}, \hat{K}_{\mathbf{y}} = \mathrm{diag}\{y_1, y_2, \ldots, y_N\}$ *and* $\nu \times N$ *zero matrix* O.

(ii) *Let* $\sharp = \mathrm{C}, \mathrm{D}$. *For* $\mathbf{x}, \mathbf{y} \in \mathbb{W}_N^{\mathrm{C}}$, $\sigma \in \mathbb{R}$,

$$\int_{\tilde{\mathrm{U}}(2N)} dU \exp\left\{ -\frac{1}{4\sigma^2} \mathrm{Tr}(\Lambda_{\mathbf{x}} - U^\dagger \Lambda_{\mathbf{y}} U)^2 \right\} = \frac{C[\sharp] \sigma^{d[\sharp]}}{h^\sharp(\mathbf{x}) h^\sharp(\mathbf{y})} \det_{1 \leqslant i,j \leqslant N} [G^\sharp(\sigma^2, y_j | x_i)],$$

where $\Lambda_{\mathbf{x}} = \mathrm{diag}\{x_1, x_2, \ldots, x_N\} \otimes \sigma_3$, $\Lambda_{\mathbf{y}} = \mathrm{diag}\{y_1, y_2, \ldots, y_N\} \otimes \sigma_3$, $\tilde{\mathrm{U}}(2N) = \mathrm{U}_2(2N)$ *for* $\sharp = \mathrm{C}$ *and* $\tilde{\mathrm{U}}(2N) = \mathrm{U}_1(2N)$ *for* $\sharp = \mathrm{D}$.

They are extensions of the Harish–Chandra (Itzykson–Zuber) formula (42). The formula (i) is found in Ref. 27.

C. Watermelon topology

Consider the N-particle system of Brownian motions starting from $\mathbf{x} \in \mathbb{W}_N^{\mathrm{A}}$ at time $t = 0$ and arriving at $\mathbf{z} \in \mathbb{W}_N^{\mathrm{A}}$ at time $T > 0$, which do not collide with each other during the time interval $[0,T]$. We denote by $g^{\mathrm{A,w}}(0,\mathbf{x};t,\mathbf{y};T,\mathbf{z})$ the probability density of the state $\mathbf{y}$ at time $t \in [0,T]$. It is given by

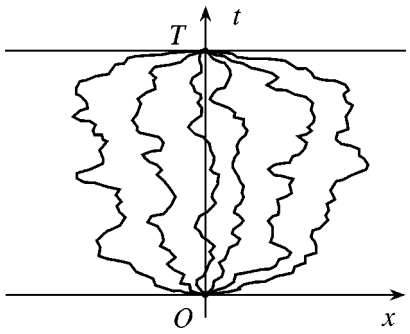

FIG. 3. Process $\mathbf{X}^{\mathrm{A,w}}(t), t\in[0,T]$, showing watermelon topology.

$$g^{\mathrm{A,\,w}}(0,\mathbf{x};t,\mathbf{y};T,\mathbf{z})=\frac{f^{\mathrm{A}}(t,\mathbf{y}|\mathbf{x})f^{\mathrm{A}}(T-t,\mathbf{z}|\mathbf{y})}{f^{\mathrm{A}}(T,\mathbf{z}|\mathbf{x})},\quad \mathbf{y}\in\mathbb{W}_N^{\mathrm{A}}, t\in[0,T]. \tag{45}$$

By using (34), we can obtain the limit $g^{\mathrm{A,\,w}}(0,\mathbf{0};t,\mathbf{y};T,\mathbf{0})=\lim_{|\mathbf{x}|\to 0,|\mathbf{z}|\to 0} g^{\mathrm{A,\,w}}(0,\mathbf{x};t,\mathbf{y};T,\mathbf{z})$. Let $\sigma_T(t)=\sqrt{t(1-t/T)}$.

Proposition 13: For $\mathbf{y}\in\mathbb{W}_N^{\mathrm{A}}$, $g^{\mathrm{A,\,w}}(0,\mathbf{0};t,\mathbf{y};T,\mathbf{0})=q^{\mathrm{GUE}}(\mathbf{y};\sigma_T(t)^2), t\in[0,T]$.

We denote by $\mathbf{X}^{\mathrm{A,\,w}}(t), t\in[0,T]$, the temporally inhomogeneous diffusion process, whose probability density is given by the above. Its path-configuration on the spatio-temporal plane is illustrated by Fig 3. Such a pattern is called *watermelon topology* in the polymer network theory.[14]

For $\nu>-1$, similar to (45) we put

$$g^{(\nu),\mathrm{w}}(0,\mathbf{x};t,\mathbf{y};T,\mathbf{z})=\frac{f^{(\nu)}(t,\mathbf{y}|\mathbf{x})f^{(\nu)}(T-t,\mathbf{z}|\mathbf{y})}{f^{(\nu)}(T,\mathbf{z}|\mathbf{x})}$$

for $\mathbf{x},\mathbf{y},\mathbf{z}\in\mathbb{W}_N^{\mathrm{C}}, t\in[0,T]$. By (33) we have the following $\mathbf{x}\to\mathbf{0}$ limit:

Proposition 14: For $\nu>-1, \mathbf{x}\in\mathbb{W}_N^{\mathrm{C}}, t\in[0,T]$,

$$g^{(\nu),\mathrm{w}}(0,\mathbf{0};t,\mathbf{x};T,\mathbf{0})=\frac{\sigma_T(t)^{-2N(N+\nu)}}{C_\nu}h^{((2\nu+1)/2)}(\mathbf{x})^2\exp\left\{-\frac{|\mathbf{x}|^2}{2\sigma_T(t)^2}\right\}.$$

In particular, if $\nu\in\mathbb{N}$, $g^{(\nu),\mathrm{w}}(0,\mathbf{0};t,\mathbf{x};T,\mathbf{0})=q_\nu^{\mathrm{chGUE}}(\mathbf{x},\sigma_T(t)^2)$, $g^{(1/2),\mathrm{w}}(0,\mathbf{0};t,\mathbf{x};T,\mathbf{0})=q^{\mathrm{C}}(\mathbf{x},\sigma_T(t)^2)$, *and* $g^{(-1/2),\mathrm{w}}(0,\mathbf{0};t,\mathbf{x};T,\mathbf{0})=q^{\mathrm{D}}(\mathbf{x},\sigma_T(t)^2)$.

We note that this expression may be formally obtained by taking $\kappa\to 2(\nu+1)$ limit of (38).

D. Banana topology

For $\varepsilon>0$, we consider a subspace of $\mathbb{W}_{2N}^{\mathrm{A}}$, $\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)=\{\mathbf{x}=(x_1,x_2,\ldots,x_{2N})\in\mathbb{W}_{2N}^{\mathrm{A}}: x_{2i}=x_{2i-1}+\varepsilon, 1\leqslant i\leqslant N\}$. For $\mathbf{x}\in\mathbb{W}_{2N}^{\mathrm{A}}$, we will use the notation $\mathbf{x}^{\mathrm{odd}}=(x_1,x_3,\ldots,x_{2N-1})$ and define $\mathcal{N}^{\mathrm{A,\,b}}(t,\mathbf{x};\varepsilon)=\int_{\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)}d\mathbf{y}^{\mathrm{odd}}f^{\mathrm{A}}(t,\mathbf{y}|\mathbf{x})$. We consider the process, whose transition probability density is given by

$$g_T^{\mathrm{A,\,b}}(s,\mathbf{x};t,\mathbf{y};\varepsilon)=\frac{f^{\mathrm{A}}(t-s,\mathbf{y}|\mathbf{x})\mathcal{N}^{\mathrm{A,\,b}}(T-t,\mathbf{y};\varepsilon)}{\mathcal{N}^{\mathrm{A,\,b}}(T-s,\mathbf{x};\varepsilon)},\quad \mathbf{x},\mathbf{y}\in\mathbb{W}_{2N}^{\mathrm{A}}, 0\leqslant s<t\leqslant T.$$

This is the $2N$-particle system of noncolliding Brownian motions in $[0,T]$ conditioned that the final state at time $t=T$ is in $\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)$. Using (34), we have

$$g_T^{\mathrm{A,\,b}}(0,\mathbf{0};t,\mathbf{y};\varepsilon)\equiv\lim_{|\mathbf{x}|\to 0}g_T^{\mathrm{A,\,b}}(0,\mathbf{x};t,\mathbf{y};\varepsilon)=\left(\frac{t}{T}\right)^{-2N^2}\frac{h^{\mathrm{A}}(\mathbf{y})e^{-|\mathbf{y}|^2/2t}\mathcal{N}^{\mathrm{A,\,b}}(T-t,\mathbf{y};\varepsilon)}{\int_{\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)}d\mathbf{z}^{\mathrm{odd}}\,h^{\mathrm{A}}(\mathbf{z})e^{-|\mathbf{z}|^2/2T}}$$

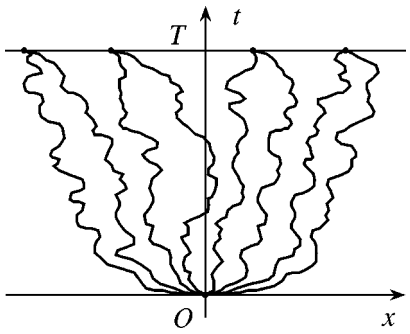

FIG. 4. Process $\mathbf{X}^{\mathrm{A},\mathrm{b}}(t), t\in[0,T]$, showing banana topology.

for $\mathbf{y}\in\mathbb{W}_{2N}^{\mathrm{A}}, t\in(0,T]$. Since $\lim_{t\to 0} f^{\mathrm{A}}(0,\mathbf{y}|\mathbf{x})=\Pi_{i=1}^{N}\delta(x_i-y_i)$, $\lim_{t\to 0}\mathcal{N}^{\mathrm{A},\mathrm{b}}(t,\mathbf{x};\varepsilon)=\mathbf{1}(\mathbf{x}\in\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon))$, and then for $\mathbf{y}\in\mathbb{W}_{2N}^{\mathrm{A}}$,

$$\lim_{t\nearrow T} g_T^{\mathrm{A},\mathrm{b}}(0,\mathbf{0};t,\mathbf{y};\varepsilon)=\frac{h^{\mathrm{A}}(\mathbf{y})e^{-|\mathbf{y}|^2/2T}}{\int_{\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)}d\mathbf{z}^{\mathrm{odd}}\,h^{\mathrm{A}}(\mathbf{z})e^{-|\mathbf{z}|^2/2T}}\mathbf{1}(\mathbf{y}\in\mathbb{B}_{2N}^{\mathrm{A}}(\varepsilon)).$$

As implied in Ref. 41 we can take the limit, $g_T^{\mathrm{A},\mathrm{b}}(s,\mathbf{x};t,\mathbf{y})=\lim_{\varepsilon\to 0} g_T^{\mathrm{A},\mathrm{b}}(s,\mathbf{x};t,\mathbf{y};\varepsilon)$, in the above formulas to have

$$g_T^{\mathrm{A},\mathrm{b}}(s,\mathbf{x};t,\mathbf{y})=\frac{f^{\mathrm{A}}(t-s,\mathbf{y}|\mathbf{x})\mathcal{N}^{\mathrm{A},\mathrm{b}}(T-t,\mathbf{y})}{\mathcal{N}^{\mathrm{A},\mathrm{b}}(T-s,\mathbf{x})}, \tag{46}$$

$$g_T^{\mathrm{A},\mathrm{b}}(0,\mathbf{0};t,\mathbf{y})=\left(\frac{T}{2}\right)^{N(2N+1)/2}\left(\frac{t}{2}\right)^{-2N^2}\frac{h^{\mathrm{A}}(\mathbf{y})}{C[\mathrm{A}'']}e^{-|\mathbf{y}|^2/2t}\mathcal{N}^{\mathrm{A},\mathrm{b}}(T-t,\mathbf{y}), \tag{47}$$

$$g_T^{\mathrm{A},\mathrm{b}}(0,\mathbf{0};T,\mathbf{y})=q^{\mathrm{GSE}}\left(\mathbf{y}^{\mathrm{odd}};\frac{T}{2}\right)\mathbf{1}(\mathbf{y}\in\mathbb{B}_{2N}^{\mathrm{A}}), \tag{48}$$

for $\mathbf{x},\mathbf{y}\in\mathbb{W}_{2N}^{\mathrm{A}}, 0\leqslant s<t<T$, where $\mathcal{N}^{\mathrm{A},\mathrm{b}}(t,\mathbf{x})=\int_{\mathbb{W}_N^{\mathrm{A}}}d\mathbf{y}\,f^{\mathrm{A},\mathrm{b}}(t,\mathbf{y}|\mathbf{x})$ with

$$f^{\mathrm{A},\mathrm{b}}(t,\mathbf{y}|\mathbf{x})=\det_{1\leqslant i\leqslant 2N,1\leqslant j\leqslant N}\left[G^{\mathrm{A}}(t,y_j|x_i)\ \ \frac{x_i}{t}G^{\mathrm{A}}(t,y_j|x_i)\right]$$

for $\mathbf{x}\in\mathbb{W}_{2N}^{\mathrm{A}}$ and $\mathbf{y}\in\mathbb{W}_N^{\mathrm{A}}$, and $\mathbb{B}_{2N}^{\mathrm{A}}=\{\mathbf{x}=(x_1,x_2,\ldots,x_{2N}):\mathbf{x}^{\mathrm{odd}}\in\mathbb{W}_N^{\mathrm{A}}, x_{2i}=x_{2i-1}, 1\leqslant i\leqslant N\}$. We define the temporally inhomogeneous process $\mathbf{X}^{\mathrm{A},\mathrm{b}}(t), t\in[0,T]$ starting from $\mathbf{0}$ or the state in $\mathbb{W}_{2N}^{\mathrm{A}}$ and ending at the state in $\mathbb{B}_{2N}$ as the diffusion process, whose transition probability density is given by (46)–(48). The path-configuration of N particles in this version of noncolliding Brownian motions on the spatio-temporal plane is illustrated by Fig. 4, which we would like to call "banana topology." An important point is that at the final time $t=T$ the particle positions are pairwise degenerated and distinct positions are identical in distribution with the Kramers doublets of eigenvalues of random matrices in GSE as claimed by (48).

Now we consider a $2N\times 2N$ Hermitian matrix-valued temporally inhomogeneous process defined by

$$\begin{aligned}\Xi_T^{\mathrm{b}}(t)=&\{s^0(t)+\sqrt{-1}a_T^0(t:O)\}\otimes\sigma_0+\{s_T^1(t:O)+\sqrt{-1}a^1(t)\}\otimes\sigma_1\\&+\{s_T^2(t:O)+\sqrt{-1}a^2(t)\}\otimes\sigma_2+\{s_T^3(t:O)+\sqrt{-1}a^3(t)\}\otimes\sigma_3,\end{aligned} \tag{49}$$

where the elements of the $N\times N$ matrices $\{s_T^\rho(t:z^\rho),(a_T^\rho:\tilde{z}^\rho)\}_{\rho=1}^3$ are given by (41). By definition, $\Xi_T^{\mathrm{b}}(T)$ distributes with the probability density of GSE. Then the same argument as Theorem 9 may prove the following:

Theorem 15: *Let* $\boldsymbol{\lambda}(t)=(\lambda_1(t),\lambda_2(t),\ldots,\lambda_{2N}(t))$ *be the eigenvalues of the process (49) with* $\lambda_1(t)\leqslant\lambda_2(t)\leqslant\cdots\leqslant\lambda_{2N}(t)$. *If* $\mathbf{X}^{\mathrm{A},\mathrm{b}}(0)=\mathbf{0}$, *then* $\boldsymbol{\lambda}(t)=\mathbf{X}^{\mathrm{A},\mathrm{b}}(t)$, $t\in[0,T]$ *in distribution*

As a corollary of this theorem, we will have the following version of Harish–Chandra formula, which is found as Eq. (3.46) in Ref. 41.

Corollary 16: Let $\mathbf{x}=(x_1,x_2,\ldots,x_{2N})\in\mathbb{W}_{2N}^{\mathrm{A}}$, $\mathbf{y}=(y_1,y_2,\ldots,y_N)\in\mathbb{W}_N^{\mathrm{A}}$. *For any* $\sigma\in\mathbb{R}$

$$\int_{U(2N)}dU\exp\left\{-\frac{1}{2\sigma^2}\mathrm{Tr}(\Lambda_{\mathbf{x}}-U^\dagger\Lambda_y U)^2\right\}=\frac{C_{2N}[\mathrm{A}]\sigma^{(2N)^2}}{h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})^4}f^{\mathrm{A},\mathrm{b}}(\sigma^2,\mathbf{y}|\mathbf{x}),$$

where $\Lambda_{\mathbf{x}}=\mathrm{diag}\{x_1,x_2,\ldots,x_{2N}\}$, $\Lambda_{\mathbf{y}}=\mathrm{diag}\{y_1,y_2,\ldots,y_N\}\otimes\sigma_0$, *and* $C_{2N}[\mathrm{A}]=(2\pi)^N\Pi_{i=1}^{2N}\Gamma(i)$.

It is easy to see by the same argument that the transition probability density given below defines the temporally inhomogeneous diffusion process $\mathbf{X}^{(\nu,\kappa),\mathrm{b}}(t),t\in[0,T],\nu>-1,\kappa\in[0,2(\nu+1))$, associated with $\mathbf{X}^{(\nu,\kappa)}$, which shows the banana topology: Let

$$f^{(\nu),\mathrm{b}}(t,\mathbf{y}|\mathbf{x})=\det_{1\leqslant i\leqslant 2N,1\leqslant j\leqslant N}[G^{(\nu)}(t,y_j|x_i)\quad G_y^{(\nu)}(t,y_j|x_i)]$$

for $\mathbf{x}\in\mathbb{W}_{2N}^{\mathrm{C}},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$, where $G_y^{(\nu)}(t,y|x)=(\partial/\partial y)G^{(\nu)}(t,y|x)$, and let $\tilde{\mathcal{N}}^{(\nu,\kappa),\mathrm{b}}(t,\mathbf{x})=\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{y}\,f^{(\nu),\mathrm{b}}(t,\mathbf{y}|\mathbf{x})\Pi_{i=1}^N y_i^{-\kappa}$ for $\mathbf{x}\in\mathbb{W}_{2N}^{\mathrm{C}}$. Then

$$g_T^{(\nu,\kappa),\mathrm{b}}(s,\mathbf{x};t,\mathbf{y})=\frac{f^{(\nu)}(t-s,\mathbf{y}|\mathbf{x})\tilde{\mathcal{N}}^{(\nu,\kappa),\mathrm{b}}(T-t,\mathbf{y})}{\tilde{\mathcal{N}}^{(\nu,\kappa),\mathrm{b}}(T-s,\mathbf{x})},$$

$$g_T^{(\nu,\kappa),\mathrm{b}}(0,\mathbf{0};t,\mathbf{y})=\frac{2^{N(4N+4\nu-1)}T^{2N^2}t^{-2N(2N+\nu)}}{\hat{C}_\nu}h^{(2\nu+1)}(\mathbf{y})e^{-|\mathbf{y}|^2/2t}\tilde{\mathcal{N}}^{(\nu,\kappa),\mathrm{b}}(T-t,\mathbf{y}),$$

$$g_T^{(\nu,\kappa),\mathrm{b}}(0,\mathbf{0};T,\mathbf{y})=\frac{1}{\hat{C}_\nu}\left(\frac{2}{T}\right)^{2N(N+\nu)}h^{((4\nu-2\kappa+3)/4)}(\mathbf{y}^{\mathrm{odd}})^4e^{-|\mathbf{y}^{\mathrm{odd}}|^2/T}\mathbf{1}(\mathbf{y}\in\mathbb{B}_{2N}^{\mathrm{C}}),\tag{50}$$

for $\mathbf{x},\mathbf{y}\in\mathbb{W}_{2N}^{\mathrm{C}},0\leqslant s<t<T$, where $\hat{C}_\nu=2^{N(2N+2\nu-1)}\Pi_{i=1}^N\{\Gamma(2i)\Gamma(2(i+\nu))\}$ and $\mathbb{B}_{2N}^{\mathrm{C}}=\{\mathbf{x}=(x_1,x_2,\ldots,x_{2N}):\mathbf{x}^{\mathrm{odd}}\in\mathbb{W}_N^{\mathrm{C}},x_{2i}=x_{2i-1},1\leqslant i\leqslant N\}$. We should notice that (50) includes the following special cases:

$$g_T^{(\nu,0),\mathrm{b}}(0,\mathbf{0};T,\mathbf{y})=q_\nu^{\mathrm{chGSE}}\left(\mathbf{y}^{\mathrm{odd}};\frac{T}{2}\right)\mathbf{1}(\mathbf{y}\in\mathbb{B}_{2N}^{\mathrm{C}})\quad\text{for}\quad\nu\in\mathbb{N},$$

$$g_T^{(-1/2,0),\mathrm{b}}(0,\mathbf{0};T,\mathbf{y})=q^{\mathrm{DIII}}\left(\mathbf{y}^{\mathrm{odd}},\frac{T}{2}\right)\mathbf{1}(\mathbf{y}\in\mathbb{B}_{2N}^{\mathrm{C}}).$$

Here

$$q_\nu^{\mathrm{chGSE}}(\boldsymbol{\kappa};t)=\frac{t^{-2N(N+\nu)}}{\hat{C}_\nu}\exp\left\{-\frac{|\boldsymbol{\kappa}|^2}{2t}\right\}\prod_{1\leqslant i<j\leqslant N}(\kappa_j^2-\kappa_i^2)^4\prod_{k=1}^N\kappa_k^{4\nu+3}$$

is the probability density of the N distinct square roots $\boldsymbol{\kappa}=(\kappa_1,\kappa_2,\ldots,\kappa_N)$ with (11) of the eigenvalues of $M^\dagger M$ conditioned that M is a $2N\times 2N$ random matrix in the chiral Gaussian symplectic ensemble (chGSE) with variance t,[54,53,27,51] and

$$q^{\mathrm{DIII}}(\boldsymbol{\omega};t)=\frac{t^{-d[\mathrm{D}'']/2}}{C[\mathrm{D}'']}\exp\left\{-\frac{|\boldsymbol{\omega}|^2}{2t}\right\}\prod_{1\leqslant i<j\leqslant N}(\omega_j^2-\omega_i^2)^4\prod_{k=1}^{N}\omega_k$$

with $d[\mathrm{D}'']=2N(2N-1), C[\mathrm{D}'']=\hat{C}_{-1/2}=2^{2N(N-1)}\Pi_{i=1}^{N}\Gamma(2i)\Gamma(2i-1)$ is the probability density of the non-negative and distinct eigenvalues $\boldsymbol{\omega}=(\omega_1,\omega_2,\ldots,\omega_N)$ with (18) of $4N\times 4N$ matrices in the ensemble in the symmetry class DIII studied by Altland and Zirnbauer.[56,1,2] (Strictly speaking, it is the DIII-even case. The DIII-odd case is obtained by setting $\nu=1/2$, $\kappa=0$ in (50).) The above implies that $\mathbf{X}^{(\nu,0),\mathrm{b}}(t)$ with $\nu\in\mathbb{N}$ and $\mathbf{X}^{(-1/2,0),\mathrm{b}}(t)$, both starting from $\mathbf{0}$, exhibit the transitions from the eigenvalue statistics of chGUE to chGSE and from the class D to the class DIII, respectively, as time t goes on from 0 to T.

A lengthy but explicit expression for the $4N\times 4N$ Hermitian matrix-valued process corresponding to $\mathbf{X}^{(-1/2,0),\mathrm{b}}(t)$ is given as

$$\begin{aligned}\Xi_T^{\mathrm{D,b}}(t)=&\sum_{\rho=0}^{2}\{\sqrt{-1}a_T^{0\rho}(t:O)\otimes(\sigma_0\otimes\sigma_\rho)+\sqrt{-1}a^{1\rho}(t)\otimes(\sigma_1\otimes\sigma_\rho)+s_T^{2\rho}(t:O)\otimes(\sigma_2\otimes\sigma_\rho)\\&+\sqrt{-1}a^{3\rho}(t)\otimes(\sigma_3\otimes\sigma_\rho)\}+\{s^{03}(t)\otimes(\sigma_0\otimes\sigma_3)+s^{13}(t)\otimes(\sigma_1\otimes\sigma_3)\\&+\sqrt{-1}a_T^{23}(t:O)\otimes(\sigma_2\otimes\sigma_3)+s_T^{33}(t:O)\otimes(\sigma_3\otimes\sigma_3)\},\end{aligned}$$

$t\in[0,T]$, where $s^{\mu\rho}(t)$, $s_T^{\mu\rho}(t:O)\in\mathcal{S}(N)$ and $a^{\mu\rho}(t)$, $a_T^{\mu\rho}(t:O)\in\mathcal{A}(N)$, $t\in[0,T]$, are defined similarly to (17) and (41). Identification of its eigenvalue process with $\mathbf{X}^{(-1/2,0),\mathrm{b}}(t)$ gives the following version of the Harish–Chandra integral,

$$\begin{aligned}&\int_{U_1(4N)}dU\exp\left\{-\frac{1}{4\sigma^2}\mathrm{Tr}(\Lambda_{\mathbf{x}}-U^{\dagger}\Lambda_{\mathbf{y}}U)^2\right\}\\&\quad=\frac{C_{2N}[\mathrm{D}]\sigma^{2N(4N+1)}}{h^{\mathrm{D}}(\mathbf{x})h^{(1/4)}(\mathbf{y})^4}\det_{1\leqslant i\leqslant 2N,1\leqslant j\leqslant N}\left[G^{\mathrm{D}}(\sigma^2,y_j|x_i)\ \frac{x_i}{\sigma^2}G^{\mathrm{C}}(\sigma^2,y_j|x_i)\right]\end{aligned}$$

for any $\sigma\in\mathbb{R}$, $\mathbf{x}=(x_1,x_2,\ldots,x_{2N})\in\mathbb{W}_{2N}^{\mathrm{C}}$, $\mathbf{y}=(y_1,y_2,\ldots,y_N)\in\mathbb{W}_N^{\mathrm{C}}$, where $\Lambda_{\mathbf{x}}=\mathrm{diag}\{x_1,x_2,\ldots,x_{2N}\}\otimes\sigma_3$, $\Lambda_{\mathbf{y}}=\mathrm{diag}\{y_1,y_2,\ldots,y_N\}\otimes(\sigma_3\otimes\sigma_0)$, and $C_{2N}[\mathrm{D}]=(\pi/2)^N\ \Pi_{i=1}^{2N}\Gamma(2i-1)$.

VI. CONCLUDING REMARKS

In the present paper we showed that the eigenvalue processes of GUE, chGUE, the class C, and the class D are realized by the temporally homogeneous noncolliding diffusion processes and then the temporally inhomogeneous noncolliding diffusion processes were introduced, which exhibit the transitions in distribution from the eigenvalue statistics of GUE to GOE, GUE to GSE, chGUE to chGOE, chGUE to chGSE, the class C to the class CI, and the class D to the class DIII. They are obtained as the special cases of the noncolliding systems of the Brownian motions and those of Yor's generalized meanders. These inhomogeneous processes are identified with the

eigenvalue processes of the inhomogeneous matrix-valued processes, some of which are regarded as the stochastic versions of two-matrix models studied by Pandey and Mehta[47,41] as demonstrated in Refs. 31, 35. We would like to put emphasis on the fact that in order to prove the identification we have not used any results by Pandey and Mehta, but used the generalized versions of Imhof relations ((4) and Proposition 8). Therefore we can give the proof for the Harish–Chandra (Itzykson–Zuber)-type integration formulas as corollaries. The present study suggests several open problems. Here we list some of them.

(i) It does not seem to be possible to realize the eigenvalue processes of the random matrix ensembles different from GUE, chGUE, the class C and the class D by any temporally homogeneous noncolliding systems of diffusion particles. Is it possible to realize them as the temporally homogeneous diffusion processes with some conditions additional to the simple noncolliding condition?

(ii) Norris, Rogers, and Williams[46] studied other matrix-valued process called Dynkin's Brownian motion $\tilde{\Xi}(t)=G(t)^T G(t)$ with $\partial G(t)=(\partial B(t))G(t)$, where ∂ denotes the Stratonovich differential; $x\partial y=xdy+dxdy/2$ for continuous semimartingales x,y. They showed that the eigenvalues of $\tilde{\Xi}(t)$ are also noncolliding systems and derived the stochastic differential equations similar to (1) for the logarithms of the eigenvalues. As mentioned by Bru (see Remark 2 in Ref. 7), $G(t)$ is a matrix-version of *multiplicative Brownian motion* in a sense, while $B(t)$ is the ordinary additional Brownian motion. Can we discuss (the logarithms of) the eigenvalue processes using the random matrix theory and noncolliding diffusion processes as well?

(iii) In the non-Hermitian random matrix ensembles, eigenvalues are distributed on the complex plane.[20,12] Is it meaningful to consider the stochastic version of non-Hermitian random matrix theory in the sense of Dyson?[10]

For the temporally inhomogeneous noncolliding Brownian motions $\mathbf{X}(t), t\in[0,T]$ with $\mathbf{X}(0)=\mathbf{0}$, the determinantal expressions for the multitime correlation functions were determined by Nagao and the present authors using the self-dual quaternion matrices[44,16,42] and the scaling limits of the infinite particles $N\to\infty$ and the infinite time-interval $T\to\infty$ were investigated.[45,30] Recently Nagao reported the similar calculation on the process, which corresponds to the process $\mathbf{X}^{(1/2,1)}$ in the present paper.[43] Calculation of the multitime correlations for the general process $\mathbf{X}^{(\nu,\kappa)}(t)$ is now in progress and the study of the infinite particle systems will be reported elsewhere.[34]

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APPENDIX A: SCHUR FUNCTION EXPANSIONS OF DETERMINANTS

Any sequence $\mu=(\mu_1,\mu_2,\ldots,\mu_N,\ldots)$ of non-negative integers in decreasing order $\mu_1\geqslant\mu_2\geqslant\cdots\geqslant\mu_N\geqslant\cdots$ is called a partition. The nonzero μ_i in μ are called the parts of μ and the number of parts is the length of μ denoted by $\ell(\mu)$. For each partition μ with $\ell(\mu)\leqslant N$, the Schur function defined by $s_\mu(\mathbf{x})=\det_{1\leqslant i,j\leqslant N}(x_i^{\mu_j+N-j})/\det_{1\leqslant i,j\leqslant N}(x_i^{N-j})$ gives a symmetric polynomial of order $|\mu|=\Sigma_{i=1}^N\mu_i$ in N variables $x_1,x_2,\ldots,x_N\in\mathbb{C}$. Note that the denominator is the Vandermonde determinant and $\det_{1\leqslant i,j\leqslant N}(x_i^{N-j})=(-1)^{N(N-1)/2}h^{\mathrm{A}}(\mathbf{x})$.[39,17,52] We can prove the following expansion formulas of the determinants with the bases of the Schur functions:[3,4,36]

$$\frac{\det_{1\leqslant i,j\leqslant N}[e^{x_i y_j}]}{h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})}=\sum_{\mu:\ell(\mu)\leqslant N} a_\mu s_\mu(\mathbf{x})s_\mu(\mathbf{y}),$$

$$\frac{\det_{1\leqslant i,j\leqslant N}[I_\nu(2\sqrt{x_i y_j})]}{\{\Pi_{i=1}^N x_i^{\nu/2}y_i^{\nu/2}\}h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})}=\sum_{\mu:\ell(\mu)\leqslant N} b_\mu^{(\nu)} s_\mu(\mathbf{x})s_\mu(\mathbf{y}),$$

where $a_\mu=1/\Pi_{i=1}^N\Gamma(\mu_i+N-i+1)$ and $b_\mu^{(\nu)}=1/\{\Pi_{i=1}^N\Gamma(\mu_i+N-i+1)\Gamma(\nu+\mu_i+N-i+1)\}$. Since $s_\mu(\mathbf{0})=\mathbf{1}(\mu=\mathbf{0})$ with $\mathbf{0}=(0,0,\ldots,0)\in\mathbb{N}^N$, from the above formulas, we have the following asymptotics of the determinants. As $|\mathbf{x}|\to 0$,

$$\det_{1\leqslant i,j\leqslant N}[e^{x_i y_j}]=\frac{h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})}{\Pi_{i=1}^N\Gamma(i)}\times(1+\mathcal{O}(|\mathbf{x}|)), \tag{A1}$$

$$\det_{1\leqslant i,j\leqslant N}[I_\nu(2\sqrt{x_i y_j})]=\left\{\prod_{i=1}^N x_i^{\nu/2}y_i^{\nu/2}\right\}\frac{h^{\mathrm{A}}(\mathbf{x})h^{\mathrm{A}}(\mathbf{y})}{\Pi_{j=1}^N\Gamma(j)\Gamma(\nu+j)}\times(1+\mathcal{O}(|\mathbf{x}|)). \tag{A2}$$

APPENDIX B: PROOF OF COROLLARY 12

By (38) of Lemma 5 (ii),

$$\begin{aligned}
g_T^{(\nu,\kappa)}(0,\mathbf{0};t,\mathbf{y})&=\frac{T^{N(N+\kappa-1)/2}t^{-N(N+\nu)}}{C_{\nu,\kappa}}\exp\left\{-\frac{|\mathbf{y}|^2}{2t}\right\}h^{(2\nu+1)}(\mathbf{y})\\
&\quad\times\int_{\mathbb{W}_N^{\mathbb{C}}}d\mathbf{z}\det_{1\leqslant i,j\leqslant N}\left[\frac{z_j^{\nu+1}}{y_i^\nu}\frac{1}{T-t}\exp\left\{-\frac{y_i^2+z_j^2}{2(T-t)}\right\}I_\nu\left(\frac{y_i z_j}{T-t}\right)\right]\prod_{k=1}^N z_k^{-\kappa}\\
&=\frac{T^{N(N+\kappa-1)/2}t^{-N(N+\nu)}}{(T-t)^N C_{\nu,\kappa}}\left(\frac{T}{t}\right)^{N(\nu+1-\kappa)}h^{(\nu+1)}(\mathbf{y})\int_{\mathbb{W}_N^{\mathbb{C}}}d\mathbf{z}\exp\left\{-\frac{T}{2t^2}\left(\frac{t}{T}\right)^2|\mathbf{z}|^2\right\}\\
&\quad\times\det_{1\leqslant i,j\leqslant N}\left[\exp\left\{-\frac{T}{2t(T-t)}\left(y_i^2+\frac{t^2}{T^2}z_j^2\right)\right\}I_\nu\left(\frac{T}{t(T-t)}y_i\times\frac{t}{T}z_j\right)\right]\\
&\quad\times\prod_{\ell=1}^N\left(\frac{t}{T}z_\ell\right)^{\nu+1-\kappa}.
\end{aligned}$$

Setting $(t/T)z_i=a_i$, $1\leqslant i\leqslant N$, $t(1-t/T)=\sigma^2$ and $T/t^2=\alpha$, we have

$$\begin{aligned}
g_T^{(\nu,\kappa)}(0,\mathbf{0};t,\mathbf{y})&=\frac{\sigma^{-2N}\alpha^{N(N+2\nu-\kappa+1)/2}}{C_{\nu,\kappa}}h^{(\nu+1)}(\mathbf{y})\\
&\quad\times\int_{\mathbb{W}_N^{\mathbb{C}}}d\mathbf{a}\,e^{-\alpha|\mathbf{a}|^2/2}\det_{1\leqslant i,j\leqslant N}\left[e^{-(y_i^2+a_j^2)/2\sigma^2}I_\nu\left(\frac{y_i a_j}{\sigma^2}\right)\right]\prod_{\ell=1}^N a_\ell^{\nu+1-\kappa}.
\end{aligned} \tag{B1}$$

Proof of (i): We write the transition probability density of the process $M_T(t)$ by $Q_T(s,m_1;t,m_2)$, $0\leqslant s<t\leqslant T$, for $m_1,m_2\in\mathcal{M}(N+\nu,N;\mathbb{C})$. Then by Theorem 9 (i) and the fact (12),

$$g_T^{(\nu,\nu+1)}(0,\mathbf{0};t,\mathbf{y})=\frac{(2\pi)^{N(N+\nu)}}{C_\nu}h^{((2\nu+1)/2)}(\mathbf{y})^2\int_{\mathrm{U}(N+\nu)\times\mathrm{U}(N)}d\mu(U,V)\,Q_T(0,O;t,U^\dagger K_{\mathbf{y}}V). \tag{B2}$$

We introduce the $\mathcal{M}(N+\nu,N;\mathbb{C})$-valued process $M^{(1)}(t)=(m_{ij}^{(1)}(t))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$ and the $\mathcal{M}(N+\nu,N;\mathbb{R})$-valued process $M^{(2)}(t)=(m_{ij}^{(2)}(t))_{1\leqslant i\leqslant N+\nu,1\leqslant j\leqslant N}$, whose elements are defined by

$$m_{ij}^{(1)}(t)=B_{ij}^0(t)-\frac{t}{T}B_{ij}^0(T)+\sqrt{-1}(\tilde{\beta}_T^0)_{ij}(t) \quad \text{and} \quad m_{ij}^{(2)}(t)=\frac{t}{T}B_{ij}^0(T).$$

Then $M_T(t)=M^{(1)}(t)+M^{(2)}(t)$. Note that $\{B_{ij}^0(t)-(t/T)B_{ij}^0(T)\}$ are Brownian bridges of duration T starting at 0 and ending at 0, which are independent of $(t/T)B_{ij}^0(T)$. Hence $M^{(1)}(t)$ is in the chiral GUE distribution and $M^{(2)}(t)$ in the chiral GOE distribution, where $M^{(1)}(t)$ and $M^{(2)}(t)$ are independent from each other. Since $E[m_{ii}^{(1)}(t)^2]=\sigma^2$ and $E[m_{ii}^{(2)}(t)^2]=1/\alpha$, $Q_T(0,O;t,M)$ for $M\in\mathcal{M}(N+\nu,N;\mathbb{C})$ can be written as

$$\begin{aligned}Q_T(0,O;t,M)&=\int_{\mathcal{M}(N+\nu,N;\mathbb{R})}\mathcal{V}(dB)\mu_\nu^{\mathrm{chGOE}}(B;1/\alpha)\mu_\nu^{\mathrm{chGUE}}(M-B;\sigma^2)\\&=\frac{\alpha^{N(N+\nu)/2}\sigma^{-N(N+\nu)}}{C_{\nu,\nu+1}(2\pi)^{N(N+\nu)}}\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{a}\,h^{(\nu)}(\mathbf{a})e^{-\alpha|\mathbf{a}|^2/2-\mathrm{Tr}(M-K_\mathbf{a})^\dagger(M-K_\mathbf{a})/2\sigma^2},\end{aligned}\tag{B3}$$

where we have used the fact (16) and the formulas (10) and (15). Combining (B1) with $\kappa=\nu+1$, (B2) and (B3), we have

$$\begin{aligned}&\frac{C_\nu\sigma^{N(N+\nu-2)}}{h^{(\nu)}(\mathbf{y})}\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{a}\,e^{-\alpha|\mathbf{a}|^2/2}\det_{1\leqslant i,j\leqslant N}\left[\exp\left\{-\frac{y_i^2+a_j^2}{2\sigma^2}\right\}I_\nu\left(\frac{y_ia_j}{\sigma^2}\right)\right]\\&\quad=\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{a}\,h^{(\nu)}(\mathbf{a})e^{-\alpha|\mathbf{a}|^2/2}\int_{\mathrm{U}(N+\nu)\times\mathrm{U}(N)}d\mu(U,V)\,e^{-\mathrm{Tr}(U^\dagger K_\mathbf{y}V-K_\mathbf{a})^\dagger(U^\dagger K_\mathbf{y}V-K_\mathbf{a})/2\sigma^2}.\end{aligned}$$

Since, for each $\sigma\in\mathbb{R}$, this equality holds for any $\alpha>0$, we have the formula (i).

Proof of (ii): By setting $(\nu,\kappa)=(1/2,1)$ and $(\nu,\kappa)=(-1/2,0)$ in (B1) we have the expressions for $\mathbf{x},\mathbf{y}\in\mathbb{W}_N^{\mathrm{C}}$,

$$g_T^{(1/2,1)}(0,\mathbf{0};t,\mathbf{x})=\frac{\alpha^{N(N+1)/2}}{C[\mathrm{C}']}h^{\mathrm{C}}(\mathbf{x})\int_{\mathbb{W}_N^{\mathrm{C}}}d\mathbf{a}\,e^{-\alpha|\mathbf{a}|^2/2}\det_{1\leqslant i,j\leqslant N}[G^{\mathrm{C}}(\sigma^2,a_j|x_i)],$$

$$g_T^{(-1/2,0)}(0,\mathbf{0};t,\mathbf{y})=\frac{\alpha^{N^2/2}}{C[\mathrm{D}']}h^{\mathrm{D}}(\mathbf{y})\int_{\mathbb{W}_N^{\mathrm{D}}}d\mathbf{a}\,e^{-\alpha|\mathbf{a}|^2/2}\det_{1\leqslant i,j\leqslant N}[G^{\mathrm{D}}(\sigma^2,a_j|y_i)].$$

Following the same argument with the proof of (i) and using the equalities (19) and (23), formulas (ii) are proved. ■

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Relativistic *N*-boson systems bound by pair potentials $V(r_{ij})=g(r_{ij}^2)$

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We study the lowest energy E of a relativistic system of N identical bosons bound by pair potentials of the form $V(r_{ij})=g(r_{ij}^2)$ in three spatial dimensions. In natural units $\hbar=c=1$ the system has the semirelativistic "spinless-Salpeter" Hamiltonian $H=\Sigma_{i=1}^{N}\sqrt{m^2+p_i^2}+\Sigma_{j>i=1}^{N}g(|\mathbf{r}_i-\mathbf{r}_j|^2)$, where g is monotone increasing and has convexity $g''\geqslant 0$. We use "envelope theory" to derive formulas for general lower energy bounds and we use a variational method to find complementary upper bounds valid for all $N\geqslant 2$. In particular, we determine the energy of the N-body oscillator $g(r^2)=cr^2$ with error less than 0.15% for all $m\geqslant 0$, $N\geqslant 2$, and $c>0$.
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I. INTRODUCTION

We consider a system of N identical bosons interacting by attractive pair potentials $V(r_{ij})$ and obeying the semirelativistic spinless Salpeter equation.[1,2] The Hamiltonian governing the dynamics of the N-particle problem is given by

$$H=\sum_{i=1}^{N}\sqrt{m^2+p_i^2}+\sum_{j>i=1}^{N}V(|\mathbf{r}_i-\mathbf{r}_j|) \tag{1.1}$$

and represents a model system having a relativistically correct expression for the kinetic energy and a static pair potential. One of the reasons for considering such a model is that the extension to the many-particle case poses no fundamental technical problems beyond what are already present in the one-body problem, namely the square root in the kinetic energy and the nonlocality that the definition[3] of the Hamiltonian entails. Our lower bounds use the necessary permutation symmetry of the N-boson problem to effect a "reduction" to an almost equivalent 2-body problem.[4,5] The purpose of the present paper is first to use envelope theory[6–10] to extend our specific energy lower bounds for the harmonic oscillator[11] to apply to smooth transformations of the oscillator having the general form $V(r)=g(r^2)$, where g is monotone increasing and of positive convexity ($g''\geqslant 0$). Secondly, we show that the earlier upper energy bounds (via a Gaussian trial function) for the oscillator $V(r)=cr^2$ can be considerably sharpened; this improvement is carried over to the larger class of pair potentials. We have already shown this[12] for the ultrarelativistic case $m=0$ of

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the pure oscillator. In this paper we shall generalize these oscillator results to $V(r)=g(r^2)$ and $m\geqslant 0$. For the oscillator $V(r)=cr^2$ itself, the new bounds are separated by less than 0.15% for all $m\geqslant 0$, $c>0$, and $N\geqslant 2$.

In Sec. II we recall some fundamental formulas concerning the one-body harmonic oscillator with Hamiltonian $\sqrt{m^2+p^2}+r^2$ and lowest energy $e(m)$. This problem does not have an exact analytical solution but can be easily solved numerically to yield $e(m)$ to arbitrary accuracy; this result is necessary for our *N*-body lower bounds. As distinct from our earlier work,[11] in this paper we eschew the *P*-representation and its concomitant scaling subtleties, and base all our lower bounds on the function $e(m)$ itself.

In Sec. III we turn to the principal topic of this paper, namely potentials which are smooth transformations $V(r)=g(r^2)$ of the oscillator potential. If g is convex ($g''\geqslant 0$), the graph of $V(r)$ lies above "tangential potentials" $V^{(t)}(r)$ with the general form $V^{(t)}(r)=a(t)+b(t)r^2$, where $t=\hat{r}^2$ is the point of contact with the potential $V(r)$ itself. As $t>0$ varies, $\{V^{(t)}(r)\}$ represents a family of shifted oscillators. Envelope theory allows one to construct energy lower bounds based on this fundamental geometrical idea. In Sec. IV we construct variational upper bounds by use of a translation-invariant Gaussian trial function. In Sec. V we look at the ultrarelativistic case $m\rightarrow 0$, and in Sec. VI we apply our general results to some examples from the family $V(r)=cr^q$, $q\geqslant 2$.

II. THE ONE-BODY OSCILLATOR PROBLEM

We consider the one-body problem with Hamiltonian

$$H_1=\sqrt{m^2+p^2}+r^2\rightarrow e(m), \tag{2.1}$$

where, for coupling $c=1$, $e(m)$ is the lowest eigenvalue as a function of the mass m. In the momentum-space representation, we have an equivalent problem with Hamiltonian

$$\tilde{H}_1=-\Delta+\sqrt{m^2+r^2}\rightarrow e(m). \tag{2.2}$$

Since this Schrödinger problem is easy to solve numerically to arbitrary accuracy, we shall take the position that $e(m)$ is "known" and at our disposal. We note that in the large-m (nonrelativistic or Schrödinger) limit, we have

$$e(m)\simeq e_{\mathrm{NR}}(m)=m+\frac{3}{\sqrt{2m}}. \tag{2.3}$$

The graph of $e(m)-m$ is shown in Fig. 1: $e(m)$ is monotone increasing with m; $e(m)-m$, however, is monotone *decreasing*, in agreement, for large m, with the Feynman–Hellmann theorem for the corresponding nonrelativistic case.

It remains now to use scaling to generalize these results. This is necessary for our later application to the *N*-body problem. For the energy of a more general one-body problem in which the kinetic-energy term is multiplied by the positive factor β, the coupling $\gamma>0$ is included, and a further parameter $\lambda>0$ is allowed for, we have, by scaling arguments,

$$H_1=\beta\sqrt{m^2+\lambda p^2}+\gamma r^2\rightarrow \epsilon(m,\beta,\gamma\lambda)=(\beta^2\gamma\lambda)^{1/3}e\left(m\left(\frac{\beta}{\gamma\lambda}\right)^{1/3}\right). \tag{2.4}$$

III. ENERGY LOWER BOUND FOR $V(r)=g(r^2)$ BY ENVELOPE THEORY

Our hypothesis is that $V(r)=g(r^2)$, where the smooth transformation function g is monotone increasing and its convexity is positive or zero. That is to say, we shall assume $g''\geqslant 0$. These assumptions imply a relation between $V(r)$ and a "tangential potential" $V^{(t)}(r)$ given explicitly by

$$V(r)\geqslant V^{(t)}(r)=g(t)-tg'(t)+g'(t)r^2=a(t)+b(t)r^2, \tag{3.1}$$

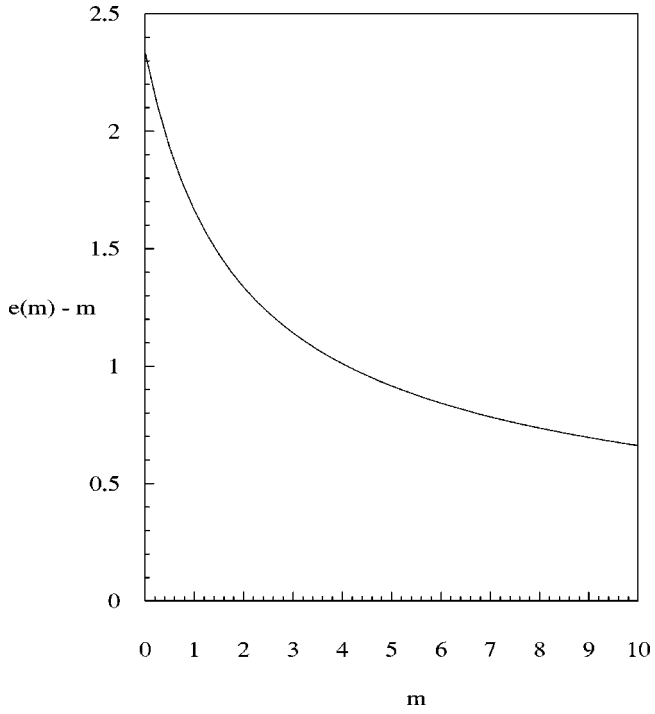

FIG. 1. The energy function $e(m)-m$ of the one-body problem defined by (2.1).

where $t=\hat{r}^2$ is the point of contact between the tangential potential and the potential. For each fixed t, the tangential potential has the form $a+br^2$ of a shifted oscillator. This potential inequality induces, in turn, a spectral inequality as an immediate consequence of the min–max characterization of the spectrum of the Hamiltonian. It is the task of envelope theory[6–10] to generate expressions for this spectral inequality.

The kinetic-energy term in the Hamiltonian H does not have the kinetic energy of the center-of-mass removed. Thus the wave function we use must satisfy two fundamental symmetries: translation invariance and boson permutation symmetry (in the individual-particle coordinates). Jacobi relative coordinates may be defined with the aid of an orthogonal matrix B relating the column vectors of the new $[\boldsymbol{\rho}_i]$ and old $[\mathbf{r}_i]$ coordinates given by $[\boldsymbol{\rho}_i]=B[\mathbf{r}_i]$. The first row of B defines a center-of-mass variable $\boldsymbol{\rho}_1$ with every entry $1/\sqrt{N}$, the second row defines a pair distance $\boldsymbol{\rho}_2=(r_1-r_2)/\sqrt{2}$, and the kth row, $k\geqslant 2$, has the first $k-1$ entries $B_{ki}=1/\sqrt{k(k-1)}$, the kth entry $B_{kk}=-\sqrt{(k-1)/k}$, and the remaining entries zero. We define the corresponding momentum variables by $[\boldsymbol{\pi}_i]=(B^{-1})^t[\mathbf{p}_i]=B[\mathbf{p}_i]$. Let us suppose that the (unknown) exact normalized boson ground-state wave function for the N-body harmonic-oscillator problem with $V(r)=cr^2$ is $\Psi=\Psi(\rho_2,\rho_3,\ldots,\rho_N)$ corresponding to energy E. Boson symmetry is a powerful constraint that greatly reduces the complexity of this problem. We immediately obtain [Ref. 11, Eq. (2.3)] the "reduction"

$$E=(\Psi,H\Psi)=\left(\Psi,\left[N\sqrt{m^2+p_N^2}+\frac{N(N-1)}{2}c|\mathbf{r}_1-\mathbf{r}_2|^2\right]\Psi\right). \tag{3.2}$$

Since $|r_1-r_2|^2=2\rho_2^2$, in terms of the Jacobi relative coordinates this becomes

$$E=\left(\Psi,\left[N\sqrt{m^2+\left(\frac{\boldsymbol{\pi}_1}{\sqrt{N}}-\sqrt{\frac{N-1}{N}}\,\boldsymbol{\pi}_N\right)^2}+N(N-1)c\rho_2^2\right]\Psi\right). \tag{3.3}$$

The lemma proved in Ref. 11 allows us to remove the term in the center-of-mass momentum operator π_1 from inside the square root. Boson permutation symmetry furthermore implies [Ref. 11, Eq. (2.5)]

$$(\Psi,\rho_2^2\Psi)=(\Psi,\rho_N^2\Psi), \tag{3.4}$$

even though the wave function Ψ may not be symmetric in the relative coordinates. These results lead to the final reduction

$$E=\left(\Psi,\left[N\sqrt{m^2+\frac{N-1}{N}\pi_N^2}+N(N-1)c\rho_N^2\right]\Psi\right). \tag{3.5}$$

If we now write $r=\rho_N$ and $p=\pi_N$, we see that the exact energy E can be written in the form $E=(\Psi,\mathcal{H}\Psi)$, in which $\mathcal{H}$ is the Hamiltonian for a one-body problem given by

$$\mathcal{H}=\beta\sqrt{m^2+\lambda p^2}+\gamma c r^2, \tag{3.6}$$

with

$$\beta=N,\quad \lambda=\frac{N-1}{N},\quad \text{and}\quad \gamma=N(N-1).$$

It follows that the exact energy E of the oscillator system is bounded below by $\mathcal{E}$, the bottom of the spectrum of the one-body Hamiltonian $\mathcal{H}$.

Thus, for the harmonic oscillator itself, we have from (3.5) and (2.4):

Theorem 1: *A lower bound to the ground-state energy eigenvalue E of the semirelativistic N-body Hamiltonian*

$$H=\sum_{i=1}^{N}\sqrt{m^2+p_i^2}+\sum_{j>i=1}^{N}c|\mathbf{r}_i-\mathbf{r}_j|^2,\quad c>0, \tag{3.7}$$

is provided by the formula

$$E\geqslant(\beta^2\gamma c\lambda)^{1/3}e\left(m\left(\frac{\beta}{\gamma c\lambda}\right)^{1/3}\right), \tag{3.8}$$

where

$$\beta=N,\quad \lambda=\frac{N-1}{N},\quad \gamma=N(N-1).$$

This lower bound yields the exact energy in the Schrödinger limit $m\to\infty$. If we consider the potential $V(r)=g(r^2)$ and use the potential lower bound (3.1), we can maximize the resulting lower bound provided by Theorem 1 to obtain:

Theorem 2: *A lower bound to the ground-state energy eigenvalue E of the semirelativistic N-body Hamiltonian*

$$H=\sum_{i=1}^{N}\sqrt{m^2+p_i^2}+\sum_{j>i=1}^{N}g(|\mathbf{r}_i-\mathbf{r}_j|^2),\quad g'>0,\quad g''\geqslant 0, \tag{3.9}$$

is provided by the formula

$$E\geqslant\max_{t>0}\left[m\beta\frac{e(\nu)}{\nu}+\frac{\gamma}{2}(g(t)-tg'(t))\right], \tag{3.10}$$

where

$$\beta=N, \quad \lambda=\frac{N-1}{N}, \quad \gamma=N(N-1), \quad \nu=m\left(\frac{\beta}{\gamma\lambda g'(t)}\right)^{1/3}.$$

If we consider the family of pure-power potentials of the form $V(r)=cr^q$, then for the harmonic oscillator $q=2$, we use Theorem 1; for more general potentials, with $q>2$, we have $V(r)=g(r^2)=g(t)=ct^{q/2}$. Consequently, we must in this case make the explicit substitutions

$$a(t)=g(t)-tg'(t)=-c\left(\frac{q}{2}-1\right)t^{q/2} \quad \text{and} \quad b(t)=g'(t)=\frac{cq}{2}t^{(q-2)/2}. \tag{3.11}$$

IV. VARIATIONAL UPPER BOUNDS

Improvement over the previous upper energy bounds[11] for the oscillator will be obtained in this paper by avoiding the loosening incurred by use of Jensen's inequality.[3,13] This goal has already been achieved[12] for the ultrarelativistic special case $m=0$ of the N-body harmonic-oscillator problem. We shall now extend this to more general problems with attractive potential $V(r)$ and $m\geqslant 0$.

We use a Gaussian wave function of the form

$$\Phi(\rho_2,\rho_3,\ldots,\rho_N)=C\exp\left(-\frac{\alpha}{2}\sum_{i=2}^{N}\rho_i^2\right), \quad \alpha>0, \tag{4.1}$$

where C is a normalization constant. The factoring property of this function, the boson-symmetry reduction leading to (3.5), and the additional fact that Φ is also symmetric under exchange of the *relative* coordinates allows us to write $r=\rho_2$, and $p=\pi_N\rightarrow\pi_2$, and finally

$$E\leqslant\beta(\phi,\sqrt{m^2+\lambda p^2}\phi)+\frac{\gamma}{2}(\phi,V(\sqrt{2}r)\phi), \tag{4.2}$$

where

$$\beta=N, \quad \lambda=\frac{N-1}{N}, \quad \gamma=N(N-1),$$

and the function $\phi(r)$ is given by

$$\phi(r)=\left(\frac{\alpha}{\pi}\right)^{3/4}\exp\left(-\frac{\alpha r^2}{2}\right). \tag{4.3}$$

The kinetic-energy integral may be written in terms of modified Bessel functions of the second kind,[14,15] which we now discuss. The calculation is best carried out in momentum space with the aid of the three-dimensional Fourier transform $\mathcal{F}$. We have

$$\phi(r)\overset{\mathcal{F}}{\rightarrow}\tilde{\phi}(k)=\left(\frac{1}{\alpha\pi}\right)^{3/4}\exp\left(-\frac{k^2}{2\alpha}\right). \tag{4.4}$$

Thus the expectation of the kinetic energy becomes

$$\langle K\rangle=\beta(\tilde{\phi},\sqrt{m^2+\lambda k^2}\tilde{\phi})=\frac{4\pi\beta}{(\alpha\pi)^{3/2}}\int_0^\infty\exp\left(-\frac{k^2}{\alpha}\right)\sqrt{m^2+\lambda k^2}k^2dk. \tag{4.5}$$

We may write this integral in the form

$$\langle K\rangle = \frac{\beta m\mu}{\sqrt{2\pi}} \exp\left(\frac{\mu^2}{4}\right) K_1\left(\frac{\mu^2}{4}\right), \quad \mu = m\left(\frac{2N}{(N-1)\alpha}\right)^{1/2}, \tag{4.6}$$

where $K_\nu(z)$ is a modified Bessel function of the second kind.[14,15]

The potential-energy integral will depend on the choice of $V(r)$. For the family $V(r) = c\ \mathrm{sgn}(q) r^q$, which we shall study in Sec. V, the integrals may be expressed in terms of the gamma function. Explicitly we have

$$\langle V\rangle = \left(\phi, \left(\frac{c\ \mathrm{sgn}(q)\gamma}{2}(r\sqrt{2})^q\right)\phi\right) = \frac{c\ \mathrm{sgn}(q)\gamma}{\sqrt{\pi}}\Gamma\left(\frac{3+q}{2}\right)\left(\frac{\mu\sqrt{\lambda}}{m}\right)^q. \tag{4.7}$$

With the results in this form we can use the parameter μ as a variational parameter. We have therefore established:

Theorem 3: *For fixed $m>0$, $q>-1$, $c>0$, $N\geqslant 2$, $\beta=N$, $\gamma=N(N-1)$, and $\lambda=(N-1)/N$, the lowest energy E of the N-boson problem for the pair potential $V(r)=c\ \mathrm{sgn}(q) r^q$ is given by the inequality*

$$E \leqslant \min_{\mu>0}\left[\frac{\beta m\mu}{\sqrt{2\pi}} \exp\left(\frac{\mu^2}{4}\right) K_1\left(\frac{\mu^2}{4}\right) + \frac{c\ \mathrm{sgn}(q)\gamma}{\sqrt{\pi}}\Gamma\left(\frac{3+q}{2}\right)\left(\frac{\mu\sqrt{\lambda}}{m}\right)^q\right]. \tag{4.8}$$

We have allowed $q>-1$ here since the upper bound easily accommodates this family of potentials in three spatial dimensions. For $q<-1$, there is no discrete spectrum. In the gravitational case $q=-1$ the minimum upper bound exists provided the coupling is not too large: specifically we require

$$\frac{c\gamma}{4\beta}\sqrt{\frac{2}{\lambda}} = \frac{c}{2}\sqrt{\frac{N(N-1)}{2}} < 1. \tag{4.9}$$

This situation is of course well known from the two-particle attractive Coulomb problem.[16,17] At present we only have close complementary lower bounds for $q\geqslant 2$.

V. THE ULTRARELATIVISTIC LIMIT

The ultrarelativistic case $m\to 0$ may be obtained from Theorems 2 and 3 as a special case. The Hamiltonian for this problem is given explicitly by

$$H = \sum_{i=1}^{N} \sqrt{p_i^2} + \sum_{j>i=1}^{N} c|\mathbf{r}_i - \mathbf{r}_j|^q, \quad c>0, \quad q\geqslant 2. \tag{5.1}$$

For the lower bound we use $g(t)=ct^{q/2}$. The upper bound may either be treated separately or taken from (4.8) by means of the limit $\lim_{z\to 0} zK_1(z)=1$. The bounds we obtain are given by

$$C\left[\frac{z_0}{3}\right]^{3q/[2(1+q)]} \leqslant E \leqslant \frac{C}{\sqrt{\pi}}\left[2\Gamma\left(\frac{3+q}{2}\right)\right]^{1/(1+q)}, \tag{5.2}$$

where $z_0 \approx 2.338\,107\,41$ is the first zero of the Airy function $\mathrm{Ai}(z)$, satisfying $\mathrm{Ai}(z_0)=0$, and the common factor C is given by

$$C = \left(\frac{cq}{2}\right)^{1/(1+q)}\left(1+\frac{1}{q}\right)(N(N-1))^{(2+q)/[2(1+q)]} 2^{3q/[2(1+q)]}.$$

As m increases from zero, the power-law bounds become closer monotonically with m; thus the $m=0$ case provides an upper bound to the error for all m. Since we have explicit formulas for the

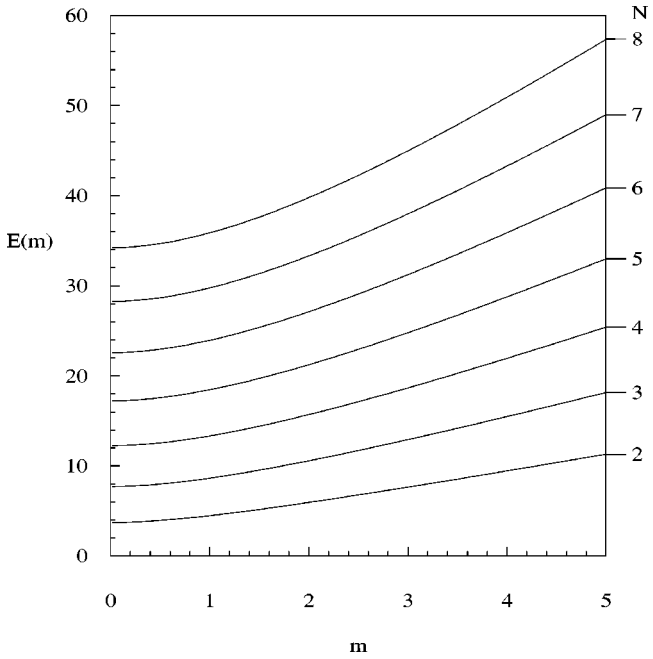

FIG. 2. The ground-state energy $E(m)$ of the relativistic N-boson harmonic-oscillator problem $V(r)=r^2$ for $N=2,3,...,8$. The figure shows the lower bounds given by Eq. (3.8): the upper bounds are everywhere less than 0.15% above these curves and are indistinguishable on the graph. In the Schrödinger limit $m\to\infty$ the upper and lower bounds coalesce to the exact energies.

bounds in terms of N, we are able to make definite statements concerning the percentage separations of the bounds for all N. If we take the energy estimate $\bar{E}$ to be the average of the bounds, the exact energy E is determined by $\bar{E}$ to within 0.15% for the harmonic oscillator $q=2$, and to 3.6% for the cubic ''oscillator'' $q=3$. In the nonrelativistic limit $m\to\infty$ the harmonic-oscillator bounds $q=2$ coalesce to the exact solution of the Schrödinger N-body problem.[11]

VI. EXAMPLES

The examples we consider are from the family $V(r)=cr^q$. In order to have a lower bound, we restrict the power to $q\geqslant 2$. We revisit the oscillator problem because we have considerably improved the upper bound since Ref. 11. Graphs of the lower bounds alone are shown in Fig. 2. The percentage separations are bounded above by the separations at $m=0$, which are there less than 0.15%. With the notation $E_N(m)$ we have explicitly, for the oscillator $q=2$, that the lower and upper estimates have numerical values $E_8^{\mathrm{L}}(1)=35.863\,83$ and $E_8^{\mathrm{U}}(1)=35.899\,53$, respectively. Thus the average of these values determines $E_8(1)$ in this case with error less than 0.05%. As we leave the oscillator and increase q beyond $q=2$, the bounds become less sharp. For $q=\frac{5}{2}$ we show the corresponding bounds in Fig. 3: here the bounds are separated for all m by less than 1.43%. The corresponding graphs for the cubic ''oscillator'' $q=3$ are shown in Fig. 4; in this case the maximum percentage separation (again for all $N\geqslant 2$ and $m\geqslant 0$) is 3.6%.

VII. CONCLUSION

The necessary permutation symmetry of the states of a system of identical particles is a powerful constraint. The approximate ''reduction'' of the N-body problem to a scaled two-body problem is most striking for systems of bosons, or for systems which are compatible with the assumption of permutation symmetry in the spatial variables alone.[4] For systems of fermions, the reduction is to a sum over two-body energies.[5] For the Schrödinger harmonic-oscillator problem, the boson reduction is complete in the sense that the N-body energy is given exactly by the energy

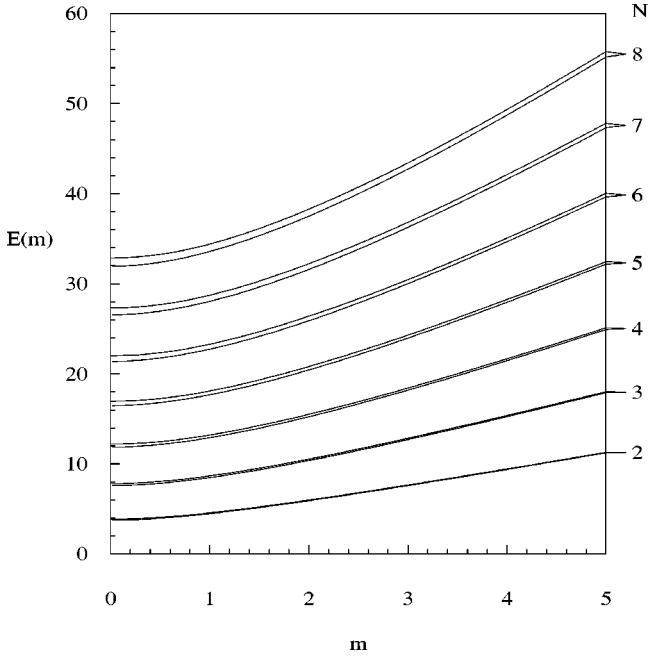

FIG. 3. Upper and lower energy bounds for the ground-state energy $E(m)$ of the relativistic N-boson problem corresponding to $V(r)=r^{5/2}$ for $N=2,3,...,8$. The percentage errors are maximum for $m=0$ where they determine the energies (for all N) with error less than 1.43%.

of a two-body problem. A lower bound by this type of reduction is possible provided either the kinetic-energy term or the potential-energy term has a quadratic form: this allows us to replace, for example, the ''mixed'' pair $\{\pi_N,\rho_2\}$ by $\{\pi_N,\rho_N\}$ in the reduced two-body Hamiltonian $\mathcal{H}$. For the Salpeter problem discussed in this paper, a quadratic form is present in the potential term of the

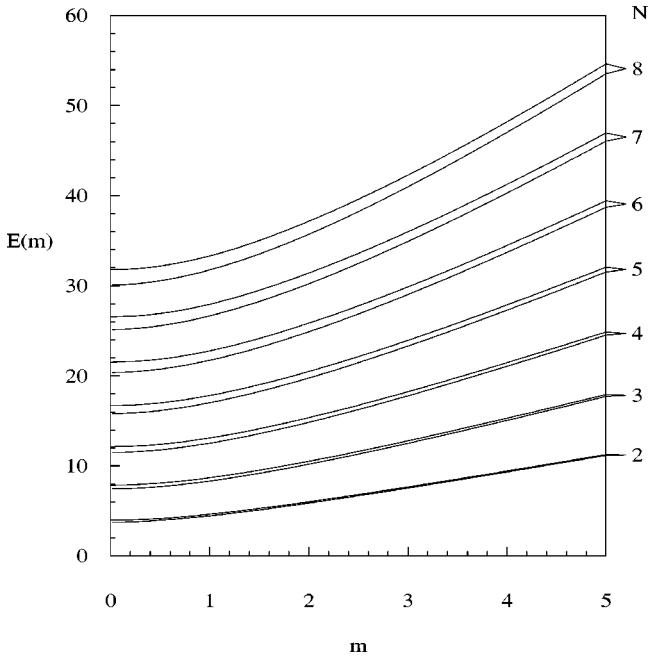

FIG. 4. Upper and lower energy bounds for the ground-state energy $E(m)$ of the relativistic N-boson problem corresponding to $V(r)=r^3$ for $N=2,3,...,8$. The percentage errors are maximum for $m=0$ where they determine the energies (for all N) with error less than 3.6%.

oscillator, and the lower bound obtained for this base problem is then applicable to other problems whose potentials $V(r)$ have the form of smooth convex transformations $g(r^2)$ of the oscillator. The extension beyond the oscillator is effected by the use of "envelope theory." A reduction is also used for our upper bound, but this reduction is allowed for general potentials and for a different reason. The trial function must be a translation-invariant boson function; but we have chosen a Gaussian trial function which has an additional symmetry, namely, it is also symmetric in the relative coordinates. It is this latter symmetry which completes the reduction in the case of the upper bound. Because of all these symmetries, what starts out as a complex many-body problem, appears in the end, for the purpose of finding energy bounds, as a one-body problem.

ACKNOWLEDGMENTS

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Langer–Cherry derivation of the multi-instanton expansion for the symmetric double well

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The multi-instanton expansion for the eigenvalues of the symmetric double well is derived using a Langer–Cherry uniform asymptotic expansion of the solution of the corresponding Schrödinger equation. The Langer–Cherry expansion is anchored to either one of the minima of the potential, and by construction has the correct asymptotic behavior at large distance, while the quantization condition amounts to imposing the even or odd parity of the wave function. This method leads to an efficient algorithm for the calculation to virtually any desired order of all the exponentially small series of the multi-instanton expansion, and with trivial modifications can also be used for nonsymmetric double wells. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767988]

I. INTRODUCTION

One of the early and most typical applications of semiclassical methods in quantum mechanics is the calculation of the exponentially small energy splitting between quasidegenerate levels in a double well, a splitting which is not captured by the usual Rayleigh–Schrödinger perturbation series for the eigenvalues around either one of the minima.[1] Almost every general-use variety of semiclassical approximation has been applied to this problem,[2–4] and many specific methods are still under active development.[5–14]

But in fact, working in the context of the large-order behavior of the coefficients of the perturbation series and partially inspired by the work of Bender and Wu,[15] already in 1981 Zinn-Justin[16,17] conjectured the form of the complete Borel-summable asymptotic expansion for the energy levels of the double well. This expansion consists of the Rayleigh–Schrödinger perturbation series plus an infinite sequence of subseries, where the kth subseries (the kth instanton contribution) is the kth power of an exponentially small factor times a sum of power series and logarithmic terms up to the power $k-1$. To be precise, the multi-instanton expansion cannot be directly summed for physical values of the coupling constant, which lie on a Stokes line of the Borel-summable asymptotic expansions, but has to be summed for, say, complex values, and followed by continuity to the positive real axis.[18–20] The multi-instanton expansion was initially derived by Wentzel–Kramers–Brillouin (WKB) methods as the solution of a modified Bohr–Sommerfeld quantization formula; a very clear and updated presentation of this quantization formula and its relation to the path integral method can be found in Ref. 21.

From a mathematical standpoint, the status of Zinn-Justin's modified quantization formula and of the ensuing multi-instanton expansion were of conjectures until the work of Delabaere, Dillinger, and Pham[22] and Delabaere and Pham.[23,24] These authors, building on previous work by Balian and Bloch,[25] Voros[26] and Écalle,[27,28] gave a rigorous set of rules whereby ''well normalized'' WKB expansions, considered as exact encodings of the true wave functions, can be analytically continued with respect to the coupling constant with a consistent and unique determination of the exponentially small terms. Although in Ref. 22 the authors deliberately emphasize the results which can be obtained without explicit computation of the WKB expansions, the double turning point connection problem pertaining to the double well is solved in terms of a ''reduced elementary connection operator'' (which in turn can be computed by the ''exact matching method'' explained in Ref. 24 and ultimately based on a form of the solution studied by Pham[29] and

Jidoumou[30]) and, besides the general proof of Zinn-Justin's conjecture, they give explicit results of the leading terms of the subseries up to the second instanton contribution for the double well $V(x)=x^4-x^2$.

The purpose of the present paper is threefold. First, to give a complete and self-contained derivation of the multi-instanton expansion for the symmetric double well based on the Langer–Cherry method to obtain Borel-summable uniform asymptotic expansions for the solutions of differential equations with turning points.[31–33] In particular we will see that the results of Cherry[33] avoid the problem of integration constants typical of WKB derivations, which is usually dealt with by regularization procedures essentially equivalent to repeated partial integrations before collapsing the integration path to the real axis.[2,34,35] Second, by using the inverse series of those used in the method of Refs. 22 and 24 we will find an explicit and efficient algorithm for the calculation of the multi-instanton expansion to any order. And third, we will show that an empirical observation made by Hoe *et al.*[36] in the context of the Stark effect can be carried over to the double well, yielding a yet more efficient algorithm which permits the calculation of virtually as many terms as desired of any instanton contribution of the quartic symmetric double well.

Furthermore, with the trivial modifications explained in the last section, the Langer–Cherry method of this paper can be used for any symmetric or nonsymmetric double well.

II. THE SYMMETRIC DOUBLE WELL

Let us briefly recall how the symmetric double well can be obtained by analytic continuation from the standard quartic anharmonic oscillator,[37] whose Schrödinger equation is

$$-\tfrac{1}{2}\Psi''(x)+(\tfrac{1}{2}x^2+Gx^4-\Lambda)\Psi(x)=0. \tag{1}$$

For real and positive values of the coupling constant G we have a well-defined self-adjoint eigenvalue problem on the real line. The spectrum consists of simple positive eigenvalues, and the Rayleigh–Schrödinger perturbation series in the coupling constant G is Borel summable to the exact eigenvalues.[38] To perform the analytic continuation to complex values of G we integrate the Schrödinger equation (1) along a straight line in the complex x plane such that at both ends there exists an exponentially decreasing solution,[39] e.g., $x=te^{-i\arg(G)/6}$ $(t\in\mathbf{R})$. The symmetric double well is reached for $\arg G=-3\pi/2$. To make contact with the usual notation in which the coupling constant g of the double well is real and positive, let

$$G=ge^{-i3\pi/2},\quad \Lambda=-iE,\quad x=ye^{i\pi/4},\quad \Psi(x)=\Phi(y).$$

The resulting equation is

$$-\tfrac{1}{2}\Phi''(y)+(gy^4-\tfrac{1}{2}y^2-E)\Phi(y)=0, \tag{2}$$

integrated along $y=te^{-i\arg(g)/6}$ $(t\in\mathbf{R})$, i.e., the integration path is the real y axis. In this form we immediately recognize the double-well potential

$$V(y)=gy^4-\tfrac{1}{2}y^2,$$

with the symmetric degenerate minima at

$$y_\pm=\pm\frac{1}{2g^{1/2}},$$

and expansions of the potential around the minima given by

$$V(y)=-\frac{1}{16g}+(y-y_\pm)^2\pm 2g^{1/2}(y-y_\pm)^3+g(y-y_\pm)^4.$$

These expansions permit a straightforward calculation of the Rayleigh–Schrödinger perturbation series around either one of the minima. To fix ideas, in the equation

$$-\frac{1}{2}\Phi''(y)+\left[(y-y_+)^2+2g^{1/2}(y-y_+)^3+g(y-y_+)^4-\frac{1}{16g}-E\right]\Phi(y)=0 \tag{3}$$

we take as unperturbed Hamiltonian the harmonic oscillator with force constant $k=2$ and unperturbed eigenvalues

$$E_n^{(0)}=\sqrt{2}(n+1/2), \tag{4}$$

and we take as perturbation the cubic and quartic terms. A parity argument shows that, aside from the trivial term $-1/(16g)$, the resulting series is a power series in g (without odd powers of $g^{1/2}$), which we write as

$$E_n=-\frac{1}{16g}+\sum_{k=0}^{\infty} g^k E_n^{(k)}. \tag{5}$$

From the usual equations of perturbation theory in the intermediate normalization it follows that the $E_n^{(k)}$ are alternatively odd and even polynomials of degree $k+1$ in $E_n^{(0)}$. With just a few lines of code (which take advantage of the fact that knowledge of the perturbed wave function to order k permits the calculation of the perturbed energy to order $2k+1$) we can calculate these perturbation coefficients $E_n^{(k)}$ to high order. To show the pattern and for later reference we list explicitly the lowest four polynomials,

$$E_n^{(1)}=-\tfrac{1}{4}-\tfrac{3}{2}(E_n^{(0)})^2, \tag{6}$$

$$E_n^{(2)}=-\tfrac{19}{8}E_n^{(0)}-\tfrac{17}{4}(E_n^{(0)})^3, \tag{7}$$

$$E_n^{(3)}=-\tfrac{131}{64}-\tfrac{459}{16}(E_n^{(0)})^2-\tfrac{375}{16}(E_n^{(0)})^4, \tag{8}$$

$$E_n^{(4)}=-\frac{22\,709}{256}E_n^{(0)}-\frac{23\,405}{64}(E_n^{(0)})^3-\frac{10\,689}{64}(E_n^{(0)})^5. \tag{9}$$

Finally, note the well-known facts that all the coefficients are negative [which precludes Borel summability of the perturbation series (5) on the real positive g axis], and that the perturbation series, being intrinsically local, does not take into account the presence of the symmetric well.

III. LANGER–CHERRY UNIFORM ASYMPTOTIC EXPANSION

In this section we discuss the calculation of a uniform (in the sense of being smooth across the classical turning points), Borel-summable asymptotic expansion for the double well. The basic strategy is the method of comparison equations[2,3] supplemented with the rigorous results on the analytic behavior of the coefficients by Langer[31,32] and Cherry,[33] and generalized by Lynn and Keller.[40] Gradual implementation of this general strategy for quantum oscillators can be traced back to the early work on the Stark effect by Silverstone *et al.*[41,42] In fact, the idea of matching two Borel-summable asymptotic expansions derived from Langer–Cherry wave functions to obtain discontinuity formulas for the eigenvalues of the quartic anharmonic oscillator with negative coupling constant is essentially contained in Ref. 42, and streamlined and carried out in detail to second order in Ref. 43. Likewise, application of similar methods to the calculation of asymptotic expansions for exponentially small splittings can be traced back at least to the work of Damburg and Propin,[44] where a symmetric double well is considered as a one-dimensional model for exchange forces in quantum chemistry, and especially to the calculation of the asymptotic expan-

sion for large distances of the energy levels of the hydrogen molecular ion by Čížek *et al.*[45] where the role of the Borel summability in the unambiguous calculation of the exponentially small subseries is carefully discussed.

As a first step we scale the independent variable to fix the position of the zeroth order double turning points, and to set g in the role, usually played by $\hbar$, of coefficient of the second-order derivative. The suitable scaling is

$$y=g^{-1/2}(z+1/2), \quad \Phi(y)=\psi(z), \tag{10}$$

which leads to the transformed equation

$$-\frac{g^2}{2}\psi''(z)+\left[z^2(1+z)^2-gE-\frac{1}{16}\right]\psi(z)=0. \tag{11}$$

We build the uniform asymptotic expansion around the minimum at $z=0$ where, aside from a constant term, the bracketed term in Eq. (11) behaves as z^2. Therefore we use as a comparison equation the Weber differential equation,[46] whose exponentially decreasing solution at large positive values of the argument [cf. Eq. (15) in the next section] is the parabolic cylinder function $D_\nu(z)$. Therefore we set

$$\psi(z)=[u'(z)]^{-1/2}D_{\nu/\sqrt{2}-1/2}[g^{-1/2}2^{3/4}u(z)], \tag{12}$$

which substituted into Eq. (11) leads to the equation for $u(z)$,

$$u(z)^2u'(z)^2=z^2(1+z)^2+g\left[\nu u'(z)^2-E(\nu)-\frac{1}{16g}\right]+\frac{g^2}{4}\{u,z\}, \tag{13}$$

where, as usual, $\{u,z\}$ stands for the Schwarzian derivative,

$$\{u,z\}=\frac{u'''(z)}{u'(z)}-\frac{3}{2}\left(\frac{u''(z)}{u'(z)}\right)^2.$$

At this point we call the reader's attention to the as yet unspecified parameter ν. In the next section we will see that the condition for the existence of eigenvalues (the modified quantization condition of Zinn-Justin) is precisely an equation for ν.

Following Langer and Cherry, we solve Eq. (13) by expanding both the function $u(z)$ and the eigenvalue $E(\nu)$ in asymptotic power series:

$$u(z)=\sum_{k=0}^{\infty}u_k(z)g^k,$$

$$E(\nu)=-\frac{1}{16g}+\sum_{k=0}^{\infty}E^{(k)}(\nu)g^k. \tag{14}$$

Substituting these asymptotic expansions into Eq. (13) and equating powers of g we arrive at a system of differential equations which can be solved recursively for the $u_k(z)$ in terms of elementary functions. We list here the first three equations, the last of which shows the general pattern because it already includes a contribution from the Schwarzian derivative,

$$\frac{\mathrm{d}}{\mathrm{d}z}[u_0(z)^2]=2z(1+z),$$

$$\frac{\mathrm{d}}{\mathrm{d}z}[u_0(z)u_1(z)]=\frac{E^{(0)}(\nu)}{2u_0(z)u_0'(z)}+\frac{\nu u_0'(z)}{2u_0(z)},$$

$$\frac{\mathrm{d}}{\mathrm{d}z}[u_0(z)u_2(z)]=\frac{E^{(1)}(\nu)}{2u_0(z)u_0'(z)}+\frac{\nu u_1'(z)}{u_0(z)}-\frac{u_0'(z)^2u_1(z)^2+u_0(z)^2u_1'(z)^2}{2u_0(z)u_0'(z)}-\frac{\{u_0,z\}}{8u_0(z)u_0'(z)}$$
$$-2u_1(z)u_1'(z).$$

Again, we draw on the results of Cherry,[33] which show that the $u_k(z)$ have to be chosen regular at $z=0$. The integration of the equation for $u_0(z)$ is immediate, yielding

$$u_0(z)=z\left(1+\frac{2z}{3}\right)^{1/2}.$$

Next, we note that for $k\geqslant 1$, if $u_k(z)$ is a solution of the corresponding differential equation, so is $u_k(z)+a/u_0(z)$ for any constant a. The integration of these equations for $k\geqslant 1$ is a two-step process: first, we fix the coefficient $E^{(k)}(\nu)$ to avoid the logarithmic singularity at $z=0$; second, we add a suitable multiple of $1/u_0(z)$ to avoid a simple pole at $z=0$ (this procedure is algorithmically easier to implement than the equivalent "integrate from 0 to z" prescription of Cherry[33]). Thus, to avoid a logarithmic singularity of $u_1(z)$ at $z=0$ we must set

$$E^{(0)}(\nu)=\nu,$$

and we get

$$2u_0(z)u_1(z)=\nu\ln[u_0(z)(1+z)/z].$$

Similarly, to avoid a logarithmic singularity in $u_2(z)$ we must set

$$E^{(1)}(\nu)=-\tfrac{1}{4}-\tfrac{3}{2}\nu^2,$$

and the corresponding regular function $u_2(z)$ is given by

$$u_1(z)^2+2u_0(z)u_2(z)=\frac{\nu u_1(z)}{u_0(z)}+\left[\frac{19}{48}-\frac{3}{16(1+z)^2}-\frac{1}{8(1+z)}-\frac{1}{4(3+2z)}\right]$$
$$+\nu^2\left[\frac{17}{8}-\frac{2}{3z}-\frac{1}{8(1+z)^2}-\frac{3}{4(1+z)}-\frac{1}{6(3+2z)}\right].$$

Although the explicit expressions of the $u_k(z)$ quickly become too unwieldy to be calculated by hand, the whole procedure can be easily programmed in a computer and carried out to high order. We list here the next three coefficients of the general asymptotic expansion for the energy $E(\nu)$,

$$E^{(2)}(\nu)=-\tfrac{19}{8}\nu-\tfrac{17}{4}\nu^3,$$

$$E^{(3)}(\nu)=-\tfrac{131}{64}-\tfrac{459}{16}\nu^2-\tfrac{375}{16}\nu^4,$$

$$E^{(4)}(\nu)=-\frac{22\,709}{256}\nu-\frac{23\,405}{64}\nu^3-\frac{10\,689}{64}\nu^5,$$

which are readily identified with the coefficients of the Rayleigh–Schrödinger perturbation series, except that the $E^{(k)}(\nu)$ are polynomials in the as yet unspecified $E_0(\nu)=\nu$.

IV. GENERALIZED QUANTIZATION CONDITION

As we mentioned in the Introduction, there are several methods to derive the generalized quantization condition, sometimes called the secular equation,[47] and there is even an ongoing discussion on whether the more general approaches are fully rigorous or contain unproved assumptions (see, for example, the discussions in Refs. 47 and 48 or the remarks after theorem 1.2.1 in Ref. 24; for yet an independent approach for polynomial potentials see Refs. 49–51).

Since our calculations are rather explicit, we will proceed in a straightforward manner. Note that, by construction, the Langer–Cherry solution (12) has the correct exponentially decreasing asymptotic behavior as z (and therefore y) tends to $+\infty$. Since the double-well potential $V(y)$ is even in y, we will impose the quantization condition by requiring that the solution (12) be even or odd in y or, on account of Eq. (10), that $\psi(-1/2)\neq 0$, $\psi'(-1/2)=0$ for the even solutions, and that $\psi(-1/2)=0$, $\psi'(-1/2)\neq 0$ for the odd solutions. To this end, we recall first the Borel-summable asymptotic expansions of the parabolic cylinder functions, and subsequently devote separate sections to the even and odd solutions. A final section deals with the solution of the generalized quantization condition.

A. Borel-summable asymptotic expansions of the parabolic cylinder functions

The sectors of Borel summability of the asymptotic expansions of the parabolic cylinder functions are ultimately determined by the branch point at $z=1$ of Gauss' hypergeometric function, and can be easily derived, for example, using the relation between the parabolic cylinder functions and the confluent hypergeometric functions.[52] The full expansions can be conveniently written in terms of the formal power series

$$ {}_2F_0(a,b;;z)=\sum_{k=0}^{\infty}(a)_k(b)_k\frac{z^k}{k!}, $$

where $(a)_k$ is the Pochhammer symbol

$$ (a)_0=1, \quad (a)_k=a(a+1)\cdots(a+k-1). $$

It turns out that the complex plane is divided into three nonoverlapping sectors separated by Stokes lines, and that within each of these sectors there is a uniquely defined Borel-summable asymptotic expansion as $z\to\infty$,

$$ D_\nu(z)\sim z^\nu e^{-z^2/4}\,{}_2F_0\left(-\frac{\nu}{2},\frac{1}{2}-\frac{\nu}{2};;-\frac{2}{z^2}\right), \quad -\frac{\pi}{2}<\arg z<\frac{\pi}{2}, \tag{15} $$

$$ \begin{aligned} D_\nu(z)\sim{}& z^\nu e^{-z^2/4}\,{}_2F_0\left(-\frac{\nu}{2},\frac{1}{2}-\frac{\nu}{2};;-\frac{2}{z^2}\right)\\ &+\frac{(2\pi)^{1/2}e^{\pm i\pi(\nu+1)}}{\Gamma(-\nu)}z^{-\nu-1}e^{z^2/4}\,{}_2F_0\left(\frac{1}{2}+\frac{\nu}{2},1+\frac{\nu}{2};;\frac{2}{z^2}\right), \quad \frac{\pi}{2}<\pm\arg z<\pi. \end{aligned} \tag{16} $$

It is worth noting that the expansions are not summable on the Stokes lines, which must be reached by continuity from either side. The validity of the subsequent formal operations with Borel-summable asymptotic expansions is established in Ref. 53.

B. Odd states

The quantization condition for odd states reads

$$ D_{\nu/\sqrt{2}-1/2}[2^{3/4}g^{-1/2}u(-1/2)]=0. \tag{17} $$

We have repeatedly noted that the negative real axis is a Stokes line for the Borel-summable asymptotic expansions of the parabolic cylinder function, and therefore we have to approach it from either side. For concreteness we give the coupling constant g a small positive argument and take

$$\arg g = \epsilon > 0, \quad \arg z = \pi.$$

The argument of the argument of the parabolic cylinder function is

$$\arg[2^{3/4} g^{-1/2} u(z)] = -\tfrac{1}{2}\arg g + \arg[u(z)] \sim -\tfrac{1}{2}\arg g + \arg[u_0(z)] \sim -\tfrac{1}{2}\arg g + \arg z = -\tfrac{1}{2}\epsilon + \pi,$$

and we have to use the plus sign in the asymptotic expansion (16). To simplify the notation, we introduce symbols for the following three formal power series in g whose coefficients are polynomials in ν:

$$u \equiv u\left(-\frac{1}{2}\right) = -\frac{1}{\sqrt{6}} + \sum_{k=1}^{\infty} c_k(\nu) g^k,$$

$$\Sigma_1 \equiv {}_2F_0\left(\frac{1}{4} - \frac{\nu}{2\sqrt{2}}, \frac{3}{4} - \frac{\nu}{2\sqrt{2}}; ; -\frac{g}{u^2\sqrt{2}}\right),$$

$$\Sigma_2 \equiv {}_2F_0\left(\frac{1}{4} + \frac{\nu}{2\sqrt{2}}, \frac{1}{4} + \frac{\nu}{2\sqrt{2}}; ; \frac{g}{u^2\sqrt{2}}\right),$$

where we have separated explicitly the constant term in u; the constant terms in Σ_1 and Σ_2 are obviously 1. Imposing the quantization condition (17) is now straightforward: we substitute the preceding series into the the right-hand side (with the plus sign) of Eq. (16) and find that the parameter ν must be a solution of the equation

$$(2^{3/4} g^{-1/2} u)^{\sqrt{2}\nu} \exp\left[-\frac{2^{1/2} u^2}{g}\right] \frac{\Sigma_1}{\Sigma_2} = -\frac{i(2\pi)^{1/2} e^{i\pi\nu/\sqrt{2}}}{\Gamma\left(\frac{1}{2} - \frac{\nu}{\sqrt{2}}\right)}.$$

To rewrite this quantization condition in a more convenient form we use the following gamma function reflection formula:

$$\Gamma\left(\frac{1}{2} + z\right)\Gamma\left(\frac{1}{2} - z\right) = \frac{\pi}{\cos(\pi z)},$$

and define a function

$$f(\nu) = \frac{i(2\pi)^{1/2}}{\Gamma\left(\frac{1}{2} + \frac{\nu}{\sqrt{2}}\right)} \left(-\frac{2^{3/4} u}{g^{1/2}}\right)^{\sqrt{2}\nu} \exp\left[-\frac{2^{1/2} u^2}{g} + \ln\frac{\Sigma_1}{\Sigma_2}\right]. \tag{18}$$

Then, the quantization condition reads

$$f(\nu) = 1 + e^{-i\pi\sqrt{2}\nu}.$$

By separating the leading behavior of u in the definition of $f(\nu)$ we can show explicitly its dependence as a function of the coupling constant g,

$$f(\nu)=\frac{i(2\pi)^{1/2}2^{3\nu/2\sqrt{2}}}{\Gamma\left(\frac{\nu}{\sqrt{2}}+\frac{1}{2}\right)}\exp\left[-\frac{1}{3\sqrt{2}}\left(\frac{1}{g}+3\nu\ln g+\sum_{k=1}^{\infty}F^{(k)}(\nu)g^{k}\right)\right], \tag{19}$$

where the $F^{(k)}(\nu)$ turn out to be polynomials in ν which can be calculated explicitly in principle to any desired order. We list here the first three, which again will be enough to show the pattern,

$$F^{(1)}(\nu)=\tfrac{19}{8}+\tfrac{51}{4}\nu^{2},$$

$$F^{(2)}(\nu)=\tfrac{459}{16}\nu+\tfrac{375}{8}\nu^{3},$$

$$F^{(3)}(\nu)=\frac{22\,709}{768}+\frac{23\,405}{64}\nu^{2}+\frac{17\,815}{64}\nu^{4}.$$

A comparison of these coefficients with the coefficients $E^{(k)}(\nu)$ shows immediately that the former can be easily written in terms of the latter,

$$F^{(k)}(\nu)=-\frac{1}{k}\frac{\partial E^{(k+1)}(\nu)}{\partial\nu}. \tag{20}$$

If we accept this conjecture, which we have checked explicitly up to $k=10$ but of which we do not have a formal proof, the expression for $f(\nu)$ can be written even more concisely in terms of the general asymptotic series for the eigenvalues $E(\nu)$ defined in Eq. (14):

$$f(\nu)=\frac{i(2\pi)^{1/2}2^{3\nu/2\sqrt{2}}}{\Gamma\left(\frac{\nu}{\sqrt{2}}+\frac{1}{2}\right)}\exp\left[\frac{1}{3\sqrt{2}}\int\frac{\partial E(\nu)}{\partial\nu}\frac{\mathrm{d}g}{g^{2}}\right].$$

From the theoretical point of view the validity of this equation would show that all the information required to calculate the complete asymptotic expansion for the energy levels in the double well is essentially contained in the coefficients of the Rayleigh–Schrödinger perturbation series when expanded as polynomials in the quantum number. Likewise, from a practical, algorithmic point of view, this relation gives an extremely simple and efficient method to calculate the $F^{(k)}(\nu)$ to very high order, avoiding the integration of the differential equation for $u(z)$; these high-order calculations have been recently of some interest for the numerical study of the Borel summation (with subsequent continuation to the real axis) of the multi-instanton series.[20] Finally, we remark that an observation equivalent to Eq. (20) was made by Hoe *et al.*[36] who, in the context of the Stark effect in hydrogenic ions, noticed that the ionization rates could be expressed in terms of the energies by a similar formula. (In fact, the Stark effect Hamiltonian, after separation in parabolic coordinates, is equivalent to a two-dimensional isotropic quartic oscillator.)

C. Even states

Although a parity argument could be invoked at this point, as a consistency check of the Langer–Cherry method we have also calculated the quantization condition for the even states directly as $\psi'(-1/2)=0$, which in terms of the parabolic cylinder and $u(z)$ functions reads

$$\frac{g^{1/2}}{2^{7/4}}\frac{u''(-1/2)}{u'(-1/2)^{2}}=\frac{D'_{\nu/\sqrt{2}-1/2}[2^{3/4}g^{-1/2}u(-1/2)]}{D_{\nu/\sqrt{2}-1/2}[2^{3/4}g^{-1/2}u(-1/2)]},$$

which using a recurrence relation[46] to eliminate the derivative of the parabolic cylinder function can be rewritten as

$$\frac{u(-1/2)}{2^{1/4}g^{1/2}}-\frac{g^{1/2}}{2^{7/4}}\frac{u''(-1/2)}{u'(-1/2)^2}=\frac{D_{\nu/\sqrt{2}+1/2}[2^{3/4}g^{-1/2}u(-1/2)]}{D_{\nu/\sqrt{2}-1/2}[2^{3/4}g^{-1/2}u(-1/2)]}. \tag{21}$$

We use the same notation of the odd case, denoting by u' and u'' the power series for $u'(-1/2)$ and $u''(-1/2)$, respectively, by σ the power series for the left-hand side of Eq. (21), i.e.,

$$\sigma=\frac{u}{2^{1/4}g^{1/2}}-\frac{g^{1/2}}{2^{7/4}}\frac{u''}{(u')^2},$$

and by Σ_3 and Σ_4 the generalized hypergeometric series corresponding to the parabolic cylinder function in the numerator of the right-hand side of Eq. (21),

$$\Sigma_3\equiv{}_2F_0\left(-\frac{1}{4}-\frac{\nu}{2\sqrt{2}},\frac{1}{4}-\frac{\nu}{2\sqrt{2}};;-\frac{g}{u^2\sqrt{2}}\right),$$

$$\Sigma_4\equiv{}_2F_0\left(\frac{3}{4}+\frac{\nu}{2\sqrt{2}},\frac{5}{4}+\frac{\nu}{2\sqrt{2}};;\frac{g}{u^2\sqrt{2}}\right).$$

Proceeding as in the odd case we arrive at the even quantization condition, whose only difference with the odd quantization condition is that in Eq. (18) we must make the replacement,

$$\ln\frac{\Sigma_1}{\Sigma_2}\to\ln\frac{\sigma\Sigma_1+\left(\frac{2^{3/2}u^2}{g}\right)\Sigma_3}{\sigma\Sigma_2+\left(\frac{1}{2}+\frac{\nu}{\sqrt{2}}\right)\Sigma_4},$$

and by substitution of the preceding power series we have checked that

$$\ln\frac{\sigma\Sigma_1+\left(\frac{2^{3/2}u^2}{g}\right)\Sigma_3}{\sigma\Sigma_2+\left(\frac{1}{2}+\frac{\nu}{\sqrt{2}}\right)\Sigma_4}=\ln\frac{\Sigma_1}{\Sigma_2}-i\pi.$$

Therefore, the generalized quantization conditions can be written in the form

$$\pm f(\nu)=1+e^{-i\pi\sqrt{2}\nu},$$

where the plus sign corresponds to odd states and the minus sign to even states. To avoid carrying this double sign, hereafter we will write explicitly the equations for the odd states. The corresponding equations for even states can be recovered immediately by reversing the sign of f and its derivatives.

D. Solution of the generalized quantization condition

In the absence of the second well, the (standard) quantization condition would simply be that the exponentially increasing term in the compound asymptotic expansion for the parabolic cylinder function $D_{\nu/\sqrt{2}-1/2}(2^{3/4}g^{-1/2}u)$ be missing, i.e., that ν be a pole of the gamma function $\Gamma(1/2-\nu/\sqrt{2})$. Then we would have $\nu=\sqrt{2}(n+1/2)=E_n^{(0)}$ $(n=0,1,2,\ldots)$, and we would recover the Rayleigh–Schrödinger perturbation theory series.

Equation (19) shows that, although different from zero, $f(\nu)$ is an exponentially small function of g for $\mathrm{Re}\,g>0$, and therefore we seek solutions of the generalized matching condition in the form

$$\nu_n=\sqrt{2}(n+\tfrac{1}{2}+\Delta n)\quad (n=0,1,2,\ldots),$$

where the correction Δn will be expanded in series of successively exponentially smaller terms. To keep track easily of the exponentially small order we introduce a parameter λ (that ultimately will be set to one) multiplying the matching function $f(\nu)$ and as the ordering parameter in the series for Δn. That is to say, we write the generalized quantization condition in the form

$$\Delta n=\frac{i}{2\pi}\ln\left[1-\lambda f\left(\sqrt{2}\left(n+\frac{1}{2}+\Delta n\right)\right)\right],$$

where

$$\Delta n=\lambda\Delta n_1+\lambda^2\Delta n_2+\lambda^3\Delta n_3+\cdots.$$

By Taylor expansion of the right-hand side of this equation we can find immediately as many corrections Δn_k as desired. Again, we list sufficiently many terms to illustrate the general pattern of the multi-instanton expansion calculated in the next section,

$$\Delta n_1=-\frac{i}{2\pi}f_n,$$

$$\Delta n_2=-\frac{i}{4\pi}f_n^2-\frac{1}{2\sqrt{2}\pi^2}f_nf_n',$$

$$\Delta n_3=-\frac{i}{6\pi}f_n^3-\frac{3}{4\sqrt{2}\pi^2}f_n^2f_n'+\frac{i}{4\pi^3}f_n(f_n')^2+\frac{i}{8\pi^3}f_n^2f_n'',$$

where the primes denote derivatives with respect to ν, and a subindex n denotes the value of the function $f(\nu)$ and its derivatives with respect to ν evaluated at $\nu=\sqrt{2}(n+1/2)$.

V. THE MULTI-INSTANTON EXPANSION

The asymptotic expansion for the eigenvalues of the symmetric double well, i.e., the multi-instanton expansion, is obtained by substitution of the values ν_n into the general asymptotic expansion $E(\nu)$ of Eq. (14). This procedure involves a composition of two Taylor expansions, and the final results are slightly simpler if the derivatives with respect to ν are replaced by derivatives with respect to n with the rule $\partial/\partial\nu=2^{-1/2}\partial/\partial n$. So, the expansion for the eigenvalues up to third exponentially small order is obtained from

$$E\sim E_n+\frac{\sqrt{2}\Delta n}{1!}E_n'+\frac{(\sqrt{2}\Delta n)^2}{2!}E_n''+\frac{(\sqrt{2}\Delta n)^3}{3!}E_n'''+\cdots,$$

which in terms of derivatives of E_n with respect to n can be rewritten as

$$E\sim E_n+\frac{\Delta n}{1!}\frac{\partial E_n}{\partial n}+\frac{(\Delta n)^2}{2!}\frac{\partial^2E_n}{\partial n^2}+\frac{(\Delta n)^3}{3!}\frac{\partial^3E_n}{\partial n^3}+\cdots.$$

Substituting in this expansion the expression for the Δn_k and collecting powers of λ, we write the multi-instanton expansion in the form

$$E\sim E_n+\Delta E_1+\Delta E_2+\Delta E_3+\cdots,$$

where we have already set $\lambda=1$, the subindex labels the exponentially small order, and the explicit expressions for the first three instanton contributions (in terms of derivatives with respect to n) are

$$\Delta E_1 = -\frac{i}{2\pi}\left(f_n \frac{\partial E_n}{\partial n}\right),$$

$$\Delta E_2 = \left[-\frac{i}{4\pi} - \frac{1}{8\pi^2}\frac{\partial}{\partial n}\right]\left(f_n^2 \frac{\partial E_n}{\partial n}\right),$$

$$\Delta E_3 = \left[-\frac{i}{6\pi} - \frac{1}{8\pi^2}\frac{\partial}{\partial n} + \frac{i}{48\pi^3}\frac{\partial^2}{\partial n^2}\right]\left(f_n^3 \frac{\partial E_n}{\partial n}\right).$$

To proceed with the evaluation of the ΔE_k, note that

$$f_n = i\frac{(2\pi)^{1/2}}{\Gamma(n+1)}\left(\frac{2\sqrt{2}}{g}\right)^{n+1/2} e^{-1/3\sqrt{2}g}\left(\sum_{k=0}^{\infty} \gamma_k g^k\right),$$

where the formal power series in the right-hand side of the last equation is defined by

$$\sum_{k=0}^{\infty} \gamma_k g^k \equiv \exp\left[-\frac{1}{3\sqrt{2}}\sum_{k=1}^{\infty} F_n^{(k)} g^k\right] = \exp\left[\frac{1}{6}\sum_{k=1}^{\infty}\frac{1}{k}\frac{\partial E_n^{(k+1)}}{\partial n} g^k\right].$$

Therefore, it is convenient to define the exponentially small coefficient,

$$\xi(n) = \frac{(2\pi)^{1/2}}{\Gamma(n+1)}\left(\frac{2\sqrt{2}}{g}\right)^{n+1/2} e^{-(1/3\sqrt{2}g)}, \tag{22}$$

and the family of power series in g (whose coefficients are again polynomials in $n+1/2$),

$$b_p(n) \equiv \exp\left[-\frac{p}{3\sqrt{2}}\sum_{k=1}^{\infty} F_n^{(k)} g^k\right]\left(\frac{\partial E_n}{\partial n}\right) = \exp\left[\frac{p}{6}\sum_{k=1}^{\infty}\frac{1}{k}\frac{\partial E_n^{(k+1)}}{\partial n} g^k\right]\left(\frac{\partial E_n}{\partial n}\right), \tag{23}$$

so that the function in which the differential operator acts in the expression of ΔE_k is

$$f_n^k \frac{\partial E_n}{\partial n} = i^k \xi(n)^k b_k(n) \quad (k = 1,2,\ldots).$$

Furthermore, we denote

$$\ell = \ln\left(\frac{g}{2\sqrt{2}}\right),$$

so that the derivative with respect to n of the exponentially small coefficient $\xi(n)$ can be written as

$$\xi'(n) = -[\psi(n+1) + \ell]\xi(n),$$

where ψ denotes the logarithmic derivative of the gamma function. [Incidentally, the coefficients of the second instanton contribution are usually[20,22] given in terms of Euler's constant γ; the relation between the two expressions is[46] $\psi(n+1) = -\gamma + \Sigma_{k=1}^{n} k^{-1}$.]

With this notation, the explicit expressions for the one-, two-, and three-instanton contributions read as

$$\Delta E_1 = \frac{\xi(n)}{2\pi} b_1(n), \tag{24}$$

$$\Delta E_2=\frac{\xi(n)^2}{8\pi^2}[b_2'(n)-2b_2(n)(\psi(n+1)+\ell)+2\pi i b_2(n)], \tag{25}$$

$$\Delta E_3=\frac{\xi(n)^3}{48\pi^3}[b_3''(n)-6b_3'(n)(\psi(n+1)+\ell)-b_3(n)[3\psi'(n+1)-9(\ell+\psi(n+1))^2+8\pi^2]$$
$$+6\pi i[b_3'(n)-3b_3(n)(\ell+\psi(n+1))]]. \tag{26}$$

This procedure can be applied without any difficulty to calculate explicitly higher exponentially small corrections. Note that, in general, the solution for Δn_k is a sum of homogeneous terms of degree k in f_n and its derivatives up to $f_n^{(k-1)}$. Since the logarithmic terms come from these derivatives, the expression for ΔE_k will contain $\ell=\ln(g/2\sqrt{2})$ up to the power $k-1$, which is precisely the structure of the multi-instanton expansion as a function of g. Note also that for $k\geqslant 3$ the expression for ΔE_k includes polygamma functions evaluated at integers or, equivalently, Riemann zeta functions.

If we rearrange the preceding expressions for ΔE_k by grouping powers of ℓ, and display explicitly all the dependence on the coupling constant g, we find expansions of the form

$$\Delta E_k=\left(\frac{2\sqrt{2}}{g}\right)^{(n+1/2)k} e^{-k/3\sqrt{2}g}\sum_{m=0}^{k-1}\left[\ln\left(\frac{g}{2\sqrt{2}}\right)\right]^m\sum_{l=0}^{\infty}c_{knml}g^l,$$

which can be easily compared with Eq. (7) of Ref. 20 in which the quantum number (here n) is denoted by N, the order of the instanton contribution (here k) is denoted by n, $g_{(\text{here})}=\sqrt{2}g_{(\text{Ref. 20})}$ and $E_{(\text{here})}=\sqrt{2}E_{(\text{Ref. 20})}$, where the latter two relations follow because we have proceeded by analytic continuation of the standard quartic anharmonic oscillator Hamiltonian [compare the Hamiltonian (1) in Ref. 20 and the Schrödinger equation (11) of the present paper]. To give some examples using only results given explicitly in this paper, from Eqs. (22) and (23) for $p=1$ and (24) as well as the explicit formulas (4)–(9) for the Rayleigh–Schrödinger coefficients as polynomials in $(n+1/2)$ we find

$$\Delta E_1=\frac{1}{2\pi}\frac{(2\pi)^{1/2}}{\Gamma(n+1)}\left(\frac{2\sqrt{2}}{g}\right)^{n+1/2}e^{-(1/3\sqrt{2}g)}\exp\left[\frac{1}{6}\sum_{k=1}^{\infty}\frac{1}{k}\frac{\partial E_n^{(k+1)}}{\partial n}g^k\right]\left(\frac{\partial E_n}{\partial n}\right)$$
$$=\frac{1}{n!\,\pi^{1/2}}\left(\frac{2\sqrt{2}}{g}\right)^{n+1/2}e^{-(1/3\sqrt{2}g)}\left[1-\left[\frac{19}{24}+6\left(n+\frac{1}{2}\right)+\frac{17}{2}\left(n+\frac{1}{2}\right)^2\right]\left(\frac{g}{\sqrt{2}}\right)-\left[\frac{5111}{1152}\right.\right.$$
$$\left.\left.+\frac{115}{8}\left(n+\frac{1}{2}\right)+\frac{2125}{48}\left(n+\frac{1}{2}\right)^2+\frac{23}{2}\left(n+\frac{1}{2}\right)^3-\frac{289}{8}\left(n+\frac{1}{2}\right)^4\right]\left(\frac{g}{\sqrt{2}}\right)^2+\cdots\right],$$

which particularized for $n=0$ reproduces (with due account of the $\sqrt{2}$ factors in the definitions of g and E and recalling that our expressions pertain to the odd states) the corresponding values reported in Eqs. (8) and (9) of Ref. 20. Or, stated directly in terms of $b_1(n)$,

$$\frac{b_1(0)}{\sqrt{2}}=1-\frac{71}{12}\left(\frac{g}{\sqrt{2}}\right)-\frac{6299}{288}\left(\frac{g}{\sqrt{2}}\right)^2-\cdots.$$

Likewise, the explicit expressions for the first three terms of $b_2(n)$ and $b_3(n)$ can be readily calculated from the definition (23) and the coefficients (4)–(9):

$$b_2(n)=\sqrt{2}\left[1-\left[\frac{19}{12}+6\left(n+\frac{1}{2}\right)+17\left(n+\frac{1}{2}\right)^2\right]\left(\frac{g}{\sqrt{2}}\right)-\left[\frac{1007}{288}+\frac{115}{4}\left(n+\frac{1}{2}\right)+\frac{289}{12}\left(n+\frac{1}{2}\right)^2\right.\right.$$
$$\left.\left.+23\left(n+\frac{1}{2}\right)^3-\frac{289}{2}\left(n+\frac{1}{2}\right)^4\right]\left(\frac{g}{\sqrt{2}}\right)^2+\cdots\right], \tag{27}$$

$$b_3(n)=\sqrt{2}\left[1-\left[\frac{19}{8}+6\left(n+\frac{1}{2}\right)+\frac{51}{2}\left(n+\frac{1}{2}\right)^2\right]\left(\frac{g}{\sqrt{2}}\right)-\left[\frac{247}{128}+\frac{345}{8}\left(n+\frac{1}{2}\right)-\frac{153}{16}\left(n+\frac{1}{2}\right)^2\right.\right.$$
$$\left.\left.+\frac{69}{2}\left(n+\frac{1}{2}\right)^3-\frac{2601}{8}\left(n+\frac{1}{2}\right)^4\right]\left(\frac{g}{\sqrt{2}}\right)^2+\cdots\right]. \tag{28}$$

And using Eqs. (25) and (27) particularized for $n=0$ and the relation $\psi(1)=-\gamma$ we can easily reproduce the rest of the coefficients in Eq. (8) of Ref. 20,

$$\frac{b_2(0)}{\sqrt{2}}=1-\frac{53}{6}\left(\frac{g}{\sqrt{2}}\right)-\frac{1277}{72}\left(\frac{g}{\sqrt{2}}\right)^2-\cdots,$$

$$\frac{b_2'(0)-2\psi(1)b_2(0)}{2\sqrt{2}}=\gamma+\left(-\frac{23}{2}-\frac{53}{6}\gamma\right)\left(\frac{g}{\sqrt{2}}\right)+\left(\frac{13}{12}-\frac{1277}{72}\gamma\right)\left(\frac{g}{\sqrt{2}}\right)^2+\cdots.$$

Note that Jentschura and Zinn-Justin state their results in terms of their $\lambda(g)=\ln(-2/g)=-\ln(g/2)+i\pi$, thus grouping formally real and formally complex terms. In our form (24)–(26) of the expressions for the instanton contributions ΔE_k we have kept explicitly separated the formally real and the formally purely imaginary parts of the expansions, among which there is a sequence of cancellations whereby the implicit imaginary parts which arise from the (continuation to the positive real axis of the) Borel sum of the formally real series are canceled by the higher order explicitly imaginary parts. These cancellations where noted by Damburg and Propin[54] in the context of the Stark effect for the hydrogen atom, who in addition conjectured their equivalence to a sequence of dispersion relations. In turn, this sequence, considered from the point of view of the Laplace transformation of ramified functions, is the hallmark of resurgent functions.[48]

The symmetric double well studied in this paper is special in that, provided the conjecture (20) is true, the complete multi-instanton expansion can be generated from the knowledge of the Rayleigh–Schrödinger perturbation theory coefficients expressed as polynomials in the quantum number. As pointed out by Zinn-Justin,[21] in general both the perturbative and one-instanton contributions (equivalently, the $E_n^{(k)}$ and $F_n^{(k)}$ coefficients) are needed to determine the complete multi-instanton expansion. We stress that the Langer–Cherry method presented in this paper is independent of this conjecture, and that it can be applied in the general case. Finally, we also point out that the same method with an obvious modification can be applied for nonsymmetric double wells: since the parity of the eigenstates is lost, the generalized quantization condition is obtained by matching under the barrier the asymptotic expansions of two Langer–Cherry wave functions anchored in the left and right well, respectively. Each one would be calculated exactly by the method of Sec. III [with its own Rayleigh–Schrödinger series and $u(z)$ function], and the matching can be implemented most easily by equating the ratio of the dominant to the subdominant parts of the respective asymptotic expansions on each well.

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On the restriction of quantum fields to a lightlike surface

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To treat the front-form Hamiltonian approach to quantum field theory, called light cone quantum field theory, in a mathematically rigorous way, the existence of a well-defined restriction of the corresponding free fields to the hypersurface $\{x^0+x^3=0\}$ in Minkowski space is of an essential necessity. However, even in the situation of a real scalar free field such a restriction does canonically not exist; this is called the restriction problem. Furthermore, since the beginning of light cone quantum field theory there is the problem of nonexistence of a well-defined Fock space expansion of a free quantum field in terms of light cone momenta which is called the zero-mode problem. In this paper we present solutions to these long outstanding problems where the study of the zero-mode problem (of the corresponding classical field) will lead us to a solution of the restriction problem. We introduce a new function space of ''squeezed'' smooth functions which can canonically be embedded into the Schwartz space $\mathcal{S}(\mathbb{R}^3)$. The restriction of the free field to $\{x^0+x^3=0\}$ is canonically definable on this function space and we show that the covariant field is uniquely determined by this ''tame'' restriction. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765746]

I. INTRODUCTION

In studying the strong coupling regime of nonperturbative QCD, quantization of a field theory on the light cone (light cone quantization) is a promising technique to overcome hard problems of classical QCD. There is vast literature on this subject and we refer the interested reader to Ref. 4, and the references therein.

The fundamental idea goes back to Dirac.[7] Let $\mathbb{M}$ denote four-dimensional Minkowski space with coordinates $x=(x^0,x^1,x^2,x^3)=(x^0,\mathbf{x})$. Usually, the dynamics of a physical observable is described by an initial value problem. For example, if $\phi(x^0,\mathbf{x})$ is the amplitude of a classical Klein–Gordon field, then the dynamics of ϕ is determined by $(\Box+m^2)\phi=0$ and by the values of ϕ and $\partial_0\phi$ on the (hyper)plane $\{x=(x^0,\mathbf{x})\in\mathbb{M}:x^0=0\}$ (initial data). As usual, $\Box=\partial^\mu\partial_\mu=\partial_0^2-\Sigma_{i=1}^3\partial_i^2$ denotes the d'Alembert operator. This form of dynamics is called the *instant form*. In Ref. 7, Dirac suggested another form of dynamics, called the *front form*, where the initial data instead are given on the null plane $\Sigma=\{x\in\mathbb{M}:x^0+x^3=0\}$ and the propagation of ϕ is parametrized by different values of $x^0+x^3=\text{const}$. The starting point of the light cone (or light front) quantization is just the use of this front form to describe the dynamics of a quantum field. Note that Σ is a so-called characteristic surface of the Klein–Gordon equation, and it is well known[11] that uniqueness of a solution cannot be guaranteed any more (we treat this problem in Ref. 21 in more detail). Introducing light cone coordinates (LC-coordinates) $\tilde{x}=(x^+,x^1,x^2,x^-)=\kappa(x)$, where $x^\pm=(1/\sqrt{2})(x^0\pm x^3)$ (we use the Kogut–Soper convention[4]) we can describe the front form dynamics of ϕ in this new coordinate system as follows:

Let $\tilde{\phi}=\tilde{\phi}(\tilde{x})=\phi\circ\kappa^{-1}$ be the transformation of ϕ to LC-coordinates. Then the front form dynamics of ϕ is given by $(\tilde{\Box}+m^2)\tilde{\phi}=0$ and by the values of $\tilde{\phi}$ (we will see that derivatives of

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$\tilde{\phi}$ are unnecessary) on the hyperplane $\{\tilde{x}=(x^+,x^1,x^2,x^-)\in\mathbb{R}^4: x^+=0\}$. Here, $\tilde{\Box}=\partial^{\tilde{\mu}}\partial_{\tilde{\mu}}=2\partial_+\partial_- -\Sigma_{i=1}^2\partial_i^2$ denotes the transformed d'Alembert operator to LC-coordinates. Thus, in the following, we are interested in the restriction of $\tilde{\phi}$ to $\{x^+=0\}$.

In this paper we will treat quantum fields in a mathematically rigorous way as operator-valued (tempered) distributions in the sense of Wightman.[20,3] Roughly spoken, a quantum field is a continuous function $f\mapsto\phi(f)$ (Ref. 22) on the test function space $\mathcal{S}(\mathbb{R}^4)$ of rapidly decreasing, smooth, complex-valued functions where, for fixed $f\in\mathcal{S}(\mathbb{R}^4)$, $\phi(f)$ is a linear operator defined on a common dense subspace of a Hilbert space $\mathcal{H}$. In addition, it is given a unitary representation of the proper Poincaré group (or the spinor Poincaré group), and all these have to fulfill the Wightman axioms. But, in this context, what should be the restriction of ϕ to $\{x\in\mathbb{M}:x^0=0\}$ or to $\Sigma=\{x\in\mathbb{M}:x^0+x^3=0\}$? The Wightman axioms do not require the existence of the restriction of a quantum field to a hypersurface.

In Ref. 16, Reed and Simon describe the restriction of a scalar free field ϕ of mass >0 to the hyperplane $\{x\in\mathbb{M}:x^0=0\}$. The restriction is defined as an operator-valued distribution on $\mathcal{S}(\mathbb{R}^3)$. If one wants to define the restriction of ϕ to the null plane $\Sigma=\{x\in\mathbb{M}:x^0+x^3=0\}$ in an analogous way, one is faced with a divergent integral of the form $\int_{x^+>0}(d^3x/2x^+)\,|g(x)|$ $(g\in\mathcal{S}(R^3))$ (Ref. 13)—notice that the function $\Theta(x^+)/x^+$ is not locally integrable. Hence the restriction $\phi|_\Sigma$ of the field ϕ to Σ cannot be defined canonically on the test function space $\mathcal{S}(\mathbb{R}^3)$. However, if one remains in an appropriate proper subspace of $\mathcal{S}(\mathbb{R}^3)$, then the restriction of ϕ to Σ can be defined in the same way as in the Minkowski case. This was done in Ref. 13, where Leutwyler *et al.* pointed out some features of fields on the null plane Σ. Among them they showed that the restrictions of two free scalar fields of different masses (>0) to Σ are unitary equivalent. This is, however, in contrast to the Minkowski case where it is well known that two free scalar fields of different masses give rise to inequivalent restrictions to $\{x^0=0\}$ (cf., e.g., Ref. 16). The reason for this difference lies in the fact that the fields on the null plane are independent of mass and hence this also holds true for the two-point function of a free scalar field on the null plane. Schlieder and Seiler[18] interpreted this feature as a hint that the test function space—a proper subspace of $\mathcal{S}(\mathbb{R}^3)$—on which the fields on the null plane are defined is too restricted. Hence the general question arises whether one throws away physical information by using the restricted test function space in the definition of the null plane fields. Since the fields on the null plane are independent of mass it is clear that the information about the (rest) mass gets lost. In this paper we will show that this is all one loses, i.e., given the mass and the restricted field on the null plane one can restore the covariant field (cf. Theorem VI.7 and Sec. VII). The keystone to prove this is the introduction of a new test function space $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ which is in our opinion the canonical choice to define the restrictions on the null plane. Since also in the covariant theory the mass is yet a parameter and has to be known *a priori*, the loss of the mass on the null plane is not really a disadvantage of the theory—the mass enters the theory through the Hamiltonian.

A systematic study of fields on the null plane was also done by Driessler.[8,9] Driessler puts his investigations on an axiomatic basement. The fields on the null plane should be defined as operator-valued distributions on the test function space $\mathcal{S}^{(1)}(\mathbb{R}^n)$ (see also Ref. 18), where for technical reasons Driessler introduced the family of test functions $\mathcal{S}^{(\nu)}(\mathbb{R}^n)=\{f\in\mathcal{S}(\mathbb{R}^n): f=\partial_{x^-}^\nu F,\ F\in\mathcal{S}(\mathbb{R}^n)\}$ and $\mathcal{T}_{0,n}=\mathcal{T}_0(\mathbb{R})\otimes\mathcal{D}(\mathbb{R}^{n-1})$, $\mathcal{T}_0(\mathbb{R})=\cap_\nu\mathcal{S}^{(\nu)}(\mathbb{R})$. It turns out that our test function space is related to Driessler's test function spaces by $\mathcal{S}_{\partial_-}(\mathbb{R}^n)=\cap_\nu\mathcal{S}^{(\nu)}(\mathbb{R}^n)$. However, Driessler uses mostly the test function spaces $\mathcal{S}^{(1)}(\mathbb{R}^n)$ and $\mathcal{S}^{(2)}(\mathbb{R}^n)$ in his assertions. In the question of using a "minimal" test function space, as e.g., $\mathcal{T}_{0,n}$, to obtain analogous results Driessler pointed out that unfortunately this lies outside the scope of his methods,[9] Sec. III 3. Nevertheless the results of Driessler are interesting, especially Driessler's no go theorem which gives sufficient conditions for a field to be a free field. However, there is still a gap between Driessler's no go theorem and an analog of Haag's theorem for fields on the null plane. Therefore Driessler suggests in Ref. 9, Sec. IV 2, to investigate the: $P(\phi)_2$:-theories on the null plane which might be possible by using the results of this paper.

In contrast to the former literature, e.g. Refs. 8, 9, 13, 18, where the test function spaces are

given by *ad hoc* definitions to guarantee convergence of the integral $\int_{x^+>0}(d^3x/2x^+)\,|g(x)|$ ($g \in \mathcal{S}(R^3)$) our test function space $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ arises in a very natural way by adapting the construction of the time zero field as in Ref. 16 to the LC-case (see the commutative diagram (20))—hence $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ should be the canonical choice to define the restriction of quantum fields to the null plane.

There are early attempts to formulate light-cone field theory in close relationship with covariant field theory, e.g. Ref. 6. However, even in the conventional formalism of quantum fields, i.e., treating fields not as operator-valued distributions, technical problems appeared. The most important one is the so-called zero-mode (or infrared) problem which states that a real scalar free field does not admit a well-defined Fock space expansion in terms of light cone momenta $\tilde{\mathbf{p}}$. To be more precise, the proposed expansion

$$\tilde{\phi}(\tilde{x}) = \frac{1}{(2\pi)^3}\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}(\tilde{a}(\tilde{\mathbf{p}})\,e^{-i(x^+\tilde{\omega}(\tilde{\mathbf{p}})+x^-p^+-\mathbf{x}_\perp\cdot\mathbf{p}_\perp)} + \tilde{a}^+(\tilde{\mathbf{p}})\,e^{i(x^+\tilde{\omega}(\tilde{\mathbf{p}})+x^-p^+-\mathbf{x}_\perp\cdot\mathbf{p}_\perp)}) \quad (1)$$

of the Klein–Gordon LC-field $\tilde{\phi}$, which is the transformation $\tilde{\phi}=\phi\circ\kappa^{-1}$ of the Klein–Gordon field ϕ, was seen to be ill-defined since the nonlocally integrable function $\Theta(p^+)/p^+$ appears in the integral. This technical insufficiency has led to pessimism in the development of light cone quantum field theory. However, on the level of Feynman graphs this problem could be avoided as was shown by Ligterink and Bakker.[15] From the point of view of conventional QFT, the restriction of $\tilde{\phi}$ to $\{x^+=0\}$ would not cause any problem if the expansion (1) has been successfully well defined; one just has to put $x^+=0$ in (1). Notice that ϕ, as a solution of the Klein–Gordon equation, has the plane wave expansion

$$\phi(x) = \frac{1}{(2\pi)^3}\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}(a(\mathbf{p})\,e^{-i(x^0\omega(\mathbf{p})-\mathbf{x}\cdot\mathbf{p})} + a^+(\mathbf{p})\,e^{i(x^0\omega(\mathbf{p})-\mathbf{x}\cdot\mathbf{p})}), \quad (2)$$

where $\omega(\mathbf{p})=\sqrt{\mathbf{p}^2+m^2}$ is locally integrable.

Since the investigation of the zero-mode problem (of the classical Klein–Gordon field) leads us in a very natural way to a solution of the restriction problem and since, afterwards, the solution of the restriction problem gives us a way to produce a well-defined Fock space expansion of the real scalar free field, i.e., a solution of the zero-mode problem of the quantized Klein–Gordon field, we treat both problems in this paper. From a general point of view these two problems are really the same. This becomes obvious if one has in view that both problems arise from the appearance of the nonlocally integrable function $\Theta(x^+)/x^+$ which causes the divergences.

The paper is organized as follows. After introducing notations from light cone physics in Sec. II, we investigate the zero-mode problem of the classical Klein–Gordon field in Sec. III. The main result of this section states that the zero-mode problem of the classical Klein–Gordon field does not really exist. We obtain a mapping, denoted ν, cf. (15), which tells us, how we have to transform the amplitudes $a(\mathbf{p})$ and $a^+(\mathbf{p})$, starting from (2), to obtain an expansion (1). This transformation is one to one and hence we may also obtain (2) starting from (1). Moreover, the mapping ν elucidates the zero-mode problem of $\tilde{\phi}$ as follows: Any occurrence of an infrared divergence in (1) is caused by an ultraviolet divergence in (2), and vice versa. Already at this point we run into a new class of functions. If the amplitudes $a(\mathbf{p})$, $a^+(\mathbf{p})$ of ϕ in (2) run through the Schwartz space $\mathcal{S}(\mathbb{R}^3)$, then the transformed amplitudes $\tilde{a}(\tilde{\mathbf{p}})$, $\tilde{a}^+(\tilde{\mathbf{p}})$ of $\tilde{\phi}=\phi\circ\kappa^{-1}$ in (1) run through $\nu^*\mathcal{S}(\mathbb{R}^3)=\{f\circ\nu \mid f\in\mathcal{S}(\mathbb{R}^3)\}$, and vice versa. The functions of $\nu^*\mathcal{S}(\mathbb{R}^3)$, however, live on the open subset $\{(p^+,p^1,p^2) \mid p^+>0\}$ of $\mathbb{R}^3$, and it is possible to embed canonically $\nu^*\mathcal{S}(\mathbb{R}^3)$ into $\mathcal{S}(\mathbb{R}^3)$. Hence, we see, that a proper subspace of $\mathcal{S}(\mathbb{R}^3)$ appears in a very natural way and is, moreover, fully equivalent to $\mathcal{S}(\mathbb{R}^3)$. This subspace is the cornerstone in our solution of the restriction problem. In Sec. IV we recall the well known construction of the (covariant) free scalar massive field ϕ, which obeys the Wightman axioms, and construct in the same way the (covariant) free scalar massive LC-field $\tilde{\phi}$. The LC-field fulfills the Wightman axioms only if we replace in

the axioms the Minkowski bilinear form by the LC-bilinear form. We call these modified axioms the LC-Wightman axioms. This is a rather trivial fact, but nevertheless we decided to write down these axioms, since especially the spectral property (LC-W2) takes on a form, which postulates two positive operators, P_+ and P_-, in contrast to the Minkowski case, where only one operator, P_0, has to be positive. This is seen to be one of the major advantages of light cone field theory. Since ϕ is really a quadruple $(\mathcal{H},U,\phi,D)$, and $\tilde{\phi}$ a quadruple $(\tilde{\mathcal{H}},\tilde{U},\tilde{\phi},\tilde{D})$ we define generally what we mean if we write $\tilde{\phi}=\kappa_*\phi=\phi\circ\kappa^{-1}$. We call $\kappa_*\phi$ the pushforward of ϕ by κ. In Sec. V we consider the problem of restricting the LC-field $\tilde{\phi}$ to $\{x^+=0\}$. Starting from the important commutative diagram (20), we again come across the function space $\nu^*\mathcal{S}(\mathbb{R}^3)$ which, for some reasons, is denoted $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$. The elements of this function space are called ''squeezed'' rapidly decreasing (smooth) functions and the elements of its dual space are called ''squeezed'' distributions. We show that the function space $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$ is isomorphic to $\mathcal{S}(\mathbb{R}^3)$ and can canonically be embedded into $\mathcal{S}(\mathbb{R}^3)$. In Sec. VI we use the preliminary work of Sec. V to define the restriction of the LC-field $\tilde{\phi}$ to $\{x^+=0\}$. Furthermore, we compute the equal-time commutator relation. As a highlight we obtain a transformation law between the restriction of $\tilde{\phi}$ to $\{x^+=0\}$ and the restrictions of ϕ and $\partial_0\phi$ to $\{x^0=0\}$. Moreover, we show that the restrictions to $\{x^+=0\}$ of two LC-fields of different masses >0 are unitary equivalent. Hence this is a special property of light cone field theory and not an artifact of a too restricted test function space as thought in Ref. 18. Quite the reverse, if one weakens slightly the definition of unitary equivalence, then it is easy to show that, even in the classical situation, the restrictions to $\{x^0=0\}$ become ''weakly unitary equivalent.'' Finally, in Sec. VII we give a rigorous Fock space expansion of $\tilde{\phi}$ and the time-zero LC-field $\tilde{\varphi}$ treating the fields as bilinear forms. The field operators are obtained by smearing the bilinear forms with test functions. This is the same approach as in the classical case (cf. Ref. 16). Hence, we present finally a solution of the zero-mode problem of the quantized Klein–Gordon field.

II. NOTATION AND CONVENTIONS

A. LC-coordinates and LC-space

We denote n-dimensional Minkowski space by $\mathbb{M}=\mathbb{M}^n$, i.e., $\mathbb{M}^n$ is $\mathbb{R}^n$ together with the symmetric bilinear form $\langle x,y\rangle_{\mathbb{M}}=x^\mu g_{\mu\nu}y^\nu$, where $G=(g_{\mu\nu})$ is the usual Minkowski metric tensor. We introduce LC-coordinates $\tilde{x}$ using the Kogut–Soper convention by $\kappa:\mathbb{R}^n\to\mathbb{R}^n$, $x\mapsto\tilde{x}=(\tilde{x^0},\ldots,\widetilde{x^{n-1}})=\kappa(x)$, where

$$\tilde{x^0}=\frac{1}{\sqrt{2}}(x^0+x^{n-1}),\quad \tilde{x^j}=x^j\quad (j=1,\ldots,n-2),\quad \widetilde{x^{n-1}}=\frac{1}{\sqrt{2}}(x^0-x^{n-1}).$$

Here, we use the so-called index-marked notation where the index carries the mark. Especially in light-cone physics, one usually writes

$$x^+:=\tilde{x^0},\quad \mathbf{x}_\perp:=(\tilde{x^1},\ldots,\widetilde{x^{n-2}}),\quad x^-:=\widetilde{x^{n-1}}$$

and chooses x^+ as the LC-time variable. Because of the Kogut–Soper convention we have $\kappa=\kappa^{-1}$. Next we transform the Minkowski metric tensor G to LC-coordinates by

$$\tilde{G}=(g_{\tilde{\mu}\tilde{\nu}}):=\kappa G\kappa,$$

then

$$\tilde{G}=\begin{pmatrix} 0 & 0 & 0 & \cdots & 1 \\ 0 & -1 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & & 0 \\ \vdots & \vdots & & -1 & \vdots \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

We define the associated bilinear form by $\langle\tilde{x},\tilde{y}\rangle_{\mathbb{L}}:=x^{\tilde{\mu}}g_{\tilde{\mu}\tilde{\nu}}y^{\tilde{\nu}}$. Note that, using the classical LC-notation, we have $\langle\tilde{x},\tilde{y}\rangle_{\mathbb{L}}=x^+y^-+x^-y^+-\mathbf{x}_\perp\cdot\mathbf{y}_\perp$. In analogy to Minkowski space $\mathbb{M}$ we define *LC-space* $\mathbb{L}=\mathbb{L}^n$ as the bilinear space $(\mathbb{R}^n,\langle-,-\rangle_{\mathbb{L}})$. It is obvious that κ preserves the bilinear forms, i.e., κ is an isomorphism (of bilinear spaces) from $\mathbb{M}$ onto $\mathbb{L}$.

Given $\tilde{x}\in\mathbb{L}$, we also define *covariant* LC-coordinates by $x_{\tilde{\mu}}=g_{\tilde{\mu}\tilde{\nu}}x^{\tilde{\nu}}$, and set $\tilde{x}^2:=x^{\tilde{\mu}}x_{\tilde{\mu}}$. A massive relativistic particle with 4-momentum p obeys the energy-momentum relation $p^2-m^2=p^\mu p_\mu-m^2=0$. In LC-coordinates this relation reads $\tilde{p}^2-m^2=p^{\tilde{\mu}}p_{\tilde{\mu}}-m^2=2p^+p^--\mathbf{p}_\perp^2-m^2=0$. Note that the transformation to LC-coordinates preserves the bilinear forms.

The relativistic energy-momentum relation $p^2-m^2=0$ is covariant under the full Lorentz group $\mathcal{L}$, where the transformed relation $\tilde{p}^2-m^2=0$, the *LC-energy-momentum relation*, is not. However, the latter is covariant under the transformed Lorentz group or *LC-Lorentz group* $\tilde{\mathcal{L}}:=\kappa\mathcal{L}\kappa$. Thus in relativistic LC-physics we have to replace the Lorentz group by the LC-Lorentz group and, as a consequence, the Poincaré group $\mathcal{P}=\{(a,\Lambda):a\in\mathbb{M},\ \Lambda\in\mathcal{L}\}$ by the LC-Poincaré group $\tilde{\mathcal{P}}=\{(\tilde{a},\tilde{\Lambda}):\tilde{a}\in\mathbb{L},\ \tilde{\Lambda}\in\tilde{\mathcal{L}}\}$. We also transform the connected component $\mathcal{L}_+^\uparrow=\{\Lambda\in\mathcal{L}:\Lambda_0^0>0,\ \det(\Lambda)=+1\}$ of $\mathcal{L}$ to LC-coordinates by

$$\tilde{\mathcal{L}}_+^\uparrow:=\kappa\mathcal{L}_+^\uparrow\kappa.$$

The coordinate transformation κ induces an isomorphism of Lie groups $\mathcal{L}\tilde{\to}\tilde{\mathcal{L}}$, $\Lambda\mapsto\kappa\Lambda\kappa$. Under this isomorphism the stability group of $\Sigma=\{x^0+x^3=0\}$, i.e., the subgroup of all $\Lambda\in\mathcal{L}$ such that $\Lambda(\Sigma)\subset\Sigma$, is mapped onto the stability group of $\{x^+=0\}$. It is well known[14] that the stability group of $\{x^0=0\}$ is not isomorphic to the stability group of Σ. Hence, the two forms of dynamics are inequivalent.

For the rest of this article we fix some notations.[23] Let

$$\Gamma_m=\{p\in\mathbb{M}^{n+1}:p^2=m^2\},\quad \tilde{\Gamma}_m=\{\tilde{p}\in\mathbb{L}^{n+1}:\tilde{p}^2=m^2\},$$

$$\Gamma_m^\pm=\{p\in\mathbb{M}^{n+1}:p^2=m^2,\ \pm p^0>0\},\quad \tilde{\Gamma}_m^\pm=\{\tilde{p}\in\mathbb{L}^{n+1}:\tilde{p}^2=m^2,\ \pm p^->0\},$$

$$V^\pm=\{p\in\mathbb{M}^{n+1}:p^2>0,\ \pm p^0>0\},\quad \tilde{V}^\pm=\{\tilde{p}\in\mathbb{L}^{n+1}:\tilde{p}^2>0,\ \pm p^->0\}.$$

It is easy to see that $\tilde{\Gamma}_m^\pm=\kappa(\Gamma_m^\pm)$ and $\tilde{V}^\pm=\kappa(V^\pm)$. In addition we will use the following (smooth) parametrizations of the (smooth) submanifolds $\Gamma_m^\pm$, $\tilde{\Gamma}_m^\pm$ of $\mathbb{R}^{n+1}$ (see Fig. 1):

$$\Omega_\pm:\mathbb{R}^n\tilde{\to}\Gamma_m^\pm\subset\mathbb{R}^{n+1},\quad \mathbf{p}\mapsto\Omega_\pm(\mathbf{p}):=(\pm\omega(\mathbf{p}),\mathbf{p})$$

$$\text{with}\ \ \omega(\mathbf{p}):=\sqrt{\mathbf{p}^2+m^2},\ \ \mathbf{p}=(p^1,p^2,\ldots,p^n),\ \ \mathbf{p}^2=\sum_{i=1}^n(p^i)^2,$$

$$\tilde{\Omega}_\pm:\mathbb{R}^n\backslash\{\mp p^+\geqslant 0\}\tilde{\to}\tilde{\Gamma}_m^\pm\subset\mathbb{R}^{n+1},\quad \tilde{\mathbf{p}}\mapsto\tilde{\Omega}_\pm(\tilde{\mathbf{p}}):=\tilde{\Omega}(\tilde{\mathbf{p}}):=(\tilde{\mathbf{p}},\tilde{\omega}(\tilde{\mathbf{p}}))$$

$$\text{with}\ \ \tilde{\omega}(\tilde{\mathbf{p}}):=\frac{\mathbf{p}_\perp^2+m^2}{2p^+},\ \ \mathbf{p}_\perp:=(\tilde{p^1},\tilde{p^2},\ldots,\widetilde{p^{n-1}}),\ \ \mathbf{p}_\perp^2=\sum_{i=1}^{n-1}(\tilde{p^i})^2,$$

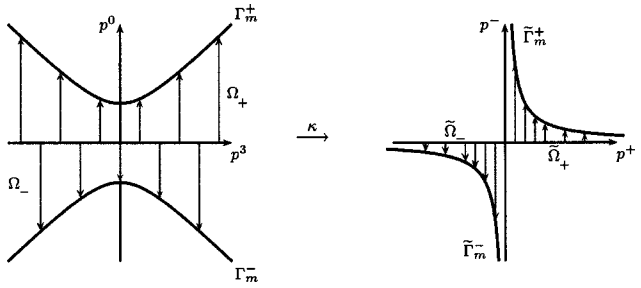


FIG. 1. Parametrizations of $\Gamma_m^{\pm}$ and $\tilde{\Gamma}_m^{\pm}$.

$$\tilde{\mathbf{p}} := (p^+, \mathbf{p}_\perp).$$

Note that $\tilde{\Omega}: \mathbb{R}^n \setminus \{p^+ = 0\} \tilde{\to} \tilde{\Gamma}_m$, $\tilde{\mathbf{p}} \mapsto (\tilde{\mathbf{p}}, \tilde{\omega}(\tilde{\mathbf{p}}))$ is a parametrization of $\tilde{\Gamma}_m$.

B. $\mathbb{M}$- and $\mathbb{L}$-Fourier transformation

In relativistic physics the Fourier transform is defined by using the Minkowski bilinear form instead of the standard Euclidean scalar product. Going over to LC-coordinates the Minkowski bilinear form transforms to LC-bilinear form $\langle -, - \rangle_{\mathbb{L}}$. To fix notations we introduce in this short subsection the so-called $\mathbb{L}$-Fourier transform and notice some properties which follow easily from the definition. Let $\mathcal{S}_n = \mathcal{S}(\mathbb{R}^n)$ denote the Schwartz space of rapidly decreasing, smooth, complex-valued functions. For $f \in \mathcal{S}_n$ define the $\mathbb{X}$-*Fourier transform* $\mathcal{F}_{\mathbb{X}}(f) = f^{\wedge \mathbb{X}}$ by

$$\mathcal{F}_{\mathbb{X}} f := \int f(x)\, e^{i\langle x, - \rangle_{\mathbb{X}}} dx,$$

where $\mathbb{X}$ stands for $\mathbb{M}$ or $\mathbb{L}$. Then $\mathcal{F}_{\mathbb{M}}$ and $\mathcal{F}_{\mathbb{L}}$ are mappings from $\mathcal{S}_n$ to $\mathcal{S}_n$. To emphasize which bilinear form we are just using we also write $\mathcal{S}(\mathbb{M})$, respectively, $\mathcal{S}(\mathbb{L})$ instead of $\mathcal{S}_n$. Thus, we have mappings $\mathcal{F}_{\mathbb{M}}: \mathcal{S}(\mathbb{M}) \to \mathcal{S}(\mathbb{M})$ and $\mathcal{F}_{\mathbb{L}}: \mathcal{S}(\mathbb{L}) \to \mathcal{S}(\mathbb{L})$. Our $\mathbb{M}$-Fourier transform is just the Fourier transform used in relativistic physics. The LC-coordinate transformation $\kappa: \mathbb{M} \to \mathbb{L}$ induces canonically a pullback/pushforward mapping $\kappa^*: \mathcal{S}(\mathbb{L}) \to \mathcal{S}(\mathbb{M})$ ($\kappa_*: \mathcal{S}(\mathbb{M}) \to \mathcal{S}(\mathbb{L})$) which canonically extends to a pullback/pushforward mapping $\kappa^*: \mathcal{S}'(\mathbb{L}) \to \mathcal{S}'(\mathbb{M})$ ($\kappa_*: \mathcal{S}'(\mathbb{M}) \to \mathcal{S}'(\mathbb{L})$), where, as usual, $\mathcal{S}'_n = \mathcal{S}'(\mathbb{R}^n) = \mathcal{S}'(\mathbb{M}) = \mathcal{S}'(\mathbb{L})$ denotes the space of tempered distributions. From the definition immediately follows

$$(\kappa^* \tilde{u})^{\wedge \mathbb{M}} = \kappa^* (\tilde{u}^{\wedge \mathbb{L}}) \quad \text{and} \quad (\kappa_* u)^{\wedge \mathbb{L}} = \kappa_* (u^{\wedge \mathbb{M}}) \tag{3}$$

for all $\tilde{u} \in \mathcal{S}'(\mathbb{L})$, $u \in \mathcal{S}'(\mathbb{M})$. Note that $|\det(\mathrm{D}\kappa)| = 1$ where $\mathrm{D}\kappa$ is the Jacobi matrix of κ. Recall that, in a canonical way, $\mathcal{S}$ is a dense linear subspace of $\mathcal{S}'$. However, $\mathcal{S}$ carries not the subspace topology of $\mathcal{S}'$, the topology on $\mathcal{S}$ is stronger.

Proposition II.1: The mapping $\mathcal{F}_{\mathbb{L}}: \mathcal{S}(\mathbb{L}) \to \mathcal{S}(\mathbb{L})$ is a $\mathbb{C}$-linear homeomorphism with inverse given by

$$f(\tilde{x}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} f^{\wedge \mathbb{L}}(\tilde{p})\, e^{-i\langle \tilde{p}, \tilde{x} \rangle_{\mathbb{L}}} d^n \tilde{p}.$$

This mapping extends uniquely to a $\mathbb{C}$-linear homeomorphism $\mathcal{F}_{\mathbb{L}}: \mathcal{S}'(\mathbb{L}) \to \mathcal{S}'(\mathbb{L})$ $u \mapsto u^{\wedge \mathbb{L}}$ by the usual formula $u^{\wedge \mathbb{L}}(f) := u(f^{\wedge \mathbb{L}})$.

III. THE KLEIN–GORDON EQUATION AND THE ZERO-MODE PROBLEM

In the canonical quantization procedure of a free scalar field of mass >0 one uses the fact that the classical field ϕ, as a solution of the Klein–Gordon equation, has a plane wave expansion of the form

$$\phi(x)=\frac{1}{(2\pi)^3}\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}(a(\mathbf{p})\,e^{-i(\omega(\mathbf{p})x^0-\mathbf{p}\cdot\mathbf{x})}+a^+(\mathbf{p})\,e^{i(\omega(\mathbf{p})x^0-\mathbf{p}\cdot\mathbf{x})}), \tag{4}$$

where $\omega(\mathbf{p})=\sqrt{\mathbf{p}^2+m^2}$.

Since the beginning of light cone QFT it was thought that there is no well-defined analogous plane wave expansion in terms of LC-momenta.[5,10] This problem is called the *zero-mode problem* (or infrared problem) which we like to explain now in more detail.

In physical literature the expansion of ϕ is obtained by transforming the Klein–Gordon equation (KG-equation) $(\Box+m^2)\phi=0$ via Fourier transformation into the algebraic equation $(p^2-m^2)\phi^{\wedge\mathbb{M}}=0$. This equation is solved by $2\pi\chi(p)\delta(p^2-m^2)$, where $\chi(p)$ is some complex-valued function on Γ_m. Using inverse Fourier transformation one obtains ϕ formally

$$\phi(x)=\frac{1}{(2\pi)^3}\int d^4p\;\chi(p)\;\delta(p^2-m^2)\,e^{-i\langle p,x\rangle_{\mathbb{M}}}.$$

To evaluate the integration over the variable p^0, one views $p^2-m^2=f(p^0)$ as a function of p^0 and uses the identity

$$\delta(f(t))=\sum_{\xi}\frac{1}{|f'(\xi)|}\delta(t-\xi), \tag{5}$$

where the sum runs over all simple roots of f. Applying this formula, yields

$$\delta(p^2-m^2)=\frac{1}{2\omega(\mathbf{p})}(\delta(p^0-\omega(\mathbf{p}))+\delta(p^0+\omega(\mathbf{p}))),$$

where $\mathbf{p}$ has to be viewed as a fixed parameter in $\mathbb{R}^3$. Now, one can evaluate the integration over p^0 by canceling the integration and substituting p^0 by $\omega(\mathbf{p})$ (resp. by $-\omega(\mathbf{p})$), so we obtain

$$\phi(x)=\frac{1}{(2\pi)^3}\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}(\chi(\Omega_+(\mathbf{p}))\,e^{-i\langle\Omega_+(\mathbf{p}),x\rangle_{\mathbb{M}}}+\chi(\Omega_-(\mathbf{p}))\,e^{-i\langle\Omega_-(\mathbf{p}),x\rangle_{\mathbb{M}}})$$

and this is the desired expansion, if we set $a(\mathbf{p})=\chi(\Omega_+(\mathbf{p}))$ and $a^+(\mathbf{p})=\chi(\Omega_-(-\mathbf{p}))$. Recall that $\Omega_\pm(\mathbf{p})=(\pm\omega(\mathbf{p}),\mathbf{p})$.

Now consider the transformed field $\tilde{\phi}=\phi\circ\kappa^{-1}$ which we call the free scalar *LC-field*. The LC-field obeys the transformed Klein–Gordon equation (LCKG-equation) $(\tilde{\Box}+m^2)\tilde{\phi}=0$—recall that $\tilde{\Box}=\partial^{\tilde{\mu}}\partial_{\tilde{\mu}}=2\partial_+\partial_--\partial_\perp^2$. Using the same strategy as in the Minkowski case, we apply $\mathbb{L}$-FT and obtain the algebraic equation $(\tilde{p}^2-m^2)\tilde{\phi}^{\wedge\mathrm{L}}=0$. Again, we solve this by $2\pi\tilde{\chi}(\tilde{p})\delta(\tilde{p}^2-m^2)$, where $\tilde{\chi}(\tilde{p})$ is some complex-valued function on $\tilde{\Gamma}_m$. To use formula (5) we have to consider $\tilde{f}(p^-)=\tilde{p}^2-m^2$ as a function in $p^-\in\mathbb{R}$. This gives

$$\delta(\tilde{p}^2-m^2)=\frac{1}{|2p^+|}\delta\left(p^--\frac{\mathbf{p}_\perp^2+m^2}{2p^+}\right), \tag{6}$$

where we have to exclude $p^+=0$. Note that $\tilde{\mathbf{p}}=(p^+,\mathbf{p}_\perp)$ in Eq. (6) has to be considered as a fixed parameter $\in\mathbb{R}^3\backslash\{p^+=0\}$. Canceling the integration over p^- and substituting p^- by $(\mathbf{p}_\perp^2+m^2)/2p^+$ yields

$$\tilde{\phi}(\tilde{x}) = \frac{1}{(2\pi)^3} \int \frac{d^3\tilde{\mathbf{p}}}{|2p^+|} \tilde{\chi}(\tilde{\Omega}(\tilde{\mathbf{p}}))\, e^{-i\langle \tilde{\Omega}(\tilde{\mathbf{p}}), \tilde{x}\rangle_{\mathrm{L}}},$$

where $\tilde{\Omega}(\tilde{\mathbf{p}}) = (\tilde{\mathbf{p}}, \tilde{\omega}(\tilde{\mathbf{p}}))$ and $\tilde{\omega}(\tilde{\mathbf{p}}) = (\mathbf{p}_\perp^2 + m^2)/2p^+$. If we set $\tilde{a}(\tilde{\mathbf{p}}) := \tilde{\chi}(\tilde{\Omega}(\tilde{\mathbf{p}}))$ and $\tilde{a}^+(\tilde{\mathbf{p}}) := \tilde{\chi}(\tilde{\Omega}(-\tilde{\mathbf{p}}))$, we get the expansion

$$\tilde{\phi}(\tilde{x}) = \frac{1}{(2\pi)^3} \int_{p^+>0} \frac{d^3\tilde{\mathbf{p}}}{2p^+} (\tilde{a}(\tilde{\mathbf{p}})\, e^{-i\langle \tilde{\Omega}(\tilde{\mathbf{p}}), \tilde{x}\rangle_{\mathrm{L}}} + \tilde{a}^+(\tilde{\mathbf{p}})\, e^{i\langle \tilde{\Omega}(\tilde{\mathbf{p}}), \tilde{x}\rangle_{\mathrm{L}}}). \tag{7}$$

Since the nonlocally integrable function $\Theta(p^+)/2p^+$ appears in (7), it was thought[5,10] that the expansion in (7) is not well-defined (as $p^+ \to 0$), and that this divergence is a special property of LC-QFT. In this section we will show that this is not the case. The denominator $2\omega(\mathbf{p})$ in (4) has not the problem to become zero anywhere, however, in classical QFT one usually uses amplitudes χ such that (4) becomes ultraviolet divergent, i.e., as $|\mathbf{p}| \to \infty$. Our analysis will show that the ultraviolet behavior of (4) determines the infrared behavior of (7), and vice versa. Or more precise, the singular behavior of (4) as $p^3 \to -\infty$ (resp. $p^3 \to \infty$) is the same as the singular behavior of (7) as $p^+ \to 0$ (resp. $p^+ \to \infty$).

The keystone to solve this problem is to consider the transformation law between $\chi\delta(p^2 - m^2)$ and $\tilde{\chi}\delta(\tilde{p}^2 - m^2)$. Since, *a priori*, it is not clear whether $\tilde{\chi}\delta(\tilde{p}^2 - m^2)$ can be viewed as a distribution depending on $\tilde{\mathbf{p}}$ as a parameter, we want to avoid formula (5) in the derivation of (4) and (7). Instead we will use the exact definitions of $\chi\delta(p^2 - m^2)$ and $\tilde{\chi}\delta(\tilde{p}^2 - m^2)$ as tempered distributions on $\mathbb{R}^4$ to derive the expansions (4) and (7).

To give a precise definition of $\chi(p)\delta(p^2 - m^2)$ and $\tilde{\chi}(\tilde{p})\delta(\tilde{p}^2 - m^2)$ we first mention that the tempered distributions $\delta(p^2 - m^2)$ and $\delta(\tilde{p}^2 - m^2)$ are well-defined as pullbacks of $\delta \in \mathcal{S}'(\mathbb{R})$ under the mapping $Q(p) = p^2 - m^2 : \mathbb{R}^4 \to \mathbb{R}$, respectively, $\tilde{Q}(\tilde{p}) = \tilde{p}^2 - m^2 : \mathbb{R}^4 \to \mathbb{R}$ (cf. Ref. 11, p. 136). Then, for all $f \in \mathcal{S}(\mathbb{R}^4)$, we have

$$(\delta(p^2 - m^2), f(p)) = \int_{\Gamma_m} \frac{f}{|\nabla Q|}\, dS \tag{8}$$

and

$$(\delta(\tilde{p}^2 - m^2), f(\tilde{p})) = \int_{\tilde{\Gamma}_m} \frac{f}{|\nabla \tilde{Q}|}\, d\tilde{S}, \tag{9}$$

where dS (resp. $d\tilde{S}$) is the canonical surface measure on Γ_m (resp. $\tilde{\Gamma}_m$). Hence, as usual, we identify $\delta(p^2 - m^2)$ with the (positive Borel-) measure $d\mu_m := dS/|\nabla Q|$ on Γ_m, and $\delta(\tilde{p}^2 - m^2)$ with the measure $d\tilde{\mu}_m := d\tilde{S}/|\nabla \tilde{Q}|$ on $\tilde{\Gamma}_m$. Because of the functoriality of the pullback operation,[11] we have $\delta(\tilde{p}^2 - m^2) = \delta(p^2 - m^2) \circ \kappa^{-1}$. This implies that the measure $\tilde{\mu}_m$ is the image measure of μ_m under the mapping $\kappa : \mathbb{M} \to \mathbb{L}$. If we define $\mu_m^\pm$ (resp. $\tilde{\mu}_m^\pm$) as the restriction of μ_m to $\Gamma_m^\pm$ (resp. $\tilde{\Gamma}_m^\pm$) then, because of $\tilde{\Gamma}_m^\pm = \kappa(\Gamma_m^\pm)$, $\tilde{\mu}_m^\pm$ is the image measure of $\mu_m^\pm$ under κ. The following lemma is an easy consequence of the transformation law between a measure and its image measure (cf., e.g., Ref. 2, 19.3).

Lemma III.1: Let ρ be a complex-valued, measurable function on $\Gamma_m^\pm$. Then ρ is $\mu_m^\pm$-integrable iff $\rho \circ \kappa^{-1}$ is $\tilde{\mu}_m^\pm$-integrable, and

$$\int_{\tilde{\Gamma}_m^\pm} \frac{\rho \circ \kappa^{-1}}{|\nabla \tilde{Q}|}\, d\tilde{S} = \int_{\Gamma_m^\pm} \frac{\rho}{|\nabla Q|}\, dS.$$

We denote by $\delta_\pm(p^2-m^2)$ (resp. $\delta_\pm(\tilde{p}^2-m^2)$) the tempered distribution induced by $\mu_m^\pm$ (resp. $\tilde{\mu}_m^\pm$), and we sometimes identify the measure with its induced distribution. Note that (as tempered distributions)

$$\delta_\pm(\tilde{p}^2-m^2)=\delta_\pm(p^2-m^2)\circ\kappa^{-1}$$

and $\delta(p^2-m^2)=\delta_+(p^2-m^2)+\delta_-(p^2-m^2)$ and $\delta(\tilde{p}^2-m^2)=\delta_+(\tilde{p}^2-m^2)+\delta_-(\tilde{p}^2-m^2)$.

When we explained the derivation of the plane wave expansion used in physical literature, we solved the associated division problem by $\chi\,\delta(p^2-m^2)$ where we have not specified the amplitude $\chi(p)$ to get a solution of the KG-equation. In the following we want to specify χ in such a way that $\chi\,\delta(p^2-m^2)$ is a well-defined tempered distribution. However, if we allow only complex-valued functions χ on Γ_m as amplitudes, we do not get all solutions of the KG-equation in $\mathcal{S}'(\mathbb{R}^4)$ because it is well known, e.g. Ref. 3, p. 60, that the general solution $u\in\mathcal{S}'(\mathbb{R}^4)$ of $(p^2-m^2)u=0$ is of the form

$$u=u_+(\mathbf{p})\,\delta_+(p^2-m^2)+u_-(\mathbf{p})\,\delta_-(p^2-m^2) \tag{10}$$

with tempered distributions $u_\pm(\mathbf{p})\in\mathcal{S}'(\mathbb{R}^3)$, where $u_\pm(\mathbf{p})\,\delta_\pm(p^2-m^2)\in\mathcal{S}'(\mathbb{R}^4)$ is defined by

$$(u_\pm(\mathbf{p})\,\delta_\pm(p^2-m^2),f(p))=\left(u_\pm(\mathbf{p}),\frac{f(\pm\omega(\mathbf{p}),\mathbf{p})}{2\omega(\mathbf{p})}\right)=\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}u_\pm(\mathbf{p})\,f(\pm\omega(\mathbf{p}),\mathbf{p}).$$

Note that the mapping $\mathcal{S}(\mathbb{R}^4)\to\mathcal{S}(\mathbb{R}^3)$, $f(p)\mapsto f(\pm\omega(\mathbf{p}),\mathbf{p})/2\omega(\mathbf{p})$ is $\mathbb{C}$-linear and continuous. If we evaluate the surface integral (8) over $\Gamma_m^\pm$ using the parametrization $\Omega_\pm:\mathbb{R}^3\tilde{\to}\Gamma_m^\pm\subset\mathbb{R}^4$, we get

$$(\delta_\pm(p^2-m^2),f(p))=\int_{\Gamma_m^\pm}\frac{f}{|\nabla Q|}\,dS=\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}f(\pm\omega(\mathbf{p}),\mathbf{p}).$$

Hence, $\delta_\pm(p^2-m^2)$ defined by the measure $\mu_m^\pm$ on $\Gamma_m^\pm$ is equal to $u_\pm(\mathbf{p})\,\delta(p^2-m^2)$ in (10) with $u_\pm(\mathbf{p})=1(\mathbf{p})$, where $1(\mathbf{p})=1$ is the constant function. For this reason we make the following definition:

Definition: (a) A function $\chi:\Gamma_m^\pm\to\mathbb{C}$ is a *multiplicator* of $\delta_\pm(p^2-m^2)$ if $\chi(\Omega_\pm(\mathbf{p}))$ is a tempered distribution $\in\mathcal{S}'(\mathbb{R}^3)$, where $\Omega_\pm$ is the introduced parametrization of $\Gamma_m^\pm$. For each such χ we define the tempered distribution $\chi(p)\,\delta_\pm(p^2-m^2)\in\mathcal{S}'(\mathbb{R}^4)$ by

$$(\chi(p)\,\delta_\pm(p^2-m^2),f(p)):=\int\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}\chi(\Omega_\pm(\mathbf{p}))\,f(\Omega_\pm(\mathbf{p}))=\int_{\Gamma_m^\pm}\frac{\chi f}{|\nabla Q|}\,dS\quad(f\in\mathcal{S}(\mathbb{R}^4)).$$

By $\mathcal{M}_\pm$ we denote the set of all multiplicators of $\delta_\pm(p^2-m^2)$.

(b) A function $\chi:\Gamma_m\to\mathbb{C}$ is called a *multiplicator* of $\delta(p^2-m^2)$ if the restrictions $\chi_\pm:=\chi|_{\Gamma_m^\pm}$ are in $\mathcal{M}_\pm$. For each such χ we define the tempered distribution $\chi(p)\,\delta(p^2-m^2)\in\mathcal{S}'(\mathbb{R}^4)$ by

$$\chi(p)\,\delta(p^2-m^2):=\chi_+(p)\,\delta(p^2-m^2)+\chi_-(p)\,\delta(p^2-m^2),$$

thus

$$(\chi(p)\,\delta(p^2-m^2),f(p))=\int_{\Gamma_m}\frac{\chi f}{|\nabla Q|}\,dS,\quad(f\in\mathcal{S}(\mathbb{R}^4)).$$

By $\mathcal{M}$ we denote the set of all multiplicators of $\delta(p^2-m^2)$.

Notice that, because the mapping $\mathcal{S}(\mathbb{R}^4)\to\mathcal{S}(\mathbb{R}^3)$, $f(p)\mapsto f(\Omega_\pm(\mathbf{p}))/2\omega(\mathbf{p})$ is $\mathbb{C}$-linear and continuous, the distributions $\chi(p)\,\delta_\pm(p^2-m^2)$ and $\chi(p)\,\delta(p^2-m^2)$ are well-defined and tempered.

As mentioned before, if we consider distributions of the form $u=\chi(p)\,\delta(p^2-m^2)$ ($\chi \in \mathcal{M}$), we do not get all solutions of $(p^2-m^2)u=0$ in $\mathcal{S}'(\mathbb{R}^4)$, and thus also not all solutions of $(p^2-m^2)\tilde{u}=0$ in $\mathcal{S}'(\mathbb{R}^4)$ (because κ induces a 1–1 correspondence between these solutions). However, we are mainly interested in the interrelation between the solutions of $(p^2-m^2)u=0$ and $(\tilde{p}^2-m^2)\tilde{u}=0$, and in studying this interrelation we will see that it is important that the definition of $\chi(p)\,\delta_\pm(p^2-m^2)$ does not depend on the chosen parametrizations (or charts) of $\Gamma_m^\pm$–only the sets $\mathcal{M}_\pm$ depend on it. It is not known to the author how to define in general $u_\pm(\mathbf{p})\,\delta_\pm(p^2-m^2)$, where $u_\pm(\mathbf{p}) \in \mathcal{S}'(\mathbb{R}^3)$, without fixing any parametrization of $\Gamma_m^\pm$.

Using the fact[17] that every function $\chi:\mathbb{R}^n \to \mathbb{C}$ such that

$$\int |(1+|x|^2)^{-N}\chi(x)|^p\, d^n x < \infty$$

for some $N \in \mathbb{N}$ and $p \in \mathbb{R}$, $p>0$, is a tempered distribution, it is easy to show that every function in $\mathcal{L}^p(\Gamma_m^\pm, d\mu_m)$ is a multiplicator of $\delta_\pm(p^2-m^2)$. If $\chi_\pm$ runs through $\mathcal{L}^2(\Gamma_m^\pm, d\mu_m)$ the solutions $\phi_\pm = \mathcal{F}_{\mathbb{M}}^{-1}(\chi_\pm(p)\,\delta_\pm(p^2-m^2))$ of the KG-equation run through all physical positive/negative energy states of a relativistic neutral particle of mass $m>0$.[19] Hence, our analysis includes all physically relevant solutions of the KG-equation. It is even possible to leave this restriction and to show that the general solution $\tilde{u}$ in $\mathcal{S}'(\mathbb{R}^4)$ of $(\tilde{p}^2-m^2)\tilde{u}=0$ is of the form

$$\tilde{u}=\tilde{u}_+(\tilde{\mathbf{p}})\,\delta_+(\tilde{p}^2-m^2)+\tilde{u}_-(\tilde{\mathbf{p}})\,\delta_-(\tilde{p}^2-m^2),$$

where $\tilde{u}_\pm(\tilde{\mathbf{p}})$ are so-called squeezed distributions, and $\tilde{u}_\pm(\tilde{\mathbf{p}})\,\delta_\pm(\tilde{p}^2-m^2)$ are defined in an analogous way as $u_\pm(\mathbf{p})\,\delta_\pm(p^2-m^2)$ in (10) (cf. Ref. 21).

Now we like to define $\tilde{\chi}(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)$ and $\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)$.

Definition: (a) Let $\tilde{\mathcal{M}}_\pm := \{\chi\circ\kappa^{-1}: \chi \in \mathcal{M}_\pm\}$. We call every function in $\tilde{\mathcal{M}}_\pm$ a *multiplicator of* $\delta_\pm(\tilde{p}^2-m^2)$. For every such $\tilde{\chi}_\pm \in \tilde{\mathcal{M}}_\pm$ we define $\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2) \in \mathcal{S}'(\mathbb{R}^4)$ by

$$(\tilde{\chi}(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2), f(\tilde{p})) := \int_{\tilde{\Gamma}_m^\pm} \frac{\tilde{\chi} f}{|\nabla \tilde{Q}|}\, d\tilde{S} \quad (f \in \mathcal{S}(\mathbb{R}^4)).$$

(b) A function $\tilde{\chi}:\tilde{\Gamma}_m \to \mathbb{C}$ is called a *multiplicator of* $\delta(\tilde{p}^2-m^2)$ if the restrictions $\tilde{\chi}_\pm := \tilde{\chi}|_{\tilde{\Gamma}_m^\pm}$ are in $\tilde{\mathcal{M}}_\pm$. For each such $\tilde{\chi}$ we define $\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2) \in \mathcal{S}'(\mathbb{R}^4)$ by

$$\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)=\tilde{\chi}_+(\tilde{p})\,\delta_+(\tilde{p}^2-m^2)+\tilde{\chi}_-(\tilde{p})\,\delta_-(\tilde{p}^2-m^2),$$

hence

$$(\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2), f(\tilde{p})) = \int_{\tilde{\Gamma}_m} \frac{\tilde{\chi} f}{|\nabla \tilde{Q}|}\, d\tilde{S} \quad (f \in \mathcal{S}(\mathbb{R}^4)).$$

By $\tilde{\mathcal{M}}$ ($=\{\chi\circ\kappa^{-1}: \chi \in \mathcal{M}\}$) we denote the set of all multiplicators of $\delta(\tilde{p}^2-m^2)$.

The next proposition shows that $\tilde{\chi}_\pm(\tilde{p})\,\delta(\tilde{p}^2-m^2)$ and $\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)$ are well-defined tempered distributions and, in addition, we obtain an easy, but important transformation law between the distributions with and without tilde.

Proposition III.2: For every $\tilde{\chi}_\pm \in \tilde{\mathcal{M}}_\pm$, $\tilde{\chi} \in \tilde{\mathcal{M}}$ *the just defined* $\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)$ *and* $\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)$ *are tempered distributions on* $\mathbb{R}^4$, *and we have*

(i) $\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)=\chi_\pm(p)\,\delta_\pm(p^2-m^2)\circ\kappa^{-1}$,
(ii) $\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)=\chi(p)\,\delta(p^2-m^2)\circ\kappa^{-1}$,

as distributions (and as complex measures), where $\chi_\pm := \tilde{\chi}_\pm\circ\kappa$ *and* $\chi := \tilde{\chi}\circ\kappa$.

Proof: Clearly (ii) follows from (i), and (i) is just applying Lemma III.1 to $\rho := \chi_\pm f$. □

Using the parametrization $\Omega_\pm$ of $\Gamma_\pm$ (resp. $\tilde{\Omega}_\pm$ of $\tilde{\Gamma}_\pm$) we can evaluate the corresponding surface integral which yields (with $f \in \mathcal{S}(\mathbb{R}^4)$)

$$(\chi_\pm(p)\,\delta_\pm(p^2-m^2), f(p)) = \int \frac{d^3\mathbf{p}}{2\,\omega(\mathbf{p})}\,\chi_\pm(\Omega_\pm(\mathbf{p}))\,f(\Omega_\pm(\mathbf{p})), \tag{11}$$

$$(\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2), f(\tilde{p})) = \int_{\pm p^+>0} \frac{d^3\tilde{\mathbf{p}}}{2|p^+|}\,\tilde{\chi}_\pm(\tilde{\Omega}_\pm(\tilde{\mathbf{p}}))\,f(\tilde{\Omega}_\pm(\tilde{\mathbf{p}})). \tag{12}$$

Remark III.3: As we have viewed $\delta_\pm(p^2-m^2)$ (resp. $\delta_\pm(\tilde{p}^2-m^2)$) as positive (Borel-) measures $\mu_m^\pm$ (resp. $\tilde{\mu}_m^\pm$) on $\Gamma_m^\pm$ (resp. $\tilde{\Gamma}_m^\pm$) we do the same with $\chi_\pm(p)\,\delta_\pm(p^2-m^2)$ (resp. $\tilde{\chi}(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)$), but these are now complex measures. From measure theory it follows that the function $\chi_\pm(p)$ (resp. $\tilde{\chi}_\pm(\tilde{p})$) is determined by the complex measure $\chi_\pm(p)\,\delta_\pm(p^2-m^2)$ (resp. $\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)$) $\mu_m^\pm$-a.e. (resp. $\tilde{\mu}_m^\pm$-a.e.).

We introduce the following sets of solutions of the KG-equation (resp. LCKG-equation):

$$\mathcal{L}_\pm := \{\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi_\pm(p)\,\delta_\pm(p^2-m^2)) : \chi_\pm \in \mathcal{M}_\pm\},$$

$$\tilde{\mathcal{L}}_\pm := \{\mathcal{F}_{\mathbb{L}}^{-1}(2\pi\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)) : \tilde{\chi}_\pm \in \tilde{\mathcal{M}}_\pm\},$$

and also define mappings

$$\alpha_\pm : \mathcal{M}_\pm \to \mathcal{L}_\pm, \quad \chi_\pm \mapsto \mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi_\pm(p)\,\delta_\pm(p^2-m^2)),$$

$$\tilde{\alpha}_\pm : \tilde{\mathcal{M}}_\pm \to \tilde{\mathcal{L}}_\pm, \quad \tilde{\chi}_\pm \mapsto \mathcal{F}_{\mathbb{L}}^{-1}(2\pi\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)).$$

The reason why there is no zero-mode problem in light cone QFT is caused by the following corollary:

Corollary III.4: Let $\phi_\pm = \mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi_\pm(p)\,\delta_\pm(p^2-m^2)) \in \mathcal{L}_\pm$ *be a solution of the KG-equation, with* $\chi_\pm \in \mathcal{M}_\pm$. *Then, if* $\tilde{\phi}_\pm = \phi_\pm \circ \kappa^{-1}$ *is the transformed solution, we have* $\tilde{\phi}_\pm = \mathcal{F}_{\mathbb{L}}^{-1}(2\pi\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2))$ *with* $\tilde{\chi}_\pm = \chi_\pm \circ \kappa^{-1}$, *i.e., the following diagram commutes*

$$\begin{array}{ccc} \mathcal{M}_\pm & \xrightarrow{\alpha_\pm} & \mathcal{L}_\pm \\ \downarrow{\scriptstyle \kappa_*} & & \downarrow{\scriptstyle \kappa_*} \\ \tilde{\mathcal{M}}_\pm & \xrightarrow{\tilde{\alpha}_\pm} & \tilde{\mathcal{L}}_\pm \end{array}$$

where $\kappa_*(f) = f \circ \kappa^{-1}$.

Notice that κ_* maps the complex vector space $\mathcal{L}^p(\Gamma_m^\pm, d\mu_m) \subset \mathcal{M}_\pm$ (isometrically) isomorphically onto the complex vector space $\mathcal{L}^p(\tilde{\Gamma}_m^\pm, d\tilde{\mu}_m) \subset \tilde{\mathcal{M}}_\pm$.

Proof: Let $u_\pm = 2\pi\chi_\pm(p)\,\delta_\pm(p^2-m^2)$ and $\tilde{u}_\pm = 2\pi\tilde{\chi}_\pm(\tilde{p})\,\delta_\pm(\tilde{p}^2-m^2)$. Then from Proposition III.2 we know $\tilde{u}_\pm = u_\pm \circ \kappa^{-1}$. Now because of (3), we get $\tilde{\phi}_\pm = \phi_\pm \circ \kappa^{-1} = \mathcal{F}_{\mathbb{M}}^{-1}(u_\pm) \circ \kappa^{-1} = \mathcal{F}_{\mathbb{L}}^{-1}(u_\pm \circ \kappa^{-1}) = \mathcal{F}_{\mathbb{L}}^{-1}(\tilde{u}_\pm)$. □

In Corollary III.4 we have considered only the positive/negative frequency part $\phi_\pm = \mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi_\pm(p)\,\delta_\pm(p^2-m^2))$ of the field

$$\phi = \mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi(p)\,\delta(p^2-m^2)), \tag{13}$$

with $\chi \in \mathcal{M}$, $\chi|_{\Gamma_m^\pm} = \chi_\pm$. But it is clear that for the transformed field $\tilde{\phi} = \phi \circ \kappa^{-1}$ we also have

$$\tilde{\phi}=\mathcal{F}_{\mathrm{L}}^{-1}(2\pi\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2)) \tag{14}$$

with $\tilde{\chi}=\chi\circ\kappa^{-1}$. We call (13) (resp. (14)) the *abstract plane wave expansion* of ϕ (resp. $\tilde{\phi}$). Because the amplitudes χ and $\tilde{\chi}$ differ only by a linear transformation, nothing gets worse if we go from the abstract plane wave expansion of ϕ to that of $\tilde{\phi}$.

To get a closer connection to the forms (4) and (7) we discuss now at the end of this section the special case, where the integrals in (4) and (7) are absolutely convergent (Lebesgue-) integrals emphasizing again the nonexistence of the zero-mode problem in light cone QFT.

Definition: A solution ϕ (resp. $\tilde{\phi}$) of the KG-equation (resp. LCKG-equation) in $\mathcal{S}'(\mathbb{R}^4)$ has a *convergent plane wave expansion* if ϕ (resp. $\tilde{\phi}$) is a regular distribution and has an integral representation of the form (4) (resp. (7)) where the integral is absolutely convergent (in the sense of Lebesgue).

If ϕ has a convergent plane wave expansion as in (4), we can write the integral as a surface integral

$$\phi(x)=\frac{1}{(2\pi)^3}\int_{\Gamma_m}\frac{\chi(p)\,e^{i\langle p,x\rangle_{\mathbb{M}}}}{|\nabla Q(p)|}dS(p)$$

if we define $\chi(p)$ on Γ_m^+ by $\chi(\Omega_+(\mathbf{p})):=a(\mathbf{p})$, and on Γ_m^- by $\chi(\Omega_-(\mathbf{p})):=a^+(-\mathbf{p})$, $(\mathbf{p}\in\mathbb{R}^3)$. To check this, just evaluate the surface integral using $\Omega_\pm$. Hence it follows $\chi\in\mathcal{L}^1(\Gamma_m,d\mu_m)$ and $\phi=\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi(p)\,\delta(p^2-m^2))$. Analogously, if $\tilde{\phi}$ has a convergent plane wave expansion as in (7), we can write the integral as a surface integral

$$\tilde{\phi}(\tilde{x})=\frac{1}{(2\pi)^3}\int_{\tilde{\Gamma}_m}\frac{\tilde{\chi}(\tilde{p})\,e^{i\langle\tilde{p},\tilde{x}\rangle_{\mathrm{L}}}}{|\nabla\tilde{Q}(\tilde{p})|}d\tilde{S}(\tilde{p})$$

if we define $\tilde{\chi}(\tilde{p})$ on $\tilde{\Gamma}_m^+$ by $\tilde{\chi}(\tilde{\Omega}(\tilde{\mathbf{p}})):=\tilde{a}(\tilde{\mathbf{p}})$, and on $\tilde{\Gamma}_m^-$ by $\tilde{\chi}(\tilde{\Omega}(-\tilde{\mathbf{p}})):=\tilde{a}^+(\tilde{\mathbf{p}})$ $(\tilde{\mathbf{p}}\in\mathbb{R}^3,p^+>0)$. As before, it follows $\tilde{\chi}\in\mathcal{L}^1(\tilde{\Gamma}_m,d\tilde{\mu}_m)$ and $\tilde{\phi}=\mathcal{F}_{\mathrm{L}}^{-1}(2\pi\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2))$. Conversely, if ϕ (resp. $\tilde{\phi}$) has an abstract plane wave expansion of the form $\phi=\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi(p)\,\delta(p^2-m^2))$ (resp. $\tilde{\phi}=\mathcal{F}_{\mathrm{L}}^{-1}(2\pi\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2))$) with $\chi\in\mathcal{L}^1(\Gamma_m,d\mu_m)$ (resp. $\tilde{\chi}\in\mathcal{L}^1(\tilde{\Gamma}_m,d\tilde{\mu}_m)$), it is easy to see—by evaluating the corresponding surface integrals using $\Omega_\pm$ (resp. $\tilde{\Omega}_\pm$)—that ϕ (resp. $\tilde{\phi}$) has a convergent plane wave expansion. Here we have used only standard facts from integration theory. Notice that, if $\chi(p)\in\mathcal{L}^1(\Gamma_m,d\mu_m)$ and $f(x)\in\mathcal{S}(\mathbb{R}^4)$, then $\chi(p)f(x)\in\mathcal{L}^1(\Gamma_m\times\mathbb{R}^4,d\mu_m(p)\otimes d^4x)$ and we can use Fubini's theorem. The same holds for $\tilde{\chi}(\tilde{p})$ (in the tilde situation). Hence we have proven the following lemma.

Lemma III.5: Let $\phi\in\mathcal{S}'(\mathbb{R}^4)$ (resp. $\tilde{\phi}\in\mathcal{S}'(\mathbb{R}^4)$) be a solution of the KG-equation (resp. LCKG-equation) which is regular (as a distribution). Then

(i) *ϕ has a convergent plane wave expansion as in* (4) *iff ϕ has an abstract plane wave expansion $\phi=\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi(p)\,\delta(p^2-m^2))$ with $\chi\in\mathcal{L}^1(\Gamma_m,d\mu_m)$. In this case $a(\mathbf{p})=\chi(\Omega_+(\mathbf{p}))$ and $a^+(\mathbf{p})=\chi(\Omega_-(-\mathbf{p}))$ $(\mathbf{p}\in\mathbb{R}^3)$.*

(ii) *$\tilde{\phi}$ has a convergent plane wave expansion as in* (7) *iff $\tilde{\phi}$ has an abstract plane wave expansion $\tilde{\phi}=\mathcal{F}_{\mathrm{L}}^{-1}(2\pi\tilde{\chi}(\tilde{p})\,\delta(\tilde{p}^2-m^2))$ with $\tilde{\chi}\in\mathcal{L}^1(\tilde{\Gamma}_m,d\tilde{\mu}_m)$. In this case $\tilde{a}(\tilde{\mathbf{p}})=\tilde{\chi}(\tilde{\Omega}(\tilde{\mathbf{p}}))$ and $\tilde{a}^+(\tilde{\mathbf{p}})=\tilde{\chi}(\tilde{\Omega}(-\mathbf{p}))$ $(\tilde{\mathbf{p}}\in\mathbb{R}^3,p^+>0)$.*

Using this lemma we can prove the following proposition:

Proposition III.6: Let $\phi\in\mathcal{S}'(\mathbb{R}^4)$ be a solution of the KG-equation which is a regular distribution. Let $\tilde{\phi}=\phi\circ\kappa^{-1}$ be the transformed solution. Then, ϕ has a convergent plane wave expansion as in (4) *iff $\tilde{\phi}$ has a convergent plane wave expansion as in* (7). *In this case $\tilde{a}(\tilde{\mathbf{p}})=a(\nu(\tilde{\mathbf{p}}))$ and $\tilde{a}^+(\tilde{\mathbf{p}})=a^+(\nu(\tilde{\mathbf{p}}))$ for all $\tilde{\mathbf{p}}\in\mathbb{R}^3$, $p^+>0$, where $\nu(\tilde{\mathbf{p}}):=\Omega_+^{-1}(\kappa^{-1}(\tilde{\Omega}(\tilde{\mathbf{p}})))$.*

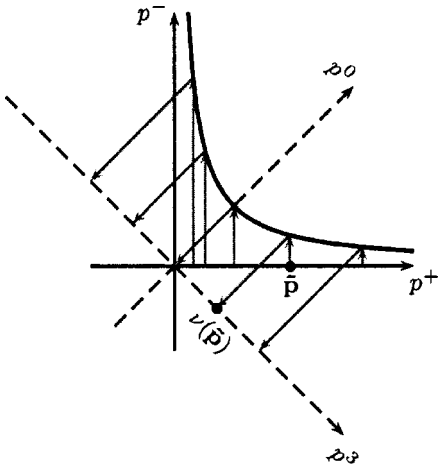


FIG. 2. The mapping $\nu:\mathbb{R}^3\backslash\{p^+\leqslant 0\}\to\mathbb{R}^3$, $\tilde{\mathbf{p}}\to\nu(\tilde{\mathbf{p}})$.

Proof: From Proposition III.2 we know that $\phi=\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi(p)\delta(p^2-m^2))$ if and only if $\tilde{\phi}=\mathcal{F}_{\mathbb{L}}^{-1}(2\pi\tilde{\chi}(\tilde{p})\delta(\tilde{p}^2-m^2))$ where $\tilde{\chi}=\chi\circ\kappa^{-1}$. Now use Lemma III.5 to get the first assertion. To obtain the second assertion write, due to Lemma III.5, $\tilde{a}(\tilde{\mathbf{p}})=\tilde{\chi}(\tilde{\Omega}(\tilde{\mathbf{p}}))$ and $\tilde{a}^+(\tilde{\mathbf{p}})=\tilde{\chi}(\tilde{\Omega}\times(-\tilde{\mathbf{p}}))$. Now use $\tilde{\chi}=\chi\circ\kappa^{-1}$, $\Omega_-(-\mathbf{p})=-\Omega_+(\mathbf{p})$ and the second assertion of Lemma III.5 (i).□

As we have seen in Lemma III.5, the integral sign in (4) (resp. (7)) only makes sense if we take the amplitude $\chi(p)$ (resp. $\tilde{\chi}(\tilde{p})$) from the proper subset $\mathcal{L}^1(\Gamma_m,d\mu_m)$ of $\mathcal{M}$ (resp. $\mathcal{L}^1(\tilde{\Gamma}_m,d\tilde{\mu}_m)$ of $\tilde{\mathcal{M}}$). In all other cases the integral sign has to be viewed only symbolically (as usual in distribution theory). If we consider in general $\chi(p)\in\mathcal{M}$ and $\tilde{\chi}(\tilde{p})\in\tilde{\mathcal{M}}$, then $a(\mathbf{p})$ and $a^+(\mathbf{p})$ in (4) are tempered distributions on $\mathbb{R}^3$, however, $\tilde{a}(\tilde{\mathbf{p}})$ and $\tilde{a}^+(\tilde{\mathbf{p}})$ are not. Later we will see that these are squeezed distributions, and therefore we have to use squeezed distributions instead of tempered distributions to define the restriction of $\tilde{\phi}$ to $\{x^+=0\}$.

The mapping ν is extremely useful because it shows us how to define squeezed distributions and, in addition, it gives us the right connection between canonical QFT and light cone QFT. In Fig. 2 we have illustrated the mapping $\nu:\mathbb{R}^3\backslash\{p^+\leqslant 0\}\to\mathbb{R}^3$ to get a better feeling of what happens; the arrays indicate the way of how the value $\nu(\tilde{\mathbf{p}})$ of $\tilde{\mathbf{p}}$ is determined. The explicit formula of ν is

$$\nu(\tilde{\mathbf{p}})=\left(\mathbf{p}_\perp,\frac{1}{\sqrt{2}}\left(p^+-\frac{\mathbf{p}_\perp^2+m^2}{2p^+}\right)\right), \tag{15}$$

where $\tilde{\mathbf{p}}=(p^+,\mathbf{p}_\perp)=(p^+,p^1,p^2)\in\mathbb{R}^3\backslash\{p^+\leqslant 0\}$.

IV. THE REAL SCALAR FREE LC-FIELD, PUSHFORWARD OF QUANTUM FIELDS

As mentioned in the Introduction, the transformed field $\tilde{\phi}=\phi\circ\kappa^{-1}$ of a given quantum field ϕ does not fit in the classical Wightman formalism because the transformation κ to LC-coordinates is not a Lorentz transformation. In this section we will define the quantum field $\tilde{\phi}_m=\phi_m\circ\kappa^{-1}$, if ϕ_m is a free scalar field of mass $m>0$, as a quadruple $(\tilde{\mathcal{H}}_m,\tilde{U}_m,\tilde{\phi}_m,\tilde{D})$ in analogy to the classical free field $(\mathcal{H}_m,U_m,\phi_m,D)$. We will show that $\tilde{\phi}_m$ satisfies a slightly modified version of the classical Wightman axioms, which we will call the LC-Wightman axioms.

Before starting the construction of $\tilde{\phi}_m$, we have to select an appropriate one-particle space $\tilde{\mathfrak{H}}_m$. The one-particle space $\mathfrak{H}_m$ of a relativistic, spinless, neutral particle (resp. antiparticle) of mass $m>0$ living in Minkowski space is $\mathcal{L}^2(\Gamma_m^+,d\mu_m)$ (resp. $\mathcal{L}^2(\Gamma_m^-,d\mu_m)$). That is because the distributions of the form $\phi_\pm=\mathcal{F}_{\mathbb{M}}^{-1}(2\pi\chi_\pm(p)\delta_\pm(p^2-m^2))$, with $\chi_\pm\in\mathcal{L}^2(\Gamma_m^\pm,d\mu_m)$, represent all physically relevant positive/negative frequency solutions of the KG-equation.[19] From Corollary

III.4 it follows that these solutions are in one-to-one correspondence—via κ—with the solutions $\tilde{\phi}_{\pm}=\mathcal{F}_{\mathbb{L}}^{-1}(2\pi\tilde{\chi}_{\pm}(\tilde{p})\delta_{\pm}(\tilde{p}^2-m^2))$, with $\tilde{\chi}_{\pm}\in\mathcal{L}^2(\tilde{\Gamma}_m^{\pm},d\tilde{\mu}_m)$, of the LCKG-equation. Hence we define:

Definition: The one-particle space of a relativistic, spinless, neutral particle (resp. antiparticle) in LC-space of mass $m>0$ is $\tilde{\mathfrak{H}}_m:=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$ (resp. $\mathcal{L}^2(\tilde{\Gamma}_m^-,d\tilde{\mu}_m)$).

Remark IV.1: The coordinate transformation $\kappa:\mathbb{M}\to\mathbb{L}$ induces a canonical isomorphism of complex Hilbert spaces $\kappa_*:\mathfrak{H}_m\tilde{\to}\tilde{\mathfrak{H}}_m$ between the one-particle spaces.

We define the real scalar free LC-field $\tilde{\phi}_m$ of mass $m>0$ in the same way as the real scalar free field ϕ_m was defined in Ref. 16 using the Segal field operator ϕ_S.

Let $\mathfrak{H}$ be a complex Hilbert space and let $\mathcal{F}_\vee(\mathfrak{H})=\oplus_{n=0}^{\infty}\mathfrak{H}^{\vee n}$ be the bosonic Fock space (over $\mathfrak{H}$). By F_0 we denote the dense linear subspace of all finite vectors ψ of $\mathcal{F}_\vee(\mathfrak{H})$, i.e., $\psi=(\psi^{(n)})_{n\in\mathbb{N}}$ such that $\psi^{(n)}=0$ for all but finitely many $n\in\mathbb{N}$. For each $f\in\mathfrak{H}$ the Segal field operator $\phi_S(f)$ is defined as a linear operator on the finite vectors F_0 by

$$\phi_S(f):=\frac{1}{\sqrt{2}}(a(f)+a^*(f)),$$

where $a(f)$ (resp. $a^*(f)$) is the annihilation (resp. creation) operator defined on F_0. Recall that on $\mathfrak{H}^{\vee n}$ (cf. Ref. 3)

$$a^*(f)(\psi_1\vee\cdots\vee\psi_n)=\sqrt{n+1}\,f\vee\psi_1\vee\cdots\vee\psi_n$$

and

$$a(f)(\psi_1\vee\cdots\vee\psi_n)=\frac{1}{\sqrt{n}}\sum_{j=1}^{n}\langle f,\psi_j\rangle\psi_1\vee\cdots\vee\widehat{\psi_j}\vee\cdots\vee\psi_n,$$

where $\widehat{\psi_j}$ means omitting ψ_j. On the finite vectors $a(f)$ is the adjoint operator of $a^+(f)$. It can be shown (Ref. 16, Theorem X.41) that $\phi_S(f)$ is essentially self-adjoint. In the following, we denote the closure of $\phi_S(f)$ also by $\phi_S(f)$. The mapping $f\mapsto\phi_S(f)$ from $\mathfrak{H}$ to the set of all self-adjoint operators on $\mathcal{F}_\vee(\mathfrak{H})$ is called the Segal quantization over $\mathfrak{H}$.

Note that $\mathcal{F}_\vee$ is a (covariant) functor on the category of complex Hilbert spaces. Hence, any linear operator u on $\mathfrak{H}$ induces a linear operator $\mathcal{F}_\vee(u)$—the second quantization of u—on $\mathcal{F}_\vee(\mathfrak{H})$. If u is unitary, then the same holds for $\mathcal{F}_\vee(u)$.

To define the real scalar free field ϕ_m of mass $m>0$, one chooses $\mathfrak{H}_m:=\mathcal{L}^2(\Gamma_m^+,d\mu_m)$ as the one-particle space. Now, let ϕ_S be the Segal quantization over $\mathfrak{H}_m$. Then on $\mathfrak{H}_m^{\vee n}$ the creation and annihilation operator are explicitly given by

$$(a^*(f)\psi)(p_1,\ldots,p_{n+1})=\frac{1}{\sqrt{n+1}}\sum_{j=1}^{n+1}f(p_j)\psi(p_1,\ldots,\widehat{p_j},\ldots,p_{n+1}),$$

$$(a(f)\psi)(p_1,\ldots,p_{n-1})=\sqrt{n}\int_{\Gamma_m^+}\overline{f(p)}\psi(p,p_1,\ldots,p_{n-1})d\mu_m(p),$$

where $\psi(p_1,\ldots,p_n)\in\mathfrak{H}_m^{\vee n}$. We denote by $\mathrm{res}:\mathcal{S}(\mathcal{M})\to\mathfrak{H}_m$ the restriction mapping $f\mapsto f|_{\Gamma_m^+}$. If $f\in\mathcal{S}(\mathbb{M})$ is real-valued, one defines

$$\phi_m(f)=\phi_S(\alpha\cdot\mathrm{res}(f^{\wedge_{\mathbb{M}}})),$$

where $\alpha:=\sqrt{2/(2\pi)^3}$ is a normalizing constant, and for general $f\in\mathcal{S}(\mathbb{M})$

$$\phi_m(f)=\phi_m(\mathrm{Re}\,f)+i\phi_m(\mathrm{Im}\,f).$$

To complete the construction of the real scalar field ϕ_m, one has to define a strongly continuous unitary representation of the restricted Poincaré group $\mathcal{P}_+^\uparrow$. This is done by

$$U_m:\mathcal{P}_+^\uparrow\to\mathcal{B}(\mathcal{F}_\vee(\mathfrak{H}_m)),\quad (a,\Lambda)\mapsto\mathcal{F}_\vee(u_m(a,\Lambda)),$$

where $u_m(a,\Lambda)\in\mathcal{B}(\mathfrak{H}_m)$ is defined by

$$(u_m(a,\Lambda)\psi)(p):=e^{i\langle a,p\rangle_{\mathbb{M}}}\psi(\Lambda^{-1}p).$$

Again we denote by F_0 the dense subspace of all finite vectors of $\mathcal{H}_m:=\mathcal{F}_\vee(\mathfrak{H}_m)$. The following theorem is proven in Ref. 16, Theorem X.42.

Theorem IV.2: *The quadruple* $(\mathcal{H}_m,U_m,\phi_m,F_0)$ *satisfies the Wightman axioms. Moreover,*

$$(\Box+m^2)\phi_m=0,$$

i.e., $\phi_m((\Box+m^2)f)=0$ *for each* $f\in\mathcal{S}(\mathbb{M})$.

If we replace in the preceding construction of ϕ_m all quantities by the corresponding tilde quantities, we obtain the real scalar free LC-field $\tilde{\phi}_m$. More precisely, let $\tilde{\phi}_S$ be the Segal quantization over $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$. The creation and annihilation operators are now given explicitly by

$$(\tilde{a}^*(f)\tilde{\psi})(\tilde{p}_1,\ldots,\tilde{p}_{n+1})=\frac{1}{\sqrt{n+1}}\sum_{j=1}^{n+1}f(\tilde{p}_j)\tilde{\psi}(\tilde{p}_1,\ldots,\widehat{\tilde{p}_j},\ldots,\tilde{p}_{n+1}),$$

$$(\tilde{a}(f)\tilde{\psi})(\tilde{p}_1,\ldots,\tilde{p}_{n-1})=\sqrt{n}\int_{\tilde{\Gamma}_m^+}\overline{f}(p)\tilde{\psi}(\tilde{p},\tilde{p}_1,\ldots,\tilde{p}_{n-1})d\tilde{\mu}_m(\tilde{p}),$$

where $\tilde{\psi}(\tilde{p}_1,\ldots,\tilde{p}_n)\in\tilde{\mathfrak{H}}_m^{\vee n}$. We denote by $\widetilde{\mathrm{res}}:\mathcal{S}(\mathbb{L})\to\tilde{\mathfrak{H}}_m$ the restriction mapping $f\mapsto f|_{\tilde{\Gamma}_m^+}$. If $f\in\mathcal{S}(\mathbb{L})$ is real-valued, we define

$$\tilde{\phi}_m(f)=\tilde{\phi}_S(\alpha\cdot\widetilde{\mathrm{res}}(f^{\wedge_{\mathbb{L}}})),$$

and for general $f\in\mathcal{S}(\mathbb{L})$

$$\tilde{\phi}_m(f)=\tilde{\phi}_m(\mathrm{Re}\,f)+i\tilde{\phi}_m(\mathrm{Im}\,f).$$

We still have to define a strongly continuous unitary representation, now, of the restricted LC-Poincaré group $\tilde{\mathcal{P}}_+^\uparrow=\kappa\mathcal{P}_+^\uparrow\kappa=\{(\kappa a,\kappa\Lambda\kappa):(a,\Lambda)\in\mathcal{P}_+^\uparrow)\}$. Let

$$\tilde{U}_m:\tilde{\mathcal{P}}_+^\uparrow\to\mathcal{B}(\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)),\quad (\tilde{a},\tilde{\Lambda})\mapsto\mathcal{F}_\vee(\tilde{u}_m(\tilde{a},\tilde{\Lambda})),$$

where $\tilde{u}_m(\tilde{a},\tilde{\Lambda})\in\mathcal{B}(\tilde{\mathfrak{H}}_m)$ is defined by

$$(\tilde{u}_m(\tilde{a},\tilde{\Lambda})\tilde{\psi})(\tilde{p}):=e^{i\langle\tilde{a},\tilde{p}\rangle_{\mathbb{L}}}\tilde{\psi}(\tilde{\Lambda}^{-1}\tilde{p}).$$

Finally, let $\tilde{F}_0$ be the dense subspace of finite vectors of $\tilde{\mathcal{H}}_m:=\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)$. Immediately from the definitions we obtain the following commutative diagrams:

$$\begin{array}{ccc} D & \xrightarrow{\phi(f)} & \mathcal{H}_m \\ {\scriptstyle \mathcal{F}_{\mathrm{V}}(\kappa_*)}\downarrow\wr & & \downarrow\wr{\scriptstyle \mathcal{F}_{\mathrm{V}}(\kappa_*)} \\ \tilde{D} & \xrightarrow[\tilde{\phi}(\tilde{f})]{} & \tilde{\mathcal{H}}_m \end{array} \qquad \begin{array}{ccc} \mathcal{H}_m & \xrightarrow{U_m(a,\Lambda)} & \mathcal{H}_m \\ {\scriptstyle \mathcal{F}_{\mathrm{V}}(\kappa_*)}\downarrow\wr & & \downarrow\wr{\scriptstyle \mathcal{F}_{\mathrm{V}}(\kappa_*)} \\ \tilde{\mathcal{H}}_m & \xrightarrow[\tilde{U}_m(\tilde{a},\tilde{\Lambda})]{} & \tilde{\mathcal{H}}_m \end{array} \tag{16}$$

with $\tilde{f}=\kappa_*(f)$, $(\tilde{a},\tilde{\Lambda})=(\kappa a,\kappa\Lambda\kappa)$, where $f\in\mathcal{S}(\mathbb{M})$, $(a,\Lambda)\in\mathcal{P}_+^\uparrow$, and $D=F_0$, $\tilde{D}=\tilde{F}_0$.

Using these commutative diagrams and Theorem IV.2, it is easy to see that the quadruple $(\tilde{\mathcal{H}}_m,\tilde{U}_m,\tilde{\phi}_m,\tilde{F}_0)$ satisfies the following axioms, called *LC-Wightman axioms* of a real scalar LC-quantum field $(\tilde{\mathcal{H}},\tilde{U},\tilde{\phi},\tilde{D})$:

LC-W1 (Relativistic invariance of the state space): $\tilde{\mathcal{H}}$ is a separable complex Hilbert space and $\tilde{U}$ is a strongly continuous unitary representation on $\tilde{\mathcal{H}}$ of the restricted LC-Poincaré group $\tilde{\mathcal{P}}_+^\uparrow$.

LC-W2 (Spectral property): The spectrum of the LC-energy-momentum operator $\tilde{P}=(P_{\tilde{\mu}})=(P_+,P_1,P_2,P_-)$ given by $\tilde{U}(\tilde{a},\mathrm{id})=e^{i\tilde{a}^{\tilde{\mu}}P_{\tilde{\mu}}}$ lies in the closed upper LC-light cone $\mathrm{cl}(\tilde{V}^+)=\{\tilde{p}\in\mathbb{L}:\tilde{p}^2\geqslant 0,\ p^-\geqslant 0\}$.

LC-W3 (Existence and uniqueness of the vacuum): There exists in $\tilde{\mathcal{H}}$ a unique (up to a phase factor) unit vector $\tilde{\psi}_0$ (also denoted by $|\tilde{0}\rangle$ and called the vacuum), which is invariant with respect to the translations $\tilde{U}(\tilde{a},\mathrm{id})$, $(\tilde{a}\in\mathbb{L})$.

LC-W4 (Domain of definition and continuity of the field):

(i) For each $f\in\mathcal{S}(\mathbb{L})$, $\tilde{\phi}(f)$ is a linear operator on $\tilde{\mathcal{H}}$ with $\tilde{D}\subset D(\tilde{\phi}(f))$, $\tilde{D}\subset D(\tilde{\phi}(f)^*)$, where $\tilde{D}$ is a dense linear subspace of $\tilde{\mathcal{H}}$.

(ii) $\tilde{\phi}(f)\tilde{D}\subset\tilde{D}$, $\tilde{\phi}(f)^*\tilde{D}\subset\tilde{D}$, $\tilde{U}(\tilde{a},\tilde{\Lambda})\tilde{D}\subset\tilde{D}$, for each $f\in\mathcal{S}(\mathbb{L})$ and $(\tilde{a},\tilde{\Lambda})\in\tilde{P}_+^\uparrow$.

(iii) The vacuum $|\tilde{0}\rangle$ is contained in $\tilde{D}$.

(iv) The mapping $\mathcal{S}(\mathbb{L})\to\tilde{\mathcal{H}}$, $f\mapsto\tilde{\phi}(f)\psi$ is linear and continuous for each $\psi\in\tilde{\mathcal{H}}$.

(v) (Hermiticity) $\tilde{\phi}(f)^*|_{\tilde{D}}=\tilde{\phi}(\overline{f})|_{\tilde{D}}$ for each $f\in\mathcal{S}(\mathbb{L})$.

LC-W5 (Poincaré invariance of the field):

$$\tilde{U}(\tilde{a},\tilde{\Lambda})\tilde{\phi}(f)\tilde{U}(\tilde{a},\tilde{\Lambda})^{-1}=\tilde{\phi}(\{\tilde{a},\tilde{\Lambda}\}.f)$$

on $\tilde{D}$ for each $f\in\mathcal{S}(\mathbb{L})$ and $(\tilde{a},\tilde{\Lambda})\in\tilde{P}_+^\uparrow$, where $\{\tilde{a},\tilde{\Lambda}\}.f(\tilde{x})=f(\tilde{\Lambda}^{-1}(\tilde{x}-\tilde{a}))$.

LC-W6 (Locality, or microcausality): If the supports of f and g in $\mathcal{S}(\mathbb{L})$ are LC-spacelike separated, i.e., if $\langle\tilde{x}-\tilde{y},\tilde{x}-\tilde{y}\rangle_{\mathbb{L}}<0$ for each $\tilde{x}\in\mathrm{supp}(f)$, $\tilde{y}\in\mathrm{supp}(g)$, then on $\tilde{D}$

$$[\tilde{\phi}(f),\tilde{\phi}(g)]=0.$$

LC-W7 (Cyclicity of the vacuum): The set of finite linear combinations of vectors of the form $\tilde{\phi}(f_1)\cdots\tilde{\phi}(f_n)|\tilde{0}\rangle$ is dense in $\tilde{\mathcal{H}}$.

Corollary IV.3: The quadruple $(\tilde{\mathcal{H}}_m,\tilde{U}_m,\tilde{\phi}_m,\tilde{F}_0)$ *satisfies the LC-Wightman axioms. Moreover,*

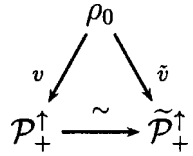
$$(\tilde{\Box}+m^2)\tilde{\phi}_m=0,$$

i.e., $\tilde{\phi}_m((\tilde{\Box}+m^2)f)=0$ *for each* $f\in\mathcal{S}(\mathbb{L})$.

Definition: The quadruple $(\tilde{\mathcal{H}}_m, \tilde{U}_m, \tilde{\phi}_m, \tilde{F}_0)$ from Corollary IV.3 is called the real scalar free LC-field of mass $m>0$.

Remark IV.4: In LC-W1–LC-W7 we have listened the LC-Wightman axioms of a real scalar LC-quantum field. Thereby we have only modified the assertions of the classical Wightman axioms which concern the Minkowski metric and replaced these by using the LC-metric.

Remark IV.5: In relativistic physics it is important to admit also two-valued representations of the restricted Poincaré group $\mathcal{P}_+^\uparrow$; for example to describe particles of half-integral spin, i.e., spinor fields. Hence, one requires in the Wightman axioms[20,3] a unitary representation of the universal covering group of $\mathcal{P}_+^\uparrow$–the Poincaré spinor group $\rho_0 := \{(a, \underset{\sim}{\Lambda}) : a \in \mathbb{M},\ \underset{\sim}{\Lambda} \in \mathrm{SL}(2,\mathbb{C})\}$ Since $\mathcal{P}_+^\uparrow \tilde{\to} \tilde{\mathcal{P}}_+^\uparrow$ $(a,\Lambda) \mapsto (\tilde{a}, \tilde{\Lambda}) := (\kappa a, \kappa \Lambda \kappa^{-1})$ is an isomorphism of complex Lie groups, the Poincaré spinor group is also the universal covering group of $\tilde{\mathcal{P}}_+^\uparrow$ and we have the following commutative diagram



where v and $\tilde{v}$ are the corresponding covering mappings and $\mathcal{P}_+^\uparrow \tilde{\to} \tilde{\mathcal{P}}_+^\uparrow$ is the above given isomorphism. Hence it is natural to generalize axiom LC-W1 by requiring that $\tilde{U}$ is a strongly continuous unitary representation of the Poincaré spinor group ρ_0. Note that $v(a, \underset{\sim}{\Lambda}) = (a, \Lambda(\underset{\sim}{\Lambda}))$ where $\mathrm{SL}(2,\mathbb{C}) \to \mathcal{L}_+^\uparrow$, $\underset{\sim}{\Lambda} \mapsto \Lambda(\underset{\sim}{\Lambda})$ is the universal covering of $\mathcal{L}_+^\uparrow$. Hence we have $\tilde{v}(a,\Lambda) = (a, \tilde{\Lambda}(\underset{\sim}{\Lambda}))$, where $\mathrm{SL}(2,\mathbb{C}) \to \tilde{\mathcal{L}}_+^\uparrow$, $\underset{\sim}{\Lambda} \mapsto \tilde{\Lambda}(\underset{\sim}{\Lambda}) = \kappa \Lambda(\underset{\sim}{\Lambda}) \kappa^{-1}$ is the universal covering mapping of the proper LC-Lorentz group $\tilde{\mathcal{L}}_+^\uparrow$.

Remark IV.6: The spectral condition LC-W2 implies (or is equivalent) that the operators P_+, P_- and $\tilde{P}^2 = 2P_+P_- - P_1^2 - P_2^2$ are positive. Note, that in the Minkowski case we have only the two positive operators P_0 and P^2. The presents of an extra positive momentum operator P_+ is one of the advantages of light cone quantum field theory.

Remark IV.7: For simplicity we have written down the LC-Wightman axioms only for a scalar LC-quantum field. But, it is trivial to generalize these axioms to multi-component LC-quantum fields $\tilde{\phi} = (\tilde{\phi}_l)$, and even to a finite or infinite collection $\{\tilde{\phi}^{(\tau)}\}$ of such fields. As in the Minkowski case (cf. Refs. 3 and 20) one has to generalize the transformation law in LC-W5 to

$$\tilde{U}(\tilde{a}, \underset{\sim}{\Lambda}) \tilde{\phi}_k^{(\tau)}(f) \tilde{U}(\tilde{a}, \underset{\sim}{\Lambda})^{-1} = \sum_l V_{kl}^{(\tau)}(\underset{\sim}{\Lambda}^{-1}) \tilde{\phi}_l^{(\tau)}(\{\tilde{a}, \tilde{\Lambda}(\underset{\sim}{\Lambda})\}.f),$$

where $V_{kl}^{(\tau)}$ is a complex or real finite-dimensional matrix representation of $\mathrm{SL}(2,\mathbb{C})$ and $\tilde{U}$ is a strongly continuous unitary representation of the Poincaré spinor group on $\tilde{\mathcal{H}}$. As in Ref. 3, p. 325, we suppose that $V^{(\tau)}(-1) = \{\pm 1\}$. If $V^{(\tau)}(-1) = 1$, then $(\tilde{\phi}_l)$ is a LC-field with integral spin (tensor LC-field), if $V^{(\tau)}(-1) = -1$, then $(\tilde{\phi}_l)$ is a LC-field with half-integral spin (spinor LC-field).

Moreover, one has to replace the commutator in LC-W6 by

$$[\tilde{\phi}_k^{(\tau)}(f), \tilde{\phi}_l^{(\tau')}(g)] = 0$$

and, if one wants to define a fermionic LC-field, one has to replace the commutator by the anticommutator.

In LC-W7 we have to require that the set of finite linear combinations of vectors of the form $\tilde{\phi}_{l_1}^{(\tau_1)}(f_1) \cdots \tilde{\phi}_{l_n}^{(\tau_n)}(f_n)|\tilde{0}\rangle$ is dense in $\tilde{\mathcal{H}}$. Hence, it should be clear how to modify the general Wightman axioms,[3] p. 324, to obtain the LC-Wightman axioms of a LC-quantum field theory, in general.

The construction of the real scalar free LC-field, especially the commutative diagrams (16), suggests the following definition.

Definition: Let $\phi=(\mathcal{H},U,(\phi_l^{(\tau)}),D)$ be a quantum field obeying the (classical) Wightman axioms. A pushforward of ϕ under $\kappa:\mathbb{M}\to\mathbb{L}$ (or pullback of ϕ under $\kappa^{-1}:\mathbb{L}\to\mathbb{M}$) is a LC-quantum field $\tilde{\phi}=(\tilde{\mathcal{H}},\tilde{U},(\tilde{\phi}_l^{(\tau)}),\tilde{D})$ obeying the LC-Wightman axioms (and transforming according to the same finite-dimensional representation $V_{kl}^{(\tau)}$ as $\phi^{(\tau)}$) together with a unitary linear operator $T:\mathcal{H}\to\tilde{\mathcal{H}}$ such that $T(D)=\tilde{D}$ and such that for each $f\in\mathcal{S}(\mathbb{M})$, $(a,\underset{\sim}{\Lambda})\in\rho_0$ the following diagrams commute

$$\begin{array}{ccc} D & \xrightarrow{\phi_l^{(\tau)}(f)} & \mathcal{H} \\ {\scriptstyle T}\downarrow & & \downarrow{\scriptstyle T} \\ \tilde{D} & \xrightarrow{\tilde{\phi}_l^{(\tau)}(\tilde{f})} & \tilde{\mathcal{H}} \end{array} \qquad \begin{array}{ccc} \mathcal{H} & \xrightarrow{U(a,\Lambda)} & \mathcal{H} \\ {\scriptstyle T}\downarrow & & \downarrow{\scriptstyle T} \\ \tilde{\mathcal{H}} & \xrightarrow{\tilde{U}(\tilde{a},\tilde{\Lambda})} & \tilde{\mathcal{H}} \end{array} \tag{17}$$

with $\tilde{a}:=\kappa a$, $\tilde{f}=\kappa_* f$ and $\tilde{\Lambda}:=\kappa\Lambda\kappa^{-1}$. For short, we write $\tilde{\phi}=\kappa_*(\phi)=(\kappa^{-1})^*(\phi)$.

We summarize the preceding by the following:

Proposition IV.8: The real scalar free LC-field $\tilde{\phi}_m=(\tilde{\mathcal{H}}_m,\tilde{U}_m,\tilde{\phi}_m,\tilde{F}_0)$ of mass $m>0$ together with the unitary operator $\mathcal{F}_\vee(\kappa_*):\mathcal{H}_m\to\tilde{\mathcal{H}}_m$ is a pushforward of the real scalar free field ϕ under $\kappa:\mathbb{M}\to\mathbb{L}$, i.e., $\tilde{\phi}_m=\kappa_*(\phi_m)$.

Remark IV.9: Let ϕ be a quantum field and $\tilde{\phi}=\kappa_*\phi$, with $T:\mathcal{H}\to\tilde{\mathcal{H}}$, a pushforward of ϕ. If $|0\rangle$ is the vacuum of ϕ then $T|0\rangle$ is the vacuum of $\tilde{\phi}$ because $T|0\rangle$ is invariant under $\tilde{U}(\tilde{a},\underset{\sim}{\Lambda})$ for each $(\tilde{a},\underset{\sim}{\Lambda})\in\rho_0$.

Remark IV.10: Given a (general) quantum field $\phi=(\mathcal{H},U,(\phi_l^{(\tau)}),D)$, it is trivial to define a pushforward of ϕ under κ. Let $\tilde{\mathcal{H}}:=\mathcal{H}$ and $\tilde{D}:=D$. Define $\tilde{\phi}_l^{(\tau)}(\tilde{f})$ and $\tilde{U}(\tilde{a},\underset{\sim}{\Lambda})$ by $\tilde{\phi}_l^{(\tau)}(\tilde{f})$ $:=\phi_l^{(\tau)}(\tilde{f}\circ\kappa)$ and $\tilde{U}(\tilde{a},\underset{\sim}{\Lambda}):=U(\kappa^{-1}\tilde{a},\underset{\sim}{\Lambda})$. It is easy to check that $\tilde{\phi}=(\tilde{\mathcal{H}},\tilde{U},(\tilde{\phi}_l^{(\tau)}),\tilde{D})$ together with $T=\mathrm{id}:\mathcal{H}\to\tilde{\mathcal{H}}$ is a pushforward of ϕ.

Remark IV.11: The definition of the pushforward $\kappa_*(\phi)$ of a quantum field ϕ can also be done for any general linear invertible mapping $\kappa:\mathbb{M}\to\mathbb{R}^4$. It is not restricted to the transformation from Minkowski- to LC-coordinates.

The next proposition concerning the (anti-)commutator of a LC-quantum field follows easily from the definition of a pushforward.

Proposition IV.12: Let $\phi=(\mathcal{H},U,(\phi_l^{(\tau)}),D)$ be a quantum field and $\tilde{\phi}=\kappa_*(\phi)$, with $T:\mathcal{H}\to\tilde{\mathcal{H}}$, a pushforward of ϕ. Then for each $f,g\in\mathcal{S}(\mathbb{M})$

$$[\tilde{\phi}_l^{(\tau)}(\kappa_* f),\tilde{\phi}_m^{(\tau')}(\kappa_* g)]_\mp = T[\phi_l^{(\tau)}(f),\phi_m^{(\tau')}(g)]_\mp T^{-1},$$

where $[\_,\_]_\mp$ denotes commutator/anticommutator.

In relativistic physics the so-called Pauli–Jordan commutation function

$$D_m(x)=\frac{1}{i(2\pi)^3}\mathcal{F}_{\mathbb{M}}(\epsilon(p^0)\delta(p^2-m^2))=\frac{1}{i(2\pi)^3}\int d^4p\ \epsilon(p^0)\delta(p^2-m^2)\,e^{i\langle p,x\rangle_{\mathbb{M}}}$$

plays an essential role. One usually splits $D_m(x)$ into its positive and negative frequency parts

$$D_m^{(\pm)}(x)=\frac{\pm 1}{i(2\pi)^3}\mathcal{F}_{\mathbb{M}}(\delta_\pm(p^2-m^2))=\frac{\pm 1}{i(2\pi)^3}\int d^4p\ \delta_\pm(p^2-m^2)\,e^{i\langle p,x\rangle_{\mathbb{M}}}$$
$$=\frac{\pm 1}{2i(2\pi)^3}\int\frac{d^3\mathbf{p}}{\omega(\mathbf{p})}e^{i(\pm\omega(\mathbf{p})x^0-\mathbf{p}\cdot\mathbf{x})},$$

then $D_m(x)=D_m^{(+)}(x)+D_m^{(-)}(x)$.

Now, let $\tilde{D}_m(\tilde{x})=\kappa_*D_m(\tilde{x})=(D_m\circ\kappa^{-1})(\tilde{x})$ be the transformation of D_m to LC-coordinates $\tilde{x}$. We also transform the positive and negative parts of D_m and obtain $\tilde{D}_m^{(\pm)}(\tilde{x})=\kappa_*D_m^{(\pm)}(\tilde{x})=(D_m^{(\pm)}\circ\kappa^{-1})(\tilde{x})$. From (3) we know that M- and L-Fourier transformation commute with κ_* and, since $\delta_\pm(\tilde{p}^2-m^2)=\kappa_*\delta_\pm(p^2-m^2)$, we obtain

$$\tilde{D}_m(\tilde{x})=\frac{1}{i(2\pi)^3}\mathcal{F}_{\mathbb{L}}(\epsilon(p^-)\delta(\tilde{p}^2-m^2))=\frac{1}{i(2\pi)^3}\int d^4\tilde{p}\ \epsilon(p^-)\delta(\tilde{p}^2-m^2)\,e^{i\langle\tilde{p},\tilde{x}\rangle_{\mathbb{L}}}$$

and

$$\tilde{D}_m^{(\pm)}(\tilde{x})=\frac{\pm 1}{i(2\pi)^3}\mathcal{F}_{\mathbb{L}}(\delta_\pm(\tilde{p}^2-m^2))=\frac{\pm 1}{i(2\pi)^3}\int d^4\tilde{p}\ \delta_\pm(\tilde{p}^2-m^2)\,e^{i\langle\tilde{p},\tilde{x}\rangle_{\mathbb{L}}}$$
$$=\frac{\pm 1}{2i(2\pi)^3}\int_{\pm p^+>0}\frac{d^3\tilde{\mathbf{p}}}{|p^+|}e^{i(\tilde{\omega}(\tilde{\mathbf{p}})x^++p^+x^--\mathbf{p}_\perp\cdot\mathbf{x}_\perp)}.$$

Hence, we also have $\tilde{D}_m(\tilde{x})=\tilde{D}_m^{(+)}(\tilde{x})+\tilde{D}_m^{(-)}(\tilde{x})$.

Corollary IV.13: Let $\tilde{\phi}_m(\tilde{x})$ be the real scalar free LC-field of mass $m>0$, i.e., the pushforward of the real scalar free field $\phi_m(x)$. Then

$$[\tilde{\phi}_m(\tilde{x}),\tilde{\phi}_m(\tilde{y})]=\frac{1}{i}\tilde{D}_m(\tilde{x}-\tilde{y}),$$

where $\tilde{D}_m(\tilde{x})=\kappa_*D_m(\tilde{x})=(D_m\circ\kappa^{-1})(\tilde{x})$.

Proposition IV.14: Let $\phi=(\mathcal{H},U,(\phi_l^{(\tau)}),D)$ be a quantum field and $\tilde{\phi}=\kappa_*(\phi)$ a pushforward of ϕ. We denote by

$$w_{l_1,\ldots,l_n}^{(\tau_1\cdots\tau_n)}(x_1,\ldots,x_n)=\langle 0|\,\phi_{l_1}^{(\tau_1)}(x_1)\cdots\phi_{l_n}^{(\tau_n)}(x_n)|0\rangle$$

the Wightman functions of ϕ and by

$$\tilde{w}_{l_1,\ldots,l_n}^{(\tau_1\cdots\tau_n)}(\tilde{x}_1,\ldots,\tilde{x}_n)=\langle\tilde{0}|\,\tilde{\phi}_{l_1}^{(\tau_1)}(\tilde{x}_1)\cdots\tilde{\phi}_{l_n}^{(\tau_n)}(\tilde{x}_n)|\tilde{0}\rangle$$

the Wightman functions of $\tilde{\phi}$. Then

$$\tilde{w}_{l_1,\ldots,l_n}^{(\tau_1\cdots\tau_n)}=w_{l_1,\ldots,l_n}^{(\tau_1\cdots\tau_n)}\circ\oplus^n\kappa^{-1}.$$

Proof: Follows immediately from the left commutative diagram of (17). □

Corollary IV.15: Let $\tilde{\phi}_m$ be the real scalar free LC-field of mass $m>0$. Then

$$\langle\tilde{0}|\,\tilde{\phi}_m(\tilde{x})\tilde{\phi}_m(\tilde{y})|\tilde{0}\rangle=\frac{1}{i}\tilde{D}_m^{(-)}(\tilde{x}-\tilde{y}).$$

Proof: Since $\langle 0|\,\phi_m(x)\phi_m(y)|0\rangle=(1/i)\,D_m^{(-)}(x-y)$, the assertion follows from Proposition IV.14. □

It should be clear that one can translate any covariant statement about Wightman quantum fields to the LC-case. All that we have to do is to rephrase a given statement by using the LC bilinear form $\langle \_,\_\rangle_{\mathbb{L}}$ instead of the Minkowski bilinear form $\langle \_,\_\rangle_{\mathbb{M}}$. In this way we obtain, for example, an analogous reconstruction theorem for LC-quantum fields. We do not want to listen all these transformed statements which can be proven trivially by using the definition of the pushforward of a quantum field. Going over from a quantum field ϕ to the corresponding LC-quantum field $\tilde{\phi}=\kappa_*\phi$ in the context of the covariant four-dimensional Wightman formalism gives, however, no additional insight into the theory. But, as mentioned in the Introduction, we are mainly interested in the use of the front form dynamics to describe the dynamics of a quantum field. So, we have to study the question whether it is possible to use in a mathematically rigorous way the nonrelativistic Hamiltonian formalism in the LC-case.

V. THE RESTRICTION PROBLEM AND SQUEEZED DISTRIBUTIONS

In this section we restrict ourselves to a real scalar free field ϕ_m of mass $m>0$. Let $\tilde{\phi}_m$ be the corresponding real scalar free LC-field. Recall that $\phi_m=(\mathcal{H}_m,U_m,\phi_m,D)$, $\tilde{\phi}_m=(\tilde{\mathcal{H}}_m,\tilde{U}_m,\tilde{\phi}_m,\tilde{D})$, where $\mathcal{H}_m=\mathcal{F}_\vee(\mathfrak{H}_m)$, $\tilde{\mathcal{H}}_m=\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)$ with $\mathfrak{H}_m=\mathcal{L}^2(\Gamma_m^+,d\mu_m)$, $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$, and that $\tilde{\phi}_m=\kappa_*\phi_m$ is a pushforward of ϕ_m under κ where the unitary operator $T=\mathcal{F}_\vee(\kappa_*):\mathcal{H}_m\to\tilde{\mathcal{H}}_m$ is induced by the canonical unitary operator $\kappa_*:\mathfrak{H}_m\to\tilde{\mathfrak{H}}_m$, $f\mapsto f\circ\kappa^{-1}$.

A. Outline of the restriction problem

The standard way to construct the time-zero field φ_m and its canonical conjugate π_m goes as follows (cf. Ref. 16, p. 215):

Let $g\in\mathcal{S}_3=\mathcal{S}(\mathbb{R}^3)$ be real valued. Since the restriction of $(\delta(x^0)\otimes g(\mathbf{x}))^{\wedge\mathbb{M}}=1\otimes\hat{g}$ to Γ_m^+ ($\hat{g}$ is the usual 3-dim. Fourier transform of g) is in $\mathfrak{H}_m=\mathcal{L}^2(\Gamma_m^+,d\mu_m)$—this is equivalent to $\hat{g}\in\mathcal{L}^2(\mathbb{R}^3,d^3\mathbf{p}/2\omega(\mathbf{p}))$—it is possible to define

$$\varphi_m(g):=\phi_m(\delta(x^0)\otimes g(\mathbf{x}))=\phi_S(\alpha\cdot\mathrm{res}_{\Gamma_m^+}(1\otimes\hat{g})).$$

Then one extends linearly the definition of φ_m to general $g\in\mathcal{S}_3$ by

$$\varphi_m(g):=\varphi_m(\mathrm{Re}\,g)+i\varphi_m(\mathrm{Im}\,g).$$

The canonical conjugate momentum π_m is defined by

$$\pi_m(g)=\frac{\partial}{\partial x^0}\phi_m(\delta(x^0)\otimes g(\mathbf{x}))=\phi_S(\alpha\cdot\mathrm{res}_{\Gamma_m^+}(-ip^0\hat{g}(\mathbf{p})))$$

for each real valued $g\in\mathcal{S}_3$ and one extends the definition to general $g\in\mathcal{S}_3$ again by linearity. Here ϕ_S denotes the Segal quantization over $\mathfrak{H}_m$. Note that π_m is well-defined because $p^0\hat{g}(\mathbf{p})$ is in $\mathfrak{H}_m$.

Now, if one tries to define the time-zero LC-field $\tilde{\varphi}_m$ (and its canonical conjugate $\tilde{\pi}_m$) in an analogous way by

$$\tilde{\varphi}_m(g)=\tilde{\phi}_m(\delta(x^+)\otimes g(\tilde{\mathbf{x}})),$$

one gets into trouble because, for general $g(\tilde{\mathbf{x}})\in\mathcal{S}_3$, the function $(\delta(x^+)\otimes g(\tilde{\mathbf{x}}))^{\wedge\mathbb{L}}$ is not in $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}^+,d\tilde{\mu}_m)$. This is easily seen by

$$\|(\delta(x^+)\otimes g(\tilde{\mathbf{x}}))^{\wedge\mathbb{L}}\|_{\tilde{\mathfrak{H}}_m}^2=\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}|g^{\sqcap}(\tilde{\mathbf{p}})|^2, \tag{18}$$

where we have denoted by $g^{\sqcap}(\tilde{\mathbf{p}})$ the partial $\mathbb{L}$-Fourier transform $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}}\to\tilde{\mathbf{p}}}(g)$ of $g(\tilde{\mathbf{x}})$ defined by

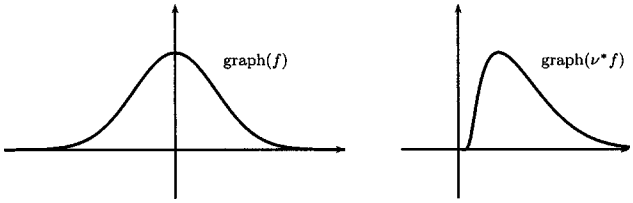


FIG. 3. Graphs of $f(p^2)=\exp(-p^2)$ and $\nu^* f(p^+)=\exp(-\frac{1}{2}(p^+-(1/2p^+))^2)$.

$$g^{\sqcap}(\tilde{\mathbf{p}}) := (\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}}\to\tilde{\mathbf{p}}} g)(\tilde{\mathbf{p}}) := \int_{\mathbb{R}^3} d^3\tilde{\mathbf{x}}\, g(\tilde{\mathbf{x}})\, e^{i(p^+x^- - \mathbf{p}_\perp\cdot\mathbf{x}_\perp)}. \tag{19}$$

To solve this restriction problem we have to drop the assumption that the restriction of a quantum field has to be defined on $\mathcal{S}(\mathbb{R}^3)$. We will see in a few moments that a completely different function space which is, however, isomorphic to $\mathcal{S}(\mathbb{R}^3)$ is the canonical candidate for a test function space to define the restriction of a LC-quantum field. Consider the following commutative diagram:

$$\begin{array}{ccccc}
\mathcal{S}(\mathbb{M}) & \xrightarrow{\text{res}} & \mathcal{L}^2(\Gamma_m^+, d\mu_m) & \xrightarrow{\Omega_+^*} & \mathcal{L}^2\left(\mathbb{R}^3, \frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}\right) \\
\downarrow{\scriptstyle \kappa_*} & & \downarrow{\scriptstyle \kappa_*} & & \downarrow{\scriptstyle \nu^*} \\
\mathcal{S}(\mathbb{L}) & \xrightarrow{\widetilde{\text{res}}} & \mathcal{L}^2(\tilde{\Gamma}_m^+, d\tilde{\mu}_m) & \xrightarrow{\tilde{\Omega}_+^*} & \mathcal{L}^2\left(\mathbb{R}_{>0}\times\mathbb{R}^2, \frac{d^3\tilde{\mathbf{p}}}{2p^+}\right)
\end{array} \tag{20}$$

Recall that κ_*, Ω_+^*, $\tilde{\Omega}_+^*$, ν^* are isomorphisms (resp. unitary mappings) and $\nu=\Omega_+^{-1}\circ\kappa^{-1}\circ\tilde{\Omega}_+$ (cf. (15)). We write briefly $\text{res}(f)$ (resp. $\widetilde{\text{res}}(f)$) instead of $\text{res}_{\Gamma_m^+}(f)$ (resp. $\text{res}_{\tilde{\Gamma}_m^+}(f)$).

It is well known that the image of $\mathcal{S}(\mathbb{M})$ under the restriction mapping is dense in $\mathcal{L}^2(\Gamma_m^+, d\mu_m)$. Essential for the definition of the time-zero field φ_m on $\mathcal{S}_3=\mathcal{S}(\mathbb{R}^3)$ is the fact that $\text{res}(\mathcal{S}(\mathbb{M}))$ equals $(\Omega_+^*)^{-1}(\mathcal{S}_3)=\{\text{res}(1(p^0)\otimes g(\mathbf{p})): g(\mathbf{p})\in\mathcal{S}_3\}$ (to see this, notice that $\text{res}(f)=\text{res}(1(p^0)\otimes f(\Omega_+(\mathbf{p})))$ and that, given $g(\mathbf{p})\in\mathcal{S}_3$, $f(p):=e^{-(p^0-\omega(\mathbf{p}))^2} g(\mathbf{p})\in\mathcal{S}_4$ and $f(\Omega_+(\mathbf{p}))=g(\mathbf{p})$).

Now, let us look at the lower row of (20). Since this diagram commutes, the image of $\mathcal{S}(\mathbb{L})$ under the restriction mapping is dense in $\mathcal{L}^2(\tilde{\Gamma}_m^+, d\tilde{\mu})$, too. Again, we can describe this image, $\widetilde{\text{res}}(\mathcal{S}(\mathbb{L}))$, as the preimage of some subspace of $\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^2, d^3\tilde{\mathbf{p}}/2p^+)$ under $\tilde{\Omega}_+$, especially we have

$$\widetilde{\text{res}}(\mathcal{S}(\mathbb{L})) = (\tilde{\Omega}_+^*)^{-1}(\nu^*(\mathcal{S}_3)) = \{\widetilde{\text{res}}(\tilde{g}(\tilde{\mathbf{p}})\otimes 1(p^-)) : \tilde{g}(\tilde{\mathbf{p}})\in\nu^*(\mathcal{S}_3)\}.$$

Hence we see that the function space

$$\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2) := \nu^*(\mathcal{S}_3) = \{g\circ\nu : g\in\mathcal{S}_3\}$$

takes on the role of $\mathcal{S}_3$, if we switch from three-dimensional $\mathbf{p}$-space to three-dimensional $\tilde{\mathbf{p}}$-space. We endow $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$ with the final topology w.r.t. $\nu^*:\mathcal{S}_3\to\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$. Then ν^* becomes an isomorphism of (complex) topological vector spaces.

Before we start to define the restriction of the free LC-field $\tilde{\phi}_m$ to $\{x^+=0\}$, we show some interesting properties of $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$. To get a first impression of what kind of functions appear in $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$ and how the mapping $\nu^*:\mathcal{S}_3\to\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$ deforms (squeezes) the functions of $\mathcal{S}_3$ we have drawn in Fig. 3, as an example, the graphs of the functions $f(p)$

$=\exp(-p^2)\in\mathcal{S}_1$ and $(\nu^* f)(p^+)$, where $\nu(p^+)=(1/\sqrt{2})(p^+-1/2p^+)$. In Fig. 3 one can see that ν^* transforms the rapidly decreasing behavior of $f(p)$ as p goes to $-\infty$ to a rapidly decreasing behavior of $\nu^* f(p^+)$ as p^+ goes to zero (from the right).

B. Squeezed distributions

Let us start to study the function space $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^2)$. We wish to do this in any dimension n, thus first we have to (re)define $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^n)$ for any $n\geqslant 0$. Also we want to consider the reflected situation and thus introduce $\mathcal{S}_{p^+}(\mathbb{R}_{<0}\times\mathbb{R}^n)$. Let $\mathbb{M}^{n+1}$ (resp. $\mathbb{L}^{n+1}$) be $(n+1)$-dimensional Minkowski space (resp. LC-space) and let $\kappa:\mathbb{M}^{n+1}\to\mathbb{L}^{n+1}$ be the transformation to LC-coordinates as introduced in Sec. II. We have introduced in Sec. II the parametrizations $\Omega_\pm:\mathbb{R}^n\tilde{\to}\Gamma_m^\pm\subset\mathbb{R}^{n+1}$ and $\tilde{\Omega}_\pm:\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1}\tilde{\to}\tilde{\Gamma}_m^\pm\subset\mathbb{R}^{n+1}$ of the smooth submanifolds $\Gamma_m^\pm$ and $\tilde{\Gamma}_m^\pm$. The *(positive/negative) squeezing mapping* $\nu_{\gtrless 0}:\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1}\to\mathbb{R}^n$ is defined by

$$\nu_{\gtrless 0}:=\Omega_\pm^{-1}\circ\kappa^{-1}\circ\tilde{\Omega}_\pm .$$

Note that the previous ν equals now $\nu_{>0}$ and that $\nu_{<0}(-\tilde{\mathbf{p}})=-\nu_{>0}(\tilde{\mathbf{p}})$ for all $\tilde{\mathbf{p}}\in\mathbb{R}_{>0}\times\mathbb{R}^{n-1}$. Furthermore $\nu_{\gtrless 0}$ is a diffeomorphism from $\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1}$ onto $\mathbb{R}^n$. If we define

$$\nu_{\neq 0}:\mathbb{R}^\times\times\mathbb{R}^{n-1}\to\mathbb{R}^n,\qquad \tilde{\mathbf{p}}=(p^+,\mathbf{p}_\perp)\mapsto\left(\mathbf{p}_\perp,\frac{1}{\sqrt{2}}\left(p^+-\frac{\mathbf{p}_\perp^2+m^2}{2p^+}\right)\right),$$

where $(\mathbb{R}^\times=\mathbb{R}\backslash 0)$, then $\nu_{\neq 0}$ is a double covering of $\mathbb{R}^n$ and the restriction of $\nu_{\neq 0}$ to $\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1}$ is $\nu_{\gtrless 0}$. The inverse mapping of $\nu_{\gtrless 0}$ is denoted by $\mu_{\gtrless 0}$, and is explicitly given by

$$\mu_{\gtrless 0}:\mathbb{R}^n\to\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1},\qquad \mathbf{p}=(p^1,\ldots,p^n)\mapsto\left(\frac{p^n\pm\omega(\mathbf{p})}{\sqrt{2}},p^1,\ldots,p^{n-1}\right),$$

where $\omega(\mathbf{p})=\sqrt{\mathbf{p}^2+m^2}$.

Definition: The (complex) topological vector space

$$\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1}):=\nu_{\gtrless 0}^*\mathcal{S}(R^n)=\{f\circ\nu_{\gtrless 0}:f\in\mathcal{S}(\mathbb{R}^n)\}$$

is called the *positive/negative squeezed Schwartz space* (of positive/negative squeezed rapidly decreasing functions), where we have endowed $\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1})$ with the final topology w.r.t. $\nu_{\gtrless 0}^*:\mathcal{S}(\mathbb{R}^n)\to\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1})$.

The next proposition deals with fundamental properties of $\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1})$ which are essential for the sequel. Recall (e.g. Ref. 1) that $\mathbb{C}[X_1,\ldots,X_n]_{X_i}$ denotes the localization of the polynomial ring $\mathbb{C}[X_1,\ldots,X_n]$ by the multiplicative set $\{X_i^k:\mathbb{Z}\ni k\geqslant 0\}$, i.e., $\mathbb{C}[X_1,\ldots,X_n]_{X_i}=\{S/X_i^k:S\in\mathbb{C}[X_1,\ldots,X_n],\ k\geqslant 0\}$. In the following we consider $\mathbb{C}[X_1,\ldots,X_n]_{X_i}$ always as a ring of functions on $\{X_i\neq 0\}$.

Lemma V.1:

(i) *Let $c\in\mathbb{R}$, $c>0$, and let $k\in\mathbb{N}$, $k>1$. Then for all $t\geqslant\max(1,3/c)$*
$$t^{k+1}+1\leqslant t^k\sqrt{t^2+c}.$$

(ii) *Assume $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$ and α is a multi-index, let $\mu_{>0}$ as above. Then there is a polynomial $R\in\mathbb{R}[\mathbf{p}]$ such that*
$$|\partial^\alpha(Q\circ\mu_{>0})(\mathbf{p})|\leqslant R(\mathbf{p})\quad\text{for all}\quad\mathbf{p}\in\mathbb{R}^n.$$

(iii) *The functions $\omega\circ\nu_{\gtrless 0}$ are (restrictions of functions) in $\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$, where $\nu_{\gtrless 0}$ is the positive/negative squeezing mapping and $\omega(\mathbf{p})=\sqrt{\mathbf{p}^2+m^2}$.*

Proof:

(i) Let $t\geqslant\max(1,3/c)$ and $k>1$. Then $2t^{k+1}+1\leqslant ct^{2k}$. Adding t^{2k+2} to both sides of this

inequality yields $(t^{k+1}+1)^2 \leqslant t^{2k}(t^2+c)$.

(ii) Clearly $\partial^\alpha(Q\circ\mu_{>0})$ is a polynomial in $1/(\omega(\mathbf{p})+p^n)$, $\omega(\mathbf{p})$, $1/\omega(\mathbf{p})$, and $\mathbf{p}$. It is enough to consider only the cases when $\partial^\alpha(Q\circ\mu_{>0})$ equals one of these functions. Thereby, the only non-trivial case is if it equals $1/(\omega(\mathbf{p})+p^n)$ (note that $\lim_{p^n\to-\infty}\omega(\mathbf{p})+p^n=0$). Let $c(\mathbf{p}') := \Sigma_{i=1}^{n-1}(p^i)^2+m^2$, where $\mathbf{p}'=(p^1,\ldots,p^{n-1})\in\mathbb{R}^{n-1}$. Fix any $k>1$, $k\in\mathbb{N}$. By (i) we have

$$(p^n)^{k+1}+1 \leqslant (p^n)^k\omega(\mathbf{p})$$

for all $\mathbf{p}\in\mathbb{R}^n$ such that $p^n \geqslant \max(1,3/c(\mathbf{p}'))$. Since $c(\mathbf{p}')$ is bounded from below, $\max(1,3/c(\mathbf{p}'))$ is bounded from above by some $C\geqslant 1$. Thus, for all $\mathbf{p}\in\mathbb{R}^n$ such that $p^n \geqslant C$, we obtain

$$\frac{1}{\omega(\mathbf{p})-p^n} \leqslant (p^n)^k.$$

If t is the supremum of $(1/(\omega(\mathbf{p})-p^n)$ on $\{\mathbf{p}\in\mathbb{R}^n : p^n\leqslant C\}$ then $R(\mathbf{p}) := (p^n)^k+t$ is the desired polynomial.

(iii) Since $\mu_{>0}\circ\nu_{>0}$ is the identity on $\mathbb{R}_{>0}\times\mathbb{R}^{n-1}$, we have

$$p^+ = \frac{1}{\sqrt{2}}\left(\omega(\nu_{>0}(\tilde{\mathbf{p}})) + \frac{1}{\sqrt{2}}\left(p^+ - \frac{\mathbf{p}_\perp^2+m^2}{2p^+}\right)\right)$$

from which the assertion follows. □

In the following we denote by $f^\vee$ the function defined by $f^\vee(p) := f(-p)$.

Proposition V.2:

(i) $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})^\vee = \mathcal{S}_{p^+}(\mathbb{R}_{<0}\times\mathbb{R}^{n-1})$.

(ii) *Assume α is a multi-index, $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$ and $f\in\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$. Then $Q\partial^\alpha f \in \mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$.*

(iii) *$\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ consists of all $f\in C^\infty(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ such that*

$$\sup_{\tilde{\mathbf{p}}\in\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1}} |Q(\tilde{\mathbf{p}})\partial^\alpha f(\tilde{\mathbf{p}})| < \infty \tag{21}$$

for all multi-indices α and $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$. Furthermore, the topology of $\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ is induced by the semi-norms in the left-hand side of (21).

Proof:

(i) is trivial and (ii) follows immediately from (iii).

(iii) It is enough to show (iii) only for $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. We write $\nu := \nu_{>0}$, $\mu := \nu^{-1}$, and $\sup'|Q\partial^\alpha f|$ for the seminorms in (21). We have defined the topology on $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$ as the final topology w.r.t. the bijection $\nu^*:\mathcal{S}(\mathbb{R}^n)\to\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. Thus the topology is induced by the family of seminorms

$$\sup_{\mathbf{p}\in\mathbb{R}^n} |R(\mathbf{p})\partial^\alpha(f\circ\mu)(\mathbf{p})|, \quad \alpha \text{ multi-index, } R \text{ polynomial.} \tag{22}$$

A smooth function f is in $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$ iff $f\circ\mu$ is in $\mathcal{S}(\mathbb{R}^n)$ which means that $\sup|R\partial^\alpha(f\circ\mu)|<\infty$ for all multi-indices α and polynomials R. Assume $f\in\mathbb{C}^\infty(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. By the chain rule $R\partial^\alpha(f\circ\mu)$ is a finite sum of terms of the form $S\mu^*(\partial^\beta f)$ where β is a multi-index and S is a polynomial in $1/\omega(\mathbf{p})$, $\omega(\mathbf{p})$, and $\mathbf{p}$. Since $1/\omega(\mathbf{p})$ is a bounded function, we can bound $|S\mu^*(\partial^\beta f)|$ by some $|R\mu^*(\partial^\beta f)|$ where R is a polynomial in $\omega(\mathbf{p})$ and $\mathbf{p}$. By Lemma V.1 (iii) $Q := R\circ\nu$ is in $\mathbb{C}[p^+,\mathbf{p}_\perp]$ and thus $|S\mu^*(\partial^\beta f)|$ is bounded by $|\mu^*(Q\partial^\beta f)|$ with $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]$. Because $\sup|\mu^*(Q\partial^\beta f)| = \sup'|Q\partial^\beta f|$, we have shown that the seminorms in (22) are continuous w.r.t. the seminorms in (21) and that $f\in\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$ whenever $\sup'|Q\partial^\alpha f|<\infty$ for all $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$ and multi-indices α.

Conversely, consider $\sup'|Q\partial^\alpha f|$, where $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$ and $f\in C^\infty(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. Let $g := f\circ\mu\in\mathbb{C}^\infty(\mathbb{R}^n)$. Then $Q\partial^\alpha(\nu^*g)$ is a finite sum of terms of the form $S\nu^*(\partial^\beta g)$ with $S\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$, β multi-index. Because $\sup'|S\nu^*(\partial^\beta g)| = \sup|(\mu^*S)\partial\beta g|$ and, by Lemma V.1 (ii), $|\mu^*S|$ is bounded by some polynomial R, we obtain $\sup|(\mu^*S)\partial^\beta g| \leqslant \sup|R\partial^\beta(f\circ\mu)|$. Es-

pecially, $\sup'|Q\partial^\alpha f|<\infty$ for all $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$ and α whenever $f\circ\mu\in\mathcal{S}(\mathbb{R}^n)$, i.e., $f\in\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. □

To study further the test function space $\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ we introduce a new space, denoted $\mathcal{S}_{p^+}(\mathbb{R}^n)$.

Definition: By $\mathcal{S}_{p^+}(\mathbb{R}^n)$ we denote the set of all $f\in C^\infty(\mathbb{R}^n)$ such that

$$\sup_{(p^+,\mathbf{p}_\perp)\in\mathbb{R}^n\setminus\{p^+=0\}}|(p^+)^k\mathbf{p}_\perp^\beta\partial^\alpha f(p^+,\mathbf{p}_\perp)|<\infty \tag{23}$$

for all $k\in\mathbb{Z}$ and all multi-indices α and β, endowed with the locally convex topology defined by the seminorms in the left-hand side of (23). The function space $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is called *squeezed Schwartz space* (of squeezed rapidly decreasing functions). The dual $\mathcal{S}'_{p^+}(\mathbb{R}^n)$ is called *space of squeezed distributions (or squeezed generalized functions).*

Note that the seminorms in the left-hand side of (23) differ only in the range of the exponent of p^+—which now can also be negative—from the seminorms that define the Schwartz space $\mathcal{S}(\mathbb{R}^n)$.

Theorem V.3:

(i) *$\mathcal{S}_{p^+}(\mathbb{R}^n)\subset\mathcal{S}(\mathbb{R}^n)$, and the topology of $\mathcal{S}_{p^+}(\mathbb{R}^n)$ coincide with the subspace topology induced by $\mathcal{S}(\mathbb{R}^n)$. Moreover, $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is a closed subspace of $\mathcal{S}(\mathbb{R}^n)$.*

(ii) *If $j(f)$ denotes extension by zero of $f\in\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ then we have a mapping $j:\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})\to\mathcal{S}_{p^+}(\mathbb{R}^n)$ which induces an isomorphism (of topological vector spaces) onto their image, denoted $\mathcal{S}_{p^+\geqslant 0}(\mathbb{R}^n)$.*

(iii) $\mathcal{S}_{p^+}(\mathbb{R}^n)=\mathcal{S}_{p^+}(\mathbb{R}_{<0}\times\mathbb{R}^{n-1})\oplus\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$.

(iv) *Consider the following filtration of $\mathcal{S}(\mathbb{R}^n)$*

$$\mathcal{S}(\mathbb{R}^n)\supset p^+\mathcal{S}(\mathbb{R}^n)\supset(p^+)^2\mathcal{S}(\mathbb{R}^n)\supset\cdots\supset(p^+)^k\mathcal{S}(\mathbb{R}^n)\supset\cdots.$$

Then $\mathcal{S}_{p^+}(\mathbb{R}^n)=\cap_{k\geqslant 0}(p^+)^k\mathcal{S}(\mathbb{R}^n)$, or, if we use categorical language,

$$\mathcal{S}_{p^+}(\mathbb{R}^n)=\varprojlim_{k\geqslant 0}(p^+)^k\mathcal{S}(\mathbb{R}^n)$$

(in the category of topological vector spaces).

(v) *If $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$, $g\in\mathcal{S}_{p^+}(\mathbb{R}^n)$, and α is a multi-index, then the mappings*

$$f\mapsto Qf,\quad f\mapsto gf,\quad f\mapsto\partial^\alpha f$$

are continuous linear mappings from $\mathcal{S}_{p^+}(\mathbb{R}^n)$ into $\mathcal{S}_{p^+}(\mathbb{R}^n)$.

Proof:

(i) That $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is a subspace of $\mathcal{S}(\mathbb{R}^n)$ follows immediately from the definition of $\mathcal{S}_{p^+}(\mathbb{R}^n)$. To show that the topology of $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is just the subspace topology induced by $\mathcal{S}(\mathbb{R}^n)$ we have to show that the seminorms $\sup|(p^+)^k\mathbf{p}_\perp^\beta\partial^\alpha f(p^+,\mathbf{p}_\perp)|$ with $k<0$ do not strengthen the topology, i.e., are continuous w.r.t. the seminorms with $k\geqslant 0$. This is easily seen by applying inductively the mean-value theorem of calculus to get $\sup|(p^+)^k g|\leqslant\sup|\partial_+^k g|$ for each $g\in\mathcal{S}_{p^+}(\mathbb{R}^n)$ and $k<0$. The last assertion follows from (iii) because $\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$ as a homeomorphic image of $\mathcal{S}(\mathbb{R}^n)$ is itself a Fréchet space and hence $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is a Fréchet space, too.

(ii) Assume $f\in\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$. We have to prove that $j(f)$ is in $\mathcal{S}_{p^+}(\mathbb{R}^n)$. First we have to show that $j(f)$ is a C^∞-function on $\mathbb{R}^n$. This is the case if we have shown, that $\lim_{p^+\to 0}\partial^\alpha f(\tilde{\mathbf{p}})=0$. However, this follows immediately from $\sup'|(1/p^+)\,\partial^\alpha f(\tilde{\mathbf{p}})|<\infty$ which holds for each multi-index α. Since $\sup'|(p^+)^k\mathbf{p}_\perp^\beta\partial^\alpha f|=\sup|(p^+)^k\mathbf{p}_\perp^\beta\partial^\alpha j(f)|$, we see $j(f)\in\mathcal{S}_{p^+}(\mathbb{R}^n)$.

Furthermore, j maps $\mathcal{S}_{p^+}(\mathbb{R}_{>0}\times\mathbb{R}^{n-1})$ homeomorphically onto its image because the family of seminorms in (23) is equivalent to the family of semi-norms $\sup_{p^+\neq 0}|Q\partial^\alpha f|$, $Q\in\mathbb{C}[p^+,\mathbf{p}_\perp]_{p^+}$, α multi-index.

(iii) Each $f\in\mathcal{S}_{p^+}(\mathbb{R}^n)$ can uniquely be written as $f=\chi_{\{p^+<0\}}f+\chi_{\{p^+>0\}}f$ where $\chi_{p^+\geqslant 0}f\in\mathcal{S}_{p^+}(\mathbb{R}_{\geqslant 0}\times\mathbb{R}^{n-1})$. (By χ_A we denote the characteristic function of a set A.)

(iv) Since $\mathcal{S}(\mathbb{R}^n)$ is closed under multiplication by polynomials, the existence of the filtration is obvious. If $f\in\mathcal{S}_{p^+}(\mathbb{R}^n)$, then $(1/(p^+)^k)\,f\in\mathcal{S}_{p^+}(\mathbb{R}^n)\subset\mathcal{S}(\mathbb{R}^n)$ for each $k\geqslant 0$ by (v) or by

Proposition V.2 (ii). Conversely, assume $f \in \cap_{k\geqslant 0}(p^+)^k\mathcal{S}(\mathbb{R}^n)$. It is enough to show that $\sup|\,(1/(p^+)^k)\,\mathbf{p}_\perp^\beta \partial^\alpha f|<\infty$ for all $k>0$ and multi-indices α, β. If l is sufficiently large, then by using the Leibniz formula we obtain $(1/(p^+)^k)\,\partial^\alpha((p^+)^l g)=\Sigma_i P_i(p^+)\partial^{\beta_i} g$ with multi-indices β_i and polynomials P_i for all $g\in\mathcal{S}(\mathbb{R}^n)$. Notice that l does not depend on g. Fix such an l and choose $g\in\mathcal{S}(\mathbb{R}^n)$ such that $f=(p^+)^l g$. Since $g\in\mathcal{S}(\mathbb{R}^n)$ we have $\sup|\,(1/(p^+)^k)\,\mathbf{p}_\perp^\beta \partial^\alpha((p^+)^l g)|<\infty$.

(v) Follows easily from the closed graph theorem.

Remark V.4: From now on we often identify $\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0}\times\mathbb{R}^{n-1})$ with $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$, i.e., we consider $\nu^*_{\gtrless 0}(f)$ $(f\in\mathcal{S}(\mathbb{R}^n))$ as functions on $\mathbb{R}^n$. Hence we have isomorphisms of Fréchet spaces

$$\nu^*_{\gtrless 0}:\mathcal{S}(\mathbb{R}^n)\tilde{\to}\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n) \tag{24}$$

with inverse mappings $(\nu^*_{\gtrless 0})^{-1}=\mu^*_{\gtrless 0}$.

Definition: The elements of the dual space $\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$ are called *positive/negative squeezed distributions*.

We identify $\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$ with the subspaces $\{u:u|_{p^+\lessgtr 0}=0\}$ of $\mathcal{S}'_{p^+}(\mathbb{R}^n)$.

Each element of $g\in\mathcal{S}_{p^+}(\mathbb{R}^n)$ can be considered in a canonical way as a (regular) squeezed distribution $f\mapsto\int gf$, also denoted g. Hence we obtain canonical inclusion mappings $\mathcal{S}_{p^+}(\mathbb{R}^n)\hookrightarrow\mathcal{S}'_{p^+}(\mathbb{R}^n)$ and $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)\hookrightarrow\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$.

Theorem V.5:

(i) $\mathcal{S}'_{p^+}(\mathbb{R}^n)=\mathcal{S}'_{p^+<0}(\mathbb{R}^n)\oplus\mathcal{S}'_{p^+>0}(\mathbb{R}^n)$.

(ii) *For each* $u\in\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$ *there is a sequence* $(u_i)_{i\in\mathbb{N}}$, $u_i\in\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$, *converging to* u *in* $\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$. *The same holds, if we replace* $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ *(resp.* $\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$*) by* $\mathcal{S}_{p^+}(\mathbb{R}^n)$ *(resp.* $\mathcal{S}'_{p^+}(\mathbb{R}^n)$*).*

(iii) *The inclusion mappings* $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)\overset{\iota_{\gtrless 0}}{\hookrightarrow}\mathcal{S}_{p^+}(\mathbb{R}^n)\overset{\iota}{\hookrightarrow}\mathcal{S}(\mathbb{R}^n)$ *induce canonical linear continuous mappings* $\mathcal{S}'(\mathbb{R}^n)\overset{\iota'}{\to}\mathcal{S}'_{p^+}(\mathbb{R}^n)\overset{\iota'_{\gtrless 0}}{\to}\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$.

(iv) *The isomorphisms* $\nu^*_{\gtrless 0}:\mathcal{S}(\mathbb{R}^n)\to\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ *extend (uniquely) to linear, sequentially continuous, bijective mappings* $\nu^*_{\gtrless 0}:\mathcal{S}'(\mathbb{R}^n)\to\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$ *by the formula* $(\nu^*_{\gtrless 0}u)(f)$ $:=u(|\det D\nu_{\gtrless 0}|^{-1}(f\circ\nu^{-1}_{\gtrless 0}))$.

(v) *The inverse mapping of* $\nu^*_{\gtrless 0}:\mathcal{S}'(\mathbb{R}^n)\to\mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n)$ *is the (unique) linear, sequentially continuous extension of* $\mu^*_{\gtrless 0}:\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)\to\mathcal{S}(\mathbb{R}^n)$, *also denoted* $\mu^*_{\gtrless 0}$, *and is explicitly given by* $(\mu^*_{\gtrless 0}u)(f)=u(|\det D\mu_{\gtrless 0}|^{-1}(f\circ\mu^{-1}_{\gtrless 0}))$.

Proof:

(i) Follows immediately from Theorem V.3.

(ii) By (iv) and (v) there is a commutative diagram

$$\begin{array}{ccc}
\mathcal{S}'(\mathbb{R}^n) & \xrightarrow{\nu^*_{\gtrless 0}} & \mathcal{S}'_{p^+\gtrless 0}(\mathbb{R}^n) \\
\uparrow{\scriptstyle incl} & & \uparrow{\scriptstyle incl} \\
\mathcal{S}(\mathbb{R}^n) & \xrightarrow{\nu^*_{\gtrless 0}} & \mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)
\end{array}$$

where the vertical arrows are inclusion mappings and the horizontal arrows are linear, sequentially continuous, bijective mappings whose inverses are also sequentially continuous. Since to any $u\in\mathcal{S}'(\mathbb{R}^n)$ there is a sequence in $\mathcal{S}(\mathbb{R}^n)$ converging to u,[11] the first part of (ii) follows from the above commutative diagram and the second part is then an easy consequence of (i) and Theorem V.3.

(iii) Is trivial.

(iv) Let $\nu := \nu_{>0}$ and $\mu := \nu^{-1}$. Then $|\det D\nu|^{-1} = (p^n/\omega(\mathbf{p})) + 1$ which can be written as $Q \circ \mu$ with some $Q \in \mathbb{C}[p^+, \mathbf{p}_\perp]_{p^+}$ by Lemma V.1(iii). The mapping $\mathcal{S}_{p^+>0}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$, $f \mapsto |\det D\nu|^{-1}(f \circ \nu^{-1}) = \mu^*(Qf)$ is well-defined and continuous by Theorem V.3(v) and remark V.4, and obviously linear. Hence the extension of ν^* to $\mathcal{S}'(\mathbb{R}^n)$ is well-defined. The linearity and sequential continuity are obvious.

(v) Let ν, μ as in (iii). By computing $|\det D\mu|^{-1}$ one sees that $Q := |\det D\mu|^{-1} \in \mathbb{C}[p^+, \mathbf{p}_\perp]_{p^+}$. As in (iii), it is enough to show that the mapping $\mathcal{S}(\mathbb{R}^n) \to \mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$, $f \mapsto |\det D\mu|^{-1}(f \circ \nu) = Q\nu^*(f)$ is well-defined, linear and continuous. But again this follows immediately from Theorem V.3(v) and remark V.4. □

We finish this section with some density results which we will use in the sequel. By $\mathcal{D}(U)$ we denote the function space of all smooth functions on $\mathbb{R}^n$ with support in an open subset $U \subset \mathbb{R}^n$, endowed with the usual topology,[17,11] i.e., $\mathcal{D}(U) = \lim_{\to K} \mathcal{D}_K$, where K runs through all compact subsets of U, and $\mathcal{D}_K$ is the space of all smooth functions with support in K endowed with the locally convex topology induced by the seminorms $\sup_{|\alpha| \leqslant l} \sup_{x \in K} |\partial^\alpha f(x)|$.

Proposition V.6:

(i) *$\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ is a dense subspace of $\mathcal{L}^2(\mathbb{R}^n, \Theta(\pm p^+) d^n\tilde{\mathbf{p}}/2|p^+|)$, and $\mathcal{S}_{p^+}(\mathbb{R}^n)$ is dense in $\mathcal{L}^2(\mathbb{R}^n, d^n\tilde{\mathbf{p}}/2|p^+|)$.*

(ii) *$\mathcal{D}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$ is dense in $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$, and $\mathcal{D}(\mathbb{R}^\times \times \mathbb{R}^{n-1})$ is dense in $\mathcal{S}_{p^+}(\mathbb{R}^n)$. Moreover, the corresponding inclusion mappings are continuous.*

(iii) *The linear subspace generated by the products $f(p^+)g(\mathbf{p}_\perp)$ where $f(p^+) \in \mathcal{S}_{p^+\gtrless 0}(\mathbb{R})$ and $g(\mathbf{p}_\perp) \in \mathcal{S}(\mathbb{R}^{n-1})$ is dense in $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$.*

(iv) *The same holds in (iii) if we replace $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ by $\mathcal{S}_{p^+}(\mathbb{R}^n)$.*

Proof:

(i) The mapping $\nu^*_{\gtrless 0}$ induces an isometric isomorphism from $\mathcal{L}^2(\mathbb{R}^n, d^n\mathbf{p}/2\omega(\mathbf{p}))$ onto $\mathcal{L}^2(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1}, d^n\tilde{\mathbf{p}}/2|p^+|)$ which maps the dense subspace $\mathcal{S}(\mathbb{R}^n)$ of $\mathcal{L}^2(\mathbb{R}^n, d^n\mathbf{p}/2\omega(\mathbf{p}))$ onto $\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$. Thus $\mathcal{S}_{p^+}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$ is a dense subspace of $\mathcal{L}^2(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1}, d^n\tilde{\mathbf{p}}/2|p^+|)$. Now apply the isometry j, i.e., trivial extension by zero. The second assertion follows then from Theorem V.3.

(ii) Because of Theorem V.3, the second assertion follows from the first. To show that $\mathcal{D}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$ is dense in $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ recall that $\mathcal{D}(\mathbb{R}^n)$ is dense in $\mathcal{S}(\mathbb{R}^n)$.[17,11] Hence, the image $\nu^*\mathcal{D}(\mathbb{R}^n) = \mathcal{D}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$ of $\mathcal{D}(\mathbb{R}^n)$ under the linear homeomorphism $\nu^*: \mathcal{S}(\mathbb{R}^n) \xrightarrow{\sim} \mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$, ($\nu := \nu_{\gtrless 0}$, see remark V.4) is a dense subspace of $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$. The continuity of the inclusion mappings is obvious since $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$ and $\mathcal{S}_{p^+}(\mathbb{R}^n)$ carry the subspace topology induced by $\mathcal{S}(\mathbb{R}^n)$.

(iii) It is well known, e.g. Ref. 11, that the linear subspace generated by the products $f(p^+)g(\mathbf{p}_\perp)$ with $f(p^+) \in \mathcal{D}(\mathbb{R}_{\gtrless 0})$ and $g(\mathbf{p}_\perp) \in \mathcal{D}(\mathbb{R}^{n-1})$ is dense in $\mathcal{D}(\mathbb{R}_{\gtrless 0} \times \mathbb{R}^{n-1})$. Hence, by (ii), it is also dense in $\mathcal{S}_{p^+\gtrless 0}(\mathbb{R}^n)$.

(iv) This follows from (iii) by Theorem V.3. □

VI. TIME-ZERO LC-FIELDS

A. Construction of the fields

After our preliminary work on squeezed distributions, it is now straightforward to define the time-zero LC-fields, i.e., the restriction of the real scalar massive LC-field $\tilde{\phi}_m$ to $\{x^+ = 0\}$ and the corresponding canonical conjugate momentum.

By the commutative diagram (20) we have seen that the function space $\nu^*(\mathcal{S}_3)$ ($\nu = \nu_{>0}$) is the adequate substitute for the space $\mathcal{S}_3 = \mathcal{S}(\mathbb{R}^3)$ if one wants to define the restriction of a real scalar free LC-field $\tilde{\phi}_m$ to the hyperplane $\{x^+ = 0\}$. Both spaces, $\mathcal{S}_3$ and $\nu^*\mathcal{S}_3$, appear completely symmetrically: $\mathcal{S}_3$ is determined by $\mathrm{res}_{\Gamma_m^+}(\mathcal{S}_4) = (\Omega_+^*)^{-1}(\mathcal{S}_3)$ and $\nu^*\mathcal{S}_3$ by $\mathrm{res}_{\tilde{\Gamma}_m^+}(\mathcal{S}_4) = (\tilde{\Omega}_+^*)^{-1}(\nu^*\mathcal{S}_3)$ where $\Omega_+ : \mathbb{R}^3 \to \Gamma_m^+$ and $\tilde{\Omega}_+ : \mathbb{R}_{>0} \times \mathbb{R}^2 \to \tilde{\Gamma}_m^+$ are the canonical parametrizations.

In the Minkowski case the time-zero field φ_m is defined by the formula $\varphi_m(g) := \phi_m(\delta(x^0) \otimes g(\mathbf{x})) = \phi_S(\alpha \cdot \mathrm{res}_{\Gamma_m^+}(1(p^0) \otimes \hat{g}(\mathbf{p})))$ if $g \in \mathcal{S}(\mathbb{R}^3)$ is real-valued, where $\hat{g}$ denotes the usual Fourier transform of g. We would like to define the time-zero LC-field $\tilde{\varphi}_m$ in the same way: $\tilde{\varphi}_m(g) := \tilde{\phi}_m(\delta(x^+) \otimes g(\tilde{x})) = \tilde{\phi}_S(\alpha \cdot \mathrm{res}_{\tilde{\Gamma}_m^+}(g^\sqcap(\tilde{\mathbf{p}}) \otimes 1(p^-)))$ if g is real valued, where $g^\sqcap$ denotes the partial $\mathbb{L}$-Fourier transform of g. In order that this definition makes sense, we first have to determine all g such that $\mathrm{res}_{\tilde{\Gamma}_m^+}(g^\sqcap(\tilde{\mathbf{p}}) \otimes 1(p^-)) \in \mathrm{res}_{\tilde{\Gamma}_m^+}(\mathcal{S}_4)$ which is equivalent to $\mathrm{res}_{p^+>0}(g^\sqcap) \in \nu^* \mathcal{S}_3$ since $\mathrm{res}_{\tilde{\Gamma}_m^+}(g^\sqcap(\tilde{\mathbf{p}}) \otimes 1(p^-)) = (\tilde{\Omega}_+^*)^{-1}(\mathrm{res}_{p^+>0}(g^\sqcap))$ and $\mathrm{res}_{\tilde{\Gamma}_m^+}(\mathcal{S}_4) = (\tilde{\Omega}_+^*)^{-1}(\nu^* \mathcal{S}_3)$. Unlike the classical Fourier transformation, which is a linear homeomorphism from $\mathcal{S}_3$ onto $\mathcal{S}_3$, the partial $\mathbb{L}$-Fourier transformation does not leave the space $\mathcal{S}_{p^+}(\mathbb{R}^3)$ invariant.

Proposition VI.1:

(i) *The partial $\mathbb{L}$-Fourier transformation $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}} \to \tilde{\mathbf{p}}}$ defined by*

$$(\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}} \to \tilde{\mathbf{p}}} g)(\tilde{\mathbf{p}}) = g^\sqcap(\tilde{\mathbf{p}}) = \int_{\mathbb{R}^n} d^n \tilde{\mathbf{x}} \; g(\tilde{\mathbf{x}}) e^{i(p^+ x^- - \mathbf{p}_\perp \cdot \mathbf{x}_\perp)} \quad (g \in \mathcal{S}(\mathbb{R}^n))$$

is a linear homeomorphism from $\mathcal{S}(\mathbb{R}^n)$ onto $\mathcal{S}(\mathbb{R}^n)$ which maps the subspace

$$\mathcal{S}_{\partial_{x^-}}(\mathbb{R}^n) := \bigcap_{m \geqslant 0} \partial_{x^-}^m \mathcal{S}(\mathbb{R}^n) = \{g : \forall m \geqslant 0 \;\; \exists h \in \mathcal{S}(\mathbb{R}^n) \quad g = \partial_{x^-}^m h\}$$

onto the subspace $\mathcal{S}_{p^+}(\mathbb{R}^n)$. We also write $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ instead of $\mathcal{S}_{\partial_{x^-}}(\mathbb{R}^n)$.

(ii) *Let*

$$\mathcal{S}_{\partial_-,r}(\mathbb{R}^n) := \{g \in \mathcal{S}_{\partial_-}(\mathbb{R}^n) : g \;\; \textit{real valued}\}.$$

Then $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}} \to \tilde{\mathbf{p}}}$ maps $\mathcal{S}_{\partial_-,r}(\mathbb{R}^n)$ onto $\{h \in \mathcal{S}_{p^+}(\mathbb{R}^n) : \overline{h} = h^\vee\}$.

Proof:

(i) The partial $\mathbb{L}$-Fourier transformation differs from the classical Fourier transformation only by a permutation and some sign changes of the coordinates, hence the first assertion follows immediately from the classical result.[17] To see the second assertion note that $\mathcal{S}_{p^+}(\mathbb{R}^3) = \cap_{m \geqslant 0} (p^+)^m \mathcal{S}(\mathbb{R}^3)$ by Theorem V.3, and that $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}} \to \tilde{\mathbf{p}}}$ maps $\partial_{x^-}^m \mathcal{S}(\mathbb{R}^n)$ onto $(p^+)^m \mathcal{S}(\mathbb{R}^n)$ for each $m \geqslant 0$.

(ii) Let $g \in \mathcal{S}_{\partial_-}(\mathbb{R}^n)$, then $\overline{g^\sqcap} = \overline{g}^{\sqcap\vee}$. Hence $\overline{g^\sqcap} = g^{\sqcap\vee}$ iff $g = \overline{g}$. □

We endow $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ with the subspace topology inherit from $\mathcal{S}(\mathbb{R}^n)$. Hence we have a linear homeomorphism

$$\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}} \to \tilde{\mathbf{p}}} : \mathcal{S}_{\partial_-}(\mathbb{R}^n) \tilde{\to} \mathcal{S}_{p^+}(\mathbb{R}^n), \quad g \mapsto g^\sqcap.$$

Furthermore,

$$\widetilde{\mathrm{res}}(\mathcal{S}(\mathbb{R}^4)) = \{\widetilde{\mathrm{res}}(g^\sqcap(\tilde{\mathbf{p}}) \otimes 1(p^-)) : g \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)\} \quad (\widetilde{\mathrm{res}} = \mathrm{res}_{\tilde{\Gamma}_m^+}), \tag{25}$$

which guarantees, among other things, that the operators $\tilde{\varphi}_m(g)$, $\tilde{\pi}_m(g)$ will be well-defined for each $g \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)$. Thus, $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ is the appropriate (smearing) test function space to define the time-zero LC-fields.

Definition: The *time-zero LC-field* (or the restriction of $\tilde{\phi}_m$ to $\{x^+ = 0\}$) $g \mapsto \tilde{\varphi}_m(g)$ and its canonical conjugate momentum $g \mapsto \tilde{\pi}_m(g)$ are defined by

$$\tilde{\varphi}_m(g) := \tilde{\phi}_m(0,g) := \tilde{\phi}_m(\delta(x^+) \otimes \mathrm{Re}\, g(\tilde{\mathbf{x}})) + i \tilde{\phi}_m(\delta(x^+) \otimes \mathrm{Im}\, g(\tilde{\mathbf{x}})),$$

$$\tilde{\pi}_m(g) := (\partial_{x^-} \tilde{\phi}_m)(0,g) = (\partial_{x^-} \tilde{\varphi}_m)(g) = \tilde{\varphi}_m(-\partial_{x^-} g),$$

where $g \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)$.

Remark VI.2: Note that $\partial_{x^-} \tilde{\phi}_m$ is a spatial derivative in contrast to the Minkowski case where the canonical momentum is defined by a time derivative. The difference results from the fact that

the Lagrangian $\tilde{\mathcal{L}}=(\partial^{\tilde{\mu}}\tilde{\phi}_m)(\partial_{\tilde{\mu}}\tilde{\phi}_m)-m^2\tilde{\phi}$ of the LC-Klein–Gordon field depends only linearly on $\partial_{x^+}\tilde{\phi}_m$, especially $\delta\tilde{\mathcal{L}}/[\,\delta(\partial_+\tilde{\phi}_m)]=2\partial_-\tilde{\phi}_m$, where $\partial_\pm=\partial_{x^\pm}$. Recall that in LC-physics the time variable is x^+.

The following theorem summarizes fundamental properties of the field $\tilde{\varphi}_m$ which follow easily from corresponding properties of the Segal quantization $\tilde{\phi}_S$, cf. Ref. 16, Theorem X.41.

Theorem VI.3:

(i) *For each real-valued $g\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$, the operator $\tilde{\varphi}_m(g)$ is essentially self-adjoint on $\tilde{F}_0$ ($\tilde{F}_0$=dense subspace of finite vectors of $\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)$, $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$).*

(ii) *The vacuum state $|\tilde{0}\rangle$ is a cyclic vector for the family $\{\tilde{\varphi}_m(g):g\in\mathcal{S}_{\partial_-}(\mathbb{R}^3),\ g$ real-valued$\}$.*

(iii) *If $g_n\to g$ in $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$, then*

$$\tilde{\varphi}_m(g_n)\psi\to\tilde{\varphi}_m(g)\psi,\quad \text{for all } \psi\in\tilde{F}_0$$

and

$$e^{i\tilde{\varphi}_m(g_n)}\psi\to e^{i\tilde{\varphi}_m(g)}\psi,\quad \text{for all } \psi\in\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m).$$

(iv) *If $g,h\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ are real-valued and $\psi\in\tilde{F}_0$, then*

$$\tilde{\varphi}_m(g)\tilde{\varphi}_m(h)\psi-\tilde{\varphi}_m(h)\tilde{\varphi}_m(g)\psi=\frac{1}{(2\pi)^3}(\langle g,h\rangle_{\mathcal{S}_{\partial_-}(\mathbb{R}^3)}-\langle h,g\rangle_{\mathcal{S}_{\partial_-}(\mathbb{R}^3)})\psi$$

and

$$e^{i\tilde{\varphi}_m(g)}e^{i\tilde{\varphi}_m(h)}=e^{(2\pi)^{-3}(\langle g,h\rangle_{\mathcal{S}_{\partial_-}(\mathbb{R}^3)}-\langle h,g\rangle_{\mathcal{S}_{\partial_-}(\mathbb{R}^3)})}e^{i\tilde{\varphi}_m(h)}e^{i\tilde{\varphi}_m(g)},$$

where $\langle g,h\rangle_{\mathcal{S}_{\partial_-}(\mathbb{R}^3)}:=\int d^3\tilde{\mathbf{p}}(\Theta(p^+)/2p^+)\overline{g^\sqcap}h^\sqcap$ $(g,h\in\mathcal{S}_{\partial_-}(\mathbb{R}^3))$ and the bar "—" means complex conjugation.

Proof: (i)–(iv) follow immediately from Ref. 16, Theorem X.41. Notice that, if $g\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ is real-valued then $\tilde{\varphi}_m(g)=\tilde{\phi}_S(\alpha\cdot\widetilde{\mathrm{res}}(g^\sqcap(\tilde{\mathbf{p}})\otimes 1(p^-)))$ and that, by (25), $\{\widetilde{\mathrm{res}}(g^\sqcap(\tilde{\mathbf{p}})\otimes 1(p^-)):g\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)\}$ is a dense subspace of $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$. □

B. Commutator relation

In order to see that we have really defined the proper time-zero LC-field, we compute the commutator of this field. At this it turns out that our result coincides with the commutator relation determined by a completely different method, namely quantization of constrained systems.[6]

Lemma VI.4: The linear subspace generated by the products $g(\mathbf{x}_\perp)h(x^-)$, where $g(\mathbf{x}_\perp)\in\mathcal{S}(\mathbb{R}^{n-1})$ and $h(x^-)\in\mathcal{S}_{\partial_-}(\mathbb{R})$ is dense in $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$.

Proof: Recall that the partial $\mathbb{L}$-Fourier transformation $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}}\to\tilde{\mathbf{p}}}$ is a linear homeomorphism from $\mathcal{S}_{\partial_-}(\mathbb{R}^n)$ onto $\mathcal{S}_{p^+}(\mathbb{R}^n)$. Moreover, $\mathcal{F}_{\mathbb{L}}^{\tilde{\mathbf{x}}\to\tilde{\mathbf{p}}}$ maps the set of products $g(\mathbf{x}_\perp)h(x^-)$ where $g(\mathbf{x}_\perp)\in\mathcal{S}(\mathbb{R}^{n-1})$, $h(x^-)\in\mathcal{S}_{\partial_{x^-}}(\mathbb{R})$ onto the set of products $h(p^+)g(\mathbf{p}_\perp)$ where $h(p^+)\in\mathcal{S}_{p^+}(\mathbb{R})$, $g(\mathbf{p}_\perp)\in\mathcal{S}(\mathbb{R}^{n-1})$. The assertion follows now from Proposition V.6. □

Proposition VI.5: The time-zero LC-field $\tilde{\varphi}_m$ fulfills the following commutator relation on the dense subspace $\tilde{F}_0$:

$$[\tilde{\varphi}_m(g),\tilde{\varphi}_m(h)]=\frac{1}{4i}(\delta(\mathbf{x}_\perp-\mathbf{y}_\perp)\otimes\epsilon(x^--y^-),g(\tilde{\mathbf{x}})\otimes h(\tilde{\mathbf{y}})),$$

with real-valued $g,h\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$.

Proof: By Theorem VI.3(iv) we have to show that

$$\frac{1}{(2\pi)^3}\int d^3\tilde{\mathbf{p}}\frac{\Theta(p^+)}{2p^+}(\overline{g^\sqcap}h^\sqcap - g^\sqcap\overline{h^\sqcap}) = \frac{1}{4i}(\delta(\mathbf{x}_\perp-\mathbf{y}_\perp)\otimes\epsilon(x^- - y^-), g\otimes h)$$

for all real-valued $g,h\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$. We know that $\delta(\mathbf{x}_\perp-\mathbf{y}_\perp)\otimes\epsilon(x^- - y^-) = \sigma^*(\delta(\mathbf{z}_\perp)\otimes\epsilon(z^-))$ is a tempered distribution on $\mathbb{R}^3\times\mathbb{R}^3$ which is defined as the pullback of $\delta(\mathbf{z}_\perp)\otimes\epsilon(z^-)$ by the mapping $\sigma:\mathbb{R}^3\times\mathbb{R}^3\to\mathbb{R}^3$, $(\tilde{\mathbf{x}},\tilde{\mathbf{y}})\mapsto\tilde{\mathbf{z}}:=\tilde{\mathbf{x}}-\tilde{\mathbf{y}}$. As a first step we prove

$$\begin{aligned}\frac{1}{4i}(\delta(\mathbf{z}_\perp)\otimes\epsilon(z^-), f(\tilde{\mathbf{z}})) &= \frac{1}{(2\pi)^3}\int d^3\tilde{\mathbf{p}}\frac{\Theta(p^+)}{2p^+}(f^\sqcap(-p^+,\mathbf{p}_\perp) - f^\sqcap(p^+,\mathbf{p}_\perp))\\ &= \frac{1}{(2\pi)^3}\int d^3\tilde{\mathbf{p}}\frac{\Theta(p^+)}{2p^+}(f^\sqcap(-\tilde{\mathbf{p}}) - f^\sqcap(\tilde{\mathbf{p}}))\end{aligned} \tag{26}$$

for all $f(\tilde{\mathbf{z}})\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$. By Lemma VI.4 it is enough to show (26) if $f(\tilde{\mathbf{z}})$ is of the form $f(\tilde{\mathbf{z}}) = f_-(z^-)f_\perp(\mathbf{z}_\perp)$ with $f_-(z^-)\in\mathcal{S}_{\partial_-}(\mathbb{R})$ and $f_\perp(\mathbf{z}_\perp)\in\mathcal{S}(\mathbb{R}^2)$. Then

$$f^\sqcap(-p^+,\mathbf{p}_\perp) - f^\sqcap(p^+,\mathbf{p}_\perp) = \widehat{f_\perp}(\mathbf{p}_\perp)(\widehat{f_-}(p^+) - \widehat{f_-}(-p^+)),$$

where the "^" means classical Fourier transformation. Hence, the right-hand side of (26) equals, except for the factor $1/2(2\pi)^3$, the product

$$\left(\int d^2\mathbf{p}_\perp\ \widehat{f_\perp}(\mathbf{p}_\perp)\right)\cdot\left(\int dp^+\frac{\Theta(p^+)}{p^+}(\widehat{f_-}(p^+) - \widehat{f_-}(-p^+))\right). \tag{27}$$

Obviously, the first factor of (27) equals $(2\pi)^2(\delta(\mathbf{x}_\perp), f_\perp(\mathbf{x}_\perp))$. To determine the second factor, note that for all $h(p^+)\in\mathcal{S}_{p^+}(\mathbb{R})$

$$\left(\mathrm{PV}\frac{1}{p^+}, h(p^+)\right) = \int dp^+\frac{\Theta(p^+)}{p^+}(h(p^+) - h(-p^+))$$

since $(1/p^+)\,h(p^+)\in\mathcal{L}^1(\mathbb{R},dp^+)$. Hence, the second factor of (27) equals $(\mathrm{PV}(1/p^+), \widehat{f_-}(p^+))$. Finally, $(\mathrm{PV}(1/p^+))^\wedge = (\pi/i)\,\epsilon(x^-)$ which follows, for example, by the Sokhotsky–Plemelj-formulas,[3] p. 55. Thus we have shown (26). Using the explicit formula of the pullback

$$(\delta(\mathbf{x}_\perp-\mathbf{y}_\perp)\otimes\epsilon(x^- - y^-), g(\tilde{\mathbf{x}})\otimes h(\tilde{\mathbf{y}})) = (\delta(\mathbf{z}_\perp)\otimes\epsilon(z^-), (g*h^\vee)(\tilde{\mathbf{z}})),$$

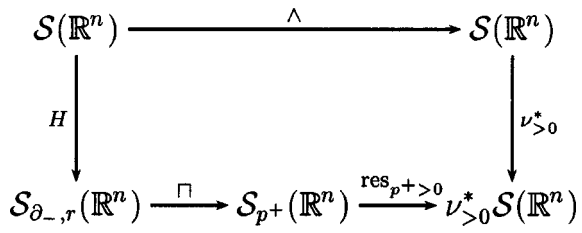
where $g*h^\vee$ denotes the convolution of g and $h^\vee$ (recall $h^\vee(\tilde{\mathbf{y}}) = h(-\tilde{\mathbf{y}})$), we yield the right formula, if we additionally take into account that $(g*h^\vee)^\sqcap = g^\sqcap h^{\vee\sqcap}$ and $h^{\vee\sqcap} = \overline{h^\sqcap} = (h^\sqcap)^\vee$ for real-valued g,h. □

C. Connection between time-zero field and time-zero LC-field

In this short subsection we will prove a transformation law between the time-zero field φ_m and the time-zero LC-field $\tilde{\varphi}_m$. By this transformation law φ_m is completely determined by $\tilde{\varphi}_m$. This shows that the time-zero LC-field, defined on the test function space $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$, carries—besides the mass—as much information as the time-zero field, defined on $\mathcal{S}(\mathbb{R}^3)$, although $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ is a proper subspace of $\mathcal{S}(\mathbb{R}^3)$. Furthermore, it is possible to recover the covariant field from the time-zero LC-field.

Let $\mathcal{S}_{\partial_-,r}(\mathbb{R}^n)$ denote the real topological (closed) subspace of all real-valued $g\in\mathcal{S}_{\partial_-}(\mathbb{R}^n)$. We need the following auxiliary lemma.

Lemma VI.6: There exists an $\mathbb{R}$*-linear homeomorphism* $H:\mathcal{S}(\mathbb{R}^n)\xrightarrow{\sim}\mathcal{S}_{\partial_-,r}(\mathbb{R}^n)$ *such that the following diagram commutes*:



Proof: Since the classical Fourier transformation "$\wedge$" and the mapping $\nu^*_{>0}$ are linear homeomorphism, we have to show that the composition $\mathrm{res}_{p^+>0} \circ \sqcap$ is bijective. Then, by the open mapping theorem, the inverse is continuous, too. By Proposition VI.1(ii) $\mathcal{F}_{\mathrm{L}}^{\tilde{\mathbf{x}}\to\tilde{\mathbf{p}}}$ maps $\mathcal{S}_{\partial_-,r}(\mathbb{R}^n)$ onto $\{g\in\mathcal{S}_{p^+}(\mathbb{R}^n): \overline{g}=g^\vee\}$. However, $\underline{\mathrm{res}}_{p^+>0}$ is one-to-one on this subspace. An inverse mapping is explicitly given by $g\mapsto j(g)^\vee + j(g)$ $(g\in\nu^*_{>0}\mathcal{S}(\mathbb{R}^n))$, where j denotes extension by zero. □

Recall that $\kappa_*:\mathfrak{H}_m\to\tilde{\mathfrak{H}}_m$ is a unitary operator between the relativistic one-particle spaces $\mathfrak{H}_m=\mathcal{L}^2(\Gamma_m^+,d\mu_m)$, $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$, and induces a unitary operator $\mathcal{F}_\vee(\kappa_*):\mathcal{F}_\vee(\mathfrak{H}_m)\to\mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)$ between the corresponding bosonic Fock spaces. The following theorem gives us a surprising transformation law between the time-zero field and the time-zero LC-field.

Theorem VI.7: *For each real-valued $g\in\mathcal{S}(\mathbb{R}^3)$, the following transformation laws hold*:

$$\varphi_m(g)=\mathcal{F}_\vee(\kappa_*)^{-1}\tilde{\varphi}_m(Hg)\mathcal{F}_\vee(\kappa_*),\quad \pi_m(g)=\mathcal{F}_\vee(\kappa_*)^{-1}\tilde{\varphi}_m(H\mathcal{F}^{-1}(\omega(\mathbf{p})\hat{g}))\mathcal{F}_\vee(\kappa_*),$$

where $H:\mathcal{S}(\mathbb{R}^3)\tilde{\to}\mathcal{S}_{\partial_-,r}(\mathbb{R}^3)$ is the $\mathbb{R}$-linear homeomorphism from Lemma VI.6 and $\mathcal{F}^{-1}$ denotes the classical inverse Fourier transformation.

Proof: Since g is real-valued, $\varphi_m(g)=\phi_S(\alpha\cdot\mathrm{res}(1\otimes\hat{g}))$. On the other hand, $\tilde{\varphi}_m(Hg)=\tilde{\phi}_S(\alpha\cdot\widetilde{\mathrm{res}}((Hg)^\sqcap\otimes 1))$ since Hg is real-valued, too. By inspecting the construction of the Segal quantization, we obtain the following transformation law between ϕ_S and $\tilde{\phi}_S$:

$$\phi_S(f)=\mathcal{F}_\vee(\kappa_*)^{-1}\tilde{\phi}_S(\kappa_* f)\mathcal{F}_\vee(\kappa_*)\quad (f\in\mathfrak{H}_m).$$

Hence, it is enough to show that $\kappa_*\mathrm{res}(1\otimes\hat{g})=\widetilde{\mathrm{res}}((Hg)^\sqcap\otimes 1)$. But this follows easily from the definition of H, i.e., from $\nu^*\hat{g}=(Hg)^\sqcap$, if one takes into account that $\mathrm{res}(1\otimes\hat{g})=(\Omega_+^*)^{-1}(\hat{g})$, $\widetilde{\mathrm{res}}((Hg)^\sqcap\otimes 1)=(\tilde{\Omega}_+^*)^{-1}((Hg)^\sqcap|_{p^+>0})$ and $\kappa_*\circ(\Omega_+^*)^{-1}=(\tilde{\Omega}_+^*)^{-1}\circ\nu^*$. Analogously, one proves the transformation law for the canonical conjugate momentum $\pi_m(g)$. □

Remark VI.8: Let $T:=\{Hg: g\in\mathcal{S}(\mathbb{R}^3),\ \text{real-valued}\}$. Then T is a proper $\mathbb{R}$-linear subspace of $\mathcal{S}_{\partial_-,r}(\mathbb{R}^3)$ by Lemma VI.6. Hence, $T+iT$ is a proper $\mathbb{C}$-linear subspace of $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$. By Theorem VI.7 $\{\tilde{\varphi}_m(h): h\in T+iT\}$ is a commuting family, i.e., the commutator $[\tilde{\varphi}_m(g),\tilde{\varphi}_m(h)]$ vanishes on $\tilde{F}_0$ for all $g,h\in T+iT$. We do not have, however, any physical explanation for this, yet.

Remark VI.9: Since in Theorem VI.7 even the canonical conjugate momentum π_m can be recovered from the time-zero LC-field $\tilde{\varphi}_m$ we see again that the canonical conjugate momentum of $\tilde{\varphi}_m$ is superfluous in LC-physics.

D. Unitary equivalence

In Ref. 13, Leutwyler *et al.* discovered the remarkable fact that the restrictions of free fields of different masses to the plane $\{x^+=\tau\}$ are unitary equivalent. We prove in this subsection an even stronger statement, namely that under a specified unitary transformation the field operators of different masses become identical.

In Sec. II we have introduced the smooth mapping $\tilde{\Omega}_+:\mathbb{R}_{>0}\times\mathbb{R}^2\to\tilde{\Gamma}_m^+$. To emphasize the mass-dependence we write $\tilde{\Omega}_{+,m}$ in the following. This mapping induces a unitary mapping $\tilde{\Omega}_{+,m}^*:\tilde{\mathfrak{H}}_m\to\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^2,d^3\tilde{\mathbf{p}}/2p^+)$, where $\tilde{\mathfrak{H}}_m=\mathcal{L}^2(\tilde{\Gamma}_m^+,d\tilde{\mu}_m)$ is the relativistic one-particle LC-space introduced in Sec. IV. We call $\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^2,d^3\tilde{\mathbf{p}}/2p^+)=:\tilde{\mathfrak{H}}_{\mathrm{nr}}$ the *nonrelativistic one-*

particle LC-space. Notice that $\tilde{\mathfrak{H}}_{\mathrm{nr}}$ does not depend on the mass m which is a special property of LC-physics and which has the following proposition as a consequence. Recall that furthermore $\tilde{\Omega}^*_{+,m}$ induces a unitary mapping $\mathcal{F}_\vee(\tilde{\Omega}^*_{+,m}):\tilde{\mathcal{H}}_m \to \tilde{\mathcal{H}}_{\mathrm{nr}}$ between the corresponding (bosonic) Fock-spaces $\tilde{\mathcal{H}}_m = \mathcal{F}_\vee(\tilde{\mathfrak{H}}_m)$ and $\tilde{\mathcal{H}}_{\mathrm{nr}} = \mathcal{F}_\vee(\tilde{\mathfrak{H}}_{\mathrm{nr}})$.

Proposition VI.10: Let $\tilde{\varphi}_{m_1}$ and $\tilde{\varphi}_{m_2}$ be time-zero LC-fields with $m_1, m_2 > 0$ and let $U_i = \mathcal{F}_\vee(\tilde{\Omega}^*_{+,m_i}):\tilde{\mathcal{H}}_{m_i} \to \tilde{\mathcal{H}}_{\mathrm{nr}}$ $(i=1,2)$ be the above unitary mappings from the relativistic to the non-relativistic Fock space. Then

$$U_1 \tilde{\varphi}_{m_1}(h) U_1^{-1} = U_2 \tilde{\varphi}_{m_2}(h) U_2^{-1}$$

for all $h \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)$.

Proof: It is enough to prove the assertion for all real-valued $h \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)$. Let $m>0$ and let $\tilde{\phi}_S$ be the Segal quantization over $\tilde{\mathfrak{H}}_m$. Then $\tilde{\varphi}_m(h) = \tilde{\phi}_S(\alpha \cdot \widetilde{\mathrm{res}}(h^\sqcap \otimes 1))$. By definition $\tilde{\phi}_S(f) = (1/\sqrt{2})\,(\tilde{a}^*(f) + \tilde{a}(f))$ where $f \in \tilde{\mathfrak{H}}_m$. Let $U := \mathcal{F}_\vee(\tilde{\Omega}^*_{+,m}):\tilde{\mathcal{H}}_m \to \tilde{\mathcal{H}}_{\mathrm{nr}}$. Because $\widetilde{\mathrm{res}}(g \otimes 1) = (\tilde{\Omega}^*_{+,m})^{-1}(g|_{p^+>0})$, we obtain

$$U\tilde{a}^*(\widetilde{\mathrm{res}}(g\otimes 1))U^{-1}(\psi_1 \vee \cdots \vee \psi_n) = \sqrt{n+1}\,(g|_{p^+>0} \vee \psi_1 \vee \cdots \vee \psi_n),$$

$$U\tilde{a}(\widetilde{\mathrm{res}}g \otimes 1))U^{-1}(\psi_1 \vee \cdots \vee \psi_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \langle g, \psi_j \rangle_{\tilde{\mathfrak{H}}_{\mathrm{nr}}} (\psi_1 \vee \cdots \vee \widehat{\psi_j} \vee \cdots \vee \psi_n)$$

for all $\psi_1 \vee \cdots \vee \psi_n \in \tilde{\mathfrak{H}}_{\mathrm{nr}}^{\vee n}$ and $g \in \mathcal{S}_{p^+}(\mathbb{R}^3)$. Since $\langle g, \psi_j \rangle_{\tilde{\mathfrak{H}}_{\mathrm{nr}}} = \int_{p^+>0} (d^3\tilde{\mathbf{p}}/2p^+)\overline{g}\psi_j$ does not depend on the mass $m>0$, the same holds for $U\tilde{\varphi}_m(h)U^{-1}$, where $h \in \mathcal{S}_{\partial_-,r}(\mathbb{R}^3)$. □

Remark VI.11: It is well known (cf., e.g., Ref. 16) that unitary equivalence fails, if we consider the restrictions of free fields of different masses $m_1 \neq m_2$ to the plane $\{x^0=0\}$, i.e., time-zero fields φ_{m_1}, φ_{m_2}. The difference to the LC-case lies in the fact that the unitary mapping $\Omega^*_{+,m}$ induced by $\Omega_{+,m}:\mathbb{R}^3 \xrightarrow{\sim} \Gamma^+_m$ maps the relativistic one-particle space $\mathcal{L}^2(\Gamma^+_m, d\mu_m)$ onto the mass-dependent space $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}/2\omega_m(\mathbf{p}))$; note that $\omega_m(\mathbf{p}) = \sqrt{\mathbf{p}^2+m^2}$. It is indeed possible to obtain a mass-independent Hilbert space by the unitary mapping $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}/2\omega_m(\mathbf{p})) \to \mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p})$, $g(\mathbf{p}) \mapsto g(\mathbf{p})/\sqrt{\omega}_m(\mathbf{p})$, however, this does not solve the problem. If $U_m = \mathcal{F}_\vee((1/\sqrt{\omega_m})\,\Omega^*_{+,m}):\mathcal{F}_\vee(\mathcal{L}^2(\tilde{\Gamma}^+_m, d\mu_m)) \to \mathcal{F}_\vee(\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}))$ then only

$$U_{m_1}\varphi_{m_1}(F_{m_1}g)U_{m_1}^{-1} = U_{m_2}\varphi_{m_2}(F_{m_2}g)U_{m_2}^{-1}$$

holds for every $g \in \mathcal{S}(\mathbb{R}^3)$, where $F_m:\mathcal{S}(\mathbb{R}^3) \xrightarrow{\sim} \mathcal{S}(\mathbb{R}^3)$ is the linear homeomorphism defined by $(F_m g)\hat{} = (1/\sqrt{\omega_m})\hat{g}$. Notice that $g \mapsto \sqrt{\omega_m}g$ is a linear homeomorphism from $\mathcal{S}(\mathbb{R}^3)$ onto $\mathcal{S}(\mathbb{R}^3)$. Hence, the fields φ_{m_1} and φ_{m_2} are "unitary equivalent modulo a linear homeomorphism" from $\mathcal{S}_3$ onto $\mathcal{S}_3$ which we call *weakly unitary equivalence*. So in both, the LC-case and the Minkowski-case, we have weakly unitary equivalence, whereas only in the LC-case weakly unitary equivalence equals unitary equivalence.

E. Completeness

Irreducibility of the time-zero LC-field was already obtained by Leutwyler *et al.* in Ref. 13. Since our function space $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ is even a proper subspace of the function space in Ref. 13, we have to reprove the irreducibility statement.

Proposition VI.12: The family of operators $\{e^{i\tilde{\varphi}_m(h)}: h \in \mathcal{S}_{\partial_-,r}(\mathbb{R}^3)\}$ is irreducible.

Proof: Let $\tilde{\phi}_S$ be the Segal quantization over $\tilde{\mathfrak{H}}_m = \mathcal{L}^2(\tilde{\Gamma}^+_m, d\tilde{\mu}_m)$. By Ref. 16, Lemma 1, p. 232, the family $\{e^{i\tilde{\phi}_S(f)}: f \in \tilde{\mathfrak{H}}_m\}$ is irreducible. For each real-valued $h \in \mathcal{S}_{\partial_-}(\mathbb{R}^3)$, we have

$\tilde{\varphi}_m(h)=\tilde{\phi}_S(\alpha\cdot\widetilde{\mathrm{res}}(h^{\sqcap}\otimes 1))$. By (25), $\{\widetilde{\mathrm{res}}(g^{\sqcap}\otimes 1): g\in\mathcal{S}_{\partial\_}(\mathbb{R}^3)\}$ is dense in $\tilde{\mathfrak{H}}_m$. Now, for each $g\in\mathcal{S}_{\partial\_}(\mathbb{R}^3)$, there exists, by Lemma VI.6, a real-valued $h\in\mathcal{S}_{\partial\_}(\mathbb{R}^3)$ such that $h^{\sqcap}|_{p^+>0}=g^{\sqcap}|_{p^+>0}$. Hence $\{\widetilde{\mathrm{res}}(h^{\sqcap}\otimes 1): h\in\mathcal{S}_{\partial\_,r}(\mathbb{R}^3)\}$ is dense in $\tilde{\mathfrak{H}}_m$, too. □

VII. ANNIHILATION AND CREATION OPERATORS, BILINEAR FORMS

In this final section we produce a closer connection to the standard terminology of LC-quantum field theory. Especially, we want to give expressions like (7) an exact meaning in the operator context. This is well known in Minkowski-case, e.g., Ref. 16, and we will use the same approach in the LC-case. First of all we have to transform our fields to fields acting on the nonrelativistic LC-Fock space $\tilde{\mathcal{H}}_{\mathrm{nr}}=\mathcal{F}_{\vee}(\tilde{\mathfrak{H}}_{\mathrm{nr}})$, where $\tilde{\mathfrak{H}}_{\mathrm{nr}}=\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^2, d^3\tilde{\mathbf{p}}/2p^+)$.

Let $U:=\mathcal{F}_{\vee}(\tilde{\Omega}^*_{+,m}):\tilde{\mathcal{H}}_m\to\tilde{\mathcal{H}}_{\mathrm{nr}}$ be the canonical, unitary mapping from the relativistic LC-Fock space $\tilde{\mathcal{H}}_m:=\mathcal{F}_{\vee}(\mathcal{L}^2(\tilde{\Gamma}^+_m, d\tilde{\mu}_m))$ to the nonrelativistic LC-Fock space $\tilde{\mathcal{H}}_{\mathrm{nr}}$. We transform the fields $\tilde{\phi}_m$ and $\tilde{\varphi}_m$ by the formulas

$$\tilde{\boldsymbol{\phi}}_m:=U\tilde{\phi}_m U^{-1},\quad \tilde{\boldsymbol{\varphi}}_m:=U\tilde{\varphi}_m U^{-1}.$$

Because of Proposition VI.10, $\tilde{\boldsymbol{\varphi}}_m$ does not depend on the mass $m>0$. Hence, we cancel the index m in the notation and write in the following $\tilde{\boldsymbol{\varphi}}$ instead of $\tilde{\boldsymbol{\varphi}}_m$. We also transform the annihilation and creation operators by

$$\tilde{\mathbf{a}}(g):=U\tilde{a}(\widetilde{\mathrm{res}}(g(\tilde{\mathbf{p}})\otimes 1(p^-)))U^{-1},\quad \tilde{\mathbf{a}}^+(g):=U\tilde{a}^+(\widetilde{\mathrm{res}}(g(\tilde{\mathbf{p}})\otimes 1(p^-)))U^{-1}$$

for every $g(\tilde{\mathbf{p}})\in\mathcal{S}_{p^+}(\mathbb{R}^3)$. The explicit action on $\tilde{\mathfrak{H}}^{\vee n}_{\mathrm{nr}}$ is given by

$$(\tilde{\mathbf{a}}^+(g)\psi)(\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_{n+1})=\frac{1}{\sqrt{n+1}}\sum_{j=1}^{n+1} g(\tilde{\mathbf{p}}_j)\psi(\tilde{\mathbf{p}}_1,\ldots,\widehat{\tilde{\mathbf{p}}_j},\ldots,\tilde{\mathbf{p}}_{n+1}),$$

$$(\tilde{\mathbf{a}}(g)\psi)(\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_{n-1})=\sqrt{n}\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}\overline{g}(\tilde{\mathbf{p}})\psi(\tilde{\mathbf{p}},\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_{n-1}),$$

where $\psi(\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_n)\in\tilde{\mathfrak{H}}^{\vee n}_{\mathrm{nr}}$ and $g\in\mathcal{S}_{p^+}(\mathbb{R}^3)$. Notice that $\tilde{\mathbf{a}}^+(g)$ is the adjoint of $\tilde{\mathbf{a}}(g)$. The fields $\tilde{\boldsymbol{\phi}}_m$ and $\tilde{\boldsymbol{\varphi}}$ can be written in terms of $\tilde{\mathbf{a}}^+$ and $\tilde{\mathbf{a}}$ as

$$\tilde{\boldsymbol{\phi}}_m(f)=\frac{\alpha}{\sqrt{2}}(\tilde{\mathbf{a}}^+(\tilde{\Omega}^*_+(f^{\wedge\mathrm{L}}))+\tilde{\mathbf{a}}(\tilde{\Omega}^*_+(f^{\wedge\mathrm{L}})))\quad (f\in\mathcal{S}(\mathbb{R}^4),\ \text{real-valued}),$$

$$\tilde{\boldsymbol{\varphi}}(g)=\frac{\alpha}{\sqrt{2}}(\tilde{\mathbf{a}}^+(g^{\sqcap})+\tilde{\mathbf{a}}(g^{\sqcap}))\quad (g\in\mathcal{S}_{\partial\_}(\mathbb{R}^3),\ \text{real-valued}).$$

Notice that, for each $f\in\mathcal{S}(\mathbb{R}^4)$, (the trivial extension by zero of) $\tilde{\Omega}^*_+(f)$ is in $\mathcal{S}_{p^+>0}(\mathbb{R}^3)$.

Recall that we often do not distinguish between functions on $\mathbb{R}_{>0}\times\mathbb{R}^{n-1}$ and there trivial extensions by zero to $\mathbb{R}^n$. In according this, recall that $\nu^*_{>0}\mathcal{S}_n=\mathcal{S}_{p^+>0}(\mathbb{R}^n)$ is dense in $\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^{n-1}, d^n\tilde{\mathbf{p}}/2p^+)=\mathcal{L}^2(\mathbb{R}^n,(\Theta(p^+)/2p^+)\,d^n\tilde{\mathbf{p}})$ by Proposition V.6. As in the relativistic case, we define $\tilde{F}_0$ as the dense subspace of all finite vectors of $\tilde{\mathcal{H}}_{\mathrm{nr}}=\mathcal{F}_{\vee}(\tilde{\mathfrak{H}}_{\mathrm{nr}})$. Let

$$\tilde{D}_0:=\{\psi=(\psi_n)_{n\geqslant 0}\in\tilde{F}_0:\psi_n\in\mathcal{S}_{p^+>0}(\mathbb{R}^{3n})\},$$

which is a dense subspace of $\tilde{\mathcal{H}}_{\mathrm{nr}}$. For each $\tilde{\mathbf{p}}\in\mathbb{R}^3$, we define an operator $\tilde{\mathbf{a}}(\tilde{\mathbf{p}}):\tilde{D}_0\to\tilde{D}_0$ by

$$(\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\psi)_n(\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_n):=\sqrt{n+1}\,\psi_{n+1}(\tilde{\mathbf{p}},\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_n)\quad (n\geqslant 0),\tag{28}$$

where $\psi=(\psi_n)_{n\geqslant 0}\in\tilde{D}_0$. Notice that $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})=0$ whenever $p^+\leqslant 0$. As in the Minkowski-case, the adjoint of $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})$ is not densely defined, however, the adjoint $\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})$ exists as bilinear form on $\tilde{D}_0\times\tilde{D}_0$, and is defined by

$$\langle\chi,\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})\psi\rangle:=\langle\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\chi,\psi\rangle\quad(\chi,\psi\in\tilde{D}_0).\tag{29}$$

Again, $\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})=0$ whenever $p^+\leqslant 0$. Notice that the brackets on the right-hand side of (29) denote the scalar product of the Fock space $\tilde{\mathcal{H}}_{\mathrm{nr}}$, whereas those on the left-hand side have to be seen only symbolically. One can easily check that

$$\tilde{\mathbf{a}}(g)=\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\overline{g}(\tilde{\mathbf{p}})\quad\text{and}\quad\tilde{\mathbf{a}}^+(g)=\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})g(\tilde{\mathbf{p}})$$

for every $g\in\mathcal{S}_{p^+}(\mathbb{R}^3)$ in the sense of integration[24] of bilinear forms. By construction, for every χ, $\psi\in\tilde{\mathcal{H}}_{\mathrm{nr}}$, the functions

$$\mathbb{R}^3\rightrightarrows\mathbb{C},\quad\tilde{\mathbf{p}}\mapsto\langle\chi,\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\psi\rangle,\quad\tilde{\mathbf{p}}\mapsto\langle\chi,\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})\psi\rangle$$

are in $\mathcal{S}_{p^+>0}(\mathbb{R}^3)$. Hence, it is possible to define bilinear forms $\tilde{\boldsymbol{\phi}}_m(\tilde{x})$ and $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})$ ($\tilde{x}\in\mathbb{R}^4$, $\tilde{\mathbf{x}}\in\mathbb{R}^3$) on $\tilde{D}_0\times\tilde{D}_0$ in the following way:

$$\tilde{\boldsymbol{\phi}}_m(\tilde{x}):=\frac{1}{(2\pi)^{3/2}}\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}(\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})\,e^{i\langle\tilde{\Omega}_+(\tilde{\mathbf{p}}),\tilde{x}\rangle_{\mathrm{L}}}+\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\,e^{-i\langle\tilde{\Omega}_+(\tilde{\mathbf{p}}),\tilde{x}\rangle_{\mathrm{L}}}),$$

$$\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}}):=\frac{1}{(2\pi)^{3/2}}\int_{p^+>0}\frac{d^3\tilde{\mathbf{p}}}{2p^+}(\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})\,e^{i(p^+x^-\,-\,\mathbf{p}_\perp\cdot\mathbf{x}_\perp)}+\tilde{\mathbf{a}}(\tilde{\mathbf{p}})\,e^{-i(p^+x^-\,-\,\mathbf{p}_\perp\cdot\mathbf{x}_\perp)}).$$

Again one easily checks that in the sense of integration of bilinear forms

$$\tilde{\boldsymbol{\phi}}_m(f)=\int d^4\tilde{x}\,\tilde{\boldsymbol{\phi}}_m(\tilde{x})f(\tilde{x}),\quad\tilde{\varphi}(h)=\int d^3\tilde{\mathbf{x}}\,\tilde{\varphi}(\tilde{\mathbf{x}})h(\tilde{\mathbf{x}})$$

for every $f\in\mathcal{S}(\mathbb{R}^4)$, $h\in\mathcal{S}_{\partial_-}(\mathbb{R}^3)$.

By the same approach, however, with $U:=\mathcal{F}_{\vee}(\Omega_+^*):\mathcal{H}_m\to\mathcal{H}_{\mathrm{nr}}$ instead of $\mathcal{F}_{\vee}(\tilde{\Omega}_+^*)$, where $\mathcal{H}_{\mathrm{nr}}=\mathcal{F}_{\vee}(\mathcal{L}^2(\mathbb{R}^3,d^3\mathbf{p}/2\omega(\mathbf{p})))$, one gets analogous formulas for the transformed free field $\boldsymbol{\phi}_m=U\phi_mU^{-1}$ and the transformed time-zero fields $\boldsymbol{\varphi}_m=U\varphi_mU^{-1}$, $\boldsymbol{\pi}_m=U\pi_mU^{-1}$:

$$\boldsymbol{\phi}_m(x):=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}(\mathbf{a}^+(\mathbf{p})\,e^{i\langle\Omega_+(\mathbf{p}),x\rangle_{\mathbb{M}}}+\mathbf{a}(\mathbf{p})\,e^{-i\langle\Omega_+(\mathbf{p}),x\rangle_{\mathbb{M}}}),$$

$$\boldsymbol{\varphi}_m(\mathbf{x}):=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\frac{d^3\mathbf{p}}{2\omega(\mathbf{p})}(\mathbf{a}^+(\mathbf{p})\,e^{-i\mathbf{p}\cdot\mathbf{x}}+\mathbf{a}(\mathbf{p})\,e^{i\mathbf{p}\cdot\mathbf{x}}),$$

$$\boldsymbol{\pi}_m(\mathbf{x}):=\frac{i}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}d^3\mathbf{p}(\mathbf{a}^+(\mathbf{p})\,e^{-i\mathbf{p}\cdot\mathbf{x}}-\mathbf{a}(\mathbf{p})\,e^{i\mathbf{p}\cdot\mathbf{x}}).$$

There, $\mathbf{a}(\mathbf{p})$ and $\mathbf{a}^+(\mathbf{p})$ are defined on $D_0:=\{\psi=(\psi_n)_{n\geqslant 0}\in F_0:\psi_n\in\mathcal{S}(\mathbb{R}^{3n})\}$ as in (28) and (29). The interrelation between $\mathbf{a}(\mathbf{p})$, $\mathbf{a}^+(\mathbf{p})$ and $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})$, $\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})$ is given as follows:

Proposition VII.1: Let $V:=\mathcal{F}_{\vee}(\nu_{>0}^*):\mathcal{H}_{\mathrm{nr}}\to\tilde{\mathcal{H}}_{\mathrm{nr}}$ *be the unitary mapping induced by* $\nu_{>0}$. *Then, in the sense of bilinear forms,*

$$\tilde{\mathbf{a}}(\tilde{\mathbf{p}})=V\mathbf{a}(\nu_{>0}(\tilde{\mathbf{p}}))V^{-1},\quad\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})=V\mathbf{a}^+(\nu_{>0}(\tilde{\mathbf{p}}))V^{-1}$$

for every $\tilde{\mathbf{p}} \in \mathbb{R}^3$, $p^+ > 0$.

Proof: This follows immediately from the fact that $V = \mathcal{F}_{\vee}(\nu^*_{>0})$ is a unitary mapping and that $\mathbf{a}(\mathbf{p})$ (resp. $\mathbf{a}^+(\mathbf{p})$) and $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})$ (resp. $\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})$) are both defined by the same kind of formula (28) (resp. (29)). □

Remark VII.2: The reader can easily verify that $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}}) = \tilde{\boldsymbol{\phi}}_m(0,\tilde{\mathbf{x}})$, i.e., $\tilde{\boldsymbol{\varphi}}$ is the restriction of $\tilde{\boldsymbol{\phi}}_m$ to $\{x^+ = 0\}$. Since, for any χ, $\psi \in \tilde{D}_0$, the functions $\tilde{\mathbf{p}} \mapsto \langle \chi, \tilde{\mathbf{a}}(\tilde{\mathbf{p}}) \rangle$ and $\tilde{\mathbf{p}} \mapsto \langle \chi, \tilde{\mathbf{a}}^+(\tilde{\mathbf{p}}) \rangle$ are in $\mathcal{S}_{p^+}(\mathbb{R}^3)$, the function $\tilde{\mathbf{x}} \mapsto \langle \chi, \tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}}) \psi \rangle$ is in $\mathcal{S}_{\partial_-}(\mathbb{R}^3)$ by the above Fock-space expansion of $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})$. Hence, it is possible to express $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})$ and $\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}})$ in terms of $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})$ by applying the partial LC-Fourier transformation which can be seen as follows: Define a bilinear form $\tilde{\mathbf{b}}(\tilde{\mathbf{p}})$ on $\tilde{D}_0 \times \tilde{D}_0$ by

$$\tilde{\mathbf{b}}(\tilde{\mathbf{p}}) := \begin{cases} \tilde{\mathbf{a}}(\tilde{\mathbf{p}}), & \text{if } p^+ > 0 \\ \tilde{\mathbf{a}}^+(-\tilde{\mathbf{p}}), & \text{if } p^+ < 0. \end{cases}$$

Then, the above Fock-space expansion of $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})$ can be rewritten as

$$\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{d^3\tilde{\mathbf{p}}}{2|p^+|} \tilde{\mathbf{b}}(\tilde{\mathbf{p}})\, e^{-i(p^+x^- - \mathbf{p}_\perp \cdot \mathbf{x}_\perp)}.$$

Applying the partial LC-Fourier transformation, we obtain

$$\tilde{\mathbf{b}}(\tilde{\mathbf{p}}) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3\tilde{\mathbf{x}}\, |p^+| \tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})\, e^{i(p^+x^- - \mathbf{p}_\perp \cdot \mathbf{x}_\perp)},$$

and hence

$$\tilde{\mathbf{a}}(\tilde{\mathbf{p}}) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3\tilde{\mathbf{x}}\, |p^+| \tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})\, e^{i(p^+x^- - \mathbf{p}_\perp \cdot \mathbf{x}_\perp)},$$

$$\tilde{\mathbf{a}}^+(\tilde{\mathbf{p}}) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3\tilde{\mathbf{x}}\, |p^+| \tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}})\, e^{-i(p^+x^- - \mathbf{p}_\perp \cdot \mathbf{x}_\perp)}.$$

This shows that $\tilde{\boldsymbol{\phi}}_m(x^+,\tilde{\mathbf{x}})$ is uniquely determined by the initial data $\tilde{\boldsymbol{\varphi}}(\tilde{\mathbf{x}}) = \tilde{\boldsymbol{\phi}}_m(0,\tilde{\mathbf{x}})$ on the hypersurface $\{x^+ = 0\}$. Since, moreover, $\boldsymbol{\phi}_m(\tilde{x})$, i.e., $\tilde{x} \mapsto \langle \chi, \boldsymbol{\phi}_m(\tilde{x})\psi \rangle$, is a solution of the LC-Klein–Gordon equation, we establish that $\tilde{\boldsymbol{\phi}}_m(\tilde{x})$ is the unique solution of the Cauchy problem of the LC-Klein–Gordon equation $(\tilde{\Box} + m^2)\tilde{u} = 0$ with initial data $\tilde{u}|_{x^+=0}$ given on $\{x^+ = 0\}$. Since the surface $\{x^+ = 0\}$ is characteristic, uniqueness of the solution cannot be guaranteed any more generally.[12] However, ambiguity is not necessary. It is even possible to show uniqueness (and existence) of the solutions in a very general situation.[21]

Notice that in the Minkowski case, the Cauchy problem of the Klein–Gordon equation with initial data given on $\{x^0 = \text{const}\}$ is always uniquely solvable (cf., e.g., Ref. 3). One needs $\boldsymbol{\varphi}_m(\mathbf{x}) = \boldsymbol{\phi}_m(0,\mathbf{x})$ and the first time-derivative $\boldsymbol{\pi}_m(\mathbf{x}) = \partial_0 \boldsymbol{\phi}_m(0,\mathbf{x})$ as initial data on $\{x^0 = 0\}$ to determine $\boldsymbol{\phi}_m(\mathbf{x})$ uniquely. This can be seen by the fact, that one also needs $\boldsymbol{\varphi}_m(\mathbf{x})$ and $\boldsymbol{\pi}_m(\mathbf{x})$ to express $\mathbf{a}(\mathbf{p})$ and $\mathbf{a}^+(\mathbf{p})$ in terms of initial data on $\{x^0 = 0\}$, e.g.,

$$\mathbf{a}(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3\mathbf{x} \left(\omega(\mathbf{p}) \boldsymbol{\varphi}_m(\mathbf{x}) + \frac{i}{2} \boldsymbol{\pi}_m(\mathbf{x}) \right) e^{-i\mathbf{p}\cdot x}.$$

The difference between Minkowski- and LC-case is not surprising since $\Box + m^2$ contains ∂_0 with exponent two, whereas in $\tilde{\Box} + m^2$ the derivative ∂_+ appears only linearly. In momentum space this situation is reflected by the fact, that $\Gamma_m \to \mathbb{R}^3$, $(p^0,\mathbf{p}) \mapsto \mathbf{p}$ is a (smooth) double covering, whereas $\tilde{\Gamma}_m \to \mathbb{R}^3 \backslash \{p^+ = 0\}$, $(\tilde{\mathbf{p}},p^-) \mapsto \tilde{\mathbf{p}}$ is a diffeomorphism.

As a final topic we consider products of $\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}})$ and $\tilde{\mathbf{a}}(\tilde{\mathbf{p}})$ $(\tilde{\mathbf{k}},\tilde{\mathbf{p}}\in\mathbb{R}^3)$ and discuss the question when these products are induced by an operator. This is essential in constructing interacting fields obeying the LC-Wightman axioms. Given $\tilde{\mathbf{k}}_1,\ldots,\tilde{\mathbf{k}}_r\in\mathbb{R}^3$ and $\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_s\in\mathbb{R}^3$, $r,s\geqslant 0$ we define the bilinear form $\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_1)\cdots\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_r)\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_1)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_s)$ on $\tilde{D}_0\times\tilde{D}_0$ by

$$\langle\chi,\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_1)\cdots\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_r)\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_1)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_s)\psi\rangle=\langle\tilde{\mathbf{a}}(\tilde{\mathbf{k}}_r)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{k}}_1)\chi,\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_1)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_s)\psi\rangle$$

for all $\chi,\psi\in\tilde{D}_0$.

Remark VII.3: In Minkowski case, $\mathbf{a}^+(\mathbf{k}_1)\cdots\mathbf{a}^+(\mathbf{k}_r)\mathbf{a}(\mathbf{p}_1)\cdots\mathbf{a}(\mathbf{p}_s)$ is defined by the same kind of formula as $\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_1)\cdots\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_r)\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_1)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_s)$.[16] Hence, it is obvious that the transformation law of Proposition VII.1 extends canonically to

$$\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_1)\cdots\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_r)\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_1)\cdots\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_s)=U\mathbf{a}^+(\nu_{>0}(\tilde{\mathbf{k}}_1))\cdots\mathbf{a}^+(\nu_{>0}(\tilde{\mathbf{k}}_r))\mathbf{a}(\nu_{>0}(\tilde{\mathbf{p}}_1))\cdots\mathbf{a}(\nu_{>0}(\tilde{\mathbf{p}}_s))U^{-1},$$

where $U:\mathcal{H}_{\mathrm{nr}}\to\tilde{\mathcal{H}}_{\mathrm{nr}}$ is as in Proposition VII.1.

Now, we can easily transfer Theorem X.44 of Ref. 16 to the LC-case. To shorten the notation we introduce the following abbreviations:

$$\tilde{\mathbf{p}}_{1\cdots r}=(\tilde{\mathbf{p}}_1,\ldots,\tilde{\mathbf{p}}_r)\in\mathbb{R}^{3r},\quad p^+_{1\cdots r}=\prod_{i=1}^{r}p_i^+,$$

$$\omega(\mathbf{p}_{1\cdots r})=\prod_{i=1}^{r}\omega(\mathbf{p}_i)=\prod_{i=1}^{r}\sqrt{\mathbf{p}_i^2+m^2},$$

$$\#(\tilde{\mathbf{p}}_{1\cdots r})=\prod_{i=1}^{r}\#(\tilde{\mathbf{p}}_i),\quad \text{where } \# \text{ represents } \mathbf{a},\mathbf{a}^+,\mathbf{a}',\mathbf{a}'^+,\tilde{\mathbf{a}} \text{ or } \tilde{\mathbf{a}}^+.$$

Recall that $\tilde{\mathfrak{H}}_{\mathrm{nr}}=\mathcal{L}^2(\mathbb{R}_{>0}\times\mathbb{R}^2,d^3\tilde{\mathbf{p}}/2p^+)$.

Theorem VII.4: *Suppose* $\tilde{W}(\tilde{k}_{1\cdots n_1},\tilde{p}_{1\cdots n_2})\in\tilde{\mathfrak{H}}_{\mathrm{nr}}^{\otimes(n_1+n_2)}$, *where* $n_1,n_2\geqslant 0$. *Then there is a unique operator* $\tilde{T}_{\tilde{W}}$ on $\tilde{\mathcal{H}}_{\mathrm{nr}}=\mathcal{F}_{\vee}(\tilde{\mathfrak{H}}_{\mathrm{nr}})$ *with the following properties*:

(i) $\tilde{D}_0\subset D(\tilde{T}_{\tilde{W}})$ *is a core for* $\tilde{T}_{\tilde{W}}$.

(ii) $\tilde{T}_{\tilde{W}}=\int_{k_1^+>0\cdots k_{n_1}^+>0}\int_{p_1^+>0\cdots p_{n_2}^+>0}(d^{3n_1}\tilde{\mathbf{k}}_{1\cdots n_1}/k^+_{1\cdots n_1})(d^{3n_2}\tilde{\mathbf{p}}_{1\cdots n_2}/p^+_{1\cdots n_2})\tilde{W}(\tilde{\mathbf{k}}_{1\cdots n_1},\tilde{\mathbf{p}}_{1\cdots n_2})\times\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_{1\cdots n_1})\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_{1\cdots n_2})$ *as bilinear forms on* $\tilde{D}_0\times\tilde{D}_0$.

(iii) *If* m_1,m_2 *are non-negative integers such that* $m_1+m_2=n_1+n_2$, then $(1+N)^{-m_1/2}\tilde{T}_{\tilde{W}}(1+N)^{-m_2/2}$ *is a bounded operator with*

$$\|(1+N)^{-m_1/2}\tilde{T}_{\tilde{W}}(1+N)^{-m_2/2}\|\leqslant C_{m_1,m_2}\|\tilde{W}\|_{\tilde{\mathfrak{H}}_{\mathrm{nr}}^{\otimes(n_1+n_2)}},$$

where N *is the number operator and* C_{m_1,m_2} *a constant (cf. Ref. 16, p. 208, 222); especially* $C_{m_1,m_2}=1$, *if* $m_1=n_1$ *and* $m_2=n_2$.

(iv) $\tilde{T}^*_{\tilde{W}}=\int_{k_1^+>0\cdots k_{n_1}^+>0}\int_{p_1^+>0\cdots p_{n_2}^+>0}(d^{3n_1}\tilde{\mathbf{k}}_{1\cdots n_1}/k^+_{1\cdots n_1})(d^{3n_2}\tilde{\mathbf{p}}_{1\cdots n_2}/p^+_{1\cdots n_2})\overline{\tilde{W}(\tilde{\mathbf{k}}_{1\cdots n_1},\tilde{\mathbf{p}}_{1\cdots n_2})}\times\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_{1\cdots n_1})\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_{1\cdots n_2})$ *as bilinear forms on* $\tilde{D}_0\times\tilde{D}_0$.

(v) *If* $(\tilde{W}_n)_{n\in\mathbb{N}}$ *converges to* $\tilde{W}$ *in* $\tilde{\mathfrak{H}}_{\mathrm{nr}}^{\otimes(n_1+n_2)}$, *then* $(\tilde{T}_{\tilde{W}_n})_{n\in\mathbb{N}}$ *converges to* $\tilde{T}_{\tilde{W}}$ *strongly on* $\tilde{D}_0$.

(vi) $\tilde{D}_0$ *is contained in* $D(\tilde{T}_{\tilde{W}})\cap D(\tilde{T}^*_{\tilde{W}})$, *and* $\tilde{T}_{\tilde{W}},\tilde{T}^*_{\tilde{W}}$ *are given on* $\tilde{D}_0$ *by the explicit formulas* $(\ell\geqslant 0)$:

$$(\tilde{T}_{\tilde{W}}\psi)_{\ell-n_2+n_1}(\tilde{\mathbf{k}}_{1\cdots\ell-n_2+n_1})=K_{\ell,n_1,n_2}S\int_{p_1^+>0\cdots p_{n_2}^+>0}\frac{d^{3n_2}\tilde{\mathbf{p}}_{1\cdots n_2}}{p^+_{1\cdots n_2}}\tilde{W}(\tilde{\mathbf{k}}_{1\cdots n_1},\tilde{\mathbf{p}}_{1\cdots n_2})$$

$$\psi_l(\tilde{\mathbf{p}}_{1\cdots n_2}, \tilde{\mathbf{k}}_{n_1+1\cdots n_1+\ell-n_2}),$$

$$(\tilde{T}_{\tilde{W}}\psi)_n = 0, \quad if \quad n < n_1 - n_2,$$

$$(\tilde{T}^*_{\tilde{W}}\psi)_{\ell-n_1+n_2}(\tilde{\mathbf{p}}_{1\cdots\ell-n_1+n_2}) = K_{\ell,n_2,n_1}\, S \int_{k_1^+>0\cdots k_{n_1}^+>0} \frac{d^{3n_1}\tilde{\mathbf{k}}_{1\cdots n_1}}{k^+_{1\cdots n_1}} \overline{\tilde{W}(\tilde{\mathbf{k}}_{1\cdots n_1}, \tilde{\mathbf{p}}_{1\cdots n_2})}$$

$$\times \psi_l(\tilde{\mathbf{k}}_{1\cdots n_1}, \tilde{\mathbf{p}}_{n_2+1\cdots n_2+\ell-n_1}),$$

$$(\tilde{T}_{\tilde{W}}\psi)_n = 0, \quad if \quad n < n_2 - n_1,$$

where S denotes the symmetrization operator and K_{ℓ,n_1,n_2} is a constant (cf. Ref. 16, p. 207).

Proof: Let $\nu = \nu_{>0}$ denote the squeezing mapping and $U := \mathcal{F}_\vee(\nu^*): \mathcal{H}_{\rm nr} \to \tilde{\mathcal{H}}_{\rm nr}$ the induced unitary operator. The annihilation and creation operators in Ref. 16 are defined by the same formulas as in (28), (29), however, on the Fock space $\mathcal{H}'_{\rm nr} = \mathcal{F}_\vee(\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}))$, which is also frequently used as the nonrelativistic one-particle space. Let us temporarily denote the creation and annihilation operators acting on $\mathcal{H}'_{\rm nr}$, as in Ref. 16, by $\mathbf{a}'(\mathbf{p})$ and $\mathbf{a}'^+(\mathbf{p})$. Let $V = \mathcal{F}_\vee(v): \mathcal{H}'_{\rm nr} \to \mathcal{H}_{\rm nr}$ be the unitary operator induced by $v: \mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}) \to \mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{p}/2\omega(\mathbf{p}))$, $g \mapsto \sqrt{2\omega(\mathbf{p})}g$. It is easy to see that

$$V\mathbf{a}'(\mathbf{p})V^{-1} = \frac{\mathbf{a}(\mathbf{p})}{\sqrt{2\omega(\mathbf{p})}} \quad \text{and} \quad V\mathbf{a}'^+(\mathbf{p})V^{-1} = \frac{\mathbf{a}^+(\mathbf{p})}{\sqrt{2\omega(\mathbf{p})}}$$

in the sense of bilinear forms for every $\mathbf{p} \in \mathbb{R}^3$. Suppose $\tilde{W} \in \tilde{\mathcal{H}}_{\rm nr}^{\otimes(n_1+n_2)}$. Then we define

$$W := (2v^{-1}\nu_*)^{\otimes(n_1+n_2)}\tilde{W} \in \mathcal{L}^2(\mathbb{R}^3, d\mathbf{p})^{\otimes(n_1+n_2)}.$$

Let T_W be the operator from Theorem X.44.[16] We define the operator $\tilde{T}_{\tilde{W}}$ by

$$\tilde{T}_{\tilde{W}} := UVT_W(UV)^{-1}.$$

Then by Theorem X.44,[16] we obtain in the sense of bilinear forms

$$\tilde{T}_{\tilde{W}} = UV\left(\int d^{3n_1}\mathbf{k}_{1\cdots n_1} \int d^{3n_2}\mathbf{p}_{1\cdots n_2} W(\mathbf{k}_{1\cdots n_1}, \mathbf{p}_{1\cdots n_2})\mathbf{a}'^+(\mathbf{k}_{1\cdots n_1})\mathbf{a}'(\mathbf{p}_{1\cdots n_2}) \right) V^{-1}U^{-1}$$

$$= U\left(\int \frac{d^{3n_1}\mathbf{k}_{1\cdots n_1}}{2^{n_1}\omega(\mathbf{k}_{1\cdots n_1})} \int \frac{d^{3n_2}\mathbf{p}_{1\cdots n_2}}{2^{n_2}\omega(\mathbf{p}_{1\cdots n_2})} (v^{\otimes(n_1+n_2)}W)(\mathbf{k}_{1\cdots n_1}, \mathbf{p}_{1\cdots n_2})\mathbf{a}^+(\mathbf{k}_{1\cdots n_1})\mathbf{a}(\mathbf{p}_{1\cdots n_2}) \right) U^{-1}$$

$$= \int_{k_1^+>0\cdots k_{n_1}^+>0} \frac{d^{3n_1}\tilde{\mathbf{k}}_{1\cdots n_1}}{k^+_{1\cdots n_1}} \int_{p_1^+>0\cdots p_{n_1}^+>0} \frac{d^{3n_2}\tilde{\mathbf{p}}_{1\cdots n_2}}{p^+_{1\cdots n_2}} \tilde{W}(\tilde{\mathbf{k}}_{1\cdots n_1}, \tilde{\mathbf{p}}_{1\cdots n_2})\tilde{\mathbf{a}}^+(\tilde{\mathbf{k}}_{1\cdots n_1})\tilde{\mathbf{a}}(\tilde{\mathbf{p}}_{1\cdots n_2})$$

since $\tilde{W} = (2^{-1}\nu^* v)^{\otimes(n_1+n_2)}W$ which proves (ii). In the same way, using the definition of $\tilde{T}_{\tilde{W}}$, we easily obtain from Ref. 16, Theorem X.44 the remaining assertions. □

VIII. CONCLUSIONS

In this paper we have shown that with the aid of squeezed distributions the technical problem of constructing a proper restriction of the free scalar massive field to the lightlike surface $\{x^0 + x^3 = 0\}$ can been solved. Such restriction problems also arise naturally in the theory of distributions and are closely related to the problem that products of distributions are not always ca-

nonically defined; the so-called wave front set plays an essential role there.[11] Hence, squeezed distributions might be helpful in constructing noncanonical restrictions and products of (tempered) distributions which occur in LC-quantum field theories.

We hope that our paper will revive the (axiomatic) development of light-cone (or light-front) quantum field theory by having eliminated some old, technical problems, see also Ref. 21. Moreover, building upon the results of this paper it might now be possible to take advantage of the front-form Hamiltonian approach in constructing explicit models of interacting (LC-)quantum fields obeying the (LC-)Wightman axioms. At least it should now be possible to investigate $:P(\phi)_2:$-theories on the light cone in a mathematically rigorous way—also to find possibly an answer to the question whether there is an analog of Haag's theorem for fields on null planes as suggested by Driessler.[9]

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The Drinfeld realization of the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$

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We construct a realization of the L-operator satisfying the RLL-relation of the face-type elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. The construction is based on the elliptic analog of the Drinfeld currents of $U_q(A_2^{(2)})$, which forms the elliptic algebra $U_{q,p}(A_2^{(2)})$. We give a realization of the elliptic currents $E(z)$, $F(z)$, and $K(z)$ as a tensor product of the Drinfeld currents of $U_q(A_2^{(2)})$ and a Heisenberg algebra. In the level-one representation, we also give a free field realization of the elliptic currents. Applying these results, we derive a free field realization of the $U_{q,p}(A_2^{(2)})$-analog of the $\mathcal{B}_{q,\lambda}(A_2^{(2)})$-intertwining operators. The resultant operators coincide with those of the vertex operators in the dilute A_L model, which is known to be a RSOS restriction of the $A_2^{(2)}$ face model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767296]

I. INTRODUCTION

An elliptic quantum group is a quasitriangular quasi-Hopf algebra obtained as a quasi-Hopf deformation of the affine quantum group $U_q(\mathfrak{g})$ by the twistor satisfying the shifted cocycle condition.[1–3] It is conjectured in Refs. 4 and 3 that the representation theory of the elliptic quantum groups of both the vertex type $\mathcal{A}_{q,p}(\widehat{\mathfrak{sl}}_N)$ and the face type $\mathcal{B}_{q,\lambda}(\mathfrak{g})$, $\mathfrak{g}$ being an affine Lie algebra, enables us to perform an algebraic analysis of the corresponding two dimensional solvable lattice models in the sense of Jimbo and Miwa.[5] In order to perform the analysis, we need to construct explicit representations of both finite and infinite dimensional. For this purpose, the Drinfeld realization of the quantum groups is known to provide a relevant framework. In the previous papers,[6–8] we constructed the Drinfeld realization of the face-type elliptic quantum group $\mathcal{B}_{q,\lambda}(\widehat{\mathfrak{sl}}_N)$ based on the elliptic algebra $U_{q,p}(\widehat{\mathfrak{sl}}_N)$. The Drinfeld generators have both finite and infinite dimensional representations suitable for the calculation of the correlation functions.

In this paper, we investigate the same problem for $\mathcal{B}_{q,\lambda}(A_2^{(2)})$, the face-type elliptic quantum group associated with the twisted affine Lie algebra $A_2^{(2)}$. We first construct the elliptic algebra $U_{q,p}(A_2^{(2)})$ as the algebra of the elliptic analog of the Drinfeld currents of $U_q(A_2^{(2)})$. Basically, the idea given in Appendix A of Ref. 7 can be applied to the twisted case. Namely, dressing the Drinfeld currents of $U_q(A_2^{(2)})$ by the bosons a_m ($m \in \mathbb{Z}_{\neq 0}$) in $U_q(A_2^{(2)})$ and taking a tensor product with a certain Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$ generated by P,Q, which commutes with $U_q(A_2^{(2)})$, we obtain the elliptic Drinfeld currents. However, we formulate the elliptic algebra $U_{q,p}(A_2^{(2)})$ in an extended form by introducing the new currents $K(u)$, which enables the RLL-formulation of $U_{q,p}(A_2^{(2)})$. Then we discuss a connection between $U_{q,p}(A_2^{(2)})$ and $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. We derive the dynamical RLL-relation of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ from the RLL-relation of $U_{q,p}(A_2^{(2)})$ by removing a half of the generator Q of the Heisenberg algebra and identifying P with the dynamical parameter in

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$\mathcal{B}_{q,\lambda}(A_2^{(2)})$. We hence find a structure of $U_{q,p}(A_2^{(2)})$ roughly given by "$\mathcal{B}_{q,\lambda}(A_2^{(2)})\otimes\mathbb{C}\{\mathcal{H}\}$," and in this sense, we regard $U_{q,p}(A_2^{(2)})$ as the Drinfeld realization of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$.

Although the above tensor structure does not preserve the coalgebra structure of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$, the same tensor structure enables us to convert the algebraic objects of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$, such as the intertwining operators, to the $U_{q,p}(A_2^{(2)})$ counterparts. Moreover, in the known cases, it is true that the $U_{q,p}(\mathfrak{g})$ counterparts of the $\mathcal{B}_{q,\lambda}(\mathfrak{g})$ intertwining operators play the role of vertex operators in the restricted solid on solid (RSOS) model associated with $\mathfrak{g}$. We call such "intertwining" operator of $U_{q,p}(\mathfrak{g})$ the vertex operator of $U_{q,p}(\mathfrak{g})$. The elliptic Drinfeld currents in $U_{q,p}(A_2^{(2)})$ admits a free field realization, which is an elliptic extension of those of $U_q(A_2^{(2)})$ obtained in Refs. 9, 10, and 11. By using such realization and applying the tensoring procedure, we derive a free field realization of the vertex operators of $U_{q,p}(A_2^{(2)})$.

The face model associated with the twisted affine Lie algebra $A_2^{(2)}$ was formulated in Ref. 12. Its RSOS restriction is known to be the dilute A_L model.[13,14] The free field formulation of the dilute A_L model was carried out in Ref. 15. There, however, the construction of the vertex operators was done by brute force based on the commutation relations among the vertex operators. We here derive the same vertex operators by using the representation theory of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ and the Drinfeld realization given by $U_{q,p}(A_2^{(2)})$.

This paper is organized as follows: In the next section, we give a summary of the basic facts on the face type elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. In Sec. III, we present a definition and a realization of the elliptic algebra $U_{q,p}(A_2^{(2)})$. New currents $K(u)$ are introduced there. In Sec. IV, we introduce a set of half currents defined from the elliptic currents in $U_{q,p}(A_2^{(2)})$ and derive their commutation relations. Section V is devoted to a construction of a L-operator and the RLL-formulation of $U_{q,p}(A_2^{(2)})$. We then derive the dynamical RLL-relation of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ from $U_{q,p}(A_2^{(2)})$. According to this result, in Sec. VI, we discuss a free field realization of the two types of vertex operators of the level one $U_{q,p}(A_2^{(2)})$-modules. The final section is devoted to discussions on some remaining problems. In addition, we have three appendixes. In Appendix A, we give a summary of the three-dimensional evaluation representation of $U_{q,p}(A_2^{(2)})$. In Appendix B, we discuss the difference equation for the twistor and give partial results on the solutions. Finally, in Appendix C, we give a proof of some formulas of commutation relations of the half currents.

II. THE ELLIPTIC QUANTUM GROUP $\mathcal{B}_{q,\lambda}(A_2^{(2)})$

In this section, we summarize some basic facts on the face-type elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ based on the results in Ref. 3.

A. Notations

Through this article, we fix a complex number $q\neq 0, 0<q<1$ and p given by

$$p=q^{2r},\quad p^*=pq^{-2c}=q^{2r^*}\quad (r^*=r-c;\ r,r^*\in\mathbb{R}_{>0}).$$

We parametrize p as follows:

$$p=e^{-2\pi i/\tau},\ p^*=e^{-2\pi i/\tau^*}\quad (r\tau=r^*\tau^*),$$

$$z=q^{2u}=e^{-2\pi i u/r\tau}.$$

We often use the following Jacobi theta functions,

$$[u]=q^{(u^2/r)-u}\Theta_p(q^{2u})=e^{-(\pi i/4)}\tau^{1/2}q^{-(r/4)}\ \vartheta_1\left(\frac{u}{r}\middle|\tau\right),$$

$$[u]_+=q^{(u^2/r)-u}\Theta_p(-q^{2u})=e^{-(\pi i/4)}\tau^{1/2}q^{-(r/4)}\ \vartheta_0\left(\frac{u}{r}\middle|\tau\right),$$

$[u]^*=[u]|_{r\to r^*,\tau\to\tau^*}$ and $[u]^*_+=[u]_+|_{r\to r^*,\tau\to\tau^*}$. Here

$$\Theta_p(z)=(z,p)_\infty(pz^{-1};p)_\infty(p;p)_\infty,$$

$$(z;t_1,\ldots,t_k)_\infty=\prod_{n_1,\cdots,n_k\geqslant 0}(1-zt_1^{n_1}\cdots t_k^{n_k}).$$

The theta functions satisfy $[-u]=-[u],[-u]_+=[u]_+$ and the quasiperiodicity property

$$[u+r]=-[u],\quad [u+r\tau]=-e^{-\pi i\tau-(2\pi iu/r)}[u], \tag{2.1}$$

$$[u+r]_+=[u]_+,\quad [u+r\tau]_+=e^{-\pi i\tau-(2\pi iu/r)}[u]_+, \tag{2.2}$$

$$\left[u+\frac{r\tau}{2}\right]=ie^{-\pi i(u/r+\tau/4)}[u]_+. \tag{2.3}$$

We use the following normalization for the contour integration:

$$\oint_{C_0}\frac{dz}{2\pi iz}\frac{1}{[-u]}=1,\quad \oint_{C_0}\frac{dz}{2\pi iz}\frac{1}{[-u]^*}=\left.\frac{[u]}{[u]^*}\right|_{u\to 0}, \tag{2.4}$$

where C_0 is a simple closed curve in the u-plane encircling $u=0$ anticlockwise.

B. Definition of the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$

Let $U_q(A_2^{(2)})$ be the standard affine quantum group, associated with the Cartan matrix

$$A=\begin{pmatrix}2 & -1\\ -4 & 2\end{pmatrix}. \tag{2.5}$$

The labels of A are $a_0=1,a_1=2$ and colabels are $a_0^\vee=2,a_1^\vee=1$. Let $B=(b_{ij})$ be the symmetrized Cartan matrix $b_{ij}=(a_i^\vee/a_i)\,a_{ij}$. We identify $\mathfrak{h}=\mathbb{C}\alpha_0^\vee\oplus\mathbb{C}\alpha_1^\vee\oplus\mathbb{C}d$ and $\mathfrak{h}^*=\mathbb{C}\alpha_0\oplus\mathbb{C}\alpha_1\oplus\mathbb{C}\Lambda_0$ via the standard invariant bilinear form $(\,,\,)$ given on $\mathfrak{h}$ and $\mathfrak{h}^*$ as follows:

$$(\alpha_i^\vee,\alpha_j^\vee)=a_{ij}\frac{a_j}{a_j^\vee}\quad(0\leqslant i,j\leqslant 1),$$

$$(\alpha_i^\vee,d)=\delta_{i,0}\quad(d,d)=0,$$

$$(\alpha_i,\alpha_j)=\frac{a_i^\vee}{a_i}a_{ij}\quad(0\leqslant i,j\leqslant 1),$$

$$(\alpha_i,\Lambda_0)=\delta_{i,0}\quad(\Lambda_0,\Lambda_0)=0.$$

The central element is given by $c=2\alpha_0^\vee+\alpha_1^\vee$. Let us set $\delta=\alpha_0+2\alpha_1$. Then the following relations hold:

$$(\delta,d)=1,\quad(\delta,\delta)=0,\quad(c,d)=2,\quad(c,c)=0.$$

The identification between $\mathfrak{h}$ and $\mathfrak{h}^*$ is given explicitly by $\alpha_i^\vee=2\alpha_i/(\alpha_i,\alpha_i)$, $c=\delta$, and $d=2\Lambda_0$. Under this, we use $\{\hat{h}_l\}_{l=1,2,3}=\{d,c,\alpha_1^\vee\}$ as a basis of $\mathfrak{h}$ and $\{\hat{h}^l\}_{l=1,2,3}=\{c/2,d/2,\alpha_1^\vee/2\}$ as its dual basis. Our conventions of coalgebra structure of $U_q(A_2^{(2)})$ follows.[3] The coproduct, counit, antipode are denoted by Δ, ε, and S, respectively.

The face-type elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ is a quasitriangular quasi-Hopf algebra obtained from $U_q(A_2^{(2)})$ by the deformation via the face-type twistor $F(\lambda)$ $(\lambda \in \mathfrak{h})$. The twistor $F(\lambda)$ is an invertible element in $U_q(A_2^{(2)}) \otimes U_q(A_2^{(2)})$ satisfying

$$(\mathrm{id} \otimes \varepsilon) F(\lambda) = 1 = F(\lambda)(\varepsilon \otimes \mathrm{id}), \tag{2.6}$$

$$F^{(12)}(\lambda)(\Delta \otimes \mathrm{id}) F(\lambda) = F^{(23)}(\lambda + h^{(1)})(\mathrm{id} \otimes \Delta) F(\lambda), \tag{2.7}$$

where $\lambda = \Sigma_l \lambda_l \hat{h}^l$ $(\lambda_l \in \mathbb{C})$, $\lambda + h^{(1)} = \Sigma_l (\lambda_l + \hat{h}_l^{(1)}) \hat{h}^l$ and $\hat{h}_l^{(1)} = \hat{h}_l \otimes 1 \otimes 1$. An explicit construction of the twistor $F(\lambda)$ is given in Ref. 3. As an associative algebra, $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ is isomorphic to $U_q(A_2^{(2)})$, but the coalgebra structure is deformed in the following way:

$$\Delta_\lambda(x) = F(\lambda) \Delta(x) F(\lambda)^{-1} \quad \forall x \in U_q(A_2^{(2)}). \tag{2.8}$$

Δ_λ satisfies a weaker coassociativity

$$(\mathrm{id} \otimes \Delta_\lambda) \Delta_\lambda(x) = \Phi(\lambda)(\Delta_\lambda \otimes \mathrm{id}) \Delta_\lambda(x) \Phi(\lambda)^{-1} \quad \forall \ x \in U_q(A_2^{(2)}), \tag{2.9}$$

$$\Phi(\lambda) = F^{(23)}(\lambda) F^{(23)}(\lambda + h^{(1)})^{-1}. \tag{2.10}$$

Let $\mathcal{R}$ be the universal R matrix of $U_q(A_2^{(2)})$. The universal R matrix of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ is given by

$$\mathcal{R}(\lambda) = F^{(21)}(\lambda) \mathcal{R} F^{(12)}(\lambda)^{-1}. \tag{2.11}$$

Definition 2.1 (Elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$): The face-type elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ is a quasitriangular quasi-Hopf algebra $(\mathcal{B}_{q,\lambda}(A_2^{(2)}), \Delta_\lambda, \varepsilon, S, \Phi(\lambda), \alpha, \beta, \mathcal{R}(\lambda))$, *where α, β are defined by*

$$\alpha = \sum_i S(k_i) l_i, \quad \beta = \sum_i m_i S(n_i). \tag{2.12}$$

Here we set $\Sigma_i k_i \otimes l_i = F(\lambda)^{-1}$, $\Sigma_i m_i \otimes n_i = F(\lambda)$.

The universal R matrix $\mathcal{R}(\lambda)$ satisfies the dynamical Yang–Baxter equation,

$$\mathcal{R}^{(12)}(\lambda + h^{(3)}) \mathcal{R}^{(13)}(\lambda) \mathcal{R}^{(23)}(\lambda + h^{(1)}) = \mathcal{R}^{(23)}(\lambda) \mathcal{R}^{(13)}(\lambda + h^{(2)}) \mathcal{R}^{(12)}(\lambda). \tag{2.13}$$

Let $(\pi_{V,z}, V_z)$, $V_z = V \otimes \mathbb{C}[z, z^{-1}]$ be a (finite dimensional) evaluation representation of U_q. Taking images of $\mathcal{R}$, we define a R-matrix $R_{VW}^+(z, \lambda)$ and a L-operator $L_V^+(z, \lambda)$ as follows:

$$R_{VW}^+(z_1/z_2, \lambda) = (\pi_{V,z_1} \otimes \pi_{W,z_2}) q^{c \otimes d + d \otimes c} \mathcal{R}(\lambda), \tag{2.14}$$

$$L_V^+(z, \lambda) = (\pi_{V,z} \otimes \mathrm{id}) q^{c \otimes d + d \otimes c} \mathcal{R}(\lambda). \tag{2.15}$$

Then from (2.13), we have the following dynamical RLL-relation:

$$R_{VW}^+(z_1/z_2, \lambda + h) L_V^+(z_1, \lambda) L_W^+(z_2, \lambda + h^{(1)}) = L_W^+(z_2, \lambda) L_V^+(z_1, \lambda + h^{(2)}) R_{VW}^+(z_1/z_2, \lambda). \tag{2.16}$$

Note that in $\mathcal{B}_{q,\lambda}(A_2^{(2)})$, $L_V^+(z, \lambda)$ and $L_V^-(z, \lambda) = (\pi_{V,z} \otimes \mathrm{id}) \mathcal{R}^{(21)}(\lambda)^{-1} q^{-c \otimes d - d \otimes c}$ are not independent operators (Proposition 4.3 in Ref. 3). Hence one dynamical RLL-relation (2.16) characterizes the algebra $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ completely in the sense of Reshetikhin and Semenov-Tian-Shansky.[16]

Through this paper, we parametrize the dynamical variable λ as

$$\lambda=(r^*+3)d+s'c+\frac{1}{2}\left(s+\frac{r\tau}{2}\right)\alpha_1^\vee \quad (r^*\equiv r-c). \tag{2.17}$$

Under this, we set $F(r^*,s)\equiv F(\lambda)$ and $\mathcal{R}(r^*,s)\equiv\mathcal{R}(\lambda)$. Since c is central, no s' dependence should appear. The dynamical shift $\lambda\to\lambda+h$ with $h=cd+(\alpha_1^\vee)^2/2$, changes the universal R-matrix $\mathcal{R}(r^*,s)$ to $\mathcal{R}(r,s+\alpha_1^\vee)$. Let us take $(\pi_{V,z},V_z)$ to be the evaluation representation associated with the vector representation $V\cong\mathbb{C}^3$ of $U_q(A_2^{(2)})$ (see Appendix A). We set

$$R^+(u,s+\alpha_1^\vee)=(\pi_{V,z_1}\otimes\pi_{V,z_2})q^{c\otimes d+d\otimes c}\mathcal{R}(r,s+\alpha_1^\vee),$$

$$L^+(u,s)=(\pi_{V,z}\otimes\mathrm{id})q^{c\otimes d+d\otimes c}\mathcal{R}(r^*,s),$$

where $z_1/z_2=q^{2u}$, $u=u_1-u_2$. From (2.11), we can obtain an explicit expression of $R^+(u,s)$, if we know the finite dimensional representation of the twistor $(\pi_{V,z_1}\otimes\pi_{V,z_2})F(r,s)$. In principle, one can obtain such representation by solving the q-difference equation for the twistor,[3] which is similar to the q-KZ equation for corresponding $U_q(\mathfrak{g})$. In the present case, the q-difference equation splits into the three parts; two 2×2 matrix parts and one 3×3 matrix part (see Appendix B). Each 2×2 matrix parts turns out to be the same as the one of the twistor for $\mathcal{B}_{q,\lambda}(A_1^{(1)})$ in the vector representation after adjusting some q-shift and sign factor, whereas we have no known solutions for the 3×3 matrix part. Writing down the solutions of the 2×2 matrix parts under the parametrization of λ (2.17), we obtain from (2.11) the corresponding matrix elements of $R^+(u,s)$ which coincide with the corresponding matrix elements of the Boltzmann weight for the $A_2^{(2)}$ face model.[12] For the remaining 3×3 matrix part, we conjecture that the same coincidence should occur. We hence assume that the R-matrix $R^+(u,s)$ is given by the following formula:

$$R^+(u,s)=\rho^+(u)\overline{R}(u,s), \tag{2.18}$$

where

$$\overline{R}(u,s)=\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & R_{+0}^{+0} & 0 & R_{+0}^{0+} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & R_{+-}^{+-} & 0 & R_{+-}^{00} & 0 & R_{+-}^{-+} & 0 & 0\\
0 & R_{0+}^{+0} & 0 & R_{0+}^{0+} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & R_{00}^{+-} & 0 & R_{00}^{00} & 0 & R_{00}^{-+} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & R_{0-}^{0-} & 0 & R_{0-}^{-0} & 0\\
0 & 0 & R_{-+}^{+-} & 0 & R_{-+}^{00} & 0 & R_{-+}^{-+} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & R_{-0}^{0-} & 0 & R_{-0}^{-0} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}, \tag{2.19}$$

$$R_{+0}^{+0}(u,s)=-\frac{[s+3/2]_+[s-1/2]_+}{[s+1/2]_+^2}\frac{[u]}{[u+1]},$$

$$R_{+0}^{0+}(u,s)=\frac{[s+1/2+u]_+[1]}{[s+1/2]_+[1+u]},$$

$$R_{0+}^{+0}(u,s)=\frac{[-s-1/2+u]_+[1]}{[-s-1/2]_+[1+u]},$$

$$R^{0+}_{0+}(u,s)=R^{-0}_{-0}(u,s)=-\frac{[u]}{[1+u]},$$

$$R^{0-}_{0-}(u,s)=-\frac{[s+1/2]_+[s-3/2]_+}{[s-1/2]^2_+}\frac{[u]}{[u+1]},$$

$$R^{-0}_{0-}(u,s)=\frac{[s-1/2+u]_+[1]}{[s-1/2]_+[1+u]},$$

$$R^{0-}_{-0}(u,s)=\frac{[-s+1/2+u]_+[1]}{[-s+1/2]_+[1+u]},$$

$$R^{+-}_{+-}(u,s)=G^+_sG^-_s\frac{[1/2+u][u]}{[3/2+u][1+u]},$$

$$R^{00}_{+-}(u,s)=-G^-_s\frac{[s+1/2]_+[-s-1-u]_+[1][u]}{[-s+1/2]^2_+[1+u][u+3/2]},$$

$$R^{-+}_{+-}(u,s)=\frac{[-2s+1-u][1]}{[-2s+1][1+u]}-G^-_s\frac{[-2s-1/2-u][u][1]}{[-2s+1][3/2+u][1+u]},$$

$$R^{-+}_{00}(u,s)=-\frac{[-s-1-u]_+[1][u]}{[s+1/2]_+[1+u][u+3/2]},$$

$$R^{-+}_{-+}(u,s)=\frac{[1/2+u][u]}{[3/2+u][1+u]},$$

$$R^{00}_{-+}(u,s)=-\frac{[s-1-u]_+[1][u]}{[-s+1/2]_+[1+u][u+3/2]},$$

$$R^{+-}_{-+}(u,s)=\frac{[2s+1-u][1]}{[2s+1][1+u]}-G^+_s\frac{[2s-1/2-u][u][1]}{[2s+1][3/2+u][1+u]},$$

$$R^{+-}_{00}(u,s)=-G^+_s\frac{[-s+1/2]_+[s-1-u]_+[1][u]}{[s+1/2]^2_+[1+u][u+3/2]},$$

$$R^{00}_{00}(u,s)=\frac{[3+u][1][3/2-u]}{[3][1+u][3/2+u]}+H_s\frac{[1][u]}{[3][1+u]}.$$

Here we have set

$$G^\pm_s=-\frac{[2s\pm2][s]_+}{[2s][s\pm1]_+},\qquad H_s=G^+_s\frac{[s-5/2]_+}{[s+1/2]_+}+G^-_s\frac{[s+5/2]_+}{[s-1/2]_+}. \tag{2.20}$$

The function $\rho^+(u)$ is given by

$$\rho^+(u)=-qz^{1/r}\frac{\{pq^2z\}\{pq^3z\}\{pq^3z\}\{pq^4z\}\{1/z\}\{q/z\}\{q^5/z\}\{q^6/z\}}{\{pz\}\{pqz\}\{pq^5z\}\{pq^6z\}\{q^2/z\}\{q^3/z\}\{q^3/z\}\{q^4/z\}}, \tag{2.21}$$

where $z=q^{2u}$ and

$$\{z\}=(z;p,q^6)_\infty. \tag{2.22}$$

The R-matrix $R^{+}{}^{*}(u,s)=(\pi_{V,z_1}\otimes\pi_{V,z_2})\mathcal{R}(r^{*},s)$ is obtained from $R^{+}(u,s)$ by the replacements $r\to r^{*}$. Hence, under the parametrization (2.17), the dynamical RLL-relation takes the form

$$R^{+(12)}(u,s+\alpha_1^{\vee})L^{+(1)}(u_1,s)L^{+(2)}(u_2,s+\alpha_1^{\vee(1)})=L^{+(2)}(u_2,s)L^{+(1)}(u_1,s+\alpha_1^{\vee(2)})R^{+*(12)}(u,s). \tag{2.23}$$

C. Intertwining operators

Let $\mathcal{F},\mathcal{F}'$ be the highest weight U_q-modules. We denote the type-I and type II intertwining operators of U_q-modules by $\Phi(z)$ and $\Psi^{*}(z)$, respectively,

$$\Phi(z):\ \mathcal{F}\to\mathcal{F}'\otimes W_z,\quad \Psi^{*}(z):\ W_z\otimes\mathcal{F}\to\mathcal{F}'. \tag{2.24}$$

Twisting these operators by $F(r^{*},s)$, we obtain the corresponding intertwining operators $\Phi(v,s)$ and $\Psi^{*}(u,s)$ of $\mathcal{B}_{q,\lambda}$-modules,

$$\Phi_W(u,s)=(\mathrm{id}\otimes\pi_{W,z})F(r^{*},s)\Phi(z), \tag{2.25}$$

$$\Psi_W^{*}(u,s)=\Psi^{*}(z)(\pi_{W,z}\otimes\mathrm{id})F(r^{*},s)^{-1}. \tag{2.26}$$

From the intertwining relation satisfied by $\Phi(z)$ and $\Psi^{*}(z)$, one can derive the following dynamical intertwining relation for the new intertwiners:[3]

$$\Phi_W^{(3)}\left(u_2+\frac{c}{2},s\right)L_V^{+(1)}(u_1,s)=R_{VW}^{+(13)}(u,s+\alpha_1^{\vee})L_V^{+(1)}(u_1,s)\Phi_W^{(3)}\left(u_2+\frac{c}{2},s+\alpha_1^{\vee(1)}\right), \tag{2.27}$$

$$L_V^{+(1)}(u_1,s)\Psi_W^{*(2)}(z_2,s+\alpha_1^{\vee(1)})=\Psi_W^{*(2)}(z_2,s)L_V^{+(1)}(u_1,s+\alpha_1^{\vee(2)})R_{VW}^{+*(12)}(u_1-u_2,s). \tag{2.28}$$

Note that (2.27) and (2.28) are the relations for the operators $V_{z_1}\otimes\mathcal{F}\to V_{z_1}\otimes\mathcal{F}\otimes W_{z_2}$ and $V_{z_1}\otimes W_{z_2}\otimes\mathcal{F}\to V_{z_1}\otimes\mathcal{F}$, respectively.

III. ELLIPTIC ALGEBRA $U_{q,p}(A_2^{(2)})$

In this section, we give a definition of the elliptic algebra $U_{q,p}(A_2^{(2)})$. We follows the idea given in Refs. 7 and 8, where the elliptic algebras $U_{q,p}(\mathfrak{g})$ with nontwisted affine Lie algebra $\mathfrak{g}$ are discussed. We first introduce the currents $e(z,p),f(z,p)$ and $\psi^{\pm}(z,p)$ of the quantum group $U_q(A_2^{(2)})$, by modifying the Drinfeld currents of $U_q(A_2^{(2)})$. We then introduce the new current $k(z)$ in $U_q(A_2^{(2)})$ which is a more basic object than the currents $\psi^{\pm}(z,p)$. Finally modifying them by taking a tensor product with Heisenberg algebra, we introduce the elliptic currents $E(u),F(u)$, $H^{\pm}(u)$, and $K(u)$ forming the elliptic algebra $U_{q,p}(A_2^{(2)})$. The current $K(u)$ plays an essential role in the RLL-formulation of $U_{q,p}(A_2^{(2)})$. Hereafter we set $h=\alpha_1^{\vee}$.

A. Drinfeld currents of $U_q(A_2^{(2)})$

Let us recall the Drinfeld currents of $U_q(A_2^{(2)})$. Let $0<q<1$. We use the standard symbol of q-integer

$$[n]_q=\frac{q^n-q^{-n}}{q-q^{-1}}. \tag{3.1}$$

Definition 3.1 (Drinfeld currents): Let $x_m^{\pm}$ $(m\in\mathbb{Z})$, $a_m(m\in\mathbb{Z}_{\neq 0})$ q^c,q^h,q^d *denote the generators of* $U_q(A_2^{(2)})$. *In terms of the generating functions*

$$x^{\pm}(z)=\sum_{m\in\mathbb{Z}}x_m^{\pm}z^{-m}, \tag{3.2}$$

$$\psi(q^{c/2}z)=q^{h/2}\exp\left((q-q^{-1})\sum_{m>0}a_m z^{-m}\right), \tag{3.3}$$

$$\varphi(q^{-c/2}z)=q^{-h/2}\exp\left(-(q-q^{-1})\sum_{m>0}a_{-m}z^{m}\right), \tag{3.4}$$

the defining relations of $U_q(A_2^{(2)})$ *are given by*

$$q^c:\text{central},\qquad q^d a_m q^{-d}=q^m a_m,\quad q^d q_m^{\pm}q^{-d}=q^m x_m^{\pm}, \tag{3.5}$$

$$q^h x^{\pm}(z)q^{-h}=q^{\pm 2}x^{\pm}(z),\quad q^d q^h=q^h q^d, \tag{3.6}$$

$$[a_m,a_n]=\delta_{m+n,0}\frac{1}{m}([2m]_q-[m]_q)q^{-c|m|}[cm]_q, \tag{3.7}$$

$$[a_m,x^{+}(z)]=\frac{1}{m}([2m]_q-[m]_q)q^{-c|m|}z^m x^{+}(z), \tag{3.8}$$

$$[a_m,x^{-}(z)]=-\frac{1}{m}([2m]_q-[m]_q)z^m x^{-}(z), \tag{3.9}$$

$$(z_1-q^{\pm 2}z_2)(z_1-q^{\mp 1}z_2)x^{\pm}(z_1)x^{\pm}(z_2)=-(q^{\pm 2}z_1-z_2)(q^{\mp 1}z_1-z_2)x^{\pm}(z_2)x^{\pm}(z_1), \tag{3.10}$$

$$[x^{+}(z_1),x^{-}(z_2)]=\frac{1}{q-q^{-1}}(\psi(q^{c/2}z_2)\delta(q^{-c}z_1/z_2)-\varphi(q^{-c/2}z_2)\delta(q^{c}z_1/z_2)), \tag{3.11}$$

$$\sum_{\sigma\in S_3}(q^{\pm 3/2}z_{\sigma(1)}-(q^{1/2}+q^{-1/2})z_{\sigma(2)}+q^{\pm 3/2}z_{\sigma(3)})x^{\pm}(z_{\sigma(1)})x^{\pm}(z_{\sigma(2)})x^{\pm}(z_{\sigma(3)})=0. \tag{3.12}$$

Here $\delta(z)$ *denotes the delta function* $\delta(z)=\Sigma_{m\in\mathbb{Z}}z^m$. *We call the generators* $h,a_m,x_m^{\pm},c,d$ *the Drinfeld generators of* $U_q(A_2^{(2)})$ *and the generating functions* $x^{\pm}(z)$, $\psi(z)$, *and* $\varphi(z)$ *the Drinfeld currents*.

B. Elliptic currents of $U_q(A_2^{(2)})$

We next consider an elliptic modification of the Drinfeld currents $x^{\pm}(z)$, $\psi(z)$, and $\varphi(z)$. Let us introduce the two auxiliary currents $u^{\pm}(z,p)$ by

$$u^{+}(z,p)=\exp\left(\sum_{m>0}\frac{a_{-m}}{[r*m]_q}q^{rm}z^m\right), \tag{3.13}$$

$$u^{-}(z,p)=\exp\left(-\sum_{m>0}\frac{a_m}{[rm]_q}q^{rm}z^{-m}\right). \tag{3.14}$$

Proposition 3.1: The following commutation relations hold:

$$u^+(z_1,p)u^-(z_2,p)$$
$$=u^-(z_2,p)u^+(z_1,p)$$
$$\times\frac{(pq^{-c-2}z_1/z_2;p)_\infty(p^*q^{c+2}z_1/z_2;p^*)_\infty(pq^{-c+1}z_1/z_2;p)_\infty(p^*q^{c-1}z_1/z_2;p^*)_\infty}{(pq^{-c+2}z_1/z_2;p)_\infty(p^*q^{c-2}z_1/z_2;p^*)_\infty(pq^{-c-1}z_1/z_2;p)_\infty(p^*q^{c+1}z_1/z_2;p^*)_\infty}, \tag{3.15}$$

$$u^+(z_1,p)x^+(z_2)=\frac{(p^*q^2z_1/z_2;p^*)_\infty(p^*q^{-1}z_1/z_2;p^*)_\infty}{(p^*q^{-2}z_1/z_2;p^*)_\infty(p^*qz_1/z_2;p^*)_\infty}x^+(z_2)u^+(z_1,p), \tag{3.16}$$

$$u^+(z_1,p)x^-(z_2)=\frac{(p^*q^{c-2}z_1/z_2;p^*)_\infty(p^*q^{c+1}z_1/z_2;p^*)_\infty}{(p^*q^{c+2}z_1/z_2;p^*)_\infty(p^*q^{c-1}z_1/z_2;p^*)_\infty}x^-(z_2)u^+(z_1,p), \tag{3.17}$$

$$u^-(z_1,p)x^+(z_2)=\frac{(pq^{-c-2}z_2/z_1;p)_\infty(pq^{-c+1}z_2/z_1;p)_\infty}{(pq^{-c+2}z_2/z_1;p)_\infty(pq^{-c-1}z_2/z_1;p)_\infty}x^+(z_2)u^-(z_1,p), \tag{3.18}$$

$$u^-(z_1,p)x^-(z_2)=\frac{(pq^2z_2/z_1;p)_\infty(pq^{-1}z_2/z_1;p)_\infty}{(pq^{-2}z_2/z_1;p)_\infty(pqz_2/z_1;p)_\infty}x^-(z_2)u^-(z_1,p), \tag{3.19}$$

$$\psi(z_1,p)u^+(z_2,p)$$
$$=u^+(z_2,p)\psi(z_1,p)$$
$$\times\frac{(q^{r^*+2}z_2/z_1;p)_\infty(q^{r^*-1}z_2/z_1;p)_\infty(q^{r^*-2}z_2/z_1;p^*)_\infty(q^{r^*+1}z_2/z_1;p^*)_\infty}{(q^{r^*-2}z_2/z_1;p)_\infty(q^{r^*+1}z_2/z_1;p)_\infty(q^{r^*+2}z_2/z_1;p^*)_\infty(q^{r^*-1}z_2/z_1;p^*)_\infty}, \tag{3.20}$$

$$\psi(z_1,p)u^-(z_2,p)$$
$$=u^-(z_2,p)\psi(z_1,p)\frac{(q^{r-2}z_1/z_2;p)_\infty(q^{r+1}z_1/z_2;p)_\infty(q^{r+2}z_1/z_2;p^*)_\infty(q^{r-1}z_1/z_2;p^*)_\infty}{(q^{r+2}z_1/z_2;p)_\infty(q^{r-1}z_1/z_2;p)_\infty(q^{r-2}z_1/z_2;p^*)_\infty(q^{r+1}z_1/z_2;p^*)_\infty},$$

$$\psi(z_1,p)x^+(z_2)$$
$$=x^+(z_2)\psi(z_1,p)\frac{(q^{r^*-2}z_2/z_1;p)_\infty(q^{r^*+1}z_2/z_1;p)_\infty(q^{r^*+2}z_1/z_2;p^*)_\infty(q^{r^*-1}z_1/z_2;p^*)_\infty}{(q^{r^*+2}z_2/z_1;p)_\infty(q^{r^*-1}z_2/z_1;p)_\infty(q^{r^*-2}z_1/z_2;p^*)_\infty(q^{r^*+1}z_1/z_2;p^*)_\infty}, \tag{3.21}$$

$$\psi(z_1,p)x^-(z_2)$$
$$=x^-(z_2)\psi(z_1,p)\frac{(q^{r+2}z_2/z_1;p)_\infty(q^{r-1}z_2/z_1;p)_\infty(q^{r-2}z_1/z_2;p^*)_\infty(q^{r+1}z_1/z_2;p^*)_\infty}{(q^{r-2}z_2/z_1;p)_\infty(q^{r+1}z_2/z_1;p)_\infty(q^{r+2}z_1/z_2;p^*)_\infty(q^{r-1}z_1/z_2;p^*)_\infty}. \tag{3.22}$$

Definition 3.2: We define "dressed" currents $e(z,p)$, $f(z,p)$, and $\psi^\pm(z,p)$ by

$$e(z,p)=u^+(z,p)x^+(z), \tag{3.23}$$

$$f(z,p)=x^-(z)u^-(z,p), \tag{3.24}$$

$$\psi^+(z,p)=u^+(q^{c/2}z,p)\psi(z)u^-(q^{-c/2}z,p), \tag{3.25}$$

$$\psi^-(z,p)=u^+(q^{-c/2}z,p)\varphi(z)u^-(q^{c/2}z,p). \tag{3.26}$$

If we introduce the auxiliary current $\psi(z,p)$ by

$$\psi(z,p)=\exp\left(\sum_{m>0}\frac{x^{cm}}{[r^*m]_q}a_{-m}z^m\right)\exp\left(-\sum_{m>0}\frac{1}{[rm]_q}a_mz^{-m}\right), \tag{3.27}$$

we have

$$\psi^{\pm}(q^{\mp(r-c/2)}z)=q^{\pm h/2}\psi(z,p). \tag{3.28}$$

Proposition 3.2: The currents $e(z,p)$, $f(z,p)$, and $\psi(z,p)$ satisfy the following commutation relations:

$$\psi(z_1,p)\psi(z_2,p)=\frac{\Theta_p(q^{-2}z_1/z_2)\Theta_p(qz_1/z_2)}{\Theta_p(q^2z_1/z_2)\Theta_p(q^{-1}z_1/z_2)}\frac{\Theta_{p^*}(q^2z_1/z_2)\Theta_{p^*}(q^{-1}z_1/z_2)}{\Theta_{p^*}(q^{-2}z_1/z_2)\Theta_{p^*}(qz_1/z_2)}\psi(z_2,p)\psi(z_1,p), \tag{3.29}$$

$$\psi(z_1,p)e(z_2,p)=\frac{\Theta_{p^*}(q^{r^*+2}z_1/z_2)\Theta_{p^*}(q^{r^*-1}z_1/z_2)}{\Theta_{p^*}(q^{r^*-2}z_1/z_2)\Theta_{p^*}(q^{r^*+1}z_1/z_2)}e(z_2,p)\psi(z_1,p), \tag{3.30}$$

$$\psi(z_1,p)f(z_2,p)=\frac{\Theta_p(q^{r-2}z_1/z_2)\Theta_p(q^{r+1}z_1/z_2)}{\Theta_p(q^{r+2}z_1/z_2)\Theta_p(q^{r-1}z_1/z_2)}f(z_2,p)\psi(z_1,p), \tag{3.31}$$

$$e(z_1,p)e(z_2,p)=(-1)\frac{\Theta_{p^*}(q^{-2}z_2/z_1)\Theta_{p^*}(q^{-1}z_1/z_2)}{\Theta_{p^*}(q^{-2}z_1/z_2)\Theta_{p^*}(q^{-1}z_2/z_1)}e(z_2,p)e(z_1,p), \tag{3.32}$$

$$f(z_1,p)f(z_2,p)=(-1)\frac{\Theta_p(q^2z_2/z_1)\Theta_p(qz_1/z_2)}{\Theta_p(q^2z_1/z_2)\Theta_p(qz_2/z_1)}f(z_2,p)f(z_1,p), \tag{3.33}$$

$$[e(z_1,p),f(z_2,p)]=\frac{1}{q-q^{-1}}(\psi^+(q^{c/2}z_2)\delta(q^{-c}z_1/z_2)-\psi^-(q^{-c/2}z_2)\delta(q^cz_1/z_2)), \tag{3.34}$$

$$\begin{aligned}&\sum_{\sigma\in S_3}\frac{(p^*q^2z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-1}z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-1}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty(p^*q^{-1}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*qz_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*qz_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty(p^*qz_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty}\\&\quad\times\left(z_{\sigma(1)}\frac{(q^2z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^2z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}-qz_{\sigma(2)}\right.\\&\quad\left.\times\frac{(p^*q^2z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^2z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}\right)e(z_{\sigma(1)},p)e(z_{\sigma(2)},p)e(z_{\sigma(3)},p)=0,\end{aligned} \tag{3.35}$$

$$\begin{aligned}&\sum_{\sigma\in S_3}\frac{(pqz_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^{-2}z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pqz_{\sigma(3)}/z_{\sigma(2)};p)_\infty(pqz_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^{-1}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pq^{-1}z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pq^{-1}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\\&\quad\times\left(z_{\sigma(1)}\frac{(q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^{-2}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^2z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\right.\\&\quad\left.-q^{-1}z_{\sigma(2)}\frac{(pq^{-2}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^2z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\right)f(z_{\sigma(1)},p)f(z_{\sigma(2)},p)f(z_{\sigma(3)},p)=0.\end{aligned} \tag{3.36}$$

C. Basic current $k(z)$

The current $\psi(z,p)$ (3.27) can be expressed by a more basic current $k(z)$. Let us modify a_m and define α_m and β_m by

$$\alpha_m=\begin{cases} a_m, & m>0, \\ \dfrac{[rm]_q}{[r^*m]_q}q^{c|m|}a_m, & m<0, \end{cases} \qquad \beta_m=\alpha_m\frac{[r^*m]_q}{[rm]_q}. \tag{3.37}$$

They satisfy the following commutation relations:

$$[\alpha_m,\alpha_n]=\delta_{m+n,0}\frac{[2m]_q-[m]_q}{m}\frac{[cm]_q[rm]_q}{[r^*m]_q}, \tag{3.38}$$

$$[\beta_m,\beta_n]=\delta_{m+n,0}\frac{[2m]_q-[m]_q}{m}\frac{[cm]_q[r^*m]_q}{[rm]_q}. \tag{3.39}$$

Then the current $\psi(z,p)$ is expressed by

$$\psi(z,p)=:\exp\left(-\sum_{m\neq 0}\frac{\alpha_m}{[rm]_q}z^{-m}\right):=:\exp\left(-\sum_{m\neq 0}\frac{\beta_m}{[r^*m]_q}z^{-m}\right):. \tag{3.40}$$

The colons : : denote the standard normal ordering.

Definition 3.3 (Basic Current): We define the current $k(z)$ by

$$k(z,p)=:\exp\left(-\sum_{m\neq 0}\frac{[m]_q}{[rm]_q([2m]_q-[m]_q)}\alpha_m z^{-m}\right):. \tag{3.41}$$

The current $\psi(z,p)$ is then expressed by $k(z)$ as follows:

$$\psi(z,p)=:k(q^{-1}z,p)k(z,p)^{-1}k(qz,p):. \tag{3.42}$$

By a straightforward calculation, we have the following commutation relations:

Proposition 3.3:

$$k(z_1,p)u^+(z_2,p)=\frac{(q^{r^*+1}z_2/z_1;p)_\infty(q^{r^*-1}z_2/z_1;p^*)_\infty}{(q^{r^*-1}z_2/z_1;p)_\infty(q^{r^*+1}z_2/z_1;p^*)_\infty}u^+(z_2,p)k(z_1,p), \tag{3.43}$$

$$k(z_1,p)u^-(z_2,p)=\frac{(q^{r-1}z_1/z_2;p)_\infty(q^{r+1}z_1/z_2;p^*)_\infty}{(q^{r+1}z_1/z_2;p)_\infty(q^{r-1}z_1/z_2;p^*)_\infty}u^-(z_2,p)k(z_1,p), \tag{3.44}$$

$$k(z_1,p)x^+(z_2)=\frac{(q^{r^*+1}z_1/z_2;p^*)_\infty(q^{r^*-1}z_2/z_1;p)_\infty}{(q^{r^*-1}z_1/z_2;p^*)_\infty(q^{r^*+1}z_2/z_1;p)_\infty}x^+(z_2)k(z_1,p), \tag{3.45}$$

$$k(z_1,p)x^-(z_2)=\frac{(q^{r-1}z_1/z_2;p^*)_\infty(q^{r+1}z_2/z_1;p)_\infty}{(q^{r+1}z_1/z_2;p^*)_\infty(q^{r-1}z_2/z_1;p)_\infty}x^-(z_2)k(z_1,p). \tag{3.46}$$

Proposition 3.4: The currents $e(z,p)$, $f(z,p)$, and $k(z,p)$ satisfy the following commutation relations:

$$k(z_1,p)k(z_2,p)=z^{-1/r^*+1/r}\rho(z_1/z_2)k(z_2,p)k(z_1,p), \tag{3.47}$$

$$k(z_1,p)e(z_2,p)=\frac{\Theta_{p^*}(q^{r^*+1}z_1/z_2)}{\Theta_{p^*}(q^{r^*-1}z_1/z_2)}e(z_2,p)k(z_1), \tag{3.48}$$

$$k(z_1,p)f(z_2,p)=\frac{\Theta_{p}(q^{r-1}z_1/z_2)}{\Theta_{p}(q^{r+1}z_1/z_2)}f(z_2,p)k(z_1,p). \tag{3.49}$$

Here we have set

$$\rho(z)=\frac{\rho^{+*}(z)}{\rho^{+}(z)}, \tag{3.50}$$

where $\rho^{+}(z)$ *is given in (2.21) and* $\rho^{+*}(z)=\rho^{+}(z)|_{r\to r^*}$.

D. Elliptic algebra $U_{q,p}(A_2^{(2)})$

Now we give a definition of the elliptic algebra $U_{q,p}(A_2^{(2)})$. For this purpose, we introduce a Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$ generated by P, Q, and $\overline{\alpha}$,

$$[P,Q]=1,\quad [Q,\overline{\alpha}]=\pi i,\quad [P,\overline{\alpha}]=0, \tag{3.51}$$

$$[P,P]=[Q,Q]=[\overline{\alpha},\overline{\alpha}]=0. \tag{3.52}$$

Definition 3.4 (Elliptic Currents): We define the elliptic (total) currents $E(z)$, $F(z)$, *and* $K(z)$ *by*

$$E(z)=e(z)e^{\overline{\alpha}}e^{-Q}z^{-P/r^*}, \tag{3.53}$$

$$F(z)=f(z)e^{-\overline{\alpha}}z^{P/r+h/2r}, \tag{3.54}$$

$$K(z)=k(z)e^{-Q}z^{(1/r-1/r^*)P+h/2r}. \tag{3.55}$$

Let us introduce the auxiliary currents $H^{\pm}(z)$ by

$$H^{\pm}(z)=H(q^{\pm(r-c/2)}z), \tag{3.56}$$

$$H(z)=\psi(z)e^{-Q}z^{(1/r-1/r^*)P+h/2r}=\kappa K(qz)K(z)^{-1}K(q^{-1}z), \tag{3.57}$$

where

$$\kappa=\frac{\{pq^8\}\{pq^5\}\{pq^3\}\{pq^4\}^2\{p\}\{p^*q^7\}^*\{p^*q\}^*\{p^*q^2\}^{*2}\{p^*q^6\}^{*2}}{\{pq^7\}\{pq\}\{pq^2\}^2\{pq^6\}^2\{p^*\}^*\{p^*q^8\}^*\{p^*q^5\}^*\{p^*q^3\}^*\{p^*q^4\}^{*2}}. \tag{3.58}$$

From the commutation relations of the currents $e(z,p)$, $f(z,p)$ and $k(z,p)$, we can verify the following relations.

Theorem 3.5: *The elliptic currents* $E(z)$, $F(z)$, *and* $K(z)$ *satisfy the following commutation relations:*

$$K(z_1)K(z_2)=\rho(z_1/z_2)K(z_2)K(z_1), \tag{3.59}$$

$$K(z_1)E(z_2)=-\frac{\left[u_1-u_2+\frac{r^*+1}{2}\right]^*}{\left[u_1-u_2+\frac{r^*-1}{2}\right]^*}E(z_2)K(z_1), \tag{3.60}$$

$$K(z_1)F(z_2)=-\frac{\left[u_1-u_2+\dfrac{r-1}{2}\right]}{\left[u_1-u_2+\dfrac{r+1}{2}\right]}F(z_2)K(z_1), \tag{3.61}$$

$$E(z_1)E(z_2)=-\frac{[u_1-u_2+1]^*[u_1-u_2-\frac{1}{2}]^*}{[u_1-u_2-1]^*[u_1-u_2+\frac{1}{2}]^*}E(z_2)E(z_1), \tag{3.62}$$

$$F(z_1)F(z_2)=-\frac{[u_1-u_2-1][u_1-u_2+\frac{1}{2}]}{[u_1-u_2+1][u_1-u_2-\frac{1}{2}]}F(z_2)F(z_1), \tag{3.63}$$

$$[E(z_1),F(z_2)]=\frac{1}{q-q^{-1}}(H^+(q^{c/2}z_2)\delta(q^{-c}z_1/z_2)-H^-(q^{-c/2}z_2)\delta(q^cz_1/z_2)). \tag{3.64}$$

Here $\rho(z)$ is given in (3.50). The elliptic currents $E(z)$ and $F(z)$ satisfy the following Serre relations:

$$\begin{aligned}&\sum_{\sigma\in S_3}\frac{(p^*q^2z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-1}z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-1}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty(p^*q^{-1}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*qz_{\sigma(3)}/z_{\sigma(1)};p^*)_\infty(p^*qz_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty(p^*qz_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty}\\&\times z_{\sigma(1)}^{-1/2r^*}z_{\sigma(2)}^{-1/r^*}\left(z_{\sigma(1)}\frac{(q^2z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^2z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}-qz_{\sigma(2)}\right.\\&\left.\times\frac{(p^*q^2z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^2z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}{(p^*q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p^*)_\infty(p^*q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p^*)_\infty}\right)E(z_{\sigma(1)})E(z_{\sigma(2)})E(z_{\sigma(3)})=0,\end{aligned} \tag{3.65}$$

and

$$\begin{aligned}&\sum_{\sigma\in S_3}\frac{(pqz_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^{-2}z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pqz_{\sigma(3)}/z_{\sigma(2)};p)_\infty(pqz_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^{-1}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pq^{-1}z_{\sigma(3)}/z_{\sigma(1)};p)_\infty(pq^{-1}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\\&\times z_{\sigma(1)}^{2/r}z_{\sigma(2)}^{1/r}\left(z_{\sigma(1)}\frac{(q^{-2}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^{-2}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^2z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\right.\\&\left.-q^{-1}z_{\sigma(2)}\frac{(pq^{-2}z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(q^{-2}z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}{(pq^2z_{\sigma(2)}/z_{\sigma(1)};p)_\infty(pq^2z_{\sigma(3)}/z_{\sigma(2)};p)_\infty}\right)F(z_{\sigma(1)})F(z_{\sigma(2)})F(z_{\sigma(3)})=0.\end{aligned} \tag{3.66}$$

Definition 3.5 (Elliptic Algebra $U_{q,p}(A_2^{(2)})$): We define the elliptic algebra $U_{q,p}(A_2^{(2)})$ to be the associative algebra generated by the currents $E(z)$, $F(z)$, and $K(z)$ satisfying the relations (3.56)–(3.66).

Corollary 3.6: The construction of $E(z)$, $F(z)$, and $K(z)$ given in (3.53)–(3.55) is a realization of the elliptic algebra $U_{q,p}(A_2^{(2)})$ in terms of the Drinfeld generator of the quantum group $U_q(A_2^{(2)})$ and the Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$.

For later convenience, let us introduce auxiliary currents $K_\epsilon(z),(\epsilon=0,\pm)$ by

$$K_+(z)=K(q^{r-2}z)=k(q^{r-2}z)e^{-Q}(q^{r-2}z)^{(1/r-1/r^*)P+h/2r}, \tag{3.67}$$

$$K_0(z)=K(q^rz)^{-1}K(q^{r-1}z)=k(q^rz)^{-1}k(q^{r-1}z)q^{(1/r^*-1/r)P-h/2r}, \tag{3.68}$$

$$K_-(z)=K(q^{r+1}z)^{-1}=k(q^{r+1}z)^{-1}(q^{r+1}z)^{(1/r^*-1/r)P-h/2r}e^Q. \tag{3.69}$$

Then one can verify the following relations:

Proposition 3.7:

$$K_+(z_1)E(z_2)=-\frac{\left[u_1-u_2+\frac{c-1}{2}\right]^*}{\left[u_1-u_2+\frac{c-3}{2}\right]^*}E(z_2)K_+(z_1), \tag{3.70}$$

$$K_0(z_1)E(z_2)=\frac{\left[u_1-u_2+\frac{c}{2}\right]^*\left[u_1-u_2+\frac{c-1}{2}\right]^*}{\left[u_1-u_2+\frac{c}{2}-1\right]^*\left[u_1-u_2+\frac{c+1}{2}\right]^*}E(z_2)K_0(z_1), \tag{3.71}$$

$$K_-(z_1)E(z_2)=-\frac{\left[u_1-u_2+\frac{c}{2}\right]^*}{\left[u_1-u_2+\frac{c}{2}+1\right]^*}E(z_2)K_-(z_1), \tag{3.72}$$

$$K_+(z_1)F(z_2)=-\frac{[u_1-u_2-\frac{3}{2}]}{[u_1-u_2-\frac{1}{2}]}F(z_2)K_+(z_1), \tag{3.73}$$

$$K_0(z_1)F(z_2)=\frac{[u_1-u_2-1][u_1-u_2+\frac{1}{2}]}{[u_1-u_2][u_1-u_2-\frac{1}{2}]}F(z_2)K_0(z_1), \tag{3.74}$$

$$K_-(z_1)F(z_2)=-\frac{[u_1-u_2+1]}{[u_1-u_2]}F(z_2)K_-(z_1), \tag{3.75}$$

$$H^{\pm}(q^{\pm c/2}z)=H(q^{\pm r}z)=\kappa K_-(z)^{-1}K_0(z)=\kappa' K_+(qz)K_0(qz)^{-1}. \tag{3.76}$$

Here μ is given in (3.58) and κ' is given by

$$\kappa'=\frac{\{pq^{10}\}\{pq^7\}\{pq^5\}\{pq^6\}^2\{pq^2\}\{p^*q^9\}^*\{p^*q^3\}^*\{p^*q^5\}^{*2}\{p^*q^8\}^{*2}}{\{pq^9\}\{pq^3\}\{pq^5\}^2\{pq^8\}^2\{p^*q^2\}^*\{p^*q^{10}\}^*\{p^*q^7\}^*\{p^*q^5\}^*\{p^*q^6\}^{*2}}. \tag{3.77}$$

IV. HALF-CURRENTS

As a preparation for the RLL-formulation of the elliptic algebra $U_{p,q}(A_2^{(2)})$ in the next section, we here introduce the half currents, and investigate their commutation relations.

Let us first summarize the commutation relations between the Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$ and the elliptic currents. From (3.53)–(3.55), we have the following relations:

Proposition 4.1:

$$[E(z),P]=E(z),\quad \left[F(z),P+\frac{h}{2}\right]=F(z), \tag{4.1}$$

$$\left[E(z),P+\frac{h}{2}\right]=0,\ [F(z),P]=0, \tag{4.2}$$

$$[K_+(z),P]=K_+(z)=\left[K_+(z),P+\frac{h}{2}\right], \tag{4.3}$$

$$[K_0(z),P]=0=\left[K_0(z),P+\frac{h}{2}\right], \tag{4.4}$$

$$[K_-(z),P]=-K_-(z)=\left[K_-(z),P+\frac{h}{2}\right]. \tag{4.5}$$

Now we define the half currents $E^+_{-,0}(u)$, $E^+_{0,+}(u)$, $E^+_{-,+}(u)$, $F^+_{0,-}(u)$, $F^+_{+,0}(u)$, $F^+_{+,-}(u)$, and $K^+_\epsilon(u),(\epsilon=0,\pm)$, by the following formulas.

Definition 4.1 (Half Currents):

$$K^+_\epsilon(u)=K_\epsilon(z), \qquad (\epsilon=0,\pm), \tag{4.6}$$

$$E^+_{-,0}(u)=a^*_{-0}\oint_{C^*_{-0}}\frac{dz'}{2\pi iz'}E(z')\frac{\left[u-u'-P+\frac{c+1}{2}\right]^*_+[1]^*}{\left[u-u'+\frac{c}{2}\right]^*\left[P-\frac{1}{2}\right]^*_+}, \tag{4.7}$$

$$E^+_{0,+}(u)=a^*_{0+}\oint_{C^*_{0+}}\frac{dz'}{2\pi iz'}E(z')\frac{\left[u-u'-P+\frac{c}{2}\right]^*_+[1]^*}{\left[u-u'+\frac{c-1}{2}\right]^*\left[P-\frac{1}{2}\right]^*_+}, \tag{4.8}$$

$$E^+_{-,+}(u)=a^*_{-+}\oint\oint_{C^*_{-+}}\frac{dz'}{z'}\frac{dz''}{z''}E(z')E(z'')\frac{[1]^{*2}}{\left[P-\frac{1}{2}\right]^*_+[2P-2]^*}$$
$$\times\frac{\left[u-u'-2P+2+\frac{c}{2}\right]^*[u'-u''-P]^*_+}{\left[u-u'+\frac{c}{2}\right]^*\left[u'-u''-\frac{1}{2}\right]^*}, \tag{4.9}$$

$$F^+_{0,-}(u)=a_{0-}\oint_{C_{0-}}\frac{dz'}{2\pi iz'}F(z')\frac{\left[u-u'+P+\frac{h-1}{2}\right]_+[1]}{[u-u']\left[P+\frac{h-1}{2}\right]_+}, \tag{4.10}$$

$$F^+_{+,0}(z)=a_{+0}\oint_{C_{+0}}\frac{dz'}{2\pi iz'}F(z')\frac{\left[u-u'+P+\frac{h}{2}-1\right]_+[1]}{\left[u-u'-\frac{1}{2}\right]\left[P+\frac{h-1}{2}\right]_+}, \tag{4.11}$$

$$F^{+}_{+,-}(u)=a_{+-}\oint\oint_{C_{+-}}\frac{dz'}{2\pi iz'}\frac{dz''}{2\pi iz''}F(z')F(z'')\frac{\left[P+\frac{h}{2}-1\right]_{+}[1]^2}{\left[P+\frac{h-3}{2}\right]_{+}\left[P+\frac{h}{2}-2\right]_{+}[2P+h-2]}$$
$$\times\frac{[u-u'+2P+h-3][u-u''+1]\left[u'-u''+P+\frac{h}{2}-1\right]_{+}}{[u-u'][u-u'']\left[u'-u''+\frac{1}{2}\right]}. \tag{4.12}$$

Here C^{*}_{-0} is a simple closed contour that encircles $pq^{c}z$ but not $q^{c}z$. We abbreviate it as C^{*}_{-0}:$|p^{*}q^{c}z|<|z'|<|q^{c}z|$. Similarly the others are given by

$$C^{*}_{-0}:\ |p^{*}q^{c}z|<|z'|<|q^{c}z|, \tag{4.13}$$

$$C^{*}_{0+}:\ |p^{*}q^{c-1}z|<|z'|<|q^{c-1}z|, \tag{4.14}$$

$$C^{*}_{-+}:\ |p^{*}q^{c}|<|z'|<|q^{c}z|,\ |p^{*}q^{c}z|<|z''|<|q^{c}z|,\ |p^{*}qz'|<|z''|<|qz'|, \tag{4.15}$$

$$C_{0-}:\ |pz|<|z'|<|z|, \tag{4.16}$$

$$C^{*}_{0+}:\ |pq^{-1}z|<|z'|<|q^{-1}z|, \tag{4.17}$$

$$C_{+-}:\ |pz|<|z'|<|z|,\ |pz|<|z''|<|z|,\ |pqz'|<|z''|<|qz'|. \tag{4.18}$$

The constants $a^{*}_{-0},a^{*}_{0+},a^{*}_{-+}$, a_{0-},a_{+0},a_{+-} are chosen to satisfy

$$\frac{\mu a_{0-}a^{*}_{-0}[1]^{*}}{q-q^{-1}}=-1=\frac{\mu' a_{+0}a^{*}_{0+}[1]^{*}}{q-q^{-1}},\quad a_{+-}=a_{0-}a_{0-},\quad a^{*}_{-+}=a^{*}_{-0}a^{*}_{-0}. \tag{4.19}$$

We then verify the following commutation relations.

Theorem 4.5: *The half-currents satisfy the following relations:*

$$K^{+}_{\pm}(u_1)K^{+}_{\pm}(u_2)=\rho(u)K^{+}_{\pm}(u_2)K^{+}_{\pm}(u_1), \tag{4.20}$$

$$K^{+}_{0}(u_1)K^{+}_{0}(u_2)=\frac{\rho(u)\rho(u)}{\rho(u+\frac{1}{2})\rho(u-\frac{1}{2})}K^{+}_{0}(u_2)K^{+}_{0}(u_1), \tag{4.21}$$

$$K^{+}_{-}(u_1)K^{+}_{+}(u_2)=K^{+}_{+}(u_2)K^{+}_{-}(u_1)\rho(u)\frac{[u_1-u_2+1][u_1-u_2+\frac{3}{2}][u_1-u_2]^{*}[u_1-u_2+\frac{1}{2}]^{*}}{[u_1-u_2][u_1-u_2+\frac{1}{2}][u_1-u_2+1]^{*}[u_1-u_2+\frac{3}{2}]^{*}}, \tag{4.22}$$

$$K^{+}_{-}(u_1)K^{+}_{0}(u_2)=\rho(u)\frac{[u_1-u_2]^{*}[u_1-u_2+1]}{[u_1-u_2+1]^{*}[u_1-u_2]}K^{+}_{0}(u_2)K^{+}_{-}(u_1), \tag{4.23}$$

$$K^{+}_{0}(u_1)K^{+}_{+}(u_2)=\rho(u)\frac{[u_1-u_2]^{*}[u_1-u_2+1]}{[u_1-u_2+1]^{*}[u_1-u_2]}K^{+}_{+}(u_2)K^{+}_{0}(u_1), \tag{4.24}$$

$$K^{+}_{-}(u_1)^{-1}E^{+}_{-,0}(u_2)K^{+}_{-}(u_1)=-E^{+}_{-,0}(u_2)\frac{[u+1]^{*}}{[u]^{*}}+E^{+}_{-,0}(u_1)\frac{[P+\frac{1}{2}+u]^{*}_{+}[1]^{*}}{[P+1/2]^{*}_{+}[u]^{*}}, \tag{4.25}$$

$$K_+^+(u_2)^{-1}E_{0,+}^+(u_1)K_+^+(u_2)=-\frac{[u+1]^*}{[u]^*}E_{0,+}^+(u_1)+\frac{[-P+\frac{1}{2}+u]_+^*[1]^*}{[-P+\frac{1}{2}]}{}_+^*[u]^*E_{0,+}^+(u_2), \tag{4.26}$$

$K_-^+(u_1)^{-1}E_{-,+}^+(u_2)K_-^+(u_1)$

$$\begin{aligned}&=E_{-,+}^+(u_2)\frac{[u+\frac{3}{2}]^*[u+1]^*}{[u+\frac{1}{2}]^*[u]^*}+K_-^+(u_1)^{-1}E_{-,0}^+(u_2)K_-^+(u_1)E_{-,0}^+(u_1)\frac{[-P-1-u]_+^*[1]^*}{[P+\frac{1}{2}]_+^*[u+\frac{1}{2}]^*}\\&\quad-E_{-,+}(u_1)\left(\frac{[-2P+1-u]^*[u+\frac{3}{2}]^*[1]^*}{[-2P+1]^*[u+\frac{1}{2}]^*[u]^*}+\frac{[2P-2]^*[P]_+^*[-2P-\frac{1}{2}-u]^*[1]^*}{[2P]^*[P-1]_+^*[-2P+1]^*[u+\frac{1}{2}]^*}\right),\end{aligned} \tag{4.27}$$

$$K_-^+(u_1)F_{0,-}^+(u_2)K_-(u_1)^{-1}=-\frac{[u+1]}{[u]}F_{0,-}^+(u_2)+\frac{\left[-P+\frac{-h+1}{2}+u\right]_+[1]}{\left[-P+\frac{-h+1}{2}\right]_+[u]}F_{0,-}^+(u_2), \tag{4.28}$$

$$K_+^+(u_2)F_{+,0}^+(u_1)K_+^+(u_2)^{-1}=-F_{+,0}^+(u_1)\frac{[u+1]}{[u]}+F_{+,0}^+(u_2)\frac{\left[P+\frac{h+1}{2}+u\right]_+[1]}{\left[P+\frac{h+1}{2}\right]_+[u]}, \tag{4.29}$$

$K_-^+(u_1)F_{+,-}^+(u_2)K_-^+(u_1)^{-1}$

$$\begin{aligned}&=\frac{\left[u+\frac{3}{2}\right][u+1]}{\left[u+\frac{1}{2}\right][u]}F_{+,-}^+(u_2)-\frac{\left[P+\frac{h}{2}-1-u\right]_+[1]}{\left[-P+\frac{-h+1}{2}\right]\left[u+\frac{1}{2}\right]}F_{0,-}^+(u_1)K_-^+(u_1)F_{0,-}^+(u_2)K_-^+(u_1)^{-1}\\&\quad-\left(\frac{\left[u+\frac{3}{2}\right][2P+h+1-u][1]}{\left[u+\frac{1}{2}\right][u][2P+h+1]}+\frac{\left[2P+h-\frac{1}{2}-u\right][1][2P+h+2]\left[P+\frac{h}{2}\right]_+}{[2P+h+1][2P+h]\left[P+\frac{h}{2}+1\right]_+\left[u+\frac{1}{2}\right]}\right)F_{+,-}^+(u_1),\end{aligned} \tag{4.30}$$

$$[E^+_{-,0}(u_1),F^+_{0,-}(u_2)]$$

$$=-K_0^+(u_2)\frac{\left[-P-\frac{1}{2}+u\right]_+^*[1]^*}{\left[-P-\frac{1}{2}\right]_+^*[u]^*}K_-^+(u_2)^{-1}+K_-^+(u_1)^{-1}\frac{\left[-P+\frac{-h+1}{2}+u\right]_+[1]}{\left[-P+\frac{-h+1}{2}\right]_+[u]}K_0^+(u_1), \tag{4.31}$$

$$[E^+_{0,+}(u_1),F^+_{+,0}(u_2)]$$

$$=-K_0^+(u_2)^{-1}\frac{\left[P+\frac{h+1}{2}+u\right]_+[1]}{\left[P+\frac{h+1}{2}\right]_+[u+1]}K_+^+(u_2)+K_+^+(u_1)\frac{\left[P-\frac{1}{2}+u\right]_+^*[1]^*}{\left[P-\frac{1}{2}\right]_+^*[u+1]^*}K_0^+(u_1)^{-1}, \tag{4.32}$$

where $u=u_1-u_2$.

Proof: The relations (4.20)–(4.24) are direct consequences of the commutation relation of the elliptic current $K(z)$. Let us consider the relations (4.25)–(4.32). These relations can be proved by reducing them to identities of the theta functions. We show the relation (4.25). The relations (4.26), (4.28), and (4.29) can be proved in the same way. From the definition of the half current (4.7) and the commutation relation of (3.72), the LHS of (4.25) yields

$$K_-^+(u_1)E^+_{-,0}(u_2)K_-^+(u_1)^{-1}$$
$$=-a^*_{-,0}\oint_{C^*_{-0}}\frac{dz'}{2\pi iz'}E(z')\frac{\left[u_1-u'+\frac{c}{2}+1\right]^*\left[u_2-u'-P+\frac{c-1}{2}\right]_+^*[1]^*}{\left[u_1-u'+\frac{c}{2}\right]^*\left[u_2-u'+\frac{c}{2}\right]^*\left[P+\frac{1}{2}\right]_+^*}. \tag{4.33}$$

Then the equality is verified by the following identity of the theta functions:

$$-\frac{\left[u_1-u'+\frac{c}{2}+1\right]^*\left[u_2-u'-P+\frac{c-1}{2}\right]_+^*}{\left[u_1-u'+\frac{c}{2}\right]^*\left[u_2-u'+\frac{c}{2}\right]^*\left[P+\frac{1}{2}\right]_+^*}=-\frac{\left[u_2-u'-P+\frac{c+1}{2}\right]_+^*[u_1-u_2+1]^*}{\left[u_2-u'+\frac{c}{2}\right]^*[u_1-u_2]^*\left[P-\frac{1}{2}\right]_+^*}$$
$$+\frac{\left[u_1-u'-P+\frac{c+1}{2}\right]_+^*\left[u_1-u_2+P+\frac{1}{2}\right]_+^*[1]^*}{\left[u_1-u'+\frac{c}{2}\right]^*[u_1-u_2]^*\left[P-\frac{1}{2}\right]_+^*\left[P+\frac{1}{2}\right]_+^*}.$$

Next, we show the relation (4.31). The relation (4.32) can be proved in the same way. Integrating the delta function appearing in (3.64) and using (3.76), we have

$$
\begin{aligned}
&(\mu a_{0-}a^{*}_{-0})^{-1}(q-q^{-1})[E^{+}_{-,0}(u_1),F^{+}_{0,-}(u_2)] \\
&\quad=\oint_{C^+}\frac{dz'}{2\pi i z'}K^{+}_{-}(u')^{-1}K^{+}_{0}(u')\frac{\left[u_1-u'-P+\frac{1}{2}\right]^{*}_{+}[1]^{*}\left[u_2-u'+P+\frac{h-1}{2}\right]_{+}[1]}{[u_1-u']^{*}\left[P-\frac{1}{2}\right]^{*}_{+}[u_2-u']\left[P+\frac{h-1}{2}\right]_{+}} \\
&\quad-\oint_{C^-}\frac{dz'}{2\pi i z'}K^{+}_{-}(u'-r)^{-1}K^{+}_{0}(u'-r) \\
&\quad\times\frac{\left[u_1-u'-P+c+\frac{1}{2}\right]^{*}_{+}[1]^{*}\left[u_2-u'+P+\frac{h-1}{2}\right]_{+}[1]}{[u_1-u'+c]^{*}\left[P-\frac{1}{2}\right]^{*}_{+}[u_2-u']\left[P+\frac{h-1}{2}\right]_{+}}.
\end{aligned}
\tag{4.34}
$$

Here the contours $C^{\pm}$ are now

$$C^{+}:\ |p^{*}z_1|,|pz_2|<|z'|<|z_1|,|z_2|, \tag{4.35}$$

$$C^{-}:\ |pz_1|,|pz_2|<|z'|<|q^{2c}z_1|,|z_2|. \tag{4.36}$$

When we change the integration variable $z'\to pz'$ in the second term, the integrand becomes the same as the first term, but the contour C^{-} is changed to $\tilde{C}^{-}$ given by

$$\tilde{C}^{-}:\ |z_1|,|z_2|<|z'|<|p^{-1}q^{2c}z_1|,|p^{-1}z_2|. \tag{4.37}$$

Taking the residues at $z'=z_1,z_2$, we get (4.31).

We give a proof of (4.27) in Appendix C. One can prove (4.30) in a similar way.

Q.E.D.

V. THE L-OPERATOR OF $U_{q,p}(A_2^{(2)})$ AND RELATION TO $\mathcal{B}_{q,\lambda}(A_2^{(2)})$

In this section, we clarify the relation between two elliptic algebras $U_{q,p}(A_2^{(2)})$ and $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. For this purpose, we first construct a L-operator which gives the RLL-formulation of $U_{q,p}(A_2^{(2)})$. Then modifying L-operator by removing the Heisenberg generators $Q,\overline{\alpha}$, we derive the dynamical RLL-relation (5.8) characterizing the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$.

A. L-operator of $U_{q,p}(A_2^{(2)})$

Definition 5.1: By using the half-currents, we define the L-operator $\hat{L}^{+}(u)\in \mathrm{End}(\mathbb{C}^3)\otimes U_{q,p}(A_2^{(2)})$ *as follows:*

$$
\hat{L}^{+}(u)=\begin{pmatrix}1 & F^{+}_{+0}(u) & F^{+}_{+-}(u)\\ 0 & 1 & F^{+}_{0-}(u)\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}K^{+}_{+}(u) & 0 & 0\\ 0 & K^{+}_{0}(u) & 0\\ 0 & 0 & K^{+}_{-}(u)\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ E^{+}_{0+}(u) & 1 & 0\\ E^{+}_{-+}(u) & E^{+}_{-0}(u) & 1\end{pmatrix}.
\tag{5.1}
$$

Here matrix elements are the half-currents given in the previous section.

By a direct comparison with the relations of the half-currents appeared in Theorem 4.2, we get the following commutation relations of the L-operator:

Theorem 5.1: *The L-operator* $\hat{L}^{+}(u)$ *satisfies the following* $RLL=LLR^{*}$ *relation:*

$$R^{+(12)}(u_1-u_2,P+h/2)\hat{L}^{+(1)}(u_1)\hat{L}^{+(2)}(u_2)$$
$$=\hat{L}^{+(2)}(u_2)\hat{L}^{+(1)}(u_1)R^{+*(12)}(u_1-u_2,P-(h^{(1)}+h^{(2)})/2). \tag{5.2}$$

The above equation should be understood as equation of the operators acting on the space $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes U_{q,p}(A_2^{(2)})$. The operator h in LHS acts on $U_{q,p}(A_2^{(2)})$, whereas the operator $h^{(1)}+h^{(2)}$ in RHS acts on $\mathbb{C}^3 \otimes \mathbb{C}^3$ as

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix} \otimes 1 + 1 \otimes \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

B. $U_{q,p}(A_2^{(2)})$ and $\mathcal{B}_{q,\lambda}(A_2^{(2)})$

Based on the above theorem, we give a relation between $U_{q,p}(A_2^{(2)})$ and $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. We argue that the RLL relation (5.2) is equivalent to the dynamical RLL relation of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. Hence we can regard the elliptic currents in $U_{q,p}(A_2^{(2)})$ as an elliptic analog of the Drinfeld currents in $U_q(A_2^{(2)})$ providing a new realization of the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. In order to show this, we consider the realization of $U_{q,p}(A_2^{(2)})$ given in (3.53)–(3.55) and modify the half-currents in such a way that they have no $Q, \bar{\alpha}$ dependence,

$$k_+(u,P)=K_+(u)e^{Q}, \quad k_0(u,P)=K_0(u) \quad k_-(u,P)=K_-(u)e^{-Q}, \tag{5.3}$$

$$f_{+,0}(u,P)=e^{\bar{\alpha}}F_{+,-}(u), \quad f_{0,-}(u,P)=e^{\bar{\alpha}}F_{0,-}(u), \quad f_{+,-}(u,P)=e^{\bar{\alpha}}F_{+,-}(u)e^{\bar{\alpha}}, \tag{5.4}$$

$$e_{0,+}(u,P)=E_{0,+}(u)e^{Q}e^{-\bar{\alpha}}, \quad e_{-,0}(u,P)=e^{Q}e^{-\bar{\alpha}}E_{-,0}(u),$$
$$e_{-,+}(u,P)=e^{Q}e^{-\bar{\alpha}}E_{-,+}(u)e^{Q}e^{-\bar{\alpha}}. \tag{5.5}$$

We regard them as the currents in $U_q(A_2^{(2)})$ with parameters P and r. Then we define a dynamical L-operator $\hat{L}^+(u,P)$ by

$$\hat{L}^+(u,P)=\begin{pmatrix} 1 & f^+_{+0}(u,P) & f^+_{+-}(u,P) \\ 0 & 1 & f^+_{0-}(u,P) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} k^+_+(u,P) & 0 & 0 \\ 0 & k^+_0(u,P) & 0 \\ 0 & 0 & k^+_-(u,P) \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & 0 & 0 \\ e^+_{0+}(u,P) & 1 & 0 \\ e^+_{-+}(u,P) & e^+_{-0}(u,P) & 1 \end{pmatrix}. \tag{5.6}$$

The two L-operators $\hat{L}^+(u)$ and $\hat{L}^+(u,P)$ are related by

$$\hat{L}^+(u,P)=\hat{L}^+(u)\begin{pmatrix} e^{Q} & & \\ & 1 & \\ & & e^{-Q} \end{pmatrix}=\hat{L}^+(u)e^{Qh^{(1)}/2}. \tag{5.7}$$

Here

$$h^{(1)}=\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix} \otimes 1.$$

Substituting this into (5.2) and moving the factor $e^{-Qh^{(j)}/2}$ $(j=1,2)$ to the right end in the both sides, we get the following statement:

Corollary 5.2: The dynamical L-operator $L^+(u,P)$ satisfies the dynamical RLL relation,

$$R^{+(12)}(u_1-u_2,P+h/2)L^{+(1)}(u_1,P)L^{+(2)}(u_2,P+h^{(1)}/2)$$
$$=L^{+(2)}(u_2,P)L^{+(1)}(u_1,P+h^{(2)}/2)R^{+*(12)}(u_1-u_2,P). \tag{5.8}$$

Comparing this with (2.23), we identify our $L^+(u,P)$ with $L^+(u,s)$ in (2.23) and s with P. We hence regard the elliptic currents $E(z)$, $F(z)$, and $K(z)$ in $U_{q,p}(A_2^{(2)})$ as the Drinfeld currents of the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$, although $U_{q,p}(A_2^{(2)})$ and $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ are different by tensoring the Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$. More precisely, $U_{q,p}(A_2^{(2)})$ is an extension of the algebra $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ by tensoring the Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$; first tensoring the generators e^Q, e^{α}, then regarding $s=P$ and imposing the commutation relations (3.51) and (3.52). Naively we regard $U_{q,p}(A_2^{(2)})$ as $\mathcal{B}_{q,\lambda}(A_2^{(2)})\otimes_{\mathbb{C}\{P\}}\mathbb{C}\{\mathcal{H}\}$.

VI. VERTEX OPERATORS

Tensoring the Heisenberg algebra breaks down the coalgebra structure of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. But we can define the $U_{q,p}(A_2^{(2)})$ counterparts of the intertwining operators of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. We call such operators the vertex operators of $U_{q,p}(A_2^{(2)})$. In this section, we study such vertex operators and compare them with those of the dilute A_L model obtained in Ref. 15.

A. Intertwining relations

We here derive the $U_{q,p}(A_2^{(2)})$ counterparts of the dynamical intertwining relations (2.27)–(2.28). In the next subsection, we use such relations to derive a free field realization of the vertex operators.

Let us first define an extension of the U_q modules by

$$\hat{\mathcal{F}}=\bigoplus_{\mu\in\mathbb{Z}}\mathcal{F}\otimes e^{\mu Q}.$$

Let $\Phi_W(u,P)$ and $\Psi_W^*(u,P)$ be the type I and type II intertwining operators of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ (2.27)–(2.28). We define type I and type II vertex operators $\hat{\Phi}_W(u),\hat{\Psi}_W^*(u)$ of $U_{q,p}(A_2^{(2)})$ as the following extensions of the corresponding intertwining operators of $\mathcal{B}_{q,\lambda}(A_2^{(2)})$:

$$\hat{\Phi}_W(u)=\Phi_W(u+c/2,P) \quad :\hat{\mathcal{F}}\to\hat{\mathcal{F}}'\otimes W_z, \tag{6.1}$$

$$\hat{\Psi}_W^*(u)=\Psi_W^*(u,P)e^{h^{(1)}Q/2} \quad :W_z\otimes\hat{\mathcal{F}}\to\hat{\mathcal{F}}'. \tag{6.2}$$

From the commutation relation of P and Q, the new operators $\hat{\Phi}_W(u)$ and $\hat{\Psi}_W^*(u)$ satisfy the following "intertwining relations":

$$\hat{\Phi}_W^{(3)}(u_2)\hat{L}_V^{+(1)}(u_1)=R_{VW}^{+(1,3)}(u_1-u_2,P+h/2)\hat{L}_V^{+(1)}(u_1)\hat{\Phi}_W^{(3)}(u_2), \tag{6.3}$$

$$\hat{L}_V^{+(1)}(u_1)\hat{\Psi}_W^{*(2)}(u_2)=\hat{\Psi}_W^{*(2)}(u_2)\hat{L}_V^{+(1)}(u_1)R_{VW}^{+*(1,2)}(u_1-u_2,P-(h^{(1)}+h^{(2)})/2). \tag{6.4}$$

Now let us restrict ourselves to the vector representation $W=V\cong\mathbb{C}v_+\oplus\mathbb{C}v_0\oplus\mathbb{C}v_-$. In this case, the R-matrix $R_{VV}^+(u,P)$ is given by $R^+(u,P)$ in (2.18), and the L-operator $\hat{L}_V^+(u,P)$ by $\hat{L}^+(u,P)$ in (5.6). Let us set the components of the vertex operators $\Phi_j(u),\Psi_j^*(u),(j=\pm,0)$ by

$$\hat{\Phi}\left(u-\frac{1}{2}\right)=\sum_{j=\pm,0}\Phi_j(u)\otimes v_j, \tag{6.5}$$

$$\hat{\Psi}*\left(u-\frac{c+1}{2}\right)(v_j\otimes\cdot)=\Psi_j^*(u), \tag{6.6}$$

and the matrix elements of the L-operator $\hat{L}^+(u)$ by

$$\hat{L}^+(u)v_j=\sum_{m=0,\pm} v_m L^+_{m,j}(u). \tag{6.7}$$

Let us investigate the relations (6.3) and (6.4) in detail. From the components $[(-,-),(j)], j=\pm,0$ of (6.3), we have

$$\Phi_-(u_2+\tfrac{1}{2})L^+_{-,j}(u_1)=\rho^+(u_1-u_2)L^+_{-,j}(u_1)\Phi_-(u_2+\tfrac{1}{2}). \tag{6.8}$$

Putting the definition $L^+_{-,j}(u)=K^+_-(u)E^+_{-,j}(u)$ into the above, we have

$$\Phi_-(u_2+\tfrac{1}{2})K^+_-(u_1)=\rho^+(u_1-u_2)K^+_-(u_1)\Phi_-(u_2+\tfrac{1}{2}), \tag{6.9}$$

$$[\Phi_-(u_1),E^+_{-,0}(u_2)]=0, \tag{6.10}$$

$$[\Phi_-(u_1),E^+_{-,+}(u_2)]=0. \tag{6.11}$$

We have the sufficient condition of (6.10) and (6.11),

$$\Phi_-(u_1)E(u_2)=E(u_2)\Phi_-(u_1), \quad [\Phi_-(z_1),P]=0. \tag{6.12}$$

From the component $[(0,-),(-)]$ of (6.3), we have

$$\begin{aligned}\Phi_-(u_2+\tfrac{1}{2})F^+_{0,-}(u_1)K^+_-(u_1)=&\rho^+(u)\overline{R}^{0-}_{0-}(u,P+h/2)F^+_{0,-}(u_1)K^+_-(u_1)\Phi_-(u_2+\tfrac{1}{2})\\&+\rho^+(u)\overline{R}^{-0}_{0-}(u,P+h/2)K^+_-(u_1)\Phi_0(u_2+\tfrac{1}{2}).\end{aligned} \tag{6.13}$$

Let us assume the operator product $K^+_-(u_1)\Phi_-(u_2+\frac{1}{2})$ has no pole at $u_1-u_2=-1-r$. Later we will check that, for $c=1$, this assumption is satisfied in a free field realization. Then from (6.9), we conclude the operator product $\Phi_-(u_2+\frac{1}{2})K^+_-(u_1)$ has zero at $u_1-u_2=-1-r$. Therefore setting $u_1-u_2=-1-r$ in (6.13), we have

$$0=\frac{[P+h/2+1/2]_+}{[P+h/2-1/2]_+}F^+_{0,-}(u_1)K^+_-(u_1)\Phi_-\left(u_2+\frac{1}{2}\right)+K^+_-(u_1)\Phi_0\left(u_2+\frac{1}{2}\right). \tag{6.14}$$

Then we have

$$\Phi_0(u)=F^+_{0,-}(u-r-\tfrac{1}{2})\Phi_-(u). \tag{6.15}$$

Substituting (6.8) and (6.15) into (6.13), we get

$$\Phi_-(u_1)F(u_2)=-\frac{[u_1-u_2+1/2]}{[u_1-u_2-1/2]}F(u_2)\Phi_-(u_1). \tag{6.16}$$

Similarly, in order to investigate the structure of the component $\Phi_+(u)$, we have, from the components of $[(+,-),(-)]$ of (6.3),

$$\Phi_-(u_2+\tfrac{1}{2})F^+_{+,-}(u_1)K^+_-(u_1)=\rho^+(u)\overline{R}^{+-}_{+-}(u,P+h/2)F^+_{+,-}(u_1)K^+_-(u_1)\Phi_-(u_2+\tfrac{1}{2})$$
$$+\rho^+(u)\overline{R}^{00}_{+-}(u,P+h/2)F^+_{0,-}(u_1)K^+_-(u_1)\Phi_0(u_2+\tfrac{1}{2})$$
$$+\rho^+(u)\overline{R}^{-+}_{+-}(u,P+h/2)K^+_-(u_1)\Phi_+(u_2+\tfrac{1}{2}). \tag{6.17}$$

On the other hand, from the component $[(+,-),(-,-)]$ of RLL relation (5.2), we have

$$K^+_-(u_2)F^+_{+,-}(u_1)K^+_-(u_2)^{-1}=R^{+-}_{+-}(u)F^+_{+,-}(u_1)+R^{00}_{+-}(u)F^+_{0,-}(u_1)K^+_-(u_1)F^+_{0,-}(u_2)K^+_-(u_1)^{-1}$$
$$+R^{-+}_{+-}(u)K^+_-(u_1)F^+_{+,-}(u_2)K^+_-(u_1)^{-1}. \tag{6.18}$$

Putting the above into (6.17), we get

$$\Phi_-(u_2+\tfrac{1}{2})F^+_{+,-}(u_1)K^+_-(u_1)=\rho^+(u)\overline{R}^{-+}_{+-}(u|P+h/2)K_-(u_1)\Phi_+(u_2+\tfrac{1}{2})$$
$$+\rho^+(u)K^+_-(u_2-r)F^+_{+,-}(u_1)K^+_-(u_2-r)^{-1}K^+_-(u_1)\Phi_-(u_2+\tfrac{1}{2})$$
$$+\rho^+(u)\overline{R}^{-+}_{+-}(u|P+h/2)K^+_-(u_1)F^+_{+,-}(u_2-r)\Phi_-(u_2+\tfrac{1}{2}). \tag{6.19}$$

Note that at the point $u_1-u_2=-1-r$, $\rho^+(u)$ has a zero, but $\rho^+(u)\overline{R}^{-+}_{+-}(u|P+h/2)$ have no zeros. In addition, under the same assumption given just below (6.13), the product $\Phi_-(u_2+\frac{1}{2})K^+_-(u_1)$ vanishes at $u_1-u_2=-1-r$. Setting $u_1-u_2=-1-r$ in (6.19), we thus have the following formula for $\Phi_+(z)$:

$$\Phi_+(u)=-F^+_{+,-}(u-r-\tfrac{1}{2})\Phi_-(u). \tag{6.20}$$

In the next section, we construct a free field realization of the type-I vertex operators using the relations (6.9), (6.12), (6.15), (6.16), and (6.20) for $c=1$. We can check that the resultant vertex operators satisfy the intertwining relation (6.3).

Similarly, the sufficient conditions for the type-II vertex operators are extracted from (6.4) as follows:

$$\Psi^*_-\left(u_2+\frac{1+c}{2}\right)K_-(u_1)\rho^{+*}(u)=K^+_-(u_1)\Psi^*_-\left(u_2+\frac{1+c}{2}\right), \tag{6.21}$$

$$\Psi^*_-(u_1)F(u_2)=F(u_2)\Psi^*_-(u_1),\quad [\Psi^*_-(u),P+h/2]=0, \tag{6.22}$$

$$\Psi^*_-(u_1)E(u_2)=-\frac{\left[u_1-u_2-\frac{1}{2}\right]^*}{\left[u_1-u_2+\frac{1}{2}\right]^*}E(u_2)\Psi^*_-(u_1), \tag{6.23}$$

$$\Psi^*_+(u)=-\Psi^*_-(u)E_{-,+}\left(u-\frac{1+c}{2}-r^*\right), \tag{6.24}$$

$$\Psi^*_0(u)=\Psi^*_-(u)E_{-,0}\left(u-\frac{1+c}{2}-r^*\right). \tag{6.25}$$

B. Free field realizations

Now we construct a free field realization of the vertex operators fixing the representation level $c=1$. For this purpose, we introduce the simple root operator α, defined by

$$[h,\alpha]=2,\ [a_m,\alpha]=0,\ [P,\alpha]=0,\ [Q,\alpha]=0,\ [\alpha,\overline{\alpha}]=0. \tag{6.26}$$

If we introduce $\hat{\alpha}$ by

$$\hat{\alpha}=\alpha+\overline{\alpha}, \tag{6.27}$$

we have

$$[h,\hat{\alpha}]=2,\ [a_m,\hat{\alpha}]=0,\ [P,\hat{\alpha}]=0,\ [Q,\hat{\alpha}]=\pi i. \tag{6.28}$$

Then the following statement holds:

Proposition 6.1: For $c=1$, we have the free field realization of the currents $E(z)$ and $F(z)$.

$$E(z)=\epsilon(q):\exp\left(-\sum_{m\neq 0}\frac{1}{[m]_q}\alpha_m z^{-m}\right):e^{\hat{\alpha}}z^{h/2+1/2}e^{-Q}z^{-P/r*}, \tag{6.29}$$

$$F(z)=\epsilon(q):\exp\left(\sum_{m\neq 0}\frac{1}{[m]_q}\beta_m z^{-m}\right):e^{-\hat{\alpha}}z^{-h/2+1/2}z^{P/r+h/2r}. \tag{6.30}$$

Here we have set

$$\epsilon(q)=(q^{1/2}+q^{-1/2})^{-1/2}. \tag{6.31}$$

Together with free field realizations of $K(z)$ (3.55), we get a free field realization of the level one elliptic algebra $U_{q,p}(A_2^{(2)})$.

Now substituting the free field realization of $E(z)$, $F(z)$, $K(z)$ into (3.53)–(3.55), we obtain a realization of the half-currents and the L-operator $\hat{L}^+(u)$ satisfying the RLL-relation (5.2) for $c=1$. Using this L-operator in the ''intertwining relations,'' (6.9), (6.12), (6.15), (6.16), (6.20), for type I and (6.21)–(6.25) for the type II, one can solve them for the vertex operators. The results are stated as follows:

Theorem 6.2: *The highest components of the type-I and type-II vertex operators $\Phi_-(u)$ and $\Psi^*_-(u)$ are realized in terms of the free field by*

$$\Phi_-(z)=:\exp\left(-\sum_{m\neq 0}\frac{1}{[2m]_q-[m]_q}\beta_m z^{-m}\right):e^{\hat{\alpha}}z^{h/2+1/2}z^{-P/r-h/2r-1/r}, \tag{6.32}$$

$$\Psi^*_-(z)=:\exp\left(\sum_{m\neq 0}\frac{[rm]_q}{[2m]_q-[m]_q}\alpha_m z^{-m}\right):e^{-\hat{\alpha}}z^{-h/2+1/2}e^{Q}z^{P/r^*+1/r^*}. \tag{6.33}$$

For the other components of type-I vertex operator $\Phi_j(u)(j=\pm,0)$, we get the following, by using (6.15) and (6.20),

$$\Phi_0(u)=a_{0,-}\oint_{C_0}\frac{dz'}{2\pi iz'}\Phi_-(u)F(z')\frac{\left[u-u'+P+\frac{h}{2}\right]_+}{\left[u-u'+\frac{1}{2}\right]\left[P+\frac{h}{2}+\frac{1}{2}\right]_+}$$

$$=-a_{0,-}\oint_{C_0}\frac{dz'}{2\pi iz'}F(z')\Phi_-(u)\frac{\left[u-u'+P+\frac{h}{2}\right]_+}{\left[u-u'-\frac{1}{2}\right]\left[P+\frac{h}{2}+\frac{1}{2}\right]_+}. \tag{6.34}$$

Here the contour C_0 is specified by the condition.

$$C_0: \quad |q^{-1}z|<|z'|<|p^{-1}q^{-1}z|.$$

The component $\Phi_+(u)$ is given by

$$\Phi_+(u)=-a_{+,-}\oint\oint_{C_+}\frac{dz'}{2\pi iz'}\frac{dz''}{2\pi iz''}\Phi_-(u)F(z')F(z'')\frac{\left[P+\frac{h}{2}\right]_+}{\left[P+\frac{h}{2}-\frac{1}{2}\right]_+\left[P+\frac{h}{2}-1\right]_+[2P+h]}$$

$$\times\frac{\left[u-u'+2P+h-\frac{3}{2}\right]\left[u'-u''+P+\frac{h}{2}\right]_+}{\left[u-u'+\frac{1}{2}\right]\left[u'-u''+\frac{1}{2}\right]}$$

$$=-a_{+,-}\oint\oint_{C^+}\frac{dz'}{2\pi iz'}\frac{dz''}{2\pi iz''}F(z')F(z'')\Phi_-(u)\frac{\left[P+\frac{h}{2}\right]_+}{\left[P+\frac{h}{2}-\frac{1}{2}\right]_+\left[P+\frac{h}{2}-1\right]_+[2P+h]}$$

$$\times\frac{\left[u-u'+2P+h-\frac{3}{2}\right]\left[u'-u''+P+\frac{h}{2}\right]_+\left[u-u''+\frac{1}{2}\right]}{\left[u-u'-\frac{1}{2}\right]\left[u-u''-\frac{1}{2}\right]\left[u'-u''+\frac{1}{2}\right]}. \tag{6.35}$$

The contour C_+ is specified by

$$C_+: \quad |q^{-1}z|<|z'|<|p^{-1}q^{-1}z|, \quad |q^{-1}z|<|z''|<|p^{-1}q^{-1}z|, \quad |pqz'|<|z''|<|qz'|.$$

Similarly, for type-II vertex operators, the component $\Psi_0^*(u)$ is given by

$$\Psi_0^*(u)=a_{-,0}^*\oint_{C_0^*}\frac{dz'}{2\pi iz'}\Psi_-^*(u)E(z')\frac{[u-u'-P]_+^*}{\left[u-u'-\frac{1}{2}\right]^*\left[P-\frac{1}{2}\right]_+^*}$$

$$=-a_{-,0}^*\oint_{C_0^*}\frac{dz'}{2\pi iz'}E(z')\Psi_-^*(u)\frac{[u-u'-P]_+^*}{\left[u-u'+\frac{1}{2}\right]^*\left[P-\frac{1}{2}\right]_+^*}. \tag{6.36}$$

The contour C_0^* satisfies

$$C_0^*: \quad |q^{-1}z|<|z'|<|qz|.$$

The component $\Psi_0^*(u)$ is given by

$$\begin{aligned}\Psi_+^*(u)=&-a_{-,+}^* \oint \oint_{C_+^*} \frac{dz'}{2\pi i z'} \frac{dz''}{2\pi i z''} \Psi_-^*(u)E(z')E(z'') \frac{1}{\left[P-\frac{1}{2}\right]_+^* [2P-2]^*} \\ &\times \frac{\left[u-u'-2P+\frac{3}{2}\right]^* [u'-u''-P]_+^*}{\left[u-u'-\frac{1}{2}\right]^* \left[u'-u''-\frac{1}{2}\right]^*} \\ =&-a_{-,+}^* \oint \oint_{C_+^*} \frac{dz'}{2\pi i z'} \frac{dz''}{2\pi i z''} E(z')E(z'')\Psi_-^*(u) \frac{1}{\left[P-\frac{1}{2}\right]_+^* [2P-2]^*} \\ &\times \frac{\left[u-u'-2P+\frac{3}{2}\right]^* [u'-u''-P]_+^* \left[u-u''-\frac{1}{2}\right]^*}{\left[u-u'+\frac{1}{2}\right]^* \left[u-u''+\frac{1}{2}\right]^* \left[u'-u''-\frac{1}{2}\right]^*}. \end{aligned} \tag{6.37}$$

Here the contour C_+^* is specified by the condition

$$C_+^*: \quad |q^{-1}z|<|z'|<|qz|, \quad |q^{-1}z|<|z''|<|qz|, \quad |q^{-1}z'|<|z''|<|qz'|.$$

In C_0^* and C_+^*, the inequality such as $|q^{-1}z|<|z'|<|qz|$ means that the integration contour encloses the pole $q^{-1}z$ but not qz.

Remark: The free field realizations of the vertex operators (6.32)–(6.37) are the same as those of the dilute A_L model obtained in Ref. 15, up to a gauge transformation.

In addition we can verify the following commutation relation:

Proposition 6.3: The highest components $\Phi_-(u)$ and $\Psi_-^*(u)$ satisfy

$$\Phi_-(u_1)\Psi_-^*(u_2)=\chi(u_1-u_2)\Psi_-^*(u_2)\Phi_-(u_1). \tag{6.38}$$

Here we have set

$$\chi(u)=-z^{-1}\frac{\Theta_{q^6}(qz)\Theta_{q^6}(q^2z)}{\Theta_{q^6}(q/z)\Theta_{q^6}(q^2/z)}. \tag{6.39}$$

C. Commutation relations of the vertex operators

We next study the commutation relations of the vertex operators and show that our realization satisfies the full intertwining relations for $c=1$.

Theorem 6.4: *The free field realizations of the type-I vertex operator $\Phi_\mu(u)$* (6.32), (6.34), (6.35), *and the type-II vertex operator $\Psi_\mu^*(u)$* (6.33), (6.36), (6.37), *satisfy the following commutation relations:*

$$\Phi_{j_2}(u_2)\Phi_{j_1}(u_1)=\sum_{j_1',j_2'=\pm,0} R_{j_1j_2}^{j_1'j_2'}(u_1-u_2,P+h)\ \Phi_{j_1'}(u_1)\Phi_{j_2'}(u_2), \tag{6.40}$$

$$\Psi^*_{j_1}(u_1)\Psi^*_{j_2}(u_2)=\sum_{j_1',j_2'=\pm,0}\Psi^*_{j_2'}(u_2)\Psi^*_{j_1'}(u_1)\ \ R^{*j_1j_2}_{j_1'j_2'}(u_1-u_2,P), \tag{6.41}$$

$$\Phi_j(u_1)\Psi^*_k(u_2)=\chi(u_1-u_2)\ \ \Psi^*_k(u_2)\Phi_j(u_1). \tag{6.42}$$

Here we set

$$R(u,P+h)=\mu(u)\overline{R}(v,P+h),\qquad R^*(u,P)=\mu^*(u)\overline{R}^*(u,P), \tag{6.43}$$

with

$$\mu(u)=z^{(1/r)-1}\frac{\{pq^4z\}\{pq^3z\}\{q^3z\}\{q^2z\}\{pq/z\}\{p/z\}\{q^6/z\}\{q^5/z\}}{\{pq^4/z\}\{pq^3/z\}\{q^3/z\}\{q^2/z\}\{pqz\}\{pz\}\{q^6z\}\{q^5z\}} \tag{6.44}$$

and $\mu^*(u)=\mu(u)|_{r\to r^*}$. *Here* $\chi(u)$ *is given by (6.39).*

The proof is similar to those of Theorem 4.2.

Now let us investigate the intertwining relation for level $c=1$. For this purpose, we construct a L-operator as a composition of type-I and type-II vertex operators.[17]

Theorem 6.5: *For* $c=1$, *the components of the* L*-operator* $\hat{L}^+(u)$ *(5.1) is given by the following product of the type-I and type-II vertex operators:*

$$L^+_{j,k}(u)=g^{-1}\Psi^*_k(u+r)\Phi_j(u+r+1/2)\quad (j,k=\pm,0). \tag{6.45}$$

Here we set

$$g=-\frac{(pq^6;q^6)_\infty(pq^5;q^6)_\infty}{(pq^3;q^6)_\infty(pq^2;q^6)_\infty}\left(\frac{\{q^2p\}\{q^3p\}\{q^3p\}\{q^4p\}}{\{p\}\{qp\}\{q^5p\}\{q^6p\}}\times(p\leftrightarrow p^*)^{-1}\right). \tag{6.46}$$

The proof is similar to the one of Theorem 6.5 in Ref. 8.

Remark: By using the commutation relations of the vertex operators (6.40)–(6.42) and the formula

$$\frac{\rho^+(u)}{\rho^{+*}(u)}=\frac{\mu(u)\chi(\frac{1}{2}-u)}{\mu^*(u)\chi(\frac{1}{2}+u)}, \tag{6.47}$$

one can prove the $RLL=LLR^*$ relation (5.2) for $c=1$ directly.

In the same way, one can verify the ''intertwining relations'' (6.3) and (6.4) of vertex operators.

Corollary 6.6: For $c=1$, *the type-I and the type-II vertex operators* $\hat{\Phi}_V(u)$, $\hat{\Psi}^*_V(u)$ *satisfy the full intertwining relations (6.3) and (6.4) with* $V=W\cong\mathbb{C}^3$.

VII. DISCUSSION

Extending the construction of the elliptic algebra to the twisted affine Lie algebra case, we have derived the elliptic algebra $U_{q,p}(A_2^{(2)})$, $p=q^{2r}$ and shown that it provides the Drinfeld realization of the elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. Based on this, we have derived the type-I and type-II vertex operators of $U_{q,p}(A_2^{(2)})$ and identified them with the vertex operators in the dilute A_L model with $r=2(L+1)/(L+2)$. Our result thus gives a representation theoretical foundation to the work.[15]

There are some open problems.

(i) We here studied the simplest twisted elliptic quantum group $\mathcal{B}_{q,\lambda}(A_2^{(2)})$ and associated elliptic algebra $U_{q,p}(A_2^{(2)})$. To generalize our consideration to the higher rank cases associated with $A_{2n}^{(2)}$ and $A_{2n+1}^{(2)}$, or moreover to other types of affine Lie algebras, is an interesting problem.

(ii) Our realization of the elliptic algebra $U_{q,p}(A_2^{(2)})$ based on the Drinfeld currents of $U_q(A_2^{(2)})$ and the Heisenberg algebra $\mathbb{C}\{\mathcal{H}\}$ is valid for a generic level c. In order to perform an algebraic analysis of the solvable lattice models, a free field realization is useful. For example, to consider a fusion of the dilute A_L model, i.e., a higher spin extension, we need a free field realization (Wakimoto construction) of the elliptic algebra $U_{q,p}(A_2^{(2)})$ in a higher level.

(iii) The Wakimoto realization of the affine quantum group $U_q(A_2^{(2)})$ itself is interesting. It should be used to solve the q-KZ equation as well as the q-difference equation for the twistor $F(r,s)$, which we have solved partly (see Appendix B). The same thing is true for the other types of affine Lie algebra and should lead us to a proof of the conjecture on the connection matrix of the q-KZ equation given by Frenkel and Reshetikhin.[18]

(iv) It is known in some cases that the generating functions of the q-deformed Virasoro or W-algebras can be obtained from a fusion of the vertex operators of corresponding elliptic algebra $U_{q,p}(\mathfrak{g})$.[19,20,15,21] It is interesting to examine the same procedure in various $U_{q,p}(\mathfrak{g})$ and derive corresponding q-W algebras. The results should be compared with those in Ref. 22.

(v) It is also an interesting problem to investigate the scaling limit of the half-currents and the L-operators of $U_{q,p}(A_2^{(2)})$ and derive the vertex operators.[19,23] The result should be applied to the Izergin–Korepin model[24] in the massless regime where a generic form of the correlation functions was studied in Ref. 25. The type-II vertex operators should provide the Zamolodchikov–Faddeev algebra for the $A_2^{(2)}$ Toda field theory with imaginary coupling constant, and enable us to derive the soliton S-matrix.

We hope to report on some of the issues listed here in the near future.

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APPENDIX A: FINITE DIMENSIONAL REPRESENTATION

The evaluation module (π_w, V_w) in terms of the Drinfeld generators, is defined by the following formulas:

$$\pi_w(h)=2(E_{++}-E_{--}), \quad \pi_w(c)=0, \tag{A1}$$

$$\pi_w(a_m)=\frac{[m]_q}{m}(w/q)^m(q^{-m}E_{++}+(1-q^m)E_{00}-q^{2m}E_{--}), \tag{A2}$$

$$\pi_w(x_k^+)=(w/q)^k(aE_{+0}+q^k bE_{0-}), \tag{A3}$$

$$\pi_w(x_k^-)=(w/q)^k(q^k b^{-1}E_{-0}+a^{-1}E_{0+}). \tag{A4}$$

Here we have used

$$E_{++}=\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix},$$

$$E_{00}=\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix},$$

and

$$E_{--}=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix},$$

etc. In what follows we set $a=b=1$. We have

$$\pi_w(x^+(z))=E_{+0}\delta(w/qz)+E_{0-}\delta(w/z), \tag{A5}$$

$$\pi_w(x^-(z))=E_{-0}\delta(w/z)+E_{0+}\delta(w/qz), \tag{A6}$$

$$\pi_w(u^+(z,p))=\frac{(pq^3z/w;p)_\infty}{(pqz/w;p)_\infty}E_{++}+\frac{(pq^2z/w;p)_\infty(pq^{-1}z/w;p)_\infty}{(pqz/w;p)_\infty(pz/w;p)_\infty}E_{00}+\frac{(pq^{-2}z/w;p)_\infty}{(pz/w;p)_\infty}E_{--}, \tag{A7}$$

$$\pi_w(u^-(z,p))=\frac{(pq^{-3}w/z;p)_\infty}{(pq^{-1}w/z;p)_\infty}E_{++}+\frac{(pqw/z;p)_\infty(pq^{-2}w/z;p)_\infty}{(pw/z;p)_\infty(pq^{-1}w/z;p)_\infty}E_{00}+\frac{(pq^2w/z;p)_\infty}{(pw/z;p)_\infty}E_{--}. \tag{A8}$$

Let us calculate finite dimensional representation of the elliptic current,

$$\pi_w(e(z,p))=\frac{(pq^3z/w;p)_\infty}{(pqz/w;p)_\infty}E_{+0}\delta(w/qz)+\frac{(pq^2z/w;p)_\infty(pq^{-1}z/w;p)_\infty}{(pqz/w;p)_\infty(pz/w;p)_\infty}E_{0-}\delta(w/z), \tag{A9}$$

$$\pi_w(f(z,p))=\frac{(pqw/z;p)_\infty(pq^{-2}w/z;p)_\infty}{(pw/z;p)_\infty(pq^{-1}w/z;p)_\infty}E_{-0}\delta(w/z)+\frac{(pq^{-3}w/z;p)_\infty}{(pq^{-1}w/z;p)_\infty}E_{0+}\delta(w/qz), \tag{A10}$$

$$\pi_w(k(z,p))=\rho^+(q^{-r+2}z/w)\left(E_{++}+\frac{\Theta_p(q^rz/w)}{\Theta_p(q^{r+2}z/w)}E_{00}+\frac{\Theta_p(q^rz/w)\Theta_p(q^{r-1}z/w)}{\Theta_p(q^{r+2}z/w)\Theta_p(q^{r+1}z/w)}E_{--}\right), \tag{A11}$$

$$\pi_w(\psi(z,p))=\frac{\Theta_p(q^{r+3}z/w)}{\Theta_p(q^{r+1}z/w)}E_{++}+\frac{\Theta_p(q^{r+2}z/w)\Theta_p(q^{r-1}z/w)}{\Theta_p(q^{r+1}z/w)\Theta_p(q^rz/w)}E_{00}+\frac{\Theta_p(q^{r-2}z/w)}{\Theta_p(q^rz/w)}E_{--}. \tag{A12}$$

APPENDIX B: TWISTOR

We here consider the difference equations of the twistor $F(\lambda)$ for $\mathcal{B}_{q,\lambda}(A_2^{(2)})$. The general framework was given in Ref. 3. Let us consider the case of the affine algebra $A_2^{(2)}$. Taking a basis $\{c,d,\alpha_1^\vee\}$ of the Cartan subalgebra $\mathfrak{h}$ of $A_2^{(2)}$. We parametrize the dynamical variable λ as

$$\lambda-\rho=r^*d+s'c+\frac{1}{2}\left(s+\frac{r\tau}{2}\right)\alpha_1^\vee, \qquad \left(\ r^*=r-c,\ \ \tau=-\frac{2\pi i}{\log q^{2r}}\ \right), \tag{B1}$$

where $\rho=3d+\frac{1}{4}\alpha_1^\vee$ is the Weyl vector. Let us set

$$\mathcal{R}(z)=\mathrm{Ad}(z^d\otimes 1)(\mathcal{R}), \tag{B2}$$

$$F(z,p,w)=\mathrm{Ad}(z^d\otimes 1)(F(\lambda)), \tag{B3}$$

$$\mathcal{R}(z;p,w)=\mathrm{Ad}(z^d\otimes 1)(\mathcal{R}(\lambda))=\sigma(F(z^{-1};p,w))\mathcal{R}(z)F(z;p,w)^{-1}, \tag{B4}$$

where $w=q^{2(s+r\tau/2)}$. In particular, for $z=0$, $q^{c\otimes d+d\otimes c}\mathcal{R}(0)$ reduces to the universal R matrix of $U_q(A_1)$. From Ref. 3, we have the difference equation for the twistor,

$$F(pq^{2c^{(1)}}z;p,w)=(\overline{\varphi_w}^{-1}\otimes id)(F(z;p,w))q^T\mathcal{R}(pq^{2c^{(1)}}z), \tag{B5}$$

$$F(0;p,w)=F_{A_1}(w), \tag{B6}$$

where $\overline{\varphi_w}=\mathrm{Ad}(q^{\alpha_1^{\vee 2}/4}w^{\alpha_1^\vee/2})$ and $T=\frac{1}{2}c\otimes d+\frac{1}{2}d\otimes c+\frac{1}{4}\alpha_1^\vee\otimes\alpha_1^\vee$.

We are interested in the vector representation (π_z,V), $V=\mathbb{C}^3$ given in Appendix A. We set

$$F_{VV}(z;p,w)=(\pi_1\otimes\pi_1)F(z;p,w)=(\pi_{z_1}\otimes\pi_{z_2})(F(\lambda)), \tag{B7}$$

$$R_{VV}(z;p,w)=(\pi_1\otimes\pi_1)\mathcal{R}(z;p,w)=(\pi_{z_1}\otimes\pi_{z_2})(\mathcal{R}(\lambda)), \tag{B8}$$

$$R_{VV}(z)=(\pi_1\otimes\pi_1)\mathcal{R}(z)=(\pi_{z_1}\otimes\pi_{z_2})\mathcal{R}, \tag{B9}$$

where $z=z_1/z_2$. The trigonometric R-matrix $R_{VV}(z)$ is given as follows:

$$R_{VV}(z)=\rho_{VV}(z)\overline{R}_{VV}(z), \tag{B10}$$

$$\overline{R}_{VV}(z)=\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & b(z) & 0 & c(z) & 0 & 0 & 0 & 0 & 0\\
0 & 0 & d(z) & 0 & e(z) & 0 & f(z) & 0 & 0\\
0 & z\ c(z) & 0 & b(z) & 0 & 0 & 0 & 0 & 0\\
0 & 0 & -q^2z\ \ e(z) & 0 & j(z) & 0 & e(z) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & b(z) & 0 & c(z) & 0\\
0 & 0 & z\ \ n(z) & 0 & -q^2z\ \ e(z) & 0 & d(z) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & z\ \ c(z) & 0 & b(z) & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix},$$

$$b(z)=-\frac{q(1-z)}{1-q^2z}, \quad c(z)=\frac{1-q^2}{1-q^2z}, \quad d(z)=\frac{(1-z)q^2(1-qz)}{(1-q^2z)(1-q^3z)},$$

$$e(z)=\frac{i(1-q^2)q^{1/2}(1-z)}{(1-q^2z)(1-q^3z)}, \quad f(z)=\frac{(1-q^2)(1+q-q^3z-qz)}{(1-q^2z)(1-q^3z)},$$

$$j(z)=-\frac{q(1-z)}{1-q^2z}+\frac{(1-q^2)(1-q^3)z}{(1-q^2z)(1-q^3z)}, \quad n(z)=\frac{(1-q^2)(1+q^2-q^3z-q^2z)}{(1-q^2z)(1-q^3z)}.$$

The function $\rho_{VV}(z)$ is given by

$$\rho_{VV}(z)=q^{-1}\frac{(1/z;q^6)_\infty(q/z;q^6)_\infty(q^5/z;q^6)_\infty(q^6/z;q^6)_\infty}{(q^2/z;q^6)_\infty(q^3/z;q^6)_\infty^2(q^4/z;q^6)_\infty}. \tag{B11}$$

Noting $\pi_1(c)=0$, we have the difference equation

$$F_{VV}(pz;p,w)^t=R_{VV}(pz)^tK(D_w\otimes 1)^{-1}F_{VV}(z;p,w)^t(D_w\otimes 1), \tag{B12}$$

where X^t means the transpose of X, and we have set

$$K=\mathrm{Diag}(q,1,q^{-1},1,1,1,q^{-1},1,q), \tag{B13}$$

$$D_w=\mathrm{Diag}(q^{-1}w^{-1},1,q^{-1}w). \tag{B14}$$

From the from of $R_{VV}(z)$, one can set

$$F(z;p,w)=f(z)\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & X_{11}^{(+)}(z) & 0 & X_{12}^{(+)}(z) & 0 & 0 & 0 & 0 & 0\\
0 & 0 & Y_{11}(z) & 0 & Y_{12}(z) & 0 & Y_{13}(z) & 0 & 0\\
0 & X_{21}^{(+)}(z) & 0 & X_{22}^{(+)}(z) & 0 & 0 & 0 & 0 & 0\\
0 & 0 & Y_{21}(z) & 0 & Y_{22}(z) & 0 & Y_{23}(z) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & X_{11}^{(-)}(z) & 0 & X_{12}^{(-)}(z) & 0\\
0 & 0 & Y_{31}(z) & 0 & Y_{32}(z) & 0 & Y_{33}(z) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & X_{21}^{(-)}(z) & 0 & X_{22}^{(-)}(z) & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}.$$

Then the q-difference Eq. (B12) is equivalent to the following equations:

$$f(pz)=q\rho_{VV}(pz)f(z), \tag{B15}$$

$$\begin{pmatrix} X_{11}^{(\pm)}(pz) & X_{12}^{(\pm)}(pz)\\ X_{21}^{(\pm)}(pz) & X_{22}^{(\pm)}(pz)\end{pmatrix}=q^{-1}\begin{pmatrix} X_{11}^{(\pm)}(z) & q^{\pm 1}wX_{12}^{(\pm)}(z)\\ q^{\mp 1}w^{-1}X_{21}^{(\pm)}(z) & X_{22}^{(\pm)}(pz)\end{pmatrix}\begin{pmatrix} b(pz) & c(pz)\\ pz\ \ c(pz) & b(pz)\end{pmatrix}, \tag{B16}$$

$$\begin{pmatrix} Y_{11}(pz) & Y_{12}(pz) & Y_{13}(pz)\\ Y_{21}(pz) & Y_{22}(pz) & Y_{23}(pz)\\ Y_{31}(pz) & Y_{32}(pz) & Y_{33}(pz)\end{pmatrix}=q^{-2}\begin{pmatrix} Y_{11}(z) & wY_{12}(z) & w^2Y_{13}(pz)\\ qw^{-1}Y_{21}(z) & qY_{22}(z) & qwY_{23}(z)\\ w^{-2}Y_{31}(z) & w^{-1}Y_{32}(z) & Y_{33}(z)\end{pmatrix}$$
$$\times\begin{pmatrix} d(pz) & e(pz) & f(pz)\\ -q^2pz\ \ e(pz) & j(pz) & e(pz)\\ pz\ \ n(pz) & -q^2pz\ \ e(pz) & d(pz)\end{pmatrix}. \tag{B17}$$

The two 2×2 matrix equations for $X_{ij}^{(\pm)}(z)$ are the same as the one appeared in the $\widehat{\mathfrak{sl}}_2$ case,[3] if we change $b(z)$ to $-b(z)$ and make the following identification:

$$q^{\pm 1}w=w_{\mathfrak{sl}_2}^{-1},\ \text{i.e.,}\quad -s_{\mathfrak{sl}_2}=s+\frac{r\tau}{2}\pm\frac{1}{2},$$

where $w_{\mathfrak{sl}_2}$ and $s_{\mathfrak{sl}_2}$ denote w and s in Ref. 3, respectively. Hence from the elliptic R matrix for $\mathcal{B}_{q,\lambda}(\widehat{\mathfrak{sl}}_2)$ ((4.18) in Ref. 3), we determine the following parts of our elliptic R-matrix:

$$\begin{pmatrix} R^{+0}_{+0} & R^{0+}_{+0} \\ R^{+0}_{0+} & R^{0+}_{0+} \end{pmatrix} = \begin{pmatrix} -\dfrac{[s+3/2]_+[s-1/2]_+}{[s+1/2]_+^2}\dfrac{[u]}{[u+1]} & e^{\pi i u/r}\dfrac{[1][s+1/2-u]_+}{[s+1/2]_+[u+1]} \\ e^{-(\pi i u/r)}\dfrac{[1][s+1/2+u]_+}{[s+1/2]_+[u+1]} & -\dfrac{[u]}{[u+1]} \end{pmatrix}, \tag{B18}$$

$$\begin{pmatrix} R^{0-}_{0-} & R^{-0}_{0-} \\ R^{0-}_{-0} & R^{-0}_{-0} \end{pmatrix} = \begin{pmatrix} -\dfrac{[s-3/2]_+[s+1/2]_+}{[s-1/2]_+^2}\dfrac{[u]}{[u+1]} & e^{\pi i u/r}\dfrac{[1][s-1/2-u]_+}{[s-1/2]_+[u+1]} \\ e^{-(\pi i u/r)}\dfrac{[1][s-1/2+u]_+}{[s-1/2]_+[u+1]} & -\dfrac{[u]}{[u+1]} \end{pmatrix}. \tag{B19}$$

By a gauge transformation, these yields the corresponding matrix elements in (2.19).

As for the 3×3 part, we have no known solutions. The Wakimoto realization of $U_q(A_2^{(2)})$ should be useful to solve the q-KZ equation for the intertwining operators (vertex operators) of $U_q(A_2^{(2)})$ as well as (B17).

APPENDIX C: PROOF OF THE RELATION (4.27)

Let us set

$$h(v) = -\frac{[v+1]^*[v-1/2]^*}{[v-1]^*[v+1/2]^*}. \tag{C1}$$

In the integrand of the half-current $E^+_{-,+}(u)$ (4.9), we call $E(z')E(z'')$ the operator part, and the ratio of the product of the theta functions the coefficient part. We keep coefficient parts in the right of operator parts. According to the relation (3.62), we have the equality

$$\oint \frac{dz'}{2\pi i z'}\frac{dz''}{2\pi i z''}E(z')E(z'')A(u,u'') = \oint \frac{dz'}{2\pi i z'}\frac{dz''}{2\pi i z''}E(z')E(z'')h(u''-u')A(u'',u'),$$

when the integration contours for z' and z'' are the same. Here we set $z'=q^{2u'}$, $z''=q^{2u''}$. We define "weak equality" in the following sense. The two coefficient functions $A(u',u'')$ and $B(u',u'')$ coupled to $E(z')E(z'')$ in integrals are equal in weak sense if

$$A(u',u'')+h(u''-u')A(u'',u') = B(u',u'')+h(u''-u')B(u'',u').$$

We write the weak equality as

$$A(u',u'') \sim B(u',u'').$$

To prove the equality (4.27), it is enough to show the equalities of coefficient parts in weak sense.

Setting $z_i=q^{2u_i}$ $(i=1,2)$ and $u=u_1-u_2$, let us consider RHS-LHS of (4.27) given as follows:

$$\oint \frac{dz'}{2\pi i z'} \oint \frac{dz''}{2\pi i z''}E(z')E(z'')F(u_1,u_2,u',u'',L),$$

where

$$
\begin{aligned}
&F(u_1,u_2,u',u'',L)\\
&=\frac{[u_2-u'-2P+2+c/2]^*[u'-u''-P]^*_+[1+u]^*[u+3/2]^*[1]^{*2}}{[u_2-u'+c/2]^*[u'-u''-1/2]^*[u]^*[2P-2]^*[P-1/2]^*_+[u+1/2]^*}\\
&\quad+\frac{[u_2-u'-P+(c+1)/2]^*_+[u_1-u'+1+c/2]^*[u_1-u''-P+(c+1)/2]^*_+[u+P+1]^*_+[1]^*}{[u_2-u'+c/2]^*[u_1-u'+c/2]^*[u_1-u''+c/2]^*[P-1/2]^{*2}_+[P+1/2]^*_+[u+1/2]^*}\\
&\quad-\frac{[u_1-u'-2P+2+c/2]^*[u'-u''-P]^*_+[1]^{*2}}{[u_1-u'+c/2]^*[u'-u''-1/2]^*[P-1/2]^*_+[u+1/2]^*}\\
&\quad\times\left(\frac{[u+2P-1]^*[1]^*[u+3/2]^*}{[u]^*[2P-1]^*[2P-2]^*}+\frac{[P]^*_+[u+2P+1/2]^*[1]^*}{[2P]^*[2P-1]^*[P-1]^*_+}\right)\\
&\quad-\frac{[u_2-u'-2P+c/2]^*[u'-u''-P-1]^*_+[u_1-u'+1+c/2]^*[u_1-u''+1+c/2]^*[1]^{*2}}{[u_2-u'+c/2]^*[u'-u''-1/2]^*[u_1-u'+c/2]^*[u_1-u''+c/2]^*[P+1/2]^*_+[2P]^*}.
\end{aligned}
$$

We will show that $F(u_1,u_2,u',u'',L)\sim 0$. For this purpose, we consider the function of u' defined by

$$F(u')=F(u_1,u_2,u',u'',L)+h(u''-u')F(u_1,u_2,u'',u',L).$$

Then it is not so hard to see that $F(u')$ is a quasiperiodic function having zeros at least at $u'=u''$ and $u'=u''+1$. The quasiperiodicity is given by

$$F(u'+\tau^*r^*)=-e^{-(2\pi i/r)(P-3/2)}F(u'),$$

$$F(u'+r^*)=F(u').$$

Therefore if we set

$$G(u')=F(u')\frac{[u'-u''-P+3/2]^*}{[u'-u'']^*},$$

$G(u')$ is a doubly periodic function of u' and $G(u''+1)=0$. It is then enough to show that $G(u')$ is an entire function.

In $G(u')$, some terms have the first order poles at $u'=u_1+c/2$, $u_2+c/2$,$u''+1/2$,$u''-1$. We checked that all the residues of the function $G(u')$ at these poles vanish. For example, at $u'=u_2+c/2$ the residue is given by

$$
\begin{aligned}
\mathrm{Res}_{u'=u_2+c/2}G(u')\frac{dz'}{2\pi iz'}&=-\frac{[u+1]^*[u_2-u''-P+c/2]^*_+[u+3/2]^*[1]^{*2}}{[u]^*[u_2-u''-1/2+c/2]^*[P-1/2]^*_+[u+1/2]^*}\\
&\quad+\frac{[u+1]^*[u_1-u''-P+(c+1)/2]^*_+[u+P+1]^*_+[1]^{*3}}{[u]^*[u_1-u''+c/2]^*[P+1/2]^*_+[P-1/2]^*_+[u+1/2]^*}\\
&\quad+\frac{[u+1]^*[u_1-u''+1+c/2]^*[u_2-u''-P-1+c/2]^*_+[1]^{*2}}{[u]^*[u_1-u''+c/2]^*[u_2-u''-1/2+c/2]^*[P+1/2]^*_+}.
\end{aligned}
$$

One can apply the following theta function identity to combine the first and the third terms,

$$
\begin{aligned}
&[u+x]^*[u-x]^*[v+y]^*_+[v-y]^*_+-[u+y]^*[u-y]^*[v+x]^*_+[v-x]^*_+\\
&\quad=-[x-y]^*[x+y]^*[u+v]^*_+[u-v]^*_+.
\end{aligned}
$$

We thus get

$$\text{first}+\text{third}=-\frac{[u+1]^*[u_1-u''-P+(c+1)/2]_+^*[u+P+1]_+^*[1]^{*3}}{[u]^*[u_1-u''+c/2]^*[P+1/2]_+^*[P-1/2]_+^*[u+1/2]^*}.$$

Therefore $\mathrm{Res}_{u'=u_2+c/2}\,G(u')\,(dz'/2\pi iz')=0$. The other cases can be treated in the similar way.

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Shouldn't there be an antithesis to quantization?

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We raise the possibility of developing a theory of constructing quantum dynamical observables independent from quantization and deriving classical dynamical observables from pure quantum mechanical consideration. We do so by giving a detailed quantum mechanical derivation of the classical time of arrival at arbitrary arrival points for a particle in one dimension. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767297]

I. INTRODUCTION

Recently we raised the problem of deriving classical dynamical observables from pure quantum mechanical consideration, and thus the problem of constructing quantum observables with classical counterparts without quantization.[1] Our motivations have been to break the circularity of quantization when invoking the correspondence principle,[2–4] and to sidestep the well-known existence of obstruction to quantization in important spaces like the Euclidean space.[5–12] The former motivation arises from the need for quantum mechanics to be internally coherent and autonomous from classical mechanics if quantum mechanics were the preponderant of the two mechanical theories. On the other hand, the later motivation arises from the need for observables to satisfy certain commutation relations in keeping with, say, the required evolution properties of the observables. Thus in Ref. 1 we have introduced the idea of *supraquantization*—the derivation of the quantum observable corresponding to a given classical observable without quantization, and the subsequent derivation of the classical observable from its quantum counterpart, as opposed to quantization which is the derivation of the quantum observable corresponding to a given classical observable by means of an associative mapping of the scalar-valued observable to an operator-valued observable.

And to illustrate our point of supraquantization and to demonstrate the general insufficiency of prescriptive quantization—particularly the Weyl quantization[13]—to satisfy required commutator values, we outlined in Ref. 1 without proof a formal quantum mechanical derivation of the local form of the classical time of arrival in the neighborhood of the origin. In this paper, we attempt to place our earlier results on a firm foundation. We do so by (1) developing the quantum mechanical framework suitable to the idea of supraquantization, and by (2) proving explicitly our earlier assertions made within the proposed framework. It is then the aim of this paper to give a quantum mechanical derivation of the classical observable

$$T_x(q,p) = -\operatorname{sgn}(p)\sqrt{\frac{\mu}{2}}\int_x^q \frac{dq'}{\sqrt{H(q,p)-V(q')}}, \tag{1}$$

where $T_x(q,p)$ is the time of arrival of a particle at some point x, whose Hamiltonian is $H(q,p)$. We will do so within the rigged Hilbert space formulation of quantum mechanics.[14–20]

This paper is organized as follows: In Sec. II we outline the quantum mechanical framework in rigged Hilbert space suitable for our purposes. In Sec. III we give a brief review of quantization and Weyl quantization in particular, and discuss the idea of supraquantization, and deal with the

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transition to the classical regime. In Sec. IV we summarize the classical solution to the classical time of arrival and introduce the concept of global and local time of arrivals. In Sec. V we formulate our quantum mechanical approach to deriving the classical time of arrival at the origin from pure quantum mechanical consideration. In Sec. VI, we explicitly supraquantize the classical time of arrivals of the harmonic oscillator and the quartic oscillator. In Sec. VII we prove, within the limits stated therein, the general result for arbitrary entire analytic potentials that the time of arrival can be derived from the supraquantization developed in Sec. V. In Sec. VIII we give the extension of our derivation for arbitrary arrival points. And in Sec. IX, we devote some discussion on the relationship between quantization and supraquantization.

In this paper, though we are concerned with the derivation of the corresponding quantum time of arrival operator, we will not delve into the important question whether one can extract quantum time of arrival distributions from the constructed operator,[21–30] nor its relevance in the quantum time problem.[31,32] We leave these issues open in the meantime.

II. THE QUANTUM MECHANICAL FRAMEWORK

A. Single Hilbert space quantum mechanics

In the generalized single Hilbert space formulation of quantum mechanics, to every quantum mechanical system is assigned a generally infinite dimensional Hilbert space $\mathcal{H}$ over the complex field; and to every pure state corresponds to a ray in $\mathcal{H}$; and to every observable corresponds to a generally maximally symmetric densely defined operator in $\mathcal{H}$.[33,34]

If the system is closed or it does not react back to its environment, its evolution is governed by a one parameter unitary group, $U_t = e^{-(i/\hbar)\mathsf{H}t}$, where H is the system Hamiltonian. In Heisenberg representation where states are stationary, observables evolve according to

$$\mathsf{A}_t = e^{i\mathsf{H}t}\mathsf{A}e^{-i\mathsf{H}t}, \tag{2}$$

$$i\hbar\dot{\mathsf{A}}_t = [\mathsf{A}_t, \mathsf{H}], \tag{3}$$

where (3) is the infinitesimal form of (2). If either H or A are unbounded, then Eqs. (2) and (3) should be properly defined to give meaning to them. In particular, Eq. (2) holds for all times t if the domain of A is invariant under $e^{-i\mathsf{H}t}$ for all t. It is possible that the evolution equation and its infinitesimal form hold only in some countable subset of the time coordinate.

While the Hilbert space formulation is successful in describing much of the quantum mechanics we know, it is not sufficient in the sense that it does not accommodate the eigenfunctions of observables with pure continuous spectrum. It is in this context that extension of quantum mechanics in a rigged Hilbert space has been proposed. Moreover, it is within the rigging of $\mathcal{H}$ that will allow us to further generalize observables to include operators that are not necessarily operators in the system Hilbert space.

B. Rigged Hilbert space extension

Let $\mathcal{H}$ be the system Hilbert space. A rigged Hilbert space (RHS) for $\mathcal{H}$ is a triplet, called a Gel'fand triplet, $\Phi^\times \supset \mathcal{H} \supset \Phi$, where Φ is a dense subspace of $\mathcal{H}$, and is a locally convex topological space and is complete with respect to its own topology; on the other hand, $\Phi^\times$ is the space of all continuous linear functionals on Φ: An element F of $\Phi^\times$ assigns to every ϕ in Φ a complex number denoted by $\langle F|\varphi\rangle$ with the properties $\langle F|a\phi_1 + b\phi_2\rangle = a\langle F|\phi_1\rangle + b\langle F|\phi_2\rangle$, for every pair ϕ_1 and ϕ_2 in Φ, and for every pair of complex numbers a and b; and $\lim_{n\to\infty}\langle F|\phi_n\rangle = 0$, for every sequence ϕ_n converging to zero in ϕ.

In extending quantum mechanics in a rigged Hilbert space, one has to specify a particular rigging. But how do we determine the necessary rigging? Our answer to this question is limited to what is relevant and useful to our present purposes. A natural choice is the one provided by the Hamiltonian of the system under consideration. Let H be the Hamiltonian and let its domain be $\mathcal{D}(\mathsf{H})$. We choose Φ in such a way that Φ is a dense subset of $\mathcal{D}(\mathsf{H})$, and that Φ is invariant under

the Hamiltonian, i.e., $\mathsf{H}:\Phi\subseteq\Phi$. Our motivation in choosing this particular rigging is for us to be able to extend the quantum evolution of observables in the rigged Hilbert space, as we will define below. Once Φ is specified, its functional space $\Phi^\times$ is automatically determined.

Given the particular rigging of $\mathcal{H}$ relative to Φ, let $\mathcal{O}$ be the set of all observables whose domains contain Φ. Let A be in $\mathcal{O}$. We define two associated operators to A: its rigged Hilbert space *extension* $\mathsf{A}^\times$, and its rigged Hilbert space *reduction* $\mathsf{A}_\times$.

Definition 1 (Rigged Hilbert space extension): $\mathsf{A}^\times$ *is the extension of* A *in the entire* $\Phi^\times$*, i.e., the operator* $\mathsf{A}^\times$: $\Phi^\times\mapsto\Phi^\times$*, such that* $\langle \mathsf{A}^\times\phi|\varphi\rangle=\langle\phi|\mathsf{A}^\dagger\varphi\rangle$ *for all* ϕ *in* $\Phi^\times$ *and* φ *in* Φ*, where* $\mathsf{A}^\dagger$ *is the adjoint of* A *in* $\mathcal{H}$.

Definition 2 (Rigged Hilbert space reduction): $\mathsf{A}_\times$ *is the reduction of* A *in* Φ*, i.e., the operator* $\mathsf{A}_\times\varphi=\mathsf{A}\varphi$ *for all* φ *in* Φ*, such that there exists a uniquely associated functional* F_A *in* $\Phi^\times$*, for which* $\mathsf{A}_\times\varphi=\langle F_\mathsf{A}|\varphi\rangle=\mathsf{A}\varphi$ *for all* φ *in* Φ*. (See Appendix A for an example and to establish our notation.)*

The rigged Hilbert space extension of A exists if $\mathsf{A}^\dagger$ is in $\mathcal{O}$ and Φ is invariant under $\mathsf{A}^\dagger$, i.e., $\mathsf{A}^\dagger$: $\Phi\subseteq\Phi$. We emphasize that the definition of the rigged Hilbert space reduction of A requires the existence of the functional F_A in $\Phi^\times$ satisfying the stated condition. Of course A will always have a reduction in Φ by restricting its domain to Φ, but it is not necessary that there is always an associated functional F_A in $\Phi^\times$. All throughout we will call F_A as the functional kernel of $\mathsf{A}_\times$.

Now eigenfunctions corresponding to the continuous part of the spectrum of an observable do not belong to the Hilbert space: they are not square integrable and the usual probabilistic interpretation of quantum mechanics fails to hold on them. But these acquire rigorous meaning within the context of a rigged Hilbert space as generalized eigenfunctions residing in the functional space $\Phi^\times$. If one can give physical significance to elements of $\Phi^\times$, it may also be possible to give physical significance to operators taking Φ into $\Phi^\times$, e.g., Hamiltonians with singular potentials in the configuration space, $V(q)\propto\delta(q-q_0)$. This motivates us to introduce the concept of generalized observable.

Definition 3 (Generalized observable): Let F *be in* $\Phi^\times$*. If for all* φ *in* Φ*,* $F(\varphi)=\langle F|\varphi\rangle$ *is in* $\Phi^\times$ *and* $\langle F(\varphi)|\varphi\rangle$ *is real valued, we call* F *to be the functional kernel of a generalized observable* $\mathcal{A}$*. The mapping* $\langle F|\cdot\rangle$: $\Phi\mapsto\Phi^\times$ *defines the generalized observable* $\mathcal{A}$: $\Phi\mapsto\Phi^\times$.

The real valuedness of $\langle F(\varphi)|\varphi\rangle$ is the generalized analogue of the symmetry condition in ordinary Hilbert space quantum mechanics, the numerical value of which is the expectation value of the generalized observable. Since we have the inclusion relation $\Phi^\times\supset\mathcal{H}\supset\Phi$, the rigged Hilbert space reduction of ordinary quantum mechanical observables is a special class of generalized observables. We say that $\mathcal{A}$ has a Hilbert space projection if there exists a dense subspace $\mathcal{D}$ of Φ such that $\langle F|\varphi\rangle$ is in $\mathcal{H}$. Its Hilbert space projection is the closure of the operator F defined by $\langle F|\varphi\rangle=\mathsf{F}\varphi$ for all φ in $\mathcal{D}$. We emphasize that the properties of generalized observables are dictated by Φ. For this reason we denote $\mathcal{O}_\Phi$ to be the set of all generalized observables defined for a given Φ.

Now we give the appropriate generalization of the evolution law for quantum observables. Let H be the system Hamiltonian, whose domain $\mathcal{D}(\mathsf{H})$ contains Φ. Let $\Phi^\times\supset\mathcal{H}\supset\Phi$ be a particular rigging of $\mathcal{H}$, where Φ is invariant under H. Given H, let $\mathsf{H}^\times$ be its RHS-extension. Let $\mathcal{A}$ be a generalized observable in $\mathcal{O}_\Phi$. If Φ is invariant under $U_t=e^{-i\mathsf{H}t}$ for all t, we then take $\mathcal{A}$ to evolve according to

$$\mathcal{A}_t=U_{-t}^\times\mathcal{A}U_t^\times, \tag{4}$$

where $U_t^\times$ is the RHS-extension of U_t in the entire $\Phi^\times$. Under the same assumption, the infinitesimal form of (4) is given by

$$\frac{d\mathcal{A}_t}{dt}=\frac{1}{i\hbar}[\mathcal{A}_t,\mathsf{H}^\times]. \tag{5}$$

Equation (4) requires that $\mathcal{A}$ evolves into a generalized observable. These equations reduce to the standard quantum evolution law when restricted to the Hilbert space. While Eqs. (4) and (5) hold for all t under the assumption that Φ is invariant under U_t, they may still hold for some times, possibly countably infinite, even when Φ is not invariant under U_t for all t.

C. Quantum mechanics in configuration space

For a spin less particle in the real line, the corresponding system Hilbert space is the space of Lebesgue square integrable functions over the real line, $\mathcal{H}=L^2(\mathfrak{R},dq)$. We assume that the particle is under the influence of an everywhere infinitely differentiable (real valued) potential, i.e., of type $C^\infty(\mathfrak{R})$. The formal Hamiltonian

$$\mathsf{H}=-\frac{\hbar^2}{2\mu}\frac{d^2}{dq^2}+V(q) \tag{6}$$

can be assigned a dense domain $\mathcal{D}(\mathsf{H})$ in which it is essentially self-adjoint. The given Hamiltonian allows several possible riggings of the Hilbert space. We choose the rigging $\Phi^\times\supset\mathcal{H}\supset\Phi$, where Φ is the space of infinitely differentiable complex valued functions with compact support in the real line, and $\Phi^\times$ its corresponding functional space. Since $V(q)$ is $C^\infty(\mathfrak{R})$, Φ is invariant under H. We note that Φ is tight enough to allow a larger $\Phi^\times$.

The convergence to zero of a sequence in Φ is defined as follows. A sequence φ_n in Φ converges to zero in Φ if all these functions vanish outside a certain fixed bounded region, the same for all of them, and converge uniformly to zero in the usual sense together with their derivatives of any order.[19,20]

With our chosen rigging, the rigged Hilbert space reduction $\mathsf{A}_\times$ of an operator A in $\mathcal{H}$ with domain containing Φ assumes the familiar form

$$(\mathsf{A}_\times\varphi)(q)=\langle F_{\mathsf{A}}(q)|\varphi\rangle=\int_{\mathfrak{R}}\langle q|\mathsf{A}_\times|q'\rangle\varphi(q')dq', \tag{7}$$

where the functional kernel F_{A} is the complex conjugate of the well-known configuration matrix elements of the operators. Generalized observables, which includes the RHS-reductions of operators in $\mathcal{H}$, assume the similar form

$$(\mathcal{A}\varphi)(q)=\int_{\mathfrak{R}}\langle q|\mathcal{A}|q'\rangle\varphi(q')dq', \tag{8}$$

where the integrations in Eqs. (7) and (8) are understood to be in the distributional sense, in particular symbolic when the integrand is singular, e.g., the Dirac delta function. We note that the functional kernel $\langle q|\mathcal{A}|q'\rangle$ must be symmetric, i.e., $\langle q|\mathcal{A}|q'\rangle=\langle q'|\mathcal{A}|q\rangle^*$, in order to ensure the real valuedness of the expectation value of $\mathcal{A}$ in Φ.

III. QUANTIZATION, SUPRAQUANTIZATION, AND THE TRANSITION TO THE CLASSICAL REGIME

A. Quantization and Weyl-quantization

Let f be a classical observable, a real valued function $f(q,p)$ in the phase space. The problem of quantization is to derive the quantum counterpart of f by some associative mapping Q of the real-valued function $f(q,p)$ to a maximally symmetric operator F in the system Hilbert space $\mathcal{H}$, i.e., $Q(f)\mapsto\mathsf{F}$. A paramount requirement, aside from other requirements, of quantization is that the Poisson bracket of two (classical) observables quantizes into the commutator of the separately quantized observables, in particular $Q(\{f,g\})=(i\hbar)^{-1}[Q(f),Q(g)]$ (for a complete discussion on the requirements of quantization, see Refs. 7, 10).

One of the earliest prescription, which has become the starting point of other quantization schemes, is the Weyl quantization Q_W. In the language of the framework outlined above, Weyl quantization is the bijective mapping of f into some functional of a particular rigging $\Phi^\times \supset \mathcal{H} \supset \Phi$ of the system Hilbert space, i.e., $Q_W: f \mapsto F \in \Phi^\times$ such that $F(\cdot)$ is a generalized observable with a nontrivial Hilbert space projection. The rigging of $\mathcal{H}$ which we have required above is appropriate for Weyl's quantization. Now Q_W is defined by the mapping

$$Q_W: \ f \mapsto \Phi^\times \ni F^* = \langle q|\mathsf{F}_\times|q'\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} f\left(\frac{q+q'}{2}, p\right)\exp\left[\frac{i}{\hbar}(q-q')p\right]dp, \tag{9}$$

where the integration is done in the distributional sense. In the standard formulation, it is assumed, though it is *not* guaranteed, that $F(\cdot)$ has a Hilbert space projection, so that $F(\cdot)$ is the rigged Hilbert reduction $\mathsf{F}_\times$ of a uniquely associated operator F in $\mathcal{H}$. The operator F is the closure of $\mathsf{F}_\times$ in $\mathcal{H}$.

Now suppose that F is the Hilbert operator corresponding to the classical operator f derived by quantization. The classical observable is recovered by mere inversion of the process. In this case one has to determine the rigged Hilbert space reduction $\mathsf{F}_\times$ of the operator F and consequently determine the functional kernel corresponding to $\mathsf{F}_\times$. Given the functional kernel, the classical observable is recovered by means of the inverse Fourier transform

$$f(q,p) = 2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}|\mathsf{F}_\times|q-\frac{v}{2}\right\rangle \exp\left(-i\frac{vp}{\hbar}\right)dv. \tag{10}$$

In this expression, taking the limit as $\hbar$ approaches zero is not required, it being just the inverse of the prescribed Weyl-quantization.

Quantization, however, is circular when invoking the correspondence principle; and this is already evident for the Weyl quantization. Moreover, there is a well known obstruction to quantization in Euclidean space (and other spaces) which says that no quantization exists that satisfies the poission-bracket-commutator correspondence requirement for all observables.[5–12] This is unsatisfactory because the said correspondence is necessary, for example, in ensuring that required evolution properties of a certain class of observables are satisfied. This handicap of quantization will be explicitly demonstrated for the Weyl quantization.

If we wish to break the inherent circularity of quantization and to sidestep the obstruction to quantization, we must then find an alternative platform upon which we can construct quantum observables without quantization, which can further allow us to derive the corresponding classical observable. It is here that the idea of supraquantization comes in.

B. Supraquantization

The idea behind supraquantization—the construction of quantum observables without quantization and the subsequent quantum mechanical derivation of its classical counterpart—is not entirely new.

It has its origin in Mackey's earlier effort of restoring the autonomy of quantum mechanics from classical mechanics.[3,4] We recall that the quantization of free particle in one dimension is accomplished by promoting its position and momentum into operators and their Poission bracket into commutator, and the energy into the Hamiltonian operator. Mackey's work obviates these quantization prescriptions by starting not from the classical description but from the axioms of quantum mechanics and the property of free space. Starting from the basic axiom that the proposition for the location of the particle in different volume elements are compatible and the fundamental homogeneity of free space, one derives the position and the momentum operators together with the canonical commutation relation they satisfy. On the other hand, requiring Galilean invariance in the lattice of propositions, one derives the free quantum Hamiltonian (see also Ref. 35). Mackey's work provides an excellent example of the existence of more than one solution to the derivation of the quantum image of a given set of classical observables. By definition Mack-

ey's construction of the position and momentum operators, together with their algebra, is a supraquantization of the classical position and momentum, and their Poisson algebra.

It may be that quantization and supraquantization yield the same results, like the position and momentum for the free particle, but they are unmistakably distinct. Quantization presupposes classical mechanics, while supraquantization upholds the autonomy of quantum mechanics; the former introduces circularity when invoking the correspondence principle, while the latter sanctions the correspondence principle as a legitimate consequence of the acknowledged preponderance of quantum mechanics over classical mechanics. In both methods of obtaining quantum observables, the classical observable plays two different roles. In quantization, it is the starting point; in supraquantization, it is a boundary condition. The correspondence principle requires that if a quantum observable corresponds to a classical observable, then the former should reduce to the latter in the limit of vanishing $\hbar$. Then if supraquantization gives the correct quantum observable, then that observable should approach its classical limit. As a consequence of the role of the classical observable as a boundary condition, supraquantization breaks the vicious circle inherent in the quantization procedure.

But how do we construct quantum observables corresponding to a given classical observable without quantization? The observable may be constructed by appealing to the *postulated properties of the observable under consideration*, or to the *postulated physical properties of the universe*, or to the *axioms of quantum mechanics*, or to *any combination of these*. Mackey's construction of the quantum position and momentum observables without quantization proceeds from the homogeneity of free space (assumed property of free space) and the commutativity of propositions for the location of a free particle (axiom of quantum mechanics).

For a specific class of classical observables, the required supraquantization may be accomplished, in addition to the aforementioned method, by referring to one of the members of the class and employing a transfer principle to the rest. The transfer principle can be expressed as follows:

Transfer Principle: Each element of a class of observables shares a common set of properties with the rest of its class such that when a particular property is identified for a specific element of the class that property can be transferred to the rest of the class without discrimination.

It is the central problem of supraquantization to determine this set of properties shared by the class of observables under consideration, together with the appropriate axioms of mechanics to impose. Obviously supraquantization treats each class of observables on a case to case basis, in contrast to quantization which gives a single rule of association between classical and quantum observables.

But how do we approach the classical limit? We can treat quantization as a first order approximation, especially in those cases where obstruction to quantization occurs, e.g., in Euclidean space, and treat its classical limit as the starting point. This is reasonable because quantization has been successful in cases where consistency is preserved. So for observables defined in $\mathcal{H}=L^2[\mathfrak{R},dq]$ or for generalized observables in a particular rigging of $\mathcal{H}$, the transition to the classical regime is still given by Eq. (10) only that one now has to specifically project the observable into the $\hbar=0$ or $\hbar=\delta$ regime. This is so as some orders of $\hbar$ now generally appear in Eq. (10). The appearance of terms in some orders of $\hbar$ indicates the failure of quantization to consistently satisfy the required commutator values, at least in Weyl's quantization. Thus for all generalized observables $\mathcal{A}$ definable relative to Φ with functional kernel $\langle q|\mathcal{A}_\times|q'\rangle^*$, the classical limit of $\mathcal{A}$ is given by

$$f(q,p)=\lim_{\hbar\to 0} 2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\middle|\mathcal{F}\middle|q-\frac{v}{2}\right\rangle \exp\left(-i\frac{vp}{\hbar}\right)dv \tag{11}$$

whenever the limit exists [Eq. (11) has already been in used, see Refs. 36, 37]. The vanishing of $\hbar$ in the above expression is the statement that classical mechanics is the projection of quantum mechanics. Because classical mechanics is a projection, there is no bijection from classical to

quantum mechanics, except in those cases where the results of quantization and supraquantization agree. This will be made clear when we consider the supraquantization of the classical time of arrival.

IV. THE OBSERVABLE ON CASE: THE CLASSICAL TIME OF ARRIVAL

Consider a particle with mass μ in one dimension whose Hamiltonian is $H(q,p)$. If at $t=0$ the particle is at the point (q,p) in the phase space, the time $t=T_x$ that the particle will arrive at the point $q(t=T_x)=x$ is given by

$$T_x(q,p)=-\mathrm{sgn}(p)\sqrt{\frac{\mu}{2}}\int_x^q \frac{dq'}{\sqrt{H(q,p)-V(q')}}, \tag{12}$$

derived by inverting the (classical) equations of motion. For a given energy the region $\Omega=\Omega_q \times\Omega_p$ in the phase space in which Eq. (12) is finite and real valued is the classically accessible region to the particle for a given arrival point x. An important property of $T_x(q,p)$ is that it evolves according to

$$\frac{dT_x(q,p)}{dt}=-1. \tag{13}$$

This property will be important to us in the supraquantization of the time of arrival.

It is the goal of this paper to show that the time of arrival (12) for entire analytic potentials can be derived within the quantum mechanical framework we have just outlined above. This we will accomplish by constructing the generalized quantum observable corresponding to $T_x(q,p)$ by supraquantization to be developed below. Before we can proceed, we must recognize that $T_x(q,p)$ is only an observable in the region of the phase space accessible to the particle. Supraquantization of $T_x(q,p)$ then must be restricted to these accessible regions. We then proceed by developing a local form of $T_x(q,p)$, i.e., an equivalent expression for $T_x(q,p)$ in some neighborhood of Ω_q, which can be assured to be finite and real valued, thus an observable. It is this local form, which we shall refer to as the local time of arrival, that we will supraquantize and show to be derivable quantum mechanically. The time of arrivals for the rest of the accessible regions are then derived by simple analytic continuation of the local time of arrival. In the following section we develop the local expression for the time of arrival for arbitrary arrival x.

The local time of arrival: Given the Hamiltonian $H=(1/2\mu)p^2+V(q,p)$, let us consider all real valued functions, $T(q,p)$, in the phase space which is canonically conjugate with the Hamiltonian, i.e.,

$$\{H(q,p),T(q,p)\}=1, \tag{14}$$

where $\{,\}$ is the Poisson bracket. The time of arrival at some specified point is one such phase space function. Out of all those $T(q,p)$'s conjugate with $H(q,p)$, let us consider those that can be parametrized by x' and h, where x' is in the configuration axis and h is a fixed function of p alone. We denote these by $T_h^{x'}(q,p)$. The parameters x' and h are defined as follows. Let $K=(1/2\mu)p^2$ be the kinetic energy, and $\mathcal{L}_K$ be the kinetic energy Liovillian operator defined by $\mathcal{L}_K\cdot g=\{K,g\}=-\mu^{-1}p\partial_q g$. The pair of parameters x' and h fixes the inverse of $\mathcal{L}_K$, $\mathcal{L}_K^{-1}$, as follows:

$$\mathcal{L}_K^{-1}\cdot f(q,p)=-\frac{\mu}{p}\int_{x'}^q f(q',p)dq'+h(p). \tag{15}$$

In other words, x' and h define the domain of $\mathcal{L}_K$ such that the inverse $\mathcal{L}_K^{-1}$ can be unambiguously defined.

Now given x' and h we construct $T_h^{x'}$ by the following prescription. Since $\{H,T_h^{x'}\}=\mathcal{L}_H \cdot T_g(q,p)=1$, we express T_h^{-1} in the following form:

$$T_h^{x'}(q,p)=\mathcal{L}_H^{-1}\cdot 1=\frac{1}{\mathcal{L}_K+\mathcal{L}_V}\cdot 1, \tag{16}$$

where K and V are the kinetic and potential energy parts of the Hamiltonian, respectively. Geometric expansion of Eq. (16) yields

$$T_g^{x'}(q,p)=\mathcal{L}_K^{-1}\cdot 1-\mathcal{L}_K^{-1}\cdot\mathcal{L}_V\cdot\mathcal{L}_K^{-1}\cdot 1+\mathcal{L}_K^{-1}\cdot\mathcal{L}_V\cdot\mathcal{L}_K^{-1}\cdot\mathcal{L}_V\cdot\mathcal{L}_K^{-1}\cdot 1\cdots, \tag{17}$$

where $\mathcal{L}_K^{-1}$ is defined by Eq. (15). Assuming that there is a neighborhood in the phase space such that the right-hand side of (17) converges, Eq. (17) can be written in series form

$$T_g^{x'}(q,p)=\sum_{k=0}^{\infty}(-1)^k T_k(q,p,x'), \tag{18}$$

where the $T_k(q,p,x')$'s satisfy the recurrence relation

$$T_0(q,p,x')=\mathcal{L}_K^{-1}\cdot 1,\quad T_k(q,p,x')=\mathcal{L}_K^{-1}\cdot\mathcal{L}_V\cdot T_{k-1}(q,p). \tag{19}$$

The system of recurrence relation (19) is equivalent to the recurrence relation $\{K,T_k\}=\{V,T_{k-1}\}$, subject to the boundary condition $\{K,T_0\}=1$. For a given x' and h, Eqs. (19) assume the explicit forms,

$$T_0(q,p,x')=-\frac{\mu}{p}(q-x')+h(p), \tag{20}$$

$$T_k(q,p,x')=-\frac{\mu}{p}\int_{x'}^{q}\left(\frac{\partial V}{\partial q'}\frac{\partial T_{k-1}}{\partial p}-\frac{\partial V}{\partial p}\frac{\partial T_{k-1}}{\partial q'}\right)dq'+h(p). \tag{21}$$

For autonomous Hamiltonian systems, i.e., $V=V(q)$, Eq. (21) reduces to

$$T_k(q,p,x')=-\frac{\mu}{p}\int_{x'}^{q}\frac{\partial V}{\partial q'}\frac{\partial T_{k-1}}{\partial p}dq'+h(p). \tag{22}$$

Of course Eq. (18) need not converge. However for some conditions to be stated below it converges to the time of arrival in some neighborhood.

Now let $h=0$, $p\neq 0$ and $V(q)$ be continuous at q where q is an interior point of Ω_q. Then there exists a neighborhood of q, $\omega_q\subseteq\Omega_q$, determined by the neighborhood $|V(q)-V(q')|<K_\epsilon\leqslant p^2/2\mu$ such that for every $x\in\omega_q$, T_0^x converges absolutely and uniformly to the classical time of arrival t_x.

We prove this assertion as follows. With $h=0$, Eqs. (20) and (22) reduce to

$$T_0(q,p;x)=-\mu\frac{(q-x)}{p}, \tag{23}$$

$$T_k(q,p,x')=-\frac{\mu}{p}\int_{x}^{q}\frac{\partial V}{\partial q'}\frac{\partial T_{k-1}}{\partial p}dq'. \tag{24}$$

Using Eq. (24) with $x'=x$, and using (23) as the initial value, the first few terms in Eq. (17) can be evaluated to aid us to infer that the kth iterate, T_k, in Eq. (18) is given by

$$T_k(q,p;x) = -\frac{(2k-1)!!}{k!}\frac{\mu^{k+1}}{p^{2k+1}}\int_x^q (V(q)-V(q'))^k dq'. \tag{25}$$

We prove Eq. (25) by induction. Shifting index $k\to(k-1)$ in (25) to get T_{k-1} and substituting T_{k-1} back into Eq. (22), we have

$$T_k(q,p;x) = -\frac{\mu}{p}\int_x^q \frac{\partial V}{\partial q'}\frac{\partial T_{k-1}}{\partial p}dq' = -\frac{(2k-3)!!}{(k-1)!}(2k-1)\frac{\mu^{k+1}}{p^{2k+1}}\int_x^q \frac{\partial V}{\partial q'}\int_x^{q'}(V(q') - V(q''))^{k-1}dq''. \tag{26}$$

Successive integration by parts evaluates the double integration into

$$\begin{aligned}\int_x^q \frac{\partial V}{\partial q'}\int_x^{q'}(V(q')-V(q''))^{k-1}dq'' &= V(q)\int_x^q (V(q)-V(q'))^{k-1}dq' \\ &\quad -\frac{(k-1)}{2}\int_x^q \frac{dV^2}{dq'}\int_x^{q'}(V(q')-V(q''))^{k-2}dq''dq' \\ &= \int_x^q \sum_{j=0}^{k-1}(-1)^j \frac{(k-1)!}{(k-1-j)!(j+1)!}V^{j+1}(q)(V(q) \\ &\quad -V(q'))^{k-1-j} + \frac{(-1)^k}{k}\int_x^q V^k(q')dq' \\ &= \frac{1}{k}\int_x^q (V(q)-V(q'))^k dq'. \end{aligned}\tag{27}$$

Substituting Eq. (27) back into Eq. (26), we get

$$T_k(q,p;x) = -\frac{(2k-3)!!}{(k-1)!}\frac{(2k-1)}{k}\int_x^q (V(q)-V(q'))^k dq', \tag{28}$$

which reproduces and validates Eq. (25). Equation (18) then reduces to the form

$$T_0^x = -\sum_{k=0}^{\infty}(-1)^k \frac{(2k-1)!!}{k!}\frac{\mu^k}{p^{2k+1}}\int_x^q (V(q)-V(q'))^k dq'. \tag{29}$$

Of course Eq. (29) does not necessarily converge. We next tackle this convergence issue.

Let us consider the neighborhood of $V(q)$ given by $|V(q)-V(q')|<K_\epsilon$ for some $K_\epsilon \leqslant p^2(2\mu)^{-1}$. By the continuity of V at q, there exists a neighborhood of q, ω_q, completely determined by the neighborhood $|V(q)-V(q')|<K_\epsilon$. Now let x be in ω_q and consider the closed interval $\Delta=[q,x]$ which is contained in ω_q. Because V is continuous in the neighborhood ω_q, it is likewise continuous in Δ. This implies that, for a fixed q, $|V(q)-V(q')|$ as function of q' in the interval Δ possesses an absolute maximum M_q. Thus we have the inequality,

$$\left|\sum_{k=0}^{\infty}(-1)^k\frac{(2k-1)!!}{k!}\frac{\mu^k}{p^{2k}}\int_q^x (V(q)-V(q'))^k dq'\right| \leqslant \sum_{k=0}^{\infty}\frac{(2k-1)!!}{k!}\frac{\mu^k}{p^{2k}}M_q^k(x-q). \tag{30}$$

The right-hand side of inequality (30) converges absolutely if and only if $\mu p^{-2}M_q<\frac{1}{2}$. Because $M_q<K_\epsilon p^2(2\mu)^{-1}$, the right-hand side of inequality (30) absolutely converges. This implies that

Eq. (18) converges absolutely for every x in ω_q. The absolute convergence of the right-hand side of inequality (30) also implies the uniform converge of Eq. (18) because we can always replace $(x-q)$ by l in (30) where l is the length of any interval containing Δ.

To show that T_g^x converges absolutely and uniformly to T_x, we must show that the indicated integration in each term of the series can be factored out. This happens when the series $\Sigma_{k=0}^{\infty}(-1)^k(2k-1)!!(k!)^{-1}\mu^k p^{-2k}(V(q)-V(q'))^k$ converges uniformly for a fixed q and for every q' in Δ. This, in fact, is ensured by the absolute convergence of (30). Pulling the integral out in Eq. (29), we arrive at

$$T_0^x(q,p) = -\int_x^q \left(\sum_{k=0}^{\infty} (-1)^k \frac{(2k-1)!!}{k!} \frac{\mu^{k+1}}{p^{2k+1}} (V(q)-V(q'))^k \right) dq'$$

$$= -\frac{\mu}{p} \int_x^q \left(\sqrt{1+\frac{2\mu(V(q)-V(q'))}{p^2}} \right)^{-(1/2)} dq'. \tag{31}$$

Writing $p=\mathrm{sgn}(p)\sqrt{|p|^2}$ in Eq. (31) finally yields

$$T_g^x(q,p) = -\mathrm{sgn}(p)\sqrt{\frac{\mu}{2}} \int_x^q \frac{dq'}{\sqrt{H(q,p)-V(q')}}, \tag{32}$$

which is just the time of arrival at x. Thus $T_g^x(q,p)=t_x(q,p)$ in $\omega\subset\Omega$.

Because $T_x(q,p)$ holds in the entire Ω by definition and $T_0^x(q,p)$ holds only in some local neighborhood ω_q of Ω_q, we have the inclusion $T_0^x(q,p)\subset T_x(q,p)$; that is, $T_x(q,p)$ is the analytic continuation of $T_0^x(q,p)$ in $\Omega\backslash\omega$. For this reason we refer to $T_0^x(q,p)$ as the *local time of arrival* at x, and $T_x(q,p)$ as the global time of arrival. As we have mentioned above it is the local form or the local time of arrival that we will derive quantum mechanically, so that the global time of arrival is only derived by extension.

V. SUPRAQUANTIZATION OF THE CLASSICAL TIME OF ARRIVAL

A. The problem

Let $\mathcal{H}$ be the system Hilbert space and $\mathsf{H}=(1/2\mu)\mathsf{p}^2+V(\mathsf{q})$ be its Hamiltonian where $V(q)$ is $C^\infty(\mathfrak{R})$. Following Sec. II C, the rigging of $\mathcal{H}$ is $\Phi^\times\supset\mathcal{H}\supset\Phi$, where Φ is the fundamental space of infinitely differentiable complex valued functions with compact support in $\mathfrak{R}$, and where $\Phi^\times$ is the corresponding functional space for Φ.

The rigged Hilbert space extension of the Hamiltonian H is then explicitly given by

$$\mathsf{H}^\times\phi = -\frac{\hbar^2}{2\mu}\frac{d^2\phi}{dq^2} + V(q)\phi \quad \text{for all} \quad \phi\in\Phi^\times. \tag{33}$$

In this paper we assume that the potential $V(q)$ is at most entire analytic in q, i.e., represented by an everywhere convergent power series in q. The entire analycity of $V(q)$ is consistent with our requirement that Φ is invariant under the action of the Hamiltonian.

Given the Hamiltonian H, our problem is to construct the corresponding generalized time of arrival operator $\mathcal{T}$ consistent with the correspondence principle: $\mathcal{T}$ reducing to the local time of arrival in the classical limit. The operator $\mathcal{T}$ is by hypothesis a generalized observable relative to the rigging provided by Φ, i.e., the operator $\mathcal{T}$: $\Phi\mapsto\Phi^\times$. This operator is then uniquely associated with a functional kernel $F_\mathcal{T}$ defined by $\mathcal{T}:\Phi=\langle F_\mathcal{T}|\cdot\rangle:\Phi$. Explicitly

$$(\mathcal{T}\varphi)(q) = \int_{-\infty}^{\infty} \langle q|\mathcal{T}|q'\rangle\varphi(q')dq', \tag{34}$$

where $\langle q|\mathcal{T}|q'\rangle^*$ is the functional kernel $F_{\mathcal{T}}$. As a generalized observable, the functional kernel must be symmetric, i.e., $\langle q|\mathcal{T}|q'\rangle=\langle q'|\mathcal{T}|q\rangle^*$. Moreover, since $\mathcal{T}$ is the quantum counterpart of the local time of arrival, it has to be that the classical local time of arrival operator is recovered by means of Eq. (11), specifically

$$t_0(q,p)=\lim_{\hbar\to 0} 2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\right|\mathcal{T}\left|q-\frac{v}{2}\right\rangle\exp\left(-i\frac{vp}{\hbar}\right)dv. \tag{35}$$

The problem of constructing $\mathcal{T}$ then reduces to the problem of determining its functional kernel $\langle q|\mathcal{T}|q'\rangle$. It is now the problem of supraquantization to determine $\langle q|\mathcal{T}|q'\rangle$ without appealing to quantization. (We leave the problem whether $\mathcal{T}$ has Hilbert space projection or none open, a problem relevant to the question whether time of arrival distributions can be extracted from $\mathcal{T}$.)

B. The construction of solution

But how do we determine the kernel $\langle q|\mathcal{T}|q'\rangle$ without resorting to quantization? We accomplish this in two steps. First is by identifying the property of $\mathcal{T}$ and implementing this property through the appropriate axiom of quantum mechanics. Being a time of arrival operator, it must at least evolve according to

$$\frac{d\mathcal{T}}{dt}=-\mathcal{I} \tag{36}$$

in which $\mathcal{I}$ is the identity in Φ. We note that it is not necessary that the above evolution law holds for all t. Fortunately, it is sufficient for us to require the condition $\dot{\mathcal{T}}(0)=-\mathcal{I}$, or $\mathcal{T}$ evolves according to Eq. (36) in the neighborhood of $t=0$. This is always satisfied because Φ is assumed to be invariant under the action of $\mathcal{H}$. Imposing this on Eq. (5), we arrive at the canonical commutation relation

$$\langle\tilde{\varphi}|[\mathsf{H}^{\times},\mathcal{T}]\varphi\rangle=i\hbar\langle\tilde{\varphi}|\varphi\rangle \tag{37}$$

satisfied by the Hamiltonian and the time of arrival operator, for all $\tilde{\varphi}$, $\varphi\in\Phi$. Equation (37) is the basic condition satisfied by $\mathcal{T}$ but it is not sufficient to completely determine $\mathcal{T}$.

The second step is by employing a kind of transfer principle we mentioned earlier. We hypothesize that each element of a class of time of arrival observables shares a common set of properties with the rest of its class such that when a particular property is identified for a specific element of the class that property can be transferred to the rest of the class without discrimination.

We exploit this in determining the kernel $\langle q|\mathcal{T}|q'\rangle$ by solving the simplest in the class of time of arrival observables, the free particle. We start by recalling that the free particle is Galilean invariant, a consequence of the homogeneity of free space. It will not matter then where we place the origin. This implies that the commutation relation (37) holds independent of the choice of origin. Because of this and because the free Hamiltonian is Galilean invariant, we require that the time kernel for the free particle must itself be Galilean invariant. Specifically if t_a is translation by a, i.e., $t_a(q)=q+a$ and if $\langle q|\mathcal{T}|q'\rangle$ is the free particle kernel, then the translated free time of arrival operator $\mathcal{T}_a=\int dq\langle t_a(q)|\mathcal{T}|t_a(q')\rangle$ must still satisfy Eq. (37). In addition to translational invariance, $\langle q|\mathcal{T}|q'\rangle$ must be symmetric, and it must be chosen such that Eq. (37) is satisfied given the free Hamiltonian $\mathsf{H}\tilde{\varphi}=-\hbar^2(2\mu)^{-1}\tilde{\varphi}''$, and it must reproduce the free time of arrival at the origin via Eq. (35). A solution satisfying all these requirements is given by

$$\langle q|\mathcal{T}|q'\rangle=\frac{\mu}{i4\hbar}(q+q')\mathrm{sgn}(q-q'). \tag{38}$$

We note though that (38) is not unique. The kernel $\hbar^{-1}\mu|a-a'|$ is dimensionally consistent with (38) and it is Galilean invariant and it commutes with the free Hamiltonian in the entire Φ.

Moreover it vanishes in the classical limit. Then real factors of it can be added to (38) without sacrificing any of the required properties of the free particle kernel. However, $\hbar^{-1}\mu|a-a'|$ arises only because of Galilean invariance which is an exclusive property of the free particle. Since we are aiming at exploiting the assumed transfer principle, we cannot carry it over to the rest of its class.

Having solved the free particle kernel, we proceed in implementing the transfer principle. We hypothesize that all time kernels assume the same form. Thus, from Eq. (38), we assume that the time kernel is given by

$$\langle q|\mathcal{T}|q'\rangle = \frac{\mu}{i\hbar} T(q,q')\mathrm{sgn}(q-q'), \tag{39}$$

where $T(q,q')$ depends on the given Hamiltonian. Inferring from the free particle time kernel, we require that $T(q,q')$ be real valued, symmetric, $T(q,q')=T(q',q)$, and analytic. We determine $T(q,q')$ by imposing condition (37) on $\mathcal{T}$. Substituting Eq. (39) back into the left-hand side of Eq. (37) and performing two successive integration by parts, we arrive at

$$\begin{aligned}\langle\tilde{\varphi}|[\mathsf{H}^{\times},\mathcal{T}]\varphi\rangle = i\hbar\int_{\Sigma}\tilde{\varphi}^{*}(q)\left(\frac{dT(q,q)}{dq}+\frac{\partial T(q',q')}{\partial q}+\frac{\partial T(q,q)}{\partial q'}\right)\varphi(q)dq \\ -i\frac{\mu}{\hbar}\int_{\Sigma}\tilde{\varphi}^{*}(q)\left[\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2}+V(q)\right)T(q,q')\right. \\ \left.-\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q'^2}+V(q')\right)T(q,q')\right]\mathrm{sgn}(q-q')\varphi(q')dq'dq,\end{aligned} \tag{40}$$

where Σ is the common support of $\varphi(q)$ and $\tilde{\varphi}(q)$. We point out that our ability to arrive at the above expression has been made possible by extending the formulation in a rigged Hilbert space.

If $\mathsf{H}^{\times}$ and $\mathcal{T}$ are to be canonically conjugate in the distributional sense, then the second term must identically vanish for all $\varphi(q)$, $\tilde{\varphi}(q)\in\Phi(\mathfrak{R})$, while the first term must identically reduce to $i\hbar\langle\tilde{\varphi}|\varphi\rangle$. Because φ and $\tilde{\varphi}$ are arbitrary and $\mathrm{sgn}(q-q)$ is not identically zero, the former is satisfied if and only if $T(q,q')$ satisfies the partial differential equation

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 T(q,q')}{\partial q^2}+\frac{\hbar^2}{2\mu}\frac{\partial^2 T(q,q')}{\partial q'^2}+(V(q)-V(q'))T(q,q')=0. \tag{41}$$

On the other hand, the later condition is satisfied if and only if $T(q,q')$ satisfies the boundary condition

$$\frac{dT(q,q)}{dq}+\left.\frac{\partial T(q,q')}{\partial q}\right|_{q=q'}+\left.\frac{\partial T(q,q')}{\partial q'}\right|_{q'=q}=1 \tag{42}$$

for all $q,q'\in\mathfrak{R}$. The boundary condition (42) defines a family of operators canonically conjugate to the extended Hamiltonian in the sense required by Eq. (37). This is a reflection of the fact that there are numerous operators that are canonically conjugate to a given Hamiltonian.

The immediate problem now is how to fix the boundary condition on $T(q,q')$ such that (41) yields a solution satisfying the quantum-classical-correspondence boundary condition (35), and at the same time satisfying the boundary condition (42). Moreover, it is appropriate to require that the solution to (41) is unique. Again we appeal to our transfer principle. We find the set of boundary conditions satisfied by the free particle kernel that ensures that the corresponding solution to the time kernel equation is unique for the free particle. For this case the time kernel equation reduces to

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 T(q,q')}{\partial q^2}+\frac{\hbar^2}{2\mu}\frac{\partial^2 T(q,q')}{\partial q'^2}=0. \tag{43}$$

The general solution to this equation is

$$T(q,q')=f(q+q')+g(q-q'). \tag{44}$$

For the free particle, we already have $T(q,q')=\frac{1}{4}(q+q')$. Now we have to identify the set of boundary conditions that isolates this known solution from the general solution.

By inspection $T(q,q')$ satisfies both (41) and (42), and it satisfies the conditions

$$T(q,q)=\frac{q}{2}, \quad T(q,-q)=0. \tag{45}$$

We now show that these two conditions, when imposed on (44) uniquely identifies the free particle solution. Note that these conditions impose that $T(q,q')$ is analytic in the neighborhood of the origin. Imposing the second condition of (45) on (44) gives $T(q,-q)=f(0)+g(2q)=0$; since this must hold for all $q\in\Re$, it must be that $g(2q)=\text{constant}=-f(0)$. On the other hand, imposing the first of (45) gives $T(q,q)=f(2q)-f(0)=\frac{1}{4}(2q)$. Since $T(q,q')$ satisfies Eq. (43), f is at least twice continuously differentiable. We can then write $f(2q)=f(0)+f'(0)(2q)+R_2$, where R_2 is the remainder in the expansion. Thus $T(q,q)=f'(0)(2q)+R_2=\frac{1}{4}(2q)$, which implies that $f'(0)=\frac{1}{4}$ and $R_2=0$. This finally implies that $T(q,q')=\frac{1}{4}(q+q')$, reproducing the solution we know for the free particle.

By our assumed transfer principle, we impose the same boundary conditions (45) on the solution to the time kernel equation (41). That the boundary conditions (45) guarantee that boundary condition (42) is satisfied and that they impose symmetry on $T(q,q')$ under the interchange of its arguments will be shown below for entire analytic potentials.

We claim that Eqs. (41) and (45) constitute the supraquantization of the local time of arrival consistent with the correspondence principle. We will explicitly demonstrate this claim in Sec. VI for the harmonic and anharmonic oscillators, and separately demonstrate in Sec. VII for entire analytic potentials.

C. Canonical form of the time kernel equation

In what follows, we will find it convenient to prove our above assertion by solving the time kernel Eq. (41) in canonical form. This is accomplished by performing a change in variable from (q,q') to $(u=q+q',\ v=q-q')$. The differential Eq. (41) and its accompanying boundary condition (45) then assume the form

$$-2\frac{\hbar^2}{\mu}\frac{\partial^2 T}{\partial u\partial v}+\left(V\left(\frac{u+v}{2}\right)-V\left(\frac{u-v}{2}\right)\right)T(u,v)=0, \tag{46}$$

$$T(u,0)=\frac{u}{4}, \quad T(0,v)=0. \tag{47}$$

The boundary conditions (47) impose that the solution to Eq. (46) is analytic in u and v. In solving for Eq. (46), we will then seek an analytic solution in powers of u and v,

$$T(u,v)=\sum_{m,n\geqslant 0}\alpha_{m,n}u^m v^n, \tag{48}$$

where the $\alpha_{m,n}$'s are constants determined by Eqs. (46) and (47) for a given potential.

Assuming a solution of the form (48), translates the boundary conditions (47) to the boundary condition on the expansion coefficients $\alpha_{m,n}$:

$$\alpha_{m,0}=\tfrac{1}{4}\delta_{m,1} \quad \alpha_{0,n}=0 \tag{49}$$

for all m and n. We arrive at them as follows. The first boundary condition gives $T(u,0)=\Sigma_m \alpha_{m0}u^m=\frac{1}{4}u$, which implies the first of Eqs. (49). And the second boundary condition gives $T(0,v)=\Sigma_n \alpha_{0n}v^n=0$, which implies the second of Eqs. (49). However, in our proof below, we will find it convenient to extend the summation in (48) to negative values of m and n; the analycity of the solution is then imposed by adjoining to (49) the condition that $\alpha_{m,n}=0$ when either m or n is negative or when both are negative.

To show the uniqueness of the solution to (46) for a given potential, we will assume the existence of two distinct solutions, say, $T_1(u,v)$ and $T_2(u,v)$. Then the function $S(u,v)=T_1(u,v)-T_2(u,v)$ satisfies the time kernel equation. $S(u,v)$ then satisfies the boundary conditions $S(u,0)=0$ and $S(0,v)=0$. Since $T_1(u,v)$ and $T_2(u,v)$ are both analytic, $S(u,v)$ must itself be analytic. Then $S(u,v)$ can be expanded in u and v in the same way that T_1 and T_2 can be expanded,

$$S(u,v)=\sum_{m,n\geqslant 0} \eta_{m,n}u^m v^n. \tag{50}$$

Now the boundary condition satisfied by the expansion coefficients are $\eta_{m,0}=0$ and $\eta_{0,n}=0$ for all m and n. The solution is unique if all the expansion coefficients are identically zero or $S(u,v)$ identically vanishes. We will show below that the solutions for entire analytic potentials are unique.

Now we can address the concern raised earlier whether the assumed properties of $T(q,q')$ are sufficient to ensure that the original boundary condition (42) is satisfied. With the assumed form of the solution (48), the solution in the original coordinates will be in the form

$$T(q,q')=\sum_{m\geqslant 1,n\geqslant 0} \alpha_{mn}(q+q')^m(q-q')^n. \tag{51}$$

Evaluating this at $q=q'$, we have $T(q,q)=2\alpha_{1,0}q$, and arrive at $T'(q,q)=\frac{1}{2}$, because of the boundary condition $\alpha_{1,0}=\frac{1}{4}$. On the other hand, we arrive at the following:

$$\left.\frac{\partial T(q,q')}{\partial q}\right|_{q=q'}=\alpha_{1,0}+\sum_{m\geqslant 1} \alpha_{m,1}2q',$$

$$\left.\frac{\partial T(q,q')}{\partial q'}\right|_{q'=q}=\alpha_{1,0}-\sum_{m\geqslant 1} \alpha_{m,1}2q.$$

However, $T(q,q')$ is symmetric, i.e., $T(q,q')=T(q',q)$, so that $\alpha_{m,n}=0$ for odd n. The second terms of the above equations then vanish and they only take contribution from the first terms. With $\alpha_{1,0}=\frac{1}{4}$ the boundary condition (42) is then satisfied. We note that we have appealed to the assumed symmetry of $T(q,q')$, but this is not totally necessary, because, as what will be shown below, the boundary conditions (45) are sufficient to impose the symmetry of $T(q,q')$.

VI. EXPLICIT EXAMPLES

Before we prove our above assertion, we will explicitly demonstrate in this section our claim for two specific systems: the harmonic and the anharmonic oscillators. We will first solve for the local time of arrival in the neighborhood of the origin using

$$t_0(q,p)=\sum_{k=0}^{\infty} (-1)^k T_k(q,p), \tag{52}$$

where the iterates T_k's are generated through the following recurrence relation:

$$T_0(q,p) = -\mu \frac{q}{p}, \tag{53}$$

$$T_k(q,p) = -\frac{\mu}{p} \int_0^q \frac{\partial V}{\partial q'} \frac{\partial T_{k-1}}{\partial p} dq', \tag{54}$$

obtained from the general expressions (23) and (24) by setting $x=0$.

We will then compare the local time of arrival with the Wigner–Weyl transform of the time kernel,

$$\mathcal{T}_\hbar(q,p) = 2\pi \int_{-\infty}^{\infty} \left\langle q + \frac{v}{2} \middle| \mathcal{T} \middle| q - \frac{v}{2} \right\rangle \exp\left(-i \frac{vp}{\hbar} \right) dv. \tag{55}$$

($\mathcal{T}_\hbar(q,p)$ is real valued and odd with respect to p.) For the harmonic oscillator we will find that the local time of arrival and $\mathcal{T}_\hbar$ coincide; and for the anharmonic oscillator it is only in the limit of vanishing or infinitesimal $\hbar$ that $\mathcal{T}_\hbar$ reproduces the local time of arrival at the origin.

A. The harmonic oscillator

1. Global and local time of arrivals

The potential for the harmonic oscillator is $V(q) = \frac{1}{2}\mu\omega^2 q^2$. Substituting the potential back into the general expression for the global time of arrival (12) yields

$$T_0(q,p) = -\frac{1}{\omega} \tan^{-1}\left(\frac{\mu\omega q}{p} \right). \tag{56}$$

We will show below that this can be derived via the local time of arrival.

Substituting the potential in Eq. (54), we generate the first two iterates of the local time of arrival,

$$T_1 = -\frac{1}{3}\mu^3\omega^2 \frac{q^3}{p^3}, \quad T_2 = -\frac{1}{5}\mu^5\omega^4 \frac{q^5}{p^5}.$$

From these iterates, we infer that for every k, the kth iterate is given by

$$T_k = -\alpha_k \mu^{2k+1} \omega^{2k} \frac{q^{2k+1}}{p^{2k+1}}, \tag{57}$$

where the α_k's are constants to be determined. These constants are determined as follows. We shift index $k \to (k-1)$ in T_k to get the expression for α_{k-1}. We then substitute T_{k-1} and the potential back in the right-hand side of Eq. (54) to yield

$$-\frac{\mu}{p} \int_0^q \frac{\partial V}{\partial q'} \frac{\partial T_{k-1}}{\partial p} dq' = -\alpha_{k-1} \frac{(2k-1)}{(2k+1)} \mu^{2k+1} \omega^{2k} \frac{q^{2k+1}}{p^{2k+1}}. \tag{58}$$

If expression (57) holds for all k, then the right-hand sides of Eqs. (57) and (58) must be equal for all k. Strict equality is then satisfied if and only if the α_k's satisfy the following recurrence relation among themselves:

$$\alpha_k = \frac{(2k-1)}{(2k+1)} \alpha_{k-1}, \tag{59}$$

subject to the initial value $\alpha_0=1$. This can in turn be solved to give $\alpha_k=(2k+1)^{-1}$. The local time of arrival is then given by

$$t_0(q,p)=-\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1}\mu^{2k+1}\omega^{2k}\frac{q^{2k+1}}{p^{2k+1}}. \tag{60}$$

$t_0(q,p)$ can be summed within its region of convergence in the phase space, and the result coincides with the global one in the same region.

In the following we will show that $\mathcal{T}_\hbar(q,p)=t_0(q,p)$, and this is just a special case of our general result on the equality of $\mathcal{T}_\hbar(q,p)$ and $t_0(q,p)$ for linear systems, i.e., systems with linear classical equations of motion.

2. Supraquantization of the local time of arrival

Substituting the potential in Eq. (46) gives the corresponding time kernel equation to solve for the harmonic oscillator,

$$-2\frac{\hbar^2}{\mu}\frac{\partial^2 T}{\partial u\partial v}(u,v)+\frac{\mu\omega^2}{2}uvT(u,v)=0, \tag{61}$$

subject to the boundary conditions (45). We assume a solution of the form

$$T(u,v)=\sum_{m,n}\alpha_{m,n}u^m v^n,$$

where the α's are constants to be determined, subject to the boundary conditions $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, $\alpha_{0,m}=0$ for all m, and $\alpha_{m,n}=0$ for $m,n<0$. Substituting the assumed solution back into Eq. (61), we arrive at

$$-2\frac{\hbar^2}{\mu}\sum_{m,n}\alpha_{m,n}mnu^{m-1}v^{n-1}+\frac{\mu\omega^2}{2}\sum_{m,n}\alpha_{m,n}u^{m+1}v^{n+1}=0.$$

Shifting indices in the second term, $m\to(m-1)$ and $n\to(n-1)$, and collecting like terms, we get

$$\sum_{m,n}\left(-2\frac{\hbar^2}{\mu}mn\alpha_{m,n}+\frac{\mu\omega^2}{2}\alpha_{m-2,n-2}\right)u^{m-1}v^{n-1}=0.$$

Since u and v are arbitrary, the quantity in the bracket must vanish for all values of u and v, dictating the coefficients to satisfy the recurrence relation

$$\alpha_{m,n}=\left(\frac{\mu^2\omega^2}{4\hbar^2}\right)\frac{1}{m\cdot n}\alpha_{m-2,n-2}. \tag{62}$$

Solving the time kernel then reduces to solving this recurrence relation among the coefficients of the assumed solution.

First for odd n. Since $\alpha_{m,n}=0$ for negative n, let us start from $n=1$. For $n=1$ we get the proportionality $\alpha_{m,2}\propto\alpha_{m-1,-1}$; but the coefficients vanish for negative n for all m; thus the right-hand side of the proportionality vanishes and consequently $\alpha_{m,1}=0$ for all m. Now if for some fixed odd n', $\alpha_{m,n'}=0$ for all m, then for the next odd $n'+2$, $\alpha_{m,n'+2}\propto\alpha_{m-1,n'}=0$ for all m. Since we have already shown that $\alpha_{m,1}=0$ for all m, it follows that $\alpha_{m,n}=0$ for all odd n, for all m. The odd powers of v then do not contribute.

We remark that the vanishing of the contributions for odd n is significant. We recall that the solution $T(q,q')$ to the time kernel equation in the original form must satisfy the boundary condition (42). And we have noted earlier in Sec. V C that if $T(q,q')=T(q',q)$ or $T(u,v)$

$=T(u,-v)$, the condition (42) is automatically satisfied as long as the boundary conditions (45) are satisfied as well. But the condition $T(u,v)=T(u,-v)$ is equivalent to the vanishing of the odd powers of v. Consequently $T(q,q')$ will automatically satisfy (42). $T(q,q')$ will then satisfy the original boundary condition (42). This will be shown to be true for the rest of the potentials considered, particularly for entire analytic potentials.

Now for even n. Since $\alpha_{m,n}=0$ for negative n and $\alpha_{m,0}$ is specified, we start with $n=2$. For $n=2$ we get the proportionality $\alpha_{m,2}\propto\alpha_{m-2,0}$; but $\alpha_{m',0}\propto\delta_{m',1}$, thus only $m=3$ contribute or $\alpha_{3,2}$ is the only nonvanishing coefficient for $n=2$. For $n=4$ we get $\alpha_{m,4}\propto\alpha_{m-2,2}$, which dictates that only $m=5$ contributes or $\alpha_{5,4}$ is the only nonvanishing coefficient for $n=4$. We see that n and m are not independent from each other, i.e., they can be index by the same letter, say k. From the first two coefficients we infer that $m=2k+1$ and $n=2k$, $k=1$, $k=2,\ldots$. We can prove this by induction. Let for some fixed k that $\alpha_{m=2k+1,n=2k}$ is the only nonvanishing coefficient for $n=2k$. Then for $k+1$, we have $\alpha_{m,2(k+1)}\propto\alpha_{m-2,2k}$; but the only nonvanishing contributions come from $m-2=2k+1$ or $m=2k+3$. Thus for $n=2(k+1)$, only $\alpha_{2k+3,2(k+1)}$ is nonzero. Thus indeed only the coefficients $\alpha_{2k+1,2k}$ are nonvanishing for all $k=1,2,\ldots$. Then the double index recurrence relation (62) reduces to the single index recurrence relation,

$$\alpha_k=\left(\frac{\mu^2\omega^2}{4\hbar^2}\right)\frac{1}{(2k+1)2k}\,\alpha_{k-1}, \tag{63}$$

subject to the initial value $\alpha_0=\alpha_{1,0}=\frac{1}{4}$. The solution to Eq. (63) is

$$\alpha_k=\frac{1}{4}\left(\frac{\mu\omega}{2\hbar}\right)^2\frac{1}{(2k+1)!}. \tag{64}$$

Substituting the nonvanishing coefficients back in the assumed solution yields the solution to time kernel equation for the harmonic oscillator,

$$T(u,v)=\frac{\hbar}{2\mu\omega}\sum_{k=0}^{\infty}\frac{1}{(2k+1)!}\left(\frac{\mu\omega}{2\hbar}\right)^{2k+1}u^{2k+1}v^{2k}. \tag{65}$$

Evidently $T(u,v)$ converges everywhere in the uv-plane. Moreover, the solution (65) is unique. This follows from the fact that $S(u,v)$ [see Eq. (50)] satisfies the time kernel equation, and it satisfies the boundary conditions $\eta_{0,n}=0$, $\eta_{m,0}=0$ for all m, n on its coefficients. The recurrence relation on the coefficients $\eta_{m,n}$ will be the same as those of the $\alpha_{m,n}$'s. Since the nonvanishing contributions in $T(u,v)$ come only from the boundary condition $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, $S(u,v)$ will be identically zero because $\eta_{m,0}=0$ for all m. The analytic solution $T(u,v)$ is then unique. This observation holds for the rest of the potentials considered here.

Transforming back to (q,q') and substituting $T(q,q')$ back into Eq. (39) yields the time kernel for the harmonic oscillator,

$$\langle q|\mathcal{T}|q'\rangle=\frac{1}{2i\omega}\,\mathrm{sgn}(q-q')\sum_{k=0}^{\infty}\frac{1}{(2k+1)!}\left(\frac{\mu\omega}{2\hbar}\right)^{2k+1}(q+q')^{2k+1}(q-q')^{2k}. \tag{66}$$

This likewise converges everywhere in the qq'-plane. Because $T(q,q')$ is everywhere absolutely convergent, $\mathcal{T}$ is a generalized observable in Φ (see Appendix). Now we can finally show that the generalized time of arrival operator reduces to the local time of arrival in the classical limit, as prescribed by Eq. (35). Using the identity[20]

$$\int_{-\infty}^{\infty}\sigma^{m-1}\,\mathrm{sgn}(\sigma)\exp(-ix\sigma)d\sigma=\frac{(m-1)!}{i^m\pi}x^{-m}, \tag{67}$$

we can perform the indicated transformation to give

$$\mathcal{T}_\hbar(q,p)=2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\middle|\mathcal{T}\middle|q-\frac{v}{2}\right\rangle\exp\left(-i\frac{vp}{\hbar}\right)dv$$

$$=2\pi\frac{1}{2i\omega}\sum_{k=0}^{\infty}\frac{1}{(2k+1)!}\left(\frac{\mu\omega}{2\hbar}\right)^{2k+1}(2q)^{2k+1}\int_{-\infty}^{\infty}v^{2k}\,\mathrm{sgn}(v)\exp\left(-i\frac{vp}{\hbar}\right)dv$$

$$=-\frac{1}{\omega}\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1}\left(\frac{\mu\omega q}{p}\right).$$

We find that $\mathcal{T}_\hbar$ coincides exactly with the local time of arrival in the neighborhood of the origin for the harmonic oscillator given by Eq. (60).

B. The anharmonic oscillator

1. Global and local time of arrivals

In the previous section the Weyl–Wigner transform of the time kernel exactly reproduces the local time of arrival at the origin. But for nonlinear systems, systems with nonlinear equations of motions, we demonstrate that only in the limit of vanishing or infinitesimal $\hbar$ that the local time of arrival (at the origin) is recovered. Let us consider the anharmonic oscillator with the potential $V=\lambda q^4$. The global time of arrival is symbolically given by

$$T_0(q,p)=-\mathrm{sgn}(p)\sqrt{\frac{\mu}{2}}\int_0^q\frac{dq'}{\sqrt{H(q,p)-\lambda q'^4}}. \tag{68}$$

The above expression can be integrated explicitly, but its exact closed integral is not important to our present purposes.

What is important to us is the local time of arrival in the neighborhood of the origin. Following the same procedure we have employed above in determining for the iterates of the harmonic oscillator, we find that the kth iterate of the local time of arrival is given by

$$T_k=\frac{1}{4}\frac{2^k\sqrt{\pi}\Gamma\left(-k-\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)\Gamma\left(-k+\frac{1}{2}\right)}\alpha_k\mu^{k+1}\lambda^k\frac{q^{4k+1}}{p^{2k+1}}. \tag{69}$$

One can prove this by induction using Eq. (54). Substituting T_k back in Eq. (18) yields the local time of arrival at the origin,

$$t_0(q,p)=\frac{1}{4}\frac{\sqrt{\pi}}{\Gamma\left(\frac{3}{4}\right)}\sum_{k=0}^{\infty}\frac{(-2)^k\Gamma\left(-k-\frac{1}{4}\right)}{\Gamma\left(\frac{1}{2}-k\right)}\mu^{k+1}\lambda^k\frac{q^{4k+1}}{p^{2k+1}}. \tag{70}$$

In the following we will show that $\mathcal{T}_\hbar(q,p)=t_0(q,p)+\mathcal{O}(\hbar^2)$. And this is just a special case of our general result on the equality of $\mathcal{T}_\hbar(q,p)$ and $t_0(q,p)$ only in the limit of vanishing or infinitesimal $\hbar$ for nonlinear systems, i.e., systems with nonlinear classical equations of motion.

2. Supraquantization of the local time of arrival

Substituting the potential equation in Eq. (46) gives the corresponding time kernel equation for the anharmonic oscillator,

$$-2\frac{\hbar^2}{\mu}\frac{\partial^2 T}{\partial v\,\partial u}+\frac{\lambda}{2}(u^3v+uv^3)T(u,v)=0, \tag{71}$$

subject to the same boundary conditions. Again we assume the most general form of the solution to the time kernel Eq. (71),

$$T(u,v)=\sum_{m,n}\alpha_{m,n}u^m v^n,$$

where the $\alpha_{m,n}$'s satisfy the boundary conditions $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$ and $\alpha_{0,n}=0$ for all m and n, and $\alpha_{m,n}=0$ for negative m and n to identify the particular solution we seek.

Substituting the assumed solution back to Eq. (71) gives the following recurrence relation for the coefficients:

$$\alpha_{m,n}=\left(\frac{\mu\lambda}{4\hbar^2}\right)\frac{1}{mn}(\alpha_{m-4,n-2}+\alpha_{m-2,n-4}). \tag{72}$$

First let us consider the coefficients for odd powers of v or for odd n. Since the coefficients vanish for negative m and n, we start from $n=1$. For $n=1$ we get the proportionality $\alpha_{m,1}\propto(\alpha_{m-4,-1}+\alpha_{m-2,-3})$. But $\alpha_{m,n}=0$ for $n<0$ for all m, so that $\alpha_{m,1}=0$ for all m. For $n=3$ we get the proportionality $\alpha_{m,3}\propto(\alpha_{m-4,1}+\alpha_{m-2,-1})$. Since $\alpha_{m,1}=0$ for all m and $\alpha_{m,n}=0$ for $n<0$, $\alpha_{m,3}=0$ for all m as well. Now if for some odd n, $\alpha_{m,n}=0$ for all m, it follows from (72) that for the next odd number $n+2$, $\alpha_{m,n+2}=0$ for all m. Thus odd powers of v vanish. This assures us that $T(q,q')$ satisfies the boundary condition (42).

Let us now consider the even powers of v. For $n=2$ we get the proportionality $\alpha_{m,2}\propto(\alpha_{m-4,0}+\alpha_{m-2,-2})$. Only $m=5$ contributes because $\alpha_{m,n}=0$ for negative n and $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$; thus for $n=2$ only $\alpha_{5,2}$ contributes. For $n=4$ we get the proportionality $\alpha_{m,4}\propto(\alpha_{m-4,2}+\alpha_{m-2,0})$. There are only two contributions: $m=3$, corresponding to $\alpha_{1,0}$, and $m=9$, corresponding to $\alpha_{5,2}$; thus for $n=4$ only $\alpha_{3,2}$ and $\alpha_{9,2}$ contribute. Continuing in this manner, we arrive at the following first few sequences of nonvanishing contributions:

$$n=0:\quad \alpha_{1,0},$$

$$n=2:\quad \alpha_{5,2},$$

$$n=4:\quad \alpha_{9,4},\ \alpha_{3,4},$$

$$n=6:\quad \alpha_{13,6},\ \alpha_{7,6},$$

$$n=8:\quad \alpha_{17,8},\ \alpha_{11,8},\ \alpha_{5,8},$$

$$n=10:\quad \alpha_{21,10},\ \alpha_{15,10},\ \alpha_{9,10}.$$

By inspection the nonvanishing coefficients can be grouped in two groups. Let $n=2j$ for $j=0,1,2,\ldots$. The contributing coefficients can then be written in the form $\alpha_{m(j),2j}$, where for

$$j=\text{odd},\quad m(j)=(j+4),\ (j+4)+6,\ (j+4)+12,\ldots,2j+1,$$

$$j=\text{even},\quad m(j)=(j+1),\ (j+1)+6,\ (j+1)+12,\ldots,2j+1.$$

Evidently for a given j there are $\{j\}$ contributing m's, in which $\{j\}=\frac{1}{2}(j-1)+1$ for $j=$odd, and $\{j\}=(\frac{1}{2}j-1)+1$ for $j=$even. This can be proved by induction.

With the arrangement above for the coefficients, we can sum along the vertical. The above results suggest that the solution can be written in the following form:

$$T(u,v)=\frac{1}{4}\sum_{k=0}^{\infty}\sum_{j=2k}^{\infty}\beta_{k,j}u^{4j+1-6k}v^{2j}, \tag{73}$$

where $\beta_{k,j}$'s are proportional to the nonvanishing coefficients, i.e., $\beta_{k,j}=4\alpha_{4j+1-6k,2j}$, $\beta_{0,0}=1$, for $k\geqslant 0$ and $j\geqslant 2k$. Substituting Eq. (73) back into Eq. (71), we get the following recurrence relation for the $\beta_{k,j}$'s:

$$\beta_{k,j}=\left(\frac{\mu\lambda}{4\hbar^2}\right)\frac{1}{(4j+1-6k)\cdot 2j}(\beta_{k,j-1}+\beta_{k-1,j-2}). \tag{74}$$

This recurrence relation (74) holds for all values of k and j restricted in the assumed solution as long as we agree to set $\beta_{k,j}=0$ when both or either of k and j is negative, or when $j<2k$.

First let us solve for $\beta_{0,j}$ for all $j\geqslant 1$ given $\beta_{0,0}=1$. Setting $k=0$ in Eq. (74) we arrive at the recurrence relation

$$\beta_{0,j}=\left(\frac{\mu\lambda}{4\hbar^2}\right)\frac{1}{(4j+1)\cdot 2j}\beta_{0,j-1}, \tag{75}$$

the $\beta_{k,j}$'s being zero for $k<0$. Let us define

$$\lambda_r^{(j,k)}=\prod_{l=0}^{r}\frac{1}{(4(j-l)+1-6k)}, \tag{76}$$

where the value $r=-1$ is allowed. Equation (75) can be solved recursively to give

$$\beta_{0,j}=\frac{1}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^j\frac{1}{(-4)^{j+1}}\frac{\Gamma\left(-j-\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} \tag{77}$$

valid for all $j\geqslant 0$. Given $\beta_{0,j}$ we can proceed in determining of the coefficients.

To solve for $\beta_{k,j}$ for arbitrary k and j, we assume that we know the solution for $(j-1)$ for all j in Eq. (74). This reduces the problem of solving the recurrence relation for some fix j. We shift index $k\rightarrow(k-1)$ in Eq. (74) and substitute it back to Eq. (74). We do this repeatedly until we arrive at the following result:

$$\beta_{k,j}=\sum_{r=0}^{j-2k}\left(\frac{\mu\lambda}{4\hbar^2}\right)^{r+1}\frac{\beta_{k-1,j-2-r}}{2^{r+1}}\frac{(j-1-r)!}{j!}\lambda_r^{(j,k)}. \tag{78}$$

This can be proven by induction. So for $k=1$, Eq. (78) yields

$$\beta_{1,j}=\frac{1}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^{j-1}\sum_{r=0}^{j-2}(j-r-1)\lambda_{j-r-3}^{(j-2-r,0)}\lambda_r^{(j,1)}=\frac{1}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^{j-1}\left[\frac{1}{2}\frac{\Gamma\left(\frac{3}{4}\right)(-1)^j\sqrt{2}\Gamma\left(-j+\frac{5}{4}\right)}{4^j\pi}\right.$$

$$\left.+\frac{1}{192}\frac{(4j-5)(2j+1)(-1)^{j-2}\Gamma\left(-j+\frac{7}{4}\right)\Gamma\left(-j+\frac{5}{4}\right)}{4^{j-2}\Gamma\left(\frac{3}{4}\right)\Gamma\left(\frac{9}{4}-j\right)}\right]. \tag{79}$$

The rest of the contributing coefficients for other k's can be determined similarly.

However, the explicit forms for $\beta_{0,j}$ and $\beta_{1,j}$ suggest a simplification for $\beta_{k,j}$. These coefficients can be explicitly written in the form

$$\beta_{k,j}=\frac{1}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^{j-k}\rho_{k,j} \tag{80}$$

for some constants $\rho_{k,j}$. These constants are found by substituting (80) back in both sides of Eq. (78), with the appropriate shifting of indices in the right-hand side. Doing so leads to the following recurrence relation:

$$\rho_{k,j}=\sum_{r=0}^{j-2k}(j-r-1)\lambda_r^{(j,k)}\rho_{k-1,j-2-r} \tag{81}$$

for all $k\geqslant 1$ and $j\geqslant 2k$. The initial value that determines all the constants $\rho_{k,j}$ is defined by (77). Comparing Eq. (77) and Eq. (80) for $k=0$ gives

$$\rho_{0,j}=\frac{1}{(-4)^{j+1}}\frac{\Gamma\left(-j-\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}, \tag{82}$$

valid for all $j\geqslant 0$. Equation (81) can be solved explicitly given the initial value. We do not need to write its explicit solution.

Substituting $\beta_{k,j}$ back in Eq. (73), the solution to the time kernel equation for the anharmonic oscillator assumes the form

$$T(u,v)=\frac{1}{4}\sum_{k=0}^{\infty}\sum_{j=2k}^{\infty}\frac{\rho_{k,j}}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^{j-k}u^{4j+1-6k}v^{2j}. \tag{83}$$

In arriving at this solution we have assumed above that the solution absolutely converges in the neighborhood of the origin in the uv-plane, so that the contributing terms can be rearranged at will. However, we can only assert at this moment absolute convergence in the entire uv-plane of the first two leading terms in the solution. Equation (83) can be written in the form

$$T(u,v)=T_0(u,v)+T_1(u,v)+\cdots, \tag{84}$$

where the subscripts denote the corresponding term for a given k. For $k=0$ and $k=1$, we have the following explicit closed forms:

$$T_0(u,v)=\frac{1}{4}u\,{}_0F_1\left(\frac{5}{4};\frac{\mu\lambda}{32\hbar^2}u^4v^2\right), \tag{85}$$

$$\begin{aligned}T_1(u,v)=&-\frac{1}{96}\left(\frac{\mu\lambda}{8\hbar^2}\right)u^3v^4\,{}_1F_2\left(1;3,\frac{7}{4};\frac{\mu\lambda}{32\hbar^2}u^4v^2\right)+\frac{5}{96}\left(\frac{\mu\lambda}{8\hbar^2}\right)u^3v^4\,{}_1F_2\left(1;3,\frac{5}{4};\frac{\mu\lambda}{32\hbar^2}u^4v^2\right)\\&+\frac{1}{720}\left(\frac{\mu\lambda}{8\hbar^2}\right)^2u^7v^6\,{}_1F_2\left(2;4,\frac{9}{4};\frac{\mu\lambda}{32\hbar^2}u^4v^2\right),\end{aligned} \tag{86}$$

where ${}_pF_q$ is the generalized hypergeometric function. ${}_pF_q$ converges everywhere if $p\leqslant q$. The first two leading terms then converge everywhere in the uv-plane.

Transforming back to (q,q'), the time kernel for the anharmonic oscillator assumes the form

$$\langle q|\mathcal{T}|q'\rangle = \frac{\mu}{4i\hbar}\,\mathrm{sgn}(q-q')\sum_{k=0}^{\infty}\sum_{j=2m}^{\infty}\frac{\rho_{k,j}}{j!}\left(\frac{\mu\lambda}{8\hbar^2}\right)^{j-k}(q+q')^{4j+1-6k}(q-q')^{2j}. \tag{87}$$

The first two groups of terms, corresponding to $k=0$ and $k=1$, converge everywhere in the qq'-plane so that they are functionals in the $\Phi^{\times}$ and define a generalized operator in Φ. We have not been able to make a conclusion on the convergence of the rest of the group of terms. We note though that, since $\langle q|\mathcal{T}|q'\rangle$ must be a functional in $\Phi^{\times}$, it is not necessary that the sum converges in the usual sense; it is sufficient that it converges in the distributional sense in $\Phi^{\times}$ (see Gel'fand and Shilov (1964), p. 368 for a discussion on the convergence of functionals in Φ). Performing the indicated transformation, we have

$$\begin{aligned}\mathcal{T}_{\hbar}(q,p) &= 2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\middle|\mathcal{T}\middle|q-\frac{v}{2}\right\rangle\exp\left(-i\frac{vp}{\hbar}\right)dv\\ &= -\frac{\mu}{2}\sum_{k=0}^{\infty}\hbar^{2k}\sum_{j=2k}^{\infty}(-1)^j\frac{\rho_{k,j}}{j!}(2j)!\left(\frac{\mu\lambda}{8}\right)^{j-k}\frac{(2q)^{4j+1-6k}}{p^{2j+1}}\\ &= \frac{1}{4}\frac{\sqrt{\pi}}{\Gamma\left(\frac{3}{4}\right)}\sum_{j=0}^{\infty}\frac{(-2)^j\Gamma\left(-\frac{1}{4}-j\right)}{\Gamma\left(\frac{1}{2}-j\right)}\mu^{j+1}\lambda^j\frac{q^{4j+1}}{p^{2j+1}}+\mathcal{O}(\hbar^2)=t_0(q,p)+\mathcal{O}(\hbar^2),\end{aligned}$$

where t_0 is the local time of arrival of the anharmonic oscillator as given by Eq. (70). Thus $\mathcal{T}_{\hbar}(q,p)$ reduces to $t_0(q,p)$ in the limit of vanishing $\hbar$ or infinitesimal $\hbar$.

VII. ENTIRE ANALYTIC POTENTIALS

In this section we prove that the local time of arrival is completely derivable from the generalized time of arrival operator for systems subject to entire analytic potentials, e.g., potentials in polynomials of q. We divide our proof for the linear (systems with linear classical equations of motions) and nonlinear (systems with nonlinear classical equations of motions) cases. In particular we will show that

$$\text{Linear Systems:}\quad \mathcal{T}_{\hbar}(q,p)=t_0(q,p), \tag{88}$$

$$\text{Nonlinear Systems:}\quad \mathcal{T}_{\hbar}(q,p)=t_0(q,p)+\mathcal{O}(\hbar^2). \tag{89}$$

Our method of proof will not follow the line used in the previous section. It will be sufficient to show that the leading term in $\mathcal{T}_{\hbar}(q,p)$, $\mathcal{T}_k^0(q,p)$, the term of order $\mathcal{O}(\hbar^0)$, can be written in the form

$$\mathcal{T}_{\hbar}^0(q,p)=\sum_{k=0}^{\infty}(-1)^k\mathcal{T}_k(q,p), \tag{90}$$

where the $\mathcal{T}_k$'s satisfy the initial value and the recurrence relation

$$\mathcal{T}_0(q,p)=-\mu\frac{q}{p}, \tag{91}$$

$$\mathcal{T}_k(q,p)=-\frac{\mu}{p}\int_0^q\frac{\partial V}{\partial q'}\frac{\partial\mathcal{T}_{k-1}}{\partial p}dq', \tag{92}$$

for all k. If they do, then, according to our result in Sec. IV, $\mathcal{T}^0_\hbar(q,p)$ converges to the local time of arrival in the neighborhood of the origin.

A. Linear systems

Now we consider the most general case for linear systems. The most general potential is given by

$$V(q)=aq+\tfrac{1}{2}bq^2, \tag{93}$$

for some constants a and b. A constant can be added to $V(q)$, but it does not change the result. Here we prove that for systems subject to the potential (93) the local time of arrival in the neighborhood of the origin is given by Eq. (88).

We first solve for the time kernel of the generalized time of arrival operator. Substituting the potential in the time kernel equations lead to solve the following partial differential equation:

$$-\frac{2\hbar^2}{\mu}\frac{\partial^2 T}{\partial u\,\partial v}+\left(av+\frac{1}{2}buv\right)T(u,v)=0, \tag{94}$$

subject to the boundary conditions $T(u,0)=\frac{1}{4}u$ and $T(0,v)=0$. We assume the most general solution of the form

$$T(u,v)=\sum_{m,n}\alpha_{m,n}u^m v^n, \tag{95}$$

where the coefficients now satisfy the conditions $\alpha_{m,n}=0$ when both or either m and n are negative, and $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, $\alpha_{0,n}=0$ for all n. Substituting the assumed solution back into Eq. (94) yields the recurrence relation among the coefficients

$$\alpha_{m,n}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{mn}\left(a\alpha_{m-1,n-2}+\frac{1}{2}b\alpha_{m-2,n-2}\right). \tag{96}$$

First let us show that odd powers of v do not contribute in the solution, i.e., $\alpha_{m,n}=0$ for all odd n for all m. For $n=1$ we have the proportionality $\alpha_{m,1}\propto(a\alpha_{m-1,-1}+\frac{1}{2}b\alpha_{m-2,-1})$. But $\alpha_{m,n}=0$ for all negative n, thus $\alpha_{m,1}=0$ for all m. Now let us assume that for some fixed odd n, $\alpha_{m,n}=0$ for all m. Then for the next odd $n'=n+2$, $\alpha_{m,n+2}\propto(a\alpha_{m-1,n}+\frac{1}{2}b\alpha_{m-2,n})$. But $\alpha_{m,n}=0$ for all m, thus $\alpha_{m,n+2}=0$ for all m. Since we have shown that $\alpha_{m,1}=0$ for all m, it then follows that $\alpha_{m,n}=0$ for all m for all odd n. The vanishing of the odd powers of v is significant because it assures us that the boundary condition (42), necessary to impose canonicality, is satisfied.

Now let us determine the coefficients for even n. For $n=2$ we have the proportionality $\alpha_{m,2}\propto(a\alpha_{m-1,0}+\frac{1}{2}b\alpha_{m-2,0})$. Since $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, only $m=2$ contributes in the first term, and $m=3$ for the second term. For $n=4$, $\alpha_{m,4}\propto(a\alpha_{m-1,2}+\frac{1}{2}b\alpha_{m-2,2})$. Only $m=3$, 4 contribute for the first term; while $m=4$, 5 for the second term. Continuing the process, we arrive at the following first few nonvanishing coefficients,

$$n=0:\quad \alpha_{1,0},$$

$$n=2:\quad \alpha_{2,2},\ \alpha_{3,2},$$

$$n=4:\quad \alpha_{3,4},\ \alpha_{4,4},\ \alpha_{5,4}.$$

We find that for every $n=2j$, for integer j, there are $j+1$ nonvanishing contributions. In particular, for a given j, we can write $\alpha_{m,n}$ in the form $\alpha_{m(j),2j}$, where $m(j)$ takes on one of the following values:

$$m(j)=(j+1),(j+2),\ldots,(2j+1).$$

This can be proven by induction.

The solution to the time kernel equation (94) can then be written in the following form:

$$T(u,v)=\sum_{j=0}^{\infty}\sum_{k=0}^{j}\alpha_{2j+1-k,2j}u^{2j+1-k}v^{2j}=\frac{1}{4}\sum_{k=0}^{\infty}\sum_{j=0}^{k}\eta_{k,j}u^{2j+1-k}v^{2j}, \tag{97}$$

where the $\eta_{k,j}$'s are constants proportional to the nonvanishing $\alpha_{m,n}$'s, with $\eta_{0,0}=1$. Substituting back the second form of the solution to the time kernel equation yields the recurrence relation

$$\eta_{k,j}=\left(\frac{\mu}{2\hbar^2}\right)\frac{\left(a\,\eta_{k-1,j-1}+\frac{1}{2}b\,\eta_{k-1,j}\right)}{2k(2k+1-j)}, \tag{98}$$

valid for all k and j as long as we set $\eta_{j,k}=0$ for all $0>j>k$. Solving this recursively yields the following form:

$$\eta_{k,j}=\left(\frac{\mu}{2\hbar^2}\right)^k\frac{1}{2^k k!}\sigma_{k,j}b^{k-j}a^j, \tag{99}$$

for some constants $\sigma_{k,j}$. Substituting Eq. (99) back into (98) gives the recurrence relation for the constants $\sigma_{k,j}$,

$$\sigma_{k,j}=\frac{1}{(2k+1-j)}\left(\sigma_{k-1,j-1}+\frac{1}{2}\sigma_{k-1,j}\right). \tag{100}$$

This can be solved recursively to give

$$\sigma_{k,j}=\sum_{r=1}^{k-j+1}\frac{\sigma_{k-r,j-1}}{2^{r-1}}\prod_{s=0}^{r-1}\frac{1}{(2(k-s)+1-j)} \tag{101}$$

with $\sigma_{0,0}=1$. We don't need to evaluate this explicitly. We will just need this recurrence relation in proving Eq. (88). The solution to the time kernel equation can now be written in the form

$$T(u,v)=\frac{1}{4}\sum_{k=0}^{\infty}\sum_{j=0}^{k}\left(\frac{\mu}{2\hbar^2}\right)^k\frac{1}{2^k k!}\sigma_{k,j}b^{k-j}a^j u^{2k+1-j}v^{2k}. \tag{102}$$

It can be shown that $T(u,v)$ is everywhere defined in the uv-plane. From the expression for $T(u,v)$, we have

$$T(q,q')=\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\mu}{2\hbar^2}\right)^k\frac{1}{2^k k!}(q-q')^{2k}\sum_{j=0}^{k}\sigma_{k,j}b^{k-j}a^j(q+q')^{2k+1-j} \tag{103}$$

in the original coordinate.

Equation (103) allows us to finally write the functional of the generalized time of arrival operator in the neighborhood of the origin,

$$\langle q|\mathcal{T}|q'\rangle=\frac{\mu}{4i\hbar}\,\mathrm{sgn}(q-q')\sum_{k=0}^{\infty}\sum_{j=0}^{k}\left(\frac{\mu}{2\hbar^2}\right)^k\frac{1}{2^k k!}\sigma_{k,j}b^{k-j}a^j(q+q')^{2k+1-j}(q-q')^{2k}. \tag{104}$$

This is a functional for fixed q in Φ. Performing the indicated transformation to go back in the classical regime, we get

$$\mathcal{T}_\hbar(q,p)=2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\right|\mathcal{T}\left|q-\frac{v}{2}\right\rangle\exp\left(-i\frac{vp}{\hbar}\right)dv$$
$$=\sum_{k=0}^{\infty}\sum_{j=0}^{k}(-1)^{k+1}\mu^{k+1}\frac{(2k)!}{k!}\frac{\sigma_{k,j}}{2^j}b^{k-j}a^j\frac{q^{2k+1-j}}{p^{2k+1}}. \tag{105}$$

We note that $\mathcal{T}_\hbar$ is to the order $\mathcal{O}(\hbar^0)$. Now to complete our proof, we write

$$\mathcal{T}_\hbar(q,p)=\sum_{k=0}^{\infty}(-1)^k\mathcal{T}_k, \tag{106}$$

where

$$\mathcal{T}_k=-\frac{(2k)!}{k!}\mu^{k+1}\sum_{j=0}^{k}\frac{\sigma_{k,j}}{2^j}b^{k-j}a^j\frac{q^{2k+1-j}}{p^{2k+1}}. \tag{107}$$

To prove our assertion that $t_0(q,p)=\mathcal{T}_\hbar(q,p)$, we need only to show that $\mathcal{T}_k$ satisfies the initial value condition $t_0(q,p)$ and the recurrence relation is satisfied by the iterates of the local time of arrival at the origin. It is straightforward to show that $\mathcal{T}_0(q,p)=t_0(q,p)$ by setting $k=0$ in Eq. (107). It only remains to show that the $\mathcal{T}_k$'s satisfy the recurrence relation (92). Shifting index $k\to k-1$ in (107) and substituting it back, together with the potential, in right-hand side of Eq. (92) yields

$$-\frac{\mu}{p}\int_0^q\frac{\partial V}{\partial q}\frac{\partial\mathcal{T}_{k-1}}{\partial p}dq=-\frac{(2(k-1))!(2k-1)}{(k-1)!}\mu^{k+1}$$
$$\times\sum_{j=0}^{k}\frac{1}{2^j}\frac{(2\sigma_{k-1,j-1}+\sigma_{k-1,j})}{(2k+1-j)}b^{k-j}a^j\frac{q^{2k+1-j}}{p^{2k+1}}, \tag{108}$$

where $\sigma_{k,j}=0$ for $0>j>k$. Equation (105) converges to the local time of arrival at the origin if and only if Eq. (108) is equal to (107) for all $k\geqslant 1$. Equating $\mathcal{T}_k$ with Eq. (108), we find that $\sigma_{k,j}$ must the satisfy the following recurrence relation if strict equality is required:

$$\sigma_{k,j}=\frac{1}{(2k+1-j)}\left(\sigma_{k-1,j-1}+\frac{1}{2}\sigma_{k-1,j}\right). \tag{109}$$

But this recurrence relation is already satisfied by the $\sigma_{k,j}$'s, as shown by Eq. (100). Thus Eq. (105) converges to the local time of arrival at the origin for the potential given.

We have thus proved what we have sought to prove that for linear systems, $\mathcal{T}_\hbar(q,p)=t_0(q,p)$.

B. Nonlinear systems

In this section we show that for entire analytic potentials of the form

$$V(q)=\sum_{s=1}^{\infty}a_sq^s, \tag{110}$$

with at least a_3 is nonvanishing, the proposed supraquantization of the time of arrival at the origin reduces only to the classical local time of arrival in the limit of vanishing or infinitesimal $\hbar$. Substituting the potential back into the time kernel equation and after some simplification, we arrive at the partial differential equation to solve

$$-2\frac{\hbar^2}{\mu}\frac{\partial^2 T}{\partial u\,\partial v}+\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{2}{2k+1}u^{s-2k-1}v^{2k+1}T(u,v)=0, \tag{111}$$

where $[s]=(s-1)/2$ for $s=$odd and $[s]=(s/2)-1$ for $s=$even, subject to the same boundary conditions.

Now let us assume an analytic solution of the form

$$T(u,v)=\sum_{m,n}\alpha_{m,n}u^m v^n, \tag{112}$$

subject to the boundary conditions $\alpha_{m,n}=0$ for $m,n<0$, $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, and $\alpha_{0,n}=0$ for all n. Substituting the assumed solution back into (111) and collecting terms of equal powers of u and v yield the following recurrence relation among the coefficients:

$$\alpha_{m,n}=\frac{\mu}{2\hbar^2}\frac{1}{mn}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{s}{2k+1}\alpha_{m-s+2k,n-2k-2}. \tag{113}$$

Imposing the boundary condition, we have the following conditions imposed upon the coefficients: $\alpha_{1,0}=\frac{1}{4}$, $\alpha_{m,n}=0$ for all $n<0$ and $m\leqslant 1$, $\alpha_{m,0}=0$ for all $m\geqslant 2$, and $\alpha_{m,1}=0$ for all m.

1. Odd powers of v

The boundary conditions impose that the $\alpha_{m,n}$'s vanish for odd n for all m. The coefficients already vanish for negative n, so we start with $n=1$. For $n=1$ Eq. (113) gives

$$\alpha_{m,1}=\frac{\mu}{2\hbar^2}\frac{1}{m\cdot 1}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{s}{2k+1}\alpha_{m-s+2k,-2k-1}.$$

Since $\alpha_{m,n}$ vanish for all negative n, $\alpha_{m,1}=0$ for all m. For $n=3$ we have

$$\alpha_{m,3}=\frac{\mu}{2\hbar^2}\frac{1}{m\cdot 3}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{s}{2k+1}\alpha_{m-s+2k,1-2k}.$$

Since $\alpha_{m,1}=0$ for all m and $\alpha_{m,n}=0$ for all negative n, it follows that $\alpha_{m,3}=0$ for all m as well. Now let $n=2j+1$, for $j=0,1,2,...$, and let $\alpha_{m,2j+1}=0$ for all m for all $j\leqslant J$. Then for $n=2(J+1)+1$,

$$\alpha_{m,2(J+1)+1}=\frac{\mu}{2\hbar^2}\frac{1}{m(2(J+1)+1)}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{s}{2k+1}\alpha_{m-s+2k,2J+1-2k}.$$

The $k=0$ term in the inner sum contains the factors $\alpha_{m-s+2k,2J+1}$, which are all vanishing because $\alpha_{m,2J+1}=0$ for all m; the $k=0$ term then does not contribute. The $k=1$ term contains the factors $\alpha_{m-s+2k,2(J-1)+1}$, which are all also vanishing because $\alpha_{m,2j+1}=0$ for all m for all $j\leqslant J$; the $k=1$ term then does not contribute.

Now for all $k\leqslant J$, the coefficients $\alpha_{m-s+2k,2J+1-2k}=\alpha_{m-s+2k,2(J-k)+1}$ vanish, again, because $\alpha_{m,2j+1}=0$ for all m for all $j\leqslant J$; and no contribution comes from them. On the other hand, for all $k>J$, the coefficients $\alpha_{m-s+2k,2(J-k)+1}$ must vanish because of the condition that $\alpha_{m,n}=0$ for all negative n. Thus $\alpha_{m,2(J+1)+1}=0$ for all m as well. We have already shown that $\alpha_{m,1}$

$=0$ and $\alpha_{m,3}=0$ for all m, and it follows that $\alpha_{m,5}=0$ for all m from what we have already shown, and so on. Thus it must be that $\alpha_{m,n}=0$ for all m for every odd n. Odd powers of v then do not contribute in the solution to the time kernel equation.

2. Even powers of v

Now we proceed in determining the nonvanishing coefficients corresponding to even powers of v or to even n. First, for $n=2$, the recurrence relation (113) reduces to

$$\alpha_{m,2}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 2}\sum_{s=1}^{\infty}\frac{a_s}{2^{2-1}}\sum_{k=0}^{[s]}\binom{s}{2k+1}\alpha_{m-2+2k,-2k}. \tag{114}$$

Since the $\alpha_{m,n}$'s vanish for all negative n, only the $k=0$ term contributes in (114). Thus

$$\alpha_{m,2}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 2}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\binom{s}{1}\alpha_{m-s,0}.$$

But $\alpha_{m',0}=\frac{1}{4}\delta_{m',1}$, so that only the $s=m-1$ term contributes in the preceding relation. Since the power of u is at least to the first order and $s\geqslant 1$, only those coefficients with $m\geqslant 2$ contribute above. Thus

$$\alpha_{m,2}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 2}\frac{a_{m-1}}{2^{m-2}}\binom{m-1}{1}\frac{1}{4}. \tag{115}$$

The nonvanishing contributions from those with $m\geqslant 2$.

For $n=4$ the recurrence relation reduces to

$$\alpha_{m,4}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 4}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{[s]}\binom{2}{2k+1}\alpha_{m-s+2k,2-2k}. \tag{116}$$

For all s only the $k=0,1$ contribute to $\alpha_{m,4}$. All of the $s\geqslant 1$ terms contribute to the $k=0$ term. However, only those for $s\geqslant 3$ contribute to the $k=1$ term. Thus

$$\alpha_{m,4}=\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 4}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\binom{s}{1}\alpha_{m-s,2}+\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 4}\sum_{s=3}^{\infty}\frac{a_s}{2^{s-1}}\binom{s}{3}\alpha_{m-s+2,0}.$$

Since $\alpha_{m',2}$ is nonvanishing only for $m'\geqslant 2$, it has to be that $(m-s)\geqslant 2$ in the first term; thus only those $1\leqslant s\leqslant(m-2)$ contribute in the sum. Since $s\geqslant 1$ only those with $m\geqslant 3$ contribute. On the other hand, only $s=m+1$ contributes in the second term. Thus, upon substituting $\alpha_{m',2}$ and $\alpha_{m',0}$,

$$\alpha_{m,4}=\left(\frac{\mu}{2\hbar^2}\right)^2\frac{1}{m\cdot 4}\sum_{s=1}^{m-2}\frac{a_s a_{m-s-1}}{2^{m-2}}\binom{s}{1}\binom{m-s-1}{1}\frac{1}{4}+\left(\frac{\mu}{2\hbar^2}\right)\frac{1}{m\cdot 4}\frac{a_{m+1}}{2^m}\binom{m+1}{3}\frac{1}{4},$$

with the first term having contribution only for $m\geqslant 3$ and the second term for all $m\geqslant 2$.

We would like now to generalize our results for arbitrary j. The explicit forms of $\alpha_{m,0}$, $\alpha_{m,2}$ and $\alpha_{m,4}$ suggest that, for some fixed j, we have

$$\alpha_{m,2j}=\sum_{s=0}^{j-1}\alpha_{m,j}^{(s)}\left(\frac{\mu}{2\hbar^2}\right)^{j-s}, \tag{117}$$

for some constants $\alpha^{(0)}_{m,j}$ independent of $\hbar$ and μ. We prove (117) by induction and consequently determine the recurrence relation satisfied by these constants that determines them uniquely. Now for $n=2j$ for some $j\geqslant 1$, the recurrence relation (113) can be written in the form

$$\alpha_{m,2j}=\frac{\mu}{2\hbar^2}\frac{1}{m\cdot 2j}\sum_{s=1}^{\infty}\frac{a_s}{2^{s-1}}\sum_{k=0}^{j-1}\binom{s}{2k+1}\alpha_{m-s+2k,2(j-k-1)}. \tag{118}$$

We have replaced $[s]$ with $j-1$ in the inner summation limit because whatever extra terms are introduced they are taken care of by the binomial factor. The order of summation can be reordered to yield

$$\begin{aligned}\alpha_{m,2j}&=\frac{\mu}{2\hbar^2}\frac{1}{m\cdot 2j}\sum_{k=0}^{j-1}\sum_{s=2k+1}^{\infty}\frac{a_s}{2^{s-1}}\binom{s}{2k+1}\alpha_{m-s+2k,2(j-k-1)}\\&=\frac{\mu}{2\hbar^2}\frac{1}{m\cdot 2j}\sum_{k=0}^{j-1}\sum_{s=2k+1}^{m+2k-1}\frac{a_s}{2^{s-1}}\binom{s}{2k+1}\alpha_{m-s+2k,2(j-k-1)}.\end{aligned} \tag{119}$$

The second line follows from the fact that $\alpha_{m-s+2k,2(j-k-1)}$ is nonvanishing only when $m-s+2k\geqslant 1$ or $m+2k-1\geqslant s$.

Now we substitute Eq. (117) back into the right-hand side of Eq. (119). This yields

$$\alpha_{m,2j}=\frac{1}{m\cdot 2j}\sum_{k=0}^{j-1}\sum_{r=0}^{j-k-1}\left(\sum_{s=2k+1}^{m+2k-1}\frac{a_s}{2^{s-1}}\binom{s}{2k+1}\alpha^{(r)}_{m-s+2k,j-k-1}\right)\left(\frac{\mu}{2\hbar^2}\right)^{j-k-r}. \tag{120}$$

We can rearrange Eq. (120) to obtain the following simplification:

$$\alpha_{m,2j}=\frac{1}{m\cdot 2j}\sum_{s=0}^{j-1}\left(\sum_{r=0}^{s}\sum_{l=2r+1}^{m+2r-1}\frac{a_l}{2^{l-1}}\binom{l}{2r+1}\alpha^{(s-r)}_{m-l+2r,j-r-1}\right)\left(\frac{\mu}{2\hbar^2}\right)^{j-s}. \tag{121}$$

Expression (117) holds if and only if it equals the right-hand side of (121) for all j. Strict equality holds if and only if the constants $\alpha^{(s)}_{m,j}$ satisfy the recurrence relation

$$\alpha^{(s)}_{m,j}=\frac{1}{m\cdot 2j}\sum_{r=0}^{s}\sum_{l=2r+1}^{m+2r-1}\frac{a_l}{2^{l-1}}\binom{l}{2r+1}\alpha^{(s-r)}_{m-l+2r,j-r-1}, \tag{122}$$

for all $0\leqslant s\leqslant(j-1)$, subject to the initial value $\alpha^{(0)}_{m,0}=\frac{1}{4}\delta_{m,1}$. Equations (120) and (122) now define the nonvanishing coefficients for even powers of v. They can be solved explicitly. In the following we are only interested in the classical limit.

C. The classical coefficients

We now identify the contributing coefficients and determine the leading order of $\hbar$ correction in the classical limit. For a fixed even $n=2j$, $j=0,1,2,...$, we have seen above that the contributing coefficients $\alpha_{m,2j}$'s are of the form

$$\alpha_{m,2j}=\sum_{s=0}^{j-1}\left(\frac{\mu}{2}\right)^{j-s}\frac{\alpha^{(s)}_{m,j}}{\hbar^{2(j-s)}}.$$

The contribution of each term is $\alpha_{m,2j}v^{2j}$ (the u^m factor is left out because it is not relevant in determining the $\hbar$-order of contribution in the classical limit). The classical contribution of this term is proportional to

$$\frac{1}{\hbar}\alpha_{m,n}\int_{-\infty}^{\infty}\mathrm{sgn}(v)v^{2j}\exp\left(-i\frac{vp}{\hbar}\right)dv\propto\sum_{s=0}^{j-1}\left(\frac{\mu}{2}\right)^{j-s}\alpha_{m,j}^{(s)}\hbar^{2s}, \tag{123}$$

where we have arrived at the left-hand side of the first line by using the prescribed classical transition and with the right-hand side using identity (67). We see immediately that the only contributing term in the classical limit corresponds to $s=0$. Moreover, we can already see that the leading $\hbar$ correction in the classical limit is $\mathcal{O}(\hbar^2)$; this corresponds to $s=1$ in Eq. (123).

Thus the coefficients contributing only in the classical limit corresponds to those for $s=0$ for a given j. And these coefficients satisfy the recurrence relation,

$$\alpha_{m,2j}^{(0)}=\frac{1}{m\cdot 2j}\sum_{s=1}^{\infty}\frac{sa_s}{2^{s-1}}\alpha_{m-s,j-1}^{(0)}. \tag{124}$$

With $\alpha_{m,0}=\frac{1}{4}\delta_{m,1}$, we can generate the following first few coefficients

$$\alpha_{m,0}^{(0)}=\tfrac{1}{4}\delta_{m,1},$$

$$\alpha_{m,1}^{(0)}=\frac{1}{2m}\sum_{s=1}^{\infty}\frac{sa_s}{2^{s-1}}\alpha_{m-s,0}^{(0)}=\frac{1}{1\cdot m}\frac{(m-1)a_{m-1}}{2^{m+1}}\quad\text{for all } m\geqslant 2,$$

$$\alpha_{m,2}^{(0)}=\frac{1}{2m}\sum_{s=1}^{\infty}\frac{sa_s}{2^{s-1}}\alpha_{m-s,1}=\frac{1}{1\cdot 2m2^{m+1}}\sum_{s=1}^{m-2}\frac{sa_s}{(m-s)}(m-s-1)a_{m-s-1}\quad\text{for all } m\geqslant 3.$$

From these few iterations, we infer that the coefficients are given by

$$\alpha_{m,j}^{(0)}=\frac{C_{m,j}}{j!\cdot 2^{m+1}m}, \tag{125}$$

where the $C_{m,j}$'s are constants, for all $m\geqslant(j+1)$. Substituting this expression back into the recurrence relation (124), yields the recurrence relation satisfied by the $C_{m,j}$'s,

$$C_{m,j}=\sum_{s=1}^{m-j}\frac{sa_s}{(m-s)}C_{m-s,j-1}. \tag{126}$$

This is uniquely solved by specifying the initial value. Setting $j=0$ in Eq. (125) and comparing it with the known value of $\alpha_{m,0}^{(0)}$ yields the initial value $C_{m,0}=\delta_{m,1}$. The recurrence relation can be solved explicitly, but we do not need to write it down.

D. The solution

The coefficients $\alpha_{m,j}^{(0)}$ give the group of contributions with the order $\mathcal{O}(\hbar^0)$ in the classical limit. For every $j\geqslant 0$, there is a contribution $T_j(u,v)$'s in the solution $T(u,v)$, which is given by

$$T_j(u,v)=\left(\frac{\mu}{2\hbar^2}\right)^j\sum_{m=j+1}^{\infty}\alpha_{m,2j}^{(0)}u^m v^{2j}=\left(\frac{\mu}{2\hbar^2}\right)^j\frac{1}{j!}\sum_{m=j+1}^{\infty}\frac{C_{[m,j]}}{m\cdot 2^{m+1}}u^m v^{2j}.$$

The solution to (46) can then be written in the form

$$T(u,v)=\sum_{j=0}^{\infty}T_j(u,v)+S(u,v), \tag{127}$$

where the second term is responsible for order $\mathcal{O}(\hbar^2)$ in the classical limit. The solution to the time kernel equation in the (q,q') coordinate then assumes the form

$$T(q,q')=\sum_{j=0}^{\infty} T_j(q,q')+S(q,q'), \tag{128}$$

in which $T_j(q,q')$ derives from $T_j(u,v)$ with the substitutions $u=(q+q')$ and $v=(q-q')$.

The functional kernel of the generalized time of arrival operator then splits in two parts

$$\langle q|\mathcal{T}|q'\rangle=\sum_{j=0}^{\infty}\langle q|\mathsf{T}_j|q'\rangle+\langle q|\Delta\mathcal{T}|q'\rangle,$$

where $\langle q|\mathsf{T}_j|q'\rangle=(\mu/i\hbar)T_j(q,q')\mathrm{sgn}(q-q')$. Each of this $\langle q|\mathsf{T}_j|q'\rangle$ contributes in the classical limit,

$$T_j(q,p)=2\pi\int_{-\infty}^{\infty}\left\langle q+\frac{v}{2}\middle|T_j\middle|q-\frac{v}{2}\right\rangle e^{(-(ipv/\hbar))}dv=-(2j-1)!!(-1)^j\frac{\mu^{j+1}}{p^{2j+1}}\sum_{m=j+1}^{\infty}\frac{C_{m,j}}{m}q^m,$$

where a simplification has been made in the second line.

To prove that $\Sigma_{j=0}^{\infty}T_j(q,p)$ converges to the local time of arrival, we write the term with leading order $\mathcal{O}(\hbar^0)$ in the form

$$\mathcal{T}_{\hbar}^{\theta}(q,p)=\sum_{k=0}^{\infty}(-1)^k\mathcal{T}_k(q,p), \tag{129}$$

$$\mathcal{T}_k=-(2k-1)!!\frac{\mu^{k+1}}{p^{2k+1}}\sum_{m=k+1}^{\infty}\frac{C_{m,k}}{m}q^m. \tag{130}$$

$\mathcal{T}_{\hbar}^{0}$ converges to the local time of arrival in the origin if the $\mathcal{T}_0$ reproduces the initial value and the remaining terms satisfy the recurrence relation for the local time of arrival. Since $C_{m,0}=\delta_{m,1}$, for $k=0$, we have

$$\mathcal{T}_0(q,p)=-\mu\frac{q}{p}, \tag{131}$$

as required.

It remains to show that the rest of the terms satisfy the recurrence relation (92). Shifting index $k\to(k-1)$ in $\mathcal{T}_k$, we have

$$\frac{\partial V}{\partial q}\frac{\partial\mathcal{T}_{k-1}}{\partial p}=(2k-1)!!\frac{\mu^k}{p^{2k}}\sum_{s=1}^{\infty}sa_sq^{s-1}\cdot\sum_{m=k}^{\infty}\frac{C_{m,k-1}}{m}q^m=(2k-1)!!\sum_{k+1}^{\infty}\sum_{r=1}^{s-r}\frac{ra_rC_{s-r,k-1}}{(s-r)}q^{s-1}, \tag{132}$$

where we have used the identity

$$\sum_{s=1}^{\infty}a_sx^s\cdot\sum_{k=m}^{\infty}b_kx^k=\sum_{l=m+1}^{\infty}\sum_{n=1}^{l-m}a_nb_{l-n}x^l$$

to arrive at the second line. Now we have

$$-\frac{\mu}{p}\int_0^q dq\frac{\partial V}{\partial q}\frac{\partial\mathcal{T}_{k-1}}{\partial p}=(2k-1)!!\sum_{k+1}^{\infty}\sum_{r=1}^{s-r}\frac{ra_rC_{s-r,k-1}}{(s-r)}\frac{q^s}{s}. \tag{133}$$

$\mathcal{T}_\hbar$ converges to the local time of arrival at the origin if and only if Eqs. (130) and (133) are strictly equal for all k. Equating them, we find that strict equality for all k holds if and only if the $C_{m,k}$'s satisfy the recurrence relation

$$C_{m,k}=\sum_{r=1}^{m-k}\frac{ra_r}{(m-r)}C_{m-r,k-1}. \tag{134}$$

But this is just the recurrence relation we have arrived at above. Thus the $\mathcal{T}_k$'s satisfy the initial value condition and the required recurrence relation. The leading term $\mathcal{T}_\hbar^0$ then converges to the local time of arrival at the origin, as what we have sought to prove.

E. Integral form of the classical term

In the above discussion, we did not bother to consider the convergence of the group of terms contributing in the classical limit, the terms with $\mathcal{O}(\hbar^0)$ when Weyl–Wigner transformed; we denote this group of terms by $\langle q|\mathcal{T}_0|q'\rangle$, and call it the classical term. Here we show that $\langle q|\mathcal{T}_0|q'\rangle$ converges everywhere in the qq'-plane. We do this by showing that it has an integral representation which is defined everywhere.

It will be sufficient for us to derive the integral form of the time kernel for the linear case, because the nonlinear case can be derived similarly. Our goal is to rewrite Eq. (103) such that it is explicitly everywhere convergent in the qq'-plane. We do this as follows. In Eq. (107), we have the following expression for $\mathcal{T}_k$:

$$\mathcal{T}_k=-\frac{(2k)!}{k!}\frac{\mu^{k+1}}{p^{2k+1}}\sum_{j=0}^{k}\frac{\sigma_{k,j}}{2^j}b^{k-j}a^jq^{2k+1-j}. \tag{135}$$

We compare this with Eq. (25) for $x=0$,

$$T_k=-\frac{(2k-1)!!}{k!}\frac{\mu^{k+1}}{p^{2k+1}}\int_0^q(V(q)-V(q'))^kdq'. \tag{136}$$

Since we already know that Eq. (106) converges absolutely to the local time of arrival at the origin, it must be that Eqs. (135) and (136) are equal for all k. Equating them and changing variables $q\to\frac{1}{2}(q+q')$ in the resulting equality gives us the following identity:

$$\sum_{j=0}^{k}\sigma_{k,j}b^{k-j}a^j(q+q')^{2k+1-j}=2^{2k+1}\frac{(2k-1)!}{(2k)!}\int_0^s(V(s)-V(q''))^kdq''|_{s=1/2(q+q')}, \tag{137}$$

which is the simplification we need in Eq. (103). Substituting Eq. (137) into Eq. (103) yields

$$\begin{aligned}T(q,q')&=\frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{\mu}{\hbar^2}\right)^k\frac{(2k-1)!!}{(2k)!k!}(q-q')^{2k}\int_0^s(V(s)-V(q''))^kdq''|_{s=1/2(q+q')}\\&=\frac{1}{2}\int_0^s dq'\,{}_0F_1\left(1;\left(\frac{\mu}{2\hbar^2}\right)(q-q')^2(V(s)-V(q''))\right)|_{s=1/2(q+q')},\end{aligned} \tag{138}$$

where ${}_pF_q$ is the generalized hypergeometric function. The integration can be pulled out of the summation because of the continuity of the potential and the absolute everywhere convergence of the hypergeometric function for $p<q$. $T(q,q')$ is consequently defined everywhere. Finally the time kernel is explicitly given by

$$\langle q|\mathcal{T}_0|q'\rangle = \frac{\mathrm{sgn}(q-q')}{2i\hbar}\int_0^{1/2(a+q')} dq''\,{}_0F_1\left(1;\frac{\mu}{2\hbar^2}(q-q')^2\left\{V\left(\frac{1}{2}(q+q')\right)-V(q'')\right\}\right). \tag{139}$$

We have arrived at Eq. (139) for linear systems, but similar working on the classical term of the solution for the nonlinear case yields the same expression (139), in which $V(q)$ is now the appropriate potential for nonlinear systems.

Since the time kernel and the classical term coincide for linear systems, the time kernel is defined everywhere, and thus a functional in $\Phi^{\times}$, and it defines a generalized observable relative to the rigging provided by Φ (see Appendix). For nonlinear systems, the leading term is likewise defined everywhere, and it defines a generalized observable relative to Φ. We have not been able to investigate the functional structure of the remaining terms for nonlinear systems. Generally the time kernels for entire analytic potentials can then be written in the form

$$\text{Linear Systems:} \quad \langle q|\mathcal{T}|q'\rangle = \langle q|\mathcal{T}_0|q'\rangle, \tag{140}$$

$$\text{Nonlinear Systems:} \quad \langle q|\mathcal{T}|q'\rangle = \langle q|\mathcal{T}_0|q'\rangle + \langle q|\Delta\mathcal{T}|q'\rangle. \tag{141}$$

Comparison of $\langle q|\mathcal{T}_0|q'\rangle$ with the Weyl quantization of the local time of arrival in the origin shows that they are equal. One can check this for himself by applying Weyl's quantization prescription (9) to the local time of arrival. Weyl quantization then agrees only with the result of supraquantization for linear systems and it fails to satisfy the required commutator value for nonlinear systems. By our results for the nonlinear system the second term in Eq. (141) is to the $\mathcal{O}(\hbar^2)$ in the classical limit.

VIII. SUPRAQUANTIZATION FOR ARBITRARY POINTS OF ARRIVAL *x*

Having solved the time of arrival supraquantization problem at the origin, now we show that our results above can be imported to solve the supraquantization at an arbitrary point *x*. Generally the classical time of arrival at a point *x* is given by Eq. (12). Changing variables in Eq. (12) to $(\tilde{q}=q-x,\ \tilde{p}=p)$, the expression for the time of arrival reduces to

$$T_x(\tilde{q},\tilde{p}) = -\,\mathrm{sgn}(\tilde{p})\sqrt{\frac{\mu}{2}}\int_0^{\tilde{q}}\frac{d\tilde{q}'}{\sqrt{H(\tilde{q}+x,\tilde{p})-V(\tilde{q}'+x)}}. \tag{142}$$

Comparing Eq. (142) with the classical time of arrival at the origin, we find that the expression is equivalent to the time of arrival at the origin under the potential $\tilde{V}(\tilde{q})=V(\tilde{q}+x)$.

The surpraquantization for arbitrary arrival points *x* then can be solved by solving the time kernel equation at the origin subject to the potential $\acute{V}(\acute{q})=V(\acute{q}+x)$. For this case the time kernel equation assumes the form

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 T_x(\tilde{q},\tilde{q}')}{\partial q^2}+\frac{\hbar^2}{2\mu}\frac{\partial^2 T_x(\tilde{q},\tilde{q}')}{\partial \tilde{q}'^2}+(V(\tilde{q}+x)-V(\tilde{q}'+x))T_x(\tilde{q},\tilde{q}')=0$$

and the solution is still subject to the same boundary conditions

$$T_x(\tilde{q},\tilde{q})=\frac{\tilde{q}}{2},\quad T_x(\tilde{q},-\tilde{q})=0. \tag{143}$$

After solving for $T_x(\overline{q},\overline{q'})$, we can transform back to the original coordinate to get the kernel for the original problem. And that completes the supraquantization of the classical time of arrival for arbitrary *x*. Note that our earlier result in the neighborhood of the origin is subsumed in the above solution by simply setting $x=0$.

IX. DISCUSSION AND CONCLUSION

In this paper we have demonstrated that the classical time of arrival can be derived quantum mechanically without solving for and inverting the classical equations of motion. Our results, albeit still needing more clarifications (especially in the nonlinear case), undoubtedly forces us to reconsider our ideas on quantization, and consider supraquantization in places where quantization fails. Generally it is known that obstruction to quantization exists, so that no quantization is possible to consistently satisfy the required commutation relations. For example, Weyl quantization cannot consistently quantize all classical observables as we have demonstrated for the class of time of arrival observables. What is generally done is to choose an elite class of the classical observable that can be consistently quantized and derive the rest of the quantum observables by expressing them in terms of this elite class. In Euclidean space, the choice is usually the Heisenberg class, the position and momentum operators, together with the identity operator. The rest of the quantum observables are then derived by expressing them in terms of this class of operators. This, however, is not wholly satisfactory because the resulting operators do not necessarily satisfy the required algebra.

Now if we strongly require consistency with the required algebra of observables in spaces where obstruction to quantization exists, then we must leave quantization and find an alternative platform. It is here that the idea of supraquantization may come in. However, its implementation may not be straightforward. As what we have discussed earlier, supraquantization may necessarily require some classification of observables, as opposed to quantization which does not classify observables. The classification is necessary, at least for the class of time of arrival observables, in identifying the characteristic properties of the class that can be used in implementing the transfer principle. The natural questions are: "*How do we get the appropriate classification and how do we identify the characteristic properties of the class?*" These may not be easily answered, but they will eventually require us to go back to the basic definition of the elements of the class and the appropriate axioms of quantum mechanics to impose on them.

Assuming that we have settled the first question, we may use quantization itself as a tool in addressing the second question. What we can do is the following: Given a class $\mathcal{C}$ of classical observables, divide $\mathcal{C}$ in two parts $\mathcal{C}_N$ and $\mathcal{C}_O$. The subclass $\mathcal{C}_N$, which we may call the nonobstructed class, consists of those observables that can be consistently quantized; and the subclass $\mathcal{C}_O$, which we may call the obstructed class, consists of those observables that cannot be consistently quantized. We can work on the $\mathcal{C}_N$ using quantization and determine the properties that can be extended to the rest of the class. Once the common property of all those in $\mathcal{C}_N$ has been determined, one can use the transfer principle in treating the obstructed class $\mathcal{C}_O$. For the class of (classical) time of arrival observables, we find that the nonobstructed class with respect to Weyl quantization consists of all linear systems, while the obstructed class consists of all nonlinear systems. Following the above suggestion, we could have arrived at the same solution by working directly with the linear system and extending the result to nonlinear systems via the appropriate transfer principle. The example of the classical time of arrival demonstrates how obstruction to quantization can be formally circumvented with the idea of supraquantization.

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APPENDIX A

To establish and to avoid possible confusion with our notation for the RHS-extensions and RHS-reductions, in particular the use of the notation $\mathsf{A}_\times\varphi=\langle F_\mathsf{A}|\varphi\rangle=\mathsf{A}\varphi$, we give an example.

Consider the momentum operator P in the Hilbert space $\mathcal{H}=L^2(\mathfrak{R},dq)$. The domain of P, $\mathcal{D}(\mathsf{P})$, consists of all vectors in $\mathcal{H}$ that are almost differentiable everywhere in the real line, and

whose first derivatives are Lesbegue square integrable. For every vector $\varphi(q)$ in $\mathcal{D}(\mathsf{P})$, the momentom operator acts as $(\mathsf{P}\varphi)(q)=-i\hbar\varphi'(q)$. By definition P is self-adjoint so that $\mathsf{P}=\mathsf{P}^\dagger$. Now we choose the rigging $\Phi^\times\supset\mathcal{H}\supset\Phi$, where Φ is the space of infinitely differentiable complex valued functions with compact support in the real line, and $\Phi^\times$ its corresponding functional space. Since Φ is contained in $\mathcal{D}(\mathsf{P})$, we can define its rigged Hilbert space extension and reduction. For every vector φ in Φ and functional ϕ in $\Phi^\times$, we can write $\langle\phi|\varphi\rangle=\int_{\mathfrak{R}}\phi^*(q)\varphi(q)dq$, where the integration is understood in the distributional sense when singular ϕ is involved, say, the Dirac delta.

Now the RHS-extension of P is found as follows: For every φ in Φ and ϕ in $\Phi^\times$, we have

$$\langle\phi|\mathsf{P}^\dagger\varphi\rangle=\int_{\mathfrak{R}}\phi^*(q)(-i\hbar\varphi'(q))dq=\int_{\mathfrak{R}}i\hbar\phi'^*(q)\varphi(q)dq$$

$$=\int_{\mathfrak{R}}(-i\hbar\phi'(q))^*\varphi(q)dq=\int_{\mathfrak{R}}(\mathsf{P}^\times\phi)(q)\varphi(q)dq,$$

where the second line follows from the definition of the derivatives of functionals. The RHS-extension of P is then given by the operator $\mathsf{P}^\times$ which acts everywhere in $\Phi^\times$ as $\mathsf{P}^\times\phi=-i\hbar\phi'$.

On the other hand, the RHS-reduction of P is found as follows: First, we have to indicate the reduction of P in Φ. Its reduction is simply the operator P_Φ, which acts only on vectors φ in Φ according to $(\mathsf{P}_\Phi\varphi)(q)=-i\hbar\varphi'(q)$. Second, we have to find the functional $F_\mathsf{P}(q)$ in $\Phi^\times$ for every q in the real line, such that $\langle F_\mathsf{P}(q)|\varphi\rangle=-i\hbar\varphi'(q)$, for all φ in Φ. By inspection, this functional is given by $F_\mathsf{P}(q)=-i\hbar\delta'(q-q')$. It is so because

$$\langle F_\mathsf{P}(q)|\varphi\rangle=\int_{\mathfrak{R}}F_\mathsf{P}(q)^*\varphi(q')dq'=\int_{\mathfrak{R}}i\hbar\delta'(q-q')\varphi(q')dq'$$

$$=\int_{\mathfrak{R}}\delta(q-q')(-i\hbar\varphi'(q'))dq'=-i\hbar\varphi'(q)=(\mathsf{P}_\Phi)(q).$$

Thus, by our definition, the uniquely associated functional to P is the functional $-i\hbar\delta'(q-q')$. The RHS-reduction of P is now symbolically given by

$$\mathsf{P}_\times=\langle F_\mathsf{P}|\cdot\rangle=\int_{\mathfrak{R}}dq'\,i\hbar\delta'(q-q'),$$

with $F_\mathsf{P}^*=i\hbar\delta(q-q')$ as the functional kernel of $\mathsf{P}_\times$.

Note that possible confusion may arise when the above notation is used, for example, in expressions like $\langle F(\varphi)|\varphi\rangle=\langle\langle F|\varphi\rangle|\varphi\rangle$, such as in the definition of generalized observables. The confusion may creep in when one interprets $\langle F|\varphi\rangle$ as a constant scalar number. While $\langle F|\varphi\rangle$ is indeed a scalar number, it may be understood to range in the complex plane, such as $\langle F_\mathsf{P}(q)|\varphi\rangle$ in the above example, so that $\langle F|\varphi\rangle$ can be understood as a vector in Φ or $\Phi^\times$, whichever the case maybe.

APPENDIX B

Let us consider the function

$$F(q,q')=\mathrm{sgn}(q-q')\sum_{k=0}^{\infty}T_k(q,q'),\tag{B1}$$

where the summation is everywhere absolutely convergent or entire analytic in the qq'-plane. Now for a fixed q, is $F(q,q')$ a functional belonging to $\Phi^\times$?

First it has to be that for all φ in Φ, $|\langle F|\varphi\rangle|<\infty$. Let us denote the sum in Eq. (B1) by $S(q,q')$. Then for all φ in Φ

$$\left|\int_{\Sigma} F(q,q')\varphi(q')dq'\right| \leqslant \sup_{\Sigma}|S(q,q')|\left|\int_{\Sigma}\varphi(q)dq\right|, \tag{B2}$$

where Σ is the support of $\varphi(q)$. The right-hand side of the above inequality is finite because $S(q,q')$ is bounded in any finite region of the qq'-plane. Second, it has to be that for every sequence φ_n in Φ converging to zero in Φ, $\langle F|\varphi_n\rangle$ converges to 0. This follows immediately because $F(q,q')$ is locally integrable. Thus $\langle q|\mathcal{T}|q'\rangle$ is a functional belonging to $\Phi^{\times}$ for a fixed q.

Now for arbitrary φ in Φ, is $G(q)=\int F(q,q')\varphi(q')dq'$ a functional belonging to $\Phi^{\times}$? For all $\phi(q)\in\Phi$,

$$\left|\int_{\Sigma'}\int_{\Sigma} F(q,q')\phi(q)^*\varphi(q')dq'dq\right| \leqslant \sup_{\Sigma\times\Sigma'}|S(q,q')|\left|\int_{\Sigma\times\Sigma'}\phi^*(q)\varphi(q')dqdq'\right|. \tag{B3}$$

The right-hand side of the inequality is finite because $S(q,q')$ is bounded in every bounded region of the qq'-plane. Now it is sufficient to show that for every sequence ϕ_n converging to zero in Φ, $\langle G|\phi_n\rangle\to 0$. This follows immediately by substituting ϕ_n in inequality (B3) for ϕ.

Thus $F(q,q')$ is the functional kernel of an operator $\mathcal{F}$: $\Phi\mapsto\Phi^{\times}$ and thus $\langle F|\varphi\rangle$ is itself a functional in $\Phi^{\times}$.

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Minimization under entropy conditions, with applications in lower bound problems

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We minimize the functional $f\mapsto\int a f d\mu$ under the entropy condition $E(f)=-\int f\log f d\mu\geqslant E$, $\int f d\mu=1$ and $f\geqslant 0$, where $E\in\mathbf{R}$ is fixed. We prove that the minimum is attained for $f=e^{-sa}/\int e^{-sa}d\mu$, where $s\in\mathbf{R}$ is chosen such that $E(f)=E$. We apply the result on minimizing problems in pseudodifferential calculus, where we minimize the harmonic oscillator. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767623]

I. INTRODUCTION

The aim of the article is to establish and prove basic results for a technique of minimization under entropy conditions which was used by von Neumann already in Ref. 9. We also give applications on minimizing pseudodifferential operators and Toeplitz operators. The entropy occurs frequently in mathematic-related topics. In statistic mechanics and quantum theory, the entropy appears as a functional acting on squares of wave functions. In statistics, such functions are interpreted as probability density functions (PDFs), and then the entropy is defined in a similar way as in quantum physics and statistic mechanics.

Roughly speaking, the entropy measures the concentration for a PDF, in the sense that the entropy is large when the PDF is not concentrated. The entropy therefore has a somewhat similar role as the variance. However, in contrast to the variance, the entropy is completely independent of the expected value and of any norm structure on the sample space.

The applications on pseudodifferential and Toeplitz operators, mentioned above, are based on the fact that Toeplitz operators may be considered as functionals acting on Wigner distributions (or coherent state transformed functions), which satisfy certain entropy conditions. The minimization result therefore applies immediately on Toeplitz operators, which in turn leads to lower bound results for pseudodifferential operators which may be approximated by Toeplitz operators.

In order to describe our results in more details, we recall the definition of the entropy. For a positive measure μ and an appropriate non-negative function $f\in L^1(d\mu)$, the entropy $E_\mu(f)$ is defined by

$$E_\mu(f)=-\int f\log f d\mu+\|f\|_{L^1(d\mu)}\log\|f\|_{L^1(d\mu)}. \tag{1.1}$$

(Cf. Ref. 7 or 8.) Here and in what follows, we let $0\log 0=0$. (We use the usual notation for function and distribution spaces, e.g., Ref. 5). It follows easily that $E_\mu(f)$ becomes large when f is not concentrated.

For an appropriate function a and real number E, we are then going to minimize the functional $f\mapsto\int a f d\mu$, when $0\leqslant f\in L^1(d\mu)$ satisfies

$$\|f\|_{L^1(d\mu)}=1,\quad E_\mu(f)\geqslant E, \tag{1.2}$$

and we prove that the minimum is attained when $f=f_s=e^{-sa}/\|e^{-sa}\|_{L^1(d\mu)}$, where s is chosen such that $E_\mu(f_s)=E$.

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It is not difficult to obtain an intuitive (but imperfect) proof of the result above. In fact, the Frechét derivatives of the left-hand sides of (1.2) are given by

$$h\mapsto\int h\,d\mu \quad \text{and} \quad h\mapsto-\int h(\log f+1)\,d\mu.$$

The Frechét derivative of the functional $f\mapsto\int af\,d\mu$ is given by $h\mapsto\int ah\,d\mu$, and it is intuitively clear that if f minimize $\int af\,d\mu$ under the conditions in (1.2) (with equality in the last condition), then the Frechét derivatives above should be linearly dependent, i.e.,

$$\int ah\,d\mu=C_1\int h\,d\mu+C_2\int h\log f\,d\mu$$

for every appropriate function h. This means that $a=C_1+C_2\log f$, and we obtain that $f=ce^{-sa}$, for some constants c and s, which are determined by (1.2).

Since the minimization result appears by such elementary computations, the method above has been used before. In fact, von Neumann used the technique already in Sec. 5.3 in Ref. 9, in order to solve certain problems in quantum mechanics. The arguments were thereafter used for example in thermodynamics. However, a strict proof that the minimum really exists and attains for $f=f_s$ seems to the author not to be well-known, hence, these missing links are presented here.

In order to describe our applications to Weyl operators and Toeplitz operators, we recall the definitions of such operators. Assume that $g\in\mathcal{S}(\mathbf{R}^n)$ is a unit vector with respect to L^2 and that $a\in\mathcal{S}(\mathbf{R}^{2n})$. Then, the Weyl and Toeplitz operators for a, $a^\omega(x,D)$ and $\mathrm{Tp}(a)=\mathrm{Tp}_g(a)$ respectively, are the continuous operators on $\mathcal{S}(\mathbf{R}^n)$, given by the formulas

$$\begin{aligned}a^\omega(x,D)f(x)&=(2\pi)^{-n}\int\int a((x+y)/2,\xi)f(y)e^{i\langle x-y,\xi\rangle}dy\,d\xi,\\(\mathrm{Tp}_g(a)f_1,f_2)&=\int a(-2X)(V_gf_1)(X)\overline{(V_gf_2)(X)}dX.\end{aligned}\tag{1.3}$$

Here, f, f_1, $f_2\in\mathcal{S}(\mathbf{R}^n)$ and $V_g:\mathcal{S}(\mathbf{R}^n)\to\mathcal{S}(\mathbf{R}^{2n})$ is the coherent state transform or the short time Fourier transform with respect to g which is defined as

$$(V_gf)(X)=(2\pi)^{-n/2}\int f(y/2-x)\overline{g(y/2+x)}e^{i\langle y,\xi\rangle}dy,\quad X=(x,\xi)\in\mathbf{R}^{2n},$$

and $(\cdot,\cdot)$ denotes the usual scalar product on $L^2(\mathbf{R}^n)$ (Ref. 1, 4, 8, 10, or 11). The definitions of $a^\omega(x,D)$ and $\mathrm{Tp}(a)$ extend to any $a\in\mathcal{S}'(\mathbf{R}^{2n})$, in which linear continuous operators from $\mathcal{S}(\mathbf{R}^n)$ to $\mathcal{S}'(\mathbf{R}^n)$ are obtained (Ref. 5, 11, or 12).

The relation which we use when approximating Weyl operators with Toeplitz operators is

$$\mathrm{Tp}_g(a)=(a*u_g)^\omega(x,D),\tag{1.4}$$

where $u_g=(2\pi)^{-n/2}V_g\check{g}$ and $\check{g}(x)=g(-x)$ (see Refs. 11 and 12). When discussing minimization for $a^\omega(x,D)$, we first use (1.4) in order to approximate $a^\omega(x,D)$ by $\mathrm{Tp}(a)$. Then, we apply the minimization properties under the entropy condition above on $\mathrm{Tp}(a)$ in (1.3) with $f=f_1=f_2$, using that $\nu=V_gf$ satisfies the entropy condition

$$\|\nu\|_{L^2}=\|f\|_{L^2},\quad \text{and}\quad E(|\nu|^2)\geqslant n(1+\log(\pi/2))\|f\|_{L^2}^2\tag{1.5}$$

(cf. Refs. 8 and 11). Here and in what follows, we use the notation E instead of E_μ when μ is the Lebesgue measure.

II. L^2-ESTIMATES FOR THE COHERENT STATE TRANSFORM

In this section, we give a review of some basic properties for the coherent state transform V_g, and sum up the results in the form of entropy inequalities. This material is included in order to make the presentation more self-contained, but all the results given here can be found in Ref. 8, for example.

We start to consider the map V_g in (1.1). We note that the map $(f,g)\mapsto V_g f$ is continuous from $\mathcal{S}(\mathbf{R}^n)\times\mathcal{S}(\mathbf{R}^n)$ to $\mathcal{S}(\mathbf{R}^{2n})$ which extends to a continuous map from $\mathcal{S}'(\mathbf{R}^n)\times\mathcal{S}'(\mathbf{R}^n)$ to $\mathcal{S}'(\mathbf{R}^{2n})$ (cf. Ref. 4 or 12). In particular, the following definition makes sense.

Definition 2.1 (see Ref. 8): Assume that $g\in L^2(\mathbf{R}^n)\backslash 0$. Then, $V_g:\mathcal{S}'(\mathbf{R}^n)\to\mathcal{S}'(\mathbf{R}^{2n})$ is called the *coherent state transform* associated with g.

In order to establish entropy conditions on functions of the type $V_g f$, we recall the following result by Lieb, which is based on sharp versions of Hausdorff–Young's inequality and Young's inequality (Ref. 2 or 3)

Theorem 2.2 (*see* Ref. 8): *Assume that $g\in L^2(\mathbf{R}^n)$, and that $q\in[2,\infty]$. Then V_g is continuous from $L^2(\mathbf{R}^n)$ to $L^q(\mathbf{R}^{2n})$, and*

$$\|V_g\|_{L^2\to L^q}\leqslant(2^{1/2}q^{-1/q}\pi^{1/q-1/2})^n. \tag{2.1}$$

Corollary 2.3: If $\nu=V_g f$ where $f,g\in L^2(\mathbf{R}^n)$ such that $\|g\|_{L^2}=1$, then the entropy $E(|\nu|^2)$ is positively homogeneous in ν of degree 2 and (1.5) *holds.*

A proof of Corollary 2.3 was essentially presented in Ref. 8. Since our choices of constants are different, here we recall the arguments.

Proof: The homogenous assertions are obvious. Since ν is bounded, by Theorem 2.2, it follows that $E(|\nu|^2)$ is defined, possibly equal to $+\infty$. Since $\epsilon\log|\nu|\leqslant|\nu|^\epsilon-1$ when $\epsilon>0$, it follows from (2.1) that

$$\int|\nu(x)|^2\log|\nu(x)|dx\leqslant\epsilon^{-1}\int(|\nu(x)|^{2+\epsilon}-|\nu(x)|^2)dx\leqslant\epsilon^{-1}((\pi/2)^{-n(1+\epsilon/2)}(\pi/(2+\epsilon))^n-1).$$

The result follows now if we let $\epsilon\to 0$.

III. MINIMIZATION UNDER ENTROPY CONDITIONS

In this section, we sum up some elementary properties of the entropy functional (see also Ref. 6), and then we discuss some minimization problems for linear functionals under entropy conditions.

Let $0\neq\mu$ be a positive σ-finite measure on the measure space $\mathcal{M}$. Then the entropy E_μ from

$$L^1_{\mu,+}=L^1_+(\mathcal{M},\mu)=\left\{0\leqslant f\in L^1(\mathcal{M},\mu);\int f\log_+ f\,d\mu<\infty\right\}$$

to $(-\infty,\infty]$ is defined by (1.1). Here, $\log_+(t)=\max(\log t,0)$. (Recall that $0\log 0=0$.) Let $\|\mu\|$ be the total mass of μ and denote by $I_\mu\subset(-\infty,\infty]$ the smallest interval which contains

$$\{\log(\mu(\Omega));\Omega\ \text{ is }\ \mu\text{-measurable and }\ \mu(\Omega)>0\}.$$

Proposition 3.1: $L^1_{\mu,+}$ is a convex cone and E_μ is positively homogeneous of degree 1 *on that set. It is concave in the sense that*

$$E_\mu(f+g)\geqslant E_\mu(f)+E_\mu(g),\quad f,g\in L^1_{\mu,+}. \tag{3.1}$$

The image under E_μ of $\{f\in L^1_{\mu,+};\|f\|=1\}$ equals I_μ.

Here and in what follows, we let $\|f\|=\|f\|_{L^1(d\mu)}$.

Proof: First, we observe that $E_\mu(tf)=tE_\mu(f)$ when $t\geqslant 0$ and $f\in L^1_{\mu,+}$. Since $t\log_+ t$ is a convex function on $\mathbf{R}_+$, it is easily seen that $L^1_{\mu,+}$ is a convex cone.

Let $f,g\in L^1_{\mu,+}$ with $\|f\|>0$, $\|g\|>0$. Jensen's inequality gives

$$\int \log(1+g/f) f d\mu/\|f\| \leqslant \log\left(\int (f+g) d\mu/\|f\| \right).$$

Hence,

$$\int f \log(f+g) d\mu - \|f\| \log\|f+g\| \leqslant \int f \log f d\mu - \|f\| \log\|f\|.$$

A similar inequality holds with the roles of f and g interchanged, and summing these inequalities and using that $\|f+g\| = \|f\| + \|g\|$, we get (3.1).

Next, we examine the values of $E_\mu(f)$ when $\|f\| = 1$. Since, by Jensen's inequality,

$$\exp\left(\int f \log(1/f) d\mu \right) \leqslant \int 1 d\mu = \|\mu\|,$$

when $\|f\| = 1$, it follows for such f that $E_\mu(f) \leqslant \log\|\mu\|$. If μ has a finite mass, then equality is obtained when f is constant. If μ has an infinite mass, then we may write $\mathcal{M}$ as a disjoint union of μ-measurable sets Ω_j, $j \geqslant 1$, of mass $\mu_j > 1$. Let $0 \leqslant t_j$ be a sequence with $\Sigma t_j = 1$ and define $f \in L^1_\mu$ by $f = t_j/\mu_j$ on Ω_j. Then $\|f\|_{L^1_\mu} = 1$ and $f \in L^1_{\mu,+}$, since $f \leqslant 1$. In order to prove that the entropy can take the value $+\infty$ we choose t_j such that $\Sigma t_j \log(\mu_j/t_j) = +\infty$. Since $\Sigma t_j \log \mu_j$ is positive this equality is fulfilled if, for example, $t_j = C/(j(\log(j+1))^2)$, where C is chosen such that $\Sigma t_j = 1$.

We now have proven that the right endpoint of I_μ is the maximal value of the entropy restricted to the set where $\|f\| = 1$. When considering lower bounds for the entropy, we first assume that $\mathcal{M}$ contains sets with arbitrarily small and positive μ-measures, such that $\inf I_\mu = -\infty$. Then, by choosing f equal to the characteristic function for sets Ω with $0 < \mu(\Omega)$ approaching 0, one finds that $\inf\{E_\mu(f)/\|f\|\}$ is also equal to $-\infty$.

If $\tau = \inf I_\mu > -\infty$, then there is a family $\{\omega_j\}$ of measurable sets in $\mathcal{M}$ such that

(1) $\mathcal{M} = \cup \omega_j$;
(2) $0 < \mu(\omega_j) < \infty$ for every j; and
(3) if $\omega_j = \omega_j^1 \cup \omega_j^2$, where ω_j^1 and ω_j^2 are μ-measurable sets, then $\mu(\omega_j^1) = \mu(\omega_j)$ or $\mu(\omega_j^2) = \mu(\omega_j)$.

In fact, if Ω is a set with finite μ-mass and Ω_j, $j = 1,...,N$, is any sequence of disjoint μ-measurable subsets of Ω with $\mu(\Omega_j) > 0$, then $\mu(\Omega) \geqslant \Sigma \mu(\Omega_j) \geqslant e^\tau N$, and the assertion follows.

Set $\mu_j = \mu(\omega_j)$ and let t_j be a sequence of nonnegative numbers with $\Sigma t_j = 1$. If $f \in L^1_{\mu,+}$ equals t_j/μ_j at x^j, then $\|f\| = 1$ and $E_\mu(f) = \Sigma t_j \log(\mu_j/t_j) \geqslant \tau$. If we choose f such that it is supported at a single set ω_j with μ-measure arbitrarily close to e^τ, we find that $\inf\{E_\mu(f)/\|f\|\} = \tau$. It is also clear that $E_\mu(f) = \tau$ for some f with $\|f\| = 1$ if and only if there is some point with μ-measure equal to e^τ.

In order to complete the proof, we observe that

$$L^1_{\mu,0} = \{f \in L^1_{\mu,+}; E_\mu(f) < \infty\}$$

is also a convex cone. This is obvious from the inequality

$$(f+g)\log(1/(f+g)) \leqslant f \log(1/f) + g \log(1/g).$$

Since $\{f \in L^1_{\mu,0}; \|f\| = 1\}$ is convex and E_μ is concave on that set, it follows that $\{E_\mu(f); \|f\| = 1\} \cap \mathbf{R}$ is connected, and the proof is complete.

In order to establish further properties for the entropy, it is convenient to use the notation

$$W_a = \{x \in \mathcal{M}; a(x) = \operatorname{ess\,inf}_\mu(a)\}, \tag{3.2}$$

where $\operatorname{ess\,inf}_\mu(a)$ is the essential infimum of a with respect to the measure μ.

Definition 3.2: $\mathcal{A}_\mu$ is the set of all real-valued and μ-measurable functions a such that $e^{-sa} \in L^1_\mu(\mathcal{M})$ for every $s>0$, and we set

$$F(s;a,\mu)=E_\mu(e^{-sa})/\|e^{-sa}\|_{L^1_\mu}, \quad s>0. \tag{3.3}$$

Note that F in Definition 3.2 makes sense since $e^{-sa}\in L^1_{\mu,+}$ when $a\in\mathcal{A}_\mu$ and $s>0$. It is easily seen that this function is smooth in s. It also follows from Proposition 2.1 that

$$F(s;a,\mu)\leqslant\log(\|\mu\|). \tag{3.4}$$

Lemma 3.3: Let $a\in\mathcal{A}_\mu$ and set $F(s)=F(s;a,\mu)$. If $\mu(W_a)=\|\mu\|$, then $F(s)\equiv\log(\|\mu\|)$. If $\mu(W_a)<\|\mu\|$ then $F(s)$ strictly decreases on $\mathbf{R}_+$ and

$$F(s)\to\log(\|\mu\|) \quad \textit{when} \quad s\to 0, \tag{3.5}$$

$$F(s)\to\log\mu(W_a) \quad \textit{when} \quad s\to+\infty. \tag{3.6}$$

Proof: We may assume that $\mu(W_a)<\|\mu\|$ since the assertion is trivial in the first case. Set $I(s)=\int e^{-sa}d\mu$ and $\vartheta(s)=\log(I(s))$ when $s>0$. Then g is smooth, convex, and

$$F(s)=\log(I(s))+\int sae^{-sa}d\mu/I(s)=\vartheta(s)-s\vartheta'(s). \tag{3.7}$$

Hence $F'(s)=-s\vartheta''(s)\leqslant 0$. Suppose that $F(s)$ is not strictly decreasing, then there are $0<s_1<s_2$ such that $F'=0$ on $[s_1,s_2]$. Hence, g is affine on this interval, and this implies that there is a constant β such that

$$\int e^{-s(a-\beta)}d\mu \text{ is constant when } s_1<s<s_2.$$

Since the second derivative of the left-hand side equals $\int(a-\beta)^2e^{-s(a-\beta)}d\mu$, it follows that $a=\beta$ a.e. with respect to μ, which contradicts the hypothesis. Hence, $F(s)$ is strictly decreasing.

Applying Lebesgue's theorem to the integral of e^{-sa} over the set where $a<0$ and the theorem of Beppo–Levi to the integral over the complement of that set, we find that $I(s)\to\|\mu\|$ as $s\to 0$. Since, by (3.7), $F(s)\geqslant\log(I(s))-\int_{a<0}e^{-2sa}d\mu/I(s)$ this gives (3.5) when $\|\mu\|=+\infty$. If instead $\|\mu\|<\infty$, then $\int sae^{-sa}d\mu\to 0$ as $s\to 0$, and this proves (3.5) again.

When proving (3.6) we set $\rho=\operatorname{ess\,inf}_\mu(a)$ and assume first that $\rho>-\infty$. Since $F(s;a,\mu)=F(s;a+C,\mu)$ for every constant C, we may assume that $\rho=0$. If $\mu(W_a)>0$, then $g(s)$ must be a bounded convex function on $(1,\infty)$, which implies that $F(s)-\vartheta(s)=-s\vartheta'(s)\to 0$ as $s\to\infty$. Since $\int e^{-sa}d\mu\to\mu(W_a)$ when $s\to+\infty$, we obtain (3.6).

If instead $\rho=\mu(W_a)=0$, then it follows from Lebesgue's theorem that $I(s)\to 0$, hence $\vartheta(s)\to-\infty$, when $s\to\infty$. Since $\mu(\{x;a(x)<\epsilon\})>0$ for every $\epsilon>0$ it follows that there are constants C_ϵ such that $\vartheta(s)\geqslant-\epsilon s-C_\epsilon$. This shows that $\vartheta(s)/s\to 0$ as $s\to\infty$. Let r be an arbitrary positive number. Then $(r+\vartheta(s))/s\to 0$ when $s\to\infty$ and $(r+\vartheta(s))/s$ is negative for large s. The derivative $(s\vartheta'(s)-\vartheta(s)-r)/s^2$ must therefore be positive for arbitrarily large values of s, and therefore for all large s since $s\vartheta'-\vartheta$ increases. Since r was arbitrary this proves that $s\vartheta'(s)-\vartheta(s)\to+\infty$ as $s\to+\infty$. Hence $F(s)\to-\infty$ as $s\to+\infty$.

It remains to consider the case when $\operatorname{ess\,inf}_\mu(a)=-\infty$. Then $\mu(W_a)=0$, and we have to prove that $F(s)\to-\infty$ as $s\to+\infty$. Assume that this is not true. Then there is a positive constant C such that $\vartheta(s)-s\vartheta'(s)\geqslant-C$, or, equivalently, $(\vartheta/s)'\leqslant C/s^2$. Hence, there is a positive constant ρ such that $\vartheta(s)\leqslant\rho s$, $s\geqslant 1$.

On the other hand, for every positive integer N we may find a constant C_N such that $\int e^{-sa}d\mu\geqslant e^{Ns}/C_N$. Hence,

$$Ns-\log(C_N)\leqslant g(s)\leqslant \rho s,\quad s\geqslant 1.$$

This gives a contradiction for large N, and the proof is complete.

Lemma 3.4: Assume that $a\in\mathcal{A}_\mu$ *and that* $f\in L^1_{\mu,+}$. *Then it is true that* $\max(-af,0)\in L^1_\mu$ *(which implies that* $\int af\,d\mu$ *is a well-defined element of* $\mathbf{R}\cup\{+\infty\}$*), and*

$$\int af\,d\mu\geqslant\frac{1}{s}\left(E_\mu(f)+\left(1-\int e^{-sa}d\mu\right)\int f\,d\mu\right),\quad s>0.$$

Proof: We may assume that $\int f\,d\mu=1$ for reasons of homogeneity. If $s>0$, then

$$af\geqslant\frac{1}{s}(f-f\log f-e^{-as}). \tag{3.8}$$

In fact, if $b=-as$ this inequality may be written $e^b-fb\geqslant f-f\log f$. The left-hand side is a convex function of b. When $f=f(x)>0$, it is stationary and equal to $f-f\log f$ when $b=\log f$. The first assertion follows now since f, $f\log_+ f$, $e^{-as}\in L^1_\mu$, and the second statement follows by integrating (3.8).

Definition 3.5: Assume that $E\in\mathbf{R}$ and $a\in\mathcal{A}_\mu$. Then, we let

$$H(E;\mu)\equiv\left\{f\in L^1_{\mu,+};\int f\,d\mu=1,E_\mu(f)\geqslant E\right\}, \tag{3.9}$$

$$m(E)=m(E;a,\mu)\equiv\inf_{f\in H(E;\mu)}\int af\,d\mu. \tag{3.10}$$

We are now ready to state the main result.

Theorem 3.6: *Let* μ *be a positive measure on* $\mathcal{M}$ *and* $a\in\mathcal{A}_\mu$. *Let* $m(E)=m(E;a,\mu)$ *be as in* (3.10) *when* $E\in\mathbf{R}$ *and set* $W_a=\{x;a(x)=\operatorname{ess\,inf}_\mu(a)\}$. *Then, the following is true*:

(i) *if* $E\leqslant\log(\mu(W_a))$ *then* $m(E)=\operatorname{ess\,inf}_\mu(a)$;

(ii) *if* $\log(\mu(W_a))<E<\log(\|\mu\|)$, *then*

$$m(E)=\int a\phi_s d\mu,$$

where $\phi_s=e^{-sa}/\int e^{-sa}d\mu$ *and* $s\in\mathbf{R}_+$ *is the unique solution to the equation* $E_\mu(\phi_s)=E$ *(cf. Lemma 3.3);*

(iii) *if* $\|\mu\|<\infty$ *and* $E=\log(\|\mu\|)$ *then*

$$m(E)=\int ad\mu/\|\mu\|,$$

and $m(E)=+\infty$ *when* $E>\log(\|\mu\|)$; and

(iv) *if* $\|\mu\|=+\infty$, *then* $m(E)$ *increases to* $+\infty$ *as* $E\to+\infty$.

The following lemmas are important for the proof of Theorem 3.6.

Lemma 3.7: If $E>\log(\|\mu\|)$, *then* $H(E;\mu)=\emptyset$, *and when* $E\leqslant\log(\|\mu\|)$ *then* $H(E;\mu)$ *is a nonempty convex set in* $L^1_{\mu,+}$.

Proof: This is an immediate consequence of Proposition 3.1.

Lemma 3.8: Let $a\in\mathcal{A}_\mu$, $s\in\mathbf{R}_+$ *and* ϕ_s *be the same as in Theorem 3.7. Assume that* E *is a real number such that* $E_\mu(\phi_s)<E$. *Then,*

$$\int a\phi_s d\mu\leqslant\int af\,d\mu\quad\forall f\in H(E;\mu). \tag{3.11}$$

We first prove Theorem 3.6, assuming that Lemma 3.8 holds, and postpone the proof of Lemma 3.8.

Proof of Theorem 3.6: (i) The condition implies that $\mu(W_a)>0$. Since this number must be less than infinity, it follows that $f\in H(E;\mu)$ if f is equal to the characteristic function of W_a divided by $\mu(W_a)$. Hence $m(E)\leqslant \int f d\mu = \operatorname{ess\,inf}_\mu(a)$. Since the opposite inequality is also fulfilled, this proves our assertion.

(ii) It follows from Lemma 3.3 that there is a unique s such that $E_\mu(\phi_s)=E$. If $t>s$ then $E_\mu(\phi_t)<E$ in view of that lemma, and it follows from Lemma 3.8 that

$$\int a\phi_t d\mu \leqslant \int af d\mu \quad \text{when} \quad f\in H(E;\mu).$$

Since $\phi_s\in H(E;\mu)$ we have proven that

$$\int a\phi_t d\mu \leqslant m(E) \leqslant \int a\phi_s d\mu,$$

and when $t\searrow s$ it follows that $m(E)=\int a\phi_s d\mu$.

(iii) It follows from Lemma 3.3 that $E_\mu(\phi_t)\nearrow \log(\|\mu\|)$ when $t\searrow 0$. Hence, by Lemma 3.8

$$\int a\phi_t d\mu \leqslant \int af d\mu$$

when $f\in H(E;\mu)$. If $f=1/\|\mu\|$ then $f\in H(E;\mu)$ and the right-hand side equals $\int a d\mu/\|\mu\|$, which is the limit of the left-hand side as $t\to 0$. Hence, $m(E)=\int a d\mu/\|\mu\|$. The second part of (iii) follows since $H(E;\mu)$ is empty when $E>\log(\|\mu\|)$ in view of Proposition 3.1.

(iv) The assertion is an immediate consequence of Lemma 3.4 with $s=1$, which shows that there is a constant $C=C_{a,\mu}$ such that $m(E)\geqslant E-C$.

Proof of Lemma 3.8: Let W_a be as in (3.2). If $\mu(W_a)=\|\mu\|$ then $\|\mu\|<\infty$, a is constant and (3.11) holds. It therefore follows from Lemma 3.3 that we may assume that $F(s)=E_\mu(\phi_s)$ is strictly decreasing. By replacing E by a smaller number if necessary, we may assume that E is an interior point of I_μ. After a change of notation we may also assume that $s=1$ and for simplicity we denote ϕ_1 by ϕ.

We first consider the case when $\mathcal{M}=\cup_1^N \omega_j$, where $N<\infty$, $\mu_j\equiv\mu(\omega_j)<\infty$ for every $j=1,...,N$, and a and f should be constant on each ω_j. For notational convenience, we will consider the numbers μ_j as the positive point masses of a measure μ on the set $\{1,...,N\}$, and we treat a and f as functions on $\{1,...,N\}$. Since the assertion of the lemma is invariant under renumbering and addition of a constant to a, we may assume that $0=a(1)\leqslant a(2)\leqslant\cdots\leqslant a(N)$.

Assume that (3.11) is not fulfilled. Then, we have for some value on E and some $f\geqslant 0$ that

$$\int af d\mu < \int a\phi d\mu, \quad \int f d\mu = 1, \quad E_\mu(\phi)<E\leqslant E_\mu(f). \tag{3.12}$$

We want to prove that (3.12) leads to a contradiction. By perturbing the $a(j)$ and μ slightly we may assume that $a(j)<a(k)$, when $j<k$. We may also assume that $\int af d\mu$ is minimal among all integrals of functions satisfying (3.12).

We shall first prove that

$$f(j)>0 \quad \text{when} \quad 1\leqslant j\leqslant N. \tag{3.13}$$

Assume that this is not true so that the set J of j with $f(j)=0$ is not empty. We claim that there is a function κ with

$$\int \kappa d\mu = 0, \quad \kappa(j)>0 \quad \text{if } j\in J \quad \text{and} \quad \int a\kappa d\mu<0. \tag{3.14}$$

Assume that such a function does not exist. Then,

$$\sum t_j = 0, \quad t_j > 0 \quad \text{when } j \in J \Rightarrow \sum a(j)t_j \geqslant 0.$$

Hence, there is a real number α and $\epsilon_j \geqslant 0$ with $\epsilon_j = 0$ when $j \notin J$ such that $a(j) = \alpha + \epsilon_j$. The condition that $0 = a(1) < a(2) \cdots < a(N)$ implies $\alpha = 0$, $\epsilon_j = a(j)$, and $J = \{2,...,N\}$. Hence $f(j) = 0$ when $j > 1$ and it follows from (3.12) that $f(1) = 1/\mu_1$. If $b = \int e^{-a} d\mu$ then

$$\int \phi(a + \log b) d\mu = E_\mu(\phi) < E \leqslant E_\mu(f) = \log \mu_1.$$

Since the left-hand side is greater than or equal to $\log b \int \phi d\mu = \log b \geqslant \log \mu_1$ we arrive at a contradiction. This proves that (3.14) has a solution.

Let κ be any solution to (3.14), ϵ be a small positive number and set

$$f_\epsilon(j) = f(j) + \epsilon\kappa(j).$$

Then, $\int f_\epsilon d\mu = 1$ and $f_\epsilon > 0$ when ϵ is small. We have $\int a f_\epsilon d\mu = \int a f d\mu + \epsilon \int a\kappa d\mu < \int a f d\mu$, which by our assumption that $\int a f d\mu$ is minimal implies that

$$E_\mu(f_\epsilon) < E \leqslant E_\mu(f). \tag{3.15}$$

On the other hand, a simple computation allows us to conclude that there are positive constants C and C' such that

$$E_\mu(f_\epsilon) - E_\mu(f) \geqslant -\sum_{j \in J} \epsilon\kappa_j \log(\epsilon\kappa_j)\mu_j - C\epsilon \geqslant \left(\sum_{j \in J} \kappa_j \mu_j \right) \epsilon \log(1/\epsilon) - C'\epsilon.$$

Since the right-hand side is positive when ϵ is sufficiently small, we again obtain a contradiction, and may assume from now on that (3.13) holds.

Let h be an arbitrary function satisfying $\int h d\mu = 0$ and set $f_\epsilon = f + \epsilon h$ when $|\epsilon|$ is sufficiently small. Then, $\int f_\epsilon d\mu = 1$. The assumptions on f allow us to conclude that

$$\frac{d}{d\epsilon} E_\mu(f_\epsilon) > 0 \quad \text{when } \epsilon = 0 \Rightarrow \frac{d}{d\epsilon} \int a f_\epsilon d\mu \geqslant 0 \quad \text{when } \epsilon = 0.$$

Computing derivatives and setting $g(j) = 1 + \log f(j)$, we may write this as

$$\sum h(j)\mu_j = 0, \quad \sum g(j)h(j)\mu_j < 0 \Rightarrow \sum a(j)h(j)\mu_j \geqslant 0.$$

This implies that there are constants λ and ρ with $\lambda \leqslant 0$ such that $a(j) = \lambda g(j) + \rho$. Since the $a(j)$ do not form a constant sequence it follows that $\lambda = -1/\sigma$ for some positive σ. This allows us to conclude that $f = \phi_\sigma$, where $\phi_\sigma = e^{-\sigma a}/I(\sigma)$ and $I(\sigma) = \int e^{-\sigma a} d\mu$.

It is now easy to complete the proof in this case. Let $F(t) = E_\mu(\phi_t)$. It follows from (3.12) that

$$I'(1)/I(1) < I'(\sigma)/I(\sigma), \quad F(1) < F(\sigma).$$

Since $I'(t)/I(t)$ increases with t in view of the convexity of $\log(I(t))$ the first inequality implies that $1 < \sigma$. This contradicts the second inequality since $F(t)$ decreases in view of Lemma 3.3. This proves the lemma in this case.

When proving the lemma in the general case, we shall reduce the proof to the discrete case, considered above. Assume that (3.11) is not fulfilled. Then, we may find $\epsilon > 0$ and $f \in H(E;\mu)$ such that

$$E_\mu(\phi)<E-\epsilon, \quad \int a f d\mu \leqslant \int a\phi d\mu - \epsilon. \tag{3.16}$$

In a first step, we want to reduce the proof to the case when μ is a bounded measure and f is a bounded function. To that end, we let Ω_j, $j=1,2,...$, be an increasing family of μ-measurable sets with characteristic functions χ_j such that $\mu(\Omega_j)<\infty$, and $\int f\chi_j d\mu \to \int f d\mu$ and $\sup \int e^{-sa}|\chi_j - 1|d\mu \to 0$ as $j\to\infty$, where the supremum is taken over all $1/2\leqslant s\leqslant 3/2$. Set (for j large)

$$\mu_j = \chi_j \mu, \quad g_j = \frac{f}{1+f/j}, \quad f_j = \frac{g_j}{\int g_j d\mu_j}, \quad \phi^j = \frac{e^{-a}}{\int e^{-a} d\mu_j}.$$

Then, $\int f_j d\mu_j = 1$ and $f_j \to f$ point wise as $j\to\infty$. We claim that

$$\liminf_{j\to\infty} E_{\mu_j}(f_j) \geqslant E, \quad \limsup_{j\to\infty} \int a f_j d\mu_j \leqslant \int a f d\mu, \tag{3.17}$$

$$\limsup_{j\to\infty} E_{\mu_j}(\phi^j) \leqslant E_\mu(\phi), \quad \liminf_{j\to\infty} \int a\phi^j d\mu_j \geqslant \int a\phi d\mu. \tag{3.18}$$

Assume that these assertions are proven. Then, $f_j \in H(E-\epsilon/2;\mu_j)$ when j is large. The inequalities in (3.16) hold then with f, μ, ϕ replaced by f_j, μ_j, ϕ^j, after ϵ and E have been replaced by some smaller numbers. Thus, when proving that (3.16) leads to a contradiction, we may assume from the beginning that f is bounded and that $\int d\mu < \infty$.

When proving the first inequality in (3.17), we consider $\int g_j(\log g_j)\chi_j d\mu$. Let $\Omega = \{x \in \mathcal{M}; f(x)>1\}$. Then, $g_j(\log g_j)\chi_j$ increases in Ω with j to $f\log f$. Hence, by Beppo–Levi's theorem,

$$\int_\Omega g_j \log g_j d\mu_j \to \int_\Omega f\log f d\mu = \int f \log_+ f d\mu.$$

In Ω^c, one has for large j

$$g_j \log g_j = \frac{f}{1+f/j}\log f + O(1/j)f,$$

which implies that $\int_{\Omega^c} g_j \log g_j d\mu_j \to \int_{\Omega^c} f\log f d\mu$. Since $f_j = g_j/c_j$, where $c_j\to 1$, the first inequality in (3.17) follows.

When proving the second inequality in (3.17), we may replace f_j by g_j, and then it suffices to prove

$$\int_{a\geqslant 0} a g_j d\mu_j \to \int_{a\geqslant 0} a f d\mu, \quad \int_{a<0} a g_j d\mu_j \to \int_{a<0} a f d\mu. \tag{3.19}$$

In the set where $a\geqslant 0$, it is true that $a g_j \chi_j$ increases to af as $j\to\infty$. The first limit in (3.19) is therefore a consequence of Beppo–Levi's theorem. If χ is the characteristic function for the set where $a<0$, then $\chi a f \in L^1_\mu$ by Lemma 3.4. Since $|\chi a g_j \chi_j| \leqslant |\chi a f|$, the second limit in (3.19) is a consequence of Lebesgue's theorem. This proves (3.17).

The assertion (3.18) follows from Lebesgue's theorem since $\phi\log\phi$ and $a\phi$ are μ-integrable.

Now we go back to (3.16), assuming as we may that $\int d\mu<\infty$ and that f is bounded. Let $a_j = a$ when $|a|<j$ and $a_j = 0$ if $|a|\geqslant j$. Set $\phi^j = e^{-a_j}/\int e^{-a_j} d\mu$. Some elementary applications of the theorems of Lebesgue and Beppo–Levi together with Lemma 3.4 show that

$$E_\mu(\phi^j)\to E_\mu(\phi) \quad \text{when } j\to\infty$$

and that $\int a_j f d\mu \leqslant \int a_j \phi^j d\mu - \epsilon/2$ for j large. After replacing ϵ by a smaller number, we may therefore assume in (3.16) that a is bounded. By another argument of approximation, we may also assume that f and a are simple functions. Then, we may also replace μ in (3.16) by a measure supported in a finite set. The first part of the proof now gives us a contradiction. Hence, (3.11) must hold, and the proof is complete.

IV. SOME APPLICATIONS OF ENTROPY ESTIMATES

In this section, we shall use the results from the previous sections and give examples of entropy estimates. We show for example that the lowest eigenvalue of the harmonic oscillator may be computed by considering entropy estimates.

As a preparation, we minimize the functional

$$L^1_+(\mathbf{R}^m)=L^1_+(\mathbf{R}^m,dx)\ni f\mapsto \int |x|^p f(x)dx, \quad p>0,$$

under the condition (1.2), with $E_\mu(f)=E(f)$. Here, we recall that $E(f)$ is the entropy with respect to the Lebesgue measure. By Theorem 3.6, the minimum is attained when

$$f(x)=\phi_s(x)=e^{-s|x|^p}/\|e^{-s|\cdot|^p}\|_{L^1},$$

and s is chosen such that $E(\phi_s)=E$. We notice that $I(s)=\int e^{-s|x|^p}dx$ is homogeneous of degree $-m/p$ in s when $s>0$. Therefore,

$$\int |x|^p \phi_s(x)dx=-I'(s)/I(s)=-\vartheta'(s)=m/sp, \tag{4.1}$$

where $\vartheta(s)=\log(I(s))$. The condition that $E(\phi_s)=E$ means that $\vartheta(s)-s\vartheta'(s)=E$. Since $\vartheta'(s)=I'(s)/I(s)=-m/sp$ this is equivalent to $\int e^{-s|x|^p}dx=e^{E-m/p}$. We may solve the last equation in s, and by straightforward computations it follows that

$$s^{-1}=(\omega_m p^{-1}\Gamma(m/p))^{-m/p}e^{Ep/m-1},$$

where ω_m is the area of the sphere S^{m-1}. By inserting this into (4.1), Theorem 3.6 gives

$$\inf_{E(f)\geqslant E}\int |x|^p f(x)dx=\int |x|^p\phi_s(x)dx=m/sp=(\omega_m p^{-1}\Gamma(m/p))^{-p/m}mp^{-1}e^{Ep/m-1}. \tag{4.2}$$

We shall now apply this result to the Toeplitz operator $\mathrm{Tp}(a)$ when $a(X)=|X|^{2p}$ and $X=(x,\xi)\in\mathbf{R}^{2n}$. We recall from the introduction that $\mathrm{Tp}(a)=\mathrm{Tp}_g(a)$ makes sense as a continuous operator from $\mathcal{S}(\mathbf{R}^n)$ to $\mathcal{S}'(\mathbf{R}^n)$ for any $a\in\mathcal{S}'(\mathbf{R}^{2n})$ and $g\in\mathcal{S}(\mathbf{R}^n)\backslash 0$.

Lemma 4.1: Assume that $f, g\in\mathcal{S}(\mathbf{R}^n)$ such that $\|f\|_{L^2}=\|g\|_{L^2}=1$, and set $a(X)=|X|^{2p}$, where $p>0$, and $X\in\mathbf{R}^{2n}$. Then,

$$\begin{aligned}(\mathrm{Tp}_g(a)f,f)&\geqslant 4^p\pi^{-p}(n/p)p^{p/n}\{\Gamma(n)/\Gamma(n/p)\}^{p/n}e^{E(|V_g f|^2)p/n-1}\\&\geqslant 2^p p^{p/n-1}\{\Gamma(n)/\Gamma(n/p)\}^{p/n}e^{p-1}n.\end{aligned} \tag{4.3}$$

Proof: We apply (4.2) when $m=2n$ and p is replaced by $2p$, observing that $a(-2X)=2^{2p}|X|^{2p}$. Since $\omega_{2n}=2\pi^n/(n-1)!$, the first inequality in (4.3) follows immediately from (1.3), (1.5), and (4.2). The second inequality follows from Corollary 2.3.

Next, we shall apply Lemma 4.1 in order to minimize the harmonic oscillator $H=\Sigma_{j=1}^n(x_j^2+D_j^2)$. We note that the Weyl symbol for H is the function $h(x,\xi)=\Sigma_{j=1}^n(x_j^2+\xi_j^2)$.

Proposition 4.2: Let $u=V_g g$, where $g\in\mathcal{S}(\mathbf{R}^n)$ is even or odd and satisfies $\|g\|_{L^2}=1$. Then,

$$(Hf,f)\geqslant 4n\pi^{-1}e^{E(|V_g f|^2)/n-1}+4^{-1}(\pi/2)^{n/2}(\Delta u)(0)\geqslant 2n+4^{-1}(\pi/2)^{n/2}(\Delta u)(0),$$

for every unit vector $f\in\mathcal{S}(\mathbf{R}^n)$. Here, $\Delta=\Delta_{(x,\xi)}=\Sigma(\partial_{x_j}^2+\partial_{\xi_j}^2)$ is the Laplace operator in the (x,ξ)-coordinates.

In the proof of Proposition 4.2, we shall use some properties for Fourier transformations. In what follows, we let $\hat{f}$ be the Fourier transform for $f\in\mathcal{S}(\mathbf{R}^n)$, given by

$$\hat{f}(\xi)=(\mathcal{F}f)(\xi)=(2\pi)^{-n/2}\int f(x)e^{-i\langle x,\xi\rangle}dx.$$

Proof: Let $\nu=(2\pi)^{-n/2}V_g\check{g}$, and let $X=(x,\xi)\in\mathbf{R}^{2n}$. Since g is even or odd, it follows easily that u and ν are even. This implies that $h*\nu=c_1h+c_2$, where

$$c_1=\int \nu(X)dX \quad\text{and}\quad c_2=\int \nu(X)|X|^2dX.$$

In order to evaluate c_1, we recall the definition of V_g. Then, an application of Fourier's inversion formula gives

$$c_1=(2\pi)^{-n}\int\int\int g(x-y/2)\overline{g(x+y/2)}e^{i\langle y,\xi\rangle}dydxd\xi=\|g\|_{L^2}^2=1.$$

In order to evaluate c_2, we note that $u(x,\xi)=(8\pi)^{n/2}\hat{\nu}(-2\xi,2x)$. It follows now by another application of Fourier's inversion formula that $c_2=-4^{-1}(\pi/2)^{n/2}(\Delta u)(0)$. Hence $h*\nu=h-4^{-1}(\pi/2)^{n/2}(\Delta u)(0)$, and we obtain the result if we combine this equality with Lemma 4.1 and (1.4). The proof is complete.

If we let $u(x,\xi)=(2/\pi)^{n/2}e^{-(|x|^2+|\xi|^2)}$ in Proposition 4.2, then it follows that $\Delta u(0)=-4n(2/\pi)^{n/2}$, which gives us the inequality $(Hf,f)\geqslant n\|f\|_2^2$, as it should.

We shall finish this section by giving a bound from below for the sum of the entropies of a function and its Fourier transform.

Proposition 4.3: Assume that $f\in\mathcal{S}(\mathbf{R}^n)$. Then

$$E(|f|^2)+E(|\hat{f}|^2)\geqslant n(1+\log\pi)\|f\|_2^2. \tag{4.4}$$

Remark 4.4: The entropy $E(g)$ is not invariant under changes of coordinates. In fact, if $0\leqslant g\in\mathcal{S}(\mathbf{R}^n)$, $\|g\|_1=1$ and $g_T(x)=\det(T)g(Tx)$, where T is an invertible linear transformation on $\mathbf{R}^n$, then

$$\int |g_T(x)|\log(|g_T(x)|)dx=\int |g(x)|\log(|g(x)|)dx+\log(|\det T|). \tag{4.5}$$

Since the Fourier transform of f_T is given by $\hat{f}_{\hat{T}}$, where $\hat{T}$ is the adjoint of T^{-1}, it follows however that the left-hand side of (4.4) is invariant under changes of coordinates.

Proof of Proposition 4.3: We may assume that $\|f\|_2=1$. Set $D_p=(2\pi)^{1/p-1/2}p^{-1/2p}p'^{1/2p'}$, where $2<p$ and $1/p+1/p'=1$. Then the sharp Hausdorff–Young's inequality gives

$$\int |\hat{f}|^p d\xi\leqslant D_p^{np}\left(\int |f|^{p'}dx\right)^{p/p'} \tag{4.6}$$

(Ref. 2 or 3). Taylor expansions give

$$D_p = 1-(1+\log\pi)(p-2)/4+O((p-2)^2),$$

$$\int |\hat{f}|^p d\xi = 1-(p-2)(E(|\hat{f}|^2)/2+O((p-2)^2),$$

$$\int |f|^{p'} dx = 1+(p-2)(E(|f|^2)/2+O((p-2)^2).$$

The proposition follows if these expansions are inserted into (4.6).

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Yang–Mills instantons with Lorentz violation

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An analysis is performed of instanton configurations in pure Euclidean Yang–Mills theory containing small Lorentz-violating perturbations that maintain gauge invariance. Conventional topological arguments are used to show that the general classification of instanton solutions involving the topological charge is the same as in the standard case. Explicit solutions are constructed for general gauge invariant corrections to the action that are quadratic in the curvature. The value of the action is found to be unperturbed to lowest order in the Lorentz-violating parameters. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767624]

I. INTRODUCTION

As is well known, solving pure Yang–Mills theory involves a complicated set of nonlinear partial differential equations. Using a series of clever arguments, some exact solutions to the pure Yang–Mills field equations formulated in four-dimensional Euclidean space were first constructed in the mid 1970s.[1] The complete set of finite action solutions was eventually classified using what is now known as the ADHM construction.[2] Subsequently, instanton physics has stimulated much research in both physics and mathematics.[3]

In pure four-dimensional Yang–Mills theory, Lorentz symmetry and renormalizability coupled with gauge invariance implies that the Lagrange density naturally takes the form of the trace of the square of the curvature tensor. If pure Yang–Mills theory arises as the low-energy limit of some more fundamental theory, it is possible that real physical fields obey a slightly modified version of the conventional equations in which some of the underlying symmetries are spontaneously broken. Specifically, Lorentz and *CPT* invariance, as well as gauge invariance can be affected.[4]

The original motivation for this possibility arose in string theory,[5] and more recently has been analyzed within the context of noncommutative geometry.[6] A framework called the standard model extension (SME) incorporates general fundamental symmetry violations that are consistent with coordinate reparametrization invariance[7] within the context of quantum field theory.[8] Usually, it is convenient to restrict the full range of possible violations to maintain certain subgroups of the original symmetry group. For instance, translational invariance, gauge invariance, and power-counting renormalizability are typically assumed to avoid many of the potential inconsistencies that may arise without these assumptions. This restriction produces a minimal version of the full SME.

The aim of this article is to analyze the instanton solutions for a Yang–Mills action in the presence of Lorentz violation. The main result is that the general classification of the instanton solutions involving the topological charge still applies when Lorentz violation is present. In addition, the value of the Euclidean action is found to be invariant to lowest order in the Lorentz-violating perturbations. Specific calculations are performed within the framework of the minimal SME, but some of the results are in fact more general. In Sec. II, the notation and conventions are described. The existence of static solutions in arbitrary dimensions is examined in Sec. III. Section IV contains the general theory of instantons with Lorentz violation, while Sec. V restricts to the specific example of SU(2) instantons with unit winding number. Section VI summarizes the

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results. The Appendix contains an exact solution for the perturbed instantons in the presence of a spatially isotropic Lorentz-violating background tensor.

II. NOTATION AND CONVENTIONS

The conventions used for the Yang–Mills gauge theory are presented in this section. Let G be a compact Lie group with Lie algebra $L(G)$. The base manifold is taken to be $M=\mathbf{R}^4$ and the gauge potential components for the principle G-bundle $P\rightarrow M$ are denoted

$$A_\mu(x)\equiv A_\mu^a(x)L_a\,, \tag{1}$$

where the L_a are hermitian generators of a Lie algebra defined by

$$[L_a\,,L_b]=iC_{abc}L_c\,, \tag{2}$$

with structure constants C_{abc} antisymmetric in all indices. The normalization of the generators is fixed by imposing

$$Tr(L_aL_b)=\tfrac{1}{2}\,\delta_{ab}\,. \tag{3}$$

The associated unitary Lie group elements that generate gauge transformations are denoted by

$$U(x)=e^{-i\omega^a(x)L_a}. \tag{4}$$

These act on the gauge fields via the transformation rule

$$A^\mu(x)\rightarrow U(x)A^\mu(x)U^{-1}(x)-\frac{i}{g}U(x)\partial^\mu U^{-1}(x). \tag{5}$$

The field strength tensor is defined as

$$F^{\mu\nu}=-\frac{i}{g}[D^\mu,D^\nu], \tag{6}$$

where the covariant derivative is taken as $D^\mu=\partial^\mu+igA^\mu$. The field strength transforms under gauge transformations as

$$F^{\mu\nu}\rightarrow U(x)F^{\mu\nu}U^{-1}(x). \tag{7}$$

The dual of F is defined as

$$\tilde{F}_{\mu\nu}\equiv\tfrac{1}{2}\epsilon_{\mu\nu\alpha\beta}F^{\alpha\beta}, \tag{8}$$

where the Levi–Civita tensor is defined such that $\epsilon^{0123}=+1$.

In four-dimensional Minkowski space, with metric $g=\mathrm{diag}(1,-1,-1,-1)$, the most general gauge invariant[9] and power counting renormalizable action is[8]

$$S_M(A)=-\frac{1}{2}\int d^4xTr\left[F^{\mu\nu}F_{\mu\nu}+(k_F)_{\mu\nu\alpha\beta}F^{\mu\nu}F^{\alpha\beta}+(k_{AF})_\kappa\epsilon_{\kappa\lambda\mu\nu}\left(A^\lambda F^{\mu\nu}-\frac{2}{3}igA^\lambda A^\mu A^\nu\right)\right], \tag{9}$$

where the k_F and k_{AF} terms are small constant background parameters. Gauge invariance fixes these parameters to be singlets under the action of the gauge group. The k_{AF} terms present theoretical difficulties associated with negative contributions to the energy[10] even in the Abelian case, and are therefore not considered further in this work. On the other hand, the k_F terms do not cause similar problems provided a concordant frame,[11] in which the parameters are small enough,

is used. The parameters k_F satisfy the symmetries of the Riemann curvature tensor[12] with vanishing total trace. This means that there are 19 independent coefficients that parameterize the violation.

III. STATIC SOLUTIONS

In the conventional case, finite-action static solutions are ruled out in all but four spatial dimensions by considering various integrals of the field strength products motivated by the form of the energy momentum tensor.[13] This result also holds in the Lorentz-violating case due to an analogous argument that will now be presented.

The partially symmetrized energy momentum tensor arising from the action in Eq. (9) generalized to n spatial dimensions is given by the expression

$$\Theta^{\mu\nu}=2Tr[-F^{\nu}{}_{\gamma}(F^{\mu\gamma}+k_F^{\mu\gamma\alpha\beta}F_{\alpha\beta})+\tfrac{1}{4}\eta^{\mu\nu}F_{\alpha\beta}(F^{\alpha\beta}+k_F^{\alpha\beta\lambda\kappa}F_{\lambda\kappa})], \tag{10}$$

and explicitly satisfies $\partial_\mu\Theta^{\mu\nu}=0$. Choosing the static gauge in which A^k is independent of time, the following constraints on finite energy solutions can be derived using the field equations

$$\int dx^n TrF_{0k}(F^{0k}+k_F^{0k\alpha\beta}F_{\alpha\beta})=0, \tag{11}$$

and

$$(n-4)\int dx^n TrF_{ij}(F^{ij}+k_F^{ij\alpha\beta}F_{\alpha\beta})=0. \tag{12}$$

Methods analogous to the ones presented in Ref. 13. have been applied to obtain the above results. These relations imply that no static solutions with nonvanishing action[14] exist when $n\neq 4$. This result is the same as the conventional situation.

IV. INSTANTON SOLUTIONS

To study the instanton solutions, the action is analytically continued to Euclidean space using imaginary time, and a new Euclidean action $S_E\equiv -iS_M$ is defined. The conventions used in this article are obtained using the replacements $x^0\rightarrow -ix_E^0$, $x^k\rightarrow x_E^k$, while the gauge field components are altered to $A^0\rightarrow iA_E^0$, and $A^k\rightarrow A_E^k$. Each time component of k_F also gets multiplied by a factor of i to define its Euclidean counterpart. The Euclidean action becomes (dropping all E subscripts)

$$S(A)=+\frac{1}{2}\int d^4xTr[(F^{\mu\nu}F^{\mu\nu})+(k_F)^{\mu\nu\alpha\beta}F^{\mu\nu}F^{\alpha\beta}], \tag{13}$$

with metric $\delta^{\mu\nu}$. The Euler–Lagrange equations of motion (for this Euclidean action) are

$$[D^\mu,F^{\mu\nu}+k_F^{\mu\nu\alpha\beta}F^{\alpha\beta}]=0, \tag{14}$$

while the Bianchi identity

$$[D^\mu,\tilde{F}^{\mu\nu}]=0, \tag{15}$$

follows from the definition of F in terms of the gauge potential.

The topological charge q is defined as in the usual case

$$q=\frac{g^2}{16\pi^2}\int d^4xTr\tilde{F}^{\mu\nu}F^{\mu\nu}, \tag{16}$$

and conventional arguments indicate that q remains an integer, even in the presence of Lorentz violation. Specifically, the identity

$$\tfrac{1}{4} Tr \tilde{F}^{\mu\nu} F^{\mu\nu} = \partial^{\mu} X^{\mu}, \tag{17}$$

where

$$X^{\mu} \equiv \frac{1}{4} \epsilon^{\mu\nu\lambda\kappa} Tr(A^{\nu} F^{\lambda\kappa} - \tfrac{2}{3} i g A^{\nu} A^{\lambda} A^{\kappa}), \tag{18}$$

ensures that the topological charge depends only on the pure-gauge boundary conditions satisfied by the potential far away from the nonvanishing curvature of the instantons. The quantity q is therefore the first Pontryagin number that corresponds to the winding number of the map from the gauge group to the three sphere at large $|x|$. The specific form of the action does not matter, provided that it is in fact gauge invariant, and that finiteness of the action restricts the curvature from contributing to the topological charge at the boundary. This means that the properties of the topological charge should be preserved, even in the more general case of the SME that includes nonrenormalizable, but gauge invariant corrections to the pure Yang–Mills sector. In particular, since any physical theory of noncommutative gauge fields is argued to be equivalent to a standard gauge theory in the context of the SME,[6] the topological charge should remain integral in realistic noncommutative Yang–Mills theories.

To make further progress, only lowest-order terms in k_F are retained. This approximation has the advantage of retaining terms that are likely to be relevant for future experiments while neglecting the theoretical complications of the nonlinearities introduced by higher-order k_F contributions. An approach that allows explicit calculation to all orders in k_F would be interesting because there is the potential of discovering novel nonperturbative features, but this is beyond the scope of the current article.

For calculational purposes, it is convenient to introduce the quantity[15]

$$F'^{\mu\nu} = F^{\mu\nu} + \tfrac{1}{2} k_F^{\mu\nu\alpha\beta} F^{\alpha\beta}. \tag{19}$$

The action then takes the conventional form in terms of F' to lowest order in k_F. Consider the inequality

$$\frac{1}{2} \int d^4x Tr(F' \mp \tilde{F}')^2 \geqslant 0. \tag{20}$$

This implies that

$$S \geqslant \pm \frac{1}{2} \int d^4x Tr\left[F^{\mu\nu} \tilde{F}^{\mu\nu} + \frac{1}{2} (k_F^{\mu\nu\alpha\beta} + \tilde{k}_F^{\mu\nu\alpha\beta}) F^{\mu\nu} \tilde{F}^{\alpha\beta} \right], \tag{21}$$

where $\tilde{k}_F^{\mu\nu\alpha\beta} \equiv \frac{1}{4} \epsilon^{\mu\nu\lambda\kappa} k_F^{\lambda\kappa\rho\sigma} \epsilon^{\rho\sigma\alpha\beta}$ is defined as the dual to k_F. The upper sign is chosen for $q > 0$ and the lower sign for $q < 0$.

The first term is proportional to the topological charge while the second term generates a correction to the lower bound on S. Provided k_F is small, the correction term will be much smaller than the topological charge term and the perturbed instantons will be close to the conventional ones. This implies that the general classification of the instanton solutions in terms of the winding number will remain unaltered.

It is evident from the form of the correction to the lower bound that splitting the coefficients k_F according to their duality properties will be useful. This decomposition is analogous to the separation of the Riemann tensor of general relativity into a Ricci tensor and a trace-free Weyl conformal tensor. The anti-self-dual k_F components correspond to the Ricci tensor components while the self-dual k_F terms correspond to the Weyl conformal tensor. For the case $k_F = -\tilde{k}_F$, the

lower bound on the action is independent of continuous perturbations of F that do not change the topological charge by an integer, and the minimum is attained for the modified duality condition

$$F' \simeq \pm \tilde{F}', \tag{22}$$

where the symbol $\simeq$ is used to denote an equality to lowest order in k_F. To construct the perturbed solutions, the potential can be expanded about the conventional ($k_F=0$) self-dual and anti-self-dual potentials, denoted by $A_{\rm SD}$ and $A_{\rm ASD}$. The corresponding field tensors are written similarly as $F_{\rm SD}$ and $F_{\rm ASD}$. It remains to show that solutions to the modified duality condition that are consistent with the Bianchi identity exist. The anti-self-duality condition on k_F implies that it must be of the form

$$k_F^{\mu\nu\alpha\beta} = \Lambda_k^{[\mu[\alpha}\delta^{\nu]\beta]}, \tag{23}$$

where $\Lambda_k^{\mu\nu} = \frac{1}{2}k_F^{\alpha\mu\alpha\nu}$ is a traceless symmetric matrix that depends on the trace components of k_F. In fact, the explicit solution can be guessed since the form of the correction to the action is related to the conventional action as described in the skewed coordinate system $\tilde{x}^\mu \equiv x^\mu + \Lambda_k^{\mu\nu}x^\nu$. These terms are exactly the ones that may be transferred to other sectors using an appropriate field redefinition,[16] so it is not surprising that they yield a conventional version of pure Yang–Mills theory when described in skewed coordinates. Note that this does not imply the absence of physical effects arising from an anti-self-dual k_F term in the action. Redefining coordinates effects all fields, not just the Yang–Mills gauge potential, so if the instantons are expressed in terms of new coordinates, the Lorentz violation will show up in the Lagrangian for other particle species that are coupled to the instantons.

The explicit form for the perturbed self-dual instanton gauge potentials are given by

$$A_+^\mu(x) \simeq A_{\rm SD}^\mu(\tilde{x}) + \Lambda_k^{\mu\nu}A_{\rm SD}^\nu(x), \tag{24}$$

yielding a perturbed field tensor

$$F_+^{\mu\nu} \simeq F_{\rm SD}^{\mu\nu}(\tilde{x}) - \Lambda_k^{[\mu\alpha}\delta^{\nu]\beta}F_{\rm SD}^{\alpha\beta}(x) \simeq F_{\rm SD}^{\mu\nu}(\tilde{x}) - \tfrac{1}{2}k_f^{\mu\nu\alpha\beta}F_{\rm SD}^{\alpha\beta}(x), \tag{25}$$

that satisfies the modified duality condition (22). Note that the approximation is in fact not necessary in this case, but the notation becomes rather cumbersome for general k_F. The exact solution for the O(3) rotationally invariant component of k_F (which is in fact anti-self-dual) is presented in the Appendix.

Next, the case $k_F = \tilde{k}_F$ is considered. This condition implies that k_F has the symmetries of the Weyl conformal tensor with vanishing single traces. In this case, the simple argument given above for anti-self-dual k_F fails because the lower bound on the action in Eq. (21) is not a topological invariant, and is therefore sensitive to small perturbations in the field strengths. In this case, there is no obvious duality condition and the equations of motion must be solved directly for the perturbed instanton solutions. A solution to lowest order in k_F always exists, since the equations reduce to a set of linear second-order elliptic partial differential equations for the gauge fields. The propagators for spin-1 particles in instanton background fields have been previously constructed[19] and are exactly what is needed to formally solve the equations. An explicit example is presented in the next section.

For general k_F, the perturbed field strength may be written as a small perturbation of either the $F_{\rm SD}$ or the $F_{\rm ASD}$ solutions. Remarkably, the approximate value of the action is the same as the conventional case. For example, an instanton that is close to self-dual yields an action of

$$S \simeq \frac{1}{2}\int d^4x Tr(F^2 + k_F^{\mu\nu\alpha\beta}F_{\rm SD}^{\mu\nu}F_{\rm SD}^{\alpha\beta}). \tag{26}$$

The first term is the conventional action and is invariant to lowest order in any perturbation of the fields due to the fact that the action is at an extremum for the self dual solutions. The O(4) symmetry of the conventional self-dual solutions imply that the second term must vanish, since only observer Lorentz-invariant components of k_F can contribute after the trace is performed. These terms are zero due to the Lorentz-violating nature of k_F. The same arguments apply to the instantons that are close to the anti-self-dual solutions. The numerical value of the action to leading order in k_F is therefore given by the conventional formula

$$S \simeq (8\pi^2/g^2)|q|, \tag{27}$$

for the general case involving arbitrary k_F values. This argument can also be generalized to nonrenormalizable corrections to the pure Yang–Mills sector involving powers of the curvature tensor. This works because any higher-order Lorentz-violating corrections must vanish when the O(4) symmetric solutions are substituted into the action. As mentioned previously, any realistic theory of noncommutative gauge fields is argued to be equivalent to a subset of the SME,[6] therefore it can be inferred that any realistic theory of noncommutative Yang–Mills fields should not affect the value of the Euclidean action for the instantons to lowest order in the noncommutative Lorentz-violating $\theta^{\mu\nu}$ parameters.

V. INSTANTONS IN SU(2)

To analyze instanton structure, an explicit map is constructed from the asymptotic three-sphere S^3 of Euclidean space into the Yang–Mills gauge group G. The winding number of this map determines the topological charge and therefore the general instanton structure according to the lower bound of the action in Eq. (21). For any simple Lie group G, a theorem by Bott[17] proves that any mapping of S^3 into G can be continuously deformed into a mapping into an SU(2) subgroup of G. It is therefore sufficient to fix SU(2) as the gauge group to construct explicit solutions that will exhibit the generic effect of Lorentz violation on the instanton structure.

Here, we work with the explicit solutions for $q=1$, or unit topological charge. The conventional solutions are denoted using the self-dual, antisymmetric tensor $\tau^{\mu\nu}$, where $\tau^{0i} \equiv \sigma^i$ and $\tau^{ij} \equiv \epsilon^{ijk}\sigma^k$, in terms of the conventional Pauli matrices σ^i. This definition provides an explicit embedding of $\mathrm{SU}(2) \rightarrow \mathrm{SU}(2) \times \mathrm{SU}(2)$ which is isomorphic to O(4). The commutation relations

$$[\tau^{\mu\nu}, \tau^{\alpha\beta}] = 2i(\delta^{\mu\alpha}\tau^{\nu\beta} - \delta^{\mu\beta}\tau^{\nu\alpha} - \delta^{\nu\alpha}\tau^{\mu\beta} + \delta^{\nu\beta}\tau^{\mu\alpha}), \tag{28}$$

and trace relations

$$Tr(\tau^{\mu\nu}\tau^{\alpha\beta}) = 2(\delta^{\mu\alpha}\delta^{\nu\beta} - \delta^{\mu\beta}\delta^{\nu\alpha} + \epsilon^{\mu\nu\alpha\beta}), \tag{29}$$

follow from the above definition. These quantities may also be expressed using the relation $\tau^{\mu\nu} = i(\tau^{\nu}\tau^{\mu\dagger} - \delta^{\mu\nu})$, where $\tau^{\mu} \equiv (i, \boldsymbol{\sigma})$. The self-dual gauge field corresponding to $q=1$ can be expressed as

$$A^{\mu}_{\mathrm{SD}} = -\frac{\tau^{\mu\nu}x^{\nu}}{g(\rho^2 + x^2)}, \tag{30}$$

and the associated field strength is

$$F^{\mu\nu}_{\mathrm{SD}} = \frac{2\rho^2}{g(\rho^2 + x^2)^2}\tau^{\mu\nu}. \tag{31}$$

The parameter ρ determines the instanton size, while the center of the instanton is taken to be at the origin for simplicity. The anti-self-dual solutions are the parity transform of the above fields. These can be expressed using $\tilde{x} = (x^0, -\mathbf{x})$ as $A^0_{\mathrm{ASD}}(x) = A^0_{\mathrm{SD}}(\tilde{x})$, $A^i_{\mathrm{ASD}}(x) = -A^i_{\mathrm{SD}}(\tilde{x})$, $F^{0i}_{\mathrm{ASD}}(x)$

$=-F^{0i}_{\rm SD}(\tilde{x})$, and $F^{ij}_{\rm ASD}(x)=F^{ij}_{\rm SD}(\tilde{x})$. This transformation may also be implemented by the transformation $\tau^{\mu\nu}\to\overline{\tau}^{\mu\nu}$ defined by $\tau^{0i}\to\overline{\tau}^{0i}=-\tau^{0i}$, and $\tau^{ij}\to\overline{\tau}^{ij}=\tau^{ij}$. A useful expression for this quantity is $\overline{\tau}^{\mu\nu}=i(\tau^{\nu\dagger}\tau^{\mu}-\delta^{\mu\nu})$.

For the case $k_F=-\tilde{k}_F$, the modified solutions have already been expressed using Eq. (24) and do not require more explicit computation. For the case $k_F=\tilde{k}_F$, the field equations (14) and (15) must be solved directly since no obvious duality condition can be determined from Eq. (21) due to the noninvariant lower bound. To accomplish this, the vector potential is expanded as a perturbation of the self-dual[18] solution $A=A_{\rm SD}+A_k$ and the linear terms in A_k are retained in the equation of motion. The Bianchi identity (15) is automatically satisfied and the equations of motion (14) become (in the Lorentz gauge $\partial^\mu A^\mu=0$)

$$[D^\nu_{\rm SD},[D^\nu_{\rm SD},A^\mu_k]]+2ig[F^{\mu\nu}_{\rm SD},A^\nu_k]-ig[D^\mu_{\rm SD},[A^\nu_{\rm SD},A^\nu_k]]=j^\mu_k, \tag{32}$$

where

$$j^\mu_k\equiv k_F^{\mu\nu\alpha\beta}[D^\nu_{\rm SD},F^{\alpha\beta}_{\rm SD}], \tag{33}$$

and $D^\mu_{\rm SD}\equiv\partial^\mu+igA^\mu_{\rm SD}$ is the covariant derivative in the conventional self-dual instanton background.

This equation can be solved by performing a convolution of j_k with the corresponding propagator for spin-1 particles in an external instanton field. This propagator has been formally constructed,[19] but the explicit form is rather unwieldy and cannot be easily expressed analytically. An alternative approach is adopted here that uses a combination of the propagator approach and a direct substitution technique. First, the solution is studied to lowest order in ρ^2/x^2, corresponding to the asymptotic region far from the self-dual instanton curvature density. This provides the general tensorial structure of the instanton correction that serves as an ansatz for general values of x^2, generating a simple form for the solution to the problem.

It is convenient to perform a gauge transformation to the singular gauge using $U(x)=-ix\cdot\tau^\dagger/x$ so that the potential is better behaved for large x. The transformed potential becomes

$$\overline{A}^\mu_{\rm SD}=-\frac{\rho^2\overline{\tau}^{\mu\nu}x^\nu}{gx^2(\rho^2+x^2)}, \tag{34}$$

with associated field strength

$$\overline{F}^{\mu\nu}_{\rm SD}=\frac{4\rho^2}{g(\rho^2+x^2)^2}\overline{\tau}^{[\mu\alpha}(1/4\,\delta^{\nu]\alpha}-x^{\nu]}x^\alpha/x^2). \tag{35}$$

In this gauge, the transformed $\overline{j_k}$ is

$$\overline{j}^\mu_k=\frac{48\rho^2}{gx^2(\rho^2+x^2)^3}k_F^{\mu\nu\alpha\beta}\overline{\tau}^{\alpha\gamma}I^{\gamma\nu\beta}(x), \tag{36}$$

where

$$I^{\gamma\nu\beta}\equiv x^\gamma x^\nu x^\beta-\tfrac{1}{6}x^2(\delta^{\nu\gamma}x^\beta+\delta^{\gamma\beta}x^\nu+\delta^{\beta\nu}x^\gamma), \tag{37}$$

is a totally symmetric tensor.

The advantage of working in the singular gauge is that the above expressions are all quadratic in ρ. This means that to lowest order in ρ^2/x^2, the propagator may be approximated by the free field Green's function

$$G_0(x,y)=\frac{1}{4\pi^2(x-y)^2}, \tag{38}$$

satisfying $\partial^\mu\partial^\mu G_0 = -\delta^{(4)}(x-y)$. The perturbed potential to lowest order in ρ^2/x^2 (in the singular gauge) is then given by

$$\overline{A}_k^\mu \simeq -\int d^4y G_0(x,y)\overline{j}_k^\mu(y). \tag{39}$$

This integral can be performed using standard field theoretic integration techniques. The result of the computation is

$$\overline{A}_k^\mu \simeq -\frac{4\rho^2}{gx^6} k_F^{\mu\nu\alpha\beta}\overline{\tau}^{\alpha\gamma} I^{\gamma\nu\beta}(x). \tag{40}$$

It can be seen that the tensorial structure of $\overline{j_k}$ has been preserved by the convolution with G_0. Some complications arise due to divergent logarithms that cancel out in the computation, but these do not cause theoretical difficulties because the validity of the solution can be verified by direct substitution into the equation of motion. It remains to check that the Lorentz gauge condition is satisfied by this solution. Direct calculation shows that this is the case provided k_F is self-dual, the current case of interest. This indicates that this solution method works for the terms that cannot be removed using a reparametrization of the coordinates.

For general values of x^2, an unknown scalar function is included in the expression (40) to produce an ansatz of the form

$$\overline{A}_k^\mu = -\frac{4\rho^2}{g} f(x^2) k_F^{\mu\nu\alpha\beta}\overline{\tau}^{\alpha\gamma} I^{\gamma\nu\beta}(x). \tag{41}$$

Remarkably, upon substitution into the equation of motion (32), the tensorial structure factors out and the following second-order linear differential equation is found for f

$$x^4(\rho^2+x^2)f'' + 5x^2(\rho^2+x^2)f' + 3\rho^2 f = -\frac{3}{(\rho^2+x^2)^2}. \tag{42}$$

This equation has a regular singular point at $x=0$, causing the homogeneous solutions to be badly behaved at the origin. Moreover, any contribution to the homogeneous equation of motion would correspond to a solution to the conventional equations of motion in an instanton background and is therefore not of interest in the present context. On the other hand, the particular solution is well behaved at the origin as can be verified using the following series expansion for f about $x=0$

$$f(x^2) = \frac{1}{\rho^6}\sum_{n=0}^{\infty} a_n \left(\frac{x^2}{\rho^2}\right)^n, \tag{43}$$

and expanding the right-hand side of Eq. (42) as

$$-\frac{3}{(\rho^2+x^2)^2} = -\frac{3}{\rho^4}\sum_{n=0}^{\infty}(-1)^n(n+1)\left(\frac{x^2}{\rho^2}\right)^n, \tag{44}$$

valid for $x^2/\rho^2<1$. The resulting recursion relation for the a_n coefficients is

$$a_{n+1} = \frac{3(-1)^n}{n+4} - \frac{n}{n+2}a_n, \tag{45}$$

with $a_0=-1$. The first few terms give

$$f(x^2)\approx 1/\rho^6\left(-1+\frac{3}{4}\left(\frac{x^2}{\rho^2}\right)-\frac{17}{20}\left(\frac{x^2}{\rho^2}\right)^2+\frac{37}{40}\left(\frac{x^2}{\rho^2}\right)^3-\cdots\right), \tag{46}$$

demonstrating the finite behavior near the origin. For large x^2, a similar expansion in ρ^2/x^2 shows that the function approaches $f(x^2)\to 1/x^6$ as expected.

Transforming the perturbed potential back to the regular gauge yields

$$A_k^\mu \simeq \frac{2\rho^2 x^2}{3g} f(x^2) k_F^{\mu\nu\alpha\beta}\tau^{\alpha\gamma}(\delta^{\gamma\nu}x^\beta+\delta^{\beta\gamma}x^\nu-\delta^{\nu\beta}x^\gamma)], \tag{47}$$

verifying that A_k is zero at the origin in the regular gauge as is required by continuity of the gauge field. The perturbation term behaves asymptotically as $\sim 1/x^3$, and therefore explicitly does not contribute to the topological charge as expected. The resulting correction to the curvature can be computed; however, the specific form is not particularly illuminating. Specifically, there seems to be no obvious generalized duality condition satisfied by F analogous to the situation for $k_F = -\tilde{k}_F$.

VI. SUMMARY

Instantons have long been studied for systems obeying strict Lorentz invariance. In this article, the structure of Yang–Mills instantons in the presence of small Lorentz-violating background fields that maintain gauge invariance is studied for the first time. No new nonzero action static solutions are present in $n\neq 4$ spatial dimensions as is apparent from Eq. (12). The gauge invariance ensures that the conventional pure-gauge asymptotic behavior maintains the same general structure as in the conventional case. This means that conventional arguments can be applied to deduce the quantization of the topological charge. The generality of the SME can then be exploited to infer similar results regarding realistic noncommutative gauge theories.

Specific perturbed instanton solutions for the action considered in this article are split into two categories that depend on the duality properties of the Lorentz-violating background tensor. For the anti-self-dual k_F case, a reparametrization of the coordinates can be used to construct deformed instantons that satisfy a modified duality condition. The perturbed theory is isomorphic to the conventional Yang–Mills theory in this case so the instanton structure is also isomorphic. The O(3) rotationally invariant term of this class is worked out exactly in the Appendix.

When k_F is self-dual, the conventional lower bound argument involving the action fails and the equations of motion must be solved directly. To lowest order in k_F, the resulting equations are linear in the correction to the vector potential and can be formally solved using the Euclidean propagator for a spin-1 particle in an instanton background. For explicit calculation, it turns out to be more practical to first deduce the general tensorial structure in the asymptotic region, then generalize the solution to arbitrary position. General arguments imply that the action is unaltered to lowest order in k_F, but it can be seen from the exact solution given in the Appendix that higher-order corrections are, in general, nonzero.

APPENDIX: EXACT SOLUTION FOR O(3) SYMMETRIC CASE

In this appendix, an exact solution (all orders in k_F) for the case of spatial rotationally invariant k_F is presented. In this case, the tensor k_F can be expressed in terms of one independent parameter $\tilde{\kappa}$ as

$$k_F^{0i0j}=-k_F^{i00j}=-k_F^{0ij0}=k_F^{i0j0}=-\frac{\tilde{\kappa}}{2}\delta^{ij}, \tag{A1}$$

and

$$k_F^{ijkl}=\tilde{\kappa}(\delta^{ik}\delta^{jl}-\delta^{il}\delta^{jk}). \tag{A2}$$

It is convenient to introduce the notation $\tilde{\kappa}=\sin 2\theta$ and the action takes the form

$$S=\frac{1}{2}\int d^4x Tr[F^{\mu\nu}F^{\mu\nu}+\sin 2\theta(F^{ij}F^{ij}-2F^{0i}F^{0i})]. \tag{A3}$$

To construct the analog of the conventional self-dual solution, consider the following inequality

$$\frac{1}{2}\int d^4x Tr\{2[\cos\theta F_{-}^{0i}-\sin\theta F_{+}^{0i}]^2+[\cos\theta F_{-}^{ij}+\sin\theta F_{+}^{ij}]^2\}\geqslant 0, \tag{A4}$$

with $F_{\pm}^{\mu\nu}\equiv F^{\mu\nu}\pm\tilde{F}^{\mu\nu}$. This can be rearranged to give the relation

$$S\geqslant\frac{8\pi^2}{g^2}q\cos 2\theta. \tag{A5}$$

The inequality is saturated when

$$\tilde{F}^{0i}=\frac{1-\tan\theta}{1+\tan\theta}F^{0i}, \tag{A6}$$

and

$$\tilde{F}^{ij}=\frac{1+\tan\theta}{1-\tan\theta}F^{ij}. \tag{A7}$$

A solution to these equations with $q=1$ is provided by the gauge potential

$$A^0=(1+\tan\theta)A^0_{\mathrm{SD}}(\tilde{x}),\quad A^i=(1-\tan\theta)A^i_{\mathrm{SD}}(\tilde{x}), \tag{A8}$$

where $\tilde{x}^\mu\equiv((1+\tan\theta)x^0,(1-\tan\theta)x^i)$. The resulting field strength is

$$F^{0i}=(1-\tan^2\theta)F^{0i}_{\mathrm{SD}}(\tilde{x}),\quad F^{ij}=(1-\tan\theta)^2F^{ij}_{\mathrm{SD}}(\tilde{x}). \tag{A9}$$

The value of the resulting action can be computed directly from the curvature, yielding the expected value

$$S=\frac{8\pi^2}{g^2}q\cos 2\theta. \tag{A10}$$

In fact, this construction applies to any conventional instanton solution, since the spatially rotational invariant k_F term corresponds to a shift in the speed of light for the gauge fields. It is therefore possible to construct the above solutions by rescaling the time and spatial coordinates appropriately. Note that this does not mean that observable effects are absent, since interactions between the instantons and other particles with conventional Lorentz properties may lead to physical effects. The action is reduced relative to the conventional case by a factor of $\cos\theta$ which is, in fact, second order in the k_F coefficients. This result is in agreement with general arguments stating that the numerical value of the action is stable to a lowest-order perturbation in k_F.

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Partially invariant solutions of models obtained from the Nambu–Goto action

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The concept of partially invariant solutions is discussed in the framework of the group analysis of models derived from the Nambu–Goto action. In particular, we consider the nonrelativistic Chaplygin gas and the relativistic Born–Infeld theory for a scalar field. Using a general systematic approach based on subgroup classification methods, nontrivial partially invariant solutions with defect structure $\delta=1$ are constructed. For this purpose, a classification of the subgroups of the Lie point symmetry group, which have generic orbits of dimension 2, has been performed. These subgroups allow us to introduce the corresponding symmetry variables and next to reduce the initial equations to different nonequivalent classes of partial differential equations and ordinary differential equations. The latter can be transformed to standard form and, in some cases, solved in terms of elementary and Jacobi elliptic functions. This results in a large number of new partially invariant solutions, which are determined to be either reducible or irreducible with respect to the symmetry group. Some physical interpretation of the results in the area of fluid dynamics and field theory are discussed. The solutions represent traveling and centered waves, algebraic solitons, kinks, bumps, cnoidal and snoidal waves. [DOI: 10.1063/1.1767625]

I. INTRODUCTION: MODELS DERIVED FROM THE NAMBU–GOTO ACTION

A few years ago, Jackiw[1] thoroughly analyzed and reviewed the subject of the motion of a d-brane in $(d+1)$ spatial dimensions moving in $(d+1,1)$-dimensional space–time, and showed that it is described by the Nambu–Goto action. This has generated quite a lot of interest (see, e.g., Refs. 2–4, and has led to the investigation of symmetry properties of relativistic and nonrelativistic models in field theory.[5] Exploiting this connection, we will extend the analysis in Ref. 5 to the case when these models admit partially invariant solutions. According to Ref. 1, we start by introducing the variables of the target space-time $X^{\mu}=(X^0,X^1,\ldots,X^d,X^{d+1})$ in which the d-brane moves, and the world-volume variables $\phi^{\alpha}=(\phi^0,\phi^1,\ldots,\phi^d)$ which parametrize the d-dimensional extended object evolving in ϕ^0. Then the motion of the d-brane is governed by the Nambu–Goto action

$$I_{\mathrm{NG}}=\int d\phi^0\, d\phi^1\cdots d\phi^d\, \sqrt{(-1)^d \det\left(\frac{\partial X^{\mu}}{\partial \phi^{\alpha}}\frac{\partial X_{\mu}}{\partial \phi^{\beta}}\right)}. \tag{1}$$

The action (1) is parametrization invariant, and different choices of parametrization lead to various

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field theory models. Recently, this concept has been applied to the theory of strings and superstrings.[6,7] In particular, it has been established that for strings moving in flat space–time, the Nambu–Goto action (1) reduces to the Polyakov action

$$S_P = -\frac{T}{2}\int d^2\xi \sqrt{-\det(g)}\, g^{\alpha\beta}\partial_\alpha X^\mu \partial_\beta X^\nu \eta_{\mu\nu}, \tag{2}$$

where $g_{\alpha\beta}$ is the world-sheet metric $g_{\alpha\beta}=\partial_\alpha X \partial_\beta X$. Varying the action with respect to the metric leads to the stress tensor

$$T_{\alpha\beta}=\partial_\alpha X \partial_\beta X - \tfrac{1}{2} g_{\alpha\beta} g^{\gamma\delta}\partial_\gamma X \partial_\delta X. \tag{3}$$

Classically, both actions are equivalent.

In particular, we are interested in the two specific cases represented by the light-cone parametrization, which leads to a nonrelativistic fluid dynamical system (Chaplygin gas), and the Cartesian parametrization, which leads to a relativistic Born–Infeld model. In both cases, we choose $(X^1,X^2,\ldots,X^d)$ to coincide with $(\phi^1,\phi^2,\ldots,\phi^d)$ and rename them for physical interpretation as the spatial position vector $\mathbf{r}$ in d dimensions. The remaining variables X^0, X^{d+1}, and ϕ^0 are treated separately for each of the two parametrizations.

A. Chaplygin gas

For the light-cone parametrization, we define

$$X^+=\frac{1}{\sqrt{2}}(X^0+X^{d+1})=t, \quad X^-=\frac{1}{\sqrt{2}}(X^0-X^{d+1})=\theta(\mathbf{r},t), \tag{4}$$

and then identify t with $\sqrt{2\lambda}\,\phi^0$, where $\lambda>0$ is a constant. The Nambu–Goto action (1) then reduces to the action[1]

$$I_\lambda = -2\sqrt{\lambda}\int dt\, d\mathbf{r}\, \sqrt{\theta_t+\tfrac{1}{2}(\nabla\theta)^2}, \tag{5}$$

which in turn leads to an Euler–Lagrange equation of the form

$$\frac{\partial}{\partial t}\left(\frac{1}{\sqrt{\theta_t+\frac{1}{2}(\nabla\theta)^2}}\right)+\nabla\cdot\left(\frac{\nabla\theta}{\sqrt{\theta_t+\frac{1}{2}(\nabla\theta)^2}}\right)=0. \tag{6}$$

Equation (6) is equivalent to the system of differential equations governing the Chaplygin gas[8]

$$\rho_t+(\nabla\rho)\cdot(\nabla\theta)+\rho\,(\nabla^2\theta)=0, \tag{7a}$$

$$\theta_t+\frac{1}{2}(\nabla\theta)^2=\frac{\lambda}{\rho^2}, \tag{7b}$$

where $\lambda>0$ is a constant. Here, $\rho(\mathbf{r},t)$ is the density and $\theta(\mathbf{r},t)$ the velocity potential of an ideal nonrelativistic fluid of zero vorticity in which the pressure P is related to the density by the polytropic relation[1]

$$P=\frac{-2\lambda}{\rho}. \tag{8}$$

The vanishing vorticity allows us to write the velocity $\mathbf{v}$ of the fluids as the gradient of the potential: $\mathbf{v}=\nabla\theta$. Here, Eqs. (7a) and (7b) correspond, respectively, to the equation of continuity

and Euler's force equation, where the current is given by $j=\rho\nabla\theta$. In the case where $\lambda\neq 0$, it is possible to eliminate the variable ρ by using Eq. (7b) to express it in terms of θ. In this way, system (7) reduces to Eq. (6).

Equations (7a) and (7b) can also be considered in the case where $\lambda=0$. In this case, the variable ρ becomes completely independent, and the Eqs. (7a) and (7b) are decoupled. The force equation (7b) can be solved for θ, and then the continuity equation (7a) solved for ρ. A detailed discussion of the symmetry group in one spatial dimension can be found in Ref. 9. This case is not derived from the Nambu–Goto d-brane. Subsequently, in this article, we will consider only the interactive case $(\lambda\neq 0)$.

B. Born–Infeld model

For the Cartesian parametrization, the variable X^0 is renamed ct, where c is the speed of light, and is also identified with $c\phi^0$. The remaining target space variable X^{d+1} is renamed $\theta(\mathbf{r},t)/c$, which is a function of $\mathbf{r}$ and t. The Nambu–Goto action (1) then reduces to the action[1]

$$I_a=-a\int dt\,d\mathbf{r}\,\sqrt{c^2-(\partial_\mu\theta)^2}, \tag{9}$$

and the corresponding Euler-Lagrange equation is found to be

$$\partial^\nu\left(\frac{1}{\sqrt{c^2-(\partial_\mu\theta)^2}}\,\partial_\nu\theta\right)=0. \tag{10}$$

Equation (10) corresponds to the equations

$$\rho_t+\nabla\cdot\left(\nabla\theta\,\sqrt{\frac{\rho^2c^2+a^2}{c^2+(\nabla\theta)^2}}\right)=0, \tag{11a}$$

$$\theta_t+\rho c^2\,\sqrt{\frac{c^2+(\nabla\theta)^2}{\rho^2c^2+a^2}}=0. \tag{11b}$$

This is the Born–Infeld theory for a scalar field θ discussed in Ref. 1. This theory is related to the nonlinear electrodynamics approach of Born and Infeld,[10,11] where the equations of motion were derived from the Lagrangian

$$L_{\mathrm{BI}}=b^2[1-\sqrt{1-(\mathbf{E}^2-\mathbf{B}^2)/b^2-(\mathbf{E}\cdot\mathbf{B})^2/b^4}]. \tag{12}$$

Here, $\mathbf{E}$ and $\mathbf{B}$ are the spatial components of the electric and magnetic fields, respectively. The connection between Lagrangians (9) and (12), in the case where $b^2=-a$, is described by the following relation:

$$\frac{\mathbf{E}^2-\mathbf{B}^2}{b^2}+\frac{(\mathbf{E}\cdot\mathbf{B})^2}{b^4}=-(c^2-(\partial_\mu\theta)^2)\pm 2\sqrt{c^2-(\partial_\mu\theta)^2}. \tag{13}$$

It should be noted that at the limit where $c\to\infty$ the relativistic Born–Infeld Lagrangian and equations reduce to the nonrelativistic Chaplygin Lagrangian and equations discussed previously, where λ is identified with $a^2/2$. A solution $\theta_{\mathrm{NR}}(\mathbf{r},t)$ of the Chaplygin equation (6) is thus related to its relativistic counterpart $\theta_R(\mathbf{r},t)$ for the Born–Infeld equation (10). This will be discussed in further detail in Sec. IV E.

The majority of known solutions in the literature for the Chaplygin and Born–Infeld equations are simple Riemann waves and their superpositions.[12] In those cases, the equations were generally solved only in the hyperbolic region

TABLE I. Commutation table for the Lie algebra L spanned by the vector fields (15).

$X\backslash Y$	$\mathbf{D_1}$	$\mathbf{D_2}$	$\mathbf{B}$	$\mathbf{Z}$	$\mathbf{P_1}$	$\mathbf{P_0}$
$\mathbf{D_1}$	0	0	B	0	$-P_1$	$-2P_0$
$\mathbf{D_2}$	0	0	$-B$	$-2Z$	$-P_1$	0
$\mathbf{B}$	$-B$	B	0	0	$-Z$	$-P_1$
$\mathbf{Z}$	0	$2Z$	0	0	0	0
$\mathbf{P_1}$	P_1	P_1	Z	0	0	0
$\mathbf{P_0}$	$2P_0$	0	P_1	0	0	0

$$c^2+(\theta_x)^2-\frac{(\theta_t)^2}{c^2}>0. \tag{14}$$

Solutions of these equations obtained from the symmetry reduction method are not necessarily required to obey differential inequality (14), as can be seen in Ref. 5.

C. Objectives and organization

Our objective in this article is to study the partially invariant solutions of the Chaplygin and Born–Infeld systems of equations based on the Lie algebra L of the group of symmetries G of the Chaplygin system. We look for new classes of solutions which are not necessarily G-invariant. Partially invariant solutions are of interest for the following reasons. They can be constructed from a simple algorithm similar to the one employed for the G-invariant case. Also, partially invariant solutions may be used to solve larger classes of initial value problems than the G-invariant solutions. Finally, once a partially invariant solution is found under a subgroup G_0, it is possible to verify whether or not it is invariant under some subgroup of the full group G. Such invariant solutions would be considerably more difficult to obtain directly from the standard symmetry reduction method, since in some cases it requires us to solve nonlinear partial differential equations (PDEs) instead of ordinary differential equations (ODEs).

This article is organized as follows. Section II is devoted to a description of the symmetry group structure of the Chalygin and Born–Infeld systems. The properties of the Chaplygin symmetry Lie algebra L are discussed, and we perform a classification of L into conjugate classes of subalgebras, having generic orbits of dimension 2. A complete list of the two-dimensional subalgebras of L is given. In Sec. III, we give a brief theoretical background needed to understand the theory of partially invariant solutions, which includes an algorithm for constructing such classes of solutions. In Sec. IV, we describe and discuss certain classes of partially invariant solutions of the Chaplygin and Born–Infeld equations. All obtained solutions are computed from two-dimensional subalgebras, and have defect structure $\delta=1$. Finally, Sec. V contains observations and a discussion of further applications of our results.

II. STRUCTURE OF THE SYMMETRY LIE ALGEBRA

A. Symmetry properties of the Chaplygin and Born–Infeld equations

The Lie algebra L of Chaplygin gas Eqs. (7a) and (7b) in one spatial dimension is spanned by the six independent vector fields:[5,9]

$$\begin{gathered} P_1=\partial_x, \quad P_0=\partial_t, \quad B=t\partial_x+x\partial_\theta, \quad Z=\partial_\theta, \\ D_1=x\partial_x+2t\partial_t+\rho\partial_\rho, \quad D_2=x\partial_x+2\theta\partial_\theta-\rho\partial_\rho. \end{gathered} \tag{15}$$

Here, P_0 and P_1 represent translations in the independent variables t and x, respectively, B consists of a Galilean boost, Z corresponds to a shift in the potential θ, and D_1 and D_2 are dilations in the dependent and independent variables. The commutation relations between the generators of the Lie algebra L are summarized in Table I.

Using the transformations of the Nambu–Goto parametrizations, we may transform the generators of the Chaplygin Lie algebra L into infinitesimal symmetries of the Born–Infeld Eqs. (11a) and (11b). We first transform the variables x, t, and θ of the Chaplygin gas equations back into the Nambu–Goto target space variables X^0, X^1, X^2:

$$X^0=\frac{1}{\sqrt{2}}(t+\theta), \quad X^1=x, \quad X^2=\frac{1}{\sqrt{2}}(t-\theta). \tag{16}$$

Thus, the derivatives may be transformed to

$$\partial_t=\frac{1}{\sqrt{2}}(\partial_{X^0}+\partial_{X^2}), \quad \partial_x=\partial_{X^1}, \quad \partial_\theta=\frac{1}{\sqrt{2}}(\partial_{X^0}-\partial_{X^2}). \tag{17}$$

Note that under this transformation, $\rho \to \infty$, so that in order to keep the transformations finite it is necessary to set $\partial_\rho=0$. We therefore obtain the generators

$$P_1=\partial_{X^1}, \quad P_0=\frac{1}{\sqrt{2}}(\partial_{X^0}+\partial_{X^2}), \quad B=\frac{1}{\sqrt{2}}(X^0+X^2)\partial_{X^1}+\frac{X^1}{\sqrt{2}}(\partial_{X^0}-\partial_{X^2}),$$

$$Z=\frac{1}{\sqrt{2}}(\partial_{X^0}-\partial_{X^2}), \quad D_1=X^1\partial_{X^1}+(X^0+X^2)(\partial_{X^0}+\partial_{X^2}), \tag{18}$$

$$D_2=X^1\partial_{X^1}+(X^0-X^2)(\partial_{X^0}-\partial_{X^2}),$$

and the commutation relations for the transformed generators (18) are identical to those given in Table I. Thus, it is possible to pass from one system of generators to another through the transformations (16). We then proceed to transform the Nambu–Goto target space variables into the equivalent Born–Infeld variables

$$t=\frac{1}{c}X^0, \quad x=X^1, \quad \theta=cX^2, \tag{19}$$

which leads to the generators

$$\widehat{P_1}=\partial_x, \quad \widehat{P_0}=\frac{1}{\sqrt{2}}\left(\frac{1}{c}\partial_t+c\partial_\theta\right), \quad \hat{B}=\frac{1}{\sqrt{2}}\left(ct+\frac{1}{c}\theta\right)\partial_x+\frac{x}{\sqrt{2}}\left(\frac{1}{c}\partial_t-c\partial_\theta\right),$$

$$\hat{Z}=\frac{1}{\sqrt{2}}\left(\frac{1}{c}\partial_t-c\partial_\theta\right), \quad \widehat{D_1}=x\partial_x+\left(ct+\frac{1}{c}\theta\right)\left(\frac{1}{c}\partial_t+c\partial_\theta\right), \tag{20}$$

$$\widehat{D_2}=x\partial_x+\left(ct-\frac{1}{c}\theta\right)\left(\frac{1}{c}\partial_t-c\partial_\theta\right).$$

As in the previous case, the commutation relations between the generators (20) are identical to those relations given in Table I.

Finally, we note that, for the Chaplygin equations, there exists an infinite number of preserved quantities[1]

$$I_n^{\pm}=\int dx\rho\left(\theta_x\pm\frac{\sqrt{2\lambda}}{\rho}\right)^n. \tag{21}$$

Consequently, we can use the transformations (16) and (19) to derive the corresponding quantities of the Born–Infeld equations

$$J_n^{\pm}=\sqrt{2\lambda}\int dx((\theta_x)^2-\theta_t)^{-1/2}\left(-\theta_x\pm\frac{1}{\sqrt{2}}((\theta_x)^2-\theta_t)^{1/2}\right)^n. \tag{22}$$

This suggests that both models are completely integrable.

B. Classification of the two-dimensional subalgebras

Here, we summarize the results obtained from the classification of the two-dimensional subalgebras of L, the Lie algebra of the Chaplygin Eqs. (7a) and (7b). This result can be extended to include the Born–Infeld equations through the reparametrizations (16) and (19). We focus exclusively on two-dimensional subalgebras because its symmetry reduction leads us mainly to solve ODEs. In order to classify the subalgebras, we can decompose the structure of L into the following solvable semidirect sum

$$L=\{\{D_1,D_2\}\supset\{B\}\} \quad \supset \quad \{Z,P_1,P_0\}. \tag{23}$$

We perform the classification in three steps, using the procedures described in Ref. 13. The full details are presented in Ref. 14.

(i) Consider first the abelian algebra $A=\{D_1,D_2\}$. Its subspaces are

$$A_1=\{0\},\quad A_2=\{D_1\},\quad A_3=\{D_2\},\quad A_4=\{D_1+aD_2,a\neq 0\},$$
$$A_5=\{D_1,D_2\}. \tag{24}$$

Since A is an abelian algebra, all of its subspaces are subalgebras, and each of them is conjugate only to itself under action by the group

$$G_A=\mathbf{e}^{\{D_1,D_2\}}=\{g=e^{\lambda Y}\ :\ Y\in\{D_1,D_2\}\}, \tag{25}$$

generated by A. For each subalgebra A_i of A, its normalizer in G_A

$$Nor(A_i,G_A)=\{g\in G_A\ :\ gXg^{-1}\in A_i,\forall X\in A_i\}, \tag{26}$$

is simply G_A.

(ii) As a next step, let us now consider the algebra

$$F=\{D_1,D_2,B\}=\{\{D_1,D_2\}\supset\{B\}\}=A\supset B. \tag{27}$$

The splitting subalgebras of F are

$$F_1=\{0\},\quad F_2=\{B\},\quad F_3=\{D_1\},\quad F_4=\{D_1,B\},$$
$$F_5=\{D_2\},\quad F_6=\{D_2,B\},\quad F_7=\{D_1+aD_2,a\neq 0\}, \tag{28}$$
$$F_8=\{D_1+aD_2,B\}_{a\neq 0},\quad F_9=\{D_1,D_2\},\quad F_{10}=\{D_1,D_2,B\}=F.$$

In addition, by considering the case of F_7 where $a=1$, we obtain the following nonsplitting subalgebra of F

$$F_{11}=\{D_1+D_2+\varepsilon B,\varepsilon=\pm 1\}. \tag{29}$$

The normalizers of these subalgebras in the group $G_F=\mathbf{e}^{\{D_1,D_2,B\}}$ are presented in Table II.

(iii) Finally, the complete Lie algebra L can be decomposed as a semidirect sum of the previouly considered algebra F and the abelian algebra N:

$$L=\{D_1,D_2,B,Z,P_1,P_0\}=F\supset N, \tag{30}$$

where $F=\{D_1,D_2,B\}$, and $N=\{Z,P_1,P_0\}$ is abelian. The two-dimensional splitting and nonsplitting subalgebras of L are summarized in Tables III and IV, respectively.

The usefulness of the classification is demonstrated in the fact that it allows us to find all corresponding reductions of the Chaplygin equations under the classified nonequivalent two-dimensional subalgebras of the symmetry algebra L. For each conjugacy class given in Tables III

TABLE II. Classes of subalgebras of $F=\{D_1,D_2,B\}$.

Subalgebra $F_i\subseteq F$	$Nor\,(F_i,G_F)$
$F_1=\{0\}$	G_F
$F_2=\{B\}$	G_F
$F_3=\{D_1\}$	$\mathbf{e}^{\{D_1,D_2\}}$
$F_4=\{D_1,B\}$	G_F
$F_5=\{D_2\}$	$\mathbf{e}^{\{D_1,D_2\}}$
$F_6=\{D_2,B\}$	G_F
$F_7=\{D_1+aD_2,a\neq 0\}$	$\begin{cases} G_F & \text{if } a=1,\\ \mathbf{e}^{\{D_1,D_2\}} & \text{if } a\neq 1 \end{cases}$
$F_8=\{D_1+aD_2,B\}_{a\neq 0}$	G_F
$F_9=\{D_1,D_2\}$	$\mathbf{e}^{\{D_1,D_2\}}$
$F_{10}=\{D_1,D_2,B\}$	G_F
$F_{11}=\{D_1+D_2+\varepsilon B,\varepsilon=\pm 1\}$	$\mathbf{e}^{\{D_1+D_2,B\}}$

and IV, we evaluate the invariants of the corresponding Lie subgroup, and also the corresponding reduced differential equations. We summarize the results in Tables V, and VI. Solutions of these equations will be analyzed in detail in Sec. IV.

III. PARTIALLY INVARIANT SOLUTIONS OF A SYSTEM OF PDEs

The concept of partially invariant solutions originates from the work of Ovsiannikov[15] and since then has been extensively developed by many authors (see, e.g., Refs. 16–22). These types of solutions can be understood as an extension of the group invariant solutions. In the case of

TABLE III. Classes of two-dimensional splitting algebras of L.

Splitting algebra $L_{i,\alpha}$	$Nor\,(L_{i,\alpha},G)$
$L_{1,6}=\{Z,P_1\}$	G
$L_{1,7}=\{Z,P_0\}$	$\mathbf{e}^{\{D_1,D_2,Z,P_1,P_0\}}$
$L_{1,8}=\{P_1,P_0\}$	$\mathbf{e}^{\{D_1,D_2,Z,P_1,P_0\}}$
$L_{1,9}=\{P_1,P_0+\varepsilon Z\}_{\varepsilon=\pm 1}$	$\mathbf{e}^{\{D_1+D_2,Z,P_1,P_0\}}$
$L_{2,2}=\{B,Z\}$	$\mathbf{e}^{\{D_1,D_2,B,Z,P_1\}}$
$L_{3,2}=\{D_1,Z\}$	$\mathbf{e}^{\{D_1,D_2,Z\}}$
$L_{3,3}=\{D_1,P_1\}$	$\mathbf{e}^{\{D_1,D_2,Z,P_1\}}$
$L_{3,4}=\{D_1,P_0\}$	$\mathbf{e}^{\{D_1,D_2,Z,P_0\}}$
$L_{4,1}=\{D_1,B\}$	$\mathbf{e}^{\{D_1,D_2,B,Z\}}$
$L_{5,2}=\{D_2,Z\}$	$\mathbf{e}^{\{D_1,D_2,Z,P_0\}}$
$L_{5,3}=\{D_2,P_1\}$	$\mathbf{e}^{\{D_1,D_2,P_1,P_0\}}$
$L_{5,4}=\{D_2,P_0\}$	$\mathbf{e}^{\{D_1,D_2,P_0\}}$
$L_{6,1}=\{D_2,B\}$	$\mathbf{e}^{\{D_1,D_2,B\}}$
$L_{7,2(a=1)}=\{D_1+D_2,Z\}$	$\mathbf{e}^{\{D_1,D_2,B,Z\}}$
$L_{7,3(a=1)}=\{D_1+D_2,P_1\}$	$\mathbf{e}^{\{D_1,D_2,P_1\}}$
$L_{7,4(a=1)}=\{D_1+D_2,P_0\}$	$\mathbf{e}^{\{D_1,D_2,P_0\}}$
$L_{7,5(a=1)}=\{D_1+D_2,P_0+\varepsilon Z\}_{\varepsilon=\pm 1}$	$\mathbf{e}^{\{D_1+D_2,P_0+\varepsilon Z\}}$
$L_{7,2(a\neq 1)}=\{D_1+aD_2,Z\}_{a\neq 0,1}$	$\begin{cases} \mathbf{e}^{\{D_1,D_2,Z,P_1\}} & \text{if } a=-1,\\ \mathbf{e}^{\{D_1,D_2,Z\}} & \text{if } a\neq -1 \end{cases}$
$L_{7,3(a\neq 1)}=\{D_1+aD_2,P_1\}_{a\neq 0,1}$	$\mathbf{e}^{\{D_1,D_2,P_1\}}$
$L_{7,4(a\neq 1)}=\{D_1+aD_2,P_0\}_{a\neq 0,1}$	$\begin{cases} \mathbf{e}^{\{D_1,D_2,P_1,P_0\}} & \text{if } a=-1,\\ \mathbf{e}^{\{D_1,D_2,P_0\}} & \text{if } a\neq -1 \end{cases}$
$L_{8,1}=\{D_1+aD_2,B\}_{a\neq 0}$	$\mathbf{e}^{\{D_1,D_2,B\}}$
$L_{9,1}=\{D_1,D_2\}$	$\mathbf{e}^{\{D_1,D_2\}}$
$L_{11,2}=\{D_1+D_2+\varepsilon B,Z\}_{\varepsilon=\pm 1}$	$\mathbf{e}^{\{D_1+D_2,B,Z\}}$

TABLE IV. Classes of two-dimensional nonsplitting algebras of L.

Splitting algebra $\mathcal{L}_{i,\alpha}$	$Nor\,(\mathcal{L}_{i,\alpha},G)$
$\mathcal{L}_{2,2}=\{B+\varepsilon P_0,Z\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_1+3D_2,B+\varepsilon P_0,Z,P_1\}}$
$\mathcal{L}_{3,3}=\{D_1+\varepsilon Z,P_1\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_1,Z,P_1\}}$
$\mathcal{L}_{3,4}=\{D_1+\varepsilon Z,P_0\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_1,Z,P_0\}}$
$\mathcal{L}_{4,1}=\{D_1+\varepsilon Z,B\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_1,B,Z\}}$
$\mathcal{L}_{5,2}=\{D_2+\varepsilon P_0,Z\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_2,Z,P_0\}}$
$\mathcal{L}_{5,3}=\{D_2+\varepsilon P_0,P_1\}_{\varepsilon=\pm1}$	$\mathbf{e}^{\{D_2,P_1,P_0\}}$
$\mathcal{L}_{7,2(a\neq1)}=\{D_1-D_2+\varepsilon P_1,Z\}_{a\neq0,1\ \varepsilon=\pm1}$	$\mathbf{e}^{\{D_1-D_2,Z,P_1\}}$
$\mathcal{L}_{7,4(a\neq1)}=\{D_1-D_2+\varepsilon P_1,P_0\}_{a\neq0,1\ \varepsilon=\pm1}$	$\mathbf{e}^{\{D_1-D_2,P_1,P_0\}}$
$\mathcal{L}_{8,1}=\{D_1+3D_2,B+\varepsilon P_0\}_{a\neq0\ \varepsilon=\pm1}$	$\mathbf{e}^{\{D_1+3D_2,B+\varepsilon P_0\}}$

partially invariant solutions, the graph of the solution Γ_f is no longer a G-invariant set (i.e., $G(\Gamma_f)\neq\Gamma_f$) but the difference between the dimensions of the manifolds $G(\Gamma_f)$ and Γ_f has to satisfy the condition

$$0<\delta=\dim G(\Gamma_f)-\dim\Gamma_f<\min(s,q), \tag{31}$$

where δ is called the defect structure of a solution with respect to the group G. Here, we assume that the transformed graph Γ_f under the action of G has a submanifold structure. We denote by s the dimension of the orbit of G and by q the number of dependent variables appearing in the considered system of m PDEs in p independent variables

$$\Delta^l(x,u^{(k)})=0,\quad l=1,\ldots,m. \tag{32}$$

For the computational purpose of constructing partially invariant solutions, it is convenient to evaluate the defect structure δ of a solution of system (32) based on the $q\times s$ characteristic matrix

$$Q_k^\alpha(x,u^{(1)})=\left(\phi_k^\alpha(x,u)-\xi_k^i(x,u)\frac{\partial u^\alpha}{\partial x^i}\right),\quad \alpha=1,\ldots,q,\quad k=1,\ldots,s, \tag{33}$$

of the infinitesimal symmetry generators

$$v_k=\xi_k^i(x,u)\partial_{x^i}+\phi_k^\alpha(x,u)\partial_{u^\alpha},\quad k=1,\ldots,s, \tag{34}$$

of s-dimensional subgroup G_0. We will assume throughout the rest of this article that each subgroup G_0 acts regularly and transversally on the space of independent and dependent variables $M=X\times U$. That is, the rank condition

$$\operatorname{rank}\{\xi_a^i(x,u)\}=\operatorname{rank}\{\xi_a^i(x,u),\phi_a^\alpha(x,u)\}=s, \tag{35}$$

is satisfied.[19] According to Ref. 20, the function $u=f(x)$ is a partially invariant solution of system (32) with defect δ if and only if

$$\operatorname{rank}Q(x,u^{(1)})=\delta. \tag{36}$$

Now, we present the algorithm for constructing partially invariant solutions with defect structure δ. The procedure involves the following steps:

(1) Construct a complete set of functionally independent invariants for a subgroup G_i of G. If the set $\{v_1,\ldots,v_r\}$ is a basis of fiber preserving infinitesimal generators of the Lie algebra $L_i=\exp(G_i)$, where

$$v_b=\xi_b^i(x)\partial_{x^i}+\phi_b^\alpha(x,u)\partial_{u^\alpha},\quad b=1,\ldots,r, \tag{37}$$

then I is an invariant of G_i if and only if $v_b(I)=0$ for all $b=1,\ldots,r$. We obtain a set of

TABLE V. Invariants of the two-dimensional subalgebras of L.

Subalgebra	Invariants	Relations and change of variable
$L_{1,6}$	$t,\ \rho$	$\rho=\rho(t)$
$L_{1,7}$	$x,\ \rho$	$\rho=\rho(x)$
$L_{1,8}$	$\theta,\ \rho$	$\theta=F(\rho)$
$L_{1,9}$	$\rho,\ \theta-\varepsilon t$	$\theta=F(\rho)+\varepsilon t$
$L_{2,2}$	$t,\ \rho$	$\rho=\rho(t)$
$L_{3,2}$	$\frac{x^2}{t},\frac{\rho}{x}$	$\rho=\sqrt{\xi}\eta F(\xi),\ \theta=\theta(\xi,\eta),\ \xi=\frac{x^2}{t},\eta=t$
$L_{3,3}$	$\theta\ \frac{\rho}{\sqrt{t}}$	$\theta=F\left(\frac{\rho}{\sqrt{t}}\right)$
$L_{3,4}$	$\theta,\frac{\rho}{x}$	$\theta=F\left(\frac{\rho}{x}\right)$
$L_{4,1}$	$\frac{\rho}{\sqrt{t}},\theta-\frac{x^2}{2t}$	$\theta=F\left(\frac{\rho}{\sqrt{t}}\right)+\frac{x^2}{2t}$
$L_{5,2}$	$t,x\rho$	$\rho=\frac{1}{x}F(t)$
$L_{5,3}$	$t,\rho^2\theta$	$\theta=\frac{F(t)}{\rho^2}$
$L_{5,4}$	$\frac{\theta}{x^2},x\rho$	$\theta=x^2F(x\rho)$
$L_{6,1}$	$t,\rho^2\left(\theta-\frac{x^2}{2t}\right)$	$\theta=\frac{F(t)}{\rho^2}+\frac{x^2}{2t}$
$L_{7,2(a=1)}$	$\frac{x}{t},\rho$	$\rho=\rho(\xi),\ \theta=\theta(\xi,\eta),\ \xi=\frac{x}{t},\eta=t$
$L_{7,3(a=1)}$	$\rho,\frac{\theta}{t}$	$\theta=tF(\rho)$
$L_{7,4(a=1)}$	$\rho,\frac{\theta}{x}$	$\theta=xF(\rho)$
$L_{7,5(a=1)}$	$\rho,\frac{1}{x}(\theta-\varepsilon t)$	$\theta=xF(\rho)+\varepsilon t$
$L_{7,2(a\neq1)}$	$\frac{t^{1+a}}{x^2},\frac{t^{1-a}}{\rho^2}$	$\rho=t^{1-a/2}F(\xi),\theta=\theta(\xi,\eta),\ \xi=\frac{t^{1+a}}{x^2},\eta=t$
$L_{7,3(a\neq1)}$	$t^{(a-1)/2}\rho,\ t^{-a}\theta$	$\theta=t^aF(t^{(a-1)/2}\rho)$
$L_{7,4(a=-1)}$	$x,\theta\rho$	$\theta=\frac{F(x)}{\rho}$
$L_{7,4(a\neq1,-1)}$	$x^{(a-1)/(a+1)}\rho,x^{-2a/(a+1)}\theta$	$\theta=x^{2a/(a+1)}F(x^{(a-1)/(a+1)}\rho)$
$L_{8,1}$	$t^{(a-1)/2}\rho,t^{-a}\left(\theta-\frac{x^2}{2t}\right)$	$\theta=t^aF(t^{(a-1)/2}\rho)+\frac{x^2}{2t}$
$L_{9,1}$	$\frac{\theta t}{x^2},\frac{\rho x}{t}$	$\theta=\frac{x^2}{t}F\left(\frac{x}{t}\rho\right)$
$L_{11,2}$	$\frac{2x}{t}-\varepsilon\ln t,\rho$	$\rho=\rho(\xi),\ \theta=\theta(\xi,\eta),\ \xi=\frac{2x}{t}-\varepsilon\ln t,\eta=t$
$\mathcal{L}_{2,2}$	$\varepsilon x-\frac{1}{2}t^2,\ \rho$	$\rho=\rho(\xi),\ \theta=\theta(\xi,\eta),\ \xi=\varepsilon x-\frac{1}{2}t^2,\eta=t$
$\mathcal{L}_{3,3}$	$\frac{\rho^2}{t},\theta-\frac{1}{2}\varepsilon\ln t$	$\theta=F\left(\frac{\rho^2}{t}\right)+\frac{1}{2}\varepsilon\ln t$
$\mathcal{L}_{3,4}$	$\frac{\rho}{x},\theta-\varepsilon\ln x$	$\theta=F\left(\frac{\rho}{x}\right)+\varepsilon\ln x$
$\mathcal{L}_{4,1}$	$\frac{\rho}{\sqrt{t}},\theta-\frac{x^2}{2t}-\frac{1}{2}\varepsilon\ln t$	$\theta=F\left(\frac{\rho}{\sqrt{t}}\right)+\frac{x^2}{2t}+\frac{1}{2}\varepsilon\ln t$
$\mathcal{L}_{5,2}$	$x\mathbf{e}^{-\varepsilon t},x\rho$	$\rho=\frac{\eta}{\xi}F(\xi),\theta=\theta(\xi,\eta),\ \xi=x\mathbf{e}^{-\varepsilon t},\ \eta=\mathbf{e}^{-\varepsilon t}$
$\mathcal{L}_{5,3}$	$\mathbf{e}^{-2\varepsilon t}\theta,\mathbf{e}^{\varepsilon t}\rho$	$\theta=\mathbf{e}^{2\varepsilon t}F(\mathbf{e}^{\varepsilon t}\rho)$
$\mathcal{L}_{7,2(a\neq1)}$	$x-\frac{1}{2}\varepsilon\ln t,\frac{\rho}{t}$	$\rho=\eta F(\xi),\ \theta=\theta(\xi,\eta),\ \xi=x-\frac{1}{2}\varepsilon\ln t,\eta=t$
$\mathcal{L}_{7,4(a\neq1)}$	$\mathbf{e}^{2\varepsilon x}\theta,\mathbf{e}^{-2\varepsilon x}\rho$	$\theta=\mathbf{e}^{-2\varepsilon x}F(\mathbf{e}^{-2\varepsilon x}\rho)$
$\mathcal{L}_{8,1}$	$\rho(\varepsilon x-\frac{1}{2}t^2)^{1/2},(\theta-\varepsilon xt+\frac{1}{3}t^3)(\varepsilon x-\frac{1}{2}t^2)^{-3/2}$	$\theta=(\varepsilon x-\frac{1}{2}t^2)^{3/2}F((\varepsilon x-\frac{1}{2}t^2)^{1/2}\rho)+\varepsilon xt-\frac{1}{3}t^3$

TABLE VI. Reduced equations obtained from the two-dimensional subalgebras of L. Splitting subalgebras are denoted by $L_{i,\alpha}$ and nonsplitting subalgebras by $\mathcal{L}_{i,\alpha}$.

Subalgebra	Reduced equation(s)
$L_{1,6}$	$-\theta_{tt}-\theta_x\theta_{xt}+2\theta_t\theta_{xx}+(\theta_x)^2\theta_{xx}=0,\ \theta_{xt}+\theta_x\theta_{xx}=0,\ \rho(t)=\sqrt{\lambda}(\theta_t+\frac{1}{2}(\theta_x)^2)^{-1/2}$
$L_{1,7}$	$2\theta_t\theta_{xx}-\theta_x\theta_{xt}=0,\ \theta_{tt}+\theta_x\theta_{xt}=0,\ \rho(x)=\sqrt{\lambda}(\theta_t+\frac{1}{2}(\theta_x)^2)^{-1/2}$
$L_{1,8}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\frac{\lambda}{\rho^3(F')^2}=0$
$L_{1,9}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda}{\rho^3(F')^2}-\frac{\varepsilon}{\rho(F')^2}\right)=0$
$L_{2,2}$	$-\theta_{tt}-\theta_x\theta_{xt}+2\theta_t\theta_{xx}+(\theta_x)^2\theta_{xx}=0,\ \theta_{xt}+\theta_x\theta_{xx}=0,\ \rho(t)=\sqrt{\lambda}(\theta_t+\frac{1}{2}(\theta_x)^2)^{-1/2}$
$L_{3,2}$	$8\xi\eta\theta_\eta\theta_{\xi\xi}+4\eta\theta_\xi\theta_\eta+4\xi(\theta_\xi)^2-2\xi\theta_\xi-\xi^2\theta_{\xi\xi}+\eta\theta_\eta-4\xi\eta\theta_\xi\theta_{\xi\eta}+\xi\eta\theta_{\xi\eta}=0,$ $4\xi\theta_\xi\theta_{\xi\eta}-\xi\theta_{\xi\eta}+\theta_\eta+\eta\theta_{\eta\eta}=0,$ $F(\xi)=\sqrt{\lambda}(2\xi^2(\theta_\xi)^2-\xi^2\theta_\xi+\xi\eta\theta_\eta)^{-1/2}$
$L_{3,3}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{\sqrt{t}}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t}{\rho^3(F')^2}+\frac{1}{2\sqrt{t}F'}\right)=0$
$L_{3,4}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{x}\frac{F''}{F'}\right)(\rho_x)^2-\left(\frac{2}{x}+\frac{2}{x^2}\rho\frac{F''}{F'}\right)(\rho_x)+\left(\frac{\lambda x^2}{\rho^3(F')^2}+\frac{3}{2x^2}\rho+\frac{1}{x^3}\rho^2\frac{F''}{F'}\right)=0$
$L_{4,1}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{\sqrt{t}}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t}{\rho^3(F')^2}+\frac{3}{2\sqrt{t}F'}\right)=0$
$L_{5,2}$	$x\theta_{tt}+x\theta_x\theta_{xt}-2x\theta_t\theta_{xx}-x(\theta_x)^2\theta_{xx}+2\theta_x\theta_t+(\theta_x)^3=0,$ $-2\theta_t+x\theta_{xt}-(\theta_x)^2+\frac{1}{2}x\theta_x\theta_{xx}=0, F(t)=\sqrt{\lambda}\left(\frac{1}{x^2}\theta_t+\frac{1}{2x^2}(\theta_x)^2\right)^{-1/2}$
$L_{5,3}$	$\rho_{xx}-\frac{5}{2\rho}(\rho_x)^2-\frac{1}{4}\rho^3\frac{F'}{F^2}+\frac{\lambda\rho^3}{4F^2}=0$
$L_{5,4}$	$\rho_{xx}+\left(\frac{1}{2\rho}+x\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{6}{x}+\frac{2\rho F''}{F'}\right)(\rho_x)+\left(\frac{\lambda}{x^6\rho^3(F')^2}+\frac{7}{2x^2}\rho+\frac{1}{x}\rho^2\frac{F''}{F'}-\frac{2}{x^4}\frac{F^2}{(F')^2}\frac{1}{\rho}\right)=0$
$L_{6,1}$	$\rho_{xx}-\frac{5}{2\rho}(\rho_x)^2-\frac{1}{2tF}\rho^3-\frac{F'}{4F^2}\rho^3+\frac{\lambda\rho^3}{4F^2}=0$
$L_{7,2(a=1)}$	$(2\eta^2\theta_\eta-\xi\eta\theta_\xi)\theta_{\xi\xi}+(\xi\eta-\eta^2)\theta_\xi\theta_{\xi\eta}+(\theta_\xi)^2\theta_{\xi\xi}-(\theta_\xi)^2\theta_{\xi\eta}+\eta(\theta_\xi)^2-\xi^2\eta^2\theta_{\xi\xi}$ $+\xi\eta^3\theta_{\xi\eta}-\xi\eta^2\theta_\xi=0,$ $\xi\eta\theta_\xi-\xi\eta^2\theta_{\xi\eta}+\eta^3\theta_{\eta\eta}-(\theta_\xi)^2+\eta\theta_\xi\theta_{\xi\eta}=0,$ $\rho(\xi)=\sqrt{\lambda}\left(-\frac{\xi}{\eta}\theta_\xi+\theta_\eta+\frac{1}{2\eta^2}(\theta_\xi)^2\right)^{-1/2}$
$L_{7,3(a=1)}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda}{t^2\rho^3(F')^2}-\frac{F}{t^2(F')^2\rho}\right)=0$
$L_{7,4(a=1)}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\frac{2}{x}\rho_x+\left(\frac{\lambda}{x^2\rho^3(F')^2}-\frac{F^2}{2x^2(F')^2\rho}\right)=0$
$L_{7,5(a=1)}$	$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\frac{2}{x}\rho_x+\left(\frac{2\lambda-\rho^2F^2-2\varepsilon\rho^2}{2x^2(F')^2\rho^3}\right)=0$
$L_{7,2(a\neq1)}$	$2\xi^3\eta^{-(1/2)(1+5a)}(\theta_\xi)^2-a(a+1)\xi\eta^{-(1/2)(1+3a)}\theta_\xi+4\xi^3\eta^{(1/2)(1-5a)}\theta_\eta\theta_{\xi\xi}+6\xi^2\eta^{(1/2)(1-5a)}\theta_\xi\theta_\eta$ $+\frac{1}{2}(1-a)\eta^{(1/2)(1-3a)}\theta_\eta-2\xi^3\eta^{(1/2)(1-5a)}\theta_\xi\theta_{\xi\eta}-\frac{1}{2}(a+1)^2\xi^2\eta^{-(1/2)(1+3a)}\theta_{\xi\xi}$ $-\frac{1}{2}(a+1)\xi\eta^{(1/2)(1-3a)}\theta_{\xi\eta}=0,$ $(1-a)\eta^{-a}\theta_\eta-a(a+1)\xi\eta^{-(a+1)}\theta_\xi+(a+1)\xi\eta^{-a}\theta_{\xi\eta}+\eta^{(1-a)}\theta_{\eta\eta}$ $-4a\xi^3\eta^{-(2a+1)}(\theta_\xi)^2+4\xi^3\eta^{-2a}\theta_\xi\theta_{\xi\eta}=0,$ $F(\xi)=\sqrt{\lambda}((a+1)\xi\eta^{-a}\theta_\xi+\eta^{(1-a)}\theta_\eta+2\xi^3\eta^{-2a}(\theta_\xi)^2)^{-1/2}$
$L_{7,3(a\neq1)}$	$\rho_{xx}+\left(\frac{1}{2\rho}+t^{(a-1)/2}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t^{(1-3a)}}{\rho^3(F')^2}-\frac{at^{-2a}F}{(F')^2\rho}+\frac{(1-a)}{2}\frac{t^{-(1/2)(1+3a)}}{F'}\right)=0$
$L_{7,4(a=-1)}$	$\rho_{xx}-\frac{3}{2\rho}(\rho_x)^2+\frac{2F'}{F}\rho_x+\left(\frac{\lambda\rho}{F^2}-\frac{(F')^2\rho}{2F^2}-\frac{F''}{F}\rho\right)=0$

TABLE VI. (*Continued.*)

Subalgebra	Reduced equation(s)
$L_{7,4(a\neq 1,-1)}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+x^{(a-1)/(a+1)}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{(6a-2)}{(a+1)}x^{-1}+\frac{(2a-2)}{(a+1)}x^{-2/(a+1)}\frac{F''}{F'}\rho\right)(\rho_x)$$ $$+\left(\frac{\lambda x^{(2-6a)/(a+1)}}{\rho^3(F')^2}-\frac{(2a)^2}{2(a+1)^2}x^{-4a/(a+1)}\frac{F^2}{(F')^2\rho}\right.$$ $$\left.+\frac{(a-1)^2}{(a+1)^2}x^{-(a+3)/(a+1)}\frac{F''}{F'}\rho^2+\frac{(7a-3)(a-1)}{2(a+1)^2}x^{-2}\rho\right)=0$$
$L_{8,1}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+t^{(a-1)/2}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t^{(1-3a)}}{\rho^3(F')^2}-\frac{(a-3)}{2}t^{-(3a+1)/2}\frac{1}{F'}-at^{-2a}\frac{F}{(F')^2\rho}\right)=0$$
$L_{9,1}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{x}{t}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{6}{x}+\frac{2}{t}\frac{F''}{F'}\rho\right)(\rho_x)$$ $$+\left(\frac{\lambda t^4}{x^6(F')^2\rho^3}+\frac{t^2(F-2F^2)}{x^4(F')^2\rho}+\frac{t}{x^3F'}+\frac{1}{xt}\frac{F''}{F'}\rho^2+\frac{7}{2x^2}\rho\right)=0$$
$L_{11,2}$	$$4\theta_\eta\theta_{\xi\xi}-2\theta_\xi\theta_{\xi\eta}+\frac{2}{\eta}(\theta_\xi)^2+\frac{1}{2}(\xi+\varepsilon+\varepsilon\ln\eta)(\eta\theta_{\xi\eta}-\theta_\xi)-\frac{1}{2}(\xi+\varepsilon+\varepsilon\ln\eta)^2\theta_{\xi\xi}=0,$$ $$\theta_{\eta\eta}+(\xi+\varepsilon+\varepsilon\ln\eta)\left(\frac{1}{\eta^2}\theta_\xi-\frac{1}{\eta}\theta_{\xi\eta}\right)-\frac{\varepsilon}{\eta^2}\theta_\xi-\frac{4}{\eta^3}(\theta_\xi)^2+\frac{4}{\eta^2}\theta_\xi\theta_{\xi\eta}=0,$$ $$\rho(\xi)=\sqrt{\lambda}\left(\theta_\eta-\frac{1}{\eta}(\xi+\varepsilon+\varepsilon\ln\eta)\theta_\xi+\frac{2}{\eta^2}(\theta_\xi)^2\right)^{-1/2}$$
$\mathcal{L}_{2,2}$	$$2\theta_\eta\theta_{\xi\xi}+\eta\theta_{\xi\eta}-\eta^2\theta_{\xi\xi}-\theta_\xi\theta_{\xi\eta}=0,$$ $$\theta_{\eta\eta}-\theta_\xi-\eta\theta_{\xi\eta}+\theta_\xi\theta_{\xi\eta}=0,$$ $$\rho(\xi)=\sqrt{\lambda}\left(\theta_\eta-\eta\theta_\xi+\frac{1}{2}(\theta_\xi)^2\right)^{-1/2}$$
$\mathcal{L}_{3,3}$	$$\rho_{xx}+\left(\frac{3}{2\rho}+\frac{2\rho}{t}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t^2}{4\rho^5(F')^2}+\frac{1}{4\rho F'}-\frac{\varepsilon t}{8\rho^3(F')^2}\right)=0$$
$\mathcal{L}_{3,4}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{x}\frac{F''}{F'}\right)(\rho_x)^2-\left(\frac{2}{x}+\frac{2\rho}{x^2}\frac{F''}{F'}\right)(\rho_x)+\left(\frac{\lambda x^2}{\rho^3(F')^2}+\frac{3\rho}{2x^2}+\frac{\rho^2}{x^3}\frac{F''}{F'}-\frac{1}{2\rho(F')^2}\right)=0$$
$\mathcal{L}_{4,1}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{\sqrt{t}}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda t}{\rho^3(F')^2}+\frac{3}{2\sqrt{t}F'}-\frac{\varepsilon}{2\rho(F')^2}\right)=0$$
$\mathcal{L}_{5,2}$	$$2\varepsilon\eta^3\theta_\eta\theta_{\xi\xi}-\varepsilon\eta^3\theta_\xi\theta_{\xi\eta}-\xi\theta_\xi+\xi^2\theta_{\xi\xi}-2\eta\theta_\eta+\xi\eta\theta_{\xi\eta}=0,$$ $$2\xi\theta_\xi+\xi\eta\theta_{\xi\eta}+3\eta\theta_\eta+\eta^2\theta_{\eta\eta}-2\varepsilon\eta^2(\theta_\xi)^2-\varepsilon\eta^3\theta_\xi\theta_{\xi\eta}=0,$$ $$F(\xi)=\sqrt{\lambda}\left(-\frac{\varepsilon\eta^2}{\xi}\theta_\xi-\frac{\varepsilon\eta^3}{\xi^2}\theta_\eta+\frac{1}{2}\frac{\eta^4}{\xi^2}(\theta_\xi)^2\right)^{-1/2}$$
$\mathcal{L}_{5,3}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\mathbf{e}^{\varepsilon t}\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda}{\mathbf{e}^{6\varepsilon t}\rho^3(F')^2}-\frac{\varepsilon}{\mathbf{e}^{3\varepsilon t}F'}-\frac{2\varepsilon F}{\mathbf{e}^{4\varepsilon t}\rho(F')^2}\right)=0$$
$\mathcal{L}_{7,2(a\neq 1)}$	$$-4\varepsilon\eta\theta_\xi+8\eta^2\theta_\eta+4\eta^2(\theta_\xi)^2+8\eta^3\theta_\eta\theta_{\xi\xi}-\eta\theta_{\xi\xi}+2\varepsilon\eta^2\theta_{\xi\eta}-4\eta^3\theta_\xi\theta_{\xi\eta}=0,$$ $$-\varepsilon\theta_\xi-\varepsilon\eta\theta_{\xi\eta}+4\eta\theta_\eta+2\eta^2\theta_{\eta\eta}+2\eta(\theta_\xi)^2+2\eta^2\theta_\xi\theta_{\xi\eta}=0,$$ $$F(\xi)=\sqrt{\lambda}\left(-\frac{\varepsilon\eta}{2}\theta_\xi+\eta^2\theta_\eta+\frac{1}{2}\eta^2(\theta_\xi)^2\right)^{-1/2}$$
$\mathcal{L}_{7,4(a\neq 1)}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\mathbf{e}^{-2\varepsilon x}\frac{F''}{F'}\right)(\rho_x)^2-(8\varepsilon+4\varepsilon\mathbf{e}^{-2\varepsilon x}F''/F'\rho)(\rho_x)$$ $$+\left(\frac{\lambda\mathbf{e}^{8\varepsilon x}}{\rho^3(F')^2}+10\rho+4\mathbf{e}^{-2\varepsilon x}\frac{F''}{F'}\rho^2-\frac{2\mathbf{e}^{4\varepsilon x}F^2}{\rho(F')^2}\right)=0$$
$\mathcal{L}_{8,1}$	$$\rho_{xx}+\left(\frac{1}{2\rho}+\left(\varepsilon x-\frac{1}{2}t^2\right)^{1/2}\frac{F''}{F'}\right)(\rho_x)^2+\left(4\varepsilon\left(\varepsilon x-\frac{1}{2}t^2\right)^{-1}+\varepsilon\left(\varepsilon x-\frac{1}{2}t^2\right)^{-1/2}\frac{F''}{F'}\rho\right)(\rho_x)$$ $$+\left(\frac{\lambda}{\left(\varepsilon x-\frac{1}{2}t^2\right)^4\rho^3(F')^2}+\frac{9}{8}\left(\varepsilon x-\frac{1}{2}t^2\right)^{-2}\rho+\frac{1}{4}\left(\varepsilon x-\frac{1}{2}t^2\right)^{-3/2}\frac{F''}{F'}\rho^2\right)$$ $$-\left(\left(\varepsilon x-\frac{1}{2}t^2\right)^{-3}\frac{1}{(F')^2\rho}+\frac{9}{8}\left(\varepsilon x-\frac{1}{2}t^2\right)^{-3}\frac{F^2}{(F')^2\rho}\right)=0$$

functionally independent invariants of the form

$$\{\eta^k(x), I^j(x,u)\}, \tag{38}$$

where $k=1,\ldots,p+\delta-s$ and $j=1,\ldots,q-\delta$. Then the rank of the Jacobian matrix J is given by

$$\operatorname{rank}(J)=\operatorname{rank}\left(\frac{\partial(I^1(x,u),\ldots,I^{q-\delta}(x,u))}{\partial(u^1,\ldots,u^q)}\right)=q-\delta. \tag{39}$$

(2) Express the $(p+\delta)$-dimensional manifold $G_i\Gamma_f$ in terms of the invariants (38). Note that $G_i\Gamma_f$ is the smallest invariant manifold containing Γ_f, with respect to the action of the group G_i. This manifold is determined by equations of the form

$$I^j(x,u)=f^j(\eta^1(x),\ldots,\eta^{p+\delta-s}(x)), \quad j=1,\ldots,q-\delta. \tag{40}$$

where f^j are arbitrary functions of their arguments.

(3) From Eq. (39) and by applying the implicit function theorem to Eq. (40), we can express $(q-\delta)$ dependent variables u^a as functions of $l\leqslant p$ independent variables x^i, of $(q-\delta)$ arbitrary functions ψ^a and of δ remaining dependent variables u^j

$$u^a=\psi^a(f^j(\eta^1(x),\ldots,\eta^{p+\delta-s}(x)),x^l,u^i), \quad a=1,\ldots,q-\delta. \tag{41}$$

(4) Substitute these $(q-\delta)$ dependent variables u^a into the original system of equations (32) and reduce the problem to a differential system of equations (so called system Δ') for δ dependent variables.

(5) Find leading derivatives among the δ dependent variables and next compute all possible compatibility conditions (modulo these leading derivatives). These conditions imply some constraints on arbitrary functions ψ^a (appearing in (41)) which form differential equations (so called system Δ/G_i) involving $(q-\delta)$ dependent variables u^a and $p+\delta-r$ independent variables.

(6) Solve the system Δ/G_i.

(7) From each solution of Δ/G_i integrate the initial system Δ. This procedure generates different classes of partially invariant solutions with given defect δ to the basic system Δ.

There is no longer a one-to-one correspondence between partially invariant solutions of the initial system Δ and solutions of the system Δ/G_i. For any solution of the system Δ/G_i we obtain, using the above procedure, a family of solutions of the original system Δ.

Note that once these computations are completed, we could check whether the obtained solutions are invariant with respect to some subgroups of the symmetry group G. A partially invariant solution $u=f(x)$, with respect to a subgroup G_i is called reducible with respect to the full group G if

(i) There exists a subgroup $G_a\subset G$ for which $u=f(x)$ is G_a-invariant, and

(ii) The dimension of the orbit of the graph Γ_f under action by G_a satisfies the inequality

$$s_1=\dim(G_a\Gamma_f)\geqslant s-\delta. \tag{42}$$

We are interested in the case of reducible partially invariant solutions, since reducible solutions can be computed from reduced systems involving $p-s_1$ independent variables, where $p-s_1\leqslant p+\delta-s$. Therefore, these reduced systems are easier to solve than the systems Δ/G_i and Δ' which we have to solve to obtain partially invariant solutions.

In order to check whether a partially invariant solution is reducible under any subalgebra of the full symmetry algebra L, one can examine the kernal K of the characteristic matrix Q of L. If a nonzero subspace of K can be generated by constant vectors, then the solution will be invariant with respect to the subalgebra identified by these vectors. In the case of the Chaplygin Eqs. (7a) and (7b), the characteristic matrix Q is

$$Q=\begin{pmatrix} -\theta_x & -\theta_t & 1 & (x-t\theta_x) & (-x\theta_x-2t\theta_t) & (2\theta-x\theta_x) \\ -\rho_x & -\rho_t & 0 & (-t\rho_x) & (\rho-x\rho_x-2t\rho_t) & (-\rho-x\rho_x) \end{pmatrix}. \tag{43}$$

Here, each constant vector $\mathbf{a}=(a_1,\ldots,a_6)$ in the kernal K corresponds to reducibility by the subalgebra

$$\mathcal{S}=\{a_1P_1+a_2P_0+a_3Z+a_4B+a_5D_1+a_6D_2\}. \tag{44}$$

In the nonreducible case, the only constant vector in the kernal K is the zero vector $\mathbf{a}=0$.

IV. PARTIALLY INVARIANT SOLUTIONS OF THE CHAPLYGIN AND BORN–INFELD EQUATIONS

In this section, we discuss the reduced PDEs and ODEs obtained in Table VI, providing partially invariant solutions of the Chaplygin Eqs. (7a) and (7b) and Born–Infeld Eqs. (11a) and (11b) where it is possible. All of these solutions have the defect $\delta=1$ and are computed from two-dimensional symmetry subalgebras of the algebra L. Here, we operate under the hypothesis that the subgroups $G_i\subset G$ are acting regularly and transversally with two-dimensional orbits. We identify the following five types of solutions.

A. Static solutions

Let us discuss some classes of static (time-independent) solutions of the Chaplygin Eqs. (7a) and (7b) which can be obtained directly from PDEs and ODEs associated to the subalgebras listed in Table VI. We discuss the results obtained individually for each subalgebra.

For the subalgebra $L_{1,8}$, the differential equation to be solved is

$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\frac{\lambda}{\rho^3(F')^2}=0, \tag{45}$$

where F is some function of ρ. We may solve this equation as an ordinary differential equation for ρ in terms of x, provided that we remember to set all constants of integration to be functions of t. We compare Eq. (45) to equation C 6.54 in Ref. 23

$$y''+f(y)y'^2+g(y)y'+h(y)=0. \tag{46}$$

Here, we identify the following functions: $f(y)=1/2y+F''/F'$, $g(y)=0$, and $h(y)=\lambda/y^3(F')^2$. We introduce the quantity $p(y)=y'(x)$, so that Eq. (46) becomes

$$pp'+\left(\frac{1}{2y}+\frac{F''}{F'}\right)p^2+\frac{\lambda}{y^3(F')^2}=0. \tag{47}$$

Setting $q=p^2$, we transform the equation again to

$$\frac{1}{2}q'+\left(\frac{1}{2y}+\frac{F''}{F'}\right)q+\frac{\lambda}{y^3(F')^2}=0. \tag{48}$$

The general solution of Eq. (48) is given by the following quadrature:

$$q(y)=\frac{1}{y}\mathbf{e}^{-2\int F''/F'\,dy}\left[K_0-2\lambda\int\frac{1}{y^2(F')^2}\mathbf{e}^{2\int F''/F'\,dy}dy\right]. \tag{49}$$

Thus, since $y'=q(y)^{1/2}$, the solution $y=y(x)$ is found implicitly through the following relation

$$\int\frac{dy}{q(y)^{1/2}}=x+c_0, \tag{50}$$

so that $\rho(x,t)$ is found by setting the constants of $y(x)$ to be functions of t, and θ is found by setting $\theta=F(\rho)$. This method can be used in general for all differential equations of the form

$$\rho_{xx}+f(\rho)(\rho_x)^2+g(\rho)=0, \tag{51}$$

which include the reduced equations corresponding to the splitting subalgebras $L_{1,9}$, $L_{3,3}$, $L_{4,1}$, $L_{5,3}$, $L_{6,1}$, $L_{7,3}$ (for all values of a), $L_{8,1}$, and the nonsplitting subalgebras $\mathcal{L}_{3,3}$, $\mathcal{L}_{4,1}$, $\mathcal{L}_{5,3}$.

To find a particular solution of Eq. (45), we set the condition $1/2\rho+F''F'=0$, so that $F(\rho)=2K_0\rho^{1/2}+K_1$. Having fixed the function $F(\rho)$, Eq. (45) reduces to

$$\rho_{xx}+\frac{\lambda}{K_0^2\rho^2}=0, \tag{52}$$

which yields the explicit solution

$$\theta(x,t)=2K_0\left(\frac{3}{2}\sqrt{\frac{2\lambda}{K_0^2}}x+K_2\right)^{1/3}+K_1,$$
$$\rho(x,t)=\left(\frac{3}{2}\sqrt{\frac{2\lambda}{K_0^2}}x+K_2\right)^{2/3}. \tag{53}$$

This is a static algebraic solution, with no singularities, and is unbounded at large values of x. It admits the gradient catastrophe since the velocity is unbounded at $x=-2/3\sqrt{K_0^2/2\lambda}K_2$.

Another class of solutions is provided from the subalgebra $L_{3,2}$. In this case, we have to solve a set of two partial differential equations for θ, in variables ξ and η, which are listed in Table VI:

$$8\xi\eta\theta_\eta\theta_{\xi\xi}+4\eta\theta_\xi\theta_\eta+4\xi(\theta_\xi)^2-2\xi\theta_\xi-\xi^2\theta_{\xi\xi}+\eta\theta_\eta-4\xi\eta\theta_\xi\theta_{\xi\eta}+\xi\eta\theta_{\xi\eta}=0, \tag{54}$$

$$4\xi\theta_\xi\theta_{\xi\eta}-\xi\theta_{\xi\eta}+\theta_\eta+\eta\theta_{\eta\eta}=0. \tag{55}$$

The second Eq. (55) corresponds to the fact that $F_\eta=0$ since $F(\xi)$ is a function of ξ only. The function F is related to θ through the formula

$$F(\xi)=\sqrt{\lambda}(2\xi^2(\theta_\xi)^2-\xi^2\theta_\xi+\xi\eta\theta_\eta)^{-1/2}. \tag{56}$$

A number of solutions $\theta(\xi,\eta)$ can be found to the system of Eqs. (54) and (55) by setting certain conditions on the derivatives of θ. By setting $\theta_{\xi\xi}=f(\eta)$, we obtain the solution of the reduced equations

$$\theta=\frac{\xi\eta}{2\eta+C_0}+C_1. \tag{57}$$

This solution however leads to an infinite value for the function F (and therefore an infinite density ρ). On the other hand, if we make the assumption that $\theta_{\xi\eta}=0$, that is $\theta=f(\xi)+g(\eta)$, then one possible solution of the reduced equations is

$$\theta=K_0\ln(\xi\eta)+K_1. \tag{58}$$

The formula (56) gives the finite value $F=\lambda/(2K_0^2)$ and so we obtain the static solution

$$\theta(x,t)=K_0\ln(x^2)+K_1,\quad \rho(x,t)=\frac{\lambda}{2K_0^2}x. \tag{59}$$

This solution is a singular solution which admits a branch point at $x=0$. Consequently, the velocity $\mathbf{v}$ of the fluid is singular there. Since the density ρ vanishes at that point, the entire line $x=0$ must be physically excluded from the domain of the fluid.

Consider the subalgebra $L_{3,4}$. In this case, the reduced differential equation to be solved is

$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{1}{x}\frac{F''}{F'}\right)(\rho_x)^2-\left(\frac{2}{x}+\frac{2}{x^2}\rho\frac{F''}{F'}\right)(\rho_x)+\left(\frac{\lambda x^2}{\rho^3(F')^2}+\frac{3}{2x^2}\rho+\frac{1}{x^3}\rho^2\frac{F''}{F'}\right)=0, \quad (60)$$

where F is a function of ρ/x. This equation is different from the one considered previously for $L_{1,8}$ in the sense that there exists a nonzero coefficient of ρ_x, in both x and ρ. Thus, Eq. (46) can no longer be used. However, in the case when $F(\xi)=K_0\xi^{1/2}+K_1$, Eq. (60) is a special case of equation C 6.70 discussed in Ref. 23:

$$y''=x^{a-2}f\left(\frac{y}{x^a},\frac{xy'}{x^a}\right), \quad (61)$$

where $a=1$ and

$$f\left(\frac{y}{x},y'\right)=y'-\frac{y}{x}-\frac{4\lambda}{K_0^2}\left(\frac{y}{x}\right)^{-2}. \quad (62)$$

Making the substitution $y(x)=x\,\eta(\xi)$, where $\xi=\ln x$, we obtain the equation

$$\eta''+\frac{4\lambda}{K_0^2\eta^2}=0, \quad (63)$$

which leads to the first integral

$$\frac{d\eta}{d\xi}=\sqrt{\frac{8\lambda}{K_0^2\eta}+K_3}. \quad (64)$$

For the special case where $K_3=0$, we obtain

$$y(x)=x\left(\frac{3}{K_0}\sqrt{2\lambda}\ln|x|+K_4\right)^{2/3}, \quad (65)$$

which leads to the static solution

$$\theta=K_0\left(\frac{3}{K_0}\sqrt{2\lambda}\ln|x|+K_4\right)^{1/3}+K_1, \quad \rho=x\left(\frac{3}{K_0}\sqrt{2\lambda}\ln|x|+K_4\right)^{2/3}. \quad (66)$$

This solution is singular with a branch point at $x=0$. Therefore, we have a situation similar to that of solution (59) above, since the entire line $x=0$ must be excluded from the domain of the solution.

For the subalgebra $L_{5,3}$, the differential equation to be solved is

$$\rho_{xx}-\frac{5}{2\rho}(\rho_x)^2-\frac{1}{4}\rho^3\frac{F'}{F^2}+\frac{\lambda\rho^3}{4F^2}=0, \quad (67)$$

where F is an arbitrary function of t. In the case where $\rho_{xx}=(2/\rho)\,(\rho_x)^2$ and $F=K_0$ is chosen to be a constant, Eq. (67) is satisfied by the static solution

$$\theta=K_0\left(K_2-\sqrt{\frac{\lambda}{2K_0^2}}x\right)^2, \quad \rho=\frac{1}{K_2-\sqrt{\frac{\lambda}{2K_0^2}}x}. \quad (68)$$

This solution has a simple pole at $x=K_2\sqrt{2K_0^2/\lambda}$. Asymptotically, it is unbounded when $x\to\pm\infty$. In general, Eq. (67) can be solved by the quadrature

$$x=\int \frac{d\rho}{\rho^2(\ln\rho)\left(\dfrac{\lambda-F'}{2F^2}-C_0\rho\right)^{1/2}}, \tag{69}$$

leading to a singular solution.

A class of solutions of (7) corresponding to the subalgebra $L_{7,2}$, $a\neq 1$, can be constructed by solving the set of two partial differential equations for θ, in the two independent variables of ξ and η, as listed in Table VI. The function F is related to θ through the relation

$$F(\xi)=\sqrt{\lambda}((a+1)\xi\eta^{-a}\theta_\xi+\eta^{(1-a)}\theta_\eta+2\xi^3\eta^{-2a}(\theta_\xi)^2)^{-1/2}. \tag{70}$$

For the case $a=-1/2$, the assumption $\theta_{\xi\xi}=0$ yields the solution of the reduced equations

$$\theta=K_0\eta^{-1/2}\xi+K_1, \quad F=\sqrt{\frac{\lambda}{2K_0^2}}\xi^{-3/2}, \tag{71}$$

which leads to the algebraic solution

$$\theta=\frac{K_0}{x^2}+K_1, \quad \rho=\sqrt{\frac{\lambda}{2K_0^2}}x^3. \tag{72}$$

This solution admits a double pole at $x=0$. Asymptotically, the velocity of the fluid flow is bounded, but the density is not.

In the case of the nonsplitting subalgebra $\mathcal{L}_{5,2}$, the function F is related to θ through the relation

$$F(\xi)=\sqrt{\lambda}\left(-\frac{\varepsilon\eta^2}{\xi}\theta_\xi-\frac{\varepsilon\eta^3}{\xi^2}\theta_\eta+\frac{1}{2}\frac{\eta^4}{\xi^2}(\theta_\xi)^2\right)^{-1/2}. \tag{73}$$

By setting $\theta_{\xi\xi}=f(\eta)$, we obtain the solution of the reduced equations

$$\theta=\frac{K_0\xi^2}{2\eta^2}+K_1, \tag{74}$$

from where we obtain the algebraic solution of the initial equations

$$\theta=\frac{1}{2}K_0x^2+K_1, \quad \rho=\frac{\sqrt{2\lambda}}{K_0x}, \tag{75}$$

admitting a simple pole at $x=0$. This solution is unbounded, but the velocity does not admit the gradient catastrophe. Note that we also obtain this solution for the subalgebra $L_{5,4}$, in the case where the function F is a constant. All of the static solutions given above are expressed in terms of elementary functions and are reducible with respect to the one-dimensional subalgebra $\{P_0\}$. The structure of the singularities consists of poles and branch points only.

B. Explicit nonstatic solutions

Let us now discuss certain classes of nonstatic solutions of the Chaplygin Eqs. (7a) and (7b) which can be obtained directly by applying the procedure presented in Sec. III to the reduced equations listed in Table VI. Here, we present only the results.

For the subalgebra $L_{1,6}$, we obtain the algebraic solution

$$\theta(x,t)=\frac{1}{2(t-t_0)}x^2+\frac{K_1}{t-t_0}x+\frac{\lambda}{3K_2^2}(t-t_0)^3+\frac{K_1^2}{2(t-t_0)}+K_3,$$
$$\rho(x,t)=\frac{K_2}{t-t_0}, \tag{76}$$

which admits a simple pole at $t=t_0$. Evaluating the characteristic matrix (43) for solution (76), we find that the only constant vectors in the kernal are multiples of the vector

$$\mathbf{a}=(t_0,0,-1,-1,0,0). \tag{77}$$

Therefore, this solution is reducible with respect to the full group G by the one-dimensional subalgebra $S_{1,6}=\{t_0P_1-K_1Z-B\}$.

Similarly, for the subalgebra $L_{2,2}$, we obtain the solution

$$\theta(x,t)=\frac{a_1x^2}{2(a_1t+a_0)}+\frac{a_2x}{(a_1t+a_0)}+\frac{1}{3}\lambda a_1^2t^3+\lambda a_1a_0t^2+\lambda a_0^2t+\frac{a_2^2}{2a_1(a_1t+a_0)}+a_3,$$
$$\rho(x,t)=\frac{1}{a_1t+a_0}. \tag{78}$$

We note that solution (78) is identical to the solution (76) found in the previous case for subalgebra $L_{1,6}$. Here, the simple pole is at $t=a_0/a_1$. We note that both solutions (76) and (78) represent centered wave-type solutions.

A similar situation to that of $L_{1,6}$ and $L_{2,2}$ occurs for the two subalgebras $L_{1,7}$ and $L_{5,2}$. In the case of $L_{1,7}$, we obtain the exponential-type solution

$$\theta(x,t)=-\frac{1}{2}\sqrt{2\lambda}K_1(x-x_0)^2\left(\frac{1+\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}{1-\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}\right)+K_2,$$
$$\mathbf{v}(x,t)=-\sqrt{2\lambda}K_1(x-x_0)\left(\frac{1+\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}{1-\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}\right),\quad \rho(x,t)=-\frac{1}{K_1(x-x_0)}. \tag{79}$$

This solution has simple poles at $x=x_0$ and $t=t_0$, and is reducible by the one-dimensional subalgebra $S_{1,7}=\{D_2-x_0P_1\}$.

In the case of subalgebra $L_{5,2}$, the solution is given by

$$\theta(x,t)=\frac{\sqrt{2\lambda}}{2C_0}x^2\left(\frac{\mathbf{e}^{2\sqrt{2\lambda}/C_0(t-t_0)}+1}{\mathbf{e}^{2\sqrt{2\lambda}/C_0(t-t_0)}-1}\right),$$
$$\mathbf{v}(x,t)=\frac{\sqrt{2\lambda}}{C_0}x\left(\frac{\mathbf{e}^{2\sqrt{2\lambda}/C_0(t-t_0)}+1}{\mathbf{e}^{2\sqrt{2\lambda}/C_0(t-t_0)}-1}\right),\quad \rho(x,t)=\frac{C_0}{x}. \tag{80}$$

Indeed, up to a translational shift in x and t, solution (80) is identical to solution (79). The pole in x is now at $x=0$. Both solutions (79) and (80) have a singularity at line $t=t_0$, as well as at line $x=x_0$ (for (79)) or $x=0$ (for (80)). When $K_1>0$, the asymptotic behavior is as follows. As $t\to\infty$, the quantity θ approaches the function $f_+(x)=a(x-x_0)^2$, and as $t\to-\infty$, it approaches the function $f_-(x)=-a(x-x_0)^2$. The density has a simple pole at $x=x_0$, and is constant in time. Both solutions correspond to kinks, and since the current for solution (79)

$$j=\rho\frac{\partial\theta}{\partial x}=\sqrt{2\lambda}\left(\frac{1+\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}{1-\mathbf{e}^{2\sqrt{2\lambda}K_1(t-t_0)}}\right), \tag{81}$$

is preserved in x, this suggests the complete integrability of system (7).

For the nonsplitting subalgebra $\mathcal{L}_{2,2}$, the density ρ is related to θ through the relation

$$\rho(\xi)=\sqrt{\lambda}(\theta_\eta-\eta\theta_\xi+\tfrac{1}{2}(\theta_\xi)^2)^{-1/2}. \tag{82}$$

The assumption $\theta_{\xi\xi}=0$ yields the polynomial solution of the reduced equations

$$\theta=\xi\eta+\tfrac{1}{6}\eta^3+K_1\eta+K_0, \tag{83}$$

which leads to the partially invariant solution

$$\theta=\varepsilon xt-\tfrac{1}{3}t^3+K_1t+K_0,\quad \mathbf{v}(x,t)=\varepsilon t,\quad \rho=\sqrt{\lambda}(\varepsilon x-\tfrac{1}{2}t^2+K_1)^{-1/2}. \tag{84}$$

This solution is reducible by the two-dimensional subalgebra $\mathcal{S}_{2,2}=\{\varepsilon P_0+\varepsilon K_1Z+B,4\varepsilon K_1P_1-6K_0Z+D_1\}$. Consequently, solution (84) can be obtained either as a partially invariant solution with $\delta=1$ with respect to the subalgebra $\mathcal{L}_{2,2}$, or as a G-invariant solution ($\delta=0$) with respect to the subalgebra $\mathcal{S}_{2,2}$.

For the subalgebra $L_{7,2}$, $a=1$, we have a set of two partial differential equations for θ listed in Table VI. The density ρ is linked to θ through the relation

$$\rho(\xi)=\sqrt{\lambda}\left(-\frac{\xi}{\eta}\theta_\xi+\theta_\eta+\frac{1}{2\eta^2}(\theta_\xi)^2\right)^{-1/2}. \tag{85}$$

We obtain two different solutions to the reduced system. First, we have

$$\theta=\tfrac{1}{2}\eta\xi^2+C_0, \tag{86}$$

which leads to an infinite density. Also, we have

$$\theta=K_0\eta+K_1, \tag{87}$$

from where we obtain the trivial constant-density solution

$$\theta=K_0t+K_1,\quad \rho=\sqrt{\frac{\lambda}{K_0}}. \tag{88}$$

Solution (88), nevertheless, has a characteristic matrix of rank 1, and is therefore partially invariant. In this case, the solution is reducible by the subalgebra $S_{7,2}=\{P_1,P_0+K_0Z,-2K_1Z+D_1+D_2\}$.

For the subalgebra $L_{11,2}$, the density ρ is related to θ through the relation

$$\rho(\xi)=\sqrt{\lambda}\left(\theta_\eta-\frac{1}{\eta}(\xi+\varepsilon+\varepsilon\ln\eta)\theta_\xi+\frac{2}{\eta^2}(\theta_\xi)^2\right)^{-1/2}. \tag{89}$$

The assumption $\theta_{\xi\eta}=K_0$ yields the solution of the reduced equations

$$\theta=K_0\xi\eta+K_0\varepsilon\eta\ln\eta+(K_1-K_0\varepsilon)\eta+K_2,\quad K_0,K_1,K_2\in\mathfrak{R}, \tag{90}$$

which leads to the constant-density solution

$$\theta(x,t)=2K_0x+(K_1-K_0\varepsilon)t+K_2,$$
$$\rho=\sqrt{\lambda}(K_1+2K_0^2-K_0\varepsilon)^{-1/2}. \tag{91}$$

This solution is reducible by the subalgebra $\mathcal{S}_{11,2}=\{P_1+2K_0Z,P_0+(K_1-K_0\varepsilon)Z,D_1+D_2-2K_2Z\}$, and represents a traveling wave.

Finally, it is interesting to note that the subalgebra $L_{7,4}$, where $a=-1$, leads to a bump-type solution. The reduced equation of the subalgebra has the form

$$\rho_{xx}-\frac{3}{2\rho}(\rho_x)^2+\frac{2F'}{F}\rho_x+\left(\frac{\lambda\rho}{F^2}-\frac{(F')^2\rho}{2F^2}-\frac{F''}{F}\rho\right)=0, \tag{92}$$

where F is a function of x. For the special case where $F=K_0$, the equation becomes

$$\rho_{xx}-\frac{3}{2\rho}(\rho_x)^2+\frac{\lambda}{F^2}\rho=0. \tag{93}$$

We can integrate Eq. (93) twice and obtain the explicit form of the bump solution

$$\rho(x,t)=-\frac{\lambda(t-t_0)}{\cosh^2(\frac{1}{2}\sqrt{2\lambda}(x+C))},$$
$$\theta(x,t)=-\frac{\cosh^2(\frac{1}{2}\sqrt{2\lambda}(x+C))}{\lambda(t-t_0)}, \tag{94}$$

which is reducible by the subalgebra $S_{7,4}=\{D_1-D_2-2t_0P_0\}$. The velocity potential θ admits a simple pole at $t=t_0$. For large values of x, the density ρ is bounded and tends to zero, but the velocity potential is unbounded. It should be noted that θ decreases with time provided that we exclude the region around the pole at t_0. Also, since the current

$$j=\sqrt{2\lambda}\tanh(\tfrac{1}{2}\sqrt{2\lambda}(x+C)), \tag{95}$$

is preserved in time t, and since there exists an infinite number of preserved quantities, the complete integrability of the Chaplygin Eqs. (7a) and (7b) is established.

C. Implicit solutions expressed in terms of elementary functions

A localized solution of (7a) and (7b) can be obtained from the subalgebra $L_{6,1}$. The reduced differential equation from Table VI takes the form

$$\rho_{xx}-\frac{5}{2\rho}(\rho_x)^2-\frac{1}{2tF}\rho^3-\frac{F'}{4F^2}\rho^3+\frac{\lambda\rho^3}{4F^2}=0, \tag{96}$$

where F is a function of t. In the case where $F(t)=1$ we can integrate Eq. (96), and this results in the solution given in implicit form

$$-\frac{1}{2K_0\rho}\sqrt{K_1\rho+2K_0}+\varepsilon\frac{K_1}{(2\varepsilon K_0)^{3/2}}\tanh^{-1}\left(\sqrt{\frac{K_1\rho+2K_0}{2\varepsilon K_0}}\right)=x+C_0, \tag{97}$$

where $K_0(t)=\lambda/4-1/(2t)$, and $\varepsilon=|K_0(t)|/K_0(t)$. This solution represents a kink in the regions where the derivatives of ρ and θ are finite and the gradient catastrophe does not occur. An analysis of the characteristic matrix (43) indicates that the only constant vector in the kernal is the zero vector. Therefore, solution (97) is irreducible with respect to the full group G.

D. Solutions in terms of Jacobi elliptic functions

We now discuss solutions which can be expressed in terms of Jacobi elliptic functions. For the subalgebra $L_{1,9}$, the basic Chaplygin system (7a) and (7b) is reduced to the following differential equation

$$\rho_{xx}+\left(\frac{1}{2\rho}+\frac{F''}{F'}\right)(\rho_x)^2+\left(\frac{\lambda}{\rho^3(F')^2}-\frac{\varepsilon}{\rho(F')^2}\right)=0. \tag{98}$$

Equation (98) has the Painlevé property (no movable singularities other than poles) if and only if

$$F(\rho)=2K_0\rho^{1/2}+K_1, \tag{99}$$

where K_0 and K_1 are functions of t. So, Eq. (98) becomes

$$\rho_{xx}+\frac{\lambda}{K_0^2\rho^2}-\frac{\varepsilon}{K_0^2}=0, \tag{100}$$

the solution of which can be expressed by quadrature

$$\int \frac{\rho d\rho}{\sqrt{\frac{2\varepsilon}{K_0^2}\rho^3+K_2\rho^2+\frac{2\lambda}{K_0^2}\rho}}=x+K_3. \tag{101}$$

Equation (101) can be solved in terms of elliptic functions[24] or degenerate cases thereof (i.e., elementary functions). We can integrate ODE (100) once and write the obtained first-order equation

$$\left(\frac{d\rho}{dx}\right)^2=\frac{1}{\rho^2}(\rho-\rho_1)(\rho-\rho_2)(\rho-\rho_3), \tag{102}$$

where the constants ρ_1, ρ_2, ρ_3 satisfy the relations

$$\begin{aligned}&\rho_1+\rho_2+\rho_3=-\tfrac{1}{2}\varepsilon K_2K_0^2,\\ &\rho_1\rho_2+\rho_2\rho_3+\rho_1\rho_3=\varepsilon\lambda,\\ &\rho_1\rho_2\rho_3=0.\end{aligned} \tag{103}$$

When all three roots ρ_i of the polynomial in Eq. (102) are different, then the solution can be expressed in terms of Jacobi elliptic functions. The results for different ordering of the roots $\rho_1<\rho_2<\rho_3$ are summarized in Table VII.

The moduli k of the Jacobi elliptic functions can be chosen in such a way that $0<k^2<1$. This ensures that the elliptic solutions possess one real and one purely imaginary period and that for real arguments x we have

$$-1\leqslant sn(x,k)\leqslant 1,\quad -1\leqslant cn(x,k)\leqslant 1,\quad \sqrt{1-k^2}\leqslant dn(x,k)\leqslant 1. \tag{104}$$

Note that nonsingular periodic solutions can be physically interpreted as kinks, bumps, cnoidal and snoidal waves, depending on the asymptotic behavior of the modulus k. Singular solutions represent static structures which develop from a point or a line into a growing sphere or cylinder.

Elementary solutions take place when two of the roots are identical, $\rho_1=\rho_2=-(1/4)\varepsilon K_2K_0^2$ and $\rho_3=0$. Then we obtain $\lambda=(1/16)\varepsilon K_2^2K_0^4$, and Eq. (102) becomes

TABLE VII. Jacobi elliptic solutions corresponding to the subalgebra $L_{1,9}$ (splitting) of the Chaplygin equation. Reduction to the ODE $\varepsilon y''+\alpha y^{-2}+\beta$, $\varepsilon=\pm 1$, where $\alpha=\lambda K_0^{-2}$, $\beta=-\varepsilon K_0^{-2}$. The function $U(\rho)$ is such that $U(\rho)=x+c_0$. Here, the constants m, n, $p_\pm$, and $q_\pm$ are defined to be $m=\frac{1}{4}K_2K_0^2+(\frac{1}{16}K_2^2K_0^4+\lambda)^{1/2}$, $n=-\lambda(\frac{1}{4}K_2K_0^2+(\frac{1}{16}K_2^2K_0^4+\lambda)^{1/2})^{-1}$, $p_\pm=-\frac{1}{4}K_2K_0^2\pm(\frac{1}{16}K_2^2K_0^4-\lambda)^{1/2}$, and $q_\pm=\lambda(-\frac{1}{4}K_2K_0^2\pm(\frac{1}{16}K_2^2K_0^4-\lambda)^{1/2})^{-1}$.

No.	Order of roots	Function $U(\rho)$	Modulus k and parameters
1	$\rho\leqslant c<0<a$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{2}{(a-c)^{1/2}}\right)$	$-1<k=\left(\frac{a}{a-c}\right)^{1/2}<1$
	$\varepsilon=-1$	$[c\,u_1+(a-c)E(u_1)+(a-c)dn(u_1)cs(u_1)]$	$sn(u_1)=\left(\frac{a-c}{a-\rho}\right)^{1/2}$
	$a=m$		
	$c=n$		
2	$\rho<c<0<a$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{2c}{(a-c)^{1/2}k'^2}\right)$	$-1<k=\left(\frac{a}{a-c}\right)^{1/2}<1$
	$\varepsilon=-1$	$[k'^2u_1-E(u_1)+dn(u_1)tn(u_1)]$	$sn(u_1)=\left(\frac{\rho-c}{\rho}\right)^{1/2}$
	$a=m$		$k'=(1-k^2)^{1/2}$
	$c=n$		
3	$c<\rho\leqslant b<0$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{2}{(-c)^{1/2}}\right)$	$-1<k=\left(\frac{b-c}{-c}\right)^{1/2}<1$
	$\varepsilon=1$	$\left[c\,u_1-\frac{(c-b)}{k^2}(u_1-E(u_1))\right]$	$sn(u_1)=\left(\frac{\rho-c}{b-c}\right)^{1/2}$
	$b=p_\pm$		
	$c=q_\pm$		
4	$c\leqslant\rho<b<0$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{2b}{(-c)^{1/2}k'^2}\right)$	$-1<k=\left(\frac{b-c}{-c}\right)^{1/2}<1$
	$\varepsilon=1$	$[E(u_1)-k^2sn(u_1)cd(u_1)]$	$sn(u_1)=\left(\frac{b-\rho}{(c-b)\rho}\right)^{1/2}$
	$b=p_\pm$		$k'=(1-k^2)^{1/2}$
	$c=q_\pm$		
5	$c<0<\rho\leqslant a$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{-2c}{(a-c)^{1/2}k'^2}\right)$	$-1<k=\left(\frac{a}{a-c}\right)^{1/2}<1$
	$\varepsilon=-1$	$[E(u_1)-k'^2u_1-k^2\,sn(u_1)cd(u_1)]$	$sn(u_1)=\left(\frac{(a-c)\rho}{a(\rho-c)}\right)^{1/2}$
	$a=m$		$k'=(1-k^2)^{1/2}$
	$c=n$		
6	$c<0\leqslant\rho<a$	$\left(\frac{K_0^2}{2}\right)^{1/2}\left(\frac{2a}{(a-c)^{1/2}k^2}\right)[E(u_1)-k'^2u_1]$	$-1<k=\left(\frac{a}{a-c}\right)^{1/2}<1$
	$\varepsilon=-1$		$sn(u_1)=\left(\frac{a-\rho}{a}\right)^{1/2}$
	$a=m$		$k'=(1-k^2)^{1/2}$
	$c=n$		
7	$c<b<0<\rho$	$\left(\frac{K_0^2}{2}\right)^{1/2}\frac{-2b}{k'^2(-c)^{1/2}}[dn(u_1)tn(u_1)-E(u_1)]$	$-1<k=\left(\frac{c-b}{c}\right)^{1/2}<1$
	$\varepsilon=1$		$sn(u_1)=\left(\frac{\rho}{\rho-b}\right)^{1/2}$
	$b=p_\pm$		
	$c=q_\pm$		

TABLE VII. (*Continued.*)

No.	Order of roots	Function $U(\rho)$	Modulus k and parameters
8	$c<b<0\leqslant\rho<\infty$	$\left(\frac{K_0^2}{2}\right)^{1/2}\frac{2c}{(-c)^{1/2}}[E(u_1)+dn(u_1)cs(u_1)]$	$-1<k=\left(\frac{c-b}{c}\right)^{1/2}<1$
	$\varepsilon=1$		$sn(u_1)=\left(\frac{c}{c-\rho}\right)^{1/2}$
	$b=p_{\pm}$		
	$c=q_{\pm}$		
9	$0<\rho$, and $b,c\in\mathcal{C}$	$\lambda^{1/4}\left(\frac{K_0^2}{2}\right)^{1/2}\left[-F(\phi,k)+2\left(u_1-E(u_1)+\frac{sn(u_1)dn(u_1)}{1+cn(u_1)}\right)\right]$	$-1<k=\left(\frac{\lambda^{1/2}-\frac{1}{4}K_0^2K_2}{2\lambda^{1/2}}\right)^{1/2}<1$
	$\varepsilon=1$		$cn(u_1)=\frac{\lambda^{1/2}-\rho}{\lambda^{1/2}+\rho}$
	$b=-\frac{K_0^2K_2}{4}\pm i\left(\lambda-\frac{K_0^4K_2^2}{16}\right)^{1/2}$		$\phi=\cos^{-1}\left(\frac{\lambda^{1/2}-\rho}{\lambda^{1/2}+\rho}\right)$
	$c=\bar{b}$		
10	$0<\rho<\infty$, and $b,c\in\mathcal{C}$	$\lambda^{1/4}\left(\frac{K_0^2}{2}\right)^{1/2}\left[u_1-2E(u_1)-2\frac{sn(u_1)dn(u_1)}{1-cn(u_1)}\right]$	$-1<k=\left(\frac{\lambda^{1/2}-\frac{1}{16}K_0^2K_2}{2\lambda^{1/2}}\right)^{1/2}<1$
	$\varepsilon=1$		$cn(u_1)=\frac{\rho-\lambda^{1/2}}{\rho+\lambda^{1/2}}$
	$b=-\frac{K_0^2K_2}{4}\pm i\left(\lambda-\frac{K_0^4K_2^2}{16}\right)^{1/2}$		$\phi=\cos^{-1}\left(\frac{\rho-\lambda^{1/2}}{\rho+\lambda^{1/2}}\right)$
	$c=\bar{b}$		

$$\left(\frac{d\rho}{dx}\right)^2=\frac{1}{\rho}\left(\rho+\frac{1}{4}\varepsilon K_2K_0^2\right)^2. \tag{105}$$

The general integral is given in implicit form

$$2\rho^{1/2}-\left(-\frac{1}{4}\varepsilon K_2K_0^2\right)^{1/2}\ln\left(\frac{\left(-\frac{1}{4}\varepsilon K_2K_0^2\right)^{1/2}+(\rho)^{1/2}}{\left(-\frac{1}{4}\varepsilon K_2K_0^2\right)^{1/2}-(\rho)^{1/2}}\right)=\pm x+C_0, \tag{106}$$

which is a singular solution admitting a branch point at $\rho=-(1/4)\varepsilon K_2K_0^2$.

By means of the nonsplitting subalgebra $\mathcal{L}_{3,4}$, the reduced equation from Table VI obtained when we set $F(\xi)=K_0\xi^{1/2}+K_1$, as in the previous cases, is

$$\rho_{xx}-\frac{1}{x}\rho_x+\frac{1}{x^2}\rho+\frac{4\lambda x}{K_0^2\rho^2}-\frac{2}{K_0^2 x}=0. \tag{107}$$

This is once again a special case of Eq. (61), except that the coefficient function is now given by

$$f\left(\frac{y}{x},y'\right)=y'-\frac{y}{x}-\frac{4\lambda}{K_0^2}\left(\frac{y}{x}\right)^{-2}+\frac{2}{K_0^2}, \tag{108}$$

where $a=1$. Making the change of variable $\rho(x)=x\,\eta(\xi)$ where $\xi=\ln x$ into (107), we obtain the first integral

$$\left(\frac{d\eta}{d\xi}\right)=\frac{8\lambda}{K_0^2\eta}+\frac{4\eta}{K_0^2}+K_3. \tag{109}$$

This leads to the quadrature

$$\int \frac{d\eta}{\sqrt{\dfrac{8\lambda}{K_0^2\eta}+\dfrac{4\eta}{K_0^2}+K_3}}=\xi+c_0, \tag{110}$$

which can be solved in terms of elliptic functions.[24] The solutions $\eta=\eta(\xi)$ are found in exactly the same manner as for the previous case $(\rho=\rho(x))$ for subalgebra $L_{1,9}$, except that the coefficients are now different. The right-hand sides of Eq. (103) in terms of η become $-(1/4)K_3K_0^2$, 2λ and 0, respectively. The coefficient ε which previously appeared for the subalgebra $L_{1,9}$ is always set to 1, which means that only those root orderings previously corresponding to the positive branch of ε are included. All implicit partially invariant solutions obtained in Sec. IV D are irreducible with respect to the full group G. This is due to the fact that the kernal of the characteristic matrix (43), built from the derivatives of ρ and θ, does not contain any nonzero constant vectors.

It should be noted that Chaplygin solutions have been found for the two-dimensional subalgebras which have not been discussed above. In order to be concise, we have omitted them from this article, and limit ourselves to a few general comments. The full details can be found in Ref. 14. In the cases of subalgebras $L_{3,3}$, $\mathcal{L}_{3,3}$, $L_{4,1}$, $\mathcal{L}_{4,1}$, $\mathcal{L}_{5,3}$, $L_{7,3}(a=1)$, $L_{7,3}(a\neq 1)$ and $L_{8,1}$, solutions of the reduced equations in Table VI were found implicitly by quadrature. As an example, we present the solution for subalgebra $L_{3,3}$:

$$\int \left(\frac{2\lambda\sqrt{t}}{K_0^2\rho}-\frac{2\rho^{3/2}}{3t^{3/4}K_0}+K_2\right)^{-1/2} d\rho=x+C_0. \tag{111}$$

For the subalgebras $L_{7,4},(a=1)$, $L_{7,5},(a=1)$, $L_{7,4},(a\neq 1)$, $L_{9,1}$, $\mathcal{L}_{7,4},(a\neq 1)$ and $\mathcal{L}_{8,1}$, G-invariant solutions have been constructed. Finally, for subalgebra $\mathcal{L}_{7,2}(a\neq 1)$, a Chaplygin solution has been determined which has infinite density. However, its equivalent Born–Infeld solution has a finite density, as will be shown in the next subsection.

E. Solutions of the Born–Infeld equations

Each solution of the nonrelativistic Chaplygin Eqs. (7a) and (7b) can where possible be used to obtain a corresponding solution of the relativistic Born–Infeld Eqs. (11a) and (11b) in one spatial dimension. Since the Chaplygin and Born–Infeld models involve two distinct parametrizations of the Nambu–Goto target space variables X^0 and X^{d+1}, we equate these variables to both their relativistic and nonrelativistic representations:

$$X^0 = ct_R = \frac{1}{\sqrt{2}}(t_{\mathrm{NR}} + \theta_{\mathrm{NR}}(t_{\mathrm{NR}}, \mathbf{r})),$$
$$X^{d+1} = \frac{1}{c}\theta(t_R, \mathbf{r}) = \frac{1}{\sqrt{2}}(t_{\mathrm{NR}} - \theta_{\mathrm{NR}}(t_{\mathrm{NR}}, \mathbf{r})). \tag{112}$$

Renaming the time variables $T = (1/c)\, t_{\mathrm{NR}}$ and $t = t_R$, we obtain the following method of solution transformation described by Jackiw.[1] If $\theta_{\mathrm{NR}}(\mathbf{r}, t)$ is a solution of the Chaplygin Eq. (6), then a solution $\theta_R(\mathbf{r}, t)$ of the Born–Infeld equation can be determined as follows. First, we determine the function $T(\mathbf{r}, t)$ from the equation

$$T + \frac{1}{c^2}\theta_{\mathrm{NR}}(\mathbf{r}, T) = \sqrt{2}t, \tag{113}$$

then, we obtain the relativistic Born–Infeld solution

$$\theta_R(\mathbf{r}, T) = \frac{1}{\sqrt{2}}c^2 T - \frac{1}{\sqrt{2}}\theta_{\mathrm{NR}}(\mathbf{r}, T) = c^2(\sqrt{2}T - t), \tag{114}$$

which is associated to the Chaplygin solution θ_{NR}. Since Eq. (113) cannot always be solved explicitly for $T(\mathbf{r}, t)$ it follows that explicit Born–Infeld solutions cannot always be found in this manner. However, the following classes of solutions of the Born–Infeld Eq. (10) can be constructed. We summarize the results as follows.

For each static solution $\theta_{\mathrm{NR}}(x)$ given in Sec. IV A, we can find the equivalent Born–Infeld solution

$$\theta_R(x, t) = c^2 t - \sqrt{2}\theta_{\mathrm{NR}}(x), \quad \rho_R(x) = \frac{a}{\sqrt{2}\left(\dfrac{d}{dx}\theta_{\mathrm{NR}}(x)\right)}, \tag{115}$$

where a is related to λ through the relation $\lambda = a^2/2$. Thus, for example, we obtain for the subalgebra $L_{1,8}$ the solution of the Born–Infeld Eq. (11) of the form

$$\theta(x, t) = c^2 t - 2\sqrt{2}K_0\left(\frac{3}{2}\sqrt{\frac{2\lambda}{K_0^2}}x + K_2\right)^{1/3} - \sqrt{2}K_1,$$
$$\rho(x, t) = \frac{1}{\sqrt{2}}\left(\frac{3}{2}\sqrt{\frac{2\lambda}{K_0^2}}x + K_2\right)^{2/3}. \tag{116}$$

For the other static solutions, the full details are given in Ref. 14. Since the coordinate transformation (112) is nonsingular, solution (116) is reducible by the subalgebra $\{\widehat{P_0}\}$ given in (20). It is to be noted that the static Chaplygin solutions are transformed to nonstationary solutions of the Born–Infeld equations.

For the subalgebras $L_{1,6}$ and $L_{2,2}$, Eq. (113) takes the following polynomial form:

$$\lambda T^4 - 4\lambda t_0 T^3 + (2c^2K_2^2 - 2\sqrt{2}c^2K_2^2 + 6\lambda t_0^2)T^2 + (2\sqrt{2}c^2K_2^2 t_0 - 2c^2K_2^2 t_0 + 2K_3K_2^2 - 4\lambda t_0^3)T$$
$$+ (\lambda t_0^4 + K_1^2K_2^2 + K_2^2x^2 + 2K_1K_2^2x - 2K_3K_2^2t_0)$$
$$= 0. \tag{117}$$

This is a quartic equation which can be solved explicitly through the method of Ferrari, by solving the resolvent cubic equation.[25] The quantity T can be expressed as a function of x and t. Since the solution has a complicated form, we will not present it here.

In the case of subalgebras $L_{1,7}$ and $L_{5,2}$, Eq. (113) has the transcendental form for T

$$T-\frac{1}{2c^2}\sqrt{2\lambda}K_1(x-x_0)^2\left(\frac{1+\mathbf{e}^{2\sqrt{2\lambda}K_1(T-t_0)}}{1-\mathbf{e}^{2\sqrt{2\lambda}K_1(T-t_0)}}\right)+\frac{K_2}{c^2}=\sqrt{2}t, \tag{118}$$

which cannot be solved explicitly as a function of x and t.

The associated Eq. (113) for the subalgebra $\mathcal{L}_{2,2}$ reduces to the cubic form

$$T^3-3(c^2+\varepsilon x+K_1)T-3(K_0-\sqrt{2}c^2t)=0. \tag{119}$$

The solution of this equation is given by Cardan's formula for the roots of a cubic

$$\begin{aligned}T(x,t)=&\left(\tfrac{3}{2}(K_0-\sqrt{2}c^2t)+\left(\tfrac{9}{4}(K_0-\sqrt{2}c^2t)^2+(c^2+\varepsilon x+K_1)^3\right)^{1/2}\right)^{1/3}\\&+\left(\tfrac{3}{2}(K_0-\sqrt{2}c^2t)-\left(\tfrac{9}{4}(K_0-\sqrt{2}c^2t)^2+(c^2+\varepsilon x+K_1)^3\right)^{1/2}\right)^{1/3},\end{aligned} \tag{120}$$

and the solution can be expressed simply as $\theta_R(x,t)=c^2(\sqrt{2}T-t)$.

For the subalgebra $L_{7,2}$,$(a=1)$, solution (88) leads to a rather trivial solution, namely,

$$\theta(x,t)=\frac{c^2((c^2+K_0)t-\sqrt{2}K_1)}{c^2-K_0},\quad \rho(x,t)=\frac{a(c^2+K_0)}{c^2\sqrt{-4K_0}}. \tag{121}$$

The associated Born–Infeld solution for the subalgebra $L_{11,2}$ takes the form

$$\theta(x,t)=\frac{c^2}{c^2-K_1+K_0\varepsilon}((c^2+K_1-K_0\varepsilon)t-2\sqrt{2}K_0x-\sqrt{2}K_2),$$

$$\rho(x,t)=\frac{a(c^2+K_1-K_0\varepsilon)}{\sqrt{c^2(c^4-(K_1-K_0\varepsilon)^2)+8c^4K_0^2}}. \tag{122}$$

Finally, for the Chaplygin bump solution (94) corresponding to the subalgebra $L_{7,4}(a=-1)$, the associated Born–Infeld solution is given by

$$\theta(x,t)=\frac{c^2t_0}{\sqrt{2}}\pm\sqrt{2}c^2\left(\frac{(t_0-\sqrt{2}t)^2}{4}+\frac{\cosh^2(\frac{1}{2}\sqrt{2\lambda}(x+C))}{c^2\lambda}\right)^{1/2}, \tag{123}$$

which is nonsingular and asymptotically unbounded. Since they correspond, respectively, to the reducible Chaplygin solutions (88), (91), and (94), the Born–Infeld solutions (121), (122), and (123) are reducible by the transformed subalgebras corresponding to $\mathcal{S}_{7,2}$, $\mathcal{S}_{11,2}$, and $\mathcal{S}_{7,4}$ respectively.

We note that the Jacobi elliptic solutions described in Sec. IV D can be transformed to hyperelliptic solutions of the Born–Infeld equations. Due to the complexity of the expressions involved, we will not include them here.

In addition to the solutions discussed above, it should be noted that certain solutions to the reduced equations in Table VI lead to Chaplygin solutions with infinite density which were not discussed previously due to physical considerations. However, these ''solutions'' can be used to determine finite-density Born–Infeld solutions. As an example, we consider the subalgebra $\mathcal{L}_{7,2}(a\neq 1)$. A solution to the reduced equations in Table VI is

$$\theta_{\mathrm{NR}}=K_0\xi+\frac{\varepsilon K_0}{2}\ln\eta-\frac{K_0^2}{2}\eta+K_1 \tag{124}$$

$$=K_0x-\frac{K_0^2}{2}t+K_1. \tag{125}$$

Since the function F is related to θ by the relation

$$F(\xi)=\sqrt{\lambda}\left(-\frac{\varepsilon\eta}{2}\theta_\xi+\eta^2\theta_\eta+\frac{1}{2}\eta^2(\theta_\xi)^2\right)^{-1/2}, \tag{126}$$

the nonrelativistic density ρ_{NR} becomes infinite. However, if we transform the nonrelativistic θ-function (125) into its relativistic (Born–Infeld) equivalent

$$\theta(x,t)=\frac{c^2}{c^2-\frac{K_0^2}{2}}\left(\left(c^2+\frac{K_0^2}{2}\right)t-\sqrt{2}K_0^2x-\sqrt{2}K_1\right), \tag{127}$$

then, we obtain a finite (though constant) density

$$\rho(x,t)=\varepsilon\left(\frac{a^2c^4\left(c^2+\frac{K_0^2}{2}\right)^2}{2K_0^2c^8(K_0^2-1)}\right)^{1/2},\quad \varepsilon=\pm1, \tag{128}$$

which represents a traveling wave similar to that of solution (122). The negative branch ($\varepsilon=-1$) could be interpreted as an antiparticle density.

V. SUMMARY AND CONCLUDING REMARKS

The main purpose of this article has been to provide a great variety of exact analytic solutions through the systematic use of the subgroup structure of the Chaplygin and Born–Infeld equations in $(1+1)$ dimensions. We concentrate exclusively on partially invariant solutions. Under the hypothesis that the subgroups $G_i\subset G$ are acting regularly with two-dimensional orbits and that the transformed graphs $G_i(\Gamma_f)$ are submanifolds, we construct and investigate partially invariant solutions with defect structure $\delta=1$. We can summarize the results which were obtained using the proposed algorithm in Sec. III, with the following cases.

(1) Elementary solutions, that is, algebraic with one or two simple poles, trigonometric, hyperbolic and logarithmic,
(2) Implicit solutions in terms of elementary functions, and
(3) Doubly periodic solutions which can be expressed in terms of Jacobi elliptic functions sn, cn, and dn.

The explicit partially invariant solutions were found to be reducible, in most cases, by one-dimensional subalgebras of L. It should be noted that these types of solutions are difficult to obtain using the standard symmetry reduction method. All implicit solutions are irreducible with respect to the full group G.

The analysis described in this article could be extended in several directions. Firstly, it should be remembered that the elimination of ρ in the equations of motion (7a), (7b), (11a) and (11b) was only made possible when the constants λ and a, respectively, do not vanish. These quantities correspond to a d-brane ''tension'' which must not vanish if the Nambu–Goto action (1) is to generate dynamics.[1] Consequently, it is reasonable to suppose that an action for a ''tensionless''

d-brane could lead to the noninteractive (free) Chaplygin and Born–Infeld theories, where $\lambda = 0$ and $a = 0$, respectively. More generally, it may be interesting to investigate partially invariant solutions of the more general form of the Nambu–Goto action.

Second, the question also arises as to whether our approach can be extended to a supersymmetric version of the Chaplygin model. Recently, such a generalization has been achieved by Jackiw and Polychronakos[26] where, in particular, the explicit representation has been derived from a supermembrane. A group analysis of this supersymmetric planar model can, through the use of Grassmann variables and the Legendre transformation, provide us with new classes of generalized solutions of this model. This work is currently undertaken.[27]

Finally, using group theoretical techniques, the authors plan to generate, in a systematic way, invariant, and partially invariant solutions of the Born–Infeld equations in $(3+1)$ dimensions. The concept of weak transversality for these types of solutions could also be investigated. This task will be undertaken in a future work.

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Quantum doubles from a class of noncocommutative weak Hopf algebras

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The concept of biperfect (noncocommutative) weak Hopf algebras is introduced and their properties are discussed. A new type of quasi-bicrossed products is constructed by means of weak Hopf skew-pairs of the weak Hopf algebras which are generalizations of the Hopf pairs introduced by Takeuchi. As a special case, the quantum double of a finite dimensional biperfect (noncocommutative) weak Hopf algebra is built. Examples of quantum doubles from a Clifford monoid as well as a noncommutative and noncocommutative weak Hopf algebra are given, generalizing quantum doubles from a group and a noncommutative and noncocommutative Hopf algebra, respectively. Moreover, some characterizations of quantum doubles of finite dimensional biperfect weak Hopf algebras are obtained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767989]

I. INTRODUCTION

In a recent work,[1] quantum doubles of finite dimensional Hopf algebras and finite groups are generalized by one of the authors to those of certain finite dimensional weak Hopf algebras and finite Clifford monoids so as to obtain singular solutions of the quantum Yang–Baxter equation. However, the procedure in Ref. 1 is not suitable for noncocommutative weak Hopf algebras. So, it is interesting to construct quantum doubles of noncocommutative weak Hopf algebras. The aim of this paper is to give one class of noncocommutative weak Hopf algebras from which their quantum doubles can be obtained.

As is known,[2] bicrossed product is a fundamental tool to construct the quantum double of a Hopf algebra. Quasi-bicrossed product plays a similar role in Ref. 1 for the construction of quantum doubles of certain weak Hopf algebras (in particular, finite Clifford monoids). In Ref. 3, the concept of weak Hopf pairs was introduced as a generalization of the Hopf pairs of Takeuchi.[4] Using the weak Hopf skew pairs, one type of quasi-bicrossed products, which lie between general quasi-bicrossed products and quantum quasidoubles, were constructed when one of the two weak Hopf algebras in the product is cocommutative. In Sec. III of this paper, we will generalize the results and construct quasi-bicrossed products of the weak Hopf skew pairs corresponding to the case where both weak Hopf algebras in the product are noncocommutative (see Theorem III.6 below).

A bialgebra H over a field k is called a *weak Hopf algebra*[1] if there exists $T \in \mathrm{Hom}_k(H,H)$ such that $\mathrm{id}*T*\mathrm{id}=\mathrm{id}$ and $T*\mathrm{id}*T=T$ where $*$ is the covolution product in $\mathrm{Hom}_k(H,H)$; T is called a *weak antipode* of H. Weak Hopf algebras lie between left (respectively, right) Hopf algebras and bialgebras. So far, two types of such weak Hopf algebras have been found, which are the monoid algebra kS of a regular monoid S (Ref. 1) and the almost quantum algebra $wsl_q(2)$ (Ref. 5) (see also Ref. 6 for weak Hopf algebras corresponding to $U_q[sl_n]$).

An application of weak Hopf algebras was found in the construction of noninvertible solutions

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of the (quantum) Yang–Baxter equation in Refs. 1 and 5. It was found that for a finite dimensional cocommutative perfect weak Hopf algebra H with an invertible weak antipode T, the quasi-bicrossed product $H^{op}{}^{*}\infty H$ [which is called the *quantum double* of H, denoted by $D(H)$], is a quasibraided almost bialgebra equipped with the quasi-R-matrix $R=\Sigma_{i=1}^{n}(1\infty e_i)\otimes(e^i\infty 1)\in D(H)\otimes D(H)$ where $\{e_i\}_{i=1}^{n}$ is a basis of H as a vector space and $\{e^i\}_{i=1}^{n}$ is its dual basis in $H^{op}{}^{*}$. Then, R is a solution of the quantum Yang–Baxter equation. In Ref. 7, it was shown that this solution R is von Neumann regular but not invertible in general. An example of this solution was constructed from the cocommutative perfect weak Hopf algebra $H=kS$ for any finite Clifford monoid S.

Although the quantum double of a finite Clifford monoid is indeed a generalization of the quantum double of a finite group, the quantum doubles in Ref. 1 cannot usually be regarded as generalizations of quantum doubles of Hopf algebras due to the cocommutativity of the weak Hopf algebras considered in Ref. 1. The goal of this paper is to overcome this so as to construct quantum doubles of noncocommutative weak Hopf algebras. We will give one class of noncocommutative weak Hopf algebras from which their quantum doubles can be obtained. First, we introduce the concept of biperfect weak Hopf algebras and discuss their properties. Then we construct a new type of quasi-bicrossed products by means of the weak Hopf skew pairs of the weak Hopf algebras which are generalizations of the Hopf pairs introduced by Takeuchi.[3] As a special case, the quantum double of a finite dimensional biperfect (noncocommutative) weak Hopf algebra is built. Examples of quantum doubles from a Clifford monoid and a noncommutative and noncocommutative weak Hopf algebra are given as generalizations of those from a group and a noncommutative and noncocommutative Hopf algebra, respectively. Moreover, we discuss some characterizations of quantum doubles of finite dimensional biperfect weak Hopf algebras.

II. PRELIMINARIES

Throughout the paper, k stands for a field. Some notations and definitions unexplained here can be found in Refs. 8, 2, 1, and 9. The word ''quantum quasidouble'' of a weak Hopf algebra in Ref. 1 will always be replaced with ''quantum double.''

We recall[1] that a linear space H is a *k-almost bialgebra* if (H,μ,η) is a k-algebra and (H,Δ,ε) is a k-coalgebra with $\Delta(xy)=\Delta(x)\Delta(y)$ for $x, y\in H$. If K is a subalgebra and also a subcoalgebra of H, then K itself is an almost bialgebra, called as an *almost sub-bialgebra* of H.

Combining formally with the definition of the weak Hopf algebras, we say in Ref. 7 that an almost bialgebra H is an *almost weak Hopf algebra* if there exists $T\in \mathrm{Hom}_k(H,H)$ such that $\mathrm{id}*T*\mathrm{id}=\mathrm{id}$ and $T*\mathrm{id}*T=T$, where T is called an *almost weak antipode* of H.

Let H be an almost bialgebra. If there exists an $R\in H\otimes H$ such that for all $x\in H$, $\Delta^{op}(x)R=R\Delta(x)$, then R is called a *universal quasi-R-matrix*; if simultaneously, $(\Delta\otimes\mathrm{id})(R)=R_{13}R_{23}$ and $(\mathrm{id}\otimes\Delta)(R)=R_{13}R_{12}$ are satisfied, then we call H a *quasibraided almost bialgebra* with a *quasi-R-matrix* R (see Ref. 1). Moreover, if H is a bialgebra and R is invertible, then H is called a *braided bialgebra*.

Let H be a bialgebra and C a coalgebra. If C is a left H-module and $\Delta(hc)=\Delta(h)\Delta(c)$ for every $h\in H$ and $c\in C$, then we call the coalgebra C a *left quasi-module-coalgebra* over H. Moreover, if $\varepsilon(hc)=\varepsilon(h)\varepsilon(c)$, then C is called a *left module-coalgebra* over H. Right quasi-module-coalgebra and right module-coalgebra can be defined similarly.

A pair (X,A) of bialgebras over a field k is called *quasimatched* (respectively, *matched*) if there exist linear maps $\alpha: A\otimes X\to X$ and $\beta: A\otimes X\to A$ which turn X into a left A-quasi-module-coalgebra (respectively, a left A-module-coalgebra) and A into a right X-quasi-module-coalgebra (respectively, a right X-module-coalgebra), such that if one sets $\alpha(a\otimes x)=a\triangleright x$, $\beta(a\otimes x)=a\triangleleft x$ then the following conditions are satisfied:

$$a\triangleright(xy)=\sum_{(a)(x)}(a'\triangleright x')((a''\triangleleft x'')\triangleright y), \tag{2.1}$$

$$a \triangleright 1 = \varepsilon(a)1, \tag{2.2}$$

$$(ab) \triangleleft x = \sum_{(b)(x)} (a \triangleleft (b' \triangleright x'))(b'' \triangleleft x''), \tag{2.3}$$

$$1 \triangleleft x = \varepsilon(x)1, \tag{2.4}$$

$$\sum_{(a)(x)} (a' \triangleleft x') \otimes (a'' \triangleright x'') = \sum_{(a)(x)} (a'' \triangleleft x'') \otimes (a' \triangleright x'), \tag{2.5}$$

for all $a, b \in A$ and $x, y \in X$, where 1 is the identity of X and of A, respectively, in (2.2) and (2.4).

For a quasimatched (respectively, matched) pair of bialgebras (X,A), we know from Refs. 1 and 2 that there exists an almost bialgebra (respectively, a bialgebra) structure on the vector space $X \otimes A$ with identity equal to $1 \otimes 1$ such that its product is given by

$$(x \otimes a)(y \otimes b) = \sum_{(a)(y)} x(a' \triangleright y') \otimes (a'' \triangleleft y'')b, \tag{2.6}$$

its coproduct by

$$\Delta(x \otimes a) = \sum_{(a)(x)} (x' \otimes a') \otimes (x'' \otimes a''), \tag{2.7}$$

and its counit by

$$\varepsilon(x \otimes a) = \varepsilon_X(x)\varepsilon_A(a) \tag{2.8}$$

for all $x, y \in X$, $a, b \in A$. Equipped with this almost bialgebra (respectively, bialgebra) structure, $X \otimes A$ is called the *quasi-bicrossed product* (respectively, *bicrossed product*) of X and A, and denoted as $X \infty A$. Furthermore, the injective maps $i_X(x) = x \otimes 1$ and $i_A(a) = 1 \otimes a$ from X and A, respectively, into $X \infty A$ are bialgebra morphisms. Also, $x \infty a = (x \infty 1)(1 \infty a)$ for $a \in A$ and $x \in X$.

III. BIPERFECT WEAK HOPF ALGEBRAS AND QUASI-BICROSSED PRODUCTS

Definition III.1: A weak Hopf algebra H is called (i) a perfect weak Hopf algebra[7] *if its weak antipode T is an anti-bialgebra morphism satisfying* $(\mathrm{id} * T)(H) \subseteq C(H)$ (*the center of H*); (ii) a coperfect weak Hopf algebra *if its weak antipode T is an anti-bialgebra morphism satisfying* $\Sigma_{(x)} x' T(x'') \otimes x''' = \Sigma_{(x)} x'' T(x''') \otimes x'$ *for any* $x \in H$; (iii) a biperfect weak Hopf algebra *if it is perfect and also coperfect.*

From Proposition 1.2 in Ref. 1, we know that if the weak antipode T of a weak Hopf algebra $H = (H, m, u, \Delta, \varepsilon, T)$ is an invertible antialgebra morphism, then $H^{op} = (H, m^{op}, u, \Delta, \varepsilon)$ and $H^{cop} = (H, m, u, \Delta^{op}, \varepsilon)$ are both weak Hopf algebras with weak antipode T^{-1}.

Lemma III.1: Suppose that $H = (H, m, u, \Delta, \varepsilon, T)$ *is a weak Hopf algebra with T invertible, then H is perfect (respectively, coperfect) if and only if* H^{op} (*respectively,* H^{cop}) *is also perfect (respectively, coperfect).*

Proof: When H is coperfect, then $\Sigma_{(x)} x' T(x'') \otimes x''' = \Sigma_{(x)} x'' T(x''') \otimes x'$ for any $x \in H$. Thus,

$$(T \otimes 1) \sum_{(x)} (x'' T^{-1}(x') \otimes x''') = (T \otimes 1) \sum_{(x)} (x''' T^{-1}(x'') \otimes x').$$

It follows that $\Sigma_{(x)}(x'' T^{-1}(x') \otimes x''') = \Sigma_{(x)}(x''' T^{-1}(x'') \otimes x')$ since T is invertible. This means that H^{cop} is coperfect on the weak antipode T^{-1}. It is similar to prove the result in the case that H is perfect.

For a finite dimensional weak Hopf algebra $H=(H,m,u,\Delta,\varepsilon,T)$, we know[1] that $H^*=(H^*,\Delta^*,\varepsilon^*,m^*,u^*,T^*)$ is a weak Hopf algebra with weak antipode T^*.

Lemma III.2: A finite dimensional weak Hopf algebra H is perfect (respectively, coperfect) if and only if its duality H is coperfect (respectively, perfect).*

Proof: "only if": When H is perfect, we need to prove that for $f\in H^*$,

$$\sum_{(f)} f'T^*(f'')\otimes f'''=\sum_{(f)} f''T^*(f''')\otimes f'.$$

In fact, for $a,\ b\in H$,

$$\begin{aligned}\left(\sum_{(f)} f'T^*(f'')\otimes f'''\right)(a\otimes b)&=\sum_{(f)} (f'T^*(f''))(a)f'''(b)\\&=\sum_{(f)(a)} f'(a')T^*(f'')(a'')f'''(b)\\&=\sum_{(f)(a)} f'(a')f''(T(a''))f'''(b)=\sum_{(a)} f(a'T(a'')b)\\&=\sum_{(a)} f(ba'T(a''))=\sum_{(f)(a)} f'(b)f''(a')f'''(T(a''))\\&=\sum_{(f)(a)} f'(b)f''(a')T^*(f''')(a'')=\sum_{(f)} f'(b)(f''T^*(f'''))(a)\\&=\sum_{(f)} (f''T^*(f''')\otimes f')(a\otimes b).\end{aligned}$$

When H is coperfect, we need to prove that $(\mathrm{id}_{H^*}*T^*)(H^*)\subseteq C(H^*)$.

In fact, for $f,\ g\in H^*,\ x\in H$,

$$\begin{aligned}(g(\mathrm{id}_{H^*}*T^*)(f))(x)&=\sum_{(x)} (g(x')(\mathrm{id}_{H^*}*T^*)(f))(x'')\\&=\sum_{(x)} g(x')\Delta^*(\mathrm{id}_{H^*}\otimes T^*)m^*(f)(x'')\\&=\sum_{(x)} g(x')(\mathrm{id}_{H^*}\otimes T^*)m^*(f)(x''\otimes x''')=\sum_{(x)} g(x')m^*(f)(x''\otimes T(x'''))\\&=\sum_{(x)} g(x')f(x''T(x'''))=\sum_{(x)} f(x'T(x''))g(x''')=((\mathrm{id}_{H^*}*T^*)(f)g)(x).\end{aligned}$$

It is easy to see that T^* is an anti-bialgebra morphism from the same fact of T.

"if": It follows from $H\cong H^{**}$.

Corollary III.3: A finite dimensional weak Hopf algebra H is biperfect if and only if its duality H is biperfect.*

Lemma III.4: Suppose that $H=(H,m,u,\Delta,\varepsilon,T)$ is a finite dimensional weak Hopf algebra and its weak antipode T is an invertible anti-bialgebra morphism. Then (i) H is perfect if and only if $(T*\mathrm{id})(H)\subseteq C(H)$; (ii) H is coperfect if and only if $\Sigma_{(x)}T(x')x''\otimes x'''=\Sigma_{(x)}T(x'')x'''\otimes x'$ for any $x\in H$.

Proof: (i) follows from Lemma 1.1 in Ref. 1.

(ii) Similar to the proof of Lemma III.2, we can prove that H satisfies $(T*\mathrm{id})(H)\subseteq C(H)$ if and only if H^* satisfies $\Sigma_{(f)}T^*(f')f''\otimes f'''=\Sigma_{(f)}T^*(f'')f'''\otimes f'$ for $f\in H^*$.

Then H is coperfect if and only if H^* is perfect, if and only if $(T^**\mathrm{id})(H^*)\subseteq C(H^*)$. But $H\cong(H^*)^*$. So, if and only if $\Sigma_{(x)}T(x')x''\otimes x'''=\Sigma_{(x)}T(x'')x'''\otimes x'$ for $x\in H$.

The concept of a Hopf pair of Hopf algebras was introduced by Takeuchi in Ref. 4, which plays a valid role in the study of the theory of quantum groups. Now, we generalize this and introduce some similar concepts corresponding to the weak Hopf algebras.

Definition III.2: (i) Suppose that A and X are weak Hopf algebras with weak antipodes S_A and S_X, respectively. We call (X,A) a weak Hopf pair, if there exists a nonsingular bilinear form $\langle,\rangle$ from $X\otimes A$ to k satisfying

$$\langle x,ab\rangle=\sum_{(x)}\langle x',a\rangle\langle x'',b\rangle, \tag{3.1}$$

$$\langle x,1_A\rangle=\varepsilon(x), \tag{3.2}$$

$$\langle xy,a\rangle=\sum_{(a)}\langle x,a'\rangle\langle y,a''\rangle, \tag{3.3}$$

$$\langle 1_X,a\rangle=\varepsilon(a), \tag{3.4}$$

$$\langle S_X(x),a\rangle=\langle x,S_A(a)\rangle, \tag{3.5}$$

where $x,\ y\in X,\ a,\ b\in A$.

(ii) In (i), moreover, if S_A is invertible and (3.1) and (3.5) are replaced with the following (3.6) and (3.7):

$$\langle x,ab\rangle=\sum_{(x)}\langle x'',a\rangle\langle x',b\rangle, \tag{3.6}$$

$$\langle S_X(x),a\rangle=\langle x,S_A^{-1}(a)\rangle, \tag{3.7}$$

respectively, we call (X,A) a weak Hopf skew-pair.

From Ref. 1, $A^{op}=(A,\mu^{op},\eta,\Delta,\varepsilon,S_A^{-1})$ is a weak Hopf algebra when S_A is invertible. Therefore (X,A) is a weak Hopf skew-pair if and only if (X,A^{op}) is a weak Hopf pair in the case where S_A is invertible.

We know from Ref. 3 that for two perfect weak Hopf algebras A and X with weak antipodes S_A and S_X, respectively, suppose that A is cocommutative, S_A is invertible and (X,A) is a weak Hopf skew-pair, then (X,A) is a quasimatched pair of bialgebra. We want to generalize this result to the case that A is noncocommutative. In fact, we have the following lemma:

Lemma III.5: For two perfect weak Hopf algebras A and X with weak antipodes S_A and S_X, respectively, suppose that S_A is invertible and (X,A) is a weak Hopf skew-pair. Then A and X are both biperfect.

Proof: For $x\in X,\ a,\ b\in A,$ since A is perfect, we have

$$\begin{aligned}\sum_{(x)}\langle x'S_X(x''),a\rangle\langle x''',b\rangle&=\sum_{(x)(a)}\langle x',a'\rangle\langle S(x''),a''\rangle\langle x''',b\rangle\\&=\sum_{(x)(a)}\langle x',a'\rangle\langle x'',S_A^{-1}(a'')\rangle\langle x''',b\rangle=\sum_{(a)}\langle x,bS_A^{-1}(a'')a'\rangle\\&=\sum_{(a)}\langle x,S_A^{-1}(a'')a'b\rangle=\sum_{(x)(a)}\langle x',b\rangle\langle x'',a'\rangle\langle x''',S_A^{-1}(a'')\rangle\\&=\sum_{(x)(a)}\langle x',b\rangle\langle x'',a'\rangle\langle S_X(x'''),a''\rangle=\sum_{(x)}\langle x''S_X(x'''),a\rangle\langle x',b\rangle,\end{aligned}$$

and hence $\Sigma_{(x)}(x'S_X(x'')\otimes x''')=\Sigma_{(x)}(x''S_X(x''')\otimes x')$. It means that X is coperfect.

Similarly, for $x,\ y\in X,\ a\in A,$ since X is perfect, we can prove

$$\sum_{(a)}\langle x,a''S_A^{-1}(a')\rangle\langle y,a'''\rangle=\sum_{(a)}\langle x,a'''S_A^{-1}(a'')\rangle\langle y,a'\rangle.$$

Hence $\Sigma_{(a)}(a''S_A^{-1}(a')\otimes a''')=\Sigma_{(a)}(a'''S_A^{-1}(a'')\otimes a')$. Thus $\Sigma_{(a)}(a'S_A(a'')\otimes a''')=\Sigma_{(a)}\times(a''S_A(a''')\otimes a')$. It follows that A is coperfect.

Theorem III.6: For two perfect weak Hopf algebras A and X with weak antipodes S_A and S_X, respectively, suppose that S_A is invertible and (X,A) is a weak Hopf skew-pair. Then (X,A) is a quasimatched pair of bialgebras with

$$a\triangleright x=\sum_{(x)}\langle x'S_X(x'''),\ a\rangle x'',$$

$$a\triangleleft x=\sum_{(a)}\langle x,\ S_A^{-1}(a''')a'\rangle a''$$

so as to get a quasi-bicrossed product $X\infty A$, denoted as $D(X,A)$.

Proof: First, we can verify easily the following:

$$\langle a\triangleright x,b\rangle=\sum_{(a)}\langle x,S_A^{-1}(a'')ba'\rangle, \tag{3.8}$$

$$\langle y,a\triangleleft x\rangle=\sum_{(x)}\langle x'yS_X(x''),a\rangle \tag{3.9}$$

for $a,\ b\in A,\ x,\ y\in X$.

Now we prove that A and X are a right X-quasi-module coalgebra and a left A-quasi-module coalgebra with the action $\triangleleft$ and $\triangleright$, respectively. In fact, for any $a\in A,\ x,\ y,\ z\in X,$ we have

$$\langle z,a\triangleleft(xy)\rangle=\sum_{(xy)}\langle(xy)''zS_X((xy)'),a\rangle=\sum_{(x)(y)}\langle x''y''zS_X(y')S_X(x'),a\rangle=\langle z,(a\triangleleft x)\triangleleft y\rangle,$$

then $a\triangleleft(xy)=(a\triangleleft x)\triangleleft y$; $\langle z,a\triangleleft 1\rangle=\langle 1zS_X(1),a\rangle=\langle z,a\rangle$, then $a\triangleleft 1=a$. Thus A is a right X-module. On the other hand,

$$\begin{aligned}\left\langle y\otimes z,\sum_{(a)(x)}(a'\triangleleft x')\otimes(a''\triangleleft x'')\right\rangle&=\sum_{(a)(x)}\langle y,a'\triangleleft x'\rangle\langle z,a''\triangleleft x''\rangle\\&=\sum_{(a)(x)}\langle x'yS_X(x''),a'\rangle\langle x'''zS_X(x^{(4)}),a''\rangle\\&=\sum_{(x)}\langle x'yS_X(x'')x'''zS_X(x^{(4)}),a\rangle\\&=\sum_{(x)}\langle x'yzS_X(x''),a\rangle=\langle yz,a\triangleleft x\rangle=\langle y\otimes z,\Delta(a\triangleleft x)\rangle,\end{aligned}$$

then $\Delta(a\triangleleft x)=\Sigma_{(a)(x)}(a'\triangleleft x')\otimes(a''\triangleleft x'')$. It means that A is a right X-quasi-module-coalgebra. Similarly, we get that X is a left A-quasi-module-coalgebra.

Moreover, we can see that (2.2) and (2.4) are trivial according to (3.4) and (3.2) and the definition of $\triangleright$ and $\triangleleft$. And, using Lemma III.5, we have

$$\left\langle \sum_{(a)(x)} (a'\triangleright x')((a''\triangleleft x'')\triangleright y), b \right\rangle = \left\langle \sum_{(a)(x)} (a'\triangleright x')(\langle x'', S_A^{-1}(a^{(4)})a''\rangle a'''\triangleright y), b \right\rangle$$

$$= \sum_{(a)(b)(x)} \langle x'', S_A^{-1}(a^{(4)})a''\rangle\langle (a'\triangleright x'), b'\rangle\langle (a'''\triangleright y), b''\rangle$$

$$= \sum_{(a)(b)(x)} \langle x'', S_A^{-1}(a^{(5)})a'''\rangle\langle x', S_A^{-1}(a'')b'a'\rangle\langle (a^{(4)}\triangleright y), b''\rangle$$

$$= \sum_{(a)(b)} \langle x, S_A^{-1}(a^{(5)})a'''S_A^{-1}(a'')b'a'\rangle\langle (a^{(4)}\triangleright y), b''\rangle$$

$$= \sum_{(a)(b)} \langle x, S_{(A)}^{-1}(a''')b'a'\rangle\langle (a''\triangleright y), b''\rangle$$

$$= \sum_{(a)(b)} \langle x, S_A^{-1}(a^{(4)})b'a'\rangle\langle y, S_A^{-1}(a''')b''a''\rangle$$

$$= \sum_{(a)} \langle xy, S_A^{-1}(a'')ba'\rangle = \langle a\triangleright(xy), b\rangle,$$

then $a\triangleright(xy)=\Sigma_{(a)(x)}(a'\triangleright x')((a''\triangleleft x'')\triangleright y)$, i.e., Eq. (2.1) holds. Similarly, we get that $(ab)\triangleleft x=\Sigma_{(b)(x)}(a\triangleleft(b'\triangleright x'))(b''\triangleleft x'')$, i.e., Eq. (2.3) holds. Moreover,

$$\sum_{(a)(x)} (a'\triangleleft x')\otimes(a''\triangleright x'') = \sum_{(a)(x)} \langle x', S_A^{-1}(a''')a'\rangle a''\otimes\langle x''S_X(x^{(4)}), a^{(4)}\rangle x'''$$

$$= \sum_{(a)(x)} \langle x', S_A^{-1}(a''')a'\rangle\langle x'', a^{(4)}\rangle\langle S_X(x^{(4)}), a^{(5)}\rangle a''\otimes x'''$$

$$= \sum_{(a)(x)} \langle x', a^{(4)}S_A^{-1}(a''')a'\rangle\langle S_X(x'''), a^{(5)}\rangle a''\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'''S_A^{-1}(a'')a'\rangle\langle S_X(x'''), a^{(5)}\rangle a^{(4)}\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle S_X(x'''), a'''\rangle a''\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle x''', S_A^{-1}(a''')\rangle a''\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle x''', S_A^{-1}(a^{(5)})a^{(4)}S_A^{-1}(a''')\rangle a''\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle x''', S_A^{-1}(a^{(5)})a'''S_A^{-1}(a'')\rangle a^{(4)}\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle x''', S_A^{-1}(a'')\rangle\langle x^{(4)}, S_A^{-1}(a^{(5)})a'''\rangle a^{(4)}\otimes x''$$

$$= \sum_{(a)(x)} \langle x', a'\rangle\langle S_X(x'''), a''\rangle\langle x^{(4)}, S_A^{-1}(a^{(5)})a'''\rangle a^{(4)}\otimes x''$$

$$= \sum_{(a)(x)} \langle x' S_X(x'''), a' \rangle \langle x^{(4)}, S_A^{-1}(a^{(4)}) a'' \rangle a''' \otimes x''$$

$$= \sum_{(a)(x)} (a'' \triangleleft x'') \otimes (a' \triangleright x'),$$

then Eq. (2.5) holds. In a word, (X,A) is a quasimatched pair of bialgebras. Hence we get a quasi-bicrossed product $X \infty A$, denoted also as $D(X,A)$.

Note that in this theorem, A is not required to be cocommutative. So, this theorem is a big improvement on the result obtained in Ref. 3.

IV. QUANTUM DOUBLES OF BIPERFECT WEAK HOPF ALGEBRAS

In Theorem III.6, when $A=H$ is a finite dimensional biperfect weak Hopf algebra with invertible weak antipode T, we set $X=H^{*cop}$ and suppose that $\langle , \rangle$ is the bilinear form of H and its dual H^* as linear spaces. It was known in Ref. 1 that $H^{*cop} = (H^*, \Delta^*, \varepsilon^*, (m^*)^{op}, u^*, (T^{*-1}))$. It is easy to see that (H^{*cop}, H) is a weak Hopf skew-pair. Then (H^{*cop}, H) is a quasimatched pair of bialgebras with $a \triangleright f = \Sigma_{(f)} \langle f' T^{*-1}(f'''), a \rangle f''$ and $a \triangleleft f = \Sigma_{(a)} \langle f, T^{-1}(a''') a' \rangle a''$ for $a \in H$ and $f \in H^{*cop}$ so as to get a quasi-bicrossed product $D(H^{*cop}, H) = H^{*cop} \infty H$, denoted briefly as $D(H)$ and called the *quantum double* of H.

Proposition IV.1: Let $H=(H,m,u,\Delta,\varepsilon,T)$ be a finite dimensional biperfect weak Hopf algebra with invertible T. Then the multiplication in $D(H)=H^{*cop} \infty H$ is given by

$$(f \infty a)(g \infty b) = \sum_{(a)} fg(T^{-1}(a''') ? a') \infty a'' b$$

for $f, g \in H^{*cop}$, $a, b \in H$.

Proof:

$$(f \infty a)(g \infty b) = \sum_{(a)(g)} f(a' \triangleright g') \infty (a'' \triangleleft g'') b$$

$$= \sum_{(a)(g)} fg'(T^{-1}(a'') ? a') \infty g''(T^{-1}(a^{(5)}) a''') a^{(4)} b$$

$$= \sum_{(a)} fg(T^{-1}(a^{(5)}) a''' T^{-1}(a'') ? a') \infty a^{(4)} b$$

$$= \sum_{(a)} fg(T^{-1}(a^{(5)}) ? a''' T^{-1}(a'') a') \infty a^{(4)} b = \sum_{(a)} fg(T^{-1}(a''') ? a') \infty a'' b.$$

Now we have the following main result.

Theorem IV.2: *Let $H=(H,m,u,\Delta,\varepsilon,T)$ be a finite dimensional biperfect weak Hopf algebra with invertible T. Then the quantum double $D(H)$ of H is quasibraided equipped with a quasi-R-matrix $R=\Sigma_{i \in I}(1 \infty e_i) \otimes (e^i \infty 1) \in D(H) \otimes D(H)$ where $\{e_i\}_{i \in I}$ is a basis of the k-vector space H together with its dual basis $\{e^i\}_{i \in I}$ in H^{*cop}. Hence R is a solution of the quantum Yang–Baxter equation.*

Proof: For $f \in H^{*cop}$, $a \in H$,

$$\Delta^{op}(f\infty a)R=\sum_{i\in I}\sum_{(f)(a)}(f''\infty a'')(1\infty e_i)\otimes(f'\infty a')(e^i\infty 1)$$

$$=\sum_{i\in I}\sum_{(f)(a)}(f''\varepsilon(T^{-1}(a^{(6)})?a^{(4)})\infty a^{(5)}e_i)\otimes(f'e^i(T^{-1}(a''')?a')\infty a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)}(f''\varepsilon(T^{-1}(a^{(6)}))\varepsilon(a^{(4)})\varepsilon\infty a^{(5)}e_i)\otimes(f'e^i(T^{-1}(a''')?a')\infty a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)}(f''\infty a^{(4)}e_i)\otimes(f'e^i(T^{-1}(a''')?a')\infty a''),$$

$$R\Delta(f\infty a)=\sum_{i\in I}\sum_{(f)(a)}(\varepsilon\infty e_i)(f'\infty a')\otimes(e^i\infty 1)(f''\infty a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)(e_i)}(\varepsilon f'(T^{-1}(e_i''')?e_i')\infty e_i''a')\otimes(e^if''(T^{-1}(1)?1)\infty 1a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)(e_i)}(f'(T^{-1}(e_i''')?e_i')\infty e_i''a')\otimes(e^if''\infty a'').$$

For every $b,\ c\in H,\ u,\ v\in H^{op*}$, let $\xi=b\otimes u\otimes c\otimes v$. Then

$$\langle\Delta^{op}(f\infty a)R,\xi\rangle=\sum_{i\in I}\sum_{(f)(a)}f''(b)u(a^{(4)}e_i)(f'e^i(T^{-1}(a''')?a'))(c)v(a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)(c)}f''(b)u(a^{(4)}e_i)f'(c')e^i(T^{-1}(a''')c''a')v(a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)(c)}f''(b)u(a^{(4)}e^i(T^{-1}(a''')c''a')e_i)f'(c')v(a'')$$

$$=\sum_{(a)(c)}f(bc')u(a^{(4)}T^{-1}(a''')c''a')v(a'')$$

$$=\sum_{(a)(c)}f(bc')u(c''a^{(4)}T^{-1}(a''')a')v(a'')$$

$$=\sum_{(a)(c)}f(bc')u(c''a'''T^{-1}(a'')a')v(a^{(4)})=\sum_{(a)(c)}f(bc')u(c''a')v(a''),$$

$$\langle R\Delta(f\infty a),\xi\rangle=\sum_{i\in I}\sum_{(f)(a)(e_i)}f'(T^{-1}(e_i''')be_i')u(e_i''a')(e^if'')(c)v(a'')$$

$$=\sum_{i\in I}\sum_{(f)(a)(e_i)(c)}f'(T^{-1}(e_i''')be_i')u(e_i''a')e^i(c')f''(c'')v(a'')$$

$$=\sum_{i\in I}\sum_{(a)(e_i)(c)}f(c''T^{-1}(e_i''')be_i')u(e_i''a')e^i(c')v(a'')$$

$$=\sum_{(a)(c)}f(c^{(4)}T^{-1}(c''')bc')u(c''a')v(a'')$$

$$\left(\text{since } \sum_{i\in I}\sum_{(e_i)} e^i(c)e_i'\otimes e_i''\otimes e_i'''=\sum_{(c)} c'\otimes c''\otimes c'''\right)$$

$$=\sum_{(a)(c)} f(c'''T^{-1}(c'')bc')u(c^{(4)}a')v(a'')=\sum_{(a)(c)} f(bc'''T^{-1}(c'')c')u(c^{(4)}a')v(a'')$$

$$=\sum_{(a)(c)} f(bc')u(c''a')v(a'')=\langle\Delta^{op}(f\infty a)R,\xi\rangle.$$

Therefore $\Delta^{op}(f\infty a)R=R\Delta(f\infty a)$. Then $H^{*cop}\infty H$ is an almost quasi-cocommutative almost bialgebra with a universal quasi-R-matrix R.

We can prove in a way similar to the proof of Theorem 2.11 in Ref. 1 that

$$(\Delta\otimes \mathrm{id}_H)(R)=R_{13}R_{23};(\mathrm{id}_H\otimes\Delta)(R)=R_{13}R_{12}.$$

It means that $H^{op*}\infty H$ is quasibraided. Thus, by Proposition 2.8 in Ref. 1, R is a quasi-R-matrix.

Note that since a cocommutative weak Hopf algebra must be coperfect, it means that Theorem IV.2 is a generalization of the one in Ref. 1 on the quantum double of a finite dimensional cocommutative perfect weak Hopf algebra.

It is easy to see that for a finite Clifford monoid $S=\{s_1,\ldots,s_n\}$ (see Refs. 8 and 1), kS is a finite dimensional biperfect weak Hopf algebra with invertible weak antipode T_S satisfying $T_S(s)=s^{-1}$ for $s\in S$. Then by Theorem IV.2, the quantum double $D(kS)$ is quasibraided equipped with a quasi-R-matrix $R=\Sigma_{i=1}^n(1\infty s_i)\otimes(s_i^*\infty 1)\in D(kS)\otimes D(kS)$ where s_i^* is the duality of s_i in $(kS)^{*cop}$. Thus, R is a solution of the quantum Yang–Baxter equation. But, this is also an example of a quantum quasidouble in Theorem 2.11 of Ref. 1 constructed from a finite dimensional cocommutative perfect weak Hopf algebra. So, it is very necessary to find an example of the quantum double from a finite dimensional biperfect weak Hopf algebra with invertible weak antipode which is not cocommutative.

For two biperfect weak Hopf algebras H and K, it is easy to prove that the tensor product $H\otimes K$ is also a biperfect weak Hopf algebra with the comultiplication $\Delta=(I\otimes T\otimes I)(\Delta_H\otimes\Delta_K)$, the multiplication $m=(m_H\otimes m_K)(I\otimes T\otimes I)$, the unit $1=1_H\otimes 1_K$, the counit $\varepsilon=\varepsilon_H\otimes\varepsilon_K$ and the weak antipode $T=T_H\otimes T_K$. $H\otimes K$ is commutative (respectively, cocommutative) if and only if H and K are so.

For a finite noncommutative Clifford monoid S, let $H=kS$ with the weak antipode T_S, then $K=(kS)^*$ is also a finite dimensional biperfect weak Hopf algebra with invertible weak antipode T_S^*. Thus, we get a finite dimensional biperfect weak Hopf algebra $A=kS\otimes(kS)^*$ with invertible weak antipode $T=T_S\otimes T_S^*$, which is indeed not a Hopf algebra unless S is a group. Since kS is noncommutative, $(kS)^*$ is noncocommutative. Hence A is noncommutative and noncocommutative. By Theorem IV.2, the quantum double $D(A)$ of A is quasibraided equipped with a quasi-R-matrix as a solution of the quantum Yang–Baxter equation. This construction is different from that of Theorem 2.11 in Ref. 1. It implies that in Theorem IV.2, the quantum double of a finite dimensional biperfect weak Hopf algebra is indeed a generalization of that of a finite dimensional Hopf algebra.

We know in Ref. 2 that the R-matrix of quantum double of a finite dimensional Hopf algebra is invertible. But, for the quasi-R-matrix in Theorem IV.2, we can only get the regularity as follows.

Proposition IV.3: For a finite dimensional biperfect weak Hopf algebra H with invertible weak antipode T, the quasi-R-matrix $R=\Sigma_{i=1}^n(\varepsilon\infty e_i)\otimes(e_i^*\infty 1)$ of its quantum quasidouble $D(H)$ is a von Neumann regular element in $D(H)\otimes D(H)$ with its inverse $\overline{R}=\Sigma_{i=1}^n(\varepsilon\infty e_i)\otimes(e_i^*T\infty 1)$ where $\{e_1,\ldots,e_n\}$ is a basis of H and $\{e_1^*,\ldots,e_n^*\}$ is the dual basis in H^*.

Proof: For any $\xi=b\otimes u\otimes c\otimes v\in H\otimes H^*\otimes H\otimes H^*$, we have

$$\langle R\overline{R}R,\xi\rangle=\sum_{i,j,l}\varepsilon(b)u(e_ie_je_l)(e_i^*(e_j^*T)e_l^*)(c)v(1)$$

$$=\varepsilon(b)v(1)\sum_{(c)}u\left(\sum_{i=1}^{n}e_ie_i^*(c')\sum_{j=1}^{n}e_je_j^*(T(c''))\sum_{l=1}^{n}e_le_l^*(c''')\right)$$

$$=\varepsilon(b)v(1)u\left(\sum_{(c)}c'T(c'')c'''\right)=\varepsilon(b)v(1)u(c)=\varepsilon(b)v(1)\sum_{i=1}^{n}u(e_i)e_i^*(c)=\langle R,\xi\rangle,$$

then $R\overline{R}R=R$. Similarly, $\langle\overline{R}R\overline{R},\xi\rangle=\langle\overline{R},\xi\rangle$, then $\overline{R}R\overline{R}=\overline{R}$.

For a left $D(H)$-module V, define $C_{V,V}^R$ satisfying $C_{V,V}^R(v\otimes w)=\tau(R(v\otimes w))$ for $v,\ w\in V$, then $C_{V,V}^R$ is a solution of the classical Yang–Baxter equation (see Ref. 7) where τ is the flip map defined as $\tau(v_1\otimes v_2)=v_2\otimes v_1$. From Propositon IV.3, it is easy to prove the following.

Corollary IV.4: For a finite dimensional biperfect weak Hopf algebra H with invertible weak antipode T, let V be a left $D(H)$-module. Then $C_{V,V}^R$ is regular in the endomorphism monoid of $V\otimes V$, with its inverse $C_{V,V}^R$ satisfying $C_{V,V}^R(v\otimes w)=\tau(\overline{R}(v\otimes w))$ for $v,\ w\in V$.

Now we discuss the representation-theoretic interpretation of $D(H)$.

Definition IV.1 (see Ref. 2): For a bialgebra H over k, a crossed H-bimodule V *is a vector space together with linear maps $\mu_V:H\otimes V\to V$ and $\Delta_V:V\to V\otimes H$ such that*

(i) *the map μ_V and Δ_V turn V into a left H-module and a right H-comodule, respectively,*
(ii) $\Sigma_{(a)(\beta)}a'\beta_V\otimes a''\beta_H=\Sigma_{(a)(a''\beta)}(a''\beta)_V\otimes(a''\beta)_Ha'$ *for all $a\in H$ and $\beta\in V$ where we set $\mu_V(a\otimes\beta)=a\beta$ and $\Delta_V(\beta)=\Sigma_{(\beta)}\beta_V\otimes\beta_H$.*

Theorem IV.5: *Suppose H is a finite dimensional biperfect weak Hopf algebra with invertible weak antipode T. Then for a k-linear space V, the following statements are equivalent*:

(i) *V is a left $D(H)$-module*;
(ii) *V is a crossed H-bimodule V and satisfies*

$$\sum_{(a)(\beta)}T^{-1}(a''')a''\beta_H\otimes a'\beta_V=\sum_{(\beta)}\beta_H\otimes a\beta_V \tag{4.1}$$

for all $a\in H$ and $\beta\in V$.

Proof: "(i)⇒(ii)": Let V be a left $D(H)$-module. Since $H^{*cop}\cong H^{*cop}\infty 1$ and $H\cong\varepsilon\infty H$ are subalgebras of $D(H)$, V is a left H-module and also a left H^*-module with $a\beta=(1\infty a)\beta$ and $x\beta=(x\infty 1)\beta$ for $a\in H$, $x\in H^*$, $\beta\in V$. Then, $(ax)(\beta)=a(x\beta)$. But, by Proposition IV.1, we get

$$ax=(1\infty a)(x\infty 1)=\sum_{(a)(x)}\langle x,T^{-1}(a''')?a'\rangle\infty a''=\sum_{(a)(x)}(\langle x,T^{-1}(a''')?a'\rangle\infty 1)(1\infty a'').$$

Hence, $a(x\beta)=\Sigma_{(a)(x)}\langle x,T^{-1}(a''')?a'\rangle(a''\beta)$.

One must show that V can be endowed with a crossed H-bimodule structure. For μ_V, we define $\mu_V(a\otimes\beta)=a\beta$.

Given a basis $\{e_1,\ldots,e_n\}$ of H and the dual basis $\{e_1^*,\ldots,e_n^*\}$ of H^*, note that $x=\Sigma_{i=1}^n x(e_i)e_i^*$ and $a=\Sigma_{i=1}^n e_i^*(a)e_i$ for $x\in H^*$, $a\in H$.

Define $\Delta_V:V\to V\otimes H$ satisfying $\Delta_V(\beta)=\Sigma_i e_i^*\beta\otimes e_i$ for any $\beta\in V$. Consider the dual Δ_V^* of Δ_V, we have that for any $\alpha\in V^*$, $\beta\in V$, $x\in H^*$,

$$\langle\Delta_V^*(\alpha\otimes x),\beta\rangle=\langle\alpha\otimes x,\Delta_V(\beta)\rangle=\sum_{i=1}^{n}\langle\alpha,e_i^*\beta\rangle\langle x,e_i\rangle=\left\langle\alpha,\left(\sum_{i=1}^{n}\langle x,e_i\rangle e_i^*\right)\beta\right\rangle=\langle\alpha,x\beta\rangle;$$

in particular, for $x=\varepsilon$ (the identity of H^*) and any $\beta\in V$,

$$\langle \Delta_V^*(\alpha\otimes\varepsilon),\beta\rangle=\langle \alpha,\beta\rangle.$$

Then $\Delta_V^*(\alpha\otimes\varepsilon)=\alpha$. It follows that, for any $y\in H^*$,

$$\langle \Delta_V^*(\Delta_V^*(\alpha\otimes x)\otimes y),\beta\rangle=\langle \Delta_V^*(\alpha\otimes x),y\beta\rangle=\langle \alpha,x(y\beta)\rangle=\langle \Delta_V^*(\alpha\otimes xy),\beta\rangle,$$

then $\Delta_V^*(\Delta_V^*(\alpha\otimes x)\otimes y)=\Delta_V^*(\alpha\otimes xy)$. Hence V^* is a right H^*-module under the action Δ_V^*. Therefore, dually, V becomes a right H-comodule under the coaction Δ_V.

For $a\in H$, $\beta\in V$, $x\in H^{*cop}$, we have

$$\begin{aligned}(\mathrm{id}\otimes x)\Big(\sum_{(a)(\beta)} a'\beta_V\otimes a''\beta_H\Big)&=\sum_{(a)}\sum_{i=1}^{n} a'(e_i^*\beta)x(a''e_i)=\sum_{(a)(x)}\sum_{i=1}^{n} a'(e_i^*\beta)x'(e_i)x''(a'')\\&=\sum_{(a)(x)} a'(x'\beta)x''(a'')=\sum_{(a)(x)} x''(a^{(4)})x'(T^{-1}(a''')?a')(a''\beta)\\&=\sum_{(a)} x(a^{(4)}T^{-1}(a''')?a')(a''\beta)=\sum_{(a)} x(?a'''T^{-1}(a'')a')(a^{(4)}\beta)\\&=\sum_{(a)} x(?a')(a''\beta)=\sum_{(a)(x)} x'(a')x''(a''\beta)\\&=\sum_{(a)(x)}\sum_{i=1}^{n} x'(a')x''(e_i)e_i^*(a''\beta)\\&=\sum_{(a)}\sum_{i=1}^{n} x(e_ia')e_i^*(a''\beta)=(\mathrm{id}\otimes x)\Big(\sum_{(a)}\sum_{i=1}^{n} e_i^*(a''\beta)\otimes e_ia'\Big)\\&=(\mathrm{id}\otimes x)\Big(\sum_{(a''\beta)(a)}(a''\beta)_V\otimes(a''\beta)_Ha'\Big).\end{aligned}$$

It follows that

$$\sum_{(a)(\beta)} a'\beta_V\otimes a''\beta_H=\sum_{(a''\beta)(a)}(a''\beta)_V\otimes(a''\beta)_Ha'. \tag{4.2}$$

Hence by Definition IV.1, V is a crossed H-bimodule.

Now, we prove the formula (4.1). With the μ_V and Δ_V as defined above, we have proved that for any $\alpha\in V^*$, $\beta\in V$, $x\in H^*$, $\langle \Delta_V^*(\alpha\otimes x),\beta\rangle=\langle \alpha,x\beta\rangle$. But,

$$\langle \Delta_V^*(\alpha\otimes x),\beta\rangle=\langle \alpha\otimes x,\beta_V\otimes\beta_H\rangle=\langle \alpha,\beta_V\rangle\langle x,\beta_H\rangle=\langle \alpha,\langle x,\beta_H\rangle\beta_V\rangle.$$

So, it follows

$$x\beta=\langle x,\beta_H\rangle\beta_V. \tag{4.3}$$

And, since V is a $D(H)$-module, we have $a(x\beta)=(ax)\beta$. However, by the formula (4.3), $a(x\beta)=\Sigma_{(\beta)}\langle x,\beta_H\rangle a\beta_V$; and by the formulas (4.3) and (4.2),

$$(ax)\beta=\left(\sum_{(a)}\langle x,T^{-1}(a''')?a'\rangle\infty a''\right)\beta=\left(\sum_{(a)}\langle x,T^{-1}(a''')?a'\rangle a''\right)\beta$$

$$=\sum_{(a)}\langle x,T^{-1}(a''')?a'\rangle(a''\beta)=\sum_{(a)(x)}\langle x''',T^{-1}(a''')\rangle\langle x',a'\rangle x''(a''\beta)$$

$$=\sum_{(a)(x)(a''\beta)}\langle x''',T^{-1}(a''')\rangle\langle x'',(a''\beta)_H\rangle\langle x',a'\rangle(a''\beta)_V$$

$$=\sum_{(a)(a''\beta)}\langle x,T^{-1}(a''')(a''\beta)_Ha'\rangle(a''\beta)_V=\sum_{(a)(\beta)}\langle x,T^{-1}(a''')a''\beta_H\rangle a'\beta_V.$$

Hence, for any $x\in H^{*cop}$, $\Sigma_{(\beta)}\langle x,\beta_H\rangle a\beta_V=\Sigma_{(a)(\beta)}\langle x,T^{-1}(a''')a''\beta_H\rangle a'\beta_V$. Then the formula (4.1) follows.

"(ii)⇒(i)": Say that V is a crossed H-bimodule about μ_V and Δ_V. Then, V is a left H-module about μ_V and a right H-comodule about Δ_V. Write $\mu_V(a\otimes\beta)=a\beta$ for $a\in H$, $\beta\in V$. For $x\in H^*$, $\beta\in V$, let $x\beta=\Sigma_{(\beta)}\langle x,\beta_H\rangle\beta_V$, where $\Delta_V(\beta)=\Sigma_{(\beta)}\beta_V\otimes\beta_H$. Since Δ_V is a right coaction, it is easy to show that $(xy)\beta=x(y\beta)$ for $y\in H^*$. Then it follows that V is a left H^{*cop}-module.

Set $(xa)\beta=x(a\beta)$ for $x\in H^{*cop}$, $a\in H$, $\beta\in V$. Then, by (4.1),

$$a(x\beta)=\sum_{(\beta)}\langle x,\beta_H\rangle a\beta_V=\sum_{(a)(\beta)}\langle x,T^{-1}(a''')a''\beta_H\rangle a'\beta_V=(ax)\beta,$$

where the first equality follows from (4.3), the second from (4.1) and the third from (4.3) and (4.2) as proved in "(i)⇒(ii)."

Therefore, V becomes a left $D(H)$-module since H and H^{*cop} are subalgebras of $D(H)$ and the multiplication of $D(H)$ is determined by the interaction of H and H^{*cop}.

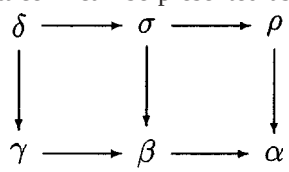
V. EXAMPLES FROM MATRIX GROUPS

Now, we give some examples from a concrete Clifford monoid. The definition of a Clifford semigroup/monoid can be found in Refs. 8 and 1.

Let $Y=\{\alpha,\beta,\gamma,\rho,\sigma,\delta\}$ be the semilattice with multiplication "$\cdot$" given by the following table:

$\cdot$	α	β	γ	ρ	σ	δ
α	α	α	α	α	α	α
β	α	β	β	α	β	β
γ	α	β	γ	α	β	γ
ρ	α	α	α	ρ	ρ	ρ
σ	α	β	β	ρ	σ	σ
δ	α	β	γ	ρ	σ	δ

The partial order in the semilattice Y can be presented as the diagram below:



Obviously, δ is the identity of Y.

For a ring R with identity, $R^{2\times 2}$ denotes the 2×2 full matrix ring over R, $U(R)$ the group consisting of all units in R. Let Z be the integer number ring. For a prime number p, Z_p is a field and $U(Z_p^{2\times 2})$ is just the 2×2 general linear group $GL_2(Z_p)$ over Z_p. Assume that $G_\alpha=\{e_\alpha\}$ and $G_\delta=\{e_\delta\}$ are the trivial groups, $G_\beta=GL_2(Z_2)$, $G_\gamma=U(Z_4^{2\times 2})$, $G_\rho=GL_2(Z_3)$, $G_\sigma=U(Z_6^{2\times 2})$. Then $G_u\cap G_v=\varnothing$ for any $u,v\in Y$, $u\neq v$. Set $S=\cup_{u\in Y}G_u$. We will define a multiplication on S such that $S=\cup_{u\in Y}G_u$ becomes a Clifford monoid related to the semilattice Y.

First, we mention the fact that over a commutative ring R with identity, an $m\times m$ matrix X is invertible if and only if $\det X$ is a unit in R.

Then, for $n=2,3,4,6$, $X=\left[\begin{smallmatrix} x & y \\ a & b\end{smallmatrix}\right]\in U(Z_n^{2\times 2})$ if and only if $\det X=xb-ay\in U(Z_n)$. It is easy to see $U(Z_6)=\{\overline{1},\overline{5}\}$, $U(Z_4)=\{\overline{1},\overline{3}\}$, $U(Z_3)=\{\overline{1},\overline{2}\}$, $U(Z_2)=\{\overline{1}\}$.

A ring homomorphism $\pi_{\sigma,\rho}:Z_6\to Z_3$ can be defined which satisfies $\pi_{\sigma,\rho}(\overline{0})=\overline{0}$, $\pi_{\sigma,\rho}(\overline{1})=\overline{1}$, $\pi_{\sigma,\rho}(\overline{2})=\overline{2}$, $\pi_{\sigma,\rho}(\overline{3})=\overline{0}$, $\pi_{\sigma,\rho}(\overline{4})=\overline{1}$, and $\pi_{\sigma,\rho}(\overline{5})=\overline{2}$.

For $X=\left[\begin{smallmatrix} x & y \\ a & b\end{smallmatrix}\right]\in U(Z_6^{2\times 2})=G_\sigma$, we have $\det X=xb-ay=\overline{1}$, or $\overline{5}$, then

$$\pi_{\sigma,\rho}(x)\pi_{\sigma,\rho}(b)-\pi_{\sigma,\rho}(a)\pi_{\sigma,\rho}(y)=\overline{1},\ \text{or}\ \overline{2}.$$

It follows

$$\begin{bmatrix} \pi_{\sigma,\rho}(x) & \pi_{\sigma,\rho}(y) \\ \pi_{\sigma,\rho}(a) & \pi_{\sigma,\rho}(b)\end{bmatrix}\in GL_2(Z_3)=G_\rho.$$

Thus, we can expand $\pi_{\sigma,\rho}$ to make it a group homomorphism from G_σ to G_ρ. For this, it is enough to define $\pi_{\sigma,\rho}:G_\sigma\to G_\rho$ satisfying

$$\pi_{\sigma,\rho}\begin{bmatrix} x & y \\ a & b\end{bmatrix}=\begin{bmatrix} \pi_{\sigma,\rho}(x) & \pi_{\sigma,\rho}(y) \\ \pi_{\sigma,\rho}(a) & \pi_{\sigma,\rho}(b)\end{bmatrix}$$

since

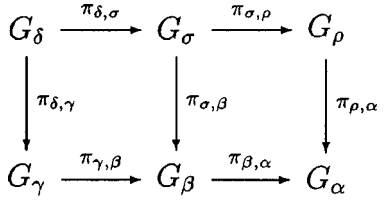
$$\pi_{\sigma,\rho}\left(\begin{bmatrix} x_1 & y_1 \\ a_1 & b_1\end{bmatrix}\begin{bmatrix} x_2 & y_2 \\ a_2 & b_2\end{bmatrix}\right)=\pi_{\sigma,\rho}\begin{bmatrix} x_1 & y_1 \\ a_1 & b_1\end{bmatrix}\pi_{\sigma,\rho}\begin{bmatrix} x_2 & y_2 \\ a_2 & b_2\end{bmatrix}$$

can be shown easily using the fact that $\pi_{\sigma,\rho}$ is a ring homomorphism from Z_6 to Z_3.

Note that $\pi_{\sigma,\rho}(\overline{5})=\overline{2}\in U(Z_3)$, so $\pi_{\sigma,\rho}$ is an epimorphism from G_σ to G_ρ.

Similarly, the ring homomorphisms $\pi_{\sigma,\beta}:Z_6\to Z_2$ and $\pi_{\gamma,\beta}:Z_4\to Z_2$ can be defined respectively satisfying $\pi_{\sigma,\beta}(\overline{0})=\overline{0}$, $\pi_{\sigma,\beta}(\overline{1})=\overline{1}$, $\pi_{\sigma,\beta}(\overline{2})=\overline{0}$, $\pi_{\sigma,\beta}(\overline{3})=\overline{1}$, $\pi_{\sigma,\beta}(\overline{4})=\overline{0}$, $\pi_{\sigma,\beta}(\overline{5})=\overline{1}$ and $\pi_{\gamma,\beta}(\overline{0})=\overline{0}$, $\pi_{\gamma,\beta}(\overline{1})=\overline{1}$, $\pi_{\gamma,\beta}(\overline{2})=\overline{0}$, $\pi_{\gamma,\beta}(\overline{3})=\overline{1}$. Moreover, the group homomorphisms $\pi_{\sigma,\beta}:G_\sigma\to G_\beta$ and $\pi_{\gamma,\beta}:G_\gamma\to G_\beta$ can be constructed in a similar way.

Finally, we define $\pi_{\beta,\alpha}:G_\beta\to G_\alpha$, $\pi_{\rho,\alpha}:G_\rho\to G_\alpha$, $\pi_{\delta,\sigma}:G_\delta\to G_\sigma$, $\pi_{\delta,\gamma}:G_\delta\to G_\gamma$ as the trivial group homomorphisms. Then one has the following diagram:



Now, we introduce the multiplication "$\cdot$" in S by $XW=\pi_{u,uv}(X)\pi_{v,uv}(W)$ if $X\in G_u$ and $W\in G_v$ for $u,v\in Y$. Then, with this multiplication, $S=\cup_{u\in Y}G_u$ becomes a Clifford monoid related to the semilattice Y, and the only element e_δ of G_δ is the identity of S.

Obviously, S is a finite and noncommutative Clifford monoid. Then for the cocommutative weak Hopf algebra kS we may obtain the quantum double $D(S)$ and its quasi-R-matrix R by using the result in Ref. 1. We have the decomposition of linear spaces as follows:

$$D(S)=(kS)^{op*}\infty(kS)=(\oplus_{u\in Y}kG_u)^{op*}\infty(\oplus_{u\in Y}kG_u)=\oplus_{u,v\in Y}((kG_u)^{op*}\infty(kG_v)),$$

where $(kG_u)^{op*}\infty(kG_v)$ means a direct summand of $D(S)$ and ∞ is the same in $D(S)$ since $(kS)^{op*}=\oplus_{u\in Y}(kG_u)^{op*}$ and $kS=\oplus_{u\in Y}kG_u$ such that for each $u\in Y$, $(kG_u)^{op*}$ is embedded into $(kS)^{op*}$ and kG_u is embedded into kS.

Any $\varphi\in(kG_u)^{op*}$ can be expanded to $\overline{\varphi}\in(kS)^{op*}$ satisfying $\overline{\varphi}(U+V)=\varphi(U)$ for any element $U+V$ of $kS=\oplus_{v\in Y}kG_v$ where $U\in kG_u$ and $V\in\oplus_{v\neq u}kG_v$.

Let $u_1, u_2, v_1, v_2\in Y$, $X\in G_{v_1}$, $W\in G_{v_2}$, $A\in G_{u_1}$, $B\in G_{u_2}$. Then their dual elements ϕ_A and ϕ_B of A and B are in $(kG_{u_1})^{op*}$ and $(kG_{u_2})^{op*}$, respectively, where

$$\phi_A(C)=\begin{cases}0 & \text{if } C\in G_{u_1},\quad C\neq A\\ 1 & \text{if } C=A\end{cases}$$

and ϕ_B is given similarly.

The multiplication of $D(S)$ can be presented by

$$(\phi_A\infty X)(\phi_B\infty W)=(\overline{\phi_A}\infty X)(\overline{\phi_B}\infty W)=\overline{\phi_A}\ \overline{\phi_B}(X^{-1}?X)\infty XW,$$

where

$$\overline{\phi_A}\ \overline{\phi_B}(X^{-1}?X)=\begin{cases}0 & \text{if } X^{-1}AX\neq B,\\ \overline{\phi_A}=\phi_A & \text{if } X^{-1}AX=B.\end{cases}$$

By Ref. 1, the quasi-R-matrix of $D(S)$ is

$$R=\sum_{s\in S}(1\infty s)\otimes_k(\overline{\phi_s}\infty 1)=\sum_{u\in Y}\sum_{g_u\in G_u}(1\infty g_u)\otimes_k(\phi_{g_u}\infty 1)\in D(S)\otimes D(S).$$

From $U(Z_6)=\{\overline{1},\overline{5}\}$, $U(Z_4)=\{\overline{1},\overline{3}\}$, $U(Z_3)=\{\overline{1},\overline{2}\}$, $U(Z_2)=\{\overline{1}\}$ and the fact that $X=\left[\begin{smallmatrix}x & y\\ a & b\end{smallmatrix}\right]\in U(Z_n^{2\times 2})$ if and only if $\det X=xb-ay\in U(Z_n)$, it is easy to compute $|G_u|$ for each $u\in Y$. We have $|G_\delta|=1,|G_\alpha|=1,|G_\beta|=6,|G_\gamma|=96,|G_\rho|=48,|G_\sigma|=288$. It follows that the number of monomials of R of $D(S)$ is $|S|=|G_\delta|+|G_\alpha|+|G_\beta|+|G_\gamma|+|G_\rho|+|G_\sigma|=440$. Therefore, from the Clifford monoid $S=\cup_{u\in Y}G_u$ we have constructed an example of the quantum doubles of cocommutative weak Hopf algebras in Ref. 1.

In the following we give an example of the quantum doubles of perfect (noncocommutative) weak Hopf algebras.

For the Clifford monoid S above, $H=kS\otimes(kS)^*$ is a finite dimensional noncommutative and noncocommutative biperfect weak Hopf algebra with invertible weak antipode $T=T_S\otimes T_S^*$ satisfying $T_S(X)=X^{-1}$ and $T_S^*(f)(X)=f(T_S(X))$ for any matrix $X\in S$ and $f\in(kS)^*$. The dimension of H is $\dim H=\dim(kS\otimes(kS)^*)=|S|^2=193\,600$. The quantum double is given by

$$D(H)=H^{op*}\infty H=(kS\otimes(kS)^*)^{op*}\infty(kS\otimes(kS)^*)=((kS)^{op*}\otimes(kS)^{cop})\infty(kS\otimes(kS)^*)$$

$$=((kS)^{op*}\otimes kS)\infty(kS\otimes(kS)^*)=\sum_{u,v,p,q\in Y}((kG_u)^{op*}\otimes kG_v)\infty(kG_p\otimes(kG_q)^*),$$

where $kG_p\otimes(kG_q)^*$ and $(kG_u)^{op*}\otimes kG_v$ are as subspaces of $kS\otimes(kS)^*$ and $(kS)^{op*}\otimes kS$. The multiplication of $D(S)$ obeys the formula in Proposition IV.1.

The quasi-R-matrix of $D(H)$ is

$$R=\sum_{p,q\in Y}\ \sum_{g_p\in G_p,g_q\in G_q}((1\otimes 1)\infty(g_p\otimes\phi_{g_q}))\otimes((\phi_{g_p}\otimes g_q)\infty(1\otimes 1)),$$

whose number of monomials is $|S|^2=193\,600$.

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Analyticity of the SRB measure of a lattice of coupled Anosov diffeomorphisms of the torus

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We consider the ''thermodynamic limit'' of a d-dimensional lattice of hyperbolic dynamical systems on the 2-torus, interacting via weak and nearest neighbor coupling. We prove that the SRB measure is analytic in the strength of the coupling. The proof is based on symbolic dynamics techniques that allow us to map the SRB measure into a Gibbs measure for a spin system on a $(d+1)$-dimensional lattice. This Gibbs measure can be studied by an extension (decimation) of the usual ''cluster expansion'' techniques. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND MAIN RESULTS

In recent years a lot of attention has been devoted to the relation between nonequilibrium statistical mechanics and dynamical systems theory. According to the point of view of Ruelle, Cohen, and Gallavotti,[21,11] a mechanical system evolving in a steady state can be described by a hyperbolic dynamical system and its properties can be deduced from the ''natural'' or SRB distribution (see below for a precise definition) associated with this dynamical system. This line of investigation has already produced several interesting results both analytical, like the ''Fluctuation Theorem'' (see Ref. 11), or numerical, like the works of Evans and Morris (see Ref. 8) and Moran and Hoover (see Ref. 18). Nonetheless, most of the work has been devoted to low dimensional dynamical system, due to their accessibility both to analytical and to numerical study. In this paper we want to study the properties of the SRB distribution for a class of simple systems in very high dimension. For more references on this kind of systems see Ref. 17. The precise model we study here is taken from Ref. 2.

We start considering a linear hyperbolic automorphism of the two-torus $\mathbb{T}^2$. To be definite, we will always consider the so called *Arnold cat map* s_0: $\mathbb{T}^2 \to \mathbb{T}^2$ defined by the action modulus 2π of the matrix

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}. \tag{1.1}$$

Note that the matrix A admits two orthogonal eigenvectors $v_\pm$ whose respective eigenvalues $\lambda_\pm$ are such that $\lambda_+ > 1 > \lambda_-$ and $\lambda_+ \lambda_- = 1$. For this reason the dynamical system s_0 is uniformly hyperbolic and the stable and unstable manifolds at any point $\phi \in \mathbb{T}^2$ are given by $W^\pm_\phi(t) = \phi + v_\pm t \bmod 2\pi$.

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From s_0 we can construct the *uncoupled* lattice dynamics by considering as phase space the Cartesian product $\mathcal{T}=(\mathbb{T}^2)^{\mathbb{Z}^d}$ (namely any point $\psi\in\mathcal{T}$ has Cartesian components $\{\psi_\xi\}_{\xi\in\mathbb{Z}^d}$), equipped with the metric $d(\psi,\psi')=\Sigma_\xi 2^{-|\xi|}\hat{d}(\psi_\xi,\psi'_\xi)$ where $\hat{d}(\psi_\xi,\psi'_\xi)$ is the usual metric on $\mathbb{T}^2$ and $|\xi|=\Sigma_{i=1}^d|\xi_i|$ for $\xi\in\mathbb{Z}^d$. On $\mathcal{T}$ the map S_0 acts simply as

$$S_0^\xi(\psi)=(S_0(\psi))_\xi=s_0(\psi_\xi). \tag{1.2}$$

Note that the stable and unstable manifold of S_0 at a point ψ are the Cartesian product of the stable and unstable manifold of s_0 for the points $\psi_\xi\in\mathbb{T}^2$, i.e., $W^\pm_{0,\psi}(\zeta)=\psi+\Sigma_\xi w^{(\xi)}_{0,\pm}\zeta_\xi \bmod 2\pi$, where $w^{(\xi)}_{0,\pm}$ is the tangent vector to $\mathcal{T}$ that has null component on the tangent space to every $\mathbb{T}^2_\eta$ but for $\mathbb{T}^2_\xi$ where it coincides with $v_\pm$. The action of S_0 on $W^\pm(\psi)$ is naturally given by a diagonal linear transformation.

We observe that the special choice of the matrix A plays no role in the following. Indeed we will show in Appendix A that our results stay true if we replace s_0 with any uniformly hyperbolic analytic automorphism of $\mathbb{T}^2$, not necessarily linear.

To add a coupling to this system we consider an analytic function g: $\mathcal{T}\to\mathbb{T}^2$ and define

$$S^\xi_\epsilon(\psi)\overset{def}{=}s_0(\psi_\xi)+\epsilon g(\rho^\xi\psi)\overset{def}{=}s_0(\psi_\xi)+\epsilon f^\xi(\psi), \tag{1.3}$$

where $(\rho^\xi\psi)_\eta=\psi_{\eta+\xi}$, i.e., ρ is the group of the translations on $\mathbb{Z}^d$. This means that the function f: $\mathcal{T}\to\mathcal{T}$, whose ξ component is $f^\xi=g\circ\rho^\xi$, is translation invariant. We want f to be short ranged: let the nearest neighbor sites of the site ξ be $nn(\xi)=\{\eta:|\xi-\eta|\leqslant 1\}$; we will assume that g depended only on $\psi_{nn(0)}$, where we have used the notation $\psi_V=\{\psi_\xi|\xi\in V\}$ for $V\subset\mathbb{Z}^d$. This implies that $S^\xi_\epsilon(\psi)$ depends only on $\psi_{nn(\xi)}$. More generally we could have assumed that g depends only on ψ_V where V is any finite subset of $\mathbb{Z}^d$ containing 0 but this would not have changed the substance of the following arguments. Moreover, we will take g analytic in all its arguments.

The dynamical system S_ϵ admits many invariant measures. Among them is the "natural" or SRB measure defined as the weak limit of the volume measure on $\mathcal{T}$ under the evolution defined by S_ϵ, when such a limit exists and is ergodic. Being that $\mathcal{T}$ is infinite dimensional, to properly define this concept we will consider finite dimensional approximations. Let $\mathcal{T}_N=(\mathbb{T}^2)^{V_N}$ where V_N is the cube of side $2N+1$ in $\mathbb{Z}^d$ centered at the origin. To define the restriction of S_ϵ to $\mathcal{T}_N$ we have to fix the boundary conditions: we choose periodic ones. To this extent note that $\mathcal{T}_N$ can be naturally identified with the submanifold of $\mathcal{T}$ formed by the points periodic of period $2N+1$. Moreover S_ϵ leaves such a manifold invariant so that we can define $S_{\epsilon,N}\overset{def}{=}S_\epsilon|_{\mathcal{T}_N}$. If no confusion can arise, we will suppress the index N.

We can now define the SRB measure for $S_{\epsilon,N}$ as $\mu_N^{\mathrm{SRB}}=\lim_{T\to\infty}(1/T)\Sigma_{t=0}^{T-1}(S^*_{\epsilon,N})^t\mu_N^0$ where the limit must be understood as a weak limit and $\mu_N^0=\Pi_{\xi\in V_N}d\psi_\xi/(2\pi)^2$ is the Lebesgue measure on $\mathcal{T}_N$. The existence of such a measure follows from rather general theorem on hyperbolic dynamical systems, if ϵ is sufficiently small (see, for example, Ref. 10 and references there). Moreover, μ_N^{SRB} is ergodic, always for small ϵ, and we have that $\mu_N^{\mathrm{SRB}}(\mathcal{O})=\lim_{T\to\infty}(1/T)\Sigma_{t=0}^{T-1}\mathcal{O}(S^t_\epsilon(\psi))$ for μ_N^0 almost every ψ, where $\mathcal{O}$ is an *observable*, i.e., a Holdër continuous function from $\mathcal{T}_N$ to $\mathbb{R}$. This means that μ_N^{SRB} is the *statistic* of S_ϵ. It is well known that the SRB measure is still well defined in the limit $N\to\infty$, for ϵ small enough. This was first proved by Bunimovich and Sinai in Ref. 6. Starting from this work, the model Eq. (1.3) (or similar models of coupled expanding automorphisms of the circle) has been widely studied in the literature (see for instance Refs. 19, 3–5, 16, 17, 1, and 15). Many properties of such systems are well known, mainly uniqueness of the SRB state in the thermodynamic limit and exponential decay of correlations (see Refs. 3–5 for a proof of these properties).

We further investigate the regularity properties of the limiting measure. We show that μ_N^{SRB} depends analytically on ϵ. This means that if we consider an analytic observable $\mathcal{O}$, i.e., an analytic function from $\mathcal{T}_N$ to $\mathbb{R}$, we have that $\mu_N^{\mathrm{SRB}}(\mathcal{O})$ is an analytic function in a domain that depends on the analyticity properties of $\mathcal{O}$.

The main point of this work is to show that such a property remains true when $N\to\infty$, i.e., we want to show that the domain of analyticity of μ_N^{SRB} does not shrink to 0 when $N\to\infty$. More precisely we say that $\mathcal{O}$: $\mathcal{T}\to\mathbb{R}$ is a *local observable* if it depends only on ψ_V for some finite $V\subset\mathbb{Z}^d$. We can summarize our main results as follows

Theorem: *Given S_ϵ as above and a local observable $\mathcal{O}$ we have*

(1) $\mu^{\mathrm{SRB}}(\mathcal{O})=\lim_{N\to\infty}\mu_N^{\mathrm{SRB}}(\mathcal{O})$ exists uniformly in ϵ for $\epsilon<\epsilon_0$ independent on $\mathcal{O}$, and

(2) if $\mathcal{O}$ is local and analytic, then $\mu^{\mathrm{SRB}}(\mathcal{O})$ is analytic in ϵ for $\epsilon<\epsilon_0(\mathcal{O})$.

The proof is mainly based on the possibility of mapping the SRB distribution into the Gibbs state of a suitable spin system on $\mathbb{Z}^{d+1}$ and on the extension of classical techniques used to study such Gibbs states (i.e., cluster expansion) to the particular ones that occur in our system. The key point in order to get analyticity of the measure is proving that the SRB potentials (i.e., the potentials of the Gibbs state the SRB measure is mapped into) are rapidly decaying. Once this decay is proved, analyticity follows via standard techniques. Analyticity of the measure and convergence of cluster expansion imply in particular uniqueness of the Gibbs measure and exponential decay in space and time of the correlations of Hölder continuous observables (see for instance Ref. 10). Our proof can also be adapted to the case of coupled analytic expanding circle map: in fact, also, these models can be mapped into spin systems, and proceeding as below one can prove that the SRB potentials satisfy the same decaying properties.

The rest of the paper is organized as follows. In Sec. II we give a brief review of the main properties of smooth uniformly hyperbolic systems and we briefly describe the construction that allows the above quoted mapping. The detailed proofs of this properties are postponed to Secs. III–V. Finally, in Sec. VI, we complete the proof of the main theorem. Appendix A contain a direct extension of our results to the case in which the uncoupled dynamics is not linear. Appendix B deals with an application. In the contest of the physical application of dynamical systems (see the beginning of this Introduction) a special status has been given to a particular observable, the *phase space contraction rate* defined as $\eta_+(\psi)=\log|\det(DS_\epsilon(\psi))|$ where DS_ϵ is the differential of S_ϵ. Being that our system is infinite, it is more interesting to study the *local* phase space contraction rate $\eta_V(\psi)$ defined by taking the determinant of a (large) minor of DS_ϵ. We show, for a large class of couplings f, that η_V has a positive average and that it obeys a large deviation principle, i.e., its large deviations are asymptotically described by a free energy functional.

II. ANOSOV SYSTEMS

A. Geometric properties

A dynamical system on a smooth compact manifold, whose dynamics is given by a uniformly hyperbolic invertible map, is called an *Anosov system*. From the general theory we know that Anosov systems are structurally stable, namely, given two Anosov diffeomorphisms S, S' on a manifold Ω that are sufficiently close in the C^2 topology, there exist a *conjugation H:* $\Omega\leftrightarrow\Omega$ such that $S\circ H=H\circ S'$.

In our situation this implies the existence of a map h_ϵ: $\mathcal{T}_N\leftrightarrow\mathcal{T}_N$ such that

$$S_\epsilon\circ h_\epsilon=h_\epsilon\circ S_0, \tag{2.1}$$

at least if ϵ is small enough (*a priori* not uniformly in N). The first step of our proof consists in showing that h_ϵ is analytic in ϵ uniformly in N. More precisely, we will construct h_ϵ directly for $N=\infty$. Its finite N version can be obtained by restricting it to $\mathcal{T}_N$. We note that h_ϵ is, in general, only Holdër continuous in the variable ψ. By this we mean that there exist constant c and β such that $d(h_\epsilon(\psi),h_\epsilon(\psi'))\leq c\,d(\psi,\psi')^\beta$. For this reason we cannot say that the SRB measure of S_ϵ is just the image under the map h_ϵ of the SRB measure for S_0, i.e., of the Lebesgue measure on $\mathbb{T}^2$. Notwithstanding, h_ϵ will play a crucial role in the construction on μ_N^{SRB}.

As we saw in the Introduction the tangent space $T_\psi\mathcal{T}$ to $\mathcal{T}$ on a point ψ can be split in two subspaces E^+_ψ and E^-_ψ such that $T_\psi\mathcal{T}=E^+_\psi\oplus E^-_\psi$. Moreover, the distributions $E^\pm$ are continuous and invariant under S_0, i.e., $(DS_0E^\pm_\psi)=E^+_{S_0\psi}$ and we have

$$\begin{aligned}\|DS_0^n w\|&\leqslant C\lambda_-^n\|w\| \quad \text{for } w\in E^-_\psi,\\ \|DS_0^{-n} w\|&\leqslant C\lambda_+^{-n}\|w\| \quad \text{for } w\in E^+_\psi.\end{aligned} \tag{2.2}$$

E^+_ψ and E^-_ψ are called the *stable* and *unstable* subspaces, respectively. In the case of S_0 all these properties are trivially true. In particular we can consider on $E^\pm_\psi$ the basis formed by the vectors $\{w^{(\xi)}_{0,\pm}\}_{\xi\in\mathbb{Z}^d}$.

We will show in Sec. IV that such a splitting can be constructed also for S_ϵ, again uniformly in N, i.e., we will prove the existence of the stable and unstable subspaces $E^\pm_{\epsilon,\psi}$ for S_ϵ. Moreover, we will show that $E^\pm_{\epsilon,h_\epsilon(\psi)}$ is an analytic function of ϵ, although it is only Holdër continuous in ψ. This will turn out to be the right regularity to study the SRB measure. To do this we will directly construct the vectors of the basis $\{w^{(\xi)}_{\epsilon,\pm}(\psi)\}_{\xi\in\mathbb{Z}^d}$ that coincide with $\{w^{(\xi)}_{0,\pm}\}_{\xi\in\mathbb{Z}^d}$ for $\epsilon=0$.

B. Symbolic dynamics

The main property that allows us to study analytically the SRB measure for an Anosov map S acting on a manifold $\mathcal{M}$ is the existence of Markov partitions. We call a collection $\mathcal{Q}_i$, $i=1,...,n$, of closed subsets of $\mathcal{M}$ a *partition* if $\cup_i\mathcal{Q}_i=\mathcal{M}$ and $\mathcal{Q}_i\cap\mathcal{Q}_j=\partial\mathcal{Q}_i\cap\partial\mathcal{Q}_j$ for every $i\neq j$. For every sequence $\sigma=\{\sigma_t\}_{t\in\mathbb{Z}}\in\{1,...,n\}^{\mathbb{Z}}$ we can define the set $\mathcal{X}(\sigma)=\cap_{t=-\infty}^{\infty}S^t(\mathcal{Q}_{\sigma_t})$. Due to the hyperbolicity properties of S, if $\mathcal{Q}_i$ are small enough, $\mathcal{X}(\sigma)$ contains at most one point. This allows us to construct a *symbolic dynamics*, i.e., a map from a subset Σ of $\{1,...,n\}^{\mathbb{Z}}$ to $\mathcal{M}$. In general, the structure of the subset Σ is very complex but for Anosov systems it is possible to construct particular partitions for which the set Σ can be described easily. Given a partition $\mathcal{Q}$ we call the $n\times n$ matrix C given by $C_{ij}=1$ if $\mathrm{int}(S\mathcal{Q}_i)\cap\mathrm{int}(\mathcal{Q}_j)\neq 0$ and 0 otherwise the compatibility matrix. We say that $\mathcal{Q}$ is a *Markov partition* if the set Σ is formed by the sequences σ such that $C_{\sigma_i,\sigma_{i+1}}=1$ for every $i\in\mathbb{Z}$. This means that the sequences that satisfy the above nearest neighbor condition code all the points of $\mathcal{M}$. In such a case we will denote $\Sigma=\{1,...,n\}^{\mathbb{Z}}_C$.

We now show how to construct a Markov partition for our model. We start with s_0. A Markov partition $Q=\{Q_i, i=1,...,n\}$ for s_0 acting on $\mathbb{T}^2$ can be easily constructed starting from its stable and unstable manifolds. Such a construction is standard and can be found, e.g., in Ref. 10. Let C be its compatibility matrix and $\hat{c}_0$ the associated symbolic dynamics.

It is important to note that $\hat{c}_0$ is Holdër continuous in the sense that there exist constants c and β such that, for any two sequences σ, $\sigma'\in\{1,...,n\}^{\mathbb{Z}}_C$, $d(\hat{c}_0(\sigma),\hat{c}_0(\sigma'))\leqslant c\tilde{d}(\sigma,\sigma')^\beta$, with $\tilde{d}(\sigma,\sigma')=e^{-\#(\sigma,\sigma')}$ where $\#(\sigma,\sigma')$ the biggest integer such that $\sigma_j=\sigma'_j$, $\forall|j|\leqslant\#(\sigma,\sigma')$. In this case we can take $\beta=\ln(\lambda_+)$. Another key property is that C is a mixing matrix; this means that there exists a *decorrelation time* $a\in\mathbb{N}$ such that C^a has all entries strictly positive. This means that we can connect any two elements of the Markov partition in a time steps.

For every point $s=\{s_\xi\}_{\xi\in\mathbb{Z}^d}\in\{1,...,n\}^{\mathbb{Z}^d}$ we can consider the Cartesian product $\mathcal{Q}_s=\times_{\xi\in\mathbb{Z}^d}Q_{s_\xi}\subset\mathcal{T}_N$. It is clear that the collection of $\mathcal{Q}_s$ with $s\in\{1,...,n\}^{\mathbb{Z}^d}$ forms a Markov partition for S_0. Note that it is natural to index the element of this partition with the element of $\{1,...,n\}^{\mathbb{Z}^d}$ so that we can associate to this partition the symbolic dynamics $c_0\colon\mathbb{Z}^d\times\mathbb{Z}=\mathbb{Z}^{d+1}\to\mathcal{T}_N$ naturally defined from $\hat{c}_0$. We can still call C the compatibility matrix and $\{1,...,n\}^{\mathbb{Z}^{d+1}}_C$ the set of possible sequences (namely $\sigma=\{\sigma_{\xi,i}\}_{\xi\in\mathbb{Z}^d,i\in\mathbb{Z}}$ is in $\{1,...,n\}^{\mathbb{Z}^{d+1}}_C$ if and only if $C_{\sigma_{\xi,i}\sigma_{\xi,i+1}}=1$ for every $\xi\in\mathbb{Z}^d$ and $i\in\mathbb{Z}$). Given any point $(\xi,i)\in\mathbb{Z}^{d+1}$ we will call ξ its *space component* and i its *time component*.

The key observation is that now the sets $h_\epsilon(\mathcal{Q}_s)$ form a Markov partition for S_ϵ. This implies that the space of symbolic sequences for S_ϵ is the same as that for S_0 and that the symbolic dynamics c_ϵ for S_ϵ is given by $c_\epsilon(\sigma)=h_\epsilon(c_0(\sigma))$. Clearly c_ϵ is still Hölder continuous. This

completes the construction of the Markov partition for S_ϵ. We thus obtained that the manifold $\mathcal{T}$ can be mapped to $\{1,...,n\}_C^{\mathbb{Z}^{d+1}}$ where d directions of the lattice $\mathbb{Z}^{d+1}$ represent the d directions of $\mathcal{T}=(\mathbb{T}^2)^{\mathbb{Z}^d}$ and the last represents the time evolution. Indeed the map S_ϵ on the space $\{1,...,n\}_C^{\mathbb{Z}^{d+1}}$ becomes the shift on the time direction, to be called τ.

C. SRB measure

Let now consider the SRB measure μ_N^{SRB} as defined in Sec. I. In this case we need to keep N finite because it is not easy to give a meaning or construct directly the SRB measure for $N=\infty$.

Let m_N^{SRB} be the measure on $\{1,...,n\}_C^{V_N\times\mathbb{Z}}$ defined as $m_N^{\mathrm{SRB}}(A)=\mu_N^{\mathrm{SRB}}(c_\epsilon^{-1}(A))$, i.e., m_N^{SRB} is the image of μ_N^{SRB} via symbolic dynamics c_ϵ. The measure m_N^{SRB} can be described efficiently through its restrictions to finite subsets of $V_N\times\mathbb{Z}$.

Given $\Lambda\subset V_N\times\mathbb{Z}$, $m_N^{\mathrm{SRB}}(\sigma_\Lambda|\sigma_{\Lambda^c})$ will denote the probability of the event $\{\sigma'|\sigma'_\Lambda=\sigma_\Lambda\}$ conditional to the event $\{\sigma'|\sigma'_{\Lambda^c}=\sigma_{\Lambda^c}\}$ w.r.t. the probability measure m_N^{SRB}, where $\Lambda^c=(V_N\times\mathbb{Z})\backslash\Lambda$ and σ_Λ is the collection of the $\sigma_{\xi,i}$ for $(\xi,i)\in\Lambda$.

From the theory of SRB measures (see Refs. 22 and 10), it follows that m_N^{SRB} is a Gibbs measure and its conditional probabilities satisfy

$$\frac{m_N^{\mathrm{SRB}}(\sigma'_\Lambda|\sigma_{\Lambda^c})}{m_N^{\mathrm{SRB}}(\sigma''_\Lambda|\sigma_{\Lambda^c})}=\lim_{K\to\infty}\left[\frac{\mathcal{D}_\epsilon^{u(2K)}(c_\epsilon(\tau^{-K}\sigma'))}{\mathcal{D}_\epsilon^{u(2K)}(c_\epsilon(\tau^{-K}\sigma''))}\right]^{-1}, \tag{2.3}$$

where σ' (resp. σ'') is the configuration coinciding with σ'_Λ (resp. σ''_Λ) on Λ and with σ_{Λ^c} on Λ^c; τ is the image of S_ϵ through c_ϵ (i.e., it is the one step shift in time direction); $\mathcal{D}_\epsilon^{u(n)}(\psi)$ measures the expansion of the volume on the unstable manifold at the point ψ. To be more precise let $\{w_{\epsilon,+}^{(\xi)}(\psi)\}_{\xi\in V_N}$ be a basis on $E_{\epsilon,\psi}^+$. We will construct one such a basis in Sec. IV. Then we have

$$\mathcal{D}_\epsilon^{u(n)}(\psi)\overset{def}{=}\sqrt{\frac{\det_{\xi\eta}[(DS_\epsilon^n w_{\epsilon,+}^{(\xi)})\cdot(DS_\epsilon^n w_{\epsilon,+}^{(\eta)})]}{\det_{\xi\eta}[w_{\epsilon,+}^{(\xi)}\cdot w_{\epsilon,+}^{(\eta)}]}}(\psi), \tag{2.4}$$

where $u\cdot v$ represent the usual scalar product in $\mathbb{R}^{V_N}$ and $\det_{\xi\eta}$ is the determinant of the expression in square brackets thought as a matrix indexed by ξ and η.

Using the invariance of E_ϵ^+ under S_ϵ and introducing the *unstable Lyapunov matrix* $\mathcal{L}(\psi)$ satisfying the equation

$$DS_\epsilon(\psi)w_{\epsilon,+}^{(\xi)}(\psi)=\sum_\eta w_{\epsilon,+}^{(\eta)}(S_\epsilon(\psi))\mathcal{L}^{\eta\xi}(\psi),$$

we can rewrite the above expression as

$$\mathcal{D}_\epsilon^{u(2K)}(S_\epsilon^{-K}(\psi))=\frac{\sqrt{\det_{\xi\eta}(w_{\epsilon,+}^{(\xi)}\cdot w_{\epsilon,+}^{(\eta)})}(S_\epsilon^K(\psi))}{\sqrt{\det_{\xi\eta}(w_{\epsilon,+}^{(\xi)}\cdot w_{\epsilon,+}^{(\eta)})}(S_\epsilon^{-K}(\psi))}\prod_{j=-K}^{K-1}|\det_{\xi\eta}[\mathcal{L}^{\xi\eta}(S_\epsilon^j\psi)]|. \tag{2.5}$$

Now the first ratio in Eq. (2.5), when inserted in Eq. (2.4), is vanishing; indeed the uniform Hölder continuity of $w_{\epsilon,+}^{(\xi)}(h_\epsilon(\psi))$ and the fact that σ' and σ'' are asymptotically identical in the past and in the future imply that

$$\lim_{K\to\pm\infty}(\ln\sqrt{\det_{\xi\eta}(w_{\epsilon,+}^{(\xi)}\cdot w_{\epsilon,+}^{(\eta)})})(c_\epsilon(\tau^K\sigma'))-(\ln\sqrt{\det_{\xi\eta}(w_{\epsilon,+}^{(\xi)}\cdot w_{\epsilon,+}^{(\eta)})})(c_\epsilon(\tau^K\sigma''))=0; \tag{2.6}$$

thus the choice of the basis in E^+ does not change the result, namely the SRB measure does not depend on the choice of the metric as is to be expected from its definition. Calling $\Lambda^{\xi}(\psi) \overset{def}{=} (\ln \mathcal{L}(h_\epsilon(\psi)))^{\xi\xi}$, we finally get

$$\frac{m_N^{\mathrm{SRB}}(\sigma'_\Lambda|\sigma_{\Lambda^c})}{m_N^{\mathrm{SRB}}(\sigma''_\Lambda|\sigma_{\Lambda^c})} = \exp\left\{ -\sum_{j=-\infty}^{+\infty} \sum_{\xi \in V_N} [\Lambda^{\xi}(c_0(\tau^j \sigma')) - \Lambda^{\xi}(c_0(\tau^j \sigma''))] \right\}. \tag{2.7}$$

Here we used the fact that $c_\epsilon = h_\epsilon \circ c_0$. Furthermore, the Hölder continuity of $\Lambda^{\xi}(c_0(\sigma'))$ implies absolute convergence of the sum in Eq. (2.7) because only points asymptotically equal both in the past and in the future are compared.

The crucial point of this construction is that the matrix $L(\psi) \overset{def}{=} \mathcal{L}(h_\epsilon(\psi))$ is analytic in ϵ due to the fact that it depends only on $w^{(\xi)}_{\epsilon,+}(h_\epsilon(\psi))$. As we already noted $w^{(\xi)}_{\epsilon,+}(h_\epsilon(\psi))$ are analytic in ϵ. We will prove this fact in Sec. IV.

In Sec. VI we will apply to Eq. (2.7) the standard methods developed in the study of Gibbs measure in statistical mechanics. To do this we will need to decompose the ''interaction'' $\Lambda^{\xi}(c_0(\sigma))$ as the sum of potentials depending only on $\sigma_X \overset{def}{=} \{\sigma_j\}_{j \in X}$ where X is a finite subset of $\mathbb{Z}^{d+1}$. More precisely, we will decompose

$$\sum_{(\xi,i) \in V_N \times \mathbb{Z}} \Lambda^{\xi}(c_0(\tau^i \sigma)) = \sum_{X \subset V_N \times \mathbb{Z}} \phi_X(\sigma_X). \tag{2.8}$$

(These two series are not convergent: they represent the formal expression for the ''Hamiltonian'' of a Gibbs measure. See Sec. V B for a more precise statement.) We shall show that we can choose ϕ_X analytic in ϵ, translationally invariant in space and time directions and decaying exponentially in the *tree distance* of the set X, namely the length of the shortest tree connecting all the lattice points in X. In this way (2.7) can be written as

$$\frac{m_N^{\mathrm{SRB}}(\sigma'_\Lambda|\sigma_{\Lambda^c})}{m_N^{\mathrm{SRB}}(\sigma''_\Lambda|\sigma_{\Lambda^c})} = \exp\left\{ -\sum_{X \cap \Lambda \neq 0} [\phi_X(\sigma'_X) - \phi_X(\sigma''_X)] \right\}, \tag{2.9}$$

so that one can finally write

$$m_N^{\mathrm{SRB}}(\sigma_\Lambda|\sigma_{\Lambda^c}) = \frac{\exp\left\{ -\sum_{X \cap \Lambda \neq \emptyset} \phi_X(\sigma_X) \right\}}{\sum_{\sigma_\Lambda} \exp\left\{ -\sum_{X \cap \Lambda \emptyset} \phi_X(\sigma_X) \right\}}. \tag{2.10}$$

This will allow us to show our analyticity claim uniformly in N.

III. PERTURBATIVE CONSTRUCTION OF THE SRB MEASURE

In this section we construct the conjugation h_ϵ and prove that it is analytic in ϵ. The technique we use consists in expanding h_ϵ as a power series in ϵ and writing a recursive relation linking the nth order coefficient to the coefficients of order i with $i<n$. This naturally leads to a tree expansion of the usual form in perturbation theory for quantum field theory, i.e., the trees we will introduce are the ''Feynmann graphs'' of our theory. See also Ref. 10 and reference therein for similar application to KAM theory.

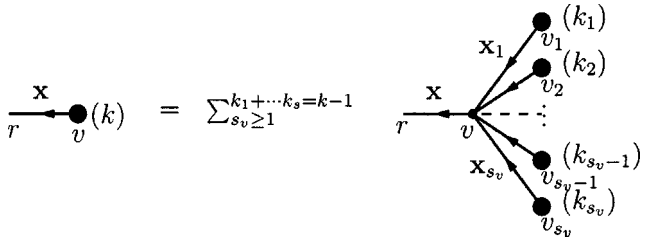

FIG. 1. Graphical interpretation of (3.6).

A. The conjugation

From now on we will identify functions from $\mathcal{T}_N$ to $\mathcal{T}_N$ with their lifts as functions from $\mathbb{R}^{2V_N}$ to $\mathbb{R}^{2V_N}$. Using the definition (2.1) and looking for h_ϵ of the form $h_\epsilon(\psi)=\psi+\delta h_\epsilon(\psi)$, we find

$$\delta h_\epsilon \circ S_0 - S_0 \circ \delta h_\epsilon = \epsilon f \circ (\mathrm{Id}+\delta h_\epsilon), \tag{3.1}$$

where Id is the identity map.

Setting $\lambda \overset{def}{=} \lambda_- = \lambda_+^{-1}$ and writing $f(\psi) \overset{def}{=} \Sigma_{\xi,\alpha} f^{\xi\alpha}(\psi) w_{0,\alpha}^{(\xi)}$ and similarly for $\delta h_\epsilon^{\xi^\pm}$, we get

$$\begin{aligned} \delta h_\epsilon^{\xi^+}(S_0\psi) - \lambda^{-1}\delta h_\epsilon^{\xi^+}(\psi) &= \epsilon f^{\xi^+}(\psi+\delta h_\epsilon(\psi)), \\ \delta h_\epsilon^{\xi^-}(S_0\psi) - \lambda\,\delta h_\epsilon^{\xi^-}(\psi) &= \epsilon f^{\xi^-}(\psi+\delta h_\epsilon(\psi)). \end{aligned} \tag{3.2}$$

Both equations can be implicitly solved by iteration:

$$\delta h_\epsilon^{\xi\alpha}(\psi) = -\alpha\epsilon \sum_{p\geq 0} \lambda^{p+\rho_\alpha} f^{\xi\alpha}(S_0^{\alpha(p+1-\rho_\alpha)}\psi + \delta h_\epsilon(S_0^{\alpha(p+1-\rho_\alpha)}\psi)), \tag{3.3}$$

where $\rho_\alpha=(1+\alpha)/2$.

It is easy to see that the series in Eq. (3.3) is absolutely convergent, since $\lambda<1$ and f is bounded. Expanding $f^{\xi^\alpha}(\psi+\delta h_\epsilon(\psi))$ in power of its argument we find

$$f^{\mathbf{x}}(\psi+\delta h_\epsilon(\psi)) = f^{\mathbf{x}}(\psi) + \sum_{k\geq 1} \epsilon^k \sum_{s=1}^{k} \sum_{\substack{k_1+\cdots+k_s=k \\ k_1,\ldots,k_s \\ k_j\geq 1}} \left(\frac{f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_{(k_1)}^{\mathbf{x}_1} \cdots \delta h_{(k_s)}^{\mathbf{x}_s} \right)(\psi), \tag{3.4}$$

where we have introduced the index $\mathbf{x}=(\xi,\alpha)$, with $\alpha=\pm$, and $f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}=\partial_{\mathbf{x}_1}\cdots\partial_{\mathbf{x}_s} f^{\mathbf{x}}$ with $\partial_{(\xi^\alpha)}$ the partial derivative in the direction of $w_{0,\alpha}^{(\xi)}$. Moreover, we use the convention of summing on twice repeated indexes. The first order coefficient of the expansion of the conjugation is then

$$\delta h_{(1)}^{\mathbf{x}}(\psi) = (-\alpha) \sum_{p\geq 0} \lambda^{p+\rho_\alpha} f^{\mathbf{x}}(S_0^{\alpha(p+1-\rho_\alpha)}\psi), \tag{3.5}$$

while the kth, $k>1$, coefficient turns out to be

$$\delta h_{(k)}^{\mathbf{x}}(\psi) = \sum_{s=1}^{k} \sum_{\substack{k_1+\cdots+k_s=k-1 \\ k_1,\ldots,k_s \\ k_j\geq 1}} (-\alpha) \sum_{p\geq 0} \lambda^{p+\rho_\alpha} \left(\frac{f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_{(k_1)}^{\mathbf{x}_1} \cdots \delta h_{(k_s)}^{\mathbf{x}_s} \right)(S_0^{\alpha(p+1-\rho_\alpha)}\psi). \tag{3.6}$$

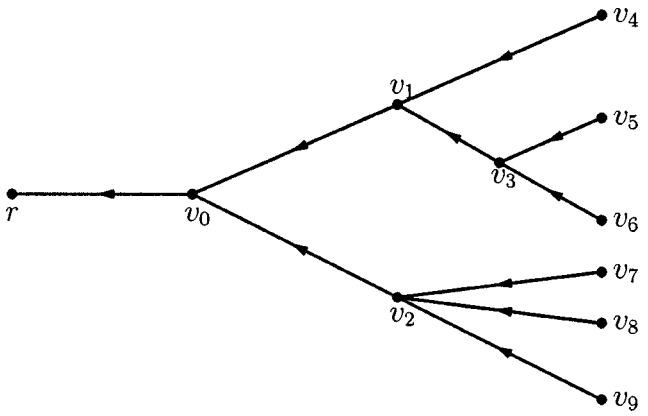

FIG. 2. A tree θ of order $k=10$ appearing in the expansion for δh_ϵ. Labels $\xi(v_i)$, $\alpha(v_i)$ and p_{v_i} are associated to all vertices v_i.

From Eq. (3.5) we see that δh_ϵ is in general nondifferentiable with respect to ψ. Indeed already differentiating $\delta h^{\xi^+}_{(1)}(\psi)$ with respect to ψ we find a nonconverging series. On the contrary, it is clear that Eq. (3.5) is Hölder continuous in ψ for every exponent $\beta<1$.

We can interpret Eq. (3.6) graphically as shown in Fig. 1.

The l.h.s. of the graphical equation in Fig. 1 represents $\delta h^{\mathbf{x}}_{(k)}(\psi)$ while the r.h.s., representing the sum in Eq. (3.6), is a "simple tree" consisting of a "root" r, a "root branch" $\lambda_v \equiv (r,v)$ coming from the "node" (or "vertex") v, and s_v branches "entering v," to be called $\lambda_{v_i} \equiv (v,v_i)$, $i=1,...,s_v$.

Even if the drawing in the figure does not carry them explicitly, we imagine that some labels are affixed to the node v: more precisely $\mathbf{x}(v)=(\xi(v),\alpha(v)) \in V_N \times \{\pm\}$ and $p_v \in \mathbb{Z}_+$. Furthermore, a label $\mathbf{x}_\lambda = (\xi_\lambda, \alpha_\lambda) \in V_N \times \{\pm\}$ is associated to each branch λ. In the figure above $\mathbf{x}_{\lambda_v} \equiv \mathbf{x}$ and $\mathbf{x}_{\lambda_{v_i}} \equiv \mathbf{x}_i$, $i=1,...,s$.

The node v symbolizes the tensor with entries

$$N_{v;\mathbf{x},\mathbf{x}_1,...,\mathbf{x}_s} \overset{def}{=} (-\alpha(v))\lambda^{p_v+\rho_{\alpha(v)}} \frac{f^{\mathbf{x},\mathbf{x}_1,...,\mathbf{x}_{s_v}}}{s_v!} (S_0^{p(v)}\psi), \tag{3.7}$$

where $p(v)=\alpha(v)(p_v+1-\rho_{\alpha(v)})$. Observe that, in order for Eqs. (3.7) and (3.6) to be nonzero, we must have $|\xi_{\lambda_{v_i}} - \xi(v)| \leq 1$, due to our definition of the coupling f.

The line λ_v exiting vertex v symbolizes the *propagator*, that is simply $\delta_{\mathbf{x}_{\lambda_v},\mathbf{x}(v)}$.

The line with label $\mathbf{x}$ exiting from the bullet of the l.h.s. with label (k) represents $\delta h^{\mathbf{x}}_{(k)}(\psi)$; the branches with labels $\mathbf{x}_i$ exiting from the bullets of the r.h.s. with label (k_i) represent $\delta h^{\mathbf{x}_i}_{(k_i)}(S_0^{p(v)}\psi)$.

Even if it is not explicitly written in the figure above, a summation over the free indices $\mathbf{x}(v)$, $\mathbf{x}_{\lambda_{v_i}}$ has to be performed [note that the summation over $\mathbf{x}(v)$ simply fixes $\mathbf{x}(v)=\mathbf{x}$, because of the presence of the propagator $\delta_{\mathbf{x}(v),\mathbf{x}}$].

Since Eq. (3.6) is multilinear in $\delta h^{\mathbf{x}_i}_{k_i}$, we can just replace each of the branches exiting from a bullet with the same graphical expression in the r.h.s. of the above figure, and so on, until the labels (k_i) on the bullets (*top nodes*) become equal to 1. In this case the end-points represent $\delta h_{(1)}$, that is a known expression, see Eq. (3.5), and we will draw these known end-points as small dots.

Thus we have represented our $\delta h^{\mathbf{x}}_{(k)}$ as a "sum over trees" with k branches and k nodes (we shall not regard the root as a node) of suitable *tree values*. In Fig. 2 we draw a typical tree θ we

get via such a procedure.

Note that a tree induces a partial ordering among its nodes: a node w precedes v (and it will be written $w<v$) if there is a path of branches connecting w and v with the arrows pointing from w to v.

Let us now summarize the discussion above. Let $\hat{\mathcal{T}}_k(\mathbf{x})$ be the set of rooted trees with k branches and k nodes, with labels $\mathbf{x}(v)$, p_v attached to their vertices and $\mathbf{x}(v_0)\equiv\mathbf{x}$, where v_0 is the last vertex preceding the root. Given $\theta\in\hat{\mathcal{T}}_k(\mathbf{x})$, let the value of θ be defined as

$$\widehat{\mathrm{Val}}(\theta,\psi)=\prod_{v\in\theta}(-\alpha(v))\lambda^{p_v+\rho_{\alpha(v)}}\frac{f^{\mathbf{x}(v),\mathbf{x}(v_1),\ldots,\mathbf{x}(v_{s_v})}}{s_v!}(S_0^{p(v)}\psi), \tag{3.8}$$

where $v_1,\ldots,v_{s_v}$ are the nodes immediately preceding v and $p(v)=\Sigma_{w\geqslant v}\alpha(v)(p_v+1-\rho_{\alpha(v)})$. With these definitions $\delta h^{\mathbf{x}}_{(k)}(\psi)$ can be calculated as $\delta h^{\mathbf{x}}_{(k)}(\psi)=\Sigma_{\theta\in\hat{\mathcal{T}}_k(\mathbf{x})}\widehat{\mathrm{Val}}(\theta,\psi)$.

B. Convergence and regularity of the perturbative expansion of the conjugation

By definition $g(\psi)$ depends only on $\psi_{nn(0)}$ so that it is analytic in $\mathcal{D}\overset{def}{=}\{\psi^i_\xi\in\mathbb{C}\,|\,|\mathrm{Im}\,\psi^j_\xi|\leqslant r_0, i=1,2,\xi\in nn(0)\}$ for some $r_0>0$. Calling G the maximum of g on $\mathcal{D}$, from Cauchy's formula we get

$$|f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi)|\leqslant G\frac{m_1!\cdots m_D!}{r_0^s}\leqslant G\frac{s!}{r_0^s}, \tag{3.9}$$

where $m_1,\ldots,m_D$ are the multiplicities of the partial derivatives with respect to the $D\overset{def}{=}2(2d+1)=2|nn(0)|$ possible variables (thus $m_1+\cdots+m_D=s$).

In the same way, if ψ and ψ' are identical on each site but $\xi'\in nn(\xi)$ and if $0<\beta\leqslant 1$, we get

$$|f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}(S_0^p\psi)-f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}(S_0^p\psi')|\leqslant G\frac{(s+1)!}{r_0^{s+1}}(2\pi^2)^{(1-\beta)/2}\lambda^{-\beta p}|\psi_{\xi'}-\psi'_{\xi'}|^\beta, \tag{3.10}$$

where we have used the periodicity of f. Next we bound the value of a tree $\theta\in\hat{\mathcal{T}}_k(\mathbf{x})$. Using Eq. (3.9), for $\theta\in\hat{\mathcal{T}}_k(\mathbf{x})$, we find

$$\|\widehat{\mathrm{Val}}(\theta,\cdot)\|_\infty\leqslant\prod_{v\in\theta}\lambda^{p_v}\frac{G}{r_0^{s_v}}=\frac{G^k}{r_0^{k-1}}\prod_{v\in\theta}\lambda^{p_v}, \tag{3.11}$$

where we used that, if $\theta\in\hat{\mathcal{T}}_k(\mathbf{x})$, $\Sigma_{v\in\theta}s_v=k-1$.

The sum over the trees can be interpreted as a sum over the topological trees and a sum over the labels attached to the trees. If Θ_k is the set of topological trees of order k, we get

$$\begin{aligned}\|\delta h^{\mathbf{x}}_{(k)}\|_\infty&\leqslant\sum_{\theta\in\Theta_k}\sum_{\substack{\mathbf{x}(v),\alpha(v)\\ v\in\theta}}\frac{G^k}{r_0^{k-1}}\sum_{\substack{p_v\\ v\in\theta}}\prod_{v\in\theta}\lambda^{p_v}=\sum_{\theta\in\Theta_k}\sum_{\substack{\xi(v),\alpha(v)\\ v\in\theta}}\frac{G^k}{r_0^{k-1}}\left(\frac{1}{1-\lambda}\right)^k\\&\leqslant\sum_{\theta\in\Theta_k}2^k(2d+1)^k\frac{G^k}{r_0^{k-1}}\left(\frac{1}{1-\lambda}\right)^k\leqslant 2^{2k}2^k(2d+1)^k\frac{G^k}{r_0^{k-1}}\left(\frac{1}{1-\lambda}\right)^k,\end{aligned} \tag{3.12}$$

where we used that:

(1) 2^k is the number of terms in the sum over the $\alpha(v)$ indices;

(2) $(2d+1)^k$ is a bound on the number of terms in the sum over the values of the $\xi(v)$ indices not making $\widehat{\mathrm{Val}}(\theta,\psi)$ vanish [observe that, given a tree θ, its value $\widehat{\mathrm{Val}}(\theta,\psi)$ is vanishing unless $|\xi(v')-\xi(v)|\leqslant 1$, where v' is the node immediately preceding v]; and
(3) 2^{2k} is a bound on the number of unlabeled rooted trees with k nodes.

In the same way we find that, if ψ and ψ' are identical on each site but ξ' and if $0<\beta<1$,

$$\frac{|\delta h^{\mathbf{x}}_{(k)}(\psi)-\delta h^{\mathbf{x}}_{(k)}(\psi')|}{|\psi_{\xi'}-\psi'_{\xi'}|^{\beta}} \leqslant \sum_{\theta\in\Theta}\left(\frac{1}{1-\lambda^{1-\beta}}\right)^k (2\pi^2)^{(1-\beta)/2}\frac{G^k}{r_0^k}2^k(2d+1)^k\sum_{v\in\theta}(s_v+1)$$
$$\leqslant 2^{2k}\left(\frac{1}{1-\lambda^{1-\beta}}\right)^k (2\pi^2)^{(1-\beta)/2}\frac{G^k}{r_0^k}2^k(2d+1)^k(2k-1). \tag{3.13}$$

So the map $h_\epsilon: \mathcal{T}_N\to\mathcal{T}_N$ exists; it is Hölder continuous w.r.t. ψ and analytic w.r.t. ϵ in the complex disc $|\epsilon|\leqslant\epsilon_\beta$, with

$$\epsilon_\beta=\left[\frac{1}{1-\lambda^{1-\beta}}2^3\frac{G}{r_0}(2d+1)\right]^{-1}. \tag{3.14}$$

In order to prove that $h_\epsilon(\psi)$ is an *homeomorphism*, we have to show that it is invertible. The proof is easy and standard. Regarding injectivity, note that two *distinct* points ψ_1, ψ_2, are necessarily far order one in the "future" or in the "past," namely there exists an integer $n\in\mathbb{Z}$ such that $|S_0^n\psi_1-S_0^n\psi_2|=O(1)$. Then $S^n_\epsilon(h_\epsilon(\psi_1))-S^n_\epsilon(h_\epsilon(\psi_2))=S^n_0(\psi_1-\psi_2)+\delta h_\epsilon(S^n_0\psi_1)-\delta h_\epsilon(S^n_0\psi_2)$ cannot vanish as the first term is order one, the other two of order ϵ; thus it cannot be but $h_\epsilon(\psi_1)\neq h_\epsilon(\psi_2)$. Regarding surjectivity, since f is a continuous injective mapping on a torus, f is necessarily surjective (the proof is trivial on $\mathbb{T}^1$ and it can be easily extended by induction to $\mathcal{T}_N$).

IV. THE UNSTABLE DIRECTION

In order to explicitly compute the SRB measure, we have to construct a basis for the unstable subspace E^+_ψ, and the expansion coefficient $\mathcal{D}^{(n)}_\epsilon$ associated to it, as explained in Sec. II B above. Note that we cannot use h_ϵ to find a basis for E^+_ψ because it is only Hölder continuous.

To find the unstable base $\{w^{(\xi)}_{\epsilon,+}(\psi)\}_{\xi\in V}$ and the *Lyapunov matrix* $\mathcal{L}(\psi)$ we have to solve the following equation:

$$(DS_\epsilon w^{(\eta)}_{\epsilon,+})(\psi)=w^{(\xi)}_{\epsilon,+}(S_\epsilon(\psi))\mathcal{L}^{\xi\eta}(\psi). \tag{4.1}$$

In general this equation cannot have solutions analytic in ϵ. In fact, from the general theory we know that the unstable vectors $\{w^{(\xi)}_{\epsilon,+}(\psi)\}_{\xi\in V}$ are not differentiable with respect to ψ. But, as we previously pointed out, to compute the SRB measure we need only to know the expansion coefficient at the point $h_\epsilon(\psi)$, i.e., $\mathcal{D}^{(n)}_\epsilon(h_\epsilon(\psi))$. Let us define $w^{(\xi)}_{\epsilon,+}(h_\epsilon(\psi))\overset{def}{=}v^{(\xi)}_\epsilon(\psi)$ for $\xi\in V$ and note that $v^{(\xi)}_\epsilon(\psi)$ satisfies the equation

$$(DS_\epsilon)(h_\epsilon(\psi))v^{(\eta)}_\epsilon(\psi)=v^{(\xi)}_\epsilon(S_0\psi)L^{\xi\eta}(\psi),\quad L(\psi)=\mathcal{L}(h_\epsilon(\psi)). \tag{4.2}$$

We will show that this equation admits a solution analytic in ϵ. Moreover, the determinant of $L(\psi)$ is all what we need to compute the SRB measure.

At this point, it is convenient to write Eq. (4.2) in components. Denoting by $\mathbf{y}$ the double index η^β (again $\mathbf{x}\overset{def}{=}\xi^\alpha$), defining $v^{(\xi)}_\epsilon(\psi)\overset{def}{=}\Sigma_\eta V^{(\xi)}_{\epsilon,\mathbf{y}}(\psi)w^{(\eta)}_{0,\beta}$ and $(DS_\epsilon w^{(\eta)}_{0,\beta})(\psi)\overset{def}{=}\Sigma_{\mathbf{x}}S^{\mathbf{x},\mathbf{y}}_\epsilon(\psi)w^{(\xi)}_{0,\alpha}$, we get

$$S_{\epsilon}^{\mathbf{x},\mathbf{y}}(h_{\epsilon}(\psi))V_{\epsilon,\mathbf{y}}^{(\rho)}(\psi)=V_{\epsilon,\mathbf{x}}^{(\zeta)}(S_0\psi)L^{\zeta\rho}(\psi). \tag{4.3}$$

Now, defining the corrections δL and δV as follows,

$$L^{\xi\eta}(\psi)\overset{def}{=}\lambda^{-1}\delta_{\xi\eta}+\delta L^{\xi\eta}(\psi),\quad V_{\epsilon,\mathbf{x}}^{(\xi)}(\psi)\overset{def}{=}V_{0,\mathbf{x}}^{(\xi)}+\delta V_{\mathbf{x}}^{(\xi)}(\psi)\quad\text{with } V_{0,\eta^+}^{(\xi)}=\delta_{\xi,\eta},\quad V_{0,\eta^-}^{(\xi)}=0, \tag{4.4}$$

we find that (4.3) is equivalent to

$$\begin{aligned}\delta L^{\xi\rho}(\psi)&=\lambda^{-1}[\delta V_{\xi^+}^{(\rho)}(\psi)-\delta V_{\xi^+}^{(\rho)}(S_0\psi)]+\epsilon f^{\xi^+,\rho^+}(h_{\epsilon}(\psi))+\epsilon f^{\xi^+,\mathbf{y}}(h_{\epsilon}(\psi))\,\delta V_{\mathbf{y}}^{(\rho)}(\psi)\\&\quad-\delta V_{\xi^+}^{(\zeta)}(S_0\psi)\,\delta L^{\zeta\rho}(\psi),\\ \lambda\,\delta V_{\xi^-}^{(\rho)}(\psi)-\lambda^{-1}\delta V_{\xi^-}^{(\rho)}(S_0\psi)&=-\epsilon f^{\xi^-,\rho^+}(h_{\epsilon}(\psi))-\epsilon f^{\xi^-,\mathbf{y}}(h_{\epsilon}(\psi))\,\delta V_{\mathbf{y}}^{(\rho)}(\psi)\\&\quad+\delta V_{\xi^-}^{(\zeta)}(S_0\psi)\,\delta L^{\zeta\rho}(\psi).\end{aligned} \tag{4.5}$$

Of course the above equations cannot determine completely the basis and its associated matrix: indeed, given a solution $\{V_{\mathbf{y}}^{(\rho)}(\psi)\}$, $\{L^{\zeta\rho}(\psi)\}$ of Eq. (4.2) and a generic invertible Hölder continuous matrix $R^{\gamma\rho}(\psi)$, also $\{V_{\mathbf{y}}^{(\gamma)}(\psi)R^{\gamma\rho}(\psi)\}$, $\{R^{-1,\zeta\delta}(S_0\psi)L^{\delta\gamma}(\psi)R^{\gamma\rho}(\psi)\}$ solve (4.2). Thus it is possible to add a constraint to $\delta V_{\mathbf{y}}^{(\rho)}(\psi)$: a possible choice, which greatly simplifies the expressions above, consists in taking $\delta V_{\rho^+}^{(\xi)}(\psi)=0$, so that (4.5) becomes

$$\begin{aligned}\delta L^{\xi\rho}(\psi)&=\epsilon f^{\xi^+,\rho^+}(h_{\epsilon}(\psi))+\epsilon f^{\xi^+,\eta^-}(h_{\epsilon}(\psi))\,\delta V_{\eta^-}^{(\rho)}(\psi),\\ \lambda\,\delta V_{\xi^-}^{(\rho)}(\psi)-\lambda^{-1}\delta V_{\xi^-}^{(\rho)}(S_0\psi)&=-\epsilon f^{\xi^-,\rho^+}(h_{\epsilon}(\psi))-\epsilon f^{\xi^-,\eta^-}(h_{\epsilon}(\psi))\,\delta V_{\eta^-}^{(\rho)}(\psi)\\&\quad+\delta V_{\xi^-}^{(\zeta)}(S_0\psi)\,\delta L^{\zeta\rho}(\psi).\end{aligned} \tag{4.6}$$

An implicit solution of (4.6) (to be inverted iteratively by a new tree expansion, see below) is

$$\begin{aligned}\delta L^{\xi\rho}(\psi)&=\epsilon f^{\xi^+,\rho^+}(h_{\epsilon}(\psi))+\epsilon f^{\xi^+,\eta^-}(h_{\epsilon}(\psi))\,\delta V_{\eta^-}^{(\rho)}(\psi),\\ \delta V_{\xi^-}^{(\rho)}(\psi)&=\sum_{j\geqslant 0}\lambda^{2j+1}[\epsilon f^{\xi^-,\rho^+}(h_{\epsilon}(S_0^{-j}\psi))+\epsilon f^{\xi^-,\eta^-}(h_{\epsilon}(S_0^{-j}\psi))\,\delta V_{\eta^-}^{(\rho)}(S_0^{-j}\psi)\\&\quad-\delta V_{\xi^-}^{(\zeta)}(S_0^{-j+1}\psi)\,\delta L^{\zeta\rho}(S_0^{-j}\psi)].\end{aligned} \tag{4.7}$$

As for the construction of the conjugation, we can expand in power series of ϵ both sides of Eq. (4.7) and equate the coefficients of the same order, thus finding an iterative solution of $\delta L_{(k)}$ and $\delta V_{(k)}$. The first order coefficients are given by

$$\begin{aligned}\delta L_{(1)}^{\xi\rho}(\psi)&=f^{\xi^+,\rho^+}(\psi),\\ \delta V_{\xi^-(1)}^{(\rho)}(\psi)&=\sum_{j\geqslant 0}\lambda^{2j+1}f^{\xi^-,\rho^+}(S_0^{-j}\psi),\end{aligned} \tag{4.8}$$

while, for $k+1\geqslant 2$,

$$\delta L^{\xi\rho}_{(k+1)}(\psi)=\sum_{s\geqslant 1,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\left(\frac{f^{\xi^+,\rho^+\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!}\,\delta h^{\mathbf{x}_1}_{(k_1)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)(\psi)$$
$$+\sum_{s\geqslant 1,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\left(\frac{f^{\xi^+,\eta^-\mathbf{x}_2,\ldots,\mathbf{x}_s}}{(s-1)!}\,\delta V^{(\rho)}_{\eta^-(k_1)}\delta h^{\mathbf{x}_2}_{(k_2)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)(\psi) \tag{4.9}$$

and

$$\delta V^{(\rho)}_{\xi^-(k+1)}(\psi)=\sum_{s\geqslant 1,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\sum_{j\geqslant 0}\lambda^{2j+1}\left(\frac{f^{\xi^-,\rho^+\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!}\,\delta h^{\mathbf{x}_1}_{(k_1)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)(S_0^{-j}\psi)$$
$$+\sum_{s\geqslant 1,\ k_i\geqslant 1}^{k_1+\cdots+k_s=k}\sum_{j\geqslant 0}\lambda^{2j+1}\left(\frac{f^{\xi^-,\eta^-\mathbf{x}_2,\ldots,\mathbf{x}_s}}{(s-1)!}\,\delta V^{(\rho)}_{\eta^-(k_1)}\delta h^{\mathbf{x}_2}_{(k_2)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)(S_0^{-j}\psi)$$
$$-\sum_{s\geqslant 1,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\sum_{j\geqslant 0}\lambda^{2j+1}\left(\frac{f^{\zeta^+,\rho^+\mathbf{x}_2,\ldots,\mathbf{x}_s}}{(s-1)!}\,(\delta V^{(\zeta)}_{\xi^-(k_1)}\circ S_0)\,\delta h^{\mathbf{x}_2}_{(k_2)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)(S_0^{-j}\psi)$$
$$-\sum_{s\geqslant 2,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\sum_{j\geqslant 0}\lambda^{2j+1}\left(\frac{f^{\zeta^+,\eta^-\mathbf{x}_3,\ldots,\mathbf{x}_s}}{(s-2)!}\,(\delta V^{(\zeta)}_{\xi^-(k_1)}\circ S_0)\,\delta V^{(\rho)}_{\eta^-(k_2)}\delta h^{\mathbf{x}_3}_{(k_3)}\cdots\delta h^{\mathbf{x}_s}_{(k_s)}\right)$$
$$\times(S_0^{-j}\psi). \tag{4.10}$$

These two relations, together with (3.6), allow a recursive construction of δL and δV. Obviously, repeating the discussion of Sec. III A, one finds that δL and δV can be expressed as sums over trees, obtained by suitably modifying the construction of previous section. It can be easily realized that the estimates for the tree values are qualitatively the same as before [see Eqs. (3.11)–(3.13)]. We point out the differences appearing in the tree expansion for δV:

(1) The nodes can be of four different types [corresponding to the four lines in Eq. (4.10)], so that the number of possible labels for a tree of order k is larger than a factor 4^k.
(2) The number D_v of derivatives acting on a node function can be either s_v or s_v+1 [see Eqs. (4.9) and (4.10)], so that $D_v!$ differs from the combinatorial factor $s_v!$ by at most s_v+1. Then the final estimate contains a factor that can be bounded by $(1/r_0)\Pi_v(s_v+1)\leqslant e^k/r_0$.

A similar discussion can be made for the tree expansion of δL.

The result is that L and V are analytic in ϵ and Hölder continuous in ψ with exponent $0<\beta<1$ in a disc $|\epsilon|\leqslant\epsilon'_\beta$, with ϵ'_β smaller than the convergence radius ϵ_β of h_ϵ [see Eq. (3.14)]. Note that also in this case ϵ'_β is independent of N.

As already explained (see Sec. II B and in particular Eq. (2.7)], in order to compute the SRB measure we need $\Lambda^\xi=(\log L)^{\xi\xi}\overset{def}{=}-\log\lambda+\delta\Lambda^\xi$, where

$$\delta\Lambda^\xi(\psi)=[\log(I+\lambda\,\delta L)]^{\xi\xi}=\sum_{s\geqslant 1}\frac{(-1)^{s+1}}{s}\lambda^s\,\delta L^{\xi\eta_1}(\psi)\cdots\delta L^{\eta_{s-1}\xi}(\psi) \tag{4.11}$$

(no summation on ξ is intended). Expanding Eq. (4.11) in series of ϵ, we get

$$\delta\Lambda^\xi_{(k)}(\psi)=\sum_{s\geqslant 1,k_i\geqslant 1}^{k_1+\cdots+k_s=k}\frac{(-1)^{s+1}}{s}\lambda^s\,\delta L^{\xi\eta_1}_{(k_1)}(\psi)\cdots\delta L^{\eta_{s-1}\xi}_{(k_s)}(\psi). \tag{4.12}$$

Again, the last equation, together with (4.10) and (3.6), allows a recursive construction of the coefficients $\delta\Lambda^{\xi}_{(k)}$ and the result is that Λ^{ξ} is a sum over (suitably modified) trees. The bounds are still qualitatively the same, so that Λ^{ξ} is analytic w.r.t. ϵ in a suitably small complex disc (independent of N) and Hölder continuous w.r.t. ψ.

V. SRB POTENTIALS

The next step towards the construction of the SRB measure and the proof of its analyticity consists in the expansion of Λ^{ξ} in potentials ϕ_X. From the analysis of previous sections it follows that Λ^{ξ}, as well as $h^{\mathbf{x}}_{\epsilon}$, $V^{(\rho)}_{\xi^-}$ and $L^{\xi\eta}$, can be expanded in convergent sums over tree values. We will discuss here how to expand h in potentials, since the analogous expansion for V, L and Λ is conceptually similar, just more involved due to the more complex structure of the trees.

We will proceed as follows. We first write the values of the trees in terms of the symbolic variables σ. We then decompose each of these values as a sum of terms only depending on the σ's on finite but arbitrary large sets. Finally, we define the associated potentials by collecting together the contributions which depend on the same σ's. Our goal is to obtain potentials defined over sets with rather arbitrary shape but decaying exponentially with the *tree distance* [see after Eq. (2.8) for a precise definition] of their support.

To begin with we expand the derivatives of the perturbation function f via a telescopic sum. Given the digits s and $s' \in \{1,...,n\}$ we can always find a sequence of digits $\Sigma(s,s') = s_1 s_2 \cdots s_{a-1}$ such that the sequence $s\Sigma(s,s')s'$ is compatible, i.e., such that $C_{s_i,s_{i+1}}=1$ for $i=0,...,a-1$, where $s_0=s$ and $s_a=s'$. Choosing a sequence $\hat{\sigma} \in \{1,...,n\}^{\mathbb{Z}}_C$ once and for all, given $\sigma \in \{1,...,n\}^{\mathbb{Z}}_C$ we can define its restriction to time j, σ^j as follows: $\sigma^j_{\xi,t}=\sigma_{\xi,t}$ if $|t|\leqslant j$, $\sigma^j_{\xi,t}=\hat{\sigma}_{\xi,t}$ if $|t|>j+a$ and the gap is filled with the sequence constructed above for $s=\sigma_{\xi,\pm j}$ and $s'=\hat{\sigma}_{\xi,\pm(j+a)}$. We can now define

$$f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}(c_0(\sigma)) = f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}(c_0(\sigma^0)) + \sum_{j\geqslant 1}\left[f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}(c_0(\sigma^j)) - f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}(c_0(\sigma^{j-1}))\right]$$

$$\stackrel{def}{=} \sum_{j\geqslant 0} f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}_{(j)}(\sigma_{nn^{(j)}(\xi)}), \tag{5.1}$$

where ξ is the spatial coordinate associated to $\mathbf{x}$ and $nn^{(j)}(\xi)=nn(\xi)\times I_j$, $I_j=[-j,j]\cap\mathbb{Z}$. Since $|c_0(\sigma^j)-c_0(\sigma^{j-1})|\leqslant c\lambda^j$ for some $c>0$, $f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}_{(j)}$ is bounded by

$$\|f^{\mathbf{x},\mathbf{x}_1,\dots,\mathbf{x}_s}_{(j)}\|_{\infty} \leqslant G\frac{(s+1)!}{r_0^{s+1}} c\lambda^j. \tag{5.2}$$

A. Decay of the potentials for the conjugation

Inserting expansion (5.1) in the definition of the value of a tree Eq. (3.8), we find

$$\widehat{\mathrm{Val}}(\theta,c_0(\sigma)) = \prod_{v\in\theta}\sum_{j_v\geqslant 0}(-\alpha(v))\lambda^{p_v+\rho_{\alpha(v)}}\frac{f^{\mathbf{x}(v),\mathbf{x}(v_1),\dots,\mathbf{x}(v_{s_v})}_{(j_v)}}{s_v!}(\tau^{p(v)}\sigma_{nn^{(j_v)}(\xi(v))}), \tag{5.3}$$

where we recall that $\rho_{\alpha(v)}=(1+\alpha(v))/2$, $p(v)=\Sigma_{w\geqslant v}\alpha(v)(p_v+1-\rho_{\alpha(v)})$ and $nn^{(j)}(\xi)=nn(\xi)\times I_j$, $I_j=[-j,j]\cap\mathbb{Z}$. The above expression can be seen as a sum over the values of a new kind of trees, identical to the ones described in Sec. III A, but with a new label $j_v\in\mathbb{N}$ attached to each node. Let $\mathcal{T}_k(\mathbf{x})$ be the set of these new trees of order k contributing to $\delta h^{\mathbf{x}}_{(k)}$, i.e., $\theta\in\mathcal{T}_k(\mathbf{x})$ is a tree with k branches and k nodes (the root is not a node) with the following labels attached to the nodes $v\in\theta$: $\xi(v)\in V$, $p_v\in\mathbb{N}$, $j_v\in\mathbb{N}$ and $\alpha(v)\in\{-1,+1\}$.

Given $\theta\in\mathcal{T}_k(\mathbf{x})$, its value is given by

$$\text{Val}\ \ \theta(\sigma)=\prod_{v\in\theta}(-\alpha(v))\lambda^{p_v+\rho_{\alpha(v)}}\frac{f_{(j_v)}^{\mathbf{x}(v),\mathbf{x}(v_1),\ldots,\mathbf{x}(v_{s_v})}}{s_v!}(\tau^{p(v)}\sigma_{nn^{(j_v)}(\xi(v))}), \tag{5.4}$$

so that we have

$$\delta h^{\mathbf{x}}_{(k)}(c_0(\sigma))=\sum_{\theta\in\mathcal{T}_k(\mathbf{x})}\text{Val}\ \ \theta(\sigma)\quad\text{with}\ \|\text{Val}\ \ \theta\|_\infty\leqslant\left(\frac{ceG}{\lambda r_0^2}\right)^k\prod_{v\in\theta}\lambda^{j_v+p_v+1}, \tag{5.5}$$

where we have used Eq. (5.2). We can now define the support $X(\theta)\subset V\times\mathbb{Z}$ of a tree $\theta\in\mathcal{T}_k(\mathbf{x})$, as the support of the spin variables on which Val θ depends in a nontrivial way, plus a *center* $(\xi,0)$. More precisely,

$$X(\theta)\overset{def}{=}\{(\xi,0)\}\cup\bigcup_{v\in 0}\mathcal{C}(\xi(v),p(v),j_v),$$

where

$$\mathcal{C}(\xi(v),p(v),j_v)\overset{def}{=}\bigcup_{\eta\in nn(\xi(v))}\ \bigcup_{|i|\leqslant j_v}(\eta,p(v)+i). \tag{5.6}$$

namely $\mathcal{C}(\xi,p,j)$ is a cylinder centered in (ξ,p), with the spatial base equal to the set of nearest neighbors of ξ and with height equal to $2j$. Then $X(\theta)$ is the union of $(\xi,0)$ and of cylinders of this kind, one for each node v of the tree. The point $(\xi,0)$ has the role of center of $X(\theta)$ and is added to $X(\theta)$ for later convenience [note in fact that Val $\theta(\sigma)$ could not depend on $\sigma_{(\xi,0)}$].

Given a set $X\subset\mathbb{Z}^{d+1}$ we can partition it in a natural way as a union of timelike segments. More precisely, given $\xi\in\mathbb{Z}^d$, let $T_\xi=\{(\xi,i)\in\mathbb{Z}^{d+1}|i\in\mathbb{Z}\}$. The intersection between T_ξ and X can be uniquely partitioned as a union of n_ξ maximal connected segments. The collection of all these segments forms a partition of X in n_X timelike segments $\{R_i(X)\}_{i=1,\ldots,n_X}$. Let now r_i be the center of $R_i(X)$. If Y is a subset of $\mathbb{Z}^{d+1}$, we call tree distance of Y, $d_t(Y)$, the length of the minimal tree connection of all the points of Y. Finally, let $d_c(X)$ be the tree distance of the set $\{r_i\}_{i=1,\ldots,n_X}$.

From the previous bound on the value of a tree $\theta\in\mathcal{T}_k(\mathbf{x})$, Eq. (5.5) can be interpreted as the tree distance decay of the contribution of order k to δh. Indeed,

$$|\epsilon|^k\|\text{Val}\ \ \theta\|_\infty\leqslant\left(\frac{ceG|\epsilon|^{1/2}}{\lambda r_0^2}\right)^k\left[\lambda^{d_c(X(\theta))}|\epsilon|^{n_{X(\theta)}/2}\prod_{i=1}^{n_{X(\theta)}}\lambda^{|R_i(X(\theta))|}\right]^{1/(2d+1)}, \tag{5.7}$$

where we have the following.

(1) The factor $\lambda^{d_c(X(\theta))}$ comes from $\Pi_{v\in\theta}\lambda^{1+p_v}$; in fact p_v is the displacement in the time direction of the cylinder associated to the node v w.r.t. the one associated to the node v' immediately following v, and 1 is their maximum displacement in spatial direction, so that $\Sigma_v(1+p_v)\geqslant d_c(X(\theta))$.
(2) We used that $n_X\leqslant(2d+1)k$ in order to bound $|\epsilon|^{k/2}$ with $|\epsilon|^{n_X/2(2d+1)}$.
(3) The factor $\Pi_{i=1}^{n_{X(\theta)}}\lambda^{|R_i(X(\theta))|}$ comes from $\Pi_{v\in\theta}\lambda^{j_v}$.
(4) The global power $1/(2d+1)$ in (5.7) comes from the size of the base of each cylinder, namely we used the fact that the number n_X of segments is less than $2d+1$ times the number of cylinders in $X(\theta)$.

Collecting together all the trees θ which have support $X(\theta)=X$ for a given X, we get

$$\delta h^{\mathbf{x}}_{\epsilon}(c_0(\sigma)) = \sum_{X \ni (\xi,0)} \delta h^{\mathbf{x}}_X(\sigma_X) \quad \text{with} \quad \delta h^{\mathbf{x}}_X(\sigma_X) \stackrel{def}{=} \sum_{k \geq 1} \epsilon^k \sum_{\theta \in \mathcal{T}_k(\mathbf{x})} \sum^{X(\theta)\equiv X} \text{Val} \quad \theta(\sigma). \tag{5.8}$$

So, using the bound (5.7) for $|\epsilon|$ small enough, $\gamma_0 = 1/2(2d+1)$, $\kappa_0 = -2\gamma_0 \log \lambda$, $\nu_0 = |\epsilon|^{\gamma_0}$ and a suitable $c > 0$, we get

$$\| \delta h^{\mathbf{x}}_X \|_\infty \leq c e^{-\kappa_0 d_c(X)} \nu_0^{n_X} \prod_{i=1}^{n_X} e^{-\kappa_0 |R_i(X)|}, \tag{5.9}$$

namely $\delta h^{\mathbf{x}}_X$ decays exponentially with the tree distance of X.

B. SRB potentials and their decay

Proceeding as above for the function $\Lambda^{\xi}(c_0(\sigma))$ we obtain that we can write it as

$$\Lambda^{\xi}(c_0(\sigma)) \stackrel{def}{=} \sum_{X \subset (V_N \times \mathbb{Z})} \phi^{(\xi,0)}_X(\sigma_X),$$

where by construction $\phi^{(\xi,0)}_X$ is different from 0 only if $(\xi,0) \in X$. The function $\phi^{(\xi,0)}_X$ is again given by a tree expansion analogous to that in Eq. (5.8). Moreover, we will set

$$\phi^{(\xi,j)}_X(\sigma_X) \stackrel{def}{=} \phi^{(\xi,0)}_{\tau^{-j}X}(\sigma_X).$$

We can define

$$\phi_X(\sigma_X) \stackrel{def}{=} \sum_{(\xi,j) \in X} \phi^{(\xi,j)}_X(\sigma_X),$$

so that we formally obtain Eq. (2.8), namely, given $I_T = [-T/2, T/2] \cap \mathbb{Z}$ (T even) and calling $\Lambda = V_N \times I_T$,

$$\sum_{(\xi,i) \in \Lambda} \Lambda^{\xi}(c_0(\tau^i \sigma)) - \sum_{X \cap \Lambda \neq \emptyset} \phi_X(\sigma_X) = O(\partial \Lambda),$$

where $\partial\Lambda$ is the boundary of Λ and the correction can be exactly computed from the definitions above.

Note the potential $\phi_X(\sigma_X)$ is invariant under time and space translations (respectively for the definition of $\phi^{(\xi,i)}_X$ and for the periodic boundary conditions), namely,

$$\phi_X(\sigma_X) = \phi_{\rho^{\xi} \tau^j X}(\sigma_X) \quad \text{for any} \quad (\xi,j) \in V_N \times \mathbb{Z}. \tag{5.10}$$

Moreover, it can be bounded by

$$\| \phi_X \|_\infty \leq c e^{-\kappa_1 d_c(X)} \nu_1^{n_X} \prod_{i=1}^{n_X} e^{-\kappa_1 |R_i(X)|}, \tag{5.11}$$

for suitable c, γ_1, $\kappa_1 > 0$ and $\nu_1 = |\epsilon|^{\gamma_1}$.

VI. ANALYTICITY OF SRB MEASURE

In the previous sections, we wrote the SRB measure as a Gibbs measure with translationally invariant potentials ϕ_X, decaying as in (5.11), and with hard core interaction in time direction.

Moreover, the potential ϕ_X is analytic in ϵ in a small disc in $\mathbb{C}$ around the origin (independent of N). A well known technique to show analyticity of the Gibbs measure w.r.t. ϵ is the so called *cluster expansion*.

If $\Lambda = V_N \times I_T$, with $I_T \overset{def}{=} [-T/2, T/2] \cap \mathbb{Z}$ for some even $T \in \mathbb{N}$, we call $\Lambda_a = V_N \times I_{T+2a}$. Given a *boundary condition* $\overline{\sigma} \in \{1,...,n\}_C^{\mathbb{Z}^{d+1}}$, we define the *pressure* P_Λ as

$$P_\Lambda \overset{def}{=} |\Lambda|^{-1} \log \sum_\sigma e^{-\Sigma_{X \cap \Lambda \neq \emptyset} \phi_X(\sigma_X)}, \tag{6.1}$$

where the sum is over all the σ that coincide with σ_Λ on Λ, to $\overline{\sigma}$ on Λ_a^c and with $\Sigma(\sigma_{\xi,T/2}, \overline{\sigma}_{\xi,T/2+a})$ in the space remaining. It is well known that the pressure P_Λ can be considered as the generating functional for the Gibbs states. From its analyticity our main theorem will follow easily, as we will see in Sec. VI D.

A. Decimation

In the presence of hard cores we cannot proceed in the standard way (Mayer's expansion), since the standard proof (see Ref. 13) requires weakness of the original interactions. We can overcome this obstacle by a *decimation* (see Ref. 7), namely considering the statistical system on scales larger than the length of decorrelation of the hard core.

1. Decimated lattice Λ_D

For each $\xi \in V_N$, we divide the time interval $I_T^\xi \overset{def}{=} \{\xi\} \times I_T$ into an alternating sequence of blocks, called "*B*-type" and "*H*-type," $B_\xi^{(0)}$, $H_\xi^{(0)}$, $B_\xi^{(1)}$, $H_\xi^{(1)}$,..., $B_\xi^{(\ell-1)}$, $H_\xi^{(\ell-1)}$, $B_\xi^{(\ell)}$, containing a number of spins respectively equal to $b=1$ and $h = h_0 a - 1$, with $h_0 \in \mathbb{N}$ to be chosen later. For this reason we choose the number of points in I_T^ξ to be $|I_T^\xi| = \ell h_0 a + 1$, namely $T = \ell h_0 a$.

Remark: The choice $b=1$ is special for the present case, in which the unperturbed potential is vanishing. In general one could treat with the same technique the case in which the unperturbed potential is order one, with a sufficiently fast decay of the tails, and in that case b should be chosen suitably large (see Ref. 7). Such a case arises, for instance, when the unperturbed system is the product of nonlinear Anosov maps on $\mathbb{T}^2$, namely in the case treated in Appendix A. The present discussion could be easily adapted to cover that case.

Let $\beta_\xi^{(i)} \overset{def}{=} \sigma_{(\xi, -T/2 + i h_0 a)}$, $\xi \in V_N$, $i = 0,...,\ell$, be the spin in the block $B_\xi^{(i)}$ and $\eta_\xi^{(i)} \overset{def}{=} \{\sigma_{(\xi,p)}\}_{(\xi,p) \in H_\xi^{(i)}}$, $\xi \in V_N$, $i = 0,...,\ell-1$, be the collection of spins belonging to the block $H_\xi^{(i)}$; it will be regarded as a sequence of h β spins: $\eta_\xi^{(i)} = (\beta_1(\eta_\xi^{(i)}), \ldots, \beta_h(\eta_\xi^{(i)}))$. The lattice obtained considering the H and B blocks as points:

$$\Lambda_D \overset{def}{=} \{B_\xi^{(p)}, H_\xi^{(q)}\}_{\xi \in V_N, p=0,...,\ell}^{q=0,...,\ell-1} \tag{6.2}$$

will be called the *decimated lattice*; on Λ_D the distances will be computed by thinking of it as having its sites spaced by 1 also in the time direction.

If $X \subset \Lambda$, $Y(X)$ will denote the corresponding subset in Λ_D, namely the smaller subset $Y \subset \Lambda_D$ such that the union of the *B*- and *H*-blocks in Y contains the set X. Defining $\Phi_Y(\beta_Y, \eta_Y) \overset{def}{=} \Sigma_{X: Y(X) = Y} \phi_X(\sigma_x)$ Eq. (6.1) can be rewritten as

$$P_\Lambda = \frac{1}{|\Lambda|} \log \sum_{\beta_\Lambda} \sum_{\eta_\Lambda} e^{-\Sigma_{Y\subset\Lambda_D} \Phi_Y(\beta_Y,\eta_Y)} \prod_{\xi\in V} \prod_{i=0}^{\ell-1} Z(\beta_\xi^{(i)}, \eta_\xi^{(i)}, \beta_\xi^{(i+1)}),$$

where

$$Z(\beta,\eta,\beta') = C_{\beta\beta_1(\eta)} C_{\beta_1(\eta)\beta_2(\eta)} \cdots C_{\beta_{h-1}(\eta)\beta_h(\eta)} C_{\beta_h(\eta)\beta'}. \tag{6.3}$$

Observe that, from Eq. (5.11), if Y does not coincide with a single H-block, Φ_Y satisfies a qualitatively equivalent bound:

$$\|\Phi_Y\|_\infty \leqslant c e^{-\tilde{\kappa} d_c(Y)} \tilde{\nu}^{n_Y} \prod_{i=1}^{n_Y} e^{-\tilde{\kappa}|R_i(Y)|}, \quad Y \neq H_\xi^{(i)}, \tag{6.4}$$

for some c, $\tilde{\kappa}$, $\tilde{\gamma}>0$ and $\tilde{\nu}=|\epsilon|^{\tilde{\gamma}}$. Whereas if $Y=H_\xi^{(i)}$ for some $\xi\in V$ and some $i=0,\ldots,\ell-1$, we have $\|\Phi_Y\|_\infty \leqslant h\tilde{\nu}$.

2. Averaging over many degrees of freedom: The Perron–Frobenius theorem

Decimation is a *renormalization group* technique, consisting in summing first on the H-type spins, thus getting an effective statistical system for the B-blocks: the idea is that if the B-blocks are sufficiently far apart, after the averaging of the η's, the β's should be *almost independent*, as if there were only small interactions among them. The technical tool we shall use to prove rigorously that the effective interactions between the β's are small is the Perron–Frobenius theorem.

Let $Z(\beta,\beta')$ be defined, with a little abuse of notation, as

$$Z(\beta,\beta') \stackrel{def}{=} \sum_\eta Z(\beta,\eta,\beta') = C^{ah_0}_{\beta\beta'}. \tag{6.5}$$

Observe that $1 \leqslant C^a_{\sigma\sigma'} \leqslant q^a$. Since C^a has strictly positive entries, we can apply the Perron–Frobenius theorem and obtain that C^a and its transpose $C^{a,T}$ admit a nondegenerate eigenvalue $l>0$ with eigenvectors π and π^*, respectively, such that π_σ, $\pi^*_\sigma>0$ for any $\sigma=1,\ldots,q$, and $\Sigma_\sigma \pi^*_\sigma \pi_\sigma = 1$. The eigenvalue l is maximal in the spectrum of C^a; namely, if we define P as the projection matrix $P_{\sigma\sigma'} = \delta_{\sigma\sigma'} - \pi_\sigma \pi^*_{\sigma'}$, we have

$$\|(l^{-1}C^a)^k P \omega\|_\infty \leqslant c_\alpha e^{-\alpha k} \|\omega\|_\infty, \tag{6.6}$$

for any $\omega \in \mathbb{R}^q$ and with

$$\alpha \stackrel{def}{=} -\log(1-[\min(C^a_{\sigma\sigma''}/C^a_{\sigma\sigma'})]^2) \geqslant q^{-2a}. \tag{6.7}$$

As a consequence,

$$Z(\beta,\beta') = C^{ah_0}_{\beta\beta'} = \sum_\sigma C^{ah_0}_{\beta\sigma}(\pi_\sigma \pi^*_{\beta'} + P_{\sigma\beta'}) = l^{h_0} \pi_\beta \pi^*_{\beta'} \left[1 + \frac{(l^{-h_0} C^{ah_0} P)_{\beta\beta'}}{\pi_\beta \pi^*_{\beta'}}\right]$$

$$\stackrel{def}{=} l^{h_0} \pi_\beta \pi^*_{\beta'} e^{-I(\beta,\beta')}, \tag{6.8}$$

with $I(\beta,\beta') = O(e^{-h_0 q^{-2a}})$. It is now clear that taking h_0 big enough we can make the two body potential $I(\beta,\beta')$ as small as needed.

Using Eq. (6.8), introducing a new effective potential W including the contributions from Φ and I, defining

$$\prod_{i=0}^{\ell} e^{-U^{(i)}(\beta_\xi^{(i)})} \overset{def}{=} \prod_{i=0}^{\ell-1} \pi_{\beta_\xi^{(i)}} \pi^*_{\beta_\xi^{(i+1)}} \tag{6.9}$$

and using $\lim_{\Lambda\to\infty}|\Lambda|^{-1}\log\Pi_{\xi,i}\Sigma_{\beta_\xi^{(i)}}e^{-U^{(i)}(\beta_\xi^{(i)})}=0$ (as it follows from the normalization condition $\Sigma_\sigma \pi^*_\sigma \pi_\sigma = 1$), we can rewrite P_Λ as

$$P_\Lambda = \frac{1}{a}\log l + \frac{1}{|\Lambda|}\log \sum_{\beta_\Lambda} \sum_{\eta_\Lambda} m(\beta_\Lambda, \eta_\Lambda) \prod_{Y\subset\Lambda} e^{-W_Y(\beta_Y,\eta_Y)}$$

with

$$m(\beta_\Lambda,\eta_\Lambda) \overset{def}{=} \prod_{\xi\in V}\prod_{i=0}^{\ell} \frac{e^{-U^{(i)}(\beta_\xi^{(i)})}}{\Sigma_{\beta_\xi} e^{-U^{(i)}(\beta_\xi)}} \prod_{i=0}^{\ell-1} \frac{Z(\beta_\xi^{(i)},\eta_\xi^{(i)},\beta_\xi^{(i+1)})}{Z(\beta_\xi^{(i)},\beta_\xi^{(i+1)})}, \tag{6.10}$$

where $m(\beta_\Lambda,\eta_\Lambda)$ is a probability density. Observe that, if one chooses $h_0 \simeq -\log\tilde{\nu}$ [so that both $h\tilde{\nu}$ and $I(\beta,\beta')$ are small], the new interaction W satisfies a bound similar to the one of Φ:

$$\|W_Y\|_\infty \leqslant c e^{-\bar{\kappa} d_c(Y)} \bar{\nu}^{n_Y} \prod_{i=1}^{n_Y} e^{-\bar{\kappa}|R_i(Y)|}, \quad \forall Y\subset\Lambda_D, \tag{6.11}$$

for some c, $\bar{\kappa}$, $\bar{\gamma}>0$, $\bar{\nu}=|\epsilon|^{\bar{\gamma}}$.

B. Mayer's expansion and polymer lattice gas

We shall now expand the small potential appearing in the expression for P_Λ, via a *Mayer's expansion*, obtaining the pressure for $\epsilon=0$ plus a correction.

It will be convenient to collect together the contributions of the potentials whose supports have the same *closure*, in the following sense: for a set formed by a unique point $H_\xi^{(i)}\in\Lambda_D$ we define its *closure* as $\overline{(H_\xi^{(i)})} \overset{def}{=} (B_\xi^{(i)}, H_\xi^{(i)}, B_\xi^{(i+1)})$ while for a set formed by a unique point $B_\xi^{(i)} \in \Lambda_D$ we define $\overline{(B_\xi^{(i)})} \overset{def}{=} (B_\xi^{(i)})$; finally for $Y\subset\Lambda_D$ we define its closure as $\bar{Y} \overset{def}{=} \cup_{G\in Y}\overline{(G)}$.

We say that a collection $\mathcal{C}=\{Y_m\}_{m=1}^n$ of sets $Y_i\subset\mathbb{Z}^{d+1}$ (think of them as *molecules*) is *connected* if, given a couple $(Y_{\rm in}, Y_{\rm fin})\in\mathcal{C}\times\mathcal{C}$, it is possible to find $\{Y_{m_j}\}_{j=1}^p$, such that $\bar{Y}_{\rm in}\cap\bar{Y}_{m_1}\neq\emptyset$, $\bar{Y}_{m_i}\cap\bar{Y}_{m_{i+1}}\neq\emptyset$ and $\bar{Y}_{m_p}\cap\bar{Y}_{\rm fin}\neq\emptyset$.

Writing $e^{-W_Y(\beta_Y,\eta_Y)}$ as the value for $\epsilon=0$ plus the correction, namely $1+(e^{-W_Y(\beta_Y,\eta_Y)}-1)$, expanding the product over $Y\subset\Lambda_D$ and collecting together the connected components, we can rewrite Eq. (6.10) as

$$P_\Lambda - \frac{1}{a}\log l = \frac{1}{|\Lambda|}\log \sum_{\beta_\Lambda}\sum_{\eta_\Lambda} m(\beta_\Lambda,\eta_\Lambda) \sum_{\Gamma\subset\Lambda_D} \Upsilon(\Gamma) \prod_{\gamma\in\Gamma} \rho(\gamma|\beta_\gamma,\eta_\gamma), \tag{6.12}$$

where

(1) γ is a subset of Λ_D, to be called in the following *polymer* (they are, indeed, the union of a connected collection of molecules);
(2) Γ is a collection of polymers: $\Gamma=(\gamma_1,\ldots,\gamma_n)$, $n\geqslant 1$ and $\Gamma\subset\Lambda_D$ means that $\gamma\subset\Lambda_D$, $\forall\gamma\in\Gamma$;
(3) $\Upsilon(\Gamma)$ is the function equal to 1 if $\gamma\cap\gamma'=\emptyset$ for every γ, $\gamma'\in X$ with $\gamma\neq\gamma'$ and 0 otherwise;

(4) $\rho(\gamma|\beta_\gamma,\eta_\gamma)$, $\gamma\subset\Lambda_D$ is defined as

$$\rho(\gamma|\beta_\gamma,\eta_\gamma)\overset{def}{=}\sum_{q\geqslant 1}\frac{1}{q!}\sum_{\substack{Y_1,\dots,Y_q\\ \cup_i Y_i=\gamma}}^{*}\prod_{i=1}^{q}(e^{-W_{Y_i}(\beta_{Y_i},\eta_{Y_i})}-1), \tag{6.13}$$

where the $*$ on the sum means that $Y_1\dots,Y_q$ is a connected collection of subsets of Λ_D; (5) the term corresponding to $\Gamma=\emptyset$ must be interpreted as equal to 1.

The key observation is that, thanks to the above definition of closure, in (6.12) we can sum over η spins before summing over the β spins. After doing this the measure $m(\beta_\Lambda,\eta_\Lambda)$ factorizes, i.e.,

$$\begin{aligned}P_\Lambda-\frac{1}{a}\log l&=\frac{1}{|\Lambda|}\log\sum_{\Gamma\subset\Lambda_D}\Upsilon(\Gamma)\prod_{\gamma\in\Gamma}\left[\sum_{\beta_\gamma}\sum_{\eta_\gamma}m(\beta_\gamma,\eta_\gamma)\rho(\gamma|\beta_\gamma,\eta_\gamma)\right]\\&\overset{def}{=}\frac{1}{|\Lambda|}\log\sum_{\Gamma\subset\Lambda_D}\Upsilon(\Gamma)\prod_{\gamma\in\Gamma}\rho(\gamma).\end{aligned} \tag{6.14}$$

Namely, we have rewritten P_Λ as the pressure for $\epsilon=0$ plus a correction having the form of the pressure of a "polymer lattice gas," with activities $\rho(\gamma)$ and hard core potentials $\Upsilon(\Gamma)$.

C. Cluster expansion and its convergence

A standard argument, exposed for instance in Ref. 13, 20, or 10, leads to

$$P_\Lambda-\frac{1}{a}\log l=\frac{1}{|\Lambda|}\log\sum_{\Gamma\subset\Lambda_D}\Upsilon(\Gamma)\rho(\Gamma)=\frac{1}{|\Lambda|}\sum_{\Gamma\subset\Lambda_D}\Upsilon^T(\Gamma)\rho(\Gamma), \tag{6.15}$$

where Υ^T is the Mayer function, defined as

$$\Upsilon^T(\gamma_1,\dots,\gamma_n)\overset{def}{=}\begin{cases}\displaystyle\sum_{g\in\mathcal{G}(n)}\prod_{(i,j)\in g}f(\gamma_i,\gamma_j) & \text{if } n>1,\\ 1 & \text{if } n=1,\end{cases} \tag{6.16}$$

where $\mathcal{G}(n)$ is the set of connected graphs which can be drawn on n vertices labeled 1,...,n by connecting with links couples of distinct vertices; the function $f(\gamma_i,\gamma_j)$ is equal to 1 if $\gamma_i\cap\gamma_j\neq\emptyset$ and 0 otherwise. By construction, $\Upsilon^T(\Gamma)$ is different from zero only if Γ is a connected collection of polymers. Observe that Γ could contain many copies of the same γ. More precisely, here Γ represents a function from the subsets of Λ_D to $\mathbb{N}$ [and we can think $\Gamma(\gamma)$ as representing the number of copies of γ] such that $\Sigma_{\gamma\subset\Lambda_D}\Gamma(\gamma)\leqslant\infty$.

A bound for $\rho(\gamma)$ can be obtained as follows:

$$|\rho(\gamma)|\leqslant\|\rho(\gamma|\cdot,\cdot)\|_\infty\leqslant\sum_{p\geqslant 1}\frac{1}{p!}\sum_{Y_i,\cup_i Y_i=\gamma}^{*}\prod_{i=1}^{p}\|W_{Y_i}\|_\infty e^{\|W_{Y_i}\|_\infty}. \tag{6.17}$$

Using the bound (6.11) (and that, if $\cup_{i=1}^p\overline{Y}_i=\gamma$, one has $\Sigma_{i=1}^p\|W_{Y_i}\|\leqslant c\overline{\nu}|\gamma|$), we find

$$|\rho(\gamma)|\leqslant e^{c\overline{\nu}|\gamma|}\sum_{p\geqslant 1}\frac{1}{p!}\sum_{Y_i,\cup_i Y_i=\gamma}^{*}\prod_{i=1}^{p}ce^{-\overline{\kappa}d_c(Y_i)}\overline{\nu}^{n_{Y_i}}\prod_{j=1}^{n_{Y_i}}e^{-\overline{\kappa}|R_j(Y_i)|}. \tag{6.18}$$

We can now use the connectedness constraint on the sum in order to extract a factor exponentially small in the size of γ. Indeed, if $\cup_{i=1}^{p}\overline{Y}_i=\gamma$, one has both $\Sigma_{i=1}^{p}d_c(Y_i)\geqslant d_c(Y_i)$ and $\Sigma_{i=1}^{p}n_{Y_i}\geqslant n_\gamma$. After extracting such a factor we can relax the constraints on the sum, so that

$$|\rho(\gamma)|\leqslant ce^{c\overline{\nu}|\gamma|}\left[e^{-(\overline{\kappa}/2)d_c(\gamma)}\overline{\nu}^{n_\gamma/2}\prod_{i=1}^{n_\gamma}e^{-(\overline{\kappa}/2)|R_i(\gamma)|}\right]\times\sum_{p\geqslant 1}\frac{1}{p!}\left(\sum_{Y\subset\gamma}e^{-(\overline{\kappa}/2)d_c(Y)}\overline{\nu}^{n_Y/2}\prod_{j=1}^{n_Y}e^{-(\overline{\kappa}/2)|R(Y)|}\right)^p. \tag{6.19}$$

It is easy to see that the last sum is bounded by $c|\gamma|\overline{\nu}^{1/4}$, so that

$$|\rho(\gamma)|\leqslant ce^{c\overline{\nu}|\gamma|}\left[e^{-(\overline{\kappa}/2)d_c(\gamma)}\overline{\nu}^{n_\gamma/2}\prod_{i=1}^{n_\gamma}e^{-(\overline{\kappa}/2)|R_i(\gamma)|}\right]\sum_{p\geqslant 1}\frac{1}{p!}(c|\gamma|\overline{\nu}^{1/4})^p$$

$$\leqslant ce^{-\kappa' d_c(\gamma)}(\nu')^{n_\gamma}\prod_{i=1}^{n_\gamma}e^{-\kappa'|R_i(\gamma)|}, \tag{6.20}$$

for some c, κ', $\gamma'>0$ and $\nu'=|\epsilon|^{\gamma'}$. Using the preceding bound we can easily prove that

$$\sup_{x\in\mathbb{Z}^{d+1}}\sum_{\delta(\gamma)\geqslant r}^{\gamma\ni x}|\rho(\gamma)|\leqslant c(\nu')^{1/2}e^{-(\kappa'/2)r}, \tag{6.21}$$

where $\delta(\gamma)$ is the diameter of the polymer γ. A standard theorem, proved for instance in Refs. 13 and 10, states that, if $\rho(\gamma)$ satisfies (6.21), then

$$\sup_{x\in\Lambda_D}\sum_{\delta(\Gamma)\geqslant r}^{\Gamma\ni x}\Upsilon^T(\Gamma)|\rho(\Gamma)|\leqslant c(\nu')^{1/4}e^{-(\kappa'/4)r}. \tag{6.22}$$

This implies that, varying Λ, P_Λ is a uniformly convergent sequence of analytic functions in a domain independent from Λ. The limit, still analytic in the same domain (thanks to Vitali's convergence theorem), is independent of the way the thermodynamic limit is performed (i.e., one can send the time side of Λ to ∞ either before the spatial side is sent to ∞ or together with it), thanks to the exponentially fast convergence of the sequence, implied by (6.22). For the same reason, the limit is also independent of the choice of boundary conditions and, because of translational invariance, it is equal to

$$P\overset{def}{=}\lim_{|\Lambda|\to\infty}P_\Lambda=\frac{1}{a}\log l+\frac{2}{h_0 a}\sum_{\Gamma\subset\mathbb{Z}^{d+1}}^{\Gamma\ni(0,0)}\frac{\Upsilon^T(\Gamma)\rho(\Gamma)}{|\Gamma|}, \tag{6.23}$$

where $|\Gamma|\overset{def}{=}|\cup_{\gamma\in\Gamma}\gamma|$ and $2/(h_0 a)=\lim_{|\Lambda|\to\infty}|\Lambda_D|/|\Lambda|$.

D. Analyticity of the mean values

The analyticity for the mean value of an analytic local observable $\mathcal{O}(\psi_V)$ (depending on the variables in the finite set $V\subset\mathbb{Z}^d$) is an easy corollary of the previous result.

We first observe that $\mu^{\mathrm{SRB}}(\mathcal{O})=\lim_{N,T\to\infty}(1/|V_N||I_T|)\Sigma_{(\xi,i)\in(V_N\times I_T)}\mu^{\mathrm{SRB}}(\mathcal{O}\circ\rho^{\xi}\circ S_\epsilon^i)$. This is true thanks to the time and space translation invariance of μ^{SRB}. Moreover, it is possible to decompose $\mathcal{O}$ as

$$\mathcal{O}(h_\epsilon(c_0(\sigma))_V)=\sum_{X\cap(V\times\{0\})=\emptyset}\mathcal{O}_X^{(0,0)}(\sigma_X).$$

This can be done expanding $\mathcal{O}(h_\epsilon)$ in power of ψ, using the representation of h_ϵ given in Secs. III and V and collecting the terms with the same support. Moreover, we will set

$$\mathcal{O}_X^{(\xi,j)}(\sigma_X)\overset{def}{=}\mathcal{O}^{(0,0)}_{\rho^{-\xi}\tau^{-j}X}(\sigma_X)$$

and

$$\mathcal{O}_X(\sigma_X)\overset{def}{=}\sum_{\substack{(\xi,j)\\ \rho^\xi V\times\{j\}\cap X\neq\emptyset}}\mathcal{O}_X^{(\xi,j)}(\sigma_X).$$

It is easy to realize that $\mathcal{O}_X$ is invariant under space and time translations, and satisfies

$$\|\mathcal{O}_X\|_\infty\leqslant c_V\nu^{n_X}e^{-\kappa d_c(X)}\prod_{i=1}^{n_X}e^{-\kappa|R_i(X)|},\tag{6.24}$$

for some κ, $\gamma>0$, $\nu=|\epsilon|^\gamma$ and some constant $c_V>0$ which depends on the size of V. Setting $\Lambda=V_N\times I_T$, the thermodynamic limit of the mean value of $\mathcal{O}(\psi_V)$ can be written as

$$\mu^{\mathrm{SRB}}(\mathcal{O})=\lim_{\Lambda\to\infty}\frac{1}{|\Lambda|}\partial_\zeta\log\frac{\Sigma_{\sigma_\Lambda}e^{-\Sigma_{X\cap\Lambda\neq\emptyset}[\phi_X(\sigma_X)-\zeta\mathcal{O}_X(\sigma_X)]}}{\Sigma_{\sigma_\Lambda}e^{-\Sigma_{X\cap\Lambda\neq\emptyset}\phi_X(\sigma_X)}}\Bigg|_{\zeta=0}\overset{def}{=}\partial_\zeta P_{\mathcal{O}}(\zeta).\tag{6.25}$$

Via a new cluster expansion we find

$$\mu^{\mathrm{SRB}}(\mathcal{O})=\lim_{\Lambda\to\infty}\frac{1}{|\Lambda|}\partial_\zeta\sum_{\Gamma\cap\Lambda_D\neq\emptyset}\Upsilon^T(\Gamma)(\rho^\zeta(\Gamma)-\rho(\Gamma))|_{\zeta=0},\tag{6.26}$$

where $\rho^\zeta(\gamma)$ are the activities corresponding to the potential $\phi_X-\zeta\mathcal{O}_X$. For $|\zeta|$ small enough, the potential $\phi_X-\zeta\mathcal{O}_X$ satisfies the same bounds of ϕ_X so that $\Sigma_{\Gamma\cap\Lambda_D\neq\emptyset}\Upsilon^T(\Gamma)(\rho^\zeta(\Gamma)-\rho(\Gamma))$ is a uniformly convergent sequence of functions, analytic in ϵ and ζ in the product of two small discs. This implies that $\mu^{\mathrm{SRB}}(\mathcal{O})$ is analytic in ϵ and given by

$$\mu^{\mathrm{SRB}}(\mathcal{O})=\frac{2}{h_0a}\sum_{\Gamma\subset\mathbb{Z}^{d+1}}^{\Gamma\ni(0,0)}\frac{\Upsilon^T(\Gamma)}{|\Gamma|}\partial_\zeta(\rho^\zeta(\Gamma)-\rho(\Gamma))|_{\zeta=0}.\tag{6.27}$$

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APPENDIX A: UNPERTURBED NONLINEAR DYNAMICS

The result about analyticity can be extended to the case in which the unperturbed dynamic is made up of independent *nonlinear* analytic Anosov systems $s_0\colon\mathbb{T}^2\to\mathbb{T}^2$. We suppose that there exist $v_\pm(\psi)$ and $\lambda_\pm(\psi)$ such that

$$(Ds_0v_+)(\phi)=\lambda_+(\phi)v_+(s_0(\phi)),\quad (Ds_0v_-)(\phi)=\lambda_-(\phi)v_-(s_0(\phi)),\tag{A1}$$

with $\phi \in \mathbb{T}^2$, $v_\pm(\phi)$ and $\lambda_\pm(\phi)$ are Hölder continuous and $|\lambda_+(\phi)|^{-1}$, $|\lambda_-(\phi)| \leqslant \lambda < 1$. Then we consider again a perturbation $f(\psi)$ on $\mathcal{T}_N$ analytic in ψ. Observe, however, that in this case the most naive example of perturbation, $f(\psi) \overset{def}{=} f^+(\psi) v_+(\psi)$, with $f^+(\psi)$ analytic, is *no longer* an analytic perturbation.

1. Conjugation

The constitutive equation for δh_ϵ, lifted on $\mathbb{R}^{2V_N}$, is

$$S_0(h_\epsilon(\psi)) + \epsilon f(h_\epsilon(\psi)) = S_0(\psi) + \delta h_\epsilon(S_0(\psi)). \tag{A2}$$

In order to exploit the hyperbolicity, it is convenient to arrange the terms as follows:

$$(DS_0 \delta h_\epsilon)(\psi) - \delta h_\epsilon(S_0(\psi)) = -\epsilon f(\psi + \delta h_\epsilon(\psi)) - [S_0(h_\epsilon(\psi)) - S_0(\psi) - (DS_0 \delta h_\epsilon)(\psi)]. \tag{A3}$$

Define

$$f^{,\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) \overset{def}{=} \frac{\partial^s}{\partial\zeta_1,\ldots,\partial\zeta_s} f(\psi + \zeta_1 w_{0,\alpha_1}^{(\xi_1)}(\psi) + \cdots + \zeta_s w_{0,\alpha_s}^{(\xi_s)}(\psi))\big|_{\zeta_1=\cdots=\zeta_s=0},$$

whereas

$$f^{\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) \overset{def}{=} \sum_{\mathbf{x}} f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) w_{0,\alpha}^{(\xi)}(S_0(\psi)) \quad \text{and} \quad S_0^{\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) \overset{def}{=} \sum_{\mathbf{x}} S_0^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) w_{0,\alpha}^{(\xi)}(S_0(\psi)).$$

Writing $\delta h_\epsilon(\psi) \overset{def}{=} \Sigma_{\mathbf{x}} \delta h_\epsilon^{\mathbf{x}}(\psi) w_{0,\alpha}^{(\xi)}(\psi)$, and $(DS_0 w_{0,\alpha}^{(\xi)})(\psi) \overset{def}{=} \Sigma_{\mathbf{y}} S_0^{\mathbf{y},\mathbf{x}}(\psi) w_{0,\beta}^{(\eta)}(S_0(\psi))$, with $S_0^{\mathbf{y},\mathbf{x}}(\psi) = \lambda_\alpha(\psi_\xi)\delta_{\mathbf{x},\mathbf{y}}$, we get

$$\lambda_\alpha \delta h_\epsilon^{\mathbf{x}}(\psi) - \delta h_\epsilon^{\mathbf{x}}(S_0(\psi)) = -\epsilon \sum_{s\geqslant 0} \left(\frac{f^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_\epsilon^{\mathbf{x}_1} \cdots \delta h_\epsilon^{\mathbf{x}_s} \right)(\psi) - \sum_{s\geqslant 2} \left(\frac{S_0^{\mathbf{x},\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_\epsilon^{\mathbf{x}_1} \cdots \delta h_\epsilon^{\mathbf{x}_s} \right)(\psi). \tag{A4}$$

Finally, the recursive equation for the Taylor coefficients of $\delta h_\epsilon^{\xi^+}(\psi)$ is

$$\begin{aligned}
\delta h_{(k+1)}^{\xi^+}(\psi) = &- \sum_{p\geqslant 0} \left(\prod_{m=0}^{p} \lambda_+^{-1}(s_0^m(\psi_\xi)) \right) \sum_{s\geqslant 0} \sum_{\substack{k_1+\cdots+k_s=k \\ k_i\geqslant 1}} \left(\frac{f^{\xi^+,\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_{(k_1)}^{\mathbf{x}_1} \cdots \delta h_{(k_s)}^{\mathbf{x}_s} \right)(S_0^p(\psi)) \\
&+ \sum_{p\geqslant 0} \left(\prod_{m=0}^{p} \lambda_+^{-1}(s_0^m(\psi_\xi)) \right) \sum_{s\geqslant 2} \sum_{\substack{k_1+\cdots+k_s=k+1 \\ k_i\geqslant 1}} \left(\frac{S_0^{\xi^+,\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} \delta h_{(k_1)}^{\mathbf{x}_1} \cdots \delta h_{(k_s)}^{\mathbf{x}_s} \right) \\
&\times (S_0^p(\psi)).
\end{aligned} \tag{A5}$$

A similar equation holds for $\mathbf{x} = \xi^-$.

From now on, the construction of the conjugation function goes on as in the linear case with similar considerations. We have only to take in account the fact that a tree of order k (w.r.t. ϵ) does not necessarily have k branches, because of the term on the last line of (1.5) (to be called a vertex of type 0). Since the number of lines entering a vertex of type 0 is $\geqslant 2$, one can easily prove that the number b_k of branches of a tree of order k is bounded by $k \leqslant b_k \leqslant 2k-1$, so that nothing qualitatively changes in the bounds and the proof of analyticity of δh_ϵ proceed as in Secs. III and VI.

2. Unstable direction

The perturbed unstable direction in the point $h_\epsilon(\psi)$ is given by the equation

$$(DS_\epsilon w^{(\xi)}_{\epsilon,+})(h_\epsilon(\psi)) = w^{(\eta)}_{\epsilon,+}(h_\epsilon(S_0(\psi)))L^{\eta\xi}(\psi). \tag{A6}$$

Setting $w^{(\xi)}_{\epsilon,+}(h_\epsilon(\psi)) \overset{def}{=} v^{(\xi)}_\epsilon(\psi)$, it is convenient to rearrange the terms of the equation in the following way:

$$\begin{aligned}(DS_0 v^{(\xi)}_\epsilon)(\psi) - \lambda_+(\psi_\xi) v^{(\xi)}_\epsilon(S_0(\psi)) = \delta L^{\eta\xi}(\psi) v^{(\eta)}_\epsilon(S_0(\psi)) - \epsilon(Df)(h_\epsilon(\psi)) v^{(\xi)}_\epsilon(\psi) \\ - [DS_0(h_\epsilon(\psi)) - DS_0(\psi)] v^{(\xi)}_\epsilon(\psi).\end{aligned} \tag{A7}$$

Defining $v^{(\eta)}_\epsilon(\psi) = \Sigma_{\mathbf{x}} V^{(\eta)}_{\epsilon,\mathbf{x}}(\psi) w^{(\xi)}_{0,\alpha}(\psi)$, and using again the considerations of Sec. IV, we finally get

$$\begin{aligned}\lambda_\alpha(\psi_\rho) V^{(\rho)}_{\epsilon,\mathbf{x}}(\psi) - \lambda_+(\psi_\rho) V^{(\rho)}_{\epsilon,\mathbf{x}}(S_0(\psi)) = &+ \delta L^{\zeta\rho}(\psi) V^{(\zeta)}_{\epsilon,\mathbf{x}}(S_0(\psi)) \\ &- \epsilon \sum_{s\geqslant 0} \left(\frac{f^{\mathbf{x},\mathbf{y}\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} V^{(\rho)}_{\epsilon,\mathbf{y}} \delta h^{\mathbf{x}_1}_\epsilon \cdots \delta h^{\mathbf{x}_s}_\epsilon \right)(\psi) \\ &- \sum_{s\geqslant 1} \left(\frac{S_0^{\mathbf{x}\mathbf{y},\mathbf{x}_1,\ldots,\mathbf{x}_s}}{s!} V^{(\rho)}_{\epsilon,\mathbf{y}} \delta h^{\mathbf{x}_1}_\epsilon \cdots \delta h^{\mathbf{x}_s}_\epsilon \right)(\psi)\end{aligned}$$

[with $(DS_0^{\mathbf{x}_1\ldots\mathbf{x}_s} w^{(\xi)}_a)(\psi) \overset{def}{=} S_0^{\mathbf{x}\mathbf{y},\mathbf{x}_1,\ldots,\mathbf{x}_s}(\psi) w^{(\eta)}_b(S_0\psi)$]. Again, because of the third term on the r.h.s. of Eq. (A7), the number of branches of a tree appearing in the construction of δV and δL is greater (in general) than the order of the tree itself. This is not a problem, since one can easily realize that, again, the number b_k of branches of a tree of order k is such that $k \leqslant b_k \leqslant 2k$.

3. SRB interactions

Following the proof in Sec. IV and, proceeding as in Secs. V and VI, one proves analyticity of the SRB distribution. In fact, the only (slight) difference in the construction of SRB potentials is in the telescopic cutting necessary to represent h, L, V and Λ as sums of local functions of spin variables. Notice that now each tree node is associated to the product of a node function $f_v(\psi)$ [e.g., in the case of a tree contributing to δh, f_v can be a derivative of f or a derivative of S_0, see (A5)] times a product of local Lyapunov exponents, like the factor $\Pi^p_{m=0}\lambda_+^{-1}(s_0^m(\psi_\xi)) \overset{def}{=} \Theta_+(p, s_0^{p(v)}(\psi_\xi))$ in (A5); the analogous expression appearing in a vertex with $\alpha(v) = -$ will be denoted by $\Theta_-(p, s_0^{p(v)}\psi_\xi)$. So the total node function associated to a vertex v will now be of the form

$$F^v(p(v), S_0^{p(v)}(\psi)) \overset{def}{=} \Theta_{\alpha(v)}(p(v), s_0^{p(v)}(\psi_{\xi_v})) f_v(S_0^{p(v)}(\psi)), \tag{A8}$$

where v' is the vertex immediately following v. The telescopic expansion (5.1) has to be done *separately* for each of the factors in the above equation [$\lambda(\psi)$ is Hölder continuous], getting in the end potentials with the same kind of decay rate. The bounds are not qualitatively changed and the subsequent analysis of Sec. V follows so that, by suitably modifying the decimation procedure, analyticity of SRB measure can be proved. We point out that a main difference in the proof of convergence of the cluster expansion is that now the unperturbed potentials are not vanishing, but have support only on timelike segments $I \subset \mathbb{Z}$, and are exponentially decaying with the diameter of I. For this reason one cannot proceed exactly as in Sec. VI. The standard way to treat this problem (see Ref. 7), is to choose a length r such that the unperturbed interactions on sets I, diam(I)

$>r$, are small enough for the cluster expansion. Then one fixes the size of the *B*-blocks $b=r$, and the size of the *H*-blocks, h, such that the Perron–Frobenius theorem is true for the *reduced partition function* $Z_r(\beta_\xi^{(p)},\eta_\xi^{(p)},\beta_\xi^{(p+1)})$, in which only the interaction on sets $I\subset(B_\xi^{(p)}\cup H_\xi^{(p)}\cup B_\xi^{(p+1)})$, $\mathrm{diam}(I)\leqslant r$, are taken in account.

APPENDIX B: GREEN–KUBO FORMULA AND LARGE DEVIATION

In this section we deal with an application. We introduce the *local phase space contraction rate*[9] on a volume $V_0\subset V_N$ averaged on a time T_0, given by

$$\eta_{\Lambda_0}(\psi)\overset{def}{=}\frac{1}{|\Lambda_0|}\sum_{j\in I_{T_0}}\log|\det(DS_\epsilon)_{V_0}(S_\epsilon^j(\psi))|, \tag{B1}$$

with $\Lambda_0=V_0\times I_0$ and $I_0\overset{def}{=}[-T_0/2,T_0/2]\cap\mathbb{Z}$. We prove a Green–Kubo formula for η_{Λ_0}, from which it will come out that generically its mean value η_+ is strictly negative. Furthermore, we can show the large fluctuations of η_{Λ_0} around η_+ satisfy a large deviation principle, namely they are asymptotically described by a strictly convex *free energy functional* $F(\eta)$: it can be obtained as the Legendre transform of the generating functional $P(\zeta)=P_{\eta_{\Lambda_0}}(\zeta)$ [see Eq. (6.25)].

For the rest of the Appendix the SRB interaction will be called $\{\phi_X^+\}_{X\subset\mathbb{Z}^{d+1}}$, to remind that they are derived from the unstable restriction of DS_ϵ.

Theorem B1: *Given S_ϵ such that $\eta_+<0$,*

(1) $P(\zeta)$ is analytic and strictly convex in ζ, for $|\epsilon|<\epsilon_0$, $|\zeta|\leqslant 1$, with ϵ_0 small enough; and
(2) the Green–Kubo formula is valid:

$$\partial_\epsilon^2 P'(0)|_{\epsilon=0}=-\tfrac{1}{2}\partial_\epsilon^2 P''(0)|_{\epsilon=0}. \tag{B2}$$

Theorem B2: *Given S_ϵ such that $\eta_+<0$,*

(1) the free energy $F(\eta)$ is analytic in η, for $|\epsilon|<\epsilon_0$, and $\eta\in[P'(-1),P'(1)]$;
(2) if $[a,b]\subset[P'(-1),P'(1)]$, then

$$\lim_{|\Lambda_0|\to\infty}\frac{1}{|\Lambda_0|}\log\mu^{\mathrm{SRB}}(\eta_{\Lambda_0}\in[a,b])=\max_{\eta\in[a,b]}-\Delta F(\eta,\eta_+), \tag{B3}$$

with $\Delta F(\eta,\eta_+)\overset{def}{=}F(\eta)-F(\eta_+)$.

1. Local phase space contraction rate

Repeating the construction of SRB potentials leading to (B8), we set

$$\eta_{\Lambda_0}(h_\epsilon(c_0(\sigma)))\overset{def}{=}\frac{1}{|\Lambda_0|}\sum_{X\subset\mathbb{Z}^{d+1}}^{X\cap\Lambda_0\neq 0}\phi_X(\sigma_X), \tag{B4}$$

for a suitable potential ϕ_X, satisfying

$$\|\phi_X\|_\infty\leqslant ce^{-\kappa d_c(X)}\nu^{n_X}\prod_{i=1}^{n_X}e^{-\kappa|R_i(X)|}, \tag{B5}$$

for some c, κ, $\gamma>0$ and $\nu=|\epsilon|^\gamma$. From the invariance under time translations of the SRB measure, we have

$$\eta_+ \overset{def}{=} \lim_{|V_0|\to\infty} \frac{1}{|V_0|}\mu^{\mathrm{SRB}}(\log|\det(DS_\epsilon)_{V_0}|) = \lim_{|\Lambda_0|\to\infty} \mu^{\mathrm{SRB}}(\eta_{\Lambda_0}) = \lim_{|\Lambda_0|\to\infty} \frac{1}{|\Lambda_0|} \sum_{X\cap\Lambda_0\neq 0} \mu^{\mathrm{SRB}}(\phi_X)$$

$$= \lim_{|\Lambda_0|\to\infty} \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda_0|}\partial_\zeta \log \frac{\Sigma_{\sigma_\Lambda} e^{-\Sigma_{X\cap\Lambda\neq\emptyset}\phi_X^+(\sigma_X)+\zeta\Sigma_{X\cap\Lambda_0\neq\emptyset}\phi_X(\sigma_X)}}{\Sigma_{\sigma_\Lambda} e^{-\Sigma_{X\cap\Lambda\neq\emptyset}\phi_X^+(\sigma_X)}}\Bigg|_{\zeta=0}. \tag{B6}$$

It is easy to show the last expression is equal to the one with the summations over $X\cap\Lambda\neq\emptyset$ and $X\cap\Lambda_0\neq\emptyset$ replaced by $X\subset\Lambda_0$ and without the limit in Λ (since the correction is only a border effect; or simply using again the cluster expansion developed in Sec. VI D). In this way, defining the *generating function* $P(\zeta)$ as

$$P(\zeta) \overset{def}{=} \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|}\log \frac{\Sigma_{\sigma_\Lambda} e^{-\Sigma_{X\subset\Lambda}(\phi_X^+ - \zeta\phi_X)(\sigma_X)}}{\Sigma_{\sigma_\Lambda} e^{-\Sigma_{X\subset\Lambda}\phi_X^+(\sigma_X)}}, \tag{B7}$$

we finally get

$$\eta_+ = P'(0). \tag{B8}$$

Analyticity is achieved by cluster expansion [we do not need ζ small, but we can take, say, $|\zeta|\leqslant 1$, since $\{\phi_X\}_X$ are $O(\epsilon)$].

2. Green–Kubo formula

Consider the case in which s_0 is the Arnold's cat map defined by (A1).

Using the definition of pressure (B7) and the fast convergence properties of the cluster expansion of $P(\zeta)$, we find

$$P(\zeta) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|}\log \frac{\mu_{N,0}^{\mathrm{SRB}}(e^{-\Sigma_{j\in I_T}\log|\det L\circ S_0^j| + \zeta\Sigma_{j\in I_T}\log|\det DS_\epsilon\circ h_\epsilon\circ S_0^j|})}{\mu_{N,0}^{\mathrm{SRB}}(e^{-\Sigma_{j\in I_T}\log|\det L\circ S_0^j|})}, \tag{B9}$$

where

(1) the matrix $L=\mathcal{L}\circ h_\epsilon$ was introduced in Sec. II B above;

(2) $\mu_{N,0}^{\mathrm{SRB}}$ is the unperturbed SRB measure: if $\mathcal{O}(\psi)$ is a local Hölder continuous observable, it is defined as

$$\mu_{N,0}^{\mathrm{SRB}}(\mathcal{O}) = \lim_{|\Lambda|\to\infty} \frac{\Sigma_{\sigma_\Lambda}\mathcal{O}(c_0(\sigma_\Lambda|\hat\sigma_{\Lambda^c}))}{\Sigma_{\sigma_\Lambda} 1}, \tag{B10}$$

and, independently of the boundary conditions, it is equal to the Lebesgue measure.

Defining U_ζ as

$$U_\zeta = \log|\det L| - \zeta\log|\det S_0^{-1}\circ DS_\epsilon\circ h_\epsilon|, \tag{B11}$$

and using that $\mu_{N,0}^{\mathrm{SRB}}$ is the Lebesgue measure on $\mathcal{T}_N$, we find

$$P(\zeta) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|}\log \frac{\int d\psi e^{-\Sigma_{j\in I_T} U_\zeta(S_0^j\psi)}}{\int d\psi e^{-\Sigma_{j\in I_T} U_0(S_0^j\psi)}}, \tag{B12}$$

so that $P'(0)$ is equal to

$$P'(0)=\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{j\in I_T}\frac{\int \mathrm{d}\psi \log|\det S_0^{-1}DS_\epsilon(h_\epsilon(S_0^j\psi))|e^{-\Sigma_{j\in I_T}U_0(S_0^j\psi)}}{\int \mathrm{d}\psi e^{-\Sigma_{j\in I_T}U_0(S_0^j\psi)}}. \tag{B13}$$

Since $P'(0)|_{\epsilon=0}$ is trivially=0, we can try to see if $\partial_\epsilon P'(0)|_{\epsilon=0}$ is different from zero [if it were, $P'(0)$ would be different from zero for $\epsilon\neq 0$ small enough]. Recalling that $f(\psi)$ is the perturbing function and $f^\xi(\psi)$ is its projection on the ξth site, we get

$$\begin{aligned}\partial_\epsilon P'(0)|_{\epsilon=0}&=\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{j\in I_T}\int\frac{\mathrm{d}\psi}{(2\pi)^{2|V_N|}}\mathrm{Tr}[S_0^{-1}Df(S_0^j\psi)]\\&=\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{j\in I_T}\sum_{\substack{\alpha=\pm\\ \xi\in V_N}}\int\frac{\mathrm{d}\psi}{(2\pi)^{2|V_N|}}\lambda^\alpha f^{\xi^\alpha,\xi^\alpha}(S_0^j\psi).\end{aligned} \tag{B14}$$

Since f is periodic we have $\partial_\epsilon P'(0)|_{\epsilon=0}=0$.

A straightforward calculation shows that

$$\begin{aligned}\frac{1}{2}\partial_\epsilon^2 P'(0)|_{\epsilon=0}=\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{j\in I_T}\int\frac{\mathrm{d}\psi}{(2\pi)^{2|V_N|}}\Bigg\{&\mathrm{Tr}[S_0^{-1}D^2f(S_0^j\psi)\,\delta h_{(1)}(S_0^j\psi)]\\&-\frac{1}{2}\mathrm{Tr}[(S_0^{-1}Df(S_0^j\psi))^2]-\sum_{j'\in I_T}\mathrm{Tr}(S_0^{-1}Df(S_0^j\psi))\mathrm{Tr}^{(u)}(S_0^{-1}Df(S_0^{j'}\psi))\Bigg\},\end{aligned} \tag{B15}$$

where $\mathrm{Tr}^{(u)}$ is the trace restricted to the (unperturbed) unstable manifold. The preceding expression can be rewritten in a more convenient way. Using the explicit expression of $\delta h_{(1)}$, Eq. (3.5), and defining $A_0=\cup_{\xi\in nn(0)}nn(\xi)$, we find that the first term in Eq. (2.15) is equal to

$$\begin{aligned}&\sum_{\substack{\alpha_i=\pm\\ |\xi|\leqslant 1}}\sum_{p\geqslant 0}\int\frac{\mathrm{d}\psi_{A_0}}{(2\pi)^{2|A_0|}}\lambda^{\alpha_1}f^{0^{\alpha_1},0^{\alpha_1}\xi^{\alpha_2}}(\psi)(-\alpha_2)\lambda^{p+\rho_{\alpha_2}}f^{\xi^{\alpha_2}}(S_0^{\alpha_2(p+1-\rho_{\alpha_2})}\psi)\\&=\sum_{\substack{\alpha_i=\pm\\ |\xi|\leqslant 1}}\sum_{p\geqslant 0}\int\frac{\mathrm{d}\psi_{A_0}}{(2\pi)^{2|A_0|}}\lambda^{\alpha_1}f^{0^{\alpha_1},0^{\alpha_1}}(\psi)\alpha_2\lambda^{\alpha_2}f^{\xi^{\alpha_2},\xi^{\alpha_2}}(S_0^{\alpha_2(p+1-\rho_{\alpha_2})}\psi).\end{aligned} \tag{B16}$$

Integrating by parts, we see that the sum of the second and third terms in Eq. (2.15) is equal to

$$-\frac{1}{2}\sum_{\substack{\alpha_i=\pm\\ |\xi|\leqslant 1}}\int\frac{\mathrm{d}\psi_{A_0}}{(2\pi)^{2|A_0|}}\lambda^{\alpha_1}f^{0^{\alpha_1},0^{\alpha_1}}(\psi)\left[\lambda^{\alpha_2}f^{\xi^{\alpha_2},\xi^{\alpha_2}}(\psi)+\lambda\sum_{p\in\mathbb{Z}}f^{\xi^+,\xi^+}(S_0^p\psi)\right]. \tag{B17}$$

Combining the three contributions, we finally find

$$\partial_\epsilon^2 P'(0)|_{\epsilon=0} = -\sum_{\substack{\alpha_i=\pm \\ |\xi|\leqslant 1}} \sum_{p\in\mathbb{Z}} \int \frac{d\psi_{A_0}}{(2\pi)^{2|A_0|}} \lambda^{\alpha_1} f^{0^{\alpha_1},0^{\alpha_1}}(\psi) \lambda^{\alpha_2} f^{\xi^{\alpha_2},\xi^{\alpha_2}}(S_0^p \psi)$$

$$= -\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \int \frac{d\psi}{(2\pi)^{2|V_N|}} \left(\sum_{j\in I_T} \mathrm{Tr}[S_0^{-1} Df(S_0^j \psi)] \right)^2 = -\frac{1}{2} \partial_\epsilon^2 P''(0)|_{\epsilon=0}, \tag{B18}$$

that is the expected Green–Kubo relation (see Ref. 14).

From Eqs. (2.18) and (2.8), we see that, for ϵ small enough, η_+ is negative and, generically, strictly negative [the condition for f to be *generic* is just that the first line in Eq. (2.18) is different from 0].

Let us now compute Eq. (2.18) in a special case, essentially the simplest possible. Let

$$f^{\xi^+}(\psi) = \sum_{\eta\in nn(\xi)} \sin(\psi_\xi^1 - \psi_\eta^1), \quad f^{\xi^-}(\psi) = 0. \tag{B19}$$

Substituting such choice in Eq. (2.18), we find

$$\partial_\epsilon^2 P'(0)|_{\epsilon=0} = -2 \sum_{|\xi|=1} \int \frac{d\psi_0}{(2\pi)^2} \frac{d\psi_\xi}{(2\pi)^2} \lambda^2 \cos^2(\psi_0^1 - \psi_\xi^1)(v_+ \cdot \hat{e}_1)^2 = -\frac{2d}{1+\lambda^{-2}}, \tag{B20}$$

where $\hat{e}_1 = (1,0)$ and we used that $v_+ = (1/\sqrt{1+\lambda^2}, -\lambda/\sqrt{1+\lambda^2})$.

So, choosing $\epsilon \in \mathbb{R}$ small enough and different from zero, $\eta_+ = P'(0) = -[d/(1+\lambda^{-2})]\epsilon^2 + O(\epsilon^3) < 0$. Furthermore, if $\zeta \in \mathbb{R}$ has modulus smaller than 1, $P(\zeta)$ is strictly convex [since $1/2P''(0) = -P'(0) > 0$ and $P(\zeta)$ is analytic for $|\zeta| \leqslant 1$ and ϵ small enough].

3. Large deviations

In the present section we shall prove a large deviations property for η_{Λ_0}. We will follow the classical strategy set up in Refs. 22 and 12 (in particular we will refer to the formulas in Sec. 5 of the latter). The proof below will hold in the case $\eta_+ < 0$, namely in the generic case or, to be definite, in the case the perturbation is chosen as in Eq. (B19).

Thanks to the convexity of $P(\zeta)$, given $\eta \in [P'(-1), P'(1)]$, there exists a unique point $Z(\eta) \in [-1,1]$ such that $P'(Z(\eta)) \equiv \eta$; considering such a point η and its neighbor of radius δ, $I_\delta(\eta)$, such that $I_\delta(\eta) \subset [P'(-1), P'(1)]$, from the "large deviation property III", Sec. 5 of Ref. 12, we get

$$\mu^{\mathrm{SRB}}(\eta_+ \in I_\delta(\eta)) = O(1) e^{O(\delta|\Lambda_0|)} e^{O(|\partial\Lambda_0|)} \exp\{[P(Z(\eta)) - P(0) - Z(\eta)\eta]|\Lambda_0|\}. \tag{B21}$$

In our case $P(0) = 0$. Still for $\eta \in [P'(-1), P'(1)]$, we define the free energy $F(\eta)$ as the Laplace transform of the generating function $P(\zeta)$:

$$F(\eta) \overset{def}{=} \max_\zeta \{\zeta\eta - P(\zeta)\} = Z(\eta)\eta - P(Z(\eta)); \tag{B22}$$

therefore, for $I_\delta(\eta) \subset [P'(-1), P'(1)]$,

$$\mu^{\mathrm{SRB}}(\eta_+ \in I_\delta(\eta)) = O(1) e^{O(\delta|\Lambda_0|)} e^{O(|\partial\Lambda_0|)} \exp\{-|\Lambda_0| \Delta F(\eta, \eta_+)\}; \tag{B23}$$

where $\Delta F(\eta, \eta_+) \overset{def}{=} F(\eta) - F(\eta_+)$ [indeed $F(\eta_+) = -P(0) = 0$].

Finally, if $[a,b]\subset[P'(-1),P'(1)]$, it is suitable to take $\delta_{\Lambda_0}=|\Lambda_0|^{-\beta}$, $0<\beta<1$, and divide the interval $[a,b]$ in $|b-a||\Lambda_0|^{\beta}$ identical disjoint subintervals centered in $\eta_n \overset{def}{=} a+(n-1/2)\delta_{\Lambda_0}$. We find

$$\mu^{\mathrm{SRB}}(\eta_{\Lambda_0}\in[a,b])=\sum_{n=1}^{|b-a||\Lambda_0|^{\beta}}\mu^{\mathrm{SRB}}(\eta_+\in I_{\delta_{\Lambda_0}}(\eta_n))$$

$$=O(1)|\Lambda_0|^{\beta}e^{O(|\Lambda_0|^{1-\beta})}e^{O(|\partial\Lambda_0|)}\exp\{|\Lambda_0|\max_{\eta\in[a,b]}[-\Delta F(\eta,\eta_+)]\},\tag{B24}$$

namely the result in the second theorem.

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Random-field quantum spherical ferroelectric model

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We study a (quenched) random-field quantum model of an anharmonic crystal for displacive structural phase transitions in spherical approximation: the random-field quantum spherical (ferroelectric) model. For stationary ergodic random fields its behavior depends on the quantum parameter of the model and on the expectation and covariance of the field. If quantum fluctuations are small enough not to destroy the phase transition, then it can be suppressed when the field fluctuations are large. For the field of independent identically distributed random variables and the short-range interaction we obtain that the *lower* critical dimensionality $d_l=4$ ($d_l=2$ for the zero-field) and that it decreases for long-range interactions. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1769103]

I. INTRODUCTION

References 19 and 20 started a rigorous study of quantum critical fluctuations in the quantum spherical ferroelectric model, known also as the quantum anharmonic crystal model in spherical approximation, see, e.g., Ref. 6. Further examination of the displacive structural (or the ferroelectric) phase transition and the critical behavior of this model shows that the quantum fluctuations are dependent not only on details of the interaction but also on small perturbations (such as an external field) breaking the symmetry of the model.[21,9]

The aim of the present note is to consider the quantum spherical ferroelectric model in quenched external random fields conjugate to particles displacements from equilibria. Since the paper of Ref. 11, it is known that the presence of randomness leads to some new features of the phase transition in the classical spherical model.

In this paper we show that the simultaneous presence of quantum and external random-field fluctuations makes the critical behavior of the random field quantum spherical ferroelectric model rather nontrivial.

In Sec. II we formulate our model and the main Theorem 2.1. There we also discuss the properties of the displacive phase transition as a function of the model parameters. We show that the randomness acts in the same direction as quantum fluctuations, i.e., it has a tendency to suppress the order parameter and the phase transition. For example, in the simplest case of the random field of independent identically distributed variables and of a short-range harmonic interaction the lower critical dimensionality is $d=4$, instead of $d=3$ for the model without the random field. The proof of the main Theorem 2.1 is given in Sec. III. Some concluding remarks are collected in Sec. IV.

II. MODEL AND MAIN THEOREM

Let $\mathbb{Z}^d$ be a d-dimensional hypercubic lattice. With each lattice site $l\in\mathbb{Z}^d$ occupied by a particle of mass m, we associate a position and momentum operators $Q_l\in\mathbb{R}^1$ and $P_l=(\hbar/i)$

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$\times(\partial/\partial Q_l)$ corresponding (for simplicity) to one-dimensional particle displacements at this site. The case of $Q_l \in \mathbb{R}^\nu, \nu \geqslant 1$, involves more symmetry, but essentially it is very similar to $\nu = 1$, see, e.g., Refs. 4, 5, or 6.

Let $\Lambda \subset \mathbb{Z}^d$ be a finite rectangular subset wrapped according to the periodic boundary conditions:

$$\Lambda := \{l \in \mathbb{Z}^d : -N_\alpha/2 < l_\alpha \leqslant N_\alpha/2\,,\ \alpha = 1,2,\ldots,d\}, \tag{2.1}$$

where we suppose $\{N_\alpha\}_{\alpha=1}^d$ to be even. Then $V := |\Lambda| = N_1 N_2 \cdots N_d$, and Λ^* be the lattice dual to Λ:

$$\Lambda^* := \{k \in \mathbb{R}^d : k_\alpha = 2\pi n_\alpha / N_\alpha, \alpha = 1,2,\ldots,d, \text{ and } \{n_\alpha\}_{\alpha=1}^d \in \Lambda\}. \tag{2.2}$$

The local Hamiltonian of the quantum spherical model in the external random field that we study in this paper is given by the operator

$$H_\Lambda(h^\omega) = \sum_{l\in\Lambda} \frac{P_l^2}{2m} + \frac{1}{4}\sum_{l,l'\in\Lambda} \phi_{l,l'}^\Lambda (Q_l - Q_{l'})^2 + \frac{a}{2}\sum_{l\in\Lambda} Q_l^2 + VW\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right) - \sum_{l\in\Lambda} h_l^\omega Q_l\,, \tag{2.3}$$

with domain in the Hilbert space $L^2(\mathbb{R}^\Lambda)$. The first term in (2.3) corresponds to the kinetic-energy operator of displacements. The second term represents a harmonic interaction between particles, which are in turn confined by the local harmonic potential with $a \geqslant 0$ described by the third term.

We suppose that the harmonic interaction matrix $\{\phi_{l,l'} = \phi_{l-l'}\}_{l,l'\in\mathbb{Z}^d}$ is positive-definite and translation-invariant. Then for any Λ the matrix $\{\phi_{l,l'}^\Lambda\}_{l,l'\in\Lambda} := \{\phi_{l-l'}^{per}\}_{l,l'\in\Lambda}$ is a restriction to Λ of periodically extended [according to the boundary conditions (2.1)] matrix $\{\phi_{l-l'}\}_{l,l'\in\mathbb{Z}^d}$, which we denoted by $\{\phi_{l-l'}^{per}\}_{l,l'\in\mathbb{Z}^d}$. Therefore, by construction the matrix $\{\phi_{l,l'}^\Lambda\}_{l,l'\in\Lambda}$ is positive-definite and translation-invariant.

The first two terms of the Hamiltonian (2.3) correspond to the one-component Debye phonons, whereas the third term creates a gap in the phonon spectrum, if $a > 0$. The fourth term in (2.3) represents a one-site lattice nonpolynomial anharmonic potential in the (mean) spherical approximation,[18,19] known also as the choquard self-consistent phonons approximation.[2,6–8] One can model this anharmonicity by $W: \mathbb{R}_+^1 \to \mathbb{R}_+^1$, monotonous decreasing to a zero function with a bounded positive second derivative $W'' > 0$, see Refs. 18–20. The last term in (2.3) describes the interaction between particles in positions $\{Q_l\}_{l\in\mathbb{Z}^d}$ and the external random field $\{h_l^\omega\}_{l\in\mathbb{Z}^d} \in \mathbb{R}^{\mathbb{Z}^d}$, where $\omega \in \Omega$, and $(\Omega, \mathcal{F}, \mathbb{P})$ is a corresponding probability space.

We denote by

$$f_\Lambda[H_\Lambda(h^\omega)] := -(\beta V)^{-1} \ln \mathrm{Tr}_{L^2(\mathbb{R}^\Lambda)} \exp\{-\beta H_\Lambda(h^\omega)\}, \tag{2.4}$$

the free-energy density associated with the Hamiltonian (2.3), where $\beta = (k_B T)^{-1}$ and T is the temperature. The main result of the present paper is the following statement:

Theorem 2.1: *Let $W: \mathbb{R}_+^1 \to \mathbb{R}_+^1$, be a monotonous decreasing to zero function with a bounded positive second derivative $W'' > 0$. If the stationary random field $h^\omega := \{h_l^\omega\}_{l\in\mathbb{Z}^d} \in \mathbb{R}^{\mathbb{Z}^d}$ on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is metrically transitive (ergodic), then the thermodynamic limit (here $\lim_\Lambda$ stays for $\Lambda \uparrow \mathbb{Z}^d$):*

$$f(\beta, h^\omega) := \lim_\Lambda f_\Lambda[H_\Lambda(h^\omega)] \tag{2.5}$$

of the free-energy (2.4) exists for $\mathbb{P}$-almost all $\omega \in \Omega$ and it has the following properties:

(a) *The limit $f(\beta, h^\omega) =: f(\beta, h)$ is $\mathbb{P}$-almost surely* (a.s.) *nonrandom;*

(b) *It coincides with the limiting free-energy density for the approximating Hamiltonian:*

$$H_\Lambda(c,h^\omega) := \sum_{l\in\Lambda}\frac{P_l^2}{2m} + \frac{1}{4}\sum_{l,l'\in\Lambda}\phi_{l,l'}(Q_l - Q_{l'})^2 + \frac{a}{2}\sum_{l\in\Lambda}Q_l^2 + W'(c)\sum_{l\in\Lambda}Q_l^2 - \sum_{l\in\Lambda}h_l^\omega Q_l + V[W(c) - cW'(c)], \tag{2.6}$$

in the sense that

$$f(\beta,h^\omega) = \text{a.s.} - \sup_{c\geqslant c^*}\lim_{\Lambda}\mathbb{E}(f_\Lambda[H_\Lambda(c,h^\omega)]). \tag{2.7}$$

Here $\mathbb{E}(\cdot)$ *is the expectation with respect to the probability* $\mathbb{P}$ *and* c^* *is defined by*

$$c^* := \inf_{c\geqslant 0}\{c : a + 2W'(c) \geqslant 0\}. \tag{2.8}$$

Remark 2.2: Since the approximating Hamiltonian (2.6) is harmonic, the corresponding free-energy density is known explicitly for any Λ *and* $c\geqslant c^*$*:*

$$f_\Lambda[H_\Lambda(c,h^\omega)] = \frac{1}{\beta V}\sum_{q\in\Lambda^*}\ln\left[2\sinh\frac{\beta\lambda\Omega_q(c)}{2}\right] - \frac{1}{2V}\sum_{q\in\Lambda^*}\frac{|h_\Lambda^\omega(q)|^2}{\Omega_q^2(c)} + [W(c) - cW'(c)]. \tag{2.9}$$

Here

$$\Omega_q(c) = (\Delta(c) + \omega_q^2)^{1/2}, \quad q\in\Lambda^* \tag{2.10}$$

is the q-mode frequency of the harmonic (self-consistent) phonons of Hamiltonian (2.6), with the non-negative gap:

$$\Delta(c) := a + 2W'(c) \geqslant 0, \tag{2.11}$$

for $c\geqslant c^*$*. The Debye phonons frequencies are defined by*

$$\omega_q^2 = \tilde{\phi}(0) - \tilde{\phi}(q), \quad q\in\Lambda^*, \tag{2.12}$$

where

$$\tilde{\phi}(q) = \sum_{l\in\mathbb{Z}^d}\phi_{l,0}\exp(-iql), \tag{2.13}$$

and similarly

$$h_\Lambda^\omega(q) := \frac{1}{V^{1/2}}\sum_{l\in\Lambda}h_l^\omega\exp(-iql). \tag{2.14}$$

The quantum parameter of the model λ *is*

$$\lambda = \frac{\hbar}{\sqrt{m}}. \tag{2.15}$$

The Proof of Theorem 2.1 is given in the next section. We conclude this section by some additional remarks concerning the properties of our model (2.3).

Remark 2.3: The simplest stationary ergodic random field $\{h_l^\omega\}_{l\in\mathbb{Z}^d}\in\mathbb{R}^{\mathbb{Z}^d}$ *corresponds to independent identically distributed random variables (i.i.d.r.v.) on the lattice* $\mathbb{Z}^d$*. Since this ran-*

dom field enters in Hamiltonians (2.3), (2.6) as an additive term, the standard self-averaging arguments (see, e.g., Refs. 10–12) for the thermodynamic limit of the free-energy density give

$$\text{a.s.}-\lim_{\Lambda} f_\Lambda[H_\Lambda(h^\omega)]=\lim_{\Lambda}\mathbb{E}f_\Lambda[H_\Lambda(h^\omega)] \tag{2.16}$$

and similarly

$$\text{a.s.}-\lim_{\Lambda} f_\Lambda[H_\Lambda(c,h^\omega)]=\lim_{\Lambda}\mathbb{E}f_\Lambda[H_\Lambda(c,h^\omega)]. \tag{2.17}$$

Corollary 2.4: Let $\{h_l^\omega\}_{l\in\mathbb{Z}^d}$ *be i.i.d.r.v. with expectation* $\mathbb{E}(h_l^\omega)=h$ *and with variance* $var(h_l^\omega)=\sigma^2$. *Then the covariance* $\mathrm{cov}(h_l^\omega,h_{l'}^\omega):=\mathbb{E}((h_l^\omega-h)(h_{l'}^\omega-h))=\sigma^2\delta_{l,l'}$ *and for any* $k\in\Lambda^*$ *one gets*

$$\mathbb{E}(|h_\Lambda^\omega(k)|^2)=\frac{1}{V}\sum_{l,l'\in\Lambda}\mathbb{E}(h_l^\omega h_{l'}^\omega)e^{-ikl}e^{ikl'}=\sigma^2+Vh^2\delta_{k,0}. \tag{2.18}$$

Then by Theorem 2.1 and by the explicit expressions (2.9), (2.18) we obtain

$$f(\beta,h)=\sup_{c\geqslant c^*} f(\beta,h,\sigma^2;c), \tag{2.19}$$

where

$$f(\beta,h,\sigma^2;c):=\frac{1}{(2\pi)^d\beta}\int_{\mathcal{B}_d}d^dq\,\ln\left[2\sinh\frac{\beta\lambda\Omega_q(c)}{2}\right]-\frac{h^2}{2\Delta(c)}-\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d}d^dq\,\frac{\sigma^2}{2\Omega_q(c)^2}$$
$$+[W(c)-cW'(c)], \tag{2.20}$$

and $\mathcal{B}_d:=(-\pi,\pi]^d$ *denotes the first Brillouin zone.*

Therefore, if $h\neq 0$, then by virtue of (2.7) and (2.19), (2.20) the value of the trial parameter c is given by the equation

$$c=\frac{h^2}{\Delta(c)^2}+\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d}d^dq\,\frac{\sigma^2}{\Omega_q(c)^4}+I_d(c,\beta,\lambda), \tag{2.21}$$

where

$$I_d(c,\beta,\lambda):=\frac{\lambda}{(2\pi)^d}\int_{\mathcal{B}_d}d^dq\,\frac{1}{2\Omega_q(c)}\coth\frac{\beta\lambda\Omega_q(c)}{2}. \tag{2.22}$$

Corollary 2.5: Our conditions on the monotone convex function $W(c)\geqslant 0$ *(see Theorem 2.1) imply that derivative* $W'(c)\leqslant 0$ *is a monotone increasing function bounded by zero. If (a priori) phonon spectrum has a gap* $a>0$ *[see (2.3), (2.6), (2.8)], we distinguish two cases:*
(**A**) $\Delta(c=0)\geqslant 0$, *i.e.*, $c^*=0$;
(**B**) $\Delta(c=0)<0$, *i.e.*, $c^*>0$.
In the case (**A**) *for any values of the parameters* β, h, σ, λ *the right-hand side of Eq. (2.21) is strictly positive and decreasing in* $c\in(0,+\infty)$. *Hence, this equation always has a unique positive solution* $\hat{c}(\beta,h,\sigma,\lambda)>0$, *which is a smooth function of those parameters. Therefore, thermodynamic properties of the system are regular, and there are no phase transitions.*

In the case (**B**) *we may have a displacive phase transition. Denote by* $c^*:=c^*(a)$ *a unique root of equation* $a+2W'(c)=0$, *cf. (2.8). By monotonicity of* $W'(c)$ *it exists and we have*: $c^*>0$ *with* $a+2W'(c)\geqslant 0$ *for* $c\geqslant c^*$. *Notice that for* $h\neq 0$ *the solution of Eq. (2.21)*: $\hat{c}(\beta,h$

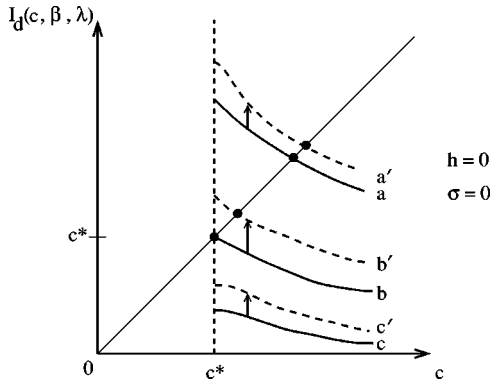

FIG. 1. (a) $\lambda>\lambda_c$, $\beta=\infty$; (a′) $\lambda>\lambda_c$, $\beta<\infty$. (b) $\lambda=\lambda_c$, $\beta=\infty$; (b′) $\lambda=\lambda_c$, $\beta<\infty$. (c) $\lambda<\lambda_c$, $\beta=\infty$; (c′) $\lambda<\lambda_c$, $\beta<\infty$.

$\neq 0,\sigma,\lambda)>c^*$, *and it is still a smooth function of the rest of parameters. This rules out phase transitions if the external field has a nonzero expectation. Thus, we may have a phase transition in the case* (***B***) *only when* $h=0$.

Notice that in the case (**B**) with $h=0$ one has to distinguish two possibilities: $\sigma=0$ and $\sigma\neq 0$. The first one means that the external field is simply absent, whereas the second one corresponds to a random field with nondegenerate distribution.

(**B1**) *Let* $h=0$ *and* $\sigma=0$. Since $c^*>0$, there exists a critical value $\lambda_c:=\lambda_c(c^*)$, of the quantum parameter, defined by Eq. (2.21) at zero temperature:

$$c^*=\lim_{\beta\to\infty} I_d(c^*,\beta,\lambda_c), \tag{2.23}$$

see Fig. 1. By monotonicity of $I_d(c^*,\beta,\lambda)$ in β and λ one gets that $I_d(c^*,\beta,\lambda)\geqslant c^*$ for all $\beta\leqslant\infty$ and $\lambda\geqslant\lambda_c$. Since $I_d(c,\beta,\lambda)$ is monotonous decreasing function of $c\geqslant c^*$, Eq. (2.21) for $h=0$, $\sigma=0$:

$$c=I_d(c,\beta,\lambda), \tag{2.24}$$

has a unique solution $\hat{c}(\beta,h=0,\sigma=0,\lambda)>c^*$ for any $\lambda\geqslant\lambda_c$, Figs. 1(a), 1(a′) and 1(b), 1(b′). The solution is a smooth function of β and λ, including the zero temperature. This phenomenon is well-known as the suppression of the displacive phase transition by large quantum fluctuations, see e.g., Refs. 13, 14, 18, 19, or the recent book (Ref. 6).

If $\lambda<\lambda_c$, then by monotonicity of the integral $I_d(c^*,\beta,\lambda)$ in β, there is $\beta_c(\lambda)$, such that

$$c^*=I_d(c^*,\beta_c(\lambda),\lambda). \tag{2.25}$$

Then for $\beta\leqslant\beta_c(\lambda)$ Eq. (2.24) has again only a unique smooth solution $\hat{c}(\beta,h=0,\sigma=0,\lambda)>c^*$. Whereas for $\beta>\beta_c(\lambda)$ one gets $c^*>I_d(c^*,\beta,\lambda>\lambda_c)$, i.e., formally Eq. (2.24) has no solution, see Figs. 1(c), 1(c′). The value $\beta_c(\lambda)^{-1}$ is the critical temperature of the model. It corresponds to the phase transition breaking the symmetry $\{Q_l\to -Q_l\}_{l\in\mathbb{Z}^d}$. To find the corresponding order parameter one has to return to Eq. (2.24) before taking the thermodynamic limit, i.e., before the corresponding finite-volume Darboux–Riemann sums give us in the limit the integral $I_d(c,\beta,\lambda)$. Another possibility is to add to the Hamiltonian a constant-field term breaking the symmetry, i.e., to put $h\neq 0$, see Refs. 18, 19, 21, 9, and Fig. 2. Using the latter trick one obtains for the displacive order parameter $M(\beta)$:

$$\pm M(\beta):=\lim_{h\to\pm 0}\lim_{\Lambda\uparrow\mathbb{Z}^d}\langle Q_l\rangle_{H_\Lambda(h)}(\beta,h,\sigma=0)=\pm\sqrt{c^*-I_d(c^*,\beta,\lambda<\lambda_c)}, \tag{2.26}$$

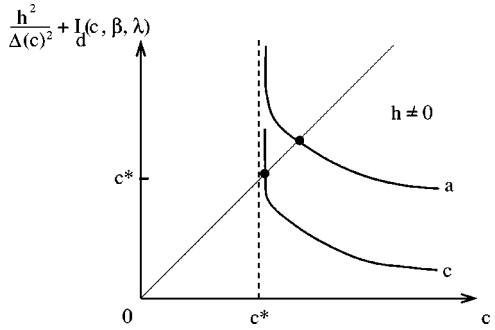

FIG. 2. (a) $\lambda>\lambda_c$, $\beta=\infty$, $h\neq 0$. (c) $\lambda<\lambda_c$, $\beta=\infty$, $h\neq 0$.

when $\beta>\beta_c(\lambda)$, and $M(\beta)=0$ for $\beta\leqslant\beta_c(\lambda)$, Fig. 3. Here $\langle\cdot\rangle_{H_\Lambda(h)}$ is the Gibbs state with Hamiltonian (2.3), for constant external field $h_l^\omega=h$.

Remark 2.6: Notice that the definition of the critical temperature given by Eq. (2.25) demands the convergence of the integral $I_d(c^*,\beta,\lambda<\lambda_c)$. *For the short-range harmonic interaction, i.e., for*

$$\phi_{l-l'}\leqslant A\|l-l'\|^{-(d+\alpha)},\quad \|l-l'\|\to\infty\,, \tag{2.27}$$

with $\alpha\geqslant 2$, *we have*

$$\tilde{\phi}(q)=\tilde{\phi}(0)+s^2\|q\|^2+o(\|q\|^2),\quad \|q\|\to 0\,, \tag{2.28}$$

for some $s>0$. *Therefore, the integral in (2.25) converges only for* $d>2$.

If we suppose that $0<\alpha<2$ *in (2.27) (long-range harmonic interaction), then*

$$\tilde{\phi}(q)=\tilde{\phi}(0)+s^\alpha\|q\|^\alpha+o(\|q\|^\alpha),\quad \|q\|\to 0. \tag{2.29}$$

Hence, the integral in (2.25) converges for $d>\alpha$.

(**B2**) *Let* $h=0$ *and* $\sigma\neq 0$. Then Eq. (2.21) takes the form

$$c=\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{\sigma^2}{\Omega_q(c)^4}+I_d(c,\beta,\lambda). \tag{2.30}$$

Now besides (2.25) we need the convergence of the integral

$$J_d(c^*,\sigma):=\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{\sigma^2}{\Omega_q(c^*)^4}. \tag{2.31}$$

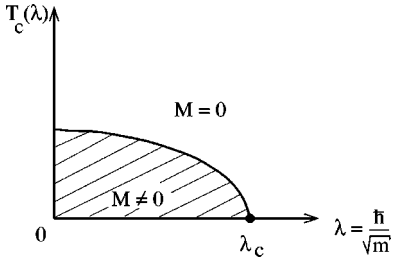

FIG. 3. Phase diagram for $\sigma=0$ $(h=0)$.

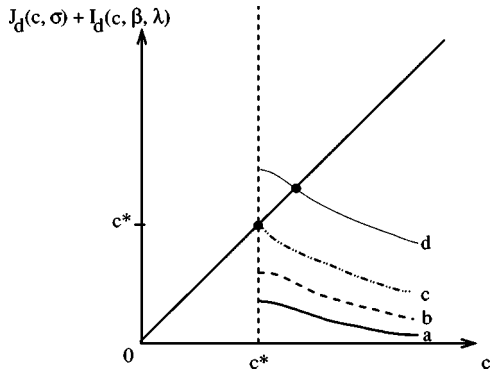

FIG. 4. (a) $\lambda<\lambda_c$, $\beta=\infty$, $\sigma=0$. (b) $\lambda<\lambda_c$, $\beta=\infty$, $\sigma>0$. (c) $\lambda<\lambda_c$, $\beta=\infty$, $\sigma=\sigma_c(\lambda)$. (d) $\lambda<\lambda_c$, $\beta=\infty$, $\sigma>\sigma_c(\lambda)$.

Indeed, if $\lim_{c\downarrow c^*} J_d(c,\sigma)=+\infty$, then Eq. (2.30) has a unique smooth solution $\hat{c}(\beta,h=0,\sigma,\lambda)>c^*$. Notice that even if the integral (2.31) converges, but

$$J_d(c^*,\sigma)+I_d(c^*,\beta=\infty,\lambda)>c^*, \tag{2.32}$$

we arrive to the same conclusion, since

$$\frac{\lambda}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{1}{2\Omega_q(c^*)}=I_d(c^*,\beta=\infty,\lambda)\leqslant I_d(c^*,\beta,\lambda)\leqslant I_d(c^*,\beta=0,\lambda), \tag{2.33}$$

see Fig. 4. Therefore, the stationary random field with zero expectation, $\mathbb{E}(h_l^\omega)=0$, rules out the phase transition if its variance verifies the following estimate from below:

$$\sigma^2>\left\{c^*-\frac{\lambda}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{1}{2\Omega_q(c^*)}\right\}\left\{\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{1}{\Omega_q(c^*)^4}\right\}^{-1}=:\sigma_c^2(\lambda). \tag{2.34}$$

Here we supposed that $\lambda<\lambda_c(c^*)$, i.e.,

$$c^*>\frac{\lambda}{(2\pi)^d}\int_{\mathcal{B}_d} d^dq\,\frac{1}{2\Omega_q(c^*)}, \tag{2.35}$$

to avoid the suppression of the phase transition by the quantum fluctuations, see (**B1**).

If the quantum fluctuations are small enough, see (2.35), and $\sigma^2<\sigma_c^2(\lambda)$, then by Eq. (2.30) we find a nontrivial critical temperature $0<\beta_c(\lambda,\sigma)<\infty$ verifying the equation:

$$c^*=J_d(c^*,\sigma)+I_d(c^*,\beta_c(\lambda,\sigma),\lambda), \tag{2.36}$$

for the symmetry breaking phase transition. Following the same method as in (2.26) we obtain for the displacive order parameter:

$$\pm M(\beta):=\lim_{h\to\pm 0}\lim_{\Lambda\uparrow\mathbb{Z}^d}\langle Q_l\rangle_{H_\Lambda(h^\omega+h)}(\beta,h,\sigma)=\pm\sqrt{c^*-J_d(c^*,\sigma)-I_d(c^*,\beta,\lambda)}, \tag{2.37}$$

when $\beta>\beta_c(\lambda,\sigma)$ and $M(\beta)=0$ for $\beta\leqslant\beta_c(\lambda,\sigma)$, see Fig. 5. Here $H_\Lambda(h^\omega+h)$ is the Hamiltonian (2.3) with shifted external field: $\{h_l^\omega+h\}_{l\in\mathbb{Z}^d}$, i.e., with $\mathbb{E}(h_l^\omega+h)=h$.

Remark 2.7: Notice that for the short-range harmonic interaction (2.27) the integral (2.31) converges only for $d>4$. This means that the external field fluctuations of i.i.d.r.v. with $\mathbb{E}(h_l^\omega)$

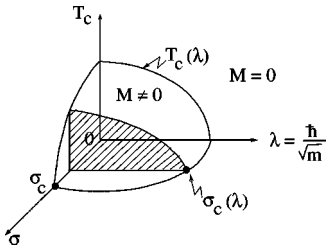

FIG. 5. Phase diagram for $\sigma \neq 0$ $(h=0)$.

$=0$, *suppress the phase transition for all lower dimensions* $d \leqslant 4$. *On the other hand, the estimates (2.32), (2.33) show that for* $d>4$ *there is a competition between external field fluctuations and quantum fluctuations to rule out the phase transition.*

For the long-range harmonic interaction (2.29) the integral (2.31) converges if $d>2\alpha$. *By virtue of Remark 2.6 and (2.33) the integral (2.25) also converges. Now, to ensure phase transition for* $d=3$ *one has to choose* $\alpha<3/2$ *and the quantum parameter* λ *verifying (2.35), together with i.i.d.r. external field variance* $\sigma^2<\sigma_c^2(\lambda)$.

III. PROOFS

The next statement generalizes one of the results from Ref. 19 to the case of random external fields.

Lemma 3.1: Let W verify conditions of the Theorem 2.1 with $b:=\sup_{c\geqslant 0} W''(c)$. *Suppose that* $\{h_l^{\omega}=h\}_{l\in\mathbb{Z}^d}$ *is a nonrandom (constant) field. Then*

$$f(\beta,h)=\lim_{\Lambda} f_{\Lambda}[H_{\Lambda}(h)]=\sup_{c\geqslant c^*}\lim_{\Lambda} f_{\Lambda}[H_{\Lambda}(c,h)]. \tag{3.1}$$

Proof: By virtue of the Bogoliubov convexity inequality (see e.g., Ref. 16 or 17) one gets

$$\frac{1}{V}\langle \delta H_{\Lambda}(c,h)\rangle_{H_{\Lambda}(h)} \leqslant f_{\Lambda}[H_{\Lambda}(h)]-f_{\Lambda}[H_{\Lambda}(c,h)] \leqslant \frac{1}{V}\langle \delta H_{\Lambda}(c,h)\rangle_{H_{\Lambda}(c,h)}, \tag{3.2}$$

where $\delta H_{\Lambda}(c,h):=H_{\Lambda}(h)-H_{\Lambda}(c,h)$, and $c>c^*$, $h\in\mathbb{R}^1$. By (2.3), (2.6) and the condition $b:=\sup_{c\geqslant 0} W''(c)>0$ we have for $\delta H_{\Lambda}(c,h)$ the following operator inequalities:

$$0\leqslant H_{\Lambda}(h)-H_{\Lambda}(c,h)\leqslant V\frac{b}{2}\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2-c\right)^2. \tag{3.3}$$

Together with (3.2) these inequalities imply the estimate

$$0\leqslant f_{\Lambda}[H_{\Lambda}(h)]-f_{\Lambda}[H_{\Lambda}(c,h)]\leqslant \frac{b}{2}\left\langle\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2-c\right)^2\right\rangle_{H_{\Lambda}(c,h)}. \tag{3.4}$$

Since we still have a freedom to choose the parameter $c>c^*$, we fix it in the right-hand side of (3.3) by the equation:

$$c=\left\langle\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right\rangle_{H_{\Lambda}(c,h)}. \tag{3.5}$$

Then the following estimate is true:

$$0 \leqslant f_\Lambda[H_\Lambda(h)] - \sup_{c>c^*} f_\Lambda[H_\Lambda(c,h)] \leqslant \frac{b}{2} \left\langle \left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2 - \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(\hat{c}_\Lambda,h)} \right)^2 \right\rangle_{H_\Lambda(\hat{c}_\Lambda,h)}, \tag{3.6}$$

where $\hat{c}_\Lambda := \hat{c}_\Lambda(\beta,h)$ is the solution of Eq. (3.5). Notice that the approximating Hamiltonian $H_\Lambda(c,h)$ is harmonic. Therefore, we can calculate the expectation in the right-hand side of (3.6) explicitly:

$$\left\langle \left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2 - \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(c,h)} \right)^2 \right\rangle_{H_\Lambda(c,h)} = \frac{2}{V^2} \sum_{q \in \Lambda^*} \left\{ \frac{\lambda}{2\Omega_q(c)} \coth\left(\frac{1}{2} \beta \lambda \Omega_q(c) \right) \right\}^2 + \frac{2}{V} \left(\frac{h}{\Delta(c)} \right)^4. \tag{3.7}$$

Similarly one gets for the self-consistency equation (3.5),

$$c = \frac{h^2}{\Delta(c)^2} + \frac{1}{V} \sum_{q \in \Lambda^*} \frac{\lambda}{2\Omega_q(c)} \coth\left(\frac{1}{2} \beta \lambda \Omega_q(c) \right). \tag{3.8}$$

Due to the first term in the right-hand side of (3.8) we obtain that solution of this equation for $h \neq 0$ is strictly greater than c^*: $\hat{c}_\Lambda(\beta,h) > c^*$, or $\Delta(\hat{c}_\Lambda(\beta,h)) > 0$. Since the value of the fluctuation (3.7) in the estimate (3.6) should be calculated for $c = \hat{c}_\Lambda(\beta,h)$, the right-hand side of (3.6) tends to zero, when $V \to \infty$, i.e., we get

$$\lim_\Lambda f_\Lambda[H_\Lambda(h \neq 0)] = \lim_\Lambda \sup_{c>c^*} f_\Lambda[H_\Lambda(c,h \neq 0)] = \sup_{c>c^*} \lim_\Lambda f_\Lambda[H_\Lambda(c,h \neq 0)]. \tag{3.9}$$

Here the last equality is due to concavity of the trial free-energy density $f_\Lambda[H_\Lambda(c,h \neq 0)]$ in c. Finely, the pointwise convergence (3.9) for $h \neq 0$ implies the convergence at $h = 0$ by convexity of $\sup_{c>c^*} f_\Lambda[H_\Lambda(c,h)]$ in h. □

Corollary 3.2: Using the explicit form of the trial free-energy density $f_\Lambda[H_\Lambda(c,h \neq 0)]$ (see (2.9) for $h_\Lambda^\omega(q) = \sqrt{V} h \delta_{q,0}$), we obtain that solution of the variational problem $\sup_{c>c^*} f_\Lambda[H_\Lambda(c,h)]$ coincides with solution $\hat{c}_\Lambda(\beta,h)$ of the self-consistency equation (3.8).

Corollary 3.3: Let $\{h_l^\omega\}_{l \in \mathbb{Z}^d}$ be a stationary ergodic random field with expectation $\mathbb{E}(h_l^\omega) = h$. Then similar to (3.6) and (3.7) we get the estimate

$$0 \leqslant f_\Lambda[H_\Lambda(h^\omega)] - \sup_{c>c^*} f_\Lambda[H_\Lambda(c,h^\omega)] \leqslant \frac{b}{2} D_\Lambda(\hat{c}_\Lambda^\omega, \beta, h^\omega). \tag{3.10}$$

Here fluctuations (3.7) for the case of random field have the form

$$D_\Lambda(c,\beta,h^\omega) := \left\langle \left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2 - \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(c,h^\omega)} \right)^2 \right\rangle_{H_\Lambda(c,h^\omega)}$$
$$= \frac{2}{V^2} \sum_{q \in \Lambda^*} \left\{ \frac{\lambda}{2\Omega_q(c)} \coth\left(\frac{1}{2} \beta \lambda \Omega_q(c) \right) \right\}^2 + \frac{2}{V} \left(\frac{h^2}{\Delta(c)^2} \right)^2 + \frac{2}{V^2} \sum_{q \in \Lambda^* \setminus \{0\}} \left(\frac{|\tilde{h}_\Lambda^\omega(q)|^2}{\Omega_q(c)^4} \right)^2, \tag{3.11}$$

and $\hat{c}_\Lambda^\omega := \hat{c}_\Lambda^\omega(\beta,h^\omega)$ is a solution of the self-consistency equation:

$$c=\frac{h^2}{\Delta(c)^2}+\frac{1}{V}\sum_{q\in\Lambda^*\setminus\{0\}}\frac{|\tilde{h}^{\omega}_{\Lambda}(q)|^2}{\Omega_q(c)^4}+\frac{1}{V}\sum_{q\in\Lambda^*}\frac{\lambda}{2\Omega_q(c)}\coth\left(\frac{1}{2}\beta\lambda\Omega_q(c)\right), \tag{3.12}$$

where $\tilde{h}^{\omega}_{\Lambda}(q)$ *is the lattice Fourier transformation (2.14) of the shifted random field* $\{\tilde{h}^{\omega}_l=h^{\omega}_l-h\}_{l\in\mathbb{Z}^d}$.

Proof (of Theorem 2.1): If $h\neq 0$, then (3.12) implies that for any configuration $\omega\in\Omega$ and uniformly in Λ the solution $\hat{c}^{\omega}_{\Lambda}\geqslant c^*+\epsilon(h)$, where $\epsilon(h)>0$ and $\lim_{h\to 0}\epsilon(h)=0$. Since in this case $\lim_{\Lambda} D_{\Lambda}(c,\beta,h^{\omega})=0$ uniformly in $c\geqslant c^*+\epsilon(h)$, the thermodynamic limit of (3.11) gives $\lim_{\Lambda} D_{\Lambda}(\hat{c}^{\omega}_{\Lambda},\beta,h^{\omega})=0$, i.e.,

$$\lim_{\Lambda} f_{\Lambda}[H_{\Lambda}(h^{\omega})]=\lim_{\Lambda}\sup_{c>c^*} f_{\Lambda}[H_{\Lambda}(c,h^{\omega})]=\sup_{c>c^*}\lim_{\Lambda} f_{\Lambda}[H_{\Lambda}(c,h^{\omega})]. \tag{3.13}$$

Since $\{\Omega^2_q(c)\}_{q\in\Lambda^*}$ are eigenvalues of the matrix $\{\phi_{l,l'}/2+\Delta(c)\delta_{l,l'}\}_{l,l'\in\Lambda}$ with eigenvectors $\{\psi_l(q):=\exp(-iql)\}_{q\in\Lambda^*}$, we can construct a nondecreasing (random) function of the real variable E:

$$\mu^{\omega}_{\Lambda}(E):=\frac{1}{V}\sum_{q\in\Lambda^*:\Omega^2_q(c)\leqslant E}\left|\sum_{l\in\Lambda}\psi_l(q)h^{\omega}_l\right|^2. \tag{3.14}$$

If the random field $\{h^{\omega}_l\}_{l\in\mathbb{Z}^d}$ is stationary and ergodic, then there exists a nonrandom nondecreasing spectral function $\mu(E)$ such that

$$\mu(E)=\text{a.s.}-\lim_{\Lambda}\mu^{\omega}_{\Lambda}(E) \tag{3.15}$$

at all their points of continuity, see e.g., Refs. 12 or 10. This means that the measure $\mu^{\omega}_{\Lambda}(dE)$ converges weakly with $\mathbb{P}$-probability 1 to the measure $\mu(dE)$, or

$$\text{a.s.}-\lim_{\Lambda}\frac{1}{V}\sum_{q\in\Lambda^*}\frac{|h^{\omega}_{\Lambda}(q)|^2}{\Omega_q(c)^4}=\text{a.s.}-\lim_{\Lambda}\int_{\Delta(c^*+\epsilon(h))}^{+\infty}\frac{\mu^{\omega}_{\Lambda}(dE)}{E^2}=\int_{\Delta(c^*+\epsilon(h))}^{+\infty}\frac{\mu(dE)}{E^2}, \tag{3.16}$$

since by virtue of $h\neq 0$ the integration in (3.16) runs over strictly positive E's. Therefore, (3.16) implies the self-averaging of the free-energy limit:

$$\text{a.s.}-\lim_{\Lambda} f_{\Lambda}[H_{\Lambda}(c,h^{\omega})]=\lim_{\Lambda}\mathbb{E}(f_{\Lambda}[H_{\Lambda}(c,h^{\omega})]). \tag{3.17}$$

This, together with (3.13), proves Theorem 2.1 for the random field when $h\neq 0$.

Now let $h=0$. Then one can use the convexity arguments for the free-energy density (as a function of h) to reach the same conclusion as in (3.17) when $h\to 0$, which by continuity coincides with the case $h=0$. □

IV. CONCLUDING REMARKS

We presented here a quenched random quantum model to study the impact of different type of fluctuations (thermal, quantum and random-field) on the second-order phase transition. Here we compare this for quantum and random-field fluctuations. Our main conclusion is that the random-field fluctuations may lift the lower critical dimensionality up to $d_l=4$ to screen the impact of quantum fluctuations for which the lower critical dimensionality is $d_l=2$, and even $d_l=1$ in the pure quantum limit $T=0$, see (2.35).

Notice that our results about suppression of the quantum phase transition by the random external fields with zero mean in some aspects are similar to those for the classical spherical model. For example, we obtain for the critical value of the variance (2.34) of the i.i.d.r. field:

$$\sigma_c^2(\lambda)=\left\{c^*-\frac{\lambda}{(2\pi)^d}\int_{\mathcal{B}_d}d^dq\,\frac{1}{2\Omega_q(c^*)}\right\}\sigma_{c,\mathrm{class}}^2, \tag{4.1}$$

where

$$\sigma_{c,\mathrm{class}}^2=\left\{\frac{1}{(2\pi)^d}\int_{\mathcal{B}_d}d^dq\,\frac{1}{\Omega_q(c^*)^4}\right\}^{-1} \tag{4.2}$$

is the corresponding threshold for the classical spherical model.[10,11] The supplementary factor in front of $\sigma_{c,\mathrm{class}}^2$, see (4.1), is due to quantum fluctuations, $\lambda\neq 0$, and due to a specific choice of the potential function W. We recover the classical result (4.2), if we put $\hbar=0$ and $c^*=1$ in (2.34). The relation (2.34) implies that the lower critical dimensionality $d_l=4$ is identical for classical and quantum random spherical models. Notice that the random field classical n-vector model also has the same lower critical dimensionality $d_l=4$, see Ref. 1. This similarity is not accidental, since the classical spherical random model can be obtained as the $n\to\infty$ limit from the corresponding random n-vector model.[10] Notice that in Refs. 4 and 5 it is shown that the $n\to\infty$ limit of a quantum n-vector crystal model with a one-site anharmonic potential, gives for the free-energy density the same result as the corresponding spherical (or Hartree–Fock) approximation, but it gives different results for fluctuations. Since the critical properties of this quantum n-vector anharmonic crystal in random fields are unknown, we have no quantum analog of the statements.[1,10]

Another open problem concerns the impact of the random field on the displacive (ferroelectric) phase transition in the anharmonic quantum crystal without spherical approximation. It is known that for a rather general class of double-well one-site anharmonic potentials the large quantum fluctuations (large parameter λ) suppress the displacive phase transition in this model,[22] and even make the Gibbs state unique.[3,15] Our conjecture is that the presence of random field will produce the same scenario as we obtained in the spherical approximation.

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Partial classification of modules for Lie-algebra of diffeomorphisms of *d*-dimensional torus

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We consider the Lie-algebra of the group of diffeomorphisms of a d-dimensional torus which is also known to be the algebra of derivations on a Laurent polynomial ring A in d commuting variables denoted by $\mathrm{Der}\,A$. The universal central extension of $\mathrm{Der}\,A$ for $d=1$ is the so-called Virasoro algebra. The connection between Virasoro algebra and physics is well known. See, for example, the book on Conformal Field Theory by Di Francesco, Mathieu, and Senechal. In this paper we classify (A, $\mathrm{Der}\,A$) modules which are irreducible and have finite dimensional weight spaces. Earlier Larsson constructed a large class of modules, the so-called tensor fields, based on $g\ell_d$ modules which are also A modules. We prove that they exhaust all (A, $\mathrm{Der}\,A$) irreducible modules. © *2004 American Institute of Physics.*
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I. INTRODUCTION

It is well known that the group of diffeomorphisms on a manifold is very important and shows up directly in many branches of physics (see, for example, Ref. 22). We are particularly interested in d-dimensional torus. The case $d=1$ is well studied by both mathematicians and physicists. The one-dimensional central extension of the Lie-algebra of diffeomorphisms of the circle is a well-known object called Virasoro algebra. The representation theory of Virasoro algebra is studied in great detail. See Ref. 14.

The Virasoro algebra acts on any (except when the level is negative of dual Coxeter number) highest weight module of the affine Lie algebra through the use of the famous Sugawara operators. It is well known that affine Lie algebras admit representation on the Fock space (see Ref. 13) and hence admits a representation of the Virasoro algebra. This classical theory is what we originally want to generalize to d-dimensional torus.

The relation to physics is well established in the book on Conformal Field Theory by Di Francesco, Mathieu, and Senechal, Ref. 5. In particular, Chaps. 13–18 explain the connection between physics and the representation theory of Virasoro and affine Kac–Moody Lie-algebras. Several important papers on these aspects have been put in one volume by Goddard and Olive in Ref. 11. The most fundamental paper in this direction is due to Belavin, Polyakov, and Zamolodchikov in Ref. 1.

The generalization of affine Lie algebra is the so-called toroidal Lie-algebra. For the first time a large class of representations are constructed in Refs. 9 and 21 through the use of vertex operators generalizing the Fock space construction to the toroidal Lie-algebras. One significant difference for the toroidal Lie-algebra is that the universal center is infinite dimensional unlike in the affine case where it is one dimensional.

So the next natural issue is to generalize Virasoro algebra and see whether the algebra acts on the Fock space. For that we first denote the Lie algebra of diffeomorphisms of d-dimensional torus by $\mathrm{Der}\,A$ (it is known that $\mathrm{Der}\,A$ is isomorphic to the derivations of Laurent polynomial ring A in d-variables). Here one should mention that several attempts have been made by physicists to give

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a Fock space representation to Der A or to its extension (see Ref. 10). They all failed to produce any interesting results due to lack of proper definition of ''normal ordering'' among other things. At this juncture an interesting result has come out from Ref. 23 which says that Der A has no nontrivial central extension for $d \geqslant 2$.

Let us go back to the vertex construction of toroidal Lie-algebra of Ref. 9. Here operators are constructed for Der A generalizing the Sugawara construction. But the corresponding extension for Der A is very wild (certainly noncentral) and not tractable (see Ref. 7). In the process an interesting Abelian extension for Der A has been created in Ref. 9 and the Abelian part is exactly the center of the toroidal Lie algebra. So the semi-direct sum of the toroidal Lie algebra and Der A with common extension has emerged as an interesting object which we will now define.

We will first define toroidal Lie algebra. Let $\mathcal{G}$ be simple finite dimensional Lie algebra and let $\langle , \rangle$ be a nondegenerate symmetric bilinear form on $\mathcal{G}$. Fix a positive integer d and let $A = \mathbb{C}[t_1^{\pm 1}, \ldots, t_d^{\pm 1}]$ be a Laurent polynomial ring in d-commuting variables.

Let Ω_A be the module of differentials which can be defined as vector space spanned by $t^r K_i$, $i = 1, \ldots, d$ and $r \in \mathbb{Z}^n$. Let d_A be the subspace spanned by $\Sigma r_i t^r K_i$ and consider the toroidal Lie algebra $\mathcal{G} \otimes A \oplus \Omega_A / d_A$ with Lie-bracket.

$$[X \otimes t^r, Y \otimes t^s] = [X, Y] \otimes t^{r+s} + \langle X, Y \rangle \Sigma r_i t^{r+s} K_i$$

Ω_A / d_A is central.

Let Der A be the derivation on A. For $u \in \mathbb{C}^d$ and $r \in \mathbb{Z}^d$ let $D(u,r) = \Sigma u_i t^r t_i (\mathrm{d}/\mathrm{d}t_i)$ where $u = (u_1, \ldots, u_d)$ and $r = (r_1, \ldots, r_d), t^r = t_1^{r_1} t_2^{r_2} \cdots t_d^{r_d} \in A$. Let $K(u,r) = \Sigma u_i t^r K_i$. Consider the Lie-algebra

$$\tau = \mathcal{G} \otimes A \oplus \Omega_A / d_A \oplus \mathrm{Der}\, A,$$

$$[D(u,r), D(v,s)] = D(w, r+s) - (u,s)(v,r) K(r, r+s),$$

where $w = (u,s)v - (v,r)u$ and $(,)$ is the standard inner product in $\mathbb{C}^d$,

$$[D(u,r), K(v,s)] = (u,s) K(v, r+s) + (u,v) K(r, r+s),$$

$$[K(u,r), K(v,s)] = 0.$$

The first issue is that can we construct a representation for τ from known methods. Several attempts have been made (Refs. 2, 3, and 9). Eventually in a remarkable paper, Billig (Ref. 4) succeeded in constructing a class of modules for τ through the use of Vertex operator algebras (VOA). In the process Billig has used the Der A modules constructed in Ref. 17 and studied in Ref. 6. One natural question is, do more modules exist for Der A so that we get a much larger class of models of τ.

In an interesting paper by Jiang and Meng (Ref. 12) it is proved that classification of irreducible integrable modules of τ can be reduced to the classification of irreducible (A, Der A) modules which the current paper settles. See also Ref. 8 for more precise results.

Let me explain the results of this paper in more detail. In Ref. 17, Larsson constructed a large class of Der A modules and some of them with finite dimensional weight spaces. In fact he constructed a functor from gl_d-modules to Der A-modules. In Ref. 6 the author proves that the image of an irreducible finite dimensional module is most often irreducible.

Further Larsson's Der A modules are A modules too and they are always irreducible as (A, Der A)-modules. Thus the purpose of the paper is to prove the converse. So we prove in Theorem 2.9 that any (A, Der A) module which is irreducible and has finite dimensional weight spaces has to come from Larsson's construction.

It will certainly be interesting to classify all irreducible Der A modules with finite dimensional weight spaces. Now some kind of highest weight modules are constructed in Refs. 2 and 3 (they are not A modules). We will also note that $GL(d, \mathbb{Z})$ acts as automorphisms on Der A and so we

can twist a Der$A$ module by $GL(d,\mathbb{Z})$. [Larsson's modules are closed under $GL(d,\mathbb{Z})$ action.] So it will be interesting to prove that any irreducible Der$A$ module with finite dimensional weight spaces is either a highest weight module or a Larsson's module up to a twist of $GL(d,\mathbb{Z})$ action. The problem is completely solved for $d=1$ by Mathieu in Ref. 20.

Our results in Ref. 9 have been reinterpreted in the language of physics by Larsson in Refs. 18 and 19. Larsson is also the first to talk about noncentral extensions in Refs. 15 and 16. Der$A$ has also been studied in Ref. 24.

II. CONSTRUCTION OF Der$A$ MODULES

(2.1) Throughout this paper we fix a positive integer $d\geqslant 2$ and a Laurent polynomial ring $A=\mathbb{C}[t_1^{\pm 1},\ldots,t_d^{\pm 1}]$ in d commuting variables. Let $\mathbb{C}^d$ be d copies of complex field $\mathbb{C}$. Let $e_1,\ldots,e_d$ be the standard basis of $\mathbb{C}^d$, and let $(,)$ be the standard form on $\mathbb{C}^d$ such that $(e_i,e_j)=\delta_{ij}$.

(2.2) Let $\Gamma=\mathbb{Z}e_1\oplus\cdots\oplus\mathbb{Z}e_d$. Throughout this paper we use m,n,r, and s to denote elements of Γ. For $r=\Sigma r_i e_i\in\Gamma$ let $t^r=t_1^{r_1}t_2^{r_2}\cdots t_d^{r_d}\in A$ and let $D^i(r)=t^r t_i(\mathrm{d}/\mathrm{d}t_i)$ be a derivation on A. Let Der$A$ be the Lie-algebra of derivations of A. It is easy to verify that $D^i(r),1\leqslant i\leqslant d,r\in\Gamma$ is a basis of Der$A$. For $u=\Sigma u_i e_i\in\mathbb{C}^d$ let $D(u,r)=\Sigma u_i D^i(r)$. Then Der$A$ has the following Lie structure:

(2.3)

$$[D(u,r),D(v,s)]=D(w,r+s),$$

where $w=(u,s)v-(v,r)u$, $r,s\in\Gamma$ and $u,v\in\mathbb{C}^d$. Let h be the subspace spanned by $D^i(0),1\leqslant i\leqslant d$, which is a maximal Abelian subalgebra of Der$A$.

(2.4) Note that $D(u,r)t^s=(u,s)t^{r+s}$. Thus $A\oplus\mathrm{Der}A$ is a Lie-algebra by extending the Lie structure in the following way:

$$[t^r,t^s]=0,$$

$$[D(u,r),t^m]=(u,m)t^{r+m}.$$

Let $\tilde{h}=\mathbb{C}\oplus h$, which is an Abelian subalgebra of $A\oplus\mathrm{Der}A$.

The purpose of this paper is to study $A\oplus\mathrm{Der}A$ modules which are weight modules for $\tilde{h}$ with finite dimensional weight spaces and to classify such modules with some natural conditions.

We first recall Der$A$ modules which are constructed and studied in Refs. 17 and 6.

(2.5) Let $g\ell_d$ be the Lie-algebra of $d\times d$ matrices with entries in $\mathbb{C}$. Let E_{ij} be the elementary matrix with (i,j)th entry 1 and zero elsewhere. Then it is well known that $g\ell_d$ is spanned by $E_{ij},1\leqslant i,j\leqslant d$ with the following Lie-bracket:

$$[E_{ij},E_{k\ell}]=\delta_{jk}e_{i\ell}-\delta_{i\ell}E_{kj}.$$

Let $g\ell_d=s\ell_d\oplus\mathbb{C}I$ where $s\ell_d$ is a Lie-subalgebra of trace zero matrices and I is the identity matrix. Let $V(\psi)$ be the irreducible finite dimensional module for $s\ell_d$ where ψ is a dominant integral weight. Let I act by scalar b on $V(\psi)$ and denote the resultant $g\ell_d$ module by $V(\psi,b)$. Let $\alpha\in\mathbb{C}^d$ and we will make $F^\alpha(\psi,b):=V(\psi,b)\otimes A$ a Der$A$ module. First denote $v\otimes t^m$ by $v(m)$ for v in $V(\psi,b)$ and m in Γ.

(2.6) *Definition* (Ref. 17):

$$D(u,r)\cdot v(m)=(u,m+\alpha)v(m+r)+\left(\sum_{i,j}u_i r_j E_{ji}v\right)(m+r),$$

where $m,r\in\Gamma,u\in\mathbb{C}^d,v\in V(\psi,b)$. We will now recall the following:

(2.7) *Theorem* (Theorem (1.9) and Proposition (5.1) of Ref. 6):
(1) $F^{\alpha}(\psi,b)$ is irreducible as $\mathrm{Der}\,A$ module if $(\psi,b)\neq(\delta_k,k),(0,b),1\leqslant k\leqslant d-1$ where δ_k is the kth fundamental weight of $s\ell_d$.
(2) $F^{\alpha}(0,b)$ is irreducible as $\mathrm{Der}\,A$ module unless $\alpha\in\Gamma$ and $b\in\{0,d\}$.

In all other cases $F^{\alpha}(\psi,b)$ is reducible and the submodule structure has been worked out in Proposition (5.1) and Theorem (5.5) of Ref. 6.

Recall that A is associative algebra with unit and $F^{\alpha}(\psi,b)$ is an A module by defining

$$t^m\cdot v(r)=v(m+r)$$

for $m,r\in\Gamma$ and $v\in V(\psi,b)$. Further it is easy to see that $F^{\alpha}(\psi,b)$ is a $A\oplus\mathrm{Der}\,A$ module.

(2.8) *Proposition:* $F^{\alpha}(\psi,b)$ is irreducible as $A\oplus\mathrm{Der}\,A$ module.

Proof: First note that $F^{\alpha}(\psi,b)$ is a weight module with respect to $\tilde{h}$ and the weight spaces are $V(\psi)\otimes t^m$. Suppose W is a nonzero $A\oplus\mathrm{Der}\,A$ submodule of $F^{\alpha}(\psi,b)$. As submodule of a weight module is a weight module, W is a weight module. From the action of A it is clear that $v(m)\in W$ implies $v(s)\in W$ for all $s\in\Gamma$. Thus $W=W_1\otimes A$ for some $W_1\subseteq V(\psi,b)$. Now choose $u=e_i,r=e_j$ and consider

$$D(u,r)v(m)=(u,m+\alpha)v(m+r)+(E_{ji}v)(m+r).$$

It now follows from the above-presented remarks that W_1 is $g\ell_d$-invariant. Since $V(\psi)$ is irreducible and W_1 is nonzero, it follows that $W_1=V(\psi)$ and hence $W=F^{\alpha}(\psi,b)$.

The purpose of this paper is to prove the converse of the above proposition. In other words we classify $A\oplus\mathrm{Der}\,A$ modules with certain natural properties.

(2.9) *Theorem:* Let V be irreducible module for $A\oplus\mathrm{Der}\,A$ which is also a weight module for $\tilde{h}$ with finite dimensional weight spaces. We further assume the following:

(1) V is an A-module as associative algebra and the Lie-module structure of A comes from associative algebra.
(2) $1.v=v,\forall v$ in V.

Then $V\cong F^{\alpha}(\psi,b)$ (for some α,ψ,b) as $A\oplus\mathrm{Der}\,A$-module.

We need to develop several lemmas to prove the theorem which will be done in Sec. III. The final proof will be given in Sec. IV.

III. FILTERATION OF CO-FINITE IDEALS

First we need to change some notation. We treat A as group algebra over Γ. For that let $k(r)$ be a symbol for $r\in\Gamma$. Let A be the linear span of $k(r),r\in\Gamma$ with multiplication defined as $k(r)\cdot k(s)=k(r+s)$.

Let U be the universal enveloping algebra of $A\oplus\mathrm{Der}\,A$. Let L be the two sided ideal of U generated by $k(r)k(s)-k(r+s)$ and $k(0)-1$.

Throughout this section the module V is as in Theorem (2.9). Since V is an A module, L acts trivially and hence V is a U/L-module. Let $V=\oplus_{r\in\Gamma}V_r$ be the weight space decomposition and $V_r=\{v\in V|D(u,0)v=(u,r+\alpha)v,\forall u \text{ in } \mathbb{C}^d\}$. Such a uniform α in $\mathbb{C}^d$ exists as V is irreducible. In fact take any weight space where h acts as linear function which can be taken as $u\mapsto(u,\alpha)$ for some $\alpha\in\mathbb{C}^d$. Because of irreducibility the action of h on the rest of the spaces is easily computed. Further each V_r is an $\tilde{h}$-module as 1 in A acts as one on the entire module.

(3.1) Let $U_1=U/L$ and let $T(u,r)=k(-r)D(u,r)-D(u,0)$ as an element of U_1 for $u\in\mathbb{C}^d$ and $r\in\Gamma$. Let T be the subspace spanned by $T(u,r)$ for all u and r.

(3.2) *Proposition:*

(1) $[T(v,s),T(u,r)]=(u,s)T(v,s)-(v,r)T(u,r)+T(w,r+s)$ where $w=(v,r)u-(u,s)v$ and hence T is a Lie-subalgebra.
(2) $[D(v,0),T(u,r)]=0$.

(3) Let $V=\oplus V_r$ be weight space decomposition. Then each V_r is T-invariant.
(4) Each V_r is T-irreducible.
(5) $V_r\cong V_s$ as T-module.

Proof: (2)

$$\begin{aligned}&[D(v,0),k(-r)D(u,r)-D(u,0)]\\&\quad=[D(v,0),k(-r)D(u,r)]=[D(v,0),k(-r)]D(u,r)+k(-r)[D(v,0),D(u,r)]\\&\quad=-(v,r)k(-r)D(u,r)+(v,r)k(-r)D(u,r)=0.\end{aligned}$$

(1) From (2) it follows that

$$\begin{aligned}[T(v,s),T(u,r)]&=[k(-s)D(v,s),k(-r)D(u,r)]\\&=[k(-s),k(-r)D(u,r)]D(v,s)+k(-s)[D(v,s),k(-r)D(u,r)]\\&=[k(-s),k(-r)]D(u,r)D(v,s)+k(-r)[k(-s),D(u,r)]D(v,s)\\&\quad+k(-s)[D(v,s),k(-r)]D(u,r)+k(-s)k(-r)[D(v,s),D(u,r)]\\&=(u,s)k(-s)D(v,s)-(v,r)k(-r)D(u,r)\\&\quad+k(-s-r)D(w,r+s)\ \text{ where }\ w=(v,r)u-(u,s)v\\&=(u,s)T(v,s)-(v,r)T(u,r)+T(w,r+s)\ \text{ where }\ w=(v,r)u-(u,s)v.\end{aligned}$$

(3) From (2) it follows that T commutes with h and hence V_r is a T-module.

(4) Let $U=\oplus_{r\in\Gamma}U_r$ where $U_r=\{v\in U|[D(u,0),v]=(u,r)v$ for $u\in\mathbb{C}^d\}$. Since V is $A\oplus\mathrm{Der}\,A$ irreducible for v,w in V_r there exists X in U_0 such that $Xv=w$. This is due to weight reasons. Now $X=\Sigma a_iX_i$ where each X_i is of the form $k(-r)D(u_0,r_1)\cdots D(u_k,r_k)$ where $\Sigma r_i=r$. We are using the fact that L acts trivially on V. Now using the fact that $k(-s)D(u,r)=D(u,r)k(s)-(u,s)D(u,r)$ and the fact that $k(r)k(s)=k(r+s)$ we see that each X_i is linear combination of elements of the form

$$k(-r_1)D(u_1,r_1)k(-r_2)D(u_2,r_2)\cdots k(-r_k)D(u_k,r_k).$$

This proves $X\in U(T)$, the universal enveloping algebra of T. Hence V_r is T irreducible.

(5) First note that $k(s-r)V_r\subseteq V_s$. Repeating the same we see that

$$V_r=k(r-s)k(s-r)V_r\subseteq k(r-s)V_s\subseteq V_r.$$

Thus $V_r=k(r-s)V_s$. Define $f:V_r\to V_s$ by $f(v)=k(s-r)v$ which is clearly injective and surjective. Now

$$f(T(u,k)v)=k(s-r)T(u,k)v=T(u,k)k(s-r)v=T(u,k)f(v).$$

Thus f is a T-homomorphism. This proves (5).

(3.3) *Notation:* For any integer $k>0,r,m_1,\ldots,m_k\in\Gamma$ define

$$T_k(u,r,m_1,\ldots,m_k)=T(u,r)-\sum_i T(u,r+m_i)+\sum_{i<j} T(u,r+m_i+m_j)\cdots(-1)^j$$

$$+\sum_{1\leqslant i_1<i_2<\cdots<i_j\leqslant k} T(u,r+m_{i_1}+\cdots+m_{i_j})\cdots(-1)^k T(u,r+m_1+m_2$$

$$+\cdots+m_k).$$

Let I_k be the linear span of $T_k(u,r,m_1,\ldots,m_k), u\in\mathbb{C}^d$ for all $r,m_1,m_2,\ldots,m_k\in\Gamma$.

(3.4) *Lemma:* (1) $T_k(u,r,m_1,\ldots,m_k)=T_k(u,r,m_{\sigma(1)},\ldots,m_{\sigma(k)})$ for any permutation σ on k-letters.
(2) $T_k(u,r,m_1,\ldots,m_k)=T_{k-1}(u,r,m_1,\ldots,m_{k-1})-T_{k-1}(u,r+m_k,m_1,\ldots,m_{k-1})$
(3) I_k is an ideal of T.
(4) $I_k\subseteq I_{k-1}$ for $k\geqslant 2$.
(5) $[I_k,I_\ell]\subseteq I_{k+\ell-1}$ for $k,\ell\geqslant 1$.

Proof: (1) Follows from definition.

(2) Collect all terms where m_k does not occur in the sum of T_k and that can be seen to be equal to $T_{k-1}(u,r,m_1,\ldots,m_{k-1})$. Sum of the rest of the terms can be seen to be equal to $-T_{k-1}(u,r+m_k,m_1,\ldots,m_{k-1})$. This is because every term contains m_k

$$(3)\ [T(v,s),T_k(u,r,m_1,\ldots,m_k)]=(u,s)\sum_{\ell=0}^{k}\binom{k}{\ell}(-1)^\ell k(-s)D(v,s)-(v,r)T_k(u,r,m_1,\ldots,m_k)$$

$$+\sum (v,m_i)T_{k-1}(u,r+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k)+(v,r)T_k(u,r$$

$$+s,m_1,\ldots,m_k)-\sum (v,m_i)T_{k-1}(u,r+s$$

$$+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k)-(u,s)T_k(v,r+s,m_1,\ldots,m_k).$$

By applying Proposition 3.2 (1) write $[T(v,s),T_k(u,r,m_1,\ldots,m_k)]=A_1+A_2+A_3$. It is easy to see that A_1 is the first term of the above-given formula. Now in A_2 look for the terms where (v,m_i) occurs and that can be seen as a component of the third term of the above-given formula. Now in A_2 the terms where no m_i occurs is equal to the second term of the above-given formula. The rest of the formula can be seen in a similar way. This proves the claim. Now note that the first term in the claim is zero. Clearly the second, fourth, and sixth terms are in I_k. Now the third and fifth terms are equal to

$$\sum (v,m_i)T_{k-1}(u,r+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k)-\sum (v,m_i)T_{k-1}(u,r+m_i+s,m_1\ldots,\widehat{m_i},\ldots,m_k)$$

$$=\sum (v,m_i)T_k(u,r+m_i,m_1,\ldots,\widehat{m_i}\ldots,m_k,s)$$

(by Lemma 3.4 (2)).
(4) Follows from (2).
(5)

$$[T_\ell(v,s,n_1,\ldots,n_\ell),T_k(u,r,m_1,\ldots,m_k)]=\sum_{t=0}^{\ell}\sum_{i_1<i_2<\cdots<i_t}(u,s+n_{i_1}+\cdots+n_{i_t}).$$

$$\sum_{b=0}^{k}\binom{k}{b}(-1)^b T(v,s+n_{i_1}+\cdots+n_{i_t})-\sum_{t=0}^{k}\sum_{j_1<\cdots<j_t}(v,r+m_{j_1}+\cdots+m_{j_t}).$$

$$\sum_{b=0}^{\ell}\binom{\ell}{b}(-1)^b T(u,r+m_{i_1}+\cdots+m_{i_t})+(v,r)T_{k+\ell}(u,r+s,m_1,\ldots,m_k,n_1,\ldots,n_\ell)$$

$$-(u,s)T_{k+\ell}(v,r+s,m_1,\ldots,m_k,n_1,\ldots,n_\ell)-\sum\ (v,m_i)T_{k+\ell-1}(u,r+s$$

$$+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k,n_1,\ldots,n_\ell)+\sum\ (u,n_j)T_{k+\ell-1}(v,r+s+n_j,m_1,\ldots,m_k,n_1,\ldots,\widehat{n_j},\ldots,n_\ell).$$

The above-presented formula can be deduced as in (3) from Proposition 2.2 (1). Now note that the first two terms are zero as

$$\sum_{b=0}^{k}\binom{k}{b}(-1)^b=0=\sum_{b=0}^{\ell}\binom{\ell}{b}(-1)^b.$$

The rest of the four terms are in $I_{k+\ell-1}$ and this proves (5).

(3.5) *Lemma:* For $u\in\mathbb{C}^d$, $0\neq m_i\in\Gamma$, $s\in\Gamma$.

(1) $T_k(u,s,m_1,\ldots,m_k)\notin I_{k+1}$ for $k\geqslant 1$.

(2) $T_k(u,s,m_1,\ldots,m_k)+T_k(u,s,n,m_2,\ldots,m_k)=T_k(u,s,m_1+n,m_2,\ldots,m_k)+I_{k+1}$.

(3) $T_k(u,s,-m_1,m_2,\ldots,m_k)=-T_k(u,s-m_1,m_1,m_2,\ldots,m_k)$

Proof: To prove the Lemma, we first interpret T_k's as certain polynomials in $A=\mathbb{C}[t_1^{\pm 1},\ldots,t_d^{\pm 1}]$. We fix a nonzero u in $\mathbb{C}^d$. Let k be a positive integer and let $m_1,m_2,\ldots,m_k\in\Gamma$. Let $P_k(m_1,\ldots,m_k)=\Pi_{1\leqslant i\leqslant k}(1-t^{m_i})$. Recall $t^{m_i}=t_1^{(m_i)_1}\cdots t_d^{(m_i)_d}$. Let J_k be the ideal in A generated by $P_k(m_1,\ldots,m_k)$ for all nonzero m_i's $\in\Gamma$. Then clearly $J_{k+1}\subseteq J_k$. It is easy to see that $T_k(u,r,m_1,\ldots,m_k)$ can be identified with polynomial $t^rP_k(m_1,\ldots,m_k)$. Recall that u is fixed.

Thus it is sufficient to prove that

Claim 1: $P_k(m_1,\ldots,m_k)\notin J_{k+1}$. Suppose

$$(*)\qquad P_k(m_1,\ldots,m_k)=\sum\ f_\ell P_{k+1}(n_{\ell_1},n_{\ell_2},\ldots,n_{\ell_{k+1}})$$

where $f_\ell\in A$. Let $Dt_i=t_i(\mathrm{d}/\mathrm{d}t_i)$. Now consider $D_{t_{i_1}}\cdots D_{t_{i_k}}P_{k+1}(n_1,\ldots,n_{k+1})$ and evaluate at $(t_1,\ldots,t_d)=(1,\ldots,1)$. This can be seen to be zero as after differentiating P_{k+1},k times, each component has at least one factor $(t^{n_i}-1)$. We will now prove that there exists $i_1,\ldots,i_k$ such that

Claim 2: $D_{t_{i_1}}\cdots D_{t_{i_k}}P_k(m_1,\ldots,m_k)|_{t=(1,\ldots,1)}$ is nonzero. Thus $*$ cannot hold. This proves claim 1. Now choose $\ell,1\leqslant\ell\leqslant d$ such that $S=\{i|(m_i)_\ell\neq 0\}$ is nonempty. Let $\#S=p$ and let $i_1,\ldots,i_p\in S$. Consider

$$(D_{t_\ell})^pP_k(m_1,\ldots,m_k)=\mu\prod_{i\in S}\ (m_i)_\ell\prod_{j\notin S}\ (1-t^{m_j})t^{m_{i_1}+m_{i_2}+\cdots+m_{i_p}}+J_{k-s+1},$$

which is not too difficult to see—where μ is a non-negative integer. Repeating the process finitely many times (choosing different index $\ell^1\neq\ell$). We see that there exists $i_1,\ldots,i_k$ such that $D_{t_{i_1}}D_{t_{i_2}}\cdots D_{t_{i_k}}.\ P_k(m_1,\cdots,m_k)=\lambda t^{m_1+\cdots+m_k}+J_1$ where λ is nonzero integer. Now evaluating at $t=(1,\ldots,1)$ we see that claim 2 is true.

To see (2) first note that

$$(1-t^m)(1-t^n)+(1-t^{m+n})=(1-t^m)+(1-t^n).$$

Thus

$$t^s\prod_{i=2}^{k}(1-t^{m_i})(1-t^{m_1})+t^s\prod_{i=2}^{k}(1-t^{m_i})(1-t^n)=t^s\prod_{i=2}^{k}(1-t^{m_i})(1-t^n)(1-t^{m_1})+t^s\prod_{i=2}^{k}(1-t^{m_i})\times(1-t^{m_1+n}).$$

This proves (2).

(3) is easy to check.

(3.6) *Lemma:*

$$(1)\quad \mathrm{Dim}(I_k/I_{k+1})\leqslant d^{k+1}, k\geqslant 1.$$

$$(2)\quad T=I_1.$$

In particular I_k is a co-finite ideal in T.

Proof: First note that from Lemma 3.4(2) we have

$$T_k(u,r,m_1,\ldots,m_k)=T_k(u,s,m_1,\ldots,m_k)\ \mod I_{k+1}$$

for all $r,s\in\Gamma$. Further

$$-T_k(u,0,m_1,\ldots,m_k)=T_k(u,0,-m_1,m_2,\ldots,m_k)\ \mod I_{k+1},$$

which follows from above and Lemma 3.5 (3). Now from additive property of Lemma 3.5(2) it follows that I_k/I_{k+1} is spanned by $T_k(u,0,e_{i_1},\ldots,e_{i_k})$ where $e_1,\ldots,e_d$ is the standard basis. Thus (1) follows. (2) follows from definitions. Now it is easy to conclude that I_k is a co-finite ideal for each k.

IV. PROOF OF THE CLASSIFICATION THEOREM

We will explain the plan of the proof of Theorem (2.9). First we will prove that $T/I_2\cong g\ell_d(\mathbb{C})$. Then we will prove that if $I_k, k\geqslant 2$ is zero on a finite dimensional irreducible module V of T then I_2 is zero on V. Thus V is a module for $T/I_2\cong g\ell_d(\mathbb{C})$. Further we prove that any co-finite ideal J of T contains I_k for large k. Thus any irreducible finite dimensional module V of T is actually a module for T/I_2. From this it will be easy to conclude Theorem 2.9 which will be explained at the end of the section.

(4.1) *Proposition:* $T/I_2\cong g\ell_d(\mathbb{C})$.

Proof: First recall that $F^\alpha(\psi,b)$ is an $A\oplus \mathrm{Der}\,A$-module and each weight space $V(\psi)\otimes t^m$ is a T-module. It is easy to verify that I_2 acts trivially on $V(\psi)\otimes t^m$. Now note that $T(e_i,e_j)v(m)=E_{ji}v(m)\neq 0$ for some ψ. From this we conclude that $T(e_i,e_j)$ is nonzero in T/I_2. Now it is easy to see that $T(u,s)+T(u,r)=T(u,r+s)\ \mathrm{mod}\, I_2$ and hence $T(e_i,e_j)$ spans T/I_2. Define $\pi: T/I_2\to g\ell_d(\mathbb{C})$,

$$\pi(T(e_i,e_j))=E_{ji}.$$

Consider

$$\begin{aligned}X=[T(e_i,e_j),T(e_k,e_\ell)]&=[k(-e_j)D(e_i,e_j),k(-e_\ell)D(e_k,e_\ell)]\\&=-\delta_{i\ell}k(-e_\ell)D(e_k,e_\ell)+\delta_{kj}k(-e_j)D(e_i,e_j)\\&\quad-\delta_{kj}k(-e_\ell-e_j)D(e_i,e_\ell+e_j)\\&\quad+\delta_{i\ell}k(-e_\ell-e_j)D(e_k,e_\ell+e_j).\end{aligned}$$

Follows from Proposition (3.2). Note that the following is true in T/I_2:

$$k(-e_\ell-e_j)D(e_s,e_\ell+e_j)=k(-e_\ell)D(e_s,e_\ell)+k(-e_j)D(e_s,e_j)-D(e_s,0)$$

for $s=i,k$. Thus $X=-\delta_{kj}(k(-e_\ell)D(e_i,e_\ell)-D(e_i,0))$

$$+\delta_{i\ell}(k(-e_j)D(e_k,e_j)-D(e_k,0))=-\delta_{kj}T(e_i,e_\ell)+\delta_{i\ell}T(e_k,e_j).$$

Thus π defines a surjective homomorphism. As $T(u,0)$ is zero it follows that $T(e_i,e_j)$ span T/I_2 which proves dim $(T/I_2)\leqslant d^2$. Thus π defines an isomorphism.

(4.2) *Lemma (Billig):* Suppose $\mathcal{G}$ is a Lie-algebra over $\mathbb{C}$ and J is an ideal with spanning set $J_\alpha, \alpha\in B$. Suppose there exists an element I in $\mathcal{G}$ such that $[I,J_\alpha]=\lambda J_\alpha$, $\lambda\neq 0$ for all $\alpha\in B$. then J acts trivially on any irreducible finite dimensional module V of $\mathcal{G}$.

Proof: Since the base field is complex numbers and V is finite dimensional, I has eigen vectors. Let $\lambda_1,\ldots,\lambda_k$ be all the eigenvalues of I on V. Choose λ_i such that $\lambda+\lambda_i$ is not an eigenvalue. Let v be eigenvector with eigenvalue λ_i for I. Consider $IJ_\alpha v=J_\alpha Iv+[I,J_\alpha]v=(\lambda_i+\lambda)J_\alpha v$. This proves $J_\alpha v=0\ \forall\alpha\in B$. Let $W=\{w\in V|J_\alpha w=0\ \forall\alpha\in B\}$. Since J is an ideal, it is easy to see that W is a $\mathcal{G}$-module. But $W\neq 0$. Since V is irreducible $W=V$ which proves that J acts trivially on V.

(4.3) *Proposition:* Suppose V is irreducible finite dimensional module for T such that I_{k+1} acts trivially on V. Then I_2 acts trivially on V.

Proof: From the proof of Lemma 3.4(3) we have

$$[T(v,s),T_k(u,r,m_1,\ldots,m_k)]=-(v,r)T_{k+1}(u,r,m_1,\ldots,m_k,s)-(u,s)T_k(v,r+s,m_1,\ldots,m_k)$$
$$+\sum(v,m_i)T_k(u,r+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k,s).$$

Let $I=\Sigma T(e_i,e_i)$ and note that I is actually identity element in $T/I_2\cong g\ell_d(\mathbb{C})$. Thus I is nonzero on T/I_{k+1} for $k\geqslant 1$.

Claim:

$$[I,T_k(u,r,m_1,\ldots,m_k)=(k-1)T_k(u,r,m_1,\ldots,m_k).$$

Consider

$$\left[\sum_j T(e_j,e_j),T_k(u,r,m_1,\ldots,m_k)\right]=-\sum u_jT_k(e_j,r+e_j,m_1,\ldots,m_k)+\sum_{i,j}(m_i)_jT_k(u,r$$
$$+m_i,m_1,\ldots,\widehat{m_i},\ldots,m_k,e_j).$$

Now we use Lemma 3.5(2) and the following facts.

(1) T_k is linear in u
(2) $T_k(u,r+m,m_1,\ldots,m_k)=T_k(u,r,m_1,\ldots,m_k)$ mod I_{k+1} (by Lemma 3.4(2)).
(3) I_{k+1} is zero on V.

From that we conclude that

$$[I,T_k(u,r,m_1,\ldots,m_k)]=-T_k(u,r,m_1,\ldots,m_k)+kT_k(u,r,m_1,\ldots,m_k),$$

which proves the claim. Now we can use Lemma (4.2) for the ideal I_k. Thus I_k is zero on V. Repeating this argument we conclude that I_2 acts trivially on V. This argument breaks down for $k=1$ as we cannot apply the Lemma 3.2.

(4.4) *Proposition:* Any co-finite ideal J of T contains I_k for large k.

Proof: Claim $J\cap I_k$ is co-finite in T for all k. For that consider $\varphi: T\mapsto T/J\oplus T/I_k$,

$$v\mapsto(v,v).$$

Clearly ker $\varphi=J\cap I_k$ and $T/J\cap I_k$ is a subalgebra of finite dimensional Lie-algebra $T/J\oplus T/I_k$. This proves the claim.

Consider $I_k/J\cap I_k \overset{\varphi_1}{\hookrightarrow} I_{k-1}/J\cap I_k \overset{\varphi_2}{\hookrightarrow} I_{k-1}/J\cap I_{k-1}$ where φ_1 is injective and φ_2 is surjective. Let $\rho_k=\varphi_2\circ\varphi_1$. Thus $\rho_k: I_k/I_k\cap J\to I_{k-1}/J\cap I_{k-1}$. Clearly ρ_k is injective. Let $t_n=\dim I_n/I_n\cap J$ and note that $t_{n+1}\leqslant t_n$. Thus $\{t_n\}_{n\in\mathbb{Z}^+}$ is a decreasing sequence of non-negative integers. Therefore $t_k=s$ for some s and for large $k>N$.

First we note the following two statements for a fixed i.

(1) For $\ell\neq i$,
$$[T(e_\ell,-e_\ell),T_k(e_i,0,e_{j_1},\ldots,e_{j_k})]=-k_\ell T_k(e_i,0,e_{j_1},\ldots,e_{j_k})$$
where k_ℓ is the number of e_ℓ that occur in $T_k(e_i,0,e_{j_1},\ldots,e_{j_k})$.

(2) Suppose the ideal J contains $\Sigma a_{m,I}T_m(e_i,0,e_{j_1},\ldots,e_{j_m})$ where the number of e_i's that occur in $T_m(e_i,0,e_{j_1},\ldots,e_{j_m})$ is the same for all m where $I=\{j_1,\ldots,j_k\}$. Then J contains $T_m(e_i,0,e_{j_1},\ldots,e_{j_m})$ for $m\ni a_{m,I}\neq 0$.

(1) Follows from the proof of Lemma 3.4(3). (2) follows from (1). We will prove the Proposition assuming $d\geqslant 3$ to avoid some computations. For a fixed i, consider the following set

$$S=\{T_k(e_i,0,e_{j_1},\ldots,e_{j_k})|j_\ell\neq i \text{ for all } \ell\}.$$

Now choose $k\ni \#S>s$ and $k>N$. Thus S is linearly dependent mod $I_k\cap J$. Thus there exist nonzero scalars $a_I(I=\{j_1,\ldots j_k\})$ such that

$$X=\sum a_I T_k(e_i,0,e_{j_1},\ldots,e_{j_k})\in J.$$

Now using (2) we conclude that

$$T_k(e_i,0,e_{j_1},\ldots,e_{j_k})\in J \text{ for some } I.$$

For $m,n\neq i$ consider

$$[T(e_m,e_n),T_k(e_i,0,e_{j_1},\ldots,e_{j_k})]=\ell\,\delta_{j_i m}T_k(e_i,e_m,e_{j_1},\ldots,\hat{e}_{j_i},\ldots,e_{j_k},e_n)\in J.$$

Now

$$T_k(e_i,e_m,e_{j_1},\ldots,\hat{e}_{j_i},\ldots,e_{j_k},e_n)=T_k(e_i,0,e_{j_1},\ldots,\hat{e}_{j_i},\ldots,e_{j_k},e_n)-T_{k+1}(e_i,0,e_{j_1},\ldots,e_{j_i},\ldots,e_{j_k},e_n).$$

Now by (2) it follows that

$$T_k(e_i,0,e_{j_1},\ldots,\hat{e}_{j_i},\ldots,e_{j_k},e_n)\in J.$$

Now repeating this process we see that

$$(*)\qquad T_k(e_i,0,e_{j_1},\ldots,e_{j_k})\in J$$

for all possible indices $j_1,\ldots,j_k$ which are all different from i. Applying $T(e_i,e_i)$ to the above vector to conclude

$$T_k(e_i,e_i,e_{j_1},\ldots,e_{j_k})\in J,$$

$$(**)\qquad T_k(e_i,0,e_{j_1},\ldots,e_{j_k})-T_k(e_i,e_i,e_{j_1},\ldots,e_{j_k})=-T_{k+1}(e_i,0,e_{j_1},\ldots,e_{j_k},e_i)\in J.$$

Fix $j\neq i$. Replacing k by $k+1$, consider the following vector which is in J by $(*)$.

$$[T(e_j,e_i),T_{k+1}(e_i,0,e_{j_1},\ldots,e_{j_{k+1}})]=P\delta_{jj_\ell}T_{k+1}(e_i,e_j,e_{j_1},\ldots,\hat{e}_{j_\ell},\ldots,e_{j_{k+1}},e_i)$$
$$-T_{k+1}(e_j,e_i,e_{j_1},\ldots,e_{j_{k+1}}).$$

Now

$$T_{k+1}(e_i,e_j,e_{j_1},\ldots,\hat{e}_{j_\ell},\ldots,e_{j_{k+1}},e_i)=T_{k+1}(e_i,0,e_{j_1},\ldots,\hat{e}_{j_\ell},\ldots,e_{j_{k+1}},e_i)$$
$$-T_{k+2}(e_i,0,e_{j_1},\ldots,e_j,\ldots,e_{j_{k+1}},e_i).$$

Now by $(**)$ both vectors are in J. Thus we conclude that

$$T_{k+1}(e_j,e_i,e_{j_1},\ldots,e_{j_{k+1}})\in J.$$

Now by (2) we see that

$$T_{k+1}(e_j,0,e_{j_1},\ldots,e_{j_{k+1}})\in J.$$

This is true for all possible indices $j_1,\ldots,j_{k+1}$ which are all different from i.

Now applying $T(e_{j_\ell},e_i)$ for $j_\ell\neq j$ we see that

$$T_{k+1}(e_j,e_{j_\ell},e_{j_1},\ldots,\hat{e}_{j_\ell},\ldots,e_{j_{k+1}},e_i)\in J.$$

Now by (2) we see that

$$T_{k+1}(e_j,0,e_{j_1},\ldots,\hat{e}_{j_\ell},\ldots,e_{j_{k+1}},e_i)\in J.$$

Repeating this process we see that $T_{k+1}(e_j,0,e_{\ell_1},\ldots,e_{\ell_{k+1}})\in J$ for all possible $\ell_1,\ldots,\ell_{k+1}$.

Now using the technique in the proof of Lemma 3.5 we see that

$$T_{k+1}(e_j,0,m_1,\ldots,m_{k+1})\in J \quad \text{for all } m_i\in\Gamma.$$

Now replacing $k+1$ by $k+2$ we see that

$$T_{k+2}(e_j,0,m_1,\ldots,m_{k+2})=T_{k+1}(e_j,0,m_1,\ldots,m_{k+1})-T_{k+1}(e_j,m_{k+2},m_1,\ldots,m_{k+1})\in J.$$

Then it follows that

$$T_{k+1}(e_j,m_{k+2},m_1,\ldots,m_{k+1})\in J.$$

Strictly speaking we have it for non-negative coefficients. But the other cases can be handled similarly. This proves $I_{k+1}\subseteq J$ and the Proposition. Further $s=0$.

Proof of Theorem (2.9): Let V be a module as in Theorem. Let $V=\oplus_{r\in\Gamma}V_r$ be the weight space decomposition where

$$V_r=\{v\in V|D(u,0)v=(u,r+\alpha)v,\ \ \forall u\in\mathbb{C}^d\}.$$

We know that $V_r\cong V_s$ as T-modules from Proposition 3.2(5). This with Proposition (4.3), Proposition (4.4) combined with the fact that some co-finite ideal of T acts trivially on V_r tells us that all V_r's are isomorphic to some $V(\psi,b)$ as $g\ell_d$-modules. Note that the isomorphism between V_r''s is given by $k(r)$ (from proof of proposition 3.2(5)). Thus if we let $V_r=V(\psi,b)\otimes t^r$ we see that $k(r)v(s)=v(s+r)$ for v in $V(\psi,b)$.

Now consider $T(u,r)$ in T/I_2 and note that it is linear in both variables.

Thus

$$T(u,r)v(s)=\sum_{i,j} u_i r_j T(e_i,e_j)v(s)=\sum_{i,j} u_i r_j E_{ji}v(s)$$

Therefore

$$k(-r)D(u,r)v(s)=D(u,0)v(s)+(\Sigma u_i v_j E_{ji}v)(s)=(u,s+\alpha)v(s)+\left(\sum u_i r_j E_{ji}v\right)(s).$$

Multiply both sides by $k(r)$ we get

$$D(u,r)v(s)=(u,s+\alpha)v(s+r)+\left(\sum_{ij} u_i r_j E_{ji}v\right)(s+r).$$

This completes the proof of the theorem.

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An algorithm for eigenvalues and eigenvectors of quaternion matrices in quaternionic quantum mechanics

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By means of complex representation and companion vector, this paper studies the problems of eigenvalues and eigenvectors of quaternion matrices, and gives a technique of computing the eigenvalues and eigenvectors of the quaternion matrices in quaternionic quantum mechanics. © *2004 American Institute of Physics*.
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I. INTRODUCTION

In quaternionic quantum mechanics (Adler and co-workers, 1995, 1996, 1997; Finkelstein *et al.*, 1962), one of the most important tasks is to solve the Schrödinger equation

$$\frac{\partial}{\partial t}|f\rangle = -\hat{H}|f\rangle, \tag{1.1}$$

with $\hat{H}$ an anti-self-adjoint real quaternion matrix, and $|f\rangle$ an eigenstate to $\hat{H}$. The quaternionic Schrödinger Eq. (1.1) plays an important role in quaternionic quantum mechanics, it is known that the study of the quaternionic Schrödinger Eq. (1.1) is reduced to the study of quaternionic eigenequation

$$\hat{H}\alpha = \alpha\lambda, \tag{1.2}$$

with $\hat{H}$ an anti-self-adjoint real quaternion matrix (time-independent). But because of the noncommutation of quaternions, the studies of the equations are more difficult. In order to solve Eqs. (1.1) and (1.2), the author (Adler, 1995) changed the quaternionic Schrödinger equations into a two-component complex Schrödinger equations, and turned the problem of quaternionic Schrödinger equation into that of complex Schrödinger equation. In this paper, by means of complex representation and companion vector, we study the problems of eigenvalues and eigenvectors of general quaternion matrices, and give a technique of computing eigenvalues and eigenvectors of the quaternion matrices in quaternionic quantum mechanics.

Let $\mathbf{R}$ denote the real number field, $\mathbf{C}=\{a+b\sqrt{-1}|a,b\in\mathbf{R}\}$ the complex number field, $\mathbf{Q}$ the quaternion number field. For any quaternion

$$x = x_0 + x_1 i + x_2 j + x_3 k, \tag{1.3}$$

$$i^2 = j^2 = k^2 = -1, \quad ij = -ji = k, \tag{1.4}$$

in which $x_i \in \mathbf{R}$, the conjugate of quaternion x is $\overline{x} = x_0 - x_1 i - x_2 j - x_3 k$. It is clear that x can be uniquely expressed as $x = y + zj$, in which y, $z \in \mathbf{C}$, and $x = y + zj$ if and only if $\overline{x} = \overline{y} - zj$. Let $\mathbf{F}^{m\times n}$ denote the set of $m\times n$ matrices on the field $\mathbf{F}$. For any $A=(a_{ij})\in\mathbf{Q}^{n\times n}$, $A^T=(a_{ji})$ and $A^H=(\overline{a}_{ji})$ denote the transpose and the conjugate transpose of the quaternion matrix A, respectively, and A is an anti-self-adjoint quaternion matrix if $A^H=-A$. Two quaternions x and y are

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said to be similar if there exists a nonzero quaternion p such that $p^{-1}xp=y$, and this is written as $x\sim y$. It is routine to check that $\sim$ is an equivalence relation on the quaternions. We denote by $[x]$ the equivalence class containing x.

II. COMPLEX REPRESENTATION AND COMPANION VECTOR

For any quaternion $x=x_0+x_1i+x_2j+x_3k=y+zj\in\mathbf{Q}$, and quaternion matrix $A=(a_{ij})\in\mathbf{Q}^{m\times n}$, the complex representation of quaternion x and A are, respectively, defined to be

$$x^f=\begin{pmatrix} x_0+x_1\sqrt{-1} & x_2+x_3\sqrt{-1} \\ -x_2+x_3\sqrt{-1} & x_0-x_1\sqrt{-1} \end{pmatrix}=\begin{pmatrix} y & z \\ -\overline{z} & \overline{y} \end{pmatrix}\in\mathbf{C}^{2\times 2}, \tag{2.1}$$

and

$$A^f=((a_{ij})^f)=\left(\begin{pmatrix} y_{ij} & z_{ij} \\ -\overline{z}_{ij} & \overline{y}_{ij} \end{pmatrix}\right)\in\mathbf{C}^{2m\times 2n}. \tag{2.2}$$

It is easy to verify the following Eqs. (2.3) and (2.4) by the definition of complex representation of quaternion matrices. That is if $A, B\in\mathbf{Q}^{m\times n}$, $r\in\mathbf{R}$, then

$$(A+B)^f=A^f+B^f,\quad (rA)^f=rA^f, \tag{2.3}$$

and if $A\in\mathbf{Q}^{m\times n}$, $B\in\mathbf{Q}^{n\times s}$, then

$$(AB)^f=A^fB^f, \tag{2.4}$$

and A is nonsingular if and only if A^f is nonsingular if $A\in\mathbf{Q}^{n\times n}$, and $(A^f)^{-1}=(A^{-1})^f$.

Next we introduce the concept of companion vector.

If $\alpha=(x_1,x_2,\ldots,x_{2n})^T\in\mathbf{C}^{2n\times 1}$, then the companion vector α^c of vector α is defined to be

$$\alpha^c=(-\overline{x}_2,\overline{x}_1,-\overline{x}_4,\overline{x}_3,\ldots,-\overline{x}_{2n},\overline{x}_{2n-1})^T\in\mathbf{C}^{2n\times 1}.$$

Let $\alpha, \beta\in\mathbf{C}^{2n\times 1}$, $\lambda\in\mathbf{C}$, $A\in\mathbf{Q}^{n\times n}$. Then we can easily get the following Eqs. (2.5) and (2.6) by the definition of companion vector and complex representation,

$$(\alpha\pm\beta)^c=\alpha^c\pm\beta^c,\quad (\alpha^c)^c=-\alpha, \tag{2.5}$$

$$(A^f\alpha)^c=A^f\alpha^c,\quad (\alpha\lambda)^c=\alpha^c\overline{\lambda}, \tag{2.6}$$

and if $\alpha\neq 0$, then α and α^c are linearly independent.

From (2.6) we have following result:

Proposition 2.1: Let $A\in\mathbf{Q}^{n\times n}$. Then the real eigenvalues of complex representation A^f appear in pairs, and the complex eigenvalues of complex representation A^f appear in conjugate pairs.

III. EIGENVALUES AND EIGENVECTORS OF A QUATERNION MATRIX

In this section, by means of complex representation and companion vector, we study the eigenvalues and eigenvectors of quaternion matrices, and give a technique of computing the eigenvalues and eigenvectors of the quaternion matrices in quaternionic quantum mechanics.

Since right and left scalar multiplications of quaternions are different, we need to define right and left eigenvalues for a quaternion matrix. Let $A\in\mathbf{Q}^{n\times n}$, a quaternion λ is said to be a right (left) eigenvalue provided that $A\alpha=\alpha\lambda(A\alpha=\lambda\alpha)$, and α is said to be an eigenvector to corresponding eigenvalue λ. In this paper we mainly focus on the right eigenvalues and eigenvectors of quaternion matrices.

Lemma 3.1 (Fuzhen, 1997): Let $x=x_0+x_1i+x_2j+x_3k$ be a real quaternion. Then there exists a quaternion p such that

$$p^{-1}\lambda p = x_0 + hi, \quad h = \sqrt{x_1^2 + x_2^2 + x_3^2} \geqslant 0, \tag{3.1}$$

namely, $x \in [x_0 + \sqrt{x_1^2 + x_2^2 + x_3^2} i]$. The complex number $\overset{a}{x} = x_0 + hi$ in (3.1) is called principal number of the class $[x]$.

Since $A\alpha = \alpha\lambda$ if and only if $A(\alpha p) = (\alpha p)(p^{-1}\lambda p)$ for any nonzero quaternion p, so λ is an eigenvalue of quaternion matrix A if and only if $p^{-1}\lambda p$ is an eigenvalue of quaternion matrix A, and α is an eigenvector to the eigenvalue λ if and only if αp is an eigenvector to the eigenvalue $p^{-1}\lambda p$ for any nonzero quaternion p.

If $A \in \mathbf{Q}^{n\times n}$, λ is an eigenvalue of quaternion matrix A and let $\overset{a}{\lambda} = p^{-1}\lambda p$ be the principal number of $[\lambda]$ for quaternion p, then

$$A\alpha = \alpha\lambda \Leftrightarrow A(\alpha p) = (\alpha p)(p^{-1}\lambda p) \Leftrightarrow A\beta = \beta\overset{a}{\lambda}, \tag{3.2}$$

where $\beta = \alpha p$ and $\overset{a}{\lambda} = p^{-1}\lambda p$ is the principal eigenvalue. By (2.4) we know that (3.2) is equivalent to

$$A^f\alpha^f = \alpha^f\lambda^f \Leftrightarrow A^f\beta^f = \beta^f\overset{a}{\lambda}^f, \tag{3.3}$$

and if we let $\beta^f = (\gamma, \gamma^c)$, then

$$A^f\beta^f = \beta^f\overset{af}{\lambda} \Leftrightarrow A^f(\gamma, \gamma^c) = (\gamma, \gamma^c)\begin{pmatrix} \overset{a}{\lambda} & 0 \\ 0 & \overline{\overset{a}{\lambda}} \end{pmatrix}, \tag{3.4}$$

i.e., $A^f\gamma = \gamma\overset{a}{\lambda}$ and $A^f\gamma^c = \gamma^c\overline{\overset{a}{\lambda}}$.

From the statement above we obtain the following result:

Theorem 3.2: Let $A \in \mathbf{Q}^{n\times n}$. Then

(1) A quaternion λ is an eigenvalue of quaternion matrix A if and only if $p^{-1}\lambda p$ (for any nonzero quaternion p) is an eigenvalue of quaternion matrix A; a quaternion vector α is an eigenvector corresponding to the eigenvalue λ if and only if αp is an eigenvector corresponding to the eigenvalue $p^{-1}\lambda p$ for any nonzero quaternion p;

(2) A quaternion λ is an eigenvalue of quaternion matrix A if and only if $\overset{a}{\lambda}$ is an eigenvalue of complex representation A^f; and α is an eigenvector corresponding to the eigenvalue λ (i.e., $A\alpha = \alpha\lambda$) if and only if γ is an eigenvector corresponding to the principal eigenvalue $\overset{a}{\lambda}$ (i.e., $A^f\gamma = \gamma\overset{a}{\lambda}$) with $(\alpha p)^f = (\gamma, \gamma^c)$, $\overset{a}{\lambda} = p^{-1}\lambda p$.

Remark: Theorem 3.2 gives a relationship between the eigenvalues and eigenvectors of a quaternion matrix and that of corresponding complex representation matrix by means of complex representation and companion vector, and turns the eigenvalues and eigenvectors of a quaternion matrix into that of a complex matrix.

IV. ALGORITHM

Now we list an algorithm for computing eigenvalues and eigenvectors of a quaternion matrix by means of complex representation and companion vector.

Algorithm: Let $A \in \mathbf{Q}^{n\times n}$.

Step 1: Find the complex representation matrix A^f and all complex eigenvalues and eigenvectors of the complex matrix A^f.

By Proposition 2.1 and (2.6), we may let the eigenvalues and corresponding eigenvectors of the complex matrix A^f be

$$\lambda_1, \overline{\lambda_1}, \lambda_2, \overline{\lambda_2}, \ldots, \lambda_n, \overline{\lambda_n},$$

$$\gamma_1, \gamma_1^c, \gamma_2, \gamma_2^c, \ldots, \gamma_n, \gamma_n^c,$$

with $A^f\gamma_i = \gamma_i\lambda_i$ and $A^f\gamma_i^c = \gamma_i^c\overline{\lambda_i}$, and $\mathrm{Im}\,\lambda_i \geqslant 0$, $i=1,2,...,n$;

Step 2: Find all principal eigenvalues and corresponding eigenvectors of the A.

By step 1, we know that $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all the principal eigenvalues of the quaternion matrix A, let $\alpha_i^f = (\gamma_i, \gamma_i^c)$, since

$$A^f(\gamma_i, \gamma_i^c) = (\gamma_i, \gamma_i^c)\begin{pmatrix} \lambda_i & 0 \\ 0 & \overline{\lambda_i} \end{pmatrix} \Leftrightarrow A^f\alpha_i^f = \alpha_i^f\lambda_i^f \Leftrightarrow A\alpha_i = \alpha_i\lambda_i,$$

so vector $\alpha_i = (\gamma_i, \gamma_i^c)^{f^{-1}}$ is an eigenvector of the A corresponding to the principal eigenvalue λ_i;

Step 3: Find all eigenvalues and corresponding eigenvectors of the A.

For any nonzero quaternion p, by Theorem 3.2 we know that $p^{-1}\lambda_i p$ are all eigenvalues of the A, and $\alpha_i p$ are all eigenvectors of the A corresponding to eigenvalue $p^{-1}\lambda_i p$, $i=1,2,...,n$.

Example: Let

$$A = \begin{pmatrix} i & 1+j \\ -1+j & -k \end{pmatrix}.$$

Find all eigenvalues and corresponding eigenvectors of the quaternion matrix A (an anti-self-adjoint matrix).

It is easy to find the A^f by the definition of complex representation of the A, and

$$A^f = \begin{pmatrix} i & 0 & 1 & 1 \\ 0 & -i & -1 & 1 \\ -1 & 1 & 0 & -i \\ -1 & -1 & -i & 0 \end{pmatrix},$$

and $|\lambda I_{2n} - A^f| = (\lambda^2 + 3)^2$. Therefore eigenvalues of the complex representation matrix A^f are $\lambda_1 = \sqrt{3}i$, $\lambda_2 = -\sqrt{3}i = \overline{\lambda_1}$, and

$$\gamma_1^T = (2i, 0, 1-\sqrt{3}, 1-\sqrt{3}), \quad \gamma_2^T = (0, -2i, -1-\sqrt{3}, 1+\sqrt{3})$$

are two eigenvectors of A^f corresponding to eigenvalues λ_1, namely, $A^f\gamma_1 = \gamma_1\lambda_1$, $A^f\gamma_2 = \gamma_2\lambda_1$, and by (2.6) we also have $A^f\gamma_1^c = \gamma_1^c\overline{\lambda_1}$ and $A^f\gamma_2^c = \gamma_2^c\overline{\lambda_1}$. Let $\alpha_1^T = (\gamma_1, \gamma_1^c)^{f^{-1}} = (2i, (1-\sqrt{3})(1-j))^T$, $\alpha_2^T = (\gamma_1, \gamma_1^c)^{f^{-1}} = (-2k, -(1+\sqrt{3})(1+j))^T$. Then $A\alpha_1 = \alpha_1\lambda_1$, $A\alpha_2 = \alpha_2\lambda_1$, and all eigenvalues of the quaternion matrix A are $p^{-1}\lambda_1 p$, and $\alpha_i p$, $i=1,2$, are the corresponding eigenvectors to $p^{-1}\lambda_1 p$, where p is an arbitrary quaternion.

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Time fractional Schrödinger equation

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The Schrödinger equation is considered with the first order time derivative changed to a Caputo fractional derivative, the time fractional Schrödinger equation. The resulting Hamiltonian is found to be non-Hermitian and nonlocal in time. The resulting wave functions are thus not invariant under time reversal. The time fractional Schrödinger equation is solved for a free particle and for a potential well. Probability and the resulting energy levels are found to increase over time to a limiting value depending on the order of the time derivative. New identities for the Mittag–Leffler function are also found and presented in an Appendix. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1769611]

I. INTRODUCTION

A Gaussian distribution for random walk problems, in the continuum limit, can be used to generate the ordinary diffusion equation (ignoring boundary conditions and sources)[1]

$$\frac{\partial}{\partial t}\mathrm{U}=c\frac{\partial^2}{\partial x^2}\mathrm{U}, \tag{1}$$

U represents the concentration of the diffusing material. c is the diffusion coefficient which is positive and whose magnitude helps determine the speed at which the diffusion takes place, and, t and x are the temporal and spatial coordinates. The diffusion coefficient may depend on the coordinates and/or the concentration. When non-Gaussian distributions are used fractional diffusion equations are produced. Diffusion that is generated by non-Gaussian distributions is typically referred to as anomalous diffusion. There is a growing body of examples of phenomena that lie outside of what is predicted by the ordinary diffusion equation (see, for example, Refs. 2–7).

Three types of fractional diffusion equations can be produced when considering non-Gaussian distributions. The first is the space fractional diffusion equation

$$\frac{\partial}{\partial t}\mathrm{U}=c\frac{\partial^\beta}{\partial x^\beta}\mathrm{U}. \tag{2}$$

Here $0<\beta\leqslant 2$ (in this paper Caputo fractional derivatives will be used, the reader is directed to Appendix A for definitions and notation conventions). In this case, the diffusion is still Markovian but only exhibits Brownian motion for $\beta=2$.

The second type is the time fractional diffusion equation

$$\frac{\partial^\alpha}{\partial t^\alpha}\mathrm{U}=c\frac{\partial^2}{\partial x^2}\mathrm{U}. \tag{3}$$

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In this case the diffusion is non-Markovian and can further be divided into sub-($0<\alpha<1$) and super-($1<\alpha<2$) diffusive behavior. Additionally, the mixed case can be considered with both space and time fractional derivatives

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}}\mathrm{U}=c\,\frac{\partial^{\beta}}{\partial x^{\beta}}\mathrm{U}. \tag{4}$$

The Schrödinger equation has the mathematical appearance of a diffusion equation and can be derived by considering probability distributions. Feynman and Hibbs used a Gaussian probability distribution in the space of all possible paths, for a quantum mechanical particle, to derive the Schrödinger equation.[8] Therefore, it is reasonable to consider the different types of Schrödinger equations that are obtainable for non-Gaussian distributions. In an earlier sequence of papers (see Refs. 9–11) Laskin constructed space fractional quantum mechanics. This was done using Feynman's path integral approach, the difference being the use of Levy distributions instead of Gaussian distributions for the set of possible paths. The Schrödinger equation that was obtained had space fractional derivatives. This is the same result that one obtains when studying diffusion processes based on Levy distributions instead of Gaussian distributions. Similarly, a time fractional Schrödinger equation would be obtained if one considered non-Markovian evolution. Laskin was able to show that the fractional Hamiltonian was Hermitian and that parity is conserved. Energy levels were also computed for the hydrogen atom and the harmonic oscillator.

In this paper, properties of the time fractional Schrödinger equation are examined. The time fractional Schrödinger equation will be constructed by rewriting the Schrödinger equation so that all derivative operators appear as dimensionless objects, the time derivative is then fractionalized, and the imaginary unit is raised to the order of the fractional time derivative. This last step is important because it ensures the same physical character of the time fractional Schrödinger equation no matter what the order.

For the time fractional Schrödinger equation there are two cases: One for the order of the time derivative being between zero and one, and another case for the order being between one and two. For the later case the resulting equation has the same draw backs as the Klein–Gordon equation, in that the initial value of the first derivative and the wave function itself must be specified.

In the following section the time fractional Schrödinger equation is constructed. Section III will show that the time fractional Schrödinger equation is equivalent to the usual Schrödinger equation but with a time dependent Hamiltonian. The solutions will not be invariant under time reversal nor will probability be conserved. In Sec. IV solutions are obtained for a free particle. In Sec. V a solution for a potential well is found. In both cases it will be shown that probability increases over time to a limiting value that depends on the order of the time derivative. Section VI presents some properties for the case of the order of the time derivative being between one and two. Concluding remarks are given in Sec. VII. There are also two Appendixes. The first is a primer on Caputo fractional calculus and a rationale of why it should be used to study physical systems instead of Riemann–Liouville fractional calculus. A second appendix presents some properties of the Mittag–Leffler function along with a new identity.

II. TIME FRACTIONAL SCHRÖDINGER EQUATION

To fractionalize the time derivative of the Schrödinger equation care must be taken to preserve the units of the wave function. To begin with, note the definitions and the relationships of the Plank units given below (Plank length, time, mass, and energy):[12]

$$L_p=\sqrt{\frac{G\hbar}{c^3}},\quad T_p=\sqrt{\frac{G\hbar}{c^5}},\quad M_p=\sqrt{\frac{\hbar c}{G}},\quad E_p=M_pc^2. \tag{5}$$

The standard form of the Schrödinger equation in one space and one time dimension is[13]

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_x^2\psi + V\psi. \tag{6}$$

This can be expressed in Plank units as follows:

$$iT_p\partial_t\psi = -\frac{L_p^2 M_p}{2m}\partial_x^2\psi + \frac{V}{E_p}\psi. \tag{7}$$

Define two dimensionless parameters; $N_m = m/M_p$ the number of Plank masses in m and $N_V = V/E_p$ the number of Plank energies in V

$$iT_p\partial_t\psi = -\frac{L_p^2}{2N_m}\partial_x^2\psi + N_V\psi. \tag{8}$$

When the time derivative is fractionalized there are two options,

$$(iT_p)^\nu \mathrm{D}_t^\nu\psi = -\frac{L_p^2}{2N_m}\partial_x^2\psi + N_V\psi, \tag{9}$$

$$i(T_p)^\nu \mathrm{D}_t^\nu\psi = -\frac{L_p^2}{2N_m}\partial_x^2\psi + N_V\psi. \tag{10}$$

In this paper, D_t^ν shall denote the Caputo fractional derivative of order ν. T_p must be raised to the same order as the fractional derivative to preserve the units of ψ.

The question of whether or not to raise i to the order of the time derivative needs more investigation. There are two reasons to choose Eq. (9) over Eq. (10), one superficial and one physical. When performing a Wick rotation the imaginary unit is raised to the same power as the time coordinate. The second reason involves the temporal behavior of the solution. When solving for the time component of Eq. (9) or Eq. (10) the Laplace transform is the preferred method. For Eq. (9), changing the order of the derivative moves the pole (from the inverse Laplace transform) up or down the negative imaginary axis. Hence, the temporal behavior of the solution will not change. For Eq. (10), changing the order of the derivative moves the pole to almost any desired location in the complex plane. Physically, this would mean that a small change in the order of the time derivative, in Eq. (10), could change the temporal behavior from sinusoidal to growth or to decay. Due to the simpler physical behavior of Eq. (9) and the role of "i" in a Wick rotation, Eq. (9) is the best candidate for a time fractional Schrödinger equation.

III. TIME DEPENDENT HAMILTONIAN AND PROBABILITY CURRENT

The order of the time derivative on the left hand side Eq. (9) is not one, therefore, the operator on the right hand side is not a Hermitian Hamiltonian. Equation (5) can be rearranged to expose a time dependent Hamiltonian. To do so, the order of the time derivative on the left hand side of Eq. (9) must be raised to order one. First note an identity for Caputo derivatives for $0<\nu<1$,

$$\mathrm{D}_t^{1-\nu}\mathrm{D}_t^\nu y(t) = \frac{\mathrm{d}}{\mathrm{d}t}y(t) - \frac{[\mathrm{D}_t^\nu y(t)]_{t=0}}{t^{1-\nu}\Gamma(\nu)}. \tag{11}$$

Now define two parameters:

$$\alpha = \frac{N_V}{T_p^\nu}, \tag{12}$$

$$\beta = \frac{(L_p)^2}{2N_m(T_p)^\nu}, \tag{13}$$

then Eq. (9) can be written as

$$\mathrm{D}_t^\nu \psi = -\frac{\beta}{i^\nu}\partial_x^2 \psi + \frac{\alpha}{i^\nu}\psi. \tag{14}$$

Using the identity for Caputo derivatives, Eq. (11), the time dependent Hamiltonian appears

$$\partial_t \psi = -\frac{\beta}{i^\nu}\partial_x^2(\mathrm{D}_t^{1-\nu}\psi) + \frac{\alpha}{i^\nu}(\mathrm{D}_t^{1-\nu}\psi) + \frac{[\mathrm{D}^\nu \psi(t)]_{t=0}}{t^{1-\nu}\Gamma(\nu)}. \tag{15}$$

Since the Hamiltonian is time dependent we should not expect probability to be conserved. Note also that the Hamiltonian is nonlocal in time, due to the integral in the formulation of the fractional derivative (see the Appendix). This nonlocal character tells us that the solutions will not be invariant under time reversal. The third term in the Hamiltonian goes to zero as time goes to infinity (recall that the order of the original fractional time derivative is less than one).

Consider the nonlocal object in Eq. (15)

$$\mathrm{D}_t^{1-\nu}\psi(t,x) = \frac{1}{\Gamma(1-\nu)}\int_0^t \left(\frac{\mathrm{d}}{\mathrm{d}\tau}\psi(\tau,x)\right)\frac{\mathrm{d}\tau}{(t-\tau)^\nu}. \tag{16}$$

For a possible interpretation of this object recall the interpretation of the first order time derivative in standard quantum mechanics,[13]

$$\frac{\partial}{\partial t} = \frac{E}{i\hbar}, \tag{17}$$

where E is viewed as the energy operator (Hamiltonian). Then the inner product (* denotes complex conjugation),

$$\int_{-\infty}^{\infty} \psi(t,x)^* \mathrm{D}_t^{1-\nu}\psi(t,x)\mathrm{d}x, \tag{18}$$

can be interpreted as being proportional to the weighted time average of the energy of the wave function, the weighting factor being $(t-\tau)^{-\nu}$. For the remainder of the paper denote $\tilde{\psi} = \mathrm{D}_t^{1-\nu}\psi$.

The probability current equation (for a free particle) can be constructed just as for the non-fractional Schrödinger equation.

$$probability\ \ density = P = \psi\psi^*, \tag{19}$$

$$\partial_t P = \partial_t \psi \psi^* + \psi \partial_t \psi^*, \tag{20}$$

$$\partial_t P = \left(-\frac{\beta}{i^\nu}\partial_x^2\tilde{\psi} + \frac{[\mathrm{D}_t^\nu \psi(t,x)]_{t=0}}{t^{1-\nu}\Gamma(\nu)}\right)\psi^* + \psi\left(-\frac{\beta}{(-i)^\nu}\partial_x^2\tilde{\psi}^* + \frac{[\mathrm{D}_t^\nu \psi(t,x)^*]_{t=0}}{t^{1-\nu}\Gamma(\nu)}\right). \tag{21}$$

This can be rearranged

$$\partial_t P+\beta\partial_x\left(\frac{\partial_x\tilde{\psi}\psi^*}{i^\nu}+\frac{\partial_x\tilde{\psi}^*\psi}{(-i)^\nu}\right)=\beta\left(\frac{\partial_x\tilde{\psi}\partial_x\psi^*}{i^\nu}+\frac{\partial_x\tilde{\psi}^*\partial_x\psi}{(-i)^\nu}\right)$$
$$+\frac{\psi^*[\mathrm{D}_t^\nu\psi(t,x)]_{t=0}+\psi[\mathrm{D}_t^\nu\psi(t,x)^*]_{t=0}}{t^{1-\nu}\Gamma(\nu)}. \tag{22}$$

If the Hamiltonian were not time dependent (i.e., if $\nu\to 1$) then the right hand side of Eq. (22) would be zero. The probability current can be identified as

$$J=\frac{\beta}{i^\nu}(\partial_x\tilde{\psi})\psi^*+\frac{\beta}{(-i)^\nu}\psi(\partial_x\tilde{\psi}^*). \tag{23}$$

The right hand side of Eq. (22) can be viewed as a source in the probability current equation. The nonzero source term in Eq. (22) confirms that probability will not be preserved for solutions of the time fractional Schrödinger equation.

$$S(x,t)=\frac{\beta}{i^\nu}\partial_x\tilde{\psi}\partial_x\psi^*+\frac{\beta}{(-i)^\nu}\partial_x\tilde{\psi}^*\partial_x\psi+\frac{\psi^*[\mathrm{D}_t^\nu\psi(t,x)]_{t=0}+\psi[\mathrm{D}^\nu\psi(t,x)^*]_{t=0}}{t^{1-\nu}\Gamma(\nu)}, \tag{24}$$

$$\partial_t P+\partial_x J=S. \tag{25}$$

Integrating Eq. (25) over all space and requiring the wave function and its first derivative go to zero at spatial infinity gives

$$\partial_t\int_{-\infty}^{\infty}P\,\mathrm{d}x=\int_{-\infty}^{\infty}S\mathrm{d}x. \tag{26}$$

IV. FREE PARTICLE SOLUTION

The time fractional Schrödinger equation for a free particle is given by

$$(iT_p)^\nu\mathrm{D}_t^\nu\psi=-\frac{L_p^2}{2N_m}\partial_x^2\psi. \tag{27}$$

To solve this equation, apply a Fourier transform on the spatial coordinate, $\mathcal{F}(\psi(x,t))=\Psi(\lambda,t)$

$$(iT_p)^\nu\mathrm{D}_t^\nu\Psi=\frac{(L_p\lambda)^2}{2N_m}\Psi. \tag{28}$$

The resulting equation can be rearranged and the results of Appendix B can be used. Namely, the identity for the Mittag–Leffler function with a complex argument

$$\mathrm{D}_t^\nu\Psi=\frac{(L_p\lambda)^2}{2N_mT_p^\nu i^\nu}\Psi, \tag{29}$$

$$\Psi=\Psi_0E_\nu(\omega(-it)^\nu), \tag{30}$$

or

$$\Psi=\frac{\Psi_0}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_\nu(\omega(-i)^\nu,t)\}, \tag{31}$$

where $\omega=(L_p\lambda)^2/2N_mT_p^{\nu}$. In Eq. (31) the first term is oscillatory, and the second is decay in the time variable. The function, F_{ν}, is defined in Appendix B. Inverse Fourier transforming gives the final solution

$$\psi(x,t)=\mathcal{F}^{-1}\Psi(\lambda,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\lambda x}\frac{\Psi_0}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}(\omega(-i)^{\nu},t)\}\mathrm{d}\lambda. \tag{32}$$

This can be broken into two parts, a Schrödinger like piece divided by ν, and a decay term that goes to zero as time goes to infinity

$$\psi_S(x,t)=\frac{1}{2\pi\nu}\int_{-\infty}^{\infty}e^{i\lambda x}\Psi_0 e^{-i\omega^{1/\nu}t}\mathrm{d}\lambda, \tag{33}$$

$$\psi_D(x,t)=\frac{-1}{2\pi}\int_{-\infty}^{\infty}e^{i\lambda x}\Psi_0 F_{\nu}(\omega(-i)^{\nu},t)\mathrm{d}\lambda, \tag{34}$$

$$\psi(x,t)=\psi_S(x,t)+\psi_D(x,t). \tag{35}$$

Note that as ν goes to one the decay term goes to zero and the Schrödinger like term becomes the nonfractional Schrödinger term.

Ψ_0 may be chosen so that the initial probability is one

$$\int_{-\infty}^{\infty}\psi(x,0)\psi^*(x,0)\mathrm{d}x=1. \tag{36}$$

Due to the decay term in the solution one may ask what happens to the total probability as time goes to infinity. Consider the following limit

$$\lim_{t\to\infty}\int_{-\infty}^{\infty}\psi(x,t)\psi^*(x,t)\mathrm{d}x \tag{37}$$

$$=\lim_{t\to\infty}\int_{-\infty}^{\infty}\mathcal{F}^{-1}\left(\frac{\Psi_0}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}(\omega(-i)^{\nu},t)\}\right)\mathcal{F}^{-1}\left(\frac{\Psi_0}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}(\omega(-i)^{\nu},t)\}\right)^*\mathrm{d}x. \tag{38}$$

Now use Parseval's identity

$$=\frac{2\pi}{\nu^2}\lim_{t\to\infty}\int_{-\infty}^{\infty}\Psi_0\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}(\omega(-i)^{\nu},t)\}(\Psi_0\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}(\omega(-i)^{\nu},t)\})^*\mathrm{d}\lambda. \tag{39}$$

In the limit that time goes to infinity F_{ν} goes to zero, this leaves

$$=\frac{2\pi}{\nu^2}\lim_{t\to\infty}\int_{-\infty}^{\infty}\Psi_0 e^{-i\omega^{1/\nu}t}\Psi_0^* e^{i\omega^{1/\nu}t}\mathrm{d}\lambda, \tag{40}$$

$$=\frac{2\pi}{\nu^2}\lim_{t\to\infty}\int_{-\infty}^{\infty}\Psi_0\Psi_0^*\mathrm{d}\lambda. \tag{41}$$

Now use Parseval's identity again

$$=\frac{1}{\nu^2}\lim_{t\to\infty}\int_{-\infty}^{\infty}\psi_0\psi_0^*\,\mathrm{d}x. \tag{42}$$

The remaining integral is unity. Hence,

$$\lim_{t\to\infty}\int_{-\infty}^{\infty}\psi(x,t)\overline{\psi}(x,t)\,\mathrm{d}x=\frac{1}{\nu^2}. \tag{43}$$

Since ν is less than one, the total probability increases over time to the limiting value of Eq. (43).

V. POTENTIAL WELL SOLUTION

Now consider a particle in a potential well

$$V(x)=\begin{cases}0, & 0<x<a\\ \infty & \text{elsewhere,}\end{cases} \tag{44}$$

$$(iT_p)^{\nu}\mathrm{D}_t^{\nu}\psi=-\frac{L_p^2}{2N_m}\partial_x^2\psi, \tag{45}$$

$$\begin{aligned}\psi(0,t)&=0,\\ \psi(a,t)&=0.\end{aligned} \tag{46}$$

This can be solved by separation of variables, $\psi=A(t)B(x)$

$$(iT_p)^{\nu}\frac{\mathrm{D}_t^{\nu}A}{A}=-\frac{L_p^2}{2N_m}\frac{\partial_x^2 B}{B}=\lambda. \tag{47}$$

Solve the spatial component first

$$B''+\lambda\frac{2N_m}{L_p^2}B=0. \tag{48}$$

The boundary conditions give

$$B_n=c_n\sin\left(\frac{n\pi}{a}x\right), \tag{49}$$

$$\lambda_n=\left(\frac{n\pi L_p}{a}\right)^2\frac{1}{2N_m}. \tag{50}$$

The time equation is

$$D_t^{\nu}A=\frac{\lambda_n}{(iT_p)^{\nu}}A. \tag{51}$$

This can be solved in terms of the Mittag–Leffler function (see Appendix B). Let $A(t=0)=1$ so that we can specify an initial wave function.

$$A=E_{\nu}(\omega_n(-it)^{\nu}), \tag{52}$$

$$A=\frac{1}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}((-i\omega)^{\nu},t)\}, \tag{53}$$

where, $\omega_n=\lambda_n/T_p^{\nu}$.

Note also that

$$\lim_{t\to\infty}|A(t)|=\frac{1}{\nu}. \tag{54}$$

The normalized spatial eigenfunctions are

$$\psi_n(x,0)=\sqrt{\frac{2}{a}}\sin(n\pi x/a), \tag{55}$$

$$\int_0^a \psi_n(x,0)\cdot\psi_n(x,0)\mathrm{d}x=1. \tag{56}$$

The solutions for all times can be written as

$$\psi_n(x,t)=\sqrt{\frac{2}{a}}\sin(n\pi x/a)\,\frac{1}{\nu}\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}((-i\omega)^{\nu},t)\}. \tag{57}$$

As in the free particle case it is interesting to compute the limit of the total probability as time goes to infinity

$$\lim_{t\to\infty}\int_0^a \psi_n(x,t)\cdot\overline{\psi}_n(x,t)\mathrm{d}x=\frac{1}{\nu^2}. \tag{58}$$

This is the same result as for the free particle. As ν is less than one, the total probability is greater than one as time goes to infinity. In fact as long as $t_1<t_2$ we have

$$\int_0^a \psi(x,t_1)\cdot\overline{\psi}(x,t_1)\mathrm{d}x<\int_0^a \psi(x,t_2)\cdot\overline{\psi}(x,t_2)\mathrm{d}x. \tag{59}$$

Probability is created as time progresses. This can also be viewed as particles are created (extracted from the potential) as time progresses.

The energy levels for the potential well can be computed. Since the Hamiltonian is time dependent the energy levels will also be time dependent.

$$\mathrm{E}_n(t)=\int_0^a \psi^* i\hbar\,\partial_t\psi\mathrm{d}x, \tag{60}$$

$$\mathrm{E}_n(t)=\frac{2i\hbar}{a\nu^2}\{e^{i\omega^{1/\nu}t}-\nu F_{\nu}((i\omega)^{\nu},t)\}\partial_t\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}((-i\omega)^{\nu},t)\}\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\mathrm{d}x, \tag{61}$$

$$\mathrm{E}_n(t)=\frac{i\hbar}{\nu^2}\{e^{i\omega^{1/\nu}t}-\nu F_{\nu}((i\omega)^{\nu},t)\}\partial_t\{e^{-i\omega^{1/\nu}t}-\nu F_{\nu}((-i\omega)^{\nu},t)\}. \tag{62}$$

The interesting result is when time goes to infinity

$$\mathrm{E}_n(\infty)=\frac{\hbar(\lambda_n)^{1/\nu}}{\nu^2 T_p}=\frac{\hbar(n\pi L_p)^{2/\nu}}{\nu^2 T_p(2a^2N_m)^{1/\nu}}. \tag{63}$$

This is the same energy spectrum that is obtained for the nonfractional Schrödinger equation except for the factor of $1/\nu^2$ and the exponent of $1/\nu$. The difference between two energy levels, say m and n, is given by

$$\mathrm{E}_m(\infty)-\mathrm{E}_n(\infty)=\frac{\hbar(\pi L_p)^{2/\nu}}{\nu^2 T_p(2a^2N_m)^{1/\nu}}(m^{2/\nu}-n^{2/\nu}). \tag{64}$$

Since ν is less than one the spacing between energy levels is greater than that given by the nonfractional Schrödinger equation. In fact the smaller the value of ν the greater the difference between energy levels. Note also that at $t=0$ the spacing between the energy levels is that same as that of the nonfractional Schrödinger equation. As time progresses the spacing between the energy levels increases to the limiting value given by Eq. (64). Hence, radiation that is emitted, say from state n to state m, at an early time will have a longer wavelength than radiation emitted at a later time.

VI. SOME PROPERTIES FOR $1<\nu\leqslant 2$

In this section the case of $1<\nu\leqslant 2$ is briefly considered. Notice that at the upper limit we have a special case of the Klein–Gordon equation. Like the Klein–Gordon equation, the initial value of the first derivative must also be specified to obtain a solution. Just as in the previous case, Eq. (14) can be recast to expose a time dependent Hamiltonian. First note an identity for Caputo fractional derivatives and integrals for $1<\nu\leqslant 2$

$$I_t^{\nu-1}\mathrm{D}_t^{\nu}f(t)=\mathrm{D}_t^1 f(t)-\mathrm{D}_t^1 f(t)\big|_{t=0}. \tag{65}$$

Applying $I_t^{\nu-1}$ to Eq. (14) yields

$$\partial_t\psi=-\frac{\beta}{i^{\nu}}\partial_x^2(I_t^{1-\nu}\psi)+\frac{\alpha}{i^{\nu}}(I_t^{1-\nu}\psi)+\partial_t\psi(t)\big|_{t=0}. \tag{66}$$

This is very similar to Eq. (15) except that the fractional derivatives are replaced with fractional integrals and the initial value term is for the first derivative.

The solution can also be written down for a free particle just like the previous case

$$\begin{aligned}(iT_p)^{\nu}\mathrm{D}_t^{\nu}\psi&=-\frac{L_p^2}{2N_m}\partial_x^2\psi,\\ \psi(x,0)&=\psi_0,\\ \frac{\mathrm{d}}{\mathrm{d}t}\psi(x,t)\bigg|_{t=0}&=\psi_1.\end{aligned} \tag{67}$$

Denote the Fourier transform (on the spatial coordinate) of the wave function and the initial conditions as

$$\begin{aligned}\Psi(\lambda,t)&=\mathcal{F}(\psi(x,t)),\\ \Psi_0&=\mathcal{F}(\psi_0),\\ \Psi_1&=\mathcal{F}(\psi_1).\end{aligned} \tag{68}$$

The solution, in Fourier space, can then be expressed as

$$\Psi=\Psi_0\left(\frac{e^{i\omega^{1/\nu}t}}{\nu}+F_\nu(\omega(-i)^\nu,t)\right)+\Psi_1\left(\frac{e^{i\omega^{1/\nu}t}}{\omega^{1/\nu}\nu}-F_{\nu-1}(\omega(-i)^\nu,t)\right), \tag{69}$$

where, $\omega=(L_p\lambda)^2/2N_mT_p^\nu$. This solution behaves just like the case of $0<\nu\leqslant 1$ in that there is an oscillatory term and a decay term. The presence of a decay term will again cause probability to increase over time.

VII. CONCLUSION

In this paper the time fractional Schrödinger equation was constructed. It was found to be equivalent to the usual Schrödinger equation but with a Hamiltonian that was time dependent and nonlocal in time. In contrast to the space fractional Schrödinger equation, probability was not conserved but found to increase over time to a limiting value depending on the order of the time derivative. Consequently, the energy of the eigenstates for the potential well were also found to increase over time to a limiting value (for $0<\nu<1$). In the limit that $t\to\infty$ the energy of the eigenstates was found to be similar to that given by the usual Schrödinger equation but divided by the order of the time derivative squared and having an exponent depending on the order of the time derivative. Initially the energy of the eigenstates is the same as for the nonfractional Schrödinger equation. As time progresses the energy of each level increases as does the spacing between the energy levels. Hence, if the spectrum of emitted radiation was monitored over time, for such a fractional well, it would be seen to blue shift and, the space between the spectral lines would also increase. In finding a solution to the time fractional Schrödinger equation a new identity for the Mittag–Leffler function was found. This identity generalizes the Euler identity for the exponential function with complex arguments.

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APPENDIX A: CAPUTO FRACTIONAL CALCULUS

The bulk of this appendix is taken from Ref. 14. The two most commonly used definitions of fractional derivatives are the Riemann–Liouville and Caputo (there are many definitions, the reader is encouraged to consult Ref. 15 for a more complete discussion). Each definition uses Riemann–Liouville fractional integration and derivatives of whole order. The difference between the two definitions is in the order of evaluation. Riemann–Liouville fractional integration of order μ is defined as

$$\mathrm{I}^\mu(f(t))=\frac{1}{\Gamma(\mu)}\int_0^t\frac{f(\tau)\mathrm{d}\tau}{(t-\tau)^{1-\mu}}. \tag{A1}$$

The next two equations define Riemann–Liouville (RL) and Caputo fractional derivatives of order ν, respectively,

$${}^{\mathrm{RL}}\mathrm{D}_t^\nu f(t)=\frac{\mathrm{d}^k}{\mathrm{d}t^k}(\mathrm{I}^{k-\nu}f(t)), \tag{A2}$$

$${}^{C}\mathrm{D}_t^\nu f(t)=\mathrm{I}^{k-\nu}\left(\frac{\mathrm{d}^k}{\mathrm{d}t^k}f(t)\right), \tag{A3}$$

where $k-1 \leqslant \nu < k$. For now, the Caputo fractional derivative will be denoted by ${}^{C}\mathrm{D}_t^{\nu}$ to maintain a clear distinction with the Riemann–Liouville fractional derivative. The Caputo fractional derivative first computes an ordinary derivative followed by a fractional integral to achieve the desired order of fractional derivative. The Riemann–Liouville fractional derivative is computed in the reverse order.

The desire to formulate initial value problems for physical systems leads to the use of Caputo fractional derivatives rather than Riemann–Liouville fractional derivatives. Consider the Laplace transform of the Riemann–Liouville fractional derivative,

$$\mathcal{L}_t\{{}^{\mathrm{RL}}\mathrm{D}_t^{\nu} f(t)\} = s^{\nu} F(s) - \sum_{k=0}^{n-1} s^k ({}^{\mathrm{RL}}\mathrm{D}_t^{\nu-k-1} f(t))\big|_{t=0}. \tag{A4}$$

The initial conditions, $({}^{\mathrm{RL}}\mathrm{D}_t^{\nu-k-1} f(t))\big|_{t=0}$ for $k=0,\ldots,n-1$, are fractional order derivatives (see Ref. 15 for a detailed discussion of these objects). When studying a physical system, initial conditions are typically conditions that can be measured or imposed on the system. As yet there is no physical interpretation for $({}^{\mathrm{RL}}\mathrm{D}_t^{\nu-k-1} f(t))\big|_{t=0}$ (see Refs. 16 and 17 for a fractal interpretation of the fractional order integral). Some authors using equations with Riemann–Liouville fractional derivatives to model physical systems have added terms to the diffusion equation to eliminate these unphysical terms (see, e.g., Ref. 18).

The Laplace transform of the Caputo fractional derivative is

$$\mathcal{L}_t\{{}^{C}\mathrm{D}_t^{\nu} f(t)\} = s^{\nu} \mathrm{F}(s) - \sum_{k=0}^{n-1} s^{\nu-k-1} (\mathrm{D}_t^k f(t))\big|_{t=0}. \tag{A5}$$

In this case the initial conditions are well understood from a physical point of view. For example if $f(t)$ represents position then $(\mathrm{D}_t^0 f(t))\big|_{t=0}$ is the initial position, $(\mathrm{D}_t^1 f(t))\big|_{t=0}$ is the initial velocity, etc. (see Podlubny Ref. 15, Sec. 2.4 for a more detailed discussion of this point).

APPENDIX B: THE MITTAG–LEFFLER FUNCTION

The Mittag–Leffler function, $E_{\nu}(t)$, is a generalization of the exponential function (see Refs. 15 and 19 for additional properties and a history)

$$e^t = \sum_{n=0}^{\infty} \frac{t^n}{n!} = \sum_{n=0}^{\infty} \frac{t^n}{\Gamma(n+1)}, \tag{B1}$$

$$E_{\nu}(t) = \sum_{n=0}^{\infty} \frac{t^n}{\Gamma(\nu n+1)}. \tag{B2}$$

One very useful formula concerning the exponential function is with a complex argument, the Euler identity

$$e^{it} = \cos(t) + i \sin(t). \tag{B3}$$

A similar identity occurs for the Mittag–Leffler function. The derivation is given below. Consider the initial value fractional differential equation

$$\begin{aligned} {}_0\mathrm{D}_t^{\nu} A &= \sigma A, \\ A(t=0) &= A_0. \end{aligned} \tag{B4}$$

The solution of this can be found by Laplace transform in two different ways

$$s^{\nu} \tilde{A} - s^{\nu-1} A_0 = \sigma \tilde{A}, \tag{B5}$$

$$\tilde{A}=\frac{s^{\nu-1}A_0}{s^{\nu}-\sigma}. \tag{B6}$$

Equation (B6) can be expressed as a power series

$$\tilde{A}=A_0\sum_{n=0}^{\infty}\frac{\sigma^n}{s^{1+\nu n}}. \tag{B7}$$

Inverting this series yields a series representation for the Mittag–Leffler function

$$A=A_0\sum_{n=0}^{\infty}\frac{\sigma^n t^{\nu n}}{\Gamma(\nu n+1)}=A_0E_{\nu}(\sigma t^{\nu}). \tag{B8}$$

The solution to

$$\begin{aligned} {}_0\mathrm{D}_t^{\nu}A&=\sigma i^{\nu}A,\\ A(t=0)&=A_0, \end{aligned} \tag{B9}$$

is then given by

$$A=A_0E_{\nu}(\sigma i^{\nu}t^{\nu}). \tag{B10}$$

To see how this breaks up into an oscillatory piece and a decay piece consider the Laplace transform of Eq. (B9)

$$\tilde{A}=\frac{s^{\nu-1}A_0}{s^{\nu}-\sigma i^{\nu}}. \tag{B11}$$

The inverse Laplace transform is given by

$$A(t)=\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{e^{st}s^{\nu-1}A_0}{s^{\nu}-\sigma i^{\nu}}\mathrm{d}s. \tag{B12}$$

The inverse Laplace transform can be evaluated using residues. This integral has a branch point at $s=0$ due to $s^{\nu-1}$ in the numerator and s^{μ} in the denominator, and a pole at $s_0=\sigma^{1/\nu}i$. Due to the branch point at the origin the usual Bromwich contour cannot be used. A branch cut along the negative Real(s) axis must be made. That is, a cut from $-\infty$ into and then around the origin in a clockwise sense and then back out to $-\infty$. The usual Bromwich contour is continued after the cut. This is referred to as a Hankel contour. The solution will then be given by the residue minus the contribution along the partial path

$$A(t)=\text{Residue}-\frac{A_0}{2\pi i}\int_{\text{Hankel}}. \tag{B13}$$

The residue is given by

$$\frac{\text{Residue}}{A_0}=\lim_{s\to s_0}\frac{(s-s_0)e^{st}s^{\nu-1}}{s^{\nu}-s_0^{\nu}}=\frac{e^{i\sigma^{1/\nu}t}}{\nu}. \tag{B14}$$

The integral along the Hankel contour only makes contributions along the branch cut. This contribution is given by

$$-\frac{A_0\sigma i^{\nu}}{\pi}\int_0^{\infty}\frac{\sin(\nu\pi)e^{-rt}r^{\nu-1}dr}{r^{2\nu}-2\sigma i^{\nu}\cos(\nu\pi)r^{\nu}+(\sigma i^{\nu})^2}. \tag{B15}$$

Combining the path and residue contributions, and doing some algebra gives

$$\frac{A}{A_0}=\frac{e^{i\sigma^{1/\nu}t}}{\nu}-\frac{\sigma i^{\nu}\sin(\nu\pi)}{\pi}\int_0^{\infty}\frac{e^{-rt}r^{\nu-1}dr}{r^{2\nu}-2\sigma i^{\nu}\cos(\nu\pi)r^{\nu}+(\sigma i^{\nu})^2}. \tag{B16}$$

The first term is oscillatory, and the second decays monotonically in the time variable. Hence, the Mittage–Leffler function, with a complex argument, can be expressed as

$$E_{\nu}(\sigma i^{\nu}t^{\nu})=\frac{e^{i\sigma^{1/\nu}t}}{\nu}-\frac{\sigma i^{\nu}\sin(\nu\pi)}{\pi}\int_0^{\infty}\frac{e^{-rt}r^{\nu-1}dr}{r^{2\nu}-2\sigma i^{\nu}\cos(\nu\pi)r^{\nu}+(\sigma i^{\nu})^2}. \tag{B17}$$

Note that as $\nu\rightarrow 1$ the above equation becomes the Euler identity.

To make this result appear more compact define a new function

$$F_{\nu}(\rho,t)=\frac{\rho\sin(\nu\pi)}{\pi}\int_0^{\infty}\frac{e^{-rt}r^{\nu-1}dr}{r^{2\nu}-2\rho\cos(\nu\pi)r^{\nu}+\rho^2}. \tag{B18}$$

This function decays monotonically in time. The following results are special cases:

$$F_{\nu}(0,t)=0, \tag{B19}$$

$$F_1(\rho,t)=0, \tag{B20}$$

$$F_{\nu}(\rho,0)=\frac{1-\nu}{\nu}, \tag{B21}$$

$$0\leqslant F_{\nu}(\rho,t)\leqslant\frac{1-\nu}{\nu}. \tag{B22}$$

Hence, a solution to ${}_0\mathrm{D}_t^{\nu}A=\sigma i^{\nu}A$, $A(t=0)=A_0$ can be written as

$$\frac{A}{A_0}=\frac{e^{i\sigma^{1/\nu}t}}{\nu}-F_{\nu}(\sigma i^{\nu},t). \tag{B23}$$

Additionally, the solution to ${}_0\mathrm{D}_t^{\nu}A=\sigma(-i)^{\nu}A$, $A(t=0)=A_0$ is given by

$$\frac{A}{A_0}=\frac{e^{-i\sigma^{1/\nu}t}}{\nu}-F_{\nu}\left(\frac{\sigma}{i^{\nu}},t\right). \tag{B24}$$

To recap, the ''Euler identity'' for the Mittag–Leffler function is

$$E_{\nu}(\sigma i^{\nu}t^{\nu})=\frac{e^{i\sigma^{1/\nu}t}}{\nu}-F_{\nu}(\sigma i^{\nu},t). \tag{B25}$$

In a similar fashion, a solution can be worked out for $1<\nu<2$

$${}_0\mathrm{D}_t^{\nu}A=\sigma i^{\nu}A,$$

$$A(t=0)=A_0, \tag{B26}$$

$$
{}_0\mathrm{D}_t^1 A(t=0)=A_1,
$$

$$
A=A_0\left(\frac{e^{i\sigma^{1/\nu}t}}{\nu}+F_\nu(\sigma i^\nu,t)\right)+A_1\left(\frac{e^{i\sigma^{1/\nu}t}}{\sigma^{1/\nu}\nu}-F_{\nu-1}(\sigma i^\nu,t)\right). \tag{B27}
$$

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The Lerch function and the thermodynamical functions of the ideal quantum gases

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The unified description of the main thermodynamical functions of the Bose and Fermi ideal gases, obtained by Lee [J. Math. Phys. **36**, 1217 (1995)] in terms of the polylogarithmic functions, can also be obtained by analytic continuation in the chemical potential owing to the analytic properties of the Lerch function that is simply related to the polylogarithmic ones. By this procedure we also show that the Fourier coefficients of the thermal Green function of the ideal Bose gas convert into those of the Fermi one. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The ideal quantum gases of Fermi and Bose[1] are two basic issues of modern physics. They yield a first rough description of the behavior of condensed matter as well as the hints for understanding superfluidity and superconductivity phenomena, the knowledge of which is actively progressing.[2,3] Even though the subject of ideal quantum gases is very old, some new interesting results were obtained in the past decade. These results point to a sort of unified description of the two systems. In fact, Lee[4] showed that the particle number density (PND) $\rho = N/V$, the pressure P, the internal energy U and the entropy S of the two ideal quantum gases can be expressed in terms of the so-called polylogarithm function[5] $\mathrm{Li}_s(z)$ [for its definition, see Eq. (17)], as follows:

$$\frac{(\lambda^D)\rho}{g} = \mathrm{sign}(\zeta)\mathrm{Li}_{D/2}(\zeta), \tag{1}$$

$$\beta P/\rho = \mathrm{Li}_{D/2+1}(\zeta)/\mathrm{Li}_{D/2}(\zeta), \tag{2}$$

$$\beta U/N = (D/2)\mathrm{Li}_{D/2+1}(\zeta)/\mathrm{Li}_{D/2}(\zeta), \tag{3}$$

$$S/Nk_{\mathrm{B}} = (D/2+1)\mathrm{Li}_{D/2+1}(\zeta)/\mathrm{Li}_{D/2}(\zeta) - \ln|\zeta|. \tag{4}$$

Here D denotes the space dimensions, $\lambda = (2\pi\beta/m)^{1/2}$ (with $\hbar = 1$) is the thermal wave-length, $\beta \equiv 1/k_{\mathrm{B}}T$ and $g = (2s+1)$, while k_{B}, T, m and s denote the Boltzman constant, the temperature, the mass and the spin of the particles, respectively. Finally, ζ is equal to z or to $-z$ depending on whether the system is respectively made up of bosons or of fermions, the fugacity z being related to the chemical potential μ of the two systems as $z \equiv e^{\beta\mu}$. The noticeable property of Eqs. (1)–(4) is that the thermodynamical quantities, scaled as reported on the left hand side (lhs) of (1)–(4), only depend on the fugacity of the system and, more importantly, that their values are given by the same analytic functions, respectively evaluated in the ranges $-\infty < \zeta \leqslant 0$ and $0 \leqslant \zeta < 1$ in the cases of the Fermi and Bose gas. A further interesting consequence of (1)–(4), valid in only the two-dimensional case, is the property that the entropy and, consequently, the specific heat at constant

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volume of the Bose gas, when expressed in terms of ρ and T, coincide with those of the fermion gas.[6–9] As recently shown by Anghel,[10] these properties generalize to 2-D systems obeying fractional exclusion statistics[11] related to the bosonization technique.[12]

The aim of this note is to present an alternative derivation of results (1)–(4) based on the mathematical trick of considering the chemical potential as a complex variable. The plan of the paper is as follows. In Sec. II we show that the product of grand-partition functions of the Bose and Fermi gases, respectively evaluated at $-z$ and z, is equal to one and that the analytic continuation of the grand-potential Ω_B of the Bose gas, with respect to the chemical potential, yields the grand-potential Ω_F of the Fermi gas with the reversed sign. This conclusion is made possible by the fact that the grand-potentials are expressed in terms of the Lerch function[13] that simply reduces to the polylogarithmic function for the samples under analysis. In Sec. III, we show that the same analytic continuation converts the Fourier coefficients of the thermal Green function of the Bose gas into those of the Fermi gas. By this result we show that the same property of analytic continuation, found for the grand-potentials, applies to the internal energy and the mean particle number. Finally, in Sec. IV we report our conclusive remarks.

II. ANALYTIC CONTINUATION OF THE GRAND-POTENTIAL

Throughout the paper we shall adopt the mathematical notation of Ref. 1. The grand-Hamiltonian of a quantum system of noninteracting particles of mass m and spin s is

$$\hat{K}=\hat{H}-\mu\hat{N}, \tag{5}$$

with

$$\hat{H}=\sum_{k,\sigma}\epsilon_k a^{\dagger}_{k,\sigma}a_{k,\sigma}, \quad \hat{N}=\sum_{k,\sigma}a^{\dagger}_{k,\sigma}a_{k,\sigma}$$

and the operator algebras

$$[a_{k,\sigma},a_{k',\sigma'}]_{\pm}=0, \quad [a_{k,\sigma},a^{\dagger}_{k',\sigma'}]_{\pm}=\delta_{k,k'}\delta_{\sigma,\sigma'}, \tag{6}$$

where $\epsilon_k=k^2/2m$ and σ denotes the spin index ranging from $-s$ to s. The case of fermions or bosons corresponds to taking the anticommutator or the commutator in (6). In contrast to standard definition, we assume now that μ can also take complex values in which the physical (or observable) chemical potential is recovered when μ is real. By so doing, $\hat{K}$ is no longer Hermitian, but we can still define the complex valued grand-canonical partition function $\mathcal{Z}_B$ and the complex valued grand-potential Ω_B of the ideal Bose gas by the relations

$$\mathcal{Z}_B(V,T,\mu)\equiv e^{-\beta\Omega_B(V,T,\mu)}\equiv \mathrm{Tr}[e^{-\beta\hat{K}}] \tag{7}$$

that coincide with the physical ones when μ is real. The explicit evaluation of the trace yields

$$\mathcal{Z}_B(V,T,\mu)=\prod_{j=0}^{\infty}\sum_{n=0}^{\infty}e^{-n\beta(\epsilon_j-\mu)},$$

where j labels the couple of indices $(\mathbf{k},\sigma)$. The series can be explicitly summed up under the condition that

$$\Re\mu<\min(\epsilon_0,\ldots,\epsilon_\infty)=\epsilon_0=0. \tag{8}$$

In this way, one gets

$$\mathcal{Z}_{\mathrm{B}}(V,T,\mu)=\tilde{\mathcal{Z}}_{\mathrm{B}}(V,T,z)\equiv\prod_{j=0}^{\infty}\frac{1}{1-ze^{-\beta\epsilon_j}}. \tag{9}$$

Equation (9) makes it evident that $\mathcal{Z}_{\mathrm{B}}(V,T,\mu)$ depends on μ through the fugacity. It will become clear later that $\tilde{\mathcal{Z}}_{\mathrm{B}}(V,T,z)$ is analytic throughout the complex z plane cut along the real half-axis from $z=1$ to $z=\infty$ [see (14)]. In the fermion case one finds that

$$\mathcal{Z}_{\mathrm{F}}(V,T,\mu)\equiv e^{-\beta\Omega_{\mathrm{F}}(V,T,\mu)}=\mathrm{Tr}[e^{-\beta\hat{K}}]=\tilde{\mathcal{Z}}_{\mathrm{F}}(V,T,z)\equiv\prod_{j=0}^{\infty}[1+ze^{-\beta\epsilon_j}] \tag{10}$$

with μ obeying the constraints $-\infty<\Re\mu<\infty$. Taking now $\mu=\mu'+i\pi/\beta$ in Eq. (9) [with $\mu'<0$ as required by (8)] and setting $z'=e^{\beta\mu'}$, one gets

$$\mathcal{Z}_{\mathrm{B}}(V,T,\mu'+i\pi/\beta)=\tilde{\mathcal{Z}}_{\mathrm{B}}(V,T,-z')=\prod_{j=0}^{\infty}\frac{1}{1+e^{\beta(\mu'-\epsilon_j)}}=\frac{1}{\mathcal{Z}_{\mathrm{F}}(V,T,\mu')}=\frac{1}{\tilde{\mathcal{Z}}_{\mathrm{F}}(V,T,z')}.$$

From this relation it follows that

$$\tilde{\mathcal{Z}}_{\mathrm{B}}(V,T,-z')\tilde{\mathcal{Z}}_{\mathrm{F}}(T,V,z')=1 \quad \text{if } 0\leqslant z'<1, \tag{11}$$

a relation already reported in Ref. 14 [see their Eq. (27)] and Ref. 15 [see their Eq. (23), where a minus sign is missed in the argument of one of the two functions]. Equation (11) shows that the grand-partition function of the Bose gas is functionally dependent on that of the Fermi gas and vice versa. Taking the logarithm of Eq. (9) and performing the sum over the spin states one finds

$$-\beta\Omega_{\mathrm{B}}(V,T,\mu)=-g\sum_{\mathbf{k}}\ln(1-ze^{-\beta\epsilon_{\mathbf{k}}}),$$

where $g=2s+1$. In the continuum limit one uses the property

$$\sum_{\mathbf{k}}\rightarrow\frac{V}{(2\pi)^D}\int k^{D-1}dkd\omega^D,$$

where $V=L^D$ is the box volume, $d\omega^D$ is the infinitesimal "surface" element of the unit radius hypersphere of R^D and k is the modulus of $\mathbf{k}$. The resulting integrand only depends on the modulus of $\mathbf{k}$ and the angular integration yields the area of the unit hypersphere, equal to[16] $2\pi^{D/2}/\Gamma(D/2)$. After converting to the new integration variable $x=\beta k^2/2m$ one gets

$$\frac{\lambda^D\beta\Omega_{\mathrm{B}}(V,T,\mu)}{gV}=\frac{1}{\Gamma(D/2)}\int_0^{\infty}x^{D/2-1}\ln(1-ze^{-x})dx. \tag{12}$$

We recall now the definition of the Lerch function $\Phi(z,s,v)$:[13]

$$\Phi(z,s,v)\equiv\sum_{n=0}^{\infty}\frac{z^n}{(v+n)^s}=\frac{1}{\Gamma(s)}\int_0^{\infty}\frac{x^{s-1}e^{-vx}}{1-ze^{-x}}dx, \quad |z|<1, \quad v=0,-1,..., \tag{13}$$

where the integral expression applies if $\Re v>0$ and either $|z|\leqslant 1$, $z\neq 1$, $\Re s>0$ or with $z=1$, $\Re s>1$. By this integral expression, Eq. (12) can be written as

$$\frac{\lambda^D\beta\Omega_{\mathrm{B}}(V,T,\mu)}{gV}=-\frac{1}{\Gamma(D/2)}\int_0^{\infty}dx\int_0^{z}\frac{x^{D/2-1}e^{-x}}{1-te^{-x}}dt=-\int_0^{z}\Phi(t,D/2,1)dt.$$

Assuming that $|z|<1$, we can use the reported power expansion of the Lerch function to evaluate the last integral. We find that

$$\frac{\lambda^D \beta \tilde{\Omega}_B(V,T,z)}{gV} = -z\Phi(z,D/2+1,1),$$

where $\tilde{\Omega}_B(V,T,z) \equiv \Omega_B(V,T,\mu)$. In the continuum limit the evaluation of the grand-potential of the fermion gas can be performed by the same procedure applied to Eq. (10). One finds that

$$-\frac{\lambda^D \beta \Omega_F(V,T,\mu)}{gV} = \frac{1}{\Gamma(D/2)} \int_0^\infty x^{D/2-1} \ln(1+ze^{-x})dx = \frac{1}{\Gamma(D/2)} \int_0^\infty dx \int_0^z \frac{x^{D/2-1}e^{-x}}{1+te^{-x}} dt$$

$$= \int_0^z \Phi(-t,D/2,1)dt$$

$$= z\Phi(-z,D/2+1,1).$$

Collecting the last results we obtain

$$\Omega_B(V,T,\mu) = \tilde{\Omega}_B(V,T,z) = -\left[\frac{gV}{\lambda^D \beta}\right] z\Phi(z,D/2+1,1), \tag{14}$$

$$\Omega_F(V,T,\mu) = \tilde{\Omega}_F(V,T,z) = -\left[\frac{gV}{\lambda^D \beta}\right] z\Phi(-z,D/2+1,1). \tag{15}$$

These relations deserve some comments. They show that the grand-potentials of the Bose and Fermi ideal gases depend on the chemical potential via the fugacity z and that their dependence on z is determined by a single function, i.e., the Lerch function $\Phi(z,s,v)$ with $v=1$ and $s=(D/2+1)$. The further dependence on V, m and the spin s (not to be confused with parameter s present in the Lerch and in the polylogarithmic functions) is fully specified by the factor within square brackets, while the dependence on T is partly determined by the aforesaid factor and partly contained in the fugacity definition. It is recalled now that the Lerch function is analytic throughout the z-plane cut along the real half-axis from $z=1$ to $z=\infty$ as it appears evident from the integral expression reported in (13) (see, also, Sec. 1.11 of Ref. 13). This property implies that $\Omega_B(V,T,\mu)$ is an analytic function of $\mu=\mu'+i\mu''$ within the strip delimited by $\mu''=0^+$ and $\mu''=2\pi/\beta$. Thus, setting $\mu=\mu'+i\pi/\beta$ with $-\infty<\mu'<\infty$ in (14) so as to have $0<\arg(1-z)<2\pi$, we find that

$$\Omega_B(V,T,\mu'+i\pi/\beta) = \tilde{\Omega}_B(V,T,-z') = \left[\frac{gV}{\lambda^D \beta}\right] z'\Phi(-z',D/2+1,1)$$

$$= -\tilde{\Omega}_F(V,T,z') = -\Omega_F(V,T,\mu'). \tag{16}$$

The knowledge of the quantity on the lhs of this relation is made possible by the analytic continuation, ensured by (14), of $\Omega_B(V,T,\mu)$ with respect to μ. At the same time, (16) shows that this analytic continuation yields the grand-potential (with the reversed sign) of the corresponding Fermi gas with chemical potential μ'. Thus, $\Omega_B(V,T,\mu)$ and $-\Omega_F(V,T,\mu)$ are the boundary values of the function $\Omega(V,T,w)=[gV/\lambda^D\beta]e^{\beta w}\Phi(e^{\beta w},D/2+1,1)$, analytic in the complex variable w, as $w\to\mu+i0$ with $\mu<0$ and as $w\to\mu+i\pi/\beta$ with $-\infty<\mu<\infty$, respectively. It should be noted that this property holds only true for $-\Omega_F(V,T,\mu)$ and that it does not apply to $\Omega_F(V,T,\mu)$. This property reflects the fact that the Bose and the Fermi ideal gases are physically different so that the grand-potential of the second cannot be obtained by a simple analytical continuation of the first,[17] but we must also add, so to say "by hand," a further change of sign. Before proceeding to evaluate further thermodynamical functions we add now two remarks. First,

it is simple to verify that results (14) and (15) make (11) fulfilled. Second, Eqs. (14) and (15) can be written in terms of the polylogarithm functions. These being defined as[5]

$$\mathrm{Li}_s(z) \equiv \sum_{n=0}^{\infty} \frac{z^{n+1}}{(n+1)^s}, \quad |z|<1, \tag{17}$$

it is evident that

$$\mathrm{Li}_s(z) = F(z,s) \equiv z\Phi(z,s,1), \tag{18}$$

where $F(z,s)$ is the notation adopted by Erdeley[13] (Sec. 1.11). Thus, Eqs. (14) and (15) also read

$$\frac{\lambda^D \beta \tilde{\Omega}_{\mathrm{B}}(V,T,z)}{gV} = -\mathrm{Li}_{D/2+1}(z), \tag{19}$$

$$\frac{\lambda^D \beta \tilde{\Omega}_{\mathrm{F}}(V,T,z)}{gV} = \mathrm{Li}_{D/2+1}(-z). \tag{20}$$

The entropies $S_{\mathrm{B}}(V,T,\mu)$ and $S_{\mathrm{F}}(V,T,\mu)$ of the two gases can easily be calculated by the thermodynamical relation $S=-\partial\Omega(V,T,\mu)/\partial T$, applied to (14) and (15). By the relation

$$\frac{\partial\Phi(z,s,v)}{\partial z} = \frac{1}{z}[\Phi(z,s-1,v) - v\Phi(z,s,v)],$$

one finds

$$S_{\mathrm{B}}(V,T,\mu) = \frac{gVk_{\mathrm{B}}}{\lambda^D}[(D/2+1)z\Phi(z,D/2+1,1) - \mu\beta z\Phi(z,D/2,1)] \tag{21}$$

for $\mu<0$ and

$$S_{\mathrm{F}}(V,T,\mu) = \frac{gVk_{\mathrm{B}}}{\lambda^D}[(D/2+1)z\Phi(-z,D/2+1,1) - \mu\beta z\Phi(-z,D/2,1)] \tag{22}$$

for $-\infty<\mu<\infty$. The mean numbers of bosons and fermions $N_{\mathrm{B}}(V,T,\mu)$ and $N_{\mathrm{F}}(V,T,\mu)$ and the relevant internal energies could be evaluated by the thermodynamical relations $N=-\partial\Omega/\partial\mu$ and $U=\Omega+TS+\mu N$. It looks, however, more interesting to determine these quantities by the thermal Green function $\mathcal{G}_{\alpha,\beta}(x,x')$.

III. ANALYTIC CONTINUATION OF THE THERMAL GREEN FUNCTION

Even in the presence of a complex chemical potential, it is formally possible to define the statistical operator as in Ref. 1, i.e., $\hat{\rho}_G = e^{\beta(\Omega-\hat{K})}$. In terms of the Schrödinger field operators $\hat{\psi}_\alpha(\mathbf{x},0)$ and $\hat{\psi}^\dagger_\alpha(\mathbf{x},0)$ the modified Heisenberg operators assume the form

$$\hat{\psi}_\alpha(\mathbf{x}\tau) = e^{\hat{K}\tau}\hat{\psi}_\alpha(\mathbf{x},0)e^{-\hat{K}\tau},$$

$$\hat{\psi}^\dagger_\alpha(\mathbf{x}\tau) = e^{\hat{K}\tau}\hat{\psi}^\dagger_\alpha(\mathbf{x},0)e^{-\hat{K}\tau}.$$

They clearly depend on μ (though this dependence is not explicitly reported) because $\hat{K}$ depends on μ [see Eq. (5)]. After denoting the set of variables $(\mathbf{x},\tau)$ by x, the thermal Green function is defined as

$$\mathcal{G}_{\alpha,\beta}(x,x')=-\mathrm{Tr}\{\hat{\rho}_G \mathrm{T}_\tau(\hat{\psi}_\alpha(x)\hat{\psi}^\dagger_\beta(x'))\}, \tag{23}$$

where the meaning of T_τ is reported in Sec. 23 of Ref. 1. One of the most important properties of the thermal Green function is the fact that its knowledge determines the mean value of any single particle operator $\hat{J}=\int \psi^\dagger_\alpha(\mathbf{x})J_{\alpha,\beta}(\mathbf{x})\psi_\beta(\mathbf{x})d^Dx$ through the relation

$$\langle\hat{J}\rangle=\mathrm{Tr}(\hat{\rho}_G\hat{J})=\pm\int \lim_{\mathbf{x}'\to\mathbf{x}} \lim_{\tau'\to\tau^+} (J_{\beta,\alpha}(\mathbf{x})\mathcal{G}_{\alpha,\beta}(\mathbf{x}\tau,\mathbf{x}'\tau'))d^Dx,$$

where the $+$ sign applies to fermions and the $-$ sign to bosons. It is straightforward to verify that, even in presence of a complex μ, the thermal Green function obeys the periodicity or the antiperiodicity condition for bosons and fermions, respectively. Therefore, by the same analysis reported in Ref. 1, one finds that the Fourier coefficients of the thermal Green function are

$$\mathcal{G}^0{}_{B,\alpha,\beta}(\mathbf{k},\omega_n,\mu)=\begin{cases}\dfrac{\delta_{\alpha,\beta}}{i\omega_n-(\epsilon^0{}_{\mathbf{k}}-\mu)} & \text{with even } n\\ 0 & \text{with odd } n,\end{cases} \tag{24}$$

for the ideal Bose gas and

$$\mathcal{G}^0{}_{F,\alpha,\beta}(\mathbf{k},\omega_n,\mu)=\begin{cases}\dfrac{\delta_{\alpha,\beta}}{i\omega_n-(\epsilon^0{}_{\mathbf{k}}-\mu)} & \text{with odd } n\\ 0 & \text{with even } n,\end{cases} \tag{25}$$

for the fermion one. In both equations, we have $\omega_n=n\pi/\beta$. Setting now $\mu=\mu'+i\pi/\beta$ in the denominator of (24), we find that

$$i\omega_n-(\epsilon^0{}_{\mathbf{k}}-\mu'-i\pi/\beta)=i(\omega_n+\pi/\beta)-(\epsilon^0{}_{\mathbf{k}}-\mu')=i\omega_{n+1}-(\epsilon^0{}_{\mathbf{k}}-\mu').$$

Thus, we find the interesting property that the Fourier coefficients of the bosonic thermal Green function, evaluated at $\mu=\mu'+i\pi/\beta$, convert into those of the fermionic Green function evaluated at $\mu=\mu'$, namely

$$\mathcal{G}^0{}_{B,\alpha,\beta}(\mathbf{k},\omega_n,\mu'+i\pi/\beta)=\mathcal{G}^0{}_{F,\alpha,\beta}(\mathbf{k},\omega_{n+1},\mu') \quad \forall n\in\mathcal{Z}. \tag{26}$$

We can now use Eqs. (26.6) and (26.7) of Ref. 1, adapted to the case of the free gases contained in a D-dimensional box, in order to evaluate the mean number of particle and the internal energy of the two ideal quantum gases. In the boson case, we find

$$N_{\mathrm{B}}(V,T,\mu)=-\frac{V_g}{\beta(2\pi)^D}\int d^Dk \sum_{n\ \mathrm{even}} \frac{e^{i\omega_n\eta}}{i\omega_n-(\epsilon^0{}_{\mathbf{k}}-\mu)},$$

which, by the identity (25.38) of Ref. 1, becomes

$$N_{\mathrm{B}}(V,T,\mu)=\frac{Vg}{(2\pi)^D}\int \frac{1}{e^{\beta(\epsilon^0{}_{\mathbf{k}}-\mu)}-1}d^Dk. \tag{27}$$

Setting $\mu=\mu'+i\pi/\beta$ in (27) and using (26) we obtain

$$N_{\mathrm{B}}(V,T,\mu'+i\pi/\beta)=-\frac{Vg}{\beta(2\pi)^D}\int d^Dk \sum_{n\ \mathrm{odd}} \frac{e^{i\omega_n\eta}}{i\omega_n-(\epsilon^0{}_{\mathbf{k}}-\mu')}$$

that, by identity (25.38) of Ref. 1, yields

$$N_{\mathrm{B}}(V,T,\mu'+i\pi/\beta)=-\frac{Vg}{(2\pi)^D}\int\frac{1}{e^{\beta(\epsilon^0_{\mathbf{k}}-\mu')}+1}d^Dk=-N_{\mathrm{F}}(V,T,\mu'). \tag{28}$$

In a similar way, we find that the internal energy of the Bose gas is [see Eq. (26.7) of Ref. 1]

$$\begin{aligned}U_{\mathrm{B}}(V,T,\mu)&=-\frac{Vg}{\beta(2\pi)^D}\int d^Dk\sum_{n\ \mathrm{even}}\frac{e^{i\omega_n\eta}}{2}\left[1+\frac{2\epsilon^0_{\mathbf{k}}}{i\omega_n-(\epsilon^0_{\mathbf{k}}-\mu)}\right]\\&=\frac{Vg}{(2\pi)^D}\int\frac{\epsilon^0_{\mathbf{k}}}{e^{\beta(\epsilon^0_{\mathbf{k}}-\mu)}-1}d^Dk,\end{aligned} \tag{29}$$

and that

$$\begin{aligned}U_{\mathrm{B}}(V,T,\mu'+i\pi/\beta)&=-\frac{Vg}{\beta(2\pi)^D}\int d^Dk\sum_{n\ \mathrm{odd}}\frac{e^{i\omega_n\eta}}{2}\left[1+\frac{2\epsilon^0_{\mathbf{k}}}{i\omega_n-(\epsilon^0_{\mathbf{k}}-\mu')}\right]\\&=-\frac{Vg}{(2\pi)^D}\int\frac{\epsilon^0_{\mathbf{k}}}{e^{\beta(\epsilon^0_{\mathbf{k}}-\mu')}+1}d^Dk=-U_{\mathrm{F}}(V,T,\mu').\end{aligned} \tag{30}$$

The integrals appearing in Eqs. (27)–(30) can be expressed in terms of the appropriate Lerch functions by the procedure reported in the previous section. In particular, from (27) it follows that

$$\frac{\lambda^D N_{\mathrm{B}}(V,T,\mu)}{gV}=\frac{\lambda^D\rho_{\mathrm{B}}(T,\mu)}{g}=z\Phi(z,D/2,1), \tag{31}$$

and from (28) that

$$\frac{\lambda^D\rho_{\mathrm{B}}(T,\mu'+i\pi/\beta)}{g}=-z'\Phi(-z',D/2,1)=-\frac{\lambda^D\rho_{\mathrm{F}}(T,\mu')}{g}. \tag{32}$$

Finally, Eqs. (29) and (30) convert into

$$\frac{\beta\lambda^D U_{\mathrm{B}}(V,T,\mu)}{gV}=(D/2)z\Phi(z,D/2+1,1) \tag{33}$$

and

$$\frac{\beta\lambda^D U_{\mathrm{B}}(V,T,\mu'+i\pi/\beta)}{gV}=-(D/2)z'\Phi(-z',D/2+1,1)=-\frac{\beta\lambda^D U_{\mathrm{F}}(V,T,\mu')}{gV}. \tag{34}$$

The comparison of these relations with Eqs. (14) and (15) shows that, as in the case of the classical ideal gas, the grand-potential and the internal energy of the ideal quantum gases are linearly related,[17] i.e.,

$$\Omega_{\mathrm{B}}(V,T,\mu)=-\frac{2U_{\mathrm{B}}(V,T,\mu)}{D}\quad\text{and}\quad\Omega_{\mathrm{F}}(V,T,\mu)=-\frac{2U_{\mathrm{F}}(V,T,\mu)}{D}, \tag{35}$$

which for both gases imply that

$$(1+D/2)PV=TS+\mu N. \tag{36}$$

[In passing, it is also noted that in the two-dimensional case Eqs. (35) and (36) were shown[10] to hold true for any fractional exclusion statistics.] Similarly to Eq. (16), from Eqs. (31) and (32) one concludes that $\lambda^D\rho_B(T,\mu)/g$ and $-\lambda^D\rho_F(T,\mu)/g$ are the boundary values of the analytic function $z\Phi(z,D/2,1)=e^{\beta w}\Phi(e^{\beta w},D/2,1)$ as $w\to\mu+i0$ with $\mu<0$ and $w\to\mu+i\pi/\beta$ with $-\infty<\mu<\infty$. The same property applies to $\beta\lambda^D U_B(V,T,\mu)/gV$ and to $-\beta\lambda^D U_F(V,T,\mu)/gV$ owing to (33) and (34). [The property is also proven by recalling that it is true for the grand-potentials and then using (35).] We now note that Eq. (1) immediately follows from (31) and (32) using (17) and (18). In a similar way, Eq. (2) is obtained by combining the two expressions obtained by dividing the left hand sides of (19) and (20) by $\lambda^D\rho_B/g$ and $\lambda^D\rho_F/g$, respectively. By the same procedure, starting from (33), (34), (21) and (22) one respectively recovers Eqs. (3) and (4). Since the right hand sides of (2) and (3) are analytic in the complex z-plane cut from $z=1$ to $z=\infty$ along the real axis, it follows that $\beta P/\rho$ for the Bose and the Fermi gases are the boundary values of the same analytic function $\mathrm{Li}_{D/2+1}(e^{\beta w})/\mathrm{Li}_{D/2}(e^{\beta w})=\Phi(e^{\beta w},D/2+1,1)/\Phi(e^{\beta w},D/2,1)$ as $w\to\mu'+i0$ with $-\infty<\mu'<0$ and $w\to(\mu'+i\pi/\beta)$ with $-\infty<\mu'<\infty$. In other words, $\beta P/\rho$ of the ideal Bose gas by analytic continuation in the chemical potential converts into $\beta P/\rho$ of the ideal Fermi gas. On the contrary, this property is neither true for the particle density (because the analytic continuation yields the opposite value of the density) nor for the entropy due to presence of the nonanalytic contribution $\log|\zeta|$. For the entropy, it should also be stressed that (21) and (22) only apply with real values of μ. In fact, the analytic continuation of (21) would yield $S_B(V,T,\mu+i\pi/\beta)=-S_F(V,T,\mu)+i\pi([gVk_B/\lambda^D]e^{\beta\mu}\Phi(-e^{\beta\mu},D/2,1)$ that does not coincide with the entropy (with the reversed sign) of the fermion system for the presence of the imaginary term. On the contrary, starting from (14) with $-\infty<\mu<\infty$, one rightly finds that $-(\partial\Omega_B(V,T,\mu+i\pi/\beta))/(\partial T)=-S_F(V,T,\mu)$ because the temperature derivative also acts on the imaginary part of the chemical potential.

A further advantage of having related the thermodynamical functions of the ideal quantum gases to the Lerch function is the possibility of determining analytically their behaviors as μ approaches the limiting points $-\infty$ and 0^- for the Bose gas and $-\infty$ and ∞ for the Fermi gas. This analysis can be found in Refs. 4 and 17 where the particle number fluctuations are also discussed.

IV. CONCLUSIONS

We have shown that the results obtained by Lee[4] can also be recast in the following way: the particle number density $\rho(T,\mu)$, the internal energy $U(V,T,\mu)$ or the grand-potential $\Omega(V,T,\mu)$ of the Bose and Fermi ideal gases confined to a D-dimensional box, aside from the trivial factors reported in Eqs. (31)–(34), (14) and (15), are the boundary values of the analytic functions $F(e^{\beta w},D/2)=e^{\beta w}\Phi(e^{\beta w},D/2,1)$ and $F(e^{\beta w},D/2+1)=e^{\beta w}\Phi(e^{\beta w},D/2+1,1)$, as $w\to\mu+i0$ with $\mu<0$ and $w\to\mu+i\pi/\beta$ with $-\infty<\mu<\infty$. Since the mentioned trivial factors depend on the bosonic or fermionic nature of the particle, the PND of the Fermi gas cannot be considered as the analytic continuation in the chemical potential of the PND of the Bose gas. The same happens for U_B and U_F. On the contrary, the analytic continuation in μ of U_B/N and P_B/ρ_B respectively yield U_F/N and P_F/ρ_F but these two functions do not fully determine the thermodynamics of the two systems since they are not expressed in terms of their natural variables. An interesting result, which to our knowledge does not seem to have been noted before, is the fact that the analytic continuation from μ to $\mu+i\pi/\beta$ of the Fourier coefficients of the bosonic thermal Green function exactly reproduces the Fourier coefficients of the fermionic function. If we recall that the general expression of the Fourier coefficients, in presence of a spin-independent interaction, is

$$\mathcal{G}_{\alpha,\beta}(\mathbf{k},\omega_n,\mu)=\frac{\delta_{\alpha,\beta}}{i\omega_n-(\epsilon^0_{\mathbf{k}}-\mu)-\Sigma^*(\mathbf{k},\omega_n,\mu)},$$

where $\Sigma^*(\mathbf{k},\omega_n,\mu)$ is the proper self-energy contribution, we realize that the aforesaid analytic continuation does not convert the boson proper self-energy into the fermion one. In fact, even though the Feynman graphs are the same and the substitution $\mu\to\mu+i\pi/\beta$ converts the free

boson propagator into the fermion one, this substitution does not reproduce the factor $(-1)^F$ related to possible fermion loops. Hence, the results illustrated in the paper are only valid in the noninteracting case. They look, however, interesting both for extracting the asymptotic behaviors of the thermodynamical functions and for the resulting unified picture of the boson and fermion free gases.

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Balian–Low phenomenon for subspace Gabor frames

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In this work, the Balian–Low theorem is extended to Gabor (also called Weyl–Heisenberg) frames for subspaces and, more particularly, its relationship with the unique Gabor dual property for subspace Gabor frames is pointed out. To achieve this goal, the subspace Gabor frames which have a unique Gabor dual of type I (resp. type II) are defined and characterized in terms of the Zak transform for the rational parameter case. This characterization is then used to prove the Balian–Low theorem for subspace Gabor frames. Along the same line, the same characterization is used to prove a duality theorem for the unique Gabor dual property which is an analogue of the Ron and Shen duality theorem. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1768621]

I. INTRODUCTION

A Gabor system is a collection of functions generated by a window function $g \in L^2(\mathbb{R})$ and by translations and modulations:

$$\mathbf{G}(\alpha,\beta,g) := \{e^{2\pi i m\alpha} g(x-n\beta) : m,n \in \mathbb{Z}\},$$

where α and β are two positive parameters. Gabor systems were first proposed by Gabor (1946) for the purpose of applications in signal processing. To ensure stable reconstruction of signals, the Gabor system needs to be a frame, a concept introduced by Duffin and Schaeffer (1952) as a generalization of Riesz bases. It is well known that the condition $\alpha\beta \leqslant 1$ is both necessary and sufficient for the existence of a window function $g \in L^2(\mathbb{R})$ such that the Gabor system $\mathbf{G}(\alpha,\beta,g)$ forms a frame for $L^2(\mathbb{R})$ (cf. Daubechies, 1990 and Rieffel, 1981). Moreover, if $\alpha\beta = 1$, then every Gabor frame $\mathbf{G}(\alpha,\beta,g)$ for $L^2(\mathbb{R})$ is Riesz basis while $\mathbf{G}(\alpha,\beta,g)$ cannot be a Riesz basis for $L^2(\mathbb{R})$ when $\alpha\beta < 1$. The following is one of the fundamental results for Gabor systems. It shows that if the system $\mathbf{G}(\alpha,\beta,g)$ forms a frame for $L^2(\mathbb{R})$, the generating function g cannot be at the same time well localized in time and frequency.

Theorem 1.1 (Balian–Low Theorem): *Assume that* $\alpha\beta = 1$ *and suppose that* $g \in L^2(\mathbb{R})$ *is such that* $\mathbf{G}(\alpha,\beta,g)$ *is a frame for* $L^2(\mathbb{R})$. *Then,*

$$\left(\int_{\mathbb{R}} |xg(x)|^2 dx \right) \left(\int_{\mathbb{R}} |\omega \hat{g}(\omega)|^2 d\omega \right) = \infty. \tag{1.1}$$

Note that the Fourier transform defined by

$$\hat{g}(\omega) = \int_{\mathbb{R}} g(x) e^{-2\pi i x\omega} dx, \quad g \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}) \tag{1.2}$$

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can be extended to all of $L^2(\mathbb{R})$ by using the isometry of the transform. The Balian–Low theorem (abbr. BLT) was first proved by Balian (1981) and Low (1985) for orthonormal bases with a gap in their proofs. The gap was later corrected and this result was generalized to Riesz bases (cf. Battle, 1988 and Daubechies, 1990). There have been, since then, some interest in generalizing the BLT to more general frameworks. For some recent progress related to different generalizations of the BLT, we refer to Benedetto *et al.* (2003a); Benedetto *et al.* (2003b); Benedetto and Powell (2004); Gröchenig *et al.* (2002), etc. In this paper we are interested in studying the BLT in the context of Gabor frames for subspaces of $L^2(\mathbb{R})$. Subspace Gabor frames have some interesting properties and, also, certain advantages. For example, the restriction $\alpha\beta\leqslant 1$ is no longer needed when working in the setting of subspace Gabor frames. To simplify the notations, we will denote by $\mathcal{M}(\alpha,\beta,g)$ the closed linear subspace generated by the Gabor system $\mathbf{G}(\alpha,\beta,g)$. We refer to Casazza and Christensen (2001); Gabardo and Han (2003a, 2001, 2003b, 2004) for some recent work on this topic. One of our goals in this paper is to prove the following generalization of the BLT:

Theorem 1.2: *Let* $\mathbf{G}(\alpha,\beta,g)$ *be a frame for* $\mathcal{M}(\alpha,\beta,g)$. *Then*

(i) *If* $\alpha\beta=1$, *then* (1.1) *always holds*.

(ii) *If* $\alpha\beta$ *is an integer larger than 1, then* (1.1) *holds whenever* $\mathbf{G}(\alpha,\beta,g)$ *is not a Riesz sequence*.

(iii) *If* $1/\alpha\beta$ *is an integer larger than 1, then* (1.1) *holds whenever the subspace* $\mathcal{M}(\alpha,\beta,g)\neq L^2(\mathbb{R})$.

We remark that the condition that $\mathbf{G}(\alpha,\beta,g)$ is not a Riesz sequence in (ii) and the condition that $\mathcal{M}(\alpha,\beta,g)\neq L^2(\mathbb{R})$ in (iii) cannot be dropped. In fact, let $g(x)=e^{-x^2}$. Then $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence when $\alpha\beta$ is an integer larger than one and $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$ if $1/(\alpha\beta)$ is an integer larger than 1 (see Example 4.8 for details). However, it is clear that

$$\left(\int_{\mathbb{R}}|xg(x)|^2dx\right)\left(\int_{\mathbb{R}}|\omega\hat{g}(\omega)|^2d\omega\right)<\infty. \tag{1.3}$$

For Theorem 1.2, we will, in fact, obtain a more general result which shows that the Balian–Low phenomenon for subspace Gabor frames is, somewhat surprisingly, related to the unique Gabor dual property, a topic that has been investigated in Gabardo and Han (2004). One of our goals, in this paper, is to further investigate the unique Gabor dual property for subspace Gabor frames. In particular, we will give a concrete characterization for those subspace Gabor frames which have the unique Gabor dual property and we will use this result to prove Theorem 1.2. This paper is organized as follows: In Sec. II, we introduce the unique Gabor dual property and discuss the main results. Since the techniques to deal with unique Gabor dual property for the rational (i.e., the case where $\alpha\beta$ is a rational number) and the irrational cases are quite different, we will first treat the rational case in Sec. III and use the Zak-transform in that case to characterize all the functions $g\in L^2(\mathbb{R})$ such that $\mathbf{G}(\alpha,\beta,g)$ has unique Gabor dual of type I or type II. In Sec. IV, we prove our main results including Theorem 1.1, the duality theorem, and the characterization theorem for the unique Gabor dual property in the case of arbitrary parameters α and β.

II. THE UNIQUE GABOR DUAL PROPERTY AND THE MAIN RESULTS

Let us first introduce some terminology and notation that will be used throughout this paper.

A family of vectors $\{x_k\}_{k\in\mathbb{N}}$ is called a *frame* for a Hilbert space H if there exist two positive constants A and B such that

$$A\|x\|^2\leqslant\sum_{k\in\mathbb{N}}|\langle x,x_k\rangle|^2\leqslant B\|x\|^2 \tag{2.1}$$

holds for all $x\in H$. The two optimal constants in (2.1) are called the *frame bounds*. When $A=B=1$, the frame is called a *normalized tight* frame. A family $\{x_k\}$ is called *Bessel* when the second inequality in (2.1) hold. A Bessel sequence $\{y_n\}$ is called a *dual* for a frame $\{x_n\}$ if

$$x=\sum_{n\in\mathbb{N}}\langle x,y_n\rangle x_n \tag{2.2}$$

holds for all $x\in H$, where the convergence of the series in (2.2) is unconditional in the Hilbert space norm.

For a frame $\{x_k\}$, we define the associated *analysis operator* T by

$$Tx=\sum_{k\in\mathbb{N}}\langle x,x_k\rangle e_k,\quad x\in H,$$

where $\{e_k\}$ is the standard orthonormal basis for $\ell^2(\mathbb{N})$. Since $\{x_k\}$ is a frame, Range(T) is a closed linear subspace of $\ell^2(\mathbb{N})$. The associated *frame operator* S is defined to be T^*T. It is a bounded, positive and invertible operator from H onto itself. By the definition of S, it is clear that $\{S^{-1}x_n\}$ is a dual of $\{x_n\}$. It is also called the *standard dual* of the frame $\{x_n\}$.

Given two positive parameter α and β, we define the collection of unitary operators on $L^2(\mathbb{R})$, $\mathcal{U}_{\alpha,\beta}$, by

$$\mathcal{U}_{\alpha,\beta}=\{\mathcal{E}_{m\alpha}\mathcal{T}_{n\beta}:m,n\in\mathbb{Z}\},$$

where the two unitary operators $\mathcal{E}_{m\alpha}$ and $\mathcal{T}_{n\beta}$ are defined by

$$(\mathcal{E}_{m\alpha}f)(x)=e^{2\pi im\alpha x}f(x)\ \text{ and }\ (\mathcal{T}_{n\beta}f)(x)=f(x-n\beta),\quad f\in L^2(\mathbb{R}).$$

For convenience, we also write $g_{m\alpha,n\beta}=\mathcal{E}_{m\alpha}\mathcal{T}_{n\beta}g$, when $g\in L^2(\mathbb{R})$.

If $\mathbf{G}(\alpha,\beta,g)$ is a frame for $\mathcal{M}(\alpha,\beta,g)$, then we say that $\mathbf{G}(\alpha,\beta,g)$ is a *subspace Gabor frame*. We also use T_g to denote the analysis operator associated with $\mathbf{G}(\alpha,\beta,g)$. Let $S=T_g^*T_g$ be the frame operator associated with a subspace Gabor frame $\mathbf{G}(\alpha,\beta,g)$. Then $S^{-1}g\in\mathcal{M}(\alpha,\beta,g)$, and $(S^{-1}g)_{m\alpha,n\beta}=S^{-1}(g_{m\alpha,n\beta})$. Therefore, $\mathbf{G}(\alpha,\beta,S^{-1}g)$ is the standard dual of $\mathbf{G}(\alpha,\beta,g)$. Since we are dealing with Gabor frames for subspaces, we can have several ways of choosing a dual frame which also has the ''Gabor form.'' In particular, we will now introduce two different type of duals, which we call type I and type II duals.

Definition 2.1: Let $\mathbf{G}(\alpha,\beta,g)$ *be a subspace Gabor frame for* $\mathcal{M}(\alpha,\beta,g)$.

(i) *If* $\mathbf{G}(\alpha,\beta,h)$ *is a Bessel sequence such that* $h\in\mathcal{M}(\alpha,\beta,g)$ *and*

$$f=\sum_{m,n}\langle f,h_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta},\ f\in\mathcal{M}(\alpha,\beta,g),$$

then $\mathbf{G}(\alpha,\beta,h)$ *is called a Gabor dual of type I for* $\mathbf{G}(\alpha,\beta,g)$

(ii) *If* $h\in L^2(\mathbb{R})$ (*not necessarily in* $\mathcal{M}(\alpha,\beta,g)$) *is such that* $\mathbf{G}(\alpha,\beta,h)$ *is a Bessel sequence,* $Range(T_h)$ *is contained in* $Range(T_g)$ *and*

$$f=\sum_{m,n}\langle f,h_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}$$

holds for every $f\in\mathcal{M}(\alpha,\beta,g)$, *then* $\mathbf{G}(\alpha,\beta,h)$ *is called a Gabor dual of type II for* $\mathbf{G}(\alpha,\beta,g)$.

Roughly speaking, for Gabor duals of type I, we are interested in the existence of a dual window function which belongs to the subspace generated by the original frame, while for Gabor dual of type II, the dual window function is not required to be in that subspace, but we require the coefficient sequence $\{\langle f,h_{m\alpha,n\beta}\rangle\}$ to be in the ''analyzing space'' Range(T_g) of the frame $\mathbf{G}(\alpha,\beta,g)$. It is obvious that there is only one Gabor dual of type I if $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence. However, this is not the only case where there could be a unique Gabor dual of type I. A similar situation occurs for the Gabor dual of type II whose uniqueness is guaranteed by the

density in $L^2(\mathbb{R})$ of the subspace generated by the original frame, even though that condition is not always necessary. In this paper, we are interested in finding conditions on g under which there is only one window function generating a Gabor dual of type I (resp. type II) for the frame $\mathbf{G}(\alpha,\beta,g)$.

For type I Gabor duals, we obtained the following characterization theorem in Gabardo and Han (2004; see also Gabardo, 2003):

Theorem 2.2: *Let $\mathbf{G}(\alpha,\beta,g)$ be a normalized Gabor tight frame for $\mathcal{M}(\alpha,\beta,g)$. Then, the following are equivalent:*

(i) *$\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I.*

(ii) *$\langle g,UVg\rangle=\langle g,VUg\rangle$ holds for all $U,V\in\mathcal{U}_{\alpha,\beta}$.*

(iii) *$e^{2\pi i(nk-m\ell)\alpha\beta}\langle g,g_{m\alpha,n\beta}\rangle=\langle g,g_{m\alpha,n\beta}\rangle$ for all m, n, k, $\ell\in\mathbb{Z}$.*

To prove Theorem 1.2, we need the following more concrete characterization for the unique Gabor dual property. Note that the assumption that $\mathbf{G}(\alpha,\beta,g)$ be a normalized tight frame is not needed here.

Theorem 2.3: *Let $\mathbf{G}(\alpha,\beta,g)$ be a subspace Gabor frame for $\mathcal{M}(\alpha,\beta,g)$.*

A. *If $\alpha\beta$ is irrational, then*

(A_1) *$\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I if and only if $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence.*

(A_2) *$\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type II if and only if $\mathbf{G}(\alpha,\beta,g)$ is a frame for the whole space $L^2(\mathbb{R})$.*

B. *Suppose that $\alpha\beta$ is rational. Let $\alpha\beta=p/q$ where p, q are positive integers with $gcd(p,q)=1$, and let $\mathcal{G}$ be the corresponding Zak-matrix associated with g (as in* (3.1)*). Then,*

(B_1) *$\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I if and only if $rank(\mathcal{G})\in\{0,q\}$.*

(B_2) *$\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type II if and only if $rank(\mathcal{G})\in\{0,p\}$.*

The well-known Ron–Shen duality principle (Ron and Shen, 1997) tells us that $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence (hence, $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I) if and only if $\mathbf{G}(1/\beta,1/\alpha,g)$ is a frame for $L^2(\mathbb{R})$ (hence, $\mathbf{G}(1/\beta,1/\alpha,g)$ has a unique Gabor dual of type II). Theorem 2.3 allows us to get the following *duality theorem* which is consistent with the Ron–Shen principle:

Theorem 2.4 (Duality Theorem): *Let $\{g_{m\alpha,n\beta}\}$ be a subspace Gabor frame. Then, $\{g_{m\alpha,n\beta}\}$ has a unique Gabor dual of type I if and only if $\{g_{m/\beta,n/\alpha}\}$ has a unique Gabor dual of type II.*

As a consequence of Theorem 2.3, we have:

Corollary 2.5: Let $\{g_{m\alpha,n\beta}\}$ be a subspace Gabor frame.

(i) *If $\alpha\beta$ is an integer, then $\{g_{m\alpha,n\beta}\}$ has a unique Gabor dual of type I.*

(ii) *If $\alpha\beta=1/q$ for some integer q, then $\{g_{m\alpha,n\beta}\}$ has a unique Gabor dual of type II.*

(iii) *If $\alpha\beta=1$, then $\{g_{m\alpha,n\beta}\}$ has a unique Gabor dual of both type I and type II.*

Proof: Statement (*i*) follows from (B_1) of Theorem 2.3 since $\mathcal{G}$ is a $1\times p$ matrix function and thus its rank can only be 0 or 1. Statement (ii) follows from (B_2) of Theorem 2.3 in a similar way and statement (iii) is deduced immediately from (i) and (ii). Note that (i) can also be obtained from Theorem 2.2, since the unitary operators in $\mathcal{U}_{\alpha,\beta}$ commute when $\alpha\beta$ is an integer, and that (ii) follows from (i) and Theorem 2.4. □

It is known that $\{g_{m\alpha,n\beta}\}$ can be a Riesz basis for all of $L^2(\mathbb{R})$ only when $\alpha\beta=1$. In this case, $\{g_{m\alpha,n\beta}\}$ has unique Gabor dual of both types. Therefore, it is natural to ask whether the unique Gabor dual property is related to the Balian–Low phenomenon. We shall prove the following:

Theorem 2.6: *Let $\{g_{m\alpha,n\beta}\}$ be a subspace Gabor frame which has a unique Gabor dual of type I. Then, one of the following must holds:*

(i) *$\{g_{m\alpha,n\beta}\}$ is a Riesz sequence.*

(ii) $(\int_{\mathbb{R}}|xg(x)|^2dx)(\int_{\mathbb{R}}|\omega\hat{g}(\omega)|^2d\omega)=\infty$.

Combining this result together with Theorem 2.4, we get

Corollary 2.7: Let $\{g_{m\alpha,n\beta}\}$ *be a subspace Gabor frame which has a unique Gabor dual of type II. Then, one of the following must hold:*

(i) $\{g_{m\alpha,n\beta}\}$ *is a frame for the whole space* $L^2(\mathbb{R})$.
(ii) $(\int_{\mathbb{R}}|xg(x)|^2dx)(\int_{\mathbb{R}}|\omega\hat{g}(\omega)|^2d\omega)=\infty$.

III. THE ZAK-TRANSFORM CHARACTERIZATION

As we mentioned in the Introduction, in order to prove our main results, different techniques are needed depending on whether $\alpha\beta$ is rational or irrational. In this section, we first deal with the rational case.

Suppose $\alpha\beta=p/q$, where p,q are positive integers with $\gcd(p,q)=1$. We will denote by $\mathcal{M}_{m,n}$ the set of $m\times n$ matrices with complex entries. If $g\in L^2(\mathbb{R})$, we denote by $\mathcal{Z}_\alpha g$ the Zak transform of g defined by

$$\mathcal{Z}_\alpha g(t,\nu)=\alpha^{-1/2}\sum_{k\in\mathbb{Z}} g\left(\frac{t-k}{\alpha}\right)e^{2\pi ik\nu},$$

and associate with g the matrix function $\mathcal{G}(t,\nu)$, taking value in $\mathcal{M}_{q,p}$, defined by

$$\mathcal{G}_{r,s}(t,\nu)=\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu+\frac{s}{p}\right),\quad 0\leqslant r\leqslant q-1,\ 0\leqslant s\leqslant p-1, \tag{3.1}$$

for a. e. (t,ν) in $[0,1)\times[0,1/p)$.

The following result will be needed. It was proved in Gabardo and Han, 2003 in the case $\alpha=1$, although the general case can be handled in a very similar way.

Proposition 3.1: Let g *and* α, β *as above. Then, the following are equivalent.*

(a) $\mathbf{G}(\alpha,\beta,g)$ *is a subspace Gabor frame for* $\mathcal{M}(\alpha,\beta,g)$.
(b) *There exist two constants* C_1, $C_2>0$ *such that*
$$C_1\mathcal{G}\mathcal{G}^*\leqslant(\mathcal{G}\mathcal{G}^*)^2\leqslant C_2\mathcal{G}\mathcal{G}^*,$$
a. e. on $[0,1)\times[0,1/p)$.
(c) *There exist two constants* C_1, $C_2>0$ *such that*
$$C_1\mathcal{G}^*\mathcal{G}\leqslant(\mathcal{G}^*\mathcal{G})^2\leqslant C_2\mathcal{G}^*\mathcal{G},$$
a. e. on $[0,1)\times[0,1/p)$.

Lemma 3.2: Let g *and* α, β *as above and let* $f\in L^2(\mathbb{R})$ *have a Zak transform denoted by* $\mathcal{Z}_\alpha f=F$. *Then, for each* m, $n\in\mathbb{Z}$ *and each* $r=0,\ldots,q-1$, *we have*

$$\langle f,g_{m\alpha,(nq+r)\beta}\rangle=\int_0^1\int_0^{1/p}e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F(t,\nu+l/p)d\nu dt.$$

Proof: First note that

$$\begin{aligned}(\mathcal{Z}_\alpha g_{m\alpha,(nq+r)\beta})(t,\nu)&=\alpha^{-1/2}\sum_{k\in\mathbb{Z}}e^{2\pi im\alpha(t-k/\alpha)}g\left(\frac{t-k}{\alpha}-(nq+r)\beta\right)e^{2\pi ik\nu}\\&=\alpha^{-1/2}\sum_{k\in\mathbb{Z}}e^{2\pi imt}g\left(\frac{t-k-(nq+r)\frac{p}{q}}{\alpha}\right)e^{2\pi ik\nu}\\&=\alpha^{-1/2}e^{2\pi imt}\sum_{k\in\mathbb{Z}}g\left(\frac{t-k-np-r\frac{p}{q}}{\alpha}\right)e^{2\pi ik\nu}\end{aligned}$$

$$= \alpha^{-1/2} e^{2\pi imt} \sum_{k\in\mathbb{Z}} g\left(\frac{t-k-r\frac{p}{q}}{\alpha}\right) e^{2\pi i(k-np)\nu}$$

$$= e^{2\pi imt} e^{-2\pi inp\nu} \mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu\right).$$

Using the unitarity of the Zak transform as a mapping from $L^2(\mathbb{R})$ to $L^2(I\times I)$, where $I=[0,1)$, we have, for $0\leqslant r\leqslant q-1$ and for $m,n\in\mathbb{Z}$,

$$\langle f, g_{m\alpha,(nq+r)\beta}\rangle = \int_{\mathbb{R}} f(x)\overline{g_{m\alpha,(nq+r)\beta}(x)}dx = \int_I\int_I F(t,\nu)e^{-2\pi imt}e^{2\pi inp\nu}\overline{\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu\right)}d\nu dt$$

$$= \int_0^1\int_0^{1/p} e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu+l/p\right)}F(t,\nu+l/p)d\nu dt$$

$$= \int_0^1\int_0^{1/p} e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F(t,\nu+l/p)d\nu dt,$$

which proves the lemma. □

The following result is known (Zibulski and Zeevi, 1997) and will be needed later.

Proposition 3.3: Let g and α, β as above. Then, the following are equivalent.

(a) $\mathbf{G}(\alpha,\beta,g)$ *is a Bessel system in* $L^2(\mathbb{R})$.

(b) *There exists* $C>0$ *such that*

$$\|\mathcal{G}(t,\nu)\|\leqslant C, \quad \text{a. e. on } [0,1)\times\left[0,\frac{1}{p}\right),$$

where $\|.\|$ *denotes the matrix-norm of a matrix in* $\mathcal{M}_{q,p}$.

(c) $\mathcal{Z}_\alpha g$ *belongs to* $L^\infty([0,1)\times[0,1))$.

We will make use of the following fact which is intuitively clear.

Lemma 3.4: If Ω *is a measure space and* $\mathcal{G}:\Omega\to\mathcal{M}_{m,n}$, *where m and n are positive integers, is measurable, then the function* $rank(G):\Omega\to\mathbb{R}$ *is also measurable.*

Proof: The measurability of rank(G) can easily be deduced from the fact that the rank of a matrix $A\neq 1$ is the unique integer $n\geqslant 0$ such that any submatrix of A of size $n+1\times n+1$ has zero determinant and such that there exists a least one submatrix of A of size $n\times n$ with a nonzero determinant. □

The following result is well known and provides a proof of the incompleteness of $\mathcal{M}(\alpha,\beta,g)$ in $L^2(\mathbf{R})$ when $\alpha\beta>1$, in the rational case (Daubechies, 1990 and Zibulski and Zeevi, 1997). We provide a proof here for the reader's comvenience.

Proposition 3.5: Let g be in $L^2(\mathbb{R})$ *and let* $\alpha\beta=p/q$ *as above. Then, the identity* $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbf{R})$ *holds if and only if*

$$rank(\mathcal{G})=p \quad a.\ e.\ on\ [0,1)\times\left[0,\frac{1}{p}\right).$$

Proof: Let f be a function in $L^2(\mathbb{R})$ with Zak transform $\mathcal{Z}_\alpha f=F\in L^2(I\times I)$. Using Lemma 3.2, we can write, for $0\leqslant r\leqslant q-1$ and for m, $n\in\mathbb{Z}$, that

$$\langle f, g_{m\alpha,(nq+r)\beta}\rangle = \int_0^1\int_0^{1/p} e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F(t,\nu+l/p)d\nu dt.$$

Since the function defined by the sum inside this last integral belongs to $L^1(I\times I)$, a function $f \in L^2(\mathbb{R})$ is orthogonal to $\mathcal{M}(\alpha,\beta,g)$ if and only if

$$\sum_{l=0}^{p-1} \overline{\mathcal{G}_{r,l}(t,\nu)}F(t,\nu+l/p)=0, \quad \text{for a. e. } (t,\nu)\in[0,1)\times[0,1/p), \tag{3.2}$$

for each $r=0,...,q-1$. Now, if $\operatorname{rank}(\mathcal{G})=p$ for a. e. $(t,\nu)\in[0,1)\times[0,1/p)$, it follows that $F(t,\nu+l/p)=0$ for a. e. $(t,\nu)\in[0,1)\times[0,1/p)$ and thus that $F=0$ as a function in $L^2(I\times I)$. Hence $f=0$ and $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$. On the other hand, if $\operatorname{rank}(\mathcal{G})<p$ on a subset of $[0,1)\times[0,1/p)$ with positive measure, then it is easy to construct a nonzero function $F\in L^2(I\times I)$ satisfying (3.2). The function $f:=\mathcal{Z}_\alpha^{-1}F$ is thus a nonzero function in $L^2(\mathbb{R})$ orthogonal to $\mathcal{M}(\alpha,\beta,g)$ which, then, must be a proper subspace of $L^2(\mathbb{R})$. □

Definition 3.6: Let $g\in L^2(\mathbb{R})$ and let α and β be positive numbers. Then we say that the system $\mathbf{G}(\alpha,\beta,g)$ has the *Riesz Property* if, whenever

$$\sum_{m,m\in\mathbb{Z}} c_{m,n}g_{m\alpha,n\beta}=0,$$

where the series converges unconditionally in $L^2(\mathbb{R})$ and $\{c_{m,n}\}\in\ell^2(\mathbb{Z}^2)$, we must have that $c_{m,n}=0$, for all $(m,n)\in\mathbb{Z}^2$.

Remark 3.7: Clearly, if the system $\mathbf{G}(\alpha,\beta,g)$ is a Riesz basis for its span, then it must have the Riesz property.

The following result is essentially known Balan *et al.* (2000). We state it in a slightly more general form that does not require the system to form a frame for its closed linear span.

Proposition 3.8: Let g be in $L^2(\mathbb{R})$ and let $\alpha\beta=p/q$ as above. Then, the system $\mathbf{G}(\alpha,\beta,g)$ has the Riesz property if and only if

$$rank(\mathcal{G})=q \quad a.\ e.\ on\ [0,1)\times\left[0,\frac{1}{p}\right).$$

Proof: Suppose that

$$\sum_{\substack{m,n\in\mathbb{Z}\\ 0\leqslant r\leqslant q-1}} c_{m,nq+r}g_{m,nq+r}=0,$$

where the series converges unconditionally in $L^2(\mathbb{R})$ and $\{c_{m,n}\}\in\ell^2(\mathbb{Z}^2)$. Then, if $f\in L^2(\mathbb{R})$ and $\mathcal{Z}_\alpha f=F$, we have

$$\begin{aligned}
0&=\sum_{\substack{m,n\in\mathbb{Z}\\ 0\leqslant r\leqslant q-1}} c_{m,nq+r}\int_{\mathbb{R}} f(x)\overline{g_{m,nq+r}(x)}dx\\
&=\sum_{\substack{m,n\in\mathbb{Z}\\ 0\leqslant r\leqslant q-1}} c_{m,nq+r}\int_0^1\int_0^1 F(t,\nu)e^{-2\pi imt}e^{2\pi inp\nu}\overline{\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu\right)}d\nu dt\\
&=\int_0^1\int_0^{1/p}\sum_{\substack{m,n\in\mathbb{Z}\\ 0\leqslant r\leqslant q-1}} c_{m,nq+r}e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\mathcal{G}_{r,l}(t,\nu)F(t,\nu+l/p)d\nu dt.
\end{aligned}$$

For $r=0,...,q-1$, let H_r be the functions in $L^2([0,1)\times[0,1/p))$ defined by the series

$$H_r(t,\nu)=\sum_{m,n\in\mathbb{Z}} c_{m,nq+r}e^{-2\pi imt}e^{2\pi inp\nu}, \quad \text{for } r=0,...,q-1,$$

and, for $0\leqslant l\leqslant p-1$, define the functions $F_l(t,\nu)=F(t,\nu+l/p)$, for $(t,\nu)\in[0,1)\times[0,1/p)$. We have thus

$$\int_0^1\int_0^{1/p}\sum_{0\leqslant r\leqslant q-1}H_r(t,\nu)\sum_{l=0}^{p-1}\mathcal{G}_{r,l}(t,\nu)F_l(t,\nu)d\nu dt=0,$$

and, since the functions F_l can be arbitrary functions in $L^2([0,1)\times[0,1/p))$, it follows that, for each $l=0,...,p-1$,

$$\sum_{0\leqslant r\leqslant q-1}H_r(t,\nu)\mathcal{G}_{r,l}(t,\nu)=0 \quad \text{a. e. on } [0,1)\times[0,1/p). \tag{3.3}$$

Therefore, the system $\mathbf{G}(\alpha,\beta,g)$ has the Riesz property if, whenever the functions $H_r\in L^2([0,1)\times[0,1/p))$, for $r=0,...q-1$, and (3.3) holds for each $l=0,...,p-1$, then $H_r=0$, for each $r=0,...,q-1$. This is clearly equivalent to $\operatorname{rank}(\mathcal{G})=q$ for a. e. $(t,\nu)\in[0,1)\times[0,1/p)$. □

Our next goal is to provides a characterization through the Zak transform for systems admitting a unique dual of type I. We note that the standard dual, $S^{-1}g$, where S is the frame operator, is always a dual of type I. Before stating the result, we need the following intermediary steps.

Lemma 3.9: Let $g,h\in L^2(\mathbb{R})$, let $\alpha\beta=p/q$ as above and consider the associated measurable functions $\mathcal{G}$ and $\mathcal{H}$ with values in $\mathcal{M}_{q,p}$ defined as in (3.1). Then, the function $h\in L^2(\mathbb{R})$ belongs to $\mathcal{M}(\alpha,\beta,g)$ if and only if there exists a measurable function $\mathcal{A}$ with values in $\mathcal{M}_{q,q}$ such that

$$\mathcal{H}(t,\nu)=\mathcal{A}(t,\nu)\mathcal{G}(t,\nu), \quad \text{for a. e. } (t,\nu)\in[0,1)\times\left[0,\frac{1}{p}\right).$$

Proof: First note that, if $h\in\mathcal{M}(\alpha,\beta,g)$, then $h_{m\alpha,n\beta}\in\mathcal{M}(\alpha,\beta,g)$ for each $m,n\in\mathbb{Z}$. Thus, $h\in\mathcal{M}(\alpha,\beta,g)$ if and only if, for any $f\in L^2(\mathbb{R})$, the fact that f is orthogonal to $\mathcal{M}(\alpha,\beta,g)$ implies that f is also orthogonal to $\mathcal{M}(\alpha,\beta,h)$. Denoting by F the Zak transform of the function $f\in L^2(\mathbb{R})$, we have, as before, that

$$\langle f,g_{m\alpha,(nq+r)\beta}\rangle=\int_0^1\int_0^{1/p}e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F(t,\nu+l/p)d\nu dt,$$

for $m,n\in\mathbb{Z}$ and $0\leqslant r\leqslant q-1$. Thus, letting for $l=0,...,p-1$, $F_l(t,\nu)=F(t,\nu+l/p)$, where $(t,\nu)\in[0,1)\times[0,1/p)$, we see that the fact that f is orthogonal to $\mathcal{M}(\alpha,\beta,g)$ is equivalent to

$$\sum_{l=0}^{p-1}\mathcal{G}_{r,l}(t,\nu)\overline{F_l(t,\nu)}=0, \quad \text{for a. e. } (t,\nu)\in[0,1)\times\left[0,\frac{1}{p}\right). \tag{3.4}$$

Similarly, f is orthogonal to $\mathcal{M}(\alpha,\beta,h)$ if and only if

$$\sum_{l=0}^{p-1}\mathcal{H}_{r,l}(t,\nu)\overline{F_l(t,\nu)}=0, \quad \text{for a. e. } (t,\nu)\in[0,1)\times\left[0,\frac{1}{p}\right). \tag{3.5}$$

Clearly, the implication (3.4)⇒(3.5) holds if and only if, for a. e. $(t,\nu)\in[0,1)\times[0,1/p)$, the rows of the matrix $\mathcal{H}(t,\nu)$ can be expressed as linear combination of those of the matrix $\mathcal{G}(t,\nu)$. This is equivalent to the existence, for a. e. such (t,ν) of a matrix $\mathcal{A}(t,\nu)$ in $\mathcal{M}_{q,q}$ such that $\mathcal{H}(t,\nu)=\mathcal{A}(t,\nu)\mathcal{G}(t,\nu)$. Since $\mathcal{A}$ must clearly be measurable, this proves the lemma. □

Lemma 3.10: Let G belong to $\mathcal{M}_{q,p}$. Then, G has the property that, whenever A belongs to $\mathcal{M}_{q,q}$, the identity $G^*AG=0$ implies that $AG=0$ if and only if $rank(G)\in\{0,q\}$.

Proof: It is clear that the property $G^*AG=0$ implies that $AG=0$ holds if $\operatorname{rank}(G)=0$, i.e., if $G=0$ and if $\operatorname{rank}(G)=q$, i.e., if the range of G is all of C^q, where we view G has a linear mapping from $\mathbf{C}^p$ to $\mathbf{C}^q$. Conversely, if $\operatorname{rank}(G)\notin\{0,q\}$, consider the subspace N of $\mathbf{C}^q$ defined by

$N=G(\mathbf{C}^p)$. Then, by assumption $N\neq\{0\}$ and $N\neq\mathbf{C}^q$. Hence, there exists a nonzero linear mapping from N to $N^{\perp}$. We can extend this mapping to a linear mapping A from C^q to itself by defining A to be 0 on $N^{\perp}$. Let **u.v** denote the standard inner product between two vectors **u** and **v** in $\mathbf{C}^p$. If **x** and **y** belong to $\mathbf{C}^p$, we have

$$G^*AG\mathbf{x}.y=AG\mathbf{x}.Gy=0,$$

so $G^*\,AG=0$, but $AG\mathbf{x}\neq 0$, for some $\mathbf{x}\in\mathbf{C}^p$ by construction, which shows that the property mentioned above cannot hold. □

Remark: The lemma above also holds for measurable matrix-valued functions G and A of the corresponding size if the equalities in the lemma are replaced by a. e. equalities, since, as can be easily shown, all the operations involved in the construction of A, in the case where $\text{rank}(G)\notin\{0,q\}$, can be made to be measurable. The same remark holds, with the obvious changes, for the analoguous Lemma 3.13.

Now we are ready to prove (B_1) of Theorem 2.3:

Theorem 3.11: *Let $\alpha\beta=p/q$ as above and suppose that the system $\mathbf{G}(\alpha,\beta,g)$ is a frame for $\mathcal{M}(\alpha,\beta,g)$. Then, the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type I (which is thus given by the standard dual) if and only if*

$$rank\ \ (\mathcal{G})\in\{0,q\}\quad \text{a. e. } on\ \ [0,1)\times\left[0,\frac{1}{p}\right).$$

Proof: The existence of two different duals of type I for the system $\mathbf{G}(\alpha,\beta,g)$ is easily seen to be equivalent to the existence of a nonzero function $h\in M$ such that the system $\mathbf{G}(\alpha,\beta,g)$ is Bessel and which satisfies

$$\sum_{m,n\in\mathbb{Z}}\langle f,g_{m\alpha,n\beta}\rangle h_{m\alpha,n\beta}=0,\quad \forall f\in L^2(\mathbb{R}),$$

or, equivalently,

$$\sum_{m,n\in\mathbb{Z}}\langle f_1,g_{m\alpha,n\beta}\rangle\overline{\langle f_2,h_{m\alpha,n\beta}\rangle}=0,\quad \forall f_1,f_2\in L^2(\mathbb{R}). \tag{3.6}$$

Let F_1 and F_2 denote the Zak transform of f_1 and f_2, respectively, and let $\mathcal{G}$ and $\mathcal{H}$ be the functions with valued in $\mathcal{M}_{q,p}$ associated with g and h, respectively, defined as in (3.1). We have

$$\begin{aligned}\sum_{m,n\in\mathbb{Z}}\langle f_1,g_{m\alpha,n\beta}\rangle\overline{\langle f_2,h_{m\alpha,n\beta}\rangle}&=\sum_{\substack{m,n\in\mathbb{Z}\\0\le r\le q-1}}\int_0^1\int_0^1 F_1(t,\nu)e^{-2\pi imt}e^{2\pi inp\nu}\overline{\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu\right)}\,d\nu dt\\&\quad\times\int_0^1\int_0^1\overline{F_2(t,\nu)}e^{2\pi imt}e^{-2\pi inp\nu}\mathcal{Z}_\alpha h\left(t-r\frac{p}{q},\nu\right)d\nu dt\\&=\sum_{\substack{m,n\in\mathbb{Z}\\0\le r\le q-1}}\int_0^1\int_0^{1/p}e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F_1(t,\nu+l/p)\,d\nu dt\\&\quad\times\int_0^1\int_0^{1/p}e^{2\pi imt}e^{-2\pi inp\nu}\sum_{l=0}^{p-1}\mathcal{H}_{r,l}(t,\nu)\overline{F_2(t,\nu+l/p)}\,d\nu dt.\end{aligned}$$

Letting $F_l^1(t,\nu)=F_1(t,\nu+l/p)$ and $F_l^2(t,\nu)=F_2(t,\nu+l/p)$ for $(t,\nu)\in[0,1)\times[0,1/p)$, we can write this last expression, using Parseval's identity as

$$\sum_{r=0}^{q-1}\int_0^1\int_0^{1/p}\sum_{l,m=0}^{p-1} F_l^1(t,\nu)\mathcal{G}_{l,r}^*(t,\nu)\mathcal{H}_{r,m}(t,\nu)\overline{F_m^2(t,\nu)}\,d\nu dt$$

$$=\int_0^1\int_0^{1/p}\sum_{l,m=0}^{p-1}(\mathcal{G}^*\mathcal{H})_{l,m}(t,\nu)F_l^1(t,\nu)\overline{F_m^2(t,\nu)}\,d\nu dt$$

Since the functions $F_l^1, F_m^2, l,m=0,\ldots,p-1$, can be arbitrary in $L^2([0,1)\times[0,1/p))$, the identity (3.6) is equivalent to $\mathcal{G}^*\mathcal{H}=0$ a.e. on $[0,1)\times[0,1/p)$. Since $h\in M$, Lemma 3.9 shows the existence of a measurable function $\mathcal{A}$ defined on $[0,1)\times[0,1/p)$ and with values in $\mathcal{M}_{q,q}$ such that $\mathcal{H}=\mathcal{A}\mathcal{G}$. Hence, it follows that $\mathcal{G}^*\mathcal{A}\mathcal{G}=0$ a.e. on $[0,1)\times[0,1/p)$. If $\operatorname{rank}(\mathcal{G})\in\{0,q\}$, Lemma 3.10 shows that $\mathcal{A}\mathcal{G}=\mathcal{H}=0$ a.e. on $[0,1)\times[0,1/p)$ and thus that $h=0$, so the dual of type I must be unique in this case. On the other hand, if $\operatorname{rank}(\mathcal{G})\notin\{0,q\}$ on a subset of $[0,1)\times[0,1/p)$ having positive measure, we can easily construct a $\mathcal{M}_{q,p}$-valued matrix function $\mathcal{A}$ such that $\mathcal{G}^*\mathcal{A}\mathcal{G}=0$ and $\mathcal{A}\mathcal{G}\neq 0$ on a set of positive measure. The function $h\in L^2(\mathbb{R})$ corresponding to $\mathcal{H}=\mathcal{A}\mathcal{G}$ is then a nonzero function in M satisfying (3.6), and adding a nonzero multiple of that function to any dual of type I produces a dual of type I different than the original one. □

Our next goal is to prove (B_2) of Theorem 2.3. We need the following two lemmas.

Lemma 3.12: Let $\alpha\beta=p/q$ as above and assume that the Gabor systems $\mathbf{G}(\alpha,\beta,g)$ and $\mathbf{G}(\alpha,\beta,h)$ are both Bessel. Consider the associated measurable functions $\mathcal{G}$ and $\mathcal{H}$ with values in $\mathcal{M}_{q,p}$ defined as in (3.1). Let $T_g:L^2(\mathbb{R})\to\ell^2(\mathbb{Z}^2)$ and $T_h:L^2(\mathbb{R})\to\ell^2(\mathbb{Z}^2)$ be the analyzing operators associated with the systems $\mathbf{G}(\alpha,\beta,g)$ and $\mathbf{G}(\alpha,\beta,h)$, respectively. Then, $\overline{Range(T_h)}$ is contained in $\overline{Range(T_g)}$ if and only if there exists a measurable $\mathcal{M}_{q,p}$-valued function $\mathcal{B}$ such that

$$\mathcal{H}(t,\nu)=\mathcal{G}(t,\nu)\mathcal{B}(t,\nu)\quad for\ a.\ e.\ (t,\nu)\in[0,1)n\left[0,\frac{1}{p}\right).$$

Proof: First note that, using Proposition 3.1, the entries of both $\mathcal{G}$ and $\mathcal{H}$ belong to $L^\infty([0,1)\times[0,1/p))$ since the systems $\mathbf{G}(\alpha,\beta,g)$ and $\mathbf{G}(\alpha,\beta,h)$ are both assumed to be Bessel. We will first give a description through the Zak transform of the sequences which are orthogonal to $\overline{\operatorname{Range}(T_g)}$. A sequence $\{a_{m,n}\}$ is orthogonal to $\overline{\operatorname{Range}(T_g)}$ if and only if

$$\sum_{\substack{m,n\in\mathbb{Z}\\0\leqslant r\leqslant q-1}} a_{m,nq+r}\langle f,g_{m\alpha,(nq+r)\beta}\rangle=0,\quad \forall f\in L^2(\mathbb{R}).$$

Letting $F=\mathcal{Z}_\alpha f$ and defining $F_l(t,\nu)=\mathcal{Z}_\alpha f(t,\nu+l/p)$, where $(t,\nu)\in[0,1)\times[0,1/p)$, for each $l=0,\ldots,p-1$, this identity can also be written, using Lemma 3.2, as

$$\int_0^1\int_0^{1/p}\sum_{0\leqslant r\leqslant q-1}\sum_{m,n\in\mathbb{Z}} a_{m,nq+r}e^{-2\pi imt}e^{2\pi inp\nu}\sum_{l=0}^{p-1}\overline{\mathcal{G}_{r,l}(t,\nu)}F_l(t,\nu)\,d\nu dt=0,$$

for each function $F_0,\ldots,F_{l-1}\in L^2([0,1)\times[0,1/p))$. If we denote by K_r the functions in $L^2([0,1)\times[0,1/p))$ defined by the series

$$K_r(t,\nu)=\sum_{m,n\in\mathbb{Z}} a_{m,nq+r}e^{-2\pi imt}e^{2\pi inp\nu},$$

for $0\leqslant r\leqslant q-1$, we can simply express the previous identity as

$$\sum_{0\leqslant r\leqslant q-1} K_r(t,\nu)\overline{\mathcal{G}_{r,l}(t,\nu)}=0\quad \text{a. e. on } [0,1)\times\left[0,\frac{1}{p}\right),\tag{3.7}$$

for each $l=0,...,p-1$. Similarly, the fact that the sequence $\{a_{m,n}\}$ is orthogonal to $\overline{\text{Range}(T_h)}$ is equivalent to

$$\sum_{0\leq r\leq q-1} K_r(t,\nu)\overline{\mathcal{H}_{r,l}(t,\nu)}=0 \quad \text{a. e. on } [0,1)\times\left[0,\frac{1}{p}\right), \tag{3.8}$$

for each $l=0,...,p-1$. Thus the inclusion $\overline{\text{Range}(T_h)}\subset\overline{\text{Range}(T_g)}$ can be rephrased by stating that, whenever functions $K_0,\ldots,K_{q-1}\in L^2([0,1)\times[0,1/p))$ exist such that (3.7) holds, then so does (3.8). This last statement is equivalent to the fact that, for a. e. (t,ν), the rows of $\mathcal{H}(t,\nu)$ are linear combinations of those of $\mathcal{G}(t,\nu)$, i.e., to the existence of a measurable $\mathcal{M}_{p,p}$-valued function $\mathcal{B}$ defined on $[0,1)\times[0,1/p)$ such that $\mathcal{H}=\mathcal{G}\mathcal{B}$ almost everywhere. □

Lemma 3.13: Let G belong to $\mathcal{M}_{q,p}$. Then, G has the property that, whenever B belongs to $\mathcal{M}_{p,p}$, the identity $GBG^*=0$ implies that $GB=0$ if and only if $rank(G)\in\{0,p\}$.

Proof: Viewing G as a linear mapping from $\mathbf{C}^p$ to $\mathbf{C}^q$ and G^* as a linear mapping from $\mathbf{C}^q$ to $\mathbf{C}^p$ and using the fact that $\text{rank}(G)=\text{rank}(G^*)$, it is clear that, if $\text{rank}(G)=p$, then $G^*(\mathbf{C}^q)=\mathbf{C}^p$, and thus $GBG^*=0$ implies $GB=0$. The same implication obviously holds if $\text{rank}(G)=0$, i.e., if $G=0$. Conversely, if $0<\text{rank}(G)<p$, then $N=G^*(\mathbf{C}^q)$ is a subspace of $\mathbf{C}^p$ different than $\{0\}$ and $\mathbf{C}^p$. There exists thus a nonzero linear mapping from N to $N^\perp$. Extending this linear mapping to all of $\mathbf{C}^p$ by defining it to be 0 on $N^\perp$, we obtain in this way a linear mapping $B:\mathbf{C}^p\to\mathbf{C}^p$ such that $GBG^*=0$ but $GB\neq 0$. This proves the lemma. □

We can now state state our Zak transform characterization for the unique dual of type II, which complete the proof of (B_2) of Theorem 2.3.

Theorem 3.14: *Let $g\in L^2(\mathbb{R})$, let $\alpha\beta=p/q$ as above and suppose that the system $\mathbf{G}(\alpha,\beta,g)$ is a frame for $\mathcal{M}(\alpha,\beta,g)$. Then, the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type II (which is thus given by the standard dual) if and only if*

$$rank\ (\mathcal{G})\in\{0,p\} \quad a.\ e.\ on\ [0,1)\times\left[0,\frac{1}{p}\right).$$

Proof: The existence of two different duals of type II for the system $\mathbf{G}(\alpha,\beta,g)$ is easily seen to be equivalent to the existence of a nonzero function $h\in L^2(\mathbb{R})$ such that the system $\mathbf{G}(\alpha,\beta,h)$ is Bessel, which satisfies $\overline{\text{Range}(T_h)}\subset\overline{\text{Range}(T_g)}$ and

$$\sum_{m,n\in\mathbb{Z}}\langle f,h_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}=0, \quad \forall f\in M,$$

or, equivalently,

$$\sum_{m,n\in\mathbb{Z}}\langle f_1,g_{m\alpha,n\beta}\rangle\overline{\langle f_2,h_{m\alpha,n\beta}\rangle}=0, \quad \forall f_1\in L^2(\mathbb{R}),\ \forall f_2\in M. \tag{3.9}$$

As in the proof of Theorem 3.11, we can write the left side of the equality (3.9) as

$$\int_0^1\int_0^{1/p}\sum_{i,j=0}^{p-1}(\mathcal{G}^*\mathcal{H})_{i,j}(t,\nu)F_i^1(t,\nu)\overline{F_j^2(t,\nu)}\,d\nu dt,$$

where $F_i^1(t,\nu)=\mathcal{Z}_\alpha f_1(t,\nu+i/p)$, $F_j^2(t,\nu)=\mathcal{Z}_\alpha f_2(t,\nu+j/p)$ for $(t,\nu)\in[0,1)\times[0,1/p)$. Furthermore, letting $f_2=g_{m,nq+r}\in M$, where $m,n\in\mathbb{Z}$, and, using the fact that

$$\mathcal{Z}_\alpha g_{m,nq+r}(t,\nu)=e^{2\pi imt}e^{-2\pi inp\nu}\mathcal{Z}_\alpha g\left(t-r\frac{p}{q},\nu\right),$$

we deduce from (3.9) that

$$\int_0^1 \int_0^{1/p} \sum_{i,j=0}^{p-1} (\mathcal{G}^*\mathcal{H})_{i,j}(t,\nu) F_i^1(t,\nu) e^{-2\pi i m t} e^{2\pi i n p \nu} \overline{\mathcal{G}_{r,j}(t,\nu)} d\nu dt = 0,$$

for every $F_0^1,\ldots,F_{p-1}^1 \in L^2([0,1)\times[0,1/p)$, for every m, $n \in \mathbb{Z}$ and for every integer r from 0 to $q-1$, which is equivalent to $\mathcal{G}^*\mathcal{H}\mathcal{G}^* = 0$ a. e. on $[0,1)\times[0,1/p)$. Since $\overline{\text{Range}(T_h)} \subset \overline{\text{Range}(T_g)}$, Lemma 3.12 shows the existence of a $\mathcal{M}_{q,p}$-valued measurable function $\mathcal{B}$ defined on $[0,1)\times[0,1/p)$ such that $\mathcal{H} = \mathcal{G}\mathcal{B}$. Hence, it follows that $\mathcal{G}^*\mathcal{G}\mathcal{B}\mathcal{G}^* = 0$ a.e. on $[0,1)\times[0,1/p)$ which is equivalent to $\mathcal{G}\mathcal{B}\mathcal{G}^* = 0$ a.e. on $[0,1)\times[0,1/p)$. If $\text{rank}(\mathcal{G}) \in \{0,p\}$, Lemma 13 shows that $\mathcal{G}\mathcal{B} = \mathcal{H} = 0$ a. e. on $[0,1)\times[0,1/p)$ and thus that $h = 0$, so the dual of type II must be unique in this case. On the other hand, if $\text{rank}(\mathcal{G}) \notin \{0,p\}$ on a subset of $[0,1)\times[0,1/p)$ having positive measure, we can easily construct a $\mathcal{M}_{p,p}$-valued function $\mathcal{B}$ such that $\mathcal{G}\mathcal{B}\mathcal{G}^* = 0$ and $\mathcal{G}\mathcal{B} \neq 0$ on a set of positive measure. The function $h \in L^2(\mathbb{R})$ corresponding to $\mathcal{H} = \mathcal{G}\mathcal{B}$ is then a nonzero function in M satisfying (3.9), and adding a nonzero multiple of that function to any dual of type II produces a dual of type II different than the original one. □

IV. PROOFS OF THE MAIN RESULTS

Proof of Theorem 2.3

Part *B* of Theorem 2.3 is proved in Theorems 3.11 and 3.14. Therefore, all that is left to prove is part *A*.

We can assume that $\mathbf{G}(\alpha,\beta,g)$ is a normalized tight Gabor frame for $\mathcal{M}(\alpha,\beta,g)$, since the system $\mathbf{G}(\alpha,\beta,g_1)$, (where $g_1 = S^{-1/2}g$ and S is the associated frame operator), is a normalized tight frame for $\mathcal{M}(\alpha,\beta,g)$ and it is easy to check that this system admits a unique dual of type I (resp. type II) if and only if the original one does.

(i) Since $\alpha\beta$ is irrational, it follows that identity (iii) of Theorem 2.2 holds for all m, n, k, $\ell \in \mathbb{Z}$ if and only if $\{g_{m\alpha,n\beta}\}$ is orthogonal. Hence, (A_1) holds.

To prove (A_2), we first assume that $\mathbf{G}(\alpha,\beta,g)$ is a frame for the whole space $L^2(\mathbb{R})$. Let $\mathbf{G}(\alpha,\beta,h)$ be a dual of type II for $\mathbf{G}(\alpha,\beta,g)$. We need to show that $g = h$. Since $\text{Range}(T_h) \subset \text{Range}(T_g)$, there exists a function $f \in L^2(\mathbb{R})$ such that $T_h(g) = T_g(f)$ which implies that $\langle g, h_{m\alpha,n\beta}\rangle = \langle f, g_{m\alpha,n\beta}\rangle$ holds for all m, $n \in \mathbb{Z}$. Also note that

$$g = \sum_{m,n\in\mathbb{Z}} \langle g, h_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}$$

and

$$f = \sum_{m,n\in\mathbb{Z}} \langle f, g_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}.$$

Thus $f = g$, which implies that

$$\langle g, h_{m\alpha,n\beta}\rangle = \langle g, g_{m\alpha,n\beta}\rangle, \quad m,n \in \mathbb{Z},$$

and so,

$$\langle g_{-m\alpha,-n\beta}, h\rangle = \langle g_{-m\alpha,-n\beta}, g\rangle, \quad m,n \in \mathbb{Z}.$$

Therefore $h = g$ since $\mathbf{G}(\alpha,\beta,g)$ is a frame for the whole space $L^2(\mathbb{R})$.

Now assume that $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type II. Let us show that $\mathcal{M}(\alpha,\beta,g) = L^2(\mathbb{R})$. Suppose, to the contrary, that $\mathcal{M}(\alpha,\beta,g) \neq L^2(\mathbb{R})$. Let P be the orthogonal projection onto M. Then $P \in \mathcal{A}'_{\alpha,\beta}$. Since $\mathcal{A}'_{\alpha,\beta}$ is a factor von Neumann algebra, and $0 \neq P \neq I$, by a standard result about in von Neumann algebra theory (cf. Takesaki, 1979), there exists a nonzero partial isometry $V \in \mathcal{A}'_{\alpha,\beta}$ with initial space contained in M and final space contained in $M^\perp$. Let $h = g + Vg$. Then $h \neq g$ since $Vg \neq 0$ (In fact, if $Vg = 0$, then $Vg_{m\alpha,n\beta} = 0$ for all m, $n \in \mathbb{Z}$, which

implies $V=0$). We claim that $\mathbf{G}(\alpha,\beta,h)$ is a type II Gabor dual of $\mathbf{G}(\alpha,\beta,g)$ which will yield a contradiction. Indeed, clearly $\mathbf{G}(\alpha,\beta,h)$ is Bessel since $V\in\mathcal{A}'_{\alpha,\beta}$. Secondly, for any $f\in L^2(\mathbb{R})$, we have

$$T_h(f)=\{\langle f,h_{m\alpha,n\beta}\rangle\}=\{\langle f,g_{m\alpha,n\beta}+(Vg)_{m\alpha,n\beta}\rangle\}=\{\langle f,(I+V)g_{m\alpha,n\beta}\rangle\}=T_g((I+V^*)f).$$

Thus, Range$(T_h)\subset$Range(T_g). Finally, note that M is orthogonal to Range(V). So

$$\sum_{m,n}\langle f,h_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}=\sum_{m,n}\langle f,g_{m\alpha,n\beta}+Vg_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}=\sum_{m,n}\langle f,g_{m\alpha,n\beta}\rangle g_{m\alpha,n\beta}=f$$

holds for every $f\in M$. Therefore, $\mathbf{G}(\alpha,\beta,h)$ is a type II Gabor dual of $\mathbf{G}(\alpha,\beta,g)$ as claimed. □

In order to prove our duality theorem (Theorem 2.4), we need a few more lemmas. The first lemma follows from the identity

$$\mathcal{F}(g_{m\alpha,n\beta})=e^{2\pi imn\alpha\beta}(\mathcal{F}g)_{-n\beta,m\alpha},\quad m,n\in\mathbb{Z}$$

(where $\mathcal{F}(h)$ denotes the Fourier transform of h) and the definition of type I and II Gabor dual property. The second one is elementary and well-known.

Lemma 4.1: Let $\mathbf{G}(\alpha,\beta,g)$ be a subspace Gabor frame for $\mathcal{M}(\alpha,\beta,g)$. Then $\mathbf{G}(\alpha,\beta,g)$ has unique Gabor dual of type I (resp. type II) if and only if $\mathbf{G}(\beta,\alpha,\hat{g})$ has unique Gabor dual of type I (resp. type II).

Lemma 4.2: Let p and q be relatively prime positive integer. For $k\in\{0,...,q-1\}$, define $\sigma(k)$ to be the unique integer in $\{0,...,q-1\}$ such that

$$kp=\sigma(k)+r(k)q,$$

where $r(k)$ in an integer. Then $\sigma:\{0,...,q-1\}\to\{0,...,q-1\}$ is a bijection.

Lemma 4.3: Let $A=(A_{k,l})_{q\times p}$, where $0\leq k\leq q-1$ and $0\leq l\leq p-1$ be a $q\times p$ matrix and let α_k, $0\leq k\leq q-1$, and β_l, $0\leq l\leq p-1$, be nonzero complex numbers. Then the rank of the matrix $B=B_{k,l}$ defined by

$$B_{k,l}=A_{k,l}\alpha_k\beta_l,\quad k=0,...,q-1,\ l=0,...p-1,$$

is the same as that of A.

Proof: This follows easily from the fact that if L is a subset of $\{0,...,p-1\}$ and c_l, $l\in L$, are complex numbers, then the implication

$$\sum_{l\in L}A_{k,l}c_l=0,\ k=0,...q-1\Rightarrow c_l=0,\ l\in L$$

is equivalent to

$$\sum_{l\in L}B_{k,l}c_l=0,\ k=0,...q-1\Rightarrow c_l=0,\ l\in L$$

□

Lemma 4.4: Let $A=(A_{k,l})_{q\times p}$, where $0\leq k\leq q-1$ and $0\leq l\leq p-1$ be a $q\times p$ matrix, let σ be a permutation of the set $\{0,...,q-1\}$ and let τ be a permutation of the set $\{0,...,p-1\}$. Then the rank of the matrix $C=C_{k,l}$ defined by

$$C_{k,l}=A_{\sigma(k),\tau(l)}\quad k=0,...,q-1,\ l=0,...p-1,$$

is the same as that of A.

Proof: This, again, follows easily from the fact that, if m is a positive integer, the implication

$$\sum_{l\in L} A_{k,l}c_l=0,\ \ k=0,...\Rightarrow c_l=0,\ \ l\in L,$$

for any subset L of $\{0,...,p-1\}$ of cardinality m is equivalent to

$$\sum_{l\in L} B_{k,l}c_l=0,\ \ k=0,...\Rightarrow c_l=0,\ \ l\in L,$$

for any subset L of $\{0,...,p-1\}$ of cardinality m. □

Now we are ready to prove Theorem 2.4.

Proof of Theorem 2.4

Case 1: $\alpha\beta$ is irrational

From Theorem 2.3, $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I if and only if $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence. Thus, using the Ron and Shen duality theorem, $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I is in turn equivalent to $\mathbf{G}(1/\beta,1/\alpha,g)$ is a Gabor frame for the whole space $L^2(\mathbb{R})$. Therefore, again by Theorem 2.3, this is equivalent to the condition that $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type II.

Case 2: $\alpha\beta=p/q$ with $\gcd(p,q)=1$ is rational

In the computations above, we use the fact that

$$\mathcal{Z}_\alpha g(t+m,\nu)=e^{2\pi im\nu}\mathcal{Z}_\alpha g(t,\nu),\quad \mathcal{Z}_\alpha g(t,\nu+m)=\mathcal{Z}_\alpha g(t,\nu),$$

and

$$\mathcal{Z}_\alpha \hat{g}(t,\nu)=e^{2\pi it\nu}\mathcal{Z}_{1/\alpha}g(-\nu,t) \tag{4.1}$$

for any $g\in L^2(\mathbb{R})$ and an integer m.

By Lemma 4.1 and Theorem 2.3 (B) we have that $G(1/\beta,1/\alpha,g)$ has a unique dual of type II if and only $G(1/\alpha,1/\beta,\hat{g})$ has a unique dual of type II, which is in turn equivalent to the condition that $\widetilde{\mathcal{G}}=(\widetilde{\mathcal{G}}_{k,l})_{p\times q}$ has a rank in $\{0,q\}$ (a.e.), where $\widetilde{\mathcal{G}}_{k,l}=\mathcal{Z}_{1/\alpha}\hat{g}(t-kq/p,\nu+l/q)$ has a rank in $\{0,q\}$ $(0\leqslant k\leqslant p-1$ and $0\leqslant l\leqslant q-1)$

From (4.1), we have that $\widetilde{\mathcal{G}}_{k,l}=e^{2\pi i(t-kq/p)(\nu+l/q)}\mathcal{Z}_\alpha g(-\nu-l/q,t-kq/p)$.

Now let σ be the permutation of $\{0,...,q-1\}$ defined by

$$l=\sigma(l)p+r(l)q,\quad l=0,....,q-1,$$

where $\sigma(l)\in\{0,...,q-1\}$ and $r(l)\in\mathbb{Z}$ (Lemma 4.2). Therefore, we have

$$\begin{aligned}
\widetilde{\mathcal{G}}_{k,l}&=e^{2\pi i(t-kq/p)(\nu+l/q)}\mathcal{Z}_\alpha g\left(-\nu-\frac{l}{q},t-k\frac{q}{p}\right)\\
&=e^{2\pi i(t-kq/p)(\nu+\sigma(l)p/q+r(l))}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q}-r(l),t-k\frac{q}{p}\right)\\
&=e^{2\pi i(t-kq/k)(\nu+\sigma(l)p/q+r(l))}e^{2\pi i(t-kq/p)(-r(l))}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q},t-k\frac{q}{p}\right)\\
&=e^{2\pi i(t-kq/p)(\nu+\sigma(l)p/q)}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q},t-k\frac{q}{p}\right)\\
&=e^{2\pi it\nu}e^{2\pi it(\sigma(l)p/q)}e^{2\pi i(-kq/p)\nu}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q},t-k\frac{q}{p}\right).
\end{aligned}$$

Now, letting τ be the permutation of $\{0,...,p-1\}$ defined by

$$-kq=\tau(k)+s(k)p, \quad k=0,...,p-1,$$

where $\tau(k)\in\{0,...,p-1\}$ and $s(k)\in\mathbb{Z}$ (Lemma 4.2), we can rewrite the matrix entry above as

$$e^{2\pi it\nu}e^{2\pi it(\sigma(l)p/q)}e^{2\pi i(\tau(k)/p+s(k))\nu}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q},t+\frac{\tau(k)}{p}+s(k)\right),$$

which is equal to

$$e^{2\pi it\nu}e^{2\pi it(\sigma(l)p/q)}e^{2\pi i(\tau(k)/p+s(k))\nu}\mathcal{Z}_\alpha g\left(-\nu-\sigma(l)\frac{p}{q},t+\frac{\tau(k)}{p}\right).$$

Using Lemmas 4.3 and 4.4, the rank of that last matrix is the same as that of the matrix with (k, l) entries:

$$\mathcal{Z}_\alpha g\left(-\nu-l\frac{p}{q},t+\frac{k}{p}\right)$$

Finally, by (B_1) of Theorem 2.3, this matrix has a rank in $\{0,q\}$ if and only if $G(\alpha,\beta,g)$ has a unique dual of type I, which proves the result. □

Our next goal is to prove Theorem 2.6 and Corollary 2.7 which state that if g is a nonzero smooth and well localized window function such that the system $\mathbf{G}(\alpha,\beta,g)$ is a frame for its closed linear span, then this system admits a unique dual of type I if and only if it is a Riesz basis for its closed linear span and the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type II if and only if its closed linear span is $L^2(\mathbb{R})$. We first need the following lemma.

Lemma 4.5: Let $g\in L^2(\mathbb{R})$ satisfy

$$\int_{\mathbf{R}}x^2|g(x)|^2dx<\infty \quad and \quad \int_{\mathbb{R}}\xi^2|\hat{g}(\xi)|^2d\xi<\infty.$$

Then, for a. e. $t\in[0,1)$, $\mathcal{Z}_\alpha g(t,.)$ is a continuous function of the second variable and for a. e. $\nu\in[0,1)$, $\mathcal{Z}_\alpha g(.,\nu)$ is a continuous function of the first variable.

Proof: To show that, for a. e. $t\in[0,1)$, $\mathcal{Z}_\alpha g(t,\nu)$ is a continuous function of ν, it is enough to show, that, as a function of ν, the series defining the Zak transform of g is an absolutely convergent Fourier series for a. e. $t\in[0,1)$. This last fact follows easily from Cauchy–Schwartz inequality since,

$$\int_{[0,1)}\sum_{k\neq 0,1}\left|g\left(\frac{t-k}{\alpha}\right)\right|=\alpha\int_{|u|\geqslant 1}|g(u)|du\leqslant\alpha\left[\int_{|u|\geqslant 1}u^2|g(u)|^2du\right]^{1/2}\left[\int_{|u|\geqslant 1}\frac{1}{u^2}du\right]^{1/2}<\infty.$$

To prove the second part of our assertion, we use the first part and the fact that

$$\mathcal{Z}_\alpha\hat{g}(t,\nu)=e^{2\pi it\nu}\mathcal{Z}_{1/\alpha}g(-\nu,t),$$

for any $g\in L^2(\mathbb{R})$. □

Remark 4.6: The previous lemma can also be proved by using well known properties of Sobolev spaces, since our assumptions on g are equivalent to the fact that $\mathcal{Z}_\alpha g$, $(\partial/\partial t)\mathcal{Z}_\alpha g$ and $(\partial/\partial\nu)\mathcal{Z}_\alpha g$ are in $L^2_{\mathrm{loc}}(\mathbb{R}^2)$ (see Daubechies, 1992).

We complete the proofs of Theorem 2.6 and Corollary 2.7 by proving the following result.

Theorem 4.7: *Let $\alpha\beta=p/q$ and let $g\in L^2(\mathbb{R})$ with $g\neq 0$. Suppose, furthermore, that the system $\mathbf{G}(\alpha,\beta,g)$ is a frame for $\mathcal{M}(\alpha,\beta,g)$ and that*

$$\int_{\mathbf{R}} |xg(x)|^2 dx < \infty \quad \text{and} \quad \int_{\mathbb{R}} |\omega \hat{g}(\omega)|^2 d\omega < \infty.$$

Then,

(a) *The system* $\mathbf{G}(\alpha,\beta,g)$ *admits a unique dual of type I if and only if it forms a Riesz basis for* $\mathcal{M}(\alpha,\beta,g)$.
(b) *The system* $\mathbf{G}(\alpha,\beta,g)$ *admits a unique dual of type II if and only if the identity* $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$ *holds.*

Proof: It is clear that if the system $\mathbf{G}(\alpha,\beta,g)$ forms a Riesz basis for M, then the standard dual is the unique dual of type I (see the statements of Proposition 3.8 and Theorem 3.11), and that, if $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$, then the standard dual is the unique dual of type II (see the statements of Proposition 3.5 and Theorem 3.14). Conversely, if g satisfies the conditions of the theorem and the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type I, let $\mathcal{G}$ be the measurable $\mathcal{M}_{q,p}$-valued function defined by (3.1) on the set $[0,1)\times[0,1/p)$. Since the system $\mathbf{G}(\alpha,\beta,g)$ is a frame for $\mathcal{M}(\alpha,\beta,g)$, the equivalence of (a) and (b) in Proposition 3.1 shows the existence of two positive constants C_1 and C_2 such that

$$C_1\mathcal{G}\mathcal{G}^* \leqslant (\mathcal{G}\mathcal{G}^*)^2 \leqslant C_2\mathcal{G}\mathcal{G}^*, \tag{4.2}$$

a. e. on $[0,1)\times[0,1/p)$. By Theorem 3.11, the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type I if and only if $\operatorname{rank}(\mathcal{G})=0$ or q a. e. on $[0,1)\times[0,1/p)$. Since the rank of $\mathcal{G}\mathcal{G}^*$ is the same as that of $\mathcal{G}$, it follows that, for a.e. $(t,\nu)\in[0,1)\times[0,1/p)$, the $q\times q$ matrix $(\mathcal{G}\mathcal{G}^*)(t,\nu)$ is either identically zero or invertible. On the set where $(\mathcal{G}\mathcal{G}^*)(t,\nu)$ is invertible, (4.1) reduces to the inequalities

$$C_1 I \leqslant \mathcal{G}\mathcal{G}^* \leqslant C_2 I, \tag{4.3}$$

where I denote the $q\times q$ identity matrix. Let $h(t,\nu)$ denote the first entry of $(\mathcal{G}\mathcal{G}^*)(t,\nu)$, i.e., $(\mathcal{G}\mathcal{G}^*)_{0,0}(t,\nu)$. Then, $\mathcal{G}\mathcal{G}^*$ is the zero $q\times q$ matrix on the set where $h=0$ and $\mathcal{G}\mathcal{G}^*$ is invertible on the set where $h\geqslant C_1$. By Lemma 4.5, $h(t,.)$ is continuous for a. e. $t\in[0,1)$. Hence, for a. e. $t\in[0,1)$, the function $\nu\mapsto h(t,\nu)$ is either identically zero or larger than C_1 for all $\nu\in[0,1/p)$. Therefore, if E is the subset of $[0,1)\times[0,1/p)$ where $\mathcal{G}\mathcal{G}^*$ is invertible, then E must thus be a Cartesian product of the form $E=E_1\times[0,1/p)$, where E_1 is a measurable subset of $[0, 1)$, modulo a set of zero measure. Similarly, since, by Lemma 4.5, the function $t\mapsto h(t,\nu)$ is continuous for a. e. $\nu\in[0,1/p)$, E must also have the form $E=[0,1)\times E_2$, where E_2 is a measurable subset of $[0,1/p)$, modulo a set of zero measure. Since $g\neq 0$, E must have positive measure and thus $E=[0,1)\times[0,1/p)$, modulo a set of zero measure, i.e., the rank of $\mathcal{G}\mathcal{G}^*$ is equal to q a. e. on $[0,1)\times[0,1/p)$. Proposition 3.5 shows then that the system $\mathbf{G}(\alpha,\beta,g)$ is a Riesz basis for $\mathcal{M}(\alpha,\beta,g)$. To prove that, under the conditions of the theorem, if the system $\mathbf{G}(\alpha,\beta,g)$ admits a unique dual of type II, then $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$, we use similar arguments and, in particular, the equivalence of (a) and (c) in Proposition (3.1) as well as Proposition 3.8. □

Proof of Theorem 1.2

By Theorem 2.3, the subspace Gabor frame $\mathbf{G}(\alpha,\beta,g)$ has a unique Gabor dual of type I whenever $\alpha\beta$ is an integer. Therefore, we can apply Theorem 2.6.

First assume that $\alpha\beta=1$. If $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$, then it is well-known that $\mathbf{G}(\alpha,\beta,g)$ is a Riesz basis for $L^2(\mathbb{R})$. Thus (1.1) holds by the Balian–Low theorem (Theorem 1.1). Otherwise, it is known that $\mathbf{G}(\alpha,\beta,g)$ cannot be a Riesz sequence (cf. Gabardo, 20xx). Therefore, we also have (1.1) by Theorem 2.5. Similarly, (ii) follows immediately from Theorem 2.6 and (iii) from Corollary 2.7 □

Finally we give an example showing that the condition in Theorem 1.2 cannot be dropped.

Example 4.8: Let $g(x)=e^{-x^2}$. Then

$$\left(\int_{\mathbb{R}} |xg(x)|^2 dx \right) \left(\int_{\mathbb{R}} |\omega \hat{g}(\omega)|^2 d\omega \right) < \infty$$

and $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence when $\alpha\beta$ is an integer larger than 1. We only need to check that $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence. We can assume that $\alpha=1$ and $\beta=n>1$. Since g is Gaussian, the Zak-transform of g has a single zero on the unit square $[0,1]\times[0,1]$ (Janssen, 1981; see also Janssen, 2003). Also, the associated Zak-transform matrix for $\mathbf{G}(\alpha,\beta,g)$ is the row matrix:

$$\mathcal{G}(t,\nu)=[Zg(t,\mu),Zg(t,\nu+1/n),\ldots,Zg(t,\nu+(n-1)/n)].$$

Hence, $\mathcal{G}\mathcal{G}^*(t,\nu)=\Sigma_{j=0}^{n-1}|Zg(t,\nu+j/n)|^2$ is a continuous function with no zeros on $[0,1]\times[0,1/n]$ (because $n>1$) and is, therefore, bounded from below. It is also true that $\mathcal{G}\mathcal{G}^*(t,\nu)$ is bounded. Thus, by Propositions 3.1 and 3.8, $\mathbf{G}(\alpha,\beta,g)$ is a Riesz sequence. Similar arguments using Propositions 3.1 and 3.5 show that, when $1/(\alpha\beta)$ is an integer larger than 1, then $\mathcal{M}(\alpha,\beta,g)=L^2(\mathbb{R})$.

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Bounds on the dragging rate of slowly and differentially rotating relativistic stars

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For relativistic stars rotating slowly and differentially with a positive angular velocity, some properties in relation to the positiveness of the rate of rotational dragging and of the angular momentum density are derived. Moreover, the proof for the bounds on the rotational mass-energy, which we have generalized (outside the slow rotation limit) in a previous paper, is briefly exposed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1767987]

I. INTRODUCTION

In a previously published paper[1] we have given general bounds on the dragging rate (angular velocity of locally nonrotating observers, or angular velocity of cumulative dragging) of a differentially rotating relativistic stellar configuration; however, the validity of these bounds depends heavily on the underlying *rotation law*, which must be compatible with the field equations.

In the prescription for calculating a *slowly* and differentially rotating relativistic stellar configuration the field equations are expanded in powers of a *fluid angular velocity parameter*, and the perturbations (around a nonrotating configuration) are calculated by retaining only first and second order terms. Hartle[2] has derived these equations of structure in the rigidly rotating case. It is remarkable that at first order the only effect of the rotation is to drag the inertial frames; at second order it also deforms the star. An expansion of the dragging rate potential in powers of the angular velocity parameter only contains odd powers. Hence, if one is interested in calculating all effects up to second order, it is then sufficient to include only the linear (first order) corrections in the dragging rate. And it turns out that up to first order there are no restrictions on the rotation profile by the field equations, more exactly, by the Euler equation, through a rotation law. Hence, the result on bounds on the dragging rate in the general (differentially) rotating case, mentioned above (Proposition 3 in Ref. 1), does not apply any more in the slow rotation limit. In the present paper the bounds on the dragging rate (including positivity of the angular momentum density) are refined for the slowly and differentially rotating case.

The first order equations of structure reduce to the time-angle field equation component (to first order), which is a partial differential equation, linear in the dragging rate potential. This linearity in the dragging rate persuades us to rewrite that equation in appropriate coordinates—in order to avoid the coordinate singularity occurring on the axis of rotation in spherical polar coordinates, generally used in the slow rotation approximation—so that in the new coordinates the equation writes in a ''regular'' form as an elliptic equation with measurable and bounded coefficients. This allows us to apply a minimum principle for generalized supersolutions in the whole domain (interior and exterior of the star). Making use of the asymptotic flatness condition, this will lead us directly to the positivity of the dragging rate, provided that the distribution of angular velocity of the fluid is non-negative everywhere (and nontrivial) and that we start from a reasonable unperturbed (nonrotating) stellar model satisfying the weak energy condition. In this case, the linearity (in the rotation) of the considered equation will guarantee a positive angular momentum density, provided that the amplitude of the rotation profile is bounded in a certain way.

The *rotational mass-energy*, derived by Hartle in Ref. 3, although accurate to second order in the angular velocity, involves only quantities which can be calculated from the first order structure equation (time-angle component of the Einstein field equations) as well. A proof of the positivity

and an upper bound on this rotational energy was given in the same paper,[3] however using an expansion in eigenfunctions (and leaving open the nontrivial mathematical problems which may arise on the existence of these eigenfunctions). We found a much simpler proof of that result, avoiding expansions in eigenfunctions (in the present paper briefly exposed) which, remarkably, was possible to generalize to the general differentially rotating case, i.e., outside the slow rotation limit (cf. Sec. V of Ref. 1).

The paper is organized as follows. After a description of the relativistic rotating stellar model in Sec. II, and a brief revision of the concepts of angular momentum density and rate of rotational dragging in Sec. III, in Sec. IV we concentrate on the slow rotation approximation, particularly on the first order perturbations of the metric (linear correction of the dragging rate, with description of the unperturbed, i.e., zero order, configuration), and explicit expressions for the expansions of the angular momentum density and of the rotational mass-energy are derived. In the same section the null contribution (at first order in the angular velocity) of the integrability condition of the Euler equation is discussed, and the time-angle component of the Einstein equations (to first order) is written in appropriate coordinates, as a background allowing to apply a minimum principle and obtain the first of the properties mentioned above and proved in Sec. V, and consequences of that one. Apart from this, we sketch here the alternative proof of the bounds on the rotational energy. Finally, in Sec. VI, concluding remarks are briefly stated.

II. THE RELATIVISTIC ROTATING STELLAR MODEL

The space–time of a rotating relativistic star is represented by a Lorentzian 4-manifold $(\mathcal{M}, \mathbf{g})$ which satisfies the following.

A. Assumptions

(i) The space–time is stationary in time and axially symmetric, which means that $\mathbf{g}$ admits two global Killing vector fields, a timelike future-directed one, $\boldsymbol{\xi}$, and a spacelike one, with closed trajectories, $\boldsymbol{\eta}$, except on a timelike 2-surface (defining the axis of rotation) where $\boldsymbol{\eta}$ vanishes;

(ii) the space–time is asymptotically flat; in particular, $\mathbf{g}(\boldsymbol{\xi},\boldsymbol{\xi})\to -1$, $\mathbf{g}(\boldsymbol{\eta},\boldsymbol{\eta})\to +\infty$, and $\mathbf{g}(\boldsymbol{\xi},\boldsymbol{\eta})\to 0$ at spatial infinity [the signature of the metric $\mathbf{g}$ being $(-+++)$];

(iii) the matter—confined in a compact region in the space (interior), with vacuum on the outside, so that (ii) holds—is perfect fluid, and therefore the energy-momentum tensor (source of the Einstein equations) is written as

$$\mathbf{T}=(\varepsilon+p)\mathbf{u}^\flat\otimes\mathbf{u}^\flat+p\,\mathbf{g}\,,$$

where ε and p denote the energy density and the pressure of the fluid, respectively; and $\mathbf{u}^\flat$ denotes the 1-form equivalent to the 4-velocity of the fluid $\mathbf{u}$ (in the exterior $\mathbf{T}\equiv 0$; hence, $\varepsilon+p=p=0$ there);

(iv) the fluid velocity is azimuthal (nonconvective) (*circularity condition*), i.e.,

$$\mathbf{u}^\flat\wedge\boldsymbol{\xi}^\flat\wedge\boldsymbol{\eta}^\flat=0\,;$$

(v) $(\mathcal{M}, \mathbf{g})$ satisfies Einstein's field equations $\mathbf{G}=8\pi\mathbf{T}$ for the energy-momentum tensor $\mathbf{T}$ of a perfect fluid (iii), where $\mathbf{G}\equiv\mathbf{Ric}-1/2\,R\,\mathbf{g}$ denotes the Einstein tensor—equations which can also be written in the form

$$\mathbf{Ric}=8\pi(\mathbf{T}-\tfrac{1}{2}tr(\mathbf{T})\,\mathbf{g})\,; \tag{1}$$

(vi) ε and p satisfy a barotropic (one-parameter) equation of state, $\varepsilon=\varepsilon(p)$;

(vii) $\varepsilon+p\geqslant 0$ (*weak energy condition* for perfect fluid, assuming $\varepsilon\geqslant 0$);[4]

(viii) the metric functions are essentially bounded.

B. Form of the metric

Assumptions (i) and (ii) imply that the two Killing fields commute, $[\boldsymbol{\xi},\boldsymbol{\eta}]=0$,[5] which is equivalent to the existence of coordinates $x^0\equiv t$ and $x^1\equiv\phi$ such that $\boldsymbol{\xi}\equiv\partial_t$ and $\boldsymbol{\eta}\equiv\partial_\phi$; moreover, by the circularity condition (iv), the space–time $\mathbf{g}$ admits 2-surfaces orthogonal to the group orbits of the Killing fields (orthogonal transitivity).[6] We may then choose the two remaining coordinates (x^2,x^3) in one of these 2-surfaces and carry them to the whole space–time along the integral curves of $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$; accordingly, the metric can be written in the form

$$\mathrm{d}s^2\equiv g_{\alpha\beta}\,\mathrm{d}x^\alpha\,\mathrm{d}x^\beta=g_{tt}\,\mathrm{d}t^2+2g_{t\phi}\,\mathrm{d}t\,\mathrm{d}\phi+g_{\phi\phi}\,\mathrm{d}\phi^2+g_{22}(\mathrm{d}x^2)^2+2g_{23}\,\mathrm{d}x^2\,\mathrm{d}x^3+g_{33}(\mathrm{d}x^3)^2\,,$$

where the metric coefficients are independent of the time $x^0\equiv t$ and azimuthal $x^1\equiv\phi$ coordinates corresponding to the two Killing fields; that is, $g_{\alpha\beta}=g_{\alpha\beta}(x^2,x^3)$.

When solving Einstein's field equations it is convenient to specify the coordinates x^2 and x^3 in such a way as to simplify the task; a particular choice, usually made when studying slowly rotating configurations,[2] is the one which makes $g_{23}=0$ and $g_{33}=g_{\phi\phi}\sin^{-2}x^3$. Hence x^2 and x^3 are chosen so that at large spatial distances the asymptotically flat metric is expressed in terms of spherical polar coordinates in the usual way. In the resulting coordinate system, with the notation $x^2\equiv r$, $x^3\equiv\theta$, and with new symbols for the metric functions, the line element reads

$$\mathrm{d}s^2=-H^2\,\mathrm{d}t^2+Q^2\,\mathrm{d}r^2+r^2K^2[\mathrm{d}\theta^2+\sin^2\theta\,(\mathrm{d}\phi-A\,\mathrm{d}t)^2]\,, \tag{2}$$

where H, Q, K, and A are functions of r and θ alone. In these coordinates ($r\geqslant 0$, $0\leqslant\theta\leqslant\pi$) the spatial infinity is given by $r\to\infty$, and the axis of rotation ($\partial_\phi\equiv\boldsymbol{\eta}=0$) is described by $\theta\to 0$ or π ($r\geqslant 0$).

Notice that the function A appears in the metric (2) as the nonvanishing of the $(t\phi)$ metric component of a rotating configuration. A is actually the *dragging rate* potential (cf. Sec. III).

C. Differential rotation

According to assumption (iv) of Sec. II A—circularity condition—the fluid 4-velocity $\mathbf{u}$ has the form

$$\mathbf{u}=u^t\partial_t+u^\phi\partial_\phi=u^t(\partial_t+\Omega\,\partial_\phi),\quad \text{where}\ \ \Omega\equiv\frac{u^\phi}{u^t}=\frac{\mathrm{d}\phi}{\mathrm{d}t}$$

is the angular velocity of the fluid measured in units of t, i.e., as seen by an inertial observer at infinity whose proper time is the same as the coordinate t (observer ∂_t), and u^t is the normalization factor, such that $\mathbf{g}(\mathbf{u},\mathbf{u})=-1$, i.e., $(u^t)^{-2}=-(g_{tt}+2\Omega g_{t\phi}+\Omega^2 g_{\phi\phi})$. The star's matter rotates then in the azimuthal direction ϕ.

We consider a star rotating differentially, with a prescribed distribution of angular velocity

$$\Omega\equiv\Omega(x^2,x^3)\equiv\Omega(r,\theta)\,,$$

an essentially bounded function. However, with the assumptions made (Sec. II A), the rotation profile of the fluid cannot be freely chosen, this shows up in the following. We consider the equation of hydrostatic equilibrium, $T^{\alpha\beta}{}_{;\beta}=0$ (integrability conditions of the field equations), particularly, its part orthogonal to the fluid 4-velocity $\mathbf{u}$, i.e., the Euler equation,

$$\mathrm{d}p=-(\varepsilon+p)\,\mathbf{a}\,, \tag{3}$$

where $\mathbf{a}$ is the 4-acceleration of the fluid, $\mathbf{a}^\sharp=\nabla_{\mathbf{u}}\mathbf{u}$, specifically,

$$\mathbf{a}=-\,\mathrm{d}\ln u^t+u^t u_\phi\,\mathrm{d}\Omega\,. \tag{4}$$

And the integrability condition of Eq. (3), taking into account (vi) of Sec. II A, $\varepsilon=\varepsilon(p)$, is d**a** $=0$; following, from (4), $\mathrm{d}(u^t u_\phi)\wedge \mathrm{d}\Omega=0$; in other words, the fluid angular velocity, Ω, is functionally related to the specific angular momentum times u^t,

$$u^t u_\phi=\mathcal{F}(\Omega)\,. \tag{5}$$

Nevertheless, as will be seen in Sec. IV B, in the slow rotation approximation, at first order in the angular velocity, Eq. (5) is no restriction on the rotation profile $\Omega(r,\theta)$.

III. ANGULAR MOMENTUM DENSITY AND DRAGGING RATE

The total angular momentum of a rotating relativistic star can be defined[7] from the variational principle for general relativity—for an isolated system which is not radiating gravitational waves—but this is shown[7] to coincide with the *geometrical* definition—from the asymptotic form of the metric at large spacelike distances from the rotating fluid—(analog to the ADM mass), which for stationary and axisymmetric (asymptotically flat) space–times is given by the Komar integral for the angular momentum,[8] a surface integral, which, when reformulated using the Gauss theorem and the Einstein equations, converts into the volume integral over the interior

$$J=\int_{\mathcal{I}} T_\alpha{}^\beta \eta^\alpha n_\beta \,\mathrm{d}v \tag{6}$$

$$=\int_{\mathcal{I}} T_\phi{}^t n_t \,\mathrm{d}v=\int_{\mathcal{I}} T_\phi{}^t(-\mathrm{g})^{1/2}\,\mathrm{d}^3x\,, \tag{7}$$

where **T** is the energy-momentum tensor of perfect fluid, $\boldsymbol{\eta}$ is the Killing field corresponding to the axial symmetry, $\mathbf{n}^\sharp$ is the unit timelike and future pointing normal to the hypersurface of constant t, i.e., $\mathbf{n}=n_t\,\mathrm{d}t$, with $n_t>0$, and $\mathrm{d}v$ is the proper volume element of the surface $t=$const, i.e., $\int_{\mathcal{I}}\mathrm{d}v=\mathrm{Vol}$, the volume of the body of the star, $\mathcal{I}\equiv$interior of the star ($t=$const). Here $g\equiv\det(\mathbf{g})$. The invariantly defined integrand of this volume integral (6), $T_\alpha{}^\beta\eta^\alpha n_\beta$, is what one would naturally define as *angular momentum density*—coinciding with the standard form in special relativity—and can be calculated as

$$\begin{aligned} T_\alpha{}^\beta\eta^\alpha n_\beta &= n_t T_\phi{}^t = n_t(\varepsilon+p)u^t u_\phi \quad [u_\phi=u^t(g_{t\phi}+\Omega g_{\phi\phi})]= n_t(\varepsilon+p)(u^t)^2(g_{t\phi}+\Omega g_{\phi\phi}) \\ &= n_t(\varepsilon+p)(u^t)^2 g_{\phi\phi}(\Omega-A), \quad \text{with } n_t=H=\left(\frac{-g_{tt}g_{\phi\phi}+g_{t\phi}^2}{g_{\phi\phi}}\right)^{1/2}, \end{aligned} \tag{8}$$

where A is the metric function [cf. (2)] such that

$$g_{t\phi}=-A\ g_{\phi\phi}\,. \tag{9}$$

It is remarkable that, since $n_t>0$, $g_{\phi\phi}\geqslant 0$, and we are assuming the energy condition $\varepsilon+p\geqslant 0$ [(vii) in Sec. II A], the sign of the angular momentum density (8) is determined by the sign of the difference $\Omega-A$.

The metric function A is indeed the angular velocity of a particle which is dragged along in the gravitational field of the star, as seen from a nonrotating observer at spatial infinity (∂_t), so that it has zero angular momentum relative to the axis, $p_\phi=0$,

$$\frac{\mathrm{d}\phi}{\mathrm{d}t}=\frac{p^\phi}{p^t}=\frac{g^{t\phi}p_t}{g^{tt}p_t}=\frac{g^{t\phi}}{g^{tt}}=\frac{-g_{t\phi}}{g_{\phi\phi}}, \quad g_{t\phi}+\left(\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)g_{\phi\phi}=0, \quad \frac{\mathrm{d}\phi}{\mathrm{d}t}=A\,.$$

A is called *angular velocity of cumulative dragging* (shortly called *dragging rate*).[9,10] One of the purposes of this work is precisely to find appropriate bounds on the uniformly non-negative

distribution of angular velocity, $\Omega \equiv \Omega(x^2,x^3) \geqslant 0$, of a slowly differentially rotating star, so that $\Omega - A \geqslant 0$ holds; from where the positivity of the angular momentum density (8) follows [property (c) in Sec. V].

Observe, in the special relativistic limit [$g_{t\phi} \to 0$, using coordinates (x^2,x^3) which go at spatial infinity to the usual flat coordinates, cf. Sec. II B], if the fluid rotates uniformly with angular velocity Ω positive (negative), then the angular momentum density, Eq. (8), is uniformly positive (negative).

IV. SLOWLY DIFFERENTIALLY ROTATING STARS: FIRST ORDER PERTURBATIONS

By slow rotation we mean that the absolute value of the angular velocity is much smaller than the critical value $\Omega_{\text{crit}} \equiv (M/R^3)^{1/2}$ (taking units $c=G=1$), where M is the total mass of the unperturbed (nonrotating) configuration, and R, its radius; $|\Omega(x^2,x^3)|/\Omega_{\text{crit}} \ll 1$. Thus, stars which rotate slowly can be studied by expanding the Einstein field equations for a fully relativistic differentially rotating star in powers of the dimensionless ratio

$$\frac{|\Omega_{\max}|}{\Omega_{\text{crit}}} =: \mu \,, \tag{10}$$

where $|\Omega_{\max}|$ is the maximum value of $|\Omega(x^2,x^3)|$ (at the interior of the star).

A. The metric and the energy density and pressure of the fluid

We assume that the star is slowly rotating, with angular velocity

$$\Omega(r,\theta) \equiv \Omega(x^2,x^3) = O(\mu) \,,$$

parameter μ given, e.g., by (10). Because the star (stationary in time and axially symmetric) rotates in the ϕ direction [(iv) of Sec. II A], a time reversal ($t \to -t$) would change the sense of rotation, as well as an inversion in the ϕ direction ($\phi \to -\phi$) would do. As a result, the metric coefficients H, Q, and K [in (2)] and the energy density will not change sign under *one of* these inversions, whereas A will do. Therefore, an expansion of H, Q, and K, as well as of the energy density, ε, and, hence, of the pressure, p, in powers of the angular velocity parameter μ will contain only even powers, while an expansion of the dragging rate, A, will have only odd ones. Hence, considering effects up to second order only the linear corrections in the dragging rate count. Indeed, the only first order $O(\mu)$ perturbation brought about by the rotation is the dragging of the inertial frames; the star is still spherical, because the ''potential functions'' which deform the shape of the star are $O(\mu^2)$. We shall keep here only the effects linear in the angular velocity. At first order, $O(\mu)$, the metric coefficients, and fluid energy density and pressure, are

$$\begin{aligned} H &= H_0 + O(\mu^2), \\ Q &= Q_0 + O(\mu^2), \\ K &= K_0 + O(\mu^2), \\ \varepsilon &= \varepsilon_0 + O(\mu^2), \\ p &= p_0 + O(\mu^2), \\ \text{but } A &= \omega + O(\mu^3), \end{aligned} \tag{11}$$

where H_0, Q_0, and K_0 are the coefficients of the unperturbed (nonrotating) configuration, and ω denotes the linear (first order) correction in μ of the dragging rate A, so that, from Eq. (9),

$$g_{t\phi} = -\omega \ (g_{\phi\phi})_0 + O(\mu^3) \,. \tag{12}$$

The (unperturbed) nonrotating configuration: The starting nonrotating equilibrium configuration is described by the spherically symmetric metric in the Schwarzschild form

$$\begin{aligned} ds^2 &= -e^{\nu(r)}\,dt^2 + e^{\lambda(r)}\,dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2) \\ &\equiv -H_0{}^2\,dt^2 + Q_0{}^2\,dr^2 + r^2K_0{}^2\,(d\theta^2 + \sin^2\theta\, d\phi^2) \quad (A_0 = 0)\,, \end{aligned} \tag{13}$$

with $\lambda(r)$, or equivalently, the mass $m(r)$ interior to a given radial coordinate r, given by

$$1 - \frac{2m(r)}{r} = e^{-\lambda(r)}\,, \tag{14}$$

and $\nu(r)$, together with the pressure $p_0(r)$, and the energy density $\varepsilon_0(r)$, solutions of the system of equations of general relativistic hydrostatics, which for a nonrotating configuration are the equation of hydrostatic equilibrium (Tolman–Oppenheimer–Volkoff equation),

$$\frac{dp_0}{dr}(r) = -\frac{[\varepsilon_0(r) + p_0(r)][m(r) + 4\pi r^3 p_0(r)]}{r^2[1 - 2m(r)/r]}\,, \tag{15}$$

the mass equation,

$$\frac{dm}{dr}(r) = 4\pi r^2 \varepsilon_0(r)\,, \tag{16}$$

and the source equation for ν,

$$\frac{d\nu}{dr}(r) = -\frac{2}{\varepsilon_0(r) + p_0(r)}\,\frac{dp_0}{dr}(r)\,, \tag{17}$$

with the initial boundary conditions

$$0 < p_0(0) = p_{0c} < \infty \quad \text{(central pressure)},$$

$$m(0) = 0\,, \quad \text{and}$$

$$\nu(0) = \nu_c \quad \text{(constant fixed by the asymptotic condition at infinity)},$$

this being the prescription for the interior of the star, that is, inside the fluid, $r \leqslant R$, $R \equiv$ radius of the surface of the star, determined by $p_0(R) = 0$. Furthermore, we assume p_0 and ε_0 related to each other by a barotropic equation of state,

$$\varepsilon_0 = \varepsilon_0(p_0)\,, \tag{18}$$

$p_0 \mapsto \varepsilon_0(p_0)$ a bounded function on any closed interval, and satisfying the weak energy condition

$$\varepsilon_0 + p_0 \geqslant 0\,. \tag{19}$$

Observe, from Eqs. (15) and (19), p_0 is a decreasing function from the center, $r = 0$, to the star's surface, $r = R$; in particular, $p_0 \geqslant 0$ and attains its maximum value p_{0c} at the center.

In the exterior (vacuum) the geometry is described by the same line element (13), but with the metric function ν specified and related to λ by

$$e^{\nu(r)} = e^{-\lambda(r)} = 1 - \frac{2M}{r}, \quad \forall r > R\,, \tag{20}$$

where $M \equiv m(R)$ is the star's total mass.

Notice that this standard form of the nonrotating metric, (13), is the limit of zero rotation of the general rotating metric in spherical polar coordinates (2),

$$H\to H_0\equiv e^{\nu/2},\quad Q\to Q_0\equiv e^{\lambda/2},\quad K\to K_0\equiv 1,\quad A\to A_0\equiv 0\,,$$

from where the effect of the rotation can be seen as given by the term $\mathrm{d}\phi - A\,\mathrm{d}t$ in the place of $\mathrm{d}\phi$.

Note, since at first order in the angular velocity there is still no effect on the pressure and on the energy density [cf. (11)], conditions (18) and (19) for the starting nonrotating configuration guarantee (vi) and (vii) of Sec. II A at first order.

B. Euler equation

It will be important to note that at first order the Ω-profile is not restricted by the field equations (through the Euler equation). That shows up in the following. Consider the first integral of the Euler equation (3), namely,

$$\int_0^{p(r,\theta)} \frac{\mathrm{d}\overline{p}}{\varepsilon(\overline{p})+\overline{p}} + \frac{1}{2}\ln[(u^t)^{-2}]\Big|_{(r,\theta)} + \int_{\Omega_0}^{\Omega(r,\theta)} \mathcal{F}(\Omega)\,\mathrm{d}\Omega = \mathrm{const}\,, \tag{21}$$

where Eqs. (4) and (5) have been used, and Ω_0 is a given constant (changing the value of Ω_0 simply modifies the value of the constant on the right-hand side). The first term in Eq. (21) is a function of the pressure, which is, to this approximation, a function of r, i.e., $O(1)$ with respect to the angular velocity; on the other hand,

$$(u^t)^{-2} = -(g_{tt}+2\Omega g_{t\phi}+\Omega^2 g_{\phi\phi}) = H^2 - K^2 r^2 \sin^2\theta\,(\Omega-A)^2 = O(1-(\Omega-A)^2)\,,$$

so the second term is $O((\Omega-A)^2)$ and, hence, $O(\mu^2)$; also, since

$$u^t u_\phi = (u^t)^2 g_{\phi\phi}(\Omega-A) = \frac{K^2 r^2 \sin^2\theta\,(\Omega-A)}{H^2 - K^2 r^2 \sin^2\theta\,(\Omega-A)^2} = O(\Omega-A)\,,$$

$\mathcal{F}(\Omega) = u^t u_\phi = O(\Omega-A)$, thus, the third term is $O((\Omega-A)^2)$ as well, and, hence, $O(\mu^2)$. Consequently, to $O(\mu)$, the Euler equation reduces to its static (nonrotating) case, and indeed we have presumably already used it to get the starting unperturbed solution. Therefore, at this order in the angular velocity, Eq. (5) is no restriction on $\Omega(r,\theta)$.

C. The angular momentum density

Using the definition of ω, linear correction of the dragging rate, via the expansion of the metric coefficient $g_{t\phi}$, Eq. (12), and the metric coefficients of the nonrotating configuration [cf. (13)], we obtain the expansion for the angular momentum density (8),

$$\begin{aligned} T_\alpha{}^\beta \eta^\alpha n_\beta = n_t T_\phi{}^t &= n_t(\varepsilon+p)(u^t)^2(g_{t\phi}+\Omega g_{\phi\phi}) \\ &= (n_t)_0(\varepsilon_0+p_0)[(-g_{tt})_0]^{-1}[-\omega\ (g_{\phi\phi})_0+\Omega\ (g_{\phi\phi})_0]+O(\mu^3) \\ &= e^{\nu/2}(\varepsilon_0+p_0)e^{-\nu}r^2\sin^2\theta(\Omega-\omega)+O(\mu^3) \\ &= (\varepsilon_0+p_0)\,e^{-\nu/2}r^2\sin^2\theta\ (\Omega-\omega)+O(\mu^3)\,. \end{aligned} \tag{22}$$

Thus showing also for the first order rotational perturbation that, since we are assuming the energy condition $\varepsilon_0+p_0\geqslant 0$, the sign of the angular momentum density (22) to $O(\mu)$ is determined by the sign of $\Omega-\omega$.

D. The rotational mass-energy

In Ref. 3 Hartle has derived the difference in total mass-energy, $M_{\rm rot}$, between a slowly and differentially rotating relativistic star and a nonrotating star with the same number of baryons and the same distribution of entropy, namely,

$$M_{\rm rot}=\frac{1}{2}\int_{\mathcal{I}}\Omega\,\mathrm{d}J+O(\mu^4)\,,$$

where $\mathrm{d}J$ is the angular momentum of a fluid element in the star (to first order in the angular velocity), i.e., from (7),

$$\mathrm{d}J=T_{\phi}{}^{t}(-\mathrm{g})^{1/2}\,\mathrm{d}^3x|_{O(\mu)}\,;$$

taking into account (22) and (13), we obtain an explicit expression for the expansion of $M_{\rm rot}$ in powers of the angular velocity parameter μ,

$$M_{\rm rot}=\frac{1}{2}\int_0^R\mathrm{d}r\int_0^{\pi}\,\mathrm{d}\theta\,2\pi(\varepsilon_0+p_0)\,r^4\,e^{(\lambda-\nu)/2}\sin^3\theta\,\Omega(\Omega-\omega)+O(\mu^4)\,. \tag{23}$$

E. The time-angle component of the Einstein equation

The $(t\phi)$ field equation component retaining only first order terms in the angular velocity (second order terms vanish), i.e., from Eq. (1),

$$R_{\phi}{}^{t}=8\pi T_{\phi}{}^{t}+O(\mu^3)\,,$$

takes the form

$$\partial_r[r^4j(r)\,\partial_r\omega]+\frac{r^2\,k(r)}{\sin^3\theta}\,\partial_\theta[\sin^3\theta\,\partial_\theta\omega]-16\pi\,r^4k(r)[\varepsilon_0(r)+p_0(r)][\omega-\Omega]=0\,, \tag{24}$$

where we have introduced the abbreviations

$$j(r)\equiv e^{-[\lambda(r)+\nu(r)]/2}\quad\text{and}\quad k(r)\equiv e^{[\lambda(r)-\nu(r)]/2}\,. \tag{25}$$

As outlined in Ref. 2, using the 0-order field equations, (14)–(17), it follows

$$4\pi\,r\,[\varepsilon_0(r)+p_0(r)]\,k(r)=-j'(r) \tag{26}$$

(where $'\equiv\mathrm{d}/\mathrm{d}r$), which, substituted into Eq. (24), yields

$$\partial_r[r^4j(r)\,\partial_r\omega]+\frac{r^2\,k(r)}{\sin^3\theta}\,\partial_\theta[\sin^3\theta\,\partial_\theta\omega]+4\,r^3j'(r)\,\omega=4\,r^3j'(r)\,\Omega(r,\theta)\,. \tag{27}$$

We write this differential equation for the dragging rate in the abbreviated form

$$\overline{L}\,\omega=-\Psi^2\Omega\,, \tag{28}$$

with the linear second order partial differential operator $\overline{L}\equiv\overline{L}_0-\Psi^2$, where

$$\overline{L}_0\omega:=\frac{1}{r^4j(r)}\,\partial_r[r^4j(r)\,\partial_r\omega]+\frac{k(r)}{r^2j(r)\sin^3\theta}\,\partial_\theta[\sin^3\theta\,\partial_\theta\omega] \tag{29}$$

and

$$\Psi^2(r) := -\frac{4}{r}\frac{j'(r)}{j(r)} = 16\pi[\varepsilon_0(r)+p_0(r)]\frac{k(r)}{j(r)} \geqslant 0 \quad \forall r \geqslant 0\,. \tag{30}$$

Equation (26) has been used in (30), and the sign follows from the assumed energy condition (19), the functions j and k [cf. (25)] are always positive. Notice, $\Psi^2 \equiv 0$ in the exterior ($\forall r \in [R,\infty[$), where vacuum [$\varepsilon_0 = p_0 = 0$, cf. (iii) in Sec. II A] is considered.

Specifically, we are only interested in solutions $\omega \equiv \omega(r,\theta)$ of Eq. (28) in $[0,\infty[\times[0,\pi]$, which satisfy the *boundary conditions*

$$\omega \quad \text{asymptotically flat} \quad \left(\lim_{r\to\infty}\omega = 0\right), \tag{31}$$

$$\omega \quad C^1 \text{ regular on the axis of rotation}, \tag{32}$$

and a *matching condition*, namely, to be at least a class C^1 function on the surface of the star—which is spherical at first order rotational perturbations—

$$\omega(.,\theta) \text{class } C^1 \text{ across } r = R\,. \tag{33}$$

Notice, (31) follows from our star model [condition (ii) in Sec. II A], and it can be easily seen that (33) follows from the equation itself, provided that $\omega(.,\theta)$ and $\Omega(.,\theta)$ are at least essentially bounded ($\in L^\infty$)—as has been assumed—i.e., even if they have a jump discontinuity.

At the star's surface, $r = R$, higher regularity of $\omega(.,\theta)$ is not guaranteed by the equation, due to a jump discontinuity of the function Ψ^2 at this point. For this reason, we shall be considering (in the following section) *generalized* ($\in W^{1,2}$) solutions ω of Eq. (28) in the whole domain (interior and exterior).

"*Coordinate change*": In order to avoid the coordinate singularity occurring on the axis in polar coordinates (r,θ), and wishing instead to have in the differential operator (29) a Lapacian in some higher dimension, we consider the following "change of coordinates." First, we introduce *isotropic* cylindrical coordinates in the meridian plane,

$$(r,\theta) \mapsto (\rho := h(r)\sin\theta,\ \ z := h(r)\cos\theta) \in \mathbb{R}_0^+ \times \mathbb{R}\,, \tag{34}$$

with the function h satisfying the following ordinary differential equation of first order with separated coefficients:

$$\frac{h'(r)}{h(r)} = \frac{e^{\lambda(r)/2}}{r} \tag{35}$$

[which makes the coefficient of the crossed derivatives in the operator (29) after the change (34) to vanish], and the *boundary condition*

$$\lim_{r\to\infty}\frac{h(r)}{r} = 1\,, \tag{36}$$

i.e., so that the *isotropic* radius $h(r) \equiv \overline{r}$ approaches r at spatial infinity, because far away from the source we assume to have Euclidean geometry. This leads us to the definition of the function [having $\omega(r,\theta)$]

$$w(\rho,z) := \omega(h^{-1}(\sqrt{\rho^2+z^2}),\ \arctan(\rho/z))\,, \tag{37}$$

or inversely, w such that

$$\omega(r,\theta) = w(h(r)\sin\theta,\ h(r)\cos\theta)\,.$$

Second (in the spirit of Ref. 11), we define [with $w(\rho,z)$] the 5-*lift of* $w:\mathbb{R}_0^+\times\mathbb{R}\to\mathbb{R}$ in flat $\mathbb{R}^5$, axisymmetric around the x_5 axis, by

$$w\mapsto\tilde{\omega}\ \text{ such that }\ \tilde{\omega}(\mathbf{x})\equiv\tilde{\omega}(x_1,x_2,x_3,x_4,x_5):=w\left(\ \rho=\left(\sum_{i=1}^{4}x_i^{\,2}\right)^{1/2},\ z=x_5\ \right), \tag{38}$$

and, for every function $\tilde{\omega}:\mathbb{R}^5\to\mathbb{R}$, the *meridional cut (in direction* x_1*) of* $\tilde{\omega}$,

$$\tilde{\omega}\mapsto w\ \text{ such that }\ w(\rho,z):=\tilde{\omega}(\rho,0,0,0,z)\,.$$

For axisymmetric functions these are isometric operations inverse to each other.[11] After considering the change of variable (34) with (37) in the differential operator $\overline{L_0}$ (29), we get [remember (25), $e^{\lambda}=k/j$]

$$\overline{L_0}\,w=\frac{e^{\lambda(r)}h(r)^2}{r^2}\left\{\partial_{\rho\rho}w+\partial_{zz}w+\frac{3}{\rho}\partial_\rho w+H(r)\,\frac{\rho\,\partial_\rho w+z\,\partial_z w}{h(r)}\right\}, \tag{39}$$

where

$$H(r):=\frac{-e^{[-\lambda(r)/2]}[-6+6\,e^{[\lambda(r)/2]}+r\,\nu'(r)]}{2\,h(r)}. \tag{40}$$

But, through the 5-lift (38), the flat Laplacian in five dimensions of the "lifted" function $\tilde{\omega}$ gives exactly

$$\Delta\tilde{\omega}\equiv\sum_{i=1}^{5}\partial_{ii}\tilde{\omega}=\partial_{\rho\rho}w+\partial_{zz}w+\frac{3}{\rho}\partial_\rho w\,, \tag{41}$$

the first three terms in the curly brackets of (39). Furthermore, as outlined in Ref. 11, n-lift and meridional cut (of *axisymmetric functions*) leave the regularity properties and the norm invariant; and *axisymmetric* operations, like multiplication, $\partial_{\overline{r}}$ [$\overline{r}\equiv h(r)=(\rho^2+z^2)^{1/2}=(\Sigma_{i=1}^5 x_i^{\,2})^{1/2}$], and scalar product, commute with n-lift and meridional cut. In particular, in the fourth term in the curly brackets of (39) the factor

$$\rho\,\partial_\rho w+z\,\partial_z w=\partial_{\overline{r}}\tilde{\omega}=\sum_{i=1}^{5}x_i\,\partial_i\tilde{\omega}\,. \tag{42}$$

Therefore, substituting (41) and (42) into (39), Eq. (28) in the form $\overline{L_0}\tilde{\omega}=-\Psi^2(\tilde{\Omega}-\tilde{\omega})$ (with $\tilde{\Omega}$ defined from Ω as it was $\tilde{\omega}$ from ω, and $\Psi^2=e^{\lambda}16\pi[\varepsilon_0+p_0]$) now writes

$$\overline{L_0}\,\tilde{\omega}\equiv\frac{e^{\lambda(r)}h(r)^2}{r^2}\left\{\Delta\tilde{\omega}+H(r)\,\frac{\Sigma_{i=1}^5 x_i\,\partial_i\tilde{\omega}}{h(r)}\right\}=e^{\lambda(r)}\{-16\pi[\varepsilon_0(r)+p_0(r)][\tilde{\Omega}-\tilde{\omega}]\}\,,$$

or, equivalently,[12]

$$\Delta\tilde{\omega}+H(r)\,\frac{\Sigma_{i=1}^5 x_i\,\partial_i\tilde{\omega}}{h(r)}=-16\pi\,\frac{r^2}{h(r)^2}[\varepsilon_0(r)+p_0(r)][\tilde{\Omega}-\tilde{\omega}]\,. \tag{43}$$

V. PROPERTIES

With the assumptions made in Sec. II A for this slowly rotating configuration [starting from a nonrotating one as described in Sec. IV A; particularly, satisfying the energy condition $\varepsilon_0+p_0\geqslant 0$], and considering only solutions of Eq. (28) satisfying the boundary and matching conditions (31), (32), and (33), the following results hold.

Property (a) (positiveness of the dragging rate): If the distribution of angular velocity of the fluid is non-negative (and nontrivial), then the dragging rate *(to first order in the fluid angular velocity) is positive everywhere,*

$$\Omega \geqslant 0, \quad \Omega \not\equiv 0 \Rightarrow \ \omega > 0 \, .$$

Proof: We have seen in the former section that, using the coordinate change (34) and the 5-lift (38), Eq. (28) for ω is equivalent to Eq. (43) for $\tilde{\omega}$, which reads

$$L\tilde{\omega} \coloneqq \Delta\tilde{\omega} + \sum_{i=1}^{5} H(r)\frac{x_i}{h(r)}\partial_i\tilde{\omega} - 16\pi[\varepsilon_0 + p_0]\frac{r^2}{h(r)^2}\tilde{\omega} = -16\pi[\varepsilon_0 + p_0]\frac{r^2}{h(r)^2}\tilde{\Omega} \, . \tag{44}$$

This equation may be obviously written *in divergence form*

$$L\tilde{\omega} \equiv \partial_i[a^{ij}(\mathbf{x})\partial_j\tilde{\omega} + a^i(\mathbf{x})\,\tilde{\omega}] + b^i(\mathbf{x})\,\partial_i\tilde{\omega} + c(\mathbf{x})\,\tilde{\omega} = g(\mathbf{x})$$

(where repeated indices denote summation over the index), with the coefficients

$$\begin{gathered} a^{ij}(\mathbf{x}) \equiv \delta_{ij} \quad (=1 \ \text{ if } \ i=j, \ \text{ and } \ =0 \ \text{ otherwise}) \, , \\ a^i(\mathbf{x}) \equiv 0 \, , \\ b^i(\mathbf{x}) = H(r)\frac{x_i}{h(r)} \quad (\forall\, i,j \in \{1,\ldots,5\}), \\ c(\mathbf{x}) = -16\pi[\varepsilon_0(r) + p_0(r)]\frac{r^2}{h(r)^2} \quad (\leqslant 0) \, , \end{gathered} \tag{45}$$

and

$$g(\mathbf{x}) = c(\mathbf{x})\,\tilde{\Omega}(\mathbf{x}) \, . \tag{46}$$

The isotropic radius $\overline{r} \equiv h(r)$ is Gaussian coordinate with respect to the star's surface, $\overline{r} = h(R)$, and, thus, $\tilde{\omega}$ is at least class C^1 across this surface; therefore, $\tilde{\omega} \in C^1(\mathbb{R}^5)$. Thus, considering the domain G defined by a ball in $\mathbb{R}^5$ centered at the origin of coordinates $\mathbf{x} = \mathbf{0}$ ($\overline{r} = 0$) and of arbitrary large radius σ,

$$G \coloneqq \mathcal{B}_\sigma(\mathbf{0}) \subset \mathbb{R}^5 \, , \tag{47}$$

the function $\tilde{\omega}$ and its (first) derivatives (continuous in $\mathbb{R}^5$) are 2-integrable in G, i.e., $\tilde{\omega} \in W^{1,2}(G) \cap C^1(G)$, and Eq. (43) is satisfied in G in a generalized sense (cf. Appendix B).

Notice, whenever $\tilde{\Omega} \geqslant 0$, we have, by (46), $g \leqslant 0$ (because $c \leqslant 0$), and, hence, $L\tilde{\omega} \leqslant 0$, specifically $\tilde{\omega}$ is a generalized supersolution relative to the operator L, in (44), and the domain G (47). We look at the requirements for a minimum principle to be applied (Appendix B). The Laplacian operator is obviously strictly elliptic, and the coefficients (45) are measurable and bounded functions on G, this shows up in the following: the mapping $r \mapsto r/h(r)$ is bounded from above and below everywhere in $[0,\infty[$ (Appendix A); $\varepsilon_0 + p_0$ is also bounded, since p_0 is bounded and $p_0 \mapsto \varepsilon_0(p_0)$ is bounded in any closed interval (Sec. IV A); consequently, the coefficient c is bounded (from above and below); the coefficients of the first derivatives, b^i, are also bounded (from above and below), because the function H is bounded everywhere (Appendix A) and since $(\forall i = 1,\ldots,5)$ ${x_i}^2 \leqslant \Sigma_{j=1}^5 {x_j}^2 = h(r)^2$, we have $[x_i/h(r)]^2 \leqslant 1$. Thus, all conditions of a minimum principle for generalized supersolutions relative to the differential operator L and the domain G hold, and, as a result of the *weak* minimum principle (Theorem 1 in Appendix B), we have

$$\inf_G \tilde{\omega} \geqslant \inf_{\partial G} \tilde{\omega}^- \quad [\tilde{\omega}^- \equiv \min(\tilde{\omega},0)]. \tag{48}$$

But, since the radius of the ball G is arbitrary, we can make it sufficiently large ($\sigma \to \infty$) so that, by asymptotic flatness [$\lim_{h(r)\to\infty} \tilde{\omega}=0$, from condition (31) and $\lim_{r\to\infty}[h(r)/r]=1$], $\tilde{\omega}$ is arbitrary small at ∂G, following, from (48), $\tilde{\omega} \geqslant 0$. Actually, the positivity is strict, because if $\tilde{\omega}(\mathbf{x}_0)=0$ for some $\mathbf{x}_0 \in G$ (interior point), then $\tilde{\omega}(\mathbf{x}_0)=\min \tilde{\omega}$ (since $\tilde{\omega} \geqslant 0$), and, by the *strong* minimum principle (Theorem 2 in Appendix B), $\tilde{\omega}$ would be constant in G; in this case, $\tilde{\omega} \equiv \text{const}=0$ in G (i.e., everywhere); but $\tilde{\omega} \equiv 0$ yields, by Eq. (44), $\tilde{\Omega} \equiv 0$, or, equivalently, $\Omega \equiv 0$, and we are assuming that Ω is nontrivial. We conclude then $\omega > 0$ everywhere. □

Property (b): Suppose we perturb the nonrotating configuration (in particular, with a given equation of state) with two (small) different distributions of angular velocity, Ω_1 and Ω_2, and integrate Eq. (28) to obtain their respective solutions for the dragging rate, ω_1 and ω_2, then

$$\Omega_1 \geqslant \Omega_2, \quad \Omega_1 \neq \Omega_2 \Rightarrow \ \omega_1 > \omega_2.$$

Proof: This follows from the linearity of Eq. (28) and Property (a). □

We are already in position to get a result about the positiveness of the difference $\Omega - \omega$, and, hence, of the *angular momentum density* (22). However, in order to first do this more specific and concrete, we shall make use of a property for the particular case of rigid rotation (RR), which can be found in Ref. 2, Sec. IV.

Property RR: For the slowly rotating configuration, if $\Omega(r,\theta) \equiv \text{const} \equiv \hat{\Omega} > 0$ ($in\ [0,R] \times [0,\pi]$) then

$$\omega(r,\theta) = \omega(r),$$

$$0 < \omega(r) < \hat{\Omega} \ \ in \ \ [0,R]$$

$$\omega > 0 \ in \ \ [0,\infty[\,, \ \ \omega' < 0 \ \ in \ \ ]0,\infty[\,, \ \ \omega'(0)=0.$$

Property (c) (positiveness of the angular momentum density): For the slowly rotating configuration, with a given equation of state, its dragging rate ω will satisfy

$$\omega(r,\theta) < \Omega(r,\theta)$$

if $\Omega \equiv \Omega(r,\theta)$ ($\geqslant 0$) is bounded in the form

$$\underline{\Omega}(\overline{\Omega}) \equiv \underline{\Omega} \ \leqslant \ \Omega(r,\theta) \ \leqslant \ \overline{\Omega}$$

(in $[0,R]\times[0,\pi]$), where $\overline{\Omega}$ is an arbitrary positive constant $0 < \overline{\Omega}$ ($\ll \Omega_{\text{crit}}$) (Sec. IV), and $\underline{\Omega} = \overline{\omega}(0)$, $\overline{\omega}$ solution of Eq. (28) with $\overline{\Omega}(r,\theta) = \text{const} = \overline{\Omega}$, and with the same 0-order coefficients (same starting nonrotating configuration) as the ones considered for our slowly rotating configuration, in particular with the same equation of state; or, more generally, if (with that notation)

$$\overline{\omega}(r) \ \leqslant \ \Omega(r,\theta) \ \leqslant \ \overline{\Omega}.$$

Notice, $\omega < \Omega$ means that the angular momentum density *to first order in the fluid angular velocity, (22), of this configuration [with the energy condition (19)] is $\geqslant 0$, vanishing on the axis.*

[Remarkably, the upper bound required on Ω is not restrictive, because for Ω continuous, Ω is essentially bounded ($\in L^\infty$) there, and $\Omega/\|\Omega\|_\infty \leqslant 1$.]

Proof: We give a practical method of construction in two steps.

First step: Consider $\overline{\Omega}(r,\theta) := \overline{\Omega} = \text{const} > 0$, and solve the corresponding Eq. (28) for $\overline{\omega}$. Then, by Property RR, the solution satisfies

$$\overline{\omega}(r,\theta) = \overline{\omega}(r), \tag{49}$$

$$0<\overline{\omega}(r)<\overline{\Omega} \text{ in } [0,R], \tag{50}$$

$$\text{and } \overline{\omega}>0 \text{ in } [0,\infty[\,, \overline{\omega}'<0 \text{ in }]0,\infty[\,, \overline{\omega}'(0)=0. \tag{51}$$

Second step: Consider a slowly rotating configuration starting from the same nonrotating configuration (as in the first step) with a fluid angular velocity distribution $\Omega(r,\theta)$ such that

$$\overline{\omega}(0)=:\underline{\Omega} \leqslant \Omega(r,\theta) \leqslant \overline{\Omega}. \tag{52}$$

Observe, we are always allowed to do this because of (50). Or, more generally, such that $\overline{\omega}(r) \leqslant \Omega(r,\theta) \leqslant \overline{\Omega}$; notice, from (51), $\overline{\omega}$ is a (positive) decreasing function; in particular, $\overline{\omega}(0) \geqslant \overline{\omega}(r)>0, \ \forall r \in [0,\infty[$.

From the second inequality in (52), i.e., from $\Omega(r,\theta) \leqslant \overline{\Omega}$, and, since we have the same starting unperturbed configuration (same 0-order coefficients) for these both slowly rotating configurations, it follows, by Property (b), that their corresponding solutions [of Eq. (28)] satisfy

$$\omega(r,\theta)<\overline{\omega}(r), \tag{53}$$

where we have used (49). On the other hand, the first inequality in (52), and (51) yield

$$\overline{\omega}(r) \leqslant \overline{\omega}(0) =: \underline{\Omega} \leqslant \Omega(r,\theta), \tag{54}$$

and consequently, from (53) and (54),

$$\omega(r,\theta) < \Omega(r,\theta).$$

□

Remark: Notice, the same argument also assures that, given a slowly rotating configuration with $\overline{\Omega}(r,\theta)$ such that the corresponding dragging rate $\overline{\omega}(r,\theta)<\overline{\Omega}(r,\theta)$, we shall have the same positivity result [property (c)] for any slowly rotating configuration, starting from the same unperturbed configuration (in particular, with the same equation of state), with an angular velocity distribution $\Omega(r,\theta)$ such that

$$\underline{\Omega}(r,\theta) =: \overline{\omega}(r,\theta) \leqslant \Omega(r,\theta) \leqslant \overline{\Omega}(r,\theta),$$

because we obtain, from the last inequality and property (b), $\omega(r,\theta)<\overline{\omega}(r,\theta)$, and hence, $\omega(r,\theta)<\Omega(r,\theta)$.

Series expansion: M_{rot}. Before we prove the next property, we first stress that, since Ω and ω transform like vectors under rotation, Eq. (27) may be separated by expanding them as

$$\Omega(r,\theta) \equiv \Omega(r,x) \sim \sum_{l=1}^{\infty} \Omega_l(r)\, y_l(x) \tag{55}$$

and

$$\omega(r,\theta) \equiv \omega(r,x) \sim \sum_{l=1}^{\infty} \omega_l(r)\, y_l(x), \tag{56}$$

with the change of variable $\theta \mapsto x := \cos\theta$, and

$$y_l(x) := \frac{d\mathcal{P}_l}{dx} \qquad \forall x \in [-1,1] (\theta \in [0,\pi]), \quad \mathcal{P}_l \equiv \text{Legendre polynomial of degree } l. \tag{57}$$

Then the equation for ω_l takes the form

$$\frac{\mathrm{d}}{\mathrm{d}r}[r^4 j(r)\ \ \omega_l']+[4\,r^3 j'(r)-r^2\,k(r)\,\lambda_l]\ \ \omega_l=4\,r^3 j'(r)\ \ \Omega_l(r)\,, \tag{58}$$

with $\lambda_l := l(l+1)-2$, $l\in\mathbb{N}$, $l\neq 0$, and j and k defined in (25).

From conditions (31) and (32) on ω, we have the respective boundary conditions on ω_l,

$$\lim_{r\to\infty}\omega_l(r)=0\,, \tag{59}$$

$$\omega_l \quad C^1 \ \text{regular at the origin}, \tag{60}$$

and, from (33), the matching condition

$$\omega_l \ \text{class}\ C^1\ \text{across}\ r=R\,. \tag{61}$$

In Sec. IV D an explicit expression for the expansion of the rotational mass-energy M_{rot} in powers or the angular velocity parameter was obtained (23), or, using Eq. (26),

$$M_{\mathrm{rot}}=-\frac{1}{4}\int_0^R \mathrm{d}r\, r^3 j'\int_0^\pi \mathrm{d}\theta \sin^3\theta\,\Omega(\Omega-\omega)+O(\mu^4)\,. \tag{62}$$

Using the series expansions of Ω and ω, (55) and (56), and the fact that the system $\{y_l\}_{l=1}^\infty$ is orthogonal in the Hilbert space $L^2_\rho([-1,1])$, with respect to the weight function $\rho(x):=1-x^2$, $x\in[-1,1]$, and have norm $\|y_l\|_\rho{}^2=2l(l+1)/(2l+1)$, the integral over θ in (62) may be expressed as the sum

$$\int_0^\pi \mathrm{d}\theta\sin^3\theta\,\Omega(r,\theta)[\Omega(r,\theta)-\omega(r,\theta)]=\sum_{l=1}^\infty \frac{2l(l+1)}{2l+1}\Omega_l(r)[\Omega_l(r)-\omega_l(r)]\,, \tag{63}$$

and, consequently, the rotational mass-energy (62) can be expressed as a sum of integrals (over r)

$$M_{\mathrm{rot}}=\sum_{l=1}^\infty \frac{l(l+1)}{2(2l+1)}M_l+O(\mu^4)\,, \tag{64}$$

with

$$M_l := \int_0^R f^2(r)\,\Omega_l(r)[\Omega_l(r)-\omega_l(r)]\,\mathrm{d}r\,,\quad f^2(r):=-r^3 j'(r)\geqslant 0\,. \tag{65}$$

Property (d) (positivity and upper bound on the rotational energy M_{rot}): We consider Eq. (58), which can be written

$$\frac{\mathrm{d}}{\mathrm{d}r}(r^4 j\,\omega_l')-r^2 k\,\lambda_l\,\omega_l=-4\,f^2\,(\Omega_l-\omega_l)\,. \tag{66}$$

The main observation is that, multiplying both sides of Eq. (66) by ω_l, integrating from $r=0$ to $r=\infty$, and taking into account that $f^2=-r^3 j'=4\pi r^4(\varepsilon_0+p_0)\,k\equiv 0\,\forall\, r>R$,

$$\int_0^\infty\left[\frac{\mathrm{d}}{\mathrm{d}r}(r^4 j\,\omega_l')\,\omega_l-r^2 k\,\lambda_l\,\omega_l{}^2\right]\mathrm{d}r=-4\int_0^R f^2\,\omega_l\,(\Omega_l-\omega_l)\,\mathrm{d}r$$

[note, the integral on the left-hand side converges, because an asymptotically flat (59) solution of Eq. (58) must behave, for $r\to\infty$, as $\omega_l=O(r^{-l-2})$, and $\omega_l'=O(r^{-l-3})$, $l\geqslant 1$]; and, after integrating once by parts the first term on the left-hand side,

$$r^4\, j\, \omega_l'\, \omega_l|_0^\infty - \int_0^\infty [r^4\, j\, (\omega_l')^2 + r^2\, k\, \lambda_l\, \omega_l{}^2]\mathrm{d}r = -4\int_0^R f^2\, \omega_l\, (\Omega_l - \omega_l)\, \mathrm{d}r\,.$$

The first term vanishes because ω_l falls off rapidly enough at $r\to\infty$, and the second term (minus the integral on the left-hand side) is nonpositive (since j and k are always positive), therefore

$$\int_0^R f^2\, \omega_l\, (\Omega_l - \omega_l)\, \mathrm{d}r \geqslant 0\,. \tag{67}$$

Using a few simple linear algebra calculations [including the Cauchy-Schwarz inequality for the bilinear form $\langle u,v\rangle_f := \int_0^R f^2(r)\, u(r)\, v(r)\, \mathrm{d}r u,v \in C^0([0,R])$], the former inequality (67) yields (see Ref. 1, Sec. V) $0 \leqslant M_l \leqslant \int_0^R f^2\, \Omega_l{}^2\, \mathrm{d}r$, which gives respective bounds on M_{rot} [cf. (64)],

$$0 \leqslant M_{\mathrm{rot}} \leqslant \sum_{l=1}^{\infty} \frac{l(l+1)}{2(2l+1)} \int_0^R f^2(r)\, \Omega_l{}^2(r)\, \mathrm{d}r + O(\mu^4)\,,$$

or, writing the sum as integral over θ [as in (63)],

$$0 \leqslant M_{\mathrm{rot}} \leqslant \frac{1}{4}\int_0^R \mathrm{d}r\, f^2(r) \int_0^\pi \mathrm{d}\theta \sin^3\theta\, [\Omega(r,\theta)]^2 + O(\mu^4)\,, \tag{68}$$

where $f^2 := -r^3\, j' = 4\pi\, r^4\, (\varepsilon_0 + p_0) e^{(\lambda-\nu)/2}$. Additionally, $\int_0^R f^2\, \omega_l{}^2\, \mathrm{d}r \leqslant \int_0^R f^2\, \Omega_l{}^2\, \mathrm{d}r$ also follows from (67), yielding the "mean values" inequality (in full general)

$$\int_0^R \mathrm{d}r\, f^2(r) \int_0^\pi \mathrm{d}\theta \sin^3\theta\, [\omega(r,\theta)]^2 \leqslant \int_0^R \mathrm{d}r\, f^2(r) \int_0^\pi \mathrm{d}\theta \sin^3\theta\, [\Omega(r,\theta)]^2 + O(\mu^4)\,. \tag{69}$$

□

VI. CONCLUDING REMARKS

Summing up, it has been seen that relativistic stars rotating slowly and differentially, with a non-negative (and nontrivial) angular velocity distribution, $\Omega(x_2,x_3) \geqslant 0\ (\not\equiv 0)$, and satisfying the energy condition $\varepsilon + p \geqslant 0$, have positive *rate of rotational dragging* $\omega > 0$ [property (a) in Sec. V]; and a restriction on the amplitude of the Ω-profile assures also the positivity of the difference $\Omega - \omega$ and, hence, of the *angular momentum density*, this later vanishes on the axis [property (c)]. We also observe that the *rotational mass-energy*, [from property (d)] non-negative and (as expected) "increased" by a (slow) angular velocity of the fluid, Ω, is "decreased" by the dragging effect (over what it would be if this effect were neglected), i.e., is decreasing with respect to dragging rate, ω, despite of [as shown in property (b)] ω being an "increasing function" of Ω. Property (b) and, hence, also property (c) are based on the linearity of the time-angle field equation component to first order in the fluid angular velocity. In the general differentially rotating case, i.e., outside the slow rotation limit, the rotation profile Ω cannot be freely chosen, but is restricted by the integrability condition of the Euler equation, i.e., by Eq. (5). This makes unlikely a generalization of Property (c) outside the slow rotation limit, other than in the form given in Ref. 1, Sec. IV B.

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APPENDIX A: BOUNDEDNESS OF SOME FUNCTIONS IN $[0,\infty[\ \ni r$

1. The ratio radius-isotropic radius $\chi(r):=r/h(r)$

We have

$$\frac{h'(r)}{h(r)}=\frac{e^{\lambda(r)/2}}{r}, \tag{A1}$$

with

$$e^{-\lambda(r)}=1-\frac{2\,m(r)}{r}, \tag{A2}$$

where

$$m(r):=\begin{cases} 4\pi\int_0^r \varepsilon_0(s)s^2\,\mathrm{d}s & :\ r\in[0,R], \\ M\equiv 4\pi\int_0^R \varepsilon_0(s)s^2\,\mathrm{d}s & :\ r\in\,]R,\infty[, \end{cases} \tag{A3}$$

if we denote the stellar radius of the static model by $R>0$. As we start with a (physically) regular (i.e., noncollapsed) static solution, we assume that $2m(r)<r$ (for all $r\in\,]0,R[$), and $2M<R$.

Integrating Eq. (A1) and using Eq. (A2) we get

$$h(r)=h(R)\exp\left(\int_R^r \frac{\mathrm{d}s}{\sqrt{s(s-2m(s))}}\right). \tag{A4}$$

[Note, the constant $h(R)$ is determined by the asymptotic condition

$$\lim_{r\to\infty}\frac{h(r)}{r}=1\,;$$

see below.] Let

$$g(r):=\int_R^r \frac{\mathrm{d}s}{\sqrt{s(s-2m(s))}} \quad \forall r>0\,. \tag{A5}$$

With this definition, the solution (A4) now writes

$$h(r)=h(R)\exp(g(r))\,. \tag{A6}$$

Due to the assumptions made for m, g is obviously a continuous function in the open interval $]0,\infty[$; consequently, by (A6), h is also a continuous function there, and, in particular, $h(r)$ cannot be zero in $]0,\infty[$ [unless $h(R)=0$, however this would contradict asymptotic flatness]; therefore $\chi: r\mapsto\chi(r):=r/h(r)$ is continuous in $]0,\infty[$ as well. Choose an $\epsilon\in\,]0,R[$ and an $\epsilon'\in\,]R,\infty[$, then χ is bounded below and above in the interval $[\epsilon,\epsilon']$ (where the upper and lower bound depend on the selected ϵ and ϵ', of course). Let us now consider the intervals $[0,\epsilon]$ and $[\epsilon',\infty[$ separately.

On $[\epsilon',\infty[$: We have

$$0\leqslant m(r)\equiv M\,.$$

Then

$$\frac{1}{s}\leqslant\frac{1}{\sqrt{s(s-2m(s))}}\equiv\frac{1}{\sqrt{s(s-2M)}}\quad\forall r\in[\epsilon',\infty].$$

As in this interval $r\geqslant R$, we find, with Eq. (A5),

$$\ln\left(\frac{r}{R}\right)=\int_R^r\frac{\mathrm{d}s}{s}\leqslant g(r)\equiv\int_R^r\frac{\mathrm{d}s}{\sqrt{s(s-2M)}}=2\ln\left(\frac{\sqrt{r}+\sqrt{r-2M}}{\sqrt{R}+\sqrt{R-2M}}\right).$$

Inserting it into Eq. (A6), yields (since exp is a monotonically increasing function)

$$\frac{h(R)}{R}r\leqslant h(r)\equiv h(R)\left(\frac{\sqrt{r}+\sqrt{r-2M}}{\sqrt{R}+\sqrt{R-2M}}\right)^2\leqslant\frac{4h(R)}{(\sqrt{R}+\sqrt{R-2M})^2}r. \tag{A7}$$

Note especially that

$$\lim_{r\to\infty}\frac{h(r)}{r}=\frac{4h(R)}{(\sqrt{R}+\sqrt{R-2M})^2},$$

but, by asymptotic flatness, $\lim_{r\to\infty}[h(r)/r]=1$; therefore $h(R)=\frac{1}{4}(\sqrt{R}+\sqrt{R-2M})^2>0$. Thus, $h(R)>0$, and, from Eq. (A7),

$$0<\frac{(\sqrt{R}+\sqrt{R-2M})^2}{4h(R)}\leqslant\chi(r)\leqslant\frac{R}{h(R)}<\infty\quad\forall r\in[\epsilon',\infty[. \tag{A8}$$

On $[0,\epsilon]$: We have

$$0\leqslant m(r)=4\pi\int_0^r\varepsilon_0(s)s^2\,\mathrm{d}s\leqslant\frac{4\pi}{3}\hat{\varepsilon}_0r^3=:\frac{c_0}{2}r^3,$$

where $\hat{\varepsilon}_0:=\sup_{r\in[0,R]}\varepsilon_0(r)>0$. Next choose $\epsilon>0$, such that $1-c_0r^2>0$ on $[0,\epsilon]$ [e.g., $\epsilon:=(2\sqrt{c_0})^{-1}$]. Then

$$\frac{1}{s}\leqslant\frac{1}{\sqrt{s(s-2m(s))}}\leqslant\frac{1}{s\sqrt{1-c_0s^2}}\quad\forall r\in[0,\epsilon],$$

and, since in this interval $r\leqslant R$, we find, with Eq. (A5),

$$\ln\left(\frac{R}{r}\right)=\int_r^R\frac{\mathrm{d}s}{s}\leqslant-g(r)\leqslant\int_r^R\frac{\mathrm{d}s}{s\sqrt{1-c_0s^2}}=\ln\left(\frac{R}{r}\right)+\ln\left(\frac{1+\sqrt{1-c_0r^2}}{1+\sqrt{1-c_0R^2}}\right).$$

Again, inserting it into Eq. (A6), yields

$$\frac{h(R)}{R}r\geqslant h(r)\geqslant\frac{h(R)}{R}\frac{1+\sqrt{1-c_0R^2}}{1+\sqrt{1-c_0r^2}}r\geqslant\frac{h(R)(1+\sqrt{1-c_0R^2})}{2R}r,$$

and, hence,

$$0<\frac{R}{h(R)}\leqslant\chi(r)\leqslant\frac{2R}{h(R)(1+\sqrt{1-c_0R^2})}<\infty\quad\forall r\in[0,\epsilon]. \tag{A9}$$

We can therefore conclude that, since $\mathbb{R}_0^+=[0,\epsilon]\cup[\epsilon,\epsilon']\cup[\epsilon',\infty[$ and χ is bounded (from above and below) in each of these subintervals, χ is bounded (from above and below) in $\mathbb{R}_0^+$. □

2. The function *H*

We have

$$H(r):=\frac{-e^{[-\lambda(r)/2]}[-6+6\,e^{[\lambda(r)/2]}+r\,\nu'(r)]}{2\,h(r)},$$

and

$$e^{-\lambda(r)/2}=\sqrt{1-\frac{2m(r)}{r}},$$

$$r\,\nu'(r)=\frac{2m(r)+8\,\pi r^3 p_0(r)}{r-2m(r)}=\frac{\dfrac{2m(r)}{r}+8\,\pi r^2 p_0(r)}{1-\dfrac{2m(r)}{r}}.$$

Thus,

$$H(r)=\frac{1}{2h(r)}\left\{6\left[\sqrt{1-\frac{2m(r)}{r}}-1\right]-\left[\frac{2m(r)}{r}+8\,\pi r^2 p_0(r)\right]\left(\sqrt{1-\frac{2m(r)}{r}}\right)^{-1}\right\}. \tag{A10}$$

Using the Cauchy–Schwarz inequality in (A10), and the following estimates in $r\in[0,\epsilon]$, for some $\epsilon\in\,]0,R[$ small (see former section in Appendix A)

$$0\leqslant m(r)\leqslant\frac{c_0}{2}r^3, \tag{A11}$$

$$0\leqslant\sqrt{1-x}\leqslant 1-\frac{x}{2}\quad\forall x\in[0,1], \tag{A12}$$

$$0\leqslant c_1 r\leqslant h(r)\leqslant c_2 r, \tag{A13}$$

$$0\leqslant p_0(r)\leqslant\hat{p}_0:=\sup_{r\in[0,R]}p_0(r)\quad\forall r\geqslant 0\,, \tag{A14}$$

where the constants $c_{i\ (i=0,\ldots,2)}$ are all strictly positive (and finite), we get

$$\begin{aligned}|H(r)|&\leqslant\frac{1}{2h(r)}\left\{6\left|\sqrt{1-\frac{2m(r)}{r}}-1\right|+\left|\frac{2m(r)}{r}+8\,\pi r^2 p_0(r)\right|\left(\sqrt{1-\frac{2m(r)}{r}}\right)^{-1}\right\}\\&\leqslant\frac{1}{2c_1 r}\left\{6\left[\frac{c_0}{2}r^2\right]+[c_0 r^2+8\,\pi\hat{p}_0 r^2](\sqrt{1-c_0\epsilon^2})^{-1}\right\}=:\frac{c_3 r^2}{c_1 r}=:c_4 r\,,\end{aligned} \tag{A15}$$

with $0<c_3\,,c_4<\infty$. Therefore H is bounded in $[0,\epsilon]$. [Especially, due to Eq. (A15), $H(0)=0$.] And, since, by Eq. (A10), H is also continuous in the open interval $]0,\infty[$ and $\lim_{r\to\infty}H(r)=0$ (because $\lim_{r\to\infty}[h(r)/r]=1$), H is bounded everywhere in $[0,\infty[$. □

APPENDIX B: THE MINIMUM PRINCIPLE FOR GENERALIZED SUPERSOLUTIONS

Consider in a domain (open and connected set) $G\subset\mathbb{R}^n$ $(n\geqslant 2)$ the differential operator with principal part of divergence form, defined by

$$Lu=\partial_i[a_{ij}(x)\partial_j u+a_i(x)\,u]+b_i(x)\,\partial_i u+c(x)\,u\,,$$

with $a_{ij}=a_{ji}$. Notice, an operator L of the general form $Lu=\tilde{a}_{ij}(x)\partial_{ij}u+\tilde{b}_i(x)\partial_i u+\tilde{c}(x)u$ may be written in divergence form provided its principal coefficients $\tilde{a}_{ij}$ are differentiable. If furthermore the $\tilde{a}_{ij}$ are constants, then even with coinciding coefficients ($a_{ij}=\tilde{a}_{ij}$, $b_i=\tilde{b}_i$, $c=\tilde{c}$) and $a_i\equiv 0$. Let us assume that

(1) L is strictly elliptic in G, i.e., $\exists$ a constant $\lambda>0$ such that $\lambda\leqslant$the minimum eigenvalue of the principal coefficient matrix $[a_{ij}(x)]$,

$$\lambda\,|y|^2\leqslant a_{ij}(x)\,y_i y_j \quad \forall y\in\mathbb{R}^n, \quad \forall x\in G\,; \tag{B1}$$

(2) a_{ij}, a_i, b_i, and c are measurable and bounded functions in G,

$$|a_{ij}|<\infty, \quad |a_i|<\infty, \quad |b_i|<\infty, \quad |c|<\infty \text{ in } G \quad (i,j\in\{1,\ldots,n\})\,. \tag{B2}$$

By definition, for a function u which is only assumed to be *weakly differentiable* and such that the functions $a_{ij}\partial_j u+a_i u$ and $b_i\partial_i u+cu$, $i=1,\ldots,n$ are locally integrable [in particular, for u belonging to the Sobolev space $W^{1,2}(G)$], u is said to satisfy $Lu=g$ in G *in a generalized (or weak) sense* (g also a locally integrable function in G) if it satisfies

$$\mathcal{L}(u,\varphi;G):=\int_G\{(a_{ij}\partial_j u+a_i u)\partial_i\varphi-(b_i\partial_i u+cu)\varphi\}\mathrm{d}x=-\int_G g\,\varphi\,\mathrm{d}x, \quad \forall\varphi\geqslant 0, \quad \varphi\in C_c^1(G)$$

[where $C_c^1(G)$ is the set of functions in $C^1(G)$ with compact support in G].

Notice, u is *generalized supersolution* relative to a differential operator L and the domain G (i.e., satisfies $Lu\leqslant 0$ in G in a generalized sense) if it satisfies $\mathcal{L}(u,\varphi;G)\geqslant 0$, $\forall\varphi\geqslant 0$, $\varphi\in C_c^1(G)$.

Theorem 1 (weak minimum principle): *Let $u\in W^{1,2}(G)$, G a bounded domain, satisfy $Lu\leqslant 0$ in G in a generalized sense with*

$$\int_G(c\varphi-a^i\partial_i\varphi)\,\mathrm{d}x\leqslant 0, \quad \forall\varphi\geqslant 0, \quad \varphi\in C_c^1(G) \tag{B3}$$

and conditions (B1) *and* (B2) *above, then*

$$\min_{\bar{G}}\,u\geqslant\min_{\partial G}u^- \quad [\,u^-\equiv\min(u,0)\,]\,.$$

(A proof of this theorem can be found in Ref. 13, Theorem 8.1.)

Theorem 2 (strong minimum principle): *Let $u\in W^{1,2}(G)\cap C^0(G)$ satisfy $Lu\leqslant 0$ in G in a generalized sense, with the operator L satisfying conditions* (B1), (B2), *and* (B3), *then u cannot achieve a nonpositive minimum in the interior of G, unless $u\equiv$*const.

(A proof of this theorem can be found in Ref. 13, Theorem 8.19.) Note that the weak minimum principle, Theorem 1, for $C^0(G)$ supersolutions is a direct consequence.

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[12] Indeed, the first order terms (in the fluid angular velocity) of the general metric, as given in Ref. 1, yield (omitting here the tilde symbol for all 5-*lifted* functions) $H(r)=(3\partial_{\bar{r}}B-4\partial_{\bar{r}}U)|_{h(r)}$, where $\bar{r}=h(r)$, given by Eq. (35). [This can be seen by a straightforward calculation, using $e^{2U(h(r))}=e^{\nu(r)}$, $h(r)^2e^{2[B(h(r))-U(h(r))]}=r^2$, and their differentiations with respect to r.] And since [from $h(r)=(\Sigma_{i=1}^{5}x_i^2)^{1/2}$] $\partial_i h(r)=x_i h(r)^{-1}$, we have $H(r)x_i h(r)^{-1}=(3\partial_i B-4\partial_i U)|_{O(\Omega)}$, and, hence, $\langle 3\nabla B-4\nabla U,\nabla\omega\rangle|_{O(\Omega)}$ as the second term in Eq. (43). Also, since to first order (spherical; $K=B$) $e^{2K}N^{-1}=e^{2(B-U)}=r^2h^{-2}$, the coefficient of the right-hand side of Eq. (43) is actually $-\Psi(r)^2e^{-\lambda(r)}r^2h(r)^{-2}=-\psi^2|_{O(\Omega)}$, in the notation of Ref. 1.
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Dirac theory within the Standard-Model Extension

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The modified Dirac equation in the Lorentz-violating Standard-Model Extension (SME) is considered. Within this framework, the construction of a Hermitian Hamiltonian to all orders in the Lorentz-breaking parameters is investigated, discrete symmetries and the first-order roots of the dispersion relation are determined, and various properties of the eigenspinors are discussed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1769105]

I. INTRODUCTION

Perhaps the most intriguing open question in present-day fundamental physics concerns a quantum theory of all fundamental interactions including gravitation. Experimental research in this field is challenging because quantum-gravitational effects are expected to be suppressed by the Planck scale $M_{\mathrm{Pl}} \simeq 10^{19}$ GeV. However, Lorentz violation is a promising candidate signature of fundamental physics that lies within the sensitivity range of experiments with current or near-future technology.[1]

At presently attainable energy scales, the effects of Lorentz violation can be described within an effective-field-theory framework called the Standard-Model Extension (SME).[2–4] At the classical level, the action of the SME incorporates, e.g., all leading-order contributions to the Lagrangian that are formed by combining Standard-Model and gravitational fields with Lorentz-breaking parameters such that coordinate independence is maintained. Nonzero parameters for Lorentz violation can arise in a variety of approaches to underlying physics including strings,[5] various nonstring models of quantum gravity,[6] noncommutative field theories,[7] varying couplings,[8,9] random dynamics,[10] multiverses,[11] and brane-world scenarios.[12] The flat-space–time limit of the SME has provided the basis for numerous investigations of Lorentz violation involving mesons,[13–15] baryons,[16–19] electrons,[20–23] photons,[24–27] muons,[28] and neutrinos.[2,29,30]

The extraction of the physical content of the SME requires an initial investigation of the quadratic sectors of its Lagrangian paralleling the conventional case. More specifically, the source-free equations of motion, the associated Hamiltonians, the dispersion relations, and, in the fermion case, the eigenspinors form a cornerstone on which further theoretical studies and comparisons with experiment rest. For example, the majority of the aforementioned analyses of Lorentz tests involve the theory of free massive fermions of the SME. Some basics of this theory have been made plausible or have been derived in certain limits as needed, but a comprehensive treatment has been lacking. The present work is intended to fill this gap.[31] More specifically, we give a more rigorous and detailed study of the general free Dirac equation and its solutions in the context of the SME. These results provide important tools for further studies of the physical implications of Lorentz violation.

The paper is organized as follows. Section II sets up the notation, reviews the basics of the modified Dirac equation, and comments on its structure. The construction of a Hermitian Hamiltonian to arbitrary order in the Lorentz-violating parameters is discussed in Sec. III. In Sec. IV, we perform a systematic analysis of discrete dispersion-relation symmetries. Explicit leading-order approximations of the fermion eigenenergies are obtained in Sec. V. Sections VI and VII contain an investigation of the eigenspinors including a discussion of their symmetries and a derivation of

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the generalized spinor projectors. A brief summary is presented in Sec. VIII.

II. BASICS

The general Lorentz-violating Lagrangian for a single spin-1/2 fermion[2] can be cast into a variety of forms. One such form reminiscent of the ordinary Dirac Lagrangian and emphasizing the derivative structure is[17]

$$\mathcal{L}=\frac{1}{2}i\overline{\psi}\Gamma^{\nu}\overleftrightarrow{\partial}_{\nu}\psi-\overline{\psi}M\psi\,, \tag{1}$$

where

$$\begin{aligned}\Gamma^{\nu}&\equiv\gamma^{\nu}+c^{\mu\nu}\gamma_{\mu}+d^{\mu\nu}\gamma_5\gamma_{\mu}+e^{\nu}+if^{\nu}\gamma_5+\frac{1}{2}g^{\lambda\mu\nu}\sigma_{\lambda\mu}\,,\\ M&\equiv m+a_{\mu}\gamma^{\mu}+b_{\mu}\gamma_5\gamma^{\mu}+\frac{1}{2}H^{\mu\nu}\sigma_{\mu\nu}\,.\end{aligned} \tag{2}$$

The gamma matrices $\{I,\gamma_5,\gamma^{\mu},\gamma_5\gamma^{\mu},\sigma^{\mu\nu}\}$ have conventional properties, and the signature of the Minkowski metric $\eta_{\mu\nu}$ is -2. The Lorentz-violating parameters a_{μ}, b_{μ}, $c_{\mu\nu}$, $d_{\mu\nu}$, e_{μ}, f_{μ}, $g_{\mu\nu\lambda}$, and $H_{\mu\nu}$ are taken as real with $c_{\mu\nu}$ and $d_{\mu\nu}$ traceless, $g_{\mu\nu\lambda}$ antisymmetric in its first two indices, and $H_{\mu\nu}$ antisymmetric. Note that a_{μ}, b_{μ}, e_{μ}, f_{μ}, and $g_{\mu\nu\lambda}$ break CPT symmetry as well. For definiteness, we assume $m>0$. However, many of our results also hold in the massless case. On phenomenological grounds, all Lorentz-violating coefficients must be minute in a certain class of inertial frames called *concordant frames*, in which the Earth moves nonrelativistically. Then, paralleling the usual Dirac case, a Hermitian Hamiltonian with two positive and two negative eigenvalues exists.[3]

For future reference, we provide an equivalent form of Lagrangian (1) emphasizing its gamma-matrix structure:[3]

$$\mathcal{L}=\overline{\psi}(S+iP\gamma_5+V^{\mu}\gamma_{\mu}+A^{\mu}\gamma_5\gamma_{\mu}+T^{\mu\nu}\sigma_{\mu\nu})\psi\,. \tag{3}$$

Here, we have defined

$$\begin{aligned}&S[i\partial]\equiv e^{\mu}i\partial_{\mu}-m\,,\quad P[i\partial]\equiv f^{\mu}i\partial_{\mu}\,,\quad V^{\mu}[i\partial]\equiv i\partial^{\mu}+c^{\mu\nu}i\partial_{\nu}-a^{\mu}\,,\quad A^{\mu}[i\partial]\equiv d^{\mu\nu}i\partial_{\nu}-b^{\mu}\,,\\ &T^{\mu\nu}[i\partial]\equiv\frac{1}{2}(g^{\mu\nu\rho}i\partial_{\rho}-H^{\mu\nu})\,,\end{aligned} \tag{4}$$

where the dependence of the introduced quantities on the quantum-mechanical four-momentum operator has been displayed for clarity. The Lagrangians (1) and (3) differ only by a total divergence, so that they are physically equivalent. Note that the replacement $i\partial\rightarrow 1/2\,i\overleftrightarrow{\partial}$ in Def. (4) renders both Lagrangians identical.

The associated modified Dirac equation is given by

$$(i\Gamma^{\mu}\partial_{\mu}-M)\psi(x)=0\,. \tag{5}$$

A Klein–Gordon-type equation can be obtained employing the following squaring procedure. Consider the modified Dirac operator $(i\Gamma^{\mu}\partial_{\mu}-M)$ and change the signs of the parameters b^{μ}, $d^{\mu\nu}$, $g^{\mu\nu\rho}$, and $H^{\mu\nu}$. Application of the resulting operator to Eq. (5) yields the desired second-order equation

$$(\check{S}+\check{P}\gamma^5+\check{V}^{\mu}\gamma_{\mu})\psi(x)=0\,, \tag{6}$$

where we have defined

$$\check{S}\equiv S^2-P^2+V^2+A^2-2T^2\ ,\quad \check{P}\equiv 2(iPS-V\cdot A-iT\tilde{T})\ ,$$

$$\check{V}^\mu\equiv 2(SV^\mu+iPA^\mu-2iT^{\mu\nu}V_\nu+2\tilde{T}^{\mu\nu}A_\nu)\ . \tag{7}$$

In the above expressions, the dependence of the various quantities on $i\partial$ is understood. The tensor $\tilde{T}^{\mu\nu}=1/2\epsilon^{\mu\nu\alpha\beta}T_{\alpha\beta}$ denotes the dual and $\epsilon^{\mu\nu\alpha\beta}$ is the totally antisymmetric symbol with $\epsilon^{0123}=+1$, as usual. The unconventional off-diagonal pieces in Eq. (6) can be eliminated with a second squaring procedure involving the application of $(\check{S}-\check{P}\gamma^5-\check{V}^\mu\gamma_\mu)$ to the Klein–Gordon-type equation (6). As expected, the resulting fourth-order operator can be expressed as the determinant of the modified Dirac operator, paralleling the conventional case:

$$\det(i\Gamma^\mu\partial_\mu-M)\psi(x)=0\ . \tag{8}$$

Thus, each individual component of a spinor solving the modified Dirac equation (5) satisfies Eq. (8).

A plane-wave ansatz $\psi(x)=\exp(-i\lambda^\mu x_\mu)W(\vec{\lambda})$ for solutions to the modified Dirac equation (5) yields

$$(\Gamma^\mu\lambda_\mu-M)W(\vec{\lambda})=0 \tag{9}$$

determining the four-component spinor $W(\vec{\lambda})$, where the four-momentum λ^μ must solve the dispersion relation

$$\det(\Gamma^\mu\lambda_\mu-M)=0\ . \tag{10}$$

With our earlier assumption, dispersion relation (10) has two positive-valued roots $\lambda^0_{+(1,2)}(\vec{\lambda})$ and two negative-valued ones $\lambda^0_{-(1,2)}(\vec{\lambda})$. The corresponding four-momenta and eigenspinors are $\lambda^\mu_{\pm(\alpha)}$ and $W^{(\alpha)}_\pm(\vec{\lambda})$, respectively. Throughout this work, indices in parentheses can take the values 1 and 2. After the usual reinterpretation of the negative-energy solutions, the four-momenta are denoted by

$$p^{(\alpha)}_u\equiv\lambda_{+(\alpha)}\ ,\quad p^{(\alpha)}_v\equiv-\lambda_{-(\alpha)}\ , \tag{11}$$

where we have omitted the Minkowski indices for brevity. The notation for the reinterpreted eigenspinors is

$$U^{(\alpha)}(\vec{p})\equiv W^{(\alpha)}_+(\vec{\lambda})\ ,\quad V^{(\alpha)}(\vec{p})\equiv W^{(\alpha)}_-(-\vec{\lambda})\ . \tag{12}$$

The spinors and the dispersion relation are discussed in more detail in subsequent sections.

For a four-momentum λ_μ that fails to satisfy dispersion relation (10), the cofactor matrix of the modified Dirac operator $(\Gamma^\mu\lambda_\mu-M)$ in λ-momentum space is given by

$$\mathrm{cof}(\Gamma^\mu\lambda_\mu-M)=\det(\Gamma^\mu\lambda_\mu-M)(\Gamma^\mu\lambda_\mu-M)^{-1}\ . \tag{13}$$

This matrix appears in many applications of our model (1), such as the anticommutator function.[3] A more explicit expression is therefore desirable. As a corollary of the above discussion of the equations of motion, we obtain

$$\mathrm{cof}(\Gamma^\mu\lambda_\mu-M)=(\check{S}-\check{P}\gamma^5-\check{V}^\mu\gamma_\mu)(S+iP\gamma_5+V^\mu\gamma_\mu-A^\mu\gamma_5\gamma_\mu-T^{\mu\nu}\sigma_{\mu\nu})\ . \tag{14}$$

As we are now working in momentum space, the according change from $i\partial$ to λ in Defs. (4) and (7) is implied. Replacing $\lambda \to i\partial$ everywhere in (14), yields the associated relation in position space, as usual.

III. HAMILTONIAN

In concordant frames, Γ^0 is invertible,[3] so that the modified Dirac equation (5) can be cast into Schrödinger form:

$$i\partial_0\psi(x) = (\Gamma^0)^{-1}(i\vec{\Gamma}\cdot\vec{\nabla} + M)\psi(x) \ . \tag{15}$$

Although the operator $\tilde{H}[i\vec{\nabla}] \equiv (\Gamma^0)^{-1}(i\vec{\Gamma}\cdot\vec{\nabla} + M)$ appearing above is reminiscent of a Hamiltonian, it fails to be Hermitian in general. This results in such undesirable features like a nonunitary time evolution. This issue can be resolved by a spinor redefinition $A\chi \equiv \psi$ chosen to eliminate the unconventional time-derivative couplings.[21] Here, A is a nonsingular space–time-independent 4×4 matrix, which exists in concordant frames.[3] This field redefinition leaves the physics unaffected because it is a canonical transformation. It amounts to a change of basis in spinor space.

The existence of A is equivalent[3] to the positive definiteness of $\gamma^0\Gamma^0$. One can then define[32] the "square root" of $\gamma^0\Gamma^0$ as the unique, positive-definite, invertible matrix $(\gamma^0\Gamma^0)^{1/2}$ that obeys $(\gamma^0\Gamma^0)^{1/2}(\gamma^0\Gamma^0)^{1/2} = \gamma^0\Gamma^0$. The matrix A can now be expressed as

$$A = (\gamma^0\Gamma^0)^{-1/2} \ . \tag{16}$$

Note that the hermiticity of $\gamma^0\Gamma^0$ yields $A = A^\dagger$. It can now be verified that the Hamiltonian H given by

$$H[i\vec{\nabla}] = (\gamma^0\Gamma^0)^{-1/2}\gamma^0(i\vec{\Gamma}\cdot\vec{\nabla} + M)(\gamma^0\Gamma^0)^{-1/2} \ , \tag{17}$$

which governs the time evolution of the redefined field χ, is Hermitian, as desired. We also point out that H and $\tilde{H}$ are related by the similarity transformation

$$H = (\gamma^0\Gamma^0)^{1/2}\tilde{H}(\gamma^0\Gamma^0)^{-1/2} \ . \tag{18}$$

The determination of the explicit form of the matrix A is challenging in general. In practice, however, it usually suffices to determine A up to a given order in the Lorentz-violating coefficients. Notice that $\gamma^0\Gamma^0$ can be split into the 4×4 identity I plus a Lorentz-breaking correction: $\gamma^0\Gamma^0 = I + \gamma^0(\Gamma^0 - \gamma^0)$. This suggests the following expansion:

$$A = I + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{(2n)!!}(I - \gamma^0\Gamma^0)^n \ . \tag{19}$$

In a basis in which $\gamma^0\Gamma^0$ is diagonal, it is straightforward to verify that the expansion (19) indeed converges and is consistent with the "square root" definition. It can therefore be used to determine A to arbitrary order.

IV. SYMMETRIES OF THE DISPERSION RELATION

An explicit expression for the single-particle dispersion relation (10) can be found by expanding the determinant:[3]

$$\begin{aligned}\det(\Gamma^\mu\lambda_\mu - M) = {} & 4(V_{[\mu}A_{\nu]} - V_\mu V_\nu + A_\mu A_\nu + PT_{\mu\nu} - S\tilde{T}_{\mu\nu} + T_{\mu\alpha}T^\alpha{}_\nu + \tilde{T}_{\mu\alpha}\tilde{T}^\alpha{}_\nu)^2 \\ & + (V^2 - A^2 - S^2 - P^2)^2 - 4(V^2 - A^2)^2 + 6(\epsilon_{\mu\nu\alpha\beta}A^\alpha V^\beta)^2 \ . \end{aligned} \tag{20}$$

Here, S, P, V^μ, A^μ, and $T^{\mu\nu}$ are given in λ-momentum space, and $V_{[\mu}A_{\nu]}=V_\mu A_\nu - A_\mu V_\nu$ denotes the antisymmetric part. Relation (20) also follows directly from Eqs. (13) and (14). The position-space version of Eq. (20) can be used to cast Eq. (8) into a more explicit form.

Further insight about the structure of dispersion relation (10) can be gained by analyzing its properties under charge conjugation C, parity inversion P, and time reversal T. For example, in the absence of explicit expressions for the eigenenergies, these investigations can be used to obtain information about their degeneracy. One such transformation, charge conjugation C, has been considered previously.[3] It was shown that the two sets of roots

$$\{\lambda^0_{-(\alpha)}(\vec{\lambda},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})\}=\{-\lambda^0_{+(\beta)}(-\vec{\lambda},m,-a^\mu,b^\mu,c^{\mu\nu},-d^{\mu\nu},-e^\mu,-f^\mu,g^{\mu\nu\rho},-H^{\mu\nu})\} \tag{21}$$

are identical. In this section, we employ the same methodology to find additional symmetries of the dispersion relation (10) and point out some subtleties regarding the labeling of the roots.

The idea is as follows. Multiplication of the modified Dirac operator $(\Gamma^\mu\lambda_\mu - M)$ with a nonsingular, λ-independent matrix contributes only a nonzero multiplicative factor to the determinant in Eq. (10) leaving this equation, and thus its roots, unchanged. The determinant remains also invariant under transposition or complex conjugation of the modified Dirac operator. The latter is true because $\det(\Gamma^\mu\lambda_\mu - M)$ is real, which follows from Eq. (20) and Def. (4).

We first consider

$$(\Gamma^\mu\lambda_\mu - M)\to\gamma^0(\Gamma^\mu\lambda_\mu - M)\gamma^0\ , \tag{22}$$

which corresponds to parity inversion P in spinor space. We remark in passing that $\det(\Gamma^\mu\lambda_\mu - M)$ remains unchanged, since the overall factor induced is $\det(\gamma^0\gamma^0)=1$. It follows that the dispersion relation (10) is invariant under

$$\{\lambda^\mu,m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu}\}\to\{\lambda_\mu,m,a_\mu,-b_\mu,c_{\mu\nu},-d_{\mu\nu},e_\mu,-f_\mu,g_{\mu\nu\rho},H_{\mu\nu}\}\ . \tag{23}$$

Hence, the two sets

$$\{\lambda^0_{+(\alpha)}(\vec{\lambda},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})\}=\{\lambda^0_{+(\beta)}(-\vec{\lambda},m,a_\mu,-b_\mu,c_{\mu\nu},-d_{\mu\nu},e_\mu,-f_\mu,g_{\mu\nu\rho},H_{\mu\nu})\}\ , \tag{24}$$

each containing the two positive-valued solutions of Eq. (10), must be identical. The result for the remaining sets of the two negative-valued roots is obtained by replacing the subscript $+$ by $-$ in Eq. (24).

Next, we investigate spinor-space time reversal given by

$$(\Gamma^\mu\lambda_\mu - M)\to i\gamma^5 C(\Gamma^\mu\lambda_\mu - M)^* iC\gamma^5\ , \tag{25}$$

where $*$ denotes complex conjugation and C is the usual charge-conjugation matrix. Again, $\det(\Gamma^\mu\lambda_\mu - M)$ is left unchanged. The resulting symmetry between the positive-valued roots of the dispersion relation (10) takes the form

$$\{\lambda^0_{+(\alpha)}(\vec{\lambda},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})\}=\{\lambda^0_{+(\beta)}(-\vec{\lambda},m,a_\mu,b_\mu,c_{\mu\nu},d_{\mu\nu},e_\mu,-f_\mu,-g_{\mu\nu\rho},-H_{\mu\nu})\}\ . \tag{26}$$

For the corresponding expression involving the negative-valued solutions, the subscript $+$ must be changed to $-$.

Note that the above arguments, which generated (21), (24), and (26), provide only equalities between *sets* of roots. In order to find relations between the individual roots, additional considerations are needed. Charge conjugation, on one hand, and parity inversion and time reversal, on the other hand, have to be treated separately.

We begin by discussing charge conjugation. Equality (21) relates positive- and negative-valued eigenenergies. It therefore follows already at this point that in principle relation (21) and the knowledge of one root suffices to construct another solution. The remaining less important question is how the subscript (α) behaves under C. If an additional conserved quantity commuting with H is known (such as a spin component or helicity in the conventional case), the subscript (α) may be used to label its eigenvalues. A definite correspondence can then be determined by investigating the behavior of this conserved quantity under C. In the present case without knowledge of such an additional conserved quantity, the label (α) becomes essentially arbitrary and can therefore be chosen freely.[33] Our conventions agree with the conventional ones in the following sense:[34] the labels of eigenvalues and eigenspinors match and change under charge conjugation. This produces after reinterpretation

$$E_v^{(1,2)}(\vec{p},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})=E_u^{(2,1)}(\vec{p},m,-a^\mu,b^\mu,c^{\mu\nu},-d^{\mu\nu},-e^\mu,-f^\mu, g^{\mu\nu\rho},-H^{\mu\nu}) , \tag{27}$$

where $E_{u,v}^{(1,2)}$ denotes the zero-components of $p_{u,v}^{(1,2)}$ defined by (11). We remark that this labeling agrees with our previous choice.[3]

We now turn to parity inversion and time reversal. The equalities (24) and (26) provide a correspondence between roots of the same sign. As opposed to the previous case for C, it is therefore unclear *a priori* whether P and T individually can be used to construct additional eigenvalues from a known one. However, the combined transformation PT should give a different root: it connects different eigenspinors,[35] and according to our above conventions, this fact should be reflected in the labels of the eigenenergies. The invariance of the dispersion relation (10) under the transformation PT yields with this choice of labeling after reinterpretation

$$E_{u,v}^{(1,2)}(\vec{p},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})=E_{u,v}^{(2,1)}(\vec{p},m,a^\mu,-b^\mu,c^{\mu\nu},-d^{\mu\nu},e^\mu,f^\mu, -g^{\mu\nu\rho},-H^{\mu\nu}) . \tag{28}$$

To determine equalities between the individual roots in (24) and (26), a definite labeling scheme is needed. Without knowledge of an additional conserved operator this becomes a matter of choice constrained only by Eq. (28). Contrary to the charge-conjugation case, there is more freedom even at the conventional level: the two customary labels, spin projection onto a fixed direction or helicity, behave differently under both P and T. For definiteness, we choose the label (α) to change under P, but not under T. This agrees with the behavior of the conventional helicity labeling.

We mention that from any other combination of C, P, and T additional correspondences can be constructed straightforwardly. However, if one eigenenergy (with functional dependence agreeing with our choice of labeling) is known explicitly, the symmetries (27) and (28) suffice to determine the remaining three. As an illustrative example, consider the following case: all Lorentz-violating parameters except a_μ and b_0 are zero. The eigenenergies are then given by[2]

$$E_u^{(\alpha)}=\sqrt{m^2+(|\vec{p}-\vec{a}|+(-1)^\alpha b_0)^2}+a_0 , \quad E_v^{(\alpha)}=\sqrt{m^2+(|\vec{p}+\vec{a}|-(-1)^\alpha b_0)^2}-a_0 . \tag{29}$$

Suppose only one of the above energies, say $E_u^{(1)}=[m^2+(|\vec{p}-\vec{a}|-b_0)^2]^{1/2}+a_0$, is known. According to Eq. (28), the eigenvalue $E_u^{(2)}$ for the other positive-energy solution can then be obtained by keeping the sign of a_μ the same, but reversing the sign of b_0 in complete agreement with Eq. (29). Similarly, the symmetry (27) permits the determination of the antiparticle energy $E_v^{(2)}$ by

keeping all signs unchanged except for the one of a_μ, which has to be reversed. Again, the result is identical to the one given by (29). The remaining antiparticle energy $E_v^{(1)}$ can be found in the same way as $E_v^{(2)}$, but starting from $E_u^{(2)}$ instead of $E_u^{(1)}$.

The above method for the construction of additional eigenvalues from a known root has to be taken with a grain of salt. It is required that the functional dependence of the given eigenenergy on the Lorentz-violating parameters is consistent with our above choice of labeling. The following example illustrates this issue. Consider a model in which Lorentz breaking can be described by a^μ and $\vec{b}$ only. The following expressions for the reinterpreted eigenenergies satisfy its dispersion relation:[2]

$$\begin{aligned} E_u^{\pm} &= [m^2+(\vec{p}-\vec{a})^2 \pm 2\sqrt{m^2\vec{b}^2+(\vec{b}\cdot(\vec{p}-\vec{a}))^2}+\vec{b}^2]^{1/2}+a_0\ , \\ E_v^{\pm} &= [m^2+(\vec{p}+\vec{a})^2 \pm 2\sqrt{m^2\vec{b}^2+(\vec{b}\cdot(\vec{p}+\vec{a}))^2}+\vec{b}^2]^{1/2}-a_0\ . \end{aligned} \tag{30}$$

Suppose again that only one of these eigenenergies, say E_u^+, were known. Employing symmetry (28), i.e., reversing the sign of $\vec{b}$, does not yield any of the other eigenenergies. This can be traced to the fact that the functional dependence in Eq. (30) does not agree with our convention that the labels should change under PT. In Eq. (30), the labels reflect the sign of a square root in the expression rather than being related to the PT transformation. We remark that a suitable labeling can be obtained by multiplying the inner square roots in Eq. (30) by a quantity D that can take the values $+1$ and -1 and changes sign when $\vec{b}$ is reversed (i.e., a possible choice would be $D=\vec{b}\cdot\vec{B}/|\vec{b}\cdot\vec{B}|$, where $\vec{B}$ is arbitrary but fixed and satisfies $\vec{b}\cdot\vec{B}\neq 0$).

The symmetries (27) and (28) can also be used to find parameter combinations yielding degenerate roots. It follows from Eq. (28) that for

$$b^\mu = d^{\mu\nu} = g^{\mu\nu\rho} = H^{\mu\nu} = 0\ , \tag{31}$$

roots of the same sign are equal. Thus, Eq. (31) provides a sufficient condition for energy equality of two (distinct) particle states of a given three-momentum. The same holds true for the antiparticles. Suppose the Lorentz-violating parameters obey

$$a^\mu = d^{\mu\nu} = e^\mu = f^\mu = H^{\mu\nu} = 0\ , \tag{32}$$

or

$$a^\mu = b^\mu = e^\mu = f^\mu = g^{\mu\nu\rho} = 0\ . \tag{33}$$

Either one of the conditions (32) and (33) is sufficient for an energy degeneracy such that for each particle there exists an antiparticle of equal four-momentum. This can be verified by using the symmetries (27) and (28). As a corollary of the above discussion we remark that if $c^{\mu\nu}$ is the only nonvanishing Lorentz-violating parameter, then all four eigenenergies become degenerate after reinterpretation.

V. FIRST-ORDER APPROXIMATION OF THE EIGENENERGIES

In principle, the dispersion relation (20) and Eq. (4) allow the determination of the exact eigenenergies at a given three-momentum in the presence of Lorentz violation. In many circumstances, however, only leading-order corrections to the conventional eigenenergies are of interest. They can be obtained with the method described below.

With the aid of generalized Foldy–Wouthuysen techniques one can find a (momentum-dependent) unitary matrix U transforming the Hamiltonian (17) into the following block-diagonal form:[17]

$$U^{\dagger}HU=\begin{pmatrix} h_{\rm rel} & 0 \\ 0 & \overline{h}_{\rm rel} \end{pmatrix}, \tag{34}$$

where the two 2×2 matrices $h_{\rm rel}$ and $\overline{h}_{\rm rel}$ are the respective Hamiltonians for the fermion and the antifermion. From the procedure it is obvious that the eigenvalues of the matrices $h_{\rm rel}$ and $\overline{h}_{\rm rel}$ are the respective particle and antiparticle energies. To make further progress, consider the expansion

$$h_{\rm rel}=h_0+\sum_{j=1}^{3} h_j\sigma_j \tag{35}$$

of $h_{\rm rel}$ with respect to the basis $\{I,\sigma_j\}$. Here, I is the 2×2 identity and σ_j are the usual Pauli matrices. The components $h_0,\ldots,h_3$ depend on the three-momentum, the mass, and the parameters for Lorentz breaking as determined by the Foldy–Wouthuysen transformation. They yield the fermion eigenenergies by means of

$$E_u^{(\alpha)}=h_0\pm\sqrt{\sum_{j=1}^{3} h_j h_j}\,. \tag{36}$$

Note that the correspondence between the energy superscript (α), $\alpha\in\{1,2\}$ and the sign of the square root in (36) is only constrained by the symmetry (28).

This method is suitable for extracting the leading-order approximation of the eigenenergies because the components $h_0,\ldots,h_3$ are known to first order in the Lorentz-violating parameters:[17]

$$\begin{aligned}
h_0&=\gamma m+\left(a_0-\frac{mc_{00}}{\gamma}-me_0\right)+[a_j-\gamma m(c_{0j}+c_{j0})-me_j]\frac{p^j}{\gamma m}-(c_{jk}-\eta_{jk}c_{00})\frac{p^jp^k}{\gamma m}\,,\\
h_j&=-\frac{1}{\gamma}b_j+md_{j0}+\frac{1}{2}\varepsilon^{kl}{}_jH_{kl}-\frac{1}{2\gamma}m\varepsilon^{kl}{}_jg_{kl0}+\Bigg[\eta_{jk}b_0+m(d_{jk}-\eta_{jk}d_{00})+\varepsilon^{l}{}_{kj}H_{0l}\\
&\quad-\gamma m\varepsilon^{lm}{}_j\left(\frac{1}{2}g_{lmk}-\eta_{km}g_{l00}\right)\Bigg]\frac{p^k}{\gamma m}+\Bigg[\frac{(\gamma-1)m}{\vec{p}^{\,2}}\left(b_k+md_{k0}+\frac{1}{2}\varepsilon^{mn}{}_kH_{mn}+\frac{1}{2}m\varepsilon^{mn}{}_kg_{mn0}\right)\eta_{jl}\\
&\quad-(d_{0k}+d_{k0})\eta_{jl}+\varepsilon^{m}{}_{lj}(g_{m0k}+g_{mk0})\Bigg]\frac{p^kp^l}{\gamma m}+\frac{(\gamma-1)}{\vec{p}^{\,2}}\Bigg[-(d_{kl}-\eta_{kl}d_{00})-\frac{1}{2}\varepsilon^{nq}{}_lg_{nqk}\Bigg]\\
&\quad\times\eta_{jm}\frac{p^kp^lp^m}{\gamma}\,,
\end{aligned} \tag{37}$$

where $\gamma\equiv\sqrt{1+\vec{p}^{\,2}/m^2}$ is the usual relativistic gamma factor, and the totally antisymmetric rotation tensor ε^{jkl} satisfies $\varepsilon_{123}=+1$ and $\varepsilon^{jkl}=-\varepsilon_{jkl}$. Note that the parameter f^{μ} does not contribute to the eigenenergies at leading order. We remark that the symmetries (27) and (28) permit the construction of the antifermion energies.

As an illustration, consider the previously considered (a_{μ},b_0) model with the eigenenergies (29). For this model, we have $h_0=\gamma m+a_0-\vec{p}\cdot\vec{a}/\gamma m$ and $h_j=b_0p_j/\gamma m$. For this case, Eq. (36) yields

$$E_u^{(1,2)}=\sqrt{m^2+\vec{p}^{\,2}}+a_0-\frac{\vec{p}\cdot\vec{a}\pm b_0|\vec{p}|}{\sqrt{m^2+\vec{p}^{\,2}}}\,. \tag{38}$$

One can verify that Eqs. (29) and (38) agree to leading order in the Lorentz-violating coefficients provided the upper and lower signs in Eq. (38) are identified with the labels $\alpha=1$ and $\alpha=2$, respectively. The corresponding antiparticle energies to first order can now be obtained with the aid of symmetry (27), as discussed previously.

VI. SYMMETRIES OF THE EIGENSPINORS

It is necessary to begin this section by introducing our conventions and some more notation. The four eigenspinors $w_{\pm}^{(\alpha)}(\vec{\lambda})$ of $H(\vec{\lambda})$ are determined by

$$(H(\vec{\lambda})-\lambda^{0}_{\pm(\alpha)})w_{\pm}^{(\alpha)}(\vec{\lambda})=0\,. \tag{39}$$

We have used that the dispersion relation (10), and thus its roots $\lambda^{0}_{\pm(\alpha)}$, remain unchanged under the field redefinition. The eigenspinors $w_{\pm}^{(\alpha)}(\vec{\lambda})$ are related to the observer-covariant momentum-space spinors $W_{\pm}^{(\alpha)}(\vec{\lambda})$ obeying Eq. (9) by

$$W_{\pm}^{(\alpha)}(\vec{\lambda})=Aw_{\pm}^{(\alpha)}(\vec{\lambda})\,, \tag{40}$$

where A is the field-redefinition matrix discussed earlier. After reinterpretation of the negative-energy solutions we denote the eigenspinors of H by $u^{(\alpha)}(\vec{p})$ and $v^{(\alpha)}(\vec{p})$ in complete analogy to Def. (12). Thus, the transformation (40) remains valid even after the reinterpretation. The four eigenspinors for a given momentum, which can be taken as orthogonal, span spinor space. Our choice of normalization is

$$u^{(\alpha)\dagger}(\vec{p})u^{(\alpha')}(\vec{p})=\delta^{\alpha\alpha'}\frac{E_u^{(\alpha)}}{m}\,,\quad v^{(\alpha)\dagger}(\vec{p})v^{(\alpha')}(\vec{p})=\delta^{\alpha\alpha'}\frac{E_v^{(\alpha)}}{m}\,,\quad u^{(\alpha)\dagger}(\vec{p})v^{(\alpha')}(-\vec{p})=0\,. \tag{41}$$

Note that the physical spinors $w_{\pm}^{(\alpha)}$, and thus $u^{(\alpha)}$ and $v^{(\alpha)}$, fail to be observer Lorentz covariant due to the frame dependence of A.

The discrete transformations C, P, and T determine correspondences between sets of spinors, paralleling the eigenenergy case. For the charge-conjugation transformation our previous result[3]

$$\{W_{-}^{(\alpha)}(\vec{\lambda},m,a^{\mu},b^{\mu},c^{\mu\nu},d^{\mu\nu},e^{\mu},f^{\mu},g^{\mu\nu\rho},H^{\mu\nu})\}\propto\{W_{+}^{(\beta)c}(-\vec{\lambda},m,-a^{\mu},b^{\mu},c^{\mu\nu},-d^{\mu\nu},-e^{\mu},-f^{\mu},g^{\mu\nu\rho},-H^{\mu\nu})\} \tag{42}$$

holds, which we provide here for completeness. The charge-conjugated spinor $W^{c}\equiv C\overline{W}^{T}$ is defined with the conventional charge-conjugation matrix C. A $\propto$ sign, such as the one in relation (42), is to be understood as follows. For each spinor in one set there exists a spinor in the other set such that the two spinors are linearly dependent.

The parity transformation (22) induces the following relation:

$$\{W_{+}^{(\alpha)}(\vec{\lambda},m,a^{\mu},b^{\mu},c^{\mu\nu},d^{\mu\nu},e^{\mu},f^{\mu},g^{\mu\nu\rho},H^{\mu\nu})\}\propto\{W_{+}^{(\beta)p}(-\vec{\lambda},m,a_{\mu},-b_{\mu},c_{\mu\nu},-d_{\mu\nu},e_{\mu},-f_{\mu},g_{\mu\nu\rho},H_{\mu\nu})\}\,, \tag{43}$$

where $W^{p}\equiv\gamma^{0}W$ denotes the parity-inverted spinor as usual. The relation for the negative-eigenvalue spinors is obtained by replacing the subscripts $+$ with $-$. The result for time reversal (25) is given by

$$\{W_{+}^{(\alpha)}(\vec{\lambda},m,a^{\mu},b^{\mu},c^{\mu\nu},d^{\mu\nu},e^{\mu},f^{\mu},g^{\mu\nu\rho},H^{\mu\nu})\}\propto\{W_{+}^{(\beta)t}(-\vec{\lambda},m,a_{\mu},b_{\mu},c_{\mu\nu},d_{\mu\nu},e_{\mu},-f_{\mu},-g_{\mu\nu\rho},-H_{\mu\nu})\}\,. \tag{44}$$

Here, $W^{t}\equiv-i\gamma^{5}CW^{*}$ is the conventional time-reversed spinor. Again, changing the subscripts from $+$ to $-$ yields the corresponding relation for the remaining eigenspinors.

To find correspondences between individual eigenspinors, a definite labeling scheme for the spinors must be selected. The associated subtleties are analogous to the eigenenergy case and do not require additional discussion. Our previous convention that the labeling of the roots and eigenspinors matches leads after reinterpretation to the symmetries

$$V^{(1,2)}(\vec{p},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})=\zeta U^{(2,1)c}(\vec{p},m,-a^\mu,b^\mu,c^{\mu\nu},-d^{\mu\nu},-e^\mu,-f^\mu,g^{\mu\nu\rho},-H^{\mu\nu}) \tag{45}$$

and

$$U^{(1)}(\vec{p},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})=\eta U^{(2)pt}(\vec{p},m,a^\mu,-b^\mu,c^{\mu\nu},-d^{\mu\nu},e^\mu,f^\mu,-g^{\mu\nu\rho},-H^{\mu\nu}) \tag{46}$$

resulting from C and PT, respectively. Here, ζ and η are (possibly spinor-dependent) proportionality factors, and the superscript pt stands for the combined spinor transformations P and T defined above. The relation arising from PT, but involving the spinors $V^{(1,2)}$ can be obtained by replacing U with V in Eq. (46). If one eigenspinor is known explicitly (with functional dependence agreeing with our choice of labeling), the symmetries (45) and (46) can in principle be used to construct the remaining three.

As an illustration, we again consider the (a_μ,b_0) model. Its eigenspinors in Pauli–Dirac representation are[2]

$$\begin{aligned} U^{(\alpha)}(\vec{p},m,a^\mu,b^0)&=\left(\frac{E_u^{(\alpha)}(E_u^{(\alpha)}-a_0+m)}{2m(E_u^{(\alpha)}-a_0)}\right)^{1/2}\begin{pmatrix}\phi^{(\alpha)}(\vec{p}-\vec{a})\\ \dfrac{-(-1)^\alpha|\vec{p}-\vec{a}|-b_0}{E_u^{(\alpha)}-a_0+m}\phi^{(\alpha)}(\vec{p}-\vec{a})\end{pmatrix},\\ V^{(\alpha)}(\vec{p},m,a^\mu,b^0)&=\left(\frac{E_v^{(\alpha)}(E_v^{(\alpha)}+a_0+m)}{2m(E_v^{(\alpha)}+a_0)}\right)^{1/2}\begin{pmatrix}\dfrac{-(-1)^\alpha|\vec{p}+\vec{a}|+b_0}{E_v^{(\alpha)}+a_0+m}\phi^{(\alpha)}(\vec{p}+\vec{a})\\ \phi^{(\alpha)}(\vec{p}+\vec{a})\end{pmatrix}, \end{aligned} \tag{47}$$

where the two-component spinors $\phi^{(\alpha)}(\vec{k})$ are given by

$$\phi^{(1)}(\vec{k})=\begin{pmatrix}\cos(\theta/2)\\ e^{i\varphi}\sin(\theta/2)\end{pmatrix},\quad \phi^{(2)}(\vec{k})=\begin{pmatrix}-e^{-i\varphi}\sin(\theta/2)\\ \cos(\theta/2)\end{pmatrix}. \tag{48}$$

Here, θ and φ are the spherical-polar angles subtended by $\vec{k}$. Suppose that only one of the spinors in Eq. (47), say $U^{(1)}(\vec{p},m,a^\mu,b^0)$, is known. With the symmetry (46) one can now construct $U^{(2)}(\vec{p},m,a^\mu,b^0)$ up to a constant: in $U^{(1)}(\vec{p},m,a^\mu,b^0)$, the sign of b^0 has to be reversed. Note that this entails changing $E_u^{(1)}$ to $E_u^{(2)}$ by virtue of Eq. (28). Complex conjugation resulting from time reversal affects only $\phi^{(1)}(\vec{p}-\vec{a})$ because all other quantities in the expression are real for this specific model. The final step is multiplication with the matrix $-i\gamma^3\gamma^1\gamma^0=\left(\begin{smallmatrix}-\sigma^2 & 0\\ 0 & \sigma^2\end{smallmatrix}\right)$, where σ^2 denotes the usual Pauli matrix associated with the two-direction. This is somewhat simplified by observing that $\sigma^2\phi^{(1)*}(\vec{k})=i\phi^{(2)}(\vec{k})$. Comparison with Eq. (47) shows that the resulting spinor is indeed $U^{(2)}(\vec{p},m,a^\mu,b^0)$ up to a factor of $-i$. The symmetry (45) determines (up to constants) the remaining two spinors $V^{(1)}(\vec{p},m,a^\mu,b^0)$ and $V^{(2)}(\vec{p},m,a^\mu,b^0)$ from $U^{(2)}(\vec{p},m,a^\mu,b^0)$ and $U^{(1)}(\vec{p},m,a^\mu,b^0)$, respectively: reverse the sign of a^μ, complex conjugate and multiply by $i\gamma^2$. This procedure yields $V^{(2)}(\vec{p},m,a^\mu,b^0)$ exactly and $V^{(1)}(\vec{p},m,a^\mu,b^0)$ up to a relative minus sign.

With an explicit labeling scheme like that selected for the eigenenergies, additional relations between the spinors can be determined using other combinations of Eqs. (42), (43), and (44). The corresponding symmetries for the physical spinors defined earlier can be obtained by replacing $U^{(1,2)}$ and $V^{(1,2)}$ in Eqs. (45) and (46) by $u^{(1,2)}$ and $v^{(1,2)}$, respectively. Note that the field-

redefinition matrix A depends on the Lorentz-violating parameters. For example, to construct $u^{(\alpha)}(\vec{p},m,-a^\mu,b^\mu,c^{\mu\nu},-d^{\mu\nu},-e^\mu,-f^\mu,g^{\mu\nu\rho},-H^{\mu\nu})$ from $U^{(\alpha)}(\vec{p},m,a^\mu,b^\mu,c^{\mu\nu},d^{\mu\nu},e^\mu,f^\mu,g^{\mu\nu\rho},H^{\mu\nu})$ and $A(c^{\mu 0},d^{\mu 0},e^0,f^0,g^{\mu\nu 0})$, the appropriate sign changes have to be implemented *both* in $U^{(\alpha)}$ and in A.

VII. GENERALIZATION OF THE CONVENTIONAL SPINOR PROJECTORS

In the ordinary Dirac case, the spinor matrices that project on the positive- and negative-energy eigenspaces

$$\pm\sum_{\alpha=1}^{2} w_{\pm}^{(\alpha)}\otimes\overline{w}_{\pm}^{(\alpha)}=\frac{\not{\lambda}_{\pm}+m}{2m} \tag{49}$$

are an indispensable tool in numerous calculations. To obtain the Lorentz-violating analog, we fix an arbitrary three-momentum $\vec{\lambda}$ and express the left-hand side of Eq. (13) in terms of the Hamiltonian (17):

$$\mathrm{cof}(\Gamma_\mu\lambda^\mu-M)=\det(\Gamma^0)\prod_{[j]}(\lambda^0-\lambda^0_{[j]})(\gamma^0\Gamma^0)^{-1/2}(\lambda^0-H)^{-1}(\gamma^0\Gamma^0)^{-1/2}\gamma^0\ . \tag{50}$$

Here and in what follows, the dependence of the eigenvalues, the eigenspinors, and the Hamiltonian on the fixed $\vec{\lambda}$ is omitted for brevity. The two positive and two negative eigenvalues $\lambda^0_{+(1,2)}$ and $\lambda^0_{-(1,2)}$ of H are denoted collectively by $\lambda^0_{[j]}$, where $[j]\in\{-(2),-(1),+(1),+(2)\}$. The product in Eq. (50) runs over all four of these eigenvalues. Since the Hamiltonian (17) is Hermitian, there exists a spinor basis in which H is diagonal. In this basis, we have explicitly

$$\mathrm{cof}(\Gamma_\mu\lambda^\mu-M)=\det(\Gamma^0)(\gamma^0\Gamma^0)^{-1/2}P_{\lambda^0}(\gamma^0\Gamma^0)^{-1/2}\gamma^0\ , \tag{51}$$

where the diagonal matrix P_{λ^0} is given by

$$P_{\lambda^0}\equiv\begin{pmatrix}(\lambda^0-\lambda^0_{+(2)})(\lambda^0-\lambda^0_{-(1)})(\lambda^0-\lambda^0_{-(2)}) & & & \cdots & 0\\ & (\lambda^0-\lambda^0_{+(1)})(\lambda^0-\lambda^0_{-(1)})(\lambda^0-\lambda^0_{-(2)}) & & & \vdots\\ \vdots & & (\lambda^0-\lambda^0_{+(1)})(\lambda^0-\lambda^0_{+(2)})(\lambda^0-\lambda^0_{-(2)}) & & \\ 0 & \cdots & & (\lambda^0-\lambda^0_{+(1)})(\lambda^0-\lambda^0_{+(2)})(\lambda^0-\lambda^0_{-(1)})\end{pmatrix}. \tag{52}$$

For $\lambda^0\to\lambda^0_{+(1)}$, the nondegenerate case $\lambda^0_{+(1)}\neq\lambda^0_{+(2)}$ and the degenerate case $\lambda^0_{+(1)}=\lambda^0_{+(2)}$ have to be distinguished.

In the nondegenerate case, the matrix P_{λ^0} simplifies to

$$P_{\lambda^0_{+(1)}}=\begin{pmatrix}(\lambda^0_{+(1)}-\lambda^0_{+(2)})(\lambda^0_{+(1)}-\lambda^0_{-(1)})(\lambda^0_{+(1)}-\lambda^0_{-(2)}) & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}, \tag{53}$$

which can be written $P_{\lambda^0_{+(1)}}=(H-\lambda^0_{+(2)})(H-\lambda^0_{-(1)})(H-\lambda^0_{-(2)})$. Thus, $P_{\lambda^0_{+(1)}}$ is proportional to the projector on the $\lambda^0_{+(1)}$ eigenspace. The above argument applied to an arbitrary nondegenerate eigenvalue $\lambda^0_{[r]}$ yields

$$\mathrm{cof}(\Gamma_\mu\lambda^\mu_{[r]}-M)=\det(\Gamma^0)(\gamma^0\Gamma^0)^{-1/2}\prod_{[j]\neq[r]}(H-\lambda^0_{[j]})(\gamma^0\Gamma^0)^{-1/2}\gamma^0\ . \tag{54}$$

The $P_{\lambda^0_{[r]}}$ can be expressed in terms of the eigenspinors in the usual way. Our normalization (41) gives explicitly

$$\prod_{[j]\neq[r]}(H-\lambda^0_{[j]})=\frac{m}{|\lambda^0_{[r]}|}w_{[r]}\otimes w^\dagger_{[r]}\prod_{[j]\neq[r]}(\lambda^0_{[r]}-\lambda^0_{[j]})\ , \tag{55}$$

where $w_{[r]}\in\{w^{(2)}_-,w^{(1)}_-,w^{(1)}_+,w^{(2)}_+\}$ is a shorthand notation for the $\lambda^0_{[r]}$ eigenspinor. One can now determine the desired projectors for the observer-invariant eigenspinors. We obtain for nondegenerate eigenvalues $\lambda^0_{[r]}$:

$$\frac{m}{|\lambda^0_{[r]}|}W_{[r]}\otimes\overline{W}_{[r]}=\frac{\mathrm{cof}(\Gamma_\mu\lambda^\mu_{[r]}-M)}{\det(\Gamma^0)\prod_{[j]\neq[r]}(\lambda^0_{[r]}-\lambda^0_{[j]})}\ . \tag{56}$$

For degenerate eigenvalues $\lambda^0_{[q]}=\lambda^0_{[r]}$, $([q]\neq[r])$, the matrix $P_{\lambda^0_{[r]}}$ vanishes. However, Eq. (51) can be modified to

$$\widehat{\mathrm{cof}}(\Gamma_\mu\lambda^\mu-M)=\det(\Gamma^0)(\gamma^0\Gamma^0)^{-1/2}\hat{P}_{\lambda^0}(\gamma^0\Gamma^0)^{-1/2}\gamma^0\ , \tag{57}$$

where a caret denotes division by the appropriate $(\lambda^0-\lambda^0_{[r]})$ factor. The existence of $\hat{P}_{\lambda^0}$ in the limit $\lambda^0\to\lambda^0_{[r]}$ is immediate from Def. (52). Note that the resulting matrix $\hat{P}_{\lambda^0_{[r]}}$ is again, up to normalization, the projector on the $\lambda^0_{[r]}$ eigenspace. By virtue of Eq. (57), $\widehat{\mathrm{cof}}(\Gamma_\mu\lambda^\mu-M)$ is also well defined for all λ^0. Considerations similar to the ones for a nondegenerate eigenvalue yield the following intermediate expression involving the eigenspinors of H:

$$\prod_{[j]\neq[q],[r]}(H-\lambda^0_{[j]})=\frac{m}{|\lambda^0_{[r]}|}\sum_{[k]=[q],[r]}w_{[k]}\otimes w^\dagger_{[k]}\prod_{[j]\neq[q],[r]}(\lambda^0_{[r]}-\lambda^0_{[j]})\ . \tag{58}$$

The final result for the case of two degenerate eigenvalues $\lambda^0_{[q]}=\lambda^0_{[r]}$, $([q]\neq[r])$ is given by

$$\frac{m}{|\lambda^0_{[r]}|}\sum_{[k]=[q],[r]}W_{[k]}\otimes\overline{W}_{[k]}=\frac{\widehat{\mathrm{cof}}(\Gamma_\mu\lambda^\mu_{[r]}-M)}{\det(\Gamma^0)\prod_{[j]\neq[q],[r]}(\lambda^0_{[r]}-\lambda^0_{[j]})}\ . \tag{59}$$

For any square matrix B, the relation $U^\dagger\mathrm{cof}(B)U=\mathrm{cof}(U^\dagger BU)$ holds, where U is unitary. Thus expressions (56) and (59) for the generalized projectors are independent of the spinor-space basis. We also remark that the projectors (49) for the ordinary Dirac case can be recovered from these results, as expected. In this case, the eigenenergies are degenerate so that Eq. (59) must be employed. Moreover, no field redefinition is necessary, so that the covariant and physical spinors are identical. The matrix of cofactors is given by $(\lambda^2-m^2)(\not{\lambda}+m)$, which can be verified directly or can be obtained from Eq. (14). Assembling everything yields Eq. (49).

As an immediate application, the generalized projector (56) permits the construction of a more explicit form of the eigenspinor in the case when there is a nondegenerate eigenvalue $\lambda^0_{[r]}$:

$$W_{[r]}(\vec{\lambda})=N_{[r]}(\vec{\lambda})\mathrm{cof}(\Gamma_\mu\lambda^\mu_{[r]}-M)W^0_{[r]}(\vec{\lambda})\ , \tag{60}$$

where $N_{[r]}(\vec{\lambda})$ is a normalization factor and $W^0_{[r]}(\vec{\lambda})$ any spinor only constrained by $W^0_{[r]}(\vec{\lambda})\notin\mathrm{Ker}[\mathrm{cof}(\Gamma_\mu\lambda^\mu_{[r]}-M)]$. The remaining spinors can be determined, e.g., with the symmetries discussed earlier. If both the negative- and the positive-valued roots are degenerate and an additional conserved quantity commuting with the Hamiltonian is unknown, no orthonormal

spinor basis spanning the eigenspaces is preferred. One can then replace cof$\rightarrow\widehat{\text{cof}}$ in Eq. (60) and in the associated requirement on $W^0_{[r]}(\check{\lambda})$. It is now possible to proceed as in the nondegenerate case.

VIII. SUMMARY

This work has discussed the theory of the Lorentz-violating Dirac equation in the Standard-Model Extension (SME). The main results include various symmetry properties of the solutions and generalizations of conventional relations. In particular, Eq. (19) permits the construction of a Hermitian Hamiltonian to arbitrary order in the Lorentz-violating parameters. Symmetries of the eigenenergies and the eigenspinors arising from the discrete C, P, and T transformations are given by Eqs. (27) and (28), and by Eqs. (45) and (46), respectively. The analog of the conventional spinor projectors is provided by Eq. (56) in the nondegenerate case or Eq. (59) in the degenerate case. These latter two equations involve the matrix of cofactors of the modified Dirac operator, which is given explicitly by Eq. (14).

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[33] Note, however, that the labeling should reflect in a consistent way the functional dependence of the roots on the three-momentum, the mass, and Lorentz-violating parameters. To illustrate this issue, consider a b_0 model with dispersion-relation roots labeled $\lambda^0_{+(\alpha)}(\vec{\lambda},m,b_0)=\sqrt{m^2+(|\vec{\lambda}|+(-1)^\alpha b_0)^2}$ and $\lambda^0_{-(\alpha)}(\vec{\lambda},m,b_0)=-\sqrt{m^2+(|\vec{\lambda}|+(-1)^\alpha|b_0|)^2}$. This labeling entails the undesirable feature that the behavior of (α) under C depends on the sign of b_0. A different choice of labels, such as $|b_0|\to b_0$ in $\lambda^0_{-(\alpha)}$, would be more natural. This issue is particularly important for the PT transformation.
[34] In the ordinary Dirac case, either helicity or spin projection with respect to a given direction in the rest frame of the particle is usually employed to characterize the degeneracy of the eigenergies. Note that under charge conjugation both of these operators change sign (Ref. 36). For the present purpose it is therefore irrelevant whether helicity or spin-projection labels are taken as the conventional ones.
[35] Suppose this were not true. In the conventional case, the arguments of the spinors, $\vec{p}$ and m, remain unchanged under the combined transformation of parity inversion and time reversal. This implies that there exist spinors W that are proportional to their PT image $-iC\gamma^5\gamma^0 W$. That this is impossible can be verified by an explicit calculation in Pauli–Dirac representation. Thus the claim holds true in the conventional case for any labeling. Assuming that in the present context the spinors depend smoothly on the Lorentz-breaking parameters as they approach zero, the result can be extended to the case of small Lorentz violation.
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Nonlinear canonical transformations in classical and quantum mechanics

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p-mechanics is a consistent physical theory which describes both classical and quantum mechanics simultaneously through the representation theory of the Heisenberg group. In this paper we describe how nonlinear canonical transformations affect *p*-mechanical observables and states. Using this we show how canonical transformations change a quantum mechanical system. We seek an operator on the set of *p*-mechanical observables which corresponds to the classical canonical transformation. In order to do this we derive a set of integral equations which when solved will give us the coherent state expansion of this operator. The motivation for these integral equations comes from the work of Moshinsky and a variety of collaborators. We consider a number of examples and discuss the use of these equations for non-bijective transformations. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Canonical transformations are at the center of classical mechanics.[5,14,18] A canonical transformation in classical mechanics is a map A defined on phase space (throughout this paper we take phase space to be $\mathbb{R}^{2n}$) which preserves the Poisson bracket. That is A: $\mathbb{R}^{2n}\rightarrow\mathbb{R}^{2n}$ such that for any two classical mechanical observables f, g

$$\{f\circ A,g\circ A\}=\{f,g\}\circ A. \tag{1}$$

It is important to note that the map A may well be non-bijective and nonlinear. A condition which is equivalent to (1) is that the map A must also preserve the symplectic form on $\mathbb{R}^{2n}$,

$$\omega(A(q,p),A(q',p'))=\omega((q,p),(q',p')), \tag{2}$$

where ω is defined as $\omega((q,p),(q',p'))=qp'-q'p$. The most advanced applications of canonical transformations in classical mechanics are the Hamilton–Jacobi theory (Ref. 14, Chap. 10, and Ref. 5, Chap. 9) and action angle variables (Ref. 18, Sec. 6.2, and Ref. 5, Chap. 9).

The passage of canonical transformations from classical mechanics to quantum mechanics has been a long journey which is still incomplete. The first person to give a clear formulation of quantum canonical transformations was Dirac; this is presented in his book.[9] Mario Moshinsky along with a variety of collaborators has published a great number of enlightening papers on the subject.[27,29,30,13,10] In these papers the aim is to find an operator, U, defined on a Hilbert space which corresponds to the canonical transformation. Moshinsky and his collaborators developed a system of differential equations which when solved gave the matrix elements—with respect to the eigenfunctions of the position or momentum operator—of U. More recently Arlen Anderson[2,3] has published some results on modeling canonical transformations in quantum mechanics using nonunitary operators.

In this paper we use *p*-mechanics to exhibit relations between classical and quantum canonical transformations. *p*-mechanics[8] describes both classical and quantum mechanics using the Heisen-

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berg group (denoted $\mathbb{H}^n$). The theory contains both observables and states which can both be realized as functions/distributions on $\mathbb{H}^n$. *p*-mechanical observables can be transformed into both quantum and classical observables using different representations of $\mathbb{H}^n$.

We derive a system of integral equations using *p*-mechanics which when solved give the coherent state expansion of an operator on the set of *p*-mechanical observables corresponding to the canonical transformation. Under representations of $\mathbb{H}^n$ this will give us the representation of canonical transformations in both classical and quantum mechanics. Our approach, unlike Moshinsky's, does not need observables to be members of the algebra generated by the position and momentum operators.

In Sec. II we give an outline of *p*-mechanics and extend it to fit the needs of this paper. In Sec. III we derive systems of integral equations for canonical transformations which when solved will give the corresponding operator on *p*-mechanical states in terms of coherent state expansions. For Hilbert space states this is presented in Sec. III A while for states realized as integration kernels these equations are derived in Sec. III B. We consider applications of these equations to nonbijective transformations in Sec. III D. Finally, we summarize the paper and suggest some interesting extensions in Sec. IV.

II. *p*-MECHANICS

The theory of *p*-mechanics has been presented in a number of papers[7,24,23]—a recent review article is Ref. 8. In this section we extend these concepts to fit the purposes of our paper. In particular we give a new definition of *p*-mechanical observables and show how the kernel states can be expanded out using coherent states.

At the heart of *p*-mechanics is the Heisenberg group.[12,34] The Heisenberg group (denoted $\mathbb{H}^n$) is the set of all triples in $\mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n$ under the law of multiplication

$$(s,x,y)\cdot(s',x',y')=(s+s'+\tfrac{1}{2}(x\cdot y'-x'\cdot y),x+x',y+y'). \tag{3}$$

The noncommutative convolution of two functions $B_1,\ B_2\in L^1(\mathbb{H}^n)$ is

$$(B_1*B_2)(g)=\int_{\mathbb{H}^n}B_1(h)B_2(h^{-1}g)dh=\int_{\mathbb{H}^n}B_1(gh^{-1})B_2(h)dh, \tag{4}$$

where dh is Haar measure on $\mathbb{H}^n$ which is Lebesgue measure $ds\,dx\,dy$ on $\mathbb{R}^{2n+1}$. In this paper the convolution algebra $L^1(\mathbb{H}^n)$ is too restrictive so we extend convolution to spaces of distributions. Spaces of interest in this paper are

(i) $\mathcal{E}'(\mathbb{H}^n)$ of distributions with compact support (Ref. 35, Thm. 24.2) on $\mathbb{H}^n$;
(ii) $\mathcal{S}'(\mathbb{H}^n)$ of tempered distributions (also known as the Schwartz space) (Ref. 35, Defn. 25.2) on $\mathbb{H}^n$; and
(iii) $\mathcal{D}'(\mathbb{H}^n)$ of all distributions (Ref. 35, and Chap. 21) on $\mathbb{H}^n$.

The convolution of two distributions is defined in a natural way (Ref. 34, Chap. 0). The spaces $\mathcal{E}'(\mathbb{H}^n)$ and $\mathcal{D}'(\mathbb{H}^n)$ are closed under convolution.

The Lie algebra of $\mathbb{H}^n$ is denoted by $\mathfrak{h}_n$ and can be realized by the left invariant vector fields

$$S=\frac{\partial}{\partial s},\quad X_j=\frac{\partial}{\partial x_j}-\frac{y_j}{2}\frac{\partial}{\partial s},\quad Y_j=\frac{\partial}{\partial y_j}+\frac{x_j}{2}\frac{\partial}{\partial s},$$

with the Heisenberg commutator relations

$$[X_i,Y_j]=\delta_{ij}S.$$

The most common representation of the Heisenberg group is the Schrödinger representation (Ref. 12, Sec. 1.3, and Ref. 34, Eq. 2.23) on $L^2(\mathbb{R}^n)$:

$$(\rho_h^S(s,x,y)\psi)(\xi)=e^{-2\pi ihs-2\pi ix\xi-\pi ihxy}\psi(\xi+hy). \tag{5}$$

Throughout this paper we do not use (5); instead we show how a representation unitarily equivalent to this can at times be advantageous. We now introduce this representation and the space on which it is defined.

Definition 2.1: We define the space $F^2(\mathcal{O}_h)$ *as*

$$F^2(\mathcal{O}_h)=\{f_h(q,p)\in L^2(\mathbb{R}^{2n}):D_h^j f_h=0,\quad \text{for } 1\leqslant j\leqslant n\}, \tag{6}$$

where the operator D_h^j *on* $L^2(\mathbb{R}^{2n})$ *is defined as* $(h/2)(\partial/\partial p_j+i\partial/\partial q_j)+2\pi(p_j+iq_j)$.

The inner product on $F^2(\mathcal{O}_h)$ is given by

$$\langle v_1,v_2\rangle_{F^2(\mathcal{O}_h)}=\left(\frac{4}{h}\right)^n\int_{\mathbb{R}^{2n}}v_1(q,p)\overline{v_2(q,p)}dqdp. \tag{7}$$

$F^2(\mathcal{O}_h)$ is a Hilbert space with this inner product (Ref. 21, Sec. 4.1). The motivation for using this space in p-mechanics originates from Kirillov's method of orbits[19,20]—this relation is discussed in Refs. 8 and 24. $F^2(\mathcal{O}_h)$ is similar to the Fock–Segal–Bargmann [Refs. 6, 12 (Sec. 1.6), and 34 (Chap. 1)] space of analytic functions on $\mathbb{C}^n$ which are square integrable with respect to the measure $e^{-2|z|^2/h}dz$. It is shown in Ref. 24, Prop. 2.6, that $f_h(q,p)$ is in $F^2(\mathcal{O}_h)$ if and only if $f_h(z)e^{|z|^2/h}$ is in the Fock–Segal–Bargmann space with $z=p+iq$. The integral kernel

$$K_I(q,p,x)=e^{2\pi iqx-\pi ipq}e^{-\pi(x-p)^2}$$

provides an isometry W: $L^2(\mathbb{R}^n)\to F^2(\mathcal{O}_h)$ by

$$\psi(x)\mapsto f(q,p)=\int_{\mathbb{R}^n}\psi(x)K_I(q,p,x)dx. \tag{8}$$

This is proved in Ref. 21, Sec. 4.2. It is also shown in Ref. 21, Sec. 4.2, that $F^2(\mathcal{O}_h)$ is a reproducing kernel Hilbert space with reproducing kernel

$$K_R(q,p,q',p')=\exp\left(-\frac{2\pi}{h}(q^2+p^2+q'^2+p'^2-2qq'-2pp'-2iq'p+2iqp')\right).$$

The representation ρ_h (Refs. 24 and 8) of $\mathbb{H}^n$ on $F^2(\mathcal{O}_h)$ is defined by

$$\rho_h(s,x,y):f_h(q,p)\mapsto e^{-2\pi i(hs+qx+py)}f_h\left(q-\frac{h}{2}y,p+\frac{h}{2}x\right), \tag{9a}$$

which is unitary with respect to the inner product defined in (7). This representation is intertwined with the Schrödinger representation by the unitary map (8)[21] and so is unitarily equivalent to the Schrödinger representation.

The crucial theorem which motivates the whole of p-mechanics is the following.

Theorem 2.1 *(The Stone–von Neumann Theorem): All unitary irreducible representations of the Heisenberg group,* $\mathbb{H}^n$*, up to unitary equivalence, are either*

(i) *of the form* ρ_h *on* $F^2(\mathcal{O}_h)$ *from Eq. (9) or*
(ii) *for* $(q,p)\in\mathbb{R}^{2n}$ *the commutative one-dimensional representations on* $\mathbb{C}=L^2(\mathcal{O}_{(q,p)})$

$$\rho_{(q,p)}(s,x,y)u=e^{-2\pi i(q\cdot x+p\cdot y)}u. \tag{9b}$$

Proof: In Ref. 12 or 34 it is shown that this holds for the Schrödinger representation. Our result follows since ρ_h is intertwined with the Schrödinger representation by the isometry W given in (8). □

We can extend both ρ_h and $\rho_{(q,p)}$ to the representation of an infinitely differentiable compactly supported function, $B \in C_0^\infty(\mathbb{H}^n)$, on $\mathbb{H}^n$ by

$$\rho(B) = \int_{\mathbb{H}^n} B(g)\rho(g)dg.$$

The representation of distributions is done in the natural way (Ref. 34, Chap 0, Eq 3.4).

The basic idea of *p*-mechanics is to choose particular functions or distributions on $\mathbb{H}^n$ which under the infinite dimensional representation will give quantum mechanical observables, while under the one dimensional representation will give classical mechanical observables. In doing this it is shown that both mechanics are derived from the same source. *p*-mechanical observables can be realized as operators (some of which are unbounded) on a subset of $L^2(\mathbb{H}^n)$ generated by convolutions of the chosen functions or distributions. To define *p*-mechanical observables properly we need to introduce a map from the set of classical observables to the set of *p*-mechanical observables. In Refs. 8 and 24 a map of *p*-mechanization, $\mathcal{P}$, from the set of classical observables to the set of *p*-mechanical observables is defined as

$$(\mathcal{P}f)(s,x,y) = \delta(s)\check{f}(x,y), \tag{10}$$

where f is any classical observable and $\check{f}$ is the inverse Fourier transform of f [that is, $\check{f}(x,y) = \int_{\mathbb{R}^{2n}} f(q,p)e^{2\pi i(qx+py)}dqdp$].

Definition 2.2 (*p*-Mechanical Observables): *The set of p-mechanical observables is the image of the set of classical observables under the map $\mathcal{P}$ from Eq. (10).*

Clearly this definition depends on how the set of classical observables is defined. Any physically reasonable classical mechanical observable can be realized as an element of $\mathcal{S}'(\mathbb{R}^{2n})$. Since the Fourier transform maps $\mathcal{S}'(\mathbb{R}^{2n})$ into itself, $\mathcal{S}'(\mathbb{H}^n)$ is a natural choice for the set of *p*-mechanical observables. It includes the image of all classical observables which are polynomials or exponentials of the variables q and p.

If we take the ρ_h representation (9) of many of the distributions described above, we would get unbounded operators. For example, the distribution $\delta(s)\delta^{(1)}(x)\delta(y)$ under the ρ_h representation will generate the unbounded operator $(h/2)(\partial/\partial p) - 2\pi iqI$. This operator is clearly not defined on the whole of $F^2(\mathcal{O}_h)$. This technical problem can be solved by the usual method of rigged Hilbert spaces (also known as Gelfand triples)[36,32,33] which uses the theory of distributions. Another approach to dealing with unbounded operators is given by using the Gårding space as explained in Ref. 34, Chap. 0.

The dynamics of a *p*-mechanical system is described in Refs. 8, 23, and 24 using the universal brackets. The universal brackets (also known as *p*-mechanical brackets) are

$$\{[B_1, B_2]\} = \mathcal{A}(B_1 * B_2 - B_2 * B_1), \tag{11}$$

where $\mathcal{A}$ is the right inverse to the vector field $S = \partial/\partial s$. It is shown in Ref. 23, Prop. 3.5, that under the one and infinite dimensional representations the universal brackets become the Poisson brackets and the quantum commutator, respectively. Hence, for a system with Hamiltonian B_H (the *p*-mechanization of the classical Hamiltonian H) solving the *p*-dynamic equation,

$$\frac{dB}{dt} = \{[B, B_H]\} \tag{12}$$

will give the quantum and classical dynamics under the infinite and one dimensional representations, respectively.

In Refs. 7 and 8, states in *p*-mechanics were introduced. They were defined as functionals on the set of *p*-mechanical observables and came in two forms—elements of a Hilbert space and integration kernels.

Definition 2.3: The Hilbert space $\mathcal{H}_h$, $h \in \mathbb{R}\backslash\{0\}$, is defined as the set of functions on $\mathbb{H}^n$,

$$\mathcal{H}_h=\{e^{-2\pi ihs}f(x,y):E_h^j f=0 \quad 1\leqslant j\leqslant n \quad \text{and} \quad f\in L^2(\mathbb{R}^{2n})\}, \tag{13}$$

where the operator $E_h^j=\pi h(y-ix)+i\partial/\partial x-\partial/\partial y$ *[this is the Fourier transform of* D_h^j *from (6)].*

The inner product on $\mathcal{H}_h$ is defined as

$$\langle v_1,v_2\rangle_{\mathcal{H}_h}=\left(\frac{4}{h}\right)^n\int_{\mathbb{R}^{2n}}v_1(s,x,y)\overline{v_2}(s,x,y)dxdy. \tag{14}$$

The set of *p*-mechanical observables acts on $\mathcal{H}_h$ by convolution. For many observables this will give rise to unbounded operators which are not defined on the whole of $\mathcal{H}_h$. This problem is solved as before by the use of rigged Hilbert spaces. It is shown in Ref. 7, Eq. 3.4, that any element $v\in\mathcal{H}_h$ is of the form $v(s,x,y)=e^{-2\pi ihs}\hat{f}(x,y)$ for some $f\in F^2(\mathcal{O}_h)$ ($\hat{f}$ denotes the Fourier transform of f).

The state corresponding to $v\in\mathcal{H}_h$ can be realized by an integration kernel

$$l(s,x,y)=\left(\frac{4}{h}\right)^n\int_{\mathbb{R}^{2n}}v((s,x,y)^{-1}(s',x',y'))\overline{v((s',x',y'))}dx'dy'. \tag{15}$$

For any *p*-mechanical observable B the following relation is proved in Ref. 7, Thm. 3.1 and Thm. 3.2:

$$\langle\rho_h(B)f,f\rangle=\langle B*v,v\rangle=\int_{\mathbb{H}^n}B(g)l(g)dg, \tag{16}$$

where f is the element of $F^2(\mathcal{O}_h)$ such that $v(s,x,y)=e^{-2\pi ihs}\hat{f}(x,y)$ and l is the kernel corresponding to v through relation (15). Equation (16) gives the expectation value of the observable B in the state corresponding to f, v and l.

In Ref. 7 an overcomplete system of coherent states in $\mathcal{H}_h$ is derived using representations of the Heisenberg group:

$$v_{(h,q,p)}(s,x,y)=\left(\frac{h}{2}\right)^n\exp\left(-2\pi ihs+\pi i(xq+yp)-\frac{\pi h}{2}\left(\left(x+\frac{p}{h}\right)^2+\left(y-\frac{q}{h}\right)^2\right)\right). \tag{17}$$

The corresponding kernel coherent states are

$$l_{(h,q,p)}=\exp\left(-2\pi i(qx+py)+2\pi ihs-\frac{\pi h}{2}(x^2+y^2)\right). \tag{18}$$

It is shown in Ref. 7 that if we choose $B=\mathcal{P}(f)$, then

$$\lim_{h\to 0}\langle B*v_{(h,q,p)},v_{(h,q,p)}\rangle=\int_{\mathbb{H}^n}Bl_{(h,q,p)}dg=f(q,p).$$

By the usual theory of coherent states (that is, wavelets),[1] in a Hilbert space any element $v\in\mathcal{H}_h$ can be written as

$$v=\int_{\mathbb{R}^{2n}}\langle v,v_{(h,q,p)}\rangle v_{(h,q,p)}dqdp. \tag{19}$$

If we define an inner product on the set of kernels as

$$\langle l_1,l_2\rangle=\int_{\mathbb{R}^{2n}}l_1(s,x,y)\overline{l_2(s,x,y)}dxdy, \tag{20}$$

this inner product will be well defined for any two kernel coherent states from (18) since the integral on the right hand side of (20) will be finite. Then we can define our space of kernels, $\mathcal{L}_h$, as the completion of the set of linear combinations of the coherent states (18). Clearly $\mathcal{L}_h$ is a Hilbert space so we can expand any kernel in $\mathcal{L}_h$ by the formula

$$l(s,x,y)=\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} l(s,x',y')\overline{l_{(h,q,p)}(s,x',y')}dx'dy'l_{(h,q,p)}(s,x,y)dqdp.$$

We now show that the $\mathcal{H}_h$ coherent states are eigenfunctions of the creation and annihilation operators. The creation and annihilation distributions are defined as

$$a^+=\frac{1}{2\pi i}(\delta(s)\delta^{(1)}(x)\delta(y)-i\delta(s)\delta(x)\delta^{(1)}(y)), \tag{21}$$

$$a^-=\frac{1}{2\pi i}(\delta(s)\delta^{(1)}(x)\delta(y)+i\delta(s)\delta(x)\delta^{(1)}(y)). \tag{22}$$

The creation and annihilation operators are convolution by the above distributions. It should be noted that a^+ and a^- are the p-mechanization of the classical observables $q-ip$ and $q+ip$, respectively. By a direct calculation it can be shown that

$$a^-*v_{(h,q,p)}=(q+ip)v_{(h,q,p)},$$

so $v_{(h,q,p)}$ is an eigenfunction for a^- with eigenvalue $(q+ip)$. By another direct calculation using (24) we have

$$\langle v_{(h,q,p)},v_{(h,q',p')}\rangle_{\mathcal{H}_h}=\exp\left(-\frac{\pi}{2h}((p-p')^2+(q-q')^2+2i(qp'-q'p))\right). \tag{23}$$

Finally, by another direct calculation we have that a^- and a^+ are adjoints of each other.

A well known equation which will be used throughout this paper is

$$\int_{\mathbb{R}}\exp(-ax^2+2bx)dx=\left(\frac{\pi}{a}\right)^{1/2}\exp\left(\frac{b^2}{a}\right), \tag{24}$$

where $a>0$. A similar equation (Ref. 15, p. 337) which we repeatedly use is

$$\int_{\mathbb{R}}x^n\exp(-ax^2+2bx)dx=\frac{1}{2^{n-1}a}\left(\frac{\pi}{a}\right)^{1/2}\frac{d^{n-1}}{db^{n-1}}\left(b\exp\left(\frac{b^2}{a}\right)\right), \tag{25}$$

providing $a>0$ and n is an integer greater than or equal to 1. This equation for the particular value of $n=1$ is well known:

$$\int_{\mathbb{R}}x\exp(-ax^2+2bx)dx=\left(\frac{\pi}{a}\right)^{1/2}\left(\frac{b}{a}\right)\exp\left(\frac{b^2}{a}\right). \tag{26}$$

III. NONLINEAR CANONICAL TRANSFORMATIONS

In Refs. 7 and 8 the p-dynamic equation (12) for the forced and harmonic oscillators are solved in p-mechanics. In doing so it was made evident that the quantum and classical pictures of the problems were generated from the same source. To solve the p-dynamic equation for more complicated problems, such as the Kepler problem, technical problems are encountered. In classical mechanics, when these problems arise the solution often lies in finding a canonical transformation to a set of coordinates in which Hamilton's equations have a more manageable form. For

example, the transformation to action-angle variables completely solves the Kepler problem (Ref. 14, Sec. 10.8). By studying canonical transformations in *p*-mechanics we have a tool which will transform the *p*-dynamic equation (12) into a more desirable form.

In studying *p*-mechanical canonical transformations we show how canonical transformations can be represented in the mathematical framework of both quantum and classical mechanics. It is stated in Ref. 3 that canonical transformations have three important roles in both quantum and classical mechanics:

(i) time evolution
(ii) physical equivalence of two theories, and
(iii) solving a system.

Taking the one and infinite dimensional representation of the *p*-mechanical system will show how these properties are exhibited in classical and quantum mechanics respectively.

There are further benefits of considering canonical transformations in *p*-mechanics. Canonical transformations can represent the symmetries of a classical mechanical system. In looking at the image of canonical transformations in quantum mechanics we can see how these symmetries are represented in quantum mechanics. In Ref. 2 Anderson shows how quantum integrability can be defined in terms of canonical transformations. In Ref. 4 it is shown that quantum canonical transformations can also help in the study of partial differential equations.

In this section we consider nonlinear canonical transformations. The role of linear canonical transformations in *p*-mechanics is straightforward and is described in Refs. 8, 24, and 22. Unfortunately, some of the most fundamental canonical transformations are nonlinear—for example, the passage to action angle variables for the harmonic and the repulsive oscillator.

For nonlinear transformations we follow an approach which is an enhancement of a method pioneered by Mario Moshinsky and a variety of collaborators.[27,29,30,13,10] In this paper we are looking at general *p*-mechanical observables as opposed to just quantum mechanical observables. We also make use of the *p*-mechanical coherent states (17) and (18).

A. Equations for nonlinear transformations involving $\mathcal{H}_h$ states

This method starts with the observation that a canonical transformation in classical mechanics described by $2n$ independent relations

$$q_i \to Q_i(q,p), \tag{27}$$

$$p_i \to P_i(q,p), \tag{28}$$

$i=1,...,n$, where $\{Q_i,P_j\}_{q,p}=\delta_{ij}$ can be realized by $2n$ functional relations

$$f_i(q,p)=F_i(Q,P), \tag{29}$$

$$g_i(q,p)=G_i(Q,P), \tag{30}$$

for $i=1,...,n$ where $\{f_i,g_i\}_{q,p}=\{F_i,G_i\}_{Q,P}$. The advantage of this approach is that the *p*-mechanization (10) of the functions in (29) and (30) may be easier to derive than the functions on the right hand side of Eqs. (27) and (28). We assume throughout the paper that the above functions of q and p are C^∞ with isolated singularities and when integrated next to an element of $\mathcal{S}(\mathbb{R}^{2n})$ will be finite. This means they can always be realized as elements of $\mathcal{S}'(\mathbb{R}^{2n})$. The isolated singularity condition means the equality in system (29) and (30) holds everywhere except at a finite number of isolated points.

We now derive an equation which will give us a clear form of an operator U on $\mathcal{H}_h$ corresponding to a canonical transformation. This equation will supply us with the matrix elements of the operator U with respect to the overcomplete set of coherent states, that is, it will give us $\langle Uv_{(h,q,p)},v_{(h,q',p')}\rangle$ for all $q, p, q', p' \in \mathbb{R}^n$.

In Dirac's original treatment of quantum canonical transformations (Ref. 9, Chap. 27) he proposed that the canonical transformation from Eqs. (27) and (28) should be represented in quantum mechanics by a unitary operator U on a Hilbert space such that

$$\tilde{Q}_i = U\tilde{q}_i U^{-1} \quad \text{and} \quad \tilde{P}_i = U\tilde{p}_i U^{-1},$$

$i=1,...,n$. Here $\tilde{Q}_i$, $\tilde{P}_i$, $\tilde{q}_i$, $\tilde{p}_i$ are the quantum mechanical observables corresponding to the classical mechanical observables Q_i, P_i, q_i, p_i, respectively.

In Ref. 27 Mello and Moshinsky suggested that in some circumstances it is easier to define the operator U by the equations

$$\tilde{F}U = U\tilde{f} \quad \text{and} \quad \tilde{G}U = U\tilde{g},$$

where $\tilde{F}$, $\tilde{G}$, $\tilde{f}$, $\tilde{g}$ are the quantum mechanical observables (that is operators on a Hilbert space) corresponding to the classical observables F, G, f, g from Eqs. (29) and (30).

We proceed to transfer this approach into p-mechnaics. We want to understand the operator U which is defined by the equations

$$\mathcal{P}(f_i(q,p)) * Uv = U\mathcal{P}(F_i(Q,P)) * v, \tag{31}$$

$$\mathcal{P}(g_i(q,p)) * Uv = U\mathcal{P}(G_i(Q,P)) * v, \tag{32}$$

where $\mathcal{P}$ is the map of p-mechanization (10) and v is any element of $\mathcal{H}_h$.

We will now divert from deriving the general equation by giving an example to illuminate these ideas. (The example we give is a linear transformation, but it must be stressed that this work holds for nonlinear transformations, too.)

Example 3.1: Consider the linear canonical transformation

$$q \to -P, \quad p \to Q.$$

This can be realized by the two equations

$$q + ip = -P + iQ, \tag{33}$$

$$q - ip = -P - iQ, \tag{34}$$

the p-mechanizations of which are

$$a^- = iA^-, \tag{35}$$

$$a^+ = iA^+, \tag{36}$$

where a^- and a^+ are defined in Eqs. (21) and (22).

We now continue to derive the equation which will help us understand the operator U. For the rest of this section we just write the equations out using f_i and F_i, but all these will still hold if they are replaced by g_i and G_i. We begin by taking the matrix elements of Eq. (31) with respect to the coherent states defined in Eq. (17); we get

$$\langle \mathcal{P}(f_i) * Uv_{(h,q,p)}, v_{(h,q',p')} \rangle = \langle U\mathcal{P}(F_i) * v_{(h,q,p)}, v_{(h,q',p')} \rangle. \tag{37}$$

We can expand $Uv_{(h,q,p)}$ using our system of coherent states

$$Uv_{(h,q,p)} = \int_{\mathbb{R}^{2n}} \langle Uv_{(h,q,p)}, v_{(h,q'',p'')} \rangle v_{(h,q'',p'')} dq'' dp''.$$

The left hand side of Eq. (37) now becomes

$$\int_{\mathbb{R}^{2n}} \langle U v_{(h,q,p)}, v_{(h,q'',p'')} \rangle \langle \mathcal{P}(f_i) * v_{(h,q'',p'')}, v_{(h,q',p')} \rangle dq'' dp''.$$

Similarly, we expand out $\mathcal{P}(F_i) * v_{(h,q,p)}$ out as

$$\mathcal{P}(F_i) * v_{(h,q,p)} = \int_{\mathbb{R}^{2n}} \langle \mathcal{P}(F_i) * v_{(h,q,p)}, v_{(h,q'',p'')} \rangle v_{(h,q'',p'')} dq'' dp'',$$

so the right hand side of (37) becomes

$$\int_{\mathbb{R}^{2n}} \langle U v_{(h,q'',p'')}, v_{(h,q',p')} \rangle \langle \mathcal{P}(F_i) * v_{(h,q,p)}, v_{(h,q'',p'')} \rangle dq'' dp''.$$

Hence, if we set $m(a,b,c,d) = \langle U v_{(h,a,b)}, v_{(h,c,d)} \rangle$, Eq. (37) becomes

$$\int_{\mathbb{R}^{2n}} m(q,p,q'',p'') \langle \mathcal{P}(f_i) * v_{(h,q'',p'')}, v_{(h,q',p')} \rangle dq'' dp''$$

$$= \int_{\mathbb{R}^{2n}} m(q'',p'',q',p') \langle \mathcal{P}(F_i) * v_{(h,q,p)}, v_{(h,q'',p'')} \rangle dq'' dp''. \tag{38}$$

Note that to get the full system of equations we need a further n equations which we get by replacing f_i and F_i with g_i and G_i. If we can solve this integral equation for m, then we can understand the effect of U on any element v of $\mathcal{H}_h$ through coherent state expansions. Even if we cannot solve the integral equation (38), we can still gain some useful insights into the nature of the canonical transformation in question.

By (19) the unitarity of U is equivalent to the following two equations holding:

$$\int_{\mathbb{R}^{2n}} \langle v_{(h,q',p')}, U v_{(h,q''',p''')} \rangle \langle U^T v_{(h,q'',p'')}, v_{(h,q''',p''')} \rangle dq''' dp''' = \langle v_{(h,q',p')}, v_{(h,q'',p'')} \rangle,$$

$$\int_{\mathbb{R}^{2n}} \langle v_{(h,q',p')}, U^T v_{(h,q''',p''')} \rangle \langle U v_{(h,q'',p'')}, v_{(h,q''',p''')} \rangle dq''' dp''' = \langle v_{(h,q',p')}, v_{(h,q'',p'')} \rangle,$$

where U^T stands for Hermitian conjugate. Since for many functions f, $\langle \mathcal{P}(f) * v_{(h,q,p)}, v_{(h,q',p')} \rangle$ is a manageable function of q, p, q', p', Eq. (38) will take a simple form for a variety of examples. For example, consider the distributions involved in Eqs. (35) and (36). Since $v_{(h,q,p)}$ is an eigenfunction of the annihilation operator a^- with eigenvalue $(q+ip)$ we have

$$\langle a^- * v_{(h,q,p)}, v_{(h,q',p')} \rangle = (q+ip) \langle v_{(h,q,p)}, v_{(h,q',p')} \rangle,$$

and hence

$$\langle \mathcal{P}(q+ip) * v_{(h,q,p)}, v_{(h,q',p')} \rangle = (q+ip) \langle v_{(h,q,p)}, v_{(h,q',p')} \rangle$$

$$= (q+ip) \exp\left(-\frac{\pi}{2h} ((p-p')^2 + (q-q')^2 + 2i(qp' - q'p)) \right). \tag{39}$$

Here we have used (23). Furthermore, since a^- is the adjoint of a^+ we have

$$\langle a^+ * v_{(h,q,p)}, v_{(h,q',p')} \rangle = \langle v_{(h,q,p)}, a^- * v_{(h,q',p')} \rangle = (q'-ip') \langle v_{(h,q,p)}, v_{(h,q',p')} \rangle,$$

hence

$$\langle \mathcal{P}(q-ip)*v_{(h,q,p)}, v_{(h,q',p')}\rangle = (q'-ip')\langle v_{(h,q,p)}, v_{(h,q',p')}\rangle$$
$$= (q'-ip')\exp\left(-\frac{\pi}{2h}((p-p')^2+(q-q')^2+2i(qp'-q'p))\right). \tag{40}$$

We are now in a position to present Eqs. (38) for the canonical transformation

$$q \to -P, \quad p \to Q.$$

Using Eqs. (33), (34), (39) and (40) we can see that Eqs. (38) must take the form

$$\int_{\mathbb{R}^{2n}} m(q,p,q'',p'')(q''+ip'')\exp\left(-\frac{\pi}{2h}[(p''-p')^2+(q''-q')^2+2i(q''p'-q'p'')]\right)dq''dp''$$
$$= \int_{\mathbb{R}^{2n}} m(q'',p'',q',p')i(q+ip)\exp\left(-\frac{\pi}{2h}[(p-p'')^2+(q-q'')^2+2i(qp''-q''p)]\right)dq''dp''$$

and

$$\int_{\mathbb{R}^{2n}} m(q,p,q'',p'')(q'-ip')\exp\left(-\frac{\pi}{2h}[(p''-p')^2+(q''-q')^2+2i(q''p'-q'p'')]\right)dq''dp''$$
$$= \int_{\mathbb{R}^{2n}} m(q'',p'',q',p')(-i(q''-ip''))\exp\left(-\frac{\pi}{2h}[(p-p'')^2+(q-q'')^2 + 2i(qp''-q''p)]\right)dq''dp''$$

for this canonical transformation. The function

$$m(q,p,q',p') = \exp\left(-\frac{\pi}{2h}(q^2+p^2+q'^2+p'^2-2iqp-2iqq'+2iqp')\right)$$

can be shown to satisfy these equations through the repeated use of formulas (26) and (24). Even though we have only looked at this equation for a linear example, it must be stressed that it holds for nonlinear examples also. We do not give any examples of this here as in the next section we derive some more manageable equations using the kernel states.

B. Equations for nonlinear transformations for states realized as kernels

In Ref. 7 we showed that *p*-mechanical states could be realized as integration kernels. In this section we derive an equation similar to (38) for the kernel states. It is shown that this equation in many circumstances is easier to solve than (38).

Let $\mathcal{U}$ denote the operator on the algebra of *p*-mechanical observables corresponding to a canonical transformation

$$\mathcal{U}B = U^{-1}BU.$$

The adjoint operator $\mathcal{U}^*$ action on a kernel l is defined by

$$\langle \mathcal{U}B, l\rangle = \langle B, \mathcal{U}^* l\rangle. \tag{41}$$

Note here that this is not an inner product, instead a functional on the right acting on a *p*-observable which is on the left. In Sec. II we showed that any kernel l can be expanded using the coherent state kernels, that is,

$$l(s,x,y)=\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} l(s,x',y')\overline{l_{(h,q,p)}(s,x',y')}dx'dy'l_{(h,q,p)}(s,x,y)dqdp.$$

We now derive an integral equation which when solved will give us $\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle$. Initially we present a lemma which will give an exact formula for the *p*-mechanization of a classical observable evaluated by a kernel coherent state.

Lemma 3.1: If f is a classical observable and $\mathcal{P}$ is the map of p-mechanization as defined in Eq. (10), then

$$\langle \mathcal{P}(f), l_{(h,q,p)}\rangle=\left(\frac{2}{h}\right)^n \exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)$$
$$\times\int_{\mathbb{R}^{2n}} f(a,b)\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb.$$

Proof: By a direct calculation

$$\langle \mathcal{P}(f), l_{(h,q,p)}\rangle=\int_{\mathbb{R}^{2n+1}}\delta(s)\int_{\mathbb{R}^{2n}} f(a,b)\exp(2\pi i(ax+by))dadb$$
$$\times\exp\left(2\pi ihs-2\pi i(qx+py)-\frac{\pi h}{2}(x^2+y^2)\right)dsdxdy,$$

which implies that

$$\langle \mathcal{P}(f), l_{(h,q,p)}\rangle=\int_{\mathbb{R}}\delta(s)\exp(2\pi ihs)ds\int_{\mathbb{R}^{4n}} f(a,b)\exp(x(2\pi i(a-q)))\exp(y(2\pi i(b-p)))$$
$$\times\exp\left(-\frac{\pi h}{2}(x^2+y^2)\right)dadbdxdy.$$

Using (24) the right hand side of the above equation becomes

$$\left(\frac{2}{h}\right)^n\int_{\mathbb{R}^{2n}} f(a,b)\exp\left(\frac{(\pi i(a-q))^2}{\pi h/2}\right)\exp\left(\frac{(\pi i(b-p))^2}{\pi h/2}\right)dadb$$
$$=\left(\frac{2}{h}\right)^n\int_{\mathbb{R}^{2n}} f(a,b)\exp\left(-\frac{2\pi}{h}[(a-q)^2+(b-p)^2]\right)dadb.$$

The result follows from a trivial rearrangement of the above equation. □

So now if we have $2n$ relations as in (29) and (30) we can define the operator $\mathcal{U}$ by the relation

$$\mathcal{U}\mathcal{P}(F_i)=\mathcal{P}(f_i).$$

Applying the kernel $l_{(h,q,p)}$ to both sides of this equation we get

$$\langle \mathcal{U}\mathcal{P}(F_i), l_{(h,q,p)}\rangle=\langle \mathcal{P}(f_i), l_{(h,q,p)}\rangle.$$

This is equivalent to

$$\langle \mathcal{P}(F_i), \mathcal{U}^* l_{(h,q,p)}\rangle=\langle \mathcal{P}(f_i), l_{(h,q,p)}\rangle. \tag{42}$$

However,

$$\mathcal{U}^* l_{(h,q,p)}=\int_{\mathbb{R}^{2n}}\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle l_{(h,q',p')}dq'dp', \tag{43}$$

where the $\langle , \rangle$ for two kernels is just $\langle l, l' \rangle = \int_{\mathbb{R}^{2n}} l\overline{l'} dxdy$. (However, if they contain an observable and a kernel, it is still the evaluation of the observable by the functional.) Substituting (43) into (42) gives us

$$\left\langle \mathcal{P}(F_i), \int_{\mathbb{R}^{2n}} \langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')} \rangle l_{(h,q',p')} dq' dp' \right\rangle = \langle \mathcal{P}(f_i), l_{(h,q,p)} \rangle,$$

which is equivalent to

$$\int_{\mathbb{R}^{2n}} \langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')} \rangle \langle \mathcal{P}(F_i), l_{(h,q',p')} \rangle dq' dp' = \langle \mathcal{P}(f_i), l_{(h,q,p)} \rangle.$$

Using Lemma 3.1 this equation becomes

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')} \rangle \left(\frac{2}{h}\right)^n \exp\left(-\frac{2\pi}{h}(q'^2+p'^2)\right) \int_{\mathbb{R}^{2n}} F_i(a,b) \exp\Bigg(-\frac{2\pi}{h}(a^2+b^2) \\ &\quad + \frac{4\pi}{h}(aq'+bp')\Bigg) dadbdq'dp' \\ &= \left(\frac{2}{h}\right)^n \exp\left(-\frac{2\pi}{h}(q^2+p^2)\right) \int_{\mathbb{R}^{2n}} f_i(a,b) \exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right) dadb, \end{aligned}$$

which can be simplified to

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')} \rangle \exp\left(-\frac{2\pi}{h}(q'^2+p'^2)\right) \int_{\mathbb{R}^{2n}} F_i(a,b) \\ &\quad \times \exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq'+bp')\right) dadbdq'dp' \\ &= \exp\left(-\frac{2\pi}{h}(q^2+p^2)\right) \int_{\mathbb{R}^{2n}} f_i(a,b) \exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right) dadb. \end{aligned} \tag{44}$$

We will now go on to show that for a number of canonical transformations this integral equation takes a clear form which is easy to solve.

C. The Hamilton transformation from the forced oscillator

We now demonstrate how Eqs. (44) can deal with a nonlinear transformation. We do this through applying it to the Hamilton transformation for the forced oscillator. This is the canonical transformation which is generated by the time evolution of phase space due to the forced oscillator. The *p*-mechanical forced oscillator is discussed in Ref. 7, for simplicity we consider the oscillator to be of unit mass and unit frequency, but forced by an arbitary function $z(t)$. The classical canonical transformation (this is for the time evolution from time 0 to time t) is defined by

$$Q = q\cos(t) + p\sin(t) + \int_0^t z(\tau)\sin(\tau)d\tau,$$

$$P = -q\sin(t) + p\cos(t) + \int_0^t z(\tau)\cos(\tau)d\tau.$$

Using Eqs. (26) and (24) we get the relations

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}} a\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb=\frac{h}{2}q,$$

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}} b\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb=\frac{h}{2}p,$$

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}} \exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb=\frac{h}{2}.$$

These relations imply that Eqs. (44) for this transformation take the form

$$\int_{\mathbb{R}^{2n}}\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle q'dq'dp' = q\cos(t)+p\sin(t)+\int_0^t z(\tau)\sin(\tau)d\tau, \tag{45}$$

$$\int_{\mathbb{R}^{2n}}\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle q'dq'dp' = -q\sin(t)+p\cos(t)+\int_0^t z(\tau)\cos(\tau)d\tau. \tag{46}$$

By observing Eqs. (26) and (24), a potential solution of Eqs. (45) and (46) is

$$\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle = \frac{1}{h}\exp\left(-\frac{\pi}{h}\left[\left(q\cos(t)+p\sin(t)+\int_0^t z(\tau)\sin(\tau)d\tau-q'\right)^2 + \left(\int_0^t z(\tau)\cos(\tau)d\tau-q\sin(t)+p\cos(t)-p'\right)^2\right]\right). \tag{47}$$

We now show that this satisfies (45):

$$\begin{aligned}
&\int_{\mathbb{R}^{2n}}\langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')}\rangle q'dq'dp' \\
&\quad=\int_{\mathbb{R}^{2n}}\frac{1}{h}\exp\left(-\frac{\pi}{h}\left[\left(q\cos(t)+p\sin(t)+\int_0^t z(\tau)\sin(\tau)d\tau-q'\right)^2\right.\right. \\
&\qquad\left.\left.+\left(\int_0^t z(\tau)\cos(\tau)d\tau-q\sin(t)+p\cos(t)-p'\right)^2\right]\right)q'dq'dp' \\
&\quad=\frac{1}{h}\exp\left(-\frac{\pi}{h}\left[\left(q\cos(t)+p\sin(t)+\int_0^t z(\tau)\sin(\tau)d\tau\right)^2\right.\right. \\
&\qquad\left.\left.+\left(\int_0^t z(\tau)\cos(\tau)d\tau-q\sin(t)+p\cos(t)\right)^2\right]\right)\int_{\mathbb{R}^{2n}}\exp\left(\frac{2\pi}{h}\left[q'\left(q\cos(t)+p\sin(t)\right.\right.\right. \\
&\qquad\left.\left.\left.+\int_0^t z(\tau)\sin(\tau)d\tau\right)+p'\left(\int_0^t z(\tau)\cos(\tau)d\tau-q\sin(t)+p\cos(t)\right)\right]\right) \\
&\qquad\times\exp\left(-\frac{\pi}{h}(q'^2+p'^2)\right)q'dq'dp'.
\end{aligned} \tag{48}$$

Using (26) and (24) this becomes

$$\int_{\mathbb{R}^{2n}} \langle \mathcal{U}^* l_{(h,q,p)}, l_{(h,q',p')} \rangle q' dq' dp'$$

$$= \frac{1}{h} \exp\left(-\frac{\pi}{h} \left[\left(q\cos(t) + p\sin(t) + \int_0^t z(\tau)\sin(\tau) d\tau \right)^2 \right.\right.$$

$$\left.\left. + \left(\int_0^t z(\tau)\cos(\tau) d\tau - q\sin(t) + p\cos(t) \right)^2 \right] \right)$$

$$\times h\left(q\cos(t) + p\sin(t) + \int_0^t z(\tau)\sin(\tau) d\tau \right) \exp\left(\frac{\pi}{h} \left[\left(q\cos(t) + p\sin(t) \right.\right.\right.$$

$$\left.\left.\left. + \int_0^t z(\tau)\sin(\tau) d\tau \right)^2 + \left(\int_0^t z(\tau)\cos(\tau) d\tau - q\sin(t) + p\cos(t) \right)^2 \right] \right)$$

$$= q\cos(t) + p\sin(t) + \int_0^t z(\tau)\sin(\tau) d\tau.$$

By a similar calculation we can show that (47) satisfies (45).

D. A note on non-bijective transformations

In Ref. 29 the problem of representing non-bijective canonical transformations in quantum mechanics is considered. The majority of canonical transformations in classical mechanics are non-bijective—one example is the action angle variables for the Kepler problem. If we can represent non-bijective canonical transformations in *p*-mechanics, we can use the infinite dimensional representations to get their representation in quantum mechanics. The physical importance of non-bijective canonical transformations in quantum mechanics is discussed in Ref. 29, Sec. 7. It is claimed that some nonlinear canonical transformations can be used to show that some elements of quantum mechanics are already contained in classical mechanics.

We now outline a method of how to deal with non-bijective canonical transformations in *p*-mechanics. Our method is best illustrated through an example—we look at the transformation into the action angle coordinates for the repulsive oscillator. This is a nonlinear, non-bijective transformation which is discussed in great detail in Ref. 29. The canonical transformation is

$$Q = \ln|p+q|, \tag{49}$$

$$P = \tfrac{1}{2}(p^2 - q^2). \tag{50}$$

The non-bijectiveness of this transformation is manifested by the points (q,p) and $(-q,-p)$ in the original phase space being mapped into the same point. Also the entire line $q+p=0$ is mapped to the single point $Q=-\infty$, $P=0$. To derive an equation for the states realized as kernels we put Eqs. (49) and (50) into the form

$$\exp(2Q) = (p+q)^2,$$

$$P = \tfrac{1}{2}(p^2 - q^2).$$

To derive Eqs. (44) for this example we need the following lemma.

Lemma 3.2: We have the following relations:

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}}\exp(2a)\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb$$
$$=\left(\frac{h}{2}\right)\exp\left(2q+\frac{h}{2\pi}\right), \tag{51}$$

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}}a^2\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb=\frac{h}{2}\left(\frac{h}{4\pi}+q^2\right). \tag{52}$$

Clearly analogous relations to these hold if we replace a by b on the left hand side and q by p on the right hand side. Furthermore, we have that

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}}ab\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb=\frac{h}{2}qp. \tag{53}$$

Proof: Equation (51) follows from a direct calculation using (24):

$$\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\int_{\mathbb{R}^{2n}}\exp(2a)\exp\left(-\frac{2\pi}{h}(a^2+b^2)+\frac{4\pi}{h}(aq+bp)\right)dadb$$
$$=\exp\left(-\frac{2\pi}{h}(q^2+p^2)\right)\left(\frac{h}{2}\right)\exp\left(\frac{2\pi p^2}{h}\right)\exp\left(\frac{((2\pi/h)q+1)^2}{2\pi/h}\right)=\left(\frac{h}{2}\right)\exp\left(2q+\frac{h}{2\pi}\right).$$

Similarly (52) can be verified by a direct calculation using (25) with $n=2$. Likewise (53) can be verified by using (26) twice. □

Using Lemma 3.2, Eqs. (44) for this example take the form

$$\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle\exp\left(2q'+\frac{h}{2\pi}\right)dq'dp'=(p+q)^2+\frac{h}{2\pi}, \tag{54}$$

$$\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle p'dq'dp'=(p^2-q^2). \tag{55}$$

The non-bijectiveness is apparent in Eqs. (54) and (55) since they are invariant under the translation $(q,p)\mapsto(-q,-p)$. Any solution of (54) and (55) will be such that

$$\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle=\langle\mathcal{U}^*l_{(h,-q,-p)},l_{(h,q',p')}\rangle. \tag{56}$$

Since

$$\mathcal{U}^*l_{(h,q,p)}=\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle l_{(h,q',p')}dq'dp'$$

it is clear that $\mathcal{U}^*l_{(h,q,p)}=\mathcal{U}^*l_{(h,-q,-p)}$. Now we show that this map $\mathcal{U}^*$: $\mathcal{L}_h\to\mathcal{L}_h$ is not a bijection. We have the formula for any kernel l

$$\mathcal{U}^*l=\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle\langle l,l_{(h,q,p)}\rangle l_{(h,q',p')}dqdpdq'dp'.$$

So $\mathcal{U}^*l=\mathcal{U}^*l'$ if and only if

$$\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle\langle l,l_{(h,q,p)}\rangle dqdp=\int_{\mathbb{R}^{2n}}\langle\mathcal{U}^*l_{(h,q,p)},l_{(h,q',p')}\rangle\langle l',l_{(h,q,p)}\rangle dqdp$$

holds for almost all q', p'. (Almost every and almost everywhere are measure theoretic terms, see Refs. 31 and 25.) By (56) this is equivalent to

$$\int_{q+p>0}(\langle l,l_{(h,q,p)}\rangle+\langle l,l_{(h,-q,-p)}\rangle)\langle \mathcal{U}^* l_{(h,q,p)},l_{(h,q',p')}\rangle dqdp$$

$$=\int_{q+p>0}(\langle l',l_{(h,q,p)}\rangle+\langle l',l_{(h,-q,-p)}\rangle)\langle \mathcal{U}^* l_{(h,q,p)},l_{(h,q',p')}\rangle dqdp.$$

This holds if and only if

$$\langle l,l_{(h,q,p)}\rangle+\langle l,l_{(h,-q,-p)}\rangle=\langle l',l_{(h,q,p)}\rangle+\langle l',l_{(h,-q,-p)}\rangle \tag{57}$$

holds for almost every q, p such that $q+p>0$. So one way of restoring bijectiveness would be to reduce the size of the original set of kernels by factoring out by the equivalence relation, $l\sim l'$, if and only if (57) holds. In the obvious way we would have a bijection from $\mathcal{L}_h/\sim$ to $\mathcal{L}_h$.

Instead of taking this approach we take the simpler approach of increasing the size of the set of kernels to which we map. In doing so we derive a bijection from $\mathcal{L}_h$ to $\mathcal{L}_h\times\mathcal{L}_h$. We do this through introducing two new operators $\mathcal{U}^{*+}$, $\mathcal{U}^{*-}$: $\mathcal{L}_h\to\mathcal{L}_h$ which are defined as

$$\mathcal{U}^{*+}l_{(h,q,p)}=\begin{cases}\mathcal{U}^* l_{(h,q,p)}, & \text{if } q+p>0\\ 0, & \text{if } q+p<0;\end{cases}$$

and

$$\mathcal{U}^{*-}l_{(h,q,p)}=\begin{cases}0, & \text{if } q+p>0\\ \mathcal{U}^* l_{(h,q,p)}, & \text{if } q+p<0.\end{cases}$$

These operators can be extended to the entire space by coherent state (i.e., wavelet) expansions. Furthermore, we define the mapping: $\tilde{\mathcal{U}}^*$: $\mathcal{L}_h\to\mathcal{L}_h\times\mathcal{L}_h$ by

$$\tilde{\mathcal{U}}^* l=[\mathcal{U}^{*+}l,\mathcal{U}^{*-}l].$$

So for any kernel l,

$$\tilde{\mathcal{U}}^* l=\int_{\mathbb{R}^{2n}}\langle l,l_{(h,q,p)}\rangle\tilde{\mathcal{U}}^* l_{(h,q,p)}dqdp$$

$$=\int_{\mathbb{R}^{2n}}\langle l,l_{(h,q,p)}\rangle[\mathcal{U}^{*+}l_{(h,q,p)},\mathcal{U}^{*-}l_{(h,q,p)}]dqdp$$

$$=\left[\int_{q+p>0}\langle l,l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp,\int_{q+p<0}\langle l,l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp\right].$$

Hence $\tilde{\mathcal{U}}^* l=\tilde{\mathcal{U}}^* l'$ if and only if

$$\int_{q+p>0}\langle l,l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp=\int_{q+p>0}\langle l',l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp$$

and

$$\int_{q+p<0}\langle l,l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp=\int_{q+p<0}\langle l',l_{(h,q,p)}\rangle\mathcal{U}^* l_{(h,q,p)}dqdp.$$

These two equations hold if and only if

$$\langle l, l_{(h,q,p)}\rangle = \langle l', l_{(h,q,p)}\rangle$$

holds for almost every q, p such that $q+p>0$ and almost every q, p such that $q+p<0$. This is equivalent to l and l' being equal. Hence we have restored bijectiveness.

The implications to quantum mechanics of this are as follows. We now have a map $\tilde{\mathcal{U}}$ (the adjoint of $\mathcal{U}^*$) which transforms p-mechanical observables corresponding to this non-bijective canonical transformation. If we take the ρ_h representation of this, we get a map for quantum observables.

This work also has classical implications. Initially looking at nonstatistical mechanics we have if the canonical transformation changes a classical observable $f(q,p)$ into $\tilde{f}(q,p)$ and the p-mechanization of f is $B(s,x,y)$, then

$$\tilde{f}(q,p) = \langle B, \mathcal{U}^* l_{(0,q,p)}\rangle = \langle B, \mathcal{U}^* l_{(0,-q,-p)}\rangle = \tilde{f}(-q,-p).$$

Hence we have a demonstration of the classical non-bijectiveness directly from p-mechanics. If we let A denote the set of classical observables, we have shown that the mapping from A→A by $f \mapsto \tilde{f}$ is non-bijective. However, we can restore bijectiveness in the classical mapping through p-mechanics. If we introduce the operator $\widetilde{\mathcal{U}^{class}}$: A→A×A by

$$\widetilde{\mathcal{U}^{class}} f(q,p) = \langle B, \widetilde{\mathcal{U}^*} l_{(0,q,p)}\rangle,$$

where B is the p-mechanization of f, then

$$\widetilde{\mathcal{U}^{class}} f(q,p) = \langle B, \tilde{\mathcal{U}}^* l_{(0,q,p)}\rangle = [\langle B, \mathcal{U}^{*+} l_{(0,q,p)}\rangle, \langle B, \mathcal{U}^{*-} l_{(0,q,p)}\rangle] = \begin{cases} [\tilde{f}(q,p),0] & \text{if } q+p>0 \\ [0,\tilde{f}(q,p)] & \text{if } q+p<0. \end{cases}$$

Now we have a map A→A×A representing this canonical transformation which is bijective. We can extend all of this to statistical mechanics[16] by using linear combinations of these coherent states.

IV. SUMMARY AND POSSIBLE EXTENSIONS

One of the main features of this work is demonstrating how using coherent states in a Segal–Bargmann–Fock-type space can sometimes be advantageous over using the matrix elements of position and momentum in $L^2(\mathbb{R}^n)$. Another feature of our equations is that they do not rely on the property that observables are elements of the algebra generated by the position and momentum operators. In Refs. 29 and 27 all the quantum mechanical operators are derived using this algebra condition—in this paper we use an integral transform instead. This integral transform at first makes our equations look less desirable, but it is shown that for many examples they take a simple form. This work has also demonstrated the advantages of representing states as integration kernels—this complements the work in Ref. 7.

The most immediate extension of this work would be to look at more complex examples, especially some more nonlinear, non-bijective examples. One possible and interesting extension would be to extend these ideas to phase spaces other than $\mathbb{R}^{2n}$. This would be to extend these ideas to a phase space which is a general symplectic manifold (Ref. 26, Chap. 5), for example T^*M for some general manifold M (Ref. 5, Chaps. 7–10, and Ref. 18, Chap. 5). Another interesting extension would be to look at the role of Egorov's theorem[22] in infinitesimal canonical transformations for p-mechanics. Egorov's theorem[11] has always been posed in the language of pseudodifferential and Fourier integral operators on $L^2(\mathbb{R}^n)$; this idea could be extended to our space $F^2(\mathcal{O}_h)$ with pseudodifferential operators being replaced by Toeplitz operators as in Ref. 17.

All these equations could be defined outside the world of p-mechanics. If the usual coherent states in $L^2(\mathbb{R}^n)$ (Ref. 28, Sec. 10.7) were used instead of the eigenfunctions of position and momentum, Moshinsky's equations would be immediately transformed into integral equations.

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Analytic representations based on su(3) coherent states and Robertson intelligent states

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Robertson intelligent states which minimize the Schrödinger–Robertson uncertainty relation are constructed as eigenstates of a linear combination of Weyl generators of the su(3) algebra. The construction is based on the analytic representations of su(3) coherent states. New classes of coherent and squeezed states are explicitly derived. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777794]

I. INTRODUCTION

The coherent states introduced as displacement of the ground state of harmonic oscillator by Schrödinger,[1] have found revived interest when it was realized that they are eigenfunctions of the annihilation operator and minimize the Heisenberg uncertainty relation. The generalization of the usual coherent states from the Weyl–Heisenberg to the other Lie algebras and from harmonic oscillator to other potentials, followed these three approaches, namely, (i) eigenstates of lowering group generator for Lie algebras or annihilation operator of exactly solvable system, (ii) as orbits of the extremal weight state, or (iii) as states minimizing the uncertainty relation. These different approaches lead to distinct sets of coherent states and coincide only in the special case of the harmonic oscillator (see Refs. 2–4 for review). Concerning the optimization of the uncertainty principle, it was observed that a relation more accurate than the Heisenberg one may be used to construct generalized coherent states and squeezed states. Indeed this relation known as Schrödinger–Robertson uncertainty inequality[5] can be minimized and gives rise to new sets of coherent and squeezed states (see the pioneering works[6–8]). The states resulting from this minimization have different names in the literature such as correlated states[6–8] or Robertson intelligent states.[9]

More recently, there has been much interest in such states for Lie algebras[9–13] as well as for quantum systems evolving in various potentials.[14–17] Robertson intelligent states for the quadrature components of Weyl generators of the algebras su(1,1) and su(2) were constructed.[9–13] They were also defined for exactly solvable quantum systems as the eigenstates of complex combination of creation and annihilation operators.[14–17]

The purpose of this paper is to further extend the classes of Robertson intelligent states for higher symmetries. In this sense, the main idea of this note is to construct the intelligent states for the quadrature components of Weyl operators of the algebra su(3). For this end, it may be useful to start by giving the explicit computation of the associated coherent states and their analytic representations. Hence, one can introduce the differential realizations for the su(3) generators. As we will see, the analytic realization enables us to convert the eigenvalue equations arising from the minimization of Schrödinger–Robertson inequality into quasilinear differential equations which provide the Robertson intelligent states.

The paper is organized as follows. In Sec. II we review the derivation of su(3) coherent states. We compute explicitly the action of unitary displacement operator on the highest weight vector of the finite dimension representation space of the algebra su(3). We give the analytic representations of the su(3) coherent states. We construct also the differential operators corresponding to the actions of the generators of su(3) on the Fock–Bargmann space. In Sec. III, we show how the

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analytic representation based on the coherent states provides us with the tool to solve the eigenvalue equations resulting from the minimization of the Schrödinger–Robertson relation and to obtain intelligent states for the quadrature components of su(3) Weyl generators. We conclude in Sec. IV after pointing out a number of interesting open problems.

II. ANALYTIC REPRESENTATIONS OF su(3)-COHERENT STATES

A. Reconstructing su(3)-coherent states

We shall begin by re-examining the construction of the coherent states associated with a quantum system of dynamical symmetry su(3). Although this subject has been considered previously in Refs. 18 and 19 (see also Refs. 20 and 21), we thought that it is always interesting to give another method based on the explicit computation of the action of the displacement operator on the highest weight state (fudicial vector) of the finite dimensional representation space of the algebra su(3). The explicit forms of such states are needed to perform their analytic representations and to give the realization of the generators of the algebra under consideration.

The algebra su(3) is defined by the generators e_i, f_i, h_i $(i=1,2)$ and the relations

$$[e_i,f_i]=\delta_{ij}h_j, \tag{1}$$

$$[h_i,e_j]=a_{ij}e_j, \quad [h_i,f_j]=-a_{ij}f_j, \tag{2}$$

$$[e_i,e_j]=0 \quad \text{for} \quad |i-j|>1, \tag{3}$$

$$e_i^2e_{i\pm1}-2e_ie_{i\pm1}e_i+e_{i\pm1}e_i^2=0, \tag{4}$$

$$f_i^2f_{i\pm1}-2f_if_{i\pm1}f_i+f_{i\pm1}f_i^2=0, \tag{5}$$

where $(a_{ij})_{i,j=1,2}$ is the Cartan matrix of su(3), i.e., $a_{ii}=2$, $a_{i,i\pm1}=-1$ and $a_{ij}=0$ for $|i-j|>1$. Many aspects of Lie algebras are best considered after choosing a special type of representation basis. Since one would write down the su(3) coherent states, the most convenient choice, in this case, is the bosonic realization. Indeed, an adapted basis is given in term of three bosonic pairs of creation and annihilation operators; they satisfy the commutation relations

$$[a_k^-,a_l^+]=\delta_{kl}, \tag{6}$$

where $k,l=1,2,3$. The operator numbers are $N_k=a_k^+a_k^-$. The Fock space is generated by the eigenstates $|n_1,n_2,n_3\rangle$ of a number of operators, namely,

$$|n_1,n_2,n_3\rangle=\frac{(a_1^+)^{n_1}}{\sqrt{n_1!}}\frac{(a_2^+)^{n_2}}{\sqrt{n_2!}}\frac{(a_3^+)^{n_3}}{\sqrt{n_3!}}|0,0,0\rangle. \tag{7}$$

In this bosonic representation, we define the generators of su(3) as

$$e_i=a_i^+a_{i+1}^-, \quad f_i=a_i^-a_{i+1}^+, \quad h_i=N_i-N_{i+1}. \tag{8}$$

The generators e_i, f_i are called step, ladder or Weyl operators. The Cartan subalgebra is generated by the elements h_i. They act on the representation space of dimension $\frac{1}{2}(j_1+1)(j_1+2)$ that is obtained from the Fock space of three harmonic oscillators by restricting the total number of quantas to $j_1=n_1+n_2+n_3$. In the present representation the state of highest weight is $|j_1,0,0\rangle$. The generators of su(3) having a nontrivial action (nonvanishing and nondiagonal) on the fudicial vector $|j_1,0,0\rangle$ are $f_1=a_1^-a_2^+$ and $f_3=[f_2,f_1]=a_1^-a_3^+$. At this stage, one can define the coherent state as

$$|z_1,z_2\rangle = D(z_1,z_2)|j_1,0,0\rangle = \exp(z_1 f_1 + z_2 f_3 - \overline{z_1}e_1 - \overline{z_2}e_3)|j_1,0,0\rangle, \tag{9}$$

where $e_3=[e_1,e_2]=a_1^+a_3^-$. Expanding the displacement operator $D(z_1,z_2)$ and using the action of creation and annihilation operators on the restricted Fock space,

$$\mathcal{F} = \{|n_1,n_2,n_3\rangle; n_1+n_2+n_3 = j_1\},$$

one obtains

$$|z_1,z_2\rangle = \sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2} z_1^{j_2} z_2^{j_3} I_{j_2}^{j_1}(|z_1|) I_{j_3}^{j_2}(|z_2|)|j_1-j_2, j_2-j_3, j_3\rangle, \tag{10}$$

where

$$I_{j_{s+1}}^{j_s}(|z_s|) = \sum_{k=0}^{\infty} \frac{(-)^k(|z_s|^2)^k}{(j_{s+1}+2k)!} P(j_{s+1}+1,k), \tag{11}$$

for $s=1,2$. The quantities P occuring in (11) are given by

$$P(j_{s+1}+1,k) = P(j_{s+1}+1,0)\sum_{l_1=1}^{j_{s+1}+1} E_s(l_1)\sum_{l_2=1}^{l_1+1} E_s(l_2)\cdots\sum_{l_k=1}^{l_{k-1}+1} E_s(l_k) \tag{12}$$

with $P(j_{s+1}+1,0)=j_s!\,j_{s+1}!/(j_s-j_{s-1})!$ and $E_s(l)=(j_s-l+1)l$. They satisfy the following recursion relation:

$$P(j_{s+1}+1,k) = \sqrt{E_s(j_{s+1})}P(j_{s+1},k) + \sqrt{E_s(j_{s+1}+1)}P(j_{s+1}+2,k-1). \tag{13}$$

Setting

$$J_{j_{s+1}}^{j_s}(|z_s|) = |z_s|^{j_s} P(j_{s+1}+1,0) I_{j_{s+1}}^{j_s}(|z_s|), \tag{14}$$

we get the first order differential equation

$$\frac{\mathrm{d}J_{j_{s+1}}^{j_s}(|z_s|)}{d|z_s|} = J_{j_{s+1}-1}^{j_s}(|z_s|) - (E_s(j_{s+1}+1))^2 J_{j_{s+1}+1}^{j_s}(|z_s|). \tag{15}$$

The solution of this equation takes the simple form

$$J_{j_{s+1}}^{j_s}(|z_s|) = \frac{1}{j_{s+1}!}(\cos(|z_s|))^{j_{s+1}-1}(\mathrm{tg}(|z_s|))^{j_{s+1}}, \tag{16}$$

and the su(3) coherent states rewrite as

$$|\zeta_1,\zeta_2\rangle = (1+|\zeta_1|^2+|\zeta_1|^2|\zeta_2|^2)^{-(j_1/2)}\sum_{j_2=0}^{j_1}\sqrt{\frac{j_1!}{j_2!\,(j_1-j_2)!}}\zeta_1^{j_2} \times\sum_{j_3=0}^{j_2}\sqrt{\frac{j_2!}{j_3!\,(j_2-j_3)!}}\zeta_2^{j_3}|j_1-j_2,j_2-j_3,j_3\rangle, \tag{17}$$

where $\zeta_s=(z_s/|z_s|)\mathrm{tg}(|z_s|)\cos(|z_{s+1}|)^{2-s}$ for $s=1,2$. They have the property of strong continuity in the label space and overcompletion in the sense that there exists a positive measure such that they solve the resolution to identity. The appropriate form of this resolution is

$$\int \mathrm{d}\mu(\zeta_1,\overline{\zeta_1},\zeta_2,\overline{\zeta_2})|\zeta_1,\zeta_2\rangle\langle\zeta_1,\zeta_2| = \sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2}|j_1-j_2,j_2-j_3,j_3\rangle\langle j_1-j_2,j_2-j_3,j_3|. \tag{18}$$

Assuming the isotropy of the measure $\mathrm{d}\mu(\zeta,\overline{\zeta})$, we set

$$\mathrm{d}\mu(\zeta_1,\overline{\zeta_1},\zeta_2,\overline{\zeta_2}) = \pi^2(1+|\zeta_1|^2+|\zeta_1|^2|\zeta_2|^2)^{j_1/2}h(|\zeta_1|^2)h(|\zeta_2|^2)|\zeta_1|d|\zeta_1||\zeta_2|d|\zeta_2|\mathrm{d}\theta_1\mathrm{d}\theta_2 \tag{19}$$

with $\zeta_s=|\zeta_s|e^{i\theta_s}$. Substituting (19) in Eq.(18), we obtain the following sum:

$$\int_0^\infty x_s^{j_{s+1}}h(x_s)\mathrm{d}x_s = \frac{j_{s+1}!\,(j_s-j_{s+1})!}{j_s!}, \tag{20}$$

which should be satisfied by the function $h(x_s=|\zeta_s|^2)$. One obtains

$$h(x_s) = \frac{j_s+1}{(1+x_s^2)^{j_s+2}}. \tag{21}$$

This result can be obtained by using the definition of Meijer's G-function and the Mellin inversion theorem.[22] The resolution to identity is necessary to build up the Fock–Bargmann space based on the set of su(3) coherent states.

B. Differential realization of the su(3) generators

It is well established that the use of the Fock–Bargmann representation is a powerful method for obtaining closed analytic expressions for various properties of coherent states. Calculation for some quantum exception values and solutions for some eigenvalue equations are simlpified by exploiting the theory of analytical entire functions. Here, we give the Fock–Bargmann representation of a su(3) quantum mechanical system. We define the Fock–Bargmann space as a space of functions which are holomorphic. The scalar product is written with an integral of the form

$$\langle f|g\rangle = \int \overline{f}(\zeta_1,\zeta_2)g(\zeta_1,\zeta_2)\mathrm{d}\mu(\zeta_1,\overline{\zeta_1},\zeta_2,\overline{\zeta_2}), \tag{22}$$

where the measure is defined above [see Eq. (19)]. Due to overcompletion of the coherent states, it is induced by the scalar product in $\mathcal{F}$. Let

$$|\psi\rangle = \sum_{n_1,n_2,n_3} a_{n_1,n_2,n_3}|n_1,n_2,n_3\rangle \tag{23}$$

be an arbitrary quantum state of $\mathcal{F}$, it can be represented as a function of the complex variables ζ_1,ζ_2 as

$$\psi(\zeta_1,\zeta_2) = (1+|\zeta_1|^2+|\zeta_1|^2|\zeta_2|^2)^{j_1/2}\langle\overline{\zeta_1},\overline{\zeta_2}|\psi\rangle. \tag{24}$$

In particular, the analytic functions associated to elements of the basis of $\mathcal{F}$ are defined as

$$\psi_{j_1,j_2,j_3}(\zeta_1,\zeta_2) = (1+|\zeta_1|^2+|\zeta_1|^2|\zeta_2|^2)^{j_1/2}\langle\overline{\zeta_1},\overline{\zeta_2}|j_1-j_2,j_2-j_3,j_3\rangle. \tag{25}$$

We now investigate the form of the action of the operators e_i, f_i, and h_i on Fock–Bargmann space. Indeed, any operator O of the algebra su(3) is represented in the space of the entire analytical functions by some differential operator $\mathcal{O}$, defined by

$$\langle\overline{\zeta_1},\overline{\zeta_2}|O|\psi\rangle = \mathcal{O}\psi(\zeta_1,\zeta_2) \tag{26}$$

for any state $|\psi\rangle$ of $\mathcal{F}$.

According to this definition, we obtain

$$e_1 = \frac{\partial}{\partial \zeta_1}, \quad e_3 = \frac{\partial}{\partial \zeta_2}, \tag{27}$$

$$f_1 = j_1\zeta_1 - \zeta_1^2\frac{\partial}{\partial \zeta_1} - \zeta_1\zeta_2\frac{\partial}{\partial \zeta_2}, \tag{28}$$

$$f_3 = j_1\zeta_2 - \zeta_2^2\frac{\partial}{\partial \zeta_2} - \zeta_1\zeta_2\frac{\partial}{\partial \zeta_1}, \tag{29}$$

$$e_2 = \zeta_1\frac{\partial}{\partial \zeta_2}, \quad f_2 = \zeta_2\frac{\partial}{\partial \zeta_1}, \tag{30}$$

$$h_1 = j_1 - 2\zeta_1\frac{\partial}{\partial \zeta_1} - \zeta_2\frac{\partial}{\partial \zeta_2}, \tag{31}$$

$$h_2 = \zeta_1\frac{\partial}{\partial \zeta_1} - \zeta_2\frac{\partial}{\partial \zeta_2}. \tag{32}$$

To obtain the above differential realization:

(i) we remark that the coherent states (17) can be also written as

$$|\zeta_1,\zeta_2\rangle = (1 + |\zeta_1|^2 + |\zeta_1|^2|\zeta_2|^2)^{-j_1/2}D(\zeta_1,\zeta_2)|j_1,0,0\rangle, \tag{33}$$

where $D(\zeta_1,\zeta_2)=\exp(\zeta_1 f_1+\zeta_2 f_3)$;

(ii) we observe that

$$\frac{\partial}{\partial \zeta_1}D(\zeta_1,\zeta_2) = f_1D(\zeta_1,\zeta_2), \quad \frac{\partial}{\partial \zeta_2}D(\zeta_1,\zeta_2) = f_3D(\zeta_1,\zeta_2); \tag{34}$$

(iii) we use the Hausdorff formula

$$e^{-B}Ae^{B} = \sum_{n\geqslant 0}\frac{1}{n!}(-\,a\mathrm{d}B)^nA, \tag{35}$$

where $(a\mathrm{d}B)A=[B,A]$;

(iv) we use also the actions of the elements of su(3) on the basis of Fock space $\mathcal{F}$, in particular the fudicial vector $|j_1,0,0\rangle$, and the structure relations (1)–(5) of the algebra su(3).

From the previous considerations, it follows that the su(3) generators act as first-order holomorphic differential operators on the space of the analytic functions generated by the elements (25). One can verify that the commutation relations (1)–(5) are preserved. This result combined with eigenvalue equations ensuring the minimization of Schrödinger–Robertson inequality provides the intelligent states as will be explained in the next section.

III. su(3) ROBERTSON STATES

As we have already mentioned, in this section, we will study the fluctuations of the quadrature components of the Weyl generators which represent creation and annihilation of states for a quantum mechanical system of su(3) symmetry. In this order, to construct the intelligent states of any pair of ladder operators e_i, f_i $(i=1,2,3)$, it is natural to introduce the quantum observables $\sqrt{2}p_i=e_i+f_i$ and $\mathbf{i}\sqrt{2}q_i=e_i-f_i$ where $\mathbf{i}^2=-1$. These observables obey

$$[p_i, q_i] = \mathbf{i}h_i. \tag{36}$$

We known that p_i and q_i satisfy, in a given state, the Robertson–Shrödinger uncertainty relation

$$(\Delta p_i)^2(\Delta q_i)^2 \geqslant \tfrac{1}{4}(\langle h_i\rangle^2 + \langle c_i\rangle^2), \tag{37}$$

where Δp_i and Δq_i are the dispersions and the Hermitian operator $c_i = \{p_i - \langle p_i\rangle, q_i - \langle q_i\rangle\}$ gives the covariance (correlation) of the observables p_i and q_i. The symbol $\{,\}$ stands for the standard definition of the anticommutator. A state $|\Phi\rangle$ providing the equality in (37) is the so-called Robertson intelligent state. It was proven that such state satisfies the following eigenvalue equation:

$$((1+\alpha)e_i + (1-\alpha)f_i)|\Phi\rangle = \lambda|\Phi\rangle, \tag{38}$$

where $\alpha \neq 0$ and $\lambda = (1+\alpha)\langle e_i\rangle + (1-\alpha)\langle f_i\rangle$ are complex parameters. Furthermore, the variances and covariance, in the intelligent state $|\Phi\rangle$, are related by

$$(\Delta p_i)^2 = |\alpha|\Delta_i, \quad (\Delta q_i)^2 = \frac{1}{|\alpha|}\Delta_i, \tag{39}$$

where $\Delta_i = \frac{1}{2}\sqrt{\langle h_i\rangle^2 + \langle c_i\rangle^2}$. Remark that they can be also expressed as

$$(\Delta p_i)^2 = \frac{|\alpha|^2}{u}\langle h_i\rangle, \quad (\Delta q_i)^2 = \frac{1}{u}\langle h_i\rangle, \quad \langle c_i\rangle = \frac{v}{u}\langle h_i\rangle, \tag{40}$$

where the real parameters u and v are such that $u^2 + v^2 = 4|\alpha|^2$. (As example, one can take $u = 2$ Re α and $v = 2$ Im α.) It is clear that the dispersions and the correlation can be obtained from the mean value of the observable h_i. The state $|\Phi\rangle$ satisfying (38) with $|\alpha| = 1$ are coherent because they satisfy $(\Delta p_i)^2 = (\Delta q_i)^2 = \Delta_i$. The fluctuations are equal and minimized in the sense of the Schrödinger–Robertson uncertainty relation. The state satisfying (38) with $|\alpha| \neq 1$ are squeezed because if $|\alpha| < 1$, we have $(\Delta p_i)^2 < \Delta_i < (\Delta q_i)^2$ and if $|\alpha| > 1$, we have $(\Delta q_i)^2 < \Delta_i < (\Delta p_i)^2$.

To solve the eigenvalues equation (38), we will use the analytic representations of coherent states as well as the differential realizations of the generators e_i and f_i given by Eqs. (27)–(30). So, let us start by deriving the eigenfunctions of Eq. (38) for the first pair e_1, f_1. By introducing the analytic function

$$\Phi_1 \equiv \Phi_1(\zeta_1, \zeta_2, \alpha, \lambda, j_1) = (1 + |\zeta_1|^2 + |\zeta_1|^2|\zeta_2|^2)^{j_1/2}\langle\overline{\zeta_1}, \overline{\zeta_2}|\Phi_1\rangle, \tag{41}$$

it can be easily checked that the eigenvalue equation (38) can be converted in the following first order differential equation:

$$(j_1\eta_1 - \lambda')\Phi_1 + (1 - \eta_1^2)\frac{\partial\Phi_1}{\partial\eta_1} - \eta_1\eta_2\frac{\partial\Phi_1}{\partial\eta_2} = 0, \tag{42}$$

where $\eta_1 = \sqrt{(1-\alpha)/(1+\alpha)}\zeta_1$, $\eta_2 = \zeta_2$ and $\lambda' = \lambda/\sqrt{1-\alpha^2}$ for $\alpha \neq \pm 1$. The function $\Phi_1(\zeta_1, \zeta_2, \alpha, \lambda, j_1)$ can be expanded as

$$\Phi_1 = \sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2} a_{j_1,j_2,j_3}\eta_1^{j_2}\eta_2^{j_3}. \tag{43}$$

Substitution of (43) in (42) yields the recursion formula

$$(j_1 - j_2 - j_3 + 1)a_{j_1,j_2-1,j_3} - \lambda' a_{j_1,j_2,j_3} + (j_2+1)a_{j_1,j_2+1,j_3} = 0, \tag{44}$$

which can be solved by the Laplace method. Indeed, we set

$$a_{j_1,j_2,j_3} = \int_{-1}^{+1} x^{j_2} f(x)\mathrm{d}x \tag{45}$$

that we introduce in (44) to obtain, after partial integration, the simple first order differential equation satisfied by the function $f(x)$,

$$(x - x^3)\frac{\mathrm{d}f}{\mathrm{d}x} + (j_1 - j_3 + 1 - \lambda' x - x^2) = 0. \tag{46}$$

The last equation is easily solvable. Replacing in (45), one obtains

$$a_{j_1,j_2,j_3} = \int_{-1}^{+1} x^{j_2 - j_1 + j_3 - 1}(1 - x)^{(-\lambda' + j_1 - j_3)/2}(1 + x)^{(\lambda' + j_1 - j_3)/2}\mathrm{d}x, \tag{47}$$

or

$$a_{j_1,j_2,j_3} = (-)^{j_2}\frac{\Gamma\left(\frac{\lambda' + j_1 - j_3}{2} + 1\right)\Gamma\left(\frac{-\lambda' + j_1 - j_3}{2} + 1\right)}{\Gamma(j_1 - j_3 + 2)} \times {}_2F_1\left(j_1 - j_3 - j_2 + 1, \frac{\lambda' + j_1 - j_3}{2} + 1, j_1 - j_3 + 2, 2\right) \tag{48}$$

using the integral representation for the hypergeometric function ${}_2F_1$.[20] Comparing the expansion (43) with the general formula (41), we have the decomposition of Robertson intelligent states over the basis of Fock space $\mathcal{F}$,

$$|\Phi_1\rangle = \sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2} a_{j_1,j_2,j_3}\left(\frac{1-\alpha}{1+\alpha}\right)^{j_2/2}\sqrt{\frac{(j_1 - j_2)\,!\,j_3\,!\,(j_2 - j_3)!}{j_1!}}|j_1 - j_2, j_2 - j_3, j_3\rangle, \tag{49}$$

where the coefficients a_{j_1,j_2,j_3} are given by Eq. (48).

Now we consider the construction of intelligent states for the second pair e_2, f_2. The eigenvalues equation (38) gives, in this case, the following quasilinear differential equation:

$$\xi_1\frac{\partial \Phi_2}{\partial \xi_2} + \xi_2\frac{\partial \Phi_2}{\partial \xi_1} - \lambda'\Phi_2 = 0, \tag{50}$$

where $\xi_1 = \sqrt{(1+\alpha)/(1-\alpha)}\zeta_1$, $\xi_2 = \zeta_2$, and $\lambda' = \lambda/\sqrt{1-\alpha^2}$. Here also, we expand the eigenfunction $\Phi_2 \equiv \Phi_2(\xi_1, \xi_2, \alpha, \lambda, j_1)$ as

$$\Phi_2 = \sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2} b_{j_1,j_2,j_3}\xi_1^{j_2}\xi_2^{j_3} \tag{51}$$

that we insert in Eq. (50) to obtain the recursion relation linking the coefficients b's,

$$(j_3 + 1)b_{j_1,j_2-1,j_3+1} - \lambda' b_{j_1,j_2,j_3} + (j_2 + 1)b_{j_1,j_2+1,j_3-1} = 0. \tag{52}$$

Setting $b_{j_1,j_2,j_3} \equiv b_{j_1,j_2-j,j}$ where $2j = j_2 + j_3$, the previous relation can be transformed to

$$(j_2 + 1)b_{j_1,j_2-j+1,j} - \lambda' b_{j_1,j_2-j,j} + (j_3 + 1)b_{j_1,j_2-j-1,j} = 0, \tag{53}$$

solvable in a similar manner as that given by the solution of the recursion formula (44), and one has

$$b_{j_1,j_2,j_3}=(-)^{j_2}\frac{\Gamma\left(\frac{\lambda'+j_2+j_3}{2}+1\right)\Gamma\left(\frac{-\lambda'+j_2+j_3}{2}+1\right)}{\Gamma(j_2+j_3+2)}$$
$$\times{}_2F_1\left(j_3+1,\frac{\lambda'+j_2+j_3}{2}+1,j_2+j_3+2,2\right). \tag{54}$$

Finally, one obtains

$$|\Phi_2\rangle=\sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2}b_{j_1,j_2,j_3}\left(\frac{1+\alpha}{1-\alpha}\right)^{j_2/2}\sqrt{\frac{(j_1-j_2)\,!\,j_3\,!\,(j_2-j_3)!}{j_1!}}|j_1-j_2,j_2-j_3,j_3\rangle. \tag{55}$$

It remains to determine the e_3, f_3 intelligent states. In this case, the Robertson states should satisfy the following equation:

$$(j_1\vartheta_2-\lambda')\Phi_3+(1-\vartheta_2^2)\frac{\partial\Phi_3}{\partial\vartheta_2}-\vartheta_1\vartheta_2\frac{\partial\Phi_3}{\partial\vartheta_1}=0, \tag{56}$$

where $\vartheta_1=\zeta_1$, $\vartheta_2=\sqrt{(1-\alpha)/(1+\alpha)}\zeta_2$ and λ' is defined above. In a similar way as that presented above, one obtains the intelligent states

$$\Phi_3=\sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2}c_{j_1,j_2,j_3}\vartheta_1^{j_2}\vartheta_2^{j_3}, \tag{57}$$

where $\Phi_3\equiv\Phi_3(\zeta_1,\zeta_2,\alpha,\lambda,j_1)$ and the constants c's are given by

$$c_{j_1,j_2,j_3}=(-)^{j_3}\frac{\Gamma\left(\frac{\lambda'+j_1-j_2}{2}+1\right)\Gamma\left(\frac{-\lambda'+j_1-j_2}{2}+1\right)}{\Gamma(j_1-j_2+2)}$$
$$\times{}_2F_1\left(j_1-j_2-j_3+1,\frac{\lambda'+j_1-j_2}{2}+1,j_1-j_2+2,2\right). \tag{58}$$

Analogously to the above cases, the intelligent states Φ_3 can be converted as follows:

$$|\Phi_3\rangle=\sum_{j_2=0}^{j_1}\sum_{j_3=0}^{j_2}c_{j_1,j_2,j_3}\left(\frac{1+\alpha}{1-\alpha}\right)^{j_3/2}\sqrt{\frac{(j_1-j_2)\,!\,j_3\,!\,(j_2-j_3)!}{j_1!}}|j_1-j_2,j_2-j_3,j_3\rangle. \tag{59}$$

To close this section, let us note that it is clear that the Fock–Bargmann representation of the coherent states provide a simplification and a "minimization" in the problem of finding intelligent states of su(3) Weyl generators. It is evident that the procedure described here can be relevant in the derivation of intelligent states for other quadrature components of type, for instance, e_i, e_j and f_i, f_j $(i\neq j)$.

IV. DISCUSSION AND OUTLOOK

In conclusion, we have developed a method for finding the Robertson intelligent states for linear combination of the Weyl operators e_i and f_i for $i=1,2,3$, corresponding to the Lie algebra su(3). The use of the analytic representation enables us to write the eigenvalue equations, satisfied by states minimizing the Schrödinger–Robertson uncertainty relation, as quasilinear first order differential equation. Interestingly, new types of coherent states for su(3) emerge for $|\alpha|=1$. Also when $|\alpha|\neq 1$, the solutions give squeezed states. As it is noted in the end of the preceding section, the approach used through this work can be applied to derive Robertson intelligent states associ-

ated to the other quadratures of the su(3) generators. In a unified scheme, they can be obtained by considering the eigenvalue problem for an operator which is a complex linear combination of all elements of su(3),

$$\sum_{i=1,2} (\alpha_i^+ e_i + \alpha_i^- f_i + \alpha_i^0 h_i)|\Phi\rangle = \lambda|\Phi\rangle. \tag{60}$$

The solutions of such a general problem give the so-called algebra eigenstates or algebraic coherent states (Ref. 13 and references therein). Taking specific constraints on the complex parameters occurring in this general eigenvalue equation, one can get various kinds of coherent and squeezed states, in particular ones that are not discussed in this paper. This constitutes the first possible prolongation of our results. Also, as a continuation, it would be interesting to apply the approach presented here to other Lie algebras like su(n) or su(p,q).

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Solutions for a fractional nonlinear diffusion equation: Spatial time dependent diffusion coefficient and external forces

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We analyze a generalized diffusion equation which extends some known equations such as the fractional diffusion equation and the porous medium equation. We start our investigation by considering the linear case and the nonlinear case afterward. The linear case is discussed taking fractional time and spatial derivatives into account in a unified approach. We also discuss the modifications that emerge by employing simple drifts and the diffusion coefficient given by $\mathcal{D}(x,t)=\mathcal{D}(t)|x|^{-\theta}$. For the nonlinear case, we study scaling behavior of the time in connection with the asymptotic behavior for the solution of the nonlinear fractional diffusion equation. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Nowadays, fractional diffusion equations (e.g., $\partial_t^\gamma \rho = \mathcal{D}\partial_x^2 \rho$) and nonlinear diffusion equations (e.g., $\partial_t \rho = \mathcal{D}\partial_x^2 \rho^\nu$) play important roles in describing anomalous diffusion due to their broadness of the physical applications. In fact, they have been applied to several physical situations such as percolation of gases through porous media,[1] thin saturated regions in porous media,[2] diffusion of dissolved solutes into immobile water zones of various sizes, a standard solid-on-solid model for surface growth, thin liquid films spreading under gravity,[3] modeling of non-Markovian dynamical processes in protein folding,[4] relaxation to equilibrium in a system (such as polymer chains and membranes) with long temporal memory,[5] and anomalous transport in disordered systems.[6] Some properties concerning the nonlinear fractional diffusion have also been investigated in Ref. 7. In this scenario, a high order diffusion-like equation such as the thin film equation,[8] which contains a fourth order derivative, has been used to describe the lubrication models for thin viscous films, spreading droplets and Hele-Shaw cells.[9] Note that the physical situations mentioned above essentially concern anomalous diffusion of the correlated type (both sub- and superdiffusion; see Ref. 10 and references therein) or of the Lévy type (superdiffusion; see Ref. 11 and references therein). The anomalous correlated diffusion usually has a finite second moment $\langle x^2\rangle \propto t^\sigma$ ($\sigma>1$, $\sigma=1$ and $0<\sigma<1$ correspond to superdiffusion, normal diffusion and subdiffusion, respectively; $\sigma=0$ corresponds basically to localization). The second type is essentially characterized by Lévy distributions and, consequently, it has no finite second moment, i.e., $\langle x^2\rangle$ diverges.

Now, let us accomplish the above situations in a unified approach based on the generalized diffusion equation

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho(x,t)=\int_0^t dt' \frac{\partial}{\partial|x|}\left\{\mathcal{D}(x,t-t')\frac{\partial^{\mu-1}}{\partial|x|^{\mu-1}}[\rho(x,t')]^\nu\right\}-\frac{\partial}{\partial x}\{F(x)\rho(x,t)\}\ , \tag{1}$$

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where $\nu,\gamma,\mu\in\mathcal{R}$, $\mathcal{D}(x,t)=\mathcal{D}(t)|x|^{-\theta}$ is a diffusion coefficient, and $F(x)\equiv -dV(x)/dx$ is an external force (*drift*) associated with the potential $V(x)$. We use the Caputo[12] operator for the time derivative. For the spatial fractional derivative we consider the Riesz–Weyl operator.[13–15] Also, we employ, in general, the initial condition $\rho(x,0)=\delta(x)$ or $\rho(x,0)=\tilde{\rho}(x)$ and the boundary condition $\rho(x\to\pm\infty,t)\to 0$ or $\rho(x\to 0,t)=\rho(x\to\infty,t)\to 0$ depend on the situation analyzed. For Eq. (1), one can prove that $\int_{-\infty}^{\infty}dx\ \rho(x,t)$ is time independent (hence, if ρ is normalized at $t=0$, it will remain so forever). Indeed, if we write Eq. (1) as $\partial_t^{\gamma}\rho=-\partial_x\mathcal{J}$ and, for simplicity, assume the boundary conditions $\mathcal{J}(\pm\infty,t)\to 0$, it can be shown that $\int_{-\infty}^{\infty}dx\ \rho(x,t)$ is a constant of motion. Note that Eq. (1) recovers, for $(\mu,\gamma,\nu)=(2,1,1)$, the standard Fokker–Planck equation in the presence of a drift taking memory effects into account. The particular case $F(x)=0$ (no drift) and $\mathcal{D}(x,t)=\mathcal{D}\delta(t)$ with $(\mu,\gamma,\theta)=(2,1,0)$ has been considered by Spohn,[16] and the case $(\mu,\gamma)=(2,1)$ has been investigated in Refs. 17 and 18. Our present investigation involves extensions of these cases by considering a wide variety of situations: Employing fractional derivatives, nonlinearity and the mixing of them. Note that Eq. (1) has also a kernel which takes a memory effect into account. In this way, we expect to bring new aspects of physical phenomena to be explored, for example, when a mixing between the fractional diffusion equations and the nonlinear diffusion equations are present. In addition, by using Eq. (1), a well-known limitation of the description of diffusion processes with the diffusion equation, i.e., the infinite velocity of information propagation inherent to a parabolic equation caused by the model assumption that the collision frequency is infinite, can be avoided.

From the previous discussion, we verify that the diffusion equations investigated in the manuscript may be useful to model several physical situations. On the other hand, exact solutions play an important role in analyzing physical situations, since they contain, in principle, precise information about the system. In particular, they can be used as a useful guide to control the accuracy of numerical solutions. For these reasons, we dedicated this work to investigate some solutions of these equations in order to give support to possible investigations of physical systems modeling by the diffusion equations studied here. The reminder of this paper goes as follows. In Sec. II, we investigate several situations for Eq. (1) by considering the linear case ($\nu=1$). In Sec. III, we discuss the nonlinear ($\nu\neq 1$) fractional diffusion equation and connect the asymptotic behavior with the distributions which emerge from the nonextensive statistics.[19,20] In Sec. IV, we present our conclusions.

II. LINEAR CASE

We start our discussion by considering the linear case, i.e., $\nu=1$, with $\mathcal{D}(x,t)=\mathcal{D}(t)$ and $\mu=2$ without external force. Thus, Eq. (1) reads

$$\frac{\partial^{\gamma}}{\partial t^{\gamma}}\rho(x,t)=\int_0^t dt'\left\{\mathcal{D}(t-t')\frac{\partial^2}{\partial x^2}\rho(x,t')\right\}. \tag{2}$$

Notice that for $\gamma=1$ Eq. (2) reduces to the one obtained from a dichotomous random process.[21] In fact, by identifying the diffusion coefficient with the normalized correlation function

$$\Phi_{\xi}(t)=\frac{\langle\xi\xi(t)\rangle}{\langle\xi^2\rangle}, \tag{3}$$

we formally recover the evolution equation for the density probability present in Refs. 14 and 21. It is also interesting to note that we can also use Eq. (2) by considering an appropriate $\mathcal{D}(t)$ as a model for the diffusion that takes a finite collision time into account. Indeed, the usual diffusion equation is an approximation only valid on time scales which are large compared to the time scale at which the diffusion-causing collisions take place. One of the most striking unphysical properties of the diffusion equation is an infinite velocity of information propagation. However, the inclusion of the finite collision frequency in the system may create additional difficulties to treat the prob-

lem; an approximation which makes the problem more tractable is discussed by Bourret,[22] and it leads to an integral equation with a correlation function in the kernel-like equation Eq. (2).

Before analyzing the solutions of Eq. (2), we obtain formal results for the time behavior of the moments, in particular, of the second moment. In this direction, by simple calculation, we obtain a dynamic equation for the nth moment:

$$\frac{d^{\gamma}}{dt^{\gamma}}\langle x^{2n}\rangle(t)=2n(2n-1)\int_0^t dt'\,\mathcal{D}(t-t')\langle x^{2n-2}\rangle(t')\ , \tag{4}$$

for $n=1,2,\ldots$. To find the nth moment related to this equation, a coupled system of equations needs to be solved. For simplicity, we consider $0<\gamma<1$. Thus, we start by evaluating the second moment and then we use this result to obtain the nth moment. By choosing $n=1$ in Eq. (4) we have an equation for the second moment whose solution is

$$\langle x^2\rangle=\frac{2}{\Gamma(\gamma+1)}\int_0^t dt'\ \ (t-t')^{\gamma}\mathcal{D}(t')\ . \tag{5}$$

Using the above result we can show that the nth moment is given by

$$\langle x^{2n}\rangle=\frac{(2n)!}{\Gamma(n\gamma+1)}\int_0^t dt^{(1)}(t-t^{(1)})^{n\gamma}\int_0^{t^{(1)}}dt^{(2)}\mathcal{D}(t^{(1)}-t^{(2)})\cdots\int_0^{t^{(n-1)}}dt^{(n)}$$
$$\times\mathcal{D}(t^{(n-1)}-t^{(n)})\mathcal{D}(t^{(n)})\ . \tag{6}$$

Now, let us investigate the solutions for Eq. (2). By employing the Laplace transform in Eq. (2), we obtain that

$$s^{\gamma}\hat{\rho}(x,s)-s^{\gamma-1}\rho(x,0)=\mathcal{D}(s)\frac{d^2}{dx^2}\hat{\rho}(x,s), \tag{7}$$

($\hat{\rho}(x,s)=\mathcal{L}\{\rho(x,t)\}$ where $\mathcal{L}\{\cdots\}=\int_0^{\infty}dte^{-st}\cdots$), whose solution, for $\rho(x,0)=\delta(x)$, is given by

$$\hat{\rho}(x,s)=\frac{1}{2s}\left(\frac{s^{\gamma}}{\mathcal{D}(s)}\right)^{1/2}\exp\left[-\left(\frac{s^{\gamma}}{\mathcal{D}(s)}\right)^{1/2}|x|\right]\ . \tag{8}$$

Note that, if we take a general diffusion coefficient into account in the above equation, the inversion of the Laplace transform becomes a hard task. However, for some cases it is possible to calculate the inverse of Laplace transform. For instance, $\mathcal{D}(s)=constant$ ($\mathcal{D}(t)=\mathcal{D}\delta(t)$), which recovers the result presented in Ref. 14, Cattaneo's case,[23] i.e., $\mathcal{D}(s)=\mathcal{D}/(1+\tau_c s)$ ($\mathcal{D}(t)=\mathcal{D}/\tau_c e^{-t/\tau_c}$), and $\mathcal{D}(s)=\mathcal{D}s^{-\alpha}$ ($\mathcal{D}(t)=\mathcal{D}t^{\alpha-1}/\Gamma(\alpha)$) which lead us to

$$\rho(x,t)=\frac{1}{\sqrt{4\mathcal{D}t^{\gamma+\alpha}}}\ \mathrm{H}_1^{\,1\ 0}_{\,1\ 1}\left[\frac{|x|}{\sqrt{\mathcal{D}t^{\gamma+\alpha}}}\middle|\begin{matrix}(1-(\gamma+\alpha)/2\,,(\gamma+\alpha)/2)\\(0,1)\end{matrix}\right]\ , \tag{9}$$

where $\mathrm{H}_p^{\,m\ n}_{\,q}[x|^{(a_1,A_1),\ldots,(a_p,A_p)}_{(b_1,B_1),\ldots,(b_q,B_q)}]$ is the FOX function.[24] In Fig. 1, we show the behavior of the above equation by considering typical values of $\gamma+\alpha$ with $0<\gamma<1$. It is interesting to note that for $\gamma+\alpha<1$ we have a unimodal distribution, similar result is reported in Ref. 14, and for $1<\gamma+\alpha<2$ we have a bimodal distribution, in according to the results present in Ref. 21. The asymptotic behavior of Eq. (9) is

$$\rho(x,t)\sim\frac{1}{\sqrt{4\pi\mathcal{D}t^{\gamma+\alpha}}}\left(\frac{|x|}{\sqrt{\mathcal{D}t^{\gamma+\alpha}}}\right)^{(-1-\gamma-\alpha)/(2-\gamma-\alpha)}\exp\left[-\mathcal{C}_{\gamma,\alpha}\left(\frac{|x|}{\sqrt{\mathcal{D}t^{\gamma+\alpha}}}\right)^{2/(2-\gamma-\alpha)}\right], \tag{10}$$

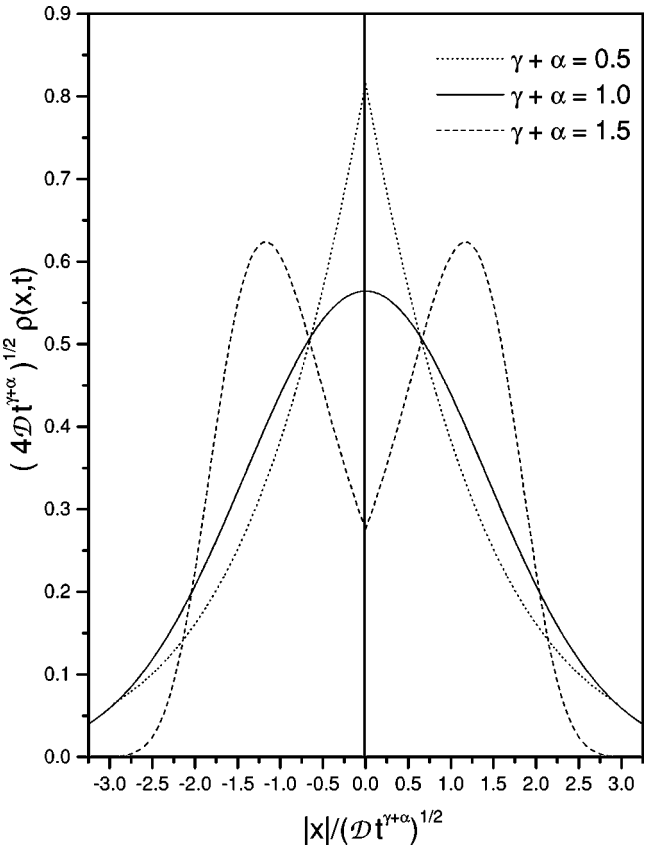

FIG. 1. In this figure, we illustrate the behavior of Eq. (9) by plotting $(4\mathcal{D}t^{\gamma+\alpha})^{1/2}\rho(x,t)$ vs $|x|/(\mathcal{D}t^{\gamma+\alpha})^{1/2}$, for typical values of for $\gamma+\alpha$ with $0<\gamma<1$.

where $\mathcal{C}_{\gamma,\alpha}=[(2-\gamma-\alpha)/2][(\gamma+\alpha)/2]^{(\gamma+\alpha)/(2-\gamma-\alpha)}$. Similar asymptotic behavior is found in homogeneous and isotropic random walk models.[25,26] Notice that Eq. (9) recovers the Gaussian distribution for $\gamma+\alpha=1$. In particular, for a general initial condition, i.e., $\rho(x,0)=\tilde{\rho}(x)$, we have that

$$\rho(x,t)=\frac{1}{\sqrt{4\mathcal{D}t^{\gamma+\alpha}}}\int_{-\infty}^{\infty}dx'\,\tilde{\rho}(x')\;\mathrm{H}_{1\;1}^{1\;0}\left[\frac{|x-x'|}{\sqrt{\mathcal{D}t^{\gamma+\alpha}}}\middle|\begin{matrix}(1-(\gamma+\alpha)/2,(\gamma+\alpha)/2)\\ \\ (0,1)\end{matrix}\right]. \tag{11}$$

In order to extend the above results, we incorporate a linear drift force, i.e., $F(x)=-\mathcal{K}x$. In this case, by employing the Fourier and Laplace transforms we can show that

$$\rho(k,s)=s^{\gamma-1}\int_0^{\infty}du\,e^{-us^{\gamma}}e^{-\mathcal{D}(s)/2\mathcal{K}|k|^2(1-e^{-2u\mathcal{K}})}\,. \tag{12}$$

The second moment obtained from the above equation is given by

$$\langle x^2\rangle=2\int_0^t dt'\mathcal{D}(t-t')t'^{\;\gamma}\mathrm{E}_{\gamma,\gamma+1}(-2\mathcal{K}t'^{\;\gamma})\,, \tag{13}$$

where $\mathrm{E}_{\alpha,\beta}(x)$ is the generalized Mittag–Leffler function

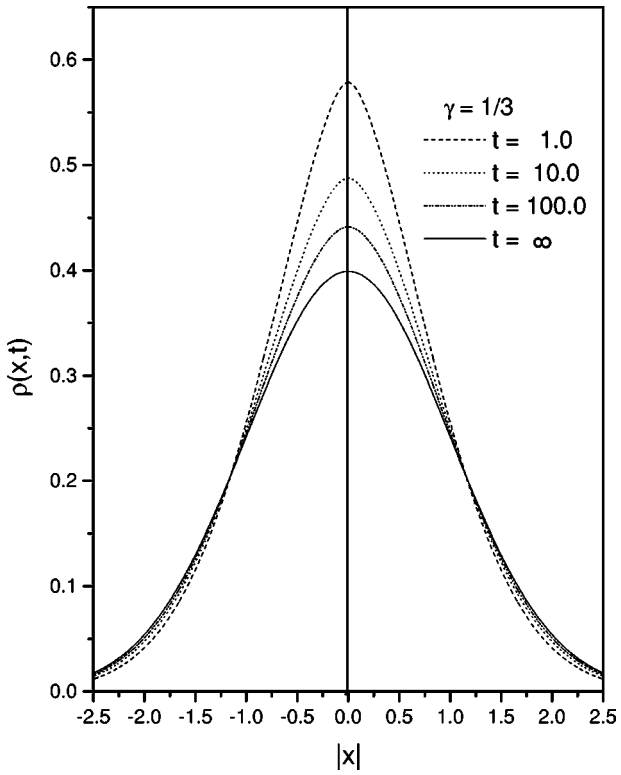

FIG. 2. In this figure, we illustrate the behavior of Eq. (15), by considering $\rho(x,t)$ vs $|x|$ for several times, with $\gamma=1/3$, $\mathcal{K}=1$, and $\mathcal{D}=1$. Note that for long times we have the Gaussian behavior for the stationary solution.

$$\mathrm{E}_{\alpha,\beta}(x)=\sum_{n=0}^{\infty}\frac{x^n}{\Gamma(n\alpha+\beta)}\,. \tag{14}$$

We notice that for $\mathcal{K}=0$ in Eq. (12) we recover Eq. (8). For simplicity, by choosing $\mathcal{D}(s)=\mathcal{D}$ in (12) we can reduce it to

$$\rho(x,t)=\sqrt{\frac{\mathcal{K}}{2\pi\mathcal{D}}}\int_0^{\infty}du\,\frac{\mathcal{W}(1-\gamma,-\gamma;-u)}{(1-e^{-2ut^{\gamma}\mathcal{K}})^{1/2}}\exp\left[-\frac{\mathcal{K}x^2}{2\mathcal{D}(1-e^{-2ut^{\gamma}\mathcal{K}})}\right], \tag{15}$$

where $\mathcal{W}(\beta,\alpha;x)$ is the Wright function[27]

$$\mathcal{W}(\beta,\alpha;u)=\frac{1}{2\pi i}\int_{Ha}d\tau\tau^{-\beta}e^{\tau+u\tau^{-\alpha}}\,, \tag{16}$$

and Ha denotes the Hankel contour and $0<\gamma<1$. In particular, $\mathcal{W}(1-\gamma,-\gamma;-u)=\mathcal{M}(\gamma,u)$, where $\mathcal{M}(\gamma,u)$ is the Mainardi function (for detail, see Ref. 28). In Fig. 2, we show the time behavior of Eq. (15) by considering $\gamma=1/3$. We verify that the time behavior is unimodal. Further, for small times Eq. (15) has a similar behavior like the one present in Fig. 1 for the case $\gamma+\alpha<1$ $(0<\gamma<1)$, and for long times the solution recovers the usual stationary solution. This behavior obtained for Eq. (15) is in accordance to the results reported in Ref. 14. Note that the solution (15) is valid for $0<\gamma<1$ (subdiffusive case). If we had considered the range $1<\gamma<2$, it would be convenient to use an extension of Eq. (15) such as presented in Ref. 14. Thus, for $1<\gamma<2$, we verify for small times a bimodal behavior, similar to the case $\alpha+\gamma>1$ $(0<\gamma<1)$ obtained in Fig. 1. Further, the bimodal behavior present for small times evolves to a unimodal

distribution in such way that for long times the unimodal Gaussian distribution is recovered. In particular, Eq. (15) always recovers the usual stationary solution $\rho(x)\sim e^{-(\mathcal{K}/2\mathcal{D})x^2}$ for long times. For the case $\mu\neq 1$ with a generic initial condition, Eq. (15) is modified to

$$\rho(x,t)=\int_0^\infty du\,\mathcal{W}(1-\gamma,-\gamma;-u)\int_{-\infty}^{\infty}dx'\,\tilde{\rho}(x-x')\mathcal{G}(x',u;t)\ ,$$

$$\mathcal{G}(x,u;t)=\frac{1}{\mu|x|}\,\mathrm{H}_{2\ 2}^{1\ 1}\left[\left(\frac{\mu\mathcal{K}}{\mathcal{D}}\right)^{1/\mu}\frac{|x|}{(1-e^{-\mu u t^{\gamma}\mathcal{K}})^{1/\mu}}\middle|\begin{matrix}(1,1/\mu) & , & (1,1/2)\\ (1,1) & , & (1,1/2)\end{matrix}\right]. \tag{17}$$

Note that the above equation, in contrast with Eq. (15), has a Lévy distribution as a stationary solution for long times.

Interesting features can be incorporated in the above scenario when we consider a spatial dependence on the diffusion coefficient, i.e., $\mathcal{D}(x,t)=\mathcal{D}(t)|x|^{-\theta}$. In particular, this kind of diffusion coefficient may be related to several physical situations, for example, diffusion on fractals,[29] turbulence[30] and fast electrons in a hot plasma in the presence of a dc electric field.[31] In this direction, the mean first passage time has also been analyzed in Ref. 32. Thus, Eq. (1) is given by

$$\frac{\partial^{\gamma}}{\partial t^{\gamma}}\rho(x,t)=\int_0^t dt'\frac{\partial}{\partial|x|}\left\{\mathcal{D}(t-t')|x|^{-\theta}\frac{\partial}{\partial|x|}\rho(x,t')\right\}, \tag{18}$$

in the absence of external force for $\mu=2$. To investigate solutions for the above equation we consider, for simplicity, x nonnegative, the boundary conditions $\rho(0,t)=\rho(\infty,t)=0$ and use the following integral transform:

$$\rho(k,t)=\int_0^\infty dx\ \ x^{1/2(1+\theta)}\mathrm{J}_{(1+\theta)/(2+\theta)}\left(\frac{2kx^{1/2(2+\theta)}}{2+\theta}\right)\rho(x,t),$$

$$\rho(x,t)=\frac{2}{2+\theta}\int_0^\infty dk\ \ kx^{1/2(1+\theta)}\mathrm{J}_{(1+\theta)/(2+\theta)}\left(\frac{2kx^{1/2(2+\theta)}}{2+\theta}\right)\rho(k,t)\ , \tag{19}$$

obtained from the Sturm–Liouville problem related to the differential equation for the spatial variable of Eq. (1) with $(\nu,\mu)=(1,2)$ and $\mathcal{D}(x,t)=\mathcal{D}|x|^{-\theta}$. By using Eq. (19), we can simplify Eq. (18) and obtain

$$\frac{d^{\gamma}}{dt^{\gamma}}\rho(k,t)=-k^2\int_0^t dt'\ \mathcal{D}(t-t')\rho(k,t')\ , \tag{20}$$

whose Laplace transform is given by

$$\rho(k,s)=\frac{s^{\gamma-1}}{s^{\gamma}+\mathcal{D}(s)k^2}\rho(k,0)\ . \tag{21}$$

By substituting the above equation in Eq. (19), we obtain that

$$\rho(x,s)=\frac{2x^{1/2(1+\theta)}}{2+\theta}\int_0^\infty dk\,\frac{s^{\gamma-1}k}{s^{\gamma}+\mathcal{D}(s)k^2}\mathrm{J}_{(1+\theta)/(2+\theta)}\left(\frac{2kx^{1/2(2+\theta)}}{2+\theta}\right)\rho(k,0)\ . \tag{22}$$

In order to invert the Laplace transform, for simplicity, we employ $\mathcal{D}(s)=\mathcal{D}s^{\alpha}$ $(\alpha<\gamma)$ and the condition $\rho(x,0)=\tilde{\rho}(x)$. Then, after some calculations, we can show that

$$\rho(x,t)=\frac{2x^{1/2(1+\theta)}}{2+\theta}\int_0^\infty du\,\mathcal{W}(1+\alpha-\gamma,\alpha-\gamma;-u)\int_0^\infty dx'\;\; x'^{1/2(1+\theta)}\tilde{\rho}(x')$$
$$\times\int_0^\infty dk\;\; k\;\; \mathrm{J}_{(1+\theta)/(2+\theta)}\left(\frac{2kx^{1/2(2+\theta)}}{2+\theta}\right)\mathrm{J}_{(1+\theta)/(2+\theta)}\left(\frac{2kx'^{1/2(2+\theta)}}{2+\theta}\right)e^{-ut^{\gamma-\alpha}\mathcal{D}k^2}\;. \quad (23)$$

By using the identity

$$\int_0^\infty dk\;\; k\;\; \mathrm{J}_\nu(\alpha k)\mathrm{J}_\nu(\beta k)e^{-a^2k^2}=\frac{1}{2a^2}e^{-\beta^2+\alpha^2/4a^2}\mathrm{I}_\nu\left(\frac{\alpha\beta}{2a^2}\right)\;, \quad (24)$$

present in Ref. 33, we may simplify Eq. (23) and obtain

$$\rho(x,t)=\frac{x^{1/2(1+\theta)}}{(2+\theta)\mathcal{D}t^{\gamma-\alpha}}\int_0^\infty\frac{du}{u}\,\mathcal{W}(1+\alpha-\gamma,\alpha-\gamma;-u)\int_0^\infty dx'\;\; x'^{1/2(1+\theta)}\tilde{\rho}(x')$$
$$\times\mathrm{I}_{(1+\theta)/(2+\theta)}\left(\frac{2x^{1/2(2+\theta)}x'^{1/2(2+\theta)}}{(2+\theta)^2\mathcal{D}ut^{\gamma-\alpha}}\right)\exp\left[-\frac{x^{2+\theta}+x'^{2+\theta}}{(2+\theta)^2\mathcal{D}ut^{\gamma-\alpha}}\right]\;, \quad (25)$$

where $\mathrm{I}_\nu(x)$ is a modified Bessel function.

III. NONLINEAR CASE

The scaling relation is remarkable in physics due to the broadness that may arise in diverse situations, for instance, the systems of the water transport in soil are related to the dependence of the concentration on distance and time,[34] and the asymptotic form of the propagator on fractals, in Sierpinski gasket.[14] In this sense, it is interesting to analyze the time scaling behavior and the asymptotic solutions for nonlinear diffusion equations taking time fractional derivative into account. Thus, we focus our attention on the following equation:

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho(x,t)=\int_0^t dt'\frac{\partial}{\partial|x|}\left\{\mathcal{D}(x,t-t')\frac{\partial}{\partial|x|}[\rho(x,t')]^\nu\right\}\;, \quad (26)$$

where $\mathcal{D}(x,t)=\mathcal{D}|x|^{-\theta}t^\alpha$. In order to investigate the scaling behavior of the above equation we assume that the solution can be written as follows:

$$\rho(x,t)=\frac{1}{\Phi(t)}\overline{\rho}\left(\frac{x}{\Phi(t)}\right)\;. \quad (27)$$

Note that this kind of solution has been considered in several situations to analyze the nonlinear diffusion equation.[7] With these considerations we proceed to obtain the time evolution equation for the second moment related to Eq. (26) and it is given by

$$\frac{d^\gamma}{dt^\gamma}\langle x^2\rangle=2(1-\theta)\mathcal{D}\int_0^t dt'\,(t-t')^\alpha\int_{-\infty}^\infty dx|x|^{-\theta}[\rho(x,t')]^\nu\;. \quad (28)$$

By substituting Eq. (27) into Eq. (28), we can obtain a nonlinear fractional differential equation for $\Phi(t)$,

$$\frac{d^\gamma}{dt^\gamma}[\Phi(t)]^2=2(1-\theta)\mathcal{D}\frac{\mathcal{I}_1}{\mathcal{I}}\int_0^t dt'\,(t-t')^\alpha[\Phi(t')]^{1-\nu-\theta}\;, \quad (29)$$

with $\mathcal{I}=\int_{-\infty}^\infty d\overline{x}\,\overline{x}^2\overline{\rho}(\overline{x})$ and $\mathcal{I}_1=\int_{-\infty}^\infty d\overline{x}\,|\overline{x}|^{-\theta}[\overline{\rho}(\overline{x})]^\nu$. In addition, we supposed $\mathcal{I}$ and $\mathcal{I}_1$ are defined. Note that our investigation about the time scaling behavior is based on the second

moment which is finite when we consider a fractional time derivative applied to the diffusion equation, in contrast to the fractional spatial derivatives. For this reason, we only consider a fractional time derivative. The solution is given by

$$\Phi(t)=\mathcal{C}t^{(1+\gamma+\alpha)/(1+\nu+\theta)}\,, \tag{30}$$

where

$$\mathcal{C}=\left[\frac{(1-\theta)\alpha\mathcal{D}\mathcal{I}_1\Gamma(\alpha)}{\overline{\alpha}\mathcal{I}\ \Gamma(2\overline{\alpha})}\,\frac{\Gamma(1+2\overline{\alpha}-\gamma)\Gamma(1+\overline{\alpha}(1-\nu-\theta))}{\Gamma(2+\alpha+\overline{\alpha}(1-\nu-\theta))}\right]^{1/(1+\nu+\theta)}\,, \tag{31}$$

with

$$\overline{\alpha}=\frac{1+\gamma+\alpha}{1+\nu+\theta}\,. \tag{32}$$

From Eq. (30), we have $\langle x^2\rangle\propto t^{2((1+\gamma+\alpha)/(1+\nu+\theta))}$, so, for $(1+\gamma+\alpha)/(1+\nu+\theta)<1/2$, $(\gamma+\alpha)/(1+\nu+\theta)=1/2$ or $(1+\gamma+\alpha)/(1+\nu+\theta)>1/2$, which characterizes the sub, normal or superdiffusive behavior. In order to investigate the asymptotic behavior of Eq. (26), we consider

$$\rho(x,t)\sim\frac{1}{\Phi(t)}\left(\frac{|x|}{\Phi(t)}\right)^{-\eta}\,. \tag{33}$$

Note that Eq. (33) is Eq. (27) with $\overline{\rho}(x)\sim|x|^{-\eta}$. By substituting the above equation into (26), we find that $\eta=(2+\theta)/(1-\nu)$. It is possible to establish a connection between the asymptotic solution obtained here and the one obtained from the nonextensive statistics. In this sense, we compare Eq. (33) with the expression $1/|x|^{2/(q-1)}$ that appears in Ref. 20 for the entropic problem in this asymptotic behavior. Thus, we have that

$$q=\frac{4-2\nu+\theta}{2+\theta}\,. \tag{34}$$

Note that for $\theta=0$ the above result recovers the usual relation $q=2-\nu$ employed in Ref. 18.

IV. SUMMARY AND CONCLUSION

In summary, we have worked on a one-dimensional generalized diffusion equation [Eq. (1)] in several situations by considering the space and time fractional derivatives in the absence or presence of an external drift. We have also employed a time and spatial dependent diffusion coefficient. In this context, we have obtained a general expression for nth moment. Further, for some cases of $\mathcal{D}(x,t)$, we have obtained the exact solution for the probability density. Some peculiar aspects related to fractional approach have been shown along the text. It is interesting to note that the fractional derivative can deal with a bimodal distribution (see Fig. 1) which is absent in the ordinary case. For the nonlinear case we have analyzed the scaling behavior of the time and employed the scaling argument, on the space and time, to obtain an asymptotic solution for the probability density. In particular, we have related our asymptotic solution to the one obtained from nonextensive statistics. Finally, we hope that the results present in this work may be applied to physical systems exhibiting nontrivial forms of anomalous diffusion.

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High energy asymptotics of the magnetic spectral shift function

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We consider the three-dimensional Schrödinger operators H_0 and H where $H_0=(i\nabla+A)^2-b$, A is a magnetic potential generating a constant magnetic field of strength $b>0$, and $H=H_0+V$ where $V\in L^1(\mathbb{R}^3;\mathbb{R})$ satisfies certain regularity conditions. Then the spectral shift function $\xi(E;H,H_0)$ for the pair of operators H, H_0 is well-defined for energies $E\neq 2qb$, $q\in\mathbb{Z}_+$. We study the asymptotic behavior of $\xi(E;H,H_0)$ as $E\to\infty$, $E\in\mathcal{O}_r$, $r\in(0,b)$, where $\mathcal{O}r:=\{E\in(0,\infty)|\mathrm{dist}(E,2b\mathbb{Z}+)>r\}$. We obtain a Weyl-type formula $\lim_{E\to\infty,E\in\mathcal{O}_r}E^{-1/2}\xi(E;H,H_0)=(1/4\pi^2)\int_{\mathbb{R}^3}V(x)dx$. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In this note we study the high energy asymptotics of the spectral shift function (SSF) for the three-dimensional Schrödinger operator with constant magnetic field, perturbed by an electric potential which decays fast enough at infinity. The note could be regarded as a supplement to the articles in Ref. 5 where the asymptotic behavior of the SSF in the strong magnetic field regime was considered, and Ref. 6 where the singularities of the SSF at the Landau levels were investigated.

Let $H_0:=(i\nabla+A)^2-b$ be the unperturbed three-dimensional magnetic Schrödinger operator, essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Here the magnetic potential $A=(-bx_2/2,bx_1/2,0)$ generates the constant magnetic field $B=\mathrm{curl}\,A=(0,0,b)$, $b>0$. It is well-known that $\sigma(H_0)=\sigma_{\mathrm{ac}}(H_0)=[0,\infty)$ (see Ref. 1), where $\sigma(H_0)$ denotes the spectrum of H_0, and $\sigma_{\mathrm{ac}}(H_0)$ its absolutely continuous spectrum. Moreover, the so-called Landau levels $2bq$, $q\in\mathbb{Z}_+:=\{0,1,\ldots\}$, play the role of thresholds in $\sigma(H_0)$.

For $\mathbf{x}=(x_1,x_2,x_3)\in\mathbb{R}^3$ we denote by $X_\perp=(x_1,x_2)$ the variables on the plane perpendicular to the magnetic field. We assume that V satisfies

$$V\not\equiv 0,\quad V\in C(\mathbb{R}^3),\quad |V(\mathbf{x})|\leqslant C_0\langle X_\perp\rangle^{-m_\perp}\langle x_3\rangle^{-m_3},\quad \mathbf{x}=(X_\perp,x_3)\in\mathbb{R}^3, \tag{1.1}$$

with $C_0>0$, $m_\perp>2$, $m_3>1$, and $\langle x\rangle:=(1+|x|^2)^{1/2}$, $x\in\mathbb{R}^d$, $d\geqslant 1$. By (1.1) and the diamagnetic inequality (see, e.g., Ref. 1), for each $E_0<0$ we have

$$|V|^{1/2}(H_0-E_0)^{-1}\in S_2, \tag{1.2}$$

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$$|V|^{1/2}(H_0 - E_0)^{-1/2} \in S_\infty, \tag{1.3}$$

where S_2 denotes the Hilbert–Schmidt class, while S_∞ denotes the class of linear compact operators. The resolvent identity combined with (1.2) implies that for each $E_0 < \inf \sigma(H) \leqslant \inf \sigma(H_0)$ we have

$$(H - E_0)^{-1} - (H_0 - E_0)^{-1} \in S_1, \tag{1.4}$$

where S_1 denotes the trace class. Then there exists a unique function $\xi(.;H,H_0) \in L^1(\mathbb{R};(1+E^2)^{-1}dE)$ which vanishes identically on $(-\infty, \inf \sigma(H))$, and satisfies the Lifshits–Krein trace formula

$$\mathrm{Tr}(\phi(H) - \phi(H_0)) = \int_{\mathbb{R}} \xi(E;H,H_0)\phi'(E)dE, \quad \phi \in C_0^\infty(\mathbb{R})$$

(see Ref. 14, Theorem 8.9.1). The function $\xi(.;H,H_0)$ is called the SSF for the pair of the operators H and H_0. For almost every $E > 0$ the SSF $\xi(E;H,H_0)$ is related to the scattering determinant $\det S(E;H,H_0)$ for the pair H, H_0 by the Birman–Krein formula

$$\det S(E;H,H_0) = e^{-2\pi i \xi(E;H,H_0)}$$

(see Ref. 3, 4, or 14, Sec. 8.4).

A priori, the SSF $\xi(E;H,H_0)$ is defined only for almost every $E \in \mathbb{R}$. In Sec. III C below we introduce a representative of the equivalence class determined by $\xi(.;H,H_0)$, defined on $\mathbb{R}\backslash 2b\mathbb{Z}_+$, which is bounded on each compact subset of the complement of the Landau levels, and is continuous on $\mathbb{R}\backslash\{2b\mathbb{Z}_+ \cup \sigma_p(H)\}$ where $\sigma_p(H)$ denotes the set of the eigenvalues of the operator H. In this note we will identify the SSF with this particular representative of its equivalence class.

The main goal of the paper is the study of the asymptotics of $\xi(E;H,H_0)$ as $E \to \infty$, $E \in \mathcal{O}_r$, where

$$\mathcal{O}_r := \{E \in (0,\infty) | \mathrm{dist}\,(E, 2b\mathbb{Z}_+) > r\}, \quad r \in (0,b). \tag{1.5}$$

The paper is organized as follows. In Sec. II we formulate our main result. In Sec. III we obtain some preliminary estimates, while the proof of our main result can be found in Sec. IV.

II. FORMULATION OF THE MAIN RESULT

Theorem 2.1: *Assume that V satisfies (1.1). Then we have*

$$\lim_{E \to \infty, E \in \mathcal{O}_r} E^{-1/2}\xi(E;H,H_0) = \frac{1}{4\pi^2}\int_{\mathbb{R}^3} V(\mathbf{x})d\mathbf{x}, \quad r \in (0,b). \tag{2.1}$$

Remarks: (i) It is essential to avoid the Landau levels in (2.1), i.e., to suppose that $E \in \mathcal{O}_r$, $r \in (0,b)$, as $E \to \infty$, since the SSF has singularities at the Landau levels, at least in the case where V has a fixed sign (see Ref. 6).

(ii) For $E \in \mathbb{R}$ set

$$\xi_{\mathrm{cl}}(E) := \int_{T^*\mathbb{R}^3} (\theta(E - |\mathbf{p} + A(\mathbf{x})|^2) - \theta(E - |\mathbf{p} + A(\mathbf{x})|^2 - V(\mathbf{x})))d\mathbf{x}d\mathbf{p}$$

$$= \frac{4\pi}{3}\int_{\mathbb{R}^3} (E_+^{3/2} - (E - V(\mathbf{x}))_+^{3/2})d\mathbf{x}$$

where

$$\theta(t) := \begin{cases} 0 & \text{if} \quad t \leqslant 0, \\ 1 & \text{if} \quad t > 0 \end{cases}$$

is the Heaviside function. Note that $\xi_{\mathrm{cl}}(E)$ is independent of the magnetic field $b \geqslant 0$. Evidently, under the assumptions of Theorem 2.1 we have

$$\lim_{E\to\infty} E^{-1/2}\xi_{\mathrm{cl}}(E) = 2\pi \int_{\mathbb{R}^3} V(\mathbf{x})d\mathbf{x}.$$

Hence, in the case $\int_{\mathbb{R}^3} V(\mathbf{x})d\mathbf{x} \neq 0$, relation (2.1) is equivalent to

$$\xi(E;H,H_0) = (2\pi)^{-3}\xi_{\mathrm{cl}}(E)(1+o(1)), \quad E\to\infty, \quad E\in\mathcal{O}_r, \quad r\in(0,b). \tag{2.2}$$

Asymptotic relations of the type (2.2) are known in the case of decaying magnetic potentials A (see, e.g., Ref. 13). However, in the last case the magnetic part $iA.\nabla + i\,\mathrm{div}\,A + |A|^2$ of the operator H_0 is a relatively compact perturbation of the Laplacian $-\Delta$, so that the resemblance with the case of a constant magnetic field, and, hence, of a linear magnetic potential, considered in the present note, is only formal. In particular, the methods of Ref. 13 are not directly applicable.

(iii) As far as the authors are informed, the high energy asymptotics of the SSF for three-dimensional Schrödinger operators with constant magnetic fields is investigated for the first time in the present note. However, we would like to mention a result contained in Ref. 9 where an axisymmetric $V=V(|X_\perp|,x_3)$ is considered. It is well-known (see, e.g., Ref. 1) that in this case the operators H and H_0 are unitarily equivalent to the orthogonal sums $\Sigma_{m\in\mathbb{Z}}\oplus H^{(m)}$ and $\Sigma_{m\in\mathbb{Z}}\oplus H_0^{(m)}$, respectively, where the operators

$$H_0^{(m)} := -\frac{1}{\varrho}\frac{\partial}{\partial\varrho}\varrho\frac{\partial}{\partial\varrho} - \frac{\partial^2}{\partial x_3^2} + \left(\frac{b\varrho}{2}+\frac{m}{\varrho}\right)^2, \quad H^{(m)} := H_0^{(m)} + V(\varrho,x_3), \quad m\in Z,$$

are self-adjoint in $L^2(\mathbb{R}_+\times\mathbb{R};\varrho d\varrho dx_3)$. For an arbitrary fixed $m\in\mathbb{Z}$ the authors of Ref. 9 studied the asymptotics as $E\to\infty$, $E\in\mathcal{O}_r$, of the SSF $\xi(E;H^{(m)},H_0^{(m)})$. Note that (2.1) cannot be deduced from the results of Ref. 9 even in the case of axial symmetry of V.

III. AUXILIARY RESULTS

A. Classes of compact operators

In this subsection we introduce some basic notations used throughout the paper. As above, we denote by S_∞ the class of linear compact operators acting in a fixed Hilbert space. Let $T=T^*\in S_\infty$. Denote by $\mathbb{P}_I(T)$ the spectral projection of T associated with the interval $I\subset\mathbb{R}$. For $s>0$ set

$$n_\pm(s;T) := \mathrm{rank}\ \mathbb{P}_{(s,\infty)}(\pm T).$$

For an arbitrary (not necessarily self-adjoint) operator $T\in S_\infty$ put

$$n_*(s;T) := n_+(s^2;T^*T), \quad s>0. \tag{3.1}$$

If $T=T^*$, then evidently

$$n_*(s;T) = n_+(s,T) + n_-(s;T), \quad s>0. \tag{3.2}$$

Further, we denote by S_p, $p\in[1,\infty)$, the Schatten–von Neumann class of compact operators for which the norm $\|T\|_p := (p\int_0^\infty s^{p-1}n_*(s;T)ds)^{1/p}$ is finite. In particular, as already indicated, S_1 stands for the trace class, and S_2 for the Hilbert–Schmidt class. If $T\in S_p$, $p\in[1,\infty)$, then the following elementary inequality,

$$n_*(s;T) \leqslant s^{-p}\|T\|_p^p, \tag{3.3}$$

holds for every $s>0$. If $T=T^* \in S_p$, $p \in [1,\infty)$, then (3.2) and (3.3) imply

$$n_\pm(s;T) \leqslant s^{-p}\|T\|_p^p, \quad s>0. \tag{3.4}$$

Finally, we define the self-adjoint operators $\mathrm{Re}\, T := \frac{1}{2}(T+T^*)$ and $\mathrm{Im}\, T := \frac{1}{2i}(T-T^*)$.

B. Index for a pair of projections

In this subsection we introduce the concepts of index of a Fredholm pair of orthogonal projections, and index for a pair of self-adjoint operators, and describe some basic properties related to these concepts which will be often used in the sequel. More details can be found in Ref. 2.

A pair of orthogonal projections P, Q is said to be Fredholm if

$$\{-1,1\} \cap \sigma_{\mathrm{ess}}(P-Q) = \emptyset\,.$$

In particular, if $P-Q \in S_\infty$, then the pair P, Q is Fredholm.

Assume that the pair of orthogonal projections P, Q is Fredholm. Set

$$\mathrm{index}(P,Q) := \dim \mathrm{Ker}\,(P-Q-I) - \dim \mathrm{Ker}\,(P-Q+I).$$

Let $\widetilde{M}$, M, be bounded self-adjoint operators. If the spectral projections $\mathbb{P}_{(-\infty,0)}(\widetilde{M})$ and $\mathbb{P}_{(-\infty,0)}(M)$ form a Fredholm pair, we shall use the short-hand notation

$$\mathrm{ind}(\widetilde{M},M) := \mathrm{index}(\mathbb{P}_{(-\infty,0)}(\widetilde{M}),\mathbb{P}_{(-\infty,0)}(M)).$$

A sufficient condition that the pair $\mathbb{P}_{(-\infty,0)}(\widetilde{M})$, $\mathbb{P}_{(-\infty,0)}(M)$ be Fredholm is $\widetilde{M}=M+A$, where M is a bounded self-adjoint operator such that $0 \notin \sigma_{\mathrm{ess}}(M)$, and $A=A^* \in S_\infty$.

Lemma 3.1 (see Ref. 12, Lemma 5.2): Let $M=M^*$, $0 \notin \sigma(M)$, $0 \leqslant A=A^* \in S_\infty$. Then for $t \in (0,\infty)$ we have

$$\mathrm{ind}(M+tA,M) = -\lim_{\varepsilon \downarrow 0} n_-(1-\varepsilon;tA^{1/2}M^{-1}A^{1/2}), \tag{3.5}$$

$$\mathrm{ind}(M-tA,M) = n_+(1;tA^{1/2}M^{-1}A^{1/2}). \tag{3.6}$$

Lemma 3.2 [see Ref. 5, Sec. 3.2, Property (g)]: Let M be a bounded self-adjoint operator such that $0 \notin \sigma(M)$. Let A and B be compact self-adjoint operators. Then for $s \in (0,\infty)$ such that $[-s,s] \cap \sigma(M)=\emptyset$ we have

$$\mathrm{ind}(M+s+B,M+s) - n_+(s;A) \leqslant \mathrm{ind}(M+A+B,M) \leqslant \mathrm{ind}(M-s+B,M-s) + n_-(s;A). \tag{3.7}$$

Lemma 3.3 (see Ref. 11, Lemma 2.1, or Ref. 5, Sec. 3.3): Let M be a bounded self-adjoint operator such that $0 \notin \sigma(M)$. Let $T_1=T_1^* \in S_\infty$ and $T_2=T_2^* \in S_1$. Then for each $s_1>0$, $s_2>0$ such that $[-s,s] \cap \sigma(M)=\emptyset$ with $s=s_1+s_2$ we have

$$\int_{\mathbb{R}} |\mathrm{ind}(M+T_1+t\,T_2,M)|\,d\mu(t) \leqslant n_*(s_1;T_1) + \frac{1}{\pi s_2}\|T_2\|_1, \tag{3.8}$$

where $d\mu(t) := (1/\pi)[dt/(1+t^2)]$.

C. Representation of the SSF

In this subsection we describe a representation of the SSF $\xi(E;H,H_0)$ which is a special case of the general representation of the SSF for a pair of lower-bounded self-adjoint operators, obtained by Gesztesy, Makarov, and Pushnitski (see Refs. 11, 8, and 12).

For $z\in\mathbb{C}$, $\operatorname{Im} z>0$, set $T(z):=|V|^{1/2}(H_0-z)^{-1}|V|^{1/2}$.

Lemma 3.4 (see Ref. 5, Lemma 3.1): Let (1.1) hold. Then for every $E\in\mathbb{R}\setminus 2b\mathbb{Z}_+$, the operator-norm limit

$$T(E):=\mathrm{n}-\lim_{\delta\downarrow 0} T(E+i\delta) \tag{3.9}$$

exists, and by (1.3) we have $T(E)\in S_\infty$. Moreover, $\operatorname{Im} T(E)\in S_1$.

Lemma 3.4 follows easily from Propositions 3.2 and 3.3 below (see Corollary 3.2).

Denote by J the multiplier by the function

$$\operatorname{sign} V(\mathbf{x})=\begin{cases}1 & \text{if } V(\mathbf{x})\geqslant 0,\\ -1 & \text{if } V(\mathbf{x})<0.\end{cases}$$

Introduce the function

$$\widetilde{\xi}(E;H,H_0)=\int_{\mathbb{R}}\operatorname{ind}(J+\operatorname{Re}T(E)+t\operatorname{Im}T(E),J)\,d\mu(t),\quad E\in\mathbb{R}\setminus 2b\mathbb{Z}_+, \tag{3.10}$$

which is well-defined by Lemmas 3.3 and 3.4.

Proposition 3.1 (see Ref. 5, Proposition 2.5): The function $\widetilde{\xi}(E;H,H_0)$ is continuous on $\mathbb{R}\setminus\{2b\mathbb{Z}_+\cup\sigma_p(H)\}$, and is bounded on every compact subset of $\mathbb{R}\setminus 2b\mathbb{Z}_+$.

Remark: Note that, in contrast to the case $b=0$, we cannot rule out the possibility of existence of embedded eigenvalues, by imposing short-range assumptions of the type of (1.1): Theorem 5.1 of Ref. 1 shows that there are axisymmetric potentials V of compact support such that below each Landau level $2bq$, $q\in\mathbb{Z}_+$, there exists an infinite sequence of eigenvalues of H which converges to $2bq$. On the other hand, generically, the only possible accumulation points of the eigenvalues of the operators H are the Landau levels [see Ref. 1, Theorem 4.7, and Ref. 7, Theorem 3.5.3 (iii)]. Further information of the location of these eigenvalues can be found in Ref. 5.

Theorem 3.1 (see Refs. 11, 8, 12, or 5, Sec. 3.3): *Let (1.1) hold. Then for almost every $E\in\mathbb{R}$ we have*

$$\xi(E;H,H_0)=\widetilde{\xi}(E;H,H_0). \tag{3.11}$$

Remark: As explained in the Introduction, we identify $\xi(E;H,H_0)$ with $\widetilde{\xi}(E;H,H_0)$. The identification on the set $\mathbb{R}\setminus\{2b\mathbb{Z}_+\cup\sigma_p(H)\}$ where $\widetilde{\xi}$ is continuous, is natural. On the other hand, the values prescribed to the SSF at the eigenvalues $E\in\sigma_p(H)$ may seem somewhat arbitrary; in any case, as Theorem 2.1 shows, these values are consistent with the asymptotics of $\xi(E;H,H_0)$ as $E\to\infty$, $E\in\mathcal{O}_r$, $r\in(0,b)$, *and* $E\notin\sigma_p(H)$.

D. Preliminary estimates

Introduce the Landau Hamiltonian

$$h(b):=\left(i\frac{\partial}{\partial x_1}-\frac{bx_2}{2}\right)^2+\left(i\frac{\partial}{\partial x_2}+\frac{bx_1}{2}\right)^2-b, \tag{3.12}$$

i.e., the two-dimensional Schrödinger operator with constant scalar magnetic field $b>0$, essentially self-adjoint on $C_0^\infty(\mathbb{R}^2)$. It is well-known that $\sigma(h(b))=\cup_{q=0}^\infty\{2bq\}$, and each eigenvalue $2bq$, $q\in\mathbb{Z}_+$, has infinite multiplicity (see, e.g., Ref. 1).

For $\mathbf{x},\mathbf{x}' \in \mathbb{R}^2$ denote by $\mathcal{P}_{q,b}(\mathbf{x},\mathbf{x}')$ the integral kernel of the orthogonal projection $p_q(b)$ onto the subspace $\mathrm{Ker}(h(b)-2bq)$, $q \in \mathbb{Z}_+$. It is well-known that

$$\mathcal{P}_{q,b}(\mathbf{x},\mathbf{x}') = \frac{b}{2\pi} L_q\left(\frac{b|\mathbf{x}-\mathbf{x}'|^2}{2}\right)\exp\left(-\frac{b}{4}(|\mathbf{x}-\mathbf{x}'|^2 + 2i(x_1x_2' - x_1'x_2))\right) \tag{3.13}$$

(see Ref. 10) where $L_q(t) := \sum_{k=0}^{q}\binom{q}{k}(-t)^k/k!$, $t \in \mathbb{R}$, $q \in \mathbb{Z}_+$, are the Laguerre polynomials. Note that

$$\mathcal{P}_{q,b}(\mathbf{x},\mathbf{x}) = \frac{b}{2\pi} \tag{3.14}$$

for each $q \in \mathbb{Z}_+$ and $\mathbf{x} \in \mathbb{R}^2$. Introduce the orthogonal projections $P_q : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $q \in \mathbb{Z}_+$, by $P_q := p_q \otimes I$ where I denotes the identity operator in $L^2(\mathbb{R}_{x_3})$. For $z \in \mathbb{C}$ with $\mathrm{Im}\, z > 0$, define the operator $R(z) := (-d^2/dx_3^2 - z)^{-1}$ bounded in $L^2(\mathbb{R})$, as well as the operators

$$T_q(z) := |V|^{1/2} P_q (H_0 - z)^{-1} |V|^{1/2}, \quad q \in \mathbb{Z}_+,$$

bounded in $L^2(\mathbb{R}^3)$. The operator $R(z)$ admits the integral kernel $\mathcal{R}_z(x_3 - x_3')$ where $\mathcal{R}_z(x) = ie^{i\sqrt{z}|x|}/(2\sqrt{z})$, $x \in \mathbb{R}$, the branch of $\sqrt{z}$ being chosen so that $\mathrm{Im}\,\sqrt{z} > 0$. Moreover, $T_q(z) = |V|^{1/2}(p_q(b) \otimes R(z-2bq))|V|^{1/2}$.

For $\lambda \in \mathbb{R}$, $\lambda \neq 0$, define $R(\lambda)$ as the operator with integral kernel $\mathcal{R}_\lambda(x_3 - x_3')$ where

$$\mathcal{R}_\lambda(x) := \lim_{\delta \downarrow 0} \mathcal{R}_{\lambda + i\delta}(x) = \begin{cases} \dfrac{e^{-\sqrt{-\lambda}|x|}}{2\sqrt{-\lambda}} & \text{if} \quad \lambda < 0, \\ \dfrac{ie^{i\sqrt{\lambda}|x|}}{2\sqrt{\lambda}} & \text{if} \quad \lambda > 0, \end{cases} \qquad x \in \mathbb{R}. \tag{3.15}$$

Evidently, if $w \in L^2(\mathbb{R})$ and $\lambda \neq 0$, then $wR(\lambda)\overline{w} \in S_2$. For $E \in \mathbb{R}$, $E \neq 2bq$, $q \in \mathbb{Z}_+$, set

$$T_q(E) := |V|^{1/2}(p_q(b) \otimes R(E - 2bq))|V|^{1/2}.$$

Proposition 3.2 (Ref. 6, Proposition 4.1 and Corollaries 4.1, 4.2): Let $E \in \mathbb{R}$, $q \in \mathbb{Z}_+$, $E \neq 2bq$. *Assume that (1.1) holds.*

(i) *We have* $T_q(E) \in S_2$, *and* $\lim_{\delta \downarrow 0} \|T_q(E + i\delta) - T_q(E)\|_2 = 0$.
(ii) *We have* $\mathrm{Im}\, T_q(E) \geqslant 0$, *and if* $E < 2bq$, *then* $\mathrm{Im}\, T_q(E) = 0$. *Moreover,* $\mathrm{Im}\, T_q(E) \in S_1$.

Proposition 3.3 (see Ref. 6, Proposition 4.2): Let $b > 0$, $E \notin 2b\mathbb{Z}_+$. *Assume that V satisfies (1.1). Then the operator series* $T_+(E + i\delta) := \sum_{l=[E/2b]+1}^{\infty} T_l(E + i\delta)$, $\delta > 0$, *and* $T_+(E) := \sum_{l=[E/2b]+1}^{\infty} T_l(E)$, *where* $[x]$ *denotes the integer part of the real number x, are convergent in* S_2. *Moreover,*

$$\|T_+(E)\|_2^2 \leqslant \frac{C_0 b}{8\pi} \sum_{l=[E/2b]+1}^{\infty} (2bl - E)^{-3/2} \int_{R^3} |V(\mathbf{x})| d\mathbf{x}. \tag{3.16}$$

Finally, $\lim_{\delta \downarrow 0} \|T_+(E + i\delta) - T_+(E)\|_2 = 0$.

Corollary 3.1: Let $r \in (0, b)$. *Then we have*

$$\|\mathrm{Re}\, T_+(E)\|_2^2 = O(1), \quad E \to \infty, \quad E \in \mathcal{O}_r. \tag{3.17}$$

Proof: Estimate (3.17) follows immediately from (3.16) since we have

$$\sum_{l=[E/2b]+1}^{\infty}(2bl-E)^{-3/2}\leqslant\sum_{p=1}^{\infty}(2bp)^{-3/2}+r^{-3/2}.$$

For sufficiently large $E\in\mathcal{O}_r$ with $r\in(0,b)$, set $T_-(E):=\Sigma_{l=0}^{[E/2b]}T_l(E)$. Propositions (3.2) and (3.3) imply the following.

Corollary 3.2: For $E\in\mathcal{O}_r$ *with* $r\in(0,b)$ *the operator-norm limit* (3.9) *exists, and* $T(E)=T_-(E)+T_+(E)$. *Moreover,* $\mathrm{Re}\,T(E)=\mathrm{Re}\,T_-(E)+T_+(E)$, *and* $\mathrm{Im}\,T(E)=\mathrm{Im}\,T_-(E)\in S_1$.

For $n=0,1$ and $E\in\mathcal{O}_r$, $r\in(0,b)$, set $\varphi_n(E):=\Sigma_{q=0}^{[E/2b]}(E-2bq)^{-1+n/2}$.

Lemma 3.5: Let $r>0$. *Then the asymptotic relations*

$$\varphi_0(E)=O(\ln E),\tag{3.18}$$

$$\varphi_1(E)=E^{1/2}\frac{1}{b}(1+o(1)),\tag{3.19}$$

hold as $E\to\infty$, $E\in\mathcal{O}_r$.

Proof: Evidently, for $E>0$ large enough,

$$\varphi_n(E)=E^{-1+n/2}\sum_{q=0}^{[E/2b]-1}\left(1-\frac{2bq}{E}\right)^{-1+n/2}+(E-2b[E/2b])^{-1+n/2},\quad n=0,1.\tag{3.20}$$

Since the functions $(0,E/2b)\ni x\mapsto(1-2bx/E)^{-1+n/2}$, $n=0,1$, are increasing, and $E\in\mathcal{O}_r$, we have

$$\begin{aligned}\sum_{q=0}^{[E/2b]-1}\left(1-\frac{2bq}{E}\right)^{-1+n/2}&\leqslant\int_0^{[E/2b]}\left(1-\frac{2bx}{E}\right)^{-1+n/2}dx\leqslant\int_0^{(E-r)/(2b)}\left(1-\frac{2bx}{E}\right)^{-1+n/2}dx\\&=\frac{E}{2b}\int_0^{1-r/E}(1-t)^{-1+n/2}dt,\quad n=0,1.\end{aligned}\tag{3.21}$$

Further,

$$\int_0^{1-r/E}(1-t)^{-1+n/2}dt=\begin{cases}\ln(E/r) & \text{if}\quad n=0,\\ 2(1-(r/E)^{1/2}) & \text{if}\quad n=1.\end{cases}\tag{3.22}$$

Finally, we estimate the second term on the r.h.s. of (3.20):

$$(E-2b[E/2b])^{-1+n/2}\leqslant r^{-1+n/2},\quad n=0,1.\tag{3.23}$$

Putting together (3.20)–(3.23), we obtain (3.18), as well as $\limsup_{E\to\infty,E\in\mathcal{O}_r}E^{-1/2}\varphi_1(E)\leqslant 1/b$. In order to prove (3.19), it remains to show that $\liminf_{E\to\infty,E\in\mathcal{O}_r}E^{-1/2}\varphi_1(E)\geqslant 1/b$, which follows immediately from

$$\begin{aligned}\varphi_1(E)&\geqslant E^{-1/2}\int_{-1}^{[E/2b]}\left(1-\frac{2bx}{E}\right)^{-1/2}dx\geqslant E^{-1/2}\int_0^{E/2b-1}\left(1-\frac{2bx}{E}\right)^{-1/2}dx=\frac{E^{1/2}}{2b}\int_0^{1-2b/E}(1-t)^{-1/2}dt\\&=\frac{E^{1/2}}{b}\left(1-\left(\frac{2b}{E}\right)^{1/2}\right).\end{aligned}$$

Corollary 3.3: Let $r\in(0,b)$. *Then the asymptotic estimate*

$$\|T_-(E)\|_2^2=O(\ln E)\tag{3.24}$$

holds as $E\to\infty$, $E\in\mathcal{O}_r$.

Proof: We have

$$\begin{aligned}\|T_-(E)\|_2^2 &= \left\| |V|^{1/2} \sum_{q=0}^{[E/2b]} (p_q \otimes R(E-2bq))|V|^{1/2} \right\|_2^2 \\ &\leqslant C_0^2 \left\| \sum_{q=0}^{[E/2b]} (p_q \langle X_\perp\rangle^{-m_\perp/2}) \otimes (\langle x_3\rangle^{-m_3/2} R(E-2bq)\langle x_3\rangle^{-m_3/2}) \right\|_2^2 \\ &= C_0^2 \sum_{q=0}^{[E/2b]} \|p_q\langle X_\perp\rangle^{-m_\perp/2}\|_2^2 \|\langle x_3\rangle^{-m_3/2} R(E-2bq)\langle x_3\rangle^{-m_3/2}\|_2^2 \\ &= C_0^2 \frac{b}{8\pi} \int_{\mathbb{R}^2} \langle X_\perp\rangle^{-m_\perp} dX_\perp \left(\int_{\mathbb{R}} \langle x_3\rangle^{-m_3} dx_3 \right)^2 \varphi_0(E) \end{aligned} \tag{3.25}$$

[see (3.13) for the definition of the integral kernel of p_q, (3.14) for its value on the diagonal, and (3.15) for the definition of the integral kernel of $R(E-2bq)$]. Bearing in mind (3.18), we find that (3.25) implies (3.24). □

Proposition 3.4: Let $r \in (0,b)$. Then we have

$$\|\mathrm{Im}\, T(E)\| = O(1), \quad E \to \infty, \quad E \in \mathcal{O}_r. \tag{3.26}$$

Proof: Estimate (3.26) follows immediately from Ref. 5, Lemma 4.2, according to which we have $\|T(E)\| \leqslant r^{-1/2}(C_0/2)\int_{\mathbb{R}}\langle x_3\rangle^{-m_3} dx_3$. □

IV. PROOF OF THE MAIN RESULT

Fix an arbitrary $\varepsilon \in (0,1)$. Applying (3.5)–(3.7), and arguing as in the proof of Ref. 5, Lemma 5.1, we easily get

$$\begin{aligned} &\frac{1}{\pi}\mathrm{Tr}\arctan((\mathrm{Im}\, T(E))^{1/2}(J+\varepsilon)^{-1}(\mathrm{Im}\, T(E))^{1/2}) - n_+(\varepsilon;\mathrm{Re}\, T(E)) \\ &\quad \leqslant \int_{\mathbb{R}} \mathrm{ind}(J + \mathrm{Re}\ T(E) + t\ \mathrm{Im}\ T(E); J) d\mu(t) \\ &\quad \leqslant \frac{1}{\pi}\mathrm{Tr}\arctan((\mathrm{Im}\, T(E))^{1/2}(J-\varepsilon)^{-1}(\mathrm{Im}\, T(E))^{1/2}) + n_-(\varepsilon;\mathrm{Re}\, T(E)). \end{aligned} \tag{4.1}$$

Set

$$G_s = G_s(E) := (\mathrm{Im}\, T(E))^{1/2}(J+s)^{-1}(\mathrm{Im}\, T(E))^{1/2}, \quad s \in (-1,1).$$

Evidently, for each $s \in (-1,1)$ we have

$$\begin{aligned} |\mathrm{Tr}\arctan G_s(E) - \mathrm{Tr}\, G_s(E)| &\leqslant \tfrac{1}{3}\|G_s(E)\|_3^3 \leqslant \tfrac{1}{3}\|G_s(E)\|_2^2\|G_s(E)\| \leqslant \tfrac{1}{3}\|(J+s)^{-1}\|^3\|\mathrm{Im}\, T(E)\|_2^2\|\mathrm{Im}\, T(E)\| \\ &\leqslant \tfrac{1}{3}(1-|s|)^{-3}\|\mathrm{Im}\, T(E)\|_2^2\|\mathrm{Im}\, T(E)\|. \end{aligned} \tag{4.2}$$

The operator $(J+s)^{-1}\,\mathrm{Im}T(E)$ admits an explicit kernel

$$\begin{aligned} &\frac{1}{2}\sum_{q=0}^{[E/2b]} (E-2bq)^{-1/2}\mathcal{P}_q(X_\perp, X'_\perp)\cos(\sqrt{E-2bq}(x_3-x'_3)) \\ &\quad \times (\mathrm{sign}(V(X_\perp,x_3)) + s)^{-1}|V(X_\perp,x_3)|^{1/2}|V(X'_\perp,x'_3)|^{1/2}, \quad (X_\perp,x_3) \in \mathbb{R}^3, \quad (X'_\perp,x'_3) \in \mathbb{R}^3 \end{aligned}$$

[see (3.13) for the definition of $\mathcal{P}_q$]. Therefore,

$$\mathrm{Tr}G_s(E) = \mathrm{Tr}((J+s)^{-1}\mathrm{Im}\,T(E)) = \frac{b}{4\pi}\sum_{q=0}^{[E/2b]}(E-2bq)^{-1/2}\int_{\mathbb{R}^3}(\mathrm{sign}(V(\mathbf{x}))+s)^{-1}|V(\mathbf{x})|d\mathbf{x}$$

$$= \frac{b}{4\pi}\varphi_1(E)\int_{\mathbb{R}^3}(\mathrm{sign}(V(\mathbf{x}))+s)^{-1}|V(\mathbf{x})|d\mathbf{x} \tag{4.3}$$

[see (3.14)]. Finally, we estimate the second terms in the first and third lines in (4.1):

$$n_{\pm}(\varepsilon;\mathrm{Re}\,T(E)) \leqslant \varepsilon^{-2}\|\mathrm{Re}\,T(E)\|_2^2 \leqslant 2\varepsilon^{-2}(\|\mathrm{Re}\,T_-(E)\|_2^2 + \|\mathrm{Re}\,T_+(E)\|_2^2), \tag{4.4}$$

using (3.4) with $p=2$. Combining (4.1)–(4.4) with (3.10), making use of (3.19), (3.24), (3.17), and (3.26), and applying our convention to identify $\tilde{\xi}(E;H,H_0)$ with $\xi(E;H,H_0)$ we find that for each $\varepsilon\in(0,1)$ we have

$$\limsup_{E\to\infty,E\in\mathcal{O}_r} E^{-1/2}\xi(E;H,H_0) \leqslant \frac{1}{4\pi^2}\int_{\mathbb{R}^3}(\mathrm{sign}(V(\mathbf{x}))-\varepsilon)^{-1}|V(\mathbf{x})|d\mathbf{x},$$

$$\liminf_{E\to\infty,E\in\mathcal{O}_r} E^{-1/2}\xi(E;H,H_0) \geqslant \frac{1}{4\pi^2}\int_{\mathbb{R}^3}(\mathrm{sign}(V(\mathbf{x}))+\varepsilon)^{-1}|V(x)|d\mathbf{x}.$$

Letting $\varepsilon\downarrow 0$, we obtain (2.1).

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Global periodic attractor for strongly damped wave equations with time-periodic driving force

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In this paper, we consider the existence of a global periodic attractor for a strongly damped nonlinear wave equation with time-periodic driving force under homogeneous Dirichlet boundary condition. It is proved that in certain parameter region, for arbitrary time-periodic driving force, the system has a unique periodic solution attracting any bounded set exponentially. This implies that the system behaves exactly as a one-dimensional system. We mention, in particular, that the obtained result can be used to prove the existence of global periodic attractor of the usual damped and driven wave equations. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In this paper, we study the following strongly damped nonlinear wave equation:

$$\frac{\partial^2 u}{\partial t^2} - \alpha\Delta\frac{\partial u}{\partial t} - \Delta u + h\left(\frac{\partial u}{\partial t}\right) + f(u) = g(x,t), \quad (x,t) \in \Omega \times R_+, \tag{1}$$

with the homogeneous Dirichlet boundary condition,

$$u(x,t)_{x\in\partial\Omega} = 0, \quad t > 0, \tag{2}$$

and the initial value conditions,

$$u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = u_1(x), \quad x \in \Omega, \tag{3}$$

where $u=u(x,t)$ is a real-valued function on $\Omega\times[0,+\infty)$, Ω is an open bounded set of $R^n(n \in N)$ with a smooth boundary $\partial\Omega$, $\alpha>0$, h, $f\in C^1(R,R)$, $u_0(x)\in H_0^1(\Omega)$, $u_1(x)\in L^2(\Omega)$, $D(-\Delta) = H_0^1(\Omega)\cap H^2(\Omega)$, $g(\cdot,t)$ is a continuous T-periodic function in t, that is,

$$g(\cdot,t+T) = g(\cdot,t), \quad t \in R, \tag{4}$$

where T is a positive constant.

Wave equations, describing a great variety of wave phenomena, occur in the extensive applications of mathematical physics. Equation (1) can be regarded as a perturbed equation of continuous Josephson junction $[f(u)=\sin u]$.[1]

Strongly damped nonlinear wave equations have been studied widely in a different context by various methods. A large part of literature is devoted to the study of the asymptotic behavior of solutions (see Refs. 2–6). For the autonomous damped and driven sine-Gordon equation (f and g are independent of t), where $\alpha=0$, $h(u_t)=\gamma u_t$, $f(u)=\beta\sin u$, Zhao and Li proved that in Ref. 8 if

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$$|\beta| < \lambda_1^{1/2} \min\left(\frac{\gamma}{4}, \frac{\lambda_1}{2\gamma}, \sqrt{\frac{\lambda_1}{2}}\right),$$

where λ_1 is the first positive eigenvalue of operator $-\Delta$, when $g(x,t)=g(x)$, the global attractor is exactly an equilibrium point, which suggests that $|\beta|$ decreases as the damping γ grows and $\lim_{\gamma\to\infty}|\beta|=0$. This implies that the system behaves as a linear one as the damping γ tends to infinity. It is difficult to comprehend from physical intuition. For the non autonomous equations, Zhou and Fan[6] considered the existence of kernel sections and obtained an upper bound of its Hausdorff dimension. The existence of global periodic attractor, under a certain parameter region, was derived by Zhu and Zhou in Ref. 7 for the damped sine-Gordon equation with time-periodic force. In this paper, our goal is to find a parameter region under which there exists a continuous periodic solution attracting exponentially any bounded sets for the equation (1), hence, the problem behaves as a one-dimensional system. According to our result, in the particular case considered by Zhao and Li,[8] it reads that the nonlinear term $\beta \sin u$ is not necessary to become zero as $\gamma\to\infty$, which conforms to the physical intuition.

We arrange this paper as follows. First we present the existence and uniqueness of solutions. Then following the idea of Ref. 6, by introducing a new norm in the phase space E which is equivalent to the usual norm in E, we obtain a parameter region under which system (1)–(3) possesses a global periodic attractor. Finally, for the special case $\alpha=0$, we discuss the existence of a global periodic attractor.

II. PRELIMINARIES

It is known that the linear operator $A=-\Delta: D(A)=H_0^1(\Omega)\cap H^2(\Omega)\to L^2(\Omega)$ is self-adjoint positive and linear, and eigenvalues $\{\lambda_i\}_{i\in N}$ of A satisfy

$$0<\lambda_1\leqslant\lambda_2\leqslant\cdots\leqslant\lambda_m\leqslant\cdots, \quad \lambda_m\to+\infty (m\to+\infty).$$

Set $E=H_0^1(\Omega)\times L^2(\Omega)$, and let

$$(u,v)=\int_\Omega uv\ \mathrm{d}x, \quad |u|=(u,u)^{1/2}, \quad \forall\, u,v\in L^2(\Omega),$$

$$((u,v))=\int_\Omega \nabla u\cdot\nabla v\ \mathrm{d}x, \quad \|u\|=((u,v))^{1/2}, \quad \forall\, u,v\in H_0^1(\Omega),$$

and

$$(Y_1,Y_2)_{H_0^1\times L^2}=((u_1,u_2))+(v_1,v_2), \quad |Y|_{H_0^1\times L^2}=(Y,Y)^{1/2}_{H_0^1\times L^2},$$

$$\forall Y_i=(u_i,v_i)^T, \quad Y=(u,v)^T\in H_0^1(\Omega)\times L^2(\Omega), \quad i=1,2,$$

denote the usual inner products and norms in $L^2(\Omega), H_0^1(\Omega)$, and E, respectively.

In what follows, we consider the system (1)–(3) and present the existence and uniqueness of its solutions. It is convenient to reduce system (1)–(3) to an evolution equation of the first order in time. Let $u_t=v$, then (1)–(3) are equivalent to the following initial value problem in the Hilbert space E:

$$\begin{aligned}&\dot{Y}=CY+F(Y,t), \quad x\in\Omega, t>0,\\ &Y(0)=Y_0=(u_0,v_0)^T\in E,\end{aligned} \tag{5}$$

where $Y=(u,v)^T$, $F(Y,t)=(0,-h(v)-f(u)+g(x,t))^T$, and

$$C = \begin{pmatrix} 0 & I \\ -A & -\alpha A \end{pmatrix}. \tag{6}$$

Massatt in Ref. 2 proved that C in (6) is a sectorial operator and generates an analytic semigroup e^{Ct} on E for $t>0$.

Let $f,h \in C^1(R,R)$, we make the following assumptions:

(i) There exists a non-negative constant $c_0 \geqslant 0$ such that

$$f(0)=0, \quad |f(u_1)-f(u_2)| \leqslant c_0|u_1-u_2|, \quad \forall\, u_1,u_2 \in R, \tag{7}$$

where $|\cdot|$ denotes the absolute value of number in R.

(ii) There exist two constants β_1,β_2 such that

$$h(0)=0, \quad -\alpha\lambda_1 < \beta_1 \leqslant h'(s) \leqslant \beta_2 < +\infty, \quad \forall\, s \in R, \tag{8}$$

where λ_1 is the first eigenvalue of the operator A on Ω under the boundary condition (2).

By the assumptions (7) and (8), it is easy to check that the function $F(Y,t):E\to E$ is continuous differentiable and globally Lipschitz continuous with respect to Y. By the classical theory concerning the existence and uniqueness of the solutions of evolution differential equations,[9] we have the following lemma (see Ref. 6 for the proof detail).

Lemma 1: If (7) and (8) hold, then, for any $Y_0 \in E$, there exists a unique continuous function $Y(\cdot)=Y(\cdot,Y_0) \in C(R_+;E)$ such that $Y(0,Y_0)=Y_0$ and $Y(t)$ satisfies the integral equation

$$Y(t,Y_0) = e^{Ct}Y_0 + \int_0^t e^{C(t-s)}F(Y(s),s)\mathrm{d}s.$$

$Y(t)$ is called a (mild) solution of (5), and $Y(t,Y_0)$ is jointly continuous in t and Y_0.

Therefore, for $u_0 \in H_0^1(\Omega)$, $u_1 \in L^2(\Omega)$, there exists unique function $u(t)$ such that

$$(u,u_t) \in C(R_+;H_0^1(\Omega)) \times [C(R_+;L^2(\Omega)) \cap L^2(0,T^*;H_0^1(\Omega))], \quad \forall\, T^*>0, \tag{9}$$

satisfies (1)–(3). From (9), we can define a map

$$S(t):Y_0=(u_0,u_1) \to (u,u_t)=Y(t,Y_0), \quad E\to E, \quad \forall\, t \geqslant 0,$$

where $Y(t,Y_0)$ is the (mild) solution of (5), then $\{S(t),t\geqslant 0\}$ is a continuous process on E. Again since $g(x,t)$ is a T-periodic function with respect to $t \in R$, $\{S(nT)|n \in N\}$ is a discrete semidynamical system in E.

III. MAIN RESULT

In this section, we will study the existence of a global periodic attractor for system (5) in E. For this purpose, we define a new weighted inner product and norm in $E=H_0^1(\Omega)\times L^2(\Omega)$ as

$$(\varphi,\psi)_E = r((u_1,u_2)) + (v_1,v_2), |\varphi|_E = (\varphi,\varphi)_E^{1/2}, \tag{10}$$

for any $\varphi=(u_1,v_1)^T$, $\psi=(u_2,v_2)^T \in E$, where r is chosen as

$$r = \frac{4+(\alpha\lambda_1+\beta_1)\alpha+\beta_2^2/\lambda_1}{4+2(\alpha\lambda_1+\beta_1)\alpha+\beta_2^2/\lambda_1} \in \left(\frac{1}{2},1\right). \tag{11}$$

Obviously, the norm $|\cdot|_E$ in (10) is equivalent to the usual norm $|\cdot|_{H_0^1\times L^2}$ in E.

Let $\varphi=(u,v)^T$, $v=u_t+\varepsilon u$, where ε is chosen as

$$\varepsilon = \frac{\alpha\lambda_1 + \beta_1}{4 + 2(\alpha\lambda_1 + \beta_1)\alpha + \beta_2^2/\lambda_1}, \tag{12}$$

and then the system (1)–(3) can be written as

$$\varphi_t + H(\varphi) = F_1(\varphi,t), \quad \varphi(0) = (u_0, u_1 + \varepsilon u_0)^T, \quad t \geqslant 0, \tag{13}$$

where

$$\begin{aligned} F_1(\varphi,t) &= \begin{pmatrix} 0 \\ -f(u) + g(x,t) \end{pmatrix}, \\ H(\varphi) &= \begin{pmatrix} \varepsilon u - v \\ Au - \varepsilon(\alpha A - \varepsilon)u + (\alpha A - \varepsilon)v \end{pmatrix} + \begin{pmatrix} 0 \\ h(v - \varepsilon u) \end{pmatrix}. \end{aligned} \tag{14}$$

Our main result in this paper is as follows.

Theorem 1: *If (4), (7), and (8) and* $\beta_2 \geqslant |\beta_1| + \min\{1/\alpha, (\alpha\lambda_1 + \beta_1)/2\}$ *hold and* c_0 *in (7) satisfies*

$$0 \leqslant c_0 \leqslant \sqrt{\lambda_1 r \sigma(\sigma + \alpha\lambda_1 + \beta_1)}, \tag{15}$$

where

$$\sigma = \frac{\lambda_1\alpha + \beta_1}{\gamma_1 + \sqrt{\gamma_1\gamma_2}}, \quad \gamma_1 = 4 + (\alpha\lambda_1 + \beta_1)\alpha + \frac{\beta_2^2}{\lambda_1}, \quad \gamma_2 = (\alpha\lambda_1 + \beta_1)\alpha + \frac{\beta_2^2}{\lambda_1}. \tag{16}$$

Then system (5) [*or (1)–(3)*] *has a unique T-periodic solution which attracts any bounded set exponentially.*

Proof: Let $\varphi_1(t), \varphi_2(t)$ be two solutions of (5) with the initial values $\varphi_{01}, \varphi_{02} \in E$ and $\varphi(t) = \varphi_1(t) - \varphi_2(t)$. We obtain from (13) that

$$\frac{\partial \varphi(t)}{\partial t} + H(\varphi_1(t)) - H(\varphi_2(t)) = F_1(\varphi_1(t),t) - F_1(\varphi_2(t),t). \tag{17}$$

Taking the scalar product of two sides of (17) with $\varphi(t) = (u,v)^T$ in E, we find

$$\frac{1}{2}\frac{d}{dt}|\varphi|_E^2 + (H(\varphi_1(t)) - H(\varphi_2(t)), \varphi)_E = (F_1(\varphi_1(t),t) - F_1(\varphi_2(t),t), \varphi)_E. \tag{18}$$

For the second term on the left-hand side of (18), according to (8), $\beta_2 \geqslant |\beta_1| + \min\{1/\alpha, (\alpha\lambda_1 + \beta_1)/2\}$ and $r = 1 - \varepsilon\alpha$, we have

$$\begin{aligned} (H(\varphi_1(t)) - H(\varphi_2(t)), \varphi)_E - \sigma|\varphi|_E^2 - \frac{\alpha\lambda_1 + \beta_1}{2}|v|^2 &\geqslant (\varepsilon - \sigma)r\|u\|^2 + \left(\frac{\alpha\lambda_1 + \beta_1}{2} - \varepsilon - \sigma\right)|v|^2 \\ &\quad - \frac{\varepsilon\beta_2}{\sqrt{\lambda_1 r}} \cdot \sqrt{r}\|u\| \cdot |v|. \end{aligned} \tag{19}$$

By (12) and (16), simple computation shows

$$4(\varepsilon - \sigma)\left(\frac{\alpha\lambda_1 + \beta_1}{2} - \varepsilon - \sigma\right) \geqslant \frac{\varepsilon^2\beta_2^2}{r\lambda_1}.$$

By (19),

$$(H(\varphi_1(t)) - H(\varphi_2(t)), \varphi)_E \geqslant \sigma|\varphi|_E^2 + \frac{\alpha\lambda_1 + \beta_1}{2}|v|^2, \tag{20}$$

where σ is as in (16). From (7), (18), and (20), we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\varphi|_E^2 &\leqslant -2\sigma|\varphi|_E^2 - \alpha\lambda_1|v|^2 - \beta_1|v|^2 + 2|f(u_1) - f(u_2)| \cdot |v| \\ &\leqslant -\sigma|\varphi|_E^2 - \sigma r\|u\|^2 - (\sigma + \alpha\lambda_1 + \beta_1)|v|^2 + \frac{2c_0}{\sqrt{\lambda_1 r}}\sqrt{r}\|u\| \cdot |v| \\ &\leqslant -\sigma|\varphi|_E^2 - \left(2\sqrt{\sigma(\sigma + \alpha\lambda_1 + \beta_1)} - \frac{2c_0}{\sqrt{\lambda_1 r}}\right)\sqrt{r}\|u\| \cdot |v| \leqslant -\sigma|\varphi|_E^2,\end{aligned}$$

which implies

$$|\varphi(t)|_E \leqslant e^{-(\sigma/2)t}|\varphi(0)|_E, \quad \forall\, t \geqslant 0. \tag{21}$$

Now considering T-mapping $S(T): E \to E$, $S(T)\varphi_0 = \varphi(T, \varphi_0)$, where $\varphi(t, \varphi_0)$ is the solution of (5), $\varphi(0, \varphi_0) = \varphi_0$. From (21), $\forall \varphi_1, \varphi_2 \in E$, we obtain

$$|S(T)\varphi_1 - S(T)\varphi_2|_E \leqslant e^{-(\sigma/2)T}|\varphi_1 - \varphi_2|_E.$$

Thus $S(T)$ is a contraction mapping. By Banach's fixed point theorem, there exists a unique fixed point φ^* for $S(T)$ in E such that $S(T)\varphi^* = \varphi^*$. At the same time, since $\{S(nT)|n \in N\}$ is a discrete semidynamical system in E, we can deduce

$$S(nT)\varphi^* = S(T)^n\varphi^*, \quad \forall\, n \in N$$

and

$$\varphi^*(t + T) = S(t)\varphi^*(T) = S(t)\varphi^* = \varphi^*(t),$$

where $\varphi^*(t)$ is the solution passing $\varphi^* \in E$. Thus $\varphi^*(t) = \varphi(t, \varphi^*)$ is a T-periodic solution of system (1)–(3). By (21), $\varphi^*(t)$ attracts any bounded set exponentially. The proof is completed.

Remark: If $g(x,t) = g(x)$ is independent of t, then the T-periodic solution in Theorem 1 is an equilibrium point.

IV. SPECIAL CASE $\alpha = 0$

When $\alpha = 0$, Eq. (1) reduces to the following damped and driven wave equation with time-periodic driving force:

$$\frac{\partial^2 u}{\partial t^2} + h\left(\frac{\partial u}{\partial t}\right) - \Delta u + f(u) = g(x,t), \quad (x,t) \in \Omega \times R_+, \tag{22}$$

endowed with the homogeneous Dirichlet boundary condition (2) and the initial value condition (3), where Ω is an open bounded domain of $R^n (n \in N)$ with a smooth boundary $\partial\Omega$. We assume that the functions $g(\cdot, t)$ and $h, f \in C^1(R, R)$ satisfy (4), (7), and (8). From Theorem 1, we have the following result.

Theorem 2: *Suppose* $0 \leqslant c_0 \leqslant \sqrt{\sigma\lambda_1(\sigma + \beta_1)}$, *where*

$$\sigma = \frac{\beta_1\lambda_1}{\sqrt{\beta_2^2 + 4\lambda_1}(\beta_2 + \sqrt{\beta_2^2 + 4\lambda_1})}.$$

Then system (22) with conditions (2) and (3) possesses a global T-periodic attractor which attracts any bounded set exponentially.

In particular, when $h(u_t)=\gamma u_t$, $f(u)=\beta \sin u$, $\gamma>0$, $\beta>0$, Eq. (22) reduces to the damped and driven sine-Gordon equation modeling the Josephson junction in superconduction,

$$\frac{\partial^2 u}{\partial t^2}+\gamma\frac{\partial u}{\partial t}-\Delta u+\beta \sin u=g(x,t), \quad u(x,t)\in R, \quad x\in R, \tag{23}$$

which was studied by many authors (see Refs. 7, 8, and 10). When $g(x,t)=I(x)+f(x)\sin \omega t$, Zhu and Zhou[7] proved the existence of global periodic solution in a certain parameter region. As a corollary of Theorem 2, we have

Corollary: Assume that $|\beta|\leqslant\sqrt{\sigma\lambda_1(\sigma+\gamma)}$, where $\sigma=\gamma\lambda_1\big/\sqrt{\gamma^2+4\lambda_1}(\gamma+\sqrt{\gamma^2+4\lambda_1})$, *then system (23) with conditions (2) and (3) has a global T-periodic attractor which attracts any bounded set exponentially*.

Remark: The main point of the present paper is to show the existence of a global periodic attractor of the system (1)–(3). Our method here is different from that in Ref. 7. Zhao and Li proved that in Ref. 8 if $|\beta|<\lambda_1^{1/2}\min(\gamma/4,\lambda_1/2\gamma,\sqrt{\lambda_1}/2)$, *when* $g(x,t)=g(x)$, *the global attractor for system (23) with conditions (2) and (3) is exactly an equilibrium point, which suggests that* $|\beta|$ *decreases as the damping* γ *grows and* $\lim_{\gamma\to\infty}|\beta|=0$. *It implies that the system behaves as a linear one as the damping* γ *tends to infinity. However, from our result, if* $|\beta|\leqslant\sqrt{\sigma\lambda_1(\sigma+\gamma)}$, *then system (23), (2), and (3) possesses a T-periodic solution for* $t\in R$, *which attracts any bounded set exponentially. In particular, we point out that* $\sqrt{\sigma\lambda_1(\sigma+\gamma)}$ *increases as the damping* γ *grows, and* $\lim_{\gamma\to+\infty}\sqrt{\sigma\lambda_1(\sigma+\gamma)}=\lambda_1/\sqrt{2}$, *thus the nonlinear term* $\beta \sin u$ *is not necessary to become zero as* $\gamma\to\infty$, *which conforms to the physical intuition*.

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Energy momentum, wave velocities and characteristic shocks in Euler's variational equations with application to the Born–Infeld theory

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We consider the Euler's variational equations deriving from a general Lagrangian $L(\partial_\alpha q^r, q^s)$. Under the assumption of convexity of energy, we write down some inequalities for the energy-momentum tensor including Hawking–Ellis energy conditions. We show that there exists the same number of positive and negative wave velocities and no velocity can change sign. Finally, we study the structure of the characteristic shocks with particular attention to the generalized Born–Infeld Lagrangian describing the electron with spin. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1780611]

I. INTRODUCTION

It is well known that a system of balance laws with a convex extension can be symmetrized in the sense of Friedrichs.[1] In Physics this additional equation corresponds to an entropy or energy law. The convexity requirement is satisfied in many physical situations and, for instance, corresponds in thermomechanics to restrictions on the constitutive functions and on the field such that stability holds: the pressure of a fluid increases with the material density, the specific heat at constant volume must be positive together with the density and the temperature. This entropy principle was used in the construction of the Extended Thermodynamics for non-equilibrium fluids.[2,3] As we shall see in nonlinear electrodynamics it imposes an upper bound for the electric field.

In a privileged set of field variables (main field) the original system is symmetric hyperbolic and is generated by a potential four-vector[4–6] (see also Ref. 7) ensuring, in particular, the local well-posedness of the Cauchy problem.[8,9]

More specifically in various physical situations there exists a variational principle. Instead of a four-vector, a *single* function, the Lagrangian, suffices to determine the corresponding Euler's system which admits *four* (instead of one) supplementary laws representing the conservation of the energy-momentum tensor.[10]

Nonlinear electrodynamics, regarded with a new interest and connected to string theory[11,12] was introduced by Born and Infeld in their 1934 celebrated paper[13] with the Lagrangian

$$L = \sqrt{-R^2 + k(2Q + k)}, \tag{1}$$

where Q and R are the electromagnetic invariants and the constant $\sqrt{k}$ (absolute field) is an upper limit for the electric field thus eliminating the Maxwell singularity at the point charge through the *BIon* (to quote Gibbons[14]) solution

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$$E = \frac{\sqrt{k}}{\sqrt{1 + (r/r_0)^4}}, \tag{2}$$

where r_0 is the radius of the electron. (See also Ref. 15.)

More generally considering a Lagrangian $L(Q,R)$ depending on Q and R, several interesting properties of nonlinear wave propagation appear. In particular by requiring that the two families of discontinuity waves never evolve into shocks (exceptionality conditions) the Lagrangian assumes the form stated in Sec. VII (exceptional Lagrangian) which includes spin and reduces to (1) in the case of a null Planck constant.[16] However, if the shock does exist at some initial time it propagates on characteristic surfaces.[7,17]

From the convexity of the energy density of a general Lagrangian some results concerning the energy-momentum tensor and the characteristic velocities are derived. In particular in Sec. III we show that the assumption $T^{0i}=T^{i0}$ implies the complete symmetry of the energy momentum tensor $T^{\alpha\beta}$ and we obtain several inequalities for its components including Hawking–Ellis energy condition.[18–20,11,21] In Sec. IV we can verify that there always exists the same number of positive and negative wave velocities and no velocity can change sign. As a consequence it is immediately seen, for instance, that the equations of fluid dynamics cannot derive from a variational principle for this very last reason.

In Sec. V we give the structure of the characteristic shocks and in particular we discuss their boundedness. Then we apply the results to the Born–Infeld model and its generalization. We verify that the characteristic shocks of the proper Born–Infeld model are unbounded while for the generalized Lagrangian several possibilities can occur.

II. EULER'S VARIATIONAL EQUATIONS

Let $q^r(x^\alpha)$, $r=1,\ldots,M$ be functions of the space-time coordinates $x^\alpha(\alpha=0,i;\ i=1,2,3;\ x^0=t)$, $q^r_\alpha \doteqdot \partial_\alpha q^r$ be the derivative of q^r with respect to x^α and $L(q^r_\alpha,q^r)$ a general Lagrangian function. Let us agree that summation occurs only for repeated indices in up and down positions. Then a classical solution of Euler's equations

$$\partial_\alpha\left(\frac{\partial L}{\partial q^s_\alpha}\right) = \frac{\partial L}{\partial q^s} \tag{3}$$

also satisfies the four additional conservation laws

$$\partial_\alpha T^\alpha_\beta = 0,$$

where T^α_β is defined by

$$T^\alpha_\beta = q^r_\beta \frac{\partial L}{\partial q^r_\alpha} - L\,\delta^\alpha_\beta. \tag{4}$$

With the field

$$\breve{\mathbf{u}} \equiv \left(\frac{\partial L}{\partial q^s_0}, q^s_i, q^s\right) \tag{5}$$

(the breve denotes the transpose) (3) can be written as a first order partial differential system of $5M$ balance laws,

$$\partial_t \mathbf{u} + \partial_i \mathbf{f}^i(\mathbf{u}) = \mathbf{f}(\mathbf{u}),$$

i.e.,

$$\partial_t\left(\frac{\partial L}{\partial q^s_0}\right) + \partial_i\left(\frac{\partial L}{\partial q^s_i}\right) = \frac{\partial L}{\partial q^s},$$

$$\partial_t q_i^s - \partial_i q_0^s = 0, \quad s = 1, \ldots, M,$$

$$\partial_t q^s = q_0^s. \tag{6}$$

Instead, if we introduce the main field[4,5]

$$\check{\mathbf{u}}' = \frac{\partial T^0{}_0}{\partial \mathbf{u}} \equiv \left(q_0^s, -\frac{\partial L}{\partial q_i^s}, -\frac{\partial L}{\partial q^s} \right),$$

(6) appears as a Friedrichs–Lax–Godunov symmetric hyperbolic system

$$\mathbf{H}'(\mathbf{u}')\partial_t \mathbf{u}' + \mathbf{A}'^i \partial_i \mathbf{u}' = \mathbf{B}'\mathbf{u}', \tag{7}$$

where the constant symmetric matrices $\mathbf{A}'^i$, satisfy a Duffin–Kemmer–Petiau relation

$$\mathbf{A}'^i\mathbf{A}'^k\mathbf{A}'^j + \mathbf{A}'^j\mathbf{A}'^k\mathbf{A}'^i = \delta^{ik}\mathbf{A}'^j + \delta^{jk}\mathbf{A}'^i \tag{8}$$

while $\mathbf{B}'$ is skew-symmetric and the Hessian matrix $\mathbf{H}' \doteq \partial \mathbf{u}/\partial \mathbf{u}'$ is positive definite provided that the energy density T_0^0 is a convex function of the field variables $\mathbf{u}$,[7] which means that

$$\delta\check{\mathbf{u}}' \cdot \delta\mathbf{u} = \delta q_0^s \delta\left(\frac{\partial L}{\partial q_0^s} \right) - \delta q_i^s \delta\left(\frac{\partial L}{\partial q_i^s} \right) - \delta q^s \delta\left(\frac{\partial L}{\partial q^s} \right) > 0. \tag{9}$$

This property (which is supposed to hold in the following) also insures a global one to one correspondence between $\mathbf{u}$ and $\mathbf{u}'$. If, as usual, the Lagrangian does not depend explicitly on q^s the last equation in (6) and the last component of the main field can be dropped and (7) becomes a system of $4M$ conservation laws without second member. It is interesting to observe that this last system is a principal subsystem of the former one following the definitions and the properties stated in Ref. 22. Similarly the Euler–Lagrange equations of analytical mechanics are another principal subsystem of (6).

III. THE SYMMETRIC ENERGY-MOMENTUM TENSOR

In terms of the $\mathbf{u}$ and $\mathbf{u}'$ fields the components of T_β^α take the form[10]

$$T_0^i = \tfrac{1}{2}\check{\mathbf{u}}'\mathbf{A}'^i\mathbf{u}', \quad T_i^0 = -\tfrac{1}{2}\check{\mathbf{u}}\mathbf{A}'^i\mathbf{u}, \quad T_j^i = T^0{}_0\delta_j^i - \check{\mathbf{u}}\mathbf{A}'^j\mathbf{A}'^i\mathbf{u}'.$$

While Physics usually requires T to be a symmetric tensor in general T is not a tensor and is not symmetric. Suppose nevertheless that we raise the lower indices with the Minkowski metric, $\eta^{\alpha\beta} = \mathrm{diag}(1,-1,-1,-1)$,

$$T^{\alpha\beta} = \eta^{\beta\gamma}T_\gamma^\alpha.$$

Then the mere condition $T^{0i} \equiv T^{i0}$ implies that $T^{ij} \equiv T^{ji}$, i.e., complete symmetry.

To see this we differentiate

$$\check{\mathbf{u}}'\mathbf{A}'^i\mathbf{u}' = \check{\mathbf{u}}\mathbf{A}'^i\mathbf{u}$$

with respect to $\mathbf{u}'$ to get

$$\check{\mathbf{u}}'\mathbf{A}'^i = \check{\mathbf{u}}\mathbf{A}'^i\mathbf{H}' \tag{10}$$

so that

$$T^{ij} \equiv T^{ji} = \check{\mathbf{u}}\mathbf{A}'^i\mathbf{H}'\mathbf{A}'^j\mathbf{u} - T^{00}\delta^{ij}. \tag{11}$$

Now for any unit vector $\vec{n}$ since

$$T^{i0} = \tfrac{1}{2}\breve{\mathbf{u}}\mathbf{A}'^{i}\mathbf{H}'\mathbf{u}'$$

and thanks to Schwarz inequality

$$(T^{i0}n_i)^2 \leqslant \tfrac{1}{2}\breve{\mathbf{u}}'\mathbf{H}'\mathbf{u}'\left(\frac{T^{ij}n_in_j + T^{00}}{2}\right),$$

$$(T^{ij})^2 \leqslant (T^{ii} + T^{00})(T^{jj} + T^{00}), \quad i \neq j.$$

From (11),

$$T^{00} + T^{ij}n_in_j \geqslant 0, \quad \vec{n}^2 = 1 \Rightarrow T^{ii} + T^{00} \geqslant 0.$$

Provided that the absolute values of the wave velocities, i.e., the eigenvalues of $\mathbf{A}'_n/\mathbf{H}'$ ($\mathbf{A}'_n \doteq \mathbf{A}'^{i}n_i$, see below), do not exceed 1, the matrices $\mathbf{H}' \pm \mathbf{A}'_n$ are semidefinite positive. Thus

$$-T^{i0}n_i = \tfrac{1}{2}\breve{\mathbf{u}}'(\mathbf{H}' - \mathbf{A}'_n)\mathbf{u}' - \tfrac{1}{2}\breve{\mathbf{u}}'\mathbf{H}'\mathbf{u}' \Rightarrow T^{i0}n_i \leqslant \tfrac{1}{2}\breve{\mathbf{u}}'\mathbf{H}'\mathbf{u}'. \tag{12}$$

With the same subluminal restriction a (weak) energy condition holds true.[18–20,11,21] Let l_α be a null vector ($l_0^2 = \vec{l}^2$)). From the Duffin–Kemmer–Petiau relation (8) we first obtain

$$\mathbf{A}'^{i}\mathbf{A}'_n\mathbf{A}'^{j}l_il_j = l_0l_i\mathbf{A}'^{i}, \quad n_k = l_k/l_0$$

from which follows

$$T^{\alpha\beta}l_\alpha l_\beta = l_il_j\breve{\mathbf{u}}\mathbf{A}'^{i}(\mathbf{H}' + \mathbf{A}'_n)\mathbf{A}'^{j}\mathbf{u} \geqslant 0.$$

Now assume T is a (symmetric) tensor. *Hawking–Ellis "dominant energy condition,"*

$$T^{\mu\nu}t_\mu s_\nu \geqslant 0 \tag{13}$$

for all pairs of future-directed timelike vectors follows with the additional restriction

$$T^{00} \geqslant \tfrac{1}{2}\breve{\mathbf{u}}'\mathbf{H}'\mathbf{u}'.$$

The invariant inequality (13) is verified in the rest frame $s_0 = 1$, $s_i = 0$,

$$T^{00}t_0 + T^{0i}t_i = t_0\{T^{00} - \tfrac{1}{2}\breve{\mathbf{u}}'\mathbf{H}'\mathbf{u}' + \tfrac{1}{2}\breve{\mathbf{u}}'(\mathbf{H}' + \mathbf{A}'^{i}t_i/t_0)\mathbf{u}'\} \geqslant 0,$$

and so in any frame. Alternatively $T^{\lambda\nu}s_\lambda$ is not a spacelike vector

$$T_{\mu\nu}s^\mu T^{\lambda\nu}s_\lambda \geqslant 0$$

for

$$T^{0\mu}T_{0\mu} = (T^{00})^2 - \sum (T^{0i})^2 \geqslant 0$$

by (12).

All these conditions are easily checked for the linear Maxwell equations where $\breve{\mathbf{u}}' = \breve{\mathbf{u}} = (\vec{E}, \vec{B})$, i.e., $\mathbf{H}' = \mathbf{I}$. As an illustration with many interesting features consider the scalar field.[7,23] The Lagrangian depends on the derivatives q_α of a single function $q(x^\alpha)$ and the condition for symmetry reads

$$T^{0i} = T^{i0} \Rightarrow q_0\frac{\partial L}{\partial q_i} + q_i\frac{\partial L}{\partial q_0} = 0$$

that implies

$$q_0\left(dL-\frac{\partial L}{\partial q_0}dq_0\right)+\frac{\partial L}{\partial q_0}d\left(\frac{1}{2}\vec{q}^2\right)=0$$

from which follows

$$L=L(Q),\quad Q=\tfrac{1}{2}(q_0^2-\vec{q}^2)=\tfrac{1}{2}\eta^{\alpha\beta}q_\alpha q_\beta,\quad T_{\alpha\beta}=L'(Q)q_\alpha q_\beta-L\,\eta_{\alpha\beta}.$$

As for convexity (9) gives

$$\delta\breve{\mathbf{u}}'\,\delta\mathbf{u}=(L'+q_0^2L'')\,\delta q_0^2+L'\,\delta\vec{q}^2-L''(\vec{q}\,.\,\delta\vec{q})^2>0,$$

which requires

$$L'>0,\quad L'+q_0^2L''>0,\quad L'-\vec{q}^2L''>0\Rightarrow(QL')'>0.$$

IV. CHARACTERISTIC VELOCITIES

Across a wave front $\varphi(x^\alpha)=0$ the second order derivatives of the functions q^r may suffer discontinuities so that by Hadamard condition $[\partial_\beta q^r_\alpha]=\partial_\alpha\varphi\partial_\beta\varphi\delta^2q^r$ and (3) yields

$$\frac{\partial^2L}{\partial q^r_\alpha\partial q^s_\beta}\partial_\alpha\varphi\partial_\beta\varphi\,\delta^2q^r=0 \tag{14}$$

giving the characteristic equation of the wave front

$$\det\left(\frac{\partial^2L}{\partial q^r_\alpha\partial q^s_\beta}\partial_\alpha\varphi\partial_\beta\varphi\right)=0. \tag{15}$$

If we define the normal (to the wave surface) velocity $\lambda(\mathbf{u},\vec{n})\vec{n}$ by $\lambda=-\partial_t\varphi/|\nabla\varphi|$, $n_i=\partial_i\varphi/|\nabla\varphi|$ and substitute in (14) we have

$$\left\{\lambda^2\frac{\partial^2L}{\partial q^r_0\partial q^s_0}-\lambda\left(\frac{\partial^2L}{\partial q^r_i\partial q^s_0}+\frac{\partial^2L}{\partial q^r_0\partial q^s_i}\right)n_i+\frac{\partial^2L}{\partial q^r_i\partial q^s_j}n_in_j\right\}\delta^2q^r=0. \tag{16}$$

The inequality (9) shows that the first matrix, coefficient of λ^2, is positive definite, and the last $(M\times M)$ matrix is negative definite. *Therefore M wave velocities are positive and M are negative and no one can change sign* [$\lambda=0$ *is not solution of* (16)] (for instance D'Alembert equation has velocities $\pm c$). As a consequence translational waves of the form $\lambda=\vec{\Lambda}(\mathbf{u})\cdot\vec{n}$, i.e., with a ray velocity $\vec{\Lambda}$ independent of $\vec{n}$ cannot be found because λ would change sign when the normal varies. It is important to remark that if such a wave exists the system cannot derive from a variational principle (in the sense of this paper). This occurs, for example, in the classical Euler's fluid dynamics where a ray velocity coincides with the fluid velocity (known as contact discontinuity or entropy wave).

Consider now the interesting case of a second order polynomial solution of (15),

$$G^{\alpha\beta}(\mathbf{u})\partial_\alpha\varphi\partial_\beta\varphi=0$$

with $G^{00}>0$. The convexity of $T^0{}_0$ implies that

$$G^{ij}n_in_j<0 \tag{17}$$

since both roots λ must be real and different from zero for every $\vec{n}$.

V. RIEMANN INVARIANTS. EXCEPTIONAL WAVES AND CHARACTERISTIC SHOCKS

In the reduction (7) the first order derivatives of the field may be discontinuous across the wave front. Making the substitution

$$\partial_t \to -\lambda\delta, \quad \partial_i \to n_i\delta$$

shows that $\delta\mathbf{u}'$ is an eigenvector and the normal velocities λ are eigenvalues of $\mathbf{A}'_n/\mathbf{H}'$. Associated with them a complete set of eigenvectors forms a basis in the field space. However zero eigenvalues (with no physical meaning) appear with a $3M$ multiplicity in the first order reduction; the associated disturbances are canceled by the differential constraints

$$\partial_i q^r_j - \partial_j q^r_i = 0, \quad \partial_i q^r = q^r_i.$$

Taking account of a possible multiplicity m^a of λ^a,

$$\begin{gathered}(\mathbf{A}'_n - \lambda^a\mathbf{H}')\mathbf{d}'_A = 0, \quad \lambda^a \neq 0, \quad A = 1,2,3,\ldots,m^a,\\ \mathbf{A}'_n\mathbf{d}'_\omega = 0, \quad \lambda = 0, \quad \omega = 1,2,3,\ldots,3M.\end{gathered} \tag{18}$$

A function $w^a(\mathbf{u}',\vec{n})$ is a Riemann invariant corresponding to a (possibly multiple) λ^a if its gradient with respect to the field $\mathbf{u}'$ is orthogonal to all corresponding eigenvectors,

$$\delta w^a = 0 \Leftrightarrow \boldsymbol{\nabla}' w^a \mathbf{d}'_A \equiv 0, \quad A = 1,2,3,\ldots,m^a.$$

In particular if this is true for λ^a itself,

$$\delta\lambda^a = 0, \tag{19}$$

the wave is said to be *exceptional* or *linearly degenerated* a concept due to Lax.[24] If all the waves are *exceptional* the field is *completely exceptional*.[17] A number of fields in Physics share this property (including, of course, the linear fields) but also in Mathematics: the Monge–Ampère equation,[25,7] the Cayley–Darboux equation.[26]

A shock is a discontinuity $[\mathbf{u}]\equiv\mathbf{u}_1-\mathbf{u}_0$ in the field itself, $\mathbf{u}_0$ is the field ahead of the shock and $\mathbf{u}_1$ the field behind the shock. It satisfies the Rankine–Hugoniot relations

$$[\mathbf{f}^i]n_i - s[\mathbf{u}] = 0.$$

In general the shock speed s differs from the wave velocities. However when a wave is exceptional a shock may exist that moves with this velocity: it is called a *characteristic shock*. Across such a shock a Riemann invariant ($\delta w=0$) is continuous $[w]=0$ so that $s=\lambda^a(\mathbf{u}_0)=\lambda^a(\mathbf{u}_1)$.

If we define the vector $\mathbf{g}^a$ by

$$\mathbf{g}^a(\mathbf{A}'_n - \lambda^a\mathbf{H}') = -\boldsymbol{\nabla}'\lambda^a, \quad \mathbf{g}^a\mathbf{H}'\mathbf{d}'_A = 0, \ A = 1,2,\ldots,m^a \tag{20}$$

we can write the jump of the main field in the explicit form

$$[\mathbf{u}'] = u^A\mathbf{d}'_A(\mathbf{u}'_0,\vec{n}) + w(u^A,\mathbf{u}'_0,\vec{n})\breve{\mathbf{g}}^a(\mathbf{u}'_0,\vec{n}),$$

where the u^A's are m^a parameters corresponding to the multiplicity of λ^a and w is a nonlinear function of the u^A. More precisely for Euler's equations

$$\alpha_0 w^2 - 2w + |u|^2 = 0,$$

where $|u|^2=\Sigma(u^A)^2$ if the eigenvectors are normalized with $\mathbf{H}'$ and α_0 is the value of

$$\alpha = \mathbf{g}^a\mathbf{A}'_n\breve{\mathbf{g}}^a/\lambda^a \tag{21}$$

for $\mathbf{u}'=\mathbf{u}'_0$. Here the jumps of $\mathbf{u}$ and $\mathbf{u}'$ are linearly related. From (7) follows

$$[\mathbf{u}] = \mathbf{A}'_n[\mathbf{u}']/\lambda^a_0 = u^A\mathbf{H}'(\mathbf{u}'_0)\mathbf{d}'_A(\mathbf{u}'_0,\vec{n}) + w\mathbf{A}'_n\breve{\mathbf{g}}^a(\mathbf{u}'_0,\vec{n})/\lambda^a_0$$

and the product of the nonlinear parts (in u^A) of $[\mathbf{u}]$ and $[\mathbf{u}']$ is just $\alpha_0 w^2$. The jump is bounded if $\alpha_0>0$.

If there are only two velocities $\lambda^+>0$, $\lambda^-<0$ of multiplicity M and therefore two shocks each function of M parameters $\mathbf{g}$ can be expanded on the basis of the eigenvectors by (20)

$$\check{\mathbf{g}}^+ = \mathbf{d}'^- + \mathbf{d}'^0,$$

where $\mathbf{d}'^-$, $\mathbf{d}'^0$ are eigenvectors for the eigenvalues λ^- and 0, respectively. As a result (21)

$$\alpha^+ = \mathbf{g}^+ \mathbf{A}'_n \check{\mathbf{g}}^+ / \lambda^+ = (\lambda^-/\lambda^+) \check{\mathbf{d}}'^- \mathbf{H}' \mathbf{d}'^- < 0.$$

The aim of Sec. VII is to evaluate the explicit expression of the characteristic shock and in particular to find the sign of α in nonlinear electrodynamics.

VI. NONLINEAR ELECTRODYNAMICS. BORN–INFELD LAGRANGIAN

After the scalar field we consider the (four-dimensional) vector field where

$$q^r \to \phi_\beta, \quad q^r_\alpha \to \phi_{\beta,\alpha}, \quad L = L(\phi_{\beta,\alpha}).$$

The field equations thus obtained

$$\partial_\alpha L^{\alpha\beta} = 0, \quad L^{\alpha\beta} = \partial L / \partial \phi_{\beta,\alpha}$$

have no tensorial character unless L only depends on the curl

$$F_{\alpha\beta} \doteqdot \phi_{\beta,\alpha} - \phi_{\alpha,\beta}$$

through its invariants

$$Q = \tfrac{1}{4} F_{\alpha\beta} F^{\alpha\beta}, \quad R = \tfrac{1}{4} F_{\alpha\beta} F^{*\alpha\beta},$$

where $F_{\alpha\beta} = \partial_\alpha \phi_\beta - \partial_\beta \phi_\alpha$ is the electromagnetic tensor and $F^{*\alpha\beta} = \eta^{\mu\nu\alpha\beta} F_{\mu\nu}/2$ its dual. This is the starting point of nonlinear electrodynamics a natural generalization of Maxwell theory [where $L(Q,R)$ is a linear function of Q and R]. Because of the electromagnetic tensor skew symmetry the field equations

$$\partial_\alpha L^{\alpha\beta} \equiv \partial_\alpha (L_Q F^{\alpha\beta} + L_R F^{*\alpha\beta}) = 0, \quad \partial_\alpha F^{*\alpha\beta} = 0$$

corresponding to $\beta = 0$ do not contain the time derivative and are called *involutive constraints* in the sense that they are true at any instant if they are satisfied at some time. It is also well known that the divergence free quantity

$$\phi_{\beta,\gamma} L^{\alpha\gamma}$$

is added to transform $-T^\alpha_\beta$ as defined by (4) into the conserved symmetric tensor

$$T^\alpha_\beta = L \delta^\alpha_\beta - L^{\alpha\gamma} F_{\beta\gamma}.$$

The two families of wave surfaces associated with the field equations are given by[11,16]

$$G^{\alpha\beta} \partial_\alpha \varphi \partial_\beta \varphi = 0, \quad G^{\alpha\beta} = \tau^{\alpha\beta} + (\zeta + Q) g^{\alpha\beta},$$

where $\tau^{\alpha\beta} = Q g^{\alpha\beta} - F^{\alpha\rho} F^\beta{}_\rho$ is the usual Maxwell tensor and $\zeta(Q,R)$ takes on two positive values $\zeta_{(1)}, \zeta_{(2)}$.

From (17) one sees that in terms of the electromagnetic field vectors

$$G^{00} = \zeta + B^2 > 0, \quad G^{ij} n_i n_j = E^2 - \zeta - E_n^2 - B_n^2 < 0,$$

which means that

$$E^2 < \min(\zeta_{(1)}, \zeta_{(2)}) \tag{22}$$

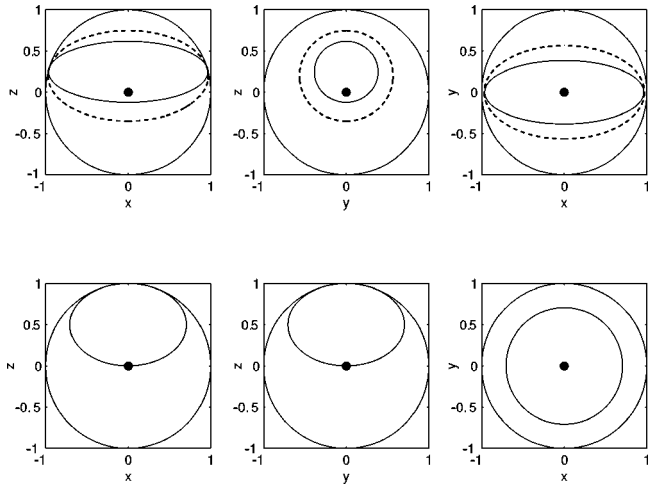

FIG. 1. Sections of the wave surface by the coordinate planes. The ellipsoids corresponding to different values $\zeta_{(1)}$, $\zeta_{(2)}$ of the absolute field are drifted along the z axis, are tangent to each other and to the light sphere in two points (upper left). Below, the limit case ($E^2=\zeta$, $Q=R=0$) of a drift velocity equals to $1/2$. See also Gibbons and Herdeiro (Ref. 11).

is a necessary condition (which turns out to be sufficient) for the *convexity of energy*.[27] The wave front issuing from the origin is no longer a sphere as in Maxwell theory but an ellipsoid drifted along its smallest axis in the direction of the Poynting vector.[16,28] This limitation of the electric field also expresses the fact that the origin stays inside the ellipsoid. Further it ensures the subluminal character of the wave and shock velocities. See Fig. 1 which also shows the limiting case (independent of the nonlinear Lagrangian) corresponding to the ellipsoid

$$x^2 + y^2 + 2(z - \tfrac{1}{2})^2 = \tfrac{1}{2}.$$

Only in the case of the Born–Infeld Lagrangian[13] do both values of ζ coincide with a positive constant k called the *absolute field*, which by (22) is an upper limit to the electric field as in (2),

$$E^2 < k.$$

Thus the Born–Infeld Lagrangian appears as the fundamental one. We consider it as the approximation of a null Planck constant as we shall see in the next section. The wave velocities being double are *exceptional* and both α's are *negative* according to the preceding section.

VII. EXCEPTIONAL LAGRANGIAN WITH SPIN

Here the covariant formulation of (19) that both wave fronts must satisfy is simply[16]

$$\partial_\alpha\varphi\partial_\beta\varphi\delta G^{\alpha\beta} = 0 \Leftrightarrow \delta\zeta = 0,$$

which is obviously true in the case of Born–Infeld since both ζ's are equal to the same constant k. All the Lagrangians yielding field equations that are *completely exceptional* have been determined. The most general one (nonconstant ζ's) has the form

$$L = F(\zeta)f + RG(\zeta) + H(\zeta), \quad f = \sqrt{-R^2 + \zeta(2Q + \zeta)}$$

with $\zeta(Q,R)$ implicitly determined by

$$\partial L/\partial\zeta = O \Rightarrow F' f^2 + (RG' + H')f + (Q + \zeta)F = 0. \tag{23}$$

This function which turns out to be a direct generalization of the Born–Infeld Lagrangian (although it is obtained in a completely different way) must be independent on the choice of $\zeta_{(1)}$ or

$\zeta_{(2)}$ to replace ζ. This condition allows for the determination of the three functions F, G, H. With (say) $\zeta_{(1)}=\zeta$ they read[16]

$$F^2=\frac{1}{s(1+\gamma^2)\zeta^2}\{\gamma^2(k^2-h^2)+2K\gamma\zeta-\zeta^2\}, \tag{24}$$

$$G\zeta=-\gamma H, \quad H^2=\frac{1}{s(1+\gamma^2)}\{h^2-(\zeta-k)^2\}, \tag{25}$$

where

$$2K=k\left(\frac{s+1}{\gamma}+\gamma(s-1)\right).$$

Four constants appear: h may be proportional to the Planck constant since $\zeta\to k$ when $h\to 0$ as can be seen from the expression of H thus giving the Born–Infeld field equations; γ is set equal to $\tan(\theta/2)$ and in the study of the electron field s appears to be equal to $1/2$ and may be associated with the spin.[29] Having solved these equations for $\zeta_{(1)}=\zeta(Q,R;k,h,s,\theta)$ the other value $\zeta_{(2)}$ (and the functions $F_{(2)}$, $G_{(2)}$, $H_{(2)}$ of this variable) immediately follow by the simple change of constants $s\to -s$, $\theta\to\theta+\pi$. For instance $\zeta_{(2)}=\zeta(Q,R;k,h,-s,\theta+\pi)$, $G_{(2)}\zeta_{(2)}=H_{(2)}/\gamma$.

VIII. JUMP OF THE ELECTROMAGNETIC TENSOR

Now let us study the characteristic shocks. Several quantities (Riemann invariants) are continuous across the shock and have already been determined: the scalar ζ and a set of four vectors

$$V^\alpha_{(\gamma)}{:}u^\alpha,\ \frac{e^\alpha}{\sqrt{\zeta}},\ \frac{(Re^\alpha+\zeta b^\alpha)}{f\sqrt{\zeta}},\ \frac{S^\alpha}{f},\ V_{(\mu)\alpha}V^\alpha_{(\nu)}=\eta_{\mu\nu}$$

containing the electric, magnetic fields, and the Poynting vector

$$e_\alpha=F_{\rho\alpha}u^\rho, \quad b_\alpha=F^*_{\rho\alpha}u^\rho, \quad S^\alpha=\eta^{\alpha\beta\gamma\delta}e_\beta b_\gamma u_\delta$$

in the frame of the ray velocity $u^\alpha\propto\{\tau^{\alpha\beta}+(\zeta+Q)g^{\alpha\beta}\}\partial_\beta\varphi$.[16] In terms of these vectors we can write

$$F_{\alpha\beta}=\sqrt{\zeta}a_{\alpha\beta}-\frac{fb^*_{\alpha\beta}}{\sqrt{\zeta}}+\frac{Ra^*_{\alpha\beta}}{\sqrt{\zeta}}, \quad F^*_{\alpha\beta}=\sqrt{\zeta}a^*_{\alpha\beta}+\frac{fb_{\alpha\beta}}{\sqrt{\zeta}}-\frac{Ra_{\alpha\beta}}{\sqrt{\zeta}},$$

where

$$a^{\alpha\beta}=V^\alpha_{(0)}V^\beta_{(1)}-V^\beta_{(0)}V^\alpha_{(1)}, \quad b^{\alpha\beta}=V^\alpha_{(0)}V^\beta_{(2)}-V^\beta_{(0)}V^\alpha_{(2)},$$

$$a^{*\alpha\beta}=V^\alpha_{(2)}V^\beta_{(3)}-V^\beta_{(2)}V^\alpha_{(3)}, \quad b^{*\alpha\beta}=V^\alpha_{(3)}V^\beta_{(1)}-V^\beta_{(3)}V^\alpha_{(1)},$$

$a^{**}_{\alpha\beta}=-a_{\alpha\beta}$, etc.

The jump follows easily

$$\sqrt{\zeta}[F_{\alpha\beta}]=[R]a^*_{\alpha\beta}-[f]b^*_{\alpha\beta}. \tag{26}$$

It can be observed that a jump of the electromagnetic field is generated by a first order discontinuity of the potential vector so that

$$[F_{\alpha\beta}]=\Phi_\beta\partial_\alpha\varphi-\Phi_\alpha\partial_\beta\varphi,$$

which is just the structure of the preceding expression since $\partial_\alpha\varphi\propto S_\alpha\propto V_{(3)\alpha}$.[16]

Since each shock velocity is single the jump must depend on a single parameter. To find the link between $[R]$ and $[f]$ we eliminate $Q+\zeta$ between

$$2\zeta(Q+\zeta) = f^2 + R^2 + \zeta^2$$

and (23) obtaining

$$\left(\frac{F\zeta}{f} + H'\right)^2 + \left(\frac{FR}{f} + G'\zeta\right)^2 = \rho^2(\zeta)$$

with

$$\rho^2(\zeta) = \zeta^2 G'^2 + H'^2 - F(F + 2\zeta F').$$

From (24) and (25) we get

$$\zeta(G^2 + F^2) = -\frac{\zeta}{s} + k\frac{1+s}{s}$$

and substituting

$$(\zeta F^2)' = -\frac{1}{s} - (\zeta G^2)'$$

in the preceding equation we obtain

$$\rho^2 = \frac{1}{s} + (\zeta G)'^2 + H'^2 = \frac{1}{s} + (1+\gamma^2)H'^2 = \frac{h^2}{s^2(1+\gamma^2)H^2}.$$

We introduce the shock parameter ω through

$$\frac{F\zeta}{f} + H' = \rho \sin\omega, \quad \frac{FR}{f} + G'\zeta = \rho\cos\omega.$$

But ζ is continuous across the shock $(\zeta_1 = \zeta_0)$ and therefore the values of f and R behind the shock front

$$f_1 = \frac{F_0\zeta_0}{\rho_0 \sin\omega - H_0'}, \quad R_1 = \zeta_0\frac{\rho_0\cos\omega - G_0'\zeta_0}{\rho_0\sin\omega - H_0'},$$

determine by (26) the jump $[F_{\alpha\beta}]$ of the electromagnetic field which is certainly bounded if $|H_0'/\rho_0| > 1$. To each value of ζ correspond two shocks with different ray velocities. From (25) we have

$$\left(\frac{H_{(1)}'}{\rho_{(1)}}\right)^2 = \frac{(\zeta_{(1)} - k)^2}{h^2(1+\gamma^2)} < 1$$

for $\zeta = \zeta_{(1)}$ which shows that the jump of the field can reach large values. For the other family of shocks, i.e., for $\zeta_{(2)}$ the different functions F, G, H are obtained with the mentioned substitution $s \to -s$, $\gamma \to -1/\gamma$ which gives

$$\left(\frac{H_{(2)}'}{\rho_{(2)}}\right)^2 = \frac{(\zeta_{(2)} - k)^2\gamma^2}{h^2(1+\gamma^2)},$$

a quantity that may or may not be smaller than 1. In fact for the spherically symmetric solution[29]

$$\zeta_{(2)} = k + h\frac{\phi + s}{\sqrt{s^2 + \phi^2 + 2s\phi\cos\theta}}, \qquad \phi = \frac{r^4}{r_0^4 + r^4},$$

$$\left|\frac{H'_{(2)}}{\rho_{(2)}}\right| = \frac{\sin\dfrac{\theta}{2}}{\sqrt{1 - \dfrac{4s\phi}{(\phi + s)^2}\sin^2\dfrac{\theta}{2}}},$$

where $s = 1/2$. When r varies from 0 to infinity this quantity has a minimum, $\sin(\theta/2)$, for $r = 0$ and a maximum, $\tan(\theta/2)$, for $r = r_o$. Hence it is less than 1 for all r only if $\theta < \pi/2$.

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On the initial boundary value problem for a shallow water equation

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In this paper, we obtain the existence and uniqueness of the local strong solutions to the initial boundary problem for a one-dimensional shallow-water equation (Camassa–Holm equation) on the half-space $\{x>0\}$ with initial data $u_o \in H^2(R^+)\cap H_0^1(R^+)$. The solution is obtained as a limit of the solutions for a class of approximation problems. We also establish the global result of the corresponding solution, provided that the initial data u_0 satisfies certain positivity condition. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1765216]

I. INTRODUCTION

In this paper we consider the existence and uniqueness of strong solutions to the initial boundary value problem for the following one-dimensional shallow-water equation on the half-space $\{x>0\}$:

$$\begin{cases} \partial_t u + u\partial_x u + \partial_x p = 0, & t>0, x>0, \\ p(t,x) = \displaystyle\int_0^\infty h(x,y)\left(u^2 + \frac{1}{2}(\partial_x u)^2\right)(t,y)\,dy, & t>0, x>0, \end{cases} \tag{1.1}$$

where

$$h(x,y) = \begin{cases} e^{-x}shy, & y\leqslant x, \\ e^{-y}shx, & y>x, \end{cases}$$

with the initial data

$$u(0,x) = u_0(x), \quad x>0, \tag{1.2}$$

and boundary value

$$u(t,0) = 0, \quad t>0, \tag{1.3}$$

which is formally equivalent to the initial boundary value problem for the Camassa–Holm equation[1] (simply denoted by C–H equation),

$$\partial_t u - \partial_t \partial_{xx} u + 3u\partial_x u = 2\partial_x u \partial_{xx} u + u\partial_{xxx} u. \tag{1.1'}$$

Here u denotes the fluid velocity at time t in the x direction (or, equivalently, the height of the water's free surface above a flat bottom).

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Equation (1.1) is derived physically by Camassa and Holm who used an asymptotic expansion directly in the Hamiltonian for Euler's equations in the shallow-water regime.[2] Equation (1.1) also proved to be formally integrable by Fuchssteiner and Fokas as a bi-Hamiltonian generalization of KDV.[3]

Many special features make (1.1) an important equation in the shallow-water regime. Besides the bi-Hamiltonian structure and the formal integrability, Camassa and Holm discovered that the solitary waves have a discontinuity in the first derivative at their peak and that soliton interactions occur for (1.1). In fact, physical water waves often break down, which cannot be predicted by the solutions for the KDV equation.[4] So Eq. (1.1) is the first model that is completely integrable and yet exhibits the remarkable finite-time breakdown phenomena as commented upon by Constantin and Escher.[5] Equation (1.1) possesses an infinite number of conservation laws due to its bi-Hamiltonian structure, but, unlike KDV, the global existence of regular solutions is guaranteed for only a special class of initial data, and the $H^k(R)$ norm is preserved for smooth solutions to (1.1) only for $k=1$. Indeed, it has been observed that finite-time breakdown of smooth solutions always occurs for a large class of initial data.[2,5,10]

Recently, after Camassa and Holm established that Eq. (1.1) also has physical meaning, numerous papers were devoted to its study. For example, Hongjun Gao *et al.* proved the local existence and property of blow-up to the initial boundary value problem of (1.1′) with initial data $u_0 \in \mathcal{B}=\{u \in H^4(0,1): u(0)=u_{xx}(0)=u(1)=u_{xx}(1)=0\}$;[17] Constantin *et al.* made sequential researches on the C–H equation, such as the well posedness, spectral problem, and inverse spectral problem, etc. (Refs. 5–9 and 11–14); Blanco established the well posedness to the Cauchy problem associated with (1.1′) with the initial data $u_0 \in H^s(R), s>\frac{3}{2}$;[22] and Zhouping Xin *et al.* obtained the existence and uniqueness of the weak solution to the Cauchy problem of (1.1′) with initial $u_0 \in H^1(R)$.[15,16] But, it is worthwhile to note that despite an abundance of literature on the C–H equation, the initial boundary value problem on the half-space $\{x>0\}$ hardly seems to have been treated except for Yang Ling'e and Guo Boling who proved the well-posedness of classical solutions to (1.1)–(1.3) with the intial data $u_0 \in H^3(R^+) \cap H_0^1(R^+)$.[23] Natural questions arise: Can a strong solution to the initial boundary value problem on the half-space $\{x>0\}$ exist? Is it local or global in time if it does? Is it unique? How about a weak solution? The aim of this paper is to prove the existence and uniqueness of the local solutions for (1.1)–(1.3) with initial data $u_0 \in H^2(R^+) \cap H_0^1(R^+)$, and to analyze the global existence and blow-up phenomena.

Before giving the precise statements of the main results, we first introduce the definition of a strong solution to the initial boundary value problem (1.1)–(1.3).

Definition: A function $u=u(t,x)$ is said to be a strong solution to the initial boundary value problem (1.1)–(1.3) if $u \in L^\infty(0,T;H^2(R^+) \cap H_0^1(R^+))$, $\partial_t u \in L^\infty(0,T;H_0^1(R^+))$, and

$$\partial_t u + u\partial_x u + \partial_x p = 0 \quad a.e.[0,T)\times R^+, \quad u(0,x)=u_0(x) \quad a.e.R^+.$$

If T is an arbitrarily given positive constant, u is said to exist globally in time.

The main results of this paper can be stated as follows:

(1) Local existence and uniqueness: Given $u_0 \in H^2(R^+) \cap H_0^1(R^+)$, there exists a $T^*>0$ depending only on $\|u_0\|_{H^2(R^+)}$ and a unique strong solution to problems (1.1)–(1.3)
$$u=u(t,x) \in C([0,T^*];H^2(R^+) \cap H_0^1(R^+)) \cap C^1([0,T^*];H_0^1(R^+)).$$
(2) Global existence and uniqueness: Suppose that $u_0 \in H^2(R^+) \cap H_0^1(R^+)$, with $V_0=(1-\partial_{xx})u_0 \geqslant 0$. Then the unique strong solution $u(t,x)$ to problems (1.1)–(1.3) exist globally in time.
(3) Blow-up: Let $u_0 \in H^2(R^+) \cap H_0^1(R^+)$, with $\partial_x u(\overline{x}) \leqslant -\sqrt{2}\|u_0\|_{H^1(R^+)}$ for some $\overline{x} \in R^+$. Then the strong solution to problems (1.1)–(1.3) blows-up in finite time.

Remark 1: The major difficulty of this work is that the domain of the problem we considered is $\{(t,x): x \in R^+\}$ and the regularity of the initial data is not good enough so that we cannot directly apply Kato's Theorem to prove the existence of the strong solution to problems (1.1)–(1.3) as in Refs. 22, 23. We prove the main results by an approximation method. We expect that

the strong solution to problems (1.1)–(1.3) can be obtained as a strong limit in $C([0,T^*];H^2(R^+)\cap H_0^1(R^+))$ of the approximations, $u^n=u^n(t,x)$, which solves the following approximation problem:

$$\begin{cases} \partial_t u^n + u^n \partial_x u^n + \partial_x p^n = 0, & t>0, x>0, \\ p^n(t,x) = \displaystyle\int_0^\infty h(x,y)\left((u^n)^2 + \frac{1}{2}(\partial_x u^n)^2 \right)(t,y)\,dy, & t>0, x>0, \\ u^n(0,x) = u_0^n(x), & x>0, \\ u^n(t,0) = 0, & t>0, \end{cases} \tag{1.4}$$

where $u_0^n \in \mathcal{B}=\{u\in H^4(R^+)\,|\,u(0)=\partial_{xx}u(0)=0\}$ is an approximation of u_0, i.e.,

$$u_0^n \to u_0, \quad \text{as} \quad n\to\infty \quad \text{in} \quad H^2(R^+)\cap H_0^1(R^+).$$

II. THE LOCAL SOLUTION FOR AN APPROXIMATION PROBLEM

In this section, we construct the approximate solution sequence $u^n=u^n(t,x)$ as solutions to the problem (1.4). The existence and uniqueness on this approximate solution sequence are given in the following theorem. For convenience we will omit the supscript n in $u^n(t,x)$ in this section.

Theorem 1: *Given $u_0\in\mathcal{B}$, there exists a maximal $T>0$ depending only on $\|u_0\|_{H^4(R^+)}$ and a unique strong solution to (1.4) such that*

$$u=u(t,x)\in C([0,T);\mathcal{B})\cap C^1([0,T);H^2(R^+)\cap H_0^1(R^+)).$$

We reformulate (1.4) as the following initial boundary value problem:

$$\begin{cases} m=(1-\partial_{xx})u, & x>0, t>0, \\ \partial_t m + u\partial_x m = -2m\partial_x u, & t>0, x>0, \\ m(0,x)=m_0(x)=(1-\partial_{xx})u_0, & x>0, \end{cases} \tag{2.1}$$

where $u_0\in\mathcal{B}$, and $m_0\in H^2(R^+)\cap H_0^1(R^+)$.

The new form is suitable to be analyzed with Kato's method for abstract quasilinear evolution equations of the hyperbolic type. For complement we state here Kato's Theorem[18] in the form appropriate for our purposes.

Consider the Cauchy problem for the abstract quasilinear evolution equation

$$\begin{cases} \dfrac{dv}{dt} + A(v)v = f(v), & t>0, \\ v(0)=v_0. \end{cases} \tag{Q}$$

Assume that:

(X) X,Y are reflexive Banach spaces, where $Y\hookrightarrow X$ continuously and densely, and there is an isomorphism S from Y onto X such that $\|\phi\|_Y=\|S\phi\|_X$, for all $\phi\in Y$. Let $W\subset Y$ be an open ball centered at 0 and with radius r.

(i) For each $y\in W$, the linear operator $A(y)$ belongs to $G(X,1,\beta)$ where β is a real number, i.e., $-A(y)$ generates a C_0 semigroup such that
$$\|e^{-tA(y)}\|\leqslant e^{\beta t}, \quad t\geqslant 0.$$

(ii) $Y\subset D(A(y))$ for each $y\in W$ (so that $A(y)|_Y\in\mathcal{B}(Y,X)$) satisfies the following Lipschitz condition:
$$\|A(y)-A(z)\|_{\mathcal{B}(Y,X)}\leqslant \mu_1\|y-z\|_X,$$
for all $y,z\in Y$.

(iii) For each $y \in W$, one has

$$SA(y)S^{-1}=A(y)+B(y),$$
$$B(y)\in\mathcal{B}(X), \quad \|B(y)\|_X\leqslant\lambda_1.$$

(iv) The function $f:W\to Y$ is bounded, i.e., there is a constant $\lambda_2>0$ such that

$$\|f(y)\|_Y\leqslant\lambda_2,$$

for all $y\in W$. The function $y\in X\to f(y)$ is Lipschitz-continuous in X, i.e.,

$$\|f(y)-f(z)\|_X\leqslant\mu_2\|y-z\|_X,$$

for all $y,z\in X$.

Here λ_1,λ_2 depend only on r; and, μ_1 and μ_2 depend only on $\max\{\|y\|_Y,\|z\|_Y\}$ and $\max\{\|y\|_X,\|z\|_X\}$, respectively.

Kato's Theorem: *Assume that* (X) *and* (i)–(iv) *hold. Given* $v_0\in Y$, *there exists a maximal* $T>0$ *depending only on* $\|v_0\|_Y$ *and a unique solution to* (Q) *such that*

$$v=v(t,x)\in C([0,T);Y)\cap C^1([0,T);X).$$

We apply Kato's Theorem to prove the following lemma.

Lemma 1: For $m_0\in H^2(R^+)\cap H_0^1(R^+)$, *there exists a maximal* $T>0$ *depending only on* $\|m_0\|_{H^2(R^+)}$ *and a unique solution to (2.1) such that*

$$m=m(t,x)\in C([0,T);H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,T),L^2(R^+)).$$

Proof: Let $X=L^2(R^+), Y=H^2(R^+)\cap H_0^1(R^+), W=\{y\in Y:\|y\|_Y\leqslant r\}$ and $S=1-\partial_{xx}$. Clearly the embedding $Y\hookrightarrow X$ is continuous and dense. Moreover, $S:Y\to X$ is an isometric isomorphism. In fact, $\forall f\in L^2(R^+)$, the well-known existence theorem of weak solution and regularity for boundary problem of elliptic equation implies that the boundary value problem

$$\begin{cases} v-\partial_{xx}v=f, \\ v(0)=v(+\infty)=0, \end{cases}$$

has a unique solution

$$v(t,x)=\int_0^{+\infty}h(x,y)f(t,y)dy$$

in $H^2(R^+)\cap H_0^+(R^+)$, where $h(x,y)=\begin{cases} e^{-x}shy, & y\leqslant x, \\ e^{-y}shx, & y>x. \end{cases}$

Rewrite problem (2.1) into an abstract form

$$\begin{cases} \dfrac{dm}{dt}+A(m)m=f(m), \quad t>0 \\ m(0)=m_0, \end{cases}$$

where $A(m)=(S^{-1}m)\partial_x$, $f(m)=-2m\partial_x(S^{-1}m)$.

To prove Lemma 1, it suffices to verify conditions (i)–(iv) of Kato's Theorem.

Step 1: Let $v=S^{-1}m\in H^2(R^+)\cap H_0^1(R^+)$, $\overline{A}=v\partial_x=A(m)$, and $A_0=\overline{A}+\frac{1}{2}\partial_x vI$. We show that the operator iA_0 is self-adjoint, i.e., $A_0^*=-A_0$. In fact,

$$D(A(m))=\{u\in X:(S^{-1}m)\partial_x u\in X\},$$

$$D(A_0)=D(\overline{A})=\{u\in X:v\partial_x u\in X\},$$

$$D(A_0^*)=\{w\in X: A_0^*w\in X\}$$
$$=\{w\in X: \text{there exists a } M_w>0,$$
$$\text{such that } |(w,A_0u)_X|\leqslant M_w\|u\|_X, \text{ for all } u\in D(A_0)\}.$$

Fix $w\in D(A_0^*)$ $\forall\phi\in\mathcal{D}(R^+)$, we deduce that $v\partial_x w\in X$:

$$(\phi,A_0^*w)_X=(A_0\phi,w)_X=\int_0^\infty (v\partial_x\phi+\tfrac{1}{2}\phi\partial_x v)w\,dx$$
$$=-\int_0^\infty (\phi\partial_x(vw)-\tfrac{1}{2}\phi w\partial_x v)dx$$
$$=-\int_0^\infty \phi(v\partial_x w+\tfrac{1}{2}w\partial_x v)dx$$
$$=-(\phi,v\partial_x w+\tfrac{1}{2}w\partial_x v)_X.$$

Since $\mathcal{D}(R^+)$ is dense in $D(A_o)$, the above formula holds for all $\phi\in D(A_0)$. Hence $-(v\partial_x w+\frac{1}{2}w\partial_x v)=A_0^*w\in X$. This implies $v\partial_x w\in X$. Thus $w\in D(A_0)$ and $A_0w=-A_0^*w$. This proves that $A_0^*\subset -A_0$.

Conversely, fix $u\in D(A_0)$ and let $u^n=\rho_n * u$, where ρ_n is the usual mollifiers on R^+. It follows from the proof of (2.3) in Ref. 6 that

$$\lim_{n\to\infty}\overline{A}(u_n)=\overline{A}(u) \text{ in } L^2(R^+).$$

Then

$$(A_0z,u)_X=\lim_{n\to\infty}(A_0z,u_n)_X=\lim_{n\to\infty}\int_0^\infty (v\partial_x z+\tfrac{1}{2}z\partial_x v)u_n=-\lim_{n\to\infty}\int_0^\infty (z\partial_x(vu_n)-\tfrac{1}{2}u_nz\partial_x v)$$
$$=-\int_0^\infty z(v\partial_x u+\tfrac{1}{2}u\partial_x v)$$
$$=-(z,A_0u).$$

Thus $u\in D(A_0^*)$ and $A_0^*u=-A_0u$. This proves that $-A_0\subset A_0^*$.

Hence $A_0^*=-A_0$, that is, iA_0 is self-adjoint in X. Stone theorem[19] implies that A_0 is the infinitesimal generator of a C_0 group unitary operators on X, and so $-A_0$ is the infinitesimal generator of a C_0 semigroup of contraction on X. In addition, $\|(A_0-A(m))w\|_X=\|\frac{1}{2}w\partial_x(S^{-1}m)\|_X\leqslant\frac{1}{2}\sup_{x\in R^+}|\partial_x(S^{-1}m)|\|w\|_X=\omega\|w\|_X$. If $\omega<\infty$, it follows from the theorem 3.1.1 in Ref. 19 that $-A(m)=(A_0-A(m))+(-A_0)$ is the infinitesimal generator of a C_0 semigroup and $\|e^{-tA(m)}\|\leqslant e^{\omega t}$.

Next, we need to estimate $\sup_{x\in R^+}|\partial_x(S^{-1}m)|$. Since $v=S^{-1}m\in H^2(R^+)\cap H_0^1(R^+)$ solves the equation $v-v_{xx}v=m$, we have

$$\int_0^\infty (v^2-2v\partial_{xx}v+(\partial_{xx}v)^2)dx=\int_0^\infty m^2(x)dx,$$

$$2\int_0^\infty v\partial_{xx}v\,dx=-\int_0^\infty (\partial_x v)^2dx.$$

Hence

$$\int_0^\infty (v^2+2(\partial_x v)^2+(\partial_{xx}v)^2)dx=\int_0^\infty m^2(x)dx,$$

and so

$$\|v\|^2_{H^2(R^+)}+\|\partial_x v\|^2_{L^2(R^+)}=\|m\|^2_{L^2(R^+)},$$

that is,

$$\|S^{-1}m\|^2_{H^2(R^+)}+\|\partial_x(S^{-1}m)\|^2_{L^2(R^+)}=\|m\|^2_{L^2(R^+)}, \tag{2.2}$$

it follows that

$$(\partial_x(S^{-1}m))^2(x)-(\partial_x(S^{-1}m)(0))^2=2\int_0^x \partial_x(S^{-1}m)\partial_{xx}(S^{-1}m)dx\leqslant\|S^{-1}m\|^2_{H^2(R^+)}\leqslant\|m\|^2_{L^2(R^+)},$$

$$|\partial_x(S^{-1}m)(0)|=\left|\int_0^\infty e^{-y}m(y)dy\right|\leqslant\|m\|_{L^2(R^+)}\|e^{-y}\|_{L^2(R^+)}=\frac{1}{\sqrt{2}}\|m\|_{L^2(R^+)},$$

and so $\forall x\in R^+$, $(\partial_x(S^{-1}m))^2(x)\leqslant\frac{3}{2}\|m\|^2_{L^2(R^+)}$,

$$\sup_{x\in R^+}|\partial_x(S^{-1}m|\leqslant\sqrt{3/2}\|m\|_{L^2(R^+)}. \tag{2.3}$$

Consequently,

$$\omega=\frac{1}{2}\sup_{x\in R^+}|\partial_x(S^{-1}m)|\leqslant\|m\|_{L^2(R^+)}\leqslant\|m\|_Y\leqslant r.$$

So the condition (i) of Kato's Theorem is verified with constant $\beta=r$.

Step 2: To check condition (ii) of Kato's Theorem.

$\forall m_1,m_2,w\in Y$,

$$\|(A(m_1)-A(m_2))w\|_X=\|(S^{-1}m_1-S^{-1}m_2)\partial_x w\|_X\leqslant\|S^{-1}(m_1-m_2)\|_{L^\infty(R^+)}\|\partial_x w\|_X$$
$$\leqslant\|m_1-m_2\|_X\|w\|_Y, \tag{2.4}$$

due to the fact that

$$(S^{-1}m)^2(x)=2\int_0^x S^{-1}m\partial_x(S^{-1}m)dy\leqslant\|S^{-1}m\|^2_{H^1(R^+)}\leqslant\|S^{-1}m\|^2_{H^2(R^+)}\leqslant\|m\|^2_{L^2(R^+)}.$$

So $\|A(m_1)-A(m_2)\|_{\mathcal{B}(Y,X)}\leqslant\|m_1-m_2\|_X$.

$\forall m\in W\subset Y$, let $m_1=m,m_2=0$ in (2.4), we have

$$\|A(m)w\|_X\leqslant\|m\|_X\|w\|_Y\leqslant r\|w\|_Y.$$

Thus $A(m)|_Y\in\mathcal{B}(Y,X)$.

Step 3: Now we check condition (iii) of Kato's Theorem.

$\forall m\in W,w\in Y$, by direct computation we obtain

$$
\begin{aligned}
SA(m)S^{-1}w &= S(S^{-1}m\partial_x(S^{-1}w)) \\
&= S^{-1}m\partial_x(S^{-1}w) - \partial_{xx}(S^{-1}m\partial_x(S^{-1}w)) \\
&= S^{-1}m\partial_x(S^{-1}w) - [\partial_{xx}(S^{-1}m)\partial_x(S^{-1}w) \\
&\quad + 2\partial_x(S^{-1}m)\partial_{xx}(S^{-1}w) + S^{-1}m\partial_{xxx}(S^{-1}w)] \\
&= S^{-1}m\partial_x(S^{-1}w) - [(S^{-1}m - m)\partial_x(S^{-1}w) \\
&\quad + 2\partial_x(S^{-1}m)(S^{-1}w - w) + S^{-1}m(\partial_x(S^{-1}w) - \partial_x w)] \\
&= m\partial_x(S^{-1}w) - 2\partial_x(S^{-1}m)(S^{-1}w - w) - S^{-1}m\partial_x(S^{-1}w) + (S^{-1}m)\partial_x w \\
&= (m - S^{-1}m)\partial_x(S^{-1}w) + 2\partial_x(S^{-1}m)(w - S^{-1}w) + A(m)w.
\end{aligned}
$$

Hence

$$
SA(m)S^{-1} = (m - S^{-1}m)\partial_x S^{-1} + 2\partial_x(S^{-1}m)(1 - S^{-1}) + A(m).
$$

Let $B(m) = (m - S^{-1}m)\partial_x S^{-1} + 2\partial_x(S^{-1}m)(1 - S^{-1})$, so that

$$
SA(m)S^{-1} = A(m) + B(m),
$$

and $B(m)$ can be extended to an operator in X. Next we show that $B(m) \in \mathcal{B}(X)$.

$\forall w \in X$,

$$
\begin{aligned}
\|B(m)w\|_X &= \|(m - S^{-1}m)\partial_x(S^{-1}w) + 2\partial_x(S^{-1}m)(w - S^{-1}w)\|_X \\
&\leqslant \|m - S^{-1}m\|_X \|\partial_x(S^{-1}w)\|_{L^\infty(R^+)} + 2\|\partial_x(S^{-1}m)\|_{L^\infty(R^+)} \|w - S^{-1}w\|_X \\
&\leqslant \sqrt{3/2}\|m\|_X \|w\|_X + 2\sqrt{3/2}\|m\|_X \|w\|_X \\
&\leqslant 6\|m\|_X \|w\|_X \\
&\leqslant 6\|m\|_Y \|w\|_X \\
&\leqslant \lambda_1 \|w\|_X,
\end{aligned}
$$

due to (2.2)–(2.3) and the fact that $m - S^{-1}m = -\partial_{xx}(S^{-1}m)$, where $\lambda_1 = 6r$. So $B(m) \in \mathcal{B}(X)$ and $\|B(m)\|_{\mathcal{B}(X)} \leqslant \lambda_1$.

Step 4: Finally we check condition (iv) of Kato's Theorem.

$\forall m \in W$, it follows from (2.3) that

$$
\begin{aligned}
\|f(m)\|_Y = 2\|m\partial_x(S^{-1}m)\|_Y &\leqslant 2\|\partial_x(S^{-1}m)\|_{L^\infty(R^+)} \|m\|_Y \\
&\leqslant 2\sqrt{3/2}\|m\|_X \|m\|_Y \leqslant 4\|m\|_Y^2 \leqslant \lambda_2,
\end{aligned}
$$

where $\lambda_2 = 4r^2$,

$\forall m_1, m_2 \in X$,

$$
\begin{aligned}
\|f(m_1) - f(m_2)\|_X &= 2\|m_1\partial_x(S^{-1}m_1) - m_2\partial_x(S^{-1}m_2)\|_X \\
&\leqslant 2\|\partial_x(S^{-1}m_1)\|_{L^\infty(R^+)} \|m_1 - m_2\|_X + 2\|m_2\|_X \|\partial_x(S^{-1}(m_1 - m_2))\|_{L^\infty(R^+)} \\
&\leqslant 2\sqrt{3/2}\|m_1\|_X \|m_1 - m_2\|_X + 2\sqrt{3/2}\|m_2\|_X \|m_1 - m_2\|_X \\
&\leqslant 4(\|m_1\|_X + \|m_2\|_X)\|m_1 - m_2\|_X \\
&\leqslant \mu_2 \|m_1 - m_2\|_X,
\end{aligned}
$$

where $\mu_2 = 8\max\{\|m_1\|_X, \|m_2\|_X\}$.

By Kato's Theorem, the proof of Lemma 1 is completed.

The proof of Theorem 1: Since $S:\mathcal{B}\to Y$ is bijective, $\forall m(t,\cdot)\in Y=H^2(R^+)\cap H_0^1(R^+)$, we can solve $u\in\mathcal{B}$ from $Su=m$ uniquely

$$u(t,x)=\int_0^\infty h(x,y)m(t,y)dy$$

$$=e^{-x}/2\int_0^x e^y m(t,y)dy+e^x/2\int_x^\infty e^{-y}m(t,y)dy-e^{-x}/2\int_0^\infty e^{-y}m(t,y)dy.$$

Consequently the result follows from this and Lemma 1.

III. THE EXISTENCE AND UNIQUENESS OF LOCAL SOLUTIONS TO PROBLEMS (1.1)–(1.3)

In this section, we consider the existence and uniqueness of the local solution to problems (1.1)–(1.3), i.e.,

$$\begin{cases} \partial_t u+u\partial_x u+\partial_x p=0, & t>0,x>0,\\ p(t,x)=\displaystyle\int_0^\infty h(x,y)\left(u^2+\frac{1}{2}(\partial_x u)\right)^2(t,y)dy, & t>0,x>0,\\ u(0,x)=u_0(x), & x>0,\\ u(t,0)=0, & t>0, \end{cases} \tag{3.1}$$

where

$$h(x,y)=\begin{cases} e^{-x}shy, & y\leqslant x,\\ e^{-y}shx, & y>x, \end{cases}$$

with $u_0\in H^2(R^+)\cap H_0^1(R^+)$. First we introduce some lemmas as follows.

Lemma 2 (Ref. 20, Lemma 4(ii)): Let $X\subset E\subset Y$ be Banach spaces, the imbedding $X\hookrightarrow E$ being compact. Then the following imbedding is compact:

$$L^\infty(0,T;X)\cap\left\{\phi:\frac{\partial\phi}{\partial t}\in L^r(0,T;Y)\right\}\hookrightarrow C([0,T];E),1<r\leqslant\infty.$$

Lemma 3 (Ref. 21, Lemma 1.4): Let X and Y be two Banach spaces such that $X\hookrightarrow Y$ with a continuous injection. If a function ϕ belongs to $L^\infty(0,T;X)$ and is weakly continuous with values in Y, then ϕ is weakly continuous with values in X.

Lemma 4 (Ref. 20, Lemma 6): Let $g\in W^{1,1}(0,T)$ and $k\in L^1(0,T)$ satisfy

$$\frac{dg}{dt}\leqslant F(g)+k,\quad \forall t\in(0,T),$$

$$g(0)\leqslant g_0,$$

where F is bounded on bounded sets from R into R, that is

$$\forall a>0,\exists A>0\quad \text{such that } |x|\leqslant a\Rightarrow|F(x)|\leqslant A.$$

Then for every $\epsilon>0$, there exists $T_\epsilon>0$ independent of g such that

$$g(t)\leqslant g_0+\epsilon,\quad \forall t\leqslant T_\epsilon.$$

Theorem 2: *Given* $u_0 \in H^2(R^+) \cap H_0^1(R^+)$, *there exists a* $T^* > 0$ *depending only on* $\|u_0\|_{H^2(R^+)}$ *and a unique solution to (3.1)*

$$u = u(t,x) \in C([0,T^*];H^2(R^+) \cap H_0^1(R^+)) \cap C^1([0,T^*];H_0^1(R^+)).$$

Proof: We begin with the proof of existence.

Since $\mathcal{B} = \{u \in H^4(R^+) | u(0) = \partial_{xx} u(0) = 0\}$ is dense in $H^2(R^+) \cap H_0^1(R^+)$, there exists a sequence $\{u_0^n\} \subset \mathcal{B}$ such that

$$u_0^n \to u_0 \quad \text{in} \quad H^2(R^+) \cap H_0^1(R^+) \quad \text{and} \quad \|u_0^n\|_{H^2(R^+)} \leqslant \|u_0\|_{H^2(R^+)}. \tag{3.2}$$

It follows from Theorem 1 that there exists a unique solution $u^n(t,x) \in C([0,T^n);\mathcal{B}) \cap C^1([0,T^n);H^2(R^+) \cap H_0^1(R^+))$ to problem (1.4), i.e.,

$$\begin{cases} \partial_t u^n + u^n \partial_x u^n + \partial_x p^n = 0, & t > 0, x > 0, \quad (3.3) \\ p^n(t,x) = \displaystyle\int_0^\infty h(x,y) \left((u^n)^2 + \frac{1}{2} (\partial_x u^n)^2 \right)(t,y)\, dy, & t > 0, x > 0, \quad (3.4) \\ u^n(0,x) = u_0^n(x), & x > 0, \quad (3.5) \\ u^n(t,0) = 0, & t > 0, \quad (3.6) \end{cases}$$

where T^n is the life span of the solution $u^n(t,x)$ in $C([0,T^n);\mathcal{B})$, then

$$\lim_{t \to T^n} \|u^n(t,\cdot)\|_{H^4(R^+)} = +\infty.$$

It follows from the proof of (2.4) in Ref. 15 that this holds if and only if

$$\lim_{t \to T^n} (\|u^n(t,\cdot)\|_{L^\infty(R^+)} + \|\partial_x u^n(t,\cdot)\|_{L^\infty(R^+)}) = +\infty.$$

Suppose that there exists a time $T^* > 0$ and a constant $C > 0$ independent of n such that $\sup_{[0,T^*)} \|u^n(t,\cdot)\|_{H^2(R^+)} \leqslant C$. This implies that $T^n \geqslant T^*$. Indeed, if this is not true one has

$$\sup_{[0,T^*)} \|u^n(t,\cdot)\|_{H^2(R^+)} \geqslant \sup_{[0,T^n)} \|u^n(t,\cdot)|_{H^2(R^+)} \geqslant \sup_{[0,T^n)} (\|u^n(t,\cdot)\|_{L^\infty(R^+)} + \|\partial_x u^n(t,\cdot)\|_{L^\infty(R^+)}) = +\infty,$$

which is a contradiction.

Next, we prove that T^* and C do exist.

Indeed, since $u^n(t,x) \in C([0,T^n);\mathcal{B})$ and satisfies Eq. (3.3):

$$\partial_t u^n + u^n \partial_x u^n + \partial_x p^n = 0,$$

then

$$\partial_t \partial_x u^n = -(\partial_x u^n)^2 - u^n \partial_{xx} u^n - \partial_{xx} p^n = -\tfrac{1}{2}(\partial_x u^n)^2 - u^n \partial_{xx} u^n + (u^n)^2 - p^n, \tag{3.7}$$

$$\partial_t \partial_{xx} u^n = -\partial_x (u^n \partial_{xx} u^n) - \partial_x p^n + 2 u^n \partial_x u^n - \partial_x u^n \partial_{xx} u^n, \tag{3.8}$$

it follows that

$$\frac{1}{2} \frac{d}{dt} \|u^n(t,\cdot)\|_{L^2(R^+)}^2 = \int_{R^+} (p^n - (u^n)^2) \partial_x u^n \, dx, \tag{3.9}$$

$$\frac{1}{2}\frac{d}{dt}\|\partial_x u^n(t,\cdot)\|^2_{L^2(R^+)} = -\frac{1}{2}\int_{R^+}(\partial_x u^n)^3 dx - \int_{R^+} u^n \partial_{xx} u^n \partial_x u^n dx + \int_{R^+}((u^n)^2 - p^n)\partial_x u^n dx$$

$$= \int_{R^+}((u^n)^2 - p^n)\partial_x u^n dx, \tag{3.10}$$

$$\frac{1}{2}\frac{d}{dt}\|\partial_{xx} u^n(t,\cdot)\|^2_{L^2(R^+)} = \int_{R^+} u^n \partial_{xx} u^n \partial_{xxx} u^n dx - \int_{R^+} \partial_x p^n \partial_{xx} u^n dx$$

$$+2\int_{R^+} u^n \partial_x u^n \partial_{xx} u^n dx - \int_{R^+} \partial_x u^n (\partial_{xx} u^n)^2 dx$$

$$= -\frac{3}{2}\int_{R^+} \partial_x u^n (\partial_{xx} u^n)^2 dx - \int_{R^+} \partial_x p^n \partial_{xx} u^n dx + 2\int_{R^+} u^n \partial_x u^n \partial_{xx} u^n dx. \tag{3.11}$$

Due to (3.9) and (3.10), we obtain

$$\frac{1}{2}\frac{d}{dt}\|u^n(t,\cdot)\|^2_{H^1(R^+)} = 0, \tag{3.12}$$

then,

$$\|u^n(t,\cdot)\|_{H^1(R^+)} = \|u_0^n\|_{H^1(R^+)} \leqslant \|u_0^n\|_{H^2(R^+)} \leqslant \|u_0\|_{H^2(R^+)}. \tag{3.13}$$

Due to (3.11) and (3.12), we obtain

$$\frac{1}{2}\frac{d}{dt}\|u^n(t,\cdot)\|^2_{H^2(R^+)} = -\frac{3}{2}\int_{R^+} \partial_x u^n (\partial_{xx} u^n)^2 dx - \int_{R^+} \partial_x p^n \partial_{xx} u^n dx + 2\int_{R^+} u^n \partial_x u^n \partial_{xx} u^n dx$$

$$\leqslant \frac{3}{2}\|\partial_x u^n(t,\cdot)\|_{L^\infty(R^+)}\|\partial_{xx} u^n(t,\cdot)\|^2_{L^2(R^+)}$$

$$+\|\partial_x p^n(t,\cdot)\|_{L^2(R^+)}\|\partial_{xx} u^n(t,\cdot)\|_{L^2(R^+)}$$

$$+\|u^n(t,\cdot)\|_{L^\infty(R^+)}\|\partial_x u^n(t,\cdot)\|^2_{H^1(R^+)}$$

$$\leqslant C\|u^n(t,\cdot)\|^3_{H^2(R^+)}, \tag{3.14}$$

where C is a constant depending on nothing, and, the imbedding $H^2(R^+) \hookrightarrow W^{1,\infty}(R^+)$ and the following facts are used:

$$\|p^n(t,\cdot)\|^2_{L^2(R^+)} \leqslant \int_0^\infty \left\{ \int_0^\infty h(x,y)|((u^n)^2 + \tfrac{1}{2}(\partial_x u^n)^2)(t,y)|^2 dy \int_0^\infty h(x,y)dy \right\} dx$$

$$\leqslant \int_0^\infty \int_0^\infty h(x,y)|((u^n)^2 + \tfrac{1}{2}(\partial_x u^n)^2)(t,y)|^2 dy dx$$

$$= \int_0^\infty |((u^n)^2 + \tfrac{1}{2}(\partial_x u^n)^2)(t,y)|^2 \left(\int_0^\infty h(x,y)dx \right) dy$$

$$\leqslant \int_0^\infty |(u^n)^2 + \tfrac{1}{2}(\partial_x u^n)^2(t,y)|^2 dy \leqslant 2\|u^n(t,\cdot)\|^4_{L^4(R^+)} + 2\|\partial_x u^n(t,\cdot)\|^4_{L^4(R^+)}$$

$$\leqslant 2\|u^n(t,\cdot)\|^2_{L^\infty(R^+)}\|u^n(t,\cdot)\|^2_{L^2(R^+)} + 2\|\partial_x u^n(t,\cdot)\|^2_{L^\infty(R^+)}\|\partial_x u^n(t,\cdot)\|^2_{L^2(R^+)}$$

$$\leqslant 4\|u^n(t,\cdot)\|^4_{H^2(R^+)}, \tag{3.15}$$

and

$$\begin{aligned}\|\partial_x p^n(t,\cdot)\|^2_{L^2(R^+)} &= \int_0^\infty |\partial_x p^n|^2 dx \\ &= -\int_0^\infty p^n \partial_{xx} p^n dx \\ &= \int_0^\infty p^n \left((u^n)^2 + \frac{1}{2}(\partial_x u^n)^2 - p^n \right) dx \\ &\leqslant \|p^n(t,\cdot)\|_{L^2(R^+)} (\|u^n(t,\cdot)\|^2_{L^4(R^+)} + \|\partial_x u^n(t,\cdot)\|^2_{L^4(R^+)} + \|p^n(t,\cdot)\|_{L^2(R^+)}) \\ &\leqslant C\|u^n(t,\cdot)\|^4_{H^2(R^+)}, \end{aligned} \tag{3.16}$$

where C is a constant depending on nothing.

It follows from (3.14) and Lemma 4 that there exists a time $T^*>0$ and a constant $C_1>0$ depending only on $\|u_0\|_{H^2(R^+)}$ such that

$$\|u^n(t,\cdot)\|_{H^2(R^+)} \leqslant C_1, \tag{3.17}$$

and so $T^n \geqslant T^*, \forall n$.

On the other hand,

$$\begin{aligned}\|\partial_t u^n\|_{L^\infty(0,T^*;L^2(R^+))} &\leqslant \|u^n \partial_x u^n\|_{L^\infty(0,T^*;L^2(R^+))} + \|\partial_x p^n\|_{L^\infty(0,T^*;L^2(R^+))} \\ &\leqslant \sup_{0<t<T^*} \|u^n(t,\cdot)\|_{L^\infty(R^+))} \|\partial_x u^n(t,\cdot)\|_{L^2(R^+)} + \sup_{0<t<T^*} \sqrt{C}\|u^n(t,\cdot)\|^2_{H^2(R^+)} \\ &\leqslant (1+\sqrt{C})C_1^2 \triangleq C_2, \end{aligned} \tag{3.18}$$

due to (3.3) and (3.16)–(3.17), where C_2 is constant depending only on $\|u_0\|_{H^2(R^+)}$.

It follows from (3.17)–(3.18) and Lemma 2 that there exist a subsequence of $\{u^n\}$, still denoted by $\{u^n\}$, and some function $u \in L^\infty(0,T^*;H^2(R^+)\cap H_0^1(R^+)) \cap C([0,T^*];C^1_{\text{loc}}(R^+)), \partial_t u \in L^\infty(0,T^*;L^2(R^+))$ such that

$$u^n \overset{*}{\rightharpoonup} u, \text{ as } n\to\infty \text{ in } L^\infty(0,T^*;H^2(R^+)\cap H_0^1(R^+)), \tag{3.19}$$

$$\partial_t u^n \overset{*}{\rightharpoonup} \partial_t u, \text{ as } n\to\infty \text{ in } L^\infty(0,T^*;L^2(R^+)), \tag{3.20}$$

$$u^n \to u, \text{ as } n\to\infty \text{ in } C([0,T^*];C^1_{\text{loc}}(R^+)), \text{ uniformly on each compact subset of } [0,T^*]\times R^+. \tag{3.21}$$

It follows from Lemma 3 that $u \in C([0,T^*];H^2(R^+)\cap H_0^1(R^+))$.

Now, $\{p^n\}$ is uniformly bounded in $L^\infty(0,T^*;H^2(R^+)\cap H_0^1(R^+))$ due to (3.15)–(3.17) and the fact $\partial_{xx} p^n = p^n - (u^n)^2 - \frac{1}{2}(\partial_x u^n)^2$. On the other hand,

$$(1-\partial_{xx})\frac{\partial}{\partial t} p^n = \partial_t((u^n)^2) + \frac{1}{2}\partial_t((\partial_x u^n)^2),$$

$\partial_t((u^n)^2) = 2u^n \partial_t u^n$ is uniformly bounded in $L^\infty(0,T^*;L^2(R^+))$, and

$$\tfrac{1}{2}\partial_t((\partial_x u^n)^2)=\partial_x u^n \partial_{xt} u^n=-\tfrac{1}{2}(\partial_x u^n)^3-u^n\partial_x u^n \partial_{xx} u^n+((u^n)^2-p^n)\partial_x u^n,$$

which is uniformly bounded in $L^\infty(0,T^*;L^2(R^+))$, consequently $\{\partial_t p^n\}$ is uniformly bounded in $L^\infty(0,T^*;L^2(R^+))$. It follows from Lemma 2 that there exists a subsequence of $\{p^n\}$, still denoted by $\{p^n\}$, and some function $p\in L^\infty(0,T^*;H^2(R^+)\cap H_0^1(R^+))\cap C([0,T^*];C^1_{\mathrm{loc}}(R^+))$ such that

$$p^n \overset{*}{\rightharpoonup} p, \quad \text{as} \quad n\to\infty \quad \text{in} \quad L^\infty(0,T^*;H^2(R^+)\cap H_0^1(R^+)), \tag{3.22}$$

$$p^n \to p, \quad \text{as} \quad n\to\infty \quad \text{in} \quad C([0,T^*];C^1_{\mathrm{loc}}(R^+)), \tag{3.23}$$

then $p\in C([0,T^*];H^2(R^+)\cap H_0^1(R^+))$ and

$$\partial_{xx}p^n=p^n-(u^n)^2-\tfrac{1}{2}(\partial_x u^n)^2\to p-u^2-\tfrac{1}{2}(\partial_x u)^2 \quad \text{as} \quad n\to\infty \quad \text{in} \quad C([0,T^*],C_{\mathrm{loc}}(R^+)).$$

Consequently,

$$\begin{cases}(1-\partial_{xx})p=u^2+\tfrac{1}{2}(\partial_x u)^2,\\ p(t,0)=p(t,\infty)=0,\end{cases}$$

and so $p(t,x)=\int_0^\infty h(x,y)(u^2+\frac{1}{2}(\partial_x u)^2)(t,y)dy$.

For any $v\in L^2(0,T^*;\mathcal{D}(R^+))$, by multiplying v to both sides of (3.3) and integrating over $[0,T^*]\times R^+$, we find

$$\int_0^{T^*}\int_0^\infty(\partial_t u^n+u^n\partial_x u^n+\partial_x p^n)v\,dx\,dt=0,$$

passing to the limit, due to (3.19) and (3.20) and (3.22), we obtain

$$\int_0^{T^*}\int_0^\infty(\partial_t u+u\partial_x u+\partial_x p)v\,dx\,dt=0,$$

that is, $\partial_t u+u\partial_x u+\partial_x p=0$ in the weak sense. Note that $u\in C([0,T^*];H^2(R^+)\cap H_0^1(R^+))$, which implies

$$\partial_t u=-u\partial_x u-\partial_x p\in C([0,T^*];H_0^1(R^+)),$$

and so

$$u\in C([0,T^*];H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,T^*];H_0^1(R^+)),$$

consequently $\partial_t u+u\partial_x u+\partial_x p=0$ a. e. $[0,T^*]\times R^+$.

It follows from $u^n(0,x)=u_0^n(x)$, (3.2) and (3.20), we obtain

$$u(0,x)=u_0(x).$$

The proof of existence is completed.

Before proving the uniqueness, we introduce the following Lemma.

Lemma 5: Let $u_0\in H^2(R^+)\cap H_0^1(R^+)$, *and* $u\in C([0,T];H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,T];H_0^1(R^+))$ *be a solution to (3.1). Then the following problem:*

$$\begin{cases} \dfrac{d\Phi^x(t)}{dt} = u(t,\Phi^x(t)), & t>0, \\ \Phi^x(0) = x, & x\geqslant 0, \end{cases}$$

has a unique solution $\Phi^x(t)\in C^1([0,T])$ *and* $x\in R^+\to\Phi^x(t)\in R^+$ *is an isomorphism.*

Proof: Let $\tilde{u}(t,x)=\begin{cases} u(t,x), & x\geqslant 0, \\ -u(t,-x), & x<0. \end{cases}$

We consider the ordinary differential equation

$$\begin{cases} \dfrac{d\Phi^x(t)}{dt} = \tilde{u}(t,\Phi^x(t)), & t>0, \\ \Phi^x(0) = x, & x\geqslant 0. \end{cases} \tag{3.24}$$

Note that $u(t,x)\in C([0,T];H^2(R^+)\cap H_0^1(R^+))$. It follows from the definition of $\tilde{u}$ and Sobolev Embedding Theorem that $\tilde{u}(t,q)$ is Lipschitz continuous with respect to q. Then for any $x\geqslant 0$, there exists a unique solution $\Phi^x(t)\in C^1([0,T])$ to (3.24). Let $q(t,x)=\Phi^x(t)$, then $q(t,x)$ solves the following problem:

$$\begin{cases} q_t = \tilde{u}(t,q), & t>0, \\ q(0,x) = x, & x\geqslant 0. \end{cases} \tag{3.25}$$

Applying ∂_x to (3.25), we have

$$\begin{cases} q_{xt} = \tilde{u}_q(t,q)q_x, & t>0, \\ q_x(0,x) = 1, & x\geqslant 0, \end{cases} \tag{3.26}$$

and so $q_x(t,x)=e^{\int_0^t \tilde{u}_q(\tau,q(\tau,x))q_x(\tau,x)d\tau}>0$. From the facts that $q(t,x)$ is continuous with respect to x and that

$$|q(t,x)-x|\leqslant \int_0^t |\tilde{u}(\tau,q(\tau,x))|d\tau \leqslant 2\|u_0\|_{H^2}t,$$

we know

(1) $q(t,x)>q(t,0)=0, t\in[0,T]$,

(2) $\lim_{x\to+\infty} q(t,x)=+\infty, t\in[0,T]$,

(3) $q(t,x)$ is a homeomorphism.

Consequently $x\in R^+\to\Phi^x(t)\in R^+$ is an isomorphism. The proof of Lemma 5 is completed.

Now, we turn to the proof of the uniqueness. Let $u_1(t,x)$ and $u_2(t,x)$ be any two solutions of (3.1). Set $W=u_1-u_2$. Then W solves

$$\begin{cases} \partial_t W + u_1\partial_x W = -\partial_x(p_1-p_2) - W\partial_x u_2, \\ W(0,x)=0, \\ W(t,0)=0. \end{cases} \tag{3.27}$$

Thus by (3.27), Lemma 5, and the characteristic method, we get

$$W(t,x) = -\int_0^t (\partial_x(p_1-p_2) + W\partial_x u_2)(s,x)ds,$$

and so

$$\|W(t,\cdot)\|_{L^\infty(R^+)} \leqslant \int_0^t \|(\partial_x(p_1-p_2) + W\partial_x u_2)(s,\cdot)\|_{L^\infty(R^+)}ds, \forall t\in[0,T]. \tag{3.28}$$

On the other hand, by the definition of P_i $(i=1,2)$, we have

$$\begin{aligned}\partial_x(p_1-p_2)&=\partial_x(1-\partial_{xx})^{-1}\{(u_1^2-u_2^2)+\tfrac{1}{2}[(\partial_x u_1)^2-(\partial_x u_2)^2]\}\\&=\partial_x(1-\partial_{xx})^{-1}\{(u_1+u_2)W+\tfrac{1}{2}\partial_x W\partial_x(u_1+u_2)\}.\end{aligned}\tag{3.29}$$

The second term on the right-hand side of (3.29) can be rewritten as

$$\begin{aligned}\partial_x(1-\partial_{xx})^{-1}(\partial_x W\partial_x(u_1+u_2))&=\partial_{xx}(1-\partial_{xx})^{-1}(W\partial_x(u_1+u_2))-\partial_x(1-\partial_{xx})^{-1}(W\partial_{xx}(u_1+u_2))\\&=-W\partial_x(u_1+u_2)+(1-\partial_{xx})^{-1}(W\partial_x(u_1+u_2))\\&\quad-\partial_x(1-\partial_{xx})^{-1}(W\partial_{xx}(u_1+u_2)).\end{aligned}$$

Hence

$$\begin{aligned}\partial_x(p_1-p_2)=&\tfrac{1}{2}\partial_x(1-\partial_{xx})^{-1}\{(u_1+u_2)W+(v_1+v_2)W\}+\tfrac{1}{2}(1-\partial_{xx})^{-1}(W\partial_x(u_1+u_2))\\&-\tfrac{1}{2}W\partial_x(u_1+u_2),\end{aligned}$$

where $v_i=(1-\partial_{xx})u_i$, $i=1,2$.

And so

$$\begin{aligned}\partial_x(p_1-p_2)+W\partial_x u_2=&\tfrac{1}{2}\partial_x(1-\partial_{xx})^{-1}\{(u_1+u_2)W+(v_1+v_2)W\}\\&+\tfrac{1}{2}(1-\partial_{xx})^{-1}(W\partial_x(u_1+u_2))-\tfrac{1}{2}W\partial_x W.\end{aligned}\tag{3.30}$$

Using the definition of $(1-\partial_{xx})^{-1}$, we have

$$\begin{aligned}&\|\partial_x(1-\partial_{xx})^{-1}((u_1+u_2)W)(t,\cdot)\|_{L^\infty(R^+)}\\&=\sup_{x\in R^+}\left|\int_0^x e^{-x}shy((u_1+u_2)W)(t,y)dy+\int_x^\infty e^{-y}chx((u_1+u_2)W)(t,y)dy\right|\\&\leqslant\sup_{x\in R^+}\left(\left(\int_0^x|e^{-x}shy|^2dy\right)^{1/2}+\left(\int_x^\infty|e^{-y}chx|^2dy\right)^{1/2}\right)\\&\quad\times\|(u_1+u_2)(t,\cdot)\|_{L^2(R^+)}\|W(t,\cdot)\|_{L^\infty(R^+)}\\&\leqslant\frac{3\sqrt{2}}{4}\|(u_1+u_2)(t,\cdot)\|_{L^2(R^+)}\|W(t,\cdot)\|_{L^\infty(R^+)}\\&\leqslant\frac{3\sqrt{2}}{4}(\|u_1(t,\cdot)\|_{L^2(R^+)}+\|u_2(t,\cdot)\|_{L^2(R^+)})\|W(t,\cdot)\|_{L^\infty(R^+)},\end{aligned}\tag{3.31}$$

$$\begin{aligned}&\|\partial_x(1-\partial_{xx})^{-1}((v_1+v_2)W)(t,\cdot)\|_{L^\infty(R^+)}\\&\leqslant\frac{3\sqrt{2}}{4}\|(v_1+v_2)(t,\cdot)\|_{L^2(R^+)}\|W(t,\cdot)\|_{L^\infty(R^+)}\\&\leqslant\frac{3\sqrt{2}}{4}\|(u_1+u_2)(t,\cdot)\|_{H^2(R^+)}\|W(t,\cdot)\|_{L^\infty(R^+)}\\&\leqslant\frac{3\sqrt{2}}{4}(\|u_1(t,\cdot)\|_{H^2(R^+)}+\|u_2(t,\cdot)\|_{H^2(R^+)})\|W(t,\cdot)\|_{L^\infty(R^+)},\end{aligned}\tag{3.32}$$

$$\|(1-\partial_{xx})^{-1}(W\partial_x(u_1+u_2))(t,\cdot)\|_{L^\infty(R^+)}$$
$$\leqslant \sup_{x\in R^+}\left(\int_0^\infty |h(x,y)|^2 dy\right)^{1/2}\|\partial_x(u_1+u_2)(t,\cdot)\|_{L^2(R^+)}\|W(t,\cdot)\|_{L^\infty(R^+)}$$
$$\leqslant\left(\frac{\sqrt{2}}{4}+\frac{1}{2}\right)(\|u_1(t,\cdot)\|_{H^2(R^+)}+\|u_2(t,\cdot)\|_{H^2(R^+)})\|W(t,\cdot)\|_{L^\infty(R^+)}, \tag{3.33}$$

$$\|(W\partial_x W)(t,\cdot)\|_{L^\infty(R^+)}\leqslant\|W(t,\cdot)\|_{L^\infty(R^+)}\|(\partial_x W)(t,\cdot)\|_{L^\infty(R^+)}$$
$$\leqslant\|W(t,\cdot)\|_{L^\infty(R^+)}\|W(t,\cdot)\|_{H^2(R^+)}\leqslant\|W(t,\cdot)\|_{L^\infty(R^+)}(\|u_1(t,\cdot)\|_{H^2(R^+)}+\|u_2(t,\cdot)\|_{H^2(R^+)}). \tag{3.34}$$

Putting all the estimates (3.28) and (3.30)–(3.34) together, we can find some constant C which depends only on $\|u_i\|_{L^\infty(0,T;H^2(R^+))}$ $(i=1,2)$, such that

$$\|W(t,\cdot)\|_{L^\infty(R^+)}\leqslant C\int_0^t\|W(s,\cdot)\|_{L^\infty(R^+)}ds,\forall t\in[0,T].$$

This yields, by Gronwall's inequality, that

$$\|W(t,\cdot)\|_{L^\infty(R^+)}=0,\forall t\in[0,T],$$

and so $W=0$, which completes the proof of the uniqueness.

Remark 2: The proof of uniqueness implies that for any $T>0$, if there exists a solution to (3.1) in $C([0,T];H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,T];H_0^1(R^+))$, then the solution must be unique.

IV. THE EXISTENCE AND UNIQUENESS OF THE GLOBAL SOLUTION TO PROBLEMS (1.1)–(1.3)

In this section we will show that the solution to (1.1)–(1.3) is global in-time provided u_0 satisfies a certain positivity condition.

Theorem 3: *Suppose that $u_0\in H^2(R^+)\cap H_0^1(R^+)$ and $V_0=(1-\partial_{xx})u_0\geqslant 0$. Then the unique strong solution to (1.1)–(1.3) exists globally in time.*

Proof: We proceed in four steps.

Step 1: First we mollify the initial data u_0.

Let $\rho(x)\in C_0^\infty(R^+):\rho(x)\geqslant 0,\int_{R^+}\rho(x)dx=1$, and $\rho_n(x)=n\rho(nx)$ be the usual mollifiers on R^+, $u_0^n=\rho_n^* u_0$, where $*$ denote the convolution. Then

$$u_0^n\to u_0 \text{ in } H^2(R^+)\cap H_0^1(R^+) \text{ and } \|u_0^n\|_{H^2(R^+)}\leqslant\|u_0\|_{H^2(R^+)}. \tag{4.1}$$

Note that $u_0\in H_0^1(R^+)$. We get $u_0^n\in\mathcal{B}$ and

$$V_0^n=(1-\partial_{xx})u_0^n=\rho_n*(1-\partial_{xx})u_0\geqslant 0.$$

For this $u_0^n\in\mathcal{B}$, it follows from Theorem 1 that there exists a unique solution to (1.4) such that

$$u^n(t,x)\in C([0,T^n);\mathcal{B})\cap C^1([0,T^n);H^2(R^+)\cap H_0^1(R^+)).$$

Let $V^n(t,x)=(1-\partial_{xx})u^n(t,x)$, then

$$u^n(t,x)=(1-\partial_{xx})^{-1}V^n(t,x)=\int_0^\infty h(x,y)V^n(t,y)dy.$$

Step 2: To prove that $V^n(t,x)\geqslant 0$.

Since $V^n(t,x)=(1-\partial_{xx})u^n(t,x)$, Eq. (3.3) can be rewritten as

$$\partial_t V^n + u^n \partial_x V^n = -2V^n \partial_x u^n. \tag{4.2}$$

It follows from Lemma 5 that the following problem:

$$\begin{cases} \dfrac{d\Phi^x(t)}{dt} = u^n(t,\Phi^x(t)), & t>0, \\ \Phi^x(0) = x, & x \geqslant 0, \end{cases}$$

has a unique solution $\Phi^x(t) \in C^1(0,T^n)$ and $x \in R^+ \to \Phi^x(t) \in R^+$ is an isomorphism. Set $S(t) = V^n(t,\Phi^x(t))$. Then $S(0) = V^n(0,x) = V_0^n(x)$ and

$$\begin{aligned} \frac{dS}{dt} = \partial_t V^n(t,\Phi^x(t)) + \partial_x V^n(t,\Phi^x(t)) \frac{d\Phi^x(t)}{dt} &= \partial_t V^n(t,\Phi^x(t)) + u^n(t,\Phi^x(t)) \partial_x V^n(t,\Phi^x(t)) \\ &= -2V^n(t,\Phi^x(t)) \partial_x u^n(t,\Phi^x(t)) \\ &= -2S \partial_x u^n(t,\Phi^x(t)), \end{aligned}$$

due to (4.2). From this and (3.26), we get

$$\partial_t \{S(t)[\partial_x \Phi^x(t)]^2\} = 0,$$

and so

$$S(t)[\partial_x \Phi^x(t)]^2 = S(0)[\partial_x \Phi^x(0)]^2 = S(0), \tag{4.3}$$

consequently $S(t) \geqslant 0$. Since $x \in R^+ \to \Phi^x(t) \in R^+$ is an isomorphism, we get that

$$V^n(t,x) \geqslant 0.$$

Step 3: To get some *a priori* estimates.
Since

$$\begin{aligned} u^n(t,x) &= \int_0^\infty h(x,y) V^n(t,y)\, dy \\ &= e^{-x}/2 \int_0^x e^y V^n(t,y)\, dy + e^x/2 \int_x^\infty e^{-y} V^n(t,y)\, dy - e^{-x}/2 \int_0^\infty e^{-y} V^n(t,y)\, dy, \end{aligned}$$

$$\partial_x u^n(t,x) = -e^{-x}/2 \int_0^x e^y V^n(t,y)\, dy + e^x/2 \int_x^\infty e^{-y} V^n(t,y)\, dy + e^{-x}/2 \int_0^\infty e^{-y} V^n(t,y)\, dy,$$

we get

$$u^n(t,x) + \partial_x u^n(t,x) = e^x \int_x^\infty e^{-y} V^n(t,y)\, dy \geqslant 0,$$

and so

$$\begin{aligned} -\partial_x u^n(t,x) \leqslant u^n(t,x) \leqslant \|u^n(t,x)\|_{L^\infty} &\leqslant \|u^n(t,x)\|_{H^1(R^+)} \\ &= \|u_0^n\|_{H^1(R^+)} \leqslant \|u_0^n\|_{H^2(R^+)} \leqslant \|u_0\|_{H^2(R^+)}. \end{aligned}$$

Then by multiplying $2V^n$ to (4.2), integrating the resulting identity over R^+ associated with x and performing integration by parts, we obtain

$$\frac{d}{dt}\|V^n(t,\cdot)\|^2_{L^2(R^+)}=-3\int_{R^+}(V^n(t,x))^2\partial_x u^n(t,x)dx\leqslant 3\|u_0\|_{H^2(R^+)}\|V^n(t,\cdot)\|^2_{L^2(R^+)}.$$

It follows from Gronwall's inequality that

$$\|V^n(t,\cdot)\|_{L^2(R^+)}\leqslant\|V_0^n\|_{L^2(R^+)}e^{3/2\|u_0\|_{H^2(R^+)}t}\leqslant\|u_0^n\|_{H^2(R^+)}e^{3/2\|u_0\|_{H^2(R^+)}t}\leqslant\|u_0\|_{H^2(R^+)}e^{3/2\|u_0\|_{H^2(R^+)}t},$$

and so

$$\|u^n(t,\cdot)\|_{H^2(R^+)}\leqslant\|V^n(t,\cdot)\|_{L^2(R^+)}\leqslant\|u_0\|_{H^2(R^+)}e^{3/2\|u_0\|_{H^2(R^+)}t}.$$

Consequently, $\forall T>0,\{u^n\}$ is uniformly bounded in $L^\infty(0,T;H^2(R^+)\cap H_0^1(R^+))$.

On the other hand,

$$\begin{aligned}\|\partial_t u^n\|_{L^\infty(0,T;L^2(R^+))}&\leqslant\|u^n\partial_x u^n\|_{L^\infty(0,T;L^2(R^+))}+\|\partial_x p^n\|_{L^\infty(0,T;L^2(R^+))}\\&\leqslant 2\sup_{0<t<T}\|u^n(t,\cdot)\|^2_{H^2(R^+)}\\&\leqslant 2\|u_0\|^2_{H^2(R^+)}e^{3\|u_0\|_{H^2(R^+)}T},\end{aligned}$$

that is, $\{\partial_t u^n\}$ is uniformly bounded in $L^\infty(0,T;L^2(R^+))$.

Step 4: Passing to the limit.

Since $\forall T>0$, $\{u^n\}$ and $\{\partial_t u^n\}$ are uniformly bounded in $L^\infty(0,T;H^2(R^+)\cap H_0^1(R^+))$ and $L^\infty(0,T;L^2(R^+))$, respectively, there exists a subsequence of $\{u^n\}$, still denoted by $\{u^n\}$, and some function $u\in L^\infty(R^+;H^2(R^+)\cap H_0^1(R^+))\cap C(R^+;C^1_{\mathrm{loc}}(R^+))$, $\partial_t u\in L^\infty(R^+,L^2(R^+))$ by the diagonal process of choice to $\{u^n\}$, such that

$$u^n\overset{*}{\rightharpoonup}u,\ \text{as}\ \ n\to\infty\ \ \text{in}\ \ L^\infty(0,T;H^2(R^+)\cap H_0^1(R^+)),\tag{4.4}$$

$$\partial_t u^n\overset{*}{\rightharpoonup}\partial_t u,\ \text{as}\ \ n\to\infty\ \ \text{in}\ \ L^\infty(0,T;L^2(R^+)),\tag{4.5}$$

$$u^n\to u,\ \text{as}\ \ n\to\infty\ \ \text{in}\ \ C([0,T];C^1_{\mathrm{loc}}(R^+)),\tag{4.6}$$

for any $T>0$. Then by the same method of passing to the limit in the proof of the existence of the local solution, we obtain $u\in C([0,T];H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,T];H_0^1(R^+))$, and

$$\partial_t u+u\partial_x u+\partial_x p=0,\ \text{a. e.}\ \ [0,T]\times R^+.$$

Since T is arbitrary, we get that $u\in C([0,\infty);H^2(R^+)\cap H_0^1(R^+))\cap C^1([0,\infty);H_0^1(R^+))$, and

$$\partial_t u+u\partial_x u+\partial_x p=0,\ \text{a. e.}\ \ [0,\infty)\times R^+,$$

which proves that the solution exists globally in time. Finally the solution must be unique due to Remark 2.

We complete the proof of Theorem 3.

Remark 3: The relation (4.3) is not accidental. It actually represents something fundamental in the periodic case, when the Camassa–Holm equation is a re-expression of geodesic flow on the diffeomorphism group of the circle endowed with the H^1-right-invariant metric; this geometric interpretation was first described by Misioek.[24] Within the geometric framework it turns out that this relation represents conservation of momentum and is a consequence of Noether's theorem.[25]

V. BLOW-UP

Theorem 4: *Let* $u_0 \in H^2(R^+) \cap H_0^1(R^+)$ *with* $\partial_x u_0(\overline{x}) \leqslant -\sqrt{2}\|u_0\|_{H^2(R^+)}$ *for some* $\overline{x} \in R^+$. *Then the strong solution to (1.1)–(1.3) blows-up in finite time.*

Proof: Let $S(t) = \partial_x u(t, x(t))$ with $x(0) = \overline{x}$. It follows from Lemma 5 that

$$\frac{dx(t)}{dt} = u(t, x(t)),$$

then

$$\frac{dS}{dt} = \partial_{xt} u + \partial_{xx} u \frac{dx(t)}{dt} = \partial_{xt} u + u \partial_{xx} u.$$

On the other hand, applying ∂_x to (1.1) we have

$$\partial_{xt} u = -(\partial_x u)^2 - u \partial_x u - \partial_{xx} p = -\tfrac{1}{2}(\partial_x u)^2 - u \partial_{xx} u - p + u^2.$$

Thus

$$\frac{dS}{dt} = -\frac{1}{2} S^2 + u^2 - p. \tag{5.1}$$

Observing that $p \geqslant 0$, expression (5.1) can be transformed in

$$\frac{dS}{dt} + \frac{1}{2} S^2 \leqslant u^2 \leqslant \|u(t, \cdot)\|^2_{L^\infty(R^+)} \leqslant \|u_0\|^2_{H^2(R^+)},$$

that is

$$\frac{dS}{dt} \leqslant \|u_0\|^2_{H^2(R^+)} - S^2/2.$$

Solving this inequality, we obtain

$$\frac{S_0 + k}{S_0 - k} e^{kt} - 1 \leqslant \frac{2k}{S - k},$$

where $k = \sqrt{2}\|u_0\|_{H^2(R^+)}$ and $S_0 = S(0) = \partial_x u(0, x(0)) = \partial_x u_0(\overline{x})$, and so

$$S \leqslant \frac{2k}{\dfrac{S_0 + k}{S_0 - k} e^{kt} - 1} + k.$$

Taking $T_0 = 1/k \ln (S_0 - k)/(S_0 + k) > 0$, we get

$$\lim_{t \to T_0^-} S(t) \leqslant \lim_{t \to T_0^-} \frac{2k}{\dfrac{S_0 + k}{S_0 - k} e^{kt} - 1} + k = -\infty,$$

which implies

$$\lim_{t \to T_0^-} \|u(t, \cdot)\|_{H^2(R^+)} = \infty,$$

since $|\partial_x u(t,x)| \leqslant \|\partial_x u(t,\cdot)\|_{L^\infty(R^+)} \leqslant \|u(t,\cdot)\|_{H^2(R^+)}$.

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Asymptotic analysis of field commutators for Einstein–Rosen gravitational waves

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We give a detailed study of the asymptotic behavior of field commutators for linearly polarized, cylindrically symmetric gravitational waves in different physically relevant regimes. We also discuss the necessary mathematical tools to carry out our analysis. Field commutators are used here to analyze microcausality, in particular the smearing of light cones owing to quantum effects. We discuss in detail several issues related to the semiclassical limit of quantum gravity, in the simplified setting of the cylindrical symmetry reduction considered here. We show, for example, that the small G behavior is not uniform in the sense that its functional form depends on the causal relationship between space–time points. We consider several physical issues relevant for this type of models such as the emergence of large gravitational effects. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Among the many symmetry reductions of general relativity that have been considered in the past, linearly polarized cylindrical waves (also known as Einstein–Rosen waves[1,2]) have been the focus of intensive study. They provide a model with an infinite number of degrees of freedom that can be exactly solved in spite of the fact that it is nonlinear. This is not only true classically but also quantum mechanically, and hence this system is a valuable tool to explore the physics that may be found if a successful quantization of full general relativity is ever achieved.[3–6]

One of the main reasons behind this success is the fact that the physical Hamiltonian is a function of the free Hamiltonian of a $2+1$ dimensional, axially symmetric, massless scalar field evolving in an auxiliary Minkowskian background.[4,5,7] In a previous paper[6] we took advantage of this fact to study the quantum corrections to the space–time structure by considering the commutator of this scalar field at different space–time points. As is well known, microcausality in quantum field theories can be discussed by looking at the commutator of quantum fields (or anticommutator in the case of fermions). In the standard examples the microcausality requirement means that this (anti)commutator must vanish for spatially separated space–time points. A similar argument can be made for vector fields, though issues of gauge invariance change some of the conclusions; in particular if one computes the commutator of the four-vector potential A_μ at two spatially separated points, it may be different from zero in some gauges, even though it is always true that the commutator of gauge invariant objects is zero for such points.

The issue of gauge invariance in the context of cylindrical gravitational waves has been discussed at length by Bičák and collaborators.[8] These authors show that is is legitimate to use the Ashtekar–Pierri gauge fixed action[3] written in terms of the scalar field that encodes the physical

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information in this model to obtain gauge invariant structures such as Dirac observables or the S matrix. This justifies the computation of the type of objects—field commutators—that we will be considering here to extract conclusions about the quantum structure of space–time.

The particular problem that we will be concerned with in this paper is the detailed study of the field commutator (given as a certain integral) and, in particular, its limiting behavior when the time and length separations are much larger than the natural length scale of the problem—the Planck length. In order to do this the procedure of expanding the integrand of the field commutator as a power series in the gravitational constant and other asymptotic parameters is not useful. In fact it will be necessary to adapt some methods developed for the asymptotic analysis of integrals and get a consistent procedure to expand the relevant objects as asymptotic series. It is possible to understand this *a posteriori* as a consequence of the fact that some limiting behaviors (i.e., in G) of the field commutator change in a nontrivial way as the space–time intervals go from spacelike to timelike or when one of the space–time points lies in the symmetry axis. Also the functional dependence in some of these parameters is highly nonpolynomial. This is not what one would expect to obtain in the familiar perturbative treatment of quantum field theories (QFT's).

The paper is divided in two main sections: A physical discussion of the behavior of the field commutator followed by a detailed description of the asymptotic methods necessary to study the different physically relevant regimes. Specifically, after this introduction we will give the different asymptotic expansions for all the relevant parameters (involving the $G\rightarrow 0$ limit and also the limits in which the difference in the time coordinates or the radial coordinates go to infinity). Using them we will discuss the main physical consequences of the quantization of this model as far as microcausality is concerned. In this respect it is particulary interesting to point out the existence of a certain type of large quantum mechanical effects (in a sense that will be made precise later) when one of the space–time points in the field commutator lies in the symmetry axis.

A technical issue that should be considered is the role of regulators in the final physical results. As is well known regulators are necessary to give sense to otherwise ill-defined objects. They must be introduced, for example, to obtain a finite norm vector by acting with the field operator on the vacuum state. Cutoffs are a simple way to regulate amplitudes. It is conceivable that physical regulators exist that restrict, for example, the integration intervals for some physical objects (such as the field commutators considered here) to finite real intervals. However, it is also possible that they are just a convenient way to render some physical objects finite in such a way that no footprint is left in the final results. This is the philosophy that one has in mind in the usual renormalization scheme where cutoffs are taken to infinity and disappear from physical quantities.

The point of view of this paper is that the un-regulated objects (integrals), when defined, are a good approximation to the regulated ones. The asymptotic analysis of regulated commutators and their relation with the un-regulated ones will be discussed elsewhere.

In the usual perturbative QFT computations Green functions, matrix elements, and similar objects are expanded as power series in the coupling constants of the model with coefficients that are usually written as regulated integrals. This is a necessary step because it is usually not possible to write them in closed form. Here the situation is different because it is possible to write down expressions for the objects of interest (field commutators in the present example) that depend on the coupling constants in a nontrivial way. This has the advantage of allowing us to use approximation techniques specially adapted to their specific form and much better suited to its study. It also permits to consider some problems that may be difficult to tackle for the usual QFT's; for example, one can try to figure out if the asymptotic behavior of some regulated object coincides with its asymptotic behavior after the regulator is removed.

A detailed technical discussion of the techniques needed to explore the relevant asymptotic regimes is presented in Sec. III. These techniques will be useful tools in order to analyze other types of physical objects (such as S-matrix elements) so they provide the necessary background for a perturbative framework properly adapted to this model; this is why we invest some time to study them here. We end the paper with a summary of the main results, comments, perspectives for future work, and several appendices. Numerical and algebraic computations have been performed with the aid of MATHEMATICA®.

II. THE FIELD COMMUTATOR

We start with a brief description of the model and introduce our conventions and notation. As is well known[1,2,9] Einstein–Rosen waves correspond to topologically trivial space–times with two linearly independent, commuting, spacelike, and hypersurface orthogonal Killing vector fields. The metric in this case can be writen as

$$ds^2 = e^{\gamma-\psi}(-dT^2+dR^2)+e^{-\psi}R^2 d\theta^2+e^{\psi}dZ^2, \tag{1}$$

where we are using coordinates (T,R,θ,Z), $T\in\mathbb{R}$, $R\in[0,\infty)$, $\theta\in[0,2\pi)$, $Z\in\mathbb{R}$, and ψ and γ are functions only of R and T. The Einstein field equations for this metric are very simple: The scalar field ψ must satisfy the wave equation for a massless, axially symmetric scalar field in three dimensions

$$\partial_T^2\psi-\partial_R^2\psi-\frac{1}{R}\partial_R\psi=0,$$

and the function γ can be expressed in terms of this field on the classical solutions[3,5] as

$$\gamma(R)=\frac{1}{2}\int_0^R d\overline{R\,R}\,[(\partial_T\psi)^2+(\partial_{\overline{R}}\psi)^2].$$

Throughout the paper we will use a system of units such that $c=\hbar=1$ and define $G\equiv\hbar G_3$, where G_3 denotes the gravitational constant per unit length in the direction of the symmetry axis.[16] The metric function $\gamma(R)$ admits a simple physical interpretation: Apart from a factor of $8G$ it is the energy of the scalar field in a ball of radius R, and $\gamma_\infty\equiv\lim_{R\to\infty}\gamma(R)$ the energy of the whole two-dimensional flat space. Furthermore, $\gamma_\infty/(8G)$ coincides with the Hamiltonian H_0 of the system obtained by linearizing the metric (1).[3,6]

In order to arrive at a unit asymptotic timelike Killing vector that allows us to introduce a physical notion of energy (per unit length) it is convenient to use coordinates (t,R,θ,Z) defined by $T=e^{-\gamma_\infty/2}t$. In these coordinates the metric takes the form[2,9]

$$ds^2=e^{\gamma-\psi}(-e^{-\gamma_\infty}dt^2+dR^2)+e^{-\psi}R^2d\theta^2+e^{\psi}dZ^2.$$

By choosing a metric function ψ with a sufficiently fast fall-off as $R\to\infty$, this metric describes asymptotically flat space–times with a certain (nonzero) deficit angle and such that ∂_t is a unit timelike Killing vector in the asymptotic region.

The Einstein field equations can be obtained from a Hamiltonian action principle[9–11] where the Hamiltonian H is a function of that corresponding to the free scalar field, H_0:

$$H=E(H_0)=\frac{1}{4G}(1-e^{-4GH_0}).$$

In the following we will refer to t as the physical time and to H as the physical Hamiltonian.

In terms of the T-time and imposing that ψ be regular at $R=0$,[3] the classical solutions for the field ψ can be written as

$$\psi(R,T)=\sqrt{4G}\int_0^\infty dk\,J_0(Rk)[A(k)e^{-ikT}+A^\dagger(k)e^{ikT}],$$

where $A(k)$ [and its complex conjugate $A^\dagger(k)$] are determined by the initial conditions.[17] The free Hamiltonian H_0 can be written now as

$$\gamma_\infty=H_0=\int_0^\infty dk\,kA^\dagger(k)A(k).$$

Using this expression, we can obtain the t-evolution of the field

$$\psi_E(R,t)=\sqrt{4G}\int_0^\infty dk\, J_0(Rk)[A(k)e^{-ikte^{-\gamma_\infty/2}}+A^\dagger(k)e^{ikte^{-\gamma_\infty/2}}].$$

The quantization can be carried out by following the usual steps. We introduce a Fock space in which $\hat{\psi}(R,0)$, the quantum counterpart of $\psi(R,0)$, is an operator-valued distribution.[12] Its action is determined by those of $\hat{A}(k)$ and $\hat{A}^\dagger(k)$, the annihilation and creation operators with nonvanishing commutators given by

$$[\hat{A}(k_1),\hat{A}^\dagger(k_2)]=\delta(k_1,k_2).$$

Explicitly,

$$\hat{\psi}(R,0)=\hat{\psi}_E(R,0)=\sqrt{4G}\int_0^\infty dk\, J_0(Rk)[\hat{A}(k)+\hat{A}^\dagger(k)].$$

Evolution in T is given by the unitary operator $\hat{U}_0(T)=\exp(-iT\hat{H}_0)$ where

$$\hat{H}_0=\int_0^\infty dk\, k\,\hat{A}^\dagger(k)\hat{A}(k)$$

is the quantum Hamiltonian operator of a three-dimensional, axially symmetric scalar field. The quantum scalar field in the Heisenberg picture is hence given by

$$\hat{\psi}(R,T)=\hat{U}_0^\dagger(T)\,\hat{\psi}(R,0)\hat{U}_0(T)=\sqrt{4G}\int_0^\infty dk\, J_0(Rk)[\hat{A}(k)e^{-ikT}+\hat{A}^\dagger(k)e^{ikT}].$$

If we choose the physical time t to define the evolution in our model, the quantum Hamiltonian is $\hat{H}=E(\hat{H}_0)=(1-e^{-4G\hat{H}_0})/(4G)$ and unitary evolution is given by $\hat{U}(t)=\exp(-it\hat{H})$. With this time evolution the annihilation and creation operators in the Heisenberg picture are

$$\hat{A}_E(k,t)\equiv\hat{U}^\dagger(t)\hat{A}(k)\hat{U}(t)=\exp[-itE(k)e^{-4G\hat{H}_0}]\hat{A}(k),$$

$$\hat{A}_E^\dagger(k,t)=\hat{A}^\dagger(k)\exp[itE(k)e^{-4G\hat{H}_0}],$$

where $E(k)=(1-e^{-4Gk})/(4G)$, and the field operator evolved with the physical Hamiltonian [that we denote as $\hat{\psi}_E(R,t)$] is given by

$$\hat{\psi}_E(R,t)=\sqrt{4G}\int_0^\infty dk\, J_0(Rk)[\hat{A}_E(k,t)+\hat{A}_E^\dagger(k,t)].$$

The field commutator $[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]$ can be computed from these expressions.[6] One of its interesting features is the fact that it is not proportional to the identity as in the case of free theories (or if we consider the quantum evolution defined by the Hamiltonian H_0 of the linearized model) but is a nondiagonal operator in the chosen basis. We are hence led to consider its matrix elements. We will concentrate here on the most relevant of these elements (at least from the perspective of the microcausality of the classical background of the model), namely the vacuum expectation value, which is explicitly given by

$$\frac{1}{8iG}\langle 0|\,[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]\,|0\rangle=\int_0^\infty dk\, J_0(R_1k)J_0(R_2k)\sin\left[\frac{t_2-t_1}{4G}(1-e^{-4Gk})\right]. \quad (2)$$

As we can see it depends on the time coordinates through their difference t_2-t_1 (which we will assume to be, e.g., positive) and depends symmetrically on R_1 and R_2. The functional dependence in G is less trivial, a fact that will require special attention when studying the limit in which the relevant lengths and time differences are much larger than the Planck length. For comparison purposes we remember that

$$\frac{1}{8iG}\langle 0|\,[\hat{\psi}(R_1,T_1),\hat{\psi}(R_2,T_2)]\,|0\rangle=\int_0^\infty dk\,J_0(R_1k)J_0(R_2k)\sin[k(T_2-T_1)]. \tag{3}$$

In the following it will be convenient to refer the dimensional parameters of the integral to another length scale that we choose as R_1. We hence define $R_2=\rho R_1$, $t_2-t_1=\tau R_1$, $\lambda=R_1/(4G)$ and rewrite (2) as

$$\frac{1}{8iG}\langle 0|\,[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]\,|0\rangle=\frac{\lambda}{R_1}\Im\left\{\int_0^\infty dq J_0(\lambda q)J_0(\rho\lambda q)e^{i\tau\lambda(1-e^{-q})}\right\}, \tag{4}$$

after introducing the new variable $k=q/(4G)$. Here $\Im$ denotes the imaginary part.

A. Asymptotic behavior in ρ: Smearing of light cones

The integral (4) can be written as a standard h-transform,[14] with asymptotic parameter ρ, by the change of variables $t=q\lambda$,

$$\frac{1}{R_1}\Im\left\{\int_0^\infty dt\,J_0(\rho t)J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})}\right\}. \tag{5}$$

In this case a straightforward Mellin transform analysis[14] (discussed in Sec. III) gives the following asymptotic behavior in the $\rho\to\infty$ limit

$$\begin{aligned}&\frac{1}{R_1}\Im\left\{\frac{1}{\rho}+\frac{1}{\rho^3}\left(\frac{1}{4}+\frac{\tau^2}{2}+\frac{i\tau}{2\lambda}\right)+\frac{9}{\rho^5}\left(\frac{1}{64}-\frac{i\tau}{24\lambda^3}+\frac{i\tau}{8\lambda}+\frac{\tau^2}{8}+\frac{i\tau^2}{4\lambda}-\frac{7\tau^2}{24\lambda^2}+\frac{\tau^4}{24}\right)+O\left[\frac{1}{\rho^7}\right]\right\}\\&\quad=\frac{1}{R_1}\left\{\frac{\tau}{2\lambda\rho^3}+\frac{1}{\rho^5}\left(\frac{9\tau}{8\lambda}-\frac{3\tau}{8\lambda^3}+\frac{9\tau^2}{4\lambda}\right)+O\left[\frac{1}{\rho^7}\right]\right\}.\end{aligned} \tag{6}$$

The asymptotic behavior in the $\rho\to\infty$ limit gives a precise and quantitative description of the smearing of (cylindrically symmetric) light cones because it shows, for example, that for fixed values of R_1 and t_2-t_1 the expectation value of the commutator (over $8iG$) falls off for large values of R_2 as

$$\frac{2G(t_2-t_1)}{R_2^3}+O\left[\frac{1}{R_2^5}\right].$$

This means that even for large spatial separations the scalar field that encodes the gravitational field does not commute with itself.

In the $\rho\to 0^+$ limit, on the other hand, we get

$$\frac{1}{R_1}\Im\left\{\int_0^\infty dt J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})}\right\}+O(\rho). \tag{7}$$

This shows that the commutator is a continuous function of ρ in $\rho=0$, a fact that will be important in the analysis of the semiclassical limit.

B. Asymptotic behavior in τ: Large quantum gravity effects

The integral in (5) has the convenient form of a h-transform if the asymptotic parameter is chosen to be ρ; however, this is no longer true if the asymptotic parameter is τ (which corresponds to considering large separations in the time coordinates). This introduces some mathematical difficulties in the asymptotic analysis that will be discussed later.

In this case one has to perform separate analyses for $\rho=0$ and $\rho\neq 0$. In $\rho=0$ one finds that the asymptotic behavior when $\tau\to\infty$ is given by

$$\frac{1}{R_1}\left[\frac{\lambda}{2\pi\log\tau}\right]^{1/2}\Im\{e^{i[\pi/4+\tau\lambda-\lambda\log(\tau\lambda)]}e^{(\pi/2)\lambda}\Gamma(i\lambda)+e^{-i[\pi/4-\tau\lambda-\lambda\log(\tau\lambda)]}e^{-(\pi/2)\lambda}\Gamma(-i\lambda)\}$$
$$+O\left[\frac{1}{(\log\tau)^{3/2}}\right], \tag{8}$$

whereas for $\rho\neq 0$ we find

$$\frac{1}{2\pi R_1\sqrt{\rho}\log\tau}\Im\{e^{i[\pi/2+\tau\lambda-\lambda(1+\rho)\log(\tau\lambda)]}e^{(\pi/2)\lambda(1+\rho)}\Gamma[i\lambda(1+\rho)]$$
$$+e^{-i[\pi/2-\tau\lambda-\lambda(1+\rho)\log(\tau\lambda)]}e^{-(\pi/2)\lambda(1+\rho)}\Gamma[-i\lambda(1+\rho)]$$
$$+e^{i[\tau\lambda-\lambda(1-\rho)\log(\tau\lambda)]}e^{(\pi/2)\lambda(1-\rho)}\Gamma[i\lambda(1-\rho)]$$
$$+e^{i[\tau\lambda-\lambda(\rho-1)\log(\tau\lambda)]}e^{(\pi/2)\lambda(\rho-1)}\Gamma[i\lambda(\rho-1)]\}+O\left[\frac{1}{(\log\tau)^2}\right]. \tag{9}$$

The most striking feature of these expressions is the unusual dependence on the asymptotic parameter τ; in fact the dependence on inverse powers of logarithms (especially on the inverse square root of $\log\tau$) cannot be obtained by direct application of the usual asymptotic expressions derived by Mellin transform techniques. It is also remarkable how slowly the commutator decays in τ—in particular in the axis $\rho=0$—a fact that is suggestive of the large quantum gravity effects discussed by Ashtekar in Ref. 4. Outside the axis the decay is quicker but still rather slow. A consequence of the different asymptotic behaviors in τ for $\rho=0$ and $\rho\neq 0$ is the impossibility to recover (8) as the limit when $\rho\to 0$ of (9). It is interesting to point out that the frequency of the oscillations of the commutator in the τ parameter is controlled by the value of λ (proportional to the inverse of G) in such a way that although the amplitude of the oscillations decays very slowly they will average to the value of the free commutator on scales much larger than the Planck length.

The $\tau\to 0$ limit is simpler to analyze. Actually we find that the series obtained by expanding $e^{i\tau\lambda(1-e^{-t/\lambda})}$ as a power series in $e^{-t/\lambda}$, exchanging integration and infinite sum, and computing the resulting integrals gives an expansion that converges to the value of the commutator.

C. Asymptotic behavior in λ: The semiclassical limit

The possibility of studying the asymptotic behaviors in ρ and τ by using the powerful mathematical tools provided by the theory of Mellin transforms relies on the fact that these integrals can be written as h-transforms of the type mentioned above. However, this is no longer possible if one wants to study the limit $\lambda\to\infty$ (corresponding to the situation when R_1 is much larger than the Planck length) because of the particular dependence of these integrals on λ. There is, however, a way out of this if one is willing to abandon Mellin transforms: writing the integral in (4) as a multiple integral by introducing the integral representation of the Bessel functions J_n $(n=0,1,\ldots)$,

$$J_n(z)=\frac{1}{2\pi i}\oint_\gamma \frac{dt}{t^{n+1}}e^{(z/2)(t-1/t)},$$

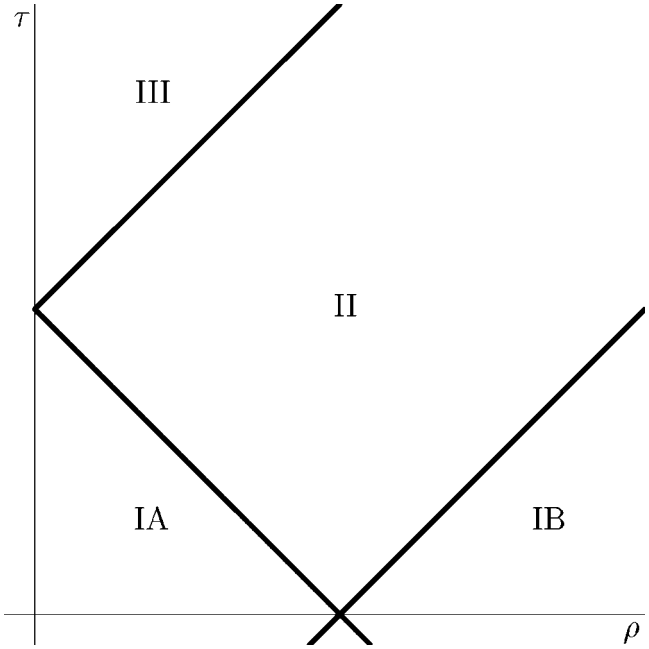

FIG. 1. Regions in the (ρ, τ) plane used in the discussion of the λ asymptotics. Region I corresponds to $0<\tau<|\rho-1|$, region II to $|\rho-1|<\tau<\rho+1$, and region III to $\rho+1<\tau$.

where γ is a closed, positively oriented, simple path in the complex plane surrounding the origin. By doing this the right hand side (r.h.s.) of (4) can be rewritten in the following form:

$$-\frac{1}{R_1}\Im\left\{\frac{\lambda e^{i\tau\lambda}}{4\pi^2}\int_0^\infty dq\oint_{\gamma_1}dt_1\oint_{\gamma_2}dt_2\frac{1}{t_1t_2}e^{\lambda[(q/2)(t_1-1/t_1)+(\rho q/2)(t_2-1/t_2)-i\tau e^{-q}]}\right\}. \tag{10}$$

Although the contours γ_1 and γ_2 may be different in principle we will take them equal in practice. Besides, we will see in the next section that it is convenient to choose them in a specific way.

As in the τ case one has to perform separate asymptotic analyses for $\rho=0$ and $\rho\neq 0$. In order to proceed it is necessary to divide the (ρ, τ) plane into the same regions that appear in the discussion of the ''free'' commutator[6] (3) which corresponds to the evolution dictated by the Hamiltonian H_0 (see Fig. 1).

In $\rho=0$ one finds that the asymptotic behavior when $\lambda\to\infty$ is given by

$$\frac{1}{R_1}\Im\left\{\frac{i}{\sqrt{\tau^2-1}}+\frac{e^{i\lambda[\tau-\log\tau-1]}}{\sqrt{\log\tau}}\right\}+O\left[\frac{1}{\lambda}\right]\quad \tau>1, \tag{11}$$

$$\frac{1}{R_1}\frac{\tau(1+2\tau^2)}{2\lambda(1-\tau^2)^{5/2}}+O\left[\frac{1}{\lambda^2}\right]\qquad \tau<1. \tag{12}$$

If $\rho\neq 0$ the asymptotic behavior in the different regions shown in Fig. 1 is the following: Regions IA and IB

$$\frac{\tau}{2\pi R_1\lambda}\left\{\frac{2[1+\rho^4+2\tau^2-3\tau^4+2\rho^2(\tau^2-1)]\sqrt{(1+\rho)^2-\tau^2}}{(1+\rho-\tau)^2(1-\rho+\tau)^2(-1+\rho+\tau)^2(1+\rho+\tau)^2}E\left(\sqrt{\frac{4\rho}{(1+\rho)^2-\tau^2}}\right)\right.$$

$$\left.-\frac{2\tau^2}{[\rho^4+(\tau^2-1)^2-2(1+\tau^2)\rho^2]\sqrt{(1+\rho)^2-\tau^2}}K\left(\sqrt{\frac{4\rho}{(1+\rho)^2-\tau^2}}\right)\right\}+O\left[\frac{1}{\lambda^2}\right]. \tag{13}$$

Region II

$$\frac{1}{\pi R_1\sqrt{\rho}}K\left(\sqrt{\frac{\tau^2-(\rho-1)^2}{4\rho}}\right)+\frac{1}{R_1}\Im\left\{\frac{e^{-i\,\pi/4}e^{i\lambda[\tau+|\rho-1|(1+\log\tau/|\rho-1|)]}}{\sqrt{2\pi\lambda\rho|1-\rho|}\log\dfrac{\tau}{|1-\rho|}}\right\}+O\left[\frac{1}{\lambda^{3/2}}\right]. \quad (14)$$

Region III

$$\frac{2}{\pi R_1}\frac{1}{\sqrt{\tau^2-(1-\rho)^2}}K\left(\sqrt{\frac{4\rho}{\tau^2-(1-\rho)^2}}\right)+\frac{1}{R_1}\Im\left\{\frac{e^{-i\,\pi/4}e^{i\lambda[\tau-|\rho-1|(1+\log\tau/|\rho-1|)]}}{\sqrt{2\pi\lambda\rho|1-\rho|}\log\dfrac{\tau}{|1-\rho|}}\right.$$
$$\left.+\frac{e^{i\pi/4}e^{i\lambda[\tau+(\rho+1)(\log(1+\rho/\tau)-1)]}}{\sqrt{2\pi\lambda\rho(1+\rho)}\log\dfrac{\tau}{1+\rho}}\right\}+O\left[\frac{1}{\lambda^{3/2}}\right]. \quad (15)$$

Here $K(k)$ and $E(k)$ denote the complete elliptic integrals of the first and second kind, respectively, defined by

$$K(k)\equiv\int_0^{\pi/2}\frac{d\theta}{\sqrt{1-k^2\sin^2\theta}},\qquad E(k)\equiv\int_0^{\pi/2}d\theta\sqrt{1-k^2\sin^2\theta}.$$

Some comments are in order now. The first is that the λ independent terms in the above expressions correspond to the commutator obtained from the free Hamiltonian H_0 both in the axis and outside the axis. The remaining terms (except when $\rho=0$ and $\tau>1$) are corrections to this free commutator that fall off to zero as $\lambda\to\infty$, and have an additional, non-polynomial dependence in $1/\lambda$. Since the free commutator defines a characteristic light cone structure these terms are responsible for the smearing of the light cones in this model. It is worthwhile pointing out that the asymptotic behavior in λ is different in regions I, II, III, and in the axis—this is the reason that explains the appearance of singularities in the borders between adjacent regions[18]—and it has a nonpolynomial dependence on $1/\lambda$. This kind of behavior cannot possibly appear in an ordinary perturbative QFT where the relevant objects (propagators, Green's functions, and so on) are expanded as power series in the coupling constants. One of the novel features of the approach that we follow in this paper is that by using more sophisticated approximation techniques, and taking advantage of the fact that we have closed explicit expressions for the objects of interest, we are able to extract such nontrivial behaviors. In the axis we notice that for $\tau>1$ there is a λ-independent contribution that corresponds to the free commutator and an oscillating contribution with a frequency that depends on λ (this term is similar to the one obtained in the asymptotic analysis for τ). For large values of λ this term oscillates very fast and averages to zero. For $\tau<1$ we get a correction to the free commutator (which is zero in region I) that goes to zero as $1/\lambda$. Outside the axis we see that the corrections to the free commutator fall-off as $1/\lambda$ in region I—outside the light cone—but only as $1/\sqrt{\lambda}$ (with the additional non-polynomial terms) in regions II and III. The presence of two oscillating terms in region III produces some interference effects that manifest themselves as a checkered pattern in plots of the commutator—especially close to the axis—which suggests a division of space–time into cells of a size governed by the value of the gravitational constant (through λ). These are shown in Fig. 2 where we plot the free commutator over $8iG$ plus the first asymptotic correction, given by the above expressions in each of the regions. For comparison we also display a plot constructed with the power series representation obtained in Ref. 6:

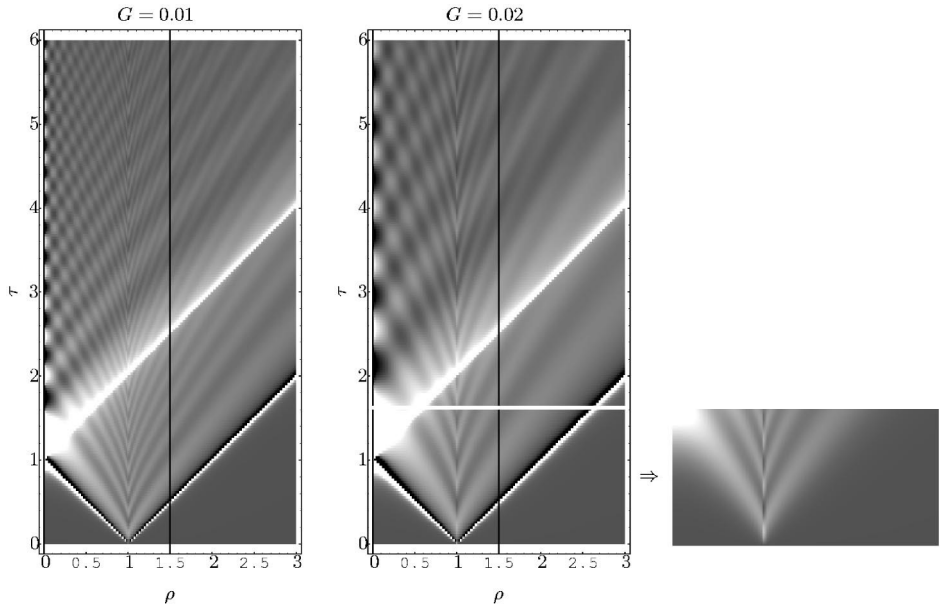

FIG. 2. Density plot of the asymptotic approximation in λ for the field commutator (over $8iG$) as a function of (ρ, τ) for $G=0.01$ and $G=0.02$. Notice the singular behavior of the approximation in the boundaries between the regions I, II, and III, and on the axis. For comparison we show part of the plot for $G=0.02$ obtained with the series expansion (16). Sections of these plots for $\rho=0$ and $\rho=1.5$ with $G=0.02$ are shown in Figs. 3 and 4.

$$\frac{1}{\pi R_1\sqrt{\rho}}\left\{\sin(\lambda\tau)\sum_{n=0}^{\infty}\frac{(-1)^n(\lambda\tau)^{2n}}{(2n)!}Q_{-1/2}[\sigma_{2n}(\rho)]\right.$$
$$\left.-\cos(\lambda\tau)\sum_{n=0}^{\infty}\frac{(-1)^n(\lambda\tau)^{2n+1}}{(2n+1)!}Q_{-1/2}[\sigma_{2n+1}(\rho)]\right\}, \tag{16}$$

where

$$\sigma_n(\rho)=\frac{n^2+\lambda^2(1+\rho^2)}{2\rho\lambda^2},$$

and $Q_{-1/2}(x)=\pi F(3/4,1/4;1;1/x^2)/\sqrt{2x}$ [for $x>1$] is the associated Legendre function of the second kind.[13] As can be seen, the result of the asymptotic approximation matches that obtained with the power series expansion (16).[19] In Figs. 3 and 4 we also plot the commutator as a function of τ for $\rho=0$ and a value of ρ different from zero. It is interesting to point out that, as τ grows, a distinctive beating pattern appears due to the interference of terms in the asymptotic expressions for region III mentioned above.

Comparison with the results of numerical integration confirm the accuracy of the approximation provided by the asymptotic expressions, as long as one is far enough from the boundary between regions. This is shown in Figs. 3 and 4, where we compare the asymptotic approximation with the result obtained by numerically computing the field commutator at $\rho=0$ and $\rho=1.5$.

The limit $\lambda\to 0$ is directly obtained by truncating (16) to the desired number of terms.

III. ASYMPTOTIC ANALYSIS: MATHEMATICAL DETAILS

We discuss in detail here the techniques used to obtain the asymptotic expansions discussed in the previous section. Even though we will be mostly employing standard techniques it is nonetheless necessary to adapt them to the different parameters that appear in the problem, (ρ, τ, λ).

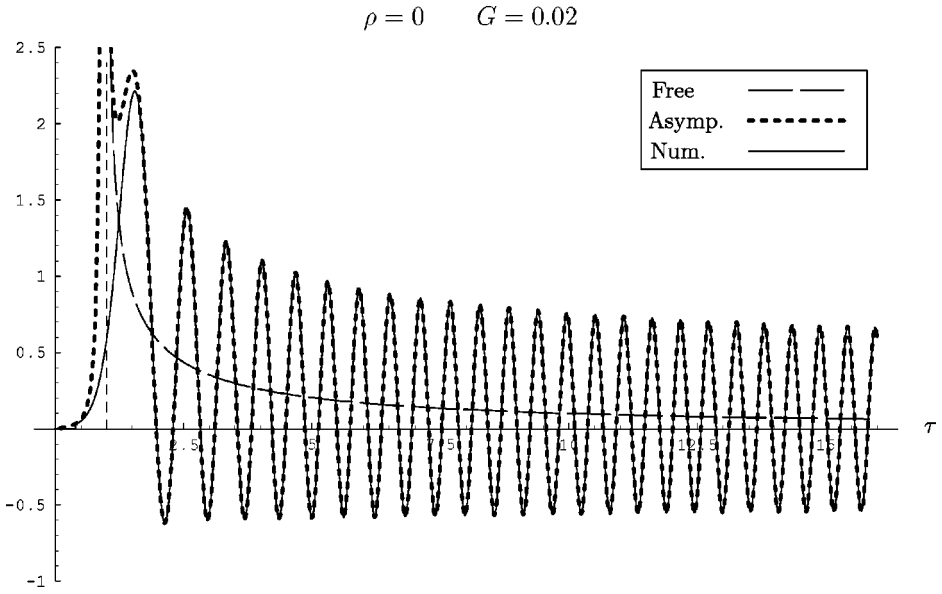

FIG. 3. Asymptotic approximation in λ for the field commutator (over $8iG$) as a function of τ for $\rho=0$ and $G=0.02$. We plot, for comparison, the commutator corresponding to the free Hamiltonian discussed in Ref. 6. The solid line corresponds to a numerical computation of (4). As can be seen the asymptotic approximation is very good for most of the values of τ.

Before studying the asymptotic expansions we present some results on Mellin transforms and explain the basics of their use to obtain the asymptotic behavior of integrals.

Whenever possible it will prove useful to write the integrals under consideration as h-transforms, i.e., objects of the type

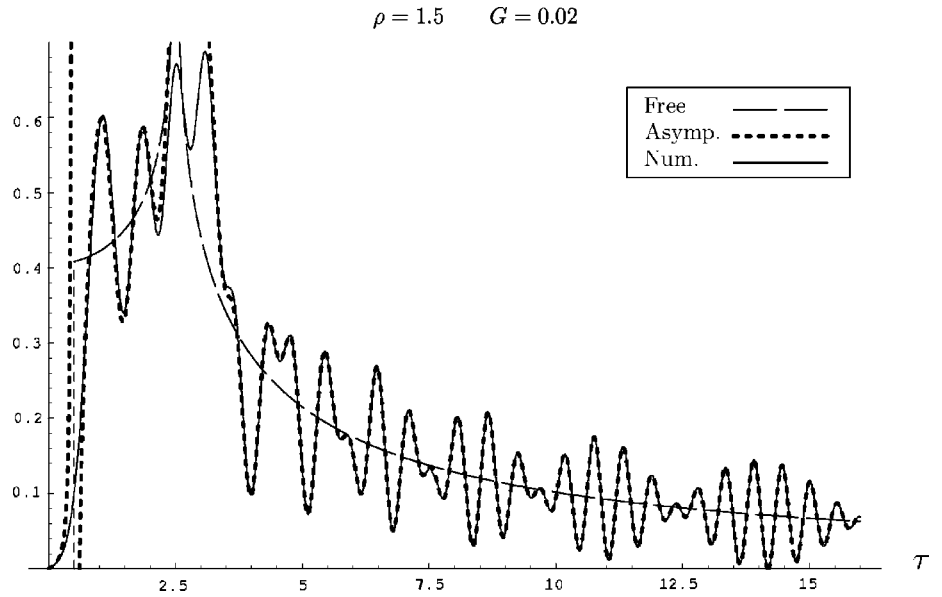

FIG. 4. Asymptotic approximation in λ for the field commutator (over $8iG$) as a function of τ for $\rho=1.5$ and $G=0.02$. We plot, as before, the contribution corresponding to the free Hamiltonian and a numerical computation of the commutator.

$$H[f;\zeta] := \int_0^\infty h(\zeta t) f(t) dt,$$

where ζ is the asymptotic parameter (that in practice approaches either 0 or ∞) and f and h are locally integrable functions in $(0,\infty)$ [functions that are integrable in every closed interval in $(0,\infty)$]. This will allow us, in many cases, to employ standard asymptotic techniques (see, e.g. Ref. 14) based on Mellin transforms[20] that can be summarized in the following.

Theorem: *Let $h:(0,\infty)\mapsto\mathbb{C}$ and $f:(0,\infty)\mapsto\mathbb{C}$ be locally integrable functions. Let us assume that they, respectively, have the following asymptotic expansions when $t\to\infty$ and $t\to 0^+$:*

$$h(t) \sim e^{-dt^\nu} \sum_{m=0}^{\infty} \sum_{n=0}^{N(m)} c_{mn} t^{-r_m} (\log t)^n \tag{17}$$

[$\Re(d)\geqslant 0$, $\nu>0$, $\Re(r_m)$ grows monotonically to ∞, and $N(m)>0$ is a finite integer for each value of m] and

$$f(t) \sim e^{-qt^\mu} \sum_{m=0}^{\infty} \sum_{n=0}^{\bar{N}(m)} p_{mn} t^{a_m} (\log t)^n \tag{18}$$

[$\Re(q)\geqslant 0$, $\mu>0$, $\Re(a_m)$ grows monotonically to ∞ and $\bar{N}(m)>0$ is a finite integer for each value of m].

Let $M[h;z]$ and $M[f;z]$ be the Mellin transforms of h and f (in the generalized sense, see Ref. 14 for details), holomorphic in the strips $\alpha<\Re(z)<\beta$ and $\gamma<\Re(z)<\delta$ that we assume overlapping. Let us suppose also that the Parseval identity holds:[21]

$$H[f;\zeta] = \frac{1}{2\pi i} \int_{r-i\infty}^{r+i\infty} dz\, \zeta^{-z} M[h;z] M[f;1-z] \equiv \frac{1}{2\pi i} \int_{r-i\infty}^{r+i\infty} dz\, \zeta^{-z} G(z), \tag{19}$$

with r in the intersection of the holomorphicity strips. If $\lim_{|y|\to\infty} G(x+iy)=0$ for each $x\in[r,R]$, $(R\in\mathbb{R})$ and $\int_{-\infty}^{\infty} dy |G(R+iy)|$ is finite then

$$H[f;\zeta] \sim -\sum_{r<\Re(z)<R} \operatorname{res}(\zeta^{-z} M[h;z] M[f;1-z]),$$

is a finite asymptotic expansion of $H[f;\zeta]$ as $\zeta\to\infty$ with respect to the asymptotic sequence $\Phi_{j,m}(\zeta)=\{\zeta^{-\alpha_j}(\log\zeta)^{n_j-m}\}$, $m=0,1,\ldots,n$, $j=0,1,\ldots$ with error $O(\zeta^{-R})$. If the previous hypotheses hold for arbitrary values of R we get an asymptotic expansion with an infinite number of terms.

In the following we will only need to consider the case when $d\neq 0$ and $q=0$. The result of the previous theorem can be written as

$$H[f;\zeta] \sim \sum_{m=0}^{\infty} \zeta^{-1-a_m} \sum_{n=0}^{\bar{N}(m)} p_{mn} \sum_{j=0}^{n} \binom{n}{j} (-\log\zeta)^j M^{(n-j)}[h;z]\big|_{z=1+a_m}, \tag{20}$$

with $M^{(k)}[h;z]$ denoting the kth derivative of the Mellin transform with respect to to z.

A. Asymptotic behavior in ρ

We write the integral that gives the field commutator in the form (5) and choose ρ as the asymptotic parameter. In order to apply the previous theorem we need the asymptotic expansion of $f(t)=J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})}$ as $t\to 0^+$ and the Mellin transform of $h(t)=J_0(t)$. From the first we get $a_k=k$ $(k=0,1,\ldots)$, $p_{00}=1, p_{10}=i\tau$, etc. The Mellin transform of h is given by

$$M[h;z]=\frac{2^{z-1}\Gamma(z/2)}{\Gamma(1-z/2)}.$$

Since $M[h;k]=0$ for even values of k, we get the asymptotic expansion in odd powers of $1/\rho$ given in (6).

In order to obtain the asymptotic expansion of the commutator when $\rho\to 0^+$ we change variables in (5) according to $s=\rho t$,

$$\frac{1}{\rho R_1}\Im\left\{\int_0^\infty ds\, J_0(s)J_0\left(\frac{s}{\rho}\right)e^{i\tau\lambda(1-e^{-s/\rho\lambda})}\right\},$$

take $1/\rho$ as the asymptotic parameter, and switch the roles[14] of f and h [$f(s)=J_0(s)$, $h(s)=J_0(s)e^{i\tau\lambda(1-e^{-s/\lambda})}$]. The Mellin transform of h is given now by

$$M[h;z]=\int_0^\infty dt\, t^{z-1}J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})},$$

which converges in the strip $0<\Re(z)<3/2$. We do not know any closed expression for this integral but it suffices to obtain the first term of the asymptotic expansion of the commutator when $\rho\to 0^+$. The asymptotic expansion of f gives now $a_k=2k$ $(k=0,1,\ldots)$, $p_{00}=1, p_{10}=-1/4$, etc. and using the theorem we obtain the expansion (7). Under mild restrictions[14] it can be shown that $M[h;z]$ admits an analytic continuation for $\Re(z)\to\infty$ which is meromorphic, at worst, in the complex plane, and that can be used to get further terms of the analytic expansion as $\rho\to 0^+$. Notice, however, that beyond the first term we cannot use the integral representation of the Mellin transform of h given above because the integral becomes divergent for $z=2k$; $k\geqslant 1$. This prevents us from getting further terms in the asymptotic expansion as $\rho\to 0^+$ by using this method.

B. Asymptotic behavior in τ

The integral in (4) is not an h-transform when τ is chosen as the asymptotic parameter but can be written as such by using the change of variables $u=\lambda e^{-t/\lambda}$. This gives

$$\frac{\lambda}{R_1}\Im\left\{e^{i\tau\lambda}\int_0^\lambda du\,\frac{e^{-i\tau u}}{u}J_0\left(\lambda\log\frac{u}{\lambda}\right)J_0\left(\rho\lambda\log\frac{u}{\lambda}\right)\right\}. \tag{21}$$

Even though this integral has now the appropriate form with $f(u)=(1/u)\,\chi_{[0,\lambda]}(u)J_0[\lambda\log(u/\lambda)]J_0[\rho\lambda\log(u/\lambda)]$ and $h(u)=e^{-iu}$, the asymptotic behavior of $f(u)$ as $u\to 0^+$ is not of the type considered in the theorem. This has some unpleasant consequences, the Mellin transform of f cannot be analytically continued as a meromorphic function on $\mathbb{C}$, and we cannot use the expressions given in the theorem for the asymptotic behavior of h-transforms. This forces us to follow a more complicated approach. We will consider the cases $\rho=0$ and $\rho\neq 0$ separately.

1. $\rho=0$

We have to study the integral

$$\frac{\lambda}{R_1}\Im\left\{e^{i\tau\lambda}\int_0^\lambda du\,\frac{e^{-i\tau u}}{u}J_0\left(\lambda\log\frac{u}{\lambda}\right)\right\}, \tag{22}$$

when $\tau\to\infty$. Let us set $h(u)=e^{-i\tau u}$ and $f(u)=\chi_{[0,\lambda]}(u)\,(1/u)\,J_0[\lambda\log(u/\lambda)]$ [remember that h-transforms are defined as integrals over $(0,\infty)$]. The Mellin transforms of these functions are

$$M[h;z]=\tau^{-z}\Gamma(z)e^{-i\pi z/2},$$

convergent in the strip $0<\Re(z)<1$, and

$$M[f;z]=\frac{\lambda^{z-1}}{\sqrt{\lambda^2+(z-1)^2}},$$

which converges in $1<\Re(z)$. Several comments are in order. First we see that the Mellin transform of f cannot be analytically continued as a meromorphic function over the complex plane because of the cuts coming from the square root. If we choose the branch[22] given by $\log(z)=\log|z|+i\arg(z)$ with $\arg(z)\in(-\pi,\pi]$ the cuts are those parts of the imaginary axis with $|z|\geqslant\lambda$. Another comment is that the regions where the Mellin transforms converge do not overlap; this fact precludes us from directly employing the Mellin–Parseval formula (19). The reason can be traced back to the behavior of $h(t)$ as $t\to 0^+$; fortunately this problem can be fixed in a straightforward way. First we rewrite (22) as

$$\frac{\lambda}{R_1}\Im\left\{e^{i\tau\lambda}\int_0^\lambda du\,\frac{(e^{-i\tau u}-1)}{u}J_0\left(\lambda\log\frac{u}{\lambda}\right)\right\}+\frac{i\lambda}{R_1}\Im\left\{e^{i\tau\lambda}\int_0^\lambda du\,\frac{1}{u}J_0\left(\lambda\log\frac{u}{\lambda}\right)\right\}$$
$$=\frac{1}{R_1}\Im\left\{e^{i\tau\lambda}\left[1+\lambda\int_0^\lambda du\,\frac{(e^{-i\tau u}-1)}{u}J_0\left(\lambda\log\frac{u}{\lambda}\right)\right]\right\}.$$

In order to study the last integral, we choose $f(u)$ as above and $h(u)=\chi_{[0,\lambda]}(u)[e^{-i\tau u}-1]$. The Mellin transform of h can be written in terms of confluent hypergeometric functions but one can work with a simpler expression by realizing that, since $f(u)$ is zero if $u>\lambda$, one can replace h with a new function $\tilde{h}$ that differs from it only for $u>\lambda$:

$$\tilde{h}:\mathbb{R}^+\to\mathbb{R}:s\mapsto\begin{cases}e^{-i\tau s}-1 & s\in(0,\lambda)\\ e^{-i\tau s} & s\in[\lambda,\infty).\end{cases}$$

The result is easily seen to be independent of this extension of h. The integral giving the Mellin transform of $\tilde{h}$ converges in the strip $-1<\Re(z)<1$ with $M[\tilde{h};z]=\tau^{-z}\Gamma(z)e^{-i\pi z/2}-\lambda^z/z$. Since we now have overlapping convergence strips we can use the Mellin–Parseval formula and obtain a Mellin–Barnes representation of our integral as

$$\frac{1}{R_1}\Im\left\{e^{i\tau\lambda}\left[1+\frac{\lambda}{2\pi i}\int_{c-i\infty}^{c+i\infty}dz\,\frac{\tau^{-z}\lambda^{-z}\Gamma(z)e^{-i\pi z/2}-1/z}{\sqrt{\lambda^2+z^2}}\right]\right\}$$
$$=\frac{1}{R_1}\Im\left\{e^{i\tau\lambda}\left[1+\frac{\lambda}{2\pi i}\int_{c-i\infty}^{c+i\infty}dz\,\frac{\tau^{-z}\lambda^{-z}\Gamma(z)e^{-i\pi z/2}}{\sqrt{\lambda^2+z^2}}\right]\right\},\qquad(23)$$

with $\Re(c)\in(-1,0)$. We have employed the fact that

$$\int_{c-i\infty}^{c+i\infty}dz\,\frac{dz}{z\sqrt{\lambda^2+z^2}}=0.$$

The analytic continuation of the integrand in the r.h.s. of (23) is immediate. It has algebraic singularities at $z=\pm i\lambda$ (see Fig. 5) with cuts in those points of the imaginary axis where $|z|>\lambda$, and simple poles on $-z\in\mathbb{N}\cup\{0\}$.

In order to study the limit $\tau\to 0^+$ we can displace the integration contour in (23) leftwards parallel to the imaginary axis.[23] A simple analysis using the asymptotics of $\Gamma(z)$ for large values of $\Im(z)$ shows that the series given by the residues of the integrand at the poles $-z\in\mathbb{N}$, namely

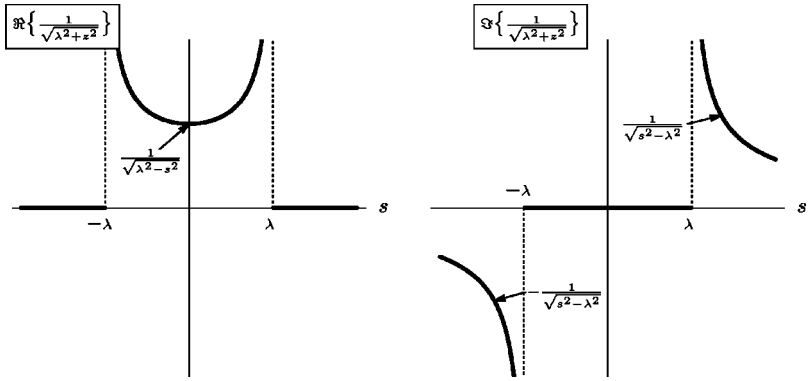

FIG. 5. Real and imaginary parts of $1/\sqrt{\lambda^2+z^2}$ on the curve $z=-0^+ + is$ (corresponding to $\rho=0$). In the vicinity of the singularities at $is=\pm i\lambda$ the real and imaginary parts of this function behave as $1/\sqrt{2\lambda(\lambda\mp s)}$ ($|s|<\lambda$) and $\pm 1/\sqrt{2\lambda(\pm s-\lambda)}$ ($|s|>\lambda$).

$$\frac{\lambda}{R_1}\mathfrak{I}\left\{ e^{i\tau\lambda}\sum_{k=0}^{\infty}\frac{(-i\lambda\tau)^k}{k!\sqrt{\lambda^2+k^2}}\right\},$$

converges to the value of the integral. This is precisely what one would get by expanding the exponential in (22), exchanging sum and integration, and computing the integrals that appear. This was the procedure used in Ref. 6.

It is not possible to directly get the asymptotic behavior in the $\tau\to\infty$ limit by displacing the integration contour rightwards because of the presence of the cut and, even worse, the absence of poles with $\Re(z)\geqslant 0$. One could consider choosing a value for c and write (23) as a real integral in the variable $y\in\mathbb{R}$ after the change $z=c+iy$. In fact, by doing that one obtains the sum of two h-transforms with asymptotic parameter $\log\tau$ that can be studied with the standard formulas. Unfortunately, proceeding in this way one gets a trivial *zero* asymptotic expansion. The reason, as we will find out later on, is that $\log\tau$ is *almost*, but not quite, the right asymptotic parameter.[24]

The solution to our problem is displacing the integration contour all the way to the cut (choosing $c\to 0^-$) as shown in Fig. 6.

The contribution of the arcs Γ_2 and Γ_4 to the integral in the r.h.s. of (23) goes to zero as $-c=\epsilon\to 0^+$. The remaining three contributions to the integral (without prefactors) are

$$\Gamma_1 \qquad -\int_{\lambda}^{\infty} dy\,\frac{e^{-iy\log(\lambda\tau)}e^{\pi y/2}\Gamma(iy)}{\sqrt{y^2-\lambda^2}},$$

$$\Gamma_3 \qquad -\frac{\pi i}{\lambda}+i\,\mathrm{P.V.}\int_{-\lambda}^{\lambda} dy\,\frac{e^{-iy\log(\lambda\tau)}e^{\pi y/2}\Gamma(iy)}{\sqrt{\lambda^2-y^2}},$$

$$\Gamma_5 \qquad \int_{-\infty}^{-\lambda} dy\,\frac{e^{-iy\log(\lambda\tau)}e^{\pi y/2}\Gamma(iy)}{\sqrt{y^2-\lambda^2}}.$$

The asymptotic expansions of these integrals can be obtained by a variety of methods, for example by steepest descents. Nonetheless, it is now possible to employ formula (20) and obtain, in principle, the asymptotics to any order.

The integral over Γ_1 can be written as the following standard h-transform by the change of variables $y=\lambda(1+s)$ with $s\in[0,\infty)$:

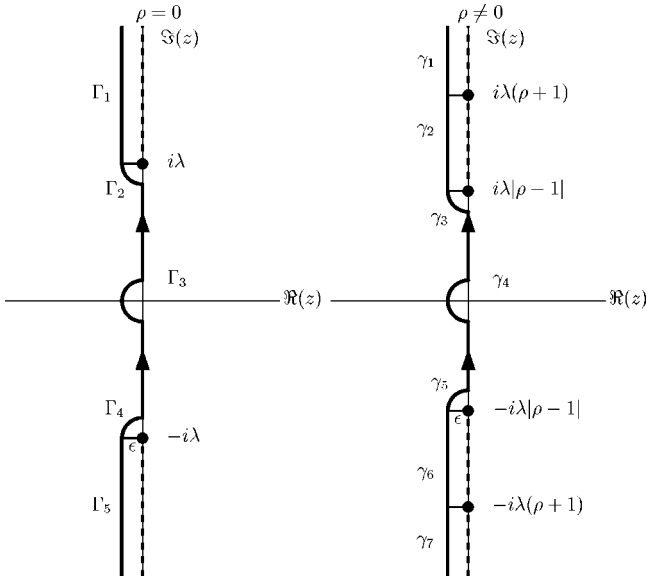

FIG. 6. Cuts and singularities of the integrand and integration contours in the complex plane for the Mellin–Barnes representation used in the asymptotic analysis for $\tau\to\infty$ in the cases $\rho=0$ and $\rho\neq 0$.

$$-e^{-i\lambda\,\log(\lambda\tau)}e^{\pi\lambda/2}\int_0^\infty ds\, e^{-i\lambda s\,\log\tau}\frac{e^{-i\lambda s\,\log\lambda}e^{\pi\lambda s/2}\Gamma[i\lambda(1+s)]}{\sqrt{s(s+2)}}.$$

Taking $h(z)=e^{-i\lambda z}$, $f(z)=e^{-i\lambda z\,\log\lambda}e^{\pi\lambda z/2}\Gamma[i\lambda(1+z)]/\sqrt{z(z+2)}$, and the asymptotic parameter $\log\tau$ we can use formulas (19) and (20). Since the asymptotic behavior of f when $z\to 0^+$ is

$$f(z)\sim\frac{\Gamma(i\lambda)}{\sqrt{2z}}+O(z^{1/2}),$$

and $M[h;z]=\lambda^{-z}e^{-\pi iz/2}\Gamma(z)$, we get for the integral over Γ_1 an asymptotic expansion in powers of $1/\sqrt{\log\tau}$ with a τ oscillating factor $e^{-i\lambda\,\log(\lambda\tau)}$, namely

$$-e^{-i\lambda\,\log(\lambda\tau)+\,\pi\lambda/2\,-\,\pi i/4}\Gamma(i\lambda)\left\{\sqrt{\frac{\pi}{2\lambda\,\log\tau}}+O\left[\frac{1}{(\log\tau)^{3/2}}\right]\right\}.$$

A similar argument can be used to calculate the asymptotic expansion of the integral over Γ_5,

$$e^{i\lambda\,\log(\lambda\tau)-\,\pi\lambda/2\,+\,\pi i/4}\Gamma(-i\lambda)\left\{\sqrt{\frac{\pi}{2\lambda\,\log\tau}}+O\left[\frac{1}{(\log\tau)^{3/2}}\right]\right\}.$$

Finally, to get the asymptotics of the integral over Γ_3 we express it in the form

$$-\frac{\pi i}{\lambda}+i\int_0^\lambda dy\,\cos[y\,\log\tau]\frac{e^{-iy\,\log\lambda}e^{\pi y/2}\Gamma(iy)+e^{iy\,\log\lambda}e^{-\pi y/2}\Gamma(-iy)}{\sqrt{\lambda^2-y^2}}$$

$$-i\int_0^\lambda dy\,\sin[y\,\log\tau]\frac{e^{iy\,\log\lambda}e^{-\pi y/2}\Gamma(-iy)-e^{-iy\,\log\lambda}e^{\pi y/2}\Gamma(iy)}{\sqrt{\lambda^2-y^2}}.$$

By introducing neutralizers, as in Ref. 14, it is possible to show that the critical points for the previous two integrals are 0 and λ. The contributions to the asymptotic expansion from both points

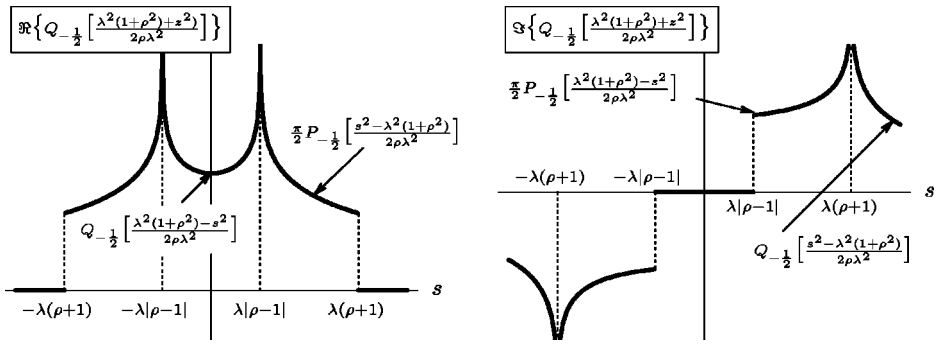

FIG. 7. Real and imaginary parts of $Q_{-1/2}[(\lambda^2(1+\rho^2)+z^2)/(2\rho\lambda^2)]$ on the curve $z=-0^+ +is$ for $\rho\neq 0$.

can be obtained in a straightforward way using formula (20). The contribution from zero is $-\pi i/\lambda$ whereas the one from λ coincides precisely with the sum of the contributions obtained before for Γ_1 and Γ_5. Summing all the terms and substituting the result in (23) we finally get the behavior in τ presented in Sec. II.

It is worth remarking that the asymptotic expansions discussed can be written as an oscillating factor that depends on $\log\tau$ multiplying an expansion in terms of inverse powers of $\sqrt{\log\tau}$. Moreover, note that the frequency of these oscillations is *exactly* that of the oscillating factor that we have already obtained.

2. $\rho\neq 0$

Consider now the integral (21). We set $h(u)=e^{-i\tau u}$ and $f(u)=\chi_{[0,\lambda]}(u)\,(1/u)\,J_0[\lambda\log(u/\lambda)]J_0[\rho\lambda\log(u/\lambda)]$. The Mellin transform of f is

$$M[f;z]=\frac{\lambda^{z-2}}{\pi\sqrt{\rho}}Q_{-1/2}\left[\frac{\lambda^2(1+\rho^2)+(z-1)^2}{2\rho\lambda^2}\right].$$

Proceeding as in the $\rho=0$ case we get the following Mellin–Barnes representation:

$$\frac{1}{\pi R_1\sqrt{\rho}}\Im\left\{e^{i\tau\lambda}\left[Q_{-1/2}\left(\frac{1+\rho^2}{2\rho}\right)+\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dz\left(\tau^{-z}\lambda^{-z}\Gamma(z)e^{-i\pi z/2}-\frac{1}{z}\right)\right.\right.$$
$$\left.\left.\times Q_{-1/2}\left(\frac{\lambda^2(1+\rho^2)+z^2}{2\rho\lambda^2}\right)\right]\right\}=\frac{1}{\pi R_1\sqrt{\rho}}\Im\left\{e^{i\tau\lambda}\left[Q_{-1/2}\left(\frac{1+\rho^2}{2\rho}\right)\right.\right.$$
$$\left.\left.+\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dz\;\tau^{-z}\lambda^{-z}e^{-i\pi z/2}\Gamma(z)Q_{-1/2}\left(\frac{\lambda^2(1+\rho^2)+z^2}{2\rho\lambda^2}\right)\right]\right\}. \tag{24}$$

The main difference with the previous case is the appearance of the associated Legendre function $Q_{-1/2}$. This function has cuts on the imaginary axis for $|\Im(z)|\geqslant\lambda|\rho-1|$. On the left of the cut the real and imaginary parts behave as shown in Fig. 7. They become singular in the neighborhood of the four points $z=\pm i\lambda|\rho-1|$ and $z=\pm i\lambda(\rho+1)$. The real functions that describe each of the continuous pieces are shown in the plots. Some of them are given by $Q_{-1/2}(x)$ evaluated on $x>1$. Quite surprisingly, the others can be written in terms of the associated Legendre function $P_{-1/2}$ [$P_{-1/2}(x)=F(1/2,1/2;1;(1-x)/2)$] with argument $x>-1$. The fundamental consequence of this is a change in the singularity structure of the integrand of (24).

The limit $\tau\to 0^+$ can be obtained as we did for $\rho=0$. The result is given by (16).

By displacing the integration contour rightwards to the cut as in the $\rho=0$ case (see Fig. 6) we can split the last integral in (24) into seven different contributions corresponding to the integration curves $\gamma_1,\ldots,\gamma_7$. It is straightforward to show that the contributions from γ_3 and γ_5 go to zero as the contour gets closer to the imaginary axis. We are then left with

$$\gamma_1 \qquad -\int_{\lambda(\rho+1)}^{\infty} dy e^{-iy\log(\lambda\tau)} e^{\pi y/2}\Gamma(iy) Q_{-1/2}\left(\frac{y^2-\lambda^2(1+\rho^2)}{2\rho\lambda^2}\right),$$

$$\gamma_2 \qquad \frac{\pi}{2} i \int_{\lambda|\rho-1|}^{\lambda(\rho+1)} dy e^{-iy\log(\lambda\tau)} e^{\pi y/2}\Gamma(iy)\left[P_{-1/2}\left(\frac{y^2-\lambda^2(1+\rho^2)}{2\rho\lambda^2}\right)+iP_{-1/2}\left(\frac{\lambda^2(1+\rho^2)-y^2}{2\rho\lambda^2}\right)\right],$$

$$\gamma_4 \qquad -i\pi Q_{-1/2}\left(\frac{1+\rho^2}{2\rho}\right)+i\,\mathrm{P.V.}\int_{-\lambda|\rho-1|}^{\lambda|\rho-1|} dy e^{-iy\log(\lambda\tau)} e^{\pi y/2}\Gamma(iy) Q_{-1/2}\left(\frac{\lambda^2(1+\rho^2)-y^2}{2\rho\lambda^2}\right),$$

$$\gamma_6 \qquad \frac{\pi}{2} i \int_{-\lambda(\rho+1)}^{-\lambda|\rho-1|} dy e^{-iy\log(\lambda\tau)} e^{\pi y/2}\Gamma(iy)\left[P_{-1/2}\left(\frac{y^2-\lambda^2(1+\rho^2)}{2\rho\lambda^2}\right)\right.$$
$$\left.-iP_{-1/2}\left(\frac{\lambda^2(1+\rho^2)-y^2}{2\rho\lambda^2}\right)\right],$$

$$\gamma_7 \qquad \int_{-\infty}^{-\lambda(\rho+1)} dy e^{-iy\log(\lambda\tau)} e^{\pi y/2}\Gamma(iy) Q_{-1/2}\left(\frac{y^2-\lambda^2(1+\rho^2)}{2\rho\lambda^2}\right).$$

All these integrals can be written as Fourier transforms whose only critical points are the integration limits. These can be isolated by using the appropriate neutralizers[14] and the integrals so obtained can be written as h-transforms by straightforward changes of variables. An interesting feature of some of the integrals that arise is the fact that the asymptotic expansion of the corresponding f functions involve logarithms precisely in the form assumed in (18). This means that in addition to the p_{m0} coefficients that appeared in the $\rho=0$ case we will have also contributions coming from the p_{mn}'s with $n\neq 0$.

In order to get the asymptotic behavior of the different f functions close to their singularities it is useful to remember the asymptotic expansions of $P_{-1/2}(x)$ and $Q_{-1/2}(x)$ at $x=-1^+$ and $x=1^+$, respectively:

$$P_{-1/2}(x)\sim \frac{5}{\pi}\log 2-\frac{1}{\pi}\log(x+1)+\cdots,$$

$$Q_{-1/2}(x)\sim \frac{5}{2}\log 2-\frac{1}{2}\log(x-1)+\cdots.$$

With the previous guidelines, and following the same steps as in the $\rho=0$ case, it is easy (albeit lengthy) to deduce (9). It is possible to arrive at the same result by different methods that are somewhat simpler (i.e., steepest descents) but they only allow to compute the first contribution to the asymptotic behavior of the field commutator. The advantage of the method employed here is that one can calculate as many terms as desired for the asymptotic expansion just by taking more terms in the asymptotic series of the function f.

C. Asymptotic behavior in λ

We will consider now integrals of the form

$$\int_B^A dq \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2\, f_{(0)}(q;t_1,t_2) e^{\lambda\Phi(q;t_1,t_2)}, \tag{25}$$

$(0\leqslant B<A)$ where q is a real variable, t_1 and t_2 are complex variables and $\gamma_{1,2}$ are closed paths (possibly different) in the complex plane. The functions $f_{(0)}$ and Φ are supposed to be holomorphic in the two complex arguments and C^n in q (with n possibly infinite) in an open neighborhood of the integration region. In the following we will use the notation $\partial_i \equiv \partial_{t_i}$, $i=1,2$, $\nabla \equiv (\partial_q, \partial_1, \partial_2)$, and $\|\nabla\Phi\|^2 \equiv \eta_q(\partial_q\Phi)^2 + \eta_{t_1}(\partial_1\Phi)^2 + \eta_{t_2}(\partial_2\Phi)^2$, where η_q, η_{t_1}, and η_{t_2} are some functions of q, t_1, and t_2 that will be chosen later in the discussion. This freedom will prove to be useful when we parametrize the curves $\gamma_{1,2}$ because it will allow us to have denominators in the integrand that are real positive functions, facilitating the analysis of the $A\to\infty$ limit. If $\|\nabla\Phi\|^2$ differs from zero for all $q\in[B,A]$, $t_1\in\gamma_1$, and $t_2\in\gamma_2$, it is possible to devise an ''integration by parts'' procedure for this type of integrals by writing them as

$$\frac{1}{\lambda}\int_B^A dq \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \left[\frac{f_{(0)}\eta_q \partial_q\Phi\,\partial_q e^{\lambda\Phi}}{\|\nabla\Phi\|^2} + \frac{f_{(0)}\eta_{t_1}\partial_1\Phi\,\partial_1 e^{\lambda\Phi}}{\|\nabla\Phi\|^2} + \frac{f_{(0)}\eta_{t_2}\partial_2\Phi\,\partial_2 e^{\lambda\Phi}}{\|\nabla\Phi\|^2} \right].$$

The contribution of the first term can be written, after integrating by parts in q, as

$$\frac{1}{\lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{f_{(0)}\eta_q\partial_q\Phi e^{\lambda\Phi}}{\|\nabla\Phi\|^2}\bigg|_B^A - \frac{1}{\lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \int_B^A dq e^{\lambda\Phi}\partial_q \frac{f_{(0)}\eta_q\partial_q\Phi}{\|\nabla\Phi\|^2}$$

(notice that the integration region is compact and the function integrable so that we can apply Fubini's theorem and freely exchange orders of integration). Integration by parts in t_1 gives

$$\frac{1}{\lambda}\int_B^A dq \oint_{\gamma_2} dt_2 \oint_{\gamma_1} dt_1 \partial_1 \frac{f_{(0)}\eta_{t_1}\partial_1\Phi e^{\lambda\Phi}}{\|\nabla\Phi\|^2} - \frac{1}{\lambda}\int_B^A dq \oint_{\gamma_2} dt_2 \oint_{\gamma_1} dt_1 e^{\lambda\Phi}\partial_1 \frac{f_{(0)}\eta_{t_1}\partial_1\Phi}{\|\nabla\Phi\|^2}.$$

If $(f_{(0)}\eta_{t_1}\partial_1\Phi e^{\lambda\Phi})\|\nabla\Phi\|^{-2}$ is a holomorphic function of t_1 in an open set containing the *closed* curve γ_1 (for all $q\in[B,A]$ and $t_2\in\gamma_2$) the first integral is zero and we are left only with the second term. The same argument applies to the integration in t_2. We finally get that (25) can be written as

$$\frac{1}{\lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{f_{(0)}\eta_q\partial_q\Phi e^{\lambda\Phi}}{\|\nabla\Phi\|^2}\bigg|_B^A - \frac{1}{\lambda}\int_B^A dq \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2\, f_{(1)}(q;t_1,t_2) e^{\lambda\Phi(q;t_1,t_2)}, \quad (26)$$

here we have introduced the notation

$$f_{(k+1)} \equiv \partial_q \frac{f_{(k)}\eta_q\partial_q\Phi}{\|\nabla\Phi\|^2} + \partial_1 \frac{f_{(k)}\eta_{t_1}\partial_1\Phi}{\|\nabla\Phi\|^2} + \partial_2 \frac{f_{(k)}\eta_{t_2}\partial_2\Phi}{\|\nabla\Phi\|^2}, \quad k=0,1,\ldots .$$

The second integral in (26) has the same structure as the original integral, so the same procedure can be applied as long as the appropriate regularity conditions are satisfied for expressions involving the successive $f_{(k)}$, $k=1,\ldots$ The strategy to obtain asymptotic expansions for the original integral consists in getting expansions for the lower dimensional boundary integrals that arise in this way, provided that the remaining nonboundary integral behaves nicely in the $\lambda\to\infty$ limit. Particularizing this argument to the case of a single complex variable t is straightforward.

In our case [see Eq. (10)] we actually want to obtain an asymptotic expansion of an improper integral. So we will also have to study the asymptotics of the limit $A\to\infty$,

$$-\frac{1}{\lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{f_{(0)}\eta_q\partial_q\Phi e^{\lambda\Phi}}{\|\nabla\Phi\|^2}\bigg|_B + \lim_{A\to\infty}\left\{ \frac{1}{\lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{f_{(0)}\eta_q\partial_q\Phi e^{\lambda\Phi}}{\|\nabla\Phi\|^2}\bigg|_A - \frac{1}{\lambda}\int_B^A dq \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2\, f_{(1)}(q;t_1,t_2) e^{\lambda\Phi(q;t_1,t_2)} \right\}. \quad (27)$$

In order to derive useful asymptotic expansions from the previous formulas it is desirable that $e^{\lambda\Phi(q;t_1,t_2)}$ be bounded by a λ-independent function.[25] This happens, for example, if $\Re[\Phi(q;t_1,t_2)]\leqslant 0$ in the integration region $[B,A]\times\gamma_1\times\gamma_2$. In fact, we will take advantage of the freedom in the choice of the integration contours $\gamma_{1,2}$ to impose this condition.

If there are points in the integration region (referred to in the following as singular points) where $\|\nabla\Phi\|^2=0$ the argument presented above to derive (26) is no longer true. In such a situation the way to proceed[14,15] is to isolate them by introducing neutralizers.[26] This allows us to divide the integration region into several pieces and study the resulting integrals by choosing the most suitable techniques. This is facilitated by the fact that neutralizers force most of the boundary integrals to be zero. In the process of obtaining asymptotic expansions from (27) it may be useful to further divide the integration region of the last integral in several pieces, by introducing additional neutralizers, in order to localize the singular points in a region that does not contain the boundary $q=A$; this simplifies the analysis of the $A\to\infty$ limit.

The freedom to choose the integration contours in (25) may be useful for other purposes. One can, for example, avoid singularities of the boundary integrals over $\{B\}\times\gamma_1\times\gamma_2$ and $\{A\}\times\gamma_1\times\gamma_2$; it may be possible to write the integrals involving the singular points as (multidimensional) Laplace or Fourier transforms for which the analysis of singular points can be carried out by standard procedures (see Ref. 14) or to improve the behavior for large values of q if one intends to study the asymptotics of the improper integral when $A\to\infty$.[27] Finally in some cases this freedom may allow us to simplify the analysis of the contribution of some of the singular points.

As in the study of the τ asymptotics, we will consider the cases $\rho=0$ and $\rho\neq 0$ separately.

1. $\rho=0$

We study the integral (10) for $\rho=0$:

$$-\frac{1}{R_1}\lim_{A\to\infty}\Im\left\{\frac{i\lambda e^{i\tau\lambda}}{2\pi}\int_0^A dq\oint_\gamma dt\,\frac{1}{t}e^{\lambda[(q/2)(t-1/t)-i\tau e^{-q}]}\right\}. \tag{28}$$

Let us discuss first the possible choices of integration contour γ. As commented above it is convenient to impose that the real part of the exponent in the integrand be less or equal to zero, i.e., $\Re(t-1/t)\leqslant 0$. It is straightforward to show that this happens when $u(u^2+v^2-1)\geqslant 0$ $(t=u+iv)$. This complex region (see Fig. 8) is given by the points inside the unit circle centered at the origin with positive real part, those outside this circle with negative real part, and the boundary of these two regions (i.e., the imaginary axis and the unit circumference centered at the origin). The integration contour can be any closed, positively oriented, simple curve contained in this region that surrounds the origin. Notice that all these contours contain the points $t=\pm i$.

If we choose $\eta_q=-1$ and $\eta_t=t^2$ we have

$$\|\nabla\Phi\|^2=\frac{1}{4}\left[q^2\left(t+\frac{1}{t}\right)^2-\left(t-\frac{1}{t}+2i\tau e^{-q}\right)^2\right].$$

At the left boundary $(q=0)$ this is zero when $t=-i\tau\pm\sqrt{1-\tau^2}$. Depending on the value of τ these points may be on the unit circumference; it is, hence, convenient to choose integration contours in the allowed part of $\mathbb{C}$ that avoid them (see Fig. 8). This will always be possible except for $\tau=1$. When $q\neq 0$ the condition $\|\nabla\Phi\|^2=0$ gives, generically, four possible solutions (depending on q and τ) that may or may not be in the integration region. If $\tau>1$, there is one of these, $(t=-i,\ q=\log\tau)$ that will be in the integration region for every possible choice of the integration contour γ. The remaining ones will or will not belong to the integration region depending on γ. In principle one would proceed by picking a certain contour, determine the values of q corresponding to these points, introduce suitable neutralizers, and study the neutralized integrals one at a time. There is, however, a simple argument that shows that it is not necessary to discuss them in detail (we assume $q\neq 0$ in the following discussion unless otherwise specified).

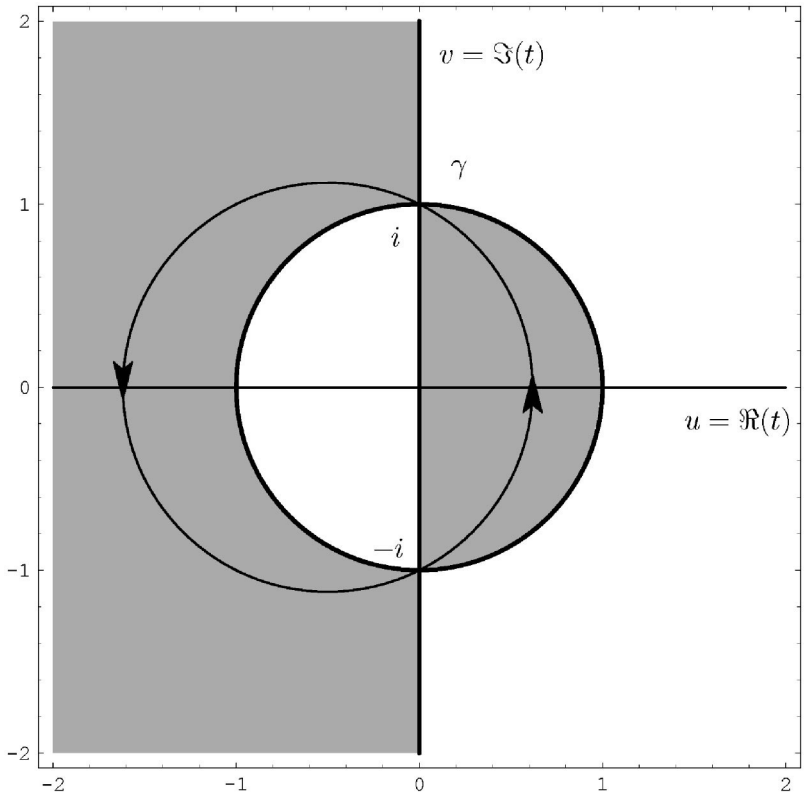

FIG. 8. The region $\Re(t-1/t)\leqslant 0$ consists of the shadowed area and its boundary. A possible choice of the integration contour γ is also shown.

The idea is to write the integral in (28) as the sum of three integrals I_j, $j=1,2,3$ and choose *different*[28] contours for each of them. These integrals are

$$I_j \equiv -\frac{1}{R_1}\Im\left\{\frac{i\lambda e^{i\tau\lambda}}{2\pi}\int_0^A dq \oint_\gamma dt\, \nu_j(q)\frac{1}{t}e^{\lambda[(q/2)(t-1/t)-i\tau e^{-q}]}\right\},$$

where we have introduced three neutralizer functions $\nu_j(q)$, $j=1,2,3$ satisfying $\nu_1+\nu_2+\nu_3=1$ in $[0, A]$ and

$$\nu_1(q)=1 \quad \text{if} \quad q\in[0,\alpha_1],$$

$$\nu_1(q)=0 \quad \text{if} \quad q\in[\alpha_2,A],$$

$$\nu_2(q)=0 \quad \text{if} \quad q\in[0,\alpha_1]\cup[\beta_2,A],$$

$$\nu_2(q)=1 \quad \text{if} \quad q\in[\alpha_2,\beta_1],$$

$$\nu_3(q)=0 \quad \text{if} \quad q\in[0,\beta_1],$$

$$\nu_3(q)=1 \quad \text{if} \quad q\in[\beta_2,A],$$

with $0<\alpha_1<\alpha_2<\beta_1<\beta_2<A$ (the specific choices for these parameters will be explained later). By doing this the effective integration regions in q are $[0,\alpha_2]$, $[\alpha_1,\beta_2]$, and $[\beta_1,A]$, respectively; notice that the boundary $q=0$ appears only in the first.

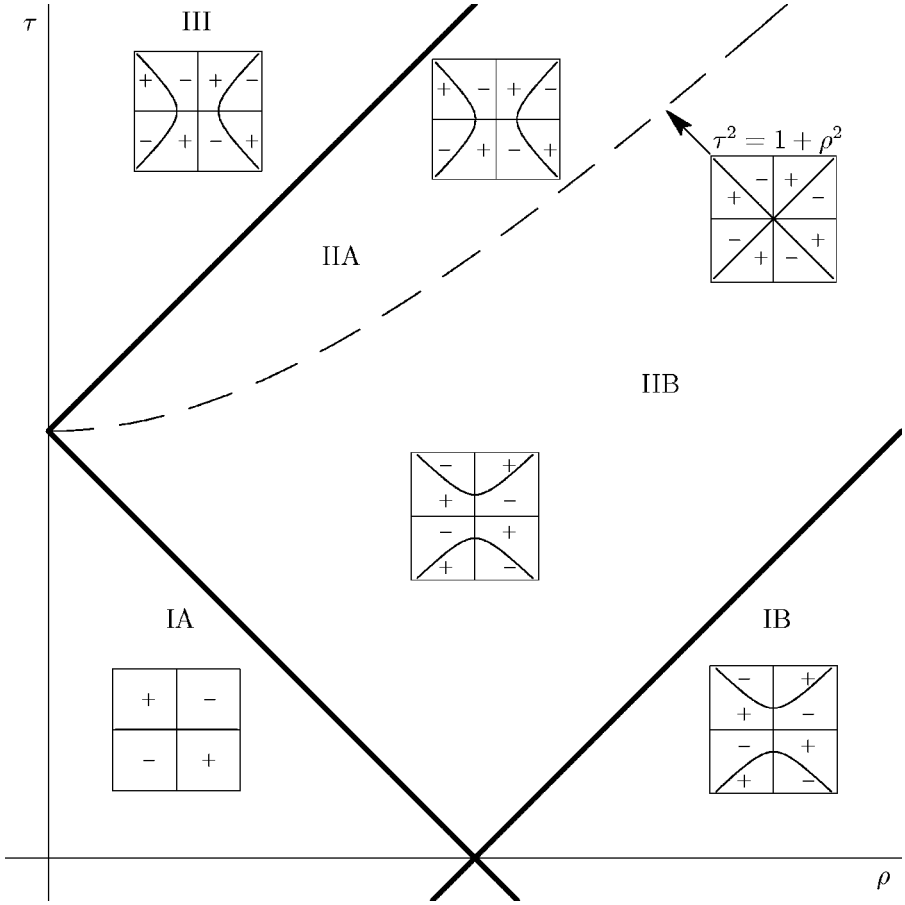

FIG. 9. Sign of $\Re[\sqrt{Q_1(s)Q_2(s)}/(is^2-i)]$ for every choice of ρ and τ. Each inset shows this sign for $s=x+iy\in\mathbb{C}$. The hyperbolas that separate some of the regions in these insets have the equation $x^2-y^2=(1+\rho^2-\tau^2)/[1-(\rho+\tau)^2]$.

Let us consider first I_1. In this case it is convenient to choose an integration contour γ that avoids the unit circumference (except at $t=\pm i$) because, if $\tau<1$, the integration by parts procedure introduced above could, otherwise, give a boundary contribution at $q=0$ involving a singular function. We pick the contour depicted in Fig. 8. In order to use integration by parts it is also necessary to show that it is possible to find α_2 such that $\|\nabla\Phi\|^2\neq 0$ in the integration region. The solutions to $\|\nabla\Phi\|^2=0$ are those satisfying the following quadratic equations

$$(1+q)t^2+2i\tau e^{-q}t-1+q=0,$$

$$(1-q)t^2+2i\tau e^{-q}t-1-q=0.$$

It can easily be shown (by using the implicit function theorem or the explicit solution of these equations in t) that the solutions are continuous at $q=0$ (if $\tau\neq 1$), i.e., the solutions for small enough q are close to $t=-i\tau\pm\sqrt{1-\tau^2}$. If $\tau\neq 1$ it is then possible to choose α_2 and γ in such a way that $\|\nabla\Phi\|^2\neq 0$ in the integration region $\gamma\times[0,\alpha_2]$.

We can use formula (27) to get an asymptotic expansion for I_1. We first note that the term corresponding to the second integral in (26) is $O(1/\lambda)$ because our choice of contour allows us to bound the absolute value of the integrand by a regular function independent of λ. The integral I_1 is then given at leading order by the contribution of the boundary terms which can be written as

$$I_1=\frac{1}{\pi R_1}\Im\left\{ i \oint_\gamma \frac{dt}{t^2+2i\tau t-1}\right\}$$

[the function $\nu_1(q)$ kills the contribution coming from the $q=\alpha_2$ boundary]. If $\tau<1$ the poles of the integrand $t=-i\tau\pm\sqrt{1-\tau^2}$ are on the unit circumference but only that with the negative real part is inside γ. The value of the residue of the integrand at this point is $-1/(2\sqrt{1-\tau^2})$ and hence

$$I_1=\frac{1}{R_1}\Im\left\{\frac{1}{\sqrt{1-\tau^2}}\right\}=0.$$

If $\tau>1$ the poles of the integrand are on the imaginary axis $t=-i\tau\pm i\sqrt{\tau^2-1}$; now only that with the positive sign in the square root is inside γ. The residue is $1/(2i\sqrt{\tau^2-1})$ and hence

$$I_1=\frac{1}{R_1}\Im\left\{\frac{i}{\sqrt{\tau^2-1}}\right\}=\frac{1}{R_1\sqrt{\tau^2-1}}. \tag{29}$$

Consider next I_2. In this case it is convenient to choose the unit circumference for γ because, parametrizing it by an angle ($t(\theta)=e^{i\theta}$, $\theta\in(-\pi,\pi]$), the exponent $\lambda\Phi(q;t)$ becomes a purely imaginary function of the two real variables q and θ,

$$i\lambda\phi(q;\theta)\equiv\lambda\Phi[q;t(\theta)]=i\lambda(q\sin\theta-\tau e^{-q}),$$

and the integral becomes a Fourier transform on a rectangular region determined by the support of the neutralizer. As is well known the critical points for Fourier transforms are given by the boundaries of the integration region and those interior points where the gradient of the *real* function ϕ is zero. In our case the $q=\alpha_1$ and $q=\beta_2$ boundaries give no contribution for this integral owing to the presence of the neutralizer. Let us then find the interior critical points. Since $\|\nabla\Phi\|^2[q;t(\theta)]$ is a sum of squares of real numbers[29] these points are precisely those where our procedure of integration by parts fails. We have to solve the following equations:

$$q\cos\theta=0,$$

$$\sin\theta+\tau e^{-q}=0.$$

The solution is $q=0$, $\theta=-\arcsin\tau$ if $\tau<1$ (these are outside the effective integration region for I_2) and $q=\log\tau$, $\theta=-\pi/2$ if $\tau>1$. The choices of $\alpha_{1,2}$ can be made in such a way that the critical point with $q>0$ (present only when $\tau>1$) always corresponds to I_2 (we also choose β_1 such that $\log\tau<\beta_1$ to avoid having critical points in I_3). The asymptotic expansion of I_2 can be now obtained by using the standard formulas[14] for the contribution of critical points. In our case this is simply

$$\frac{1}{R_1}\Im\left\{\frac{e^{i\lambda(\tau-\log\tau-1)}}{\sqrt{\log\tau}}\right\}+O\left[\frac{1}{\lambda}\right], \tag{30}$$

for $\tau>1$ and 0 if $\tau<1$. We do not need to discuss the limit $A\to\infty$ of I_1 and I_2 because the integrand has compact support independent of A; we have only assumed that $\log\tau<A$. However this is no longer true for I_3.

Let us analyze, finally, $\lim_{A\to\infty} I_3$. We choose again the unit circumference for γ (with the same parametrization) and write

$$\lim_{A\to\infty} I_3 = \Im\left\{ \frac{\lambda e^{i\tau\lambda}}{2\pi R_1} \lim_{A\to\infty} \int_{\beta_1}^{A} dq \int_{-\pi}^{\pi} d\theta\, \nu_3(q) e^{i\lambda\phi(q;\theta)} \right\}.$$

Using formula (27) with $\eta_q = -1$, $\eta_t = t^2$, and taking into account that $\nu_3(\beta_1) = 0$, this expression becomes

$$\Im\left\{ \frac{\lambda e^{i\tau\lambda}}{2\pi R_1} \lim_{A\to\infty}\left[\frac{-i}{\lambda} \int_{-\pi}^{\pi} d\theta \frac{(\tau e^{-A} + \sin\theta) e^{i\lambda\phi(A;\theta)}}{A^2\cos^2\theta + (\tau e^{-A} + \sin\theta)^2} + \frac{i}{\lambda}\int_{\beta_1}^{A} dq \int_{-\pi}^{\pi} d\theta\, \nu_3(q) e^{i\lambda\phi(q;\theta)} g_1(q;\theta) \right] \right\}. \tag{31}$$

Here[30]

$$g_1(q;\theta) \equiv i e^{i\theta} f_{(1)}[q; t(\theta)] = \frac{(\tau e^{-q} + \sin\theta)^2 (\tau e^{-q} - q\sin\theta) + q\cos^2\theta[(q^2-4)\sin\theta - \tau(q+4)e^{-q}]}{[q^2\cos^2\theta + (\tau e^{-q} + \sin\theta)^2]^2}.$$

We have disregarded in Eq. (31) a term containing derivatives of $\nu_3(q)$ because it can be shown to be $O(1/\lambda^R)$ for every $R>0$. We want to show that (31) does not contribute to the asymptotic expansion at the order in λ considered. Note that it is difficult to prove that the limit of the last integral is zero when $\lambda\to\infty$ by using an argument inspired in the Riemann–Lebesgue lemma, because changing variables to write it as a Fourier transform introduces singularities in the integrand that are not easy to deal with. To study the asymptotics of (31) we will follow instead several steps:

(i) Use integration by parts to further decompose the second integral in (31) as a surface term and a double integral in q and θ;
(ii) split each of the integrands obtained in this way in two pieces; one with a simpler denominator and another whose limit $A\to\infty$ vanishes. After this step we will be left with two integrals in q and a double integral;
(iii) split in two the double integral by writing the exponential term as

$$e^{i\lambda\phi(q;\theta)} = e^{i\lambda[q\sin\theta - \tau e^{-q}]} = e^{i\lambda q\sin\theta}(e^{-i\lambda\tau e^{-q}} - 1) + e^{i\lambda q\sin\theta},$$

(iv) show that the contribution coming from $e^{i\lambda q\sin\theta}(e^{-i\lambda\tau e^{-q}} - 1)$ vanishes sufficiently fast when $\lambda\to\infty$ by using the Hölder inequality;
(v) finally, show that the remaining terms have a simple asymptotic behavior.

Step (i): After an additional integration by parts (31) becomes

$$\Im\left\{ \frac{\lambda e^{i\tau\lambda}}{2\pi R_1} \lim_{A\to\infty}\left[-\frac{i e^{-i\lambda\tau e^{-A}}}{\lambda} \int_{-\pi}^{\pi} d\theta \frac{(\tau e^{-A} + \sin\theta) e^{i\lambda A\sin\theta}}{A^2\cos^2\theta + (\tau e^{-A} + \sin\theta)^2} + \frac{e^{-i\lambda\tau e^{-A}}}{\lambda^2} \int_{-\pi}^{\pi} d\theta \frac{(\sin\theta - \tau e^{-A}) e^{i\lambda A\sin\theta}}{A^2\cos^2\theta + (\tau e^{-A} + \sin\theta)^2} g_1(A;\theta) - \frac{1}{\lambda^2}\int_{\beta_1}^{A} dq \int_{-\pi}^{\pi} d\theta \nu_3(q) e^{i\lambda\phi(q;\theta)} g_2(q;\theta) \right] \right\}.$$

Step (ii): All the integrands that appear in the first step have factors of the type

$$\frac{1}{[q^2\cos^2\theta+(\tau e^{-q}+\sin\theta)^2]^N} \quad N=1,2,\ldots$$

that can be written as

$$\frac{1}{[q^2\cos^2\theta+\sin^2\theta]^N}+\frac{\Sigma_{j=1}^{2N}\tau^j e^{-jq}P_j(q,\sin\theta,\cos\theta)}{[q^2\cos^2\theta+(\tau e^{-q}+\sin\theta)^2]^N[q^2\cos^2\theta+\sin^2\theta]^N} \quad N=1,2,\ldots$$

with $P_j(q,\sin\theta,\cos\theta)$ a polynomial of degrees $2(N-1)$, $2(N-1)$, and $2N-1$ in q, $\cos\theta$, and $\sin\theta$ respectively. For fixed values of q larger than a certain $Q>\log\tau$ the maximum of the function $y(\theta)=[q^2\cos^2\theta+(\tau e^{-q}+\sin\theta)^2]^{-1}$ is $(1-\tau e^{-q})^{-2}$, so we have,[31] for $N=1,2,...$,

$$\left|\frac{\Sigma_{j=1}^{2N}\tau^j e^{-jq}P_j(q,\sin\theta,\cos\theta)}{[q^2\cos^2\theta+(\tau e^{-q}+\sin\theta)^2]^N[q^2\cos^2\theta+\sin^2\theta]^N}\right|\leqslant\frac{\Sigma_{j=1}^{2N}\tau^j e^{-jq}\tilde{P}_j(q)}{(1-\tau e^{-q})^{2N}(q^2\cos^2\theta+\sin^2\theta)^N},$$

where $\tilde{P}_j(q)$ is the polynomial in q obtained from $P_j(q,\sin\theta,\cos\theta)$ by taking the absolute value of the coefficients and substituting $\sin\theta=1$, $\cos\theta=1$. This formula, and the fact that

$$\int_{-\pi}^{\pi}d\theta\frac{1}{[A^2\cos^2\theta+\sin^2\theta]^N}\sim 2\frac{\sqrt{\pi}}{A}\frac{\Gamma(N-1/2)}{\Gamma(N)} \quad \text{as } A\to\infty,$$

allows us to show that the first two integrals obtained in step (i) can be substituted by

$$-\frac{i}{\lambda}\int_{-\pi}^{\pi}d\theta\frac{\sin\theta}{A^2\cos^2\theta+\sin^2\theta}e^{i\lambda A\sin\theta}+\frac{1}{\lambda^2}\int_{-\pi}^{\pi}d\theta\frac{A(A^2-4)\sin^2\theta\cos^2\theta-A\sin^4\theta}{[A^2\cos^2\theta+\sin^2\theta]^3}e^{i\lambda A\sin\theta}.$$

Let us consider now the double integral appearing in step (i). The function $g_2(q;\theta)$ can be written as the sum of two pieces $h_2(q;\theta)$ and $G_2(q;\theta)$. The first one is

$$h_2(q;\theta)=\frac{q^4(q^2-4)\cos^6\theta+q^2(40-23q^2+3q^4)\cos^4\theta\sin^2\theta-(4-23q^2+8q^4)\cos^2\theta\sin^4\theta+(q^2-1)\sin^6\theta}{(q^2\cos^2\theta+\sin^2\theta)^4},$$

and $G_2(q;\theta)$ is a sum of factors $(\tau e^{-q})^N$ $(N=1,2,\ldots)$ times quotients of polynomials in q, $\sin\theta$, and $\cos\theta$ divided by products of powers of $[q^2\cos^2\theta+\sin^2\theta]$ and $[q^2\cos^2\theta+(\tau e^{-q}\sin\theta)^2]$ (notice that these functions never vanish in the integration region). The integral becomes

$$-\frac{1}{\lambda^2}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta\,\nu_3(q)e^{i\lambda\phi(q;\theta)}[h_2(q;\theta)+G_2(q;\theta)].$$

The absolute value of the integrand involving $G_2(q;\theta)$ is an integrable function owing to the decreasing exponential factors and the fact that they multiply terms that grow polynomially at worst in q. Hence its contribution to the total integral is $O(1/\lambda^2)$ even after taking the limit $A\to\infty$. We thus conclude that (31) behaves asymptotically as

$$\Im\Bigg\{\frac{\lambda e^{i\tau\lambda}}{2\pi R_1}\lim_{A\to\infty}\Bigg[-\frac{i}{\lambda}\int_{-\pi}^{\pi}d\theta\frac{\sin\theta}{A^2\cos^2\theta+\sin^2\theta}e^{i\lambda A\sin\theta}$$
$$+\frac{1}{\lambda^2}\int_{-\pi}^{\pi}d\theta\frac{A(A^2-4)\sin^2\theta\cos^2\theta-A\sin^4\theta}{[A^2\cos^2\theta+\sin^2\theta]^3}e^{i\lambda A\sin\theta}$$
$$-\frac{1}{\lambda^2}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda\phi(q;\theta)}\nu_3(q)h_2(q;\theta)\Bigg]\Bigg\}+O\left[\frac{1}{\lambda}\right]. \tag{32}$$

Step (iii): Note that we have already managed to substitute the exponential factor $e^{i\lambda\phi(A;\theta)}$ by $e^{i\lambda\sin\theta}$ within the integrals over θ. However, it is not possible to remove the function $\phi(q,\theta)$ from the double integral. We instead proceed to rewrite it as

$$-\frac{1}{\lambda^2}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda q\sin\theta}[e^{-i\lambda\tau e^{-q}}-1]\nu_3(q)h_2(q;\theta)$$
$$-\frac{1}{\lambda^2}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda q\sin\theta}\nu_3(q)h_2(q;\theta).$$

Step (iv): Consider the first of these integrals in the limit $A\to\infty$,

$$-\frac{1}{\lambda^2}\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda q\sin\theta}[e^{-i\lambda\tau e^{-q}}-1]\nu_3(q)h_2(q;\theta). \tag{33}$$

This integral converges because $(e^{-i\lambda\tau e^{-q}}-1)$ falls off exponentially as $q\to\infty$. Let us define now the functions $f(q,\theta)=q^{\sigma}(e^{-i\lambda\tau e^{-q}}-1)$ and $g(q,\theta)=q^{-\sigma}e^{i\lambda q\sin\theta}\nu_3(q)h_2(q;\theta)$ with σ chosen so that $f,g\in L^2([\beta_1,\infty)\times[-\pi,\pi))$. For example, we set $\sigma=3$. The Hölder inequality gives

$$\left|\frac{1}{\lambda^2}\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda q\sin\theta}[e^{-i\lambda\tau e^{-q}}-1]\nu_3(q)h_2(q;\theta)\right|$$
$$\leqslant\frac{1}{\lambda^2}\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta|f(q,\theta)g(q,\theta)|$$
$$\leqslant\frac{1}{\lambda^2}\left\{\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta|f(q,\theta)|^2\right\}^{1/2}\left\{\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta|g(q,\theta)|^2\right\}^{1/2}.$$

The integral involving $|g(q,\theta)|^2$ is convergent and independent of λ and the one involving $|f(q,\theta)|^2$ satisfies

$$\left\{\int_{\beta_1}^{\infty}dq\int_{-\pi}^{\pi}d\theta\left|f(q,\theta)\right|^2\right\}^{1/2}\leqslant 2\sqrt{2\pi}\left\{\int_0^{\infty}dqq^6\sin^2\left(\frac{\tau\lambda}{2}e^{-q}\right)\right\}^{1/2}$$
$$=2\sqrt{2\pi}\left\{\int_0^1 dt\frac{1}{t}(\log t)^6\sin^2(\Lambda t)\right\}^{1/2},$$

after changing variables ($t=e^{-q}$) and defining $\Lambda=\tau\lambda/2$. As we show in Appendix A this last integral is $O(\log^7\lambda)$ and, hence, the term (33) is $O(\log^{7/2}\lambda/\lambda^2)$. So in expression (32) we obtain

$$\Im\Bigg\{\frac{\lambda e^{i\tau\lambda}}{2\pi R_1}\lim_{A\to\infty}\Bigg[-\frac{i}{\lambda}\int_{-\pi}^{\pi}d\theta\frac{\sin\theta}{A^2\cos^2\theta+\sin^2\theta}e^{i\lambda A\sin\theta}$$
$$+\frac{1}{\lambda^2}\int_{-\pi}^{\pi}d\theta\frac{A(A^2-4)\sin^2\theta\cos^2\theta-A\sin^4\theta}{[A^2\cos^2\theta+\sin^2\theta]^3}e^{i\lambda A\sin\theta}$$
$$-\frac{1}{\lambda^2}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta e^{i\lambda q\sin\theta}\nu_3(q)h_2(q;\theta)\Bigg]\Bigg\}+O\left[\frac{1}{\lambda}\right]+O\left[\frac{\log^{7/2}\lambda}{\lambda}\right]. \tag{34}$$

The reason why we had to integrate by parts in the first step is to get an additional factor of λ dividing the powers of $\log\lambda$.

Step (v): Using integration by parts twice one can check that the terms in the square brackets in (34) can be written when $A\to\infty$ as

$$2\pi\lim_{A\to\infty}\int_{\beta_1}^{A}dq\,\nu_3(q)J_0(\lambda q)=\lim_{A\to\infty}\int_{\beta_1}^{A}dq\int_{-\pi}^{\pi}d\theta\,\nu_3(q)e^{i\lambda q\sin\theta}, \tag{35}$$

plus an extra contribution coming from derivatives of $\nu_3(q)$ that does not contribute at this asymptotic order. In Appendix B we show that (35) is $O(1/\lambda^R)$ for all $R>0$. We, therefore, conclude that (31) is $O(\log^{7/2}\lambda/\lambda)$. In our proof we have used integration by parts twice to arrive at (34). Actually by using it repeatedly and applying the five-steps procedure explained above it is possible to argue that $\lim_{A\to\infty}I_3$ is, in fact, $O(1/\lambda^R)$ for all $R>0$.

We hence conclude that the first terms in the asymptotic expansion of (28) are given by the contributions (29) and (30), and therefore, by (11) when $\tau>1$. In order to get the first nonzero term in the asymptotics for $\tau<1$ it is necessary to perform integration by parts twice and follow the steps detailed above. This leads to the contribution for $\tau<1$ shown in (12),

$$-\frac{1}{2\pi R_1}\Im\left\{\frac{i}{\lambda}\oint_{\gamma}dt\frac{8i\tau t^2}{(t^2+2i\tau t-1)^3}\right\}=\frac{1}{R_1}\frac{\tau(1+2\tau^2)}{2\lambda(1-\tau^2)^{5/2}}.$$

The $\lambda\to0^+$ limit, on the other hand, can be obtained by using Taylor's theorem to write

$$e^{-i\tau\lambda e^{-t/\lambda}}=\sum_{k=0}^{N}\frac{(-i\tau\lambda)^k}{k!}e^{-kt/\lambda}+\frac{(-i\tau\lambda)^{(N+1)}}{(N+1)!}e^{-i\xi(t)}e^{-(N+1/\lambda)t},$$

with $0<\xi(t)<\tau\lambda e^{-t/\lambda}$. Substituting this in (5) (with $\rho=0$) we get

$$\frac{1}{R_1}\Im\left\{e^{i\tau\lambda}\int_0^{\infty}dtJ_0(t)\left[\sum_{k=0}^{N}\frac{(-i\tau\lambda)^k}{k!}e^{-kt/\lambda}+\frac{(-i\tau\lambda)^{(N+1)}}{(N+1)!}e^{-i\xi(t)}e^{-(N+1/\lambda)t}\right]\right\}.$$

The contribution of the last term can be easily bounded

$$\left|\frac{e^{i\tau\lambda}(-i\tau\lambda)^{N+1}}{(N+1)!}\int_0^{\infty}dt\,J_0(t)e^{-i\xi(t)}e^{-(N+1/\lambda)t}\right|\leqslant\frac{(\tau\lambda)^{N+1}}{(N+1)!}\int_0^{\infty}dt\,e^{-(N+1/\lambda)t}=\frac{\tau^{N+1}\lambda^{N+2}}{(N+1)(N+1)!}$$
$$=O(\lambda^{N+2}).$$

So we find that the asymptotics of (5) in this limit is given by

$$\frac{\lambda}{R_1}\Im\left\{e^{i\tau\lambda}\sum_{k=0}^{N}\frac{(-i\tau\lambda)^k}{k!\sqrt{k^2+\lambda^2}}\right\}+O(\lambda^{N+2}).$$

2. $\rho \neq 0$

We study now the integral (10) for $\rho \neq 0$. We will basically follow the same steps of the $\rho = 0$ case so we will skip some details. We choose $\eta_q = -1$, $\eta_{t_1} = t_1^2$, and $\eta_{t_2} = t_2^2$, obtaining

$$\|\nabla\Phi\|^2 = \frac{1}{4}\left\{ q^2\left[\left(t_1 + \frac{1}{t_2}\right)^2 + \rho^2\left(t_2 + \frac{1}{t_2}\right)^2\right] - \left[t_1 - \frac{1}{t_1} + \rho\left(t_2 - \frac{1}{t_2}\right) + 2i\tau e^{-q}\right]^2\right\}.$$

As we did above we introduce neutralizers ν_j, $j = 1, 2, 3$ and write (10) as a sum of the tree integrals

$$I_j \equiv -\frac{1}{R_1}\Im\left\{ \frac{\lambda e^{i\tau\lambda}}{4\pi^2}\int_0^\infty dq \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{\nu_j(q)}{t_1 t_2} e^{\lambda[(q/2)(t_1 - 1/t_1) + (\rho q/2)(t_2 - 1/t_2) - i\tau e^{-q}]}\right\}.$$

Starting with I_1 we fix $\gamma_{1,2}$ as in Fig. 8. Integrating by parts we find that only the boundary term contributes at leading order. This contribution can be written as

$$\frac{1}{R_1}\Im\left\{ \frac{1}{2\pi^2} \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{1}{\rho t_1(t_2^2 - 1) + t_2(t_1^2 + 2i\tau t_1 - 1)}\right\}. \tag{36}$$

This integral can be computed exactly (see Appendix C) and, in fact, it is equal to the free commutator given in Ref. 6; in particular it is zero in the regions IA and IB of Fig. 1. This means that we will have to use integration by parts again, as in the $\rho = 0$ case, to get the first significant asymptotic term when $\lambda \to \infty$ for these regions. After doing this we get the double integral

$$-\frac{1}{R_1}\Im\left\{ \frac{2i\tau}{\pi^2\lambda} \oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{t_1^2 t_2^2}{[\rho t_1(t_2^2 - 1) + t_2(t_1^2 + 2i\tau t_1 - 1)]^3}\right\}. \tag{37}$$

It can be easily checked that this reproduces the result obtained above for $\rho = 0$. This integral, in the considered regions outside the light cone, can be written in terms of complete elliptic integrals of the first and second kind, as shown in Appendix D. The result is just the $1/\lambda$ contribution appearing in Eq. (13).

Though it is also possible to compute the integral I_1 in the remaining regions, we will not do so because their contributions are subdominant with respect to those coming from the critical points of I_2.

Consider then I_2 and take as before the unit circumference as the integration path $\gamma_{1,2}$. We parametrize this curve according to $t_1(\theta_1) = e^{i\theta_1}$, $t_2(\theta_2) = e^{i\theta_2}$, $\theta_{1,2} \in (-\pi, \pi]$. Now we have

$$i\lambda\phi(q; \theta_1, \theta_2) \equiv \lambda\Phi[q; t_1(\theta_1), t_2(\theta_2)] = i\lambda[q(\sin\theta_1 + \rho\sin\theta_2) - \tau e^{-q}],$$

so that the critical points are given by the solutions to the equations

$$\sin\theta_1 + \rho\sin\theta_2 + \tau e^{-q} = 0,$$

$$q\cos\theta_1 = 0,$$

$$q\rho\cos\theta_2 = 0.$$

Since we are computing I_2 we are only interested in solutions with $q \neq 0$. Therefore, we must have $\cos\theta_1 = 0$ and $\cos\theta_2 = 0$, i.e. $\theta_1 = \pm\pi/2$ and $\theta_2 = \pm\pi/2$. For $\theta_1 = \theta_2 = \pi/2$, the remaining equation implies $1 + \rho + \tau e^{-q} = 0$, which has no solutions for $q \in \mathbb{R}$. If $\theta_1 = -\theta_2 = \pi/2$ we get $1 - \rho + \tau e^{-q} = 0$; this equation has solutions $q = \log\tau/(\rho - 1)$ in the integration region $q > 0$ only if $\tau > \rho - 1 > 0$. If $\theta_1 = -\theta_2 = -\pi/2$, we must have $-1 + \rho + \tau e^{-q} = 0$, and there exists a critical point $q = \log\tau/(1 - \rho)$ in the integration region only if $\tau > 1 - \rho > 0$. Finally if $\theta_1 = \theta_2 = -\pi/2$ we obtain $-1 - \rho + \tau e^{-q} = 0$, which is solved by $q = \log\tau/(1 + \rho)$; in this case $q > 0$ only when $\tau > 1 + \rho$. As

we see when (τ, ρ) are in the regions IA and IB of Fig. 1 there are no critical points for I_2, if (τ, ρ) is in region II there is only one critical point, and if (τ, ρ) is in region III there are two critical points. The contribution of these critical points to the asymptotics of I_2, that can be obtained with the standard formulas,[14] are the following in regions II and III, respectively:

$$\frac{1}{R_1}\Im\left\{\frac{e^{-i\,\pi/4}e^{i\lambda[\tau+|\rho-1|(1+\log\tau/|\rho-1|)]}}{\sqrt{2\pi\lambda\rho|1-\rho|}\log\dfrac{\tau}{|1-\rho|}}\right\}+O\left[\frac{1}{\lambda^{3/2}}\right],$$

$$\frac{1}{R_1}\Im\left\{\frac{e^{-i\,\pi/4}e^{i\lambda[\tau-|\rho-1|(1+\log\tau/|\rho-1|)]}}{\sqrt{2\pi\lambda\rho|1-\rho|}\log\dfrac{\tau}{|1-\rho|}}+\frac{e^{i\,\pi/4}e^{i\lambda[\tau+(\rho+1)(\log(1+\rho/\tau)-1)]}}{\sqrt{2\pi\lambda\rho(1+\rho)}\log\dfrac{\tau}{1+\rho}}\right\}+O\left[\frac{1}{\lambda^{3/2}}\right].$$

These, together with the contribution of the boundary term, provide (14) and (15).

Finally it is possible to prove that $\lim_{A\to\infty} I_3$ gives no contribution by essentially following the same steps as when $\rho=0$.

It is interesting to comment on the singularities that appear in the borders between the different regions I–III, and the axis $\rho=0$. Their presence is a manifestation of the fact that the asymptotic behavior in λ changes abruptly between adjacent regions. Notice, nonetheless, that the behavior is continuous in the border between the portion of the axis with $\tau<1$ and region IA, where the leading terms of the asymptotic expansion in λ are both $O(1/\lambda)$.

To conclude let us point out that the limit $\lambda\to 0^+$ can be obtained as in the $\rho=0$ case. The result is

$$\frac{1}{\pi R_1\sqrt{\rho}}\Im\left\{e^{i\tau\lambda}\sum_{k=0}^{N}\frac{(-i\tau\lambda)^k}{k!}Q_{-1/2}\left[\frac{\lambda^2(1+\rho^2)+k^2}{2\rho\lambda^2}\right]\right\}+O(\lambda^{N+2}).$$

IV. CONCLUSIONS AND COMMENTS

We have analyzed in detail the issue of microcausality for linearly polarized cylindrical waves by looking at the commutator of the axially symmetric scalar field that encodes the physical degrees of freedom of the system. We have been able to show several interesting effects that appear in the model. The first is a smearing of the cylindrical light cones. This is especially obvious if one studies the behavior of the commutator (divided by $8iG$) at two points with coordinates (t_1,R_1) and (t_2,R_2) when λ (the quotient of R_1 and the Planck length) is large. If R_2 is not too close to the axis one gets, in this limit, the discontinuous, cylindrical light cone structure defined by the free commutator. In particular, outside the region defined by this light cone the commutator is zero and, hence, observables would commute as in ordinary perturbative QFT. If, instead, one looks at the behavior when $R_2=0$ one finds a peculiar behavior as $\lambda\to\infty$; now superimposed to the free contribution, the commutator shows a characteristic oscillating behavior when the variable $\tau=(t_2-t_1)/(4G)$ grows. The frequency of this oscillation is controlled by the value of λ but the amplitude is *independent* of it, and turns out to decrease very slowly with τ in such a way that one recovers the value given by the free commutator only for very large values of τ. Nonetheless, there is a sense in which the free propagator is recovered if one averages over time intervals sufficiently larger than $4G$.

In our study we have had to find the most efficient methods to obtain the relevant asymptotic behaviors. Though this has not required the introduction of completely novel techniques it has been necessary to extend to our situation the usual Mellin transform methods and those employed for the analysis of multiple integrals. We have needed also to take into account that the integrals that define the commutator are, actually, improper.

Several issues are worth discussing in more detail. One is the problem of introducing regulators in the field operators and compare the results with those derived here. Though it is clear that

the approximation provided by the improper integrals considered in this work must be good in certain regimes, at some point the existence of a physical cutoff might manifest itself in the behavior of the field commutator, especially in the asymptotic regimes that we have explored. Another task that can be confronted with the techniques that we have developed here is the computation of other matrix elements for the commutator. It would also be interesting to consider other Green functions and some related objects, such as S matrix elements. We plan to do that in the future.

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APPENDIX A: ASYMPTOTICS OF THE INTEGRAL IN STEP (iv)

We want to investigate the asymptotic behavior of $\int_0^1 dt\,[(\log t)^m/t]\sin^2\Lambda t$, $m\in\mathbb{N}$, when $\Lambda\to\infty$. This can be found by a straightforward use of the Mellin–Parseval formula (19) in order to get a Mellin–Barnes representation for the integral. Defining $h(t)=\sin^2 t$ and $f(t)=(\log t)^m/t$ we get the Mellin transforms

$$M[h;z]=-\frac{\Gamma(z)\cos\frac{\pi z}{2}}{2^{1+z}},\quad -2<\Re(z)<0,$$

$$M[f;1-z]=-\frac{\Gamma(m+1)}{z^{m+1}},\quad 1<\Re(z),$$

so that

$$\int_0^1 dt\,\frac{(\log t)^m}{t}\sin^2\Lambda t=\frac{m!}{2\pi i}\int_{c-i\infty}^{c+i\infty}dz\,\Lambda^{-z}\frac{\Gamma(z)\cos\frac{\pi z}{2}}{2^{1+z}z^{m+1}},\qquad c\in(-2,0).$$

The integrand in this last expression can be analytically extended as a meromorphic function to $\mathbb{C}$ with poles in $z=-2n$, $n=0,1,\ldots$. By displacing the integration contour to the right of the pole at $z=0$, we get

$$\int_0^1 dt\,\frac{(\log t)^m}{t}\sin^2\Lambda t=-\operatorname{res}\left[\Lambda^{-z}\frac{m!\Gamma(z)\cos\frac{\pi z}{2}}{2^{1+z}z^{m+1}},z=0\right]+\frac{m!}{2\pi i}\int_{x_0-i\infty}^{x_0+i\infty}dz\,\Lambda^{-z}\frac{\Gamma(z)\cos\frac{\pi z}{2}}{2^{1+z}z^{m+1}}\tag{A1}$$

($x_0>0$) whenever the integral converges and provided we can neglect the contributions from the segments needed to close the integration contour at large values of $\Im(z)$. Writing $z=x_0+iy$ we have

$$\left|\frac{m!}{2\pi i}\int_{x_0-i\infty}^{x_0+i\infty}dz\,\Lambda^{-z}\frac{\Gamma(z)\cos\frac{\pi z}{2}}{2^{1+z}z^{m+1}}\right|\leqslant\frac{m!}{4\pi(2\Lambda)^{x_0}}\int_{-\infty}^{\infty}dy\left|\frac{\Gamma(x_0+iy)\cos\frac{\pi}{2}(x_0+iy)}{(x_0+iy)^{m+1}}\right|,$$

and using $\lim_{|y|\to\infty}(1/\sqrt{2\pi})\,|\Gamma(x+iy)|e^{\pi|y|/2}|y|^{-x+1/2}=1$ we find that

$$\left|\frac{\Gamma(x_0+iy)\cos\frac{\pi}{2}(x_0+iy)}{(x_0+iy)^{m+1}}\right| \sim \sqrt{\frac{\pi}{2}}|y|^{x_0-m-3/2}.$$

Hence, the integral in (38) is absolutely convergent if $x_0<m+1/2$ and its contribution is $O[1/\Lambda^{x_0}]$. It is straightforward to show that the residue at the pole $z=0$ is an $m+1$ degree polynomial in $\log\Lambda$ with the higher degree term given by $[(-1)^{m+1}/(2m+2)](\log\Lambda)^{m+1}$. This proves that, for $m\in\mathbb{N}$,

$$\int_0^1 dt\,\frac{(\log t)^m}{t}\sin^2\Lambda t = O[(\log\Lambda)^{(m+1)}].$$

APPENDIX B: ASYMPTOTICS OF THE INTEGRAL IN STEP (v)

Let us analyze the asymptotic behavior of $2\pi\int_{\beta_1}^{\infty}dq\;\nu_3(q)J_0(\lambda q)$ when $\lambda\to\infty$. After changing variables according to $k=\lambda q$ this integral becomes

$$\frac{2\pi}{\lambda}\int_{\lambda\beta_1}^{\infty}dk\;\nu_3\left(\frac{k}{\lambda}\right)J_0(k).$$

Taking into account that $J_0(k)=[-(1/k)(d\ /dk)-d^2/dk^2]J_0(k)$, this can be written as

$$\frac{2\pi}{\lambda}\int_{\lambda\beta_1}^{\infty}dk\;\nu_3\left(\frac{k}{\lambda}\right)\left[-\frac{1}{k}\frac{d}{dk}-\frac{d^2}{dk^2}\right]^N J_0(k),$$

with $N\in\mathbb{N}$. It is straightforward to prove by induction that

$$\left[-\frac{1}{k}\frac{d}{dk}-\frac{d^2}{dk^2}\right]^N=\sum_{j=1}^{2N}\frac{a_j}{k^{2N-j}}\frac{d^j}{dk^j},$$

for certain coefficients $a_j\in\mathbb{Z}$. Since all the derivatives of $(1/k^{2N-j})\,\nu_3(k/\lambda)$ at $k=\lambda\beta_1$ cancel, by integrating by parts j times and changing variables according to $k=q\lambda$ we obtain for our integral the following expression:

$$\frac{2\pi}{\lambda}\sum_{j=1}^{2N}(-1)^j a_j\int_{\lambda\beta_1}^{\infty}dk\,\frac{d^j}{dk^j}\left[\frac{1}{k^{2N-j}}\nu_3\left(\frac{k}{\lambda}\right)\right]J_0(k)=\frac{2\pi}{\lambda^{2N}}\sum_{j=1}^{2N}(-1)^j a_j\int_{\beta_1}^{\infty}dq\,\frac{d^j}{dq^j}\left[\frac{\nu_3(q)}{q^{2N-j}}\right]J_0(\lambda q).$$

Using that $J_0(x)\leqslant 1$ for all $x\in\mathbb{R}$, we hence get

$$\left|\frac{2\pi}{\lambda}\int_{\lambda\beta_1}^{\infty}dk\;\nu_3\left(\frac{k}{\lambda}\right)J_0(k)\right|\leqslant\frac{2\pi}{\lambda^{2N}}\sum_{j=1}^{2N}|a_j|\int_{\beta_1}^{\infty}dq\left|\frac{d^j}{dq^j}\left[\frac{\nu_3(q)}{q^{2N-j}}\right]\right|,$$

with all the integrals in the last sum being convergent. We conclude that, for all $N\in\mathbb{N}$,

$$\frac{2\pi}{\lambda}\int_{\lambda\beta_1}^{\infty}dk\;\nu_3\left(\frac{k}{\lambda}\right)J_0(k)=O\left[\frac{1}{\lambda^{2N}}\right].$$

APPENDIX C: COMPUTATION OF (36)

It is possible to show that choosing $\gamma_{1,2}$ as in Fig. 8 its denominator is always different from zero except for those exceptional values of ρ and τ corresponding to the borders between regions I and II, and II and III. We can use Fubini's theorem and exchange orders of integration. To integrate in t_1 we fix a value of t_2 on γ. The poles of the integrand are

$$t_1^{\pm}=\frac{1}{2t_2}[\rho-\rho t_2^2-2i\pi t_2\pm\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\pi t_2)^2}].$$

One of them is always inside γ and the other outside. For a fixed value of t_2 we find that t_1^- is inside γ when

$$\Re\left[\frac{1}{t_2}\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\pi t_2)^2}\right]>0,$$

or in certain exceptional cases when $\Re(t_1^-)=0$. Analogously t_1^+ is inside γ when

$$\Re\left[\frac{1}{t_2}\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\pi t_2)^2}\right]<0,$$

or, again, in certain exceptional occasions with $\Re(t_1^+)=0$ (in this last case t_1^- is outside γ). The residues at these poles are

$$t_1^+\to\frac{1}{\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\pi t_2)^2}},$$

$$t_1^-\to\frac{-1}{\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\pi t_2)^2}},$$

and integrating in t_1, (36) becomes

$$\Im\left\{-\frac{i}{\pi R_1}\oint_\gamma dt\,\frac{\operatorname{sgn}\Re[\sqrt{4t^2+(-\rho+\rho t^2+2i\pi t)^2}/t]}{\sqrt{4t^2+(-\rho+\rho t^2+2i\pi t)^2}}\right\}. \tag{C1}$$

Let us define $A=-1+\rho-\tau$, $B=1+\rho+\tau$, $C=1+\rho-\tau$, and $D=-1+\rho+\tau$. It is not difficult to check that

$$4t^2+(-\rho+\rho t^2+2i\pi t)^2=\tfrac{1}{4}[A(t-i)^2+B(t+i)^2][C(t-i)^2+D(t+i)^2],$$

and, hence, the integral (C1) is

$$\Im\left\{-\frac{2i}{\pi R_1}\oint_\gamma dt\,\frac{\operatorname{sgn}\Re[\sqrt{[A(t-i)^2+B(t+i)^2][C(t-i)^2+D(t+i)^2]}/t]}{\sqrt{[A(t-i)^2+B(t+i)^2][C(t-i)^2+D(t+i)^2]}}\right\}. \tag{C2}$$

In the following we restrict γ to be a positively oriented circumference going through $\pm i$ and parametrize it as $z(\theta)=-a+\sqrt{1+a^2}e^{i\theta}$, with $\theta\in[0,2\pi)$ and $a>0$ a constant. Changing variables according to the Möbius transformation $s(t)=(t+i)/(t-i)$ and denoting $Q_1(s)=A+Bs^2$, $Q_2(s)=C+Ds^2$ we can write (C2) in the form

$$\Im\left\{ -\frac{1}{\pi R_1}\int_{s(\gamma)} ds\, \frac{\operatorname{sgn}\Re\left[\dfrac{s-1}{i(s+1)}\sqrt{\dfrac{Q_1(s)Q_2(s)}{(s-1)^4}}\right]}{(s-1)^2\sqrt{\dfrac{Q_1(s)Q_2(s)}{(s-1)^4}}}\right\}$$

$$=\Im\left\{ -\frac{1}{\pi R_1}\int_{s(\gamma)} ds\, \frac{\operatorname{sgn}\Re\left[\dfrac{\sqrt{Q_1(s)Q_2(s)}}{i(s^2-1)}\right]}{\sqrt{Q_1(s)Q_2(s)}}\right\}\equiv \Im(I), \tag{C3}$$

where $s(\gamma)$–the image of the circumference γ–is a straight line through the origin with slope $-1/a<0$. The sign in the numerator in the last integral, for each $s\in\mathbb{C}$, is shown in Fig. 9 in the different regions in the (ρ,τ) parameter space.

We now proceed to compute the integral I appearing in (C3) for the regions IA, IB, IIA, IIB, and III, and for the hyperbola $\tau^2=\rho^2+1$.

Region IA: Here $A<0$, $B>0$, $C>0$, $D<0$, and the sign in the integrand is positive. We choose $a\to 0$ and parametrize $s(\gamma)$ as $s=\sigma(i-\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$. We have

$$I=-\frac{i}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A-B\sigma^2)(C-D\sigma^2)-i\varepsilon}},$$

with $\varepsilon\to 0^+$. Recalling our choice of branch for the square root, changing variables according to $u=\sqrt{-(B/A)}\sigma$, and noticing that $0<AD/(BC)<1$, this integral can be written as

$$I=\frac{1}{\pi R_1}\frac{1}{\sqrt{BC}}\int_{\mathbb{R}}\frac{du}{\sqrt{(1+u^2)\left(1+\dfrac{AD}{BC}u^2\right)}}=\frac{2}{\pi R_1}\frac{1}{\sqrt{(1+\rho)^2-\tau^2}}K\left(\sqrt{\frac{4\rho}{(1+\rho)^2-\tau^2}}\right). \tag{C4}$$

Region IB: Here $A>0$, $B>0$, $C>0$, $D>0$, and the sign in the integrand is positive. We choose $a\to\infty$ and parametrize $s(\gamma)$ as $s=\sigma(-1+i\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$. Then

$$I=\frac{i}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A+B\sigma^2)(C+D\sigma^2)-i\varepsilon}},$$

with $\varepsilon\to 0^+$. After the change of variables $u=\sqrt{(B/A)}\sigma$ (and since $0<AD/(BC)<1$) this integral becomes exactly (C4).

Region IIA: Here $A<0$, $B>0$, $C>0$, $D>0$, and the sign in the integrand is negative. Letting $a\to 0$ and parametrizing $s(\gamma)$ as $s=\sigma(i-\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$ we obtain (with $\varepsilon\to 0^+$)

$$I=\frac{i}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A-B\sigma^2)(C-D\sigma^2)+i\varepsilon}}.$$

This last integral can be split in two pieces:

$$I=\frac{2}{\pi R_1}\int_0^{\sqrt{C/D}}\frac{d\sigma}{\sqrt{(-A+B\sigma^2)(C-D\sigma^2)}}+\frac{2i}{\pi R_1}\int_{\sqrt{C/D}}^{\infty}\frac{d\sigma}{\sqrt{(A-B\sigma^2)(C-D\sigma^2)}}.$$

We find then [see formulas (3.152-3) and (3.152-6) of Ref. 13]

$$I=\frac{1}{\pi R_1\sqrt{\rho}}K\left(\sqrt{\frac{(1+\rho)^2-\tau^2}{4\rho}}\right)+\frac{i}{\pi R_1\sqrt{\rho}}K\left(\sqrt{\frac{\tau^2-(\rho-1)^2}{4\rho}}\right). \tag{C5}$$

Region IIB: Here $A<0$, $B>0$, $C>0$, $D>0$, and the sign in the integrand is positive. With the choice $a\to\infty$ and the parametrization $s=\sigma(-1+i\epsilon)$ $[\sigma\in\mathbb{R}]$ for $s(\gamma)$ we arrive at

$$I=\frac{1}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A+B\sigma^2)(C+D\sigma^2)-i\varepsilon}},$$

with $\varepsilon\to 0^+$. This can be written as

$$I=\frac{2i}{\pi R_1}\int_0^{\sqrt{-A/B}}\frac{d\sigma}{\sqrt{-(A+B\sigma^2)(C+D\sigma^2)}}+\frac{2}{\pi R_1}\int_{\sqrt{-A/B}}^{\infty}\frac{d\sigma}{\sqrt{(A+B\sigma^2)(C+D\sigma^2)}},$$

which gives again (C5).

Boundary between regions IIA and IIB: This is the hyperbola $\tau^2=1+\rho^2$. Parametrizing $s(\gamma)$ as $s=\sigma(i-\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$ we get

$$I=\frac{i}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A-B\sigma^2)(C-D\sigma^2)+i\varepsilon}}$$

(with $\varepsilon\to 0^+$) which reduces to the previous two cases. Substituting $\tau^2=1+\rho^2$ we thus obtain

$$I=\frac{1+i}{\pi R_1\sqrt{\rho}}K\left(\frac{1}{\sqrt{2}}\right)=\frac{1+i}{4\pi R_1\sqrt{\pi\rho}}\left[\Gamma\left(\frac{1}{4}\right)\right]^2.$$

Region III: Here $A<0$, $B>0$, $C<0$, $D>0$, and the sign in the integrand is negative. Letting $a\to 0$ and parametrizing $s(\gamma)$ as $s=\sigma(i-\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$ we obtain (with $\varepsilon\to 0^+$)

$$I=\frac{i}{\pi R_1}\int_{\mathbb{R}}\frac{d\sigma}{\sqrt{(A-B\sigma^2)(C-D\sigma^2)-i\varepsilon}}.$$

With the change of variables $u=\sqrt{-(D/C)}\sigma$ and noticing that $0<BC/(AD)<1$, this becomes

$$I=\frac{i}{\pi R_1}\frac{1}{\sqrt{-AD}}\int_{\mathbb{R}}\frac{du}{\sqrt{(1+u^2)\left(1+\dfrac{BC}{AD}u^2\right)}}=\frac{2i}{\pi R_1}\frac{1}{\sqrt{\tau^2-(1-\rho)^2}}K\left(\sqrt{\frac{4\rho}{\tau^2-(1-\rho)^2}}\right).$$

APPENDIX D: COMPUTATIONS OF THE DOUBLE INTEGRAL (37)

In order to do this we first integrate in t_1. Fixing t_2 we find that the poles coincide with those of (36). The arguments showing whether they are inside or outside γ are the same as in Appendix C. The residues are now

$$t_1^+\to\frac{t_2^2[\rho^2(t_2^2-1)^2+4i\rho\tau t_2(t_2^2-1)-2(1+2\tau^2)t_2^2]}{[4t_2^2+(-\rho+\rho t_2^2+2i\tau t_2)^2]\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\tau t_2)^2}},$$

$$t_1^-\to-\frac{t_2^2[\rho^2(t_2^2-1)^2+4i\rho\tau t_2(t_2^2-1)-2(1+2\tau^2)t_2^2]}{[4t_2^2+(-\rho+\rho t_2^2+2i\tau t_2)^2]\sqrt{4t_2^2+(-\rho+\rho t_2^2+2i\tau t_2)^2}}.$$

Integrating in t_1, (37) becomes then

$$\Im\Bigg\{-\frac{4\tau}{\pi R_1\lambda}\times\oint_\gamma dt\,\frac{\operatorname{sgn}\Re\Big[\frac{1}{t}\sqrt{4t^2+(-\rho+\rho t^2+2i\tau t)^2}\Big]\big[\rho^2(t^2-1)^2+4i\rho\tau t(t^2-1)-2(1+2\tau^2)t^2\big]t^2}{\big[4t^2+(-\rho+\rho t^2+2i\tau t)^2\big]^2\sqrt{4t^2+(-\rho+\rho t^2+2i\tau t)^2}}\Bigg\}. \tag{D1}$$

The same Möbius transformation used above allows us to write (D1) as

$$\Im\Bigg\{-\frac{i\tau}{2\pi R_1\lambda}\int_{s(\gamma)}ds\,\operatorname{sgn}\Re\Big[\frac{\sqrt{Q_1(s)Q_2(s)}}{i(s^2-1)}\Big]\times\frac{(s^2-1)^2[2\rho^2(1+s^2)^2+4\rho\tau(s^4-1)+(1+2\tau^2)(s^2-1)^2]}{Q_1^2(s)Q_2^2(s)\sqrt{Q_1(s)Q_2(s)}}\Bigg\}.$$

We compute it only in regions IA and IB, remembering that the sign in the integrand is that shown in Fig. 9.

Region IA: Here $A<0$, $B>0$, $C>0$, $D<0$, and the sign is positive. We choose $a\to 0$ and parametrize $s(\gamma)$ as $s=\sigma(i-\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$ getting

$$\Im\Bigg\{\frac{i\tau}{2\pi R_1\lambda}\int_{\mathbb{R}}d\sigma\,\frac{(1+\sigma^2)^2[2\rho^2(1-\sigma^2)^2+4\rho\tau(\sigma^4-1)+(1+2\tau^2)(\sigma^2+1)^2]}{(A-B\sigma^2)^2(C-D\sigma^2)^2\sqrt{-(A-B\sigma^2)(C-D\sigma^2)}}\Bigg\}.$$

The integrand consists of a rational function of σ divided by the square root of a fourth degree polynomial and the integration extends over the real axis; hence, it can be written in terms of complete elliptic integrals. The way to proceed now is to perform a partial fraction decomposition of the rational part and write it as a sum of integrals of the four following types

$$\int_{\mathbb{R}}\frac{dx}{\sqrt{(a^2+x^2)(b^2+x^2)^3}},\quad\int_{\mathbb{R}}\frac{dx}{\sqrt{(a^2+x^2)^3(b^2+x^2)}},$$

$$\int_{\mathbb{R}}\frac{dx}{\sqrt{(a^2+x^2)(b^2+x^2)^5}},\quad\int_{\mathbb{R}}\frac{dx}{\sqrt{(a^2+x^2)^5(b^2+x^2)}}.$$

These integrals can be found in Ref. 13 [see Eqs. (3.158-2), (3.158-4), (3.162-4), and (3.162-2) in that reference]. The result is the $1/\lambda$ contribution appearing in Eq. (13).

Region IB: Here $A>0$, $B>0$, $C>0$, $D>0$, and the sign in the integrand is positive. With the choice $a\to 0$ and the parametrization $s=\sigma(-1+i\epsilon)$ $[\sigma\in\mathbb{R},\epsilon\to 0^+]$ we obtain

$$\Im\Bigg\{\frac{i\tau}{2\pi R_1\lambda}\int_{\mathbb{R}}d\sigma\,\frac{(\sigma^2-1)^2[2\rho^2(1+\sigma^2)^2+4\rho\tau(\sigma^4-1)+(1+2\tau^2)(\sigma^2-1)^2]}{(A+B\sigma^2)^2(C+D\sigma^2)^2\sqrt{(A+B\sigma^2)(C+D\sigma^2)}}\Bigg\}.$$

It can be shown that this integral gives again the result found in region IA.

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[16] Notice that in this system of units G has dimensions of length.
[17] Throughout the paper improper integrals are understood in the Riemann sense $\int_a^\infty = \lim_{A\to\infty} \int_a^A$.
[18] As shown in Ref. 6 the only real singularity that appears now corresponds to $\rho = 1$.
[19] The very slow convergence of this oscillating series for large values of τ or large values of λ makes it impractical for numerical computations. This is the reason why we only give the lower portion of the plot in Fig. 2.
[20] The Mellin transform of a locally integrable function f in $(0, \infty)$ is given by $\int_0^\infty dt t^{z-1} f(t)$. It is a holomorphic function defined on the strip $\alpha < \Re(z) < \beta$ of the complex plane where the integral is absolutely convergent.
[21] Conditions for this identity to hold can be found in Ref. 14.
[22] We will use this choice throughout the paper.
[23] Formula (20) is obtained, precisely, by displacing the integration contour parallel to the imaginary axis. For functions with the asymptotic behaviors considered in the theorem the only singularities are poles whose residues give the asymptotic expansion.
[24] More precisely, an asymptotic sequence given by inverse powers of $\log \tau$ is appropriate to capture the behavior of our integral in τ.
[25] The asymptotic analysis of multiple integrals is greatly simplified by the identification of the *critical points*, those points that give the dominant contributions. For Laplace or Fourier types of integrals these are easy to identify and, in practice, they are just a finite number of isolated points that can be singled out and studied by using neutralizers.
[26] These are real, positive, $C^\infty(\mathbb{R})$ functions $\nu(q;\alpha_1,\alpha_2;\beta_1,\beta_2)$ satisfying $\nu(q;\alpha_1,\alpha_2;\beta_1,\beta_2) = 0$ if $q \in (-\infty,\alpha_1] \cup [\alpha_2,\infty)$ and $\nu(q;\alpha_1,\alpha_2;\beta_1,\beta_2) = 1$ if $q \in [\beta_1,\beta_2]$ (some of the parameters $\alpha_1,\alpha_2,\beta_1,\beta_2$ may be taken to be infinite). In several variables $q_1,\ldots,q_n$ it is sometimes useful to consider neutralizers that depend only on $\|q\|$.
[27] It is important to point out that the asymptotic behavior of an improper integral over $[0,\infty)$ may be very different from the limit of the asymptotic expansion of the integral over $[0, A]$ when $A \to \infty$.
[28] The reason why we use neutralizers depending only on q is, precisely, to exploit this freedom.
[29] This is no longer true for other choices of γ for which $\|\nabla\Phi\|^2$ is, in general, complex. In these cases $\|\nabla\Phi\|^2$ may be zero even though the partial derivatives of Φ are different from zero.
[30] In the following we will denote $g_k(q;\theta) \equiv i e^{i\theta} f_{(k)}[q;t(\theta)]$, the $i e^{i\theta}$ factor comes from the measure in the integral.
[31] We choose $\beta_1 > Q > \log \tau$ in the neutralizers introduced before.

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Integral representation of one-dimensional three particle scattering for δ function interactions

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The Schrödinger equation, in hyperspherical coordinates, is solved in closed form for a system of three particles on a line, interacting via pair delta functions. This is for the case of equal masses and potential strengths. The interactions are replaced by appropriate boundary conditions. This leads then to requiring the solution of a free-particle Schrödinger equation subject to these boundary conditions. A generalized Kontorovich–Lebedev transformation is used to write this solution as an integral involving a product of Bessel functions and pseudo-Sturmian functions. The coefficient of the product is obtained from a three-term recurrence relation, derived from the boundary condition. The contours of the Kontorovich–Lebedev representation are fixed by the asymptotic conditions. The scattering matrix is then derived from the exact solution of the recurrence relation. The wavefunctions that are obtained are shown to be equivalent to those derived by McGuire. The method can clearly be applied to a larger number of particles and hopefully might be useful for unequal masses and potentials.
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I. INTRODUCTION

Three-body systems and processes are of fundamental interest in physics.[1] One of these, with which a number of us have been concerned, is the recombination of three-particles to a dimer plus a free particle, in a many body system forming a Bose–Einstein condensate.[2] The condensate is not the lowest state of the system, but a metastable state. The three-body recombination is the dominant mechanism for cooling and lowering the overall energy of the system.

Experimental and theoretical studies have shown that this recombination rate depends mainly on the two-body scattering length a,[2–6] as the collision energy is low and the interaction is weak—owing to large interparticle distances, and on the bound state energies.

This would suggest that zero-range potentials (ZRP), defined in terms of the scattering length[7]

$$\lim_{r\to 0}\left[\frac{1}{r\psi}\frac{\partial(r\psi)}{\partial r}\right]=-1/a. \tag{1}$$

can be applied to model the interaction between the particles of the condensate. It has been shown by Nielsen and Macek using the hidden crossing technique that the ZRP describes properly the recombination transition in a system of three ^{4}He atoms.[2] Also, Gasaneo and Macek showed that the ZRP gives a quite good representation for the adiabatic potential of the same system.[8] A closed form solution for a system of three-particles interacting via a ZRP has been recently presented by Gasaneo *et al.*[9] The fragmentation process $^4\mathrm{He}_2+{}^4\mathrm{He}\rightarrow{}^4\mathrm{He}+{}^4\mathrm{He}+{}^4\mathrm{He}$ was studied and relatively good agreement was found when compared with the hidden crossing calculations. In the nuclear physics area we just want to mention the study of the $1+2$ elastic scattering of nnp and Λnp systems,[10] in which, besides the scattering length, it is included the effective range and the shape parameter in the boundary conditions. Recently, there has been several applications of the ZRP model in one dimension. The study of ion–atom collision have been done by Burgdörfer[11] and the photo-double ionization processes has been studied by Le Rouzo.[12] The use of one dimensional model to bosons has been considered by Muda and Snider using periodic boundary conditions and to the dynamics of fermions systems by McGuire.[13]

In this paper, we seek to apply our techniques to a famous model: Three particles in one dimension, subject to pair delta–function interactions. For this model, introduced by McGuire,[14] one can obtain exact solutions for the wave functions, the scattering matrix and the binding energies, in the case of particles of identical masses and equally weighted interactions. As such it has been extended to a larger number of particles,[15] using Bethe's Ansatz,[16] and also found to be exceedingly useful when used as a test-bed for the development of a number of different methods (pertubative, Faddeev, hyperspherical adiabatic, etc.).[17]

Here, we note that using ZRP and (1), in three-dimensions, leads to the Thomas effect and the collapse of the three-body ground state.[18] However, in one dimension, an equation similar to (1)—with a not the scattering length—provides boundary conditions which correctly characterizes the wave functions and replace the use of the δ-function interactions, and should, therefore, again give us exact results. One of these, though, is that the recombination rate, for this model, is exactly zero.

In Sec. II we propose a solution, written in integral form, for the free particle Schrödinger equation, written in hyperspherical coordinates. A linear combination of free particle solutions can then be found to satisfy the boundary condition that we alluded to earlier, and thus provide us with the solution of the problem with interaction. The requirement that the wave function satisfy the boundary conditions leads us to one of the important results of this paper, namely that the weight of the free particle solutions, in the integral form, satisfies a recurrence relation similar to that obtained in Refs. 19 and 9.

In Sec. III the method is applied to a particular case in which two of the particles are bound. It is shown that the recurrence relation, defining the coefficient of the free-particle expansion, can be solved in closed form and, thus, the scattering matrix is also obtained in a closed form. This allows us to have a detailed test of our method. In this section it is also shown that the wave function obtained is equivalent to the McGuire plane wave solution, and that our expression for the $\mathcal{S}$ matrix is the matrix obtained by McGuire, in the particular case discussed in this paper. In Sec. IV the relation between the hyperspherical adiabatic approach and the present one is discussed.

In Appendix A, the pseudo-Sturmian functions are derived. In Appendix B, the wave function is written as the symmetric wave plane in cartesian coordinates.

II. EXACT INTEGRAL REPRESENTATION

To begin the study of the three identical–particle system (therefore, with equal masses), consider the center of mass and Jacobi coordinates

$$r=\tfrac{1}{3}(x_1+x_2+x_3),$$

$$\eta=\sqrt{\tfrac{1}{2}}(x_1-x_2), \tag{2}$$

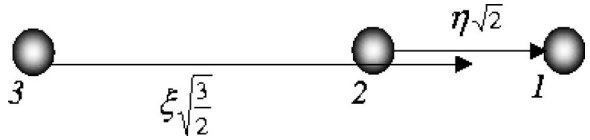

FIG. 1. One of three sets of Jacobi coordinates for the three particles.

$$\xi = \sqrt{\frac{2}{3}}\left(\frac{x_1 + x_2}{2} - x_3\right),$$

the x_i give us the locations of the 3 particles along the line, see Fig. 1. Using polar coordinates, the 2 Jacobi variables allow us to define, in turn, a hyper radius R and an angle θ as

$$\eta = R\cos\theta, \qquad \xi = R\sin\theta, \tag{3}$$

where $-\pi < \theta \leqslant \pi$ and $0 \leqslant R < \infty$. In terms of these coordinates the Schrödinger equation for the "relative" system can be written as

$$H\Psi(R,\theta) = \left(\frac{2m}{\hbar^2}\right) E\Psi(R,\theta), \tag{4}$$

where

$$H = -\left(\frac{1}{R}\frac{\partial}{\partial R}R\frac{\partial}{\partial R} + \frac{1}{R^2}\frac{\partial^2}{\partial\theta^2}\right) + \frac{1}{R}C(\theta). \tag{5}$$

The function $C(\theta)$ is defined by

$$C(\theta) = \frac{\pi}{3}c\sum_{j=0}^{5}\delta(\theta - \theta_j), \tag{6}$$

where the coefficient c equals $(3/\pi\sqrt{2})(2m/\hbar^2)g$, g being the strength of the interactions. This c is negative for attractive interactions and positive for repulsive ones. The angles θ_j equal $(2j+1)\pi/6$. The lines $\theta = \theta_j$ divide the (ρ,θ) plane in six regions. In each region the order of particles is fixed, so that between θ_4 and θ_5, $x_1 < x_2 < x_3$, etc. A different permutation of particles is associated to each region. From now on, we will choose the units such that $2m = 1$ and $\hbar = 1$. In each sector, we now seek a free particle solution that satisfies the boundary condition that will replace the effect of the potential, i.e.,

$$\lim_{\theta^- \to \theta_j}\left[\frac{1}{R\Psi(R,\theta)}\frac{\partial\Psi(R,\theta)}{\partial\theta}\right] = -\frac{1}{a}, \tag{7}$$

where $\theta^- = \theta < \theta_j$, $j = 0,1,\ldots,5$. In Eq. (7) $a = (6/\pi c)$ does not depend on j because all the strengths of the interactions and all the masses are equal. Writing a solution for the free particle system as the product $\psi_{\text{free}}(R,\theta) = \Theta(\nu,\theta)R^{1/2}\mathcal{R}_\nu(\mathrm{K}R)$, where $\mathrm{K}^2 = E$, leads to the set of free particle equations

$$\frac{R^2}{R^{-1/2}Z_\nu(\mathrm{K}R)}\left[\frac{\partial^2}{\partial R^2} + \mathrm{K}^2\right]R^{-1/2}Z_\nu(\mathrm{K}R) = \frac{-1}{\Theta(\nu,\theta)}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{4}\right)\Theta(\nu,\theta) = \nu^2 - \frac{1}{4}, \tag{8}$$

where $Z_\nu(\mathrm{K}R) = R^{1/2}\mathcal{R}_\nu(\mathrm{K}R)$ is a Bessel function and ν a separation constant. If for the $\Theta(\nu,\theta)$ functions we choose the pseudo-Sturmian functions $S(\nu,\theta)$, defined, for fixed ν, as the solutions of

$$-\left[\frac{\partial^2}{\partial\theta^2}+\frac{1}{4}-\rho(\nu)C(\theta)\right]S(\nu,\theta)=\left(\nu^2-\frac{1}{4}\right)S(\nu,\theta), \tag{9}$$

then the functions $\psi_{\text{free}}(\theta,R)=S(\nu,\theta)Z_\nu(\mathrm{K}R)$ are solutions of the Schrödinger equation Eq. (4) for values of $\rho(\nu)=R$. Note that Eq. (9) may be replaced by the relation

$$\left[\frac{\partial^2}{\partial\theta^2}+\nu^2\right]S(\nu,\theta)=0, \tag{10}$$

subject to the boundary conditions

$$\lim_{\theta^-\to\theta_j}\left[\frac{1}{\rho(\nu)}\,\frac{1}{S(\nu,\theta)}\,\frac{\partial S}{\partial\theta}(\nu,\theta)\right]=-\frac{1}{a},\quad j=0,1,\ldots,5. \tag{11}$$

In the last equation, we assumed that $S(\nu,\theta)$ is symmetric about each line $\theta=\theta_j$.

We now propose to write the general wave function of the system as a Kontorovich–Lebedev transform, in terms of the base functions just discussed, that is, as

$$\Psi(R,\theta)=\int_{\mathrm{s}} d\nu A(\nu)S(\nu,\theta)Z_\nu(\mathrm{K}R), \tag{12}$$

provided that its derivative satisfies the boundary conditions, i.e., Eq. (7). The contour of integration must be chosen so that the wave function has the correct asymptotic behavior.

Following the reasoning of Gasaneo *et al.*,[8] we will now show that the boundary conditions, Eq. (7), can be transformed into a recurrence relation for $A(\nu)$. First, we substitute Eq. (12) into Eq. (7), and then interchange the order in which the integral and the derivative are taken, to obtain for each j

$$\lim_{\theta^-\to\theta_j}\int_{\mathrm{s}} d\nu A(\nu)\left[\frac{1}{R}Z_\nu(\mathrm{K}R)\,\frac{\partial S(\nu,\theta)}{\partial\theta}+\frac{1}{a}S(\nu,\theta)Z_\nu(\mathrm{K}R)\right]=0. \tag{13}$$

Second, we use Eq. (11) and the identity $(2\nu/z)Z_\nu(z)=Z_{\nu+1}(z)-Z_{\nu-1}(z)$ to transform the equation to

$$\lim_{\theta^-\to\theta_j}\left\{\int_{\mathrm{s}} d\nu A(\nu)\frac{1}{\nu}[-\rho(\nu)/a]S(\nu,\theta)\times[Z_{\nu+1}(KR)-Z_{\nu-1}(KR)]\right.$$
$$\left.+\frac{2}{Ka}\int_{\mathrm{s}} d\nu A(\nu)S(\nu,\theta)Z_\nu(KR)\right\}=0. \tag{14}$$

We assumed in the previous equation that $\mathrm{K}=iK$ and $K\geqslant 0$, because we are mainly interested in negative energies. By selecting the appropriate contours we can now transform the last equation to

$$\lim_{\theta^-\to\theta_j}\int_{\mathrm{s}} d\nu\left[A(\nu-1)\frac{1}{\nu-1}\rho(\nu-1)S(\nu-1,\theta)-A(\nu+1)\frac{1}{\nu+1}\rho(\nu+1)S(\nu+1,\theta)\right.$$
$$\left.-\frac{2}{K}A(\nu)S(\nu,\theta)\right]Z_\nu(KR)=0. \tag{15}$$

Since the set of Bessel functions forms a complete set of basis functions, the function within the square brackets should be zero at the limit. We arrive, finally, at the recurrence relation that we are looking for

$$B(\nu-1)\rho(\nu-1)S(\nu-1,\theta_j)-B(\nu+1)\rho(\nu+1)S(\nu+1,\theta_j)=\frac{2\nu}{K}B(\nu)S(\nu,\theta_j), \tag{16}$$

where $B(\nu)=A(\nu)/\nu$. In the following section, we will apply this approach to a particular case of this three body system and show that we can obtain the wave function and the $\mathcal{S}$-matrix.

III. 2+1 SYSTEM

Consider now the case where two of the particles are bound. The wave function $\psi(R,\theta)$ can still be written in terms of the Kontorovich–Lebedev representation, Eq. (12). The unnormalized angle pseudo-Sturmian function $S(\nu,\theta)$, a six-fold symmetric function, is defined by the Eqs. (10) and (11). As can be seen in Appendix A, the function $S(\nu,\theta)$ may be written as

$$S(\nu,\theta)=\cos\left[\left(\theta-j\frac{\pi}{3}\right)\nu\right], \quad \left|\theta-j\frac{\pi}{3}\right|<\frac{\pi}{6}, \tag{17}$$

with $j=0,1,\ldots,5$, where $\rho(\nu)$ satisfies the relation

$$\nu\tan\left(\nu\frac{\pi}{6}\right)=\frac{1}{(6/\pi c)}\rho(\nu). \tag{18}$$

From the previous section, we can immediately conclude that $A(\nu)$ satisfies the recurrence relation

$$A(\nu+1)\sin\left[(\nu+1)\frac{\pi}{6}\right]-A(\nu-1)\sin\left[(\nu-1)\frac{\pi}{6}\right]=-\frac{\pi c}{3K}A(\nu)\cos\left[\nu\frac{\pi}{6}\right]. \tag{19}$$

A. Solution of the recurrence relation

The recurrence relation, displayed in Eq. (19), can be written as

$$e^{i(\pi/6)\nu}\left[A(\nu+1)e^{i(\pi/6)}-A(\nu-1)e^{-i(\pi/6)}+\frac{i\pi c}{3K}A(\nu)\right]+e^{-i(\pi/6)\nu}\left[-A(\nu+1)e^{-i(\pi/6)}\right.$$
$$\left.+A(\nu-1)e^{i(\pi/6)}+\frac{i\pi c}{3K}A(\nu)\right]=0. \tag{20}$$

An inspection, of the solution of the recurrence relation—Eq. (25) in Ref. 8, leads us to propose a coefficient in the form of the series

$$A(\nu)=e^{-\beta\nu}[e^{-i(\pi/3)\nu}+\mathcal{S}e^{i(\pi/3)\nu}+\mathcal{S}_1e^{-i(\pi/6)\nu}+\mathcal{S}_2e^{i(\pi/6)\nu}+\mathcal{S}_3]. \tag{21}$$

Substituting this expression in Eq. (20), and equating to zero the coefficients of exponentials, with different arguments that depend on ν, we obtain the following values for the parameters:

$$\mathcal{S}=\tan\left(\frac{\pi}{6}-i\beta\right)\cot\left(\frac{\pi}{6}+i\beta\right),$$

$$\mathcal{S}_3=-\cot\frac{\pi}{6}\cot\left(\frac{\pi}{6}+i\beta\right), \tag{22}$$

$$\cos(i\beta)=-\frac{\pi c}{6K},$$

$$\sin(i\beta)=i\frac{k}{K}. \tag{23}$$

Consequently, the solution for the coefficient can be written as

$$A(\nu)=e^{-\beta\nu}(e^{(-i\pi/3)\nu}+\mathcal{S}e^{(i\pi/3)\nu}+\mathcal{S}_3), \tag{24}$$

or

$$A(\nu)=2\,e^{-\beta\nu}\left[\cos\left(\frac{\pi}{3}\nu+\delta\right)+\alpha\right], \tag{25}$$

where

$$\mathcal{S}=e^{2i\delta} \tag{26}$$

and

$$\alpha=-\frac{1}{2}\cot\frac{\pi}{6}\sqrt{\cot\left(\frac{\pi}{6}-i\beta\right)\cot\left(\frac{\pi}{6}+i\beta\right)}. \tag{27}$$

In the next section, we demonstrate that $\mathcal{S}$ represents the scattering matrix and, accordingly, δ the phase shift. We should stress the remarkable fact that the S-matrix appears explicitly in the solution of the recurrence relation. In the next subsection it is shown that the expression obtained for $\mathcal{S}$ in this work is equivalent to the formula for the exact symmetric $\mathcal{S}$-matrix for the $2+1$ process, given in Ref. 21.

B. Asymptotic wave function

To be specific we will restrict the following discussion to the case of total negative energies, and will write $K=\sqrt{(\pi c)^2/36-k^2}\geqslant 0$, in which $-(\pi c)^2/36$ is the two-body bound energy and k^2 is the effective energy. Next, we will show that the imaginary axis is the appropriate contour to obtain the correct asymptotic behavior of the wave function. Substituting the coefficients $A(\nu)$ defined in Eqs. (22) and (24), the pseudo-Sturmian functions given in Eq. (17) and the modified Bessel functions $K_\nu(KR)$, into Eq. (12), as well as choosing the imaginary axis as the contour of integration, we find

$$\begin{aligned}\Psi=&\int_\varsigma d\nu(\cosh[(i\pi/3+\beta)\nu]-\sinh[(i\pi/3+\beta)\nu])\times\cos\left[\left(\theta-j\frac{\pi}{3}\right)\nu\right]K_\nu(KR)\\&+\mathcal{S}\int_\varsigma d\nu(\cosh[(i\pi/3-\beta)\nu]+\sinh[(i\pi/3-\beta)\nu])\cos\left[\left(\theta-j\frac{\pi}{3}\right)\nu\right]K_\nu(KR)\\&+\mathcal{S}_3\int_\varsigma d\nu(\cosh[\beta\nu]-\sinh[\beta\nu])\cos\left[\left(\theta-j\frac{\pi}{3}\right)\nu\right]K_\nu(KR).\end{aligned} \tag{28}$$

Note that in the above expression the exponentials in the coefficients have been written in terms of hyperbolic functions. The integral over the odd terms vanishes, leaving only the even terms in the integrand. After a trigonometric identity, this leads to

$$\Psi=\frac{1}{2}\Bigg\{\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[\beta+i\Bigg(\theta-[j-1]\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)K_{\nu}(KR)+\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[-\beta$$
$$+i\Bigg(\theta-[j+1]\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)K_{\nu}(KR)+\mathcal{S}\Bigg[\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[-\beta+i\Bigg(\theta-[j-1]\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)K_{\nu}(KR)$$
$$+\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[\beta+i\Bigg(\theta-[j+1]\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)K_{\nu}(KR)\Bigg]+\mathcal{S}_3\Bigg[\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[-\beta+i\Bigg(\theta-j\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)$$
$$\times K_{\nu}(KR)+\int_{\varsigma}d\nu\cosh\Bigg(\Bigg[\beta+i\Bigg(\theta-j\frac{\pi}{3}\Bigg)\Bigg]\nu\Bigg)K_{\nu}(KR)\Bigg]. \tag{29}$$

Using the Kontorovich–Lebedev Transforms,[20] we obtain

$$\Psi=\frac{i\pi}{2}\Bigg(\exp\Bigg\{-KR\cosh\Bigg(\beta+i\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}+\exp\Bigg\{-KR\cosh\Bigg(-\beta+i\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}$$
$$+\mathcal{S}\Bigg[\exp\Bigg\{-KR\cosh\Bigg(\beta+i\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}+\exp\Bigg\{-KR\cosh\Bigg(-\beta+i\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}\Bigg]$$
$$+\mathcal{S}_3\Bigg[\exp\Bigg\{-KR\cosh\Bigg(-\beta+i\Bigg[\theta-j\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}+\exp\Bigg\{-KR\cosh\Bigg(\beta+i\Bigg[\theta-j\frac{\pi}{3}\Bigg]\Bigg)\Bigg\}\Bigg]. \tag{30}$$

Introducing β from Eq. (23) into this expression, yields

$$\Psi=\frac{i\pi}{2}\Bigg(\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]-ikR\sin\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]\Bigg\}$$
$$+\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]+ikR\sin\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]\Bigg\}+\mathcal{S}\Bigg[\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]$$
$$-ikR\sin\Bigg[\theta-(j+1)\frac{\pi}{3}\Bigg]\Bigg\}+\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]+ikR\sin\Bigg[\theta-(j-1)\frac{\pi}{3}\Bigg]\Bigg\}\Bigg]$$
$$+\mathcal{S}_3\Bigg[\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-j\frac{\pi}{3}\Bigg]+ikR\sin\Bigg[\theta-j\frac{\pi}{3}\Bigg]\Bigg\}+\exp\Bigg\{\frac{\pi c}{6}R\cos\Bigg[\theta-j\frac{\pi}{3}\Bigg]$$
$$-ikR\sin\Bigg[\theta-j\frac{\pi}{3}\Bigg]\Bigg\}\Bigg]\Bigg),\quad j=0,1,\ldots,5. \tag{31}$$

From Eq. (17) it is easily seen that this wave function is fully symmetric under the interchange of particles. The function is invariant under the addition of $\pi/3$ to θ, together with the addition of one unit to j, which is what should be done to move from one region in the (ρ,θ) plane to its next counterclockwise neighbor. Remember that for each region there is a specific order of the particles.

We can also see that the real part of each of the exponential arguments is negative, except when $\theta-(j\mp1)\pi/3=\pm\pi/2$, that is on the lines $\theta=\theta_j$, where its value is zero. Thus, when R is large, the wave function is negligible except near the lines $\theta=\theta_j$. Note that only the first four terms give a significant contribution in the asymptotic region. We can conclude that the form of the wave function is that of products of bound state functions, associated with two particles, with oscillatory functions, which describe the location of the third particle with respect to the 2 bound ones. Evaluating, then, the wave function for large values of R, its asymptotic form can be written as

$$\Psi(R,\theta') \sim e^{\{\pi c/6\, R\cos\theta'\}}(e^{\{-ikR\sin\theta'\}} + \mathcal{S}\, e^{\{ikR\sin\theta'\}}) \tag{32}$$

where $\pi/6 < \theta' = \theta - (j-1)\,\pi/3 < \pi/2$, $j = 0,1,\ldots,5$. This asymptotic expression consists of a wave representing a two particles bound state multiplied by an incoming wave, together with an outgoing wave multiplied by $\mathcal{S}$.

From the expression in Eq. (22) the matrix $\mathcal{S}$ can be written as

$$S = \frac{\sin\left(\frac{\pi}{6}+i\beta\right)\cos\left(\frac{\pi}{6}-i\beta\right)}{\cos\left(\frac{\pi}{6}+i\beta\right)\sin\left(\frac{\pi}{6}-i\beta\right)} = \frac{\sin\frac{\pi}{3}-\sin(-2i\beta)}{\sin\frac{\pi}{3}+\sin(-2i\beta)} = \frac{\sin\frac{\pi}{3}+2\sin(i\beta)\cos(i\beta)}{\sin\frac{\pi}{3}-2\sin(i\beta)\cos(i\beta)}. \tag{33}$$

In terms of K

$$\cos(i\beta)\sin(i\beta) = -\frac{\pi c}{6K}\frac{ik}{K} = \frac{-i\pi ck}{6(\pi^2c^2/36-k^2)}. \tag{34}$$

Therefore

$$\mathcal{S} = \frac{1-36(k/\pi c)^2 - i(24/\sqrt{3})(k/\pi c)}{1-36(k/\pi c)^2 + i(24/\sqrt{3})(k/\pi c)}. \tag{35}$$

This is, precisely, the scattering matrix

$$S = \frac{[-1-i(6\sqrt{3}/\pi c)k][3+i(6\sqrt{3}/\pi c)k]}{[3+i(6\sqrt{3}/\pi c)k][-1+i(6\sqrt{3}/\pi c)k]}, \tag{36}$$

given as Eq. (61) in Ref. 21. It corresponds to the symmetric S matrix calculated for the specific process $2+1$.

The matrix $\mathcal{S}_3$, see again (22), has the following form as a function of k

$$\mathcal{S}_3 = \frac{3+i(6\sqrt{3}/\pi c)k}{-1+i(6\sqrt{3}/\pi c)k}. \tag{37}$$

$\mathcal{S}_3$ multiplies the shorter ranged part of the exact wave function, that goes to zero when R goes to ∞.

Additional insight can be gained, by following the reasoning of McGuire.[14] The scattering of 3 asymptotically free particles, to 3 also asymptotically free particles, requires 3 (successive) collisions, and yields the part of the wave function associated with the calculation of the S-matrix. Intermediate stages, associated with fewer collisions, give rise to the shorter ranged part of the wave functions. A similar reasoning holds for the $2+1$ processes.

In conclusion, we have shown that this integration contour, and the choice of Bessel functions, have imparted the correct asymptotic behavior. Furthermore, we can deduce from the asymptotic expression that the coefficient $\mathcal{S}$ represents the S-matrix.

IV. RELATION TO ADIABATIC THEORY

The eigenfunctions of the following eigenvalue equation[21] form a complete set of orthogonal hyperspherical adiabatic basis functions. Changing, a bit, the usual notation:

$$\left[\frac{1}{R'^2}\left(\frac{\partial^2}{\partial\theta^2}+\frac{1}{4}\right) - \frac{1}{R'}C(\theta) + \Lambda_\kappa(R')\right]B_\kappa(\theta;R') = 0, \tag{38}$$

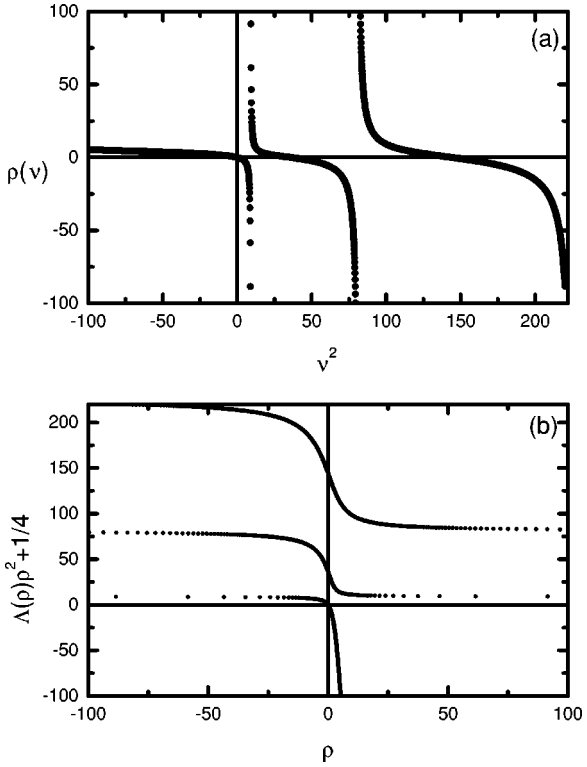

FIG. 2. Plot of the pseudo-Sturmian eigenvalue $\rho(\nu)$. In (a) we plot $\rho(\nu)$ as a function of ν^2. In (b) the plot of (a) is rotated and flipped to give ν^2 as a function of ρ. For ρ positive, $\nu^2=\Lambda(\rho)\rho^2+\frac{1}{4}$.

where R', a real parameter in this equation, is held fixed; $\kappa=0,6,12,\ldots$ and $\Lambda_\kappa(R')\rightarrow(\kappa^2-1/4)/R'^2$ as the interaction is turned off. The unnormalized eigenfunctions

$$B_\kappa(\theta;R')=\cos\left[q_\kappa\left(\theta-\frac{j\pi}{3}\right)\right], \tag{39}$$

where j is an integer such that $|\theta-j(\pi/3)|<\pi/6$ and q_κ satisfies

$$q_\kappa\tan\left(\frac{\pi}{6}q_\kappa\right)=\frac{\pi R'c}{6}. \tag{40}$$

In the adiabatic approach the parameter R' is identified with the hyper radius R. For $E<0$ there is only one open channel, labeled by $\kappa=0$. For large R, the channel function is concentrated along the lines defined by $\theta=\theta_j$. Accordingly it can represent the two-body bound state. For $E>0$, there is an infinite number of open channels, labeled by the successive numbers κ, equal and greater than zero. They describe, asymptotically, three free particles or a two-body bound state, together with a free particle.

Note that the function $\rho(\nu)$, Eq. (18), is a real function if, and only if, ν takes on values along the imaginary or the real axis, see Fig. 2. It can be seen that the pseudo-Sturmian function defined in Eq. (9) coincides, apart from normalization constants, with the lowest adiabatic function $B_0(\theta;R')$ when $\nu=q_0$ is an imaginary number and $\rho(\nu)=R'(q_0)$. Also, if $\nu=q_\kappa$ are in the real intervals $(3+[\kappa-6],9+[\kappa-6])$ with $\kappa=6,12,\ldots$, then $\rho(\nu)=R'(q_\kappa)$ and the pseudo-Sturmian functions become equal, except for the normalization constants, to the adiabatic eigenfunctions $B_\kappa(\theta;R')$.

Thus, in the case of the example considered in this paper, that is $E<0$ and the $2+1$ system, the integral Eq. (12), along the imaginary axis in the complex ν plane, can be written in terms of the lowest adiabatic function as

$$\Psi(R,\theta)=\int_{\varsigma} d\nu A(\nu)B_0(\theta;R'(\nu))Z_\nu(KR), \tag{41}$$

where ν runs from $-i\infty$ to $i\infty$. The most important contribution of the adiabatic functions to the integral, at large R, comes from the lines $\theta=\theta_j$, where two of the particles are joined. When these adiabatic functions are multiplied by the appropriate Bessels functions, their linear combination [Eq. (41)] should have the correct asymptotic behavior, and will represent a two-body bound system in the colliding with a third particle.

V. CONCLUSIONS AND OUTLOOK

We have shown that the integral representation approach within the hyperspherical context, when applied to McGuire's model, offers a reliable tool to study the collisional dynamics of the three-body system. We have obtained several interesting results, namely:

(i) an exact solution to the corresponding Schrödinger equation;
(ii) a closed form for the angular basis for this system, the pseudo-Sturmian functions;
(iii) a recurrence relation for the coefficients, in the expansion of the wave function in terms of the free-particle basis;
(iv) the S-matrix, obtained directly from the solution of the recurrence relation;
(v) the relation of the present approach to the traditional adiabatic approach;
(vi) the relation of the present solution to the known plane wave exact solution.

The simplicity of the approach as compared with the adiabatic one, promises to be very useful in extending it to more complicated situations, like the system with different masses and systems with more particles, currently under research, or systems in three dimensions modeled by ZRP potentials. In the last case, the method can be applied to a wide kind of systems to obtain asymptotic solutions which can be matched to solutions obtained with methods like the R-matrix one, simplifying substantially the calculations.

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APPENDIX A: PSEUDO-STURMIAN FUNCTIONS

Fixing ν, the general solution for the eigenvalue equation

$$\left[\frac{\partial^2}{\partial\theta^2}+\nu^2\right]\varphi(\theta)=\left[\rho(\nu)\frac{\pi c}{3}\sum_{j=0}^{5}\delta(\theta-\theta_j)\right]\varphi(\theta), \tag{A1}$$

with $\theta_j=(2j+1)\pi/6$, can be written as the free angular wave solution $\varphi(\theta)=D_\nu\cos[\nu(\theta-\gamma_j)]$, $j=0,1,\ldots,5$, provided that it be continuous through the boundary lines $\theta=\theta_j$, that is,

$$\cos[\nu(\theta_j-\gamma_{j+1})]=\cos[\nu(\theta_j-\gamma_j)], \tag{A2}$$

and satisfies the boundary conditions

$$\lim_{\zeta\to 0}\ \int_{\theta_j-\zeta}^{\theta_j+\zeta}\left\{ d\theta\left[\frac{\partial^2}{\partial\theta^2}+\nu^2\right]\varphi(\theta)-\left[\rho(\nu)\frac{\pi c}{3}\sum_{l=0}^{5}\ \delta(\theta-\theta_l)\right]\varphi(\theta)\right\}=0, \tag{A3}$$

with $j=0,1,\ldots,5$. D_ν, which does not depend on j for the symmetric solution, determined by normalizing the wave function.[22] The requirement of continuity leads to the conditions $\gamma_j+\gamma_{j+1}=2\theta_j=(j+[j+1])\pi/3$ or to $\gamma_{j-1}=\gamma_j$. The second condition does not satisfy (A3) so we shall use the first one, which can be written as $\gamma_j=j\ \ \pi/3$. Now to focus on Eq. (A3). Continuity implies that the integral of the second term gives zero. For each j, the first and the third terms give

$$\lim_{\zeta\to 0}\left(\frac{\partial}{\partial\theta}(\cos\nu[\theta-\gamma_{j+1}])_{\theta=\theta_j+\varsigma}-\frac{\partial}{\partial\theta}(\cos\nu[\theta-\gamma_j])_{\theta=\theta_j-\varsigma}\right)-\rho(\nu)\frac{\pi c}{3}\cos\nu[\theta_j-\gamma_j]=0. \tag{A4}$$

If we select a symmetric solution, then

$$-\frac{\partial}{\partial\theta}\ \cos(\nu[\theta_j+\varsigma-\gamma_{j+1}])=\frac{\partial}{\partial\theta}\ \cos(\nu[\theta_j-\varsigma-\gamma_j]), \tag{A5}$$

and taking the limit in Eq. (A4), we obtain the desired form of the boundary condition

$$\lim_{\theta^-\to\theta_j}\ \frac{1}{\rho(\nu)\cos(\nu[\theta-\gamma_j])}\frac{\partial}{\partial\theta}\ \cos(\nu[\theta-\gamma_j])=-\frac{\pi c}{6}, \tag{A6}$$

where $j=0,1,\ldots,5$. Calculating the derivative and the limit in Eq. (A6) yields

$$\frac{6}{\pi c}v\tan\nu\pi/6=\rho(\nu). \tag{A7}$$

We conclude that $\cos[\nu(\theta-j\pi/3)]$, $j=0,1,\ldots,5$, satisfies Eq. (A1), provided that $\rho(\nu)$ satisfies Eq. (A7).

APPENDIX B: DERIVATION OF THE PLANE WAVE REPRESENTATION IN TERMS OF CARTESIAN COORDINATES

For the $2+1$ system, and aside from an ultimate normalization, the incoming wave function from Eq. (31) can be written in terms of Cartesian coordinates, as

$$\begin{aligned}\psi^i=\exp\Bigg\{&\frac{\pi c}{6}\left(\frac{x_1-x_2}{\sqrt{2}}\cos\left[(j-1)\frac{\pi}{3}\right]+\frac{x_1+x_2-2x_3}{\sqrt{6}}\sin\left[(j-1)\frac{\pi}{3}\right]\right)\\&-ik\left(\frac{x_1+x_2-2x_3}{\sqrt{6}}\cos\left[(j-1)\frac{\pi}{3}\right]-\frac{x_1-x_2}{\sqrt{2}}\sin\left[(j-1)\frac{\pi}{3}\right]\right)\Bigg\}\\&+\exp\Bigg\{\frac{\pi c}{6}\left(\frac{x_1-x_2}{\sqrt{2}}\cos\left[(j+1)\frac{\pi}{3}\right]+\frac{x_1+x_2-2x_3}{\sqrt{6}}\sin\left[(j+1)\frac{\pi}{3}\right]\right)\\&+ik\left(\frac{x_1+x_2-2x_3}{\sqrt{6}}\cos\left[(j+1)\frac{\pi}{3}\right]-\frac{x_1-x_2}{\sqrt{2}}\sin\left[(j+1)\frac{\pi}{3}\right]\right)\Bigg\}.\end{aligned} \tag{B1}$$

Evaluating the trigonometric functions for $j=0$ in the above expression, the argument of the first exponential function takes the form

$$i\left[-\frac{2}{\sqrt{6}}kx_1+\left(i\frac{\pi c}{6\sqrt{2}}+\frac{k}{\sqrt{6}}\right)x_2+\left(-i\frac{\pi c}{6\sqrt{2}}+\frac{k}{\sqrt{6}}\right)x_3\right]. \tag{B2}$$

By labeling the particle wave numbers as in Ref. 21,

$$k_1=i\frac{\pi c}{6\sqrt{2}}-\frac{1}{\sqrt{6}}k,$$

$$k_2=-i\frac{\pi c}{6\sqrt{2}}-\frac{1}{\sqrt{6}}k, \tag{B3}$$

$$k_3=\sqrt{\frac{2}{3}}k,$$

the incoming wave takes the form

$$\psi^i=\exp\{-i(k_3x_1+k_2x_2+k_1x_3)\}_{j=0}+\exp\{i(k_2x_1+k_3x_2+k_1x_3)\}_{j=0}.$$

The outgoing wave for $j=0$ can be obtained from the incoming one by substituting k by $-k$, which in turns means interchanging $k_1\leftrightarrow k_2$ and inverting the sign of the whole argument within all exponentials, that is,

$$\mathcal{S}[\exp\{-i(k_1x_1+k_3x_2+k_2x_3)\}_{j=0}+\exp\{i(k_3x_1+k_1x_2+k_2x_3)\}_{j=0}].$$

The wave associated to the factor $\mathcal{S}_3$ can be written as

$$\exp\{-i(k_1x_1+k_2x_2+k_3x_3)\}_{j=0}+\exp\{i(k_2x_1+k_1x_2+k_3x_3)\}_{j=0}].$$

The above results correspond to the sector $j=0$ in the (ρ,θ) plane, in which the order of particles is given by $x_2<x_3<x_1$. The waves in different sectors can be obtained by the appropriate permutation of the set of coordinates $\{x_1,x_2,x_3\}$. The completely symmetric wave plane may then be written as

$$\begin{aligned}\psi=\Sigma_p[&\{\exp[-i(k_3x_1+k_2x_2+k_1x_3)]_{j=j_p}+\exp[i(k_2x_1+k_3x_2+k_1x_3)]_{j=j_p}\}\\&+\mathcal{S}(p)\{\exp[-i(k_1x_1+k_3x_2+k_2x_3)]_{j=j_p}+\exp[i(k_3x_1+k_1x_2+k_2x_3)]_{j=j_p}\}\\&+\mathcal{S}_3(p)\{\exp[-i(k_1x_1+k_2x_2+k_3x_3)]_{j=j_p}+\exp[i(k_2x_1+k_1x_2+k_3x_3)]_{j=j_p}\}],\end{aligned} \tag{B4}$$

where the sum runs over all permutations of the set $\{x_1,x_2,x_3\}$.

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On the general structure of Ricci collineations for type B warped space–times

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A complete study of the structure of Ricci collineations for type B warped space–times is carried out. This study can be used as a method to obtain these symmetries in such space–times. Special cases as 2+2 reducible space–times, and plane and spherical symmetric space–times are considered specifically. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1775875]

I. INTRODUCTION

In the last years, symmetries in general relativity have been studied in depth because of their interest from both a mathematical and a physical viewpoint. In fact, symmetries are important not only because of their classical physical significance, but also because they simplify Einstein equations and provide a classification of the space–times according to the structure of the corresponding Lie algebra. They are described by vector fields X on the space–time which satisfy a relation of the form

$$\pounds_X \Phi = \Lambda,$$

where Φ is any of the quantities g_{ab}, R_{ab}, R^a_{bcd}, etc, Λ is a tensor with the same index symmetries as Φ, and $\pounds$ represents the Lie derivative. Depending on Φ and Λ, there are different classes of symmetries (the relation between them was studied in Ref. 9). For example, if $\Phi = g_{ab}$ and $\Lambda = \psi g_{ab}$, with ψ a function, then X is a Killing vector field if $\psi = 0$, a homothetic vector field if $\psi_{,a} = 0$, a special conformal vector field if $\psi_{;ab} = 0$, and a conformal vector field if ψ is arbitrary. A symmetry will be called proper if it does not belong to any of its subtypes, otherwise it will be said improper.

In this paper we will concentrate on Ricci collineations, that is, the case when $\Phi = R_{ab}$ and $\Lambda = 0$. These symmetries are interesting because, among other things, they provide information about the energy-momentum tensor via the Einstein equations (although Ricci collineations are not usually matter collineations). In order to ensure that Ricci collineations form a Lie algebra with the usual bracket operation, we shall assume that they are smooth vector fields. Recall that this algebra naturally contains all the special conformal vector fields (and thus, all the homothetic and Killing vector fields). Regarding the Ricci tensor, we shall consider (up to Sec. V) that it is nondegenerate,

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i.e., rank 4; in particular, this ensures that the corresponding Lie algebra is finite dimensional, with maximal dimension being 10. Further information on dimensionality and degenerate Ricci tensors can be found, for example, in Refs. 5 and 8.

In Ref. 3 the general form and classification of Ricci collineations of Robertson–Walker space–times is provided in detail. Afterwards, in Ref. 2 the authors compute Ricci collineations of metrics g_{ab} which are conformal to $1+(n-1)$ decomposable metrics by using an interesting technique. Roughly speaking, they construct the generic metric G_{ab} defined from the symmetry group of g_{ab}. Then, proper Ricci collineations are the Killing vector fields of G_{ab} which are not Killing vector fields of g_{ab}. This method provides the Ricci collineations of Robertson–Walker space–times without any further calculations.

A few years ago, the problem of determining all Ricci collineations of type B warped space–times was considered in Ref. 6. This class of space–times is important because its structure is satisfied by multiple examples of interest in Physics as Schwarzschild, Robertson–Walker, etc. Unfortunately, the conclusion obtained there cannot be considered the solution of the problem, because it does not give *all* Ricci collineations of such space–times. In fact, two simple counterexamples to the main result in Ref. 6 were given in Ref. 1. On the other hand, the technique introduced in Ref. 2 does not seem to be applicable directly to these space–times. In conclusion, this problem remains still open.

Our aim in this paper is to describe in a general context the structure of all Ricci collineations of type B warped space–times. In fact, after a study of the equations which define these symmetries in such space–times, we classify them according to their structure. This classification can be considered a method to obtain all Ricci collineations. In particular, the counterexamples given in Ref. 1 are clearly contained in our results, Remark 4.3 (1). This paper is organized as follows.

After some preliminaries on type B warped space–times, in Sec. II we obtain two conclusions (Propositions 2.1 and 2.3) on the structure of Killing vector fields and Ricci collineations of such space–times. In Sec. III, these results are applied systematically. Ricci collineations are classified according to having or not having mixed variables and, in each case, according to their vertical component. As consequence, an exhaustive description of the structure of these symmetries is obtained. In Sec. IV, $2+2$ reducible space–times (Sec. IV A) and plane and spherical symmetric space–times (Sec. IV B) are studied specifically. Finally, the case when Ricci tensor is degenerate is briefly considered in Sec. V.

II. PRELIMINARIES

Let (M_1,g_1) and (M_2,g_2) be semi-Riemannian manifolds, and $\phi>0$ a smooth function on M_1. A warped product with base (M_1,g_1), fiber (M_2,g_2), and warping function $\phi>0$ is the product manifold $M=M_1\times M_2$ endowed with the metric tensor:

$$g^{\phi}=\pi_1^{*}g_1+(\phi\circ\pi_1)^2\pi_2^{*}g_2\equiv g_1+\phi^2 g_2,$$

where π_1 and π_2 are the natural projections of $M_1\times M_2$ onto M_1 and M_2, respectively. If, additionally, (M,g^{ϕ}) is a connected time-oriented four-dimensional Lorentzian manifold, then we say that (M,g^{ϕ}) is a warped space–time. In this case, a classification can be made according to the respective dimensions of M_1 and M_2 (see Ref. 4 and references therein for a general discussion).

In this paper we will concentrate on the study of type B warped space–times, that is, the case when M_1 and M_2 are both of dimension 2. In this case, and whenever we work locally, we can assume

$$g^{\phi}=g_{AB}(x^C)\mathrm{d}x^A\mathrm{d}x^B+\phi^2(x^C)g_{\alpha\beta}(x^{\gamma})\mathrm{d}x^{\alpha}\mathrm{d}x^{\beta},\quad \begin{matrix}A,B,C=0,1,\\ \alpha,\beta,\gamma=2,3,\end{matrix}$$

where g_{AB} and $g_{\alpha\beta}$ are the components of g_1 and g_2 in certain charts $(U_1\subseteq M_1,x^0,x^1)$, $(U_2\subseteq M_2,x^2,x^3)$, respectively.

Let X be a vector field on M and consider its horizontal and vertical components X_1, X_2; that is,

$$X_1(x^A,x^\alpha) = \mathrm{d}\pi_1(X)(x^A,x^\alpha), \quad X_2(x^A,x^\alpha) = \mathrm{d}\pi_2(X)(x^A,x^\alpha).$$

Then, the Lie derivative of g^ϕ with respect to X is

$$(\pounds_X g^\phi)_{AB} = (\pounds_{X_1} g_1)_{AB}, \tag{2.1}$$

$$(\pounds_X g^\phi)_{A\alpha} = g_{AC} X^C_{1,\alpha} + \phi^2 g_{\alpha\beta} X^\beta_{2,A}, \tag{2.2}$$

$$(\pounds_X g^\phi)_{\alpha\beta} = \phi^2 (\pounds_{X_2} g_2)_{\alpha\beta} + \phi^2_{,C} X^C_1 g_{\alpha\beta}. \tag{2.3}$$

In order to find the Killing vector fields of (M,g^ϕ), (2.1)–(2.3) must be set equal to zero. Condition (2.1) equal to zero is equivalent to the following: for every $p_2 \in M_2$ the restriction of X_1 to $M_1 \times p_2$ is a Killing vector field (perhaps zero) of $(M_1 \times p_2, g_1)$. On the other hand, (2.3) equal to zero is equivalent to the following: for every $p_1 \in M_1$ the restriction of X_2 to $p_1 \times M_2$ is a conformal vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ with conformal factor

$$\psi = -\frac{1}{2}\frac{\phi^2_{,C} X^C_1}{\phi^2}.$$

These simple facts are summarized in the following way.

Proposition 2.1: Let (M,g^ϕ) be a type B warped space–time with base (M_1,g_1), fiber (M_2,g_2) and warping function $\phi>0$. A vector field $X \not\equiv 0$ on M is Killing of (M,g^ϕ) if and only if the following statements hold:

(i) *for every $p_1 \in M_1$, X_2 is a conformal vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ with conformal factor ψ,*

(ii) *for every $p_2 \in M_2$, X_1 is a Killing vector field (perhaps zero) of $(M_1 \times p_2, g_1)$, which satisfies*

$$\phi^2_{,C} X^C_1 = -2\psi\phi^2, \tag{2.4}$$

(iii) *components (2.2) are equal to zero.*

A direct computation provides the following components R_{ab} of the Ricci tensor $\mathbf{R}$ of a type B warped space–time:

$$R_{AB} = \tfrac{1}{2} R_1 g_{AB} - \frac{2}{\phi}\phi_{A;B},$$

$$R_{A\alpha} = 0,$$

$$R_{\alpha\beta} = \tfrac{1}{2}(R_2 - (\phi^2)^A_{;A}) g_{\alpha\beta} \equiv F g_{\alpha\beta}, \tag{2.5}$$

where, obviously, $F := \frac{1}{2}(R_2 - (\phi^2)^A_{;A})$, R_1 and R_2 are the scalar curvatures of g_1 and g_2, respectively, and the semicolon indicates the covariant derivative with respect to g^ϕ.

Remark 2.2: Although the terms $\phi_{A;B}$ and $(\phi^2)^A_{;A}$ in (2.5) include covariant derivatives with respect to all the metric g^ϕ, a direct computation shows that they are independent of the variables x^γ of M_2. In fact,

$$\phi_{A;B} = \phi_{,AB} - \frac{g^{CD}}{2}(g_{DB,A} + g_{DA,B} - g_{AB,D})\phi_{,C},$$

$$(\phi^2)^A_{;A} = g^{AB}\phi^2_{,AB} - \frac{g^{AB}g^{CD}}{2}(g_{DB,A} + g_{DA,B} - g_{AB,D})\phi^2_{,C}.$$

The Lie derivative of $\mathbf{R}$ with respect to X is

$$(\pounds_X \mathbf{R})_{AB} = R_{AB,C}X^C_1 + R_{AC}X^C_{1,B} + R_{CB}X^C_{1,A}, \tag{2.6}$$

$$(\pounds_X \mathbf{R})_{A\alpha} = R_{AC}X^C_{1,\alpha} + R_{\alpha\beta}X^\beta_{2,A}, \tag{2.7}$$

$$(\pounds_X \mathbf{R})_{\alpha\beta} = F(\pounds_{X_2} g_2)_{\alpha\beta} + F_{,C}X^C_1 g_{\alpha\beta} + F_{,\gamma}X^\gamma_2 g_{\alpha\beta}. \tag{2.8}$$

In the following, our aim will be to find the Ricci collineations of (M, g^ϕ); that is, the vector fields $X \not\equiv 0$ on M such that (2.6)–(2.8) are equal to zero.

As commented in the Introduction, we will assume that $\mathbf{R}$ is nondegenerate. Therefore, $F \neq 0$ everywhere. Moreover, from (2.5) and Remark 2.2, R_{AB} can be seen as the components of a metric tensor g_R defined on M_1. Then, reasoning as in Proposition 2.1, condition (2.6) equal to zero is equivalent to the following: for every $p_2 \in M_2$ the restriction of X_1 to $M_1 \times p_2$ is a Killing vector field (perhaps zero) of $(M_1 \times p_2, g_R)$. On the other hand, (2.8) equal to zero is equivalent to the following: for every $p_1 \in M_1$ the restriction of X_2 to $p_1 \times M_2$ is a conformal vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ with conformal factor

$$\psi = -\frac{1}{2}\frac{F_{,C}X^C_1 + F_{,\gamma}X^\gamma_2}{F}. \tag{2.9}$$

Equation (2.9) can be simplified by using the classical expression of the Lie derivative of the Ricci $\mathbf{R}_h$ of a semi-Riemannian manifold (N, h) with respect to a conformal vector field Y of conformal factor ξ (see Ref. 7); that is,

$$(\pounds_Y \mathbf{R}_h)_{ab} = -(n-2)\xi_{|ab} - (\Delta_h \xi)h_{ab}, \tag{2.10}$$

where $n = \dim N$ and $\Delta_h \xi = \xi_{|cd}h^{cd}$ is the Laplacian of ξ with respect to h (obviously, the stroke denotes the covariant derivative with respect to h). In fact, assume that X_2 is a conformal vector field of $(p_1 \times M_2, g_2)$ with conformal factor ψ. Then, from (2.10) we obtain

$$(\pounds_{X_2} \mathbf{R}_{g_2})_{\alpha\beta} = -(\Delta_{g_2}\psi)g_{\alpha\beta}.$$

But, obviously,

$$\pounds_{X_2}(\mathbf{R}_{g_2})_{\alpha\beta} = \pounds_{X_2}(\tfrac{1}{2}R_2 g_2)_{\alpha\beta} = \tfrac{1}{2}(R_{2,\gamma}X^\gamma_2 + 2\psi R_2)g_{\alpha\beta};$$

thus

$$R_{2,\gamma}X^\gamma_2 + 2\psi R_2 = -2\Delta_{g_2}\psi. \tag{2.11}$$

On the other hand, by replacing in (2.9) the expression of F we have

$$2\psi(R_2 - (\phi^2)^A_{;A}) = (\phi^2)^A_{;A,C}X^C_1 - R_{2,\gamma}X^\gamma_2. \tag{2.12}$$

Therefore, from (2.11) and (2.12) we obtain

$$(\phi^2)^A_{;A,C}X^C_1 = -2\psi(\phi^2)^A_{;A} - 2\Delta_{g_2}\psi. \tag{2.13}$$

These facts are summarized in the following result.

Proposition 2.3: Let (M,g^{ϕ}) *be a type B warped space–time with base* (M_1,g_1)*, fiber* (M_2,g_2) *and warping function* $\phi>0$*. A vector field* $X\not\equiv 0$ *on* M *is a Ricci collineation of* (M,g^{ϕ}) *if and only if the following statements hold:*

(i) *for every* $p_1\in M_1$*,* X_2 *is a conformal vector field (perhaps zero) of* $(p_1\times M_2,g_2)$ *with conformal factor* ψ*,*
(ii) *for every* $p_2\in M_2$*,* X_1 *is a Killing vector field (perhaps zero) of* $(M_1\times p_2,g_R)$*, which satisfies (2.13), and*
(iii) *components (2.7) are equal to zero.*

In the next section, Propositions 2.1 and 2.3 will be exploited in order to describe the general structure of Ricci collineations of (M,g^{ϕ}).

III. RICCI COLLINEATIONS OF TYPE B WARPED SPACE–TIMES

For simplicity, first we will classify these symmetries in two families. In the first family, we will include Ricci collineations whose variables are not mixed, that is, when the corresponding vector field X can be written as

$$X(x^A,x^{\alpha})=X_1(x^A)+X_2(x^{\alpha}).$$

Our study is completed by including in a second family Ricci collineations such that either $\partial X_1/\partial x^{\alpha}\neq 0$ or $\partial X_2/\partial x^A\neq 0$.

Family 1: Ricci collineations with nonmixed variables.

Notice that, in this case, statements (iii) in Propositions 2.1 and 2.3 always hold. On the other hand, from Proposition 2.3, we can distinguish four types in this family attending to the vertical component X_2 of X.

Type 1.1: X_2 is a Killing vector field (perhaps zero) of (M_2,g_2).

From Proposition 2.3 (ii), $X\not\equiv 0$ will be a Ricci collineation if, additionally, X_1 is a Killing vector field (perhaps zero) of (M_1,g_R) with $(\phi^2)^A_{;A,C}X_1^C=0$. Therefore, Ricci collineations $X\not\equiv 0$ of type 1.1 are

$$X=X_1+X_2=\sum_{i=1}^{k_R}a_i^1X_1^i+\sum_{j=1}^{k_2}a_j^2X_2^j,$$

where

(i) $\{X_1^i\}_{i=1}^{k_R}$ is the algebra of Killing vector fields of (M_1,g_R),
(ii) $\{X_2^j\}_{j=1}^{k_2}$ is the algebra of Killing vector fields of (M_2,g_2), and
(iii) coefficients $\{a_i^1\}_{i=1}^{k_R}$ satisfy

$$\sum_{i=1}^{k_R}a_i^1(\phi^2)^A_{;A,C}X_1^{i\ C}=0. \tag{3.1}$$

Additionally, from Proposition 2.1 X is not a Killing vector field of (M,g^{ϕ}) if,
(iv) either $\phi^2_{,C}X_1^C\neq 0$ or X_1 is not a Killing vector field of (M_1,g_1) (in particular, $X_1\not\equiv 0$).

Remark 3.1: As dim $M_i=2$, $i=1,2$, necessarily $k_R,k_2=0,1,3$. But, from (iv), (M,g^{ϕ}) admits proper Ricci collineations of type 1.1 only if $k_R=1,3$. Therefore, in this case, if the curvature of (M_1,g_R) is not constant, necessarily $k_R=1$, and thus, Eq. (3.1) reduces to $(\phi^2)^A_{;A,C}X_1^{1\ C}=0$.

Type 1.2: X_2 is a proper homothetic vector field of (M_2,g_2).

Obviously, this type of collineations only exists if the curvature of (M_2,g_2) is not a constant different from zero. In this case, X will be a Ricci collineation if, additionally, X_1 is a Killing vector field (perhaps zero) of (M_1,g_R) with

$$(\phi^2)^A_{;A,C}X_1^C = -2\lambda(\phi^2)^A_{;A}, \tag{3.2}$$

where $\lambda \neq 0$ is the homothetic factor of X_2. From (3.2), recall that if $X_1=0$ then, necessarily $(\phi^2)^A_{;A}=0$.

In conclusion, Ricci collineations $X \not\equiv 0$ of type 1.2 are

$$X = X_1 + X_2 = \sum_{i=1}^{k_R} a_i^1 X_1^i + \sum_{j=1}^{k_2} a_j^2 X_2^j + \lambda Y,$$

where

(i) as before, $\{X_1^i\}_{i=1}^{k_R}$, $\{X_2^j\}_{j=1}^{k_2}$ are the algebras of Killing vector fields of (M_1,g_R), (M_2,g_2), respectively,
(ii) Y is the homothetic vector field of (M_2,g_2) with homothetic factor 1, and
(iii) coefficients $\{a_i^1\}_{i=1}^{k_R}$ and $\lambda \neq 0$ satisfy

$$\sum_{i=1}^{k_R} a_i^1 (\phi^2)^A_{;A,C} X_1^{i\ C} = -2\lambda(\phi^2)^A_{;A}.$$

Additionally, X is not a Killing vector field of (M,g^ϕ) if,
(iv) either $\phi^2_{,C}X_1^C \neq -2\lambda\phi^2$ or X_1 is not a Killing vector field of (M_1,g_1).

Type 1.3: X_2 is a proper special conformal vector field of (M_2,g_2).

This type of collineations only exists if $(\phi^2)^A_{;A}=0$. In fact, now the conformal factor ψ associated to X_2 is a nonconstant function of x^α with $\Delta_{g_2}\psi=0$. Therefore, if we assume that (2.13) holds, and derive it with respect to x^γ, we deduce that $(\phi^2)^A_{;A}=0$.

Under this restriction, all Ricci collineations $X \not\equiv 0$ of type 1.3 are given by

$$X = X_1 + X_2 = \sum_{i=1}^{k_R} a_i^1 X_1^i + \sum_{j=1}^{s_2} a_j^2 X_2^j,$$

where

(i) $\{X_1^i\}_{i=1}^{k_R}$ is the algebra of Killing vector fields of (M_1,g_R),
(ii) $\{X_2^j\}_{j=1}^{s_2}$ is the algebra of special conformal vector fields of (M_2,g_2) and,
(iii) some of the coefficients $\{a_j^2\}_{j=h_2+1}^{s_2}$ are different from zero, being h_2 the dimension of the algebra of homothetic vector fields of (M_2,g_2).

Moreover, these collineations are not Killing vector fields of (M,g^ϕ) because they do not satisfy (2.4).

Remark 3.2: Notice that condition $(\phi^2)^A_{;A}=0$ implies that proper homothetic and special conformal vector fields of (M_2,g_2) are also Ricci collineations of (M,g^ϕ) of types 1.2 and 1.3, respectively. Moreover, they are not Killing vector fields of (M,g^ϕ) [since they do not satisfy (2.4)].

Type 1.4: X_2 is a proper conformal vector field of (M_2,g_2).

This type of collineations only exists if $(\phi^2)^A_{;A}$ remains constant wherever ψ is not constant. In fact, if we assume that (2.13) holds, and derive it with respect to x^γ, we deduce that

$$\Delta_{g_2}\psi = -(\phi^2)^A_{;A}\cdot\psi = -\text{const}\cdot\psi \tag{3.3}$$

on such a domain.

In conclusion, Ricci collineations $X \not\equiv 0$ of type 1.4 satisfy the expression

$$X = X_1 + X_2 = \sum_{i=1}^{k_R} a_i^1 X_1^i + \sum_{j=1}^{c_2} a_j^2 X_2^j,$$

where

(i) $\{X_1^i\}_{i=1}^{k_R}$ is the algebra of Killing vector fields of (M_1, g_R),
(ii) $\{X_2^j\}_{j=1}^{c_2}$ is the conformal algebra of (M_2, g_2) and,
(iii) coefficients $\{a_j^2\}_{j=k_2+1}^{c_2}$ are such that the conformal factor of X_2,

$$\psi = \sum_{j=k_2+1}^{c_2} a_j^2 \psi_2^j,$$

satisfies (2.13) [in particular, satisfies (3.3) wherever ψ is not constant], where $\{\psi_2^j\}_{j=k_2+1}^{c_2}$ are the corresponding conformal factors of $\{X_2^j\}_{j=k_2+1}^{c_2}$, and some of the coefficients $\{a_j^2\}_{j=s_2+1}^{c_2}$ must be different from zero.

Again, these collineations are not Killing vector fields of (M, g^ϕ) because they do not satisfy (2.4).

Family 2: Ricci collineations with mixed variables.

In this family, the dependence of X_1 and X_2 is not restricted to x^A and x^α, respectively. Therefore, (iii) in Propositions 2.1 and 2.3 must be also taken into account in order to find these symmetries. Summarizing, Ricci collineations $X \not\equiv 0$ are given now by

$$X = X_1 + X_2 = \sum_{i=1}^{k_R} a_i^1(x^\alpha) X_1^i + \sum_{j=1}^{c_2} a_j^2(x^A) X_2^j,$$

where

(i) $\{X_1^i\}_{i=1}^{k_R}$ is the algebra of Killing vector fields of (M_1, g_R),
(ii) $\{X_2^j\}_{j=1}^{c_2}$ is the conformal algebra of (M_2, g_2), and
(iii) functions $\{a_i^1(x^\alpha)\}_{i=1}^{k_R}$, $\{a_j^2(x^A)\}_{j=1}^{c_2}$ satisfy

$$\sum_{i=1}^{k_R} a_i^1(x^\alpha)(\phi^2)^A_{;A,C} X_1^{i\,C} = -2\left(\sum_{j=k_2+1}^{c_2} a_j^2(x^A)\psi_2^j\right)(\phi^2)^A_{;A} - 2\sum_{j=s_2+1}^{c_2} a_j^2(x^A)\Delta_{g_2}\psi_2^j, \tag{3.4}$$

$$\sum_{i=1}^{k_R} \frac{da_i^1(x^\gamma)}{dx^\alpha} R_{AC} X_1^{iC} + \sum_{j=1}^{c_2} \frac{da_j^2(x^C)}{dx^A} R_{\alpha\beta} X_2^{j\beta} = 0, \quad A = 0,1, \quad \alpha = 2,3 \tag{3.5}$$

(the indexes k_2, s_2 are again the dimensions of the homothetic and special conformal algebras). Additionally, X is not a Killing vector field of (M, g^ϕ) if
(iv) any of the statements of Proposition 2.1 do not hold.

Analogously to Family 1, we classify these collineations in four types.

Type 2.1: For every $p_1 \in M_1$, X_2 is a Killing vector field (perhaps zero) of $(p_1 \times M_2, g_2)$.

In this case the only functions which can be different from zero are $\{a_i^1(x^\alpha)\}_{i=1}^{k_R}$, $\{a_j^2(x^A)\}_{j=1}^{k_2}$. As a consequence, Eq. (3.4) reduces to

$$\sum_{i=1}^{k_R} a_i^1(x^\alpha)(\phi^2)^A_{;A,C} X_1^{i\,C} = 0.$$

Type 2.2: For every $p_1 \in M_1$, X_2 is a homothetic vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ which is not always Killing.

This type of collineations only exists if the curvature of (M_2, g_2) is not a constant different from zero. In this case, only the functions $\{a_i^1(x^\alpha)\}_{i=1}^{k_R}$, $\{a_j^2(x^A)\}_{j=1}^{k_2}$, $a_{k_2+1}^2(x^A) \equiv \lambda(x^A)$ can be different from zero, and they must satisfy

$$\sum_{i=1}^{k_R} a_i^1(x^\alpha)(\phi^2)^A_{;A,C} X_1^{i\ C} = -2\lambda(x^A)(\phi^2)^A_{;A},$$

where we have assumed the homothetic factor $\psi_2^{k_2+1}$ normalized to 1.

Type 2.3: For every $p_1 \in M_1$, X_2 is a special conformal vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ which is not always homothetic.

In this case, only the functions $\{a_i^1(x^\alpha)\}_{i=1}^{k_R}$, $\{a_j^2(x^A)\}_{j=1}^{s_2}$ can be different from zero. As a consequence, Eq. (3.4) reduces now to

$$\sum_{i=1}^{k_R} a_i^1(x^\alpha)(\phi^2)^A_{;A,C} X_1^{i\ C} = -2\left(\sum_{j=k_2+1}^{s_2} a_j^2(x^A)\psi_2^j\right)(\phi^2)^A_{;A}.$$

Type 2.4: For every $p_1 \in M_1$, X_2 is a conformal vector field (perhaps zero) of $(p_1 \times M_2, g_2)$ which is not always special. In general, we cannot simplify the structure of these Ricci collineations.

In the following section a brief application of our study to some examples of type B warped space–times is carried out. Without any further calculations, we obtain interesting information about the particular structure of their symmetries.

IV. EXAMPLES

In this section we will apply our point of view to the following families of type B warped space–times: 2+2 reducible space–times, and plane and spherical symmetric space–times.

A. 2+2 reducible space–times

In this case the product manifold $M = M_1 \times M_2$ is endowed with the metric tensor

$$g = \pi_1^* g_1 + \pi_2^* g_2 \equiv g_1 + g_2.$$

Therefore, these space–times are type B warped space–times with $\phi^2 = 1$ and, thus, we can apply our previous study. First, take into account that now $g_R = 1/2R_1 g_1 = \mathbf{R}_{g_1}$. Thus, Killing vector fields X_1 of (M_1, g_R) are just the conformal vector fields of (M_1, g_1) with conformal factors satisfying $\Delta_{g_1}\psi_1 = 0$ [recall (2.10)]. Therefore, if we apply Proposition 2.3 to these space–times, we obtain the following consequences.

Corollary 4.1: Ricci collineations $X \not\equiv 0$, with nonmixed variables, of a 2+2 reducible space–time (M, g) are the vector fields $X = X_1 + X_2$ such that, X_l are conformal vector fields of (M_l, g_l) with conformal factors ψ_l satisfying

$$\Delta_{g_l}\psi_l = 0, \quad l = 1,2.$$

Corollary 4.2: Ricci collineations $X \not\equiv 0$, with mixed variables, of a 2+2 reducible space–time (M, g) are the vector fields

$$X = X_1 + X_2 = \sum_{i=1}^{c_1} a_i^1(x^\alpha) X_1^i + \sum_{j=1}^{c_2} a_j^2(x^A) X_2^j,$$

where $\{X_1^i\}_{i=1}^{c_1}$, $\{X_2^j\}_{j=1}^{c_2}$ are the conformal algebras of (M_1, g_1), (M_2, g_2), respectively, and functions $\{a_i^1(x^\alpha)\}_{i=1}^{c_1}$, $\{a_j^2(x^A)\}_{j=1}^{c_2}$ satisfy

$$\sum_{i=s_1+1}^{c_1} a_i^1(x^\alpha)\Delta_{g_1}\psi_1^i = \sum_{j=s_2+1}^{c_2} a_j^2(x^A)\Delta_{g_2}\psi_2^j = 0,$$

$$\sum_{i=1}^{c_1} \frac{\mathrm{d}a_i^1(x^\gamma)}{\mathrm{d}x^\alpha} R_{AC} X_1^{iC} + \sum_{j=1}^{c_2} \frac{\mathrm{d}a_j^2(x^C)}{\mathrm{d}x^A} R_{\alpha\beta} X_2^{j\beta} = 0, \quad A = 0,1, \quad \alpha = 2,3,$$

being $\{\psi_1^i\}_{i=1}^{c_1}$, $\{\psi_2^j\}_{j=1}^{c_2}$ *the corresponding conformal factors.*

Remark 4.3: (1) Counterexamples given in Ref. 1 are clearly contained in these results. In fact, $M=\mathbb{R}^2\times\mathbb{R}^2$ endowed with

$$g = e^{t^2/2}(-\mathrm{d}t^2 + \mathrm{d}x^2) + e^{-y^2/2}(\mathrm{d}y^2 + \mathrm{d}z^2)$$

is a 2+2 reducible space–time and, both, $X=\partial_t+\partial_y$, $Y=z\partial_t+\partial_y+t\partial_z$ are Ricci collineations which satisfy hypotheses of corollaries 4.1 and 4.2, respectively.

(2) From Eqs. (2.5), it is clear that both corollaries also hold for space–times not necessarily 2+2 reducible, but satisfying $\phi_{A;B}=(\phi^2)^A_{;A}\equiv 0$.

B. Plane and spherical symmetric space–times

Consider now the family of space–times $M=\mathbb{R}^2\times M_2$ endowed with the metric tensor

$$g^\phi = -e^{2v}\mathrm{d}t^2 + e^{2w}\mathrm{d}x^2 + \phi^2 g_2,$$

where v, w, and ϕ are each functions of t and x, and

$$(M_2,g_2) = \begin{cases} \mathbb{R}^2 \\ \mathbb{S}^2 \end{cases}$$

endowed with their corresponding usual metrics (if we also include the hyperbolic space, g^ϕ can be characterized by admitting a group G_3 acting multiply-transitively on spacelike orbits V_2, see Ref. 10). To avoid the vanishing of F, and thus, the degeneracy of Ricci tensor **R** [recall (2.5)], we will also assume

$$(\phi^2)^A_{;A} \neq R_2 \quad \text{for all} \quad (t,x) \in \mathbb{R}^2. \tag{4.1}$$

From Sec. III, the component X_1 of a Ricci collineation $X\not\equiv 0$ of these space–times is different from zero only if (M_1,g_R) admits some Killing vector fields. In this case, the dimension k_R of the corresponding algebra must be 3 or 1, depending on if v, w, and ϕ makes (R^2,g_R) being maximally symmetric or not. To study the structure of X_2, we must consider the two cases separately.

1. Plane symmetry

The conformal algebra of the plane $(\mathrm{R}^2,\mathrm{d}y^2+\mathrm{d}z^2)$ is the (infinite-dimensional) *Virasoro algebra*, which has the following special conformal vector fields:

$$X_2^1 = \partial_y, \quad \psi_2^1 = 0,$$

$$X_2^2 = \partial_z, \quad \psi_2^2 = 0,$$

$$X_2^3 = z\partial_y - y\partial_z, \quad \psi_2^3 = 0,$$

$$X_2^4 = y\partial_y + z\partial_z, \quad \psi_2^4 = 1,$$

$$X_2^5 = (y^2 - z^2)\partial_y + 2yz\partial_z, \quad \psi_2^5 = 2y,$$

$$X_2^6 = 2yz\partial_y + (z^2 - y^2)\partial_z, \quad \psi_2^6 = 2z.$$

Therefore, $k_2=3$, $h_2=4$, $s_2=6$ (and $c_2=\infty$). In this case, we can establish the following:

(i) The vertical component X_2 of a Ricci collineation $X \not\equiv 0$ of type 1.1 is a linear combination of the $k_2=3$ Killing vector fields of the plane. On the other hand, the horizontal component X_1 satisfies the equation in k_R variables (3.1).

(ii) The component X_2 of a Ricci collineation of type 1.2 is a linear combination of the $h_2=4$ homothetic vector fields of the plane. On the other hand, the horizontal component X_1 satisfies Eq. (3.2). If $k_R=0$, there are not Ricci collineations of this type since, in this case, (3.2) reduces to $(\phi^2)^A_{;A}=0$, which contradicts (4.1).

(iii) There are not Ricci collineations of type 1.3. Moreover, there are collineations of type 1.4 only if $(\phi^2)^A_{;A}=\text{const}\neq 0$.

(iv) Ricci collineations in Family 2 must satisfy Eqs. (3.4) and (3.5), which are in general complicated. If $k_R=0$ and we consider collineations of type 2.3, these equations reduce to

$$a_4^2 + 2y\ a_5^2 + 2z\ a_6^2 = 0$$

and

$$a_{1,t}^2 + z\ a_{3,t}^2 + y\ a_{4,t}^2 + (y^2 - z^2)a_{5,t}^2 + 2yz\ a_{6,t}^2 = 0,$$

$$a_{2,t}^2 - y\ a_{3,t}^2 + z\ a_{4,t}^2 + 2yz\ a_{5,t}^2 + (z^2 - y^2)a_{6,t}^2 = 0,$$

$$a_{1,x}^2 + z\ a_{3,x}^2 + y\ a_{4,x}^2 + (y^2 - z^2)a_{5,x}^2 + 2yz\ a_{6,x}^2 = 0,$$

$$a_{2,x}^2 - y\ a_{3,x}^2 + z\ a_{4,x}^2 + 2yz\ a_{5,x}^2 + (z^2 - y^2)a_{6,x}^2 = 0.$$

2. Spherical symmetry

In this case, the second space (M_2, g_2) is the unitary bidimensional sphere $\mathbb{S}^2$. The *local* conformal algebra of $\mathbb{S}^2$, like that of the plane, is the Virasoro algebra. In order to single out a finite-dimensional subalgebra from it, we will impose that conformal vectors must be *globally* defined on $\mathbb{S}^2$. Then, a well-known computation shows that the only *global* conformal vector fields of $\mathbb{S}^2$ expressed in spherical coordinates are

$$X_2^1 = \cos\ \varphi\partial_\theta - \sin\ \varphi\ \cot\ \theta\partial_\varphi, \quad \psi_2^1 = 0,$$

$$X_2^2 = \sin\ \varphi\partial_\theta + \cos\ \varphi\ \cot\ \theta\partial_\varphi, \quad \psi_2^2 = 0,$$

$$X_2^3 = \partial_\varphi, \quad \psi_2^3 = 0,$$

$$X_2^4 = \sin\ \theta\partial_\theta, \quad \psi_2^4 = \cos\ \theta,$$

$$X_2^5 = \cos\theta\ \cos\varphi\partial_\theta - \frac{\sin\ \varphi}{\sin\ \theta}\partial_\varphi, \quad \psi_2^5 = -\sin\ \theta\ \cos\varphi,$$

$$X_2^6 = \cos\ \theta\ \sin\ \varphi\partial_\theta - \frac{\cos\ \varphi}{\sin\ \theta}\partial_\varphi, \quad \psi_2^6 = -\sin\ \theta\ \sin\ \varphi.$$

(Nevertheless, recall that other conformal vectors—necessarily *locally* defined—can appear as vertical components of a Ricci collineation of a spherically symmetric space–time.)

In conclusion, $k_2=h_2=s_2=3$ and $c_2=6$. Therefore, we obtain the following:

(i) The vertical component X_2 of a Ricci collineation $X \not\equiv 0$ of type 1.1 is a linear combination of the $k_2=3$ Killing vector fields of $\mathbb{S}^2$. On the other hand, the horizontal component X_1 satisfies the equation in k_R variables (3.1).

(ii) As the curvature of $\mathbb{S}^2$ is a constant different from zero, there are not Ricci collineations of types 1.2, 2.2. Even more, as $s_2-h_2=0$, there are not Ricci collineations of types 1.3, 2.3 either.

(iii) A simple computation shows that $\Delta_{g_2}\psi_2^j=-2\psi_2^j$, $j=4,5,6$. But then, (3.3) implies $(\phi^2)^A_{;A}=R_2=2$, which contradicts (4.1). Therefore, there are not Ricci collineations of type 1.4.

(iv) Ricci collineations in Family 2 must satisfy Eqs. (3.4) and (3.5), which are in general complicated. If $k_R=0$, there are not Ricci collineations in this family. In fact, in this case (3.4); [or, equivalently, (2.13)] implies again $(\phi^2)^A_{;A}=R_2=2$, in contradiction with (4.1).

V. THE DEGENERATE CASE

For completeness, we briefly analyse here the cases when Ricci tensor is degenerate. From (2.5), the Ricci tensor of a type B warped space–time is degenerate if $F\equiv 0$ or $\phi_{A;B}\equiv(\phi/4)R_1 g_{AB}$ (if both identities hold, the Ricci tensor is zero and any vector field is a Ricci collineation).

Consider the case $F\equiv 0$ [or, equivalently, $(\phi^2)^A_{;A}\equiv R_2=0$]. Then, Eqs. (2.6)–(2.8) show that a vector field $X=X_1+X_2\not\equiv 0$ is a Ricci collineation of the space–time if and only if X_1 is a Killing vector field (perhaps zero) of $(M_1\times p_2, g_R)$ satisfying $R_{AC}X^C_{1,\alpha}=0$ for every $p_2\in M_2$. In particular, any Killing vector field of (M_1,g_R) is always a Ricci collineation of the space–time. Moreover, the group of Ricci collineations becomes infinity, since every vector field $X\not\equiv 0$ with horizontal component $X_1\equiv 0$ generates a Ricci collineation. That is, the vertical component (which is just the component where Ricci tensor degenerates) of these Ricci collineations is largely arbitrary (see Ref. 3 Sec. II, for a similar property in Robertson–Walker space–times).

The situation is more complicated when the source of degeneracy is the identity $\phi_{A;B}\equiv(\phi/4)R_1 g_{AB}$. In this case, Proposition 2.3 shows that a vector field $X=X_1+X_2\not\equiv 0$ is a Ricci collineation of the space–time if and only if X_2 is a conformal vector field (perhaps zero) of $(p_1\times M_2, g_2)$ satisfying $R_{\alpha\beta}X^\beta_{2,A}=0$ for every $p_1\in M_1$ and, additionally, X_1 satisfies (2.13) for every $p_2\in M_2$. So, in this case we have restrictions on both, the vertical and horizontal components of X. This is due to the dependence of F on both components, and breaks the similarities with respect to the Robertson–Walker case.

VI. CONCLUSION

By analyzing the equations which characterize Ricci collineations of type B warped space–times, we have determined the structure of these symmetries. They have been classified in eight types according to having or not mixed variables, and according to their vertical component. As a consequence, several examples of interest have been considered, and new information about their collineations has been provided. This study must be understood as an initial point to begin a systematic computation of Ricci collineations for a wide family of space–times of this class.

As a final remark we would like to point out that it would be very useful to use computer algebra packages to automate the search of symmetries. Nevertheless, as far as we know, the available algorithms can only check if a given vector field is a symmetry or not (at least this is the case of GRTensor with which we have some familiarity).

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On a theorem by Treves

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According to a theorem by Treves [Duke Math. J. **108**, 251 (2001)], the conserved functionals of the KdV equation vanish on each formal Laurent series $1/x^2+u_0+\Sigma_{k=2}^{+\infty}u_k x^k$. We propose a new, very simple geometrical proof for this statement. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777795]

I. INTRODUCTION

In 2001, Treves obtained a new characterization for the conserved quantities of the Korteweg–de Vries (KdV) equation. Roughly speaking, his result concerns functionals which are integrals of differential polynomials, and their evaluation on formal Laurent series with complex coefficients in one variable x (defining the integral as the residue in x). For each functional h of this kind on the Laurent series, Treves[1] proved the equivalence between (a) and (b):

(a) *h is a conserved functional for the KdV equation;*
(b) *$h(u)=0$ for each Laurent series of the form* $u=1/x^2+u_0+\Sigma_{k=2}^{+\infty}u_k x^k$ $(u_0,u_2,u_3,\ldots\in\mathbb{C})$.

Subsequently, Treves obtained a similar result for the modified KdV equation and derived the analogue of (a)⇒(b) for the conserved functionals of the nonlinear Schrödinger equation.[2]

In all cases analyzed by Treves, the proof of either (a)⇒(b) or (b)⇒(a) is very long. A simple, alternative derivation of (a)⇒(b) for the KdV case was given by Dickey,[3] using the dressing method for the Lax operator; this author also derived an analogue of this implication for the Boussinesq theory.

We became aware of the above results very recently, due to a talk given in Milano by Professor Treves,[4] and we soon developed an interest in a further simplification of the proofs. We investigated in particular the implication (a)⇒(b), concentrating for brevity on the KdV case and trying to isolate a *single geometrical property* of the conserved functionals, sufficient to derive the thesis. The conclusion of our analysis is described in this paper: here we propose a proof of (a)⇒(b) for the KdV, different from the ones of Treves and Dickey and possessing in our opinion the previously asked feature; the same approach could be probably used for other integrable systems.

Our argument can be described in very few lines, in the following way.

(I) The conserved KdV functionals are known to be invariant under the Bäcklund transformation (often called auto-Bäcklund) $M\circ R\circ M^{-1}$, where M and R are the Miura and reflection transformations, respectively. This is the geometrical property from which everything follows.
(II) Any Laurent series $u=1/x^2+u_0+\Sigma_{k=2}^{+\infty}u_k x^k$ is the Bäcklund transform of a series $w=w_0+\Sigma_{k=2}^{\infty}w_k x^k$.

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(III) If h is a conserved KdV functional and u, w are as before, we have $h(u)=h(w)$; on the other hand, $h(w)=0$ for a trivial reason: in fact, this is the integral of a series with no negative powers of x and thus with zero residue. The conclusion is $h(u)=0$.

The rest of the paper is simply a rigorous formulation of items (I)–(III). In Sec. II, to fix the language we give some background on differential polynomials, functionals, KdV theory and state precisely the Treves theorem; in Sec. III, we review the Bäcklund transformation and formalize statement (I) in the framework of the Laurent series. Expert readers can skip most of the preliminaries in these two sections, and concentrate on Eqs. (2.14) and (2.15) describing the space of Laurent series; Eqs. (3.3)–(3.6) on the Bäcklund transformation and the invariance of KdV functionals. In Sec. IV, we prove (II) and show (a)$\Rightarrow$(b) along the lines of (III).

Let us point out how the idea (I)–(III) could be employed in relation to other integrable equations. First of all, one needs a Bäcklund transformation leaving invariant the conserved functionals. Trivially, all functionals of the theory vanish on the subspace of formal series with no negative powers of x. One should start from this subspace or a subset of it, and characterize its image under the Bäcklund transformation; the latter is made of nontrivial Laurent series, on which the conserved functionals are again zero. In the KdV case, the starting set and its Bäcklund image consist, respectively, of the series w, u mentioned in (II).

Some terminology: All vector spaces considered in this paper are over $\mathbb{C}$. By a differential algebra, we mean an associative and *commutative* algebra equipped with a derivation, i.e., with a linear map of the algebra into itself having the Leibnitz property with respect to the product. A morphism of differential algebras is an algebraic morphism respecting the derivations.

II. FORMAL VARIATIONAL CALCULUS, KdV AND THE TREVES THEOREM

In all concrete manipulations, the KdV equation $(d/dt)q=q_{xxx}-12qq_x$ is understood as a vector field on some "space" $\mathcal{Q}$, whose elements q are "functions of one variable x." The analysis of this vector field is greatly simplified if one assumes $\mathcal{Q}$ to be closed under pointwise sums and products, and under the operation $q\mapsto q_x$ of derivation with respect to x; in this case, $\mathcal{Q}$ is a differential algebra.

Investigations in this area soon made clear that the striking features of KdV are largely independent of the choice of the differential algebra $\mathcal{Q}$; the same can be said for other integrable PDEs, discovered shortly after it. To take this fact into account, Gelfand and Dickey (see Ref. 5 and the bibliography therein) invented a *formal variational calculus*, allowing to describe the KdV and similar systems within a very pure algebraic setting. Hereafter we illustrate some facts about this calculus, in a fashion convenient for our purposes (and partly inspired by the setting of Ref. 1).

Formal variational calculus for KdV theory can be based on the commutative algebra

$$\mathfrak{F} := \mathbb{C}[\boldsymbol{\xi}, \boldsymbol{\xi}_x, \boldsymbol{\xi}_{xx}, \dots]_0, \tag{2.1}$$

made of complex polynomials in infinitely many indeterminates $\boldsymbol{\xi}, \boldsymbol{\xi}_x, \boldsymbol{\xi}_{xx}, \dots$ without a constant term. $\mathfrak{F}$ becomes a differential algebra, when equipped with the unique derivation $\boldsymbol{\partial}$ such that[6]

$$\boldsymbol{\partial}\boldsymbol{\xi} = \boldsymbol{\xi}_x, \quad \boldsymbol{\partial}\boldsymbol{\xi}_x = \boldsymbol{\xi}_{xx}, \quad \dots . \tag{2.2}$$

We write $\boldsymbol{F}, \boldsymbol{G}$, etc. for the elements of $\mathfrak{F}$, and $\boldsymbol{FG}$ for their product as polynomials. The *composition product* $\boldsymbol{F}\circ\boldsymbol{G}\in\mathfrak{F}$ is the polynomial obtained from the expression of $\boldsymbol{F}$ replacing $\boldsymbol{\xi}, \boldsymbol{\xi}_x, \dots$ with $\boldsymbol{G}$, $\boldsymbol{\partial G}, \dots$.[7] For each fixed $\boldsymbol{G}$, the mapping $\boldsymbol{F}\mapsto\boldsymbol{F}\circ\boldsymbol{G}$ is the unique automorphism of the differential algebra $\mathfrak{F}$ sending $\boldsymbol{\xi}$ into $\boldsymbol{G}$. The operation $\circ$ is associative, so $(\mathfrak{F}, \circ)$ is a monoid with unit $\boldsymbol{\xi}$.

Let us consider any differential algebra $(\mathcal{Q}, \cdot_x)$ (of elements $q, p, \dots$, with a derivation $q \in \mathcal{Q}\mapsto q_x\in\mathcal{Q}$; this notation for the derivation is purely conventional). Then, we can represent the elements of $\mathfrak{F}$ as *transformations of* $\mathcal{Q}$ into itself. More precisely, if $\boldsymbol{F}\in\mathfrak{F}$ and $q\in\mathcal{Q}$, let us denote with $F(q)\in\mathcal{Q}$ the element obtained from the expression of $\boldsymbol{F}$ substituting the symbols

$\boldsymbol{\xi}, \boldsymbol{\xi}_x, \ldots$ with q, q_x, etc. In this way, $\boldsymbol{F}$ induces a map of polynomial type[8]

$$F: \mathcal{Q} \to \mathcal{Q}, \quad q \mapsto F(q). \tag{2.3}$$

We point out the remotion of bold typeface to distinguish this map from $\boldsymbol{F}$; in particular, the transformation $\xi: \mathcal{Q} \to \mathcal{Q}$ induced by $\boldsymbol{\xi}$ is just the identity map $q \mapsto q$. As $\boldsymbol{F}$ ranges over the whole $\boldsymbol{\mathfrak{F}}$, we get a correspondence

$$\boldsymbol{F} \to \mathrm{Pol}(\mathcal{Q}, \mathcal{Q}), \quad \boldsymbol{F} \mapsto F. \tag{2.4}$$

Now, the set $\mathrm{Pol}(\mathcal{Q}, \mathcal{Q})$ of polynomial maps $\mathcal{Q} \to \mathcal{Q}$ is itself a commutative algebra, with all the operations defined pointwisely: for $K, L: \mathcal{Q} \to \mathcal{Q}$ and $\lambda \in \mathbb{C}$, $K+L$, λK, $KL: \mathcal{Q} \to \mathcal{Q}$ are the maps $q \mapsto K(q)+L(q)$, $q \mapsto \lambda K(q)$, $q \mapsto K(q)L(q)$. Furthermore, $\mathrm{Pol}(\mathcal{Q}, \mathcal{Q})$ becomes a differential algebra with the derivation $\partial: K \mapsto \partial K$ such that $(\partial K)(q) := K(q)_x$ for all $q \in \mathcal{Q}$. One easily recognizes that (2.4) is a morphism of differential algebras: for all $\boldsymbol{F}, \boldsymbol{G} \in \boldsymbol{\mathfrak{F}}$ and $\lambda \in \mathbb{C}$, the transformations corresponding to $\boldsymbol{F}+\boldsymbol{G}$, $\lambda \boldsymbol{F}$, $\boldsymbol{FG}$, $\boldsymbol{\partial F}$ are $F+G$, λF, FG, ∂F.

$\mathrm{Pol}(\mathcal{Q}, \mathcal{Q})$ is also a monoid with the usual composition of maps $F \circ G: q \mapsto F(G(q))$ and the identity map as unit; it turns out that (2.4) is a monoid morphism between $(\boldsymbol{\mathfrak{F}}, \circ)$ and $(\mathrm{Pol}(\mathcal{Q}, \mathcal{Q}), \circ)$.

Due to the previous facts, it is helpful for intuition *to think the elements of* $\boldsymbol{\mathfrak{F}}$ *as transformations, even when no differential algebra* $(\mathcal{Q}, \cdot_x)$ *is specified.*

The next step in formal variational calculus is the introduction of *functionals*, which are "integrals" of transformations. The only property needed for the integral is to vanish on a derivative; for this reason Gelfand and Dickey defined this operation as the quotient map

$$\int : \boldsymbol{\mathfrak{F}} \to \boldsymbol{\mathfrak{F}} / \mathrm{Im}\ \boldsymbol{\partial}, \tag{2.5}$$

and called functionals the elements of $\boldsymbol{\mathfrak{F}} / \mathrm{Im}\ \boldsymbol{\partial}$; each of them has the form

$$\boldsymbol{f} = \int \boldsymbol{F}\ (\boldsymbol{F} \in \boldsymbol{\mathfrak{F}}). \tag{2.6}$$

For any "transformation" $\boldsymbol{G} \in \boldsymbol{\mathfrak{F}}$, the functional

$$\boldsymbol{f} \circ \boldsymbol{G} := \int (\boldsymbol{F} \circ \boldsymbol{G}) \in \boldsymbol{\mathfrak{F}} / \mathrm{Im}\ \boldsymbol{\partial} \tag{2.7}$$

is well defined (i.e., independent on the choice of $\boldsymbol{F}$ within the equivalence class $\boldsymbol{f}$); we call this the *composition* between $\boldsymbol{f}$ and $\boldsymbol{G}$. One easily checks the linearity of the map $\boldsymbol{f} \mapsto \boldsymbol{f} \circ \boldsymbol{G}$, and the associative property $(\boldsymbol{f} \circ \boldsymbol{G}) \circ \boldsymbol{G}' = \boldsymbol{f} \circ (\boldsymbol{G} \circ \boldsymbol{G}')$ for $\boldsymbol{f}, \boldsymbol{G}$ as before and $\boldsymbol{G}' \in \boldsymbol{\mathfrak{F}}$.

To get concrete counterparts of functionals, consider any differential algebra $(\mathcal{Q}, \cdot_x)$, and define an *integration* for it to be any linear map

$$\int : \mathcal{Q} \to \mathbb{C} \quad \text{such that} \quad \int q_x = 0\ \forall\ q \in \mathcal{Q}; \tag{2.8}$$

the triple $(\mathcal{Q}, \cdot_x, \int)$ will then be called an *integral-differential algebra*. If $\boldsymbol{f} = \int \boldsymbol{F} \in \boldsymbol{\mathfrak{F}} / \mathrm{Im}\ \boldsymbol{\partial}$, define

$$f: \mathcal{Q} \to \mathbb{C}, \quad q \mapsto f(q) := \int F(q); \tag{2.9}$$

this definition is well posed, and gives a linear correspondence

$$\mathfrak{F}/\mathrm{Im}\ \boldsymbol{\partial} \to \mathrm{Pol}(\mathcal{Q},\mathbb{C}), \quad \boldsymbol{f} \mapsto f; \tag{2.10}$$

for all $\boldsymbol{f}$ as above and $\boldsymbol{G} \in \mathfrak{F}$, the map $\mathcal{Q} \to \mathbb{C}$ induced by $\boldsymbol{f} \circ \boldsymbol{G}$ is the usual composition $f \circ G: q \mapsto f(G(q))$.

One can then go on at the level of $\mathfrak{F}$, defining notions such as *vector fields* (identifiable with elements of $\mathfrak{F}$), and the (Lie) *derivative* of a functional $\boldsymbol{h}$ along a vector field $\boldsymbol{X}$; if the latter vanishes, we say that $\boldsymbol{h}$ is *conserved by* $\boldsymbol{X}$ (see Ref. 5 and the bibliography therein).

All this machinery is designed to discuss topics such as the *KdV vector field* and its conserved functionals, i.e.,

$$\boldsymbol{X}_{\mathrm{KdV}} := \boldsymbol{\xi}_{xxx} - 12\boldsymbol{\xi}\boldsymbol{\xi}_x, \tag{2.11}$$

$$\mathfrak{Z}_{\mathrm{KdV}} := \{\boldsymbol{h} \in \mathfrak{F}/\mathrm{Im}\boldsymbol{\partial} | \boldsymbol{h} \text{ is a conserved by } \boldsymbol{X}_{\mathrm{KdV}}\}. \tag{2.12}$$

An outstanding feature of KdV theory is that $\mathfrak{Z}_{\mathrm{KdV}}$ is *infinite dimensional* (as a vector space over $\mathbb{C}$). A basis for it is well known and consists of countably many functionals $(\boldsymbol{h}_k)_{k=1,2,\ldots}$, for which several equivalent constructions are available: for example, one can use the Magri–Lenard recursion scheme,[9] or the method of fractional powers.[5] The first elements are

$$\boldsymbol{h}_1 := -\tfrac{1}{4}\int \boldsymbol{\xi}, \quad \boldsymbol{h}_2 := \tfrac{1}{2}\int \boldsymbol{\xi}^2, \quad \boldsymbol{h}_3 := -\int (2\boldsymbol{\xi}^3 + \tfrac{1}{2}\boldsymbol{\xi}_x^2), \quad \boldsymbol{h}_4 := \int (10\boldsymbol{\xi}^4 + 10\boldsymbol{\xi}\boldsymbol{\xi}_x^2 + \tfrac{1}{2}\boldsymbol{\xi}_{xx}^2). \tag{2.13}$$

We finally come to the Treves theorem, concerning the KdV conserved functionals and their representation on a particular integral-differential algebra $(Q, \cdot_x, \int)$. By definition, this is made of formal Laurent series in one indeterminate x and complex coefficients, i.e.,

$$\mathcal{Q} := \left\{ q = \sum_k q_k x^k \,\middle|\, k \in \mathbb{Z}, q_k \in \mathbb{C}\ \forall\, k, q_k = 0 \text{ for } k \leqslant k_* = k_*(q) \right\}; \tag{2.14}$$

$\mathcal{Q}$ is a commutative algebra with the usual Cauchy product; it carries the derivation and integration

$$\cdot_x: \mathcal{Q} \to \mathcal{Q}, \quad q \mapsto q_x := \sum_k k q_k x^{k-1}; \qquad \int: \mathcal{Q} \to \mathbb{C}, \quad q \mapsto \int q := q_{-1}. \tag{2.15}$$

Clearly, $\int q = 0$ iff $q = p_x$ for some $p \in \mathcal{Q}$; of course, the definition of $\int q$ as the "residue" q_{-1} suggests to interpret it as a loop integral about zero.

With the previous notations, the Treves theorem reads as follows.

Proposition 2.1 (see Ref. 1): For any $\boldsymbol{h} \in \mathfrak{F}/\mathrm{Im}\ \boldsymbol{\partial}$, *statements (a) and (b) are equivalent*:

(a) $\boldsymbol{h} \in \mathfrak{Z}_{\mathrm{KdV}}$;
(b) $h(u) = 0$ *for each* $u \in Q$ *of the form* $u = 1/x^2 + u_0 + \sum_{k=2}^{+\infty} u_k x^k$.

As anticipated, the rest of the paper is a new geometrical proof of the implication (a) $\Rightarrow$ (b).

III. A REVIEW OF THE MIURA AND BÄCKLUND TRANSFORMATIONS

The basic facts on these transformations can be stated in the language of formal variational calculus; so, we consider the algebra $\mathfrak{F}$ of the preceding section, and state the following.

Definition 3.1: The Miura and reflection transformations are

$$\boldsymbol{M} := \boldsymbol{\xi}_x + 2\boldsymbol{\xi}^2; \quad \boldsymbol{R} := -\boldsymbol{\xi}. \tag{3.1}$$

Both $\boldsymbol{M}, \boldsymbol{R}$ are elements of $\mathfrak{F}$, so they can be composed as explained previously; of course $\boldsymbol{M} \circ \boldsymbol{R} = -\boldsymbol{\xi}_x + 2\boldsymbol{\xi}^2$. We can as well compose functionals $\in \mathfrak{F}/\mathrm{Im}\boldsymbol{\partial}$ with these transformations; for

example, composing the first KdV conserved functionals (2.13) with the Miura transformation we obtain

$$\boldsymbol{h}_1 \circ \boldsymbol{M} = -\tfrac{1}{2}\int \boldsymbol{\xi}^2, \quad \boldsymbol{h}_2 \circ \boldsymbol{M} = \int (2\boldsymbol{\xi}^4 + \tfrac{1}{2}\boldsymbol{\xi}_x^2), \quad \boldsymbol{h}_3 \circ \boldsymbol{M} = -\int (16\boldsymbol{\xi}^6 + 20\boldsymbol{\xi}^2\boldsymbol{\xi}_x^2 + \tfrac{1}{2}\boldsymbol{\xi}_{xx}^2),$$

$$\boldsymbol{h}_4 \circ \boldsymbol{M} = \int (160\boldsymbol{\xi}^8 + 560\boldsymbol{\xi}^4\boldsymbol{\xi}_x^2 + 18\boldsymbol{\xi}_x^4 + 96\boldsymbol{\xi}\boldsymbol{\xi}_x^2\boldsymbol{\xi}_{xx} + 28\boldsymbol{\xi}^2\boldsymbol{\xi}_{xx}^2 + \tfrac{1}{2}\boldsymbol{\xi}_{xxx}^2). \tag{3.2}$$

The following facts are known from the very beginning of KdV history.

Proposition 3.2: For each $\boldsymbol{h} \in \mathfrak{Z}_{\mathrm{KdV}}$:

(i) $\boldsymbol{h}\circ\boldsymbol{M}$ *is a conserved functional for the modified KdV vector field* $\boldsymbol{X}_{\mathrm{mKdV}} := \boldsymbol{\xi}_{xxx} - 24\boldsymbol{\xi}^2\boldsymbol{\xi}_x$.

(ii) $\boldsymbol{h}\circ\boldsymbol{M}$ *is invariant under reflection*: $(\boldsymbol{h}\circ\boldsymbol{M})\circ\boldsymbol{R} = \boldsymbol{h}\circ\boldsymbol{M}$.

References for the proof: For (i), see the original papers by Miura *et al.*[10] (ii) is proved recursively for all elements $(\boldsymbol{h}_k)_{k=1,2,\ldots}$ in the basis of $\mathfrak{Z}_{\mathrm{KdV}}$, using the Magri–Lenard recursion relations[9] connecting $\boldsymbol{h}_k\circ\boldsymbol{M}$ to $\boldsymbol{h}_{k+1}\circ\boldsymbol{M}$: these relations are reflection invariant. ■

For our purposes, (ii) is the essential feature of $\boldsymbol{M}$ and $\boldsymbol{R}$; now we represent this result on any integral-differential algebra $(\mathcal{Q}, \cdot_x, \int)$. Let us consider the maps of Q into itself induced by $\boldsymbol{M}, \boldsymbol{R}$ according to the framework of the preceding section; these are

$$M: \mathcal{Q} \to \mathcal{Q}, \quad p \mapsto M(p) = p_x + 2p^2; \quad R: \mathcal{Q} \to \mathcal{Q}, \quad p \mapsto R(p) = -p \tag{3.3}$$

(the letter p for elements of $\mathcal{Q}$ is used here for future convenience). The above maps will be called the *Miura and reflexion transformations* on $\mathcal{Q}$. Let us also recall that any functional $\boldsymbol{f} \in \mathfrak{F}/\mathrm{Im}\boldsymbol{\partial}$ induces a map $f: \mathcal{Q} \to \mathbb{C}$; in particular, considering the KdV conserved functionals we infer from Proposition 3.2 (ii) that

$$(h \circ M) \circ R = h \circ M \quad \text{for each } \boldsymbol{h} \in \mathfrak{Z}_{\mathrm{KdV}}, \tag{3.4}$$

with $\circ$ the usual composition of maps.

We go on and introduce the Bäcklund transformation on $\mathcal{Q}$; essentially, this is the composition of maps $M\circ R\circ M^{-1}$, leaving invariant any conserved KdV functional due to Eq. (3.4). However, M is typically noninvertible on the full space $\mathcal{Q}$: to overcome this difficulty, we use the following.

Definition 3.3: Consider the set $2^{\mathcal{Q}}$ *of the parts of* $\mathcal{Q}$ (*i.e., the collection of all subsets of* $\mathcal{Q}$). *The Bäcklund transformation on* $\mathcal{Q}$ *is the set-valued map*

$$B: \mathcal{Q} \to 2^{\mathcal{Q}}, \quad q \mapsto B(q) := \{(M \circ R)(p) | p \in \mathcal{Q}, M(p) = q\}. \tag{3.5}$$

With this definition, Eq. (3.4) implies the following.

Proposition 3.4: Let $\boldsymbol{h} \in \mathfrak{Z}_{\mathrm{KdV}}$; *then the map* $h: \mathcal{Q} \to \mathbb{R}$ *is Bäcklund invariant, in the following sense: for all* $q, r \in \mathcal{Q}$,

$$r \in B(q) \quad \Rightarrow \quad h(r) = h(q). \tag{3.6}$$

IV. THE IMPLICATION (a)⇒(b) IN PROPOSITION 2.1: A NEW PROOF

The simple geometrical proof we propose is based on the scheme (I)–(III) of the Introduction. Item (I) has been treated in the preceding section; here we formalize (II) and (III). From now on, $(Q, \cdot_x, \int)$ is the integral-differential algebra (2.14) and (2.15) of the formal Laurent series.

Definition 4.1: We set

$$\mathcal{W}:=\left\{ w\in\mathcal{Q}\,\middle|\, w=w_0+\sum_{k=2}^{+\infty} w_k x^k\right\};\quad \mathcal{V}:=\left\{ v\in\mathcal{Q}\,\middle|\, v=\frac{1}{2x}+v_1x+\sum_{k=3}^{+\infty} v_k x^k\right\};$$

$$\mathcal{U}:=\left\{ u\in\mathcal{Q}\,\middle|\, u=\frac{1}{x^2}+u_0+\sum_{k=2}^{+\infty} u_k x^k\right\}. \tag{4.1}$$

Lemma 4.2: Consider the Miura and reflections transformations M,R of Eq. (3.3). *Then*

(i) *M is one to one between $\mathcal{V}$ and $\mathcal{W}$;*
(ii) *$M\circ R$ is one to one between $\mathcal{V}$ and $\mathcal{U}$.*

Proof: (i) For all $v\in\mathcal{V}$, an elementary computation gives

$$M(v)=v_x+2v^2=3v_1+(5v_3+2v_1^2)x^2+6v_4x^3+(7v_5+4v_1v_3)x^4+(8v_6+4v_1v_4)x^5$$
$$+\sum_{k=6}^{\infty}\left((k+3)v_{k+1}+4v_1v_{k-1}+2\sum_{j=3}^{k-3}v_jv_{k-j}\right)x^k; \tag{4.2}$$

from here, we see that $M(v)\in\mathcal{W}$. Now, let us consider any $w\in\mathcal{W}$ and show that the equation $M(v)=w$ has a unique solution $v\in\mathcal{V}$. In fact, $M(v)=w$ is equivalent to $3v_1=w_0$, $5v_3+2v_1^2=w_2$, etc., giving

$$v_1=\tfrac{1}{3}w_0,\quad v_3=-\tfrac{2}{5}v_1^2+\tfrac{1}{5}w_2=-\tfrac{2}{45}w_0^2+\tfrac{1}{5}w_2,\quad v_4=\tfrac{1}{6}w_3,$$

$$v_5=\tfrac{8}{945}w_0^3-\tfrac{4}{105}w_0w_2+\tfrac{1}{7}w_4,\quad v_6=-\tfrac{1}{36}w_0w_3+\tfrac{1}{8}w_5,$$

$$v_{k+1}=-\frac{2}{k+3}\left(2v_1v_{k-1}+\sum_{j=3}^{k-3}v_jv_{k-j}\right)+\frac{w_k}{k+3}\quad\text{for all } k\geqslant 6; \tag{4.3}$$

the equation in the last line is a recursion formula, determining uniquely v_k for all $k\geqslant 7$.

(ii) For all $v\in\mathcal{V}$, we find

$$(M\circ R)(v)=-v_x+2v^2=\frac{1}{x^2}+v_1+(-v_3+2v_1^2)x^2-2v_4x^3+(-3v_5+4v_1v_3)x^4+(-4v_6+4v_1v_4)x^5$$
$$+\sum_{k=6}^{\infty}\left((1-k)v_{k+1}+4v_1v_{k-1}+2\sum_{j=3}^{k-3}v_jv_{k-j}\right)x^k; \tag{4.4}$$

this shows that $(M\circ R)(v)\in\mathcal{U}$. For all $u\in\mathcal{U}$, the equation $(M\circ R)(v)=u$ has a unique solution $v\in\mathcal{V}$, given by

$$v_1=u_0,\quad v_3=2u_0^2-u_2,\quad v_4=-\tfrac{1}{2}u_3,$$

$$v_5=\tfrac{8}{3}u_0^3-\tfrac{4}{3}u_0u_2-\tfrac{1}{3}u_4,\quad v_6=-\tfrac{1}{2}u_0u_3-\tfrac{1}{4}u_5,$$

$$v_{k+1}=\frac{2}{k-1}\left(2v_1v_{k-1}+\sum_{j=3}^{k-3}v_jv_{k-j}\right)-\frac{u_k}{k-1}\quad\text{for all } k\geqslant 6. \tag{4.5}$$

■

Of course, the previous Lemma implies the following.

Corollary 4.3: Define a restricted Bäcklund transformation

$$B_0:\mathcal{W}\to\mathcal{U},\quad B_0:=((M\circ R)\restriction\mathcal{V})\circ(M\restriction\mathcal{V})^{-1};\tag{4.6}$$

then, B_0 is one to one between $\mathcal{W}$ and $\mathcal{U}$.

The final step in our argument is trivial.

Lemma 4.4: Consider any functional $\boldsymbol{f}\in\mathfrak{F}/\mathrm{Im}\,\boldsymbol{\partial}$; then f vanishes on the "holomorphic subspace,"

$$\mathcal{Z}:=\left\{z\in\mathcal{Q}\;\middle|\;z=\sum_{k=0}^{\infty}z_k x^k\right\}.\tag{4.7}$$

Proof: $\mathcal{Z}$ is a differential subalgebra of $\mathcal{Q}$, and $\int$ clearly vanishes on $\mathcal{Z}$. Consider any functional $\boldsymbol{f}=\int\boldsymbol{F}$. For all $z\in\mathcal{Z}$ we have $F(z)\in\mathcal{Z}$ and $f(z)=\int F(z)=0$. ■

We are finally ready to prove the following.

Proof of the implication $(a)\Rightarrow(b)$ in the Treves theorem: Consider a functional $\boldsymbol{h}\in\mathfrak{Z}_{\mathrm{KdV}}$, and any Laurent series $u\in\mathcal{U}$. By the previous Corollary, there is a unique $w\in\mathcal{W}$ such that $u=B_0(w)$; of course this implies $u\in B(w)$, with B the (set-valued) Bäcklund transformation (3.5). These facts give

$$h(u)=h(w)=0.\tag{4.8}$$

The first equality above is ensured by the Bäcklund invariance of h (Proposition 3.4); the second one follows from Lemma (4.4) and the evident inclusion $\mathcal{W}\subset\mathcal{Z}$. ■

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[6] One occasionally needs the full algebra $\mathbb{C}[\boldsymbol{\xi},\boldsymbol{\xi}_x,\boldsymbol{\xi}_{xx},\ldots]$, including polynomials with constant term. This is an algebra with unity, containing $\mathfrak{F}$ as an ideal and identifiable with $\mathfrak{F}\oplus\mathbb{C}$ as a vector space; the derivation $\boldsymbol{\partial}$ is extended to this larger algebra setting $\boldsymbol{\partial}1:=0$. However, this enlargement plays no role in our construction.
[7] For example, if $\boldsymbol{F}=\boldsymbol{\xi}+\boldsymbol{\xi}_x^2$ and $\boldsymbol{G}=\boldsymbol{\xi}^4+\boldsymbol{\xi}_{xx}$, we have $\boldsymbol{FG}=\boldsymbol{\xi}^5+\boldsymbol{\xi}^4\boldsymbol{\xi}_x^2+\boldsymbol{\xi}\boldsymbol{\xi}_{xx}+\boldsymbol{\xi}_x^2\boldsymbol{\xi}_{xx}$; $\boldsymbol{F}\circ\boldsymbol{G}=\boldsymbol{G}+(\boldsymbol{\partial G})^2=(\boldsymbol{\xi}^4+\boldsymbol{\xi}_{xx})+(4\boldsymbol{\xi}^3\boldsymbol{\xi}_x+\boldsymbol{\xi}_{xxx})^2=\boldsymbol{\xi}^4+16\boldsymbol{\xi}^6\boldsymbol{\xi}_x^2+\boldsymbol{\xi}_{xx}+8\boldsymbol{\xi}^3\boldsymbol{\xi}_x\boldsymbol{\xi}_{xxx}+\boldsymbol{\xi}_{xxx}^2$.
[8] A map $K:\mathcal{S}\to\mathcal{T}$, where $\mathcal{S}$ and $\mathcal{T}$ are vector spaces, is said to be of polynomial type if there are m-linear maps $K_m:\times^m\mathcal{S}\to\mathcal{T}$ $(m=0,\ldots,n)$ such that $K(s)=\sum_{m=0}^n K_m(s,\ldots,s)$ for all $s\in\mathcal{S}$. We will write $\mathrm{Pol}(\mathcal{S},\mathcal{T})$ for the maps of polynomial type between $\mathcal{S}$ and $\mathcal{T}$.
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The canonical perfect Bose gas in Casimir boxes

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We study the problem of Bose–Einstein condensation in the perfect Bose gas in the canonical ensemble, in anisotropically dilated rectangular parallelepipeds (Casimir boxes). We prove that in the canonical ensemble for these anisotropic boxes there is the same type of generalized Bose–Einstein condensation as in the grand-canonical ensemble for the equivalent geometry. However the amount of condensate in the individual states is different in some cases and so are the fluctuations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777402]

I. INTRODUCTION

Many calculations in the grand-canonical ensemble (GCE) show a dependence of Bose–Einstein condensation (BEC) on the way the infinite volume limit is taken. For example, in Refs. 14 and 16 the authors study the perfect boson gas (PBG) in the GCE in rectangular parallelepipeds whose edges go to infinity at different rates (*Casimir boxes*, see Ref. 4). They showed that this *anisotropic dilation* can modify the standard ground-state BEC, converting it into a *generalized* BEC of type II or III. For a short history of the notion of *generalized* BEC we refer the reader to Refs. 14 and 16.

On the other hand, due to the lack of (*strong*) equivalence of ensembles, the PBG in the canonical ensemble (CE) and in the GCE gives different expectations and fluctuations for many observables. For example, it was shown in Ref. 3 that for the *isotropic dilation* of the *canonical* PBG the distribution of ground-state occupation number is *different* from the one in the GCE. The same is true for the fluctuations of the occupation numbers, which are shape dependent and are not normal or Gaussian. Therefore this lack of equivalence of ensembles does not allow us to deduce the same shape dependence for BEC in the CE as for its grand-canonical counterpart and so far the question of whether it is true in the CE has not been considered except in a special case.[2]

Our aim in the present paper is to fill this gap. We study the problem of BEC in the PBG in the CE, in anisotropically dilated rectangular boxes. We shall prove that in the CE for these anisotropic boxes there is the same type of generalized BEC as in the GCE for the equivalent geometry. However the amount of condensate in the individual states is different in some cases and so are the fluctuations.

We would like to note that there is a renewed interest in *generalized* BEC both from the theoretical[9,11,18] and experimental[5,13] points of view. This due to recent experiments which produce "fragmentation" of BEC (see, e.g., Refs. 6 and 10), that is, the single state condensation can be "smeared out" over two or more quantum states. We return to this point in Sec. IV.

The structure of the present paper is as follows. In the rest of this section we give the mathematical setting. In Sec. II we collect together the results about PBG in the GCE that we shall

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need. In Sec. III we study the PBG in the CE for the system of anisotropic parallelepipeds. We start by giving some results which are common to the three cases corresponding to the three characteristic ways of taking the thermodynamic limit. These are determined by how fast the longest edge grows: (a) faster than the square root of the volume, (b) like the square root of the volume and (c) slower than the square root of the volume. In the three subsections of Sec. III we study these cases separately. In Sec. IV we discuss the results.

We finish this section by establishing the general setting and notation.

Let Λ_V be a rectangular parallelepiped of volume V:

$$\Lambda_V := \{x \in \mathbb{R}^3 : 0 \leqslant x_j \leqslant V^{\alpha_j}, j = 1,2,3\}, \tag{1.1}$$

where

$$\alpha_1 \geqslant \alpha_2 \geqslant \alpha_3 > 0, \quad \text{and} \quad \alpha_1 + \alpha_2 + \alpha_3 = 1. \tag{1.2}$$

The space of one-particle wave-functions is $\mathcal{H}_V = L^2(\Lambda_V)$ and the one-particle Hamiltonian t_V is the self-adjoint extension of the operator $-\Delta/2$ determined by the Dirichlet boundary conditions on $\partial\Lambda_V$. We denote by $\{E_k(V)\}_{k=1}^{\infty}$ the ordered eigenvalues of t_V:

$$0 < E_1(V) < E_2(V) \leqslant E_3(V) \leqslant \cdots.$$

We also introduce the boson Fock space on $\mathcal{H}_V$ defined by $\mathcal{F}(\mathcal{H}_V) := \oplus_{n=0}^{\infty} \mathcal{H}_{V,\mathrm{symm}}^n$, where $\mathcal{H}_{V,\mathrm{symm}}^n := (\otimes_{j=1}^n \mathcal{H}_V)_{\mathrm{symm}}$ stands for the space of n-particle symmetric functions. Then $T_V^{(n)}$ denotes the n-particle free Hamiltonian determined by $t_V \equiv T_V^{(1)}$ on $\mathcal{H}_{V,\mathrm{symm}}^n$, and T_V the corresponding Hamiltonian in the Fock space.

Now the expectations for the PBG in the canonical ensemble at temperature β^{-1} and density $\rho = n/V$ are defined by the Gibbs state,

$$\langle - \rangle_V^{\mathcal{C}}(\rho) := (Z_V(n))^{-1} \mathrm{Tr}_{\mathcal{H}_{V,\mathrm{symm}}^n} (-) e^{-\beta T_V^{(n)}}, \tag{1.3}$$

where

$$Z_V(n) := \mathrm{Tr}_{\mathcal{H}_{V,\mathrm{symm}}^n} e^{-\beta T_V^{(n)}} \tag{1.4}$$

is the n-particle canonical partition function. As usual we put $Z_V(0) = 1$. The grand-canonical Gibbs state is defined by

$$\langle - \rangle_V^{\mathcal{GC}}(\mu) := (\Xi_V(\mu))^{-1} \mathrm{Tr}_{\mathcal{F}(\mathcal{H}_V)} (-) e^{-\beta(T_V - \mu N_V)}, \tag{1.5}$$

where μ is the corresponding chemical potential. Here N_V is the particle number operator, that is, $N_V := \Sigma_{k \geqslant 1} N_k$ where N_k denotes the operator for the number of particles in the k-th one-particle state. The grand-canonical partition function at chemical potential $\mu < E_1(V)$ is

$$\Xi_V(\mu) := \mathrm{Tr}_{\mathcal{F}(\mathcal{H}_V)} e^{-\beta(T_V - \mu N_V)}. \tag{1.6}$$

Because of their commutative nature it is useful to think of N_V and $\{N_k\}_{k \geqslant 1}$ as random variables rather than operators.

Notice that the one-particle Hamiltonian spectrum $\sigma(t_V) = \{E_k(V)\}_{k=1}^{\infty}$ coincides with the set

$$\left\{ \epsilon_{\mathbf{n},V} = \frac{\pi^2}{2} \sum_{j=1}^{3} \frac{n_j^2}{V^{2\alpha_j}} : n_j = 1,2,3, \ldots, \ j = 1,2,3 \right\}, \tag{1.7}$$

described by the multi-index $\mathbf{n} = (n_1, n_2, n_3)$. Then and the ground-state eigenvalue $E_1(V) = \epsilon_{(1,1,1),V}$.

Let $\{\eta_k(V) := E_k(V) - E_1(V)\}_{k \geqslant 1}$. For a given V we define $F_V : \mathbb{R} \to \mathbb{R}_+$ by

$$F_V(\eta) := \frac{1}{V}\#\{k: \eta_k(V) \leqslant \eta\}. \tag{1.8}$$

Note that F_V is a nondecreasing function on $\mathbb{R}$ with $F_V(\eta)=0$ for $\eta<0$. $F_V(\eta-E_1(V))$ is the distribution of the eigenvalues (*integrated density of states*) of the one-particle Hamiltonian t_V. One can prove in many ways, for example, by using Lemma 3.1 or by taking the Laplace transform, that

$$F(\eta) := \lim_{V\to\infty} F_V(\eta) = (\sqrt{2}/3\pi^2)\eta^{3/2}, \quad \eta \geqslant 0. \tag{1.9}$$

We shall show (see Lemma 3.1) that $F_V(\eta)\leqslant(\sqrt{2}/3\pi^2)\eta^{3/2}$ if $\eta>C/V^{2\alpha_3}$ for some $C>0$. This bound and (1.9) imply that the *critical* density of the PBG,

$$\rho_c := \lim_{\varepsilon\downarrow 0}\lim_{V\to\infty}\int_{(\varepsilon,\infty)}\frac{1}{e^{\beta\eta}-1}F_V(d\eta) = \int_0^\infty \frac{1}{e^{\beta\eta}-1}F(d\eta) < \infty, \tag{1.10}$$

is finite for any nonzero temperature.

By (1.5) the mean occupation number of the PBG in the grand-canonical ensemble in the state k is given by

$$\langle N_k\rangle_V^{\mathcal{G}C}(\mu) = \frac{1}{e^{\beta(E_k(V)-\mu)}-1}. \tag{1.11}$$

Let $\mu_V(\rho)<E_1(V)$ be the unique root of the equation

$$\rho = \frac{1}{V}\langle N_V\rangle_V^{\mathcal{G}C}(\mu), \tag{1.12}$$

for a given V. Then a standard result[16] shows that the boundedness of the critical density (1.10) implies the existence of *generalized* BEC with condensate density, ρ_0, given by

$$\rho_0 := \lim_{\varepsilon\downarrow 0}\lim_{V\to\infty}\frac{1}{V}\sum_{\{k:E_k(V)<\varepsilon\}}\langle N_k\rangle_V^{\mathcal{G}C}(\mu_V(\rho)) = \rho-\rho_c, \quad \text{for } \rho>\rho_c. \tag{1.13}$$

Following the van den Berg–Lewis–Pulé classification, Refs. 14 and 16, it is useful to identify three categories of generalized BEC.

(I) The condensation is of type I when a *finite* number of single-particle states are macroscopically occupied.
(II) It is of type II when an *infinite* number of states are macroscopically occupied.
(III) It is of type III when *none* of the states is macroscopically occupied.

For a specific geometry we have more detailed information at our disposal. In the next section we collect the results from Ref. 14 that we shall need later about the GCE in the case of the anisotropically dilated parallelepipeds (1.1).

Remark 1.1: Though we have chosen here to work with Dirichlet boundary conditions, the proofs in this paper can be adapted without difficulty to periodic or Neumann boundary conditions.

Remark 1.2: Note that according to the classification presented above the condensate "fragmentation" is nothing but a generalized BEC of type I or II.

II. GENERALIZED BOSE–EINSTEIN CONDENSATION OF THE PERFECT BOSE GAS IN THE GRAND-CANONICAL ENSEMBLE

Proposition 2.1 (Ref. 14, Theorem 1): *Let* $\overline{\mu_V}(\rho)=\mu_V(\rho)-E_1(V)$. *Then the behavior of* $\overline{\mu_V}(\rho)$ *is as follows.*

(1) *For* $\rho \leqslant \rho_c$, $\lim_{V\to\infty}\overline{\mu}_V(\rho)=\overline{\mu}(\rho)$ *where* $\overline{\mu}(\rho)<0$ *is the unique root* $\overline{\mu}(\rho)<0$ *of the equation*

$$\rho = \lim_{V\to\infty}\frac{1}{V}\langle N_V\rangle_V^{\mathcal{GC}}(\mu) = \int_0^\infty \frac{1}{e^{\beta(\eta-\mu)}-1}F(d\eta). \tag{2.1}$$

(2) *For* $\rho>\rho_c$, $\lim_{V\to\infty}\overline{\mu}_V(\rho)=0$ *and for* $V\to\infty$,

$$\overline{\mu}_V(\rho) = -\{\beta V(\rho-\rho_c)\}^{-1} + \mathrm{O}(1/V), \text{ if } \alpha_1 < 1/2; \tag{2.2}$$

$$\overline{\mu}_V(\rho) = -\{\beta V A(\rho)\}^{-1} + \mathrm{O}(1/V), \text{ if } \alpha_1 = 1/2; \tag{2.3}$$

$$\overline{\mu}_V(\rho) = -\{2\beta V^{2(1-\alpha_1)}(\rho-\rho_c)^2\}^{-1} + \mathrm{O}(1/V), \text{ if } \alpha_1 > 1/2, \tag{2.4}$$

where $A(\rho)$ *is the unique root of the equation*

$$(\rho-\rho_c) = \sum_{j=1}^{\infty}\left[\frac{\pi^2}{2}(j^2-1)+A^{-1}\right]^{-1}. \tag{2.5}$$

The next statement by the same authors shows that there are different *types* of generalized BEC corresponding to different asymptotics (2.2)–(2.4).

Proposition 2.2 (Ref. 14): *For* $\rho\leqslant\rho_c$ *there is no generalized BEC and therefore no BEC of any type.*

For $\rho>\rho_c$ *there is generalized BEC and all three types of BEC occur.*

(1) *For* $\alpha_1<1/2$ *only the ground-state is macroscopically occupied (BEC of type I):*

$$\lim_{V\to\infty}\frac{1}{V}\langle N_{\mathbf{n}}\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases}\rho-\rho_c, & \text{for } \mathbf{n}=(1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(1,1,1).\end{cases} \tag{2.6}$$

(2) *For* $\alpha_1=1/2$ *there is macroscopic occupation of an infinite number of low-lying levels (BEC of type II):*

$$\lim_{V\to\infty}\frac{1}{V}\langle N_{\mathbf{n}}\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases}\{(n_1^2-1)\pi^2/2+A^{-1}\}^{-1}, & \text{for } \mathbf{n}=(n_1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(n_1,1,1).\end{cases} \tag{2.7}$$

(3) *Finally, for* $\alpha_1>1/2$ *no single-particle state is macroscopically occupied (BEC of type III):*

$$\lim_{V\to\infty} V^{-1}\langle N_{\mathbf{n}}\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = 0, \tag{2.8}$$

$$\lim_{V\to\infty} V^{2(\alpha_1-1)}\langle N_{\mathbf{n}}\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases}2(\rho-\rho_c)^2, & \text{for } \mathbf{n}=(n_1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(n_1,1,1).\end{cases} \tag{2.9}$$

We shall need an easy generalization of the foregoing proposition to obtain the distribution of the random variables N_k through their Laplace transform.

Theorem 2.1: *Let* $\rho>\rho_c$. *Then we have the following.*

(1) *For* $\alpha_1<1/2$,

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_{\mathbf{n}}}{V}\right)\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases}\dfrac{1}{1+\lambda(\rho-\rho_c)}, & \text{for } \mathbf{n}=(1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(1,1,1).\end{cases} \tag{2.10}$$

(2) *For* $\alpha_1=1/2$,

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_{\mathbf{n}}}{V}\right)\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases} \dfrac{(n_1^2-1)\pi^2/2 + A^{-1}}{(n_1^2-1)\pi^2/2 + A^{-1} + \lambda}, & \text{for } \mathbf{n} = (n_1,1,1), \\ 0, & \text{for } \mathbf{n} \neq (n_1,1,1). \end{cases} \tag{2.11}$$

(3) *For* $\alpha_1 > 1/2$,

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_{\mathbf{n}}}{V}\right)\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = 1, \tag{2.12}$$

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_{\mathbf{n}}}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \begin{cases} \dfrac{1}{1+2\lambda(\rho-\rho_c)^2}, & \text{for } \mathbf{n} = (n_1,1,1), \\ 0, & \text{for } \mathbf{n} \neq (n_1,1,1). \end{cases} \tag{2.13}$$

Proof: This follows easily from Proposition 2.1 and the identity

$$\langle \exp(-\lambda N_k)\rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \frac{1-e^{-\beta(\eta_k(V)-\bar{\mu}_V(\rho))}}{1-e^{-\beta(\eta_k(V)-\bar{\mu}_V(\rho)+\lambda/\beta)}}. \tag{2.14}$$

□

We shall require some properties of the *Kac distribution* $\mathbb{K}_\Lambda(\mu;d\rho)$, see, e.g., Refs. 7, 14, 16, and 19. The Kac distribution relates the canonical (1.3) and grand-canonical (1.5) expectations in a finite volume:

$$\langle - \rangle_V^{\mathcal{GC}}(\mu) = \int_{[0,\infty)} \langle - \rangle_V^{\mathcal{C}}(x)\mathbb{K}_V(\mu;dx). \tag{2.15}$$

The *limiting* Kac distribution gives the decomposition of the limiting grand-canonical state $\langle - \rangle^{\mathcal{GC}}(\mu)$ into limiting canonical states $\langle - \rangle^{\mathcal{C}}(\rho)$. In the particular case of the PBG it is more convenient to define the Kac distribution in terms of the mean particle density, rather then the chemical potential. Therefore we define

$$\tilde{\mathbb{K}}_V(\rho;dx) := \mathbb{K}_V(\mu_V(\rho);dx), \tag{2.16}$$

so that

$$\langle - \rangle_V^{\mathcal{GC}}(\mu_V(\rho)) = \int_{[0,\infty)} \langle - \rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho;dx). \tag{2.17}$$

The next proposition proved in Ref. 14 gives the limiting Kac density for anisotropically dilated parallelepipeds.

Proposition 2.3: Let

$$\tilde{\mathbb{K}}(\rho;dx) := \lim_{V\to\infty} \tilde{\mathbb{K}}_V(\rho;dx). \tag{2.18}$$

If $\rho \leqslant \rho_c$, *then the PBG limiting Kac distribution has the one-point support:*

$$\tilde{\mathbb{K}}(\rho;dx) = \delta_\rho(dx). \tag{2.19}$$

If $\rho > \rho_c$, *then we have the following.*

(1) *For* $\alpha_1 < 1/2$,

$$\tilde{\mathbb{K}}(\rho;dx)=\begin{cases}0, & \text{for } x<\rho_c,\\ \dfrac{1}{\rho-\rho_c}\exp\left(-\dfrac{x-\rho_c}{\rho-\rho_c}\right)dx, & \text{for } x>\rho_c.\end{cases} \tag{2.20}$$

(2) *For* $\alpha_1=1/2$,

$$\tilde{\mathbb{K}}(\rho;dx)=\begin{cases}0, & \text{for } x<\rho_c,\\ \dfrac{\pi^2\sinh(2/A-\pi)^{1/2}}{(2/A-\pi)^{1/2}}\displaystyle\sum_{n=1}^{\infty}(-1)^{n-1}n^2\exp\left(-(x-\rho_c)\frac{\pi^2}{2}\left(n^2+\frac{2}{A\pi^2}-1\right)\right)dx, & \text{for } x>\rho_c.\end{cases} \tag{2.21}$$

(3) *For* $\alpha_1>1/2$,

$$\tilde{\mathbb{K}}(\rho;dx)=\delta_\rho(dx). \tag{2.22}$$

III. GENERALIZED BOSE–EINSTEIN CONDENSATION AND FLUCTUATIONS OF THE PERFECT BOSE GAS IN THE CANONICAL ENSEMBLE

In this section we prove results for the CE analogous to those for the GCE. We are forced to use different methods for the three regimes, so we treat them in separate subsections. But first we give some results which will be useful in all three cases. The basic identity for the canonical expectations at density $\rho=n/V$ of the occupation numbers is [see Ref. 3, Eq. (10)]:

$$\langle\exp(-\lambda N_k)\rangle_V^{\mathcal{C}}(\rho)=e^{\lambda}-(e^{\lambda}-1)Z_V(n)^{-1}\sum_{m=0}^{n}e^{-(\beta E_k+\lambda)(n-m)}Z_V(m). \tag{3.1}$$

The canonical expectations are notoriously difficult to calculate and are only accessible through the grand-canonical expectations. In the two cases $\alpha_1<1$ and $\alpha_1=1$ we shall exploit the fact that the sum on the right-hand side of Eq. (3.1) is very similar to the grand-canonical partition function.

The next theorem shows that the canonical expectations are monotonic increasing in the density. Note that this theorem holds for the PBG with any one-particle spectrum.

Theorem 3.1: *For fixed* $k\geqslant 1$ *and fixed,* V*, the canonical expectations for the PBG,* $\langle\exp(-\lambda N_k)\rangle_V^{\mathcal{C}}(\rho)$*, are monotonic decreasing functions of the density* ρ *for* $\lambda>0$ *while the moments* $\langle N_k^r\rangle_V^{\mathcal{C}}(\rho)$*,* $r\geqslant 1$ *are monotonic increasing functions of the density.*

Proof: From (3.1) we get

$$\langle\exp(-\lambda N_k)\rangle_V^{\mathcal{C}}((n+1)/V)-\langle\exp(-\lambda N_k)\rangle_V^{\mathcal{C}}(n/V)=-(e^{\lambda}-1)\left\{e^{-(\beta E_k+\lambda)(n+1)}Z_V(n+1)^{-1}+\sum_{m=0}^{n}e^{-(\beta E_k+\lambda)(n-m)}\left(\frac{Z_V(m+1)}{Z_V(n+1)}-\frac{Z_V(m)}{Z_V(n)}\right)\right\}. \tag{3.2}$$

Since

$$\left(\frac{Z_V(m+1)}{Z_V(n+1)}-\frac{Z_V(m)}{Z_V(n)}\right)=\frac{Z_V(m)}{Z_V(n+1)}\left(\frac{Z_V(m+1)}{Z_V(m)}-\frac{Z_V(n+1)}{Z_V(N)}\right),$$

by the inequalities (see Ref. 7)

$$\frac{Z_V(m+1)}{Z_V(m)} \geqslant \frac{Z_V(m+2)}{Z_V(m+1)} \geqslant \cdots \geqslant \frac{Z_V(n+1)}{Z_V(n)},$$

and by (3.2) we get the monotonicity

$$\langle \exp(-\lambda N_k)\rangle_V^{\mathcal{C}}((n+1)/V) - \langle \exp(-\lambda N_k)\rangle_V^{\mathcal{C}}(n/V) \leqslant 0. \tag{3.3}$$

By differentiating (3.2) r times with respect to λ at $\lambda=0$,

$$\langle N_k^r\rangle_V^{\mathcal{C}}((n+1)/V) - \langle N_k^r\rangle_V^{\mathcal{C}}(n/V) = \{n^r-(n-1)^r\}e^{-\beta E_k(n+1)}Z_V(n+1)^{-1} + \sum_{m=0}^{n}\{(n-m)^r-(n-m-1)^r\}e^{-\beta E_k(n-m)}\left(\frac{Z_V(m+1)}{Z_V(n+1)}-\frac{Z_V(m)}{Z_V(n)}\right), \tag{3.4}$$

which is positive by the same argument. □

Remark: In this paper whenever we take the limit

$$\lim_{V\to\infty}\langle - \rangle_V^{\mathcal{C}}(\rho); \tag{3.5}$$

we shall mean that we take the system with n particles in a container of volume $V_n = n\rho$ and then let $n\to\infty$, that is,

$$\lim_{n\to\infty}\langle - \rangle_{np}^{\mathcal{C}}(\rho). \tag{3.6}$$

The next theorem is valid for containers of any geometry and not just for rectangular boxes.

Theorem 3.2: *For $\rho \geqslant \rho_c$ the generalized condensate in the CE at density ρ is equal to $\rho - \rho_c$, that is*

$$\lim_{\varepsilon\downarrow 0}\lim_{V\to\infty}\sum_{\eta_k<\varepsilon}\langle N_k/V\rangle_V^{\mathcal{C}}(\rho) = \rho - \rho_c. \tag{3.7}$$

Proof: The statement is true for the imperfect (mean-field) Bose gas in the GCE; see Ref. 15. Since the mean-field term in the CE is irrelevant, the theorem follows from monotonicity and the fact that the Kac density for the imperfect Bose gas has one-point support. □

In the next theorem we shall make certain assumptions that are clearly satisfied for the parallelepipeds we are considering. We believe that in fact they hold much more generally.

Theorem 3.3: *Suppose that* $\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{GC}}(\mu_\Lambda(\rho'))$ and $\tilde{\mathbb{K}}(\rho';[\rho,\infty))$ *are continuous in ρ' at ρ and that* $\tilde{\mathbb{K}}(\rho;[\rho,\infty)) \neq 0$. *Then* $\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{GC}}(\mu_V(\rho))=0$ *implies that* $\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{C}}(\rho)=0$.

Proof: Using the decomposition (2.17) and monotonicity we get for any $\varepsilon>0$:

$$\begin{aligned}\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{GC}}(\mu_\Lambda(\rho+\varepsilon)) &= \lim_{V\to\infty}\int_{[0,\infty)}\langle N_k/V\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\varepsilon;dx)\\ &\geqslant \lim_{V\to\infty}\int_{[\rho,\infty)}\langle N_k/V\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\varepsilon;dx)\\ &\geqslant \limsup_{V\to\infty}\{\langle N_k/V\rangle_V^{\mathcal{C}}(\rho)\tilde{\mathbb{K}}_V(\rho+\varepsilon;[\rho,\infty))\}\\ &= \limsup_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{C}}(\rho)\tilde{\mathbb{K}}(\rho+\varepsilon;[\rho,\infty)).\end{aligned}$$

Since $\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{GC}}(\mu_\Lambda(\rho'))$ and $\tilde{\mathbb{K}}(\rho';[\rho,\infty))$ are continuous in ρ', letting ε tend to zero, we get

$$\lim_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{G}C}(\mu_\Lambda(\rho)) \geqslant \limsup_{V\to\infty}\langle N_k/V\rangle_V^{\mathcal{C}}(\rho)\widetilde{\mathbb{K}}(\rho;[\rho,\infty)),$$

and because $\widetilde{\mathbb{K}}(\rho;[\rho,\infty))$ does not vanish the result follows. □

Remark: Note that this lemma implies that for $\rho \leqslant \rho_c$, there is never BEC in the CE.

Before looking at the three cases $\alpha_1 < 1/2$, $\alpha_1 = 1/2$ and $\alpha_1 > 1/2$ we first obtain lower and upper bounds on the density of states.

Lemma 3.1:

$$\frac{\sqrt{2}}{3\pi^2}(\eta^{1/2} - CV^{-\alpha_3})^3 < F_V(\eta) < \frac{\sqrt{2}}{3\pi^2}(\eta + E_1(V))^{3/2}, \tag{3.8}$$

for some C.

Proof:

$$VF_V(\eta - E_1(V)) = \#\left\{\mathbf{n}|\mathbf{n}\in\mathbb{N}^3, \frac{\pi^2}{2}\sum_{j=1}^{d=3}\frac{n_j^2}{V^{2\alpha_j}} < \eta\right\}, \tag{3.9}$$

that is, $VF_V(\eta - E_1(V))$ is the number of points of $\mathbb{N}^3$ inside the ellipsoid,

$$\frac{x^2}{2V^{2\alpha_1}\eta/\pi^2} + \frac{y^2}{2V^{2\alpha_2}\eta/\pi^2} + \frac{z^2}{2V^{2\alpha_3}\eta/\pi^2} = 1. \tag{3.10}$$

If we associate the point $\mathbf{n}$ with the volume of the unit cube centered at $\mathbf{n} - \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ we see that this number is less the volume of the ellipsoid in the first octant which is equal to $\pi(2V^{2\alpha_1}\eta/\pi^2)^{1/2}(2V^{2\alpha_2}\eta/\pi^2)^{1/2}(2V^{2\alpha_3}\eta/\pi^2)^{1/2}/6 = \sqrt{2}\eta^{3/2}V/3\pi^2$. Thus

$$VF_V(\eta - E_1(V)) < \frac{\sqrt{2}}{3\pi^2}\eta^{3/2}V, \tag{3.11}$$

and so

$$F_V(\eta) < \frac{\sqrt{2}}{3\pi^2}(\eta + E_1(V))^{3/2}. \tag{3.12}$$

Let $a > b > c > 0$, let $\lambda = 1 - 3/c$ and $a' = \lambda a$, $b' = \lambda b$, and $c' = \lambda c$. If the point in the first quadrant (x,y,z) satisfies $x^2/a'^2 + y^2/b'^2 + z^2/c'^2 \leqslant 1$, then it satisfies $(x+1)^2/a^2 + (y+1)^2/b^2 + (z+1)^2/c^2 \leqslant 1$. That is, each point inside the first quadrant of the ellipsoid $x^2/a'^2 + y^2/b'^2 + z^2/c'^2 = 1$ lies in a unit cube with the corner $\mathbf{n} \in \mathbb{N}^3$ (with $n_1 > x$, $n_2 > y$ and $n_3 > y$) inside the ellipsoid $x^2/a^2 + y^2/b^2 + z^2/c^2 = 1$. Therefore

$$VF_V(\eta - E_1(V)) > \frac{\sqrt{2}}{3\pi^2}V\left(\eta^{1/2} - \frac{3\pi}{\sqrt{2}V^{\alpha_3}}\right)^3, \tag{3.13}$$

yielding

$$F_V(\eta) > \frac{\sqrt{2}}{3\pi^2}\left((\eta + E_1(V))^{1/2} - \frac{3\pi}{\sqrt{2}V^{\alpha_3}}\right)^3 > \frac{\sqrt{2}}{3\pi^2}V\left(\eta^{1/2} - \frac{3\pi}{\sqrt{2}V^{\alpha_3}}\right)^3. \tag{3.14}$$

□

A. Case $\alpha_1 > 1/2$

We study this case first because it is the simplest since the limiting Kac distribution is a delta measure concentrated at ρ and we have strong equivalence of ensembles (see Proposition 2.3). We

shall use this fact together with the monotonicity properties of Theorem 3.1 to show that in this case the limiting canonical and grand-canonical expectations are identical.

Lemma 3.2: For $\alpha_1 > 1/2$ *and* $\lambda > 0$ *the following inequalities hold:*

$$\begin{aligned}\liminf_{\varepsilon\downarrow 0}\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{G}C}(\mu_V(\rho-\varepsilon)) &\geqslant \limsup_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho)\\ &\geqslant \liminf_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho)\\ &\geqslant \limsup_{\epsilon\downarrow 0}\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{G}C}(\mu_\Lambda(\rho+\varepsilon)).\end{aligned} \tag{3.15}$$

Proof: We start with the first inequality. Using the decomposition (2.17) we get for any $\varepsilon > 0$:

$$\begin{aligned}\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{G}C}(\mu_V(\rho-\varepsilon)) &= \lim_{V\to\infty}\int_{[0,\infty)}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho-\varepsilon;dx)\\ &\geqslant \lim_{V\to\infty}\int_{[0,\rho)}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho-\varepsilon;dx)\\ &\geqslant \limsup_{V\to\infty}\left\{\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho)\tilde{\mathbb{K}}_V(\rho-\varepsilon;[0,\rho))\right\}\\ &= \limsup_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho).\end{aligned} \tag{3.16}$$

In the penultimate inequality we have used the monotonicity established in Theorem 3.1 and in the last one we have used (2.19) and (2.22). The last inequality in (3.15) is proved similarly:

$$\begin{aligned}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{G}C}(\mu_V(\rho+\varepsilon)) &= \int_{[0,\infty)}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\varepsilon;dx)\\ &= \int_{[0,\rho)}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\varepsilon;dx)\\ &\quad+\int_{[\rho,\infty)}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\varepsilon;dx)\\ &\leqslant \tilde{\mathbb{K}}_V(\rho+\varepsilon;[0,\rho))\\ &\quad+\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho)\tilde{\mathbb{K}}_V(\rho-\varepsilon;[\rho,\infty)).\end{aligned} \tag{3.17}$$

Therefore

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{G}C}(\mu_V(\rho+\varepsilon)) \leqslant \liminf_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho). \tag{3.18}$$

□

The following theorem and corollary give the distribution and the mean of $N_{\mathbf{n}}/V^{2(1-\alpha_1)}$ and therefore they give the fluctuations about the mean.

Theorem 3.4: *If* $\alpha_1 > 1/2$ *and* $\rho > \rho_c$ *then the limiting distribution in the canonical ensemble of* $N_{\mathbf{n}}/V^{2(1-\alpha_1)}$ *has Laplace transform for* $\lambda > 0$ *given by*

$$\lim_{V\to\infty}\left\langle \exp\left(-\lambda\frac{N_k}{V^{2(1-\alpha_1)}}\right)\right\rangle_V^{\mathcal{C}}(\rho)=\begin{cases}\dfrac{1}{1+2\lambda(\rho-\rho_c)^2}, & \text{for } \mathbf{n}=(n_1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(n_1,1,1).\end{cases} \tag{3.19}$$

Proof: This follows from the preceding lemma and Theorem 2.1. □

Corollary 3.1: If $\alpha_1>1/2$ *and* $\rho>\rho_c$ *then*

$$\lim_{V\to\infty}\left\langle \frac{N_{\mathbf{n}}}{V^{2(1-\alpha_1)}}\right\rangle_V^{\mathcal{C}}(\rho)=\begin{cases}2\lambda(\rho-\rho_c)^2, & \text{for } \mathbf{n}=(n_1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(n_1,1,1).\end{cases} \tag{3.20}$$

Proof: We have to check that there exists $K<\infty$ such that for all V,

$$\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{C}}(\rho)<K. \tag{3.21}$$

Then the corollary follows from the preceding theorem. We have again for any $\varepsilon>0$,

$$\begin{aligned}\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho+\epsilon))&=\int_{[0,\infty)}\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\epsilon;dx)\\ &\geqslant\int_{[\rho,\infty)}\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{C}}(x)\tilde{\mathbb{K}}_V(\rho+\epsilon;dx)\\ &\geqslant\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{C}}(\rho)\tilde{\mathbb{K}}_V(\rho+\epsilon;[\rho,\infty))\geqslant\frac{1}{2}\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{C}}(\rho),\end{aligned} \tag{3.22}$$

if V is large enough. This implies the existence of K as above since

$$\left\langle\left(\frac{N_k}{V^{2(1-\alpha_1)}}\right)^2\right\rangle_V^{\mathcal{GC}}(\mu_V(\rho+\epsilon)), \tag{3.23}$$

converges as $V\to\infty$. □

Corollary 3.2: When $\alpha_1>1/2$, *there is type III BEC in the canonical ensemble.*

Proof: From the preceding corollary or from Theorem 3.3 we can deduce immediately that

$$\lim_{V\to\infty}\left\langle\frac{N_k}{V}\right\rangle_V^{\mathcal{C}}(\rho)=0, \tag{3.24}$$

for any $\rho>\rho_c$. □

B. Case $\alpha_1=1/2$

For this case BEC into the ground state is treated in Ref. 2. Here we extend the result to higher levels.

Because for $\alpha_1=1/2$ the spectral series (1.7) corresponding to $n_1=1,2,3,\ldots$, has the *smallest* energy spacing $\pi^2/2V$, it plays a specific role in calculations of the limiting occupation densities. Let

$$\epsilon_n:=\pi^2n^2/2,\quad \eta_{m,n}:=\beta(\epsilon_m-\epsilon_n),\quad b_{m,n}:=\eta_{m,n}^{-1}\prod_{\{m'\neq n,m'\neq m\}}(1-\eta_{m,n}/\eta_{m',n})^{-1}, \tag{3.25}$$

for $m\neq n$.

In Ref. 2 the following result was proved.

Let $\alpha_1=1/2$. *Then for* $\rho>\rho_c$,

$$\lim_{V\to\infty}\left\langle \frac{N_1}{V}\right\rangle_V^{\mathcal{C}}(\rho)=\frac{\sum_{m=2}^{\infty} b_{m,1}\{\eta_{m,1}(\rho-\rho_c)-1+\exp[-\eta_{m,1}(\rho-\rho_c)]\}}{\sum_{m=2}^{\infty} b_{m,1}\eta_{m,1}\{1-\exp[-\eta_{m,1}(\rho-\rho_c)]\}}. \tag{3.26}$$

Here we give an extension of (3.26) to other k's. Note that by Theorem 3.3 and a comparison with the GCE, in this case there can only be condensation in states corresponding to $\mathbf{n}=(n_1,1,1)$. The main tool in the technique developed in Refs. 2 and 3 is the following identity.

Let $\{K_{k,V}(dx)\}_{k\geqslant 1}$ be (non-normalized) measures whose distributions are the functions

$$K_{k,V}(x)=\begin{cases} Z_V(r)\exp\{-\beta(V_{pk}-rE_k(V))\}, & \text{for } r/V<x\leqslant (r+1)/V,\\ 0, & \text{for } x\leqslant 0,\end{cases} \tag{3.27}$$

for $r=0,1,2,\ldots$, and some $\{p_k\}_{k\geqslant 1}$. Then we can re-write Eq. (3.1) as follows:

$$\begin{aligned}\langle\exp\{-\lambda N_k/V\}\rangle_V^{\mathcal{C}}(\rho)&=e^{-\lambda\rho}\int_{[0,\rho+1/V]} e^{\lambda x}K_{k,V}(dx)/K_{k,V}(\rho+1/V)\\ &=e^{-\lambda/V}-\lambda e^{-\lambda\rho}\int_0^{\rho+1/V} K_{k,V}(x)e^{\lambda x}dx/K_{k,V}(\rho+1/V).\end{aligned} \tag{3.28}$$

We shall use this identity to calculate the thermodynamic limit of its left-hand side for a given density and $k\geqslant 1$. From (3.27) we can calculate the Laplace transformation of the measure $K_{k,V}(dx)$:

$$\int_{\mathbb{R}} e^{-\lambda x}K_{k,V}(dx)=(1-e^{-\lambda/V})e^{-V\beta_{pk}}\Xi_V(E_k(V)-\lambda/\beta V), \tag{3.29}$$

where for the PBG the grand-canonical partition function (1.6) has the explicit form

$$\Xi_V(\mu)=\prod_{k=1}^{\infty}\{1-e^{-\beta(E_k(V)-\mu)}\}^{-1}.$$

Now we fix the p_k's which are still arbitrary by defining

$$p_k:=-\frac{1}{\beta V}\sum_{j\neq k}\ln|1-e^{-\beta(E_j(V)-E_k(V))}| \tag{3.30}$$

and prove the following lemma. We put

$$\tilde{K}_{n,V}:=K_{(n,1,1),V}. \tag{3.31}$$

Lemma 3.3: Let $\alpha_1=1/2$. *Then*

$$\tilde{K}_n(x):=\lim_{V\to\infty}\tilde{K}_{n,V}(x)=\begin{cases}0, & \text{for } x\leqslant\rho_c,\\ (-1)^{(n-1)}\sum_{m=1,m\neq n}^{\infty} b_{m,n}\eta_{m,n}\{1-\exp[-\eta_{m,n}(x-\rho_c)]\}, & \text{for } x>\rho_c.\end{cases} \tag{3.32}$$

Proof: Let $\lambda>V(E_k-E_1)$. From the definitions (3.29) and (3.30) we get

$$\int_{\mathbb{R}} e^{-\lambda x}K_{k,V}(dx)=\prod_{j\neq k}\frac{|1-e^{-\beta(E_j(V)-E_k(V))}|}{1-e^{-\beta(E_j(V)-E_k(V)+\lambda/\beta V)}}=\exp\left\{-\sum_{j\neq k}\ln\left|1+\frac{1-e^{-\lambda/V}}{e^{\beta(E_j(V)-E_k(V))}-1}\right|\right\}.$$

For $k \geqslant 1$ and $\eta \geqslant \eta_1(V) - \eta_k(V)$ we define the *shifted* integrated density of states; cf. (1.8):

$$F_{k,V}(\eta \geqslant 0) := \frac{1}{V} \#\{j : \eta_j(V) \leqslant \eta + \eta_k(V), j \neq k\} = F_V(\eta + \eta_k(V)) - \frac{1}{V}\mathbf{1}_{[0,\infty)}(\eta). \tag{3.33}$$

For $b > a$, let

$$I_{k,V}(a,b) := V \int_{[a,b)} \ln \left| 1 + \frac{1 - e^{-\lambda/V}}{e^{\beta\eta} - 1} \right| F_{k,V}(d\eta). \tag{3.34}$$

Then

$$\sum_{j \neq k} \ln \left| 1 + \frac{1 - e^{-\lambda/V}}{e^{\beta(E_j(V) - E_k(V))} - 1} \right| = V \int_{[\eta_1(V) - \eta_k(V), \infty)} \ln \left| 1 + \frac{1 - e^{-\lambda/V}}{e^{\beta\eta} - 1} \right| F_{k,V}(d\eta) = I_{k,V}(\eta_1(V) - \eta_k(V), \infty). \tag{3.35}$$

We can write

$$I_{k,V}(\eta_1(V) - \eta_k(V), \infty) = I_{k,V}(\eta_1(V) - \eta_k(V), 1/V^{2\alpha_3}) + I_{k,V}(1/V^{2\alpha_3}, \infty). \tag{3.36}$$

Since $\lim_{V \to \infty} \eta_k(V) = 0$, by Lemma 3.1 we have

$$\lim_{V \to \infty} F_{k,V}(\eta) = \lim_{V \to \infty} F_V(\eta + \eta_k(V)) = F(\eta) \tag{3.37}$$

and

$$F_{k,V}(\eta) \leqslant C' \eta^{3/2}, \tag{3.38}$$

for $\eta > 1/V^{2\alpha_3}$; using the estimate $x - x^2/2 \leqslant \ln(1+x) \leqslant x$ we get

$$\lim_{V \to \infty} I_{k,V}(1/V^{2\alpha_3}, \infty) = \lambda \rho_c. \tag{3.39}$$

On the lower part of the spectrum we need to scale $F_{k,V}$. Let

$$G_{k,V}(\xi) := V F_{k,V}(\xi/V). \tag{3.40}$$

Then

$$I_{k,V}(\eta_1(V) - \eta_k(V), 1/V^{2\alpha_3}) = \int_{[V(\eta_1(V) - \eta_k(V)), V^{1-2\alpha_3}]} \ln \left| 1 + \frac{1 - e^{-\lambda/V}}{e^{\beta\xi/V} - 1} \right| G_{k,V}(d\xi). \tag{3.41}$$

Now let $E_k(V)$ correspond to $\epsilon_{(n,1,1),V}$. Then in the limit, $G_{k,V}$ gives a nontrivial point measure concentrated on the set $\{\beta^{-1}\eta_{m,n}, m \neq n\}$:

$$\lim_{V \to \infty} G_{k,V}(\xi > 0) = \#\{m : \beta^{-1}\eta_{m,n} \leqslant \xi, m \neq n\}. \tag{3.42}$$

Therefore, by (3.41) and (3.42) we get

$$\lim_{V \to \infty} \{I_{k,V}(V(\eta_1(V) - \eta_k(V)), 1/V^{2\alpha_3}\} = \sum_{m \neq n} \ln \left| 1 + \frac{\lambda}{\eta_{m,n}} \right|. \tag{3.43}$$

Thus for $\lambda > |\eta_{1,n}|$,

$$\lim_{V \to \infty} \int_0^\infty K_{k,V}(dx) e^{-\lambda x} = \exp\{-\lambda \rho_c\} \exp\left\{ - \sum_{m \neq n} \ln \left| 1 + \frac{\lambda}{\eta_{m,n}} \right| \right\}, \tag{3.44}$$

and the lemma follows by inverting the Laplace transform. □

Theorem 3.5: *Let $\rho>\rho_c$ and $\alpha_1=1/2$. Let $E_k(V)$ correspond to $\epsilon_{(n,1,1),V}$. Then*

$$\lim_{V\to\infty}\langle\exp\{-\lambda N_k/V\}\rangle_V^{\mathcal{C}}(\rho)=\frac{\sum_{m=1,m\neq n}^{\infty}b_{m,n}\frac{\eta_{m,n}^2}{\eta_{m,n}-\lambda}\{\exp[\lambda(\rho-\rho_c)]-\exp[-\eta_{m,n}(\rho-\rho_c)]\}}{\sum_{m=1,m\neq n}^{\infty}b_{m,n}\eta_{m,n}\{1-\exp[-\eta_{m,n}(\rho-\rho_c)]\}}. \tag{3.45}$$

Proof: The identity (3.28) gives

$$\lim_{V\to\infty}\langle\exp\{-\lambda N_k/V\}\rangle_V^{\mathcal{C}}(\rho)=1-\frac{\lambda e^{-\lambda\rho}\int_0^{\rho}K_k(x)e^{\lambda x}dx}{K_k(\rho)}. \tag{3.46}$$

From the preceding lemma and for $\lambda>0$,

$$\begin{aligned}&\frac{\lambda e^{-\lambda\rho}\int_0^{\rho}K_k(x)e^{\lambda x}dx}{K_k(\rho)}\\&=\frac{\sum_{m\neq n}^{\infty}b_{m,n}\eta_{m,n}\lambda e^{-\lambda\rho}\int_{\rho_c}^{\rho}e^{\lambda x}\{1-\exp[-\eta_{m,n}(x-\rho_c)]\}dx}{\sum_{m\neq n}b_{m,n}\eta_{m,n}\{1-\exp[-\eta_{m,n}(\rho-\rho_c)]\}}\\&=-\frac{\sum_{m\neq n}b_{m,n}\frac{\eta_{m,n}}{\eta_{m,n}-\lambda}\{\eta_{m,n}\exp[-\lambda(\rho-\rho_c)]-\lambda\exp[-\eta_{m,n}(\rho-\rho_c)]-(\eta_{m,n}-\lambda)\}}{\sum_{m\neq n}b_{m,n}\eta_{m,n}\{1-\exp[-\eta_{m,n}(\rho-\rho_c)]\}}.\end{aligned} \tag{3.47}$$

This gives (3.45). □

We are now in a position to prove that in this case there is BEC of type II for $\rho>\rho_c$.

Theorem 3.6: *For $\rho>\rho_c$ and for $\alpha_1=1/2$ all states with $\mathbf{n}=(n,1,1)$ are macroscopically occupied (BEC of type II) while all the other states are not. The occupation density is given by*

$$\lim_{V\to\infty}\left\langle\frac{N_{(n,1,1)}}{V}\right\rangle_V^{\mathcal{C}}(\rho)=\frac{\sum_{m=1,\neq n}^{\infty}b_{m,n}\{\eta_{m,n}(\rho-\rho_c)-1+\exp[-\eta_{m,n}(\rho-\rho_c)]\}}{\sum_{m=1,m\neq n}^{\infty}b_{m,n}\eta_{m,n}\{1-\exp[-\eta_{m,n}(\rho-\rho_c)]\}}.$$

Proof: It is sufficient to check that there exists $K<\infty$ such that for all V,

$$\langle(N_k/V)^2\rangle_V^{\mathcal{C}}(\rho)<K. \tag{3.48}$$

Then the theorem follows from the preceding one. We have

$$\langle (N_k/V)^2\rangle_V^{\mathcal{G}C}(\mu_V(\rho)) = \int_{[0,\infty)} \langle (N_k/V)^2\rangle_V^{\mathcal{C}}(x)\widetilde{\mathbb{K}}_V(\rho;dx) \geqslant \int_{[0,\infty)} \langle (N_k/V)^2\rangle_V^{\mathcal{C}}(x)\widetilde{\mathbb{K}}_V(\rho;dx)$$

$$\geqslant \langle (N_k/V)^2\rangle_V^{\mathcal{C}}(\rho)\widetilde{\mathbb{K}}_V(\rho;[\rho,\infty)). \quad (3.49)$$

This implies the existence of K as above since $\langle (N_k/V)^2\rangle_V^{\mathcal{G}C}(\mu_V(\rho))$ converges as $V\to\infty$ and $\widetilde{\mathbb{K}}_V(\rho;[\rho,\infty))$ converges to a nonzero limit. □

C. Case $\alpha_1 < 1/2$

In Ref. 3 the canonical PBG in parallelepipeds,

$$\Lambda_V := \{x\in\mathbb{R}^3 : 0\leqslant x_j\leqslant a_j V^{1/3}, j=1,2,3\}, \quad a_1a_2a_3 = 1, \quad (3.50)$$

was considered. It was proved that for this system there is BEC of *type I*. In particular the following was proved.

Proposition 3.1 (Ref. 3, Theorem 1): *For the PBG in parallelepipeds (3.50), the following limits hold when* $\lambda\in\mathbb{R}$:

$$\lim_{V\to\infty}\langle \exp\{-\lambda N_k/V\}\rangle_V^{\mathcal{C}}(\rho) = \begin{cases} \exp\{-\lambda(\rho-\rho_c)\}, & \text{for } k=1,\\ 1, & \text{for } k>1, \end{cases} \quad (3.51)$$

if $\rho>\rho_c$, *and*

$$\lim_{V\to\infty}\langle \exp\{-\lambda V^{\gamma}N_k/V\}\rangle_V^{\mathcal{C}}(\rho) = 1, \quad (3.52)$$

for any $0\leqslant\gamma<1$ *and* $k\geqslant 1$, *if* $\rho\leqslant\rho_c$.

Note that in Ref. 3, Theorem 1, $\lambda\leqslant 0$, but this is not necessary.

In this section we shall prove a similar result to Proposition 3.1 for the case of the rectangular parallelepipeds (1.1) with $\alpha_1<1/2$, that is, we shall show that in this case there is also *type I* BEC. It is sufficient to show that there is condensation in the ground state since by Theorem 3.3 no other state can be macroscopically occupied.

Let $K_{1,V}(dx)$ be as in (3.27) in Sec. III B.

Lemma 3.4: Let $\alpha_1<1/2$. *Then*

$$\lim_{V\to\infty} K_{1,V}(dx) = \delta_{\rho_c}(dx). \quad (3.53)$$

Proof: The proof is almost identical to that of Lemma 3.3. The only difference is that since $\eta_j(V)-\eta_1(V)\geqslant a_{j,k}/V^{2\alpha_1}$, (3.40) implies that

$$G_{1,V}(\xi>0) = \#\{j : \eta_j(V)-\eta_1(V)\leqslant \xi/V\}\to 0, \quad \text{when } V\to\infty, \quad (3.54)$$

for $\alpha_1<1/2$, and the lemma follows. □

We can now prove that in this case there is BEC of type I for $\rho>\rho_c$.

Theorem 3.7: *For* $\rho>\rho_c$ *and for* $\alpha_1<1/2$ *only the ground-state is macroscopically occupied (BEC of type I):*

$$\lim_{V\to\infty}\frac{1}{V}\langle N_{\mathbf{n}}\rangle_V^{\mathcal{C}}(\rho) = \begin{cases} \rho-\rho_c & \text{for } \mathbf{n}=(1,1,1),\\ 0, & \text{for } \mathbf{n}\neq(1,1,1). \end{cases} \quad (3.55)$$

Proof: From the preceding lemma and the identity (3.28) we have for $\lambda>0$,

$$\lim_{V\to\infty}\langle\exp(-\lambda N_{\mathbf{n}}/V)\rangle_V^{\mathcal{G}C}(\rho)=\exp(-\lambda(\rho-\rho_c)). \tag{3.56}$$

It is sufficient to show the second moment is bounded, that is, there exists $K<\infty$ such that for all V,

$$\langle(N_k/V)^2\rangle_V^{\mathcal{C}}(\rho)<K. \tag{3.57}$$

The bound can be obtained by the same argument as in Theorem 3.6. □

In the rest of this subsection we study the fluctuations of N_1/V. We need the shifted integrated density of states in d dimensions $F_1^{(d)}$, $d=1,2,3$, in the unit boxes $[0,1]^d$:

$$F_1^{(d)}(\eta):=\#\left\{\mathbf{n}|\mathbf{n}\in\mathbb{N}^d,\frac{\pi^2}{2}\sum_{j=1}^{d}(n_j-1)^2\leqslant\eta\right\}. \tag{3.58}$$

Theorem 3.8: *Suppose* $\alpha_1<1/2$ *and let* $\gamma=1-2\alpha_1>0$. *Then for* $\rho>\rho_c$,

$$\lim_{V\to\infty}\langle\exp\{\lambda V^{\gamma}(N_1/V-\langle N_1/V\rangle_V^{\mathcal{C}}(\rho))\}\rangle_V^{\mathcal{C}}(\rho)$$
$$=\begin{cases}\exp(g_1(\lambda)), & \text{if } \alpha_3<\alpha_2<\alpha_1<1/2,\\ \exp(2g_1(\lambda)+g_2(\lambda)), & \text{if } \alpha_3<\alpha_2=\alpha_1<1/2,\\ \exp(3g_1(\lambda)+3g_2(\lambda)+g_3(\lambda)), & \text{if } \alpha_3=\alpha_2=\alpha_1=1/3,\end{cases} \tag{3.59}$$

where

$$g_1(\lambda)=\int_{(0,\infty)}\left[-\ln\left(1+\frac{\lambda}{\beta\eta}\right)+\frac{\lambda}{\beta\eta}\right]F_1^{(1)}(d\eta),$$

$$g_2(\lambda)=\int_{(0,\infty)^2}\left[-\ln\left(1+\frac{\lambda}{\beta(\eta_1+\eta_2)}\right)+\frac{\lambda}{\beta(\eta_1+\eta_2)}\right]F_1^{(2)}(d\eta_1,d\eta_2),$$

$$g_3(\lambda)=\int_{(0,\infty)^3}\left[-\ln\left(1+\frac{\lambda}{\beta(\eta_1+\eta_2+\eta_3)}\right)+\frac{\lambda}{\beta(\eta_1+\eta_2+\eta_3)}\right]F_1^{(3)}(d\eta_1,d\eta_2,d\eta_3). \tag{3.60}$$

Remark: Note that $3g_1(\lambda)+3g_2(\lambda)+g_3(\lambda)$ is the same as $g(\lambda)$ in Ref. 3.

Proof: Let

$$L_V(x):=\begin{cases}Z_V(r)\exp\{-\beta(Vp_1-rE_k(V))\}, & \text{for } V^{\gamma}(r/V-\rho_c^V)<x\leqslant V^{\gamma}((r+1)/V-\rho_c^V),\\ 0, & \text{for } x\leqslant -V^{\gamma}\rho_c^V,\end{cases}$$

for $r=0,1,2,\ldots$, where p_1 is as in (3.30),

$$\rho_c^V:=\int_{(0,\infty)}\frac{1}{e^{\beta\eta}-1}F_V(d\eta), \tag{3.61}$$

and where we put $Z_V(0)=1$. Then

$$\langle\exp\{\lambda V^{\lambda}(N_1/V-(\rho-\rho_c^V))\}\rangle_V^{\mathcal{C}}(\rho)=\int_{(-\infty,\delta_V)}e^{-\lambda x}L_V(dx)/K_{1,V}(\rho+1/V), \tag{3.62}$$

where $\delta_V=V^{\gamma}(\rho-\rho_c^V)+V^{-2\alpha_1}$. By Lemma 3.4 for $\rho>\rho_c$, $\lim_{V\to\infty}K_{1,V}(\rho+1/V)=1$ and therefore

$$\langle \exp\{\lambda V^{\lambda}(N_1/V-(\rho-\rho_c^V))\}\rangle_V^{\mathcal{C}}(\rho)=\lim_{V\to\infty}\int_{(-\infty,\infty)}e^{-\lambda x}L_V(dx). \tag{3.63}$$

Now

$$\begin{aligned}\ln\int_{(-\infty,\infty)}e^{-\lambda x}L_V(dx)&=V\int_{(0,\infty)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta\eta}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta\eta}-1}\right]F_V(d\eta)\\&=\sum_{\mathbf{n}\neq(1,1,1)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right].\end{aligned} \tag{3.64}$$

Consider first the case $\alpha_3<\alpha_2<\alpha_1<1/2$. We split up the last sum into two parts, the first corresponds to the eigenvalues that go to zero like $V^{-2\alpha_1}$ and the second to the rest:

$$\ln\int_{(-\infty,\infty)}e^{-\lambda x}L_V(dx)=A_V+B_V, \tag{3.65}$$

where

$$A_V=\sum_{n_1\neq 1}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \tag{3.66}$$

and

$$B_V=\sum_{(n_2,n_3)\neq(1,1)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right]. \tag{3.67}$$

Note that by definition (3.58),

$$A_V=\int_{(0,\infty)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right]F_1^{(1)}(d\eta). \tag{3.68}$$

Using the bounds [obtained from the inequality $-x<-\ln(1+x)<\frac{1}{2}x^2-x$]:

$$0<\frac{\lambda-1+e^{-\lambda}}{e^x-1}<-\ln\left(1+\frac{1-e^{-\lambda}}{e^x-1}\right)+\frac{\lambda}{e^x-1}<\frac{1}{2}\left(\frac{1-e^{-\lambda}}{e^x-1}\right)^2+\frac{\lambda-1+e^{-\lambda}}{e^x-1}<\frac{c\lambda^2}{x^2}, \tag{3.69}$$

we get using the Dominated Convergence Theorem,

$$\lim_{V\to\infty}A_V=g_1(\lambda). \tag{3.70}$$

Using the same inequality,

$$\begin{aligned}0<B_V&\leqslant\frac{\lambda^2}{\beta^2V^{4\alpha_1}}\sum_{(n_2,n_3)\neq(1,1)}\frac{1}{(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})^2}\\&=\frac{4\lambda^2}{\pi^4\beta^2V^{4\alpha_1}}\sum_{(n_2,n_3)\neq(1,1)}\frac{1}{\left(\frac{(n_1^2-1)}{V^{2\alpha_1}}+\frac{(n_2^2-1)}{V^{2\alpha_2}}+\frac{(n_3^2-1)}{V^{2\alpha_3}}\right)^2}\\&=\frac{4\lambda^2}{\pi^4\beta^2}\sum_{(n_2,n_3)\neq(1,1)}\frac{1}{((n_1^2-1)+(n_2^2-1)V^{2(\alpha_1-\alpha_2)}+(n_3^2-1)V^{2(\alpha_1-\alpha_2)})^2}.\end{aligned} \tag{3.71}$$

Now the summand in the last sum tends to zero as $V\to\infty$ and it is bounded above by

$$\frac{1}{((n_1^2-1)+(n_2^2-1)+(n_3^2-1))^2}. \tag{3.72}$$

Since

$$\sum_{(n_2,n_3)\neq(1,1)} \frac{1}{((n_1^2-1)+(n_2^2-1)+(n_3^2-1))^2} < \infty, \tag{3.73}$$

$B_V\to 0$ as $V\to\infty$ by the same theorem.

Next we consider the case $\alpha_3<\alpha_2=\alpha_1<1/2$. Now we take

$$A_V = \sum_{(n_1,n_2)\neq(1,1)} \left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \tag{3.74}$$

and

$$B_V = \sum_{n_3\neq 1} \left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{\mathbf{n},V}-\epsilon_{(1,1,1),V})}-1}\right]. \tag{3.75}$$

In this case by definition (3.58),

$$\begin{aligned} A_V &= 2\sum_{n_1\neq 1}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \\ &\quad + \sum_{n_1\neq 1,n_2\neq 1}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \\ &= 2\int_{(0,\infty)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right] F_1^{(1)}(d\eta) \\ &\quad + \int_{(0,\infty)^2}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2)}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2)}-1}\right] F_1^{(2)}(d\eta_1,d\eta_2). \end{aligned} \tag{3.76}$$

By the same argument as above,

$$\lim_{V\to\infty} A_V = 2g_1(\lambda)+g_2(\lambda), \tag{3.77}$$

and

$$\lim_{V\to\infty} B_V = 0. \tag{3.78}$$

Finally, for $\alpha_3=\alpha_2=\alpha_1=1/3$,

$$\begin{aligned} \int_{(-\infty,\infty)} L_V(dx)e^{-\lambda x} &= 3\sum_{n_1\neq 1}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,1,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \\ &\quad + 3\sum_{n_1\neq 1,n_2\neq 1}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta(\epsilon_{(n_1,n_2,1),V}-\epsilon_{(1,1,1),V})}-1}\right] \\ &= 3\int_{(0,\infty)}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right) + \frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}\eta}-1}\right] F_1^{(1)}(d\eta) \end{aligned}$$

$$+3\int_{(0,\infty)^2}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2)}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2)}-1}\right]F_1^{(2)}(d\eta_1,d\eta_2)$$
$$+\int_{(0,\infty)^3}\left[-\ln\left(1+\frac{1-e^{-\lambda V^{-2\alpha_1}}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2+\eta_3)}-1}\right)+\frac{\lambda V^{-2\alpha_1}}{e^{\beta V^{-2\alpha_1}(\eta_1+\eta_2+\eta_3)}-1}\right]$$
$$\times F_1^{(3)}(d\eta_1,d\eta_2,d\eta_3). \tag{3.79}$$

Thus

$$\lim_{V\to\infty}\ln\int_{(-\infty,\infty)}e^{-\lambda x}L_V(dx)=3g_1(\lambda)+3g_2(\lambda)+g_3(\lambda). \tag{3.80}$$

We have therefore proved that

$$\lim_{V\to\infty}\langle\exp\{\lambda V^{\gamma}(N_1/V-(\rho-\rho_c^V))\}\rangle_V^{\mathcal{C}}(\rho)=\begin{cases}\exp(g_1(\lambda)), & \text{if } \alpha_3<\alpha_2<\alpha_1<1/2,\\ \exp(2g_1(\lambda)+g_2(\lambda)), & \text{if } \alpha_3<\alpha_2=\alpha_1<1/2,\\ \exp(3g_1(\lambda)+3g_2(\lambda)+g_3(\lambda)), & \text{if } \alpha_3=\alpha_2=\alpha_1=1/3.\end{cases}$$

To finish the proof we center the distribution about $\langle N_1/V\rangle_V^{\mathcal{C}}(\rho)$. From (3.62) we get

$$\langle\{\lambda V^{\gamma}(N_1/V-(\rho-\rho_c^V))\}^2\rangle_V^{\mathcal{C}}(\rho)=\int_{(-\infty,\alpha_V)}x^2L_V(dx)/K_{1,V}(\rho+1/V)\leqslant 2\int_{(-\infty,\infty)}x^2L_V(dx).$$

Using (3.64) this gives

$$\langle[V^{\gamma}(N_1/V-(\rho-\rho_c^V))]^2\rangle_V^{\mathcal{C}}(\rho)\leqslant V^{1-4\alpha_1}\int_{(-\infty,\infty)}\left\{\frac{1}{2(e^{\beta\eta}-1)}+\frac{1}{(e^{\beta\eta}-1)^2}\right\}F_V(d\eta)$$
$$\leqslant\frac{3V^{1-4\alpha_1}}{2}\int_{(-\infty,\infty)}\frac{1}{\eta^2}F_V(d\eta). \tag{3.81}$$

Thus by the same arguments as we used above for dealing with the expression in (3.64), this second moment is bounded. Since $g_1'(0)=g_2'(0)=g_3'(0)$ we then have

$$\lim_{V\to\infty}V^{\gamma}(\langle N_1/V\rangle_V^{\mathcal{C}}(\rho)-(\rho-\rho_c^V))=\lim_{V\to\infty}\langle V^{\gamma}(N_1/V-(\rho-\rho_c^V))\rangle_V^{\mathcal{C}}(\rho)=0, \tag{3.82}$$

completing the proof. □

IV. CONCLUSION

(a) Since the paper by Buffet and Pulé,[3] it has been known that there are differences in the fluctuations of the PBG condensate in the canonical and grand-canonical ensembles. We have shown that the picture becomes even more complicated if one passes to the case of Casimir boxes where there is already generalized BEC in the GCE.

We have shown in general that there is a kind of *stability principle* relating the two ensembles: condensation in the GCE is more stable than in the CE. In fact we proved (Theorem 3.3) that the absence of the macroscopically occupied single-particle states in GCE implies the same in the CE, whereas the converse is not necessarily true. However in the case of the Casimir boxes considered here the two ensembles exhibit the same types of BEC for the same geometry. What varies in some cases is the fluctuations and the amount of condensate in the individual levels.

(b) As we have mentioned in Sec. I, BEC of *types* I and II is also known in the literature describing the experiments with trapped bosons as "fragmentation" of the condensate.[5,6,13] In these papers the authors relate this phenomenon to the interaction properties of the Bose gas, arguing that it is the exchange interaction that causes bosons with repulsive interaction to condense into a

single one-particle state whereas for attractive interactions the condensate may be "fragmented" into a number of degenerate or nearly degenerate single particle states; see Refs. 11 and 17. Here we have shown that BEC of type II occurs in the *noninteracting* Bose gas and that this is due simply to a geometric anisotropy of the boxes known since Casimir.[4] On the other hand, there are exactly soluble models (in cubic boxes) showing that some truncated repulsive interactions are able to convert BEC in the ground state into a generalized condensation of type III (see Refs. 1 and 8). In Ref. 12 an even simpler repulsive interaction than in Refs. 1 and 8 is proposed that produces type I condensation in a few degenerate single-particle states.

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Evaluation of phase-modulated lattice sums

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An exact evaluation of two-dimensional phase-modulated lattice sums of the form $\Sigma' \exp(i\mathbf{G}\cdot x)|\mathbf{G}|^{-2}$ is presented in terms of the Jacobian theta functions. The result generalizes the identity derived by M. L. Glasser [J. Math. Phys. **15**, 188 (1974)] to allow for evaluation on nonrectangular lattices. The generalized identity is also applied to a problem in vortex dynamics. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777403]

I. INTRODUCTION

A number of problems in mechanics and mathematical physics involve evaluation of two-dimensional phase-modulated lattice sums of the form

$$\Phi = \sum_{\mathbf{G}\neq 0} \frac{e^{i\mathbf{G}\cdot \mathrm{x}}}{|\mathbf{G}|^2}, \tag{1}$$

where $\mathbf{G}$ is a (nonzero) lattice vector. Problems of interest come from various fields, including electrostatics,[1] superconductivity,[2] fluid turbulence,[3] and vortex dynamics.[4] This sum is slowly and conditionally convergent, and numerous formulations have been presented to facilitate its rapid computation.[5]

When the lattice defined by $\mathbf{G}$ is square or rectangular, the evaluation of these sums can be accomplished very elegantly using an identity derived by Glasser.[6] This identity provides an exact representation of the sum in terms of the Jacobian theta functions, which allows for rapid computation and enables mathematical analysis. However, the application of Glasser's identity is somewhat limited by the restriction to square or rectangular lattices, as many physical situations require consideration of a more general lattice structure. For example, a triangular lattice of identical point vortices is more energetically favorable than a square lattice.[7] The analysis presented in Sec. II generalizes the identity derived by Glasser to include all possible two-dimensional lattices that can be generated by two (unique) vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. A brief look at how the generalized identity can be used is shown in Sec. III with an example from vortex dynamics.

II. THE IDENTITY

Consider a general two-dimensional lattice generated by the vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ as shown in Fig. 1. The magnitudes of these vectors are a and b, respectively, and the angle between the vectors is φ. Without any loss of generality, $\mathbf{e}_1$ can be restricted to lie along the x axis and the angle can be restricted to $0<\varphi\leqslant\pi$. Any point in the basic parallelogram spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$ can be represented as $\mathbf{x}=\xi\,\mathbf{e}_1+\eta\mathbf{e}_2$ for $0\leqslant\xi,\eta<1$, where

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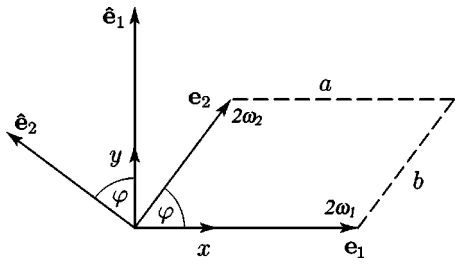

FIG. 1. Lattice vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and reciprocal lattice vectors $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ defining the basic periodic parallelogram with sides of length a and b. In the complex plane the basic parallelogram is defined by the half-periods ω_1 and ω_2.

$$\xi = \frac{x \sin\varphi - y\cos\varphi}{a \sin\varphi} \quad \text{and} \quad \eta = \frac{y}{b \sin\varphi}. \tag{2}$$

The vector $\mathbf{G}$ from Eq. (1) can then be given in terms of the reciprocal lattice vectors $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ as

$$\mathbf{G} = \frac{2\pi}{\Delta}(n\hat{\mathbf{e}}_1 - m\hat{\mathbf{e}}_2), \quad m,n = 0, \pm 1, \pm 2, \ldots, \tag{3}$$

where $\Delta = ab \sin\varphi$ is the area of the basic parallelogram spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$.

The evaluation of phase-modulated lattice sums presented here for general two-dimensional lattices parallels, in large part, the analysis of Glasser.[6] The details of the analysis are included here for completeness.

Rewriting the sum in Eq. (1) using the notation introduced above gives

$$\Phi = \left(\frac{a \sin\varphi}{2\pi}\right)^2 \sum_{(m,n)\neq(0,0)} \frac{\exp[2\pi i(m\xi + n\eta)]}{m^2 + (a/b)^2 n^2 - 2(a/b)mn\cos\varphi}, \tag{4}$$

which can be evaluated by first applying the identity

$$x\int_0^\infty e^{-xt}\mathrm{d}t = 1 \tag{5}$$

and then separating out the term $n=0$ from the double sum to obtain

$$\Phi = \left(\frac{a \sin\varphi}{2\pi}\right)^2 \int_0^\infty \mathrm{d}t \left\{ \sum_{m\neq 0} \exp(-tm^2 + 2\pi i m\xi) + \sum_{\substack{m \\ n\neq 0}} \exp\left[-t\left(\frac{a}{b}\right)^2 n^2 + 2\pi i n\eta\right] \exp\left[-tm^2 + 2\pi i m\left(\xi - itn\frac{a\cos\varphi}{\pi b}\right)\right]\right\}. \tag{6}$$

By Jacobi's imaginary transformation, namely[8,9]

$$\sum_u \exp(-tu^2 + 2\pi i u x) = \sqrt{\frac{\pi}{t}} \sum_u \exp\left[\frac{-\pi^2(x-u)^2}{t}\right], \tag{7}$$

the lattice sum in (6) becomes

$$\Phi = \left(\frac{a\sin\varphi}{2\pi}\right)^2 \left\{ \sum_{m\neq 0} \exp(2\pi i m\xi) \int_0^\infty \mathrm{d}t \, \exp(-tm^2) \right.$$
$$+ \sqrt{\pi} \sum_{\substack{m \\ n\neq 0}} \exp\left[2\pi i\left(n\eta + (\xi - m)\frac{an\cos\varphi}{b}\right)\right]$$
$$\left. \times \int_0^\infty \mathrm{d}t \, \sqrt{t} \exp\left[-t\left(\frac{an\sin\varphi}{b}\right)^2\right] \exp\left[\frac{-\pi^2(\xi-m)^2}{t}\right] \right\}. \tag{8}$$

This form of the lattice sum can be rewritten using the identity[10]

$$\int_0^\infty \mathrm{d}t \, t^{-1/2} e^{-pt} e^{-q/t} = 2\left(\frac{q}{p}\right)^{1/4} \mathrm{K}_{1/2}(2\sqrt{pq}), \tag{9a}$$

where K_s is the modified Bessel function. By the definition of the Basset function[11] this identity becomes

$$\int_0^\infty \mathrm{d}t \, t^{-1/2} e^{-pt} e^{-q/t} = \sqrt{\pi/p} \exp(-2\sqrt{pq}). \tag{9b}$$

Using Eq. (9) and the identity in Eq. (5), the sum Φ can now be written as

$$\Phi = \frac{a^2\sin^2\varphi}{2\pi^2} \sum_{m=1}^\infty \frac{\cos(2\pi m\xi)}{m^2} + \frac{ab\sin\varphi}{4\pi} \sum_{n=1}^\infty \frac{1}{n} \left\{ \exp\left[2\pi n\left((-\sin\varphi + i\cos\varphi)\frac{a}{b}\xi + i\eta\right)\right] + \text{c.c.} \right\}$$
$$+ \frac{ab\sin\varphi}{4\pi} \sum_{m=1}^\infty \sum_{n=1}^\infty \frac{1}{n} \left\{ \exp\left[-2\pi mn\frac{a}{b}(\sin\varphi + i\cos\varphi)\right] \right.$$
$$\times \left\{ \exp\left[2\pi n\left((\sin\varphi + i\cos\varphi)\frac{a}{b}\xi - i\eta\right)\right] \right.$$
$$\left. \left. + \exp\left[2\pi n\left((-\sin\varphi - i\cos\varphi)\frac{a}{b}\xi + i\eta\right)\right] \right\} + \text{c.c.} \right\}, \tag{10}$$

where c.c. denotes the complex conjugate.

At this point in his analysis, Glasser changes variables to[12]

$$q = \exp\left[-\pi\frac{a}{b}(\sin\varphi - i\cos\varphi)\right], \quad \alpha = \eta + \frac{a}{b}(\cos\varphi + i\sin\varphi)\xi. \tag{11}$$

Alternatively, choose

$$q = e^{-\pi i/\tau} \text{ and } \alpha = \frac{ibz}{a\tau}, \tag{12}$$

where $\tau = (b/a)(\cos\varphi + i\sin\varphi)$ and $z = x + iy$. Then, Eq. (10) can be expressed as

$$\Phi = \frac{a^2\sin^2\varphi}{2\pi^2} \sum_{m=1}^\infty \frac{\cos(2\pi m\xi)}{m^2} + \frac{ab\sin\varphi}{4\pi} \sum_{n=1}^\infty \frac{1}{n}[e^{-2\pi n\alpha/b} + \text{c.c.}]$$
$$+ \frac{ab\sin\varphi}{4\pi} \sum_{m=1}^\infty \sum_{n=1}^\infty \frac{1}{n}[q^{2mn}(e^{2\pi n\alpha/b} + e^{-2\pi n\alpha/b}) + \text{c.c.}]. \tag{13}$$

This form of the sum allows the analysis to continue to parallel that of Glasser[6] despite the

alternative change of variables. The sums over n are evaluated with the identity[13]

$$\sum_{n=1}^{\infty} \frac{x^n}{n} = -\ln(1-x), \tag{14}$$

giving

$$\Phi = \frac{a^2 \sin^2 \varphi}{2\pi^2} \sum_{m=1}^{\infty} \frac{\cos(2\pi m\xi)}{m^2} - \frac{ab \sin \varphi}{2\pi} \ln\left|1 - e^{-2\pi\alpha/b}\right| - \frac{ab \sin \varphi}{2\pi} \sum_{m=1}^{\infty} \ln\left|\left(1 - q^{2m} e^{2\pi\alpha/b}\right)\left(1 - q^{2m} e^{-2\pi\alpha/b}\right)\right|. \tag{15}$$

The first term in Eq. (15) is the well-know Fourier series[14]

$$\frac{a^2 \sin^2 \varphi}{2\pi^2} \sum_{m=1}^{\infty} \frac{\cos(2\pi m\xi)}{m^2} = \frac{a^2 \sin^2 \varphi}{2} \left(\xi^2 - \xi + \tfrac{1}{6}\right). \tag{16}$$

After a few manipulations the second term in Eq. (15) can be written as

$$\frac{-ab \sin \varphi}{2\pi} \ln\left|1 - e^{-2\pi\alpha/b}\right| = \frac{a^2 \sin^2 \varphi}{2} \xi - \frac{ab \sin \varphi}{2\pi} [\ln 2 + \ln|\sin(\pi i\alpha/b)|]. \tag{17}$$

The third term in Eq. (15) can be simplified by introducing the Jacobi ϑ_1-function[15]

$$\vartheta_1(z;q) = 2\mathcal{G} q^{1/4} \sin \pi z \prod_{u=1}^{\infty} (1 - 2q^{2u} \cos 2\pi z + q^{4u}), \tag{18a}$$

where[16]

$$\mathcal{G} = \prod_{u=1}^{\infty} (1 - q^{2u}), \quad \vartheta_1'(0;q) = 2\mathcal{G} q^{1/4} \prod_{u=1}^{\infty} (1 - q^{2u})^2, \tag{18b}$$

so that

$$\prod_{u=1}^{\infty} (1 - 2q^{2u} \cos 2\pi z + q^{4u}) = \frac{2^{-2/3} q^{-1/6}}{\sin \pi z} \frac{\vartheta_1(z;q)}{[\vartheta_1'(0;q)]^{1/3}}. \tag{19}$$

Note that the result on the right-hand side of Eq. (19) disagrees with Glasser's result by a factor of 2.[17] Using the identity in Eq. (19), the third term in Eq. (15) can be written as

$$\frac{-ab \sin \varphi}{2\pi} \sum_{m=1}^{\infty} \ln\left|(1 - q^{2m} e^{2\pi\alpha/b})(1 - q^{2m} e^{-2\pi\alpha/b})\right| = \frac{-a^2 \sin^2 \varphi}{12} + \frac{ab \sin \varphi}{2\pi} \left\{ \frac{2 \ln 2}{3} + \ln\left|\sin\left(\frac{\pi i\alpha}{b}\right)\right| - \ln\left|\frac{\vartheta_1(i\alpha/b;q)}{[\vartheta_1'(0;q)]^{1/3}}\right| \right\}. \tag{20}$$

By Jacobi's imaginary transformation[8,9]

$$\vartheta_1(z;q) \equiv \vartheta_1\left(z; -\frac{1}{\tau}\right) = -i \sqrt{\frac{\tau}{i}}\, e^{i\tau z^2/\pi} \vartheta_1(z\tau;\tau), \tag{21a}$$

$$\vartheta_1'(0;q) \equiv \vartheta_1'\left(0;-\frac{1}{\tau}\right) = \left(\frac{\tau}{i}\right)^{3/2}\vartheta_1'(0;\tau), \tag{21b}$$

so that

$$\frac{\vartheta_1(i\alpha/b;q)}{[\vartheta_1'(0;q)]^{1/3}} = -i\exp\left[(\sin\varphi - i\cos\varphi)\frac{\pi\alpha^2}{ab}\right]\frac{\vartheta_1(i\alpha\tau/b;\tau)}{\left[\vartheta_1'(0;\tau)\right]^{1/3}}. \tag{22}$$

Applying Eq. (22) to Eq. (20), the third term in Eq. (15) becomes

$$\begin{aligned}&\frac{-ab\sin\varphi}{2\pi}\sum_{m=1}^{\infty}\ln\left|(1-q^{2m}e^{2\pi\alpha/b})(1-q^{2m}e^{-2\pi\alpha/b})\right| \\ &\quad = \frac{a^2\sin^2\varphi}{2}\left[\left(\frac{b}{a}\right)^2\eta^2 - \xi^2 - \tfrac{1}{6}\right] + \frac{ab\sin\varphi}{2\pi}\left[\frac{2\ln 2}{3} + \ln\left|\sin\left(\frac{\pi i\alpha}{b}\right)\right| - \ln\left|\frac{\vartheta_1(i\alpha\tau/b;\tau)}{[\vartheta_1'(0;\tau)]^{1/3}}\right|\right].\end{aligned} \tag{23}$$

Thus, combining Eqs. (16), (17), and (23) with the notation from Eqs. (2) and (12) gives the result

$$\Phi = \sum_{\mathbf{G}\neq 0}\frac{e^{i\mathbf{G}\cdot\mathbf{x}}}{|\mathbf{G}|^2} = \frac{y^2}{2} - \frac{\Delta}{6\pi}\ln 2 - \frac{\Delta}{2\pi}\ln\left|\frac{\vartheta_1(z/a;\tau)}{[\vartheta_1'(0;\tau)]^{1/3}}\right|. \tag{24}$$

III. AN APPLICATION IN VORTEX DYNAMICS

The generalized identity in Eq. (24) allows for a new, independent derivation of the equations of motion for point vortices arranged in a doubly-periodic lattice. Incidentally, this problem provided the motivation for establishing the generalized result.

Consider a system of N point vortices arranged within the basic parallelogram spanned by the vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. Let vortex α $(=1,2,\ldots,N)$ have strength Γ_α and position $\mathbf{x}_\alpha=(x_\alpha,y_\alpha)$ or $z_\alpha = x_\alpha + iy_\alpha$. The equations of motion for these vortices can be cast in Hamiltonian form[18] by taking

$$\frac{\mathrm{d}x_\alpha}{\mathrm{d}t} = \frac{1}{\Gamma_\alpha}\frac{\mathrm{d}H}{\mathrm{d}y_\alpha}, \quad \Gamma_\alpha\frac{\mathrm{d}y_\alpha}{\mathrm{d}t} = \frac{\mathrm{d}H}{\mathrm{d}x_\alpha}, \tag{25}$$

where x_α are the generalized coordinates and $\Gamma_\alpha y_\alpha$ are the generalized momenta. In a fluid with density ρ, the quantity ρH gives the "interaction energy" of the fluid within the basic parallelogram;[19] that is, it gives the energy of the fluid less the (infinite) contribution to the energy from the fluid in the neighborhood of each point vortex. The Fourier representation of the interaction energy is well known to be[3]

$$E = \frac{\rho}{\Delta}\sum_{\alpha=1}^{N}\sum_{\beta=\alpha+1}^{N}\Gamma_\alpha\Gamma_\beta\sum_{\mathbf{G}\neq 0}\frac{\exp[i\mathbf{G}\cdot(\mathbf{x}_\alpha - \mathbf{x}_\beta)]}{|\mathbf{G}|^2}. \tag{26}$$

By applying Eq. (24) to Eq. (26), the Hamiltonian for this vortex system can be written as

$$\begin{aligned}H &= -\frac{1}{2\pi}\sum_{\alpha=1}^{N}\sum_{\beta=\alpha+1}^{N}\Gamma_\alpha\Gamma_\beta\left\{\ln\left|\frac{\vartheta_1[(z_\alpha - z_\beta)/a;\tau]}{[\vartheta_1'(0;\tau)/2]^{1/3}}\right| - \frac{\pi(y_\alpha - y_\beta)^2}{\Delta}\right\} \\ &= -\frac{1}{2\pi}\sum_{\alpha=1}^{N}\sum_{\beta=\alpha+1}^{N}\Gamma_\alpha\Gamma_\beta\left\{\ln|\sigma(z_\alpha - z_\beta)| - \mathrm{Re}\left[\frac{\eta_1(z_\alpha - z_\beta)^2}{2\omega_1}\right] - \frac{\pi(y_\alpha - y_\beta)^2}{\Delta}\right\} \\ &\quad - \frac{1}{3\pi}\left(\sum_{\alpha=1}^{N}\sum_{\beta=\alpha+1}^{N}\Gamma_\alpha\Gamma_\beta\right)\ln\left|\frac{\vartheta_1'(0;\tau)}{2\omega_1^{3/2}}\right|,\end{aligned} \tag{27}$$

where $\sigma(z;\omega_1,\omega_2)$ is the Weierstrass σ-function defined in terms of the half-periods ω_1 and ω_2 (see Fig. 1), $\eta_1=\zeta(\omega_1;\omega_1,\omega_2)$ is the Weierstrass ζ-function evaluated at the half-period ω_1, and the last term in Eq. (27) is a constant. This Hamiltonian can then be differentiated according to Eq. (25) to give the equations of motion

$$\frac{d\overline{z_\alpha}}{dt}=\frac{1}{2\pi i}\sum_{\beta=1}^{N}{}'\,\Gamma_\beta\left[\zeta(z_\alpha-z_\beta)-\frac{\eta_1}{\omega_1}(z_\alpha-z_\beta)-\frac{2\pi}{\Delta}(y_\alpha-y_\beta)\right], \tag{28}$$

where the overbar denotes complex conjugation and the sum is over all $\beta\neq\alpha$. This result confirms previous derivations[20] that determined the vortex velocities directly in terms of the Weierstrass ζ-function.

It would be interesting to examine the impact of the generalization in Eq. (24) on other results that use Glasser's identity, such as the set of lattice sum identities derived by McPhedran and co-workers.[21,22]

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Reduction of the classical MICZ-Kepler problem to a two-dimensional linear isotropic harmonic oscillator

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The classical MICZ-Kepler problem is shown to be reducible to an isotropic two-dimensional system of linear harmonic oscillators and a conservation law in terms of new variables related to the Ermanno–Bernoulli constants and the components of the Poincaré vector. An algorithmic route to linearization is shown based on Lie symmetry analysis and the reduction method [Nucci, J. Math. Phys. **37**, 1772 (1996)]. First integrals are also obtained by symmetry analysis and the reduction method [Marcelli and Nucci,J. Math. Phys. **44**, 2111 (2002)]. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1781748]

I. INTRODUCTION

The classical MICZ-Kepler problem was introduced and studied by McIntosh and Cizneros[35]—hence the MIC—and independently by Zwanziger[54]—whence the Z. The equation of motion is

$$\ddot{\mathbf{r}} + \frac{\lambda \mathbf{L}}{r^3} + \left(\frac{\mu}{r^2} + \frac{2\nu}{r^3}\right)\hat{\mathbf{r}} = 0, \tag{1}$$

in which $\mathbf{r}$ is the position vector, of magnitude r and unit vector $\hat{\mathbf{r}}$, in $\Re^3$, the overdot denotes differentiation with respect to time, $\mathbf{L}(:=\mathbf{r}\times\dot{\mathbf{r}})$ is the reduced angular momentum, λ, μ, and ν are constants and the three forces are due to a magnetic monopole, the Newtonian gravitational potential and a Newton–Cotes potential, respectively.

In the case of a particle moving in the field of a magnetic monopole, indifferently to the presence or absence of a central force, the angular momentum is not conserved. However, Poincaré,[49] writing on an experiment of Kristian Birkeland, the pioneer investigator of the Aurora Borealis, showed that there does exist a related conserved vector, now known as the Poincaré's vector. In the literature relating to magnetic monopoles Poincaré's vector is termed the *total* angular momentum to distinguish it from the mechanical angular momentum which is called the orbital angular momentum. In this paper we use the notation and terminology to be found in the general literature of Mechanics. If one takes the vector product of $\mathbf{r}$ with (1),

$$0 = \mathbf{r}\times\ddot{\mathbf{r}} + \lambda\frac{\mathbf{r}\times\mathbf{L}}{r^3} = \mathbf{r}\times\ddot{\mathbf{r}} - \lambda\dot{\hat{\mathbf{r}}} \Rightarrow \mathbf{P}: = \mathbf{L} - \lambda\hat{\mathbf{r}}. \tag{2}$$

One notes that both P and L are constants. Specifically they are given by

$$L^2 = r^4(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta) \quad \text{and} \quad P^2 = L^2 + \lambda^2. \tag{3}$$

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In the same spirit as adopted for the calculation of the Laplace–Runge–Lenz vector of the classical Kepler problem[4,5] we take the vector product of (1) with **P** (rather than the **L** as in the case of the Kepler Problem) to obtain

$$\ddot{\mathbf{r}} \times \mathbf{P} + \frac{\lambda}{r^3}\left(\mathbf{L} + \frac{2\nu}{\lambda}\hat{\mathbf{r}}\right) \times \mathbf{P} + \frac{\mu}{r^2}\hat{\mathbf{r}} \times \mathbf{P} = 0. \tag{4}$$

If we restrict 2ν to $-\lambda^2$, (4) becomes

$$\ddot{\mathbf{r}} \times \mathbf{P} + \frac{\lambda}{r^3}\mathbf{P} \times \mathbf{P} + \frac{\mu}{r^2}\hat{\mathbf{r}} \times \mathbf{L} = 0. \tag{5}$$

The middle term of (5) vanishes and the third term reduces to $r^2\dot{\hat{\mathbf{r}}}$ when $\dot{\mathbf{r}}$ is written as $\dot{r}\hat{\mathbf{r}}+r\dot{\hat{\mathbf{r}}}$. We integrate (5) to obtain a conserved vector of Laplace–Runge–Lenz-type, *videlicet*

$$\mathbf{J} = \dot{\mathbf{r}} \times \mathbf{P} - \mu\hat{\mathbf{r}}. \tag{6}$$

This vector can equally be written as

$$\mathbf{J} = \dot{\mathbf{r}} \times \mathbf{L} - \mu\hat{\mathbf{r}} + \frac{\lambda\mathbf{L}}{r}, \tag{7}$$

which emphasizes the add-on effect of the magnetic monopole to the standard form of the Laplace–Runge–Lenz vector.

There is a vast literature devoted to the analysis of (1) and its higher dimensional analogues (see, for example, the original papers of Manton,[33] Gibbons and Manton,[14] Fehér and Horváthy,[12] Gibbons and Ruback,[15] Cordani *et al.*,[6] and Cordani *et al.*,[7] and also those of Iwai and Sunako;[22] Odzijewicz and Świçtochowski;[46] Iwai *et al.*;[23] Pletyulhov and Tolkachov;[47] Pletyulhov and Tolkachov;[48] Lambert and Kibler;[29] Kibler and Winternitz;[26] Mladenov and Tsanov[37]) much of it related to the embedding of the problem in a space of greater dimension in which the nonlinear problem is reduced to an oscillator under constraint. The latter connection in the case of the quantum mechanical problem was reported by Niederer.[39] A more recent extension into the Chern–Simons field theory has been given by Duval *et al.*[9]

In this article we show how (1) (with $2\nu=-\lambda^2$) can be reduced to a two-dimensional linear isotropic oscillator plus a conservation law. The method used is an application of the method of reduction of order developed by Nucci[42] to show how the nonlocal symmetries of the Kepler problem derived by Krause[27,28] could be obtained by local methods. The method has been applied successfully to a variety of problems resembling the Kepler problem, such as the Kepler problem with drag[8,24,30,36] to obtain their nonlocal symmetries and, by accident as it were, to show that these problems are all related by means of generalized transformations.[43,44]

II. LIE SYMMETRIES: FIRST INTEGRALS AND LINEARIZATION

The equation of motion (1) with $2\nu=-\lambda^2$ has the radial, polar, and azimuthal components

$$\ddot{r} - r\dot{\theta}^2 - r\dot{\phi}^2 \sin^2\theta = -\frac{\mu}{r^2} + \frac{\lambda^2}{r^3}, \tag{8a}$$

$$r\ddot{\theta} + 2\dot{r}\dot{\theta} - r\dot{\phi}^2 \sin\theta\cos\theta = \frac{\lambda\dot{\phi}}{r}\sin\theta, \tag{8b}$$

$$(r\ddot{\phi} + 2\dot{r}\dot{\phi})\sin\theta + 2r\dot{\theta}\dot{\phi}\cos\theta = -\frac{\lambda\dot{\theta}}{r}, \tag{8c}$$

respectively.

The Cartesian components of **P** and **J** are

$$P_x = -r^2[\dot{\theta}\sin\phi + \dot{\phi}\sin\theta\cos\theta\cos\phi] - \lambda\sin\theta\cos\phi,$$

$$P_y = r^2[\dot{\theta}\cos\phi - \dot{\phi}\sin\theta\cos\theta\sin\phi] - \lambda\sin\theta\sin\phi, \tag{9}$$

$$P_z = r^2\dot{\phi}\sin^2\theta - \lambda\cos\theta,$$

and

$$J_x = \left(\frac{L^2}{r} - \mu\right)\sin\theta\cos\phi - r^2\dot{r}(\dot{\theta}\cos\theta\cos\phi - \dot{\phi}\sin\theta\sin\phi) - \lambda r(\dot{\theta}\cos\phi - \dot{\phi}\sin\theta\cos\theta\sin\phi),$$

$$J_y = \left(\frac{L^2}{r} - \mu\right)\sin\theta\sin\phi - r^2\dot{r}(\dot{\theta}\cos\theta\sin\phi - \dot{\phi}\sin\theta\cos\phi) - \lambda r(\dot{\theta}\sin\phi - \dot{\phi}\sin\theta\cos\theta\cos\phi), \tag{10}$$

$$J_z = \left(\frac{L^2}{r} - \mu\right)\cos\theta + r^2\dot{r}\dot{\theta}\sin\theta + \lambda r\dot{\phi}\sin^2\theta,$$

respectively.

We examine the system (8) algorithmically in an approach based upon the underlying Lie symmetries of the integrals and equations of motion and hence use the assistance of a suitable symbolic manipulation code. We use the interactive package developed by Nucci.[40,41]

The algorithm is designed to calculate Lie symmetries[42] and first integrals[34] and in the process determining parabolic partial differential equations arise the characteristics of which are "useful variables" and consequently reduce the amount of branching in the algorithm.

A system of first-order equations has an infinite number of Lie point symmetries and the calculation of a subset of them requires the imposition of some constraint on the structure of the symmetries sought. Although there are instances, such as in systems of linear equations,[20,21,45] for which a prescribed structure can be argued to be sensible, such a prescription is not so obvious in the case of systems of nonlinear equations as we have here. The introduction of one or more second-order equations reduces the number of point symmetries and these can then be computed using Lie's algorithm.[42]

We write the system of equations (8), as the set of six first-order equations

$$\dot{w}_1 = w_4, \tag{11a}$$

$$\dot{w}_2 = w_5, \tag{11b}$$

$$\dot{w}_3 = w_6, \tag{11c}$$

$$\dot{w}_4 = w_1 w_5^2 + w_1 w_6^2\sin^2 w_2 - \frac{\mu}{w_1^2} + \frac{\lambda^2}{w_1^3}, \tag{11d}$$

$$\dot{w}_5 = -2\frac{w_4 w_5}{w_1} + w_6^2\sin w_2\cos w_2 + \frac{\lambda w_6}{w_1^2}\sin w_2, \tag{11e}$$

$$\dot{w}_6 = -2\frac{w_4 w_6}{w_1} - 2w_5 w_6 \cot w_2 - \frac{\lambda w_5}{w_1^2 \sin w_2}, \tag{11f}$$

where $w_1 = r$, $w_2 = \theta$, and $w_3 = \phi$. To make the process of the determination of the symmetries of (11) finite we convert the system of six first-order equations to one of four first-order equations plus a second-order equation. We use (11a) to eliminate w_4 and now we have the system

$$\ddot{w}_1 = w_1 w_5^2 + w_1 w_6^2 \sin^2 w_2 - \frac{\mu}{w_1^2} + \frac{\lambda^2}{w_1^3},$$

$$\dot{w}_2 = w_5,$$

$$\dot{w}_3 = w_6,$$

$$\dot{w}_5 = -2\frac{\dot{w}_1 w_5}{w_1} + w_6^2 \sin w_2 \cos w_2 + \frac{\lambda w_6}{w_1^2} \sin w_2,$$

$$\dot{w}_6 = -2\frac{\dot{w}_1 w_6}{w_1} - 2w_5 w_6 \cot w_2 - \frac{\lambda w_5}{w_1^2 \sin w_2}. \tag{12}$$

Note that we have not changed the independent variable which is the standard procedure in the method of reduction of order.[42,43] We are actually trying to find first integrals by using the Lie symmetries in the manner described in Ref. 34. If we apply Lie symmetry analysis to system (13), i.e., we look for a Lie symmetry of the form $\Gamma = V(w_1, w_2, w_3, w_5, w_6, t)\partial_t$, then, as was shown in Ref. 34, the algorithm leads to a parabolic equation in V the characteristics of which, in this case $w_1^2 w_5$ and $w_1^2 w_6$, provide the new set of dependent variables, i.e., u_5 and u_4, respectively. Also, in order to avoid the ill-behavior of the computer algebra system in the presence of trigonometric functions, we introduce the transformation $w_2 = 2\arctan(u_2)$ and thereby render the system of equations in rational form. So we define a new set of dependent variables and list their differential equations, *videlicet*

$$\begin{aligned}
&u_1 = w_1 && \ddot{u}_1 = \frac{\lambda^2(u_2^2+1)^2 - \mu u_1 (u_2^2+1)^2 + 4u_2^2 u_4^2 + u_5^2 (u_2^2+1)^2}{u_1^3 (u_2^2+1)^2},\\
&u_2 = \tan(w_2/2) && \dot{u}_2 = \frac{u_5 (u_2^2+1)}{2u_1^2},\\
&u_3 = w_3 && \dot{u}_3 = u_4 u_1^{-1},\\
&u_4 = w_1^2 w_6 && \dot{u}_4 = \frac{u_5(-\lambda u_2^2 - \lambda + 2u_2^2 u_4 - 2u_4)}{2u_1^2 u_2},\\
&u_5 = w_1^2 w_5 && \dot{u}_5 = \frac{2u_2 u_4 (\lambda u_2^2 + \lambda - u_2^2 u_4 + u_4)}{u_1^2 (u_2^2+1)}.
\end{aligned} \tag{13}$$

If we apply Lie symmetry analysis to system (13), i.e., we again look for a Lie symmetry of the form $\Gamma = V(u_1, u_2, u_3, u_4, u_5, t)\partial_t$, then we obtain the following partial differential equation for V:

$$u_5^2 (u_2^2+1)^3 \frac{\partial V}{\partial u_2} + 2u_2 u_4 (u_2^2+1)^2 \frac{\partial V}{\partial u_3} - u_5((u_2^2+1)\lambda - 2(u_2^2-1)u_4)(u_2^2+1)^2 \frac{\partial V}{\partial u_4} + 4u_2^2 u_4 (\lambda u_2^2 + \lambda - u_2^2 u_4 + u_4)\frac{\partial V}{\partial u_5} = 0 \tag{14}$$

with now $V = V(u_2, u_3, u_4, u_5)$. There are three characteristics to be obtained from (14), each of

which is a first integral.[34] The characteristics are found from the associated Lagrange's system

$$\frac{\mathrm{d}u_2}{u_2u_5(u_2^2+1)^3}=\frac{\mathrm{d}u_3}{2u_2u_4(u_2^2+1)^2}=\frac{\mathrm{d}u_4}{-u_5((u_2^2+1)\lambda-2(u_2^2-1)u_4)(u_2^2+1)^2}$$
$$=\frac{\mathrm{d}u_5}{4u_2^2u_4(\lambda u_2^2+\lambda-u_2^2u_4+u_4)}. \tag{15}$$

We use MAPLE 7 to facilitate the solution of (15). We obtain

$$I_1=\frac{2u_2^2u_4-\lambda u_2^2-\lambda}{2(u_2^2+1)^2}, \tag{16}$$

which evidently comes from the first and third of (15) since u_5 is a common factor of the two denominators,

$$I_2=\frac{u_5^2(u_2^2+1)^4+2\lambda^2u_2^2(u_2^2+1)^2-4\lambda u_2^6u_4+4\lambda u_2^2u_4+4u_2^2u_4^2+4u_2^6u_4^2}{(u_2^2+1)^4} \tag{17}$$

and

$$I_3=u_3+\frac{1}{2}\arctan\left(\frac{u_5^2(u_2^2+1)^3+4u_2^2u_4\lambda(u_2^2+1)-4u_2^4u_4^2+4u_2^2u_4^2}{2u_2u_5(1+u_2^2)(2u_2^2u_4-\lambda u_2^2-\lambda)}\right)$$
$$-\frac{1}{2}\arctan\left(\frac{u_5^2(u_2^2+1)^3-4u_2^2u_4\lambda(u_2^2+1)+4u_2^4u_4^2-4u_2^2u_4^2}{2u_2u_5(\lambda u_2^2+\lambda+2u_4)(1+u_2^2)}\right). \tag{18}$$

It is perhaps of some interest to express the three integrals in terms of the known physical quantities of this problem. After some algebraic simplification we find that

$$I_1=\tfrac{1}{4}(P_z-\lambda),$$

$$I_2=\tfrac{1}{2}(P_x^2+P_y^2+L^2),$$

$$I_3=\frac{1}{2}\arctan\left\{\frac{2P_xP_y}{P_x^2-P_y^2}\right\}. \tag{19}$$

In the case of I_3 we have used the formulas for the addition of arctans to combine the expressions found in (18) which has the nature of a relationship of phases. When we express the three integrals in terms of known physical quantities, as in (19), we see quite clearly the effect of the requirement that a variable be absent from the integral. We recall that the absent variable is $w_4=\dot{r}$. The three integrals are all combinations of components of the Poincaré vector, which are individually conserved, and the magnitude of the angular momentum. (The magnitude of the angular momentum is conserved, but the individual components are not conserved.) These conserved quantities are all free of $\dot{r}$. One also notes that the expressions are not simple. In an arbitrary problem, for which one does not have a preknowledge of the conserved quantities, one can only expect something to be presented as an integral which is not necessarily a "physical" conserved quantity. This means that the algorithm finds first integrals if they exist with the only limitation being the absence of one of the variables, in this case w_4. There is no essential difference in the working of the algorithm if we wish to take one of the other variables absent.

In Ref. 31 we found a transformation which reduced the Kepler Problem to a two-dimensional linear isotropic harmonic oscillator and also found the complete symmetry group of this problem as described by Krause.[27,28] Here we show how to reduce the Kepler problem to a two-dimensional linear isotropic harmonic oscillator using Lie symmetries and the reduction method.

Then we show how to do the same for the MICZ-Kepler problem. Thus the algorithm of Lie point symmetries and the reduction method reveal the physical property underlying the model. As far as we know such a reduction has never been described before.

The Kepler system of equations can be written as the set of six first-order equations,

$$\dot{w}_1 = w_4,$$

$$\dot{w}_2 = w_5,$$

$$\dot{w}_3 = w_6,$$

$$\dot{w}_4 = w_1 w_5^2 + w_1 w_6^2 \sin^2 w_2 - \frac{\mu}{w_1^2},$$

$$\dot{w}_5 = -2\frac{w_4 w_5}{w_1} + w_6^2 \sin w_2 \cos w_2,$$

$$\dot{w}_6 = -2\frac{w_4 w_6}{w_1} - 2 w_5 w_6 \cot w_2, \tag{20}$$

where $w_1 = r$, $w_2 = \theta$, and $w_3 = \phi$. We use the method of reduction of order by choosing $y = w_3$ as the new independent variable to obtain the reduced system

$$w_1' = \frac{w_4}{w_6}, \tag{21a}$$

$$w_2' = \frac{w_5}{w_6}, \tag{21b}$$

$$w_4' = \frac{w_1 w_5^2}{w_6} + w_1 w_6 \sin^2 w_2 - \frac{\mu}{w_1^2 w_6}, \tag{21c}$$

$$w_5' = -2\frac{w_4 w_5}{w_1 w_6} + w_6 \sin w_2 \cos w_2, \tag{21d}$$

$$w_6 = -2\frac{w_4}{w_1} - 2 w_5 \cot w_2. \tag{21e}$$

If we eliminate w_5 from (21b) and search for Lie symmetries we obtain the first integral $\xi = w_6 w_1^2 \sin(w_2)^2$, i.e., the "$z$-component" of the angular momentum, as the characteristic curve of a parabolic determining equation. Finally we convert the system of six first-order equations to two second-order equations, *videlicet*

$$w_4'' = (2\cos(w_2) w_4' w_2' - \sin(w_2)^3 w_4 - \sin(w_2) w_4 w_2'^2)/\sin(w_2),$$

$$w_2'' = (\cos(w_2)(\sin(w_2)^2 + 2 w_2'^2))/\sin(w_2), \tag{22}$$

by eliminating $w_6 = \xi/(\sin^2(w_2) w_1^2)$ from the integral obtained, $w_5 = w_2' \xi/\sin^2(w_2) w_1^2$ from (21b) and $w_1 = \xi^2(w_2'^2 + \sin^2(w_2))/(\sin^2(w_2)(w_4' \xi + \sin^2(w_2)\mu))$ from (21c). Using the interactive REDUCE pro-

grams developed by Nucci[40,41] we obtain a 15-dimensional Lie symmetry algebra, isomorphic to $\mathrm{sl}(4,\mathbb{R})$,[13] generated by the following 15 operators:

$$X_1 = \mathrm{cosec}(w_2)\cos(y)w_4\partial_y + \cos(w_2)\sin(y)\partial_{w_2} - \sin(w_2)\sin(y)w_4^2\partial_{w_4},$$

$$X_2 = \mathrm{cosec}(w_2)\sin(y)w_4\partial_y - \cos(w_2)\cos(y)w_4\partial_{w_2} + \sin(w_2)\cos(y)w_4^2\partial_{w_4},$$

$$X_3 = w_4\sin(w_2)\partial_{w_2} + \cos(w_2)w_4^2\partial_{w_4},$$

$$X_4 = -\cot(w_2)\sin(y)\partial_y + \cos(y)\partial_{w_2},$$

$$X_5 = \cot(w_2)\cos(y)\partial_y + \sin(y)\partial_{w_2},$$

$$X_6 = \cos(w_2)\partial_{w_4},$$

$$X_7 = \sin^2(w_2)\sin(y)\partial_{w_2} + \sin(w_2)\cos(w_2)\sin(y)w_4\partial_{w_4},$$

$$X_8 = \sin^2(w_2)\cos(y)\partial_{w_2} + \sin(w_2)\cos(w_2)\cos(y)w_4\partial_{w_4},$$

$$X_9 = \partial_y,$$

$$X_{10} = \sin(y)\cos(y)\partial_y - \sin(w_2)\cos(w_2)\cos^2(y)\partial_{w_2} + (1-\cos^2(w_2))\cos^2(y)w_4\partial_{w_4},$$

$$X_{11} = \cos^2(y)\partial_y + \sin(w_2)\cos(w_2)\sin(y)\cos(y)\partial_{w_2} - (1-\cos^2(w_2))\sin(y)\cos(y)w_4\partial_{w_4},$$

$$X_{12} = \sin(w_2)\cos(w_2)\partial_{w_2} + \cos^2(w_2)w_4\partial_{w_4},$$

$$X_{13} = w_4\partial_{w_4},$$

$$X_{14} = \sin(w_2)\sin(y)\partial_{w_4},$$

$$X_{15} = \cos(y)\sin(w_2)\partial_{w_4}. \tag{23}$$

In order to find the linearizing transformation we need to find a four-dimensional Abelian subalgebra of rank 2.[50] Following Soh and Mahomed's classification of four-dimensional Lie algebras in the real space,[51] we have to transform this four-dimensional subalgebra into the canonical form

$$\partial_{\tilde{v}_1}, \quad \partial_{\tilde{v}_2}, \quad f(y)\partial_{\tilde{v}_1} + g(y)\partial_{\tilde{v}_2}, \quad h(y)\partial_{\tilde{v}_1} + k(y)\partial_{\tilde{v}_2}, \quad [f'(y)k'(y) \neq g'(y)h'(y)]$$

with $\tilde{v}_1$ and $\tilde{v}_2$ the new dependent variables. We find that one such subalgebra is that generated by X_7, X_8, X_{14}, X_{15} for which we make the mapping $X_{14} \to \partial_{\tilde{v}_1}, X_7 \to \partial_{\tilde{v}_2}, X_{15} \to \cot(y)\partial_{\tilde{v}_1}, X_8 \to -\cot(y)\partial_{\tilde{v}_2}$. Then it is easy to derive that

$$\tilde{v}_1 = \frac{w_4}{\sin(y)\sin(w_2)}, \quad \tilde{v}_2 = \frac{\cot(w_2)}{\sin(y)} \tag{24}$$

and system (22) becomes

$$\tilde{v}_1'' + 2\cot(y)\tilde{v}_1' = 0,$$

$$\tilde{v}_2'' + 2\cot(y)\tilde{v}_2' = 0, \tag{25}$$

which is not the equation of motion of a free particle in two dimensions as was claimed it would be in Ref. 51.

Nevertheless we note that, if we take the y-independent version of transformation (24), i.e.,

$$v_1 = \frac{w_4}{\sin(w_2)}, \quad v_2 = \cot(w_2),$$

then system (22) becomes

$$v_1'' + v_1 = 0,$$

$$v_2'' + v_2 = 0, \tag{26}$$

i.e., the two-dimensional harmonic oscillator.

Now we return to system (11) and mimic the same procedure as used for the Kepler problem by taking $y=w_3$ as the new independent variable. If we again eliminate w_4, then the Lie group analysis yields the substitutions $w_5=u_5/w_1^2$, $w_6=u_4/w_1^2$ from the determining parabolic partial differential equation. Then, after replacing $w_2=2\arctan(u_2)$ for the reason based on the workings of symbolic manipulation in a computer given above, deriving u_4 from I_1, i.e., $u_4=(u_2^2+1)\times(2I_1u_2^2+\lambda+2I_1)/(2u_2^2)$ and eliminating u_5 from the system, i.e., $u_5=-(\lambda u_2^2-\lambda-u_2^2I_1-I_1)u_2'/(2u_2^2)$, we find that the system (11) is reduced to the following three differential equations:

$$u'' = -\frac{(\lambda u^2+\lambda-I_1u^2+I_1)u^2+2(\lambda+I_1)u'^2}{(\lambda u^2-\lambda-I_1u^2-I_1)u}, \tag{27}$$

$$w_1' = -\frac{4u^2w_1^2w_4}{(\lambda u^2-\lambda-I_1u^2-I_1)(u^2+1)}, \tag{28}$$

$$w_4' = -\frac{(u^2+1)^2I_1^2-4\mu u^2w_1+(\lambda u^2+\lambda-2I_1u^2+2I_1)(u^2+1)\lambda}{(\lambda u^2-\lambda-I_1u^2-I_1)(u^2+1)w_1} - \frac{(\lambda u^2-\lambda-I_1u^2-I_1)u'^2}{(u^2+1)u^2w_1}, \tag{29}$$

where prime denotes derivative with respect to y and $u=u_2$. Equation (27) admits an eight-dimensional Lie symmetry algebra of point symmetries and therefore is linearizable by means of a point transformation.[32] The eight symmetries are

$$\Omega_1 = -\cos(y)\frac{u^2}{\lambda+I_1-(\lambda-I_1)u^2}\partial_u,$$

$$\Omega_2 = \sin(y)\frac{u^2}{\lambda+I_1-(\lambda-I_1)u^2}\partial_u,$$

$$\Omega_3 = -\frac{(\lambda u^2+\lambda-I_1u^2+I_1)u}{(\lambda+I_1-(\lambda-I_1)u^2)(\lambda-I_1)}\partial_u,$$

$$\Omega_4 = \partial_y,$$

$$\Omega_5 = \cos(y)\frac{\lambda u^2 + \lambda - I_1 u^2 + I_1}{u}\partial_y + \sin(y)\frac{(\lambda^2 + \lambda I_1 + I_1^2)(u^4+1) - (3u^4-1)\lambda I_1}{\lambda + I_1 - (\lambda - I_1)u^2}\partial_u,$$

$$\Omega_6 = -\sin(y)\frac{\lambda u^2 + \lambda - I_1 u^2 + I_1}{u}\partial_y + \cos(y)\frac{(\lambda^2 + \lambda I_1 + I_1^2)(u^4+1) - (3u^4-1)\lambda I_1}{\lambda + I_1 - (\lambda - I_1)u^2}\partial_u,$$

$$\Omega_7 = \cos(2y)\partial_y + \sin(2y)\frac{(\lambda u^2 + \lambda - I_1 u^2 + I_1)u}{\lambda + I_1 - (\lambda - I_1)u^2}\partial_u,$$

$$\Omega_8 = -\sin(2y)\partial_y + \cos(2y)\frac{(\lambda u^2 + \lambda - I_1 u^2 + I_1)u}{\lambda + I_1 - (\lambda - I_1)u^2}\partial_u. \tag{30}$$

In order to find the linearizing transformation we have to look for a two-dimensional Abelian intransitive subalgebra and, following Lie's classification of two-dimensional algebras in the real plane,[32] we have to transform the subalgebra into the canonical form

$$\partial_{\tilde{u}}, \quad \tilde{y}\partial_{\tilde{u}} \tag{31}$$

with $\tilde{u}$ and $\tilde{y}$ the new dependent and independent variables, respectively. We find that one such subalgebra is that generated by Ω_1 and Ω_2, which yields the following point transformation:

$$\tilde{u} = \frac{\lambda u^2 + \lambda - I_1 u^2 + I_1}{\cos(y)u}, \quad \tilde{y} = -\frac{\sin(y)}{\cos(y)} \tag{32}$$

and Eq. (27) becomes

$$\frac{\mathrm{d}^2\tilde{u}}{\mathrm{d}\tilde{y}^2} = 0. \tag{33}$$

The transformation which takes the free particle equation (33) into a harmonic oscillator, i.e.,

$$\frac{\mathrm{d}^2 x}{\mathrm{d}\tau^2} + x = 0$$

is (see, for example, Whittaker,[53] p. 307)

$$x = \frac{1}{\sqrt{\tilde{u}^2 + \tilde{y}^2}}, \quad \tau = \arctan\left(-\frac{\tilde{u}}{\tilde{y}}\right)$$

and vice versa

$$\tilde{u} = \frac{\sin(\tau)}{x}, \quad \tilde{y} = -\frac{\cos(\tau)}{x}.$$

Therefore we obtain a harmonic oscillator if we make the transformation

$$x = \frac{\cos(y)u}{\sqrt{(\lambda u^2 + \lambda - I_1 u^2 + I_1)^2 + \sin(y)^2 u^2}},$$

$$\tau = \arctan\left(\frac{\lambda u^2 + \lambda - I_1 u^2 + I_1}{\sin(y)u}\right). \tag{34}$$

The reduced system, (27)–(29), is separated into the second-order ordinary differential equation (27) containing the single dependent variable $u(y)$ and the pair of nonlinear first order ordi-

nary differential equations (28) and (29). Given the solution of (27) we may rewrite (28) and (29) as a pair of nonautonomous first-order ordinary differential equations. We eliminate w_4 from (29) using (28) to obtain a nonlinear second-order ordinary differential equation for w_1. The symmetry analysis of this equation shows that it has eight Lie point symmetries. Consequently it is linearizable by means of a point transformation. Thus we have shown how to reduce (21) to a two-dimensional linear isotropic harmonic oscillator plus a conservation law by using Lie symmetries and the reduction method.

III. ALGEBRAIC CONSIDERATIONS

The richness of the Lie algebraic structure of the symmetries suggests the following algebraic approach.

We obtain the Ermanno–Bernoulli constants—so named to give the discoverers[3,11,19] of the Laplace–Runge–Lenz vector at least a footnote in the history of the Kepler problem—as

$$J_{\pm} = J_x \pm iJ_y = \left[\left(\frac{L^2}{r} - \mu \right) \sin\ \theta - r^2 \dot{r} \dot{\theta} \cos\ \theta - \lambda r \dot{\phi} \sin\ \theta \cos\ \theta \pm i(-r^2 \dot{r} \dot{\phi} \sin\ \theta + \lambda r \dot{\theta}) \right] e^{\pm i\phi}, \tag{35}$$

which can be written in the more compact form

$$J_{\pm} = (v_1 \pm iv_1') e^{\pm i\phi}, \tag{36}$$

where

$$v_1 = \left(\frac{L^2}{r} - \mu \right) \sin\ \theta - r^2 \dot{r} \dot{\theta} \cos\ \theta - \lambda r \dot{\phi} \sin\ \theta \cos\ \theta,$$

$$v_1' = -r^2 \dot{r} \dot{\phi} \sin\ \theta + \lambda r \dot{\theta}$$

with the prime denoting differentiation with respect to the azimuthal angle, ϕ. The new variable, v_1, satisfies

$$v_1'' + v_1 = 0. \tag{37}$$

Equation (37), that of a simple harmonic oscillator with independent variable ϕ, replaces the radial equation (8a).

The introduction of the standard integrating factor, $r \sin\ \theta$, makes (8c) exact, *videlicet*

$$\frac{d}{dt}(r^2 \dot{\phi} \sin^2\ \theta - \lambda \cos\ \theta) = 0 \tag{38}$$

and one recognizes that this simply represents the conservation of P_z, the z-component of Poincaré's vector. To maintain a uniformity of notation we define

$$v_3 = r^2 \dot{\phi} \sin^2\ \theta - \lambda \cos\ \theta \tag{39}$$

and replace (8c) with the conservation law

$$v_3' = 0. \tag{40}$$

In a manner analogous to that used to obtain the Ermanno–Bernoulli constants we define

$$P_{\pm} = -[P_x \pm iP_y] = [r^2 \dot{\phi} \sin\ \theta \cos\ \theta + \lambda \sin\ \theta \pm i(-r^2 \dot{\theta})] e^{\pm i\phi} = (v_2 \pm iv_2') e^{\pm i\phi},$$

where

$$v_2 = r^2\dot{\phi}\sin\theta\cos\theta + \lambda\sin\theta \tag{41}$$

satisfies the second order ordinary differential equation for a second simple harmonic oscillator, *videlicet*

$$v_2'' + v_2 = 0. \tag{42}$$

Equally this equation may be obtained directly from the polar and azimuthal equations. One multiplies (8b) and (8c) by r and $r\sin\theta$, respectively, to give

$$\frac{\mathrm{d}}{\mathrm{d}t}(r^2\dot{\theta}) - \dot{\phi}(r^2\dot{\phi}\sin\theta\cos\theta + \lambda\sin\theta) = 0, \tag{43}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(r^2\dot{\phi}\sin\theta\cos\theta + \lambda\sin\theta) + r^2\dot{\theta}\dot{\phi} = 0,$$

and on replacement of time by the new independent variable, ϕ, (43) is just the system of two first order equations equivalent to (42) since

$$v_2 = r^2\dot{\phi}\sin\theta\cos\theta + \lambda\sin\theta,$$

$$v_2' = -r^2\dot{\theta}. \tag{44}$$

Consequently we have reduced the MICZ-Kepler problem, (1) with $2\nu = -\lambda^2$, from the sixth-order nonlinear system (8) to a fifth-order system comprising a linear isotropic harmonic oscillator plus a conservation law, *videlicet*

$$v_1'' + v_1 = 0, \tag{45a}$$

$$v_2'' + v_2 = 0, \tag{45b}$$

$$v_3' = 0, \tag{45c}$$

by virtue of using the conserved vectors **J** and **P**. We note that the reduced system is still autonomous.

The reduced system is a two-dimensional isotropic linear harmonic oscillator plus a conservation law. The system (45) possesses 16 Lie point symmetries comprising 15 for the pair of oscillators and an additional one for the conservation law. (One should note that the first-order ordinary differential equation for the conservation law has an infinite number of Lie point symmetries. However, we are considering a system of three equations and that infinity has to be reduced somewhat in number to be consistent with the two other equations.) They are[16]

$$\Gamma_1 = \partial_\phi, \quad \Gamma_{7\pm} = \mathrm{e}^{\pm i\phi}\partial_{v_1},$$

$$\Gamma_2 = v_1\partial_{v_1}, \quad \Gamma_{8\pm} = \mathrm{e}^{\pm i\phi}\partial_{v_2},$$

$$\Gamma_3 = v_1\partial_{v_2}, \quad \Gamma_{9\pm} = \mathrm{e}^{\pm 2i\phi}[\partial_\phi \pm i(v_1\partial_{v_1} + v_2\partial_{v_2})],$$

$$\Gamma_4 = v_2\partial_{v_1}, \quad \Gamma_{10\pm} = v_1\mathrm{e}^{\pm i\phi}[\pm i\partial_\phi + v_1\partial_{v_1} + v_2\partial_{v_2}],$$

$$\Gamma_5 = v_2\partial_{v_2}, \quad \Gamma_{11\pm} = v_2\mathrm{e}^{\pm i\phi}[\pm i\partial_\phi + v_1\partial_{v_1} + v_2\partial_{v_2}],$$

$$\Gamma_6 = \partial_{v_3}, \tag{46}$$

which is a representation of the algebra $A_1 \oplus \mathrm{sl}(4,R)$ and Γ_6 is the symmetry associated with the conservation law and the contributor of the A_1 part of the algebra given above. The original system (8) (with $2\nu = -\lambda^2$) possesses just the four Lie point symmetries

$$X_1 = \partial_t, \quad X_2 = \partial_\phi, \quad X_{3\pm} = \mathrm{e}^{\pm i\phi}(\pm i \cot\theta \partial_\phi + \partial_\theta), \tag{47}$$

i.e., a representation of $A_1 \oplus \mathrm{so}(3)$. (In the absence of the Newtonian gravitational potential (1) is an instance of a generalized Ermakov system[10] with so(3) imposed[17] which possesses the six-dimensional algebra $\mathrm{sl}(2,R) \oplus \mathrm{so}(3)$—Mladenov[37] prefers $\mathrm{so}(2,1) \oplus \mathrm{so}(3)$—so that the addition of the Kepler potential has the effect of symmetry-breaking. As is evident from the work reported in this note, the symmetry-breaking is at the level of point symmetries.)

From the set of symmetries (46) one can extract the representation of the complete symmetry group of the MICZ-Kepler problem. In general there are several equivalent representations of the complete symmetry group of systems of oscillators.[2] The generic isotropic oscillator in n dimensions is completely specified by the $(2n+1)$-dimensional algebra $A_1 \oplus_s (2n) A_1$, i.e., a representation of the group of the semidirect product of dilations and translations in $(2n)$-dimensional space. However, there are some anomalies.[2] In the case of dimension four there are two distinct complete symmetry groups. In the cases of dimensions two and three the anomalous group has one element fewer than the generic group and so is the sole representative of the complete symmetry group for the isotropic oscillator. Consequently for (45) we select Γ_1, $\Gamma_{9\pm}$ and $\tilde{\Gamma} = \Gamma_3 - \Gamma_4$—the conservation law, (45c), does not require any additional symmetry—with the algebra $\mathrm{sl}(2,R) \oplus \mathrm{so}(2)$,[31] which is the direct sum of $\mathrm{sl}(2,R)$ with the algebra of rotations in two dimensions.

To this set of symmetries one adds ∂_t to obtain a representation of the complete symmetry group of the MICZ-Kepler problem, *videlicet* $A_1 \oplus \mathrm{sl}(2,R) \oplus \mathrm{so}(2)$.

Of some interest is that the reduction of the MICZ-Kepler problem to the system (45) parallels that of the Kepler problem and its variations.[44] In the case of the latter systems a critical feature for the success of this reduction appears to be the possession of a conserved vector of Laplace–Runge–Lenz-type and in the introduction of Ermanno–Bernoulli constants. We have seen how the method of reduction of order leads to the reduction of the system to that of an isotropic two-dimensional oscillator plus a conservation law. In the case of the MICZ-Kepler problem we had such a vector in (7) and we obtained the results presented above. We emphasize that the algorithmic derivation of the reduction to the system of two oscillators plus a conservation law did not require any preknowledge of the physical problem described by the equations for the MICZ-Kepler problem, but was simply a consequence of the general procedure.

The solution of the system (45) is

$$v_1 = J_+ \mathrm{e}^{-i\phi} + J_- \mathrm{e}^{i\phi},$$

$$v_2 = P_+ \mathrm{e}^{-i\phi} + P_- \mathrm{e}^{i\phi},$$

$$v_3 = P_z, \tag{48}$$

in which the constants of integration are expressed in terms of the Ermanno–Bernoulli constants and the corresponding constants for the Poincaré vector.

IV. CONCLUSION

One recalls that the Poisson bracket relation for the monopole is not standard. The Hamiltonian[38] for the equation of motion (1) is

$$H = \frac{1}{2}\left(\mathbf{p}\cdot\mathbf{p} + \frac{\lambda^2}{r^2}\right) - \frac{\mu}{r}, \tag{49}$$

where the momentum is $\mathbf{p}=\dot{\mathbf{r}}$ and the fundamental Poisson Bracket relations are

$$[x_i,x_j]_{\mathrm{PB}} = 0, \quad [x_i,p_j]_{\mathrm{PB}} = \delta_{ij}, \quad [p_i,p_j]_{\mathrm{PB}} = \lambda\epsilon_{ijk}\frac{x_k}{r^3} \tag{50}$$

with $r=|\mathbf{r}|$, $x_ix_i=r^2$ and δ_{ij} and ϵ_{ijk} are Kronecker's delta and epsilon, respectively. The Poisson bracket relations of the components of the conserved vectors, **P** and **J**, are

$$[P_i,P_j]_{\mathrm{PB}} = \epsilon_{ijk}P_k, \quad [P_i,J_j]_{\mathrm{PB}} = \epsilon_{ijk}J_k, \quad [J_i,J_j]_{\mathrm{PB}} = -2H\epsilon_{ijk}P_k, \tag{51}$$

which provides a representation of the algebras so(4), e(3), and so(3,1) depending upon whether H is negative, zero, or positive which is a result well-known in the literature. These are exactly the same algebras as are found for the Kepler problem. We note that the Poisson bracket algebras of the first integrals and the Lie point symmetries of the underlying systems of ordinary differential equations which model the problems have different provenances. The former is based on the symplectic space of the Hamiltonian system and the latter on the invariance of the differential equations of the system under infinitesimal transformation. The Lie point symmetries of the equations of motion differ for the two problems being $A_1 \oplus \mathrm{so}(3)$ for the MICZ-Kepler problem and $A_2 \oplus \mathrm{so}(3)$ for the Kepler problem. However, the algebras become identical in the reduced system since the reduced systems are identical.

In general the Lie point symmetries of the reduced system (45) are nonlocal symmetries for the source system when expressed in terms of the coordinates of the original system. It is a matter of some curiosity that the majority of elements of the complete symmetry group should be represented by nonlocal symmetries, but not an isolated instance. A classic example is the equation (see Ref. 25, Chap. 6, p. 542ff)

$$y'' = \frac{y'^2}{y} + f'(x)y^{p+1} + pf(x)y'y^p, \tag{52}$$

which has no Lie point symmetries for general $f(x)$ and yet is trivially integrable.[52] By means of the nonpoint transformation

$$X = x \quad Y = \log\left\{-py^p \exp\left[-\int pf(x)y^p\mathrm{d}x\right]\right\}, \tag{53}$$

(52) is transformed to the trivial $\mathrm{d}^2Y/\mathrm{d}X^2=0$ for which three point symmetries with the algebra $A_{3,3}$ ($\Leftrightarrow D\oplus_s T_2$) provide the representation of the complete symmetry group. These point symmetries become horribly nonlocal when expressed in terms of the variables of (52).[1]

Since the elements of the complete symmetry algebra are the minimal set of symmetries required to specify completely the system concerned, the importance of nonlocal symmetries is further highlighted. One has the distinct impression that nonlocal symmetries come in two varieties, useful and nonuseful. (This statement is probably true of all symmetries, but one tends to attach a special value to point and contact symmetries.[18]) A possible definition of utility in this instance is that there is some transformation of dependent and independent variables which renders the nonlocal symmetry into the more comfortable point form. The technique of reduction of order[42,43] provides a systematic algorithmic procedure to identify these desirable transformations and thereby provides greater information and the potential for greater understanding of these systems.

In this paper we have approached the question of the possible linearization of the MICZ-Kepler problem on a purely algorithmic basis using a combination of the method of reduction of order and the Lie point symmetry analysis. We have shown that the MICZ-Kepler problem is essentially the same problem has the well-known Kepler problem, the reduction of which we have

also given. In terms of the natural coordinates for the description of each problem the Lie point symmetries of the equations of motion differ in number so that in terms of these coordinates the problems appear to be algebraically different. Nevertheless we have demonstrated their essential oneness in an appropriate coordinate system. The attraction of the algorithmic procedure we have demonstrated here is that there is no necessity to have a deep knowledge of the system being described. In our provision of an alternate derivation of the reduction through manipulation of the equations of motion we highlighted the approach which one can take if one is very familiar with the way these systems possess conserved quantities. Such systems are rare. We do not deny that elegant treatments are possible for certain problems. Rather our concern is for those systems for which these elementary manipulations are not obvious or perhaps even possible and yet which have a very simple structure in a suitable coordinate system. The method which we have presented here is designed for the nonobvious.

Our considerations here have been confined to the three-dimensional MICZ-Kepler problem since it is susceptible to a very transparent treatment. The extension of the application of the method of reduction of order to the higher-dimensional problems of this type of interest in the literature is intended to be the subject of a future report.

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The existence problem for dynamics of dissipative systems in quantum probability

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Motivated by existence problems for dissipative systems arising naturally in lattice models from quantum statistical mechanics, we consider the following C^*-algebraic setting: A given Hermitian dissipative mapping δ is densely defined in a unital C^*-algebra $\mathfrak{A}$. The identity element in $\mathfrak{A}$ is also in the domain of δ. Completely dissipative maps δ are defined by the requirement that the induced maps, $(a_{ij}) \to (\delta(a_{ij}))$, are dissipative on the n-by-n complex matrices over $\mathfrak{A}$ for all n. We establish the existence of different types of maximal extensions of completely dissipative maps. If the enveloping von Neumann algebra of $\mathfrak{A}$ is injective, we show the existence of an extension of δ which is the infinitesimal generator of a quantum dynamical semigroup of completely positive maps in the von Neumann algebra. If δ is a given well-behaved $*$-derivation, then we show that each of the maps $\pm\delta$ is completely dissipative. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777401]

I. INTRODUCTION

Recent applications of the operator-theoretic approach to dissipative quantum systems include Refs. 22 and 37. For a more systematic approach, see Ref. 36. Suppose we are given a one-parameter group of automorphisms $\alpha_t: a \mapsto e^{itH} a e^{-itH}$ which acts on some set of observables a, specified as a dense "local" subalgebra of a completed C^*-algebra. If we then differentiate at $t=0$, we get the derivation $\delta: a \mapsto i[H,a] = i(Ha - aH)$ which takes the form of a formal commutator. The issue is complicated by the fact that the Hamiltonian H is typically an unbounded operator in statistical models, say infinite lattice spin systems. In applications, it is H that is given, and the process must be run in reverse. By analogy to boundary value problems from partial differential equations, we then expect to encounter an existence problem for reconstructing the dynamics of the system from knowing only a formula for H.

We adopt the C^*-W^*-formalism for the dynamics of infinite quantum systems.[10,14,18,20,21,24,31,33] For the special case of quantum spin systems it is believed that the dynamics in the time-reversible case is given by an unbounded derivation of a suitable algebra $\mathfrak{A}$ of observables.[31] Depending on the range of the interaction, and the number of dimensions of the spin lattice, it is possible to exponentiate the infinitesimal derivation to a one-parameter group of automorphisms α_t $(-\infty < t < \infty)$ of $\mathfrak{A}$, or of the enveloping W^*-algebra $\mathfrak{A}''$ (see Ref. 35), or the W^*-algebra generated by a given invariant state.[10,17,26,29,32,33]

It is known that (open) irreversible systems may be obtained as restrictions of time-reversible systems, and it follows[20] that the dynamics of the open system is given mathematically by a semigroup τ_t $(0 \leqslant t < \infty)$ of completely positive mappings of the C^*-algebra $\mathfrak{A}$, or W^*-algebra $\mathfrak{A}''$. The corresponding infinitesimal generator is completely dissipative. Completely positive semigroups also play a role in quantum computing algorithms.[27] The philosophy is that noise in the quantum processes dictates the dissipative systems, as opposed to the conservative ones (which are governed by one-parameter groups of automorphisms).

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But in high lattice dimensions, or for long-range interaction, there are difficulties in exponentiating the infinitesimal generators. The determination of the time evolutions α_t (respectively, τ_t) seems to require "extra boundary conditions."[7,10,26,32,33] It is therefore a meaningful foundational question, for a given completely dissipative infinitesimal transformation δ in a C^*-algebra $\mathfrak{A}$, to ask if it is always possible to extend δ to a transformation $\tilde{\delta}$ which is the infinitesimal generator for a quantum dynamical semigroup. Under the assumption that δ is Hermitian, and that the W^*-algebra $\mathfrak{A}''$ is injective, we establish the existence of a generator extension $\tilde{\delta}$. Our extension is thus an algebraic parallel to Friederichs's extension for semibounded operators in Hilbert space, or an analogue of Phillips's[30] maximal dissipative extension of the general dissipative operator in Hilbert space.

In earlier articles[7,10,28,31] the uniqueness problem was considered for the generator extension, $\delta \subset \tilde{\delta}$. But, just as the case for operators in Hilbert space (Friedrichs, Phillips), the extension is generally not unique, reflecting the possibility of different "boundary conditions" at infinity.

We refer the reader to Refs. 14, 18, and 33, for details on the mathematical foundations of algebraic quantum theory.

The issues centering around the existence problem for the dynamical one-parameter groups, or semigroups, of quantum statistical mechanics are perhaps best known in the setup of *quantum spin systems*, as they are treated in Refs. 9, 25, and 34.

Example I.1: The mathematical framework is rather general such as to allow a wide variety of applications, including recent ones to nonequilibrium statistical mechanics.[34] A countably infinite set L (say a lattice; it may be $\mathbb{Z}^\nu$ where ν is the lattice rank, or dimension) is specified at the outset. Points $s \in L$ are sites at which quantum spins are located. For each $s \in L$, let $\mathcal{H}_s$ be a finite-dimensional complex Hilbert space, i.e., the spin vectors at site s; and for a finite $\Lambda \subset L$, set

$$\mathcal{H}_\Lambda := \bigotimes_{s \in \Lambda} \mathcal{H}_s.$$

Then let $\mathfrak{A}_\Lambda$ be the $*$-algebra of all (bounded) operators on $\mathcal{H}_\Lambda$. With the natural embedding

$$\mathfrak{A}_{\Lambda_1} \subset \mathfrak{A}_{\Lambda_2} \text{ for } \Lambda_1 \subset \Lambda_2$$

given by

$$\mathfrak{A}_{\Lambda_1} \mapsto \mathfrak{A}_{\Lambda_1} \otimes 1_{\Lambda_2 \setminus \Lambda_1} \subset \mathfrak{A}_{\Lambda_2},$$

we get the usual inductive limit C^*-algebra $\lim_\Lambda \mathfrak{A}_\Lambda =: \mathfrak{A}$. A function $\Lambda \mapsto \Phi(\Lambda) = \Phi(\Lambda)^* \in \mathfrak{A}_\Lambda$ defined on the finite subsets Λ of L is called an *interaction*, and

$$H_\Phi(\Lambda) = \sum_{X \subset \Lambda} \Phi(X) \tag{1.1}$$

is the associated local *Hamiltonian*, where in (1.1), the summation is over all finite subsets X of Λ. Since $\mathfrak{A}_{\Lambda_1}$ and $\mathfrak{A}_{\Lambda_2}$ commute when $\Lambda_1 \cap \Lambda_2 = \emptyset$, it follows that

$$\delta(a) = \lim_\Lambda [H(\Lambda), a] \tag{1.2}$$

is well defined for all local observables a in the dense $*$-subalgebra,

$$\mathfrak{A}_0 = \bigcup_{\Lambda \text{ fin}} \mathfrak{A}_\Lambda \text{ in } \mathfrak{A},$$

where $[\cdot, \cdot]$ in (1.2) denotes the usual commutator $[b, a] := ba - ab$. Ruelle proved that, if Φ is translationally invariant, and if, for some $\lambda > 0$,

$$\sum_{n=0}^{\infty} e^{n\lambda} \sup_{s\in L} \sum_{\substack{s\in X \text{ fin} \\ \text{card } X=n+1}} \|\Phi(X)\| < \infty , \tag{1.3}$$

then the $*$-derivation δ defined in (1.2) is the infinitesimal generator of a one-parameter subgroup of $*$-automorphisms $\{\alpha_t\}_{t\in\mathbb{R}} \subset \mathrm{Aut}(\mathfrak{A})$, which then satisfies

$$\alpha_t(a) = \lim_{\Lambda \nearrow L} e^{itH(\Lambda)} a e^{-itH(\Lambda)} \tag{1.4}$$

for all $a\in\mathfrak{A}$ and $t\in\mathbb{R}$, i.e., it is approximately inner. This means that, if $a\in\mathfrak{A}_0$, then

$$\lim_{\substack{t\to 0 \\ t\neq 0}} t^{-1}(\alpha_t(a) - a) = \delta(a). \tag{1.5}$$

Moreover, δ is, when extended from $\mathfrak{A}_0$, a closed $*$-derivation, in the sense that the graph of δ is closed in $\mathfrak{A}\times\mathfrak{A}$. But if Φ is not translationally invariant, or if (1.3) is not known to hold, then no such conclusion is within reach, and the issue of extensions of δ arises. We then ask if some extension $\tilde{\delta}$ of δ to a generator of a one-parameter group of automorphisms, or a semigroup of dissipations (see details below), exists.

II. DEFINITIONS AND TERMINOLOGY

Let X and Y be Banach spaces. Then the space of bounded linear operators from X to Y is denoted $L(X,Y)$. The *conjugate* (i.e., *dual*) Banach space to X is $L(X,\mathbb{C})$, and is denoted X'. If $\mathcal{H}$ is a Hilbert space, the C^*-algebra of all bounded operators on $\mathcal{H}$ is denoted $B(\mathcal{H})$. Let $\mathcal{L}$ be a linear subspace of $B(\mathcal{H})$ which is self-adjoint and contains the identity operator I. With the order inherited from $B(\mathcal{H})$, the subspace $\mathcal{L}$ gets the structure of an *operator system*, in the terminology of Effros.[11] The full matrix algebra M_n of all complex n-by-n matrices is also an operator system, and so is $\mathcal{L}_n = \mathcal{L}\otimes M_n$. The elements in $\mathcal{L}_n$ may be realized as n-by-n matrices with entries from $\mathcal{L}$, $(a_{ij})_{i,j=1}^n$, $a_{ij}\in\mathcal{L}$. If $\mathcal{L}$ and $\mathcal{R}$ are operator systems and $\varphi:\mathcal{L}\to\mathcal{R}$ is a linear mapping, then the induced map $(a_{ij})\to(\varphi(a_{ij}))$ of $\mathcal{L}_n$ into $\mathcal{R}_n$ is denoted φ_n. It is, in fact, $\varphi\otimes \mathrm{id}_n$. We say[2] that φ is *completely positive* (respectively, *completely contractive*) if φ_n is positive (respectively, contractive) for all n. We say that $\mathcal{R}$ is *injective* if for every pair of operator systems, $\mathcal{L}\subset\mathcal{L}_1$, and every completely positive map $\varphi:\mathcal{L}\to\mathcal{R}$, there is a completely positive extension $\psi:\mathcal{L}_1\to\mathcal{R}$. That is, $\psi(x)=\varphi(x)$ for all $x\in\mathcal{L}$. If $\mathcal{R}$ is a von Neumann algebra in a Hilbert space $\mathcal{H}$, it is known[13,38] that $\mathcal{R}$ is injective iff there is a norm-one projection of $B(\mathcal{H})$ onto $\mathcal{R}$.

If $\mathfrak{A}$ is a C^*-algebra, it is known[12] that $\mathfrak{A}$ is nuclear iff the double conjugate (dual) $\mathfrak{A}''$ is injective as a W^*-algebra. Connes showed[13] that a factor $\mathcal{R}$ on a separable Hilbert space is injective iff it is matricial.

III. DISSIPATIVE TRANSFORMATIONS

An operator δ in a Banach space X is said to be dissipative[29] if one of the following three equivalent conditions is satisfied:

(i) For all x in the domain $D(\delta)$ of δ, there is an element $f\in X'$, depending on x, such that $\|f\|=1$, $f(x)=\|x\|$, and $\mathrm{Re}\, f(\delta(x))\leqslant 0$.

(ii) For all x in $\mathcal{D}(\delta)$, and all $f\in X'$ satisfying $\|f\|=1$, and $f(x)=\|x\|$, the inequality $\mathrm{Re}\, f(\delta(x)) \leqslant 0$ is valid.

(iii) For all x in $\mathcal{D}(\delta)$, and all $\alpha\in\mathbb{R}_+$, the inequality $\|x-\alpha\delta(x)\|\geqslant\|x\|$ holds.

The proof of the equivalence can be found, for example, in Ref. 7, but the equivalence can also be shown to be a consequence of the approximation idea in Sec. IX and Proposition X.2 in the present paper.

If X is an operator system, we say that δ is *completely dissipative* if the induced mapping δ_n

in X_n is dissipative for all $n=1,2,\ldots$. Recall that $X_n = X \otimes M_n$, and $\delta_n:(x_{ij}) \to (\delta(x_{ij}))$, with domain $\mathcal{D}(\delta_n)=\{(x_{ij}) \in X_n : x_{ij} \in \mathcal{D}(\delta)\}$.

Finally we say that the transformation δ is *Hermitian* if the domain $\mathcal{D}(\delta)$, in the operator system X, is invariant under the $*$-involution of X, and if $\delta(x^*)=\delta(x)^*$ for all $x \in \mathcal{D}(\delta)$.

If $\delta: X \to Y$ is merely a linear transformation between Banach spaces X and Y, with domain $\mathcal{D}(\delta)$ dense in X, then the transposed (or conjugate) transformation δ' is well defined as a linear transformation $\delta': Y' \to X'$ with domain $\mathcal{D}(\delta')=\{f \in Y' : \exists g \in X'$ s.t. $f(\delta(x))=g(x)$ for all $x \in \mathcal{D}(\delta)\}$. For $f \in \mathcal{D}(\delta')$, $\delta'(f)=g$. The domain $\mathcal{D}(\delta')$ is weak*-dense in Y' iff δ is closable. It is known[29] that dissipative operators are closable.

IV. COMPLETELY POSITIVE SEMIGROUPS (QUANTUM DYNAMICAL SEMIGROUPS)

Let M be a W^*-algebra with predual M_*. Let τ_t be a family of completely positive mappings of M into itself, indexed by the time parameter $t \in [0,\infty)$. Assume that τ_0 is the identity transformation in M, and that $\tau_t(\mathbb{1})=\mathbb{1}$ for all $t \in [0,\infty)$, where $\mathbb{1}$ denotes the unit element of the W^*-algebra M in question. We assume further that the semigroup law holds, $\tau_{t_1+t_2}=\tau_{t_1}\circ\tau_{t_2}$ for $t_1,t_2 \in [0,\infty)$, and finally that each τ_t is a normal mapping in M. Recall that normality is equivalent to the requirement that the conjugate semigroup τ_t' (Ref. 16) of M' leaves invariant the subspace M_*. Finally we require continuity of each scalar function, $t \to \varphi(\tau_t(a))$, for all $\varphi \in M_*$ and $a \in M$. A semigroup which satisfies all the requirements above is called a *completely positive semigroup*. Because of the relevance to quantum dynamics, we shall also call it a quantum dynamical semigroup.[21]

The *infinitesimal generator* of a given completely positive semigroup (τ_t, M) is a, generally unbounded, transformation, denoted by ζ, in M. The domain of the generator ζ is given by

$$\mathcal{D}(\zeta) = \left\{ a \in M : \exists\, b \in M \text{ s.t. for all } t,\ \tau_t(a) - a = \int_0^t \tau_s(b)\mathrm{d}s \right\}.$$

By definition $\zeta(a)=b$. It is easy to see[16] that $\zeta(a)=(\mathrm{d}/\mathrm{d}t)\tau_t(a)|_{t=0}$, where the derivative is taken in the $\sigma(M,M^*)$-topology. Finally note that infinitesimal generators are completely dissipative.

Example IV.1: It is known that the generator δ of a completely positive semigroup $\{\tau_t\}_{t\in\mathbb{R}_+}$ on a C^*-algebra $\mathfrak{A}$ is completely dissipative on a dense subspace $\mathcal{D}$ in $\mathfrak{A}$; see Ref. 4. The following is a "canonical" example of this: it is built on the C^*-algebra over the canonical commutation relations (CCR); see Ref. 8. Specifically, let $\mathcal{H}$ be a complex Hilbert space. Then there is a C^*-algebra $\mathfrak{A}=\mathfrak{A}(\mathcal{H})$ which is generated by the identity element $\mathbb{1}$ and a family of unitary elements $\{u_\xi | \xi \in \mathcal{H}\setminus\{0\}\}$ such that

$$u_\xi u_\eta = e^{(i/2)\mathrm{Im}\langle\xi|\eta\rangle} u_{\xi+\eta}$$

for all $\xi,\eta \in \mathcal{H}$, with the understanding that $u_0=\mathbb{1}$. Then it follows that there is a unique, completely positive semigroup $\{\tau_t\}_{t\in\mathbb{R}_+}$ in $\mathfrak{A}$, such that

$$\tau_t(u_\xi) = e^{-t\|\xi\|_{\mathcal{H}}^2} u_\xi \text{ for } \xi \in \mathcal{H}.$$

Hence the subalgebra $\mathcal{D} \subset \mathfrak{A}$ spanned by the elements $\{u_\xi | \xi \in \mathcal{H}\}$ is contained in the domain of the generator δ, and

$$\delta(u_\xi) = -\|\xi\|_{\mathcal{H}}^2 u_\xi. \tag{4.1}$$

It follows from the observation in Refs. 3 and 5 that this δ is completely dissipative with dense domain $\mathcal{D}$ in the C^*-algebra $\mathfrak{A}$. That is, δ defined by

$$\delta(a) = \lim_{t\to 0_+} t^{-1}(\tau_t(a) - a) \quad \text{(norm limit)}$$

is well defined for $a = u_\xi \in \mathcal{D}$, and (4.1) holds.

We now turn to the general existence problem.

Theorem IV.2: *Let $\mathfrak{A}$ be a C*-algebra with unit $\mathbb{1}$, and let δ be a completely dissipative transformation in $\mathfrak{A}$ with dense domain $\mathcal{D}(\delta)$. Assume $\mathbb{1} \in \mathcal{D}(\delta)$, $\delta(\mathbb{1}) = 0$, and further that δ is Hermitian. Moreover assume that the double conjugate (dual) $\mathfrak{A}''$ is an injective W*-algebra. Then δ has an extension $\tilde{\delta}$ to an ultraweakly densely defined transformation in $\mathfrak{A}''$ which is at the same time the infinitesimal generator of a completely positive semigroup of normal unital transformations in $\mathfrak{A}''$.*

We have divided the proof of Theorem IV.2 into two main sections: one is concerned with the analysis of the family of extensions of the *partial resolvent operator* $(I-\delta)^{-1}$. This analysis leads to a distinguished set of contractive, and maximal, extensions which is associated with a set of extensions $\tilde{\delta}$ of δ. But $\tilde{\delta}$ turns out to be an operator in the enveloping W*-algebra of $\mathfrak{A}$. The generation properties of $\tilde{\delta}$ are analyzed in the second section of the proof, Sec. VI below.

V. EXTENSIONS OF $(I-\delta)^{-1}$

We may assume that δ is in fact a closed operator in $\mathfrak{A}$. (If not, it would be possible to replace δ by the closure $\tilde{\delta}$, and $\tilde{\delta}$ will have the properties which were listed for δ.)

This means that the linear space $\mathcal{S} = \mathrm{Ran}(I-\delta) = \{x - \delta(x) : x \in \mathcal{D}(\delta)\}$ is closed in $\mathfrak{A}$. In view of the (Hermitian) assumption on δ we note that $\mathcal{S}$ is also self-adjoint, and that $\mathbb{1} \in \mathcal{S}$. The operator $R : \mathcal{S} \to \mathfrak{A}$ defined by $x - \delta(x) \to x$, and denoted by $(I-\delta)^{-1}$, is completely positive (Ref. 2, Prop. 1.2.8). Clearly $R(\mathbb{1}) = \mathbb{1}$.

We now consider the double dual to $\mathfrak{A}$, denoted by $\mathfrak{A}''$, as a W*-algebra M, and make the appropriate identification (via the universal *-representation for $\mathfrak{A}$) such that $\mathfrak{A}$ is regarded as a C*-subalgebra of $\mathfrak{A}''$, and the predual of $\mathfrak{A}''$ is identified with the dual $\mathfrak{A}'$ of $\mathfrak{A}$. (The reader is referred to Ref. 35 Sec. 1.17, p. 42 for details.) Since $M = \mathfrak{A}''$ (with the Arens multiplication) is injective as a W*-algebra, by the assumption, it follows that a completely positive extension mapping $E : M \to M$ exists. If we regard $\mathfrak{A}$ as a subalgebra of M (as we shall), then the extension property is given by the identity

$$R(s) = E(s) \quad \text{for all } s \in \mathcal{S}. \tag{5.1}$$

Note that $\mathcal{S} \subset \mathfrak{A}$, so that $\mathcal{S}$ becomes a subspace of M with the above-mentioned identification.

The completely positive transformations of M into itself will be denoted by $CP(M)$, and the space $L(M)$ of completely bounded linear transformations in M gets an ordering arising from the cone $CP(M)$. Indeed, for $F \in L(M)$ we define $E \leqslant F$ by the requirement that $F - E \in CP(M)$. Among all the particular extensions F of R, $F \in L(M)$, such that $E \leqslant F$, we choose by Zorn a maximal element F_0. [For the basic facts on topologies on $CP(M)$ which are needed, the reader is referred to Ref. 2, Chap. 1.]

This extension F_0, described above, has the special property of being 1–1. We first consider the restriction of F_0 to the positive elements in M, M_+, that is. More precisely, we have the implication

$$x \in M_+, \ F_0(x) = 0 \Rightarrow x = 0. \tag{5.2}$$

Let $\eta : M \to M/\mathcal{S}$ be the canonical linear quotient mapping, and consider the cone $\mathcal{C}$ in the normed quotient space $\mathcal{E} = \mathcal{M}/\mathcal{S}$ given by $\mathcal{C} = \eta(M_+)$.

If the element x in (5.2) belongs to $\mathcal{S}$, then the conditions $R(x) = F_0(x) = 0$ imply $x = 0$, since $R = (I-\delta)^{-1}$. Hence, we shall assume that x is not in $\mathcal{S}$. This means that $\eta(x) \in \mathcal{C}$ defines a one-dimensional subspace $\{k\eta(x) : k \in \mathbb{C}\}$ in $\mathcal{E}$, and the functional $f : k\eta(x) \to k$ is nonzero and positive. By Krein's theorem (Ref. 1, Theorem 1, Chap. 3, p. 157) f extends to a positive functional $\tilde{f}$ on $\mathcal{E}$, and we may define

$$F_1(y) = F_0(y) + \tilde{f}(\eta(y))\mathbb{1} \text{ for } y \in M. \tag{5.3}$$

We claim that F_1 is one of the extensions considered in the Zorn process which was described above. But $F_0 \leqslant F_1$, and $F_0 \neq F_1$, contradicting the maximality of F_0—and so, we must have $x = 0$, concluding the proof of (5.2). [Note that in (5.3), instead of the identity element $\mathbb{1}$ on the right-hand side of the equation, we could have used any nonzero element in M_+. The corresponding F_1-transformation would properly majorize F_0, and have its range contained in M, since the range of F_0 falls in M.]

Since F_0 is completely positive, we have, in particular, $F_0(x^*) = F_0(x)^*$. So, to establish the identity $N(F_0) = \{x \in M : F_0(x) = 0\} = 0$, it is enough to show that the Hermitian part of $N(F_0)$ is zero. Since we have already considered positive elements, it only remains to consider $x = x^* \in N(F_0)$ satisfying $x \notin \mathcal{S}$. Choose a positive real number k such that $x_k = x + k\mathbb{1} \in M_+$. We then have $F_0(x_k) = k$ and $x_k \notin \mathcal{S}$. It is possible, therefore, by Krein's theorem, to choose a positive functional $\tilde{f}$ on $\mathcal{E} = M/\mathcal{S}$ satisfying $\tilde{f}(\eta(x_k)) = l > 0$. Then define $F_2(y) = F_0(y) + \tilde{f}(\eta(y))\mathbb{1}$ for $y \in M$. It is a simple matter to check that F_2 is one of the Zorn extensions. Indeed, $F_0 \leqslant F_2$ since $\tilde{f}$ is chosen positive. Finally $F_2(x_k) = F_0(x_k) + l\mathbb{1} > F_0(x_k)$. This contradiction to the maximality of F_0 concludes the proof. Since $N(F_0) = 0$, the inverse F_0^{-1} is defined on $F_0(M) = \{F_0(x) : x \in M\}$.

We proceed to show that $F_0(M)$ is in fact dense in the $\sigma(M, \mathfrak{A}')$-topology of M: First note that the extension property (5.1) for F_0 translates into

$$F_0(x - \delta(x)) = x \text{ for } x \in \mathcal{D}(\delta), \tag{5.4}$$

and the corresponding transposed mappings in $\mathfrak{A}'$ therefore satisfy

$$(I - \delta')F_0' = I \text{ (the identity operator in } \mathfrak{A}'). \tag{5.5}$$

Hence F_0' is 1–1, and the desired density of $F_0(M)$ follows from the bipolar theorem applied to the $\mathfrak{A}' - M$ duality. Note that in fact every extension of R has dense range, because condition (5.5) is satisfied for the most general such extension.

Since F_0 is an extension of $(I - \delta)^{-1}$ it is clear that $\tilde{\delta} = I - F_0^{-1}$ is therefore an extension of δ.

VI. GENERATION PROPERTIES OF $\tilde{\delta}$

The operator $\tilde{\delta}$ is closed and densely defined in the σ-topology of M. But $(I - \tilde{\delta})^{-1} = F_0$, so we also have $\|x - \tilde{\delta}(x)\| \geqslant \|x\|$ for all $x \in \mathcal{D}(\tilde{\delta})$. We proceed to show that in fact

$$\|kx - \tilde{\delta}(x)\| \geqslant k\|x\| \tag{6.1}$$

for all $k > 0$ and $x \in \mathcal{D}(\tilde{\delta})$. Indeed, let Λ denote the set of $k > 0$ such that the inequality (6.1) is satisfied for all $x \in \mathcal{D}(\tilde{\delta})$. Then we have seen that $k = 1$ belongs to Λ. It turns out that Λ is both open and closed as a subset of $\mathbb{R}_+$, and our result follows by connectedness.

To show openness, suppose first that $k_0 \in \Lambda$, and that $k \in \mathbb{R}_+$ satisfies $|k - k_0| < k_0$. We then use (6.1), for k_0, in estimating the terms in the Neumann expansion for $(kI - \tilde{\delta})^{-1}$, taken around the point k_0. Due to the assumption $|k - k_0| < k_0$, the Neumann series is convergent, and does indeed define a bounded inverse $R(k, \tilde{\delta})$ to $kI - \tilde{\delta}$. Termwise estimation gives $\|R(k, \tilde{\delta})\| \leqslant k^{-1}$, and it follows that (6.1) is satisfied in a neighborhood of k_0.

Consider next a convergent sequence of points $k_n \to k_0$ with $k_n \in \Lambda$ and $k_0 \in \mathbb{R}_+$. By assumption the resolvent operators $R(k_n, \tilde{\delta}) = (k_n I - \tilde{\delta})^{-1}$ exist, and they therefore satisfy the resolvent identity

$$R(k_n,\tilde{\delta}) - R(k_m,\tilde{\delta}) = (k_n - k_m)R(k_n,\tilde{\delta})R(k_m,\tilde{\delta}),$$

as well as the estimate $\|R(k_n,\tilde{\delta})\| \leqslant k_n^{-1}$. It follows that the norm-limit $\tilde{R} = \lim_n R(k_n,\tilde{\delta}) \in L(M)$ exists, and it is trivial to check that $\tilde{R}$ defines a bounded inverse to $k_0 I - \tilde{\delta}$. The estimate (6.1) for k_0 is now implied in the limit by $\|\tilde{R}\| \leqslant k_0^{-1}$. Hence Λ is closed, and the argument is completed.

We have shown that the operator $\tilde{\delta}$ in M is dissipative and closed in the $\sigma(M,\mathfrak{A}')$-topology. It is, of course, also closed in the norm topology, and it can be shown that $\mathcal{D}(\tilde{\delta})$ is norm dense. It follows by semigroup theory[23,29] that $\tilde{\delta}$ is the infinitesimal generator of a strongly continuous semigroup τ_t $(0 \leqslant t < \infty)$ of contraction operators in the Banach space M.

To show that each τ_t is a normal transformation we consider the adjoint semigroup τ_t' (cf. Ref. 16) in the norm-dual M' and show that τ_t' leaves $\mathfrak{A}'$ invariant. Note that $\mathfrak{A}'$ is being identified with the predual of the W^*-algebra M, so that we may regard it as a subspace of M'.

Let $\tilde{\delta}'$ (respectively, F_0') denote the transposed operators to $\tilde{\delta}$ (respectively, F_0) with respect to the $M-M'$ duality. It follows by operator theory that $\tilde{\delta}'$ is the generator of τ_t', and that $(I - \tilde{\delta}')^{-1} = F_0'$. From the construction of F_0 we now deduce that $\mathfrak{A}'$ is invariant under F_0'. Indeed, recall that δ' denotes the transposed transformation to δ with respect to the $\mathfrak{A}-\mathfrak{A}'$ duality. By definition $\mathcal{D}(\delta') = \{a' \in \mathfrak{A}' : \exists\, b' \in \mathfrak{A}', \langle b', x\rangle = \langle a', \delta(x)\rangle \text{ for all } x \in \mathcal{D}(\delta)\}$. But for $a' \in \mathfrak{A}'$ and $x \in \mathcal{D}(\delta)$ we have $\langle F_0'(a'), x - \delta(x)\rangle = \langle a', x\rangle$. Hence, $F_0'(a') \in \mathcal{D}(\delta') \subset \mathfrak{A}'$ by (5.5).

An application of the Neumann expansion to $[I - (t/n)\tilde{\delta}']^{-1}$ shows that $\mathfrak{A}'$ is also invariant under this operator for all $t \geqslant 0$, $n \in \mathbb{Z}_+$. But τ_t' is obtained as a weak*-limit of these operators $(n \to \infty)$, and the desired invariance $\tau_t'(\mathfrak{A}') \subset \mathfrak{A}'$ follows.

A final application of the Neumann series, now to the operators $[I - (t/n)\tilde{\delta}]^{-1}$, shows that τ_t is completely positive in M for all $t \geqslant 0$. Indeed $[I - (t/n)\tilde{\delta}]^{-1}$ may be expanded in a norm-convergent power series in the completely positive operator $F_0 = (I - \tilde{\delta})^{-1}$, and $\tau_t = \lim_{n\to\infty}[I - (t/n)\tilde{\delta}]^{-1}$.

VII. THE INEQUALITY $\delta(x^*x) \geqslant \delta(x)^*x + x^*\delta(x)$

It was shown in Ref. 19 that if δ is a bounded Hermitian linear map in a C^*-algebra $\mathfrak{A}$, then the following two conditions are equivalent:

$$e^{t\delta}(x * x) \geqslant e^{t\delta}(x *)e^{t\delta}(x), \quad \forall\, x \in \mathfrak{A},\ t \in \mathbb{R}_+, \tag{7.1}$$

and

$$\delta(x * x) \geqslant \delta(x *)x + x * \delta(x), \quad \forall\, x \in \mathfrak{A}. \tag{7.2}$$

For unbounded $\mathfrak{A}$ the situation is not as well understood. It is therefore of interest to study the connection between the property (7.2) for δ, and the other conditions which are customarily used in the applications of unbounded dissipative mappings in operator algebras to quantum dynamics.

Theorem VII.1: *Let $\mathfrak{A}$ be a C^*-algebra with unit $\mathbb{1}$, and let δ be a completely dissipative transformation in $\mathfrak{A}$ with dense domain $\mathcal{D}(\delta)$. Assume $\mathbb{1} \in \mathcal{D}(\delta)$, and $\delta(\mathbb{1}) = 0$.*

(a) *Let $x \in \mathcal{D}(\delta)$ and assume that $x^*x \in \mathcal{D}(\delta)$. Then*

$$\delta(x * x) \geqslant \delta(x) * x + x * \delta(x). \tag{7.3}$$

(b) *Suppose both x and x^* belong to $\mathcal{D}(\delta)$. Then $\delta(x^*) = \delta(x)^*$.*

The following results are corollaries to the proofs of Theorems IV.2 and VII.1.

Corollary VII.2: Let $\mathfrak{A}$ be a C^*-algebra with unit $\mathbb{1}$, and let δ be completely dissipative in $\mathfrak{A}$ with dense domain $\mathcal{D}(\delta)$, $\mathbb{1} \in \mathcal{D}(\delta)$, $\delta(\mathbb{1}) = 0$.

(a) *If $\mathfrak{A} \subset B(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, then there is a sequence of completely positive maps $E_n : \mathfrak{A} \to B(\mathcal{H})$, $E_n(\mathbb{1}) = \mathbb{1}$, such that the following norm convergence holds:*

(i)

$$E_n(x) \to x \quad \text{for } x \in \mathfrak{A},$$

and

(ii)

$$n(E_n(x) - x) \to \delta(x) \quad \text{for } x \in \mathcal{D}(\delta).$$

(b) *If $\mathcal{D}(\delta)$ is Hermitian, then δ is Hermitian as well, i.e., $\delta(x^*) = \delta(x)^*$ for all $x \in \mathcal{D}(\delta)$, and it is then possible, for each n, to choose E_n* to be 1–1 *with dense range.*

(c) *Let δ and $\mathfrak{A}$ be as in* (a), *and let $\pi: \mathfrak{A} \to B(\mathcal{K})$ be a representation of $\mathfrak{A}$ in a Hilbert space $\mathcal{K}$. Then there exists a sequence $E_n \in CP(\mathfrak{A}, B(\mathcal{K}))$ such that the following norm convergence holds:*

(i′)

$$E_n(x) \to \pi(x) \quad \text{for } x \in \mathfrak{A},$$

and

(ii′)

$$n(E_n(x) - \pi(x)) \to \pi(\delta(x)) \quad \text{for } x \in \mathcal{D}(\delta).$$

Proofs: We consider again the range subspace $\mathcal{S} = \text{Ran}(I - \delta) = \{x - \delta(x) : x \in \mathcal{D}(\delta)\}$. As in the proof of Theorem IV.2 note that $R = (1 - \delta)^{-1} : \mathcal{S} \to \mathfrak{A}$ is completely contractive, and $R(\mathbb{1}) = \mathbb{1}$. If $\mathfrak{A}$ is considered as a subalgebra of $B(\mathcal{H})$, where $\mathcal{H}$ is the Hilbert space of the universal representation, then there is, by Arveson's extension theorem (Ref. 2, Theorem 1.2.9) a completely positive mapping $E: \mathfrak{A} \to B(\mathcal{H})$ such that

$$R(s) = E(s) \quad \text{for all } s \in \mathcal{S}. \tag{7.4}$$

If for each $n = 1, 2, \ldots$ the operator δ is replaced by $n^{-1}\delta$, then the above argument yields a completely positive map $E_n: \mathfrak{A} \to B(\mathcal{H})$ such that E_n is an extension of the partially defined operator $(I - n^{-1}\delta)^{-1}$.

We claim that the sequence (E_n) satisfies conditions (i) and (ii) which are listed in Corollary VII.2(a). Indeed, for x in dense $\mathcal{D}(\delta)$ we have $E_n(x - n^{-1}\delta(x)) = x$, and therefore

$$E_n(x) = n^{-1}E_n(\delta(x)) + x \tag{7.5}$$

and

$$E_n(\delta(x)) = n(E_n(x) - x). \tag{7.6}$$

Passing to the limit in (7.5), we get (i) for the special case $x \in \mathcal{D}(\delta)$, but then also for all x in $\mathfrak{A}$ by a 3-ε argument since each E_n is contractive. The result (ii) of Corollary VII.2(a) is now an immediate consequence of (7.6).

Returning to the proof of Theorem VII.1, we note that (b) is trivial from (ii). Indeed, for x and x^* in $\mathcal{D}(\delta)$ we have

$$\delta(x^*) = \lim n(E_n(x^*) - x^*) = \lim_n (n(E_n(x) - x))^* = \delta(x)^*.$$

The proof of Theorem VII.1(a) is based on both (i) and (ii), together with the Kadison–Schwarz inequality for E_n: Suppose $x \in \mathcal{D}(\delta)$ and $x^*x \in \mathcal{D}(\delta)$. Then $\delta(x^*x) = \lim n(E_n(x^*x) - x^*x)$. For each term on the right-hand side we have

$$n(E_n(x*x)-x*x) \geqslant n(E_n(x)*E_n(x)-x*x)$$
$$= \tfrac{1}{2}((n(E_n(x)-x))*(E_n(x)+x)+(E_n(x)+x)*n(E_n(x)-x))$$
$$\to \tfrac{1}{2}(\delta(x)*(2x)+(2x)*\delta(x)) = \delta(x)*x+x*\delta(x), \tag{7.7}$$

where the last convergence $\to$ is based on (i) and (ii) from Corollary VII.2(a). Since $\delta(x*x)$ is obtained in the limit on the left, the desired inequality (7.3) in (a) of Theorem VII.1 follows.

Only part (b) of the corollary remains. The technique from the proof of Theorem IV.2 is applied here. We go back to the extension E from (7.4) in the beginning of the present proof. Consider the ordering on all the extensions F of R, $F \in L(\mathfrak{A}, B(\mathcal{H}))$, which is induced by the cone $CP(\mathfrak{A}, B(\mathcal{H}))$, and choose by Zorn a particular extension F, $E \leqslant F$, which is maximal. The argument from the proof of Theorem IV.2 then shows that F is 1–1, and the range $\mathrm{Ran}(F)$ is dense. It follows that the operator $\tilde{\delta} = I - F^{-1}: \mathrm{Ran}(F) \to \mathfrak{A}$ exists and satisfies $\tilde{\delta}(x) = \delta(x)$ for all $x \in \mathcal{D}(\delta)$.

If α is a positive real number, then the same construction may be carried out for the transformation $\alpha\delta$, instead of δ. Hence we get completely positive unital maps F_α such that the inverse F_α^{-1} exists for each α, and the domain of $I - F_\alpha^{-1}$ contains $\mathcal{D}(\delta)$. Moreover $\tilde{\delta}_\alpha = I - F_\alpha^{-1}$ satisfies $\tilde{\delta}_\alpha(x) = \delta(x)$ for $x \in \mathcal{D}(\delta)$. To get a sequence of mappings satisfying the conditions in Corollary VII.2(b), we need only take $E_n = F_{n^{-1}}$ in the special case $\alpha = n^{-1}$.

The proof of part (c) in the corollary is parallel to (a) with the following modification: Arveson's extension theorem is now applied to the mapping $\pi \circ (I - \delta)^{-1}: \mathcal{S} \to B(\mathcal{K})$. □

VIII. THE IMPLEMENTATION PROBLEM

The conclusion (ii′) in Corollary VII.2(c) is of interest when one wants to implement the transformation δ by a dissipative operator in Hilbert space. In particular, one is interested in implementing a completely dissipative δ-operator by a dissipative Hilbert-space operator. We shall establish a clear two-way connection between the dissipative notion for δ, and for the implementing Hilbert-space operator.

Theorem VIII.1: *Let $\mathfrak{A}$ be a C*-algebra with unit $\mathbb{1}$, and let δ be a completely dissipative transformation in $\mathfrak{A}$ with dense domain $\mathcal{D}(\delta)$. Assume $\mathbb{1} \in \mathcal{D}(\delta)$ and $\delta(\mathbb{1}) = 0$. Let ω be a state of $\mathfrak{A}$, and let $(\pi_\omega, \mathcal{K}_\omega, \Omega)$ be the corresponding GNS representation of $\mathfrak{A}$. Let $\tilde{\omega}$ be the vector state on $B(\mathcal{K}_\omega)$ given by the cyclic vector Ω, i.e., $\tilde{\omega}(X) = \langle X\Omega | \Omega \rangle$ for $X \in B(\mathcal{K}_\omega)$, and assume that it is possible to choose the sequence $(E_n) \subset CP(\mathfrak{A}, B(\mathcal{K}_\omega))$ from Corollary VII.2(c) in such a manner that*

$$\tilde{\omega}(E_n(x)) = \omega(x) \quad \textit{for all } x \in \mathfrak{A}. \tag{8.1}$$

Then there is a dissipative operator L_ω in $\mathcal{K}_\omega$ such that

$$\pi_\omega(\delta(x))\Omega = L_\omega(\pi_\omega(x)\Omega) \quad \textit{for all } x \in \mathcal{D}(\delta). \tag{8.2}$$

Proof: Let $\pi = \pi_\omega$, $\mathcal{K} = \mathcal{K}_\omega$, and let $(E_n) \subset CP(\mathfrak{A}, B(\mathcal{K}))$ be a sequence which, along with the conditions listed in Corollary VII.2(c), also fulfills the invariance restriction (8.1) of the present theorem. For each n define an operator C_n in $\mathcal{K}$ as follows:

$$C_n(\pi(x)\Omega) = E_n(x)\Omega, \quad x \in \mathfrak{A}.$$

Then

$$\|C_n\pi(x)\Omega\|^2 = \|E_n(x)\Omega\|^2$$
$$= \tilde{\omega}(E_n(x)*E_n(x)) \leqslant \tilde{\omega}(E_n(x*x)) = \omega(x*x) = \langle \pi(x*x)\Omega | \Omega \rangle = \|\pi(x)\Omega\|^2,$$

where the norm is that of $\mathcal{K}$, and where the Schwarz inequality is applied to E_n. It follows that C_n is well defined, and that it extends by limits (in $\mathcal{K}$) to a contraction operator, $C_n \in B(\mathcal{K})$, $\|C_n\| \leqslant 1$.

By Corollary VII.2(c) (ii′), we then have

$$\pi(\delta(x))\Omega = \lim n(E_n(x)\Omega - \pi(x)\Omega)$$
$$= \lim n(C_n(\pi(x)\Omega) - \pi(x)\Omega) = \lim n(C_n - I)\pi(x)\Omega \quad \text{for } x \in \mathcal{D}(\delta).$$

As a consequence, the following quadratic form on $\mathcal{K}$:

$$\pi(x)\Omega, \pi(y)\Omega \to \lim\langle n(C_n - I)\pi(x)\Omega | \pi(y)\Omega\rangle_{\mathcal{K}}$$

is well defined. Using the contractive property of C_n, it is easy to show that this quadratic form is given by a dissipative operator L; that is to say

$$\lim\langle n(C_n - I)\pi(x)\Omega | \pi(y)\Omega\rangle = \langle L\pi(x)\Omega | \pi(y)\Omega\rangle.$$

Since the limit on the left-hand side is also equal to the inner product

$$\langle \pi(\delta(x))\Omega | \pi(y)\Omega\rangle,$$

the identity (8.2) of the theorem follows. □

IX. A CONDITION FOR COMPLETE DISSIPATIVENESS

In applications[18,24,33] it is often possible to determine the derivation δ in a particular representation. If moreover the derivation is known to be implemented by a dissipative operator in the corresponding Hilbert space, then it follows in special cases that δ itself is completely dissipative.

Theorem IX.1: *Let $\mathfrak{A}$ be a C*-algebra with unit $\mathbb{1}$ and let δ be a densely defined transformation in $\mathfrak{A}$ such that $\mathbb{1} \in \mathcal{D}(\delta)$ and $\delta(\mathbb{1}) = 0$. Let ω be a state on $\mathfrak{A}$ such that δ is implemented by a dissipative Hilbert-space operator L in the representation π_ω. Assume moreover that π_ω is faithful, and that $L\Omega = 0$ where Ω denotes the cyclic vector in the GNS representation. Then δ is completely dissipative on its domain.*

Proof: Let $\mathcal{H} = \mathcal{H}_\omega$ be the Hilbert space of the faithful representation π_ω and let L be the operator in $\mathcal{H}$ which is assumed to exist, satisfying conditions (i) and (ii) below:

(i) The domain of L is $\pi_\omega(\mathcal{D}(\delta))\Omega$, and L is a dissipative operator in the Hilbert space $\mathcal{H}$;
(ii) L implements δ in the representation π_ω, which is equivalent to the requirement that L^* is defined on $\pi_\omega(\mathcal{D}(\delta))\Omega$, and that on this domain the following operator identiy is valid:

$$\pi(\delta(a)) = L\pi(a) + \pi(a)L^* \quad \text{for all } a \in \mathcal{D}(\delta). \tag{9.1}$$

We show first that δ must necessarily be a dissipative operator. Indeed, by Phillips's theorem (Ref. 30, Theorem 1.1.3) an extension $\tilde{L}$ of L exists which is the infinitesimal generator of a strongly continuous semigroup $S(t)$ of contraction operators in the Hilbert space $\mathcal{H}$. We note that $S(t)$ implements a semigroup $\sigma(t)$ of positive mappings in $B(\mathcal{H})$, given by

$$\sigma(t)(A) = S(t)AS(t)^* \tag{9.2}$$

for all $t \in [0, \infty)$ and $A \in B(\mathcal{H})$. By semigroup theory we note that the generator (ζ say) of $\sigma(t)$ is dissipative, so the following estimate holds:

$$\|A - \alpha\zeta(A)\| \geqslant \|A\| \tag{9.3}$$

for all $\alpha \in [0, \infty)$ and $A \in \mathcal{D}(\zeta)$.

If δ_ω denotes the operator $\pi_\omega(a) \to \pi_\omega(\delta(a))$ with domain $\pi_\omega(\mathcal{D}(\delta))$, then we claim (easy proof) that

$$\delta_\omega(A) = \zeta(A) \quad \text{for all } A \in \mathcal{D}(\delta_\omega), \tag{9.4}$$

and the known estimate (9.3) above then implies

$$\|\pi_\omega(a) - \alpha\pi_\omega(\delta(a))\| \geqslant \|\pi_\omega(a)\| \tag{9.5}$$

for $a \in \mathcal{D}(\delta)$ and $\alpha \in [0,\infty)$. But π_ω is faithful (and hence isometric), so (9.5) is in fact equivalent to the dissipation estimate

$$\|a - \alpha\delta(a)\| \geqslant \|a\|$$

for the operator δ itself.

For each $n=1,2,\ldots$, we now consider the tensor-product construction of the C^*-algebra $\mathfrak{A}$ with the n-by-n complex matrices M_n; and we define $\mathfrak{A}_n=\mathfrak{A}\otimes M_n$, $\delta_n=\delta\otimes \mathrm{id}_n$, the operator obtained by application of δ to each entry a_{ij} in the matrix representation of elements in $\mathfrak{A}_n$, $\omega_n=\omega\otimes \mathrm{tr}_n$ where tr_n denotes the normalized trace on M_n, π_{ω_n}: the GNS representation of $\mathfrak{A}_n$ associated to ω_n.

The problem is to show that each of the operators δ_n is dissipative. We show that in fact δ_n is implemented by a dissipative Hilbert-space operator in the representation π_{ω_n}. Hence, the first part of the proof applies and yields the conclusion of the claim since each representation π_{ω_n} is faithful, being the tensor product of faithful representations.

Let $\mathcal{H}_n$ denote the representation Hilbert space of π_{ω_n}. We proceed to find a dissipative operator L_n in $\mathcal{H}_n$ such that δ_n is implemented by L_n. In view of (9.1) this means that

$$\pi_{\omega_n}(\delta_n(a)) = L_n\pi_{\omega_n}(a) + \pi_{\omega_n}(a)L_n^*$$

for all $a \in \mathcal{D}(\delta_n)=\mathcal{D}(\delta_n)\otimes M_n$ (algebraic tensor product) $\subset\mathfrak{A}_n$ as an operator identity on $\pi_{\omega_n}(\mathcal{D}(\delta_n))\Omega_n \subset \mathcal{H}_n$. Here Ω_n denotes the cyclic vector for the representation π_{ω_n}, i.e.,

$$\omega_n(a) = \langle \pi_{\omega_n}(a)\Omega_n|\Omega_n\rangle \text{ for all } a \in \mathfrak{A}_n. \tag{9.6}$$

Our next step is the verification of the following:

$$\mathrm{Re}\ \omega_n(a^*\delta_n(a)) \leqslant 0 \text{ for all } a \in \mathcal{D}(\delta_n), \tag{9.7}$$

$$L_n\Omega_n = 0, \tag{9.8}$$

$$\omega_n(a^*\delta_n(a)) = \langle L_n\pi_{\omega_n}(a)\Omega_n|\pi_{\omega_n}(a)\Omega_n\rangle \text{ for } a \in \mathcal{D}(\delta_n). \tag{9.9}$$

It will follow from (9.7) and (9.9) that an implementing operator L_n satisfying (9.8) must necessarily be dissipative.

Note that (9.8) is verified for $n=1$ by assumption. Hence $\omega(a^*\delta(a))=\langle\pi(\delta(a))\Omega|\pi(a)\Omega\rangle = \langle L\pi(a)\Omega+\pi(a)L^*\Omega|\pi(a\Omega)\rangle$. Substitution of $L^*\Omega=-L\Omega=0$ into this identity yields identity (9.9) for the case $n=1$.

Let T_n denote the trace vector for the trace representative τ_n of M_n. Then $\pi_{\omega_n}=\pi\otimes\tau_n$, and therefore

$$\begin{aligned}\langle \pi_{\omega_n}(a\otimes b)\Omega\otimes T_n|\Omega\otimes T_n\rangle &= \langle \pi(a)\Omega\otimes\tau_n(b)T_n|\Omega\otimes T_n\rangle \\ &= \langle\pi(a)\Omega|\Omega\rangle\langle\tau_n(b)T_n|T_n\rangle = \omega(a)\mathrm{tr}_n(b) = \omega\otimes\mathrm{tr}_n(a\otimes b) = \omega_n(a\otimes b)\end{aligned}$$

for all $a\in\mathfrak{A}$ and $b\in M_n$. Hence $\Omega_n=\Omega\otimes T_n$. If we can show that a simple tensor operator L_n implements δ_n in π_{ω_n}, then identity (9.9), for arbitrary n, follows from the case $n=1$ which was established above.

However, it is easy to see that the operator $L_n=L\otimes I_n$ satisfies the requirements which were listed above. Indeed

$$\begin{aligned}\pi_{\omega_n}(\delta_n(a\otimes b)) &= \pi_\omega(\delta(a))\otimes\tau_n(b)\\ &= (L\pi_\omega(a)+\pi_\omega(a)L^*)\otimes\tau_n(b)\\ &= L_n\pi_\omega(a)\otimes\tau_n(b)+\pi_\omega(a)\otimes\tau_n(b)L_n^* = L_n\pi_{\omega_n}(a\otimes b)+\pi_{\omega_n}(a\otimes b)L_n^*\end{aligned}$$

for all $a\in\mathfrak{A}$ and $b\in M_n$. It follows that L_n implements δ_n in π_{ω_n}.

Only the verification of (9.7) for $n>1$ then remains. Let $a_{ij}\in\mathfrak{A}$ be the matrix entries in some $a\in\mathfrak{A}_n=\mathfrak{A}\otimes M_n$. Then the (i,j)th entry c_{ij} in $a^*\delta_n(a)$ is $\Sigma_{k=1}^n a_{ki}^*\delta(a_{kj})$. Hence

$$\omega_n(a^*\delta_n(a)) = (\omega\otimes\mathrm{tr}_n)(c_{ij}) = \sum_{i=1}^n \omega(c_{ii}) = \sum_i\sum_k \omega(a_{ki}^*\delta(a_{ki})).$$

Since $\mathrm{Re}\,\omega(a_{ki}^*\delta(a_{ki}))\leqslant 0$, (9.7) follows. □

Remark IX.2: In the foundations of irreversible statistical thermodynamics,[14,20,21,24,28] the most conclusive results have been obtained for dynamical semigroups which are described mathematically as strongly continuous, completely positive, contraction semigroups T_t on the Banach space $\mathcal{T}(\mathcal{H})$ of all trace-class operators on a given separable ∞-dimensional Hilbert space $\mathcal{H}$. Lindblad[28] found a formula for the infinitesimal generator

$$W = \left.\frac{\mathrm{d}}{\mathrm{d}t}T_t\right|_{t=0}$$

in the case of norm-continuous semigroups, and Davies[15] extended the results to strongly continuous T_t (i.e., unbounded generator W), satisfying certain side conditions. The condition of relevance to our paper is the invariance assumption of Ref. 15 that

$$T_t'(\mathcal{C}(\mathcal{H}))\subset\mathcal{C}(\mathcal{H})$$

for all $t\in[0,\infty)$, where $\mathcal{C}(\mathcal{H})$ denotes the compact operators, and T_t' the conjugate semigroup on $B(\mathcal{H})$. Our Theorem IV.2 does not apply to the algebra $\mathfrak{A}=B(\mathcal{H})$ since $B(\mathcal{H})''$ is known not to be injective.[11] [Of course, $B(\mathcal{H})$ is injective by Arveson's theorem.]

However, Theorem IV.2 combined with the above results suggests that a W^*-algebra, properly smaller than $B(\mathcal{H})$, is suitable for quantum dynamics. On the one hand, $B(\mathcal{H})$ [or $\mathcal{T}(\mathcal{H})$ in the conjugate (dual) formulation] is too big to accommodate the extensions; and, on the other hand, the requirement that $\mathcal{C}(\mathcal{H})$ contain the domain of the generator also appears to be too restrictive.

X. UNBOUNDED *-DERIVATIONS

Let $\mathfrak{A}$ be a unital C^*-algebra, and let $\mathcal{D}(\delta)$ be a dense $*$-subalgebra containing the identity $\mathbb{1}$. A linear transformation $\delta:\mathcal{D}(\delta)\to\mathfrak{A}$ is said to be a (unbounded) *-derivation if $\delta(ab)=\delta(a)b+a\delta(b)$ for $a,b\in\mathcal{D}(\delta)$, and $\delta(a^*)=\delta(a)^*$ for $a\in\mathcal{D}(\delta)$.

Since, for $*$-derivations, one is primarily interested in extensions which are also $*$-derivations, it is natural to work with a two-sided condition in place of the dissipative notions which were studied in the preceding sections for more general operators. The following such two-sided condition was suggested by Sakai,[36] and adopted by several authors in subsequent research on unbounded $*$-derivations.

Definition X.1: A $*$-derivation $\delta:\mathcal{D}(\delta)\to\mathfrak{A}$ is said to be well behaved if for all positive $a\in\mathcal{D}(\delta)$ there is a state ϕ on $\mathfrak{A}$ such that $\phi(a)=\|a\|$ and $\phi(\delta(a))=0$.

The argument in the preceding section yields the following.

Proposition X.2: Let $\delta:\mathcal{D}(\delta)\to\mathfrak{A}$ be a $*$-derivation. Then the following four conditions are equivalent:

(i) *δ is well behaved.*

(ii) *For all positive $a\in\mathcal{D}(\delta)$, and for all states ϕ on $\mathfrak{A}$ satisfying $\phi(a)=\|a\|$, we have $\phi(\delta(a))=0$.*

(iii) *Each of the operators* $\pm\delta$ *is dissipative.*
(iv) $\|a+\alpha\delta(a)\| \geqslant \|a\|$ *for all* $\alpha \in \mathbb{R}$ *and all* $a \in \mathcal{D}(\delta)$.

Definition X.3: A $*$-derivation $\delta: \mathcal{D}(\delta) \to \mathfrak{A}$ is said to be well behaved in the *matricial sense* if, for each $n=1,2,\ldots$, the $*$-derivation $\delta_n = \delta \otimes \mathrm{id}_n : \mathcal{D}(\delta) \otimes M_n \to \mathfrak{A} \otimes M_n$ is well behaved. Recall that δ_n may be regarded as a transformation on n-by-n matrices with entries in $\mathfrak{A}$. For such a matrix $a=(a_{ij})$, $i, j=1,\ldots,n$, we have $\delta_n(a)=(\delta(a_{ij}))$.

Theorem X.4: *Every well-behaved *-derivation is also well behaved in the matricial sense (i.e., completely well behaved).*

Lemma X.5: Let $\delta: \mathcal{D}(\delta) \to \mathfrak{A}$ *be a well-behaved *-derivation, and let* $a \in \mathcal{D}(\delta)$ *be positive. Then there is a state* ϕ *on* $\mathfrak{A}$ *such that* $\phi(a)=\|a\|$, *and* $\phi(\delta(b))=0$ *for a dense set of elements* $b \in C^*(a) \cap \mathcal{D}(\delta)$. [*Here* $C^*(a)$ *denotes the Abelian C*-subalgebra generated by a; and every element in* $C^*(a)$ *can be approximated in norm by a sequence of elements b satisfying the conclusion of the lemma.*]

Proofs: The implication (i)$\Rightarrow$(ii) in Proposition X.2 is the key to the proof of Lemma X.5. Since functional calculus is also applied, we shall assume in fact that δ is closed. By a result of Kishimoto–Sakai[36] this is no loss of generality. Let a be a positive element in $\mathcal{D}(\delta)$. Note that the Gelfand transform sets up an isomorphism between the C^*-algebras $C^*(a)$ and $C(\mathrm{sp}(a))$, continuous functions on the spectrum of a. Let $\lambda_0 = \mathrm{l.u.b.sp}(a)$. Then the state $c \to c(\lambda_0)$ on $C(\mathrm{sp}(a))$ corresponds to a state on $C^*(a)$ via the Gelfand transform. The latter state is then extended to $\mathfrak{A}$ by Krein's theorem, and the extended state is denoted by ϕ. It has the multiplicative property: $\phi(b_1 b_2)=\phi(b_1)\phi(b_2)$ for $b_1, b_2 \in C^*(a)$.

Now let g be a nondecreasing (monotone) continuous real function defined on $\mathrm{sp}(a)$. Then the Gelfand transform of $g(a)$ achieves its maximum at the point λ_0 since the transform of a does. But it is known that if g is also of class C^2 (two continuous derivatives) then $g(a) \in \mathcal{D}(\delta) \cap C^*(a)$. Hence $\phi(g(a))=\|g(a)\|$. An application of Proposition X.2, (i)$\Rightarrow$(ii), then yields the conclusion

$$\phi(\delta(g(a))) = 0.$$

The restriction of an arbitrary monomial λ^n to $\mathrm{sp}(a)$ satisfies the conditions listed for g. Hence, by Stone–Weierstrass there is a dense set of elements $b \in C^*(a) \cap \mathcal{D}(\delta)$ satisfying the conclusion of the lemma. [Alternatively, every positive function f in C^4 may be written in the form $f=g_1-g_2$, with g_1 and g_2 both having the properties listed above for g, we conclude that $\phi(\delta(f(a))) = \phi(\delta(g_1(a))) - \phi(\delta(g_2(a))) = 0$.]

Now, for each fixed element $a \in \mathcal{D}(\delta)_+$ we choose a state $\phi=\phi_a$ and a dense $*$-subalgebra $\mathfrak{B}=\mathfrak{B}_a$ of $C^*(a)$ according to Lemma X.5; i.e., we require that $\phi_a(\delta(b))=0$ for $b \in \mathfrak{B}_a$, as well as $\phi_a(a)=\|a\|$. Consider the GNS representation of the algebra $\mathfrak{B}$, respectively, $\mathfrak{A}$, with representation space $\mathcal{H}_\phi$, respectively, $\mathcal{K}_\phi$, and define

$$\mathcal{H} = \sum\nolimits^{\otimes} \mathcal{H}_\phi, \text{ respectively, } \mathcal{K} = \sum\nolimits^{\otimes} \mathcal{K}_\phi. \tag{10.1}$$

Then $\mathcal{H}$ is a closed subspace of the Hilbert space $\mathcal{K}$, and we can then define an operator S with dense domain from $\mathcal{H}$ to $\mathcal{K}$ as follows:

$$S\pi_\phi(b)\Omega_\phi = \pi_\phi(\delta(b))\Omega_\phi \text{ for } b \in \mathfrak{B}_\phi. \tag{10.2}$$

For vectors ξ_1 and ξ_2 in the domain of S we have

$$\langle S\xi_1 | \xi_2 \rangle + \langle \xi_1 | S\xi_2 \rangle = 0. \tag{10.3}$$

The verification of (10.3) may be based on the direct-sum decomposition (10.1) above. If $\xi_i = \Sigma_\phi^{\otimes} \pi(b_i)\Omega_\phi$ for $i=1, 2$ and $b_i \in \mathfrak{B}_\phi$, then identity (10.3) reduces to

$$\sum \langle \pi_\phi(\delta(b_1))\Omega_\phi | \pi_\phi(b_2)\Omega_\phi \rangle + \sum \langle \pi_\phi(b_1)\Omega_\phi | \pi_\phi(\delta(b_2))\Omega_\phi \rangle = 0.$$

The individual terms work out to be

$$\phi(b_2^*\delta(b_1)) + \phi(\delta(b_2)^* b_1) = \phi(\delta(b_2^* b_1)) = 0.$$

Hence, the symmetry condition (10.3) is hereby reduced to the conclusion of Lemma X.5 for a given well-behaved derivation δ.

If P denotes the orthogonal projection in $\mathcal{K}$ with range $\mathcal{H}$, identity (10.3) implies that the operator $\xi \to PS\xi$ may in fact be regarded as a skew symmetric operator in the Hilbert space $\mathcal{H}$, with dense domain there. We shall also denote this operator by S. The verification of the identity

$$\pi(\delta(b)) = S\pi(b) - \pi(b)S$$

is left to the reader.

Following the idea of Sec. IX, we now consider the *-derivations $\delta_n = \delta \otimes \mathrm{id}_n$ (for each $n = 1, 2, \ldots$) introduced in Definition X.3. For a given *-algebra $\mathfrak{C}$ we denote by $\mathfrak{C}_n$ the *-algebra $\mathfrak{C} \otimes M_n$. Correspondingly, *-algebras $\mathcal{D}(\delta)_n$, $\mathfrak{A}_n$, and $\mathfrak{B}_n$ are defined for each n. Application of the GNS representation to each $\phi_n = \phi \otimes \mathrm{tr}_n$ yields sequences of Hilbert spaces

$$\mathcal{H}^{(n)} \subset \mathcal{K}^{(n)}$$

as in (10.1) with each $\mathcal{H}^{(n)}$, respectively, $\mathcal{K}^{(n)}$, a direct sum of GNS representation spaces associated to ϕ_n.

The calculations in Sec. IX show that the operator $S_n = S \otimes I_n$ satisfies the nth-order version of (10.2), that is, (10.2) holds with the quadruple S, π, $\mathfrak{B}$, δ replaced by S_n, π_n, $\mathfrak{B}_n$, δ_n. Similarly $\langle S_n \xi_1^{(n)} | \xi_2^{(n)} \rangle + \langle \xi_1^{(n)} | S_n \xi_2^{(n)} \rangle = 0$ for vectors $\xi_i^{(n)}$, $i = 1, 2$, in the respective domains.

Hence Theorem IX.1 in Sec. IX implies that each of the operators $\pm\delta_n$ for $n = 1, 2, \ldots$ is dissipative. By Proposition X.2, (iii) $\Rightarrow$ (i), it follows that δ_n is well behaved, concluding the proof of Theorem X.4. □

As an application of the theorem we get the following existence result for generator extensions of well-behaved $*$-derivations $\delta: \mathcal{D}(\delta) \to \mathfrak{A}$ in *nuclear* C^*-algebras $\mathfrak{A}$. Indeed, if δ is such a $*$-derivation, each of the operators $\pm\delta$ is completely dissipative. Hence, by Theorem IV.2, there are extensions $\widetilde{\delta}_\pm \supset \pm\delta$ to infinitesimal generators of dynamical semigroups $a_t^{(\pm)}$ in the enveloping W^*-algebra $\mathfrak{A}''$.

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Extremal covariant quantum operations and positive operator valued measures

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We consider the convex sets of QO's (quantum operations) and POVM's (positive operator valued measures) which are covariant under a general finite-dimensional unitary representation of a group. We derive necessary and sufficient conditions for extremality, and give general bounds for ranks of the extremal POVM's and QO's. Results are illustrated on the basis of simple examples. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777813]

I. INTRODUCTION

The need for miniaturization and the new quantum information technology[1] has recently motivated a search for new quantum devices with maximum control at the quantum level. Among the many problems posed by the new technology there is the need of engineering quantum devices which perform specific measurements[2–5] or particular state transformations—the so-called *quantum operations*[6–8]—which are optimized with respect to some given criterion. In most cases such optimal quantum measurements/operations are *covariant*[9] with respect to a group of physical transformations. For the case of a quantum measurement, "group-covariant" means that there is an action of the group on the probability space which maps events into events, in such a way that when the quantum system is transformed according to a group transformation, the probability of the given event becomes the probability of the transformed event. This situation is very natural, and occurs in most practical applications. (See Refs. 10 and 11.) For example, the heterodyne measurement[12,13] is covariant under the group of displacements of the complex field, which means that if we displace the state of radiation by an additional complex averaged field, then the output photocurrent will be displaced by the same complex quantity.

In quantum mechanics the probabilities for a given apparatus for all possible states are described by positive operator valued measures (POVM),[3] and we will say that the measurement is covariant when its POVM is covariant under a unitary group representation.[2,10] For quantum operations (QO), on the other hand, covariance means that the output of a group-transformed input state is simply the transformed output state—a situation again quite common in practice. Typically covariance means that the apparatus is required to work equally well on a full set of states which is invariant under a group of transformations. For instance, if one wants to engineer an eavesdropping apparatus for a BB84 cryptographic scheme[14,15] that clones equally well all equatorial qubits, then the optimal cloning operation must be covariant under the group $\mathbf{G}=\mathbb{Z}_4$ of $\pi/2$ rotations of the Bloch sphere around its polar axis, which is a subgroup of the group of all axial rotations $\mathbf{G}=\mathbb{U}(1)$.[16] Similarly, if one wants to engineer a QO which works equally well on all pure states, then the operation must be covariant under the full $\mathbb{SU}(d)$ group, where d is the dimension of the Hilbert space of the quantum system.

It is easy to see that all POVM's covariant under some group representation make a convex set, which describes the complete class of possible covariant apparatuses. The same obviously

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holds for group-covariant QO's. Typically in most applications the optimization resorts to minimize a concave function on the convex set of covariant machines (in quantum estimation theory[3] actually such function is generally linear), whence the optimal machine will correspond to an extremal element of the convex set. For such purpose it is convenient to classify all extremal covariant POVM's and QO's, and this is precisely the subject of the present paper.

For finite dimensional Hilbert space, a characterization of all noncovariant extremal QO's was given in Ref. 17, whereas a characterization of all extremal POVM's can be found in Refs. 18 and 19 for discrete finite probability space. On the other hand, no classification of the extremal QO's or POVM's is available yet under a covariance constraint, since, as we will see, this constraint makes the classification problem much harder. Coincidentally, in many applications the optimal QO/POVM is restricted to be rank-one from the special form of the optimization function (this is the case, for example, of optimal phase estimation for pure states,[2,3,20] or of phase covariant optimal cloning of pure states[16]), and this has lead to a widespread belief that optimality is synonym of rank-one. However, as we will see in this paper, for sufficiently large dimension the extremal QO's/POVM's can easily have rank larger than one: this can actually happen for optimization with mixed input states, such as in the case of optimal phase estimation with phase-coherent mixed states.[21]

In this paper we provide a classification for finite dimensions of all extremal POVM's and QO's that are covariant under a general unitary group representation. We will generally consider continuous Lie groups, since then all results will also apply to the case of discrete groups as well, with just a little change of notation. We provide necessary and sufficient conditions for extremality, along with simple necessary conditions, which allow to "sieve" the extremal QO's/POVM's. From these conditions general bounds for the rank of the extremal QO's/POVM's easily follow as corollaries.

The paper is organized as follows. In Sec. II we briefly review the concept of POVM and that of covariant POVM based on the Holevo's theorem.[2] In Sec. III we recall the necessary concepts about QO's, including their operator form introduced in Ref. 22, which allows to easily classify the covariant QO's as non-negative operators in the commutant of a suitable representation of the group. Section IV is entirely devoted to some technical lemmas which will be used in the classification of both POVM's and QO's. Finally Secs. V and VI contains the classification theorem of extremal group covariant POVM's and QO's, respectively, with some simple explicit examples, in particular with application to phase-covariant estimation and phase-covariant optimal cloning.

II. POSITIVE OPERATOR VALUED MEASURES

In the following we will denote by $\boldsymbol{B}(\mathcal{K},\mathcal{H})$ the linear space of bounded operators from the Hilbert space $\mathcal{K}$ to the Hilbert space $\mathcal{H}$, and by $\boldsymbol{B}(\mathcal{H}) \doteq \boldsymbol{B}(\mathcal{H},\mathcal{H})$ the algebra of bounded operators on $\mathcal{H}$. By $\boldsymbol{T}_1(\mathcal{H})$ we will denote the trace-class operators on $\mathcal{H}$, and by $\boldsymbol{T}_1^+(\mathcal{H})$ its positive elements.

A general measurement is described by a probability space $\mathfrak{X}$ equipped with a sigma-algebra structure $\sigma(\mathfrak{X})$ of measurable subsets $B \in \sigma(\mathfrak{X})$. The measurement returns a random outcome $x \in \mathfrak{X}$. In quantum mechanics the probability that the outcome belongs to a subset $B \in \sigma(\mathfrak{X})$ depends on the state $\rho \in \boldsymbol{T}_1^+(\mathcal{H})$ of the system in a way which is distinctive of the measuring apparatus according to the Born rule

$$p(B) = \mathrm{Tr}[P(B)\rho], \tag{1}$$

where P is a function on $\sigma(\mathfrak{X})$ which is positive-operator valued in $\boldsymbol{B}(\mathcal{H})$, with the normalization condition

$$P(\mathfrak{X}) = I_{\mathcal{H}}. \tag{2}$$

Positivity of P is needed for positivity of probabilities for every state ρ, whereas Eq. (2) guarantees normalization of probabilities. In synthesis, P is a positive operator valued measure (POVM) on the probability space $\mathfrak{X}$. In a sense the POVM P represents our knowledge of the measuring

apparatus from which we can infer information on the state ρ from probabilities. The linearity of the Born rule (1) in both arguments ρ and P is consistent with the intrinsically statistical nature of the measurement, in which our partial knowledge of both the system and the apparatus reflects in convex structures for both states and POVM's. This means that not only states, but also POVM's can be "mixed," namely there are POVM's that give probability distributions that are equivalent to choose randomly among different apparatuses.

Group covariant POVM's: Let us consider now the general scenario in which a group of physical transformations $\mathbf{G}$ can act on the probability space $\mathcal{X}$. We will write gx for the action of the group element $g \in \mathbf{G}$ on the point $x \in \mathcal{X}$, and gB for the action of g on a whole subset $B \subseteq \mathcal{X}$. We will always consider the case in which $\mathbf{G}$ acts transitively on $\mathcal{X}$, namely for any two points on $\mathcal{X}$ there is always a group element which connects them. A consequence of transitivity is that $\mathcal{X}$ can be always regarded as the homogeneous factor space $\mathcal{X} = \mathbf{G}/\mathbf{G}_x$, $\mathbf{G}_x$ denoting the stability group of any point $x \in \mathcal{X}$.

A POVM P on $\mathcal{H}$ for the probability space $\mathcal{X}$ is covariant under the unitary representation $g \to U_g$ of the group $\mathbf{G}$ when for every set $B \in \sigma(\mathcal{X})$ one has

$$U_g^\dagger P(B) U_g = P(g^{-1}B). \tag{3}$$

The following general theorem by Holevo[2] classifies all group-covariant POVM's.

Theorem 1 (Holevo): *For square-integrable representations, a POVM P on the probability space $\mathcal{X}$ is covariant with respect to the unitary representation $g \to U_g$ on $\mathcal{H}$ of the group $\mathbf{G}$ of transformations of $\mathcal{X}$ if and only if it admits a density of the form*

$$\mathrm{d}P_x = U_{g_x}^\dagger \Xi U_{g_x} \mathrm{d}x, \quad g_x \in \mathbf{G} : g_x x_0 = x, \tag{4}$$

where $\mathrm{d}x$ *is an invariant measure on* $\mathcal{X}$, *with* $\Xi \geqslant 0$ *in the commutant* $\mathbf{G}'_{x_0}$ *of the isotropy group* $\mathbf{G}_{x_0}$ *of* x_0, *satisfying the constraint*

$$\int_{\mathbf{G}} \mathrm{d}g \; U_g^\dagger \Xi U_g = I_{\mathcal{H}}, \tag{5}$$

with $\mathrm{d}g$ *invariant measure on* $\mathbf{G}$.

In the case in which the POVM is designed to estimate the group element itself $g \in \mathbf{G}$ corresponding to an unknown transformation U_g, then the stability group is the identity, whence $\mathcal{X} = \mathbf{G}$ and the POVM P is covariant if and only if it admits a density of the form

$$\mathrm{d}P_g = U_g^\dagger \Xi U_g \, \mathrm{d}g, \quad g \in \mathbf{G} \tag{6}$$

for any $\Xi \geqslant 0$ satisfying the constraint (5). The possible *seed* operators $\Xi \geqslant 0$ satisfying the constraint (5) form a convex set. In Sec. V we will classify all extremal elements Ξ of such convex set.

III. QUANTUM OPERATIONS

The mathematical structure that describes the most general state change in quantum mechanics—such as the evolution of an open system or the state change due to a measurement—is the *quantum operation* (QO) of Kraus.[1,6] Such abstract theoretical evolution has a precise physical counterpart in its implementations as a unitary interaction between the system undergoing the QO and a part of the apparatus—the so-called *ancilla*—which after the interaction is read by means of a conventional quantum measurement. We can consider generally different input and output Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, respectively, allowing the treatment of very general quantum machines, e.g., of the kind of quantum optimal cloners.[22,23] For example, in the cloning from one to n copies one has input space $\mathcal{H}$ and output space $\mathcal{K} = \mathcal{H}^{\otimes n}$, or its symmetric version $\mathcal{K} = (\mathcal{H}^{\otimes n})_+$ for symmetric cloning. Within the present paper we will only consider finite-dimensional Hilbert spaces. In the Heisenberg picture the QO evolves observables, and will be denoted by a map $\mathcal{M}$ from $\boldsymbol{B}(\mathcal{K})$ to

$\boldsymbol{B}(\mathcal{H})$. In the Schrödinger picture the QO evolves states, and it is given by the dual map $\mathcal{M}^\tau: \boldsymbol{T}_1(\mathcal{H}) \to \boldsymbol{T}_1(\mathcal{K})$, the dualism being determined by the equivalence of the two pictures in terms of the trace inner product, namely $\mathrm{Tr}[\mathcal{M}(X)\rho] = \mathrm{Tr}[\mathcal{M}^\tau(\rho)X]$ for all $\rho \in \boldsymbol{T}_1(\mathcal{H})$ and for all $X \in \boldsymbol{B}(\mathcal{K})$. The maps $\mathcal{M}$ and $\mathcal{M}^\tau$ are linear *completely positive* (CP), namely they preserve positivity of the input operator for any trivial extension $\mathcal{M} \otimes \mathcal{I}$ on a larger Hilbert space that includes any possible additional quantum system, $\mathcal{I}$ denoting the identity map on the additional system. In the Schrödinger picture the CP property physically means that the map $\mathcal{M}^\tau$ from $\boldsymbol{T}_1(\mathcal{H})$ to $\boldsymbol{T}_1(\mathcal{K})$ preserves positivity of any input state of the quantum system (with Hilbert space $\mathcal{H}$) entangled with any possible additional quantum system. The map $\mathcal{M}^\tau$ of a QO must also be trace-not-increasing, with the trace $\mathrm{Tr}[\mathcal{M}^\tau(\rho)] \leqslant 1$ representing the probability that the transformation occurs, and the input and output states being connected as follows:

$$\rho \mapsto \rho' = \frac{\mathcal{M}^\tau(\rho)}{\mathrm{Tr}[\mathcal{M}^\tau(\rho)]}. \tag{7}$$

By denoting with $I_\mathcal{H}$ the identity operator on the Hilbert space $\mathcal{H}$, we see that the trace-not-increasing condition along with positivity of the map are equivalent to the constraint

$$\mathcal{M}(I_\mathcal{K}) = K \in \boldsymbol{B}(\mathcal{H}), \quad 0 \leqslant K \leqslant I_\mathcal{H}. \tag{8}$$

For finite-dimensional Hilbert spaces it is convenient to represent the maps $\mathcal{M}$ from $\boldsymbol{B}(\mathcal{K})$ to $\boldsymbol{B}(\mathcal{H})$ as operators $R_\mathcal{M}$ on $\mathcal{K} \otimes \mathcal{H}$ using the following one-to-one correspondence:

$$R_\mathcal{M} = \mathcal{M}^\tau \otimes \mathcal{I}(|I\rangle\langle I|), \quad \mathcal{M}^\tau(\rho) = \mathrm{Tr}_\mathcal{H}[(I_\mathcal{K} \otimes \rho^\tau)R_\mathcal{M}], \tag{9}$$

where $|I\rangle = \Sigma_n |n\rangle \otimes |n\rangle$ is a fixed vector in $\mathcal{H} \otimes \mathcal{H}$, $\{|n\rangle \otimes |m\rangle\}$ denotes an orthonormal basis for $\mathcal{H} \otimes \mathcal{H}$, and the transposition τ for operators is defined with respect to the orthonormal basis $|n\rangle\langle m|$ for $\boldsymbol{B}(\mathcal{H})$ taken as real. One can easily check the correspondence (9), and injectivity follows from linearity. In addition, the operator $R_\mathcal{M}$ is non-negative if and only if the map $\mathcal{M}$ is CP, and the constraint (8) in terms of the operator K rewrites as follows:

$$\mathrm{Tr}_\mathcal{K}[R_\mathcal{M}] = K, \quad 0 \leqslant K \leqslant I_\mathcal{H}. \tag{10}$$

The positive operators $R_\mathcal{M}$ satisfying the constraint (10) make a convex set, which is the operator counterpart of the convex set of the corresponding QO's $\mathcal{M}$.

Group covariant CP-maps: We call the map $\mathcal{M}$ from $\boldsymbol{B}(\mathcal{K})$ to $\boldsymbol{B}(\mathcal{H})$ **G**-covariant, when

$$\mathcal{M}(V_g^\dagger X V_g) = U_g^\dagger \mathcal{M}(X) U_g, \quad \forall\, g \in \mathbf{G}, \tag{11}$$

$\{U_g\}$ and $\{V_g\}$ denoting unitary representations of **G** over the input and output spaces $\mathcal{H}$ and $\mathcal{K}$, respectively. The Schrödinger picture version of identity (11) is

$$\mathcal{M}^\tau(U_g \rho U_g^\dagger) = V_g \mathcal{M}^\tau(\rho) V_g^\dagger, \quad \forall\, g \in \mathbf{G}, \tag{12}$$

where $\mathcal{M}^\tau$ goes from $\boldsymbol{T}_1(\mathcal{H})$ to $\boldsymbol{T}_1(\mathcal{K})$.

The operator form $R_\mathcal{M}$ for maps $\mathcal{M}$ simplifies the classification of QO's that are covariant under a group **G**, resorting to the Wedderburn's decomposition of the commutant of the representation. It is easy to show that the map $\mathcal{M}$ is **G**-covariant [i.e., it satisfies Eq. (11)] if and only if its corresponding operator $R_\mathcal{M}$ is invariant under the representation $V_g \otimes U_g^*$.[22] In fact, from Eq. (9) using invariance of partial trace under cyclic permutation of operators acting only on the traced space one has

$$0 = \mathcal{M}^\tau(\rho) - V_g^\dagger \mathcal{M}^\tau(U_g \rho U_g^\dagger) V_g = \mathrm{Tr}_\mathcal{H}\{(I_\mathcal{K} \otimes \rho^\tau)[R_\mathcal{M} - (V_g^\dagger \otimes U_g{}^\tau) R_\mathcal{M} (V_g \otimes U_g^*)]\}, \tag{13}$$

and, since Eq. (9) is a one-to-one correspondence between maps and operators, one concludes that

$$[R_{\mathcal{M}}, V_g \otimes U_g^*] = 0, \quad \forall\, g \in \mathbf{G}. \tag{14}$$

Therefore, the problem of classifying covariant CP-maps resorts to that of classifying positive elements of the commutant of the representation $V_g \otimes U_g^*$ on $\mathcal{K} \otimes \mathcal{H}$. By labeling with k the generic equivalence class of the representation, with multiplicity m_k, the Wedderburn's decomposition of the representation space is written as follows:[24]

$$\mathcal{K} \otimes \mathcal{H} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k}). \tag{15}$$

Then, since $R_{\mathcal{M}}$ must be a positive operator in the commutant of the representation it must have the general form

$$R_{\mathcal{M}} = \oplus_k (I_{\mathcal{H}_k} \otimes w_k^\dagger w_k) = W^\dagger W, \quad W \doteq \oplus_k (I_{\mathcal{H}_k} \otimes w_k), \tag{16}$$

where w_k is any operator on $\mathbb{C}^{m_k}$, i.e., a $m_k \times m_k$ matrix. Therefore, the classification of covariant trace-not-increasing QO's with $\mathcal{M}(I_{\mathcal{K}}) = \mathcal{K} \leqslant I_{\mathcal{H}}$ is equivalent to classify the operators $R_{\mathcal{M}}$ of the form (16) with the constraint

$$\sum_k \mathrm{Tr}_{\mathcal{K}}[(I_{\mathcal{H}_k} \otimes w_k^\dagger w_k)] = K \leqslant I_{\mathcal{H}}. \tag{17}$$

The constraint (17) is generally quite involved, due to the subspace mismatch between the tensor product $\mathcal{K} \otimes \mathcal{H}$ and the Wedderburn's decomposition: its simplification will be the main task of Sec. VI.

IV. TECHNICAL LEMMAS

This section will be entirely devoted to technical lemmas, which will be used for the classification of both extremal covariant POVM's and QO's. The lemmas connect conditions on the vanishing of partial traces with linear spannings.

In the following we will make use of the following simple fact for any linear space $\mathcal{L}$ and a subspace $\mathcal{S} \subseteq \mathcal{L}$: if the only vector of $\mathcal{L}$ that is orthogonal to the whole subspace $\mathcal{S}$ is the null vector, then one has $\mathcal{S} = \mathcal{L}$. Moreover, since orthogonality to a set s of vector implies orthogonality to its linear span $\mathsf{Span}(\mathsf{s})$, then the previous assertion holds also for subsets $\mathsf{s} \subseteq \mathcal{L}$ (not necessarily subspace), namely if the only vector orthogonal to the subset s is the null vector, than one has $\mathcal{L} \equiv \mathsf{Span}(\mathsf{s})$. From now we will also make use of the following natural notation

$$X(\boldsymbol{B}(\mathcal{A}) \otimes I_B)Y^\dagger \doteq \mathsf{Span}\{X(A \otimes I_B)Y^\dagger, A \in \boldsymbol{B}(\mathcal{A})\}, \tag{18}$$

for X, Y any operators with domain $\mathcal{A} \otimes \mathcal{B}$.

Lemma 1: *Let $B \in \boldsymbol{B}(\mathcal{B}_2 \otimes \mathcal{B}_1, \mathcal{A})$, $\mathcal{A}$ and $\mathcal{B}_{1,2}$ denoting arbitrary finite-dimensional Hilbert spaces. Then, the injectivity of the linear CP map $\mathcal{W}(A) = \mathrm{Tr}_{B_1}[B^\dagger A B]$ on $\boldsymbol{B}(\mathcal{A})$ is equivalent to the spanning condition*

$$\boldsymbol{B}(\mathcal{A}) = B(\boldsymbol{B}(\mathcal{B}_2) \otimes I_{B_1})B^\dagger. \tag{19}$$

Proof: The injectivity of the map $\mathcal{W}(A) = \mathrm{Tr}_{B_1}[B^\dagger A B]$ on $\boldsymbol{B}(\mathcal{A})$ means that

$$\forall A \in \boldsymbol{B}(\mathcal{A}), \quad \mathrm{Tr}_{B_1}[B^\dagger A B] = 0 \Rightarrow A = 0. \tag{20}$$

The condition $\mathrm{Tr}_{\mathcal{B}_1}[B^\dagger A B] = 0$ is equivalent to $\mathrm{Tr}[C\ \mathrm{Tr}_{B_1}[B^\dagger A B]] = 0\ \forall C \in \boldsymbol{B}(\mathcal{B}_2)$. Therefore, since one has

$$\mathrm{Tr}[C\ \mathrm{Tr}_{\mathcal{B}_1}[B^\dagger A B]] = \mathrm{Tr}[(C \otimes I_{B_1})B^\dagger A B] = \mathrm{Tr}[B(C \otimes I_{B_1})B^\dagger A] \tag{21}$$

condition (20) is then equivalent to

$$\forall A \in \boldsymbol{B}(\mathcal{A}), \quad \mathrm{Tr}[B(\boldsymbol{B}(\mathcal{B}_2) \otimes I_{B_1})B^\dagger A] = 0 \Rightarrow A = 0, \tag{22}$$

where we used notation (18). Equation (22) says that the only operator $A \in \boldsymbol{B}(\mathcal{A})$ orthogonal to the operator space $B(\boldsymbol{B}(\mathcal{B}_2) \otimes I_{B_1})B^\dagger \subseteq \boldsymbol{B}(\mathcal{A})$ is the null operator, which means that $B(\boldsymbol{B}(\mathcal{B}_2) \otimes I_{B_1})B^\dagger$ is actually the full linear space $\boldsymbol{B}(\mathcal{A})$, namely condition (22) is equivalent to condition (19). ■

The above theorem leads immediately to the following corollaries.

Corollary 1: A necessary condition for injectivity of the map $\mathcal{W}(A) = \mathrm{Tr}_{B_1}[B^\dagger AB]$ *on* $\boldsymbol{B}(\mathcal{A})$ *is*

$$\dim(\mathcal{A}) \leqslant \min\{\dim(\mathcal{B}_2), \mathrm{rank}(B)\}. \tag{23}$$

Corollary 2: The injectivity of the map $\mathcal{W}(A) = \mathrm{Tr}_{B_1}[B^\dagger AB]$ *on* $\boldsymbol{B}(\mathcal{A})$ *is equivalent to the existence of a linear injective map* $\mathcal{V}$ *from* $\boldsymbol{B}(\mathcal{A})$ *to* $\boldsymbol{B}(\mathcal{B})$ *such that*

$$\forall A \in \boldsymbol{B}(\mathcal{A}), \quad B(\mathcal{V}(A) \otimes I_{\mathcal{B}_1})B^\dagger = A. \tag{24}$$

The relation between the maps $\mathcal{W}$ *and* $\mathcal{V}$ *is given by*

$$\mathcal{W}(A) = \mathrm{Tr}_{\mathcal{B}_1}[B^\dagger B(\mathcal{V}(A) \otimes I_{\mathcal{B}_1})B^\dagger B]. \tag{25}$$

Proof: The spanning condition (19)—equivalent to the injectivity of the map $\mathcal{W}(A) = \mathrm{Tr}_{\mathcal{B}_1}[B^\dagger AB]$ on $\boldsymbol{B}(\mathcal{A})$—guarantees that for each $A \in \boldsymbol{B}(\mathcal{A})$ there exists an element, say V_A, of $\boldsymbol{B}(\mathcal{B})$ such that $B(V_A \otimes I_{\mathcal{B}_1})B^\dagger = A$. Consider now an orthonormal basis A_j for $\boldsymbol{B}(\mathcal{A})$, and denote by V_j any element of $\boldsymbol{B}(\mathcal{B})$ such that $B(V_j \otimes I_{\mathcal{B}_1})B^\dagger = A_j$. It is clear that the $\{V_j\}$ can be chosen as linearly independent. Now, for every element $A \in \boldsymbol{B}(\mathcal{A})$ define $\mathcal{V}(A) = \Sigma_j \mathrm{Tr}[A_j^\dagger A]V_j$. This map is clearly linear and injective. The map $\mathcal{V}(A)$ corresponds to a nonorthogonal change of basis (from $\{A_j\}$ to $\{V_j\}$) which compensates the nonorthogonal change of basis $B(V_j \otimes I_{\mathcal{B}_1})B^\dagger = A_j$. Equation (25) follows by substituting Eq. (24) into the map $\mathcal{W}$. ■

We have also the additional lemma.

Lemma 2: As in Lemma 1, *the injectivity of the map* $\mathcal{W}(A) = \mathrm{Tr}_{\mathcal{B}_1}[B^\dagger AB]$ *on* $\boldsymbol{B}(\mathcal{A})$ *is equivalent to the linear independence of the set of operators* $\{W_i^\dagger W_j\}$, *where* $W_i \in \boldsymbol{B}(\mathcal{B}_1, \mathcal{B}_2)$ *are defined from the singular value decomposition* $B = \Sigma_i |V_i\rangle\langle W_i|$ *through the identity* $|W_i\rangle = (W_i \otimes I_{\mathcal{B}_1})|I\rangle$, $|I\rangle \in \mathcal{B}_1^{\otimes 2}$ *denoting the fixed vector* $|I\rangle = \Sigma_l |l\rangle \otimes |l\rangle$, *for* $\{|l\rangle \otimes |m\rangle\}$ *arbitrary orthonormal basis of* $\mathcal{B}_1^{\otimes 2}$.

Proof: First, notice that the identity $|X\rangle = (X \otimes I_{\mathcal{B}_1})|I\rangle$ sets a bijection between vectors $|X\rangle \in \mathcal{B}_2 \otimes \mathcal{B}_1$ and operators $X \in \boldsymbol{B}(\mathcal{B}_1, \mathcal{B}_2)$. Then, using the singular value decomposition $B = \Sigma_i |V_i\rangle\langle W_i|$, with $|V_i\rangle \in \mathcal{A}$ and $|W_i\rangle \in \mathcal{B}_2 \otimes \mathcal{B}_1$, the partial trace in Eq. (20) becomes

$$\mathrm{Tr}_{\mathcal{B}_1}[B^\dagger AB] = \sum_{ij} \langle V_i|A|V_j\rangle \mathrm{Tr}_{\mathcal{B}_1}[|W_i\rangle\langle W_j|] = \sum_{ij} \langle V_i|A|V_j\rangle W_i^\tau W_j^*, \tag{26}$$

where τ denotes the transposition for which $(X \otimes I_{\mathcal{B}_1})|I\rangle = (I_{\mathcal{B}_1} \otimes X^\tau)|I\rangle$, and * denotes complex conjugation, i.e., $X^\dagger = (X^\tau)^*$. By taking the complex conjugate of the last equation and introducing the matrix $A_{ij} \doteq \langle V_i|A|V_j\rangle^* \in \mathsf{M}_N(\mathbb{C})$ where $N = \mathrm{rank}(B)$ (N^2 is the cardinality of the set $\{W_i^\dagger W_j\}$), the statement (20) is equivalent to

$$\{A_{ij}\} \in \mathsf{M}_N(\mathbb{C}), \quad \sum_{ij} A_{ij} W_i^\dagger W_j = 0 \Rightarrow A_{ij} = 0, \quad \forall\, i,j, \tag{27}$$

namely the operators $\{W_i^\dagger W_j\}$ are linearly independent. ■

In the following we will need the following generalization of Lemma 1.

Lemma 3: Let $B \in \boldsymbol{B}(\oplus_k(\mathcal{B}_2^{(k)} \otimes \mathcal{B}_1^{(k)}), \mathcal{A})$, *and denote by* P_k *the orthogonal projector over* $\mathcal{B}_2^{(k)} \otimes \mathcal{B}_1^{(k)}$, $\mathcal{A}$ *and* $\mathcal{B}_{1,2}^{(k)}$ *being arbitrary finite-dimensional Hilbert spaces*.

The following implication,

$$A \in \boldsymbol{B}(\mathcal{A}), \quad \mathrm{Tr}_{\mathcal{B}_2^{(k)}}[P_k B^\dagger ABP_k] = 0 \ \forall\, k \Rightarrow A = 0, \tag{28}$$

is equivalent to

$$\boldsymbol{B}(\mathcal{A}) = \mathrm{Span}\{B[\oplus_k(\boldsymbol{B}(\mathcal{B}_2^{(k)}) \otimes I_{\mathcal{B}_1^{(k)}})]B^\dagger\}, \tag{29}$$

and necessary conditions are

$$\dim(\mathcal{A})^2 \leqslant \sum_k \dim(\mathcal{B}_2^{(k)})^2, \tag{30}$$

$$\dim(\mathcal{A}) \leqslant \mathrm{rank}(B). \tag{31}$$

Proof: The condition $\mathrm{Tr}_{\mathcal{B}_1^{(k)}}[P_k B^\dagger A B P_k] = 0 \ \forall k$ is equivalent to say that for any $C_k \in \boldsymbol{B}(\mathcal{B}_2^{(k)})$ one has $\mathrm{Tr}[P_k C_k \mathrm{Tr}_{\mathcal{B}_1^{(k)}}[P_k B^\dagger A B P_k]] = 0 \ \forall k$. Since one has

$$\mathrm{Tr}[C_k \mathrm{Tr}_{\mathcal{B}_1^{(k)}}[P_k B^\dagger A B P_k]] = \mathrm{Tr}[(C_k \otimes I_{\mathcal{B}_1^{(k)}}) P_k B^\dagger A B P_k] = \mathrm{Tr}[B P_k (C_k \otimes I_{\mathcal{B}_1^{(k)}}) P_k B^\dagger A], \tag{32}$$

and, therefore, condition (28) is equivalent to

$$A \in \boldsymbol{B}(\mathcal{A}), \quad \mathrm{Tr}[B P_k (\boldsymbol{B}(\mathcal{B}_2^{(k)}) \otimes I_{\mathcal{B}_1^{(k)}}) P_k B^\dagger A] = 0 \ \forall \ k \Rightarrow A = 0. \tag{33}$$

The last condition says that the only operator in $\boldsymbol{B}(\mathcal{A})$ which is orthogonal to the set $B P_k (\boldsymbol{B}(\mathcal{B}_2^{(k)}) \otimes I_{\mathcal{B}_1^{(k)}}) P_k B^\dagger \ \forall k$ is the null operator, or, in other words that the set spans the full operator space $\boldsymbol{B}(\mathcal{A})$, namely Eq. (29). The necessary conditions then follow trivially. ■

We are now ready to classify the extremal group covariant POVM's and QO's in the following sections. In order to classify extremal elements of convex sets, we will use the method of perturbations. We will call a non-null operator B a *perturbation* for an operator A in a convex set if both $A \pm tB$ are still in the convex set for some (sufficiently small) $t > 0$. Then, clearly A is not extremal in the convex set if and only if it has a perturbation.

V. EXTREMAL COVARIANT POVM'S

We have seen that the covariant POVM for the estimation of a group element g of an unknown unitary transformation U_g is of the general form

$$\mathrm{d}P_g = \mathrm{d}g \ U_g^\dagger \Xi U_g^\dagger, \tag{34}$$

with probability space $\mathcal{X} = \mathbf{G}$, and with

$$\int_{\mathbf{G}} \mathrm{d}_g \ U_g^\dagger \Xi U_g = I_{\mathcal{H}}. \tag{35}$$

The Wedderburn's decomposition (15) of the representation space here rewrites as follows:

$$\mathcal{H} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k}), \tag{36}$$

where we remind that k labels the equivalence class of irreducible components, and m_k denotes its multiplicity. The integral in the normalization condition (35) belongs to the commutant of the representation, whence it can be rewritten as follows:

$$\int_{\mathbf{G}} \mathrm{d}g \ U_g^\dagger \Xi U_g = \bigoplus_k d_{\mathcal{H}_k}^{-1} [I_{\mathcal{H}_k} \otimes \mathrm{Tr}_{\mathcal{H}_k}(P_k \Xi P_k)] = I_{\mathcal{H}}, \tag{37}$$

P_k denoting the orthogonal projector on the subspace $\mathcal{H}_k \otimes \mathbb{C}^{m_k}$. Equation (37) follows from the simple fact that for an irreducible representation on the space say $\mathcal{L}$, one has $\int_{\mathbf{G}} \mathrm{d}g \ U_g^\dagger Z U_g = d_{\mathcal{L}}^{-1} \mathrm{Tr}[Z] I_{\mathcal{L}}$ for measure $\mathrm{d}g$ normalized to unit on $\mathbf{G}$. Equation (37) allows to split the constraint (35) into the following set of constraints:

$$\mathrm{Tr}_{\mathcal{H}_k}(P_k \Xi P_k) = d_{\mathcal{H}_k} I_{m_k}, \quad \forall\, k, \tag{38}$$

where by I_{m_k} we denote the identity matrix over $\mathbb{C}^{m_k}$. We then conclude that the classification of extremal **G**-covariant POVM's is equivalent to find the extremal Ξ within the convex set of operators $\Xi \geqslant 0$ satisfying the constraints (38). For such purpose we have the following theorem.

Theorem 2: Let Ξ be an element of the convex set of positive operators on $\mathcal{H}$ satisfying the constraints

$$\mathrm{Tr}_{\mathcal{H}_k}(P_k \Xi P_k) = d_{\mathcal{H}_k} I_{m_k}, \quad \forall\, k \in \mathsf{S}, \tag{39}$$

where S *denotes the set of equivalence classes of irreducible components in the representation. Write Ξ in the form $\Xi = X^\dagger A X$ with $A \geqslant 0$, choosing* $\mathsf{Rng}(X) = \mathsf{Supp}(A) \doteq \mathsf{Ker}(A)^\perp$. *Then*

(1) *Θ is a perturbation of Ξ if and only if Θ is Hermitian, with* $\mathrm{Tr}_{\mathcal{H}_k}(P_k \Theta P_k) = 0\ \forall k \in \mathsf{S}$, *and* $\Theta = X^\dagger B X$ *for some nonzero Hermitian B with* $\mathsf{Supp}(B) \subseteq \mathsf{Supp}(A)$.
(2) *For the specific choice of the form of A as* $A = \oplus_k A_k$, *with* $A_k \in B(\mathcal{H}_k \otimes \mathbb{C}^{m_k})$, *one has* $B = \oplus_k B_k$, $B_k \in \boldsymbol{B}(\mathcal{H}_k \otimes \mathbb{C}^{m_k})$ *and* $\mathsf{Supp}(B_k) \subseteq \mathsf{Supp}(A_k)$, $\forall k \in \mathsf{S}$;
(3) *$\Xi = X^\dagger X$ is extremal if and only if*

$$\boldsymbol{B}(\mathsf{Rng}(X)) = \mathsf{Span}\{X[\oplus_k (I_{\mathcal{H}^{(k)}} \otimes \boldsymbol{B}(\mathbb{C}^{m_k}))]X^\dagger\}. \tag{40}$$

Proof:

(1) Let Θ Hermitian, with $\mathrm{Tr}_{\mathcal{H}_k}(P_k \Theta P_k) = 0$, and $\Theta = X^\dagger B X$ for some nonzero Hermitian $B \in \boldsymbol{B}(\mathcal{H})$ and with $\mathsf{Supp}(B) \subseteq \mathsf{Supp}(A)$. Then for $\mathrm{rank}(B) > 0$ Θ is necessarily nonzero, and since $A \geqslant 0$, both constraints $A \pm tB \geqslant 0$ and $\mathrm{Tr}_{\mathcal{H}_k}(P_k(\Xi \pm t\Theta)P_k) = d_{\mathcal{H}_k} I_{m_k}\, \forall k$ are satisfied for some $t > 0$, whence Θ is a perturbation for Ξ. Conversely, suppose $\Theta \in \boldsymbol{B}(\mathcal{H})$ is a perturbation for Ξ. Since we must have $\Xi \pm t\Theta \geqslant 0$ and $Tr_{\mathcal{H}_k}[P_k(\Xi \pm t\Theta)P_k] = d_{\mathcal{H}_k} I_{m_k}$ for some $t > 0$, then Θ is Hermitian with $\mathrm{Tr}_{\mathcal{H}_k}(P_k \Theta P_k) = 0\ \forall k \in \mathsf{S}$. Moreover, if we write Ξ in the form $\Xi = X^\dagger A X$ with nonnegative $A \in \boldsymbol{B}(\mathcal{H})$, and $\mathsf{Rng}(X) = \mathsf{Supp}(A)$, then also Θ can be written in the same form $\Theta = X^\dagger B X$ for some nonzero Hermitian $B \in \boldsymbol{B}(\mathcal{H})$ and $\mathrm{Tr}_{\mathcal{H}_k}[P_k(\Xi \pm t\Theta)P_k] = d_{\mathcal{H}_k} I_{m_k}$. In fact, if X is not invertible, it can be always completed to an invertible operator $Z = X + Y$ by adding an operator Y with $\mathsf{Rng}(Y) = \mathsf{Ker}(A)$, and one can equivalently write $\Xi = Z^\dagger A Z$. Now we can write also the perturbation operator in the form $\Theta = Z^\dagger B Z$. However, since $A \pm tB \geqslant 0$ for some t, then necessarily B must have $\mathsf{Supp}(B) \subseteq \mathsf{Supp}(A) = \mathsf{Rng}(X)$, whence $Z^\dagger B Z = X^\dagger B X$.
(2) First it is obvious that a choice of the form $A = \oplus_k A_k$, with $A_k \in \boldsymbol{B}(\mathcal{H}_k \otimes \mathbb{C}^{m_k})$ is always possible. Then, in order to have $A \pm tB \geqslant 0$ for some $t > 0$, one must have $B = \oplus_k B_k$, each B_k Hermitian, with $\mathsf{Supp}(B_k) \subseteq \mathsf{Supp}(A_k)$, $\forall k \in \mathsf{S}$.
(3) Since $\mathsf{Supp}(A) \subseteq \mathsf{Rng}(X)$ and $A \geqslant 0$, we can always merge $\sqrt{A}$ into X by substituting $X \to \sqrt{A}X$. Then, since Ξ is not extremal iff it has a perturbation, by part (1) one sees that Ξ is extremal iff for Hermitian $B \in \boldsymbol{B}(\mathcal{H})$ with $\mathsf{Supp}(B) \subseteq \mathsf{Rng}(X)$, one has

$$\mathrm{Tr}_{\mathcal{H}_k}(P_k X^\dagger B X P_k) = 0\ \forall\, k \in \mathsf{S} \quad \Rightarrow \quad B = 0, \tag{41}$$

whence via Cartesian decomposition of B we have the equivalent statement

$$B \in \boldsymbol{B}(\mathsf{Rng}(X)), \quad \mathrm{Tr}_{\mathcal{H}_k}(P_k X^\dagger B X P_k) = 0\ \forall\, k \in \mathsf{S} \quad \Rightarrow \quad B = 0. \tag{42}$$

Then, by Lemma 3 this is equivalent to condition (40). ■

Corollary 3: A necessary condition for extremality of the seed Ξ of a group covariant representation as in Theorem 2 is

$$\mathrm{rank}(\Xi)^2 \leqslant \sum_k m_k^2. \tag{43}$$

Proof: Equation (43) is a trivial consequence of the necessary condition (40). ■

Corollary 4: Every rank-one POVM is extremal.

Proof: For $\mathrm{rank}(X)=1$ the iff condition (40) is trivially satisfied. ■

Theorem 3: *For* S *containing only a single equivalence class, say* h*, with multiplicity* $m_h \geqslant 1$*, the extremality of a covariant POVM on the Hilbert space* $\mathcal{H}=\mathcal{H}_h\otimes\mathbb{C}^{m_h}$ *is equivalent to the linear independence of the set of operators* $\{W_i^\dagger W_j\}$*, where* $W_i\in\boldsymbol{B}(\mathbb{C}^{m_h},\mathcal{H}_h)$ *are defined from the spectral decomposition* $\Xi=\sum_i |W_i\rangle\langle W_i|$ *of the seed* Ξ *of the POVM through the identity* $|W_i\rangle = (W_i\otimes I_{m_h})|I\rangle$*,* $|I\rangle\in(\mathbb{C}^{m_h})^{\otimes 2}$ *denoting the fixed vector* $|i\rangle=\sum_l |l\rangle\otimes|l\rangle$*, for* $\{|l\rangle\otimes|m\rangle\}$ *arbitrary orthonormal basis of* $(\mathbb{C}^{m_h})^{\otimes 2}$*. Extremal POVM's with any rank* $\mathrm{rank}(\Xi)\leqslant m_h$ *are admissible.*

Proof: For S containing a single equivalence class h with multiplicity $m_h\geqslant 1$ the seed Ξ of the POVM must satisfy the single constraint

$$\mathrm{Tr}_{\mathcal{H}_h}(\Xi) = d_{\mathcal{H}_h} I_{m_h}. \tag{44}$$

Now, write Ξ in the form $\Xi=X^\dagger AX$ with $X\in\boldsymbol{B}(\mathcal{H}_h\otimes\mathbb{C}^{m_h},\mathcal{A})$, and $\mathsf{Rng}(X)=\mathsf{Supp}(A)$, A being a Hilbert space such that $\mathsf{Supp}(A)\subseteq\mathcal{A}\subseteq\mathcal{H}_h\otimes\mathbb{C}^{m_h}$, and which can be chosen as $\mathcal{A}\simeq\mathsf{Rng}(X)$. Then, according to Theorem 2 Θ is a perturbation for Ξ iff it is of the form $\Theta=X^\dagger BX$, with B Hermitian, $\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)$, and $\mathrm{Tr}_{\mathcal{H}_h}(X^\dagger BX)=0$. This means that the extremality of Ξ is equivalent to the injectivity of the map $\mathcal{W}(B)=\mathrm{Tr}_{\mathcal{H}_h}(X^\dagger BX)$ over the set of Hermitian operators B with $\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)$, which is equivalent to injectivity of the same map on $\boldsymbol{B}(\mathsf{Rng}(X))$. We are thus in the situation of Lemma 2, with $\mathcal{A}=\mathsf{Rng}(X)$, $\mathcal{B}_1=\mathbb{C}^{m_h}$ and $\mathcal{B}_2=\mathcal{H}_h$. Therefore, by writing the singular value decomposition of $X=\sum_i |V_i\rangle\langle W_i|$, with $\mathsf{Span}\{||V_i\rangle\}=\mathsf{Rng}(X)=\mathsf{Supp}(A)$ the injectivity of the map $\mathcal{W}(B)=\mathrm{Tr}_{\mathcal{H}_h}[X^\dagger BX]$ on $\boldsymbol{B}(\mathsf{Rng}(\mathcal{X}))$ is equivalent to the linear independence of the set of operators $\{W_i^\dagger W_j\}$, where $W_i\in\boldsymbol{B}(\mathbb{C}^{m_h},\mathcal{H}_h)$ are defined through the identity $|W_i\rangle=(W_i\otimes I_{m_h})|I_i\rangle$, $|I\rangle\in(\mathbb{C}^{m_h})^{\otimes 2}$ denoting the fixed vector $|I\rangle=\sum_l |l\rangle\otimes|l\rangle$, with $\{|l\rangle\otimes|m\rangle\}$ arbitrary orthonormal basis of $(\mathbb{C}^{m_h})^{\otimes 2}$. Now, the maximum rank of the POVM is given by the maximum number of operators W_i such that the set of operators $\{W_i^\dagger W_j\}$ in $\boldsymbol{B}(\mathbb{C}^{m_h})$ is linearly independent. Since we can have at most m_h^2 linearly independent operators in $\boldsymbol{B}(\mathbb{C}^{m_h})$, the maximum cardinality of the set $\{W_i\}$ is m_h. ■

Corollary 5: A POVM which is covariant under an irreducible representation is extremal: *If and only if iff it is rank one.*

Proof: For S containing a single equivalence class h with multiplicity $m_h=1$ the iff condition (40) rewrites

$$\boldsymbol{B}(\mathsf{Rng}(X)) = \mathsf{Span}\{X(I_{\mathcal{H}^{(h)}}\otimes\mathbb{C}^1)X^\dagger\} = \mathsf{Span}\{XX^\dagger\}, \tag{45}$$

which is satisfied iff $\mathrm{rank}(X)=1$. As an alternative proof, the present corollary corresponds to the situation of Theorem 3 for multiplicity $m_h=1$. ■

A. Example

Consider a POVM on $\mathcal{H}$ with $\dim(\mathcal{H})=d$ covariant under $\mathbf{G}=\mathbb{U}(1)$, with

$$U_\phi = \exp(i\phi N), \quad N=\sum_{n=0}^{d-1} n|n\rangle\langle n|. \tag{46}$$

Here we have d one-dimensional irreducible representations with characters $\chi_k(\phi)=\exp(ik\phi)$, $k=0,\ldots,d-1$, namely they are all inequivalent, whence with unit multiplicity. Therefore, the necessary condition (43) bounds the rank of the POVM as follows:

$$\mathrm{rank}(\Xi)^2 \leqslant \dim(\mathcal{H}), \tag{47}$$

and in order to have $\mathrm{rank}(\Xi)=2$ one must have $\dim(\mathcal{H})\geqslant 4$. According to Theorem 2 the extremal POVM's have seed of the form $\Xi=X^\dagger X$ satisfying the identity

$$\boldsymbol{B}(\mathsf{Rng}(X)) = \mathsf{Span}\{|X_k\rangle\langle X_k| : 0 \leqslant k \leqslant \dim(\mathcal{H})\}, \tag{48}$$

where $|X_k\rangle = X|k\rangle$, $\{|k\rangle\}$ denoting any orthonormal basis for $\mathcal{H}$. Notice that in the present example the operator Ξ corresponds to a so-called *correlation matrix*, namely a positive matrix with all ones on the diagonal. This follows from the constraint (38), which in our case is simply $\langle k|\Xi|k\rangle = 1, \forall k$. Therefore, the present classification of extremal POVM's coincides with the classification of extremal correlation matrices given in Ref. 25.

B. Example

Consider a POVM for n qubits on the Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ covariant under the tensor representation $U_\phi^{\otimes n}$ of $\mathbf{G} = \mathbb{U}(1)$, with

$$U_\phi = \exp(i\phi|1\rangle\langle 1|), \tag{49}$$

where $\{|0\rangle, |1\rangle\}$ is a orthonormal basis for $\mathbb{C}^2$. Here we have $n+1$ one-dimensional irreducible representations with characters $\chi_k(\phi) = \exp(ik\phi)$, $k = 0, \ldots, n$, and with multiplicity $m_k = \binom{n}{k}$. An orthonormal basis of each subspace $\mathbb{C}^{m_k}$ of $\mathcal{H} = \oplus_k \mathbb{C}^{m_k}$ is given by

$$\{|j\rangle_k\} = \{P_j^{(n,k)}|\underbrace{00\cdots0}_{n-k}\underbrace{11\cdots1}_{k}\rangle\}, \tag{50}$$

where $P_j^{(n,k)}$ denotes the jth permutation of k qubits in the state $|1\rangle$ in the tensor product of n qubits in total, with all other qubits in the state $|0\rangle$. In the present example, the iff condition for extremality (40) requires that $\Xi = X^\dagger X$ satisfies the identity

$$\boldsymbol{B}(\mathsf{Rng}(X)) = \mathsf{Span}\{X|i\rangle_{kk}\langle j|X^\dagger, k \in \mathsf{S}, i, j = 1, \ldots, m_k\}, \tag{51}$$

where now $\{|i\rangle_k\}$ denotes any orthonormal basis for $\mathbb{C}^{m_k}$. The necessary condition (43) bounds the rank of the POVM as follows:

$$\mathrm{rank}(\Xi)^2 \leqslant \sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}. \tag{52}$$

Here, in order to have $\mathrm{rank}(\Xi) \geqslant 2$ one needs $n \geqslant 2$ qubits. For $n = 2$ according to the previous example, one necessarily must have at least two inequivalent classes, since each of the irreducible components has less than four dimensions (the same is true also for $n = 3$). The previous example is also recovered by considering the special case in which $\mathsf{Rng}(X) \subseteq ((\mathbb{C}^2)^{\otimes n})_+$, i.e., containing only the subrepresentation of $U_\phi^{\otimes n}$ on the symmetric subspace $((\mathbb{C}^2)^{\otimes n})_+$, with multiplicity 1.

C. Example

Consider a POVM on $\mathcal{H}^{\otimes 2}$ which is covariant under the group representation $U_g \otimes I_{\mathcal{H}}$, where U_g is an irreducible representation of $\mathbf{G}$ on $\mathcal{H}$. Here, we trivially have a single equivalence class, say h, (corresponding to the irreducible representation U_g) with multiplicity $m_h = \dim(\mathcal{H})$, i.e., the Hilbert space $\mathcal{H}$ coincides with the multiplicity space $\mathcal{H} \simeq \mathbb{C}^{m_h}$. This is exactly the case considered in Theorem 3. Therefore, the extremality of the POVM is equivalent to the linear independence of the set of operators $\{W_i^\dagger W_j\}$, where $W_i \in \boldsymbol{B}(\mathcal{H})$ are defined from the spectral decomposition $\Xi = \Sigma_i |W_i\rangle\langle W_i|$ of the seed Ξ of the POVM through the identity $|W_i\rangle = (W_i \otimes I_{\mathcal{H}})|I\rangle$, as in Theorem 3. Therefore, we can have extremal POVM's with any $\mathrm{rank}(\Xi) \leqslant \dim(\mathcal{H})$. Notice that there cannot be more than a single maximally entangled vector $|W_i\rangle$ in the decomposition of Ξ, since, otherwise, at least two operators W_i would be proportional to unitary operators, and then the set $\{W_i^\dagger W_j\}$ would be necessarily linearly dependent (two products would be both proportional to the identity). The rank-one case with a single maximally entangled projector corresponds to a so-called *Bell POVM*.

VI. EXTREMAL COVARIANT QUANTUM OPERATIONS

In the following we will denote shortly by $\boldsymbol{A}_{\mathbf{G}}$ the operator algebra generated by the group representation $V_g \otimes U_g^*$, by $\boldsymbol{A}'_{\mathbf{G}}$ its commutant, and finally by $\boldsymbol{H}'_{\mathbf{G}}$ the Hermitian operators in the commutant. The following theorem classifies all extremal **G**-covariant maps $\mathcal{M}$ in the convex set given by Eq. (17).

Theorem 4: *Let R be an element of the convex set of positive operators in the commutant $\boldsymbol{A}'_{\mathbf{G}}$ of the operator algebra $\boldsymbol{A}_{\mathbf{G}}$ generated by the group representation $V_g \otimes U_g^*$ on $\mathcal{K} \otimes \mathcal{H}$, i.e., of the form*

$$R = \oplus_k (I_{\mathcal{H}_k} \otimes w_k^\dagger w_k) = W^\dagger W, \quad W \doteq \oplus_k (I_{\mathcal{H}_k} \otimes w_k), \tag{53}$$

satisfying the constraint

$$\sum_k \mathrm{Tr}_{\mathcal{K}}[(I_{\mathcal{H}_k} \otimes w_k^\dagger w_k)] = K \leqslant I_{\mathcal{H}}, \tag{54}$$

where

$$\mathcal{H} \otimes \mathcal{K} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k}) \tag{55}$$

is the Wedderburn's decomposition of the representation space, k labeling the equivalence class of representations, with multiplicity m_k. Denote by P_k the orthogonal projector over the space $\mathcal{H}_k \otimes \mathbb{C}^{m_k}$ of the equivalence class. Write R in the form $R = X^\dagger Q X$ with $Q, X \in \boldsymbol{A}'_{\mathbf{G}}$ and $\mathsf{Rng}(X) = \mathsf{Supp}(Q)$. Then:

(1) *S is a perturbation of R if and only if $S \in \boldsymbol{H}'_{\mathbf{G}}$, with $\mathrm{Tr}_{\mathcal{K}}[S] = 0$, and $S = X^\dagger O X$ for some nonzero $O \in \boldsymbol{H}'_{\mathbf{G}}$ with $\mathsf{Supp}(O) \subseteq \mathsf{Rng}(X)$. Specifically, writing $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$ and $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$, one has $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $\mathsf{Supp}(O_k) \subseteq \mathsf{Rng}(X_k)\ \forall k$.*

(2) *One can always write R in the form $R = X^\dagger X$, with $X \in \boldsymbol{A}'_{\mathbf{G}}$ of the form $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$. Denote by S the set of equivalence classes k for which $X_k \neq 0$. Then, a necessary and sufficient condition for extremality of $R = X^\dagger X$ with $\mathrm{Tr}_{\mathcal{K}}[R] = K$ is the injectivity of the map $\mathcal{T}(O) = \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X]$ on $\boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X))$, namely*

$$O \in \boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X)), \quad \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X] = 0 \Rightarrow O = 0, \tag{56}$$

which is equivalent to

$$\oplus_{k \in \mathsf{S}} \boldsymbol{B}(\mathsf{Rng}(X_k)) = \oplus_{k \in \mathsf{S}} X_k \mathrm{Tr}_{\mathcal{H}_k}[P_k (I_{\mathcal{K}} \otimes \boldsymbol{B}(\mathcal{H})) P_k] X_k^\dagger. \tag{57}$$

Proof:

(1) Let $S \in \boldsymbol{H}'_{\mathbf{G}}$, with $\mathrm{Tr}_{\mathcal{K}}[S] = 0$, and $S = X^\dagger O X$ for some nonzero Hermitian O with $\mathsf{Supp}(O) \subseteq \mathsf{Supp}(Q)$. Then for $\mathrm{rank}(O) > 0$ $S \in \boldsymbol{H}'_{\mathbf{G}}$ is necessarily nonzero, and since $\boldsymbol{H}'_{\mathbf{G}} \ni Q \geqslant 0$, all constraints: $Q \pm tO \in \boldsymbol{H}'_{\mathbf{G}}$, $Q \pm tO \geqslant 0$, and $\mathrm{Tr}_{\mathcal{K}}[R \pm tS] = K$ are satisfied for some $t > 0$, whence S is a perturbation for R. Conversely, suppose that $S \in \mathcal{K} \otimes \mathcal{H}$ is a perturbation for R. Since we must have $\boldsymbol{H}'_{\mathbf{G}} \ni R \pm tS \geqslant 0$ and $\mathrm{Tr}_{\mathcal{K}}[R \pm tS] = K$ for some $t > 0$, then $S \in \boldsymbol{H}'_{\mathbf{G}}$ with $\mathrm{Tr}_{\mathcal{K}}[S] = 0$. Moreover, if we write R in the form $R = X^\dagger Q X$ with $\mathsf{Rng}(X) = \mathsf{Supp}(Q)$, then also S can be written in the form $S = X^\dagger O X$ for some nonzero Hermitian $O \in \boldsymbol{H}'_{\mathbf{G}}$. In fact, if X is not invertible, it can be always completed to an invertible operator $Z = X + Y$ by adding an operator $Y \in \boldsymbol{A}'_{\mathbf{G}}$ of the form $Y = \oplus_k (I_{\mathcal{H}_k} \otimes Y_k)$ with $\mathsf{Rng}(Y_k) = \mathsf{Ker}(Q_k)$ [where $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$], and one can equivalently write $R = Z^\dagger Q Z$ with $Q \in \boldsymbol{H}'_{\mathbf{G}}$ and $Z \in \boldsymbol{A}'_{\mathbf{G}}$. Now we can write also the perturbation operator in the form $S = Z^\dagger O Z$. However, since for some t the operator $Q \pm tO \geqslant 0$ must belong to the commutant $\boldsymbol{A}'_{\mathbf{G}}$, then necessarily $O \in \boldsymbol{H}'_{\mathbf{G}}$ and $\mathsf{Supp}(O) \subseteq \mathsf{Supp}(Q) = \mathsf{Rng}(X)$, with $Z^\dagger O Z = X^\dagger O X$. Specifically, writing $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$, one has $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $\mathsf{Supp}(O_k) \subseteq \mathsf{Supp}(Q_k) = \mathsf{Rng}(X_k)\ \forall k$.

(2) As in part (1) we can always take Q as the identity, and redefine $X \to \sqrt{Q}X$, since $Q \geqslant 0$, keeping X of the form $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$, since both operators in the product $\sqrt{Q}X$ belong to the algebra $\boldsymbol{A}'_{\mathbf{G}}$. From part (1) we then see that $R = X^\dagger X$ with $X \in \boldsymbol{A}'_{\mathbf{G}}$ is extremal if and only if

$$O \in \boldsymbol{H}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X)), \quad \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X] = 0 \Rightarrow O = 0, \tag{58}$$

and via Cartesian decomposition this is equivalent to

$$O \in \boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X)), \quad \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X] = 0 \Rightarrow O = 0. \tag{59}$$

Since $O \in \boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X))$ can be decomposed as $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $O_k \in \boldsymbol{B}(\mathsf{Rng}(X_k))$ $\forall k \in \mathsf{S}$, then the statement (59) is equivalent to

$$\forall k \in \mathsf{S}\ O_k \in \boldsymbol{B}(\mathsf{Rng}(X_k)),$$

$$\sum_{k \in \mathsf{S}} \mathrm{Tr}_{\mathcal{K}}[(I_{\mathcal{H}_k} \otimes X_k)^\dagger (I_{\mathcal{H}_k} \otimes O_k)(I_{\mathcal{H}_k} \otimes X_k)] = 0 \Rightarrow O_k = 0\ \forall\ k \in \mathsf{S}, \tag{60}$$

or else

$$\forall k \in \mathsf{S} \quad O_k \in \boldsymbol{B}(\mathsf{Rng}(X_k)),$$

$$\mathrm{Tr}_{\mathcal{K}}[\oplus_{k \in \mathsf{S}} (I_{\mathcal{H}_k} \otimes X_k)^\dagger (I_{\mathcal{H}_k} \otimes O_k)(I_{\mathcal{H}_k} \otimes X_k)] = 0 \Rightarrow O_k = 0\ \forall\ k \in \mathsf{S}, \tag{61}$$

The vanishing of the partial trace can be written as the vanishing of the trace $\mathrm{Tr}[\oplus_{k \in \mathsf{S}} (I_{\mathcal{H}_k} \otimes X_k)^\dagger (I_{\mathcal{H}_k} \otimes O_k)(I_{\mathcal{H}_k} \otimes X_k)(I_{\mathcal{K}} \otimes C)]$ for any $C \in \boldsymbol{B}(\mathcal{H})$, namely the vanishing of $\mathrm{Tr}\{\oplus_{k \in \mathsf{S}} O_k X_k\, \mathrm{Tr}_{\mathcal{H}_k}[P_k (I_{\mathcal{K}} \otimes C) P_k] X_k^\dagger\}$ for any $C \in \boldsymbol{B}(\mathcal{H})$, and upon defining $S = \oplus_{k \in \mathsf{S}} O_k$, the statement (61) rewrites

$$S \in \oplus_{k \in \mathsf{S}} \boldsymbol{B}(\mathsf{Rng}(X_k)), \quad \mathrm{Tr}\{S \oplus_{k \in \mathsf{S}} X_k\, \mathrm{Tr}_{\mathcal{H}_k}[P_k (I_{\mathcal{K}} \otimes \boldsymbol{B}(\mathcal{H})) P_k] X_k^\dagger\} = 0 \Rightarrow S = 0, \tag{62}$$

namely, since the only operator in the linear space $\oplus_{k \in \mathsf{S}} \boldsymbol{B}(\mathsf{Rng}(X_k))$ orthogonal to the subspace $\oplus_{k \in \mathsf{S}} X_k\, \mathrm{Tr}_{\mathcal{H}_k}[P_k (I_{\mathcal{K}} \otimes \boldsymbol{B}(\mathcal{H})) P_k] X_k^\dagger$ is the null operator, one has

$$\oplus_{k \in \mathsf{S}} \boldsymbol{B}(\mathsf{Rng}(X_k)) = \oplus_{k \in \mathsf{S}} X_k\, \mathrm{Tr}_{\mathcal{H}_k}[P_k (I_{\mathcal{K}} \otimes \boldsymbol{B}(\mathcal{H})) P_k] X_k^\dagger. \tag{63}$$

■

Corollary 6: As in Theorem 4, a necessary condition for extremality is

$$\sum_{k \in \mathsf{S}} \mathrm{rank}(X_k)^2 \leqslant \dim(\mathcal{H})^2. \tag{64}$$

Corollary 7: Any rank-one covariant QO is extremal.

Proof: For $\mathrm{rank}(X) = 1$ the set S must contain only one equivalence class, and the iff condition (57) of Theorem 4 is then trivially satisfied. ■

Corollary 8: For an irreducible representation any extremal covariant QO must be rank-one.

Corollary 9 (Choi): In the noncovariant case, a QO $\mathcal{M}$ from $\boldsymbol{B}(\mathcal{K})$ to $\boldsymbol{B}(\mathcal{H})$ is extremal iff it can be written in the form $\mathcal{M}(O) = \Sigma_i\, W_i^\dagger O W_i$, with $W_i \in \boldsymbol{B}(\mathcal{H}, \mathcal{K})$ and the set of operators $\{W_i^\dagger W_j\}$ linearly independent.

Proof: The noncovariant case corresponds to the trivial covariance group $\mathbf{G} = \mathbf{I}$, i.e., the group containing only the identity element. This corresponds to have just a single equivalence class, with multiplicity equal to $\dim(\mathcal{H} \otimes \mathcal{K})$. Then, as in the proof of point (2) of Theorem 4 the extremality of $R = X^\dagger X \in \boldsymbol{B}(\mathcal{H} \otimes \mathcal{K})$ is equivalent to the injectivity of the map $\mathcal{W}(A) = \mathrm{Tr}_{\mathcal{K}}[X^\dagger A X]$ on $\boldsymbol{B}(\mathsf{Rng}(X))$. According to Lemma 2, using the singular value decomposition $X = \Sigma_i\, |V_i\rangle\langle W_i|$, with $|V_i\rangle$ orthonormal basis for $\mathsf{Rng}(X)$ and $|W_i\rangle \in \mathcal{K} \otimes \mathcal{H}$, one has $\mathcal{M}(O) = \Sigma_i\, W_i^\dagger O W_i$ for $O \in \boldsymbol{B}(\mathcal{K})$, and $\mathcal{W}(A) = \Sigma_{ij}\, \langle V_i | A | V_j \rangle W_i^\tau W_j^*$ for $A \in \boldsymbol{B}(\mathsf{Rng}(X))$, and injectivity of $\mathcal{W}$ is equivalent to linear

TABLE I. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the kth equivalence class of irreducible representations for 1 to 2 phase-covariant cloning. The orthonormal basis are chosen as subsets of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{H}$.

k	$\lvert k_i\rangle \otimes \lvert h_j\rangle$
−1	$\lvert 001\rangle$
0	$\lvert 101\rangle, \lvert 011\rangle, \lvert 000\rangle$
1	$\lvert 100\rangle, \lvert 010\rangle, \lvert 111\rangle$
2	$\lvert 110\rangle$

independence of the set of operators $\{W_i^\dagger W_j\}$. ■

Corollary 9 is the same as Choi theorem.[17] Notice that differently from the case of QO's, for POVM's the noncovariant case cannot be recovered as a special case of the covariant classification, since the group itself (or, more generally, the homogeneous factor space) coincides with the probability space $\mathcal{X}$ of the POVM, whence trivializing **G** also trivializes $\mathcal{X}$.

A. Example

Consider the phase-covariant cloning[16,22] for equatorial qubits from 1 to 2 copies. This corresponds to $\mathbf{G} = \mathbb{U}(1)$, with representations $U_\phi = e^{i\phi |1\rangle\langle 1|_0}$ and $V_\phi = e^{i\phi \Sigma_{s=1}^2 |1\rangle\langle 1|_s}$ where $s=0$ denotes the input qubit and $s=1,2$ the output ones. Here $\mathcal{H} = \mathbb{C}^2$ and $\mathcal{K} = \mathcal{H}^{\otimes 2}$. We first need to decompose the representation $V_\phi \otimes U_\phi^*$. This is made of one-dimensional representations, with characters $e^{ik\phi}$, with $k = -1, 0, 1, 2$ and multiplicities $m_{-1}=1$, $m_0=3$, $m_1=3$, and $m_2=1$. The necessary condition (64) in the present case becomes $\Sigma_{k\in \mathsf{S}} \operatorname{rank}(X_k)^2 \leqslant \dim(\mathcal{H})^2 = 4$, which means that we can have either a single equivalence class with $\operatorname{rank}(X_k) \leqslant 2$, or two equivalence classes with $\operatorname{rank}(X_k) = 1$ each. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the kth equivalence class of irreducible representations are reported in Table I as subset of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{H}$.

The operators $R = \Sigma_{k\in \mathsf{S}} R_k = \Sigma_{k\in \mathsf{S}} \Sigma_l \lvert\psi_l^{(k)}\rangle\langle\psi_l^{(k)}\rvert$ satisfying the necessary conditions and the trace-preserving condition are reported in Table II. It is easy to check that the case of $\operatorname{rank}(X_k) = 2$, which would be possible only for $k=0$ or $k=1$, does not satisfy the iff condition (56). Therefore it is possible to have only rank-one operators X_k.

As a specific optimization problem, let us consider the maximization of the fidelity averaged over the two outputs

TABLE II. Cloning from 1 to 2 copies: classification of operators $R = \Sigma_{k\in \mathsf{S}} R_k = \Sigma_{k\in \mathsf{S}} \Sigma_l \lvert\psi_l^{(k)}\rangle\langle\psi_l^{(k)}\rvert$ satisfying the necessary condition.

$\mathsf{S} \doteq \{k\}$	$\{\lvert\psi_l^{(k)}\rangle\}$	$\{\lvert\psi_l^{(k')}\rangle\}$	
$\{-1,2\}$	$\lvert 001\rangle$	$\lvert 110\rangle$	
$\{0,1\}$	$a\lvert 000\rangle + b\lvert 011\rangle + c\lvert 101\rangle$	$a'\lvert 111\rangle + b'\lvert 100\rangle + c'\lvert 010\rangle$	$\lvert a\rvert^2 + \lvert b'\rvert^2 + \lvert c'\rvert^2 = 1$
			$\lvert a'\rvert^2 + \lvert b\rvert^2 + \lvert c\rvert^2 = 1$
$\{0,-1\}$	$\lvert 000\rangle + a\lvert 011\rangle + b\lvert 101\rangle$	$c\lvert 001\rangle$	$\lvert a\rvert^2 + \lvert b\rvert^2 + \lvert c\rvert^2 = 1$
$\{1,-1\}$	$a\lvert 100\rangle + b\lvert 010\rangle + c\lvert 111\rangle$	$d\lvert 001\rangle$	$\lvert a\rvert^2 + \lvert b\rvert^2 = 1$
			$\lvert c\rvert^2 + \lvert d\rvert^2 = 1$
$\{1,2\}$	$a\lvert 100\rangle + b\lvert 010\rangle + \lvert 111\rangle$	$d\lvert 110\rangle$	$\lvert a\rvert^2 + \lvert b\rvert^2 + \lvert d\rvert^2 = 1$
$\{0,2\}$	$a\lvert 000\rangle + b\lvert 011\rangle + c\lvert 101\rangle$	$d\lvert 110\rangle$	$\lvert a\rvert^2 + \lvert d\rvert^2 = 1$
			$\lvert b\rvert^2 + \lvert c\rvert^2 = 1$
$\{0\}$	$1/\sqrt{2}\lvert 101\rangle + 1/\sqrt{2}\lvert 011\rangle, \lvert 000\rangle$		
$\{1\}$	$1/\sqrt{2}\lvert 010\rangle + 1/\sqrt{2}\lvert 100\rangle, \lvert 111\rangle$		

TABLE III. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the kth equivalence class of irreducible representations for 1 to 3 phase-covariant cloning. The orthonormal basis are chosen as subsets of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{H}$.

k	$\lvert k_i\rangle \otimes \lvert h_j\rangle$
−1	$\lvert 0001\rangle$
0	$\lvert 1001\rangle, \lvert 0101\rangle, \lvert 0011\rangle, \lvert 0000\rangle$
1	$\lvert 1000\rangle, \lvert 0100\rangle, \lvert 0010\rangle, \lvert 1101\rangle, \lvert 1011\rangle, \lvert 0111\rangle$
2	$\lvert 1100\rangle, \lvert 1010\rangle, \lvert 0110\rangle, \lvert 1111\rangle$
3	$\lvert 1110\rangle$

$$F = \langle\psi|\tfrac{1}{2}\{\mathrm{Tr}_1[\mathcal{M}^\tau(|\psi\rangle\langle\psi|)] + \mathrm{Tr}_2[\mathcal{M}^\tau(|\psi\rangle\langle\psi|)]\}|\psi\rangle = \mathrm{Tr}\left[\tfrac{1}{2}(I \otimes |\psi\rangle\langle\psi| + |\psi\rangle\langle\psi| \otimes I)\mathcal{M}^\tau(|\psi\rangle\langle\psi|)\right] \tag{65}$$

and for equatorial qubits we can choose $|\psi\rangle = |+\rangle$, where $|\pm\rangle \doteq (1/\sqrt{2})(|0\rangle \pm |1\rangle)$. Then the fidelity rewrites as

$$F = \mathrm{Tr}[W R_{\mathcal{M}}], \tag{66}$$

$$W = |+\rangle\langle+|^{\otimes 3} + \tfrac{1}{2}(|-\rangle\langle-| \otimes |+\rangle\langle+| + |+\rangle\langle+| \otimes |-\rangle\langle-|) \otimes |+\rangle\langle+|. \tag{67}$$

One can see that W is invariant for permutations over the output copies, and, by construction, also all vectors in Table II have the same symmetry. Due to the special form of the fidelity, the optimal map [satisfying $\mathcal{M}(I_{\mathcal{K}}) = I_{\mathcal{H}}$] is obtained for $\mathsf{S} = \{0, 1\}$ with corresponding rank-two operator $R_{\mathcal{M}}$ given by

$$R_{\mathcal{M}} = |\psi^{(0)}\rangle\langle\psi^{(0)}| + |\psi^{(1)}\rangle\langle\psi^{(1)}|,$$

$$|\psi^{(0)}\rangle - = \frac{1}{\sqrt{2}}\left(|000\rangle + \frac{1}{\sqrt{2}}|011\rangle + \frac{1}{\sqrt{2}}|101\rangle\right),$$

$$|\psi^{(1)}\rangle - = \frac{1}{\sqrt{2}}\left(|111\rangle + \frac{1}{\sqrt{2}}|100\rangle + \frac{1}{\sqrt{2}}|010\rangle\right), \tag{68}$$

B. Example

Consider the phase-covariant cloning[16,22] for equatorial qubits from 1 to 3 copies. This correspond to $\mathbf{G} = \mathbb{U}(1)$, with representations $U_\phi = e^{i\phi|1\rangle\langle 1|_0}$ and $V_\phi = e^{i\phi\Sigma_{s=1}^3 |1\rangle\langle 1|_k}$ where $s = 0$ denotes the input qubit and $s = 1, 2, 3$ the output ones. Here $\mathcal{H} = \mathbb{C}^2$ and $\mathcal{K} = \mathcal{H}^{\otimes 3}$. We first need to decompose the representation $V_\phi \otimes U_\phi^*$. This is made of one-dimensional representations, with characters $e^{ik\phi}$, with $k = -1, 0, 1, 2, 3$ and multiplicities $m_{-1} = 1$, $m_0 = 4$, $m_1 = 6$, $m_2 = 4$, and $m_3 = 1$. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the kth equivalence class of irreducible representations are reported in Table III as subset of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{H}$. Again, since $\dim(\mathcal{H}) = 2$, the necessary condition (64) says that we can have only one equivalence class k with $\mathrm{rank}(X_k) \leqslant 2$, or two equivalence classes both with $\mathrm{rank}(X_k) = 1$. In Ref. 22 it is shown that the map which optimizes the averaged equatorial fidelity is actually given by the rank-one map for $\mathsf{S} = \{1\}$ with corresponding operator $R_{\mathcal{M}}$ given by

$$R_{\mathcal{M}} = |\psi^{(1)}\rangle\langle\psi^{(1)}|,$$

$$|\psi^{(1)}\rangle = \frac{1}{\sqrt{3}}(|1000\rangle + |0100\rangle + |0010\rangle + |1101\rangle + |1011\rangle + |0111\rangle). \tag{69}$$

Notice that, as a consequence of the specific symmetric form of the chosen fidelity criterion, the cloning maps of the examples in Secs. VI A and VI B are both symmetrical, namely the output Hilbert space is indeed restricted to the symmetric tensor space $(\mathcal{H}^{\otimes n})_+$. Clearly, with the same method also nonsymmetric types of cloning can be analyzed well.

C. Example

Consider a generic covariant QO with $\mathcal{K} \simeq \mathcal{H}$, $V_g = U_g$, and $\mathbf{G} = \mathrm{SU}(d)$, where $d = \dim(\mathcal{H})$. In this case the representation $U_g \otimes U_g^*$ has two irreducible components, one which is one dimensional, corresponding to the invariant vector $|I\rangle \in \mathcal{H}^{\otimes 2}$, and one on the orthogonal complement, and the two components will be denoted by $k=0$ and $k=1$, respectively. Since both the irreducible components of the representation have unit multiplicity, the operator $R = X^\dagger X$ must have $X = \Sigma_{k\in \mathsf{S}}\, c_k P_k$, $c_k \in \mathbb{C}$, P_k denoting the orthogonal projector on the invariant space of the irreducible component k, and the necessary condition (64) is trivially satisfied. On the other hand, one can see that the iff condition (56) is satisfied for the irreducible representations $\mathsf{S} = \{0\}$ and $\mathsf{S} = \{1\}$, whereas for the reducible one $\mathsf{S} = \{0,1\}$ the map $\mathcal{T}(O) = \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X]$ is never injective on $\boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X))$ [one has $\mathrm{Tr}_{\mathcal{K}}[X^\dagger O X] = (1/d)[|c_0|^2 a_0 + (d^2-1)|c_1|^2 a_1] I_{\mathcal{H}}$ for $O = a_0 P_0 + a_1 P_1$, $a_0, a_1 \in \mathbb{C}$]. Therefore, the only trace-preserving optimal maps are those corresponding to the operators $R = |I\rangle\langle I|$ and $R = [d/(d^2-1)](I^{\otimes 2} - (1/d)|I\rangle\langle I|)$, corresponding to the trivial map $\mathcal{M} = \mathcal{J}$ and to the so-called isotropic depolarizing channel $\mathcal{M}(O) = [d/(d^2-1)]\mathrm{Tr}[O] I_{\mathcal{H}} - [1/(d^2-1)]\rho$. Finally, notice that in the present example the optimal covariant maps are compatible only with (multiple of) the trace-preserving condition, since both partial traces $\mathrm{Tr}_{\mathcal{K}}[P_k]$ are proportional to the identity.

D. Example

We consider now the same problem as in the previous example, but now with $V_g = U_g^*$. In this case we need to consider the positive operators R which are invariant under $U_g^* \otimes U_g^*$. It will be easier to consider the representation $U_g \otimes U_g$ and then take the complex conjugate of R at the end. Now we have again two irreducible inequivalent components, say $k = \pm$ with invariant spaces $(\mathcal{H}^{\otimes 2})_\pm$, the symmetric and the antisymmetric spaces. As in the previous example, the general form of $R = X^\dagger X$ is $X = \Sigma_{k\in \mathsf{S}}\, c_k P_k$, $c_k \in \mathbb{C}$, and $P_\pm = \frac{1}{2}(I_{\mathcal{H}}^{\otimes 2} \pm E)$, where E is the swap operator on the tensor product. However, the map $\mathcal{T}(O) = \mathrm{Tr}_{\mathcal{K}}[X^\dagger O X]$ is injective on $\boldsymbol{A}'_{\mathbf{G}} \cap \boldsymbol{B}(\mathsf{Rng}(X))$ only for representations with a single irreducible component. One can see that $\mathrm{Tr}_{\mathcal{H}}[P_\pm] = \frac{1}{2}(d \pm 1) I_{\mathcal{H}}$, and only trace-preserving (or multiplying by a constant) QO's are compatible with the present covariance. In conclusion, the only extremal covariant operators are $R_\pm = (d \pm 1)^{-1}(I^{\otimes 2} \pm E)$, corresponding to the channels $\mathcal{M}_\pm(O) = (d \pm 1)^{-1}[\mathrm{Tr}(O) I_{\mathcal{H}} \pm O^\tau]$. The map $\mathcal{M}_+$ is the optimal transposition map of Ref. 26.

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Derivation of the supersymmetric Harish-Chandra integral for UOSp($k_1/2k_2$)

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The previous supersymmetric generalization of the unitary Harish-Chandra integral prompted the conjecture that the Harish-Chandra formula should have an extension to superspaces. We prove this conjecture for the unitary orthosymplectic supermanifold UOSp($k_1/2k_2$). To this end, we construct and solve an eigenvalue equation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1781746]

I. INTRODUCTION

Harish-Chandra[1] gave a closed formula for a class of group integrals. Let $\mathcal{G}$ be a compact semisimple Lie group and let a and b fixed elements in the Cartan subalgebra $\mathcal{H}_0$ of $\mathcal{G}$. Harish-Chandra's formula then reads

$$\int_{U\in\mathcal{G}} \exp(\mathrm{tr}\ U^{-1}aUb)d\mu(U) = \frac{1}{|\mathcal{W}|}\sum_{w\in\mathcal{W}} \frac{\exp(\mathrm{tr}\ w(a)b)}{\Pi(a)\Pi(w(b))}, \tag{1.1}$$

where $d\mu(U)$ stands for the properly normalized invariant measure and $\Pi(a)$ for the product of all positive roots of $\mathcal{H}_0$. Moreover, $\mathcal{W}$ is the Weyl reflection group of $\mathcal{G}$ and $|\mathcal{W}|$ is the number of its elements. We notice that the integrals (1.1) should not be confused with Gelfand's spherical functions.[2–5] They are defined by a group integral which looks at first sight just like the one in Eq. (1.1), however, for Gelfand's spherical functions, a and b are not in the Cartan subalgebra. Thus, Gelfand's spherical functions are very different objects. Only in the case of $\mathcal{G}=\mathrm{SU}(N)$, the Harish-Chandra integral (1.1) coincides with the unitary spherical function of Gelfand. It is known as the Itzykson–Zuber integral.[6] A very handy diffusion equation method was developed in Ref. 6 to derive this unitary case.

A supersymmetric generalization of the Itzykson–Zuber integral, i.e., the extension of the Harish-Chandra integral to the case of the unitary supermanifold U(k_1/k_2), was first obtained in Ref. 7 by generalizing the Itzykson–Zuber diffusion equation method to supersymmetry. In its most general form, this integral was obtained in Ref. 8 as an application of Gelfand–Tzetlin coordinates for U(k_1/k_2) and also in Ref. 9 by employing the methods as given in Ref. 7.

Serganova[10] and Zirnbauer[11] conjectured that Harish-Chandra's formula should not only have a supersymmetric extension in the unitary case, but also generalize to all classical supermanifolds $\mathcal{SG}$ which can be viewes as certain extensions of the ordinary Lie groups. Thus, one would expect a result of the following form to hold,

$$\int_{u\in\mathcal{SG}} \exp(\mathrm{trg}\ u^{-1}sur)d\mu(u) = \frac{1}{|\mathcal{SW}|}\sum_{w\in\mathcal{SW}} \frac{\exp(\mathrm{trg}\ w(s)r)}{\pi(s)\pi(w(r))}, \tag{1.2}$$

where s and r are in the Cartan subalgebra $\mathcal{SH}_0$ of $\mathcal{SG}$. The Weyl reflection group $\mathcal{SW}$ and the root system $\pi(s)$ have to be properly generalized to superspace, $|\mathcal{SW}|$ is the number of elements in $\mathcal{SW}$. The extension of the Harish-Chandra integral to the case of the unitary supermanifold U(k_1/k_2) is certainly of the form (1.2). The most interesting remaining case is the unitary ortho-

symplectic supermanifold $\mathrm{UOSp}(k_1/2k_2)$. For this case, we present a proof of the conjecture (1.2) in this note. In Sec. II, we state and derive the supersymmetric Harish-Chandra integral for $\mathrm{UOSp}(k_1/2k_2)$. We summarize and conclude in Sec. III.

II. THE SUPERMANIFOLD INTEGRAL AND ITS DERIVATION

After briefly summarizing properties of the supermanifold $\mathrm{UOSp}(k_1/2k_2)$ and introducing our notation in Sec. II A, we state the supermanifold integral in Sec. II B. The solution is sketched in the following two sections. In Sec. II C, we formulate an eigenvalue equation for the integral. It is solved by separation in Sec. II D.

A. The supermanifold $\mathrm{UOSp}(k_1/2k_2)$

Kac[12,13] gave a classification of the classical superalgebras similar to Cartan's classification of the Lie algebras in ordinary space. In principle, to each classical superalgebra a supergroup is associated by the exponential mapping. However, the classification pattern of the supergroups is usually somewhat coarser.[14,15] If one omits the supergroup stemming from the exceptional superalgebras, one is left with only four different types of subgroups of the general linear supergroup $\mathrm{GL}(k_1/k_2)$, namely the unitary supergroup $\mathrm{U}(k_1/k_2)$ the orthosymplectic supergroup $\mathrm{OSp}(k_1/2k_2)$ and the supergroups associated with the strange superalgebras $\mathrm{P}(k)$ and $\mathrm{Q}(k)$. The supergroup $\mathrm{OSp}(k_1/2k_2)$ consists of the elements u in $\mathrm{GL}(k_1/2k_2)$ which leave invariant the metric

$$L = \mathrm{diag}(1_{k_1}, J), \tag{2.1}$$

such that $u^T L u = L$. Here, J is the symplectic metric

$$J = \tau^{(1)} \otimes 1_{k_2} = \begin{bmatrix} 0 & 1_{k_2} \\ -1_{k_2} & 0 \end{bmatrix}, \quad \text{with} \quad \tau^{(1)} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{2.2}$$

Especially important in physical applications are the supergroup $\mathrm{U}(k_1/k_2)$ and the supermanifold $\mathrm{UOSp}(k_1/2k_2)$, formed by the elements of $\mathrm{OSp}(k_1/2k_2)$ which fulfill the additional condition $u^\dagger u = 1$. It contains the compact ordinary groups $\mathrm{O}(k_1)$ and $\mathrm{USp}(2k_2)$ as subgroups. However, it is strictly speaking not a compact real form of $\mathrm{OSp}(k_1/2k_2)$, see Appendix A and Refs. 16 and 17. While the fermionic dimension $2k_2$ of $\mathrm{UOSp}(k_1/2k_2)$ is always even, the bosonic dimension k_1 can be even or odd, eventually resulting in some slight differences for the supermanifold integral. One can also define the superalgebra $\mathrm{uosp}(k_1/2k_2)$ connected as usual to the supermanifold $\mathrm{UOSp}(k_1/2k_2)$ via the exponential mapping.[15] For $\sigma \in \mathrm{uosp}(k_1/2k_2)$ we have $u = \exp(\sigma) \in \mathrm{UOSp}(k_1/2k_2)$. These generators σ span the superalgebra. An element of this superalgebra can be written as

$$\sigma = \begin{bmatrix} \sigma^{(\mathrm{o})} & \sigma^{(\mathrm{a})\dagger} & & -\sigma^{(\mathrm{a})T} \\ \sigma^{(\mathrm{a})} & & & \\ & & \sigma^{(\mathrm{usp})} & \\ \sigma^{(\mathrm{a})*} & & & \end{bmatrix}. \tag{2.3}$$

The $k_1 \times k_1$ matrix $\sigma^{(\mathrm{o})}$ is antisymmetric, it is in the algebra $\mathrm{o}(k_1)$ and generates the ordinary group $\mathrm{O}(k_1)$. The $2k_2 \times 2k_2$ matrix $\sigma^{(\mathrm{usp})}$ is in the algebra $\mathrm{usp}(2k_2)$ and generates the ordinary group $\mathrm{USp}(2k_2)$, i.e. in the basis defined by Eq. (2.1) it is of the form

$$\sigma^{(\mathrm{usp})} = \begin{bmatrix} \sigma^{(\mathrm{usp},1)} & -\sigma^{(\mathrm{usp},2)} \\ \sigma^{(\mathrm{usp},2)\dagger} & -\sigma^{(\mathrm{usp},1)T} \end{bmatrix}. \tag{2.4}$$

Here $\sigma^{(\mathrm{usp},1)}$ is a skew–Hermitian matrix and $\sigma^{(\mathrm{usp},2)}$ is complex symmetric. The $k_2 \times k_1$ matrix $\sigma^{(\mathrm{a})}$ in Eq. (2.3) contains $k_1 k_2$ independent complex anticommuting variables, it is in the sector $\mathrm{usop}(k_1/2k_2) - \mathrm{o}(k_1) - \mathrm{usp}(2k_2)$. The asterisk denotes the complex conjugate of the second kind for

Grassmann variables. One uses the supertrace denoted by trg to define an invariant bilinear form on the superalgebra. Although the algebra uosp$(k_1/2k_2)$ defined by the matrices σ in Eq. (2.3) is closely related to the algebra of the orthosymplectic group osp$(k_1/2k_2)$ we avoid the notation of a real form of osp$(k_1/2k_2)$ since it cannot be derived from osp$(k_1/2k_2,R)$ by an involutive automorphism.[17]

Particularly important in the present context is the Cartan subalgebra uosp$^{(0)}(k_1/2k_2)$ of uosp$(k_1/2k_2)$. As in the theory of Lie–algebras in ordinary space there is a difference for the orthogonal group in even or odd dimension. We introduce the notation $[k_1/2]$ for the integer part of $k_1/2$. Then, for even bosonic dimension $[k_1/2]=k_1/2$, the elements of uosp$^{(0)}(k_1/2k_2)$ are the matrices

$$\sigma^{(0)} = \mathrm{diag}(s_{11}\tau^{(1)}, \ldots, s_{[k_1/2]1}\tau^{(1)}, is_{12}, \ldots, is_{k_2 2}, -is_{12}, \ldots, -is_{k_2 2}), \tag{2.5}$$

while for odd bosonic dimension $[k_1/2]=(k_1-1)/2$, the Cartan subalgebra uosp$^{(0)}(k_1/2k_2)$ consists of the matrices

$$\sigma^{(0)} = \mathrm{diag}(s_{11}\tau^{(1)}, \ldots, s_{[k_1/2]1}\tau^{(1)}, 0, is_{12}, \ldots, is_{k_2 2}, -is_{12}, \ldots, -is_{k_2 2}). \tag{2.6}$$

Thus, uosp$^{(0)}(k_1/2k_2)$ is the direct sum of the Cartan subalgebras o(k_1) and usp$(2k_2)$. We could now work with the superalgebra as defined above. However, we redefine it by a procedure similar to a Wick rotation. In most of the physics literature, this is done to ensure convergence of the integrals in superspace, see for example Ref. 21. Although the Wick rotation is not necessary in the present context, we decided to redefine the superalgebra to keep with the notation in the physics literature and in previous work on the unitary supergroup.[7–9] Hence, we proceed as follows. The Killing–Cartan form of the supermatrices defined in Eqs. (2.5) and (2.6) is not negative definite. We define another set of diagonal supermatrices by

$$s = \begin{bmatrix} i & 0 \\ 0 & 1 \end{bmatrix} \sigma^{(0)}, \tag{2.7}$$

such that always trg $s^2>0$. In the sequel we use exclusively the set of supermatrices s. We denote it also by uosp$^{(0)}(k_1/2k_2)$. By the same token we refer to its orbits under the group action $\sigma = u^{-1}su$, $u \in \mathrm{UOSp}(k_1/2k_2)$ as the superalgebra uosp$(k_1/2k_2)$. We emphasize once more that this redefinition has no direct impact in the present context.

A remark is in order for the mathematically oriented reader. The object UOSp$(k_1/2k_2)$ defined above is not included in the usual classification of symmetric superspaces. However, it still is a group in the naive, but in the present context crucial, sense that it describes generalized rotations in a superspace. It belongs to a class of supermanifolds which have been termed cs manifolds in Ref. 18. We refer the reader to the literature for further reading on the classification of supermanifolds[12–16,19,20] and to Appendix A. For this reason we refer to UOSp$(k_1/2k_2)$ defined above always as *supermanifold*.

B. Statement of the supermanifold integral

We can now write formula (1.2) for the case of the supermanifold UOSp$(k_1/2k_2)$ more explicitly. For two fixed elements s and r of the Cartan subalgebra uosp$^{(0)}(k_1/2k_2)$, we have

$$\int_{u\in \mathrm{UOSp}(k_1/2k_2)} \exp(i\ \mathrm{trg}\ u^{-1}sur)d\mu(u) = \frac{1}{[k_1/2]!\,k_2!} \frac{(\det[\cos(2s_{p1}r_{q1})] + \det[i\ \sin(2s_{p1}r_{q1})])\det[-2i\ \sin(2s_{p2}r_{q2})]}{B_{k_1 2k_2}(s)B_{k_1 2k_2}(r)} \tag{2.8}$$

for k_1 even and

$$\int_{u\in \mathrm{UOSp}(k_1/2k_2)} \exp(i\ \mathrm{trg}\ u^{-1}sur)d\mu(u) = \frac{1}{[k_1/2]!\,k_2!}\frac{\det[i\ \sin(2s_{p1}r_{q1})]\det[2\ \cos(2s_{p2}r_{q2})]}{B_{k_1 2k_2}(s)B_{k_1 2k_2}(r)} \tag{2.9}$$

for k_1 odd. We introduced the function $B_{k_1 2k_2}(s)$ which is given by

$$B_{k_1 2k_2}(s) = 2^{k_2}\frac{\prod_{p<q}(s_{p1}^2 - s_{q1}^2)\prod_{p<q}(s_{p2}^2 - s_{q2}^2)\prod_{p=1}^{k_2} s_{p2}}{\prod_{p,q}(s_{p1}^2 + s_{q2}^2)} \tag{2.10}$$

for even bosonic dimension k_1 and by

$$B_{k_1 2k_2}(s) = 2^{k_2}\frac{\prod_{p<q}(s_{p1}^2 - s_{q1}^2)\prod_{p<q}(s_{p2}^2 - s_{q2}^2)\prod_{p=1}^{[k_1/2]} s_{p1}}{\prod_{p,q}(s_{p1}^2 + s_{q2}^2)} \tag{2.11}$$

for odd bosonic dimension k_1. These two formulas differ only in the last terms of the numerators.

Formulas (2.8) and (2.9) contain, as special cases, the ordinary orthogonal and unitary symplectic Harish-Chandra integrals for $\mathcal{G}=\mathrm{SO}(k_1)$ and for $\mathcal{G}=\mathrm{USp}(2k_2)$, if we set $k_2=0$ or $k_1=0$, respectively. Thus, the derivation of the supersymmetric integral to follow also includes a rederivation of those ordinary integrals. For equal bosonic and fermionic dimension, formula (2.8) was conjectured in Ref. 11 and used to calculate the correlation functions in a certain circular random matrix ensemble.

We mention in passing that the invariant measure $d\mu(u)$ and its normalization relate to nontrivial questions of certain boundary contributions in superanalysis[22] which are highly important in applications. In the present context, however, we do not need to go into this.

C. Eigenvalue equation

The main idea for the derivation of formulas (2.8) and (2.9) is to properly modify the supersymmetric extension[7] of the Itzykson–Zuber diffusion equation method[6] to the present case. It turns out that it is somewhat more convenient to construct the eigenvalue equation associated with the diffusion equation. The two equations are related by Fourier expansion. Such an eigenvalue equation for the ordinary case of SU(N) as originally discussed by Itzykson and Zuber[6] was constructed by Brézin.[23] Berezin and Karpelevich[24] had studied such an eigenvalue equation to calculate the twofold group integral named after them, see also Ref. 25. To construct the eigenvalue equation needed to derive formulas (2.8) and (2.9), we adjust the steps made in Refs. 26 and 27, where a supersymmetric eigenvalue equation was employed for the extension of the Berezin–Karpelevich integral.

We introduce the Laplace operator over the superalgebra $\mathrm{uosp}(k_1/2k_2)$

$$\Delta = \frac{1}{2}\sum_{p<q}^{k_1}\frac{\partial^2}{\partial\,\sigma_{pq}^{(\mathrm{o})2}} + \sum_{p,q}^{2k_2}\frac{1+\delta_{pq}}{4}\frac{\partial^2}{\partial\,\sigma_{pq}^{(\mathrm{usp})}\,\partial\,\sigma_{pq}^{(\mathrm{usp})*}} + \frac{1}{2}\sum_{p=1}^{k_1}\sum_{q=1}^{k_2}\frac{\partial^2}{\partial\,\sigma_{pq}^{(\mathrm{a})}\,\partial\,\sigma_{pq}^{(\mathrm{a})*}}. \tag{2.12}$$

Its eigenfunctions are the plane waves $\exp(i\ \mathrm{trg}\ \sigma\rho)$ with both matrices $\sigma,\rho\in\mathrm{uosp}(k_1/2k_2)$. Thus, we have

$$\Delta\ \exp(i\ \mathrm{trg}\ \sigma\rho) = -\ \mathrm{trg}\ \rho^2\ \exp(i\ \mathrm{trg}\ \sigma\rho). \tag{2.13}$$

We now diagonalize both matrices according to $\sigma=u^{-1}su$ and $\rho=v^{-1}rv$, where u and v are in the supermanifold $\mathrm{UOSp}(k_1/2k_2)$ and s and r are in the Cartan subalgebra $\mathrm{uosp}^{(0)}(k_1/2k_2)$, i.e., given

by Eq. (2.5) or Eq. (2.6), respectively. Integrating both sides over v and using the invariance of the measure $d\mu(v)$, we arrive at the radial eigenvalue equation

$$\Delta_s \chi_{k_1 2k_2}(s,r) = -\operatorname{trg} r^2 \chi_{k_1 2k_2}(s,r), \tag{2.14}$$

where, now using u instead of v again, the function

$$\chi_{k_1 2k_2}(s,r) = \int_{u \in \mathrm{UOSp}(k_1/2k_2)} \exp(i \operatorname{trg} u^{-1} s u r) d\mu(u) \tag{2.15}$$

is the integral we want to calculate. The operator Δ_s in Eq. (2.14) is the radial part of Δ. The term radial refers to the Cartan subalgebra. This usage which is common in mathematics should not lead to confusions with the radial operators used, for example, in Refs. 28–31 where quite different spaces were studied. To obtain the radial operator Δ_s, we need the Jacobian, or Berezinian, of the variable transformation $\sigma = u^{-1} s u$. This Berezinian is given by the the functions $B^2_{k_1 2k_2}(s)$ of Eqs. (2.10) and (2.11). It was not possible for us to find out where this Berezinian was first obtained, and we do not claim originality for its calculation. In any case, to make the paper self-contained, we sketch the calculation in Appendix B. Hence, the radial part of the Laplacian over $\mathrm{uosp}(k_1/2k_2)$ reads

$$\Delta_s = \frac{1}{2} \sum_{p=1}^{[k_1/2]} \frac{1}{B^2_{k_1 2k_2}(s)} \frac{\partial}{\partial s_{p1}} B^2_{k_1 2k_2}(s) \frac{\partial}{\partial s_{p1}} + \frac{1}{2} \sum_{p=1}^{k_2} \frac{1}{B^2_{k_1 2k_2}(s)} \frac{\partial}{\partial s_{p2}} B^2_{k_1 2k_2}(s) \frac{\partial}{\partial s_{p2}}. \tag{2.16}$$

The number of bosonic eigenvalues is $[k_1/2]$, i.e., identical for the pairs $\mathrm{uosp}(k_1/2k_2)$ and $\mathrm{uosp}(k_1+1/2k_2)$ with k_1 even. However, the operator Δ_s is not the same in these two cases, because the functions (2.10) and (2.11) differ.

D. Solution by separation

The Laplacian (2.16) is separable. We make an ansatz for the supermanifold integral which separates off the square roots of the Berezinians,

$$\chi_{k_1 2k_2}(s,r) = \frac{\omega_{k_1 2k_2}(s,r)}{B_{k_1 2k_2}(s) B_{k_1 2k_2}(r)}. \tag{2.17}$$

A tedious but straightforward calculation then yields the trivial eigenvalue equation

$$\frac{\partial^2}{\partial \vec{s}^2} \omega_{k_1 2k_2}(s,r) = -\operatorname{trg} r^2 \omega_{k_1 2k_2}(s,r) \tag{2.18}$$

for the function $\omega_{k_1 2k_2}(s,r)$. Here we introduced the gradient

$$\frac{\partial}{\partial \vec{s}} = \left(\frac{\partial}{\partial s_{11}}, \ldots, \frac{\partial}{\partial s_{[k_1/2]1}}, \frac{\partial}{\partial s_{12}}, \ldots, \frac{\partial}{\partial s_{k_2 2}} \right), \tag{2.19}$$

which also defines the flat Laplacian $\partial^2/\partial \vec{s}^{\,2}$ appearing in the eigenvalue equation (2.18). A crucial feature of the square root of the Berezinian enters the derivation of Eq. (2.18). It satisfies the harmonic equation

$$\frac{\partial^2}{\partial \vec{s}^{\,2}} B_{k_1 2k_2}(s) = 0, \tag{2.20}$$

which we prove in Appendix C. Any linear combination of products of exponentials solves the eigenvalue equation (2.18). However, as the supermanifold integral and the eigenvalue equations are obviously invariant under permutations of the variables in the $\mathrm{o}(k_1)$ sector

$s_{p1}, p=1,\ldots,[k_1/2]$ or, equivalently, $r_{p1}, p=1,\ldots,[k_1/2]$ and under permutations of the variables in the uosp$(2k_2)$ sector $is_{p2}, p=1,\ldots,k_2$ or, equivalently, $ir_{p2}, p=1,\ldots,k_2$, the desired solution must have the same property. Moreover, there is a symmetry under a parity transformation for the variables $is_{p2}, p=1,\ldots,k_2$ and $ir_{p2}, p=1,\ldots,k_2$. That is, the solution must be invariant under the substitution $s_{p2}\rightarrow -s_{p2}$ and $r_{p2}\rightarrow -r_{p2}$. For k_1 odd, the same symmetry must hold also for $s_{p1}, p=1,\ldots,[k_1/2]$ and $r_{p1}, p=1,\ldots,[k_1/2]$ respectively. By these symmetries the solution of Eq. (2.18) for k_1 odd is up to normalization uniquely determined,

$$\omega_{k_1 2k_2}(s,r)=\frac{1}{[k_1/2]!\,k_2!}\det[i\,\sin(2s_{p1}r_{q1})]\det[2\,\cos(2s_{p2}r_{q2})]. \tag{2.21}$$

For k_1 even, the part antisymmetric under the parity transformation has to be kept and we find

$$\omega_{k_1 2k_2}(s,r)=\frac{1}{[k_1/2]!\,k_2!}(\det[\cos(2s_{p1}r_{q1})]+\det[i\,\sin(2s_{p1}r_{q1})])\det[-2i\,\sin(2s_{p2}r_{q2})]. \tag{2.22}$$

These results give, together with the ansatz (2.17), the desired supermanifold integrals (2.8) and (2.9). As already mentioned, our derivation of the supersymmetric group integral contains as special cases a rederivation of the ordinary orthogonal and unitary symplectic Harish-Chandra integrals for $k_2=0$ or $k_1=0$, respectively.

III. SUMMARY AND CONCLUSIONS

We calculated the supersymmetric Harish-Chandra integral for the unitary orthosymplectic supermanifold, thereby proving a conjecture.[10,11] Our derivation uses a diffusion equation or, equivalentely, eigenvalue equation method. It is based on the separability of the Laplacian. Our present contribution is a further extension of this technique, which, to the best of our knowledge, has previously only been used for group integrals over the unitary group: orginally, it was introduced for the Harish-Chandra integral over the ordinary unitary group,[6,23] then extended for the supersymmetric Harish-Chandra integral over the unitary supermanifold.[7] Already in 1958, Berezin and Karpelevich[24] had developed such a technique for an integral over two unitary groups, see also Ref. 25. This was also extended to the supersymmetric case.[26,27] Here, we considered the unitary orthosymplectic supermanifold and adjusted the eigenvalue equation method to this case. As the unitary orthosymplectic supermanifold contains the ordinary orthogonal and unitary symplectic groups as subgroups and special cases, we automatically also extended the eigenvalue equation method to these two ordinary groups.

We are aware of only two methods which could be an alternative: character expansions and Gelfand–Tzetlin coordinates. Balantekin developed the character expansion method for the unitary ordinary and supermanifold[32,33] and obtained various group integrals. Recently, this method was further extended and employed in Ref. 34. Similar considerations are also of interest if one studies the Itzykson–Zuber integral for matrices of large dimension.[35] Moreover, character expansions could also be developed for the calculation of certain integrals over the ordinary orthogonal and unitary symplectic group,[36] but Harish-Chandra integrals have so far not been tackled with this approach. Gelfand–Tzetlin coordinates[37,38] allow one to compute the ordinary[39] and supersymmetric[8] Itzykson–Zuber integral directly, i.e., without using a diffusion or eigenvalue equation. This method has not been applied yet to work out Harish-Chandra integrals for the ordinary orthogonal or unitary symplectic or the supersymmetric unitary orthosymplectic manifold. However, it has been employed for Gelfand's spherical functions.[28–31]

Considering all the cases, in which nontrivial group integrals could be obtained for the first time or in which known results could be rederived faster, the diffusion or eigenvalue equation method used and further extended here shows a remarkably wide range of applicability.

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APPENDIX A: ON THE SUPERMANIFOLD UOSp($k_1/2k_2$)

The real form of a complex supergroup $\mathcal{G}$ is obtained by acting with some involutive antilinear automorphism s onto the group. Then the set $\mathcal{G}_s$ of fixed points of s is a real form of $\mathcal{G}$. Since the number of antilinear involutive automorphisms is limited, so is the number of inequivalent real forms. Indeed, the real forms of all complex superalgebras (and therefore of the supergroups) have been classified in Refs. 16 and 17. In particular, there it has been shown that the complex supergroup $\mathrm{OSp}(k_1/2k_2)$ has only two real forms. They are most conveniently characterized by the restriction of $\mathcal{G}_s$ to its even part $\mathcal{G}_{s0}$. For $\mathrm{OSp}(k_1/2k_2)$ this even part $\mathcal{G}_{s0}$ has to be a product of some real forms of $\mathrm{O}(k_1,C)$ and $\mathrm{Sp}(2k_2,C)$. The only two possibilities for $\mathcal{G}_{s0}$ are $\mathrm{O}(r,k_1-r)\otimes\mathrm{Sp}(k_2,R)$ and in addition, for k_1 even, $\mathrm{O}^*(k_1)\otimes\mathrm{Sp}(r,k_2-r)$. The corresponding automorphisms can also be found in Refs. 16 and 17. That is, both real forms are noncompact supergroups. Since we wish to generalize Harish-Chandra's formula for ordinary compact groups we have to relax the definition above and seek for a class of automorphisms of the algebra that allow for compact manifolds. Therefore we consider automorphisms t which are involutive only on the even elements $t^2g_0=g_0$ and antiinvolutive $t^2g_0=-g_0$ on the odd elements. For $\mathrm{osp}(k_1/2k_2)$ such an automorphism is given by $tg=g^\dagger$ with $g\in\mathrm{osp}(k_1/2k_2)$. Now we can construct a functor from the pair $\mathbf{(}\mathrm{osp}(k_1/2k_2),t\mathbf{)}$ to a supermanifold. The so constructed object is, however not a real supermanifold since the functor is not defined on the set of real supercommutative algebrae. It falls into the class of cs (complex supersymmetric) -manifolds.[18] It is, however a frequently arising object in physics[21,40] and has an intuitive meaning in terms of the matrices as defined in Sec. II A with the usual anticommutator as product.

APPENDIX B: CALCULATION OF THE BEREZINIAN

We use the standard procedure of obtaining the metric tensor g whose superdeterminant is the square of the Berezinian. The variation of the element $\sigma=u^{-1}su\in\mathrm{uosp}(k_1/2k_2)$ reads

$$d\sigma=u^{-1}(ds+[s,\delta\tilde{u}])u,\quad \text{where}\quad \delta\tilde{u}=duu^{-1} \tag{B1}$$

is also in the superalgebra $\mathrm{uosp}(k_1/2k_2)$. Thus, the invariant length element is given by

$$\begin{aligned}\mathrm{trg}\ d\sigma^2=\mathrm{trg}\ (ds+[s,\delta\tilde{u}])^2=\mathrm{trg}\ ds^2+\mathrm{trg}\ [s,\delta\tilde{u}]^2=&\sum_{p=1}^{[k_1/2]}ds_{p1}^2+\sum_{p=1}^{k_2}ds_{p2}^2+\sum_n(\alpha_n^{(\mathrm{o})})^2(\delta\tilde{u}_{(\mathrm{o})}^n)^2\\&+\sum_n(\alpha_n^{(\mathrm{usp})})^2(\delta\tilde{u}_{(\mathrm{usp})}^n)^2+\sum_n(\alpha_n^{(\mathrm{a})})^2(\delta\tilde{u}_{(\mathrm{a})}^n)^2.\end{aligned} \tag{B2}$$

In the last step, we expanded the traces, the metric g can then be read of from the coefficients in front of the squared variation differentials. We split the contribution from the commutator in three terms and introduced a new index n, labelling the roots and the variation differentials stemming from $\delta\tilde{u}$. There are three types of roots, corresponding to the $\mathrm{o}(k_1)$ and the $\mathrm{usp}(2k_2)$ subalgebras and the remaining sector $\mathrm{uosp}(k_1/2k_2)-\mathrm{o}(k_1)-\mathrm{usp}(2k_2)$ containing the anticommuting degrees of freedom. For even bosonic dimension $2k_1$, there are $2k_1(k_1-1)$ roots $\alpha_n^{(\mathrm{o})}$ of $\mathrm{o}(2k_1)$, given by $\pm s_{p1}\pm s_{q1}$ with independent signs and $p<q$. For odd bosonic dimension $2k_1+1$, there are $2k_1$ additional roots $\pm s_{p1}$ which are needed for the complete root system of $\mathrm{o}(2k_1+1)$. The roots $\alpha_n^{(\mathrm{usp})}$ of $\mathrm{usp}(2k_2)$ are $\pm is_{p2}\pm is_{q2}$ with independent signs and $p<q$, and furthermore $\pm 2is_{p2}$, all together $2k_2^2$ roots. Finally, we have the $2k_1k_2$ roots $\alpha_n^{(\mathrm{a})}$ from $\mathrm{uosp}(k_1/2k_2)-\mathrm{o}(k_1)-\mathrm{usp}(2k_2)$, which read

$\pm s_{p1} \pm i s_{q2}$ with independent signs and indices p,q. For odd bosonic dimension we have $2k_1$ additional roots $\alpha_n^{(a)} = \pm i s_{p2}$. Collecting everything, the superdeterminant detg g of the metric g is the product of all roots from $o(k_1)$ and $usp(2k_2)$, divided by the product of all roots from $uosp(k_1/2k_2) - o(k_1) - usp(2k_2)$. The square root of $\det g$ then gives the Berezinians (2.10) and (2.11).

APPENDIX C: SQUARE ROOT OF THE BEREZINIAN AS A HARMONIC FUNCTION

The result (2.20) is crucial for the separation ansatz and for the derivation of the ensuing eigenvalue equations. It is tedious, but elementary to prove it by explicit calculation. We consider even k_1, the case of odd k_1 is treated in the same way. Using relations such as

$$\sum_{p\neq q} \frac{1}{s_{p1}^2 - s_{q1}^2} = 0 \quad \text{and} \quad \sum_{p\neq q\neq t} \frac{s_{p1}^2}{(s_{p1}^2 - s_{q1}^2)(s_{p1}^2 - s_{t1}^2)} = 0, \tag{C1}$$

we find

$$\frac{1}{B_{k_1 2k_2}(s)} \sum_{p=1}^{[k_1/2]} \frac{\partial^2}{\partial s_{p1}^2} B_{k_1 2k_2}(s) = \sum_{p,q,t} \frac{4s_{p1}^2}{(s_{p1}^2 + s_{q2}^2)(s_{p1}^2 + s_{t2}^2)} - \sum_{p\neq q,t} \frac{8s_{p1}^2}{(s_{p1}^2 - s_{q1}^2)(s_{p1}^2 + s_{t2}^2)} - \sum_{p,q} \frac{6}{s_{p1}^2 + s_{q2}^2} + \sum_{p,q} \frac{4s_{p1}^2}{(s_{p1}^2 + s_{q2}^2)^2}. \tag{C2}$$

Similarly, we obtain

$$\frac{1}{B_{k_1 2k_2}(s)} \sum_{p=1}^{k_2} \frac{\partial^2}{\partial s_{p2}^2} B_{k_1 2k_2}(s) = \sum_{p,q,t} \frac{4s_{p2}^2}{(s_{p2}^2 + s_{q1}^2)(s_{p2}^2 + s_{t1}^2)} - \sum_{p\neq q,t} \frac{8s_{p2}^2}{(s_{p2}^2 - s_{q2}^2)(s_{p2}^2 + s_{t1}^2)} - \sum_{p,q} \frac{2}{s_{p1}^2 + s_{q2}^2} + \sum_{p,q} \frac{4s_{q2}^2}{(s_{p1}^2 + s_{q2}^2)^2}. \tag{C3}$$

Combining these two intermediate results, we arrive at

$$\begin{aligned}
\frac{1}{B_{k_1 2k_2}(s)} \frac{\partial^2}{\partial \vec{s}^{\,2}} B_{k_1 2k_2}(s) &= \sum_{p\neq q,t} \left(\frac{4s_{t2}^2}{(s_{p1}^2 + s_{t2}^2)(s_{q1}^2 + s_{t2}^2)} - \frac{8s_{p1}^2}{(s_{p1}^2 - s_{q1}^2)(s_{p1}^2 + s_{t2}^2)} \right) \\
&\quad + \sum_{p\neq q,t} \left(\frac{4s_{t1}^2}{(s_{t1}^2 + s_{p2}^2)(s_{t1}^2 + s_{q2}^2)} - \frac{8s_{p2}^2}{(s_{p2}^2 - s_{q2}^2)(s_{p2}^2 + s_{t1}^2)} \right) + \sum_{p,q} \left(\frac{8s_{p1}^2}{(s_{p1}^2 + s_{q2}^2)^2} \right. \\
&\quad \left. + \frac{8s_{q1}^2}{(s_{q1}^2 + s_{p2}^2)^2} \right) - \sum_{p,q} \frac{8}{s_{p1}^2 + s_{q2}^2} \\
&= \sum_{p\neq q,t} \left(\frac{4s_{t2}^2}{(s_{p1}^2 + s_{t2}^2)(s_{q1}^2 + s_{t2}^2)} - \frac{4s_{p1}^2}{(s_{p1}^2 - s_{q1}^2)(s_{p1}^2 + s_{t2}^2)} - \frac{4s_{q1}^2}{(s_{q1}^2 - s_{p1}^2)(s_{q1}^2 + s_{t2}^2)} \right) \\
&\quad + \sum_{p\neq q,t} \left(\frac{4s_{t1}^2}{(s_{t1}^2 + s_{p2}^2)(s_{t1}^2 + s_{q2}^2)} - \frac{4s_{p2}^2}{(s_{p2}^2 - s_{q2}^2)(s_{p2}^2 + s_{t1}^2)} - \frac{4s_{q2}^2}{(s_{q2}^2 - s_{p2}^2)(s_{q2}^2 + s_{t1}^2)} \right) \\
&= 0,
\end{aligned} \tag{C4}$$

which is Eq. (2.20).

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An Ising model with three competing interactions on a Cayley tree

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In this paper we consider an Ising model with three competing restricted interactions on the Cayley tree $J^2(J^3)$. The translation invariant and periodic Gibbs measures for these models are investigated and the problem of the phase transition in these classes is solved. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The Ising model, which was originally regarded as a ferromagnetic model, has found some applications in many other physical, biological, and chemical systems, and even in sociology. The model we considered in (Ref. 6) is a natural generalization of the Ising model, and a model of the similar form has recently been investigated by Monroe[11,12] to understand the physical aspects associated with the Husimi tree or the Kagome lattice. On a similar note, the topic of statistical mechanics on nonamenable graphs is a modern growing field.[2,10] In the same paper,[6] we have presented the exact solution of an Ising model with competing restricted interactions and zero external magnetic field on the Cayley tree for J^2 order 2.

In this paper we consider the Ising model with three competing interactions on the Cayley tree which is defined by the following Hamiltonian:

$$H(\sigma) = -J_3 \sum_{\langle x,y,z\rangle} \sigma(x)\sigma(y)\sigma(z) - J\sum_{\rangle x,y\langle} \sigma(x)\sigma(y) - J_1\sum_{\langle x,y\rangle} \sigma(x)\sigma(y) - h\sum_{x\in V} \sigma(x), \tag{1}$$

where the sum in the first term ranges all triples of neighbors, the second sum ranges all second neighbors, the third sum ranges all nearest neighbors and the spin variables $\sigma(x)$ assume the values ± 1. (See Ref. 7 for models with competing interactions, and see Refs. 2 and 10–12 for the physical motivation underlying the study of these models.)

The various partial cases of this model have been investigated in numerous works, for example, the case $J_3=h=0$ was considered in Refs. 11, 12, and 6. In Ref. 6, the exact solution of an Ising model with competing restricted interactions with zero external field was presented. The case $J=h=0$ was considered in Refs. 12 and 5. In Ref. 5, the exact solution was found for the problem of phase transitions in the Ising model for competing ternary and binary interactions.

Note: Let us connect all pairs vertices (x,y) of J^2 with the same level for which $d(x,y)=2$. Then the Cayley tree J^2 is transformed to a graph $\hat{J}^2$ (see Fig. 1). Assume that the interaction

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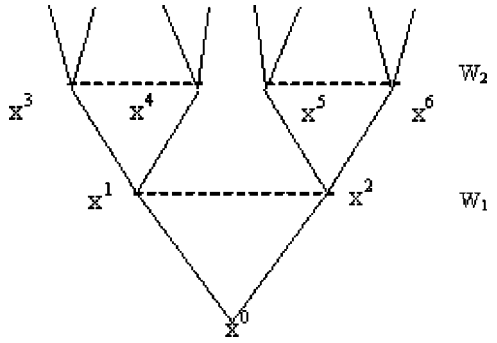

FIG. 1. A semi-infinite Cayley tree J^2 of order 2.

between nearest neighbors $\langle x,y\rangle$ in $\hat{J}^2$ is defined by constant J, if vertices x and y have distinct level and by constant J_1, if vertices x and y have the same level. The Hamiltonian of Ising model on graph $\hat{J}^2$ is the same as a modification to the Hamiltonian (1) with $J_3=0$ which we will define later. Thus the result which is proved for modification to the Hamiltonian (1) will be also valid for Ising model on the graph $\hat{J}^2$. When we let $J_1=J$, we found a critical point, $\beta J=\frac{1}{4}\ln 5$, which is the critical value found by Monroe for the special case $J_3=h=0$.[11]

In this paper we also consider restricted ternary and binary interactions. Exact definitions of such restricted interactions will be given later. The general part of our results were proven in the Cayley tree of order 2, but some parts of the results were proven also in the Cayley tree of order 3.

We end this section by some necessary definitions and preliminary results. The Cayley tree J^q (see Ref. 1) of order $q\geqslant 1$ is an infinite tree, i.e., a graph without cycles, from each vertex of which exactly $q+1$ edges issue. Let $J^q=(V,L,i)$, where V is the set of vertices of J^q, L is the set of edges of J^q, and i is the incidence function associating each edge $l\in L$ with its end points $x,y\in V$. If $i(l)=\{x,y\}$, then x and y are called nearest neighbouring vertices and we write $l=\langle x,y\rangle$. The distance $d(x,y)$, $x,y\in V$ on the Cayley tree is defined by the formula $d(x,y)=\min\{d|x=x_0,x_1,\ldots,x_{d-1},x_d=y\in V$ such that the pairs $\langle x_0,x_1\rangle,\ldots,\langle x_{d-1},x_d\rangle$ are neighboring vertices$\}$.

For the fixed $x^0\in V$ we set

$$W_n=\{x\in V|d(x,x^0)=n\},$$

$$V_n=\cup_{m=0}^{n}W_m=\{x\in V|d(x,x^0)\leqslant n\},$$

$$L_n=\{l=\langle x,y\rangle\in L|x,y\in V_n\}.$$

A collection of the pairs $\langle x,x_1\rangle,\ldots,\langle x_{d-1},y\rangle$ is called a path from x to y. We write $x<y$ if the path from x^0 to y goes through x. We call the vertex y a direct successor of x, if $y>x$ and x,y are nearest neighbors. The set of the direct successors of x is denoted by $S(x)$, i.e.,

$$S(x)=\{y\in W_{n+1}|d(x,y)=1\},\quad x\in W_n.$$

We observe that for any vertex $x\neq x^0$, x has q direct successors and x^0 has $q+1$.

The vertices x and y are called second neighbor which is denoted by $\rangle x,y\langle$, if there exists a vertex $z\in V$ such that x,z and y,z are nearest neighbors. Three vertices x,y and z are called a triple of neighbors and they are denoted by $\langle x,y,z\rangle$, if $\langle x,y\rangle$ and $\langle y,z\rangle$ are nearest neighbors and $x\neq z$. The fixed vertex x^0 is called the 0 th level and the vertices in W_n are called the nth level.

Proposition 1 (Ref. 3): There exists a one-to-one correspondence between the set V of the

vertices of the Cayley tree of order $q \geqslant 1$ *and the group* G_q *of the free products of* $q+1$ *cyclic groups of the second order with generators* $a_1, a_2, \ldots, a_{q+1}$.

Let us define a group structure on the J^q as follows. Vertices which correspond to the "words" $g, h \in G_q$ are called nearest neighbors and are connected by an edge if either $g = ha_i$ or $h = ga_j$ for some i or j. The graph thus defined is a Cayley tree of order q. Consider a left (resp. right) transformation shift on G_q defined as follows: for $g_o \in G_q$ we put

$$T_{g_0} h = g_0 h (\text{resp. } T_{g_0} h = g_0 h) \; \forall \; h \in G_q.$$

Then the set of all left (resp. right) shifts on G_q is isomorphic to the group G_q.

A semi-infinite Cayley tree J^q for order q is a infinite tree that is a graph having no cycles, from each vertex of which, except on vertex x^0, which is the root of the tree, emanates q edges (see Fig. 1). Here, just as before, we will use the same notation which is defined for the Cayley tree.

II. THE RECURRENT EQUATIONS FOR PARTITION FUNCTIONS IN THE ISING MODEL WITH RESTRICTED INTERACTIONS

There are several approaches to derive the equation describing the limiting Gibbs measures for lattice models on the Cayley tree. One approach is based on properties of Markov random fields on the Cayley tree (Refs. 16 and 13). Another approach is based on recurrent equations for partition functions.[8] Naturally both approaches lead to the same equation. However, the latter is more suitable for models with competing interactions. For the sake of completeness, we repeat the necessary notations.

From the beginning, we consider a semi-infinite Cayley tree J^k. Let Λ be a finite subset of V. Assume $\Omega(\Lambda)$ is the set of all configuration on Λ, that is the functions $\{\sigma(x), x \in \Lambda\}$. Let $\overline{\sigma}(V \setminus \Lambda)$ be a fixed boundary configuration. The total energy of configuration $\sigma(\Lambda) \in \Omega(\Lambda)$ under condition $\overline{\sigma}(V \setminus \Lambda)$ is defined as

$$\begin{aligned} H(\sigma(\Lambda)|\overline{\sigma}(V \setminus \Lambda)) = &- J_3 \sum_{\substack{\langle x,y,z \rangle \\ x,y,z \in \Lambda}} \sigma(x)\sigma(y)\sigma(z) - J \sum_{\substack{\rangle x,y \langle \\ x,y \in \Lambda}} \sigma(x)\sigma(y) - J_1 \sum_{\substack{\langle x,y \rangle \\ x,y \in \Lambda}} \sigma(x)\sigma(y) - h \sum_{x \in \Lambda} \sigma(x) \\ &- J_3 \sum_{\substack{\langle x,y,z \rangle \\ x \in \Lambda, y \notin \Lambda, z \notin \Lambda \text{ or} \\ x \in \Lambda, y \in \Lambda, z \notin \Lambda}} \sigma(x)\sigma(y)\sigma(z) - J \sum_{\substack{\rangle x,y \langle \\ x \in \Lambda, y \notin \Lambda}} \sigma(x)\overline{\sigma}(y) - J_1 \sum_{\substack{\langle x,y \rangle \\ x \in \Lambda, y \notin \Lambda}} \sigma(x)\overline{\sigma}(y). \end{aligned}$$

When all boundary points $\{\overline{\sigma}(y), y \in V \setminus \Lambda\}$ are fixed as +1, we have the positive boundary condition and when they are fixed as −1, we have negative boundary condition. The free boundary condition corresponds to the case when the last three sums in the above are absent, that is formally all boundary points are fixed as 0.

The partition function $Z_\Lambda(\overline{\sigma}(V\Lambda))$ in volume Λ under boundary condition $\overline{\sigma}(V \setminus \Lambda))$ is defined as

$$Z_\Lambda = \sum_{\sigma(\Lambda) \in \Omega(\Lambda)} \exp(-\beta H(\sigma(\Lambda))|\overline{\sigma}(V \setminus \Lambda)),$$

where $\beta = 1/kT$ is the inverse temperature. Then the conditional Gibbs measure μ_Λ in volume Λ under boundary condition $\overline{\sigma}(V \setminus \Lambda)$ is defined as

$$\mu_\Lambda(\sigma(\Lambda)) = \frac{\exp(-\beta H(\sigma(\Lambda))|\overline{\sigma}(V \setminus \Lambda))}{Z_\Lambda}.$$

We consider the configurations $\sigma(V_n)$, the partition functions Z_{V_n} and conditional Gibbs measure μ_{Λ_n} in volume V_n where $V_n = \cup_{i=0}^{n} W_i$ and for brevity we denote it as σ_n, $Z^{(n)}$ and μ_n, respectively.

Definition 1: The second neighbors $\rangle x, y \langle$ *will be named one-level neighbors and is denoted by*

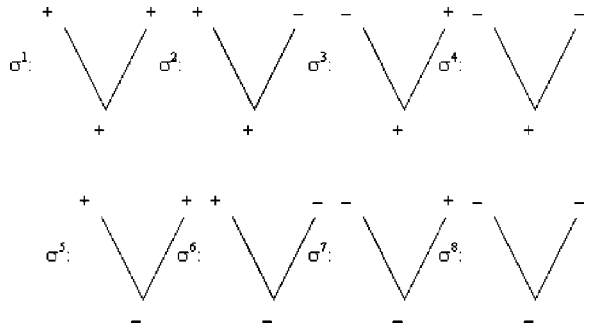

FIG. 2. All possible configurations on $V_1=\{x^0,x^1,x^2\}$.

$\overline{\rangle x,y\langle}$, *if vertices x and y belong to* W_n *for some n, that is if they are situated on the same level.*

Definition 2: The neighbors $\langle x,y,z\rangle$ *will be named two-level neighbors and is denoted by* $\overline{\langle x,y,z\rangle}$, *if vertices x and z belong to* W_n *for some n, that is if they are situated on the same level where as x and y, z, and y are nearest neighbors.*

Definition 3: The Ising model with competing restricted ternary and binary interactions on the Cayley tree is defined by the Hamiltonian

$$H(\sigma) = -J_3 \sum_{\overline{\langle x,y,z\rangle}} \sigma(x)\sigma(y)\sigma(z) - J\sum_{\overline{\rangle x,y\langle}} \sigma(x)\sigma(y) - J_1\sum_{\langle x,y\rangle} \sigma(x)\sigma(y) - h\sum_{x\in V} \sigma(x), \tag{2}$$

where the sum in the first term is taken over two-level triples of neighbors, the second term is taken over one-level second neighbors and the third term is taken over nearest neighbors.

We set

$$\theta_3 = \exp(\beta J_3), \quad \theta = \exp(\beta J), \quad \theta_1 = \exp(2\beta J_1)\,\theta_2 = \exp(\beta h)$$

and

$$u_n(x^0) = \frac{Z_+^{(n)}(x^0)}{Z_-^{(n)}(x^0)},$$

where

$$Z_+^{(n)} = \sum_{\sigma_n\in\Omega(V_n):\sigma_n(x^0)=+1} \exp(-\beta H_n(\sigma_n))$$

and

$$Z_-^{(n)} = Z^{(n)} - Z_+^{(n)}.$$

Proposition 2: For $q=2$, *the sequence* $\{u_n(x^0)\}$ *satisfies the following recurrent equation:*

$$u_n(x^0) = \theta_2^2 \frac{\theta_3^2\theta^2\theta_1^2 u_{n-1}^2(x^0) + 2\theta_1 u_{n-1}(x^0) + \theta^2\theta_3^2}{\theta^2\theta_1^2 + 2\theta_1\theta_3^2 u_{n-1}(x^0) + \theta^2 u_{n-1}^2(x^0)}, \quad n = 2,3,\ldots, \tag{3}$$

where $u_1(x^0)=\theta_1^2\theta_2^2\theta_3^2$ *for the positive boundary,* $u_1(x^0)=\theta_2^2\theta_3^2/\theta_1^2$ for the negative boundary and $u_1(x^0)=\theta_2^2[\theta^2\theta_3^2(1+\theta_1)+2\theta_1]/[\theta^2(1+\theta_1)+2\theta_1\theta_3^2]$ for the free boundary.

Proof: Consider the set of all configurations on $V_1=\{x^0,x^1,x^2\}$ and enumerate them as shown in Fig. 2. We divide the partition function $Z^{(n)}$ into eight sums

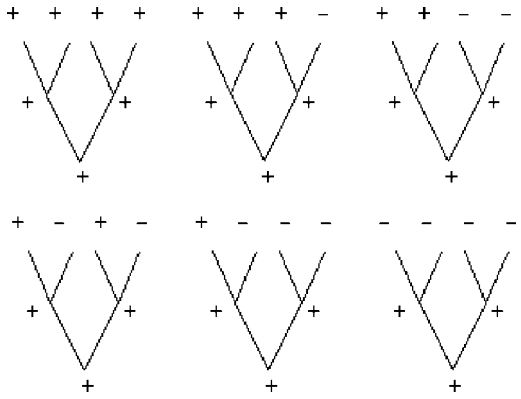

FIG. 3. Six essentially different possibilities at the second level for σ^1.

$$Z^{(n)} = \sum_{i=1}^{8} Z_i^{(n)},$$

where

$$Z_i^{(n)} = \sum_{\sigma_n \in \Omega(V_n):\sigma_n|=\sigma^i} \exp(-\beta H_n(\sigma_n)).$$

Next, we consider all the possibilities for the second level W_2 of our tree J^2 with σ^i on the $V_1, i=1,2,\ldots,8$. For example, there are a total of six different possibilities at the second level for σ^1 as shown in Fig. 3.

It is not hard to deduce the following system

$$Z_1^{(n)} = \theta_3\theta\theta_1\theta_2[Z_1^{(n-1)} + 2Z_2^{(n-1)} + Z_4^{(n-1)}]^2,$$

$$Z_2^{(n)} = Z_3^{(n)} = \theta_3^{-1}\theta^{-1}\theta_2[Z_1^{(n-1)} + 2Z_2^{(n-1)} + Z_4^{(n-1)}] \cdot [Z_5^{(n-1)} + 2Z_6^{(n-1)} + Z_8^{(n-1)}],$$

$$Z_4^{(n)} = \theta_3\theta\theta_1^{-1}\theta_2[Z_5^{(n-1)} + 2Z_6^{(n-1)} + Z_8^{(n-1)}]^2,$$

$$Z_5^{(n)} = \theta_3^{-1}\theta\theta_1^{-1}\theta_2^{-1}[Z_1^{(n-1)} + 2Z_2^{(n-1)} + Z_4^{(n-1)}]^2,$$

$$Z_6^{(n)} = Z_7^{(n)} = \theta_3\theta^{-1}\theta_2^{-1}[Z_1^{(n-1)} + 2Z_2^{(n-1)} + Z_4^{(n-1)}] \cdot [Z_5^{(n-1)} + 2Z_6^{(n-1)} + Z_8^{(n-1)}],$$

$$Z_8^{(n)} = \theta_3^{-1}\theta\theta_1\theta_2^{-1}[Z_5^{(n-1)} + 2Z_6^{(n-1)} + Z_8^{(n-1)}]^2.$$

We briefly describe how the first of the equations is obtained. According to Fig. 3, as $Z_2^{(n)} = Z_3^{(n)}$ and $Z_6^{(n)} = Z_7^{(n)}$, we have

$$Z_1^{(n)} = \theta_3\theta\theta_1\theta_2[(Z_1^{(n-1)})^2 + 4Z_1^{(n-1)}Z_2^{(n-1)} + 2Z_1^{(n-1)}Z_4^{(n-1)} + 4(Z_2^{(n-1)})^2 + 4Z_2^{(n-1)}Z_4^{(n-1)} + (Z_4^{(n)})^2],$$

where the coefficient $\theta_3\theta\theta_1\theta_2$ in front of the square bracket is taken into account for the interactions on σ^1. Here we do not take into account the interactions of the second neighbors $\langle x^0, x^3\rangle$, $\langle x^0, x^4\rangle$, $\langle x^0, x^5\rangle$, and $\langle x^0, x^6\rangle$ and also the interactions of triples of neighbors that are not two-level. The other equations are obtained similarly. Then,

$$u_n(x^0)=\frac{Z_+^{(n)}(x^0)}{Z_-^{(n)}(x^0)}=\frac{\theta_3\theta\theta_1\theta_2[Z_+^{(n-1)}]^2+2\theta_3^{-1}\theta^{-1}\theta_2Z_+^{(n-1)}Z_-^{(n-1)}+\theta_3\theta\theta_1^{-1}\theta_2[Z_-^{(n-1)}]^2}{\theta_3^{-1}\theta\theta_1^{-1}\theta_2^{-1}[Z_+^{(n-1)}]^2+2\theta_3\theta^{-1}\theta_2^{-1}Z_+^{(n-1)}Z_-^{(n-1)}+\theta_3^{-1}\theta\theta_1\theta_2^{-1}[Z_-^{(n-1)}]^2}$$
$$=\theta_2^2\frac{\theta_3^2\theta^2\theta_1^2u_{n-1}^2(x^0)+2\theta_1u_{n-1}(x^0)+\theta^2\theta_3^2}{\theta^2\theta_1^2+2\theta_1\theta_3^2u_{n-1}(x^0)+\theta^2u_{n-1}^2(x^0)},\quad n=2,3,\ldots.$$

Here we have the initial data $u_1=\theta_1^2\theta_2^2\theta_3^2$ for positive boundary and $u_1=\theta_2^2\theta_3^2/\theta_1^2$ for negative boundary. For the free boundary we have $u_1(x^0)=\theta_2^2[\theta^2\theta_3^2(1+\theta_1)+2\theta_1]/[\theta^2(1+\theta_1)+2\theta_1\theta_3^2]$.

Evidently,

$$u_n(x^0)=\frac{\mu_n(\sigma_n(x^0)=1)}{\mu_n(\sigma_n(x^0)=-1)}.$$

If we can find the limit of $u_n(x^0)$ as n tends to infinity, we will find the ratio for probability of a $+1$ to the probability of a (-1) at the root of the limiting Gibbs measure.

Now we give the construction of a special class of limiting Gibbs measures for our model (2). We consider a Cayley tree J^k below.

Let $H_n(\sigma_n)$ be the total energy of σ_n with respect to the free boundary condition.

Let $h:x\to R$ be a real valued function of $x\in V$. Given $n=1,2,\ldots$, consider the probabiity measure $\mu^{(n)}$ on $\{-1,+1\}^{V_n}$ which is defined by

$$\mu^{(n)}(\sigma_n)=Z_n^{-1}\exp\left\{-\beta H(\sigma_n)+\sum_{x\in W_n}h_x\sigma(x)\right\}.$$

Here, as before, $\beta=1/kT$ and $\sigma_n:x\in V_n\to\sigma_n(x)$ and Z_n is the corresponding partition function

$$Z_n=\sum_{\tilde{\sigma}_n\in\Omega(V_n)}\exp\left\{-\beta H(\tilde{\sigma}_n)+\sum_{x\in W_n}h_x\sigma(x)\right\}.$$

The consistency condition for $\mu^{(n)}(\sigma_n)$, $n\geqslant 1$ is

$$\sum_{\sigma^{(n)}}\mu^{(n)}(\sigma_{n-1},\sigma^{(n)})=\mu^{(n-1)}(\sigma_{n-1}),\tag{4}$$

where $\sigma^{(n)}=\{\sigma(x),x\in W_n\}$.

Let $V_1\subset V_2\subset\cdots,\cup_{n=1}^{\infty}V_n=V$ and $\mu_1,\mu_2,\ldots$ be a sequence of the probability measures on $\Phi^{V_1},\Phi^{V_2},\ldots$ satisfying the consistency condition, where $\Phi=\{-1,+1\}$. Then, according to the Kolmogorov theorem (see, e.g., Ref. 14), there is a unique limit Gibbs measure μ_h on Ω such that for every $n=1,2,\ldots$ and $\sigma_n\in\Phi^{V_n}$ the following equality holds:

$$\mu\left(\left\{\sigma\big|_{V_n}=\sigma_n\right\}\right)=\mu^{(n)}(\sigma_n).$$

The following statement describes the conditions on h_x which guarantee the consistency condition of measures $\mu^{(n)}(\sigma_n)$.

Proposition 3: The measure $\mu^{(n)}(\sigma_n)$, $n=1,2,\ldots$ satisfies the consistency condition (4) if and only if for any $x\in V$ the following equation holds:

$$h_x=\frac{1}{2}\log\left(\theta_2^2\frac{\theta_3^2\theta^2\theta_1^2e^{2(h_y+h_z)}+2\theta_1(e^{2h_y+2h_z})+\theta^2\theta_3^2}{\theta^2\theta_1^2+2\theta_1\theta_3^2(e^{2h_y}+e^{2h_z})+\theta^2e^{2(h_y+h_z)}}\right).\tag{5}$$

Here $S(x)=\{y,z\}$ and $\langle y,x,z\rangle$ is a two level ternary neighbor.

Proof: Necessity. According to the consistency condition (4) we have

$$\frac{Z_{n-1}}{Z_n}\sum_{\sigma^{(n)}}\exp\Bigg\{-\beta H_{n-1}(\sigma_{n-1})+\beta J_1\sum_{\substack{x\in W_{n-1},\\ y,z\in S(x)}}\sigma(x)(\sigma(y)+\sigma(z))+\beta J\sum_{\substack{x\in W_{n-1},\\ y,z\in S(x)}}\sigma(y)\sigma(z)$$
$$+\beta J_3\sum_{\substack{x\in W_{n-1},\\ y,z\in S(x)}}\sigma(x)\sigma(y)\sigma(z)+\sum_{x\in W_{n-1}}\beta h\sigma(x)+\sum_{x\in W_{n-1}}h_x(\sigma(x))\Bigg\}$$
$$=\exp\Bigg\{-\beta H_{n-1}(\sigma_{n-1})+\sum_{x\in W_{n-1}}h_x(\sigma(x))\Bigg\}.$$

After simplification we have

$$\frac{Z_{n-1}}{Z_n}\sum_{\sigma^{(n)}}\prod_{x\in W_{n-1}}\exp\{\beta J_1\sigma(x)(\sigma(y)+\sigma(z))+\beta J\sigma(y)\sigma(z)+\beta J_3\sigma(x)\sigma(y)\sigma(z)+\beta h\sigma(x)+h_y\sigma(y)$$
$$+h_z\sigma(z)\}=\prod_{x\in W_{n-1}}\exp\{h_x\sigma(x)\}.$$

Let $x\in W_{n-1}$ and $S(x)=\{y,z\}$, $\sigma_x^{(n)}=\{\sigma(y),\sigma(z)\}$. As $\sigma^{(n)}=\cup_{x\in W_{n-1}}\sigma_x^{(n)}$, then

$$\frac{Z_{n-1}}{Z_n}\prod_{x\in W_{n-1}}\sum_{\sigma_x^{(n)}}\exp\{\beta J_1\sigma(x)(\sigma(y)+\sigma(z))+\beta J\sigma(y)\sigma(z)+\beta J_3\sigma(x)\sigma(y)\sigma(z)+\beta h\sigma(x)+h_y\sigma(y)$$
$$+h_z(z)\}=\prod_{x\in W_n}\exp\{h_x\sigma(x)\}. \tag{6}$$

Now fix $x\in W_{n-1}$ and rewrite (6) for the cases $\sigma(x)=1$ and $\sigma(x)=-1$. If $\sigma(x)=1$, we have

$$N=\sum_{\sigma_x^{(n)}=\{\sigma(y),\sigma(z)\}}\exp\{\beta J_1(\sigma(y)+\sigma(z))+\beta J\sigma(y)\sigma(z)+\beta J_3\sigma(y)\sigma(z)+\beta h\sigma(x)+h_y\sigma(y)+h_z\sigma(z)\}$$
$$=\exp\{h_x\};$$

and if $\sigma(x)=-1$, then

$$D=\sum_{\sigma_x^{(n)}=\{\sigma(y),\sigma(z)\}}\exp\{-\beta J_1(\sigma(y)+\sigma(z))+\beta J\sigma(y)\sigma(z)\}+\beta J_3\sigma(y)\sigma(z)+\beta h\sigma(x)+h_y\sigma(y)+h_z\sigma(z)$$
$$=\exp\{-h_x\}.$$

So that

$$\frac{N}{D}=\exp\{2h_x\}. \tag{7}$$

The numerator N of the left-hand side is equal to

$$N=\exp(2\beta J_1+\beta J+\beta J_3+\beta h+h_y+h_z)+\exp(-\beta J-\beta J_3+\beta h-h_y+h_z)+\exp(-\beta J-\beta J_3+\beta h$$
$$+h_y-h_z)+\exp(-2\beta J_1+\beta J+\beta J_3+\beta h-h_y-h_z)$$

while the denumerator D is equal to

$$D=\exp(-2\beta J_1+\beta J+\beta J_3-\beta h+h_y+h_z)+\exp(-\beta J-\beta J_3-\beta h-h_y+h_z)+\exp(-\beta J-\beta J_3-\beta h$$
$$+h_y-h_z)+\exp(2\beta J_1+\beta J+\beta J_3-\beta h-h_y-h_z).$$

Then the equality $N/D=\exp\{2h_x\}$ implies (5).

Sufficiency. Assume that (5) is valid, then we have (7). From (7) we get

$$\sum_{\sigma_x^{(n)}=\{\sigma(y),\sigma(z)\}} \exp\{\beta J_1\sigma(x)(\sigma(y)+\sigma(z)) + \beta J\sigma(y)\sigma(z) + \beta J_3\sigma(x)\sigma(y)\sigma(z) + \beta h\sigma(x) + h_y\sigma(y) + h_z\sigma(z)\} = a(x)\exp\{\sigma(x)h_x\},$$

where $\sigma(x)=\pm 1$. This equality implies

$$\prod_{x\in W_{n-1}}\sum_{\sigma_x^{(n)}=\{\sigma(y),\sigma(z)\}} \exp\{\beta J_1\sigma(x)(\sigma(y)+\sigma(z)) + \beta J\sigma(y)\sigma(z) + \beta J_3\sigma(x)\sigma(y)\sigma(z) + \beta h\sigma(x) + h_y\sigma(y) + h_z\sigma(z)\} = \prod_{x\in W_{n-1}} a(x)\exp\{\sigma(x)h_x\}. \tag{8}$$

Denoting $A_n(x)=\Pi_{x\in W_{n-1}} a(x)$, we have from (8)

$$Z_{n-1}A_{n-1}\mu^{(n-1)}(\sigma_{n-1}) = Z_n\sum_{\sigma^{(n)}} \mu^{(n)}(\sigma_{n-1},\sigma^{(n)}).$$

As $\mu^{(n)}$, $n\geqslant 1$ is a probability, we have

$$\sum_{\sigma_{n-1}}\sum_{\sigma^{(n)}} \mu^{(n)}(\sigma_{n-1},\sigma^{(n)}) = \sum_{\sigma_{n-1}} \mu^{n-1}(\sigma_{n-1}) = 1.$$

From these equalities we get $Z_{n-1}A_{n-1}=Z_n$, which means that (4) holds.

According to Proposition 3 the problem of describing the Gibbs measures is reduced to the description of the solutions of the functional Eq. (5).

Let $\Omega=\{-1,+1\}^V$. According to Proposition 1 any transformation S of the group G_q induces a shift automorphism $\tilde{S}:\Omega\to\Omega$ by

$$(\tilde{S}\sigma)(h) = \sigma(Sh), h\in G_q, \sigma\in\Omega.$$

By G_q we denote the set of all shifts on Ω. We say that a Gibbs measure μ on Ω is translation-invariant if for any $T\in G_q$ the equality $\mu(T(A))=\mu(A)$ is valid for all $A\in\mathbb{F}$, where $\mathbb{F}$ is a standard σ-algebra of subsets of Ω generated by cylinder subsets.

The analysis of the solution of (5) is rather tricky. It is nartural to begin with the translation-invariant solutions where $h_x=h$ is constant for all $x\in V$. It is evident that a Gibbs measure corresponding to this solution is translation-invariant. In this case from (5), we have

$$u = \theta_2^2\frac{\theta_3^2\theta^2\theta_1^2u^2 + 2\theta_1u + \theta^2\theta_3^2}{\theta^2\theta_1^2 + 2\theta_1\theta_3^2u + \theta^2u^2}, \tag{9}$$

where $u=e^{2h}$.

Note that this equation describes the fixed points of Eq. (4). If there is more than one positive solution for Eq. (9), then there is more than one tranlation-invariant Gibbs measure corresponding to these solutions. We say that a phase transition occurs for model (2), if Eq. (9) has more than one positive solution. The number of the solutions of Eq. (3) naturally depends on the parameter $\beta=1/kT$. The phase transition usually occurs for low temperature. If it is possible to find an exact value of temperature T^* such that a phase transition occurs for all $T<T^*$, where T^* is called a critical value of temperature.

Finding the exact value of the critical temperature for some models means to exactly solve the models.

III. THE PROOF OF EXISTENCE OF PHASE TRANSITIONS FOR ZERO EXTERNAL FIELD

For the case $h=0$, Eq. (9) has the following form:

$$u = \frac{\theta_3^2\theta^2\theta_1^2u^2 + 2\theta_1u + \theta^2\theta_3^2}{\theta^2\theta_1^2 + 2\theta_1\theta_3^2u + \theta^2u^2}, \tag{10}$$

which is equivalent to the cubic equation

$$u^3 + \beta\alpha u^2 - \alpha u - \beta = 0, \tag{11}$$

where $\beta = \theta_3^2$ and $\alpha = (2\theta_1 - \theta_1^2\theta^2)/\theta^2$.

By changing the variable $u = v - (\alpha\beta/3)$, we obtain as cubic equation[9] as follows:

$$v^3 + pv + q = 0,$$

where

$$p = -\frac{\alpha^2\beta^2 + 3\alpha}{3} \quad \text{and} \quad q = \frac{2\alpha^3\beta^3}{27} + \frac{\alpha^2\beta}{3} - \beta.$$

It is well known (see, e.g., Ref. 9) that Eq. (11) has three real roots if $Q < 0$, where

$$Q = -\frac{4\alpha^3\beta^4 + (\alpha^4 + 18\alpha^2 - 27)\beta^2 + 4\alpha^3}{108}.$$

In Ref. 5, it was proven that $Q < 0$ for all $(\theta_1, \theta, \theta_3)$ such that $\theta_1^2 > 3$, $\theta^2 > 2\theta_1/(\theta_1^2 - 3)$ and $\theta_3^* < \theta_3 < \theta_3^{**}$, where

$$\theta_3^* = \sqrt{\frac{27 - 18\alpha^2 - \alpha^4 + (\alpha^2 - 9)\sqrt{\alpha^4 - 10\alpha^2 + 9}}{8\alpha^3}}$$

and

$$\theta_3^{**} = \sqrt{\frac{27 - 18\alpha^2 - \alpha^4 - (\alpha^2 - 9)\sqrt{\alpha^4 - 10\alpha^2 + 9}}{8\alpha^3}}.$$

Proposition 4 (Ref. 5): If $\theta_1^2 > 3$ *and* $\theta^2 > 2\theta_1/(\theta_1^2 - 3)$, *then* Eq. (11) *has three positive roots for all* $\theta, \theta_1, \theta_3$ *such that* $Q < 0$.

We write PR-domain to denote the set of all $(\theta, \theta_1, \theta_3)$ such that $\theta_1^2 > 3$, $\theta^2 > 2\theta_1/(\theta_1^2 - 3)$ and $Q < 0$ (see Fig. 4).

Now, we investigate the function

$$\psi(u) = \frac{\theta_3^2\theta^2\theta_1^2u^2 + 2\theta_1u + \theta^2\theta_3^2}{\theta^2\theta_1^2 + 2\theta_1\theta_3^2u + \theta^2u^2}$$

for $u > 0$. Let $u_1^* < u_2^* < u_3^*$ be the fixed points of Eq. (10). It is not hard to show by simple calculus that for all $(\theta_1, \theta, \theta_3)$ in the PR-domain (see Fig. 5), the function $\psi(u)$ will be increasing and will have a single positive point of inflection in the interval $(1, u_3^*)$, where u_3^* is the largest fixed point.

It is easy to show diagrammatically (see Fig. 5), that if $0 < u_1 < u_1^*$, u_n in Eq. (3) will monotonically increase to u_1^*, the smallest fixed point. For values $u_1^* < u_1 < u_2^*$, u_n will decrease monotonically to u_1^*. For values $u_2^* < u_1 < u_3^*$, u_n will increase monotonically to u_3^*. Finally, if $u_1 > u_3^*$, u_n will decrease monotonically to u_3^*.

As $\theta_1^2 > 3$, then $\theta^2\theta_3^2/\theta_1^2 < \theta^2\theta_1^2\theta_3^2$ so that the smallest fixed point gives the limiting probability ratio for the negative boundary condition and the largest fixed point gives the limiting probability ratio for the positive boundary condition.

We have thus proven the following theorem:

Theorem 1: *For the Ising model with ternary and binary interactions in Hamiltonian (2), and with zero external field, the PR-domain is the region of phase transition.*

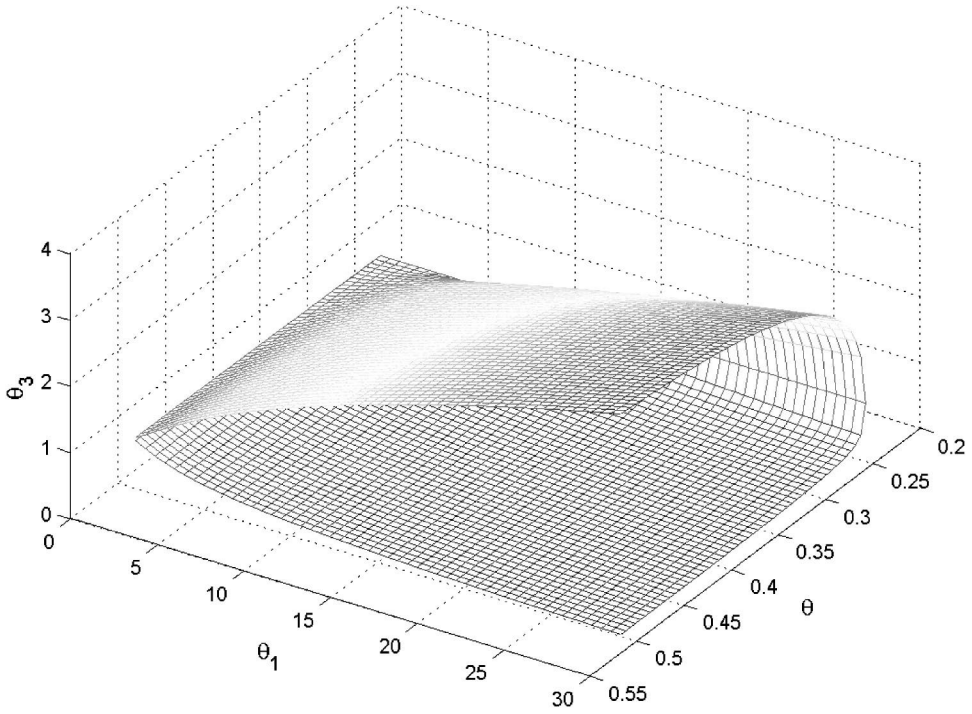

FIG. 4. For all $(\theta_1, \theta, \theta_3)$ inside the surface, a phase transition occurs.

The particular case of this theorem for $J=0$ was proven in Ref. 5 and the theorem for $J_3=0$ was proven in Ref. 6.

For $q=3$, we have the following theorem:

Theorem 2: *For the Ising model (2) with* $J_3=h=0$ *and* $q=3$, *the curve* $\theta^*=3\theta_1/(\theta_1^2-2)$ *in the plane* (θ_1, θ) *is a critical curve for phase transitions, namely, for an arbitrary pair of parameters* (θ_1, θ) *above the critical curve the phase transition takes place and for any pair of parameters on or below the critical curve there occurs a single Gibbs state*.

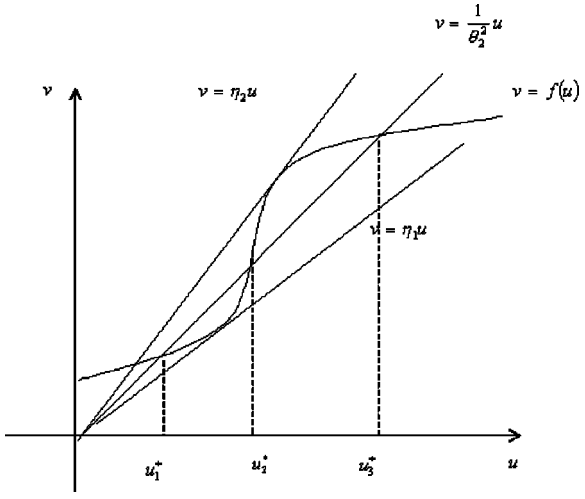

FIG. 5. The largest fixed point u_3^* and the smallest fixed point u_1^*.

IV. THE PERIODIC GIBBS MEASURES

The notions of periodic Gibbs measures, periodic Hamiltonians, and periodic configuration are introduced in Ref. 15. Let G_q be a free product of $q+1$ cyclic groups of order 2. According to Proposition 1 there is a one-to-one correspondence between the set of vertices V of the Cayley tree J^q and the group G_q. Let $\tilde{G}_q \subset G_q$ be a normal subgroup of finite index.

Definition 4: We say that $h=\{h_x : x \in G_q\}$ is $\tilde{G}_q$*-periodic if* $h_{yx}=h_x$ *for all* $x \in G_q$ *and* $y \in \tilde{G}_q$. *A Gibbs measure is called* $\tilde{G}_q$*-periodic if it corresponds to* $\tilde{G}_q$*-periodic function* h.

Observe that a translation-invariant Gibbs measure is G_q-periodic.

Let $\tilde{G}_2$ be the subgroup in G_2 consisting of all words of even length. Clearly, $\tilde{G}_2$ is a normal subgroup of index 2. In this section we consider $\tilde{G}_2$-periodic Gibbs measure, that is periodic measures of period 2 only. The description of periodic extreme Gibbs measures on some lattice models on the Cayley tree was given in Ref. 4. Here we consider a similar problem for our model. To describe the periodic Gibbs measure, we begin by investigating the following equation:

$$\psi(\psi(u)) = u,$$

where

$$\psi(u) = \frac{\theta_3^2\theta^2\theta_1^2u^2 + 2\theta_1 u + \theta^2\theta_3^2}{\theta^2\theta_1^2 + 2\theta_1\theta_3^2 u + \theta^2 u^2}.$$

Evidently the positive roots of the equation

$$\frac{\psi(\psi(u)) - u}{\psi(u) - u} = 0$$

describe the periodic nontranslation-invariant states.

As we are looking for positive roots this equation has a following form:

$$\theta^2\theta_1^2(\theta^2 + \theta^2\theta_1^2\theta_3^4 + 2\theta_1\theta_3^4)u^2 + \theta_3^2(\theta^4\theta_1^4 + 4\theta^2\theta_1^3 + 4\theta_1^2 - \theta^4)u + \theta_1^2\theta^2(\theta^2\theta_3^4 + \theta^2\theta_1^2 + 2\theta_1) = 0. \tag{12}$$

The discriminant Δ of (12) is equal to

$$\Delta = -4\theta^6\theta_1^5(\theta^2\theta_1 + 2)\theta_3^8 + A\theta_3^4 - 4\theta^6\theta_1^5(\theta^2\theta_1 + 2),$$

where

$$A = (-3\theta_1^8 - 6\theta_1^4 + 1)\theta^8 - 8\theta_1^3(\theta_1^4 + 1)\theta^6 - 8\theta_1^2(1 - \theta_1^4)\theta^4 + 32\theta_1^5\theta^2 + 16\theta_1^4.$$

Equation (12) has two positive roots if $\Delta > 0$ and $\theta^4(1-\theta_1^4) - 4\theta_1^3\theta^2 - 4\theta_1^2 > 0$. Evidently the last inequality is valid for $\theta_1 < 1$ and $\theta^2 > (2\theta_1/1-\theta_1^2)$.

The roots of equation $\Delta = 0$ with respect to θ_3, have the same sign. So they are positive when $A > 0$ and $A^2 - 64\theta^{12}\theta_1^{10}(\theta^2\theta_1+2)^2 > 0$, that is $A > 8\theta^6\theta_1^5(\theta^2\theta_1+2)$. After subsituting the value of A, the last inequality has the following form:

$$(1 - 3\theta_1^2)(\theta_1^2 + 1)^3\theta^8 - 8\theta_1^3(\theta_1^2 + 1)^2\theta^6 + 8\theta_1^2(\theta_1^4 - 1)\theta^4 + 32\theta_1^5\theta^2 + 16\theta_1^4 > 0.$$

Factorizing the left hand side, we have

$$(1 - 3\theta_1^2)(\theta_1^2 + 1)\left(\theta^2 - \frac{2\theta_1}{1 - 3\theta_1^2}\right)\left(\theta^2 - \frac{2\theta_1}{1 + \theta_1^2}\right)^2\left(\theta^2 + \frac{2\theta_1}{1 + \theta_1^2}\right) > 0.$$

This inequality has a solution when $1-3\theta_1^2 > 0$ and it follows that $\theta^2 > 2\theta_1/(1-3\theta_1^2)$ is the corresponding solution. Evidently from condition $\theta^2 > 2\theta_1/(1-3\theta_1^2)$ we have condition $\theta^2 > 2\theta_1/(1 - \theta_1^2)$. Thus if $\theta_1 < 1/\sqrt{3}$ and $\theta^2 > 2\theta_1/(1-3\theta_1^2)$, then the equation $\Delta = 0$ with respect to θ_3 has two

positive roots θ_3^* and θ_3^{**} where $\theta_3^* < \theta_3^{**}$. In this case Eq. (12) has 2 positive roots when $\theta_1 < 1/\sqrt{3}$, $\theta^2 > 2\theta_1/(1-3\theta_1^2)$ and $\theta_3^* < \theta_3 < \theta_3^{**}$.

Therefore, the following theorem is proven:

Theorem 3: *For an Ising model (2) with zero external field, a phase transition occurs for arbitrary* $(\theta, \theta_1, \theta_3)$ *such that* $0 < \theta_1 < 1/\sqrt{3}$, $\theta^2 > 2\theta_1/(1-3\theta_1^2)$ *and* $\theta_3^* < \theta_3 < \theta_3^{**}$, where θ_3^* *and* θ_3^{**} *are the positive solutions of the equation* $\Delta = 0$.

Similarly, we have found the following assertion for the same model with $q=3$:

Theorem 4: *For an Ising model (2) with* $J_3 = h = 0$ *and* $q=3$, *for* $\theta_1 < 1/\sqrt{2}$, *the curve* $\theta^* = 3\theta_1/(1-2\theta_1^2)$ *in the plane* (θ_1, θ) *is a critical curve for phase transitions, such that for an arbitrary pair of parameters* (θ_1, θ) *above the critical curve the phase transition takes place.*

V. THE PROOF OF EXISTENCE OF PHASE TRANSITIONS FOR NONZERO EXTERNAL FIELD

Here we solve the problem of phase transition for Ising model (2) for arbitrary external magnetic field h when $J_3 = 0$. Then the Eq. (9) is reduced to the equation

$$u = \theta_2^2 \frac{\theta^2\theta_1^2u^2 + 2\theta_1 u + \theta^2}{\theta^2\theta_1^2 + 2\theta_1 u + \theta^2 u^2}. \tag{13}$$

First of all, we prove the following lemma which is a generalization of Proposition 10.7 in Ref. 13.

Lemma: The equation

$$\frac{1}{\theta_2^2} \cdot u = \frac{\theta^2\theta_1^2u^2 + 2\theta_1 u + \theta^2}{\theta^2\theta_1^2 + 2\theta_1 u + \theta^2 u^2} \tag{14}$$

(*with* $u > 0$) *has a unique solution if* $\theta \leqslant \sqrt[4]{4/(\theta_1^2+1)}$.

If $\theta > \sqrt[4]{4/(\theta_1^2+1)}$, *then there are numbers* $\eta_1(\theta,\theta_1), \eta_2(\theta,\theta_1)$ *with* $0 < \eta_1(\theta,\theta_1) < \eta_2(\theta,\theta_1)$ *such that Eq. (14) has three roots, when* $\eta_1(\theta,\theta_1) < 1/\theta_2^2 < \eta_2(\theta,\theta_1)$; *it has two roots if either* $1/\theta_2^2 = \eta_1(\theta,\theta_1)$ *or* $1/\theta_2^2 = \eta_2(\theta,\theta_1)$ *and a unique solution if* $1/\theta_2^2 \in [\eta_1(\theta,\theta_1), \eta_2(\theta,\theta_1)]$.

The numbers $\eta_i, i = 1,2$ *are defined from the formula below:*

$$\eta_i(\theta,\theta_1) = \frac{1}{u_i} \cdot \frac{\theta^2\theta_1^2u_i^2 + 2\theta_1 u_i + \theta^2}{\theta^2\theta_1^2 + 2\theta_1 u_i + \theta^2 u_i^2},$$

where u_1, u_2 *are the solutions of the following equation:*

$$\theta_1^2\theta^4u^4 + 4\theta_1\theta^2u^3 + (3\theta^4 - \theta^4\theta_1^4 + 4\theta_1^2)u^2 + 4\theta_1\theta^2u + \theta_1^2\theta^4 = 0. \tag{15}$$

Proof: We first define

$$f(u) = \frac{\theta^2\theta_1^2u^2 + 2\theta_1 u + \theta^2}{\theta^2\theta_1^2 + 2\theta_1 u + \theta^2 u^2}.$$

It is easy to check that there is more than one solution to (14) if and only if there is at least one solution to the equation $x \cdot f'(x) = f(x)$ which is the same as

$$\theta_1^2\theta^4u^4 + 4\theta_1\theta^2u^3 + (3\theta^4 - \theta^4\theta_1^4 + 4\theta_1^2)u^2 + 4\theta_1\theta^4u + \theta_1^2\theta^4 = 0.$$

It is a symmetric one. So, after substitution of $u + (1/u) = t$, it reduces to the following:

$$\theta_1^2\theta^4t^2 + 4\theta_1\theta^2t - [(\theta^4(\theta_1^4 + 2\theta_1^2 - 3) - 4\theta_1^2)] = 0.$$

This equation has a positive root larger than 2 and, respectively, Eq. (14) has two positive roots u_1 and u_2, when $\theta_1^2 > 3$ and $\theta^2 > 2\theta_1/(\theta_1^2-3)$. Solving the inequality

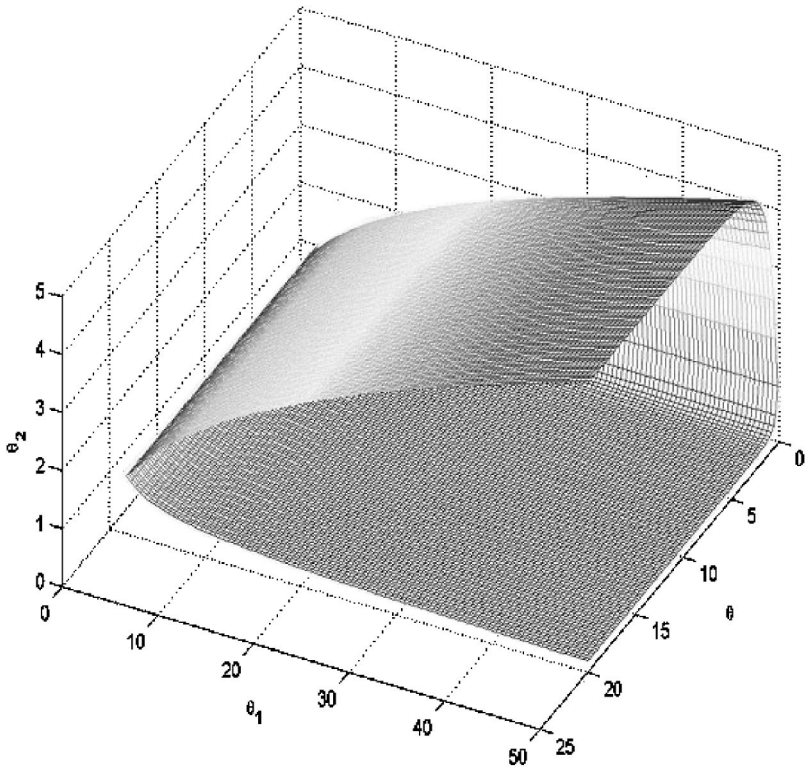

FIG. 6. For all $(\theta_1, \theta, \theta_2)$ inside the surface, a phase transition occurs.

$$\frac{2\theta_1\theta^2 + \sqrt{4\theta_1^2\theta^4 + \theta_1^2\theta^4[\theta^4(\theta_1^4 + 2\theta_1^2 - 3) - 4\theta_1^2]}}{\theta_1^2\theta^4} > 2,$$

we have

$$\theta^4(\theta_1^2 - 3)(\theta_1^2 + 1) - 8\theta^2\theta_1 - 4\theta_1^2 > 0.$$

Evidently $\theta_1^2 > 3$. Now solving this quadratic inequality with respect to θ^2, we have $\theta^2 > 2\theta_1/(\theta_1^2 - 3)$.

Since u_1 and u_2 are solutions of the equation $u^2 - tu + 1 = 0$, so $u_1 \cdot u_2 = 1$ and then $\eta_1(\theta, \theta_1) \cdot \eta_2(\theta, \theta_1) = 1$.

Theorem 5: *For Ising model (2) with $J_3 = 0$ and nonzero external magnetic field, a phase transition occurs when $\theta_1^2 > 3$, $\theta^2 > 2\theta_1/(\theta_1^2 - 3)$ and for θ_2 which satisfies the following inequalities:*

$$\eta_1(\theta, \theta_1) < \theta_2^2 < \eta_2(\theta, \theta_1),$$

where $\eta_1(\theta, \theta_1)$ and $\eta_2(\theta, \theta_1)$ are defined in the Lemma above.

Proof: According to the Lemma, Eq. (14) has three positive different roots u_1^*, u_2^*,and u_3^*. It is easy to show diagramatically (see Fig. 5) that if $0 < u_1 < u_1^*$, u_n in Eq. (3) will monotonically increase to u_1^*, the smallest root of Eq. (14). For value $u_1^* < u_1 < u_2^*$, u_n will decrease monotonically to u_1^*. For value $u_2^* < u_1 < u_3*$, u_n will monotonically increase to u_3^*. Finally if $u_1 > u_3^*$, u_n will decrease monotonically to u_3^*. Therefore, the roots u_1^* and u_3^* of Eq. (14) are two stable fixed points of the recurrent equation (3). The smallest (resp. largest) fixed point gives the limiting probability ratio for the negative (resp. positive) boundary. Hence the theorem is proven.

In Fig. 6, it is shown that the surface such that for all $(\theta_1, \theta, \theta_2)$ inside it, the conditions of Theorem 5 are valid.

VI. CONCLUSIONS

From Theorem 1 and Theorem 5, it follows that in the class of the translation-invariant state, a phase transition occurs when $\theta_1 > 1$, that is, the model (2) is a ferromagnetic one with respect to the binary interaction J_1 of the nearest neighboring vertices, namely $J_1 > 0$. From Theorem 3, it follows that in the case of nontranslation-invariant periodic state with period 2, a phase transition occurs when $\theta_1 < 1$, that is, the model (2) is an antiferromagnetic one with respect to the same binary interactions J_1, namely $J_1 < 0$.

ACKNOWLEDGMENT

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Finite size universe or perfect squash problem

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We give a physical notion to all self-adjoint extensions of the operator id/dx in the finite interval. It appears that these extensions realize different nonunitary equivalent representations of CCR and are related to the momentum operator viewed from different inertial systems. This leads to the generalization of Galilei equivalence principle and gives a new insight into the quantum correspondence rule. It is possible to get transformation laws of the wave function under Galilei transformation for any scalar potential. This generalizes the mass superselection rule. There is also given a new and general interpretation of a momentum representation of the wave function. It appears that consistent treatment of this problem leads to the time-dependent interactions and to the abrupt switching-off of the interaction. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1782671]

I. INTRODUCTION

A square well potential, although this is the simplest analytically solvable quantum model, can be used as a tool to investigate more involved quantum peculiarities. It was used recently for such different phenomena as quantum fractals,[1,2] quantum chaos[3] or wave-function revivals.[4,5] It can also be used as an approximation to experimentally realized semiconductor quantum well lasers or micromaser cavities with atomic rubidium.[6,7]

The Schrödinger equation with a square well potential can also be considered as a model of a quantum squash. An infinite well corresponds to perfectly rigid and perfectly resistant side walls. A finite square well potential corresponds to perfectly rigid but not perfectly resistant side walls—a high energy squash ball breaks through the wall. A physicist is here like a passive player. He or she [=(s)he] can use a racket only as a measurement apparatus—to register the energy or the momentum of the ball.

A simplicity of the model may be misleading. A closer inspection (see, e.g., Refs. 8–10) shows that the infinite potential well has mathematical traps which, when neglected, lead to contradictions or misinterpreted results.

The aim of this paper is to study physical consequences of different self-adjoint extensions of the "momentum" operator for a quantum squash. The "momentum" means here the differential operator $-i\hbar\nabla$. In the case of square integrable functions on $\mathbb{R}^n$ $(n=1,2,3)$ this operator is self-adjoint—so it is interpreted as the momentum operator. A situation is much more involved for a particle in a box. There are infinitely many self-adjoint extensions of the "momentum" operator. Different extensions correspond to different boundary conditions of functions from the domain of the operator and they have different spectra. A question arises which of these extensions is the physical momentum operator and what are physical notions of other self-adjoint extensions of the operator $-i\hbar\boldsymbol{\nabla}$?

It will be shown that all those self-adjoint extensions have physical meanings. They are closely related to the Galilei transformed reference frames moving with different velocities with respect to the primary frame. The primary frame is chosen as the frame with a time-independent

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potential. This means that our squash play does not move on the squash field. When (s)he changes this passive strategy and starts to run (with a constant velocity of course) then (s)he observes shifted momenta of the squash ball. This picture is in a perfect agreement with a physical "classical" intuition. It appears also that when (s)he solves corresponding Schrödinger equation then a transformed wave function behaves according to projective representations of the Galilei group.

A role of projective representations of the Galilei group was well established long ago.[11–16] All results were then obtained with Galilei-invariant potentials. For one particle this was equivalent to a free-particle case. It appears that basic results, the Bargmann superselection rule including, can be reproduced for any potential.

Finally, we are going to clarify the momentum representation puzzle. Let us consider a squash player confined to the finite region bounded by perfectly rigid and perfectly resistant side walls. For the player this squash-room is like a finite Universe. The spectrum of the momentum operator is discrete in this Universe. Since according to basic rules of quantum mechanics the only possible results of the momentum measurement are eigenvalues of the corresponding observable the momentum distribution should be a discrete one. However, there is a common procedure (see, e.g., Refs. 17 and 18) to take the Fourier integral transform of the wave function. This Fourier transform is interpreted as the momentum representation. This inconsistency was also observed in Ref. 8 but authors did not push the problem further.

One can show that both momentum representations have well established physical interpretations, although both describe different physical situations. The Fourier integral transformation of the wave function is simply related to the abrupt switch-off of the potential. As the infinite square well potential can be used as a model for the perfect squash so the Fourier integral of the harmonic oscillator wave function can be used for the quantum sling theory.

We begin by consideration of the notion of momentum distributions. It appears that a momentum distribution of the wave function understood as a Fourier transform is directly related to the solution of Schrödinger equation with a time-dependent interaction. The Fourier transform $\Phi(\vec{p},t)$ of the wave function $\Psi(\vec{r},t)$ is the probability amplitude to measure at time $t>0$ the momentum $\vec{p}$ when an interaction was switch-off at $t=0$. This gives also a new insight into a David–Goliath fight, as is presented in Sec. II B.

In Sec. III some necessary mathematical preliminaries are given. These are related to self-adjoint extensions of differential operators id/dx and d^2/dx^2. This material does not pretend to give a new insight into the problem, but collects some mathematical facts not always known to the physical community. An analysis of stationary solutions of the infinite square well potential is given as an example in Sec. III A.

Section IV deals with a physical interpretation of self-adjoint extensions of the operator $-id/dx$ in the Hilbert space of square integrable functions on a finite interval. First an analysis of the notion of the quantum momentum observable is performed. An operator can be identified with the physical momentum only if it transforms under Galilei transformation similarly to the classical momentum. This assumption allows one to add physics to all self-adjoint extensions of the operator $-id/dx$. These extensions correspond to momenta seen by moving observers from different inertial systems. It will be shown that those different extensions realize different nonunitary equivalent representations of Canonical Commutation Relations.

A natural problem which arises at that moment is to find how different moving observers see quantum mechanics from their systems. It is well known since the papers of Bargmann, Inönu and Wigner[11,12] that the free Schrödinger equation is Galilei invariant provided that wave function transforms under a projective representation of the Galilei group. Section V deals with this problem and generalizes a concept of Galilean covariance to any scalar potential. Now, a problem of the momentum distribution is reexamined. Solutions of the infinite potential well are taken as examples. It appears that momentum distributions are more tricky as it seemed before. In particular, a mathematical identity,

$$\sin x = \frac{1}{2i}(e^{ix} - e^{-ix}),$$

is not so obvious in a quantum word. This is explained in Sec. V C.

Final conclusions are given in Sec. VI.

II. MOMENTUM DISTRIBUTIONS

It is common knowledge that there is the discrete energy spectrum of a quantum particle placed in an infinite square well potential. A one-dimensional potential of the form

$$U(x) = \begin{cases} 0 & \text{for } 0 \leqslant x \leqslant a, \\ \infty & \text{for } x \text{ everywhere else,} \end{cases} \tag{1}$$

with boundary conditions

$$\psi(0) = \psi(a) = 0, \tag{2}$$

leads to the solutions

$$\psi_N(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{N\pi}{a} x & \text{for } 0 \leqslant x \leqslant a, \\ 0 & \text{for } x \text{ everywhere else,} \end{cases} \tag{3}$$

where N is an arbitrary positive integer.

Corresponding energy levels are

$$E_N = \frac{\pi^2 \hbar^2}{2ma^2} N^2. \tag{4}$$

Let us consider the Fourier integral of the wave function (3),

$$\tilde{\psi}_N(k) = \frac{1}{\sqrt{2\pi}} \int_0^a dx \psi_N(x) e^{-ikx}. \tag{5}$$

One gets

$$\tilde{\psi}_N(k) = -\sqrt{\pi a} \frac{2N}{a^2k^2 - N^2\pi^2} e^{-iak/2} \begin{cases} i \sin \frac{ak}{2} & \text{for } N \text{ even,} \\ \cos \frac{ak}{2} & \text{for } N \text{ odd.} \end{cases} \tag{6}$$

This mathematical expression is usually (see, e.g., Refs. 17 and 18 and a lot of other textbooks) interpreted as the physical momentum (with $p = \hbar k$) representation of the wave function. According to such an interpretation the probability distribution of the measurement of the momentum yielding a result between p and $p+dp$ is

$$\mathcal{P}_N(p) = \frac{4\pi a \hbar^3 N^2}{(a^2p^2 - \hbar^2 N^2 \pi^2)^2} \begin{cases} \sin^2 \frac{ap}{2\hbar} & \text{for } N \text{ even,} \\ \cos^2 \frac{ap}{2\hbar} & \text{for } N \text{ odd.} \end{cases} \tag{7}$$

This gives an average value of the momentum equal to zero, and an average value of the squared momentum is

$$\langle p^2\rangle_N = \int_{-\infty}^{+\infty} dp p^2 \mathcal{P}_N(p) = \frac{N^2\pi^2\hbar^2}{a^2}. \tag{8}$$

This is in agreement (on average) with (4). This is, however, not an answer for the question about the squash ball momentum. Besides that, there is a question about the energy conservation: how is it possible to get any value of the momentum in the state with a given value of the energy (4)?

For the player in h(is)er finite Universe $0 \leqslant x \leqslant a$ the only allowed values of a momentum are those which are eigenvalues of the corresponding self-adjoint observable. Using the trivial identity

$$\psi_N(x) = \sqrt{\frac{2}{a}}\,\sin\frac{N\pi}{a}x = \frac{1}{2i}\sqrt{\frac{2}{a}}(e^{(i\pi N/a)x} - e^{-(i\pi N/a)x}), \tag{9}$$

one gets a simple conclusion that allowed values of momenta are $\pm N\pi\hbar/a$. This is of course in perfect agreement (not only on average) with (4).

Such kinds of contradictions led recently to the conclusion[8] that the Fourier integral "is just a mathematically equivalent version of the same object, *not* the momentum representation wave function."

As we will see later, the use of Eq. (9) as a plane waves superposition is an oversimplification of the problem. There is, however, a surprisingly simple answer to a question about the physical notion of Eq. (6).

A. General momentum distribution

Let us consider a time-dependent Hamiltonian,

$$\hat{H} = \begin{cases} \dfrac{\hbar^2}{2m}\Delta + U(\vec{r}) & \text{for } t \leqslant 0, \\ -\dfrac{\hbar^2}{2m}\Delta & \text{for } t > 0. \end{cases} \tag{10}$$

Let ψ be any solution of the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + U(\vec{r})\psi.$$

A general form of the free Schrödinger equation is a wave packet,

$$\int d^3p g(\vec{p}) e^{-i(p^2/2m\hbar)t} e^{(i/\hbar)\vec{p}\cdot\vec{r}}.$$

A function

$$\Psi(\vec{r},t) = \begin{cases} \psi(\vec{r},t) & \text{for } t \leqslant 0, \\ \displaystyle\int d^3p g(\vec{p}) e^{-i(p^2/2m\hbar)t} e^{(i/\hbar)\vec{p}\cdot\vec{r}} & \text{for } t > 0, \end{cases} \tag{11}$$

is a solution of the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi,$$

and the wave function $\Psi(\vec{r},t)$ is continuous at $t=0$. This continuity condition gives

$$\psi(\vec{r},0) = \int d^3p g(\vec{p}) e^{(i/\hbar)\vec{p}\cdot\vec{r}}. \tag{12}$$

If a function ψ is a stationary solution then

$$\psi_E(\vec{r},t) = \phi_E(\vec{r}) e^{-(iE/\hbar)t},$$

with ϕ_E satisfying a stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\phi_E + U(\vec{r})\phi_E = E\phi_E.$$

Equation (12) now gives

$$\phi_E(\vec{r}) = \int d^3p g(\vec{p}) e^{(i/\hbar)\vec{p}\cdot\vec{r}}. \tag{13}$$

So we have gotten a general interpretation of the Fourier transform of a wave function. This gives the momentum distribution of a particle which was influenced by a potential and at time $t=0$ was suddenly freed. There is no question here about the energy conservation because of the time-dependency of the Hamiltonian (10).

Let us take as an example a well known Biblical story.

B. How Goliath was defeated by David

David's sling can be considered as a two-dimensional quantum rotator with a potential,

$$U(\vec{r}) = \frac{1}{2}m\omega^2(x^2+y^2).$$

Stationary solutions corresponding to the energy

$$E_{n_1,n_2} = \hbar\omega(n_1+n_2+1)$$

are given by

$$\phi_{n_1,n_2}(x,y) = C_{n_1,n_2} e^{-(m\omega/2\hbar)(x^2+y^2)} H_{n_1}\left(x\sqrt{\frac{m\omega}{\hbar}}\right) H_{n_2}\left(y\sqrt{\frac{m\omega}{\hbar}}\right). \tag{14}$$

If Goliath were hit directly by a stone still on a cord then he would absorb an impact energy E_{n_1,n_2}. But if a stone was freed from the sling then its momentum distribution was given by the Fourier transform of the function (14). So the probability distribution to have a stone with a momentum between p and $p+dp$ is proportional to

$$e^{-(p_x^2+p_y^2)/m\omega\hbar} H_{n_1}^2\left(\frac{p_x}{\sqrt{m\omega\hbar}}\right) H_{n_2}^2\left(\frac{p_y}{\sqrt{m\omega\hbar}}\right). \tag{15}$$

The corresponding impact energy is $p^2/2m$, in general, different from E_{n_1,n_2}. It is easy to check that it is more probable to get the impact energy *lower* than E_{n_1,n_2}. However there is a finite, although exponentially decreasing, probability that a high momentum stone would be thrown. One should notice that such an effect is impossible for a classical (i.e., not-quantum) sling. An exponentially small probability was not a problem in the considered case taking into account David's Protector. The crucial point was here a quantum nature of the sling.

III. MATHEMATICAL PRELIMINARIES

A cornerstone of quantum mechanics is a precise mathematical interpretation to the notion of observables. To each observable there corresponds a self-adjoint operator in the Hilbert state.[19] For unbounded symmetric operators there was a nontrivial problem to find all self-adjoint extensions but it was solved long ago.[20–22] To give a careful mathematical definition of operators related to observables is not a matter of a mathematical pedantry. Even in the simplest case of one dimensional infinite square well a lack of precision leads to obvious paradoxes.[9]

Let us consider a differential operator $-id/dx$ in the Hilbert space $L_2(0,a)$. Since

$$\int_0^a dx \bar{f}\frac{dg}{dx} = \bar{f}g|_0^a - \int_0^a dx \frac{d\bar{f}}{dx} g,$$

there are infinitely many self-adjoint extensions of the operator $-id/dx$. These extensions are parametrized by a continuous parameter $\sigma \in [0, 2\pi)$ and are defined on domains

$$\mathcal{D}_\sigma = \{f : f(a) = e^{i\sigma} f(0)\}. \tag{16}$$

The corresponding eigenvalues are

$$\lambda_n^{(\sigma)} = \frac{\sigma}{a} + \frac{2\pi n}{a}, \tag{17}$$

and normalized eigenfunctions,

$$f_n^{(\sigma)}(x) = \begin{cases} \dfrac{1}{\sqrt{a}} e^{i(\sigma/a)x} e^{i(2\pi n/a)x} & \text{for } 0 \leqslant x \leqslant a, \\ 0 \quad \text{for } x \text{ everywhere else}, \end{cases} \tag{18}$$

where $n = 0, \pm 1, \pm 2, \ldots$.

Self-adjoint operators,

$$\hat{p}_{(\sigma)} = -i\hbar \frac{d}{dx},$$

defined on the domains $\mathcal{D}_\sigma$ will henceforth be called the σ-momentum operator. Standard solutions of the infinite potential well take as the "physical momentum" the operator $\hat{p}_{(0)}$ and other extensions are simply rejected. We are going to show that other σ-momenta have an also well established physical meaning.

To consider the energy operator one should look for a self-adjoint extension of the operator d^2/dx^2. Here the situation is more involved. It was shown[23,24] that domains of self-adjoint extensions are given by a set of boundary conditions,

$$\alpha_{11} f(0) + \beta_{11} f(a) - \alpha_{12} f'(0) - \beta_{12} f'(a) = 0, \tag{19a}$$

$$\alpha_{21} f(0) + \beta_{21} f(a) - \alpha_{22} f'(0) - \beta_{22} f'(a) = 0, \tag{19b}$$

with coefficients α_{ij} and β_{kl} satisfying

$$\alpha_{11}\bar{\alpha}_{12} - \alpha_{12}\bar{\alpha}_{11} = \beta_{11}\bar{\beta}_{12} - \beta_{12}\bar{\beta}_{11}, \tag{20a}$$

$$\alpha_{21}\bar{\alpha}_{22} - \alpha_{22}\bar{\alpha}_{21} = \beta_{21}\bar{\beta}_{22} - \beta_{22}\bar{\beta}_{21}. \tag{20b}$$

In the case of the infinite potential well (1) a natural choice is to impose on the wave functions boundary conditions

$$f(0) = f(a) = 0, \tag{21a}$$

which are consistent with the continuity of the wave function. This choice corresponds to coefficients α_{ij} and β_{kl},

$$\alpha_{11} = 1, \quad \beta_{11} = -1, \quad \alpha_{12} = 0, \quad \beta_{12} = 0, \tag{21b}$$

$$\alpha_{21} = 1, \quad \alpha_{22} = 0, \quad \beta_{21} = 0, \quad \beta_{22} = 0. \tag{21c}$$

This means that functions satisfying boundary conditions (21a) form a domain $\mathcal{D}_{\Pi}$ of the self-adjoint extension of the operator d^2/dx^2. In the case of a particle on a circle a natural choice is to impose on the wave functions boundary conditions

$$f(0) = f(a), \quad f'(0) = f'(a). \tag{22a}$$

This choice corresponds to coefficients α_{ij} and β_{kl},

$$\alpha_{11} = 1, \quad \beta_{11} = -1, \quad \alpha_{12} = 0, \quad \beta_{12} = 0, \tag{22b}$$

$$\alpha_{21} = 0, \quad \alpha_{22} = 1, \quad \beta_{21} = 0, \quad \beta_{22} = -1. \tag{22c}$$

It is remarkable that the intersection of all admissible domains of σ-momenta is

$$\bigcap_{\sigma} \mathcal{D}_{\sigma} = \{f : f(a) = f(b) = 0\} = \mathcal{D}_{\Pi}. \tag{23}$$

This property makes the extension (21a) exceptional, at least from the point of view of momentum operators. A kinetic term d^2/dx^2 with this domain is well defined in (not *on*!) domains of all σ-momenta.

$\mathcal{D}_{\Pi}$ is a dense set in the Hilbert space $L_2(0,a)$ as the domain of a self-adjoint operator. This set is too small, however, to define on it a self-adjoint extension of the operator id/dx. But the property (23) together with the general theorem,[25] *any function from the domain of a self-adjoint operator $\mathcal{A}$ can be expanded in a uniformly convergent series of eigenfunctions of this operator*, allows us to write the following corollary.

Corollary 1: *Any energy eigenfunction (3) can be expanded in a uniformly convergent series of eigenfunctions of any σ-momentum.*

We also have the following corollary.

Corollary 2: *σ-momentum eigenfunctions (18) cannot be represented as uniformly convergent series of energy eigenfunctions.*

Both corollaries can be stated as follows.

In the infinite potential well σ-momentum representations of stationary states are always uniformly convergent. Energy representations of σ-momentum eigenfunctions are not uniformly convergent.

Let us make a mathematical exercise to calculate the following.

A. σ-momentum representation of stationary states

We have

$$\sqrt{\frac{2}{a}} \sin\frac{N\pi}{a}x = e^{i(\sigma/a)x}\frac{1}{\sqrt{a}}\sum_{n=-\infty}^{+\infty} c_n(\sigma)e^{i(2\pi n/a)x}. \tag{24}$$

Coefficients $c_n(\sigma)$ are given here as

$$\frac{\sqrt{2}}{a}\int_0^a dx\, e^{-i(\sigma/a+2\pi n/a)x}\sin\frac{\pi N}{a}x=\pi N\sqrt{2}\frac{e^{-i\sigma}(-1)^N-1}{(\sigma+2\pi n)^2-\pi^2N^2}. \tag{25}$$

It is convenient to discuss cases of even and odd N separately.

If $N=2r$ we can write

$$c_n(\sigma)=-4i\pi r\sqrt{2}e^{-i(\sigma/2)}\frac{\sin\frac{\sigma}{2}}{(\sigma+2\pi n)^2-4\pi^2r^2}. \tag{26}$$

A special care is needed when the nominator of this expression is equal to zero. For $\sigma=0$ one gets then

$$c_n(0)=\frac{1}{i\sqrt{2}}\begin{cases}1 & \text{for } n=r,\\ -1 & \text{for } n=-r,\\ 0 & \text{in other cases.}\end{cases} \tag{27}$$

After substitution to Eq. (24) this gives a consistency check,

$$\psi_{2r}(x)=\frac{1}{2i}\sqrt{\frac{2}{a}}(e^{i(2\pi r/a)x}-e^{-i(2\pi r/a)x}). \tag{28}$$

For nonzero σ we have

$$\psi_{2r}(x)=-4\pi ir\sqrt{\frac{2}{a}}e^{-i(\sigma/2)}e^{i(\sigma/a)x}\sin\frac{\sigma}{2}\sum_{n=-\infty}^{+\infty}\frac{e^{i(2\pi r/a)x}}{(\sigma+2\pi n)^2-4\pi^2r^2}. \tag{29}$$

If $N=2r+1$ we can write Eq. (25) as

$$c_n(\sigma)=-2\pi(2r+1)\sqrt{2}e^{-i(\sigma/2)}\frac{\cos\frac{\sigma}{2}}{(\sigma+2\pi n)^2-\pi^2(2r+1)^2}. \tag{30}$$

For $\sigma=\pi$ one gets similarly, like in Eq. (27),

$$c_n(\pi)=\frac{1}{i\sqrt{2}}\begin{cases}1 & \text{for } n=r,\\ -1 & \text{for } n=-r-1,\\ 0 & \text{in other cases.}\end{cases} \tag{31}$$

This gives, similarly like in Eq. (28),

$$\psi_{2r+1}(x)=\frac{1}{2i}\sqrt{\frac{2}{a}}(e^{i[2(r+1)\pi/a]x}-e^{-i[2(r+1)\pi/a]x}). \tag{32}$$

For $\sigma\neq\pi$ we have

$$\psi_{2r+1}(x)=-2\pi(2r+1)\sqrt{\frac{2}{a}}e^{-i(\sigma/2)}e^{i(\sigma/a)x}\cos\frac{\sigma}{2}\sum_{n=-\infty}^{+\infty}\frac{e^{i(2\pi n/a)x}}{(\sigma+2\pi n)^2-\pi^2(2r+1)^2}. \tag{33}$$

All these mathematical expansions from Eqs. (28), (29), (32), and (33), would have a physical meaning with a satisfactory physical interpretation of σ-momenta. This will be done in the next section. It should be now noted that the choice $\sigma=0$ gives expansions of the potential well stationary states into momentum eigenfunctions. The momentum spectrum is given then by Eq. (17) with $\sigma=0$. An elusively simple equation (9) *is not always* a momentum expansion because $N\pi/a$ are allowed momenta only for even N. Only in such cases a stationary state can be visual-

ized as the superposition of two waves with opposite momenta. For odd N the momentum expansion is

$$\psi_{2r+1}(x) = -2\pi(2r+1)\sqrt{\frac{2}{a}}\sum_{n=-\infty}^{+\infty}\frac{e^{i(2\pi n/a)x}}{4\pi^2n^2-\pi^2(2r+1)^2}, \tag{34}$$

with a much richer structure.

A more detailed analysis of this problem will be performed in Sec. V C.

IV. MOMENTUM SEEN FROM THE MOVING REFERENCE FRAME

We are going to find the physical meaning of different self-adjoint extensions of the operator $-id/dx$. It is a standard procedure to identify this operator with the translation generator. It is not enough, however, to relate this to the physical momentum. The same differential operator can be also related to a component of the angular momentum even for the same boundary conditions.

Let us consider as an example the operator $-i\hbar d/dx$ in the Hilbert space $L_2(0,2\pi)$ defined on the domain

$$\mathcal{D}_0 = \{f: f(2\pi) = f(0)\}. \tag{35}$$

A spectrum of this operator,

$$\lambda_n^{(0)} = n\hbar, \tag{36}$$

and normalized eigenfunctions,

$$f_n^{(0)}(x) = \frac{1}{\sqrt{2\pi}}e^{inx}, \tag{37}$$

are the same both for the momentum in the interval $(0,2\pi)$ as for the third component of the angular momentum when the variable $x \in (0,2\pi)$ is interpreted as an angular variable.

To get a momentum operator proper transformation properties are needed, specific for the corresponding classical variable. Let us consider two coordinate systems $\mathcal{O}(x,t)$ and $\mathcal{O}'(\zeta,\tau)$ related by the Galilei transformation

$$x = \zeta + V\tau; \quad t = \tau. \tag{38}$$

The following discussion is based on the "passive point of view" when the same system is observed by different observers A in $\mathcal{O}$ and A' in $\mathcal{O}'$ having different relations to the system.

Let $-i\hbar d/dx$ be a momentum operator in the system $\mathcal{O}$ and let f_λ be an eigenfunction of the momentum operator associated with the eigenvalue λ. The momentum operator should fulfill the following conditions.

(i) A momentum operator has the same structure in all inertial systems, i.e.,

$$-i\hbar d/d\zeta \text{ is a momentum operator in the coordinate system } \mathcal{O}'. \tag{39a}$$

(ii) A physical state with a defined momentum in one inertial system has a definite momentum in any inertial system, i.e.,

$$f_\lambda \text{ is transformed into } \tilde{f}_{\tilde{\lambda}}: -i\hbar\frac{d\tilde{f}_{\tilde{\lambda}}}{d\zeta} = \tilde{\lambda}\tilde{f}_{\tilde{\lambda}}. \tag{39b}$$

(iii) Eigenvalues of the momentum operator transform under the Galilei transformation like their classical counterparts, i.e.,

$$\tilde{\lambda} = \lambda - mV. \tag{39c}$$

We make an ansatz,

$$\tilde{f}_{\lambda}(\zeta,\tau) = e^{ig(\zeta,\tau)} f(\zeta + V\tau). \tag{40}$$

This gives

$$-i\hbar\frac{d\tilde{f}}{d\zeta} = \hbar\frac{dg}{d\zeta}e^{ig}f - i\hbar e^{ig}\frac{df_{\lambda}}{dx} = \hbar\frac{dg}{d\zeta}\tilde{f} + \lambda\tilde{f} = \tilde{\lambda}\tilde{f}. \tag{41}$$

The correspondence rule (39c) gives

$$\hbar\frac{dg}{d\zeta} + \lambda = \lambda - mV. \tag{42}$$

A general solution has a form

$$g(\zeta,\tau) = -\frac{mV}{\hbar}\zeta + T(\tau), \tag{43}$$

where T is an arbitrary function of the variable τ.

Starting from the consistency conditions (39a)–(39c) we have obtained a general transformation rule for momentum eigenfunctions under the Galilei transformation

$$\tilde{f}_{\lambda-mV}(\zeta,\tau) = e^{-i((mV/\hbar)\zeta - T(\tau))} f_{\lambda}(\zeta + V\tau). \tag{44}$$

Because of properties of self-adjoint operators this rule gives transformation rules for any vector from the Hilbert space.

If the momentum operator has a point spectrum, then its eigenfunctions form a base in a Hilbert space. This is a case for the $L_2(0,a)$ space. Any element u of this space can be expanded as

$$u(x) = \sum_{\lambda} c_n \tilde{f}_{\lambda}(x). \tag{45}$$

It follows from this that an observer from the Galilei transformed reference frame (38) sees this vector as

$$\tilde{u}(\zeta,\tau) = e^{-i(mV/\hbar\zeta - T(\tau))}\sum_{\lambda} c_n f_{\lambda}(\zeta + V\tau) = e^{-i(mV/\hbar\zeta - T(\tau))} u(\zeta + V\tau). \tag{46}$$

A function T is fixed by subsidiary conditions fulfilled by the function u. It will be shown in Sec. V that for one particle Schrödinger equation a function $T(\tau)$ has a form $-mV^2\tau/2$.

A result (46) can be easily generalized to the case of a continuous spectrum of the momentum operator. That is a standard mathematical procedure[21,22,26] equivalent to the replacement of the sum in Eq. (45) by the Fourier integral.

For the moment we restrict ourselves to the following.

A. Momentum inside the infinite potential well

The momentum observable "at rest" is $-i\hbar d/dx$ with the domain

$$\mathcal{D}_0 = \{f : f(a) = f(0)\}. \tag{47}$$

Boundary conditions in the moving reference frame $\mathcal{O}'(\zeta,\tau)$ are given at points $\zeta = -V\tau$ and $\zeta = -V\tau + a$. Using transformations rules given by Eqs (41) and (43) one gets the boundary conditions for the function $\tilde{f}$,

$$\tilde{f}(-V\tau + a, \tau) = e^{-i(mV/\hbar)a}\tilde{f}(-V\tau, \tau). \tag{48}$$

This gives us a direct interpretation of σ-momenta: *σ-momentum is the momentum observable measured by the observer moving with a velocity V such that*

$$\sigma = -\frac{mV}{\hbar}a \mod 2\pi. \tag{49}$$

To make the σ-momentum a real quantum mechanical momentum one should check the validity of Canonical Commutation Relations (CCR) of a momentum and a position operator in our system. In general, a problem of CCR on the finite interval is far from being obvious.[27] As opposed to the entire real line case where both position $\hat{X}$ and momentum $\hat{P}$ operators are unbounded, here the operator $\hat{X}$ is bounded in the Hilbert space $L_2(0,a)$ whereas the operator $\hat{P} = -i\hbar\partial$ is unbounded. This leads to technical troubles related to the domain $\mathcal{D}([\hat{X},\hat{P}])$ of the commutator $[\hat{X},\hat{P}]$. The domain where CCR are fulfilled is

$$\mathcal{D}(\hat{P}\hat{X}) \cap \mathcal{D}(\hat{X}\hat{P}), \tag{50}$$

where $\mathcal{D}(\hat{P}\hat{X})$ and $\mathcal{D}(\hat{X}\hat{P})$ are domains of operator products $\hat{P}\hat{X}$ and $\hat{X}\hat{P}$ correspondingly.

The domain $\mathcal{D}(\hat{P}\hat{X})$ is

$$\mathcal{D}(\hat{P}\hat{X}) = \{f : (\hat{X}f) \in \mathcal{D}(\hat{P})\}, \tag{51}$$

and the domain of the product $\hat{X}\hat{P}$ is equal here to the domain of the momentum operator because of the boundedness of the position operator.

For the σ-momentum $\hat{p}_{(\sigma)}$ the domain $\mathcal{D}_\sigma$ is given by (16). Then

$$\mathcal{D}([\hat{X},\hat{p}_{(\sigma)}]) = \{f : (\hat{X}f)(a) = e^{i\sigma}(\hat{X}f)(0)\} \cap \{f : f(a) = e^{i\sigma}f(0)\} = \{f : f(a) = f(b) = 0\}. \tag{52}$$

So CCR are realized on the dense domain in $L_2(0,a)$. This domain does not depend on the σ-realization of the momentum operator and coincides with the domain D_Π (23) of the energy operator.

Different σ-momenta, as corresponding to unitary nonequivalent projective representation of the Galilei group, correspond to different unitary nonequivalent representations of CCR although all are realized on the same dense domain D_Π.

Coming back to our quantum squash model: a player running with the velocity V sees a squash ball having σ-momentum. σ is given here by Eq. (49). H(is)er momentum eigenfunctions take on the form

$$\tilde{f}_n(\zeta,\tau) = e^{-i(mV/\hbar)\zeta}e^{i(2\pi n/a)(\zeta+V\tau)} = e^{(i/\hbar)(2\pi n/a - mV)\zeta}e^{i(2\pi n/a)V\tau}. \tag{53}$$

It is also interesting to look for solutions of the infinite potential well observed by a running player. This will be the subject of the next section.

V. SCHRÖDINGER EQUATION SEEN FROM THE MOVING REFERENCE FRAME

Let us consider a particle subjected to the influence of a time-dependent potential U. In the coordinate system $\mathcal{O}(x,t)$ the Schrödinger equation takes on the form

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{\partial x^2} + U(x,t)\Psi. \tag{54}$$

This equation is obviously not Galilei-invariant unless the potential is a trivial constant. A typical procedure is to investigate physical consequences of the symmetry group starting from the symmetry-invariant equations. In the case of the Galilei (or Poincaré) group this leads to a free

particle wave function realizing a unitary representation of the group. For the Galilei group and the Schrödinger equation one gets[11–14] that only nontrivial projective representations are physical realizations of the symmetry.

We are going to consider a more general approach based on the equivalence of all inertial coordinate systems. This Galilean equivalence principle demands that all laws of physics take the same form in different frames connected by the Galilei (or Poincaré for relativistic theory) transformations. We derive from the postulates that "the Galilei transformation is true" and "the Schrödinger equation is true" the transformation law of wave function for any scalar potential. So we do what Galilei would do, "if Galilei had know quantum mechanics."[28]

An observer in the reference frame $\mathcal{O}'(\zeta,\tau)$ sees the potential U as

$$\tilde{U}(\zeta,\tau)=U(\zeta+V\tau,\tau). \tag{55}$$

It is assumed here that the potential is a scalar with respect to the Galilei transformation (38). The equivalence principle demands that a wave function $\tilde{\Psi}(\zeta,\tau)$ viewed by an observer A' in the coordinate system $\mathcal{O}'$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial\tilde{\Psi}}{\partial\tau}=-\frac{\hbar^2}{2m}\frac{d^2\tilde{\Psi}}{\partial\zeta^2}+\tilde{U}(\zeta,\tau)\Psi. \tag{56}$$

An ansatz,

$$\tilde{\Psi}(\zeta,\tau)=e^{iu(\zeta,\tau)}\Psi(\zeta+V\tau,t), \tag{57}$$

gives

$$\frac{\partial\tilde{\Psi}}{\partial\tau}=ie^{iu}\frac{\partial u}{\partial\tau}\Psi+e^{iu}\frac{\partial\Psi}{\partial x}V+e^{iu}\frac{\partial\Psi}{\partial\tau},$$

$$\frac{\partial\tilde{\Psi}}{\partial\zeta}=ie^{iu}\frac{\partial u}{\partial\zeta}\Psi+e^{iu}\frac{\partial\Psi}{\partial x},$$

$$\frac{\partial^2\tilde{\Psi}}{\partial\zeta^2}=ie^{iu}\frac{\partial^2u}{\partial\zeta^2}\Psi-e^{iu}\left(\frac{\partial u}{\partial\zeta}\right)^2\Psi+2ie^{iu}\frac{\partial u}{\partial\zeta}\frac{\partial\Psi}{\partial x}+e^{iu}\frac{\partial^2\Psi}{\partial x^2}.$$

We see that Eq. (56) is fulfilled if

$$i\hbar\frac{\partial\Psi}{\partial x}V=-\frac{\hbar^2}{2m}2i\frac{\partial u}{\partial\zeta}\frac{\partial\Psi}{\partial x}, \tag{58a}$$

and

$$-\hbar\frac{\partial u}{\partial\tau}=\frac{\hbar^2}{2m}\frac{m^2}{\hbar^2}V^2. \tag{58b}$$

A solution of Eqs (58a) and (58b) takes on the form

$$u(\zeta,\tau)=-\frac{m}{\hbar}V\zeta-\frac{mV^2}{2\hbar}\tau+C(V). \tag{59}$$

So wave functions in different inertial reference frames connected by the Galilei transformation (38) are connected (up to the constant phase factor e^{iC}) by the relation

$$\tilde{\Psi}(\zeta,\tau)=e^{-(i/\hbar)(mV\zeta+(mV^2/2)\tau)}\Psi(x,t). \tag{60}$$

We have obtained the same factor as obtained by Bargmann[12] for a free Schrödinger particle subjected to the Galilei transformation. This factor leads to the mass-superselection rule which is mathematically due to the fact that projective (ray) representations of the Galilei group are not unitary equivalent to the usual representations.[13]

A. Stationary states seen from the moving reference frame

Let us consider now a particle in a static potential $U(x)$ described by a stationary wave function,

$$\Psi_n(x,t)=\psi_n(x)e^{-(i/\hbar)E_nt}, \tag{61}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2}+U(x)\psi_n(x)=E_n\psi_n(x). \tag{62}$$

According to the general rule (60), this state when viewed by a moving observer from the reference frame $\mathcal{O}'(\zeta,\tau)$ is described by a wave function,

$$\tilde{\Psi}_n(\zeta,\tau)=e^{-(i/\hbar)mV\zeta}\psi_n(\zeta+V\tau)e^{-(i/\hbar)(E_n+mV^2/2)\tau}. \tag{63}$$

One should note that this is not an energy eigenstate. This follows, at least formally, from the fact that Galilei transformed potential $\tilde{U}(\zeta,\tau)$ is now time dependent. The energy, however, is still conserved. To check this let us calculate an average value of the energy for the state described by the wave function (63). It is given as

$$\langle E\rangle_n=i\hbar\int d\zeta\tilde{\Psi}_n^*(\zeta,\tau)\frac{\partial}{\partial\tau}\tilde{\Psi}_n(\zeta,\tau). \tag{64}$$

Taking into account that solutions of Eq. (62) are real one obtains then

$$\langle E\rangle_n=E_n+\frac{mV^2}{2}. \tag{65}$$

This result seems to be surprising even in the simplest case of a free particle with the momentum p. Taking into account that the energy $E=p^2/2m$ and the momentum is Galilei transformed to $p-mV$ one should expect in Eq. (65) a subsidiary term of the form $-pV$. However, this not the case. Energy $p^2/2m$ is "produced" by a particle with the momentum $\pm p$. A real stationary state is a superposition of two waves corresponding to opposite momenta $\pm p$. They are Galilei transformed to $p\mp mV$ correspondingly and give contributions to the energy $p^2/2m+mV^2/2\mp pV$. These are additive contributions to the total energy so terms $\pm pv$ cancel each other. This remark gives a perfect agreement of Eq. (65) with our classical intuition although, as we will see later, does not always agree with a quantum reality.

B. Infinite potential well seen from the moving reference frame

When the potential well (1) is observed from the moving reference frame $\mathcal{O}'$ it is seen as

$$U(\zeta+V\tau)=\begin{cases}0 & \text{if } -V\tau\leqslant\zeta\leqslant a-V\tau,\\ \infty & \text{if } \zeta\notin\langle -V\tau,a-V\tau\rangle.\end{cases} \tag{66}$$

The wave function satisfies boundary conditions

$$\tilde{\Psi}(-V\tau,\tau)=\tilde{\Psi}(a-V\tau,\tau)=0. \tag{67}$$

The solution (63) has now a form

$$\tilde{\Psi}_N(\zeta,\tau)=\begin{cases}\sqrt{\dfrac{2}{a}}e^{-(i/\hbar)mV\zeta}\sin\dfrac{N\pi}{a}(\zeta+V\tau)e^{-(i/\hbar)((\pi^2\hbar^2/2ma^2)N^2+mV^2/2)\tau} & \text{if } -V\tau\leqslant\zeta\leqslant a-V\tau,\\ 0 \quad \text{if } \zeta\notin\langle -V\tau, a-V\tau\rangle.\end{cases} \tag{68}$$

where $N=1,2,\ldots$.

This solution can be written in the region $-V\tau\leqslant\zeta\leqslant a-V\tau$ as a superposition of two plain waves:

$$\tilde{\Psi}_N(\zeta,\tau)=\psi_{(+),N}(\zeta,\tau)-\psi_{(-),N}(\zeta,\tau), \tag{69a}$$

where

$$\psi_{(+),N}(\zeta,\tau)=\frac{1}{2i}\sqrt{\frac{2}{a}}e^{\frac{i}{\hbar}(N\pi\hbar/a-mV)\zeta}e^{-(i/2m\hbar)(N\pi\hbar/a-mV)^2\tau}, \tag{69b}$$

$$\psi_{(-),N}(\zeta,\tau)=\frac{1}{2i}\sqrt{\frac{2}{a}}e^{-(i/\hbar)(N\pi\hbar/a+mV)\zeta}e^{-(i/2m\hbar)(N\pi\hbar/a+mV)^2\tau}. \tag{69c}$$

This decomposition confirms our semiclassical understanding of the quantum problem. Alas, our semiclassical understanding does not quite agree with the mathematics behind the scene.

C. Moving observer measures momentum in the well

A measurement of an observable is mathematically equivalent to the spectral decomposition of the wave function into corresponding eigenfunctions. A general mathematical decomposition into momentum eigenfunctions was done in Sec. III A. A physical problem "what are possible momenta measured by a moving observer in the infinite potential well?," will be solved when h(is)er wave function $\tilde{\Psi}_N(\zeta,\tau)$ (68) will be expanded into h(is)er momentum eigenfunctions $\tilde{f}_n(\zeta,\tau)$ (53),

$$\tilde{\Psi}_N(\zeta,\tau)=\sum_{n=-\infty}^{+\infty}c_n^{(N)}(\tau)\tilde{f}_n(\zeta,\tau). \tag{70}$$

Coefficients $c_n^{(N)}$ are calculated as

$$\begin{aligned}c_n^{(N)}(\tau)&=\frac{\sqrt{2}}{a}e^{-\frac{i}{\hbar}((\pi^2\hbar^2/2ma^2)N^2+mV^2/2)\tau}\int_{-V\tau}^{-V\tau+a}d\zeta\,\sin\frac{N\pi}{a}(\zeta+V\tau)e^{-i(2\pi n/a)(\zeta+V\tau)}\\ &=e^{(-i/\hbar)(\pi^2\hbar^2/2ma^2)N^2+mV^2/2\tau}\times\begin{cases}-\dfrac{2N\sqrt{2}}{(4n^2-N^2)\pi} & \text{for odd } N,\\ \pm\dfrac{1}{i\sqrt{2}} & \text{for even } N, n=\pm N/2,\\ 0 \quad \text{for even } N, n\neq N/2.\end{cases}\end{aligned} \tag{71}$$

This gives *for even N* a simple expression, consistent with a semiclassical approach,

$$\tilde{\Psi}_N(\zeta,\tau)=\frac{1}{2i}\sqrt{\frac{2}{a}}[e^{(i/\hbar)(\pi N\hbar/a-mV)\zeta}e^{-(im/2\hbar)(V-\pi\hbar N/ma)^2\tau}-e^{-(i/\hbar)(\pi N\hbar/a+mV)\zeta}e^{-(im/2\hbar)(\pi\hbar N/ma+V)^2\tau}]. \tag{72}$$

The case *for odd N* is more involved and the momentum expansion (70) takes on the form

$$\tilde{\Psi}_N(\zeta,\tau)=\frac{2}{\pi N}\sqrt{\frac{2}{a}}e^{-i(mV/\hbar)\zeta}e^{-(i/\hbar)((\pi^2\hbar^2/2ma^2)N^2+mV^2/2)\tau}$$
$$-\frac{2N}{\pi}\sqrt{\frac{2}{a}}e^{-i(mV/\hbar)\zeta}e^{-(i/\hbar)((\pi^2\hbar^2/2ma^2)N^2+mV^2/2)\tau}\sum_{n=1}^{+\infty}\frac{1}{4n^2-N^2}[e^{i(2\pi n/a)(\zeta+V\tau)}+e^{-i(2\pi n/a)(\zeta+V\tau)}]. \tag{73a}$$

This can be also written as

$$\tilde{\Psi}_N(\zeta,\tau)=\frac{4N}{\pi}\sqrt{\frac{2}{a}}\sum_{n=-\infty}^{+\infty}\frac{e^{-i(\pi^2\hbar/2ma^2)(N^2-4n^2)\tau}}{N^2-4n^2}\,e^{(i/\hbar)(2\pi\hbar n/a-mV)\zeta}e^{-(im/2\hbar)(2\pi\hbar n/ma-V)^2\tau}, \tag{73b}$$

where contributions from stationary plane waves states are explicitly selected. We shall call from this time on a "stationary plane wave state" a plain wave with an explicit time dependence, i.e., a function of the form

$$e^{-i(p^2/2m\hbar)t}e^{(i/\hbar)\vec{p}\cdot\vec{r}}. \tag{74}$$

There is a striking difference in the behavior of odd- and even-N states $\tilde{\Psi}_N$. Any even N state is a superposition of two stationary plane waves states, while an odd-N state cannot be represented as a superposition of stationary plane wave states. An underlying mechanism is the same which made difference between Eqs (28) and (34)—allowed momenta in the infinite well are not always the same as formal arguments of the energy eigenfunctions (3).

This can be changed with a change of boundary conditions (2). If they are replaced by periodic-type conditions (22a),

$$\psi(0)=\psi(a),\quad \psi'(0)=\psi'(a), \tag{75}$$

then eigenfunctions of the Hamiltonian are

$$\sqrt{\frac{2}{a}}\sin\frac{2N\pi}{a}x,\quad \sqrt{\frac{2}{a}}\cos\frac{2N\pi}{a}x. \tag{76}$$

We see that for such boundary conditions allowed momenta in the infinite well are always the same as formal arguments of energy eigenfunctions and any state (76) is a superposition of two plane waves with the definite momenta. So, in a sense, a situation of periodic boundary conditions is "better" than for boundaries (3).

It is easy to create a "worse" situation. To this end it is enough to take antiperiodic-type boundary conditions,

$$\psi(0)=-\psi(a),\quad \psi'(0)=-\psi'(a). \tag{77}$$

Then eigenfunctions of the Hamiltonian are

$$\sqrt{\frac{2}{a}}\sin\frac{(2N+1)\pi}{a}x, \quad \sqrt{\frac{2}{a}}\cos\frac{(2N+1)\pi}{a}x. \tag{78}$$

For such boundary conditions allowed momenta in the infinite well are never the same as formal arguments of energy eigenfunctions and there is no state (78) as a superposition of two plane waves with the definite momenta.

VI. CONCLUSIONS

We performed a careful analysis of the notion of an observable related to the physical momentum. For the beginning one should identify a self-adjoint operator connected to this notion. In quantum mechanics defined on a finite interval a situation is more complicated than in the case of an unrestricted theory on $\mathbb{R}$ because there is a continuum (16) of self-adjoint extensions of the differential operator id/dx.

If you want to go beyond an argument that $-i\hbar d/dx$ is a physical momentum when it is assigned to the letter "p," and it is an angular momentum when assigned to the sign "l_z," then appropriate transformation properties must be taken into account. In a similar manner, three numbers can be a finite three-elements set or components of a three dimensional vector. A choice depends on assumed transformation properties with respect to rotations. In the momentum case, transformation properties are given (in a nonrelativistic approach) by the Galilei group as was done by conditions (39a)–(39c). All this together, supplemented with the equivalence of all inertial coordinate systems, led to different realizations of the momentum operator in the finite volume—in Sec. V C. Those different realizations have different spectra. This is quite obvious from the physical point of view.

Such an approach, based on a generalized correspondence principle (39a)–(39c), gave a physical interpretation of all self-adjoint extensions of the operator $-i\hbar d/dx$. It was also shown that those different extensions realize different nonunitary equivalent representations of CCR on the universal dense domain.

Obtained results can be generalized for a three dimensional rectangular box and the momentum operator $-i\hbar\nabla$.

Results of Sec. V show that important physical properties, related to transformation laws of wave functions, can be obtained under a much weaker assumption than was done in the past. A condition of Galilei invariance, widely used to obtain the mass superselection rule, is replaced by a (generalized) Galilei equivalence principle. This allows us to go beyond a free particle theory and gives results also for an arbitrary scalar potential.

The transformation law (63) can be treated as a realization of different self-adjoint extensions of the Hamiltonian. This is clearly visible in the infinite potential well where Eqs. (19) and (20) give different self-adjoint extensions of the operator d^2/dx^2. However, a situation here is not so simple as in the case of momentum operators. A structure of self-adjoint extensions of the operator d^2/dx^2 is much richer than in the case of the momentum operator. Only a part of those extensions can be related to the Galilei transformations and these are done by Eq. (68).

Results related to the momentum distribution, obtained in Secs. II and V C, need some comments. We have shown that the Fourier integral of the stationary wave function is directly related to the time-dependent dynamics given by Eq. (10). This gives a direct interpretation of that, which is usually called the "momentum representation of the wave function" or the "wave function in momentum space." This interpretation is different from what is usually found in textbooks. A simple statement that a wave function in momentum space,

$$\Phi(\vec{p},t) = \int d^3r \Psi(\vec{r},t) e^{-(i/\hbar)\vec{p}\cdot\vec{r}}, \tag{79}$$

is a probability amplitude to measure the momentum $\vec{p}$ at time t *is simply not true!* It sometimes reasonable, for technical reasons, to use a momentum representation of the wave function but only because of its mathematical equivalence to the wave function.

There is an exception in the "finite Universe" with dynamics defined on a finite interval. Let us introduce here two notions of momentum representation. The first is analogous to the previous one. You take the Fourier integral and you obtain a dynamics as in Eq. (10). This means that at $t=0$ all impenetrable walls vanish and you are left with a free particle. Such a situation is used in the HBT effect,[29] originally invented to determine the dimensions of distant astronomical objects. This method is widely used in high energy hadronic interaction to obtain information about the geometric properties of the source. Multi-pion and photon spectra provide precise information about reaction space time geometry in hadron–hadron and heavy ion collisions.[30,31]

Another concept of momentum representation—let us call it the "momentum distribution"—means to expand a wave function into stationary plane wave states (74). It was shown in Eq. (72) that this was possible for even-N states and impossible for odd-N states.

Such a momentum distribution in the "infinite Universe" would mean that

$$\Psi(\vec{r},t)=\int d^3p\Phi(\vec{p},t)e^{(i/\hbar)\vec{p}\cdot\vec{r}}e^{-i(p^2/2m\hbar)t}, \tag{80}$$

which is in general not possible.

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Semiclassical limit for multistate Klein–Gordon systems: almost invariant subspaces, and scattering theory

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By using the method of Helffer and Sjöstrand to construct Moyal projections, we extend the almost invariant subspace theory to the semiclassical context. Applications to the semiclassical limit for two component Klein–Gordon Hamiltonian are given. More precisely, under the conditions that the potential is analytic and its eigenvalues never cross we prove that the scattering matrix is block diagonal up to exponentially small errors. Also, we show how the existence of almost invariant subspaces leads to the existence of quasimodes with exponentially long lifetimes. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1782279]

I. INTRODUCTION

This paper is concerned with the semiclassical limit for matricial Klein–Gordon operators. More precisely we consider the two component Klein–Gordon Hamiltonian, acting in $\mathcal{H}=L^2(\mathbf{R}^n)^{\oplus 2}=L^2(\mathbf{R}^n)\oplus L^2(\mathbf{R}^n)$,

$$H_\epsilon=(\sqrt{\epsilon^2\Delta+1}-1)\mathbf{1}_2+V(x), \tag{1.1}$$

where $V(x)$ is a 2×2 Hermitian matrix valued function. At the heuristic level, under the conditions that $V(x)$ is smooth enough and its eigenvalues never cross, one expects (much like in the Born–Oppenheimer approximation) that the spectral and scattering problems for (1.1) can be reduced, up to some small errors, to the corresponding ones for two "scalar" effective Hamiltonians. Although the semiclassical limit can be viewed as a perturbation theory, it is a highly singular one so perturbed invariant subspaces do not exist and then one has to look for *almost* invariant subspaces as in the case of singular perturbation theory or adiabatic expansions [see Nenciu (2002), Nenciu (1993)]. The aim of this paper is to substantiate the heuristic picture by showing that the almost invariant subspace theory developed in Nenciu (2002) can be extended to the case at hand and in this respect the present paper can be considered as a direct continuation of Nenciu (2002).

The key point of the theory is to construct orthogonal projections,

$$\Pi_\epsilon^{\,2}=\Pi_\epsilon=\Pi_\epsilon^*,$$

satisfying

$$\|[\Pi_\epsilon,H_\epsilon]\|\leqslant s(\epsilon), \tag{1.2}$$

with $s(\epsilon)$ as small as possible so that with respect to the decomposition

$$L^2(\mathbf{R}^n)^{\oplus 2}=\Pi_\epsilon(L^2(\mathbf{R}^n)^{\oplus 2})\oplus(1-\Pi_\epsilon)(L^2(\mathbf{R}^n)^{\oplus 2}),$$

H_ϵ takes an almost diagonal form

$$H_\epsilon = H_\epsilon^D + H_\epsilon^{OD},$$

where

$$H_\epsilon^D = \Pi_\epsilon H_\epsilon \Pi_\epsilon + (1-\Pi_\epsilon) H_\epsilon (1-\Pi_\epsilon),$$

$$H_\epsilon^{OD} = (1-2\Pi_\epsilon)[\Pi_\epsilon, H_\epsilon],$$

with

$$\|H_\epsilon^{OD}\| \leqslant s(\epsilon).$$

As well known, the natural framework for the semiclassical limit is the theory of pseudodifferential operators and indeed our construction of the almost invariant subspaces rely heavily on pseudodifferential operators techniques, more exactly on the construction of Moyal projections, i.e., of orthogonal projections in the algebra of formal symbols which (at the formal symbols level) commutes with the symbol of the Hamiltonian. There are at least two different methods of constructing Moyal projections [Helffer and Sjöstrand (1990), Emmrich and Weinstein (1996), Brummelhuis and Nourrigat (1999)] and we shall follow the method of Helffer and Sjöstrand (1990) which is close in spirit with the Rellich–Kato perturbation theory. Then we follow Nenciu (2002) to construct, out of the formal Moyal projection, a bona fide orthogonal projection which almost commutes with the Hamiltonian.

We use the existence of almost invariant subspaces to prove the following results on scattering and spectral theory for matricial Klein–Gordon Hamiltonian:

(i) Under appropriate analytic and decay conditions on the potential, the scattering operator has, up to exponentially small errors, a block diagonal structure. This means that a state prepared at $t \to -\infty$ to have zero lower component will have as $t \to \infty$ only an exponentially small lower component.

(ii) The *existence* and the control on the (exponentially long) lifetime of metastable states (quasimodes). More precisely, suppose that the diagonal part, H_ϵ^D has discrete spectrum of one of the "channels" embedded into the continuous spectrum of the other channel. Then the (small) off diagonal part H_ϵ^{OD} turns these bound (stable) states into metastable states whose time life is controlled by the size of H_ϵ^{OD}. Let us mention here that in many instances [see, e.g., Stefanov (1999)] one can make the connection with the resonances defined as poles of the resolvent of scattering operator. In the cases when this connection can be made this implies that the imaginary part of the resonances is exponentially small.

The content of the paper is as follows. In Sec. II we give, at a general heuristic level, the construction of almost invariant subspaces. The reason for this is that we expect the methods developed here to be relevant and lead to a systematic theory for a much broader class of problems such as Born–Oppenheimer approximation [see, e.g., Littlejohn and Weigert (1993), Hagedorn and Joye (2000), Hagedorn and Joye (2001)], dynamics of crystal electrons in weak external fields [see, e.g., Blount (1962), Nenciu (1991), Hövermann, Spohn, and Teufel (2001)], dynamics of Pauli–Fierz model [see Teufel and Spohn (2002)], semiclassical limit of the Dirac operator [see, e.g., Littlejohn (1993), Spohn (2000)], etc. [Indeed after this paper appeared in the preprint form the almost invariant subspaces framework of this paper has been used in some recent papers on these subjects: Martinez and Sordoni (2002), Panati, Spohn, and Teufel (2003), Sordoni (2003), Bolte and Glaser (2004). For a comprehensive review of all these new developements we send the interested reader to the recent monograph Teufel (2003).]

Section III contains the technicalities for the case of analytic matricial Klein–Gordon operators as well as the applications to spectral and scattering theory. The technicalities are somewhat heavy for two reasons. First, in order to check the power of the method, we want to push the estimations up to exponential order, i.e., [see (1.2)], $s(\epsilon) \sim e^{-ct/\epsilon}$. The reader interested only in powerlike errors can skip most ot the technicalities and only the elementary pseudodifferential

operators theory is needed [see Teufel (2003) for further discussion]. Second, the application to the scattering theory is somewhat subtle since the perturbed Hamiltonian is almost diagonal with repect to a *ϵ-dependent* decomposition while the free one is diagonal with respect to the *canonical* decomposition given by

$$P_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{1.3}$$

Accordingly one must rotate the perturbed Hamiltonian so that the rotated one is almost diagonal with respect to the canonical decomposition and to prove that the rotation does not affect the scattering matrix. So besides the fact that one must prove that as $x \to \infty$ the rotated Hamiltonian approaches the free one sufficiently quick one needs also to prove that the rotation is close to the identity for states localized far away (see Remark II.4).

In the Appendix we collect, in an appropriate form, the results we need on pseudodifferential operators with analytic symbols. For a readable account of basic pseudodifferential operators theory we send the reader to Martinez (2002). Further details and references to pseudodifferential operators with matrix valued symbols can be found in Teufel (2003), Bolte and Glaser (2003, 2004).

We end with a few comments on earlier results on spectral and scattering theory for the matricial Klein–Gordon Hamiltonian in the semiclassical limit. Results on almost diagonal structure of the scattering matrix at *fixed* energy were obtained before in Nakamura (1994), Benchaou (1998), Benchaou and Martinez (1999), Martinez, Nakamura, and Sordoni (2002) both for Klein–Gordon and Schrödinger cases, by the method of phase space tunnelling developed by Martinez (1994) [see also Martin and Nenciu (1995) where almost invariant subspaces at fixed energies were constructed in the case of the one-dimensional Schrödinger operator, for energies above the potential barrier]. We would like to stress that aside from more restrictive conditions on the potential the results quoted above were proved *only* for nontrapping energies a condition which implies, in particular, the absence of resonances close to real axis and it is not valid in general at low energies (which are the most interesting from the physical point of view). Without entering the technicalities [we send the interested reader to Jecko (1998), Jecko (2004) for details and extended bibliography] we remind that an energy is nontrapping if *all* the trajectories of the corresponding classical system (i.e., the classical Hamiltonian is the symbol of the quantum Hamiltonian) are not bounded. Notice that at the heuristic level on intervals of trapping energies one expects bound states and/or quasimodes to exist. In some sense our results on the existence of quasimodes are extensions of the shape resonance theory to the matricial case. As for the scattering theory it seems that our result is the first one valid also for the trapping energies. In the same time it is weaker in the sense that involve an averaging over intervals of energies (see Sec. III for precise formulation and a heuristic discussion of its significance).

The results have been announced in Nenciu (2004).

II. GENERALITIES. MOYAL PROJECTIONS, ALMOST INVARIANT SUBSPACES AND BLOCK DIAGONALIZATION

We start by fixing some terminology and notations. In what follows, $x,\ \xi \in \mathbf{R}^n$, $n \geqslant 1$, $\epsilon \in [0, \epsilon_0]$, $\epsilon_0 > 0$, and $h(x,\xi;\epsilon)$ are C^∞, $m \times m$ Hermitian matrix valued functions on $\mathbf{R}^{2n} \times [0, \epsilon_0]$ [actually by adding the necessary technicalities one can consider the case when $h(x,\xi;\epsilon)$ are C^∞ self-adjoint operator valued functions]. If h and its derivatives satisfies suitable estimates (see Appendix), then associated to $h(x,\xi;\epsilon)$ one can consider the (essentially self-adjoint under appropriate conditions) operator H_ϵ obtained as the Weyl quantization of $h(x,\xi;\epsilon)$ (called the symbol of H_ϵ), i.e., for $\phi \in (S(\mathbf{R}^n))^{\oplus m}$,

$$(H_\epsilon \phi)(x) = (\mathrm{Op}^w_\epsilon(h)\phi)(x) = \left(\frac{1}{2\pi\epsilon}\right)^n \int e^{i[(x-y)\xi/\epsilon]} h\left(\frac{x+y}{2}, \xi; \epsilon\right) \phi(y) \mathrm{d}y\, \mathrm{d}\xi.$$

If $h(x,\xi;\epsilon)$ has an asymptotic expansion (as $\epsilon \to 0$)

$$h(x,\xi;\epsilon) \sim \sum_{j=0}^{\infty} h_j(x,\xi)\epsilon^j, \tag{2.1}$$

we say that $\Sigma_{j=0}^{\infty} h_j(x,\xi)\epsilon^j$ is the formal symbol of H_ϵ. Given another symbol b and denoting by $B_\epsilon = \mathrm{Op}_\epsilon^w(b)$, then as is well known [see Martinez (2002)], the operator multiplication corresponds to the Moyal product of symbols

$$H_\epsilon B_\epsilon = \mathrm{Op}_\epsilon^w(h\#b),$$

where $h\#b$ is given by the oscillatory integral

$$(h\#b)(x,\xi;\epsilon) = \frac{1}{2\pi\epsilon}^{2n} \int e^{i\varphi(x,y,v,\xi,\eta,\theta)/\epsilon} h\left(\frac{x+u}{2},\eta;\epsilon\right) b\left(\frac{x+v}{2},\theta;\epsilon\right) \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}\eta\,\mathrm{d}\theta, \tag{2.2}$$

with $\varphi(x,y,v,\xi,\eta,\theta) = (\xi-\eta)(v-x)+(\xi-\theta)(x-v)$. At the level of formal symbols by expanding the oscillatory integral (2.2), one can obtain that $h\#b \sim \Sigma_{j=0}^{\infty}(h\#b)_j\epsilon^j$, where

$$(h\#b)_j(x,\xi) = \sum_{|\alpha|+|\beta|+k+l=j} \Gamma(\alpha,\beta)\partial_\xi^\alpha D_x^\beta h_k(x,\xi)\partial_\xi^\beta D_x^\alpha b_l(x,\xi) \tag{2.3}$$

and

$$\Gamma(\alpha,\beta) := \frac{(-1)^{|\beta|}}{\alpha!\beta!2^{|\alpha|}2^{|\beta|}}.$$

As already mentioned, we are looking for almost invariant subspace for H_ϵ in the semiclassical limit, $\epsilon \to 0$. The basic idea is to construct first Moyal projections, i.e., formal symbols

$$\pi(x,\xi;\epsilon) \sim \sum_{j=0}^{\infty} \pi_j(x,\xi;\epsilon)\epsilon^j \tag{2.4}$$

satisfying (at a formal series level)

$$\pi \sim \pi^* \sim \pi\#\pi, \tag{2.5}$$

$$\pi\#h - h\#\pi \sim 0 \tag{2.6}$$

[here by $\pi^*(x,\xi;\epsilon)$ we mean the adjoint of the matrix $\pi(x,\xi;\epsilon)$]. The proposition below says that one can always construct Moyal projections corresponding to isolated parts of the spectrum of the principal symbol $h_0(x,\xi)$ of $h(x,\xi;\epsilon)$,

$$h(x,\xi;\epsilon) = h_0(x,\xi) + \mathcal{O}(\epsilon). \tag{2.7}$$

Let $\sigma(x,\xi)$ be the spectrum of $h_0(x,\xi)$ and suppose that, for some $(x_0,\xi_0) \in \mathbf{R}^{2n}$,

$$\sigma(x_0,\xi_0) = \sigma_1(x_0,\xi_0) \cup \sigma_2(x_0,\xi_0),$$

$$\mathrm{dist}(\sigma_1(x_0,\xi_0),\sigma_2(x_0,\xi_0)) := \mathrm{d}(x_0,\xi_0) > 0. \tag{2.8}$$

Then by perturbation theory there exists a neighborhood $\mathcal{U}(x_0,\xi_0)$ of (x_0,ξ_0) such that, for $(x,\xi) \in \mathcal{U}(x_0,\xi_0)$ the spectrum of $h_0(x,\xi)$ is well separated, i.e., (2.8) is satisfied on $\mathcal{U}(x_0,\xi_0)$ with $\mathrm{d}(x,\xi) \geqslant \mathrm{d}(x_0,\xi_0)/2$, and there exists a contour Γ_{x_0,ξ_0} [not depending upon $(x,\xi) \in \mathcal{U}(x_0,\xi_0)$] enclosing $\sigma_1(x,\xi)$ and satisfying

$$\mathrm{dist}(\Gamma_{x_0,\xi_0},\sigma(x,\xi)) \geqslant \mathrm{d}(x_0,\xi_0)/2. \tag{2.9}$$

Proposition II.1: Suppose (2.8) holds true. Then, for $(x,\xi) \in \mathcal{U}(x_0,\xi_0)$, *there exist unique*

$\pi_j(x,\xi)$, $j=0,1,\ldots$, such that $\pi_0(x,\xi)$ is the spectral projection of $h_0(x,\xi)$ corresponding to $\sigma_1(x,\xi)$ and the formal symbol $\Sigma_{j=0}^{\infty}\pi_j(x,\xi)\epsilon^j$ satisfies (2.5) and (2.6).

The result in Proposition II.1 was found independently by different authors in different contexts and actually Proposition II.1 appeared many times in the literature, e.g., Helffer and Sjöstrand (1990), Emmrich and Weinstein (1996), Brummelhuis and Nourrigat (1999) [see also Sjöstrand (1993) where the earlier construction in Nenciu (1993) and Joye and Pfister (1993) of adiabatic projections corresponding to the case $h(x,\xi;\epsilon)=\xi+H_\epsilon(x)$ was obtained in the framework of the theory of pseudodifferential operators]. There are essentially two methods of proof. The first one, Nenciu (1993), Emmrich and Weinstein (1996), Brummelhuis and Nourrigat (1999), is a recurrent construction for π_j solving the equations coming from (2.5) and (2.6). The second one, Helffer and Sjostrand (1990), Sjöstrand (1993) is close in spirit to Rellich–Kato perturbation theory [see, e.g., Kato (1980)]: due to (2.9), for all $z\in\Gamma_{x_0,\xi_0}$, one can construct [see Robert (1987), Martinez (2002)] the parametrix

$$q(x,\xi;\epsilon,z)\sim\sum_{j=0}^{\infty}q_j(x,\xi;z)\epsilon^j,$$

satisfying (at a formal series level)

$$q\#(h-z)\sim(h-z)\#q\sim 1, \tag{2.10}$$

and then obtain $\pi_j(x,\xi)$ from Riesz formula for spectral projection,

$$\pi(x,\xi;\epsilon)=\frac{i}{2\pi}\int_{\Gamma_{x_0,\xi_0}}q(x,\xi;\epsilon,z)\mathrm{d}z, \tag{2.11}$$

i.e.,

$$\pi_j(x,\xi)=\frac{i}{2\pi}\int_{\Gamma_{x_0,\xi_0}}q_j(x,\xi;z)\mathrm{d}z. \tag{2.12}$$

In what follows, we shall use the second method since, on the one hand, it gives explicit formulas for π_j and, on the other hand, allows a much easier control on $\pi_j(x,\xi)$ and their derivatives than the recurrent construction [compare for example the estimations in Nenciu (1993) with those in Martinez and Nenciu (1995) in the adiabatic case].

Remarks:

II.1. If $h_0(x,\xi)$ has a part of the spectrum which remains isolated for all $(x,\xi)\in\mathbf{R}^{2n}$, then, from Proposition II.1, one obtains $\pi_j(x,\xi)$ defined on all $\mathbf{R}^{2n}$. Moreover $\pi_j(x,\xi)$ are C^∞ and if $h_j(x,\xi)$ are real analytic $\pi_j(x,\xi)$ are also real analytic.

II.2. It is known [Helffer and Sjöstrand (1990)] that the existence of $\pi(x,\xi)$ satisfying (2.5) and (2.6) is equivalent with the block diagonalization of $h(x,\xi;\epsilon)$ at a formal level [see, e.g., Nirenberg (1973), Taylor (1981)], i.e., with the existence of a formal symbol

$$u(x,\xi;\epsilon)\sim\sum_{j=0}^{\infty}u_j(x,\xi)\epsilon^j,$$

satisfying (at the formal symbol level)

$$u\#u^*\sim u^*\#u\sim 1$$

such that, setting

$$\tilde{h}:\sim u^*\#h\#u,$$

then

$$\pi_0 \# \tilde{h} - \tilde{h} \# \pi_0 \sim 0.$$

It is worth mentioning that the formal block diagonalization appeared also in the physical literature, see e.g., Blount (1962), Littlejohn and Weigert (1993) and references therein. Let us remark that, unlike π_j, u_j (and then u and $\overline{h}$) are not unique. A somewhat canonical choice is the one mimicking the reduction scheme of Rellich–Kato perturbation theory, i.e., writing $u(x,\xi;\epsilon)$ as the Sz–Nagy matrix [see (2.25)] corresponding to the pair $\pi(x,\xi;\epsilon)$, $\pi_0(x,\xi)$,

$$u \sim (\pi \# \pi_0 + (1-\pi) \# (1-\pi_0)) \# \left(1 + \sum_{j=1}^{\infty} \frac{(2j-1)!!}{2^j j!} (\pi - \pi_0)^{\#2j}\right).$$

Let us stress that Proposition II.1 gives $\pi(x,\xi;\epsilon)$ only at the formal symbol level, that is the series $\Sigma_{j=0}^{\infty} \pi_j(x,\xi)\epsilon^j$ is not convergent in general. As a consequence (2.5) and (2.6) do not imply the existence of a corresponding orthogonal projection which commutes with H_ϵ. However, by resummation [Martinez (2002)], there exist symbols $\hat{\pi}(x,\xi;\epsilon)$ [unique modulo $\mathcal{O}(\epsilon^\infty)$] which are asymptotically equivalent with the formal symbol $\Sigma_{j=0}^{\infty} \pi_j \epsilon^j$ and satisfy (2.5) and (2.6) [where now # means the Weyl product in (4.6)] up of errors smaller than any power of ϵ, i.e., (2.5) and (2.6) hold modulo $\mathcal{O}(\epsilon^\infty)$. In addition, the ressumation can be chosen (see Appendix) as to insure that $\hat{\pi}(x,\xi;\epsilon) = \hat{\pi}^*(x,\xi;\epsilon)$.

We turn now to the construction, out of the formal symbol $\Sigma_{j=0}^{\infty} \pi_j \epsilon^j$ of almost invariant subspaces for the H_ϵ. Suppose that $\pi_j(x,\xi)$ are globally defined on $\mathbf{R}^{2n}$ and are uniformly bounded together with their derivatives. Then, by resummation, one can obtain [unique up to $\mathcal{O}(\epsilon^\infty)$] $\hat{\pi}(x,\xi;\epsilon)$ which is also bounded together with its derivatives uniformly on $\mathbf{R}^{2n} \times [0, \epsilon_0]$, for some $\epsilon_0 > 0$. Then, by Calderon–Vaillancourt theorem (see Appendix),

$$\hat{\Pi}_\epsilon = \mathrm{Op}_\epsilon^w(\hat{\pi}(x,\xi;\epsilon)) \tag{2.13}$$

is bounded and satisfies

$$\hat{\Pi}_\epsilon^2 - \hat{\Pi}_\epsilon = \mathcal{O}(\epsilon^\infty), \quad \hat{\Pi}_\epsilon^* = \hat{\Pi}_\epsilon. \tag{2.14}$$

For applications to spectral and scattering theory one would like to construct almost invariant subspaces which amounts to construct out of π_j an orthogonal projection Π_ϵ,

$$\Pi_\epsilon^2 = \Pi_\epsilon = \Pi_\epsilon^*, \tag{2.15}$$

satisfying

$$\|[\Pi_\epsilon, H_\epsilon]\| \leqslant s(\epsilon) \tag{2.16}$$

with $s(\epsilon) \geqslant 0$ as small as possible [if the series in (2.4) is nonconvergent one cannot have in general $s(\epsilon) = 0$ in (2.16)]. Of course, such a construction is not unique and we shall follow the one of Nenciu (1993), Nenciu (2002). Since $\hat{\Pi}_\epsilon^2 - \hat{\Pi}_\epsilon = \mathcal{O}(\epsilon^\infty)$, for ϵ sufficiently small the spectrum of $\hat{\Pi}_\epsilon$ is concentrate near 0 and 1 and then one can define Π_ϵ by

$$\Pi_\epsilon = \frac{i}{2\pi} \int_{|z-1|=1/2} (\hat{\Pi}_\epsilon - z)^{-1} \, dz. \tag{2.17}$$

Obviously Π_ϵ given by (2.17) satisfies (2.15). By a straightforward computation [Nenciu (1993), Nenciu (2002)], it is easy to see that, for ϵ sufficiently small, we have

$$\|[\Pi_\epsilon, H_\epsilon]\| \leqslant 2\|[\hat{\Pi}_\epsilon, H_\epsilon]\|. \tag{2.18}$$

Since it turns out that (2.6) implies that

$$[\hat{\Pi}_\epsilon, H_\epsilon] = \mathcal{O}(\epsilon^\infty), \tag{2.19}$$

we obtain almost invariant subspace modulo $\mathcal{O}(\epsilon^\infty)$. It turns out that

$$\|\hat{\Pi}_\epsilon - \Pi_\epsilon\| = \mathcal{O}(\epsilon^\infty)$$

so Π_ϵ is close to a pseudodifferential operator [actually, the results in Dimassi and Sjöstrand (1999) implies that Π_ϵ is a pseudodifferential operator]. Moreover, under appropriate analyticity properties of $h(x,\xi;\epsilon)$, one can choose a resummation of the analytic formal symbol $\Sigma_{j=0}^\infty \pi_j(x,\xi)\epsilon^j$ (see Appendix) in order to obtain an almost invariant subspace modulo $\mathcal{O}(e^{-c/\epsilon})$ for some positive constant $c>0$ independent of ϵ, i.e., one can take $s(\epsilon)=Ce^{-c/\epsilon}$ in (2.16). With respect to the decomposition

$$L^2(\mathbf{R}^n)^{\oplus m} = \Pi_\epsilon(L^2(\mathbf{R}^n)^{\oplus m}) \oplus (1-\Pi_\epsilon)(L^2(\mathbf{R}^n)^{\oplus m}),$$

H_ϵ takes an almost diagonal form,

$$H_\epsilon = H_\epsilon^{\,D} + H_\epsilon^{\,OD}, \tag{2.20}$$

where

$$H_\epsilon^{\,D} = \Pi_\epsilon H_\epsilon \Pi_\epsilon + (1-\Pi_\epsilon)H_\epsilon(1-\Pi_\epsilon), \tag{2.21}$$

$$H_\epsilon^{\,OD} = (1-2\Pi_\epsilon)[\Pi_\epsilon, H_\epsilon], \tag{2.22}$$

with

$$\|H_\epsilon^{\,OD}\| \leqslant s(\epsilon). \tag{2.23}$$

If $\pi_0(x,\xi)=\pi_0(x)$ does not depend upon ξ (as is the case of the Klein–Gordon or Schrödinger operators) then $\Pi_0=\mathrm{Op}_\epsilon^w(\pi_0)$ is just a multiplication matrix valued operator. Since

$$\lim_{\epsilon\to 0}\|\Pi_\epsilon - \Pi_0\| = 0, \tag{2.24}$$

for sufficiently small ϵ one can write down the Sz–Nagy transformation matrix corresponding to the pair Π_ϵ, Π_0 [see Kato (1980)],

$$U_\epsilon = (1-(\Pi_\epsilon-\Pi_0)^2)^{-1/2}(\Pi_\epsilon\Pi_0 + (1-\Pi_\epsilon)(1-\Pi_0)) \tag{2.25}$$

having the properties

$$U_\epsilon^{\,*}U_\epsilon = U_\epsilon U_\epsilon^{\,*} = 1, \tag{2.26}$$

$$\Pi_\epsilon = U_\epsilon \Pi_0 U_\epsilon^{\,*}. \tag{2.27}$$

From (2.20)–(2.23), (2.26), and (2.27) one gets that

$$\tilde{H}_\epsilon = U_\epsilon^{\,*} H_\epsilon U_\epsilon \tag{2.28}$$

has an almost diagonal form $\tilde{H}_\epsilon=\tilde{H}_\epsilon^{\,D}+\tilde{H}_\epsilon^{\,OD}$ with respect to the ϵ independent decomposition

$$L^2(\mathbf{R}^n)^{\oplus m} = \Pi_0(L^2(\mathbf{R}^n)^{\oplus m}) \oplus (1-\Pi_0)(L^2(\mathbf{R}^n)^{\oplus m})$$

with

$$\|\tilde{H}_\epsilon^{OD}\| \leqslant s(\epsilon). \tag{2.29}$$

Further, since $\mathbf{R}^n$ is contractible, one can find $Q(x)$ (see Lemma III.5 for an explicit construction in our case) unitary in $\mathbf{C}^n$ and satisfying

$$\Pi_0(x) = Q(x)P_0Q^*(x)$$

with $P_0 = \left(\begin{smallmatrix} \mathbf{1}_p & 0 \\ 0 & 0 \end{smallmatrix}\right)$ where $p = \dim \Pi_0(x)$ (which does not depend upon x) and then

$$H_\epsilon^{\text{eff}} = Q\tilde{H}_\epsilon Q^* \tag{2.30}$$

has an almost block diagonal form with respect to the *canonical* decomposition

$$L^2(\mathbf{R}^n)^{\oplus m} = L^2(\mathbf{R}^n)^{\oplus p} \oplus L^2(\mathbf{R}^n)^{\oplus(m-p)}.$$

In this way, up to a unitary transformation and errors of order $s(\epsilon)$ the study of H_ϵ in $L^2(\mathbf{R}^n)^{\oplus m}$ is reduced to the study of two operators in $(L^2(\mathbf{R}^n))^{\oplus p}$ and $(L^2(\mathbf{R}^n))^{\oplus(m-p)}$, respectively. If one assumes that all the m eigenvalues of $h_0(x,\xi)$ remain isolated over all $\mathbf{R}^{2n}$, one can make a complete diagonalization which reduces [up to errors of order $s(\epsilon)$] the study of the m-states Hamiltonian H_ϵ to the study of m scalar operators in $L^2(\mathbf{R}^n)$.

Remarks:

II.4. For the scattering theory the estimates (2.16) or (2.34) have to be improved at $|x| \to \infty$; for example, in the Klein–Gordon case one has to replace (2.16) by (we use the notation $\langle x\rangle = \sqrt{1+x^2}$)

$$\|\langle x\rangle^{t\delta}[\Pi_\epsilon, H_\epsilon]\langle x\rangle^{(1-t)\delta}\| \leqslant s(\epsilon), \quad t \in [0,1] \tag{2.31}$$

for some $\delta > 1$. At the technical level this amounts to show that the decay of $V(x)$ [see (3.3) below] "propagates" through the construction of Π_ϵ.

II.5. The above construction works nicely if $\pi_j(x,\xi)$ are bounded as it is the case for Klein–Gordon or Dirac operators. Unfortunately, this is not the case in the Schrödinger case where $\pi_j(x,\xi)$ behaves like $\langle\xi\rangle^j$ as $|\xi| \to \infty$ irrespective of how nice the potential is. As a consequence a block diagonalization valid on the whole $L^2(\mathbf{R}^n)^{\oplus m}$ seems not to exist (in concordance with the physical arguments saying that the adiabatic decoupling becomes poorer and poorer as energy increases) [see also the remarks in Martin and Nenciu (1995)]. However one can still hope to have it as far as the energy (and then $|\xi|$) remains bounded. One can show [see Sordoni (2003)] that this is indeed the case and the idea is to replace $\hat{\Pi}_\epsilon$ with

$$\hat{\Pi}_\epsilon^\Phi = \Phi(H_\epsilon)\hat{\Pi}_\epsilon + (1-\Phi(H_\epsilon))\hat{\Pi}_\epsilon\Phi(H_\epsilon) + (1-\Phi(H_\epsilon))\Pi_0(1-\Phi(H_\epsilon)), \tag{2.32}$$

where Φ is a smooth cutoff function on $\mathbf{R}$. Then the whole procedure works and, defining

$$\Pi_\epsilon^\Phi := \frac{i}{2\pi}\int_{|z-1|=1/2} (\hat{\Pi}_\epsilon^\Phi - z)^{-1}\,dz, \tag{2.33}$$

gives instead of (2.16),

$$\|\chi(H_\epsilon)[\Pi_\epsilon^\Phi, H_\epsilon]\| \leqslant s(\epsilon), \tag{2.34}$$

for any cutoff function χ such that $\chi^\Phi = \chi$.

III. TWO COMPONENT KLEIN–GORDON SYSTEMS. EXPONENTIAL ESTIMATES

In this section we prove the existence of invariant subspaces up to exponential small errors as $\epsilon \to 0$, for two component Klein–Gordon systems, and apply this to spectral and scattering theory. Consider the two-component Klein–Gordon Hamiltonian,

$$H_\epsilon = a(\epsilon D_x)\mathbf{1}_2 + V(x) \tag{3.1}$$

acting on $\mathcal{H}=L^2(\mathbf{R}^n)^{\oplus 2}:=L^2(\mathbf{R}^n)\oplus L^2(\mathbf{R}^n)$. Here $a(\xi)=(\sqrt{\xi^2+1}-1)$,$\mathbf{1}_2$ is the 2×2 identity matrix and $V(x)$ is a 2×2 Hermitian matrix valued function that admits an analytic extension in some strip

$$\Gamma_a = \{x \in \mathbf{R}^n; |\mathrm{Im}\, x| < a\}, \quad a > 0. \tag{3.2}$$

Moreover, since we have in mind application to scattering theory we assume $V(x)$ to be short range, i.e., there exists a Hermitian 2×2 matrix V_∞ such that

$$\sup_{x\in\Gamma_a} \langle x\rangle^\delta |V(x) - V_\infty| < \infty \tag{3.3}$$

uniformly on Γ_a with $\delta > 1$. Without loss of generality we can assume that

$$V_\infty = \begin{pmatrix} \lambda_{1,\infty} & 0 \\ 0 & \lambda_{2,\infty} \end{pmatrix}. \tag{3.4}$$

Concerning the spectrum of $V(x)$, we assume that the two real eigenvalues $\lambda_i(x)$, satisfy

$$\inf_{x\in\mathbf{R}^n} (\lambda_1(x) - \lambda_2(x)) = 2d > 0. \tag{3.5}$$

By eventually shrinking Γ_a, one can suppose that

$$\inf_{x\in\Gamma_a} |\lambda_1(x) - \lambda_2(x)| \geqslant d. \tag{3.6}$$

It follows that on Γ_a

$$V(x) = \lambda_1(x)\pi_0(x) + \lambda_2(x)(1 - \pi_0(x)),$$

where $\pi_0(x)$ is a bounded projection in $\mathbf{C}^2$, analytic in Γ_a and self-adjoint for $x \in \mathbf{R}^n$. Due to (3.4), $\pi_0(\infty) = \lim_{|x|\to+\infty} \pi(x) = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$, and from (3.3),

$$\sup_{x\in\Gamma_a} \langle x\rangle^\delta |\pi_0(x) - \pi_0(\infty)| < \infty. \tag{3.7}$$

In what follows, "for ϵ sufficiently small" is short hand for "there exists $\epsilon_0 > 0$ such that for $0 < \epsilon \leqslant \epsilon_0$." A finite number of finite, strictly positive constants independent of ϵ will appear in this section; they are all denoted by c or C. For an operator A and $\eta > 0$ we shall denote

$$\|A\|_\eta = \sup_{t\in[0,1]} \|\langle x\rangle^{t\eta} A \langle x\rangle^{(1-t)\eta}\|.$$

In the following we denote by Π_0 the operator in $\mathcal{H}$ acting as multiplication by the matrix $\pi_0(x)$.

Theorem III.1: *Assume (3.2), (3.3), and (3.5) hold true. Then, for sufficiently small ϵ, there exists an orthogonal projection Π_ϵ in $\mathcal{H}$ satisfying*

$$\|[\Pi_\epsilon, H_\epsilon]\|_\delta = \mathcal{O}(e^{-c/\epsilon}), \tag{3.8}$$

$$\epsilon^{-1}\|\Pi_\epsilon - \Pi_0\|_\delta = \mathcal{O}(1) \tag{3.9}$$

uniformly with respect to $\epsilon \in (0, \epsilon_0]$.

Proof: As already said in Sec. II, the main step in the proof of Theorem III.1 is the construction of Moyal projections for

$$h_0(\xi, x) = a(\xi)\mathbf{1}_2 + V(x). \tag{3.10}$$

Lemma III.2: There exists a formal analytic symbol

$$\pi(x,\xi;\epsilon) = \pi_0(x) + \sum_{j=1}^{\infty} \pi(x,\xi)\epsilon^j, \tag{3.11}$$

that satisfies (2.5) and (2.6), and, in addition, such that $\pi(x,\xi;\epsilon) - \pi_0(x) \in S_A^0(\langle x\rangle^{-\delta})$ *[see Appendix for the definition of* $S_A^0(1)$ *and* $S_A^0(\langle x\rangle^{-\delta})$*].*

Proof: Let $x_0,\ \xi_0 \in \mathbf{R}^n,\ 0<\eta<d/4$ and $\Gamma_{x_0,\xi_0,d,\eta}=\{z\in\mathbf{C}; d/2-\eta<|z-a(\xi_0)-\lambda_1(x_0)|<d/2+\eta\}$. Since $V(x)$ is analytic and uniformly bounded on Γ_a, $a(\xi)$ is analytic on Γ_1 and in addition $\partial_\xi^\alpha a(\xi)$, $|\alpha|=1$ are uniformly bounded on Γ_1, there exists $b>0$, $M>0$ independent on x_0, $\xi_0 \in \mathbf{R}^n$ such that for all $z\in\Gamma_{x_0,\xi_0,d,\eta}$,

$$q_0(x,\xi,z) = (h_0(x,\xi)-z)^{-1}$$

is analytic in $|x-x_0|<b$, $|\xi-\xi_0|<b$ and in addition

$$\operatorname*{Sup}_{|x-x_0|<b,|\xi-\xi_0|<b,z\in\Gamma_{x,\xi,d,\eta}} |q_0(x,\xi,z)| < M. \tag{3.12}$$

Then from Cauchy inequalities there exists $C>0$ such that for any $\alpha,\ \beta\in\mathbf{N}^n$,

$$\operatorname*{Sup}_{x,\xi\in\mathbf{R}^n,z\in\Gamma_{x,\xi,d,\eta}} |\partial_\xi^\alpha\partial_x^\beta q_0(x,\xi,z)| \leqslant C^{|\alpha|+|\beta|+1}\alpha!\beta! \tag{3.13}$$

and in addition [see (3.3)], if $|\beta|\neq 0$,

$$\operatorname*{Sup}_{x,\xi\in\mathbf{R}^n,z\in\Gamma_{x,\xi,d,\eta}} |\langle x\rangle^\delta\partial_\xi^\alpha\partial_x^\beta q_0(x,\xi,z)| \leqslant C^{|\alpha|+|\beta|+1}\alpha!\beta!. \tag{3.14}$$

Define now for $x,\ \xi\in\mathbf{R}^n$, $z\in\Gamma_{x,\xi,d,\eta}$ the formal analytic symbol

$$r = \sum_{j=1}^{\infty} r_j(x,\xi;z)\epsilon^j$$

by

$$(h_0(x,\xi)-z)\,\#\,q_0(x,\xi;z) = 1 - r(x,\xi;\epsilon,z).$$

Notice that $r_0(x,\xi)=0$. Taking into account (3.13) and (3.14) and that, for all $\alpha,\ \beta\in\mathbf{N}^n$, $|\beta|\neq 0$,

$$\operatorname*{Sup}_{(x,\xi)\in\mathbf{R}^n} |\langle x\rangle^\delta\partial_\xi^\alpha\partial_x^\beta h_0(x,\xi)| \leqslant C^{|\alpha|+|\beta|+1}\alpha!\beta!, \tag{3.15}$$

from the composition rule, Leibnitz formula and Lemma IV.4 one obtains that, for all $j=0,1,\ldots$, and $\alpha,\ \beta\in\mathbf{N}^n$,

$$\operatorname*{Sup}_{x,\xi\in\mathbf{R}^n,z\in\Gamma_{x,\xi,d,\eta}} |\langle x\rangle^\delta\partial_\xi^\alpha\partial_x^\beta r_j(x,\xi,z)| \leqslant C^{j+|\alpha|+|\beta|+1}\alpha!\beta!j!. \tag{3.16}$$

If we define the formal symbol $q(x,\xi;\epsilon,z)$ by

$$q = q_0 + q_0\,\#\sum_{j=1}^{\infty} r^{\#j}, \tag{3.17}$$

then q satisfy an estimate like (3.16). More exactly we have the following.

Lemma III. 3: There exists C such that for all $j=1,2,\ldots$, *and* $\alpha,\ \beta\in\mathbf{N}^n$,

$$\operatorname*{Sup}_{x,\xi\in\mathbf{R}^n,z\in\Gamma_{x,\xi,d,\eta}} |\langle x\rangle^\delta\partial_\xi^\alpha\partial_x^\beta q_j(x,\xi,z)| \leqslant C^{j+|\alpha|+|\beta|+1}\alpha!\beta!j!. \tag{3.18}$$

Proof: Replace the supremum over $(x,\xi)\in\Gamma_{a'}\times\Gamma_{b'}$ in (4.5) with the supremum over $x,\ \xi$

$\in \mathbf{R}^n$, $z \in \Gamma_{x,\xi,d,\eta}$ and mimic the proof of Lemmas IV.4 and IV.5 in the Appendix.

From (2.10) it follows that, for x, $\xi \in \mathbf{R}^n$, $z \in \Gamma_{x,\xi,d,\eta}$, $q(x,\xi;\epsilon,z)$ satisfies the resolvent equation

$$q(x,\xi;\epsilon,z) - q(x,\xi;\epsilon,z') = (z - z')q(x,\xi;\epsilon,z) \# q(x,\xi;\epsilon,z'). \tag{3.19}$$

Mimicking the proof of the Riesz formula for the spectral projection [see, e.g., Kato (1980)] one obtains that the formal symbol $\Sigma_{j=0}^{\infty}\pi_j(x,\xi)\epsilon^j$ defined by

$$\pi_j(x,\xi) = \frac{i}{2i\pi}\int_{\Gamma_{x,\xi}} q_j(x,\xi,z)\, dz, \tag{3.20}$$

where $\Gamma_{x,\xi}=\{z \in \mathbf{C}; |z-a(\xi)-\lambda_1(x)|=d/2\}$ satisfies (2.5) and (2.6).

We can now finish the proof of Lemma III.2: plug the estimation (3.18) into (3.20).

End of the proof of Theorem III.1: Let $\hat{\pi}_N$ be a resummation of the formal analytic symbol as given in the Appendix, i.e., $\hat{\pi}_N(x,\xi;\epsilon)=\Sigma_{j=0}^{N}\pi_j(x,\xi)\epsilon^j$. From Lemmas IV.6 and III.2, it follows that

$$\hat{\pi}_N \# \hat{\pi}_N(x,\xi;\epsilon) = \hat{\pi}_N(x,\xi;\epsilon) + r_N(x,\xi;\epsilon) \tag{3.21}$$

with

$$|||r_N|||_{p,\delta} \leqslant (C\epsilon)^{N+1}(N+1)!$$

for a new constant C. Consider now $h_0\#\hat{\pi}_N - \hat{\pi}_N\#h_0$. Since h_0 is unbounded, at the first sight, one cannot use directly Lemmas IV.6 and III.2 to obtain a similar bound. However, due to the fact that *all* the derivatives of h_0 are bounded and that since we consider a commutator so that the term without derivatives vanish one can still apply the stationary phase theorem and obtain the estimation

$$|||h\# \hat{\pi}_N - \hat{\pi}_N\#h|||_{p,\delta} \leqslant (C\epsilon)^{N+1}(N+1)!.$$

Then, taking $N=[1/B\epsilon]$ with B sufficiently large and denoting

$$\hat{\pi}^B := \sum_{j=0}^{[1/B\epsilon]} \pi_j\epsilon_j,$$

by Stirling formula, one has

$$|||\hat{\pi}^B\#\hat{\pi}^B - \hat{\pi}^B|||_{p,\delta} + |||h_0\#\hat{\pi}^B - \hat{\pi}^B\#h_0|||_{p,\delta} \leqslant Ce^{-c/h} \tag{3.22}$$

for some constants c, $C>0$ independent of ϵ. Let now

$$\hat{\Pi}_\epsilon = \mathrm{Op}_\epsilon^w(\hat{\pi}^B). \tag{3.23}$$

Then from (3.22), Lemma IV.6 and Calderon–Vaillancourt theorem (see Theorem IV.7) $\hat{\Pi}_\epsilon$ is bounded uniformly with respect to ϵ, and in addition,

$$\|\hat{\Pi}_\epsilon^2 - \hat{\Pi}_\epsilon\|_\delta = \mathcal{O}(e^{-c/\epsilon}), \tag{3.24}$$

$$\|[\hat{\Pi}_\epsilon, H_\epsilon]\|_\delta = \mathcal{O}(e^{-c/\epsilon}) \tag{3.25}$$

for some constant $c>0$ independent of $\epsilon \in (0,\epsilon_0]$. Then [see Sec. II and Nenciu (1993), Nenciu (2002) for details], if Π_ϵ is given by

$$\Pi_\epsilon = \frac{i}{2\pi}\int_{|z-1|=1/2} (\hat{\Pi}_\epsilon - z)^{-1}\, dz$$

the only thing to be verified is the $\langle x\rangle^{-\delta}$ decay as $|x|\to\infty$. By a simple computation [see Appendix in Nenciu (2002)],

$$(\hat{\Pi}_\epsilon - z)^{-1} = \frac{\hat{\Pi}_\epsilon + z - 1}{z(z-1)}\left[1 + \frac{\Delta_\epsilon}{z(1-z)}\right]^{-1}, \tag{3.26}$$

where

$$\Delta_\epsilon = \hat{\Pi}_\epsilon^2 - \hat{\Pi}_\epsilon. \tag{3.27}$$

Expanding in (3.26) and using (3.24), one has uniformly for sufficiently small ϵ,

$$\|(\hat{\Pi}_\epsilon - z)^{-1}\|_\delta = \mathcal{O}(1). \tag{3.28}$$

Again by a simple computation

$$\Pi_\epsilon - \hat{\Pi}_\epsilon = -\Delta_\epsilon \frac{i}{2\pi}\oint_{|z-1|=1/2} \frac{1}{z(1-z)}\left(\frac{\hat{\Pi}_\epsilon}{z(1-z)} + 1\right)\left(1 + \frac{\Delta_\epsilon}{z(1-z)}\right)^{-1} dz,$$

which together with (3.24) and (3.28) gives

$$\|\Pi_\epsilon - \hat{\Pi}_\epsilon\|_\delta \leqslant Ce^{-c/\epsilon}, \tag{3.29}$$

which implies (3.9). For (3.8) use

$$[H_\epsilon, \Pi_\epsilon] = -\frac{i}{2\pi}\oint_{|z-1|=1/2} (\hat{\Pi}_\epsilon - z)^{-1}[H_\epsilon, \hat{\Pi}_\epsilon](\hat{\Pi}_\epsilon - z)^{-1}\, dz,$$

(3.28) and (3.25).

Remarks:

III.1. From (3.29), Π_ϵ is exponentially close to $\hat{\Pi}_\epsilon$ which is a pseudodifferential operator with an analytic symbol. Actually, by using the results in Dimassi and Sjöstrand (1999) on functional calculus for pseudodifferential operators, one can show that Π_ϵ is a pseudodifferential operator with symbol $\hat{\pi} \in S_A^0(1)$ given by (3.11) and such that $\hat{\pi} - \pi_0 \in S_A^0(\langle x\rangle^{-\delta})$.

We turn now to applications to spectral and scattering theory for H_ϵ. Consider the scattering problem for the pair H_ϵ and

$$H_{\epsilon,0} := a(\epsilon D_x)\mathbf{1}_2 + \begin{pmatrix} \lambda_{1,\infty} & 0 \\ 0 & \lambda_{2,\infty} \end{pmatrix}. \tag{3.30}$$

We need the following elementary propagation estimate.

Lemma III.4: Let $\phi \in \mathcal{H}$, $\hat{\phi}$(= the Fourier transform of ϕ) $\in C_0^\infty(\mathbf{R}^n\setminus\{0\})^{\oplus 2}$. Then there exists $K(\phi) > 0$ such that, uniformly for sufficiently small ϵ,

$$\|\langle x\rangle^{-\delta} e^{-itH_{\epsilon,0}}\phi\| \leqslant K(\phi)\epsilon^{-2\delta}\langle t\rangle^{-\delta}. \tag{3.31}$$

Proof: The proof is standard stationary phase estimates [see, e.g., Appendix to XI.3 in Reed and Simon (1979)] and the only thing to do is to control their ϵ dependence. For this, write

$$\sqrt{\epsilon^2 k^2 + 1} - 1 = \epsilon^2 K_\epsilon(k)$$

and observe that

$$\mathrm{Inf}_{\epsilon\in(0,\epsilon_0]}|\mathbf{grad}\, K_\epsilon(k)| = \frac{|k|}{\sqrt{\epsilon_0^2 k^2+1}}$$

and

$$K_\epsilon(k) = \frac{k^2}{2} + \mathcal{O}(\epsilon^2 k^4).$$

From Lemma III.4, by the standard Cook argument, the wave operators

$$W_\pm(H_\epsilon, H_{\epsilon,0}) = s - \lim_{t\to\pm\infty} e^{itH_\epsilon} e^{-itH_{\epsilon,0}} \tag{3.32}$$

exist for $\delta>1$. As for completeness, if $\delta>n$, it follows by a direct application of Birman's theorem [see Reed and Simon (1979)], Theorem XI.10 [mimic the proof of Theorem XI.30 in Reed and Simon (1979)]. Actually the completeness holds true for $\delta>1$; one can prove it [see Simon (1979)] using Enss method. The same argument applies to all the wave operators appearing in this section so in what follows we shall assume that all of them exist and are complete. Let S be the scattering operator corresponding to the pair H_ϵ, $H_{\epsilon,0}$,

$$S = W_+(H_\epsilon, H_{\epsilon,0})^* W_-(H_\epsilon, H_{\epsilon,0}). \tag{3.33}$$

One expects that (3.8) implies that S has an almost block diagonal structure with respect to the decomposition given by Π_ϵ, and indeed one can prove (see the proof of Theorem III.8 below) that if $\phi_1\in\mathcal{H}$, $\phi_2\in(1-\Pi_\epsilon)(\mathcal{H})$ and $\hat{\phi}_j\in\mathcal{C}_0^\infty(\mathbf{R}^n\backslash\{0\})^{\oplus 2}$ then

$$|(\phi_2, S\phi_1)| \leqslant K(\phi_1,\phi_2)e^{-c/\epsilon}.$$

What we shall prove below [under an additional condition on $V(x)$, see Lemma III.5 below] that S has an almost diagonal form with respect to the *canonical* decomposition of $\mathcal{H}$, i.e., the decomposition given by

$$P_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

We start with the following elementary lemma.

Lemma III.5: Suppose that either

$$\mathrm{Sup}_{x\in\Gamma_a}\|\pi_0(x) - P_0\| < 1 \tag{3.34}$$

or, for $x\in\mathbf{R}^n$, *that*

$$V_{ij}(x) = \overline{V_{ij}(x)}, \tag{3.35}$$

i.e., $V(x)$ *has real entries for* $x\in\mathbf{R}^n$. *Then there exists a matrix* $Q(x)$ *bounded with bounded inverse uniformly in* Γ_a, *unitary for* $x\in\mathbf{R}^n$ *and satisfying*

$$\pi_0(x) = Q(x)P_0Q(x)^{-1} \tag{3.36}$$

and

$$\mathrm{Sup}_{x\in\mathbf{R}^n}|(Q(x)-\mathbf{1}_2)\langle x\rangle^\delta| < \infty. \tag{3.37}$$

Proof: If (3.34) holds true, one can take as $Q(x)$ the Sz–Nagy transformation matrix corresponding to the pair $\pi_0(x)$, $\pi_0(\infty)=P_0$.

Suppose now (3.35) holds true. For $x=(x',x_n)\in\Gamma_a$, let us set $x_n=y_n+i\eta$, $y_n\in\mathbf{R}$ and define $Q(x)$ by

$$Q(x) = 1 + \int_{-\infty}^{y_n} (1 - 2\pi_0(x', s + i\eta)) \left(\frac{\mathrm{d}}{\mathrm{d}s} \pi_0(x', s + i\eta) \right) Q(x', s + i\eta) \mathrm{d}s. \tag{3.38}$$

Notice that the integral in (3.38) is convergent since $(\mathrm{d}/\mathrm{d}s)\pi_0(x', s+i\eta) = \mathcal{O}(\langle s \rangle^{-\delta})$. Now [see, e.g., Kato (1980), Reed and Simon (1978)] $Q(x)$ is analytic and uniformly bounded in Γ_a and satisfies (3.36) since

$$\lim_{y_n \to +\infty} \pi_0(x', y_n + i\eta) = \pi(\infty) = P_0. \tag{3.39}$$

Since (3.38) implies that for $x \in \mathbf{R}^n$, $Q(x) = \overline{Q(x)}$, from (3.36) and (3.7) one obtains

$$Q_{1,1}^2(x) - 1 = \mathcal{O}(\langle x \rangle^{-\delta}),\ Q_{1,1}(x) Q_{1,2}(x) = \mathcal{O}(\langle x \rangle^{-\delta}). \tag{3.40}$$

This implies that as $|x| \to +\infty$, $Q_{1,1}(x) \to \pm 1$. By continuity the choice is the same for all directions. Since, for $x_n \to -\infty$, $Q(x) \to \mathbf{1}_2$, it follows that $\lim_{|x| \to +\infty} Q_{1,1}(x) = 1$ which together with (3.40) finishes the proof.

Let now U_ϵ be the Sz–Nagy transformation matrix corresponding to the pair Π_ϵ, Π_0 [see (2.25)] and consider the rotated Hamiltonian [see (2.28) and (2.30)]:

$$H_\epsilon^{\mathrm{eff}} = Q * U_\epsilon^* H U_\epsilon Q, \tag{3.41}$$

where Q is the operator of multiplication with $Q(x)$.

Corollary III.6: Under assumptions (3.2), (3.3), (3.5), and (3.34) or (3.35) we have

$$H_\epsilon^{\mathrm{eff}} = \begin{pmatrix} a(\epsilon D_x) + \lambda_1(x) & 0 \\ 0 & a(\epsilon D_x) + \lambda_2(x) \end{pmatrix} + \epsilon B_\epsilon, \tag{3.42}$$

where $B_{\epsilon,ii}$; $i, j = 1, 2$ are bounded operators satisfying

$$\|B_{\epsilon,ii}\|_\delta = \mathcal{O}(1), \tag{3.43}$$

$$\|B_{\epsilon,12}\|_\delta = \|B_{\epsilon,21}\|_\delta = \mathcal{O}(e^{-c/\epsilon}), \tag{3.44}$$

uniformly with respect to sufficiently small ϵ.

Proof: Write

$$H_\epsilon^{\mathrm{eff}} = Q * (H_\epsilon + U_\epsilon^* [H_\epsilon, U_\epsilon] Q) = \begin{pmatrix} a(\epsilon D_x) + \lambda_1(x) & 0 \\ 0 & a(\epsilon D_x) + \lambda_2(x) \end{pmatrix} + Q * [a(\epsilon D_x)\mathbf{1}_2, Q] + Q * U_\epsilon^* [H_\epsilon, U_\epsilon] Q. \tag{3.45}$$

The fact that, uniformly for ϵ sufficiently small,

$$\epsilon^{-1} \| \mathcal{O} * [a(\epsilon D_x)\mathbf{1}_2, Q] \|_\delta = \mathcal{O}(1) \tag{3.46}$$

follows from the fact that $\langle x \rangle^\delta$ commutes with Q, (3.37) and Lemma IV.6. Analogously

$$\epsilon^{-1} \| [H_\epsilon, \Pi_0] \|_\delta = \mathcal{O}(1). \tag{3.47}$$

Since $\langle x \rangle^\delta$ commutes with Π_0 from (3.9) one has

$$\| \langle x \rangle^\delta \Pi_\epsilon \langle x \rangle^{-\delta} \| = \mathcal{O}(1). \tag{3.48}$$

Hence, from the Sz–Nagy formula for U_ϵ, (3.8), (3.47), and (3.48) one has

$$\epsilon^{-1} \| [H_\epsilon, U_\epsilon] \|_\delta = \mathcal{O}(1), \tag{3.49}$$

$$\epsilon^{-1}\|U_\epsilon - 1\|_\delta = \mathcal{O}(1), \tag{3.50}$$

uniformly for small ϵ. From (3.49) and (3.50),

$$\epsilon^{-1}\|Q^* U_\epsilon^*[H_\epsilon, U_\epsilon]Q\|_\delta, \tag{3.51}$$

which together with (3.46) finishes the proof of (3.43). Now from (3.36) and $\Pi_\epsilon = U_\epsilon \Pi_0 U_\epsilon^*$ it follows that

$$\Pi_\epsilon = U_\epsilon Q P_0 Q^* U_\epsilon^*$$

and then

$$[H_\epsilon^{\text{eff}}, P_0] = Q^* U_\epsilon^*[H_\epsilon, \Pi_\epsilon]U_\epsilon Q, \tag{3.52}$$

which together with (3.8) and (3.50) gives

$$\|[H_\epsilon^{\text{eff}}, P_0]\|_\delta = \mathcal{O}(e^{-c/\epsilon}). \tag{3.53}$$

Taking into account that

$$\epsilon B_{\epsilon,12} + \epsilon B_{\epsilon,21} = (1 - 2P_0)[H_\epsilon^{\text{eff}}, P_0],$$

(3.53) implies (3.44).

Let us stress here that the constructive proof above provides the means to compute effectively the formal symbol of H_ϵ^{eff}.

Remarks:

III.2. As in the case of Π_ϵ, from (3.45) one sees that H_ϵ^{eff} is exponentially close to a pseudodifferential operator and again the results in Dimassi and Sjöstrand (1999) enables to show that in fact H_ϵ^{eff} is a pseudodifferential operator.

The following lemma allows to replace H_ϵ by H_ϵ^{eff} when computing the scattering operator.

Lemma III.7: Let $\tilde{S}$ be the scattering operator corresponding to the pair H_ϵ^{eff} $H_{\epsilon,0}$. Then for sufficiently small ϵ,

$$S = \tilde{S}. \tag{3.54}$$

Proof: Let $\Omega_\epsilon = QU_\epsilon$. From (3.37) and (3.50),

$$\|(\Omega_\epsilon - 1)\langle x\rangle^\delta\| = \mathcal{O}(1). \tag{3.55}$$

Now [see (3.41)]

$$W_\pm(H_\epsilon^{\text{eff}}, H_{\epsilon,0}) = \Omega_\epsilon^*(s - \lim_{t\to\pm\infty} \Omega_\epsilon e^{itH_\epsilon^{\text{eff}}} e^{-itH_{\epsilon,0}}) = \Omega_\epsilon^* W_\pm(H_\epsilon, H_{\epsilon,0}) + (s - \lim_{t\to\pm\infty} \Omega_\epsilon^* e^{itH_\epsilon}(\Omega_\epsilon - 1)e^{-itH_{\epsilon,0}}).$$

Let now $\phi \in \mathcal{H}$, $\hat{\phi} \in \mathcal{C}_0^\infty(\mathbf{R}^n \setminus \{0\})^{\oplus 2}$. Then from Lemma III.4 and (3.55),

$$\|\Omega_\epsilon^* e^{itH_\epsilon}(\Omega_\epsilon - 1)e^{-itH_{\epsilon,0}}\phi\| \leq C(\phi)\epsilon^{-2\delta}\langle t\rangle^{-\delta}.$$

Sending $|t| \to \infty$ (at fixed ϵ!), by density we get

$$s - \lim_{t\to\pm\infty} \Omega_\epsilon^* e^{itH_\epsilon}(\Omega_\epsilon - 1)e^{-itH_{\epsilon,0}} = 0,$$

which gives

$$W_\pm(H_\epsilon^{\text{eff}}, H_{\epsilon,0}) = \Omega_\epsilon^* W_\pm(H_\epsilon, H_{\epsilon,0})$$

and the proof of the lemma is finished.

We are now in position to state one of the main results of the paper.

Theorem III.8: *Let, for* $j=1,2$,

$$H^{\text{eff}}_{\epsilon,j}=a(\epsilon D_x)+\lambda_j(x)+\epsilon B_{\epsilon,ii},\ \ H_{\epsilon,j,0}=a(\epsilon D_x)+\lambda_{j,\infty} \tag{3.56}$$

acting in $L^2(\mathbf{R}^n)$ *and* S_j *the scattering operator corresponding to the pair* $H^{\text{eff}}_{\epsilon,j}$, $H_{\epsilon,j,0}$. *Then, there exists* $c>0$ *independent of* ϵ, *such that, for any* $\phi_k\in\mathcal{H}$, $\hat{\phi}_k\in\mathcal{C}^\infty_0(\mathbf{R}^n\backslash\{0\})^{\oplus 2}$, $k=1,2$ *and* $\epsilon\in(0,\epsilon_0]$ *sufficiently small, we have*

$$\left|\left(\phi_2,\left(S-\begin{pmatrix}S_1&0\\0&S_2\end{pmatrix}\right)\phi_1\right)\right|\leqslant C(\phi_1,\phi_2)e^{-c/\epsilon} \tag{3.57}$$

for some constant $C(\phi_1,\phi_2)>0$ *depending on* ϕ_1,ϕ_2 *but not on* ϵ.

Proof: Write

$$D_\epsilon=\begin{pmatrix}H^{\text{eff}}_{\epsilon,1}&0\\0&H^{\text{eff}}_{\epsilon,2}\end{pmatrix},\ \ R_\epsilon:=H^{\text{eff}}_\epsilon-D_\epsilon$$

and let $\phi\in\mathcal{H}$, $\hat{\phi}\in\mathcal{C}^\infty_0(\mathbf{R}^n\backslash\{0\})^{\oplus 2}$. By the usual Cook argument, for $T>0$, we have

$$\|(W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-e^{iTH^{\text{eff}}_\epsilon}e^{-iTH_{\epsilon,0}}\phi\,\|=\left\|\int_T^\infty e^{itH^{\text{eff}}_\epsilon}(H^{\text{eff}}_\epsilon-H_{\epsilon,0})e^{-itH_{\epsilon,0}}\phi\right\|\leqslant C(\phi)\epsilon^{-2\delta+1}T^{1-\delta} \tag{3.58}$$

and

$$\|(W_+(D_\epsilon,H_{\epsilon,0})-e^{iTD_\epsilon}e^{-iTH_{\epsilon,0}}\phi\,\|=\left\|\int_T^\infty e^{itD_\epsilon}(D_\epsilon-H_{\epsilon,0})e^{-itH_{\epsilon,0}}\phi\right\|\leqslant C(\phi)\epsilon^{-2\delta+1}T^{1-\delta}. \tag{3.59}$$

For the last inequality we used Lemma III.4 and the fact that (see Corollary III.6) $\|H^{\text{eff}}_\epsilon-H_{\epsilon,0}\|_\delta+\|D_\epsilon-H_{\epsilon,0}\|_\delta=\mathcal{O}(\epsilon)$. On the other hand, from Duhamel's formula,

$$e^{iTH^{\text{eff}}_\epsilon}=e^{iTD_\epsilon}+i\int_0^T e^{i(T-s)D}\text{Re}^{isH^{\text{eff}}_\epsilon}\,\text{d}s, \tag{3.60}$$

which together with (3.44) gives

$$\|e^{iTH^{\text{eff}}_\epsilon}e^{-iTD_\epsilon}-\mathbf{1}_2\|\leqslant C'\epsilon Te^{-c/\epsilon}. \tag{3.61}$$

From (3.58), (3.59), and (3.61) one obtains

$$\|(W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-W_+(D_\epsilon,H_{\epsilon,0}))\phi\|\leqslant 2C(\phi)\epsilon^{-2\delta+1}T^{1-\delta}+C'\epsilon Te^{-c/\epsilon}. \tag{3.62}$$

By choosing $T=\epsilon^{-2-1/\delta}e^{c/\delta\epsilon}$ in (3.62) one obtains

$$\|(W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-W_+(D_\epsilon,H_{\epsilon,0}))\phi\|\leqslant C_1(\phi)e^{-c/\epsilon} \tag{3.63}$$

for some c', $0<c'\leqslant c$, and $C=C(\phi)>0$ independent of ϵ. In the same manner

$$\|(W_-(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-W_-(D_\epsilon,H_{\epsilon,0}))\phi\|\leqslant C_2(\phi)e^{-c/\epsilon}. \tag{3.64}$$

Writing

$$\begin{aligned}S(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-S(D_\epsilon,H_{\epsilon,0})&=(W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})^*-W_+(D_\epsilon,H_{\epsilon,0})^*)W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})\\&\quad+W_+(D_\epsilon,H_{\epsilon,0})^*(W_+(H^{\text{eff}}_\epsilon,H_{\epsilon,0})-W_+(D_\epsilon,H_{\epsilon,0}))\end{aligned}$$

and using (3.63) and (3.64) and Lemma III.7, (3.57) follows.

Since $\tilde{S}$ commutes with $H_{\epsilon,0}$, one can define the scattering matrix at fixed energy $\tilde{S}(\lambda)$. Let us stress that Theorem III.8 does not imply the corresponding result for $\tilde{S}(\lambda)$; when shrinking the supports of ϕ_1 and ϕ_2 the constant $C(\phi_1,\phi_2)$ may blow up. At the heuristic level the reason for this blowing up is clear: Corollary III.6 (via the Duhamel's formula) implies that the transitions *per unit time* between the two levels is exponentially small, but if, at the given energy, there is a resonance very (exponentially) close to the real axis, it has an exponentially long lifetime and during this time considerable transitions can take place. Accordingly, one expects exponentially block diagonalization of $\tilde{S}(\lambda_0)$ only if there are no resonances around λ_0 or in other words if $\tilde{S}(\lambda)$ is smooth in a neighborhood of λ_0 and this is true if λ_0 is nontrapping.

Remarks:

III.3. For nontrapping energies the block diagonal structure (up to exponentially small errors) of $\tilde{S}(\lambda_0)$ has been proved in the papers quoted in the Introduction. Let us point out that one can prove similar results [see Sordoni (2003)] by using Corollary III.6 and resolvent estimates [see, e.g., Jensen and Nakamura (1992), Wang (1988)].

We turn now to some direct applications of Corollary III.6 to spectral theory. We shall discuss H_ϵ^{eff} but all the results apply to H_ϵ also, since they are unitarily equivalent. If

$$\operatorname*{Inf}_{x\in\mathbf{R}^n} \lambda_2(x) = m_2 < \lambda_{2,\infty}$$

then H_ϵ^{eff} has discrete spectrum in the interval $(m_2,\lambda_{2,\infty})$ which, up to exponentially small errors, equals the union of the (discrete) spectra of $H_{\epsilon,j}^{\text{eff}}$ in this interval [see Nenciu (2002) for details]. Suppose now

$$\operatorname*{Inf}_{x\in\mathbf{R}^n} \lambda_1(x) = m_1 < \lambda_{1,\infty}.$$

Then $H_{\epsilon,1}^{\text{eff}}$ has bound states in the interval $(m_1,\lambda_{1,\infty})$ and as a consequence, D_ϵ has bounded states embedded in the continuum spectrum in the interval $(\text{Max}\{m_1,\lambda_{2,\infty}\},\lambda_{1,\infty})$. The small off-diagonal term, R_ϵ, turns (generically) these bound (stable) states into metastable states. Let Ψ be an eigenfunction of such a bound state, i.e.,

$$H_{\epsilon,1}^{\text{eff}}\Psi = E\Psi, \quad E \in (\text{Max}\{m_1,\lambda_{2,\infty}\},\lambda_{1,\infty}).$$

Then from Corollary III.6,

$$\|(H_\epsilon^{\text{eff}} - E)\Psi\| \leqslant Ce^{-c/\epsilon},$$

i.e., Ψ, E, are pseudoeigenvectors and pseudoeigenvalues [see Kato (1980)] of exponential order for H_ϵ^{eff} (the name quasimodes is also used). A more physical picture is given by Duhamel formula (3.60) which together with Corollary III.6 gives the following.

Corollary III.9:

$$|(\Psi, e^{-itH_\epsilon^{\text{eff}}}\Psi)| \geqslant 1 - C|t|e^{-c/\epsilon}. \tag{3.65}$$

As it stands Corollary III.9 gives the *existence* and the control on the (exponentially long) lifetime of metastable states (quasimodes) in the semiclassical limit. However in many instances [see, e.g., Stefanov (1999)] one can make the connection with the resonances (defined as poles of the resolvent of scattering operator). In the cases when this connection can be made Corollary III.9 says that the imaginary part of the resonances is exponentially small. The same argument applies to other bound states and/or resonances of D in the interval $(\lambda_{1,\infty},\infty)$ (as far as they exist).

APPENDIX A: ANALYTIC SYMBOLS

We recall here in an appropriate form, besides some standard facts about pseudodifferential operators, the results we need for analytic symbols. For more details and proofs see Robert (1987), Dimassi and Sjostrand (1999), Martinez (2002), Taylor (1981), Boutet de Monvel and Kree (1967).

We consider matrix valued symbols so the product and the modulus are the standard product and matrix norm, respectively. We employ the standard notations concerning the derivatives, factorial, etc. Also for $y \in \mathbf{C}^n$, $\langle y\rangle = (1+|y|^2)^{1/2}$, and for $a,b>0$

$$\Gamma_a \times \Gamma_b = \{(x,\xi) \in \mathbf{C}^{2n},\ |\mathrm{Im}\, x| < a |\mathrm{Im}\, \xi| < b\}.$$

Symbols $a(x,\xi;\epsilon)$ are smooth matrix valued functions of $(x,\xi) \in \mathbf{R}^{2n}$ or Γ_a, depending on $\epsilon \in (0,\epsilon_0]$, as a parameter.

Definition IV.1: A function $a(x,\xi;\epsilon)$ defined on $\mathbf{R}^{2n}\times(0,\epsilon_0]$, is said to be a symbol in $S^m(\langle x\rangle^{-\delta})$, for some $m,\delta \in \mathbf{R}$ if a is a smooth function of (x,ξ) and, for all $\alpha,\beta \in \mathbf{N}^n$, there exist $C_{\alpha,\beta}>0$ such that

$$\sup_{(x,\xi)\in\mathbf{R}^{2n},\epsilon\in(0,\epsilon_0]} |\langle\xi\rangle^{-m}\langle x\rangle^{\delta}\partial_x^{\alpha}\partial_{\xi}^{\beta}a(x,\xi,\epsilon)| \leqslant C_{\alpha,\beta}.$$

In particular $S^0(1)$ is the set of $a(x,\xi,\epsilon)$ which are uniformly bounded together with all their derivatives. For $a \in \mathcal{S}^0(\langle x\rangle^{-\delta})$ and $p \in \mathbf{N}$ we set

$$|||a|||_{p,\delta} = \sup_{(x,\xi)\in\mathbf{R}^{2n},\epsilon\in(0,\epsilon_0]} \sum_{|\alpha|+|\beta|\leqslant p} |\langle x\rangle^{\delta}\partial_x^{\alpha}\partial_{\xi}^{\beta}a(x,\xi;\epsilon)|. \tag{4.1}$$

Definition IV.2: A function $a(x,\xi,\epsilon)$, $(x,\xi)\in\Gamma_a\times\Gamma_b$, $\epsilon\in(0,\epsilon_0]$ is called an analytic symbol of class $\mathcal{S}_A^m(\langle x\rangle^{-\delta})$ for some m, $\delta\in\mathbf{R}$ if it is analytic in $\Gamma_a\times\Gamma_b$ and, for any $a'<a, b'<b$, there exists $K>0$ such that

$$\sup_{(x,\xi)\in\Gamma_{a'}\times\Gamma_{b'},\epsilon\in(0,\epsilon_0]} |\langle\xi\rangle^{-m}\langle x\rangle^{\delta}a(x,\xi,\epsilon)| \leqslant K. \tag{4.2}$$

Definition IV.3: Given a family $a_j(x,\xi)\in\mathcal{S}_A^m(\langle x\rangle^{-\delta})$, $j\in\mathbf{N}$, analytic on $\Gamma_a\times\Gamma_b$ such that, for any $a'<a, b'<b$, there exists a constant $C>0$ independent of j such that

$$\sup_{(x,\xi)\in\Gamma_{a'}\times\Gamma_{b'}} |\langle\xi\rangle^{m}\langle x\rangle^{\delta}a_j(x,\xi)| \leqslant C^{j+1}j! \tag{4.3}$$

we call $a_f=\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ a formal analytic symbol of class $\mathcal{S}_A^0(\langle x\rangle^{-\delta})$ on $\Gamma_a\times\Gamma_b$.

We say that a symbol $a(x,\xi;\epsilon)\in\mathcal{S}_A^m(\langle x\rangle^{-\delta})$ is asymptotic equivalent to the formal analytic symbol $\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ and we write

$$a \sim \sum_{j=0}^{\infty} \epsilon^j a_j(x,\xi)$$

if there exists a constant $C>0$ such that for any $N\in\mathbf{N}$ and any $a'<a, b'<b$,

$$\sup_{(x,\xi)\in\Gamma_{a'}\times\Gamma_{b'},\epsilon\in(0,\epsilon_0]} \left| \langle\xi\rangle^{-m}\langle x\rangle^{\delta}\left(a(x,\xi;\epsilon) - \sum_{j=0}^{N} \epsilon^j a_j(x,\xi)\right)\right| \leqslant C^{N+1}\epsilon^{N+1}(N+1)!. \tag{4.4}$$

If $\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ *is a formal analytic symbol, and $T>0$ is sufficiently large then one can define $a^T(x,\xi;\epsilon)=\Sigma_{j=0}^{[1/T\epsilon]}\epsilon^j a_j(x,\xi)$ (unique modulo $\mathcal{O}(e^{-c/\epsilon})$) satisfying (4.4). The symbol $a^T(x,\xi;\epsilon)$ is called a resummation of the formal analytic symbol $\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ and any symbol a that can be written as such a resummation up to error $O(e^{-c/\epsilon})$ is an analytic representation of the formal analytic symbol $\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$.*

Let us notice [see Boutet de Monvel and Kree (1967)] that a formal symbol $a=\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ belongs to $S_A^{m_1}(\langle x\rangle^{-\delta_1})$ on $\Gamma_a\times\Gamma_b$ if and only if, for any $a',b'>0, a'<a, b'<b$, the series

$$N_{\delta_1}^{m_1}(a,T)=\sum_{j=0}^{\infty}T^j\left(\sum_{|\alpha|+|\beta|+2k=j}c_{k,\alpha}^{\beta}A_{k,\alpha,\delta_1}^{\beta,m_1}\right),$$

where

$$A_{k,\alpha,\delta_1}^{\beta,m_1}:=\sup_{(x,\xi)\in\Gamma_{a'}\times\Gamma_{b'}}\left|\langle x\rangle^{\delta_1}\langle\xi\rangle^{-m_1}\partial_x^{\alpha}\partial_\xi^{\beta}a_k\right|\leqslant C^{k+|\alpha|+|\beta|+1}k!\alpha!\beta! \tag{4.5}$$

and

$$c_{k,\alpha}^{\beta}=\frac{2(2n)^{-k}k!}{(k+|\alpha|)!(k+|\beta|)!}$$

has a nonzero radius of convergence as a series in T.

If $a_f=\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ and $b_f=\Sigma_{j=0}^{\infty}\epsilon^j b_j(x,\xi)$ are two formal analytic symbols on $\Gamma_a\times\Gamma_b$, we define, as usual, the Weyl product

$$a_f\# b_f\equiv r_f=\sum_{m=0}^{\infty}\epsilon^m r_m, \tag{4.6}$$

where

$$r_m=\sum_{|\gamma|+|\theta|+l+s=m}\Gamma(\gamma,\theta)D_x^{\gamma}\partial_\xi^{\theta}a_l D_x^{\theta}\partial_\xi^{\gamma}b_l \tag{4.7}$$

and $\Gamma(\alpha,\beta)=(1)^{\beta}/\alpha!\beta!2^{|\alpha|}2^{|\beta|}$.

The basic result [Boutet de Monvel and Kree (1967)] about the class of formal analytic symbols is that it is closed under Mpyal multiplication. More precisely, using Lemma 1.2 in Boutet de Monvel and Kree (1967), one can prove that

$$N_{\delta_1^+\delta_2}^{m_1+m_2}(r,T)\lll N_{\delta_1}^{m_1}(p,T)N_{\delta_2}^{m_2}(q,T),$$

where $\lll$ means that the coefficient of T^j in the first member is less than the same in the second member. As a consequence we have the following.

Lemma IV.4: Let $a_f=\Sigma_{j=0}^{\infty}\epsilon^j a_j(x,\xi)$ and $b_f=\Sigma_{j=0}^{\infty}\epsilon^j b_j(x,\xi)$ two formal analytic symbol on $\Gamma_a\times\Gamma_b$, then $a_f\# b_f$ is a formal analytic symbol on $\Gamma_a\times\Gamma_b$ in the class $S_A^{m_1+m_2}(\langle x\rangle^{-\delta_1-\delta_2})$.

Moreover, we have the following.

Lemma IV.5: Let $r_f=\Sigma_{j=1}^{\infty}\epsilon^j r_j$ is a formal analytic symbol in the class $S_A^0(\langle x\rangle^{-\delta_1})$ on $\Gamma_a\times\Gamma_b$. Then $\Sigma_{j=1}^{\infty}r_f^{\#j}$ is a formal analytic symbol in the class $S_A^0(\langle x\rangle^{-\delta_1})$ on $\Gamma_a\times\Gamma_b$.

Proof: It is sufficient to observe that

$$N_\delta^0\left(\sum_{j=1}^{\infty}r^{\#j},T\right)\lll N_\delta^0(r,T)\sum_{j=0}^{\infty}N_0^0(r,T)^j=N_\delta^0(r,T)(1-N_0^0(r,T))^{-1}.$$

[The last series is a convergent for sufficiently small $\langle T\rangle$ since $N_0^0(r,T)$ is, for sufficiently small T, a convergent series and has no constant term.]

We are now in position to state the basic result on composition of pseudodifferential operators [see, e.g., Martinez (2002)]. Given a symbol $a\in S_A^m(\langle x\rangle^{-\delta})$ we denote by $\mathrm{Op}_\epsilon^w(q(x,\xi;\epsilon))$ we denote the ϵ-pseudodifferential operator which, for $\phi\in C_0^{\infty}(\mathbf{R}^n,\mathbf{R}^{\oplus k})$ is defined by the oscillatory integral

$$\mathrm{Op}_\epsilon^w(a(x,\xi;\epsilon))\phi=(2\pi\epsilon)^{-n}\int e^{i(x-y)\xi/\epsilon}a\left(\frac{x+y}{2},\xi;\epsilon\right)\phi(y)\mathrm{d}y\,\mathrm{d}\xi. \tag{4.8}$$

Lemma IV.6: Let $a(x,\xi,\epsilon)\epsilon S^{m_1}(\langle x\rangle^{-\delta_1})$, $b(x,\xi,\epsilon)\in S^{m_2}(\langle x\rangle^{-\delta_2})$, m_i,δ_i, $i=1,2$. *Then* $a\#b$ *given by the oscillatory integral (2.2) belong to* $S^{m_1+m_2}(\langle x\rangle^{-(\delta_1+\delta_2)})$.

Moreover, if $a(x,\xi,\epsilon)\sim\Sigma_{j=0}^{\infty}a_j(x,\xi)\epsilon^j\in S_A^{m_1}(\langle x\rangle^{-\delta_1})$, $b(x,\xi,\epsilon)\sim\Sigma_{j=0}^{\infty}b_j(x,\xi)\epsilon^j\in S_A^{m_2}(\langle x\rangle^{-\delta_2})$ *then* $a\#b\in S_A^{m_1+m_2}(\langle x\rangle^{-(\delta_1+\delta_2)})$ *and*

$$a\#b\sim\left(\sum_{j=0}^{\infty}a_j(x,\xi)\epsilon^j\right)\#\left(\sum_{j=0}^{\infty}b_j(x,\xi)\epsilon^j\right),\tag{4.9}$$

where # is the Weyl composition of formal symbol defined in (4.6) and (4.7).

The last result we collect is the Calderon–Vaillancourt theorem.

Theorem IV.7: *Let* $a(x,\xi;\epsilon)\in S^0(\langle x\rangle^{-\delta})$. *Then, there exists* $M>0$, $p\in\mathbf{N}$ *depending only on* n,m,δ *such that*

$$\|\mathrm{Op}_\epsilon^w(a)\|_\delta\leqslant M|||a|||_{p,\delta}.\tag{4.10}$$

For the proof of the theorem see, for example, Robert (1987), Martinez (2002).

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INTRODUCTION

Quantum groups are a remarkable generalization of conventional groups using an algebraic language by now quite well-known to mathematical physicists. One replaces the notion of a Lie algebra symmetry by a "quantum enveloping algebra" which generalizes the usual enveloping algebra of a Lie algebra. Or one may replace the coordinate algebra of functions on a conventional group by a more general algebra, typically noncommutative or "quantum." In either case, the natural formulation of the more general object is a "Hopf algebra," a notion that had been proposed in the 1940s by pure mathematicians but without truly representative examples. It is now about 20 years since the subject exploded with the discovery of such quantum groups in mathematical physics, mainly in the theory of quantum inverse scattering (the quantum groups $U_q(g)$ of Drinfeld and Jimbo) but also in Planck-scale physics (the less well-known bicrossproduct quantum groups based on Lie group factorizations). The latter have provided some of the first models of noncommutative space–time with potentially measurable quantum/gravity corrections.

Remarkably, it is also about 20 years since the serious development of "noncommutative geometry" in the form of cyclic cohomology as a means of capturing geometric information about a space in terms of its algebra of functions, while making sense for more general algebras. Here again the roots of the subject go back on the mathematics side to theorems of Gelfand and Naimark in the 1940s and 1950s followed by the development of K-theory and K-homology in the 1970s. From a physicists point of view the "general idea" of replacing classical coordinates such as x, p on a classical phase space by noncommuting operator variables $\mathbf{x}$, $\mathbf{p}$ dates back to the birth of quantum mechanics itself; many authors, starting with Dirac in the 1920s, have asked how far "geometry" could be extended to such operator variables. Again, convincing examples were an issue, with the papers of Connes and of Connes-Rieffel on the differential structure of, and Yang–Mills theory over, a noncommutative torus in the 1980s probably a turning point.

Both fields have matured considerably over the intervening 20 years and two things could be said to be emerging. First of all, noncommutative geometry and quantum groups *should* be intimately related and this is slowly beginning to be explored; the cyclic cohomology of (for example, bicrossproduct) quantum groups has been computed while conversely quantum groups methods such as "Drinfeld cotwisting" are being applied to construct geometry on noncommutative tori and their cousins. The process is still in its infancy; for example the q-deformed quantum groups do not fit well into usual cyclic cohomology, which has to be generalized. Secondly, and more importantly for this volume, 20 years has been long enough for mathematical physicists to absorb the new ideas and algebraic methods and, now finding them routine, begin actually to use them in genuine physical situations. As with supersymmetry before it, it could be considered that the "wave of algebraic methods" encompased by quantum groups and noncommutative geometry has swept through the general mathematical physics community and left it enriched with powerful new tools which were not widely known before.

In this special issue on **Quantum groups and noncommutative geometry** it is certainly not possible to do justice to all the new directions which are opening up in the light of such developments. Rather, the volume aims to provide a partial snapshot of a few of the more exciting aspects looking forward. Most of the articles are research articles but two are major reviews. Bearing in mind that both quantum groups and noncommutative geometry are already covered in existing textbooks (such as my 1995 book from the Hopf algebras perspective and Connes's 1994 book from the cyclic cohomology perspective), the review articles are intended to give more exposure to other important points of view. The review article on the deformation theory view of quantum groups contains much that is accessible to physicists while providing a self-contained clean presentation of results which are otherwise scattered or vaguely formulated as well as some new results. The other review article is part of an approach to noncommutative algebraic geometry and introduces the reader to powerful homological methods which have an emerging role in mirror symmetry, string theory, BRST quantization and other topics.

The research articles meanwhile fall into three groups reflecting a broad interpretation both of noncommutative geometry and of the role of quantum groups and related objects. The first group of papers consists of several articles involving quantum groups or Hopf algebras in their mature form. Two of them are applications to actual physics, to renormalization in quantum field theory and to anyons. Two more are q-deformation papers of the "classical" style in quantum group theory, here relating to noncompact quantum groups which is a topic currently on the cutting edge. The remaining article in the group is about the famous "quantum Yang–Baxter equations," but now on finite sets which is another active frontier. New algebraic structures emerge in connection with these famous equations, linked to finite group bicrossproducts among other things.

The second group of papers is centered on categorical methods and two themes which we consider important for future developments in both physics and mathematics: 2-categories on the one hand and nonassociative algebras such as the octonions on the other. If quantum groups has taught us one thing, it is perhaps that categorical issues impinge directly on what is "natural" in physics and can be used to create and organize correct structures. Quantum group methods enter in the form of quasi-Hopf algebras, monoidal categories, and in the foundations of the theory of 2-categories, for example. While three of the papers are quite mathematical, three others relate to the potential physics of quite a concrete nature in the areas of nonstandard statistics and quarks, parallel transport on surfaces in higher gauge theory, and the possible role of the octonions in the standard model.

The last group of papers contains work on Fedosov quantization, mirror symmetry, and groupoids, all aspects of the broader noncommutative geometry of manifolds. We may stress again that the special issue covers only a small and incomplete sample of the rapidly developing literature.

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Quantum groups and deformation quantization: Explicit approaches and implicit aspects

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Deformation quantization, which gives a development of quantum mechanics independent of the operator algebra formulation, and quantum groups, which arose from the inverse scattering method and a study of Yang–Baxter equations, share a common idea abstracted earlier in algebraic deformation theory: that algebraic objects have infinitesimal deformations which may point in the direction of certain continuous global deformations, i.e., "quantizations." In deformation quantization the algebraic object is the algebra of "observables" (functions) on symplectic phase space, whose infinitesimal deformation is the Poisson bracket and global deformation a "star product," in quantum groups it is a Hopf algebra, generally either of functions on a Lie group or (often its dual in the topological vector space sense, as we briefly explain) a completed universal enveloping algebra of a Lie algebra with, for infinitesimal, a matrix satisfying the modified classical Yang–Baxter equation (MCYBE). Frequently existence proofs are known but explicit formulas useful for physical applications have been difficult to extract. One success here comes from "universal deformation formulas" (UDFs), expressions built from a Lie algebra which deform any algebra on which the Lie algebra operates as derivations. The most famous of these is the Moyal product, a special case of a class in which the Lie algebra is Abelian. Another comes from recognition that the Belavin–Drinfel'd solutions to the MCYBE are, in fact, infinitesimal deformations for which, in the case of the special linear groups, it is possible to give explicit formulas for the corresponding quantum Yang–Baxter equations. This review paper discusses, necessarily in brief, these and related topics, including "twisting" as a form of UDF and finding formulas for "preferred deformations" of Hopf algebras in which the multiplication or comultiplication is rigid and must be preserved in the course of deformation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1786681]

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I. INTRODUCTION

Mathematics arose as an abstraction of the physical world and thenceforth often became something entirely different. Still, the physical origin of many mathematical notions can be traced and is implicit in many developments. That is what we call physical *mathematics*. On the other hand, mathematics is the main language of theoretical physics, albeit used with a very peculiar accent, and the "mathematics toolbox" is crucial in *mathematical physics*. That mutual interaction appears as a watermark throughout many works, including the present paper.

It can be said that quantum groups arose "experimentally" in the Leningrad LOMI group of Ludwig Faddeev around 1980 [see, e.g., Kulish and Reshetikhin (1981) and Faddeev *et al.* (1988)], during attempts to quantize two-dimensional integrable models by methods coming from inverse scattering and a study of what they called Yang–Baxter equations. *A posteriori* it was discovered that some aspects (e.g., q-special functions in the 19th century) were present much earlier and that the notion is of importance in various areas of physics, including solid state. A recent primer of quantum groups from the physical viewpoint is Majid (2002).

Significant steps forward were made shortly afterwards, in particular when Jimbo (1985) systematized these attempts in his study of quantized enveloping algebras. Even more so when Drinfel'd (1987) made explicit the underlying Hopf algebra structures and, relating the dual aspect to deformation quantization, coined the expression "quantum groups."

Deformation quantization was certainly "in the back of the mind" of many almost since the beginning of quantum mechanics ["wave mechanics" in de Broglie (1928)] and its avatars developed since 1925 by Heisenberg ("matrix mechanics"), Schrödinger (with his celebrated equation) and especially Weyl with his quantization procedure [Weyl (1931) and Wigner (1932)]. But the relation with deformation theory [Gerstenhaber (1964)] and its role in physics [see, e.g., Flato (1982)] was made only in Bayen *et al.* (1978).

Already in the formulation of Drinfel'd (1987), it is clear that quantum groups are an avatar of deformation quantization, when the category of Hopf algebras is taken into account. But one aspect remained imprecise: the duality between the two aspects, deformations of (functions over) Poisson–Lie groups, and quantized enveloping algebras. That was, at least in the compact and semisimple cases, made clear later [Bonneau *et al.* (1994) and Bidegain and Pinczon (1996)], using natural topologies on the corresponding Hopf algebras.

There is another duality which remains largely unexplored. The Gelfand isomorphism theorem, by which commutative algebras can be considered as algebras of functions over some space (their spectrum), expresses a "duality" between a commutative algebra and a topological space. Now, on one hand, commutative algebras are deformed into noncommutative (associative or Hopf) algebras. On the other hand, differentiable manifolds, characterized, e.g., by some algebraic properties, are deformed into noncommutative ones. And manifolds have symmetries that often can be quantized. These related aspects are so far developed separately, to a large extent. A natural question is thus to study their relations. A very abstract attempt can be found in Kontsevich and Rosenberg (2000). In view of the present rapid developments in noncommutative manifolds [see, e.g., Kontsevich and Rosenberg (2000), Connes and Landi (2001), and Connes and Dubois-Violette (2003)] one should probably start with specific examples and see if a pattern arises, hence the need for explicit approaches.

In mathematics an abstract existence proof [such as the one in Etingof and Kazhdan (1998)] is perfectly satisfactory, even more so when an algorithmic construction is given [such as in Fedosov (1994)]. But for physical applications one needs to perform explicit calculations and few realizations are truly explicit. In the compact case, the ideas underlying Bonneau *et al.* (1994) were tested in the basic example of SU(2) where explicit formulas were obtained [Bonneau *et al.* (1992)]. We shall present here that example with this fact in mind. We also present the only known explicit formulas expressing the preferred deformation of a standard quantum algebra. Namely, the preferred *-products for the quantum linear spaces associated with the standard q-deformation of the special linear group $\mathrm{SL}(n)$. These approaches show that deformation quantization is implicit in most aspects of quantum groups theory.

Now, for deformation quantization, the paradigm of the Moyal star product is explicit enough,

and so are a number of related integral formulas in $\mathbb{R}^{2n}$ and a few manifolds. Some examples can be found in Bieliavsky and Maeda (2002). But for general symplectic, even more so Poisson, manifolds one has mainly existence theorems which are not easily made explicit. At its origin 25 years ago and again much more recently [Frønsdal (1979)], some explicit formulas were and are being developed. A somewhat explicit formula for many coadjoint orbits was recently developed (Alekseev and Lachowska) in terms of a pairing for generalized Verma modules. Related formulas can be found in Donin and Mudrov (2002), Enriquez *et al.* (2004), and Karolinsky *et al.* (2003). Part of this paper will be devoted to explicit approaches in that underlying aspect of quantum groups theory. In particular we shall see that quantum groups techniques may produce explicit (strict) deformation quantizations on the basis of what we call universal deformation formulas (UDFs). These come from mathematical entities living within a given algebraic structure S and they produce explicit deformations of any algebra which is also an S-module.

We start this paper (Sec. II) with a short presentation of deformation theory, mostly following Gerstenhaber. That somewhat arid presentation will be balanced by complements and, in Sec. III, by a survey of how quantum mechanics *is* a deformation of classical mechanics, with some explicit examples. Section IV begins with the explicit example [the case of $\mathrm{SU}_q(2)$] that triggered the general theory (presented afterwards) of both approaches to quantum groups (functions on a Poisson–Lie group and quantized enveloping algebras) as dual topological Hopf algebras, at least in the semisimple case. The latter theory being (in the general case) not explicit enough we devote Sec. V to a variety of explicit formulas for deformation quantization (star products), in particular for symmetric spaces and related universal deformation formulas. Section VI discusses the implications of the preceding study for obtaining explicit formulas for quantum groups, via star products or R matrices.

This paper contains only a brief review of some of the rapid developments in deformation quantization since its introduction in Bayen *et al.* (1978). André Weil's prediction near the end of the last century that deformation theory would be a major topic in the 21st so far seems justified.

II. PRELIMINARIES

A. The Gestenhaber theory of deformations of algebras

A concise formulation of a Gerstenhaber deformation of an algebra (associative, Lie, bialgebra, etc.) is [Gerstenhaber (1963, 1964) and Bonneau *et al.* (1994)]:

Definition: A deformation of an algebra A over a field $\mathbb{K}$ with deformation parameter ν is a $\mathbb{K}[[\nu]]$-algebra $\tilde{A}$ such that $\tilde{A}/\nu\tilde{A} \approx A$, where A is here considered as an algebra over $\mathbb{K}[[\nu]]$ by base field extension. Two deformations $\tilde{A}$ and $\tilde{A}'$ are called equivalent if they are isomorphic over $\mathbb{K}[[\nu]]$ (by a deformation which reduces to the identity modulo ν, which will always be tacitly understood). A deformation $\tilde{A}$ is said to be trivial if it is isomorphic to the original algebra A (considered by base field extension as a $\mathbb{K}[[\nu]]$-algebra).

Whenever we consider a topology on A, $\tilde{A}$ is supposed to be topologically free. The above definition can [cf., e.g., Kontsevich (1999) and Kontsevich and Soibelman (2000)] be extended to operads, so as to apply to the Assoc, Lie, Bialg and maybe Gerst operads, and also to the Hopf category (which can not be described by an operad), all possibly with topologies. In the present mathematical physics paper we shall not probe these sophistications, but the reader should keep such powerful possibilities in mind.

For associative (resp. Lie) algebras, the above definition tells us that there exists a new product * (resp. bracket $[\cdot,\cdot]$) such that the new (deformed) algebra is again associative (resp. Lie). Denoting the original composition laws by ordinary product (resp. $\{\cdot,\cdot\}$) this means that, for $u_1, u_2 \in A$ (we can extend this to $A[[\nu]]$ by $\mathbb{K}[[\nu]]$-linearity) we have

$$u_1 * u_2 = u_1 u_2 + \sum_{r=1}^{\infty} \nu^r C_r(u_1, u_2), \tag{1}$$

$$[u_1,u_2]=\{u_1,u_2\}+\sum_{r=1}^{\infty}\nu^r B_r(u_1,u_2), \tag{2}$$

where the C_r are Hochschild 2-cochains and the B_r (skew-symmetric) Chevalley–Eilenberg 2-cochains, such that for $u_1,u_2,u_3\in A$ we have $(u_1*u_2)*u_3=u_1*(u_2*u_3)$ and $\mathcal{S}[[u_1,u_2],u_3]=0$, where $\mathcal{S}$ denotes summation over cyclic permutations.

For a (topological) *bialgebra* (an associative algebra A where we have in addition a coproduct $\Delta:A\to A\otimes A$ and the obvious compatibility relations), denoted by $\otimes_\nu$ the tensor product of $\mathbb{K}[[\nu]]$-modules we can identify $\tilde{A}\hat{\otimes}_\nu\tilde{A}$ with $(A\hat{\otimes}A)[[\nu]]$, where $\hat{\otimes}$ denotes the algebraic tensor product completed with respect to some topology (e.g., projective for Fréchet nuclear topology on A). We similarly have a deformed coproduct $\tilde{\Delta}=\Delta+\Sigma_{r=1}^{\infty}\nu^r D_r$, $D_r\in \mathrm{L}(A,A\hat{\otimes}A)$, satisfying $\tilde{\Delta}(u_1*u_2)=\tilde{\Delta}(u_1)*\tilde{\Delta}(u_2)$. In this context appropriate cohomologies can be introduced [Gerstenhaber and Schack (1990) and Bonneau (1992)]. There are natural additional requirements for Hopf algebras.

Equivalence means that there is an isomorphism $T_\nu=I+\Sigma_{r=1}^{\infty}\nu^r T_r$, $T_r\in \mathrm{L}(A,A)$ so that $T_\nu(u_1*'u_2)=(T_\nu u_1*T_\nu u_2)$ in the associative case, denoting by * (resp. *′) the deformed laws in $\tilde{A}$ (resp. $\tilde{A}'$;) and similarly in the Lie, bialgebra and Hopf cases. In particular we see (for $r=1$) that a deformation is trivial at order 1 if it starts with a 2-cocycle which is a 2-coboundary. More generally, exactly as above, we can show [Bayen *et al.* (1978)] [Gerstenhaber and Schack (1988) and Bonneau (1992) in the Hopf case] that if two deformations are equivalent up to some order t, the condition to extend the equivalence one step further is that a 2-cocycle (defined using the T_k, $k\leqslant t$) is the coboundary of the required T_{t+1} and therefore *the obstructions to equivalence lie in the 2-cohomology*. In particular, if that space is null, all deformations are trivial.

Unit: An important property is that a *deformation of an associative algebra with unit* (what is called a unital algebra) is again unital, and *equivalent to a deformation with the same unit*. This follows from a more general result of Gerstenhaber (for deformations leaving unchanged a subalgebra) and a proof can be found in Gerstenhaber and Schack (1988).

Remark 1: In the case of (topological) *bialgebras* or *Hopf* algebras, *equivalence* of deformations has to be understood as an isomorphism of (topological) $\mathbb{K}[[\nu]]$-algebras, the isomorphism starting with the identity for the degree 0 in ν. A deformation is again said to be *trivial* if it is equivalent to that obtained by base field extension. For Hopf algebras the deformed algebras may be taken (by equivalence) to have the same unit and counit, but in general not the same antipode.

B. Complements

1. A brief historical survey: Contractions and deformations

The discovery, about 2000 years ago, of the nonflat nature of Earth is probably the first empirical introduction of the notion of deformation in our description of the universe. Closer to us, the paradox coming from the Michelson and Morley experiment (1887) was resolved in 1905 by Einstein with the special theory of relativity: in our context, one can express that by saying that the Galilean geometrical symmetry group of Newtonian mechanics is deformed to the Poincaré group, the deformation parameter being c^{-1}, where c is the velocity of light in vacuum.

Curiously, it is the (less precisely defined) inverse notion of contraction of symmetries that was first introduced in mathematical physics [Segal (1951), Inönü and Wigner (1953), Saletan (1961)]. Contractions, "limits of Lie algebras" as they were called in the first examples, can be viewed as an inverse of deformations—but not necessarily of Gerstenhaber-type deformations (see Sec. II B 3 below). We shall not expand here on that "inverse" notion but, for completeness, give its flavor. A (finite dimensional) Lie algebra can be described in a given basis L_i $(i=1,\ldots,n)$ by its structure constants $C_{i,j}^k$. The equations governing the skew symmetry of the Lie bracket and the Jacobi identity insure that the set of all structure constants lies on an algebraic variety in that n^3 dimensional space [Lévy-Nahas (1967)]. A contraction is obtained, e.g., when one makes a simple basis change of the form $L_i'=\varepsilon L_i$ on some of the basis elements, and then lets $\varepsilon\to 0$. Take, for

example, $n=3$ and restrict to the three-dimensional subspace of the algebraic variety of three-dimensional Lie algebras with commutation relations $[L_1,L_2]=c_3L_3$ and cyclic permutations. The semi-simple algebras $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ are obtained in the open set $c_1c_2c_3\neq 0$. A contraction gives the Euclidean algebras, where one c_i is 0. The "coordinate axes" (two of the c_i's are 0) give the Heisenberg algebra and the origin is the Abelian Lie algebra. This is of course a partial picture (e.g., solvable algebras are missing) but it is characteristic. The passage from the Poincaré Lie algebra to the Galilean is a higher dimensional version of it. Dirac constraints [mathematically, a restriction from $\mathbb{R}^{2n}$ to a symplectic or Poisson submanifold, see, e.g., Lichnerowicz (1975)] can give such contractions and be interpreted in terms of star products [Arnal and Cortet (1979)].

An implicit mathematical example of deformations (in a geometric context) was introduced in mid-19th century by Riemann who counted the number of "moduli" or parameters of Riemann surfaces. Teichmüller (1939) ["It does not of necessity follow that, if the work delights you with its grace, the one who wrought it is worthy of your esteem," cf. Lipman Bers (1998) (p. 324, after Plutarch, Pericles 2.1; Lives, Loeb's Classical Library 3, p. 5) who however, with André Weil, despite personal abhorrence of someone who helped drive Jewish mathematicians from Nazi Germany, fully credited his work] made deformations of Riemann surfaces explicit and identified infinitesimal deformations as quadratic differentials. The correct definition, applicable to complex manifolds of arbitrary dimension, is in the short but ground breaking note of Frölicher and Nijenhuis (1957). They showed that if all infinitesimal deformations vanished then the manifold was rigid ("stable" in their terminology), i.e., possessed no global deformations. This was the impetus for the deep and comprehensive work of Kodaira and Spencer (1958). Curiously, however, the possibility of obstructions to infinitesimal deformations (which cannot occur in the case of Riemann surfaces because of the low dimension) was not originally understood, and appeared in the words of Kodaira and Spencer as an "experimental fact."

Now, when one has an action on a geometrical structure, it is natural to try and "linearize" it by inducing from it an action on an algebra of functions on that structure. That is implicitly what Gerstenhaber (1964) did with his definition and thorough study of deformations of rings and algebras. We shall encounter the concept of contraction more explicitly as it relates to quantum groups later in Sec. VI D.

2. Homotopy of deformations

For reasons that are related to the so-called Donald–Flanigan conjecture, two of us considered [see Gerstenhaber and Giaquinto (1998) and Gerstenhaber *et al.* (2001)] the question of (formal) *compatibility* of deformations, a kind of homotopy in the variety of algebras between two deformations (1) with parameters ν and ν' and cochains C_r and C'_r. By this he means a 2-parameter deformation of the form

$$u_1 \tilde{*} u_2 = u_1u_2 + \nu C_1(u_1,u_2) + \nu' C'_1(u_1,u_2) + \sum_{r=2}^{\infty} \Phi_r(u_1,u_2;\nu,\nu'), \tag{3}$$

where each Φ_r is a polynomial of total degree r in ν and ν', which reduces to the first one-parameter deformation when $\nu'=0$ and to the second when $\nu=0$. At the first order the condition for this to hold (e.g., for associative algebras) is that the Gerstenhaber bracket [Gerstenhaber (1964)] $[C_1,C'_1]_G$ is a 3-coboundary, and here also there are higher obstructions. As an example, it follows from Hochschild *et al.* (1962) that the Weyl algebra and the quantum plane are formally **(**but nonanalytically [Giaquinto and Zhang (1995)]**)** compatible nonequivalent deformations of the polynomial algebra $\mathbb{C}[x,y]$. Below we shall see another appearance of such a 2-parameter deformation in a physical context [Basart *et al.* (1984)].

3. More general deformations

Deformations that are more general than the "DrG-deformations" of Gerstenhaber can (and have been) introduced, where, e.g., the deformation "parameter" may act on the algebra.

Nambu (1973) published some calculations which he had made a dozen years before: with quarks in the back of his mind he started with a kind of "Hamilton equations" on $\mathbb{R}^3$ with two "Hamiltonians" g, h functions of r. In this new mechanics the evolution of a function f on $\mathbb{R}^3$ is $df/dt=\partial(f,g,h)/\partial(x,y,z)$, a 3-bracket, where the right-hand side is the Jacobian of the mapping $\mathbb{R}^3\to\mathbb{R}^3$ given by $(x,y,z)\mapsto(f,g,h)$. That expression was easily generalized, e.g., to n functions f_i, $i=1,\ldots,n$.

In order to quantize the Nambu bracket a natural idea is to replace, in the definition of the Jacobian, the pointwise product of functions by a deformed product. For this to make sense, the deformed product should be Abelian, so we are lead to consider commutative DrG-deformations of an associative and commutative product. But the commutative part of Hochschild cohomology (called Harrison cohomology) is trivial, at least in the absence of singularities [see however Frønsdal (2002)]. So in Dito *et al.* (1997) a kind of "second quantization" procedure was used, where the deformation parameter behaves as if it was nilpotent (like Pauli matrices).

This triggered Pinczon (1997) and Nadaud (1998) to generalize the Gerstenhaber theory to the case of a deformation parameter which *does not commute with the algebra*, but acts on it. Though this generalization of deformations does not (yet) give Nambu mechanics quantization, it opens a whole new direction of research for deformation theory. In particular [Pinczon (1997)], while the Weyl algebra W_1 (generated by the Heisenberg Lie algebra h_1) is known to be DrG-rigid, it can be nontrivially deformed in such a *supersymmetric deformation theory* to the supersymmetry enveloping algebra $\mathcal{U}(\mathfrak{osp}(1,2))$. Also [Nadaud (1998)] on the polynomial algebra $\mathbb{C}[x,y]$ in 2 variables, Moyal-type products of a new type were discovered. All these deformations give the original algebra by a contraction, when the parameter goes to 0. So there is life outside the DrG framework, even if that is so far largely unexplored.

III. QUANTUM MECHANICS AS A DEFORMATION

A. The setting

Intuitively, classical mechanics is the limit of quantum mechanics when $\hbar=h/2\pi$ goes to zero. But how can this be realized when in classical mechanics the observables are functions over phase space (a Poisson manifold) and not operators? The deformation philosophy promoted by Flato shows the way: one has to look for deformations of algebras of classical observables, functions over Poisson manifolds, and realize there quantum mechanics in an *autonomous* manner.

What we call "deformation quantization" relates to (and generalizes) what in the conventional (operatorial) formulation are the Heisenberg picture and Weyl's quantization procedure. In the latter [Weyl (1931)], starting with a classical observable $u(p,q)$, some function on phase space $\mathbb{R}^{2\ell}$ (with $p,q\in\mathbb{R}^{\ell}$), one associates an operator (the corresponding quantum observable) $\Omega(u)$ in the Hilbert space $L^2(\mathbb{R}^{\ell})$ by the following general recipe:

$$u\mapsto\Omega_w(u)=\int_{R^{2\ell}}\tilde{u}(\xi,\eta)\exp(i(P\cdot\xi+Q\cdot\eta)/\hbar)w(\xi,\eta)d^{\ell}\xi d^{\ell}\eta, \tag{4}$$

where $\tilde{u}$ is the inverse Fourier transform of u, P_α and Q_α are operators satisfying the canonical commutation relations $[P_\alpha,Q_\beta]=i\hbar\delta_{\alpha\beta}$ $(\alpha,\beta=1,\ldots,\ell)$, w is a weight function and the integral is taken in the weak operator topology. What is called in physics normal (or antinormal) ordering corresponds to choosing for weight $w(\xi,\eta)=\exp\left(-\frac{1}{4}(\xi^2\pm\eta^2)\right)$. Standard ordering (the case of the usual pseudodifferential operators in mathematics) corresponds to $w(\xi,\eta)=\exp(-(i/2)\xi\eta)$ and the original Weyl (symmetric) ordering to $w=1$. An inverse formula was found shortly afterwards by Eugene Wigner (1932) and maps an operator into what mathematicians call its symbol by a kind of trace formula. For example Ω_1 defines an isomorphism of Hilbert spaces between $L^2(\mathbb{R}^{2\ell})$ and Hilbert–Schmidt operators on $L^2(\mathbb{R}^{\ell})$ with inverse given by

$$u = (2\pi\hbar)^{-\ell}\,\mathrm{Tr}[\Omega_1(u)\exp((\xi\cdot P+\eta\cdot Q)/i\hbar)] \tag{5}$$

and if $\Omega_1(u)$ is of trace class one has $\mathrm{Tr}(\Omega_1(u))=(2\pi\hbar)^{-\ell}\int u\omega^{\ell}\equiv \mathrm{Tr}_M(u)$, the "Moyal trace," where ω^{ℓ} is the (symplectic) volume dx on $\mathbb{R}^{2\ell}$. Looking for a direct expression for the symbol of a quantum commutator, Moyal (1949) found what is now called the Moyal bracket:

$$M(u_1,u_2)=\nu^{-1}\sinh(\nu P)(u_1,u_2)=P(u_1,u_2)+\sum_{r=1}^{\infty}\frac{\nu^{2r}}{(2r+1)!}P^{2r+1}(u_1,u_2), \tag{6}$$

where $2\nu=i\hbar$, $P^r(u_1,u_2)=\Lambda^{i_1j_1}\cdots\Lambda^{i_rj_r}(\partial_{i_1\cdots i_r}u_1)(\partial_{j_1\cdots j_r}u_2)$ is the rth power ($r\geqslant 1$) of the Poisson bracket bidifferential operator P, $i_k,j_k=1,\ldots,2\ell$, $k=1,\ldots,r$ and $(\Lambda^{i_kj_k})=\left(\begin{smallmatrix}0 & -I\\ I & 0\end{smallmatrix}\right)$. To fix ideas we may assume here $u_1,u_2\in\mathcal{C}^{\infty}(\mathbb{R}^{2\ell})$ and the sum is taken as a formal series. A corresponding formula for the symbol of a product $\Omega_1(u)\Omega_1(v)$ can be found in Groenewold (1946) and may now be written more clearly as a (Moyal) *star product:*

$$u_1{}^{*}{}_{M}u_2=\exp(\nu P)(u_1,u_2)=u_1u_2+\sum_{r=1}^{\infty}\frac{\nu^{r}}{r!}P^r(u_1,u_2). \tag{7}$$

The formal series may be deduced [see, e.g., Bieliavsky (2002)] from an integral formula of the type

$$(u_1*u_2)(x)=c_{\hbar}\int_{\mathbb{R}^{2\ell}\times\mathbb{R}^{2\ell}}u_1(x+y)u_2(x+z)e^{-(i/\hbar)\Lambda^{-1}(y,z)}dydz. \tag{8}$$

Other integral formulas are known for quite some time [Rieffel (1993) and Maillard (1986) where the Weyl correspondence between bounded operators in $L^2(\mathbb{R}^l)$ and bounded twisted convolution operators of $L^2(\mathbb{R}^{2l})$ is also described]. It was noticed, however after deformation quantization was introduced, that the composition of symbols of pseudodifferential operators (ordered, like differential operators, "first q, then p") is a star product.

One recognizes in (7) a special case of (1), and similarly for the bracket. So, via a Weyl quantization map, the algebra of quantized observables can be viewed as a deformation of that of classical observables.

But the deformation philosophy tells us more. Deformation quantization is not merely "a reformulation of quantizing a mechanical system" [Douglas and Nekrasov (2001)], e.g., in the framework of Weyl quantization: *The process of quantization itself is a deformation*. In order to show that explicitly it was necessary to treat in an *autonomous* manner significant physical examples (in effect, those for which a complete and rigorous spectral theory exists), without recourse to the traditional operatorial formulation of quantum mechanics. That was achieved in Bayen *et al.* (1978) with the paradigm of the harmonic oscillator and more, including the angular momentum and the hydrogen atom.

In particular what plays here the role of the unitary time evolution operator of a quantized system is the "star exponential" of its classical Hamiltonian H (expressed as a usual exponential series but with "star powers" of $tH/i\hbar$, t being the time, and computed as a distribution both in phase space variables and in time); in a very natural manner, the spectrum of the quantum operator corresponding to H is the support of the Fourier-Stieltjes transform (in t) of the star exponential (what Laurent Schwartz had called the spectrum of that distribution). It is worth mentioning that our definition of spectrum permits to define a spectrum even for symbols of nonspectrable operators, such as the derivative on a half-line which has different deficiency indices; this corresponds to an infinite potential barrier. That is one of the many advantages of our autonomous approach to quantization. Further examples were (and are still being) developed, in particular in the direction of field theory.

B. Quantum mechanics without operators: Harmonic oscillator, angular momentum, and hydrogen atom

In quantum mechanics it is preferable to work (for $X=\mathbb{R}^{2\ell}$) with the Moyal product, which has maximal symmetry, i.e., has $\mathfrak{sp}(\mathbb{R}^{2\ell})\cdot\mathfrak{h}_\ell$ as what we call (see Sec. IV C 2 below) algebra of preferred observables. One indeed finds [Bayen *et al.* (1978)] that star powers of these preferred observables H (polynomials of order $\leqslant 2$) are usual polynomials in H (not only in p and q), and as a consequence their star exponential is proportional to the usual exponential and a function of H. More precisely, if $H=\alpha p^2+\beta pq+\gamma q^2\in\mathfrak{sl}(2)$ with $p,q\in\mathbb{R}^\ell$, $\alpha,\beta,\gamma\in\mathbb{R}$, setting $d=\alpha\gamma-\beta^2$ and $\delta=|d|^{1/2}$ one gets by summing the star exponential (with deformation parameter $\nu=i\hbar/2$) and then taking its Fourier (or Fourier–Stieltjes) development, the sums and integrals appearing in the various expressions of the star exponential being convergent as distributions, in phase-space variables and in t or λ:

$$\exp(Ht)=\begin{cases}(\cos\ \delta t)^{-l}\exp((H/i\hbar\delta)\tan(\delta t)) & \text{for } d>01\\ \exp(Ht/i\hbar) & \text{for } d=01\\ (\cosh\ \delta t)^{-l}\exp((H/i\hbar\delta)\tanh(\delta t)) & \text{for } d<0,\end{cases}\tag{9}$$

$$\exp(Ht)=\begin{cases}\displaystyle\sum_{n=0}^{\infty}\Pi_n^{(\ell)}e^{(n+(\ell/2))t} & \text{for } d>0\\ \displaystyle\int_{-\infty}^{\infty}e^{\lambda t/i\hbar}\Pi(\lambda,H)d\lambda & \text{for } d<0.\end{cases}\tag{10}$$

We thus get the discrete spectrum $(n+(\ell/2))\hbar$ of the harmonic *oscillator* and the continuous spectrum $\mathbb{R}$ for the dilation generator pq. The eigenprojectors $\Pi_n^{(\ell)}$ and $\Pi(\lambda,H)$ are given [Bayen *et al.* (1978)] by known special functions on phase-space (generalized Laguerre and hypergeometric, multiplied by some exponential). Formulas (9) and (10) can, by analytic continuation, be given a sense outside singularities and even (as distributions) for values of t for which the expressions are singular.

Other orderings give similar formulas [Maillard (2004)] and other examples can be brought to this case, in particular by functional manipulations [Bayen *et al.* (1978)]. For instance the Casimir element C of $\mathfrak{so}(\ell)$ representing *angular momentum*, which can be written $C=p^2q^2-(pq)^2-\ell(\ell-1)(\hbar^2/4)$, has $n(n+(\ell-2))\hbar^2$ for spectrum. For the *hydrogen atom*, with Hamiltonian $H=\frac{1}{2}p^2-|q|^{-1}$, the Moyal product on $\mathbb{R}^{2\ell+2}$ ($\ell=3$ in the physical case) induces a star product on $X=T^*S^\ell$; the energy levels, solutions of $(H-E)*\phi=0$, are found from (10) and the preceding calculations for angular momentum to be (as they should, with $\ell=3$) $E=\frac{1}{2}(n+1)^{-2}\hbar^{-2}$ for the discrete spectrum, and $E\in\mathbb{R}^+$ for the continuous spectrum.

We thus have recovered, in a completely autonomous manner entirely within deformation quantization, the results of "conventional" quantum mechanics in these typical examples (and many more can be treated similarly). It is worth noting that the term $\ell/2$ in the harmonic oscillator spectrum, obvious source of divergences in the infinite-dimensional case, disappears if the normal star product is used instead of Moyal—which is one of the reasons it is preferred in field theory.

C. Modern developments

Since the original papers in 1976–1978 [Flato *et al.* (1976) and Bayen *et al.* (1978)] deformation quantization has been extended considerably. It now includes general symplectic and Poisson (finite dimensional) manifolds, with further results for infinite dimensional manifolds, for "manifolds with singularities" and for algebraic varieties, and has many far reaching ramifications in both mathematics and physics [see, e.g., a brief overview in Dito and Sternheimer (2002)]. As in quantization itself [Weyl (1931)], symmetries (group theory) play a special role and an autonomous theory of star representations of Lie groups was developed, in the nilpotent and solvable cases of course (due to the importance of the orbit method there), but also in significant other

examples. The presentation that follows can be seen as an extension of the latter, when one makes full use of the Hopf algebra structures and of the "duality" between the group structure and the set of its irreducible representations.

It goes without saying (but mentioning it will not hurt) that deformation theory and Hopf algebras are seminal in a variety of problems ranging from theoretical physics to algebraic geometry, number theory and more. We shall not insist here on the manifold applications of quantum groups, certainly treated in many contributions to this special issue. In theoretical physics one finds now applications (see, e.g., Connes and Kreimer (1999), Dito *et al.* (1997), Tamarkin (2003)] to renormalization and Feynman integrals and diagrams. Noncommutativity is a staple in modern theoretical physics [Douglas and Nekrasov (2001)] (including string theory and its avatars) even at the level of space–time; deformation quantization (in particular Moyal products) is an important tool there, at least at the formal level. But the applications (and by-products therefrom to physics) extend as far as algebraic geometry and number theory [see, e.g., Kontsevich (2001) and Kontsevich and Zagier (2001)] including algebraic curves à la Zagier [cf. Connes and Moscovici (2004), Connes and Marcoli, and Connes's lectures at Collège de France, Winter 2003 and 2004).

IV. QUANTUM GROUPS AS DEFORMATIONS

In this section we explore in detail the concept of viewing quantum groups as Hopf algebra deformations of $\mathcal{U}\mathfrak{g}$ and $\mathcal{C}^\infty(G)$. We restrict to the case where G is a semisimple Lie group with Lie algebra $\mathfrak{g}$.

A. Formal deformations

We begin with a summary of important considerations regarding *formal deformations*: all vector spaces, tensor products, etc. being complete in the ν-adic topology. This is a purely algebraic approach with no consideration to any topological or convergence questions. All of what follows can be extracted from Drinfel'd (1989a, 1989b), Gerstenhaber and Schack (1990a, 1990b).

Recall that a bialgebra is called *rigid* it every deformation is trivial. Neither $\mathcal{U}\mathfrak{g}$ nor $\mathcal{C}^\infty(G)$ is rigid but, as the theorem below asserts, each is *half-rigid* in the following sense: $\mathcal{U}\mathfrak{g}$ is rigid as an algebra and $\mathcal{C}^\infty(G)$ is rigid as a coalgebra. This means that for any deformation $\mathcal{U}_\nu(\mathfrak{g})$, there is an equivalent one in which the original multiplication $\mu_0: \mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g}\to\mathcal{U}\mathfrak{g}$ is preserved and so $\mathcal{U}_\nu(\mathfrak{g}) \cong (\mathcal{U}\mathfrak{g}[[\nu]], \mu_0, \tilde{\Delta})$ for some coassociative $\tilde{\Delta}$. Similarly, any deformation $\mathcal{C}^\infty_\nu(G)$ is equivalent to one in which the comultiplication $\Delta_0: \mathcal{C}^\infty(G)\to\mathcal{C}^\infty(G)$ is preserved on all elements. Thus $\mathcal{C}^\infty_\nu(G) \cong (\mathcal{C}^\infty(G)[[\nu]], *, \Delta_0)$ for some associative *-product. Such deformations in which one of the original structure maps is preserved are called *preferred*.

The structure of the deformed comultiplication of $\mathcal{U}\mathfrak{g}$ and the deformed multiplication $\mathcal{C}^\infty(G)$ are produced via certain elements of $(\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]$. For $F\in(\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]$ and $u\in\mathcal{U}\mathfrak{g}$, define $\Delta_F(u)=F\Delta_0(u)F^{-1}$. In a dual sense, we can define $f*_F g$ for $f,g\in\mathcal{C}^\infty(G)$. To define $*_F$ we need some notation first. For $x\in\mathfrak{g}$, let x_λ and x_ρ be the left invariant and right invariant, respectively, derivations of $\mathcal{C}^\infty(G)$ arising from the corresponding left and right invariant vector fields on G associated with x. Taking the tensor product and extending linearly, we associate to every $F \in (\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]$ two formal sums of bidifferential operators F_λ and F_ρ. With this, we define $f*_F g=\mu_0\circ(F_\lambda\circ F_\rho^{-1})(f\otimes g)$. Note that if $F\cong 1\otimes 1 \bmod \nu$, then $\Delta_F(u)$ and $f*_F g$ are series whose constant terms are the original structure maps $\Delta_0(u)$ and $f\cdot g$. However, Δ_F will not generally be coassociative and $*_F$ will not generally be associative. The appropriate condition for F to satisfy is given by the following important result.

Theorem IV.1 [Drinfel'd (1989a, 1989b), Gerstenhaber and Schack (1992)]: *Let G be a semisimple Lie group with Lie algebra $\mathfrak{g}$, and suppose that $F\in(\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]$ with $F\cong 1\otimes 1 \bmod \nu$.*

Then $(\mathcal{U}\mathfrak{g}[[\nu]], \mu_0, \Delta_F)$ and $(\mathcal{C}^\infty(G)[[\nu]], *_F, \Delta_0)$ are deformations if and only if

$$F_{12}(\Delta_0\otimes 1)F = \Phi F_{23}(1\otimes\Delta_0)F \tag{11}$$

for some $\Phi \in (\mathcal{U}\mathfrak{g} \otimes \mathcal{U}\mathfrak{g} \otimes \mathcal{U}\mathfrak{g})^{\mathfrak{g}}$. *Moreover, every deformation of* $\mathcal{U}\mathfrak{g}$ *and* $\mathcal{C}^{\infty}(G)$ *is equivalent to one defined by such an* F.

Note that (11) is an equation which must hold in the triple tensor product $\mathcal{U}\mathfrak{g} \otimes \mathcal{U}\mathfrak{g} \otimes \mathcal{U}\mathfrak{g}$. (The comultiplication Δ_0 in this equation is that of $\mathcal{U}\mathfrak{g}$.) The half-rigidity of $\mathcal{U}\mathfrak{g}$ was first proved in Drinfel'd (1989a) and it was derived for $\mathcal{C}^{\infty}(G)$ in Gerstenhaber and Schack (1992). The specific form of the deformations can be deduced from Drinfel'd (1989b).

If $\Phi = 1 \otimes 1 \otimes 1$ (a trivial $\mathfrak{g}$-invariant), then F is called a *twisting element* and, if Φ is a nontrivial invariant, then F is a *modified twisting element*. In either case, we say the deformation is given by a "twist."

From the viewpoint of deformation quantization, it may seem that Theorem IV.1 settles the story. In a way it does, but it opens up many more questions which we will address throughout the remainder of this survey. The most basic question is to find elements F which solve Eq. (11). This task is easier said than done. Indeed, no modified twisting elements are explicitly known for any simple Lie algebra $\mathfrak{g}$—even for the rank 1 case of $\mathfrak{sl}(2)$! The situation is different for twisting elements—there is a handful which are explicitly known, and we will exhibit some of them later in Sec. VI B.

There is an interesting irony here concerning the infinitesimals (or first order terms) of the two types of twisting elements. The possible infinitesimals of modified twisting elements are all constructively classified in the famous paper of Belavin and Drinfel'd (1984). In contrast, such a classification for the infinitesimals of the twisting elements is an intractable problem. (It would require, in particular, a constructive classification of all Abelian subalgebras of $\mathfrak{g}$, a question which is known to be too broad to solve as stated.)

B. Topological preliminaries

In the next few sections, we describe a "topological" approach to quantum groups via deformation quantization. Instead of working formally over complete power series rings, we consider other topologies which have more desirable properties, especially in terms of dualization. The theory was initiated in Bonneau (1994) and its generalizations can be found in Bidegain and Pinczon (1996).

1. Example: The SU(2) case

First we will investigate in detail the example that the general theory is based on. It is interesting and merits special attention because apart from giving the main ideas, it differs in two crucial points: it is *explicit* and *convergent*. The main reference is Bonneau *et al.* (1992).

We start with Jimbo's definition of $\mathcal{U}_q\mathfrak{sl}(2)$ [Jimbo (1985)]. As an algebra, $\mathcal{U}_q\mathfrak{sl}(2)$ has generators E, F, $K^{\pm 1}$ and the relations

$$KEK^{-1} = qE, \quad KFK^{-1} = q^{-1}F, \quad EF - FE = \frac{K^2 - K^{-2}}{q - q^{-1}}.$$

The coalgebra structure on $\mathcal{U}_q\mathfrak{sl}(2)$ is given by

$$\Delta(E) = E \otimes K^{-1} + K \otimes E, \quad \Delta(F) = F \otimes K^{-1} + K \otimes F, \quad \Delta(K) = K \otimes K.$$

Remark IV.1:

(1) *One may view* $\mathcal{U}_q\mathfrak{sl}(2)$ *as an algebra over* $\mathbb{K}$ (*with* $q \in \mathbb{K}^*$) *or over the rational function field* $\mathbb{K}(q)$ (*with* q *an indeterminate*). *For what follows it will be convenient to view* $q = e^{i\nu} \in \mathbb{C}$.

(2) *Note that, as presented,* $\mathcal{U}_q\mathfrak{sl}(2)$ *is not a deformation of* $\mathcal{U}\mathfrak{sl}(2)$. *If one formally sets* $K = q^{H/2}$ (*where* $[E,F] = H$ *in* $sl(2)$) *and completes the algebra with respect to the* ν*-adic topology, then one indeed has a genuine deformation of* $\mathcal{U}\mathfrak{sl}(2)$. *This fact, however, is not obvious from looking at just the relations. It is usually proved by analyzing the representation theory of the algebras involved.*

Even though $\mathcal{U}_q\mathfrak{sl}(2)$ is undefined at $q=1$, one may make sense of it as q approaches 1. Specifically, under the linear change of generators,

$$S = \frac{K - K^{-1}}{q - q^{-1}},$$

$$C = \frac{K + K^{-1}}{2},$$

one has the following set of relations:

$$EF - FE = 2SC, \quad SC = CS,$$

$$ES = (S\cos\nu - C)E, \quad EC = (C\cos\nu + S\sin^2\nu)E,$$

$$FS = (S\cos\nu + C)F, \quad FC = (C\cos\nu - S\sin^2\nu)F,$$

$$C^2 + S^2\sin^2\nu = 1. \tag{12}$$

This new system of generators and relations is well-defined for all ν, and it turns out that $\mathcal{U}_1\mathfrak{sl}(2) \cong \mathcal{U}\mathfrak{sl}(2) \otimes \mathbb{K}[X]/(X^2-1)$. The element X is called a *parity*. The Jimbo quantum groups $\mathcal{U}_q\mathfrak{g}$ have, in general, r parities, where r is the rank of $\mathfrak{g}$ and so they are clearly not a formal deformation of $\mathcal{U}\mathfrak{g}$, notwithstanding the aforementioned rigidity result of Theorem IV.1.

The algebra $\mathcal{A}$: Let $\{(\pi_n, V_n)\}_{n\in(1/2)\mathbb{N}}$ be the finite dimensional irreducible representations of $\mathfrak{sl}(2)$ [or SU(2), as they are the same]. Let $\mathcal{A} = \Pi_{n\in(1/2)\mathbb{N}}\mathrm{End}(V_n)$. We consider the product topology on $\mathcal{A}$ (Fréchet). We have embeddings $\mathcal{U}\mathfrak{sl}(2) \hookrightarrow \mathcal{A}$ and $\mathbb{C}G \hookrightarrow \mathcal{A}$ by $u \mapsto (\pi_n(u))$ and $x \mapsto (\pi_n(x))$. These maps are injective because $\{(\pi_n, V_n)\}$ is a complete set of representations for $\mathfrak{sl}(2)$ [or SU(2)].

Let π be the representation of $\mathcal{U}\mathfrak{sl}(2)$ [or SU(2)] defined by $\Sigma_{n\in(1/2)\mathbb{N}}\pi_n$. Then $\mathcal{A}$ coincides with the bicommutant of π and, by semisimplicity of π and the density theorem of Jacobson, we get

$$\overline{\mathcal{U}\mathfrak{sl}(2)} = \mathcal{A} \quad \text{and} \quad \mathbb{C}\overline{G} = \mathcal{A}.$$

Since the set $\{(\pi_n, V_n)\}_{n\in(1/2)\mathbb{N}}$ is also a complete set of representations for $\mathcal{U}_q\mathcal{G}$ we have the following similar results:

$$\mathcal{U}_q\, sl(2) \hookrightarrow \mathcal{A} \quad \text{and} \quad \overline{\mathcal{U}_q\mathfrak{sl}(2)} = \mathcal{A}, \quad \text{for all} \quad \nu \notin 2\pi\mathbb{Q}.$$

Details can be found in Bonneau *et al.* (1992).

Thus, both $\mathcal{U}\mathfrak{sl}(2)$ and $\mathcal{U}_q\mathfrak{sl}(2)$ are dense subalgebras of $\mathcal{A}$. We denote by A_ν the subalgebra of $\mathcal{A}$ isomorphic to $\mathcal{U}_q\mathfrak{sl}(2)$. Since $A_\nu \cong A_{\nu'}$ if and only if $\nu' = \pm\nu + 2k\pi, k \in \mathbb{Z}$, it follows that A_ν is a deformation of A_0.

By a standard density argument, the coproduct Δ_ν of $A_\nu, \nu \notin 2\pi\mathbb{Q}$, can be extended to the whole algebra $\mathcal{A}$; the same holds true for the antipode. Thus we have a preferred deformation of $\mathcal{A}$ as the coalgebra structure varies with a fixed algebra structure. In fact, this deformation of $\mathcal{A}$ has the same form as any preferred deformation of $\mathcal{U}\mathfrak{g}$. Specifically, there is an invertible element $F \in \mathcal{A}\hat{\otimes}\mathcal{A}$ such that $\Delta_\nu = F\Delta_0 F^{-1}$. The element F is constructed component by component using equivalences of representations, see Bonneau *et al.* (1992) for details. A consequence is that all the Hopf structures on $\mathcal{A}$ induced by various A_ν are isomorphic as quasi-Hopf algebras [see Drinfel'd (1989)].

So far we have not used the topology on $\mathcal{A}$, but it will play a crucial role as we now want to consider its dualization. The strong topological dual of $\mathcal{A} = \Pi_{n\in(1/2)\mathbb{N}}\ \mathrm{End}\ (V_n)$ is $\mathcal{A}^* = \mathcal{H}$

$=\oplus_{n\in(1/2)\mathbb{N}}\ \mathrm{End}\ (V_n)$, the coefficient Hopf algebra of polynomial functions on SU(2). Since $(\mathcal{A}\hat{\otimes}\mathcal{A})^*=\mathcal{H}\hat{\otimes}\mathcal{H}$, we obtain a Hopf algebra on $\mathcal{A}^*$, which we denote $\mathcal{H}_\nu$.

Proposition IV.1: $\mathcal{H}_\nu$ coincides precisely with the deformation of the function Hopf algebra $\mathbb{C}[SL_2]$, the quantum group $\mathbb{C}[SL_2]$, given in Faddeev et al. (1988).

Thus we have shown that there is an explicit embedding of the Jimbo quantum group $\mathcal{U}_q\mathfrak{sl}(2), q\in\mathbb{C}$ ($q^n\neq 1$ for all $n\in\mathbb{N}$) in the $\mathbb{C}$-Hopf algebra $\mathcal{A}$.

In the general case that will not be possible. We shall have to use the $\mathbb{C}[[\nu]]$-Hopf algebra $\mathcal{A}[[\nu]]$ and the nonexplicit Drinfel'd isomorphisms.

2. Some topological Hopf algebras (well-behaved Hopf algebras)

We shall now briefly review applications of the deformation theory of algebras in the context of Hopf algebras endowed with appropriate topologies and in the spirit of deformation quantization. That is, we shall consider Hopf algebras of functions on Poisson–Lie groups (or their topological duals) and their deformations, and show how this framework is a powerful tool to understand the standard examples of quantum groups, and more. In order to do so we first recall some notions on topological vector spaces and apply them to our context.

Definition IV.1: A topological vector space (tvs) V is said well-behaved if V is either nuclear and Fréchet, or nuclear and dual of Fréchet [Grothendieck (1955) and Trèves (1967)].

Proposition IV.2: If V is a well-behaved tvs and W a tvs, then

$$(i)V^{**}\simeq V,\quad (ii)(V\hat{\otimes}V)^*\simeq V^*\hat{\otimes}V^*,\quad (iii)\mathrm{Hom}_{\mathbb{K}}(V,W)\simeq V^*\hat{\otimes}W,$$

where V^* denotes the strong topological dual of V, $\hat{\otimes}$ the projective topological tensor product and the base field $\mathbb{K}$ is $\mathbb{R}$ or $\mathbb{C}$.

Definition IV.2: $(A,\mu,\eta,\Delta,\varepsilon,S)$ is a WB (well-behaved) Hopf algebra [Bonneau et al. (1994)] if

(1) A is a well-behaved topological vector space;
(2) The multiplication $\mu:A\hat{\otimes}A\to A$, the coproduct $\Delta:A\to A\hat{\otimes}A$, the unit η, the counit ε, and the antipode S are continuous;
(3) $\mu,\eta,\Delta,\varepsilon$, and S satisfy the usual axioms of a Hopf algebra.

Corollary IV.1: If $(A,\mu,\eta,\Delta,\varepsilon,S)$ is a WB Hopf algebra, then $(A^*,{}^t\Delta,{}^t\varepsilon,{}^t\mu,{}^t\eta,{}^tS)$ is also a WB Hopf algebra.

Examples IV.1: Let G be a semisimple Lie group and $\mathfrak{g}$ its complexified Lie algebra.

(1) $\mathcal{C}^\infty(G)$, the algebra of the smooth functions on G, is a WB Hopf algebra (Fréchet and nuclear).
(2) $\mathcal{D}(G)=\mathcal{C}^\infty(G)^*$, the algebra of the compactly supported distributions on G, is a WB Hopf algebra (dual of Fréchet and nuclear). The product is the transposed map of the coproduct of $\mathcal{C}^\infty(G)$ that is, the convolution of distributions.
(3) $\mathcal{H}(G)$, the algebra of coefficient functions of finite dimensional representations of G (or polynomial functions on G) is a WB Hopf algebra, the Hopf structure being that induced from $\mathcal{C}^\infty(G)$.

A short description of that algebra is as follows: We take a set $\hat{G}$ of irreducible finite dimensional representations of G such that there is *one and only one* element for each equivalence class, and, if $\pi\in\hat{G}$, its contragredient $\check{\pi}$ is also in $\hat{G}$. We define

$$C_\pi=\mathrm{vect}\{\text{coefficient functions of } \pi\}\overset{\text{Burnside}}{\simeq}\mathrm{End}(V_\pi)\ \text{for}\ \pi\in\hat{G}.$$

Then $\mathcal{H}(G)\overset{\text{alg.}}{\simeq}\oplus_{\pi\in\hat{G}}C_\pi\overset{\text{v.s.}}{\simeq}\oplus_{\pi\in\hat{G}}\mathrm{End}\ (V_\pi)$. So we take on $\mathcal{H}(G)$ the "direct sum" topology. Then $\mathcal{H}(G)$ is dual of Fréchet and nuclear and so is WB.

(4) Let $\mathcal{A}(G)$, the algebra of "generalized distributions," be defined by $\mathcal{A}(G)=\mathcal{H}(G)^{*}\overset{\text{alg.}}{\simeq}\Pi_{\pi\in\hat{G}}\,\mathrm{End}\,(V_\pi)$. The (product) topology is Fréchet and nuclear, and therefore $\mathcal{A}(G)$ is WB.

Proposition IV.3 [Bidegain and Pinczon (1996) and Bonneau et al. (1994)]: We denote by $\mathcal{U}\mathfrak{g}$ the universal enveloping algebra of $\mathfrak{g}$ and by $\mathbb{C}G$ the group algebra of G. All the following inclusions are inclusions of Hopf algebras. $\Subset$, $\ni$, $\Cup$, $\Subset$ mean a dense inclusion,

$$\begin{array}{ccccccc} \mathcal{U}\mathfrak{g} & \Subset & \mathcal{A}(G) & \underset{\ni}{\overset{(*)}{}} & \mathbb{C}G & & \mathcal{H}(G) \\ & & \Cup(*) & & & & \Subset(*) \\ \mathcal{U}\mathfrak{g} & \subset & \mathcal{D}(G) & \ni & \mathbb{C}G & & \mathcal{C}^{\infty}(G) \end{array}$$

(*) *is true if and only if G is linear (i.e., with a faithful finite dimensional representation).*

C. Topological quantum groups

We shall now deform the preceding topological Hopf algebras and indicate how this explains various models of quantum groups. For clarity of the exposition, throughout this section and the remainder of the paper, we shall limit to a minimum the details concerning the Hopf algebra structures other than product and coproduct. But whenever we write Hopf algebras and not only bialgebras, the relevant structures are included in the discussion and dealing with them is quite straightforward. Note that the results which pertain only to the formal aspect of the theory were already mentioned in Sec. IV A.

1. Topological quantization

If $\mathcal{U}_\nu\mathfrak{g}$ is a deformation of $\mathcal{U}\mathfrak{g}$, then an isomorphism (it is not unique!) $\varphi:\mathcal{U}_\nu\mathfrak{g}\to\mathcal{U}\mathfrak{g}[[\nu]]$ guaranteed to exist by Theorem IV.1 will be called a *Drinfel'd isomorphism*.

Theorem IV.2 [Bonneau *et al.* (1994) and Bidegain and Pinczon (1996)]: *Let G be a connected semisimple Lie group and $\mathfrak{g}$ be its complexified Lie algebra.*

(1) *If $\mathcal{U}_\nu\mathfrak{g}$ is a deformation of $\mathcal{U}\mathfrak{g}$ (a "quantum group") then there exists $F\in(\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]$ such that $(\mathcal{U}_\nu\mathfrak{g},\mu_\nu,\Delta_\nu)\simeq(\mathcal{U}\mathfrak{g}[[\nu]],\mu_0,F\Delta_0F^{-1})$.*

(2) *$\mathcal{A}_\nu(G):=(\mathcal{A}(G)[[\nu]],\mu_0,F\cdot\Delta_0\cdot F^{-1})$ is a Hopf deformation of $\mathcal{A}(G)$ and $\mathcal{U}_\nu\mathfrak{g}\overset{\text{Hopf}}{\subset}\mathcal{A}_\nu(G)$.*

(3) *$\mathcal{D}_\nu(G):=(\mathcal{D}(G)[[t]],\mu_0,F\cdot\Delta_0\cdot F_\nu^{-1})$ is a Hopf deformation of $\mathcal{D}(G)$ and $\mathcal{U}_\nu\mathfrak{g}\overset{\text{Hopf}}{\subset}\mathcal{D}_\nu(G)$.*

(4) *$\mathcal{C}^{\infty}_\nu(G):=\mathcal{D}_\nu(G)^{*}$ and $\mathcal{H}_\nu(G):=\mathcal{A}_\nu(G)^{*}$ are quantized algebras of functions. They are Hopf deformations of $\mathcal{C}^{\infty}(G)$ and $\mathcal{H}(G)$.*

Similar results hold for other WB Hopf algebras (e.g., constructed with infinite dimensional representations) [Bidegain (1996)].

Proof: Linear case: Item (1) is a direct consequence of Theorem IV.1. To prove item (2), observe that $F\in(\mathcal{U}\mathfrak{g}\otimes\mathcal{U}\mathfrak{g})[[\nu]]\subset(\mathcal{A}(G)\hat{\otimes}\mathcal{A}(G))[[\nu]]$ and coassociativity follows from the dense inclusion $\mathcal{U}\mathfrak{g}\Subset\mathcal{A}(G)$. Item (3) it true by restriction of (2), and item (4) holds by simple dualization from (2) and (3).

Nonlinear case: Here, as $\mathcal{D}(G)\not\subset\mathcal{A}(G)$ we have to treat $\mathcal{D}(G)$ and $\mathcal{A}(G)$ separately.

(a) Since we can prove [see Bidegain and Pinczon (1996)] that "there exists a compact connected Lie group K such that $\mathcal{H}(G)=\mathcal{H}(K)$," we have $\mathcal{A}(G)=\mathcal{A}(K)$ and we can apply the linear case.

(b) To treat $\mathcal{D}(G)$ we use the density of $\mathbb{C}G$ in $\mathcal{D}(G)$ and go from $\mathcal{U}\mathfrak{g}$ to $\mathbb{C}G$ by exponentiating [Bidegain and Pinczon (1996)]. ■

Remark IV.2: "Hidden group structure" in a quantum group. All the deformations constructed here are *preferred*, that is, the product on $\mathcal{D}_\nu(G)$ and on $\mathcal{A}_\nu(G)$ [resp. the coproduct on $\mathcal{C}^{\infty}_\nu(G)$ and

on $\mathcal{H}_\nu(G)$] is not deformed and the basic structure is still the product on the group G. So this approach gives an interpretation of the Tannaka–Krein philosophy in the case of quantum groups: it has often been noticed that, in the generic case, finite dimensional representations of a quantum group are (essentially) representations of its classical limit. So the algebras involved should be the same, which is justified by the above mentioned rigidity result of Drinfel'd. This shows that the initial classical group is still there, acting as a kind of "hidden variables" in this quantum group theory, which is exactly what we see in this quantum group theory. This fact was implicit in Drinfel'd's work. The Tannaka–Krein interpretation of the twisting of quasi-Hopf algebras can be found in Majid [see, e.g., Majid (1992)]. It was made explicit, within the framework exposed here, in Bonneau *et al.* (1994).

Thus, for any connected Lie group G and for any deformation of the universal enveloping algebra of $\mathfrak{g}=\mathrm{Lie}_{\mathbb{C}}(G)$, we obtain a star product * on $\mathcal{C}^\infty(G)$ and $\mathcal{H}(G)$. For noncompact groups see Bidegain and Pinczon (1995). The next result shows that these deformation quantizations induce other ones on some quotients of G:

Proposition IV.4: Let H be a closed normal subgroup of G.

(1) ** induces a star product on $\mathcal{C}^\infty(G/H)$.*
(2) *If G is linear, * induces a star product on $\mathcal{H}(G/H)$.*

2. Unification of models and generalizations

a. Drinfel'd models: We call "Drinfel'd model of quantum group" a deformation of $\mathcal{U}\mathfrak{g}$ for $\mathfrak{g}$ simple, as given in Drinfel'd (1987)). We have seen in the preceding section that from any Drinfel'd model $\mathcal{U}_\nu\mathfrak{g}$ of a quantum group (which can be generalized to any deformation of the Hopf algebra $\mathcal{U}\mathfrak{g}$), we obtain a deformation of $\mathcal{D}(G)$ and $\mathcal{A}(G)$ that contains $\mathcal{U}_\nu\mathfrak{g}$ as a sub-Hopf algebra. So $\mathcal{D}_\nu(G)$ and $\mathcal{A}_\nu(G)$ are quantum group models that describe Drinfel'd models. By duality, $\mathcal{C}^\infty_\nu(G)$ and $\mathcal{H}_\nu(G)$ are "quantum group deformations" of $\mathcal{C}^\infty(G)$ and $\mathcal{H}(G)$. The deformed product on $\mathcal{H}(G)$ is the restriction of that on $\mathcal{C}^\infty(G)$. Furthermore, as we shall see, these deformations coincide with the usual "quantum algebras of functions." Let us look more in detail at $\mathcal{H}_\nu(G)$:

b. Faddeev–Reshetikhin–Takhtajan (FRT) models: In Faddeev *et al.* (1988) quantized algebras of functions are defined in terms of generators and relations, the key relation being given by the star-triangle (Yang–Baxter) equation, $R(T\otimes \mathtt{Id})(\mathtt{Id}\otimes T)=(\mathtt{Id}\otimes T)(T\otimes \mathtt{Id})R$, for a given R-matrix $R\in \mathtt{End}(V\otimes V)$ and for $T\in \mathtt{End}(V)$, V being a finite dimensional vector space.

As our deformations are given by a twist F, it is not surprising, from a structural point of view [Majid (1992)] that, dually, we obtain in each case a Yang–Baxter relation and so a "FRT-type" quantized algebra of functions. Our Fréchet-topological context permits us to write precisely such a construction for the infinite-dimensional Hopf algebras involved.

c. Linear case: If G is semisimple and linear, there exists π a finite dimensional representation of G such that $\mathcal{H}(G)\simeq\mathbb{C}[\pi_{ij};1\leqslant i,j\leqslant N]$ where the π_{ij} are the coefficient functions of π. Denote by $(\mathcal{H}_\nu(G),*)$ the deformation of $\mathcal{H}(G)$ obtained in this way and by T the matrix $[\pi_{ij}]$. Define $T_1:=T\otimes Id$ and $T_2:=Id\otimes T$. Then we have

Proposition IV.5 [Bonneau et al. (1994) and Bidegain and Pinczon (1996)]:

(1) *$\{\pi_{ij};1\leqslant i,j\leqslant N\}$ is a topological generator system of the $\mathbb{C}[[\nu]]$-algebra $\mathcal{H}(G)_\nu$.*
(2) *There exists an invertible $\mathcal{R}\in\mathcal{L}(V_\pi\otimes V_\pi)[[t]]$ such that $\mathcal{R}\cdot T_1 * T_2 = T_2 * T_1\cdot\mathcal{R}$ (so $\mathcal{H}_\nu(G)$ is a "quantum algebra of functions" of type FRT).*
(3) *We recover every quantum group given in [FRT] by this construction.*

Sketch of proof:

(1) Perform a precise study of the deformed tensor product of representations.
(2) Since the deformations $\mathcal{A}_\nu(G)$ are given by a twist F, $\mathcal{A}_\nu(G)$ is quasicocommutative, i.e., there exists $R\in(\mathcal{A}(G)\hat{\otimes}\mathcal{A}(G))[[\nu]]$ such that $\sigma\circ\Delta_\nu(a)=R\Delta_F(a)R^{-1}$ with $\sigma(a\otimes b)=b\otimes a$. Standard computations give the result.

(3) We want to follow the ideas used in Drinfel'd (1987) to link Drinfel'd to FRT models. Since the main point here is that our deformations are obtained through a Drinfel'd isomorphism, we therefore have to show:

(a) There exists a specific Drinfel'd isomorphism deforming the standard representation of $\mathfrak{g}$ into the representation of $\mathcal{U}_\nu\mathfrak{g}$ used in Drinfel'd (1987).
(b) Two Drinfel'd isomorphisms give equivalent deformations. ■

For instance, the FRT quantization of SL(n) can be seen as a Hopf deformation of $\mathcal{H}(\mathrm{SU}(n))$ (with nondeformed coproduct). Moreover, this Hopf deformation extends to $\mathcal{C}^\infty(G)$.

Remark IV.3:

(1) This proposition justifies the terminology "deformation," often employed but never justified in these cases. See, e.g., Gerstenhaber *et al.* (1990), where it is shown that relations of type $\mathcal{R}T_1T_2=T_2T_1\mathcal{R}$ need not define a deformation, even if $\mathcal{R}$ is Yang–Baxter.
(2) Starting from Drinfel'd models, our construction produces FRT models also, e.g., $G=\mathrm{Spin}(n)$ and for exceptional Lie groups. In addition, at least some multiparameter deformations [Reshetikhin (1990)] can be easily treated in this way [Bonneau *et al.* (1994)].

d. Nonlinear case:

Proposition IV.6 [Bidegain and Pinczon (1996)]: If G is semisimple with finite center, there exists a dense subalgebra of $(\mathcal{C}^\infty_\nu(G),*)$ *generated by the coefficient functions of a finite number of (possibly infinite dimensional) representations.*

e. Jimbo-type models: The Jimbo models [Jimbo (1985)] have generators $E_i^\pm$, K_i, and K_i^{-1}. As stated earlier (Sec. IV B 1) these are not deformations in our sense due to the presence of parities.

The $G=\mathrm{SU}(2)$ case was developed in Sec. IV B 1. Similarly, for $G=\mathrm{SL}(2,\mathbb{C})$, Martin and Zouagui (1996) realize $\mathcal{U}_\nu\mathfrak{sl}(2,\mathbb{C})$ as a dense sub-Hopf algebra of $\mathcal{A}(G)$, $\forall t\in\mathbb{C}\backslash 2\pi\mathbb{Q}$ (with $q=\hat{e}^\nu$). Then, for the Lorentz algebra $\mathfrak{sl}(2,\mathbb{C})$, this unifies [Martin and Zouagui (1996)] all the models proposed so far in the literature for a quantum Lorentz group. We obtain here *convergent* deformations as in the above example of the SU(2) case.

For $\mathfrak{sl}(2,\mathbb{C})$, it was first proposed in Podleś and Woronowicz (1990) to consider the quantum double [Drinfel'd (1987)] of $\mathcal{U}_q\,\mathfrak{su}(2)$ as the q-deformed Lorentz group. It was known from Reshetikhin and Semenov-Tian-Shansky (1989) that in such cases the double, as an algebra, is the tensor product of two copies of $\mathcal{U}_\nu\mathfrak{su}(2)$. See also Ogievetsky *et al.* (1991), Schmidke *et al.* (1991), and Majid (1993) for a dual version and another semidirect product form.

f. Deformation quantization: From the main construction, using deformations of $\mathcal{U}\mathfrak{g}$, we deduce the following general theorem:

Theorem IV.3 [Bidegain and Pinczon (1996)]: *Let G be a semisimple connected Lie group with a Poisson–Lie structure. There exists a deformation* $(\mathcal{C}^\infty_\nu(G),*)$ *of* $\mathcal{C}^\infty(G)$ *such that * is a (differential) star product.*

Remark IV.4: Techniques similar to those indicated here can be applied to other q-algebras [more general quantum groups such as those in Frønsdal (1997) and more recent examples, Yangians, etc.]. In particular those used in the case of the Jimbo models should be applicable to q-algebras defined by generators and relations. That direction of research has not yet been developed.

Since from any Drinfel'd quantum group we obtain a star product, and since any FRT quantum group can be seen as a restriction of such a star product, we have showed that the data of a "semisimple" quantum group is equivalent to the data of a star product on $\mathcal{C}^\infty(G)$ satisfying $\Delta(f*g)=\Delta(f)*\Delta(g)$.

Actually the functorial existence results of Etingof and Kazhdan (1996) on the quantization of Lie bialgebras [see also Enriquez (2002)] show that the latter is true also for "nonsemisimple" quantum groups.

In our framework, we obtained a result in this direction about preferred deformations:

Theorem IV.4 [Bidegain and Pinczon (1996)]: *Let G be a simply connected Poisson–Lie group such that its associated Lie bialgebra has a preferred quantization. Then there exists a*

deformation $(\mathcal{C}^\infty_\nu(G),*)$ *of* $\mathcal{C}^\infty(G)$ *such that* * *is a (differential) star product.*

This can be applied, for example, when Lie (G) is the double of some Lie algebra, since there exists a preferred quantization [Etingof and Kazhdan (1996)].

It is important to remark that the proof of this theorem does not use the preceding construction. The main argument is an integrability result concerning formal deformations [Lesimple and Pinczon (1993)].

V. TOWARDS EXPLICIT REALIZATIONS. I

A. Star exponentials and star representations

Let G be a Lie group (connected and simply connected), acting by symplectomorphisms on a symplectic manifold X (e.g., coadjoint orbits in the dual of the Lie algebra $\mathfrak{g}$ of G). The elements $x,y\in\mathfrak{g}$ will be supposed to be realized by functions u_x,u_y in $\mathcal{C}^\infty(X)$ so that their Lie bracket $[x,y]_\mathfrak{g}$ is realized by $\{u_x,u_y\}$.

We define $(g.u.)(\xi)=u(g^{-1}\cdot\xi)$ the induced action of G on $\mathcal{C}^\infty(X)$. A very natural problem is the existence of a star product * on $\mathcal{C}^\infty(X)$ such that $g.u.*g.v.=g.(u*v),\forall u,v\in\mathcal{C}^\infty(X),\forall g\in G$, that is, a G-invariant star product. Explicit examples of such star products will be given later (on some symmetric spaces). But in general, even for a nilpotent G acting on a coadjoint orbit, an invariant star product does not always exists.

This leads to consider a weaker condition: we say that * is *covariant* if there exists a deformation τ of $.(\tau_g(u)=g\cdot u+\nu\cdots)$ such that * is invariant under τ. It can be shown [Arnal and Cortet (1985)] that is equivalent to ask that $\{u_x,u_y\}=[u_x,u_y]\equiv(u*v-v*u)/2\nu$.

Now take a G-covariant star-product *, then the map $\mathfrak{g}\ni x\mapsto(2\nu)^{-1}u_x\in\mathcal{C}^\infty(X)$ is a Lie algebra morphism. The appearance of ν^{-1} here and in the trace (see 2.2.1) cannot be avoided and explains why we have often to take into account both ν and ν^{-1}. We can now define the *star exponential*

$$E(e^x)=\exp(x)\equiv\sum_{n=0}^{\infty}(n)^{-1}(u_x/2\nu)^{*n},\tag{13}$$

where $x\in\mathfrak{g}$, $e^x\in G$ and the power $*n$ denotes the nth star-power of the corresponding function. By the Campbell–Hausdorff formula one can extend E to *a group homomorphism* $E:G\to(\mathcal{C}^\infty(X)\times[[\nu,\nu^{-1}]],*)$ where, in the formal series, ν and ν^{-1} are treated as independent parameters for the time being. Alternatively, the values of E can be taken in the algebra $(\mathcal{P}[[\nu^{-1}]],*)$, where $\mathcal{P}$ is the algebra generated by $\mathfrak{g}$ with the *-product (it is a representation of the enveloping algebra).

A star representation [Bayen *et al.* (1978)] of G is a distribution $\mathcal{E}$ (valued in Im E) on X defined by

$$D\ni f\mapsto\mathcal{E}(f)=\int_G f(g)E(g^{-1})dg,$$

where D is some space of test-functions on G. The corresponding *character* χ is the (scalar-valued) distribution defined by $D\ni f\mapsto\chi(f)=\int_X\mathcal{E}(f)d\mu$, $d\mu$ being a quasi-invariant measure on X.

The character is one of the tools which permit a comparison with usual representation theory. For semisimple groups it is singular at the origin in irreducible representations, which may require caution in computing the star exponential (13). In the case of the harmonic oscillator that difficulty was masked by the fact that the corresponding representation of $\mathfrak{sl}(2)$ generated by (p^2,q^2,pq) is integrable to a double covering of $\mathrm{SL}(2,\mathbb{R})$ and decomposes into a sum $D(\frac{1}{4})\oplus D(\frac{3}{4})$: the singularities at the origin cancel each other for the two components.

This theory is now very developed, and parallels in many ways the usual (operatorial) representation theory. A detailed account of all the results would take us too far, but among the most notable one may quote:

(i) An exhaustive treatment of *nilpotent* or *solvable exponential* [Arnal and Cortet (1985)] and

even general solvable Lie groups [Arnal *et al.* (1995) and Arnal and Cortet (1990)]. The coadjoint orbits are there symplectomorphic to $\mathbb{R}^{2\ell}$ and one can lift the Moyal product to the orbits in a way that is adapted to the Plancherel formula. Polarizations are not required, and "star-polarizations" can always be introduced to compare with usual theory. Wavelets, important in signal analysis, are manifestations of star-products on the (two-dimensional solvable) affine group of $\mathbb{R}$ or on a similar three-dimensional solvable group [Bertrand and Bertrand (1998)].

(ii) For *semisimple* Lie groups an array of results exists. Some explicit and autonomous formulas for star exponentials [Frønsdal (1979)] are available. In [Arnal *et al.* (1988) and Moreno (1986)] a complete treatment of the *holomorphic discrete series* (this includes the case of compact Lie groups) was made, using a kind of Berezin dequantization. Similar techniques have also been used [Cahen *et al.* (1995) and Karabegov (1998)] to find invariant star-products on Kähler and Hermitian symmetric spaces (convergent for an appropriate dense subalgebra). Note however, as shown by recent developments of unitary representations theory [see, e.g., Schmid (1997)], that for semisimple groups the coadjoint orbits alone are no more sufficient for the unitary dual and one needs far more elaborate constructions.

(iii) For semidirect products, and in particular for the Poincaré and Euclidean groups, an autonomous theory has also been developed [see, e.g., Arnal *et al.* (1980)].

Comparison with the usual results of "operatorial" theory of Lie group representations can be performed in several ways, in particular by constructing an invariant Weyl transform generalizing (4), finding "star-polarizations" that always exist, in contradistinction with the geometric quantization approach (where at best one can find complex polarizations), study of spectra (of elements in the center of the enveloping algebra and of compact generators) in the sense of (2.2.3.1), comparison of characters, etc. Note also in this context that the pseudodifferential analysis and (non autonomous) connection with quantization developed extensively by Unterberger, first in the case of $\mathbb{R}^{2\ell}$, has been extended to the above invariant context [Unterberger (1984) and Unterberger and Upmeier (1994)]. But our main insistence is that the theory of star representations is an *autonomous* one that can be formulated completely within this framework, based on coadjoint orbits (and some additional ingredients when required).

B. Universal deformation formulas

For an endomorphism ϕ of an algebra A, write a^{ϕ} for the right action of ϕ on $a \in A$. It was noticed early in deformation theory [see Gerstenhaber (1968)] that if ϕ and ψ are commuting derivations of A, then the product

$$a * b = ab + \nu a^{\phi} b^{\psi} + \frac{\nu^2}{2} a^{\phi^2} b^{\psi^2} + \cdots + \frac{\nu^n}{n!} a^{\phi^n} b^{\psi^n} + \cdots$$

defines an associative multiplication. This deformation can simply be written as

$$a * b = \mu_0((a \otimes b)^{\exp\ \nu(\phi \otimes \psi)})$$

and can be generalized to any sum of commuting derivations. The Moyal product can be realized in this fashion: take $A = \mathcal{C}^{\infty}(\mathbb{R}^{2n})$ and $\Sigma_{i<j} \partial_{x_i} \wedge \partial_{x_j}$ as the infinitesimal.

The first explicit deformation formula involving noncommuting derivations appeared in Coll *et al.* (1989). Suppose that ϕ and ψ are derivations satisfying $[\phi, \psi] = \psi$, and let $\phi^{(n)} = \phi(\phi + 1) \cdots (\phi + n - 1)$. Then,

$$a * b = ab + \nu a^{\phi} b^{\psi} + \frac{\nu^2}{2} a^{\phi^{(2)}} b^{\psi^2} + \cdots + \frac{\nu^n}{n!} a^{\phi^{(n)}} b^{\psi^n} + \cdots \tag{14}$$

is associative. As an exponential, this deformation may be written as

$$a * b = \mu_0((a \otimes b)^{\exp(\phi \otimes \ln(1+\nu\psi))}).$$

As we will see, it is this formula that produces the "Jordanian" quantization of $\mathcal{C}^\infty(\mathrm{SL}_2)$. Related *-products are given in Bieliavsky and Maeda (2002).

These are examples of *universal deformation formulas*, a construction of formal deformations inspired by Drinfel'd's twisting concept of introduced in Drinfel'd (1989a, 1989b). The basic idea is that one has a deformation solely based upon information about the Lie algebra of derivations, and the formula is independent of the actual algebra in question. Such constructions are examples of a mutual feedback between Hopf algebraic techniques in quantum groups and deformation quantization. The following subsections provide further examples.

Definition V.1: An element $F \in B \otimes B$ is a twisting element (based on a bialgebra B with comultiplication Δ_B and counit ε_B) if

(1) $(\varepsilon_B \otimes \mathrm{Id})F = 1 \otimes 1 = (\mathrm{Id} \otimes \varepsilon_B)F$, *and*
(2) $F_{12}[(\Delta_B \otimes \mathrm{Id})(F)] = F_{23}[(\mathrm{Id} \otimes \Delta_B)(F)]$.

The virtue of having such an F is that it can be used to twist the entire category of right B-module algebras and left B-module coalgebras in a uniform way. The following result from Giaquinto and Zhang (1998) is based on the fundamental ideas from Drinfel'd (1989b).

Theorem V.1: *Let $F \in B \otimes B$ be a twisting element:*

(1) *If A is a right B-module algebra, then $A_F = A(\mu_A \circ F_r, 1_A)$ is an associative algebra*;
(2) *If C is a left B-module coalgebra, then $C_F = C(F_l \circ \Delta_C, \varepsilon_C)$ is a coassociative coalgebra*;
(3) *If F is invertible and $\Delta'_B = F_l \circ F_r^{-1} \circ \Delta_B$, then $B_F = B(\mu_B, \Delta'_B, 1_B, \varepsilon_B)$ is a k-bialgebra*;
(4) *If F is invertible A is a right B-module algebra, then A_F is a right B_F-module algebra*;
(5) *If F is invertible and C is a left B-module coalgebra, then C_F is a left B_F-module coalgebra.*

The connection between twisting elements and deformations is the following:

Definition V.2: A universal deformation formula (UDF) based on a bialgebra B is a twisting element F based on $B[[\nu]]$ of the form

$$F = 1 \otimes 1 + \nu F_1 + \nu^2 F_2 + \cdots + \nu^n F_n + \cdots,$$

where each $F_i \in B \otimes B$.

If F is a UDF then it is clear that A_F, C_F, and B_F as constructed in the theorems above are all deformations. It is clear that the twisting elements defined after Theorem (IV.1) are UDFs with $B = \mathcal{U}\mathfrak{g}[[\nu]]$.

Example V.1:

(1) *The most basic UDF is based on the bialgebra $B = \mathcal{U}\mathfrak{a}$ where $\mathfrak{a}$ is an Abelian Lie algebra. The UDF is the classic exponential formula $F = \exp \nu b$, where $b \in \mathfrak{a} \otimes \mathfrak{a}$ is arbitrarily chosen. An example of a deformation arising from this UDF arise is the Moyal deformation of $\mathcal{C}^\infty(\mathbb{R}^{2n})$. Another example is the deformation of the standard quantum group $\mathcal{C}_q^\infty(SL(n))$ to the multi-parameter family first introduced in Reshetikhin (1990).*
(2) *$\mathfrak{s}$ is the two-dimensional solvable Lie algebra with basis $\{\phi, \psi\}$ and relation $[\phi, \psi] = \psi$, and set $B = \mathcal{U}\mathfrak{s}$. Then $F = \exp(\phi \otimes \ln(1 + \nu\psi))$ is a UDF.*
(3) *Other specific examples of UDF's, including ones not based on enveloping algebras, can be found in Bieliavsky et al. (2003), Caldararu et al. (2004), Connes and Moscovici (2004), Kulish et al. (1999), Lyakhovsky and Samsonov (2002), Giaquinto and Zhang (1998).*

Note that, according to Theorems (IV.1) and (V.1), a UDF based on $\mathcal{U}\mathfrak{g}$ produces a preferred deformation $\mathcal{U}\mathfrak{g}$ and matching "covariant" deformations of $\mathcal{C}^\infty(M)$ for every manifold which admits an action of the Lie group G. We shall discuss this topic in more detail later on.

C. Crossed products

The literature on Hopf algebras and quantum groups contains a large collection of what we can call generically semidirect products, or crossed products. These constructions make crucial use of the comultiplication and we will use the standard Sweedler notation for the coproducts [Sweedler (1969)]: in a coalgebra (H,Δ), $\Delta(x)=\Sigma_{(x)}x_{(1)}\otimes x_{(2)}$ and, by coassociativity, $(\mathrm{Id}\otimes\Delta)\Delta(x)=(\Delta\otimes\mathrm{Id})\Delta(x)=\Sigma_{(x)}x_{(1)}\otimes x_{(2)}\otimes x_{(3)}$. See also Abe (1980) for generalities on Hopf algebras.

Considering crossed products gives explicit, concise and workable formulas. The properties of these structures, as well as for semidirect products of groups or Lie algebras, may be deduced from the ones of the two original structures. So we can hope to obtain interesting results on, for example, cohomology or representation theories.

We will investigate two original examples: the topological quantum double and the deformation quantizations of some symmetric spaces.

But first, let us give a general idea of what it is. The simplest example of these crossed products is usually called the smash product [see Sweedler (1968) and Molnar (1977)].

Definition V.3: Let B be a bialgebra and C a B-module algebra. The smash product $C\sharp B$ is the algebra constructed on the vector space $C\otimes B$ where the multiplication is defined by

$$(f\otimes a)\overset{\rightharpoonup}{*}(g\otimes b)=\sum_{(a)}f(a_{(1)}\rightharpoonup g)\otimes a_{(2)}b \tag{15}$$

for $f,g\in C$ and $a,b\in B$.

Remark V.1:

(1) (a) Let H and K be groups and let $\tau:K\to\mathrm{Aut}(H)$ be an action of K on H. This induces a $\mathbb{C}K$-module algebra structure on $\mathbb{C}H$. Then $\mathbb{C}H\sharp\mathbb{C}K\cong\mathbb{C}(H\rtimes K)$, $H\rtimes K$ denoting the semidirect product of H by K.
(b) Similarly, for Lie algebras $\mathfrak{h}$ and $\mathfrak{k}$, a Lie algebra homomorphism $\sigma:\mathfrak{k}\to\mathrm{Der}(\mathfrak{h})$ induces a $\mathcal{U}\mathfrak{k}$-module algebra structure on $\mathcal{U}\mathfrak{h}$. Then $\mathcal{U}\mathfrak{h}\sharp\mathcal{U}\mathfrak{k}\cong\mathcal{U}(\mathfrak{h}\rtimes\mathfrak{k})$.

(2) The smash product can be seen as the algebraic version of what is called "crossed product" in the C^*-algebra literature [Drabant *et al.* (1999) and Pedersen (1979)]. Note that this is an important structure in this context, extensively used, for example, in the works around the Baum-Connes conjecture.

Now let us describe some generalizations:

This product can be seen in the cohomological interpretation of Sweedler (1968) as a representative of the trivial class of a theory of extensions. The formula of the smash product can be "twisted" a little more by some 2-cocycle from $B\otimes B$ to C and is called a crossed product.

If B and C are bialgebras, C a B-module algebra and B a C-module algebra, with some compatibilities between the two actions, one can write some kind of more "symmetric" formula. Majid has called double crossproduct the resulting algebra [Majid (1990)]. This definition leads to a good description of the structure of quantum double introduced by Drinfel'd in 1987 (see below for details).

If C is a bialgebra and B is cocommutative, the natural tensor coproduct on $C\otimes B$ yields a bialgebra structure on $C\sharp B$. If everything is Hopf, $C\sharp B$ can be made Hopf as well [Molnar (1977)].

By dualizing Definition V.3, one gets a coalgebra called the cosmash product. Combining smash and cosmash in order to form a bialgebra leads to the notion of bicrossproduct [Majid (1990)].

Before introducing a new and useful generalization of this kind of definitions let us go back to an application of the double crossproduct to the notion of quantum double in the context of topological Hopf algebras.

1. Topological quantum double

Drinfel'd (1987) defined the quantum double of $\mathcal{U}_\nu\mathfrak{g}$ [see also Semenov-Tian-Shansky (1994)]. This can be adapted to the context of topological Hopf algebras [Bonneau (1994)].

For this subsection A will denote $\mathcal{D}(G), \mathcal{A}(G), \mathcal{D}_\nu(G)$, or $\mathcal{A}_\nu(G)$.

Definitions: If A is described by (A, μ, Δ, S) then $A^* = (A^*, {}^t\Delta, {}^t\mu, {}^tS)$. Define $A^0 = A^{*co-op} = (A^*, {}^t\Delta, {}^t\mu^{op}, {}^tS^{op})$, where $\mu^{op}(x \otimes y) := \mu(y \otimes x)$ and S^{op} is the antipode compatible with μ^{op} and Δ.

If we consider the vector space $A^* \otimes A$, Drinfel'd (1987) defines the quantum double as follows:

(i) $D(A) \simeq A^0 \otimes A$ as coalgebras,
(ii) $(f \otimes Id_A) \cdot (Id_{A^0} \otimes b) = f \otimes b$,
(iii) $(Id_{A^0} \otimes e_s) \cdot (e^t \otimes Id_A) = \Delta_s^{kjn} \mu_{plk}^t S'^p_n (e^l \otimes Id_A)(Id_{A^0} \otimes e_j)$, where $\{e_s\}$ is a basis of A and $\{e^t\}$ the dual basis.

The Drinfel'd double was expressed [Majid (1990)] in a Sweedler form for dually paired Hopf algebras as an example of a theory of 'double smash products.' Adapting that formulation to our topological context we can now define the double as

Definition V.4: The double of A, D(A), is the topological Hopf algebra $(A^* \overline{\otimes} A, \mu_D, {}^t\mu^{op} \otimes \Delta, {}^tS^{op} \otimes S)$ *with*

$$\mu_D((f \otimes a) \otimes (g \otimes b)) = \sum_{(a)} f\langle g, S^{op}(a_{(3)}) \,?\, a_{(1)}\rangle \otimes a_{(2)}b$$

$$= \sum_{(a)(g)} \langle g_{(1)}, a_{(1)}\rangle \langle {}^tS^{op}(g_{(3)}), a_{(3)}\rangle f g_{(2)} \otimes a_{(2)}b,$$

where $\langle , \rangle$ *denotes the pairing* A^*/A, *"?" stands for a variable in A and* $\overline{\otimes}$ *is the completed inductive tensor product.*

As topological vector spaces we have $D(A) = A^* \overline{\otimes} A$. Thus $D(A)^* = A \hat{\otimes} A^*$ and $D(A)^{**} = D(A)$. So $D(A)$ is "almost self-dual" (it is self-dual up to a completion) and is reflexive.

Extension theory:

If A is cocommutative then the product μ_D of $D(A)$ is the smash product $\overline{\mu}^{\rightharpoonup}$ on $A^0 \overline{\otimes} A$

$$\overline{\mu}^{\rightharpoonup}((f \otimes a) \otimes (g \otimes b)) = \sum_{(a)} f(a_{(1)} \rightharpoonup g) \otimes a_{(2)}b$$

where $\rightharpoonup$ denotes the coadjoint action of A on A^0, $\langle a \rightharpoonup f, b\rangle = \Sigma_{(a)} \langle f, S(a_{(1)}) b a_{(2)}\rangle$. This product is the "zero class" of an extension theory, defined by Sweedler (1968), classified by a space of 2-cohomology $H^2_{sw}(A, A^0)$. The products are of the form, for τ a 2-cocycle,

$$\overline{\mu}^{\rightharpoonup}_\tau((f \otimes a) \otimes (g \otimes b)) = \sum_{(a)(b)} f(a_{(1)} \rightharpoonup g) \tau(a_{(2)} \otimes b_{(2)}) \otimes a_{(3)}b_{(2)}.$$

The coproduct of $D(A)$ is a smash coproduct for the trivial co-action. We can dualize the theory and, putting the two things together, we obtain an extension theory for bialgebras which is classified by a cohomology space $H^2_{\text{bisw}}(A^0, A)$.

So we can ask the following question: are there other possible definitions of the double as an extension of A^0 by A?

We get a partial answer:

Proposition V.1 [Bonneau (1994)]: $H^2_{\text{bisw}}(\mathcal{D}(G), \mathcal{C}^\infty(G)) = \{0\}$ *so* $D(\mathcal{D}(G))$ *is the unique extension of* $\mathcal{C}^\infty(G)$ *by* $\mathcal{D}(G)$.

2. L-R smash product

In order to shed light on the general definition which follows, we return to the simplest case of deformation quantization: the Moyal product on $\mathbb{R}^2$. We look at $\mathbb{R}^2$ as $T^*\mathbb{R} \equiv \mathbb{R} \times \mathbb{R}^*$ and therefore can write $\mathcal{C}^\infty(\mathbb{R}^2) \simeq \mathcal{C}^\infty(\mathbb{R}) \hat{\otimes} \mathcal{C}^\infty(\mathbb{R}^*)$. We consider first two functions of a special kind in this algebra: $u(x) = u(x_1, x_2) = f(x_1)P(x_2)$ and $v(x) = v(x_1, x_2) = g(x_1)Q(x_2)$ where $f, g \in \mathcal{C}_0^\infty(\mathbb{R})$ and P, Q are polynomials in $\mathsf{Pol}(\mathbb{R}^*) \simeq \mathsf{S}\mathbb{R}$. We can then write the usual coproduct on the symmetric algebra $\mathsf{S}\mathbb{R}$ as $\Delta(P)(x_2, y_2) = P(x_2 + y_2) \overset{\text{notation}}{=} \Sigma_{(P)} P_{(1)}(x_2) P_{(2)}(y_2))$.

We now look at formula (8) for the Moyal star product on $\mathbb{R}^2$ and perform on it some formal calculations (we do not discuss the convergence of the integrals involved). Up to a constant (depending on ν) we get

$$
\begin{aligned}
(u * v)(x) &= \int_{\mathbb{R}^2 \times \mathbb{R}^2} u(x+y) v(x+z) e^{-(i/\nu)\Lambda^{-1}(y,z)} dy dz \\
&= \int_{\mathbb{R}^2 \times \mathbb{R}^2} f(x_1 + y_1) P(x_2 + y_2) g(x_1 + z_1) Q(x_2 + z_2) e^{-(i/\nu)(y_1 z_2 - y_2 z_1)} dy_1 dy_2 dz_1 dz_2 \\
&= \int_{\mathbb{R}^2} f(x_1 + y_1) Q(x_2 + z_2) e^{-(i/\nu) y_1 z_2} dy_1 dz_2 \cdot \int_{\mathbb{R}^2} g(x_1 + z_1) P(x_2 + y_2) e^{(i/\nu) y_2 z_1} dy_2 dz_1 \\
&= \sum_{(P)(Q)} (\partial^+_{Q_{(1)}} f)(x_1) Q_{(2)}(x_2) \cdot (\partial^-_{P_{(1)}} g)(x_1) P_{(2)}(x_2) \quad \text{(up to a constant)}
\end{aligned}
$$

with $\partial^\pm_{Q_{(1)}} = Q_{(1)}(\mp i\nu \partial_{x_1})$ (the same for P), since $F^\mp_\nu(\alpha F^\pm_\nu(h)(\alpha))(x) = \mp i\nu \partial_x h(x)$ for $h \in \mathcal{C}_0^\infty(\mathbb{R})$ with $F^\pm_\nu(h)(\alpha)$ defined as $\int_{\mathbb{R}} h(x) e^{\mp (i/\nu) x\alpha} dx$. This suggests the following small generalization of the smash product:

Definition V.5: Let B be a cocommutative bialgebra and C a B-bimodule algebra (i.e., a B-module algebra for both, left and right, B-module structures). The **L-R-smash product** *$C \natural B$ is the algebra constructed on the vector space $C \otimes B$ where the multiplication is defined by*

$$
(f \otimes a) * (g \otimes b) = \sum_{(a)(b)} (f \leftharpoonup b_{(1)})(a_{(1)} \rightharpoonup g) \otimes a_{(2)} b_{(2)} \tag{16}
$$

for $f, g \in C$ and $a, b \in B$.

Proposition V.2: The L-R smash product is associative.

In the same spirit, one has

Lemma V.1: If C is a B-bimodule bialgebra, the natural tensor product coalgebra structure on $C \otimes B$ defines a bialgebra structure to $C \natural B$.

If C and B are Hopf algebras, $C \natural B$ is a Hopf algebra as well, defining the antipode by

$$
\begin{aligned}
J_*(f \otimes a) &= \sum_{(a)} J_B(a_{(1)}) \rightharpoonup J_C(f) \leftharpoonup J_B(a_{(2)}) \otimes J_B(a_{(3)}) \\
&= \sum_{(a)} (1_C \otimes J_B(a_{(1)})) * (J_C(f) \otimes 1_B) * (1_C \otimes J_B(a_{(2)})).
\end{aligned} \tag{17}
$$

Now by a careful computation, one proves

Proposition V.3: Let B be a cocommutative bialgebra, C a B-bimodule algebra and $(C \natural B, *)$ their L-R-smash product.

Let S be a linear automorphism of C (as a vector space). We define

(i) *the product $\bullet^S$ on C by*

$$
f \bullet^S g = S^{-1}(S(f) \cdot S(g)); \tag{18}
$$

(ii) *the left and right B-module structures,* $\overset{S}{\rightharpoonup}$ and $\overset{S}{\leftharpoonup}$, by

$$a\overset{S}{\rightharpoonup} f := S^{-1}(a \rightharpoonup S(f)) \quad \text{and} \quad f\overset{S}{\leftharpoonup} a := S^{-1}(S(f) \leftharpoonup a); \tag{19}$$

(iii) *the product,* $*^S$, *on* $C\otimes B$ *by*

$$(f\otimes a)*^S(g\otimes b) = T^{-1}(T(f\otimes a) * T(g\otimes b)), \tag{20}$$

where $T := S\otimes \mathrm{Id}$.

Then $(C, \bullet^S)$ *is a B-bimodule algebra for* $\overset{S}{\rightharpoonup}$ *and* $\overset{S}{\leftharpoonup}$ *and* $*^S$ *is the L-R-smash product defined by these structures.*

Moreover, if $(C, ., \Delta_C, J_C, \rightharpoonup, \leftharpoonup)$ *is a Hopf algebra and a B-bimodule bialgebra, then*

$$C_S := (C, \bullet^S, \Delta_C^S := (S^{-1}\otimes S^{-1})\circ\Delta_C\circ S, J_C^S := S^{-1}\circ J_C\circ S, \overset{S}{\rightharpoonup}, \overset{S}{\leftharpoonup})$$

is also a Hopf algebra and a B-bimodule bialgebra. Therefore, by Lemma V.1,

$$(C_S \sharp B, *^S, \Delta^S = (23)\circ(\Delta_C^S\otimes\Delta_B), J_*^S),$$

is a Hopf algebra for Δ^S *the natural tensor product coalgebra structure on* $C_S \natural B$ (with (23): $C\otimes C\otimes B\otimes B \to C\otimes B\otimes C\otimes B, c_1\otimes c_2\otimes b_1\otimes b_2 \mapsto c_1\otimes b_1\otimes c_2\otimes b_2$) *and* J_*^S *the antipode given on* $C_S \natural B$ *by Lemma V.1. Also, one has*

$$\Delta^S = (T^{-1}\otimes T^{-1})\circ(23)\circ(\Delta_C\otimes\Delta_B)\circ T \quad \textit{and} \quad J_*^S = T^{-1}\circ J_*\circ T$$

with $T = S\otimes \mathrm{Id}$.

3. Examples in deformation quantization on $T^*(G)$

Let G be a Lie group with Lie algebra $\mathfrak{g}$ and $T^*(G)$ its cotangent bundle. We denote by $\mathcal{U}\mathfrak{g}$, $\mathsf{T}\mathfrak{g}$ and $\mathsf{S}\mathfrak{g}$, respectively, the enveloping, tensor, and symmetric algebras of g. Let $\mathsf{Pol}(\mathfrak{g}^*)$ be the algebra of polynomial functions on $\mathfrak{g}^*$. We have the usual identifications:

$$\mathcal{C}^\infty(T^*G) \simeq \mathcal{C}^\infty(G\times\mathfrak{g}^*) \simeq \mathcal{C}^\infty(G)\hat{\otimes}\mathcal{C}^\infty(\mathfrak{g}^*) \supset \mathcal{C}^\infty(G)\otimes\mathsf{Pol}(\mathfrak{g}^*) \simeq \mathcal{C}^\infty(G)\otimes\mathsf{S}\mathfrak{g}.$$

First we deform $\mathsf{S}\mathfrak{g}$ via the "parametrized version," $\mathcal{U}_\nu\mathfrak{g}$, of $\mathcal{U}\mathfrak{g}$ defined by

$$\mathcal{U}_\nu\mathfrak{g} = \frac{\mathsf{T}\mathfrak{g}[[\nu]]}{\langle XY - YX - \nu[X,Y]; X, Y\in\mathfrak{g}\rangle}.$$

$\mathcal{U}_\nu\mathfrak{g}$ is naturally a Hopf algebra with $\Delta(X) = 1\otimes X + X\otimes 1$, $\varepsilon(X) = 0$ and $S(X) = -X$ for $X\in\mathfrak{g}$. For $X\in\mathfrak{g}$, we denote by $\widetilde{X}$ (resp. $\overline{X}$) the left- (resp. right-) invariant vector field on G such that $\widetilde{X}_e = \overline{X}_e = X$. We consider the following $\mathbb{K}[[\nu]]$-bilinear actions of $B = \mathcal{U}_\nu\mathfrak{g}$ on $C = \mathcal{C}^\infty(G)[[\nu]]$, for $f\in C$ and $\lambda\in[0,1]$:

(i) $(X\rightharpoonup f)(x) = \nu(\lambda - 1)(\widetilde{X}\cdot f)(x)$,

(ii) $(f\leftharpoonup X)(x) = \nu\lambda(\overline{X}\cdot f)(x)$.

One then has

Lemma V.2: C is a B-bimodule algebra w.r.t. the above left and right actions (i) and (ii).

Definition V.6: We denote by $*_\lambda$ *the star product on* $(\mathcal{C}^\infty(G)\otimes\mathsf{Pol}(\mathfrak{g}^*))[[\nu]]$ *given by the L-R-smash product on* $\mathcal{C}^\infty(G)[[\nu]]\otimes\mathcal{U}_\nu\mathfrak{g}$ *constructed from the bimodule structure of the preceding lemma.*

Proposition V.4: For $G = \mathbb{R}^n$, $*_{\frac{1}{2}}$ *is the Moyal star product (Weyl ordered),* $*_0$ *is the standard*

ordered star product, and $*_1$ *the antistandard ordered one. In general* $*_\lambda$ *yields the* λ*-ordered quantization, within the notation of M. Pflaum (1999).*

Remark V.2: In the general case, it would be interesting to compare our λ-ordered L-R smash product with classical constructions of star products on $T^*(G)$ with Gutt's product as one example [Gutt (1983)].

4. Hopf structures

We have discussed (see Lemma V.1) the possibility of having a Hopf structure on $C \natural B$. Let us consider the particular case of $\mathcal{C}^\infty(\mathbb{R}^n)[[\nu]] \natural \mathcal{U}_\nu \mathbb{R}^n = \mathcal{C}^\infty(\mathbb{R}^n)[[\nu]] \natural \mathsf{S}\mathbb{R}^n$ ($\mathbb{R}^n$ is commutative). $\mathsf{S}\mathbb{R}^n$ is endowed with its natural Hopf structure but we also need a Hopf structure on $\mathcal{C}^\infty(\mathbb{R}^n) \times[[\nu]] = \mathcal{C}^\infty(\mathbb{R}^n) \otimes \mathbb{R}[[\nu]]$. We will not use the usual one. Our alternative structure is defined as follows:

Definition V.7: We endow $\mathbb{R}[[\nu]]$ *with the usual product, the coproduct* $\Delta(P)(t_1,t_2) := P(t_1 + t_2)$*, the co-unit* $\varepsilon(P) = P(0)$ *and the antipode* $J(\nu) = -\nu$*. We consider the Hopf algebra* $(\mathcal{C}^\infty(\mathbb{R}^n), \cdot, \mathbf{1}, \Delta_C, \varepsilon_C, J_C)$*, with pointwise multiplication, the unit* $\mathbf{1}$ *(the constant function of value* 1*), the coproduct* $\Delta_C(f)(x,y) = f(x+y)$*, the co-unit* $\varepsilon(f) = f(0)$ *and the antipode* $J_C(f)(x) = f(-x)$*. The tensor product of these two Hopf algebras then yields a Hopf algebra denoted by*

$$(\mathcal{C}^\infty(\mathbb{R}^n)[[\nu]], \cdot, \mathbf{1}, \Delta_\nu, \varepsilon_\nu, J_\nu).$$

Note that Δ_ν *and* J_ν *are not linear in* ν*. We then define, on the L-R smash* $\mathcal{C}^\infty(\mathbb{R}^n)[[\nu]] \natural \mathsf{S}\mathbb{R}^n$*,*

$$\Delta_* := (23) \circ (\Delta_\nu \otimes \Delta_B), \varepsilon_* := \varepsilon_\nu \otimes \varepsilon_B \text{ and } J_*$$

as in Lemma V.1.

Proposition V.5: $(\mathcal{C}^\infty(\mathbb{R}^n)[[\nu]] \natural \mathsf{S}\mathbb{R}^n, *_\lambda, \mathbf{1} \otimes 1, \Delta_*, \varepsilon_*, J_*)$ *is a Hopf algebra.*

Remark V.3: The case $\lambda = \frac{1}{2}$ yields the usual Hopf structure on the enveloping algebra of the Heisenberg Lie algebra.

D. UDFs revisited and quantization of symmetric spaces

1. Introduction

The previous discussion of universal deformation formulas was purely formal. However, the ideas can be extended to include geometric considerations, which allows for more flexibility in the applications.

Let G be a group acting on a set M. Denote by $\tau: G \times M \to M: (g,x) \mapsto \tau_g(x)$ the (left) action and by $\alpha: G \times \mathrm{Fun}(M) \to \mathrm{Fun}(M)$ the corresponding action on the space of (complex valued) functions (or formal series) on M ($\alpha_g := \tau^*_{g^{-1}}$). Assume that on a subspace $\mathbb{A} \subset \mathrm{Fun}(G)$, one has an associative $\mathbb{C}$-algebra product $*^G_{\mathbb{A}}: \mathbb{A} \times \mathbb{A} \to \mathbb{A}$ such that

(i) $\mathbb{A}$ is invariant under the (left) regular action of G on $\mathrm{Fun}(G)$;
(ii) the product $*^G_{\mathbb{A}}$ is left-invariant as well, i.e., for all $g \in G; a,b \in \mathbb{A}$, one has

$$(L^*_g a) *^G_{\mathbb{A}} (L^*_g b) = L^*_g (a *^G_{\mathbb{A}} b). \tag{21}$$

(In Hopf algebra language, this means that $(\mathbb{A}, *^G_{\mathbb{A}})$ is a $\mathbb{C}G$-module algebra.)

Given a function on M, $u \in \mathrm{Fun}(M)$, and a point $x \in M$, one denotes by $\alpha^x(u) \in \mathrm{Fun}(G)$ the function on G defined as

$$\alpha^x(u)(g) := \alpha_g(u)(x). \tag{22}$$

Then one readily observes that the subspace $\mathbb{B} \subset \mathrm{Fun}(M)$ defined as

$$\mathbb{B} := \{u \in \mathrm{Fun}(M) \,|\, \forall x \in M: \alpha^x(u) \in \mathbb{A}\} \tag{23}$$

becomes an associative $\mathbb{C}$-algebra when endowed with the product $*^M_{\mathbb{B}}$ given by

$$u *_{\mathbb{B}}^{M} v(x) := (\alpha^x(u) *_{\mathbb{A}}^{G} \alpha^x(v))(e) \tag{24}$$

(e denotes the neutral element of G). Of course, all this can be defined for right actions as well.

Definition V.8: A pair $(\mathbb{A}, *_{\mathbb{A}}^{G})$ *is called a (left) universal deformation of* G*, while formula* (24) *is called the associated* universal deformation formula (*briefly* UDF).

In the present article, we will be concerned with the case where G is a Lie group. The function space $\mathbb{A}$ will be either a functional subspace (or a topological completion) of $\mathcal{C}^\infty(G,\mathbb{C})$ containing the smooth compactly supported functions in which case we will talk about *strict deformation* (following Rieffel (1989); or, the space $\mathbb{A}=\mathcal{C}^\infty(G)[[\nu]]$ of formal power series with coefficients in the smooth functions on G in which case, we will speak about *formal deformation*. In any case, we will assume the product $*_{\mathbb{A}}^{G}$ admits an asymptotic expansion of star-product type:

$$a *_{\mathbb{A}}^{G} b \sim ab + \frac{\nu}{2i}\mathbf{w}(\mathrm{d}u,\mathrm{d}v) + o(\nu^2) \quad (a,b \in \mathcal{C}_c^\infty(G)),$$

where $\mathbf{w}$ denotes some (left-invariant) Poisson bivector on G [Bayen *et al.* (1978) and Drinfel'd (1993)]. In the strict cases considered here, the product will be defined by an integral three-point kernel $K \in \mathcal{C}^\infty(G\times G\times G)$:

$$a *_{\mathbb{A}}^{G} b(g) := \int_{G\times G} a(g_1)b(g_2)K(g,g_1,g_2)\mathrm{d}g_1\mathrm{d}g_2 \quad (a,b \in \mathbb{A}),$$

where dg denotes a normalized left-invariant Haar measure on G. Moreover, our kernels will be of *WKB type* [Weinstein (1994) and Karasev (1994)], i.e.,

$$K = Ae^{(i/\nu)\Phi},$$

with A (the *amplitude*) and Φ (the *phase*) in $\mathcal{C}^\infty(G\times G\times G,\mathbb{R})$ being invariant under the (diagonal) action by left-translations.

Note that in the case where the group G acts smoothly on a smooth manifold M by diffeomorphisms: $\tau: G\times M\to M:(g,x)\mapsto \tau_g(x)$, the first-order expansion term of $u *_{\mathbb{B}}^{M} v$, $u,v \in C^\infty(M)$ defines a Poisson structure $\mathbf{w}^M$ on M which can be expressed in terms of a basis $\{X_i\}$ of the Lie algebra $\mathfrak{g}$ of G as

$$\mathbf{w}^M = [\mathbf{w}_e]^{ij} X_i^* \wedge X_j^*, \tag{25}$$

where X^* denotes the fundamental vector field on M associated to $X \in \mathfrak{g}$.

2. Elementary solvable symplectic symmetric spaces and their strict quantization

a. Symmetric spaces: Definition V.9 [Bieliavsky (1995)]: A symplectic symmetric space is *a triple* (M,ω,s)*, where* (M,ω) *is a smooth connected symplectic manifold and* $s: M\times M\to M$ *is a smooth map such that*

(i) *For all* x *in* M*, the partial map* $s_x: M\to M: y\mapsto s_x(y) := s(x,y)$ *is an involutive symplectic diffeomorphism of* (M,ω) *called the* symmetry *at* x;
(ii) *For all* x *in* M*,* x *is an isolated fixed point of* s_x;
(iii) *For all* x *and* y *in* M*, one has* $s_x s_y s_x = s_{s_x(y)}$.

Two symplectic symmetric spaces (M,ω,s) *and* (M',ω',s') *are* isomorphic *if there exists a symplectic diffeomorphism* $\varphi:(M,\omega)\to(M',\omega')$ *such that* $\varphi s_x = s'_{\varphi(x)}\varphi$.

We denote by G the *transvection group* of (M,s) (i.e., the subgroup of $\mathtt{Aut}(M,\omega,s)$ generated by $\{s_x\circ s_y; x,y\in M\}$).

Definition V.10: Let $(\mathfrak{g},\sigma)$ *be an* involutive algebra*, that is,* $\mathfrak{g}$ *is a finite dimensional real Lie algebra and* σ *is an involutive automorphism of* $\mathfrak{g}$*. Let* Ω *be a skewsymmetric bilinear form on* $\mathfrak{g}$*. Then the triple* $(\mathfrak{g},\sigma,\Omega)$ *is called a symplectic triple if the following properties are satisfied:*

(1) *Let* $\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{p}$, *where* $\mathfrak{k}$ *(resp.* $\mathfrak{p}$*) is the* $+1$ *(resp.* -1*) eigenspace of* σ. *Then* $[\mathfrak{p},\mathfrak{p}]=\mathfrak{k}$ *and the representation of* $\mathfrak{k}$ *on* $\mathfrak{p}$, *given by the adjoint action, is faithful.*

(2) Ω *is a Chevalley 2-cocycle for the trivial representation of* $\mathfrak{g}$ *on* $\mathbb{R}$ *such that* $\forall X\in\mathfrak{k}$, $i(X)\Omega=0$. *Moreover, the restriction of* Ω *to* $\mathfrak{p}\times\mathfrak{p}$ *is nondegenerate.*

The dimension of $\mathfrak{p}$ *defines the dimension of the triple. Two such triples* $(\mathfrak{g}_i,\sigma_i,\Omega_i)$ $(i=1,2)$ *are* isomorphic *if there exists a Lie algebra isomorphism* $\psi:\mathfrak{g}_1\to\mathfrak{g}_2$ *such that* $\psi\circ\sigma_1=\sigma_2\circ\psi$ *and* $\psi^*\Omega_2=\Omega_1$.

Proposition V.6 [Bieliavsky (1995)]: There is a bijective correspondence between the isomorphism classes of simply connected symplectic symmetric spaces (M,ω,s) *and the isomorphism classes of symmetric triples* $(\mathfrak{g},\sigma,\Omega)$.

Proposition V.7: To each symplectic symmetric space (corresponding to a class $[(\mathfrak{g},\sigma,\Omega)]$, *we can associate another triple* $\tau=(\mathfrak{h}(\mathfrak{g}),\sigma,\Omega)$ *such that*

(a) $\mathfrak{h}(\mathfrak{g})$ *is a one-dimensional central extension of* $\mathfrak{g}$;

(b) $(\mathfrak{h}(\mathfrak{g}),\sigma)$ *is an involutive Lie algebra such that if* $\mathfrak{h}(\mathfrak{g})=\mathfrak{l}\oplus\mathfrak{p}$ *is the decomposition w.r.t.* σ *one has* $[\mathfrak{p},\mathfrak{p}]=\mathfrak{l}$;

(c) Ω *is a Chevalley 2-coboundary (i.e.,* $\Omega=\delta\xi,\xi\in\mathfrak{h}(\mathfrak{g})^*$*) such that* $i(\mathfrak{l})\Omega=0$ *and* $\Omega|_{\mathfrak{p}\times\mathfrak{p}}$ *is symplectic.*

Such a triple is called exact triple.

b. Elementary solvable symplectic symmetric spaces: In Definition V.11 below, we define a particular type of solvable symmetric spaces which we call elementary. It has been proven [Bieliavsky (1998), Proposition 3.2] that every solvable symmetric space is realized through a sequence of split extensions by Abelian (flat) factors successively taken over an elementary solvable symmetric space. We therefore consider elementary solvable symmetric spaces as the "first induction step" when studying solvable symmetric spaces.

Definition V.11: A symplectic symmetric space (M,ω,s) *is called an elementary solvable symplectic symmetric space if its associated exact triple* $(\mathfrak{h}(\mathfrak{g}),\sigma,\Omega=\delta\xi)$ *(see Lemma V.7) is of the following type:*

(i) *The Lie algebra* $\mathfrak{h}(\mathfrak{g})$ *is a split extension of Abelian Lie algebras* $\mathfrak{a}$ *and* $\mathfrak{b}$:

$$0\to\mathfrak{b}\to\mathfrak{h}(\mathfrak{g})\to\mathfrak{a}\to 0.$$

(ii) *The automorphism* σ *preserves the splitting* $\mathfrak{h}(\mathfrak{g})=\mathfrak{b}\oplus\mathfrak{a}$.

Such an exact triple (associated to an elementary solvable symplectic symmetric space) is called an elementary solvable exact triple.

Observe that, since $\mathfrak{a}\cap\mathfrak{k}\subset\mathfrak{a}\cap[\mathfrak{h}(\mathfrak{g}),\mathfrak{h}(\mathfrak{g})]=0$, one has $\mathfrak{a}\subset\mathfrak{p}$. Therefore $\mathfrak{b}=\mathfrak{k}\oplus\mathfrak{l}$, with $\mathfrak{l}\subset\mathfrak{p}$. Moreover, since $\mathfrak{l}$ and $\mathfrak{a}$ are Abelian and Ω is nondegenerate, the subspaces $\mathfrak{a}$ and $\mathfrak{l}$ of $\mathfrak{p}$ are dual Lagrangians.

Now let (M,ω,s) be an elementary solvable symplectic symmetric space with associated exact triple $(\mathfrak{h}(\mathfrak{g}),\sigma,\Omega=\delta\xi)$ as above. In a neighborhood U of the origin, the map

$$\mathfrak{p}=\mathfrak{a}\times\mathfrak{l}\to M:(a,l)\mapsto\exp(a)\exp(l)\,.\,o \tag{26}$$

turns out to be a Darboux chart when $U\subset\mathfrak{p}$ has the symplectic structure $\Omega=\delta\xi$. Moreover, there exists a unique immersion $\phi:U\cap\mathfrak{a}\to\mathfrak{a}$ such that in the local coordinate system (26), one has the following linearization property:

$$\xi(\sinh(a)l)=\xi[\phi(a),l], \tag{27}$$

where, for $a\in\mathfrak{a}$ we set $\sinh(a):=\frac{1}{2}((\exp(\rho(a))-\exp(-\rho(a)))\in\mathrm{End}(b)$. This immersion is called the *twisting map*.

Proposition V.8: An elementary solvable symplectic symmetric space is strictly geodesically convex if and only if its associated twisting map extends to $\mathfrak{a}$ *as a global diffeomorphism of* $\mathfrak{a}$. *In*

this case, the Darboux chart (26) extends as a global symplectomorphism $(\mathfrak{p},\Omega)\to(M,\omega)$.

Quantization: Associated to the twisting map one has a three-point function $S\in\mathcal{C}^\infty(M\times M\times M,\mathbb{R})$ called the WKB-phase of the elementary solvable symplectic symmetric space

$$S(x_0,x_1,x_2):=\xi\left(\oint_{0,1,2}\sinh(a_0-a_1)l_2\right), \tag{28}$$

where $\oint_{0,1,2}$ stands for cyclic summation and where $x_i=(a_i,l_i)$ $(i=0,1,2)$. The phase S turns out to be invariant under the (diagonal) action of the symmetries $\{s_x\}_{x\in M}$ on $M\times M\times M$. This will be the essential constituent of the associative oscillatory kernel defining a symmetry-invariant strict quantization on every elementary solvable symplectic symmetric space. We now recall this construction as in [Bieliavsky (2002)].

Definition V.12: For a compactly supported function $u\in C_c^\infty(\mathfrak{p})$, *identifying* $\mathfrak{l}^*$ with $\mathfrak{a}$, *we denote by* $\tilde{u}\in\mathcal{C}^\infty(\mathfrak{a}\times\mathfrak{a})$ *its partial Fourier transform*

$$\tilde{u}(a,\alpha):=\int_{\mathfrak{l}}e^{i\Omega(\alpha,l)}u(a,l)\mathrm{d}l. \tag{29}$$

We also denote by $\phi_\nu:\mathfrak{a}\to a$ *the one-parameter family of twisting maps*

$$\phi_\nu(a):=\frac{2}{\nu}\phi\left(\frac{\nu}{2}a\right). \tag{30}$$

For $u,v\in C_c^\infty(\mathfrak{p})$, *we set*

$$\langle u|v\rangle_\nu:=\int_{\mathfrak{a}\times\mathfrak{a}}\tilde{u}(a,\alpha)\overline{\tilde{v}(a,\alpha)}|Jac_{\phi^{-1}}(\alpha)|\mathrm{d}a\mathrm{d}\alpha. \tag{31}$$

The pair $(\mathcal{C}^\infty(\mathfrak{p}),\langle,\rangle_\nu)$ *is a pre-Hilbert space, and we denote by* $\mathcal{H}_\nu$ *its Hilbert completion.*

The Hilbert product $\langle,\rangle_\nu$ turns out to be symmetry-invariant on $\mathcal{C}_c^\infty(M)$. The action of the transvection group then extends by continuity to an isometric action on $\mathcal{H}_\nu$.

Theorem V.2 [Bieliavsky (2002)]: *Let* (M,ω,s) *be a strictly geodesically convex elementary solvable symplectic symmetric space. Realize it symplectically as* $(\mathfrak{p}=\mathfrak{a}\times\mathfrak{l},\Omega)$, *and define the two-point function* $A\in\mathcal{C}^\infty(M\times M)$ *by*

$$A(x_1,x_2):=|Jac_\phi(a_1-a_2\,.\,)|. \tag{32}$$

This function is called the WKB-amplitude *and turns out to be symmetry-invariant. In this notation, one has the following:*

(i) *For all* $\nu\in\mathbb{R}\setminus\{0\}$ *and* $u,v\in\mathcal{C}_c^\infty(M)$, *the formula*

$$u*_\nu v(x_0):=\int_{M\times M}u(x_1)v(x_2)A(x_1,x_2)e^{\frac{i}{\nu}S(x_0,x_1,x_2)}\mathrm{d}x_1\mathrm{d}x_2 \tag{33}$$

extends as an associative product on $\mathcal{H}_\nu$ ($\mathrm{d}x$ *denotes some normalization of the symplectic volume on* (M,ω)). *Moreover (for suitable* u,v and x_0*) the stationary phase method yields a power series expansion of the form*

$$u*_\nu v(x_0)\sim uv(x_0)+\frac{\nu}{2i}\{u,v\}(x_0)+o(\nu^2), \tag{34}$$

where $\{,\}$ *denotes the symplectic Poisson bracket on* (M,ω).

(ii) *The pair* $(\mathcal{H}_\nu,*_\nu)$ *is a topological Hilbert algebra which the transvection group of* (M,ω,s) *acts on by automorphisms.*

A classical procedure then produces a similar result in the C^*-context, see Bieliavsky (2002) for details.

Remark V.4: Whether a symmetric space is strictly geodesically convex is of course entirely encoded in the spectral content of the splitting endomorphism $\rho:\mathfrak{a}\to\mathrm{End}(\mathfrak{b})$. This is discussed in detail in Bieliavsky (2002).

Before applying these results, let us discuss heuristically the ideas that led to this quantization. Denote by $\tilde{G}$ the group naturally obtained from the Lie algebra $\mathfrak{h}(\mathfrak{g})$. Proposition V.8 gives a global Darboux chart from $\mathfrak{p}\simeq\mathfrak{a}\times\mathfrak{l}\simeq M$ to the coadjoint orbit $\mathcal{O}=Ad^*(\tilde{G}).\xi\subset\mathfrak{h}(g)^*$. Denote by $\lambda_X\in\mathcal{C}^\infty(\mathfrak{p})$ the Hamiltonian function associated with the infinitesimal action of $X\in\mathfrak{h}(\mathfrak{g})$ and by $*_\nu^M$ the standard Moyal star product on $(\mathfrak{p},\Omega)$. So, using ideas coming from star representation theory (see Sec. V A) we remark that $[\lambda_X,\lambda_Y]_{*_\nu^M}=(\nu/i)\{\lambda_X,\lambda_Y\}$, that is, $*_\nu^M$ is $\mathfrak{h}(\mathfrak{g})$-covariant. This covariance allows us to define a representation of $\mathfrak{h}(\mathfrak{g})$ on the space $\mathcal{C}^\infty(\mathcal{O})[[\nu]]$, $\rho_\nu(X)u=(i/\nu)\times[\lambda_X,u]_{*_\nu^M}$.

Through the partial Fourier transform F (29) ($F(u):=\tilde{u}$) we obtain a representation on $\mathcal{C}^\infty(\mathfrak{a}\times\mathfrak{a})[[\nu]]$, $\tilde{\rho}_\nu$ s.t. $\tilde{\rho}_\nu(X)\tilde{u}=X_{\mathfrak{a}}.\tilde{u}+c_\nu(X)\tilde{u}$. The expression of the cocycle c_ν is very similar to the one of the "twisting map" ϕ_ν (30). So now let us consider a deformation of the partial Fourier transform defined by $Z_\nu(u)(a,\alpha)=\tilde{u}(a,\phi_\nu(\alpha))$. Defining the commutative product $\bullet_\nu$ on $\mathcal{C}^\infty(\mathfrak{a}\times\mathfrak{a})[[\nu]]$ by $f\bullet_\nu g=Z_\nu(Z_\nu^{-1}(f)\cdot Z_\nu^{-1}(g))$, calculations show that $\bullet_\nu$ is invariant under $\tilde{\rho}_\nu$.

More, we have $Z_\nu^{-1}\circ\tilde{\rho}_\nu(X)\circ Z_\nu=X^*$, X^* being the vector field induced on M by the action of $\mathfrak{h}(\mathfrak{g})$. That means that the action of $\mathfrak{h}(\mathfrak{g})$ on the "underlying manifold" M_ν of $(\mathcal{C}^\infty(\mathfrak{a}\times\mathfrak{a})[[\nu]],\bullet_\nu)$ is equivalent to the one of $\mathfrak{h}(\mathfrak{g})$ on M. So, "going back" to M by F^{-1} we define $T_\nu=F^{-1}\circ Z_\nu$ and we get a formal product on $\mathcal{C}^\infty(\mathfrak{p})[[\nu]]$ defined by

$$u*_\nu v = T_\nu^{-1}(T_\nu u *_\nu^M T_\nu v) \tag{35}$$

which is invariant under the coadjoint action of $\tilde{G}$ on $\mathcal{O}=\mathfrak{p}$.

3. UDF and Hopf algebra structure

In Bieliavsky *et al.* (2003) we define a specific class of Lie groups called elementary solvable presymplectic Lie groups. Let g be a group in this class. By the quantification of elementary solvable symmetric spaces described above, we get a left G-invariant star product on a G-invariant (under the regular action of G) algebra of functions on G, $\mathbb{A}$. That is, we get a UDF $(\mathbb{A},*_{\mathbb{A}}^G)$ (see definition V.8) for every group G in this class. The formulas are convergent (strict deformation quantization). By asymptotic expansion we obtain also a formal UDF on $\mathcal{C}^\infty(G)[[\nu]]$.

Now, at the formal level, we will obtain compatible coproducts and antipode, seeing the above quantization as a L-R smash product (definition V.5).

To do that let us recall that the obtained star products are of the form

$$u*_\nu v = T_\nu^{-1}(T_\nu u *_\nu^M T_\nu v)$$

with $T=F^{-1}\circ(\mathrm{Id}\otimes\phi_\nu^*)\circ F$. But F does not act on the $\mathfrak{a}$ variable, so we can see it as a map from $\mathcal{C}^\infty(\mathfrak{l})$ to $\mathcal{C}^\infty(\mathfrak{a})$. So we have $T=\mathrm{Id}\otimes S$ with $S=F^{-1}\circ\phi_\nu^*\circ F$. Considering that

$$\mathcal{C}^\infty(M)\simeq\mathcal{C}^\infty(\mathfrak{p})\simeq\mathcal{C}^\infty(\mathfrak{a})\hat{\otimes}\mathcal{C}^\infty(\mathfrak{l})\underset{a\simeq\mathfrak{l}^*}{\simeq}\mathcal{C}^\infty(\mathfrak{l}^*)\hat{\otimes}\mathcal{C}^\infty(\mathfrak{l})\supset Pol(\mathfrak{l}^*)\otimes\mathcal{C}^\infty(\mathfrak{l})\underset{\mathfrak{l}\text{ Abelian}}{\simeq}\mathcal{U}\mathfrak{l}\otimes\mathcal{C}^\infty(\mathfrak{l}),$$

it is easy to show

Proposition V.9: The formal version of the invariant WKB-quantization of an elementary solvable symplectic symmetric spaces defined in Theorem V.2 is a L-R-smash product of the form $*^S$ (*cf. Proposition V.3*).

Corollary V.1: The UDF's for elementary solvable pre-symplectic Lie groups admit compatible coproducts and antipodes.

Then Bieliavsky (2003) gives a UDF and an associated Hopf algebra structure for every three dimensional solvable Lie group. The dressing action of the "book" group on SU(2) is particularly investigated.

VI. TOWARDS EXPLICIT REALIZATIONS. II

In the next sections, we revisit in more detail the ideas that were hinted upon in Sec. IV A. Recall that any formal deformation of $\mathcal{U}\mathfrak{g}$ or $\mathcal{C}^\infty(G)$ is preferred and all are produced by modified twisting elements [solutions of (11) with nontrivial Φ] or twisting elements [solutions of (11) with $\Phi=1\otimes 1\otimes 1$]. In both cases, $F=1\otimes 1+\nu r+O(\nu^2)$. We will be particularly interested in the infinitesimal r.

The deformation of $\mathcal{U}\mathfrak{g}$ or $\mathcal{C}^\infty(G)$ is called "triangular" if F is a twisting element. A standard cohomological equivalence argument can be invoked to ensure that the infinitesimal r lies in $\mathfrak{g}\wedge\mathfrak{g}$ and satisfies the *classical Yang-Baxter equation* (CYBE)

$$[r_{12},r_{13}]+[r_{12},r_{23}]+[r_{13},r_{23}]=0. \tag{36}$$

We will frequently call this type of infinitesimal a *triangular r-matrix*.

The deformation of $\mathcal{U}\mathfrak{g}$ or $\mathcal{C}^\infty(G)$ is called *quasitriangular* if F is a modified twisting element. A deep result of Drinfel'd (1989b) asserts that, in the quasitriangular case, the element Φ is uniquely determined up to a certain natural equivalence. The element Φ is known as the *associator* and it has deep connections to the theory of quasi-Hopf algebras, the Kniznik–Zamolodchikov equations, and a theorem of Kohno regarding certain representations of braid groups. It also enters in a crucial way in the operadic demonstration [Tamarkin (1998), Hinich (2003)] of the Kontsevich formality theorem [Kontsevich (2003)] (which gives the existence of a star-product on every Poisson manifold).

We do not have the time to discuss these matters in this survey. In this case however, the infinitesimal r still satisfies the CYBE but $r\in\mathfrak{g}\otimes\mathfrak{g}$ is no longer skew. Instead, we have $r+r_{21}=\Omega$ where Ω is the Casimir element in $\mathfrak{g}\otimes\mathfrak{g}$ chosen with respect to some fixed invariant bilinear form on $\mathfrak{g}$. In this case, the infinitesimal r is called a *quasitriangular r*-matrix, and it necessarily follows that $\tilde{r}=r-(\Omega/2)\in\mathfrak{g}\wedge\mathfrak{g}$ will satisfy the *modified classical Yang-Baxter equation* (MCYBE)

$$[\tilde{r}_{12},\tilde{r}_{13}]+[\tilde{r}_{12},\tilde{r}_{23}]+[\tilde{r}_{13},\tilde{r}_{23}]\in(\mathfrak{g}\wedge\mathfrak{g}\wedge\mathfrak{g})^{\mathfrak{g}}. \tag{37}$$

Given an r-matrix of either type, it is natural to seek the twisting element F [guaranteed to exist by Drinfel'd (1985, 1989)] whose infinitesimal is r. In the explicit sense, the results are quite scarce. Indeed, as previously mentioned, F is unknown for all quasitriangular r-matrices including, in particular, the "standard" solution which serves as the infinitesimal for the quantum groups $\mathcal{U}_q(\mathfrak{g})$ and $\mathcal{C}_q^\infty(G)$.

A. Preferred *-products for the standard quantum *n*-space

Since the F is unknown, it should be no surprise that the preferred *-products have not been exhibited even for $\mathcal{C}_q^\infty(\mathrm{SL}(n))$. However, we do have the preferred *-products for the covariant quantization, $\mathcal{C}_q^\infty(\mathbb{C}^n)$, of the function algebra $\mathcal{C}^\infty(\mathbb{C}^n)$. If x_i are the coordinate functions on $\mathbb{C}^n$, then $\mathcal{C}_q^\infty(\mathbb{C}^n)$ is characterized by the relations $x_ix_j=qx_jx_i$ for $i<j$. In the classical case, the action of the group SL_n on $\mathbb{C}^n$ makes $\mathcal{C}^\infty(\mathbb{C}^n)$ into an $\mathcal{C}^\infty(\mathrm{SL}(n))$-comodule algebra. This means that $\mathcal{C}^\infty(\mathbb{C}^n)$ is an $\mathcal{C}^\infty(\mathrm{SL}(n))$-comodule with the compatibility condition that the coaction map is an algebra homomorphism. The same is true at the quantized level: $\mathcal{C}_q^\infty(\mathbb{C}^n)$ is an $\mathcal{C}_q^\infty(\mathrm{SL}(n))$-comodule algebra. A preferred covariant deformation in this case is a *-product on $\mathcal{C}^\infty(\mathbb{C}^n)$ which is compatible with both the original unchanged (on all elements) comodule structure map (on all elements) and the preferred quantization of $\mathcal{C}^\infty(\mathrm{SL}(n))$ to $\mathcal{C}_q^\infty(\mathrm{SL}(n))$.

In order to describe the preferred *-products for the quantum linear space, we need some combinatorial notation. Define the q-factorial to be

$$m!_q = \frac{(1-q^m)(1-q^{m-1})\cdots(1-q)}{(1-q)^m}$$

and for $\lambda \in \mathbb{N}^n$ with $|\lambda| = \lambda_1 + \cdots + \lambda_n$ let

$$\langle \lambda \rangle_q = \frac{|\lambda|!_q}{\lambda_1!_q \cdots \lambda_n!_q}$$

be the q-multinomial coefficient. Without the subscript, $\langle \lambda \rangle$ will denote the usual multinomial coefficient. The symbol X^λ will denote the monomial $x_1^{\lambda_1}\cdots x_n^{\lambda_n}$. Note that by linearity, it is only necessary to consider the product of monomials. The ordinary commutative multiplication is simply expressible as $X^\lambda X^\nu = X^{\lambda+\nu}$. Finally, for $\lambda, \nu \in \mathbb{N}^n$ set

$$(\lambda : \nu) = \sum_{i=1}^{n} \sum_{j>i} \lambda_i \nu_j.$$

Theorem VI.1 [Gerstenhaber *et al.* (1990) and Giaquinto (1992)]: *The preferred deformation for the quantum linear space $\mathcal{C}_q(\mathbb{C}^n)$ is given by*

$$X^\lambda * X^\nu = \left(\frac{\langle \lambda \rangle_{q^2} \langle \nu \rangle_{q^2} \langle \lambda + \nu \rangle}{\langle \lambda \rangle \langle \nu \rangle \langle \lambda + \nu \rangle_{q^2}} \right)^{1/2} q^{(\lambda:\nu)} X^{\lambda+\nu}. \tag{38}$$

The presence of the factor $q^{(\lambda:\nu)}$ is clear as it comes directly from the defining relations $x_i x_j = q x_j x_i$ of $\mathcal{C}_q^\infty(\mathbb{C}^n)$. The other numerical factor in the formula may be viewed as a ratio of norms and its necessity is less obvious. Note that some of the products in (38) are undefined when q is a root of unity which helps explain from the deformation quantization viewpoint that the standard quantum groups at roots of unity have different behavior than at generic specializations of q. Upon seeing this formula in 1990, Ludwig Faddeev was startled and claimed that, within a year, we would have the preferred *-products on all of $\mathcal{C}_q^\infty(\mathrm{SL}(n))$. Unfortunately, time has not been kind to his prediction as this problem is unfortunately still open.

Formula (38) of Theorem VI.1 was recently rediscovered by Blohmann (2003) using q-Clebsch–Gordan coefficients.

B. Triangular *r*-matrices and twists

Suppose that r is a triangular r-matrix [a solution of (VI)]. Drinfel'd has given a procedure in Drinfel'd (1985) which, given a triangular r, produces the twisting F. It is generally difficult though to extract the exact form of F since the construction uses, among other things, the Campbell–Baker–Hausdorff formula for the series of $\ln(e^x e^y)$, where $x, y \in \mathfrak{g}$. In the "strong" explicit sense, the twisting F is known only for certain classes of r-matrices including the "Jordanian" solution for $\mathfrak{sl}(2)$ and several of its generalizations.

Let us recall the basic classification scheme [see Belavin and Drinfel'd (1982)] for triangular r-matrices. Our formulation follows that of Stolin (1991). A Lie algebra $\mathfrak{f}$ is quasi-Frobenius if there exists a nondegenerate two-cocycle $\phi : \mathfrak{f} \wedge \mathfrak{f} \to \mathbb{C}$. The connection to triangular r-matrices is that the cocycle condition for the bilinear form ϕ is equivalent to ϕ^{-1} (the element of $\mathfrak{f} \wedge \mathfrak{f}$ whose matrix of coefficients is the inverse of the matrix of ϕ) satisfying the classical Yang–Baxter equation. The problem of finding triangular r-matrices up to equivalence is then reduced to listing the quasi-Frobenius Lie algebras, their normalizers, and calculating the second cohomology group $H^2(\mathfrak{f}, \mathbb{C})$. A simple Lie algebra $\mathfrak{g}$ is never quasi-Frobenius but if $r \in \mathfrak{g} \wedge \mathfrak{g}$ is classical r-matrix, then there is a unique quasi-Frobenius "carrier" subalgebra $\mathfrak{f} \subset \mathfrak{g}$ for which $r \in \mathfrak{f} \wedge \mathfrak{f}$. Note that such an $\mathfrak{f}$ is necessarily even-dimensional. This approach does not give a constructive classification of triangular r-matrices as there is no effective way to find all quasi-Frobenius Lie subalgebras of $\mathfrak{g}$.

The easiest example of the foregoing is when $\mathfrak{f}$ is an Abelian subalgebra of $\mathfrak{g}$. Then any $r \in \mathfrak{f} \wedge \mathfrak{f}$ is a classical r-matrix and it is elementary to check that the corresponding twisting element is $F = \exp(\nu r)$. We have already seen that this twisting element (=UDF) produces, in particular, the Moyal deformation.

Perhaps the most well known example of a triangular r-matrix is based on the Borel subalgebra of $\mathfrak{sl}(2)$ which is generated by h and e with $[h,e]=2e$. The r-matrix $h \wedge e$ is the infinitesimal of the "Jordanian" quantization of $\mathcal{C}^\infty(\mathrm{SL}(2))$, which is its unique (up to equivalence) triangular quantization. The twisting element can be derived using (14) and comes out to be $F = \exp((h/2) \otimes \ln(1+\nu e))$. Note that the infinitesimal is $h \otimes e$ and not $h \wedge e$. These are equivalent r-matrices and the twisting element with infinitesimal $h \wedge e$ is given in Giaquinto and Zhang (1998).

There are various extensions of the Jordanian r-matrix to $\mathfrak{sl}(n)$ with $n > 2$. In particular, the triangular r-matrix

$$r = (e_{11} - e_{nn}) \wedge e_{1n} + 2\sum_{j=2}^{n-1} e_{1j} \wedge e_{jn}$$

was exhibited in Gerstenhaber *et al.* (1990). The element F for this family has been called an *extended Jordanian* twist and was derived independently in Giaquinto and Zhang (1995) and Kulish *et al.* (1999), although the latter reference has the following more compact form of the twisting element

$$F = \exp\left\{ 2\nu \sum_{i=2}^{n-1} e_{1i} \otimes e_{in} e^{-\sigma} \right\} \exp\{(e_{11} - e_{nn}) \otimes \sigma\},$$

where $\sigma = \frac{1}{2} \ln(1+2\nu e_{1n})$. Note that the carriers for this family are contained in the Borel subalgebra of $\mathfrak{sl}(n)$, and are hence solvable.

Another interesting generalization of the Jordanian twist is a family of r-matrices whose carriers, in contrast with the above examples, are nonsolvable subalgebras of $\mathfrak{sl}(n)$. In particular, the carrier algebra is the (Frobenius) Lie algebra $\mathfrak{p}_1$ which denotes the maximal parabolic subalgebra generated by all simple positive root vectors $e_{i,i+1}$, the Cartan subalgebra of traceless matrices, and the simple negative root vectors $e_{i+1,i}$ *except* e_{21}. For example, when $n=3$, this Lie algebra consists of all traceless matrices of the form

$$\begin{pmatrix} * & * & * \\ 0 & * & * \\ 0 & * & * \end{pmatrix}.$$

The r-matrix with carrier $\mathfrak{p}_1 \subset \mathfrak{sl}(n)$ was discovered in Gerstenhaber and Giaquinto (1997). For $n=3$ the explicit form is

$$r = (2e_{11} - e_{22} - e_{33}) \wedge e_{12} + (e_{11} + e_{22} - 2e_{33}) \wedge e_{23} + e_{13} \wedge e_{32}.$$

The twist for this family is only known in the case of $n=3$; it has the form of a product of an extended Jordanian twist (as illustrated above) with a "deformed" Jordan type twist. Details of this interesting twist can be found in Lyakhovsky and Samsonov (2002).

C. Quasitriangular *r*-matrices: The Belavin–Drinfel'd classification

We now turn to the case of quasitriangular r-matrices. First, some good news. There is a complete constructive classification of all such $r \in \mathfrak{g} \otimes \mathfrak{g}$ when $\mathfrak{g}$ is simple. This is the famous Belavin–Drinfel'd classification, see Belavin and Drinfel'd (1984). To describe this classification we need some notation. Let $\mathfrak{h}$ be a Cartan subalgebra of $\mathfrak{g}$. The root system will be denoted by Δ and Γ will be a set of simple roots. Let $\Omega_0 \in \mathfrak{g} \otimes \mathfrak{g}$ be the restriction of the Casimir element Ω to $\mathfrak{h} \otimes \mathfrak{h}$.

Definition VI.1: A Belavin–Drinfel'd triple for $\mathfrak{g}$ *is a triple* (Γ_1, Γ_2, T), *where* Γ_i *are subsets of*

the positive simple roots of $\mathfrak{g}$ *and* $T:\Gamma_1\to\Gamma_2$ *is a bijection which preserves the invariant bilinear form and for all* $\alpha\in\Gamma_1$, *there exists* $k>1$ *such that* $T^k\notin\Gamma_1$.

Given such a triple (henceforth simply denoted T), an element $s\in\mathfrak{h}\otimes\mathfrak{h}$ is called T-admissible if

$$s+s_{21}=\Omega_0 \quad \text{and} \quad (T(\alpha)\otimes 1)s+(1\otimes\alpha)s=\Omega_0$$

for all $\alpha\in\Gamma_1$. A T-admissible s is always of the form $s=\tilde{s}+\Omega_0/2$, where $\tilde{s}\in\mathfrak{h}\wedge\mathfrak{h}$. The set of all admissible $\tilde{s}$ forms a linear subvariety of $\mathfrak{h}\wedge\mathfrak{h}$ whose dimension is $\binom{d}{2}$ where $d=\#(\Gamma-\Gamma_1)$.

The map T can be extended to an isomorphism of Lie subalgebras $T:\mathfrak{g}_1\to\mathfrak{g}_2$ where $\mathfrak{g}_i$ is the Lie subalgebra of $\mathfrak{g}$ generated by the simple roots in Γ_i. Choose $e_\alpha\in\mathfrak{g}_\alpha$ such that $(e_\alpha,e_{-\alpha})=1$ and $T(e_\alpha)=e_{T\alpha}$ and define an ordering on Δ by $\alpha\prec\beta$ if $T^k\alpha=\beta$ for some positive integer k. View $\mathfrak{g}\wedge\mathfrak{g}$ as a subset of $\mathfrak{g}\otimes\mathfrak{g}$ according to the identification $x\wedge y=1/2(x\otimes y-y\otimes x)$. The spectacular result of Belavin and Drinfel'd is the content of the next theorem.

Theorem VI.2 [Belavin and Drinfel'd (1984)]: Let $\mathfrak{g}$ *be a simple complex Lie algebra and suppose that T is a triple. Then for every admissible s, the element*

$$r=s+\sum_{\alpha>0}e_{-\alpha}\otimes e_\alpha+2\sum_{\substack{\alpha,\beta>0\\ \alpha\prec\beta}}e_{-\alpha}\wedge e_\beta$$

is a quasitriangular solution to the Yang–Baxter equation satisfying $r_{12}+r_{21}=\Omega$. *Moreover, every such solution is of this form up to the adjoint action of* $\mathfrak{g}$ *on* $\mathfrak{g}\otimes\mathfrak{g}$.

The standard solution, $r_{st}=\Omega_0+\Sigma_{\alpha>0}\,e_{-\alpha}\otimes e_\alpha$, corresponds to the empty triple (with $\Gamma_i=\emptyset$) and $\tilde{s}=0$. It is the infinitesimal for the quantum groups $\mathcal{U}_q(\mathfrak{g})$ and $\mathcal{C}_q^\infty(G)$. For this triple, any $s=\Omega_0+\tilde{s}$ with $\tilde{s}\in\mathfrak{h}\wedge\mathfrak{h}$ is admissible so the dimension of this family of solutions is $\binom{l}{2}$ where l is the rank of $\mathfrak{g}$.

At the other extreme, there are certain triples for which there is a unique T-admissible element. For $\mathfrak{g}=\mathfrak{sl}_n$, these are the *generalized Cremmer–Gervais* triples, see Gerstenhaber and Giaquinto (1997). If $\{\alpha_1,\ldots,\alpha_{n-1}\}$ are the simple positive roots and i is relatively prime to n, then the triple T_i with

$$\Gamma_1=\Gamma-\{\alpha_{n-i}\},\quad \Gamma_2=\Gamma-\{\alpha_m\},\quad T(\alpha_j)=\alpha_{i+j \mod n} \tag{39}$$

is a generalized Belavin-triple. The r-matrix where $m=1$ serves as the infinitesimal of the Cremmer-Gervais R-matrix, see Cremmer and Gervais (1990). The original approach of Cremmer–Gervais made no mention of the Belavin–Drinfel'd triple; the connection was first made in Gerstenhaber *et al.* (1993).

D. Boundary solutions of the classical Yang–Baxter equation

Suppose $r\in\mathfrak{g}\wedge\mathfrak{g}$ is a solution of the modified classical Yang–Baxter equation (VI) $[r_{12},r_{13}]+[r_{12},r_{23}]+[r_{13},r_{23}]=c\omega$, where ω is a $\mathfrak{g}$-invariant element in $\mathfrak{g}\wedge\mathfrak{g}\wedge\mathfrak{g}$ and c is a scalar. It should be intuitively clear that as c tends to zero, r tends to a solution of the classical Yang–Baxter equation. This theory of this type of "degeneration" was made precise in Gerstenhaber and Giaquinto (1997), and it is essentially the concept of contraction which was elaborated upon earlier in this paper.

Let $\mathcal{M}$ be the set of all solutions to the modified classical Yang–Baxter equation in the projective space $\mathbb{P}(\mathfrak{g}\wedge\mathfrak{g})$ of lines in $\mathfrak{g}\wedge\mathfrak{g}$. Similarly, $\mathcal{C}$ will denote the solutions to the classical Yang-Baxter equation in $\mathbb{P}(\mathfrak{g}\wedge\mathfrak{g})$.

Theorem VI.3 [Gerstenhaber and Giaquinto (1997)]:

(1) *The set* $\mathcal{M}$ *is a quasiprojective variety (i.e., an open subset of* $\overline{\mathcal{M}}$, *its closure);*
(2) *Any element in the closure of* $\mathcal{M}$ *not lying in* $\mathcal{M}$ *is contained in* $\mathcal{C}$;
(3) *There exist elements of* $\mathcal{C}$ *which are not in* $\overline{\mathcal{M}}$.

In light of the theorem, call an r which lies in $\overline{\mathcal{M}}$ but not $\mathcal{M}$ a *boundary solution* of the classical Yang–Baxter equation.

Question VI.1: Is there a reasonable constructive classification of the boundary r-matrices? As stated earlier, no such classification seems likely for all triangular r-matrices. But the relation of the boundary solutions to the constructively known set $\mathcal{M}$ gives plausibility to a positive answer to this question.

An easy way to construct boundary r matrices is the following: Take an ad-nilpotent element $x \in \mathfrak{g}$ and any modified classical r-matrix r. Then $\exp(\xi \mathrm{ad}_x)\cdot r$ is necessarily of the form $r+\xi r_1 + \cdots + \xi^m r_m$. Dividing the result by ξ^m and letting ξ approach zero then shows that r_m must be a boundary solution of the classical Yang–Baxter equation. The extended Jordanian and parabolic triangular r-matrices discussed earlier were first realized with this construction. The extended Jordanian r lies in the boundary of an orbit of the standard solution to the modified classical Yang–Baxter equation, see Gerstenhaber *et al.* (1990). The more interesting example is the parabolic r-matrix. It lies in the closure of an orbit of the Cremmer–Gervais solution to the modified classical Yang–Baxter equation. What is striking here is that both the parabolic solution and the Cremmer–Gervais solution are uniquely determined by the first root of $\mathfrak{sl}(n)$. The parabolic subalgebra is the unique r-matrix with carrier $\mathfrak{p}_1$ (determined by deleting the first negative root), and the Cremmer–Gervais triple is the unique one whose Γ_2 omits only the first root. There should be a parallel situation with the modified Cremmer–Gervais triples, each of which is uniquely determined by an integer relatively prime to n. Elashvili (1982) has proved that the parabolic subalgebra $\mathfrak{p}_i$ of $\mathfrak{sl}(n)$ determined by deleting $\alpha_i = e_{i+1,i}$ is quasi-Frobenius if and only if i and n are relatively prime.

Conjecture VI.1: Suppose i is relatively prime to n. Then the triangular r-matrix whose carrier is the maximal parabolic subalgebra $\mathfrak{p}_i$ lies in the closure of the orbit of the modified Cremmer–Gervais quasitriangular r-matrix determined by the triple T_i [defined in formula (VI.3)].

In unpublished work, the second and third authors have verified this conjecture by direct computation in the case $n=5$ and $i=2$.

E. The GGS "magic" formula

The central aspect of the FRT approach is a quantum Yang–Baxter matrix $R \in \mathrm{End}(V \otimes V)$ where V is the vector representation of G. The matrix R is used to provide commutation relations for the generators which define the quantized Hopf algebra of functions. Given a solution r to the classical Yang–Baxter equation (triangular or quasitriangular), a natural question is quantize it to an R-matrix of the form $R = 1 + \nu r + \nu^2 r_2 + \cdots$ which satisfies the quantum Yang–Baxter equation $R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}$ (QYBE).

If r is triangular and F is its corresponding twisting element, then $\mathcal{R} = FF_{21}^{-1}(\mathcal{U}\mathfrak{g} \otimes \mathcal{U}\mathfrak{g})[[\nu]]$ is a universal solution to the QYBE. Specializing to the vector representation then gives a quantum Yang–Baxter matrix. However, it is hard to be explicit here because the F is unknown in the strong explicit sense, except in some cases previously mentioned. However, if r is quasitriangular, there is the Belavin–Drinfel'd classification and an interesting question is to quantize these r-matrices. For general simple $\mathfrak{g}$ there is no satisfactory answer as of yet, but for $\mathfrak{sl}(n)$ there is a remarkable explicit quantization called the *GGS Formula*, see Gerstenhaber *et al.* (1993). Our esteemed colleague Yvette Kosmann–Schwarzbach calls this the magic formula because of its simplicity and the remarkable fact that such a simple formula can work for all quasitriangular r-matrices.

For the standard solution r_{st} the corresponding R-matrix

$$R_{\mathrm{st}} = q\sum_i e_{ii} \otimes e_{ii} + \sum_{i \neq j} e_{ii} \otimes e_{jj} + (q - q^{-1})\sum_{i>j} e_{ij} \otimes e_{ji} \tag{40}$$

is well-known. In addition to the quantum Yang–Baxter equation, PR_{st} satisfies the Hecke relation $(PR-q)(PR+q^{-1})=0$, where P is the matrix representing the interchange of factors in $V \otimes V$. If $\tilde{s} \in \mathfrak{h} \wedge \mathfrak{h}$ then recall that $r_{\mathrm{st}} + \tilde{s}$ is a quasitriangular r-matrix associated with the empty triple. Its quantization has the elementary form $q^{\tilde{s}} R_{\mathrm{st}} q^{\tilde{s}}$ and was first given in Reshetikhin (1990), a paper

which initiated a flurry of activity in the area of multiparameter quantum groups.

Until 1993, the only other specific R-matrix was that given by Cremmer and Gervais (1990). Then a conjecture was made by Gerstenhaber, Giaquinto, and Schack which gave a formula which was conjectured to produce an R-matrix from each Belavin–Drinfel'd r-matrix for $\mathfrak{sl}(n)$. This became known as the "GGS conjecture." Evidence of the conjecture's validity was confirmed by computer programs for all triples up through $\mathfrak{sl}(5)$ in Giaquinto and Hodges (1998), and for all triples up through $\mathfrak{sl}(12)$ in Schedler (1999). Up to a natural notion of equivalence, there are 210,300 triples for $\mathfrak{sl}(12)$.

To describe the GGS formula, we need some notation. Let $r_{\mathrm{st}}+s+a$ be a Belavin–Drinfel'd quasitriangular r-matrix. Recall that $s=\tilde{s}+\Omega_0/2$ with $\tilde{s}\in\mathfrak{h}\otimes\mathfrak{h}$. Set

$$\varepsilon = ar_{\mathrm{st}} + r_{\mathrm{st}}a + a^2.$$

For $M\in M_n(\mathbb{C})\otimes M_n(\mathbb{C})$ we use the Kronecker notation $M=\Sigma M_{ik}^{jl}e_{ij}\otimes e_{kl}$. Define

$$\tilde{a} = \sum a_{ij}^{kl} q^{a_{ij}^{kl}\varepsilon_{ij}^{kl}} e_{ij}\otimes e_{kl}.$$

Theorem VI.4 [Gerstenhaber *et al.* (1993) and Schedler (2000)]: *Let $r_{\mathrm{st}}+s+a$ be a Belavin–Drinfel'd quasitriangular r-matrix, and define*

$$R_{GGS} = q^{\tilde{s}}(R_{\mathrm{st}} + (q-q^{-1})\tilde{a})q^{\tilde{s}}. \tag{41}$$

Then R_{GGS} satisfies the quantum Yang–Baxter equation which quantizes r, and PR_{GGS} satisfies the Hecke relation.

The proof of the conjecture is due to Schedler (2000) and is rather complicated. In related work, Etingof, Schedler, and Schiffmann gave an (explicit) quantization of the so-called dynamical r-matrices for simple Lie algebras [Etingof *et al.* (2000)]. A special case of their construction gives a universal quantization of any quasi-triangular r-matrix. Even though the construction is "explicit," it is a formidable task to perform computations with the universal quantization in a specific representation. Indeed, Schedler begins his proof of the GGS conjecture with the ESS universal quantization and then he proceeds to evaluate it in the tensor square of the vector representation. After 25 pages of lengthy combinatorial computations, he finds out that the result is exactly the GGS matrix! Something is wanting, however, for a more elementary proof as the statement of the GGS conjecture is just an assertion about specific linear transformation of a finite dimensional vector space.

Question VI. 2:

(1) *Find a similar GGS-type formula which quantizes the quasitriangular r-matrices for the other classical series (B,C,D) of simple Lie algebras. So far, no progress has been made in this direction.*
(2) *Find a "boundary GGS formula." By this, we mean formula which quantizes the boundary r-matrices. For example, it was proved in Gerstenhaber and Giaquinto (1998) that for any triangular r-matrix in $\mathfrak{sl}(n)\wedge\mathfrak{sl}(n)$ which lies in the boundary of the standard solution $\Sigma_{i>j}\, e_{ij}\wedge e_{ji}$ to the MCYBE, then $\exp(\xi r)$ is a boundary solution to the QYBE.*

In a matter related to the second question, Endelman and Hodges (2000) have shown that the Cremmer–Gervais R-matrix degenerates to a QYBE matrix which quantizes the parabolic triangular r-matrix associated to the parabolic subalgebra $\mathfrak{p}_1$ of $\mathfrak{sl}(n)$. This may be seen as the quantum version of the degeneration of the Cremmer–Gervais quasitriangular r-matrix to the triangular parabolic r-matrix.

F. Quantizing in representation space

Let V be the vector representation of a simple complex Lie algebra $\mathfrak{g}$. In the last section, we exhibited a canonical QYBE matrix $R\in\mathrm{End}(V\otimes V)$ associated with each Belavin–Drinfel'd infinitesimal for $\mathfrak{sl}(n)$. The FRT formalism then may be used to produce commutation relations for

the generators of a quantization $\mathbb{C}_R[\mathrm{SL}(n)]$ of the coordinate Hopf algebra of $\mathrm{SL}(n)$. Each R-matrix also enjoys many other nice properties. For example, the operator $\hat{R}=PR$ has eigenvalues q and $-q^{-1}$ with multiplicities $(n^2+n)/2$ and $(n^2-1)/2$, respectively. These numbers coincide with the multiplicities of the eigenspaces corresponding to the eigenvalues ± 1 of the permutation operator P.

What the R-matrix does not do, however, is *quantize* the module $V\otimes V$—that is, transform the $+1$-eigenspace for P to the q-eigenspaces for $\hat{R}$ and the—1-eigenspace for P to the $-q^{-1}$-eigenspace for $\hat{R}$. Some explanation is in order to explain more precisely what we mean here. In the classical $(q=1)$ case the module $V\otimes V$ splits into a direct sum $V^+\oplus V^-$, where V^+ consists of the symmetric vectors (eigenvalue -1 for P) and V^- is the space of skew-symmetric vectors (eigenvalue -1 for P). In the quantized case the same idea holds. Specifically, $V\otimes V\cong V_q^+\oplus V_q^-$, where V_q^+ is the space of q-symmetric vectors (eigenvalue q for $\hat{R}$) and V_q^- is the space of q-skew-symmetric vectors (eigenvalue $-q^{-1}$) for $\hat{R}$. What we seek is a *quantizing transformation* $Q\in \mathsf{End}(V\otimes V)$ which takes V^+ to V_q^+ and V^- to V_q^-. If the Belavin–Drinfel'd infinitesimal of R is r, then it is known that any possible quantizing transformation Q has infinitesimal $\tilde{r}=r-(\Omega/2)$, the solution to the MCYBE associated with r. Ideally we would like to have a canonical (explicit of course!) simple formula for the quantizing transformation Q as a function of $\tilde{r}$.

For the standard solution R_{st}, we do have a pleasant description of Q which we now describe. The solution to the MCYBE associated to r_{st} is $\tilde{r}_{\mathrm{st}}=\Sigma_{i>j}\, e_{ij}\wedge e_{ji}$. Let $e_1,\ldots,e_n$ be the standard basis of $V\cong\mathbb{C}^n$. It will be convenient to use the inner product on V defined by $(e_i,e_j)=\delta_{ij}$. This extends to one on $V\otimes V$ in which the set of all $e_i\otimes e_j$ forms an orthonormal basis. Then an elementary calculation shows that

$$V_q^+=\left\{\{\, e_i\otimes e_i \,|\, 1\leqslant i\leqslant n\}\cup\left\{\left.\frac{qe_i\otimes e_j+e_j\otimes e_i}{\sqrt{1+q^2}}\right|\, i<j\right\}\right\}$$

and

$$V_q^-=\left\{\left\{\left.\frac{e_i\otimes e_j-qe_j\otimes e_i}{\sqrt{1+q^2}}\right|\, i<j\right\}\right\}.$$

Note that these are orthogonal bases and that setting $q=1$ gives orthogonal bases for the eigenspaces $V^{\pm}$ of P.

Theorem VI.5 [Gerstenhaber *et al.* (1990)]: *Let* $Q=\exp(\nu\tilde{r}_{\mathrm{st}})$ *and* $q=\sec\nu-\tan\nu$. *Then* $Q(e_i\otimes e_i)=e_i\otimes e_i$ *for each* i *and for all* $i<j$

$$Q\left[\frac{e_i\otimes e_j+e_j\otimes e_i}{\sqrt{2}}\right]=\frac{qe_i\otimes e_j+e_j\otimes e_i}{\sqrt{1+q^2}},\quad \textit{and}\quad Q\left[\frac{e_i\otimes e_j-e_j\otimes e_i}{\sqrt{2}}\right]=\frac{e_i\otimes e_j-qe_j\otimes e_i}{\sqrt{1+q^2}}$$

and

$$\hat{R}_{\mathrm{st}}=\frac{1}{\cos\,\nu}(Q^{-1}PQ-\sin\,\nu).$$

Thus Q is an orthogonal quantizing transformation and $\hat{R}_{\mathrm{st}}$ (and hence also R_{st}) is easily recoverable from Q. In fact, the transformation Q performs the quantization eigenvector by eigenvector, which is quite desirable. In the simplest case of $n=2$, Q is a rotation in the plane spanned by $e_1\otimes e_2$ and $e_2\otimes e_1$. The striking aspect of this theorem is that Q, being just an exponential, is produced in a very elementary way solely based on infinitesimal data. Thus we recover R_{st} in a particularly simple way. Also note that the choice of $q=\sec\nu-\tan\nu$ is absolutely necessary for the theorem. From the viewpoint of deformation quantization, it turns out that this seems to be the natural choice for the parameter q, and not e^{ν}, or $e^{i\nu}$ as many (including us!) authors tend to use.

It was shown in Gerstenhaber *et al.* (1990) [see also Blohmann (2003)] that if $\mathcal{F} \in \mathcal{U}(\mathfrak{sl}(n)) \otimes U(\mathfrak{sl}(n))[[\nu]]$ is the modified twisting element which gives the preferred deformation of $\mathcal{C}^\infty(\mathrm{SL}(n))$ to $\mathcal{C}_q^\infty(\mathrm{SL}(n))$, then $(\rho \otimes \rho)F = Q^{-1}$ where $\rho : \mathfrak{sl}(n) \to \mathsf{End}(V)$ is the vector representation. Thus, the inverse of the quantizing transformation Q coincides with the image of the modified twisting element in the vector representation.

Optimally, we would like to have such an elementary quantizing transformation as a simple function of the corresponding $\tilde{r}_{\mathrm{st}}$ for the orthogonal and symplectic Lie algebras. Recent work of second and third authors shows that this is indeed possible, but the construction is more subtle. The difficulty lies in the fact that for these Lie algebras, $V \otimes V$ contains a one-dimensional g-module, a vector which represents the defining bilinear form of $\mathfrak{g}$. For the orthogonal Lie algebras, this vector splits off of the symmetric vectors and in the symplectic case it splits off of the skew vectors. A similar decomposition occurs in the quantized cases. This difficulty is paralleled in fact that the operator $\hat{R}_{\mathrm{st}}$ has three eigenvalues. For type B_n, they are q, $-q^{-1}$, and q^{1-N} where $N = 2n+1$, and the remaining types of C_n and D_n have a similarly formed third eigenvalue. Unfortunately, space prohibits a detailed description of the quantizing transformation in these cases. We can just say what it is not: unlike the A_n series, the exponential of $\tilde{r}_{\mathrm{st}}$ does not produce the quantizing transformation. Nevertheless, like many deformation problems, the exponential function plays a substantial role in the construction of the quantizing transformation.

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Mirror symmetry and noncommutative geometry of A_∞-categories

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Homological mirror symmetry aims to explain the phenomenon of mirror symmetry in the language of A_∞-categories and their deformation theory. In these notes I discuss various aspects of this approach from the point of view of noncommutative algebraic geometry in the tensor category of graded vector spaces. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1789282]

I. INTRODUCTION

This review article is an extended version of my lectures at a workshop at UCLA. My aim was to discuss one aspect of mirror symmetry, namely, the categorical one. It is known as homological mirror symmetry, and was suggested by Maxim Kontsevich in 1993 (see Kontsevich, 1994). Mirror symmetry of course has many other aspects related to string theory, algebraic geometry, differential equations, differential geometry, and symplectic geometry. In order to have a more general picture the interested reader should look at the literature [see, for example, the list of references in Cox and Katz (1999)]. The homological approach is characterized by restating the symplectic and complex geometry of mirror symmetry in terms of so-called A_∞-categories. The latter are homotopy versions of ordinary categories. Thus, for example, A-branes (Lagrangian submanifolds equipped with flat bundles) become objects of the so-called Fukaya category (see Kontsevich, 1994; Fukaya *et al.*, 2000). Interaction between A-branes is interpreted in terms of morphisms in the Fukaya category. In the simplest case the interaction between two A-branes is "measured" by the vector space spanned by their intersection points. On the other hand, B-branes (holomorphic vector bundles) are naturally objects of the derived category of coherent sheaves. The duality between the A and B sides of mirror symmetry then becomes an equivalence of the corresponding A_∞-categories assigned to dual Calabi–Yau manifolds. All numbers (for example, the number of rational curves on a Calabi–Yau manifold) become a part of categorical data. Conversely, one expects that the numbers which appear in mirror symmetry can be recovered from the categorical data intrinsically. This opens a way to generalize mirror symmetry to the world of noncommutative spaces.

It is clear after Kontsevich (1994) that homological mirror symmetry is closely related to the deformation theory of A_∞-categories. Therefore one needs the language which fits well to homological algebra and deformation theory. This language is briefly explained in Secs. III and VI.

Another conceptual point of discussion is the geometric framework of homological mirror symmetry. Currently, the only way to formulate rigorously homological mirror conjecture from Kontsevich (1994) is to consider degenerating *families* of Calabi–Yau manifolds. In this paper we follow the ideas of Kontsevich and Soibelman (2000a) where the relevant geometry was formulated in terms of Gromov–Hausdorff collapse. In the simplest example of such a collapse a complex elliptic curve collapses to its equator circle. In general, various structures inherited by such a limit can be axiomatized. Subsequently the geometric portion of mirror symmetry admits an easy formulation in terms of limiting data (see Sec. II).

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The nontrivial part of the story is to formulate instanton corrections (i.e., the structure of A_∞-category on A-branes) in terms of the limiting data. This is done in Sec. V. A_∞-category of B-branes is explained in Sec. IV.

Sections VII and VIII are devoted to the language suitable for generalization to noncommutative Calabi–Yau manifolds (we give the definition of the latter in Sec. VII).

The paper has two appendixes. In the first one we recall the picture of Kontsevich and Soibelman (2000a) of the collapse of conformal field theories. It makes a striking parallel to the purely mathematical picture of Gromov–Hausdorff collapse. Appendix B is devoted to the language of saturated A_∞-categories. It is appropriate for the pure categorical definition of the notion of smooth projective variety, and hence works for noncommutative Calabi–Yau manifolds as well.

I should say that there are many topics within homological mirror symmetry which I do not discuss in this review. Here are few examples of what is missing:

(a) noncommutative periods (Barannikov and Kontsevich, 1997; Barannikov, 1999, 2000),
(b) homological mirror symmetry for Fano and general type varieties (Kontsevich, Kapustin, Katzarkov, Seidel),
(c) homological mirror symmetry for noncommutative spaces (see Bressler and Soibelman, 2002;, Kapustin and Orlov, 2001; Soibelman, 2000), and
(d) moduli space of stability structures (Bridgeland, 2002).

II. COMMUTATIVE CALABI–YAU MANIFOLDS

A. Calabi–Yau manifolds and their moduli spaces

Definition 1: *Let k be a field. A Calabi–Yau manifold over k is a smooth projective variety X having the trivial canonical bundle* $K_X = \wedge^{top} T_X^*$.

Example 1: *An Abelian variety over k is a Calabi–Yau manifold.*

For the purposes of mirror symmetry the most interesting cases are

(a) $k = \mathbf{C}$;
(b) k is a complete non-Archimedean local field, for example, $k = \mathbf{C}((q))$.

In the case (a) of the field of complex numbers one can study Calabi–Yau manifolds by means of differential geometry due to the following theorem of Yau.

Theorem 1: *Let X be a compact complex manifold,* $dim_{\mathbf{C}} X = n$, *with the trivial canonical bundle. Let* g_X *be a Kähler metric on X and* ω_X *the corresponding Kähler form. There exists a unique Kähler metric* g_X^{CY} *with the holonomy in* $SU(n)$ *such that the cohomology classes of the Kähler forms* ω_X *and* ω_X^{CY} *are the same.*

In Yau's theorem X does not have to be algebraic. The metric g_X^{CY} is called *Calabi–Yau metric*. It has vanishing Ricci curvature, i.e., in local coordinates one has $Ricci(g_X^{CY}) = \partial\overline{\partial}(\log(det(g_{ij}^{CY}))) = 0$. One can see that X admits a holomorphic volume form vol_X (trivialization of K_X) such that the wedge product $vol_X \wedge \overline{vol}_X$ coincides (up to a known scalar factor) with the Riemannian volume form given by the Kähler metric. With these properties in mind one can speak even about noncompact Calabi–Yau manifolds (unless we say otherwise, all complex Calabi–Yau manifolds will be assumed compact).

Formal deformations of the complex structure of X are described by the deformation functor $Def_X : Artin_{\mathbf{C}} \to Sets$ from the category of Artinian local algebras to the category of sets. Namely, for an Artinian local algebra A with the maximal ideal m the set $Def_X(A)$ consists of isomorphism classes of families of Calabi–Yau manifolds over $Spec(A)$ such that the fiber over $\mathbf{C} = Spec(A/m) \subset Spec(A)$ is isomorphic to X. It follows from the Bogomolov–Tian–Todorov theorem (see Bogomolov, 1978; Tian, 1987; Todorov, 1989) that this functor is pro-represented by the completed local algebra of a point of a complex manifold. In particular, the formal moduli space is unobstructed and smooth. This is true for nonformal deformations as well. In other words, the deformation functor which describes isomorphism classes of *analytic* families of Calabi–Yau manifolds, such that X is the fiber over a marked point, is represented by the germ of a complex

manifold. The structure of the global moduli space is more complicated. In the case of complex projective Calabi–Yau manifolds the moduli space is an orbifold.

One of the ideas behind homological mirror symmetry is the suggestion to extend this picture to the deformations of X within the class of "noncommutative" Calabi–Yau manifolds. Before discussing the details I would like to make few motivating comments.

(1) With a complex Calabi–Yau manifold X which has " very large volume" physicists suggest to associate two "theories" denoted by $A(X)$ and $B(X)$ (A-model and B-model). The precise meaning of these words is not important for us at this time. Roughly speaking, the theory $A(X)$ depends on the symplectic structure of X, while the theory $B(X)$ depends on the complex structure of X. It is believed that for an algebraic X there is a "dual" (or mirror symmetric) one denoted by $X^\vee$, which satisfies the following property:

The theory $A(X)$ is equivalent to the theory $B(X^\vee)$, and the theory $B(X)$ is equivalent to the theory $A(X^\vee)$.

Construction of the dual Calabi–Yau manifold $X^\vee$ is known for many X, but not in general.

The equivalence of the theories is an incarnation of mirror symmetry. Moreover, according to Witten (1999) the graded tangent space to the moduli space $\mathcal{M}^A(X)$ of formal deformations of $A(X)$ is naturally isomorphic to the cohomology space $H^\bullet(X,\mathbf{C})=\oplus_{n\geqslant 0}H^n(X,\mathbf{C})$, while the graded tangent space to the moduli space $\mathcal{M}^B(X)$ of formal deformations of $B(X)$ is isomorphic to $H^\bullet(X,\mathbf{C})=\oplus_{p,q\geqslant 0}H^p(X,\wedge^q T_X)$. Notice that the former tangent space contains $H^2(X,\mathbf{C})$ (which is the tangent space to the moduli space of deformations of complexified symplectic structure), while the latter one contains $H^1(X,T_X)$ (the tangent space to the moduli space of complex structures). Therefore $\mathcal{M}^A(X)$ and $\mathcal{M}^B(X)$ can be treated as "generalized" moduli spaces of the corresponding structures. "Mirror map" identifies $\mathcal{M}^A(X)$ with $\mathcal{M}^B(X^\vee)$, interchanging "stupid" and Hodge filtrations on the cohomology.

(2) Mathematically these observations can be (roughly) encoded in the following way (see Kontsevich, 1994; Kontsevich and Soibelman, 2000a, 2004a). To a "maximally degenerate" family $\mathcal{X}=(X_q)_{q\to 0}$ of complex Calabi–Yau manifolds one associates two "noncommutative spaces" over a non-Archimedean field k, often $k=\mathbf{C}((q))$. Let us denote these spaces by $F(\mathcal{X})$ and $D(\mathcal{X})$. The former depends on the symplectic structure of the canonically defined (singular) torus fibration, while the latter depends on the structure of rigid analytic space over k on the base of this torus fibration. The mirror dual family $\mathcal{X}^\vee=(X_q^\vee)_{q\to 0}$ defines another pair of noncommutative spaces $F(\mathrm{X}^\vee)$ and $D(\mathrm{X}^\vee)$, which are associated with the dual torus fibration. Then the homological mirror conjecture is a statement about the equivalences of noncommutative spaces

$$F(\mathcal{X})\simeq D(\mathcal{X}^\vee),$$

$$D(\mathcal{X})\simeq F(\mathcal{X}^\vee).$$

As we will see below, the noncommutative spaces $F(\mathcal{X})$ and $D(\mathcal{X})$ are described in terms of the so-called A_∞-categories, and the above statement claims an equivalence of A_∞-categories. More precisely one should take triangulated envelopes of these categories, which are in fact saturated A_∞-categories with Serre functor (see below and Kontsevich and Soibelman, 2004b).

Mirror map identifies the moduli spaces of formal deformations of $F(\mathcal{X})$ and $D(\mathcal{X}^\vee)$ [resp. $D(\mathcal{X})$ and $F(\mathcal{X}^\vee)$], and there is a cohomological description of the tangent spaces to these moduli spaces.

B. Maximal degenerations of Calabi–Yau manifolds: Algebro-geometric description

We start with the geometric side of the story following Kontsevich and Soibelman (2000a).

Let $\mathbf{C}_q^{mer}=\{f=\Sigma_{n\geqslant n_0}a_nq^n\}$ be the field of germs at $q=0$ of meromorphic functions in one complex variable and $\mathcal{X}_{mer}$ be an algebraic n-dimensional Calabi–Yau manifold over $\mathbf{C}_q^{mer}$ (i.e., $\mathcal{X}_{mer}$ is a smooth projective manifold over $\mathbf{C}_q^{mer}$ with the trivial canonical class: $K_{\mathcal{X}_{mer}}=0$). We fix

an algebraic nonvanishing volume element $vol \in \Gamma(\mathcal{X}_{mer}, K_{\mathcal{X}_{mer}})$. The pair $(\mathcal{X}_{mer}, vol)$ defines a one-parameter analytic family of complex Calabi–Yau manifolds $(X_q, vol_q), 0<|q|<r_0$, for some $r_0>0$.

Let $[\omega] \in H^2_{DR}(\mathcal{X}_{mer})$ be the cohomology class in the ample cone. Then for every q, such that $0<|q|<r_0$, it defines a Kähler class ω_q on X_q. By Yau's theorem, there exists a unique Calabi–Yau metric $g^{CY}_{X_q} := g_{X_q}$ on X_q with the Kähler class $[\omega_q]$.

It follows from the resolution of singularities that as $q \to 0$, one has the following formula:

$$\int_{X_q} vol_q \wedge \overline{vol}_q = C(\log|q|^m |q|^{2k}(1 + o(1))$$

for some $C \in \mathbf{C}^*, k \in \mathbf{Z}, 0 \leqslant m \leqslant n = dim\ (\mathcal{X}_{mer})$.

Definition 2: *We say that $\mathcal{X}_{mer}$ has maximal degeneration at $q=0$ if in the above formula we have $m=n$.*

This definition is equivalent to the algebro-geometric one, given in terms of variations of Hodge structures (see, for example, Morrison, 1993). More precisely, the following result holds.

Proposition 1 (Kontsevich and Soibelman, 2000a): The Calabi–Yau manifold $\mathcal{X}_{mer}$ has maximal degeneration iff for all sufficiently small q there exists a vector $v \in H^n(X_q, \mathbf{C})$ such that $(T - Id)^{n+1} v = 0$ and $(T - id)^n v \neq 0$, where T is the monodromy operator.

C. Differential-geometric description

The Gromov–Hausdorff metric ρ_{GH} is a metric on the set of isometry classes of compact metric spaces. We say that two metric spaces M_1 and M_2 are ε-close with respect to ρ_{GH} if there exists a metric space M containing both M_1 and M_2 as metric subspaces, such that M_1 belongs to the ε-neighborhood of M_2 and vice versa. Then $\rho_{GH}(M_1, M_2)$ is given by the infimum of such ε.

Let us rescale the Calabi–Yau metric: $g^{new}_{X_q} = g_{X_q} / diam(X_q, g_{X_q})^2$. Thus we obtain a one-parameter family of Riemannian manifolds $X^{new}_q = (X_q, g^{new}_{X_q})$ of diameter 1. Motivated by Gromov's theory of collapsing Riemannian manifolds (see, for example, Cheeger and Colding, 1997) and some considerations from conformal field theory (see Kontsevich and Soibelman, 2000a) we proposed the following conjecture.

Conjecture 1 (Gross and Wilson, 2000; Kontsevich and Soibelman, 2000a): If $\mathcal{X}_{mer}$ has maximal degeneration at $q=0$, then there exists a limit $(\overline{Y}, g_{\overline{Y}})$ of X^{new}_q in the Gromov–Hausdorff metric such that the following hold.

(a) *$(\overline{Y}, g_{\overline{Y}})$ is a compact metric space, which contains a smooth oriented Riemannian manifold (Y, g_Y) of dimension $n=dim(\mathcal{X}_{mer})$ as a dense open metric subspace. The Hausdorff dimension of $Y^{sing} = \overline{Y} \setminus Y$ is less than or equal to $n-2$.*

(b) *Y carries an integral affine structure, i.e., a torsion-free flat connection ∇ with the holonomy contained in $SL(n, \mathbf{Z})$.*

(c) *The metric g_Y has a potential, i.e., it is locally given in affine coordinates by a symmetric matrix $(g_{ij}) = (\partial^2 K / \partial x_i \partial x_j)$, where K is a smooth function (defined modulo adding an affine function, i.e., the sum of a linear function and a constant).*

(d) *In affine coordinates the metric volume element is constant, i.e., $det(g_{ij}) = det(\partial^2 K / \partial x_i \partial x_j) = const$ (the latter is called real Monge–Ampère equation).*

Example 2: *Let $E_q = \mathbf{C}^*/q^{\mathbf{Z}}, q \to 0$ be a maximally degenerate family of elliptic curves. Then $\overline{Y} = Y = \mathbf{R}/2\pi\mathbf{Z}$. Similarly, in the case of complex Abelian varieties of dimension n one gets $\overline{Y} = Y$ = flat n-dimensional torus. In the case of K3 surfaces $\overline{Y} \simeq S^2$, while Y is obtained from the sphere S^2 by removing 24 points.*

D. Monge–Ampère manifolds and geometric mirror symmetry

In this section we propose mathematical language for the geometric counterpart of mirror symmetry, which is understood as a duality of torus fibrations over the same base. We start with axiomatization of the Gromov–Hausdorff limits of Calabi–Yau manifolds discussed above [more on this "real" analog of Kähler geometry see in Kontsevich and Soibelman (2000a)].

Definition 3: *A Monge–Ampère manifold is a triple* (Y,g,∇), *where* (Y,g) *is a smooth Riemannian manifold with the metric* g, *and* ∇ *is a torsion-free flat connection on* T_Y *such that we have the following*.

(a) ∇ *defines an affine structure on* Y.
(b) *Locally in affine coordinates* $(x_1,\ldots,x_n)$ *the matrix* $((g_{ij}))$ *of* g *is given by* $((g_{ij}))=((\partial^2 K/\partial x_i \partial x_j))$ *for some smooth real-valued function* K.
(c) *The Monge–Ampère equation* $det((\partial^2 K/\partial x_i \partial x_j))=const$ *is satisfied*.

Monge–Ampère manifolds were studied (under a different name) in Cheng and Yau (1982) where it was proved that if Y is *compact*, then it is a finite cover of a torus.

Proposition 2: *For a given Monge–Ampère manifold* (Y,g_Y,∇_Y) *there is a canonically defined dual Monge–Ampère manifold* $(Y^\vee,g_Y^\vee,\nabla_Y^\vee)$ *such that* (Y,g_Y) *is identified with* $(Y^\vee,g_Y^\vee)$ *as Riemannian manifolds, and the local system* $(T_{Y^\vee},\nabla_Y^\vee)$ *is naturally isomorphic to the local system dual to* (T_Y,∇_Y).

Corollary 1: *If* ∇_Y *defines an integral affine structure on* Y *(i.e., the holonomy of* ∇_Y *belongs to* $GL(n,\mathbf{Z})$*), then* $\nabla_Y^\vee$ *defines an integral affine structure on* $Y^\vee$. *As the dual covariant lattice one takes the lattice* $(T_Y^{\mathbf{Z}})^\vee$, *which is dual to* $T_Y^{\mathbf{Z}}$ *with respect to the metric* g_Y.

Let us call *integral* Monge–Ampère manifolds with integral affine structure. Now we can state the geometric counterpart of the mirror symmetry conjecture.

Conjecture 2: *Let* X *and* $\mathrm{X}^\vee$ *be dual families of Calabi–Yau manifolds, which have maximal degeneration at* $q=0$. *Let* $M=(Y,g_Y,\nabla_Y)$ *and* $M'=(Y',g_{Y'},\nabla')$ *be smooth parts of their Gromov–Hausdorff limits (see Conjecture 1). Then* M *and* M' *are dual integral Monge–Ampère manifolds*.

Reversing the logic, one can use our conjectures as a mathematical definition of dual families of Calabi–Yau manifolds.

Remark 1: *If* $M=(Y,g_Y,\nabla_Y,T_Y^{\mathbf{Z}})$ *is an integral Monge–Ampère manifold then the total space of the torus fibration* $p:T_Y/T_Y^{\mathbf{Z}}\to Y$ *carries a canonical structure of the complex Calabi–Yau manifold (noncompact if* Y *is noncompact). It is easy to see that passing from* M *to* $M^\vee$ *amounts to the passing from the torus fibration* p *to the dual torus fibration* $p^\vee:T_Y^*/(T_Y^{\mathbf{Z}})^\vee\to Y$. *The dual potential function* $K^\vee$ *is the Legendre transform (in affine coordinates) of the potential function* K. *This picture should be compared with Strominger et al. (1996), where the special Lagrangian torus fibration structure of Calabi–Yau manifolds near the "large complex structure limit" was suggested. Our point of view is different in the following sense: we suggest to work with the limiting Monge–Ampère manifolds and their singularities. All the quantities appearing in the mirror symmetry story (like the number of rational curves on a Calabi–Yau manifold) should be computed in terms of the limiting data*.

III. A_∞-CATEGORIES AND NONCOMMUTATIVE SCHEMES

Here we only outline the geometric language A_∞-categories. See Kontsevich and Soibelman (2004b) for the details.

Let k be a commutative unital ring and $\mathcal{C}$ be a k-linear Abelian tensor category. The category of (commutative) affine schemes $Aff_{\mathcal{C}}$ is by definition the one opposite to the category $Comm_{\mathcal{C}}$ of commutative unital algebras in $\mathcal{C}$. Similarly, the category of noncommutative affine schemes in $\mathcal{C}$ (notation $NAff_{\mathcal{C}}$) is the category opposite to the category of associative unital algebras $Alg_{\mathcal{C}}$. For an algebra $A\in Ob(Alg_{\mathcal{C}})$ the corresponding noncommutative affine scheme is denoted by $Spec(A)$. Every affine scheme can be considered as a noncommutative affine scheme, so we use the same notation $Spec(A)$ for a commutative algebra A. To save the space we will discuss below mainly noncommutative affine schemes. The reader can make obvious changes for commutative affine

schemes (see also Kontsevich and Soibelman, 2004a, 2004b). Morphisms of noncommutative schemes correspond to homomorphisms of unital algebras. Our main example from now on will be the tensor category $\mathcal{C}=Vect_k^{\mathbf{Z}}$, where k is a field of characteristic zero [here we have the Quillen rule of signs: $a_ib_j=(-1)^{ij}b_ja_i$, where i and j are degrees of a_i and b_j, respectively]. Noncommutative *ind-affine* schemes by definition correspond to projective systems $((A_i)_{i\in I},\phi_{ji})$ of unital algebras in $\mathcal{C}$, such that the morphisms $\phi_{ji}:A_i\to A_j$ are surjective homomorphisms of unital algebras. Equivalently, a noncommutative ind-affine scheme is an inductive system $((X_i)_{i\in I},\psi_{ji})$ of noncommutative affine scheme, such that the morphisms $\psi_{ji}:X_i\to X_j$ are closed embeddings. Since any counital coalgebra B in $Vect_k^{\mathbf{Z}}$ is a union of finite-dimensional counital subcoalgebras, we can assign to B a noncommutative ind-affine scheme X_B.

Example 3: *(a) Let V be a $\mathbf{Z}$-graded k-vector space. Then the formal neighborhood of zero in the noncommutative affine space V_{NC}, by definition, corresponds to the cofree tensor coalgebra $T(V)=\oplus_{n\geqslant 0}V^{\otimes n}$.*

(b) Replacing $T(V)$ by $S(V)=\oplus_{n\geqslant 0}S^n(V)$ (sum of symmetric tensor powers) we arrive at the definition of the formal neighborhood of zero in the (commutative) affine space V.

This example can be generalized further. Indeed the cofree coalgebra $T(V)$ is the coalgebra of the quiver with one vertex and $N=dim_kV$ loops. Let Q be an arbitrary quiver in $Vect_k^{\mathbf{Z}}$ with the set of vertices I. Then the coalgebra B_Q of Q gives rise to a noncommutative ind-affine scheme X_{B_Q}. It contains a noncommutative closed ind-subscheme X_I of disjoint points (vertices of Q), corresponding to the direct sum of trivial coalgebras $\oplus_I k$. If I is finite, then X_{B_Q} is smooth in the sense of Cuntz and Quillen (1995). In general it is an inductive limit of noncommutative smooth affine schemes (we can call them ind-smooth for short). In any case we can speak about vector fields on X_{B_Q}. A vector field of degree n is a derivation of B_Q of degree n. Clearly vector fields on X_{B_Q} form a differential-graded Lie algebra.

Let now $X\simeq X_{B_Q}$ be an ind-affine scheme corresponding to a quiver Q, and let d be a vector field on X_Q of degree +1 which vanishes on the subscheme X_I, commutes with the natural morphisms $X\to X_I$ (projection) and $X_I\to X$ (closed embedding), and satisfies the condition $[d,d]=0$.

Definition 4: *We say that the pair (X,d) defines a noncommutative differential-graded (dg for short) ind-manifold with marked points X_I.*

Equivalently we say that X is a (nonlinear) small A_∞-*category* with the set of objects I. Assume Q has only one vertex i and N loops of various degrees. Then the coalgebra B_Q is generated by a $\mathbf{Z}$-graded N-dimensional vector space $A=\oplus_{m\in Z}A^m$ of loops $i\to i$ (degree of the trivial loop is zero, other degrees are arbitrary). Let $A[-1]$ denote the vector space A with the grading shifted by one: $A[-1]^n=A^{n-1}$. Then we say that $A[-1]$ is an A_∞-*algebra*. It is easy to see that Taylor coefficients of d at the marked point define a sequence of linear maps

$$m_n:A^{\otimes n}\to A[2-n],\quad n\geqslant 1,$$

of degree $n-2$ (higher products) satisfying a system of quadratic equations.

Analogously, a small A_∞-category $\mathcal{A}$ is defined by the set of objects I, $\mathbf{Z}$-graded spaces of morphisms $Hom_{\mathcal{A}}(X,Y)$ and a collection of higher composition maps

$$m_n:Hom_{\mathcal{A}}(X_0,X_1)\otimes\cdots\otimes Hom_{\mathcal{A}}(X_{n-1},X_n)\to Hom_{\mathcal{A}}(X_0,X_n)[2-n]$$

satisfying a system of quadratic equations (see, for example, Kontsevich and Soibelman, 2000a).

Therefore an A_∞-category is a nonlinear A_∞-category with the choice of affine structure (i.e., a quiver Q and an isomorphism $X\simeq X_{B_Q}$).

Remark 2: *For any collection of objects $(X_0,X_1,\ldots,X_r)$ the sequence $m_n, n\geqslant 1$, defines a structure of an A_∞-algebra on $\oplus_{0\leqslant i,j\leqslant r}Hom_{\mathcal{A}}(X_i,X_j)$. This A_∞-structure is compatible with inclusions of collections of objects. Then one can derive many results about A_∞-categories from similar results about A_∞-algebras.*

In the above version of A_∞-categories the space of morphisms $Hom_{\mathcal{A}}(M,N)$ is well-defined for any two objects M and N. Furthermore, for any object M there is an identity morphism $id_M\in Hom_{\mathcal{A}}(M,M)$. There are various versions of A_∞-categories in which these (or other) conditions

are weakened [for example, one can work with the identity morphisms which exist only in cohomology $H^{\bullet}(Hom_{\mathcal{A}}(M,M),m_1)$]. Moreover, there is a version of nonlinear A_∞-categories where I is a (commutative) dg ind-manifold. If we drop the condition that the vector field d vanishes at the marked points, we obtain the notions of *generalized* A_∞-algebra and A_∞-category. In this case one can have a nontrivial element m_0. See Fukaya *et al.* (2000) and Kontsevich and Soibelman (2000a, 2004a, 2004b) for some details. For simplicity of the exposition we will disregard all these difficulties below.

For two noncommutative dg ind-manifolds X and Y which correspond to the A_∞-categories $\mathcal{A}$ and $\mathcal{B}$, respectively, one can define a noncommutative dg ind-manifold $Maps(X,Y)$ of morphisms $X\to Y$. Algebraically it corresponds to the A_∞-category of A_∞-functors $Funct(\mathcal{A},\mathcal{B})$. There are explicit formulas for the A_∞-structure on $Funct(\mathcal{A},\mathcal{B})$ given in terms of the summation over the set of trees (see Kontsevich and Soibelman, 2004b).

In the next two sections we are going outline constructions of $F(\mathcal{X})$ and $D(\mathcal{X})$ (see the Introduction) in the simplest case when $\overline{Y}=Y$ (i.e., the torus fibration is nonsingular). The construction in the general case is not known.

IV. NONCOMMUTATIVE SPACE $D(\mathcal{X})$

Let $(Y,g_Y,\nabla_Y,T_Y^{\mathbf{Z}})$ be an integral Monge–Ampère manifold of dimension n. The construction consists of several steps [see Kontsevich and Soibelman (2000a) for the details].

(1) Using the affine structure on Y one defines a sheaf $\mathcal{O}_Y$ of algebras over the field $\mathbf{C}_\varepsilon$: $=\{\Sigma_{i\geqslant 0}a_i e^{-\lambda_i/\varepsilon}\,|\,a_i\in\mathbf{C},\lambda_i\in\mathbf{R},\lambda_i\to+\infty\}$. For an open chart $U\subset\mathbf{R}^n$ the algebra $\mathcal{O}_{\mathbf{R}^n}(U)$ is a vector space over $\mathbf{C}_\varepsilon$ consisting of formal Laurent series

$$f=\sum_{k_1,\ldots,k_n\in\mathbf{Z}^n} a_{k_1\cdots k_n}z_1^{k_1}\cdots z_n^{k_n},$$

where $z_1,\ldots,z_n$ are formal variables, $a_{k_1\cdots k_n}\in\mathbf{C}_\varepsilon$, and for any $(y_1,\ldots,y_n)\in U$ we have $\lim_{\Sigma_i|k_i|\to\infty}(v(a_{k_1\cdots k_n})+\Sigma_i k_i y_i)=+\infty$. Here we denote by $v:\mathbf{C}_\varepsilon\to\mathbf{R}\cup\{+\infty\}$ a (nondiscrete) valuation such that $v(\Sigma_{\lambda_1<\lambda_2<\ldots}c_i e^{-\lambda_i/\varepsilon})=\lambda_1$ if $c_1\neq 0$ and $v(0)=+\infty$.

(2) The sheaf $\mathcal{O}_Y$ admits a resolution $\hat{\Omega}_Y^*$ by a soft sheaf of dg-algebras. Locally, for a small open $U\subset Y$, sections of $\hat{\Omega}_*^Y$ are given by sums $\alpha=\Sigma_{i_1,\ldots,i_n}c_{i_1\cdots i_n}z_1^{i_1}\cdots z_n^{i_n}$ where $c_{i_1\cdots i_n}=\Sigma_j c_{j,i_1\cdots i_n}e^{-\lambda_{j,i_1\cdots i_n}/\varepsilon}$, $c_{j,i_1\cdots i_n}\in\Omega^*(U)$ (de Rham differential forms), with the same convergence conditions as for the sheaf $\mathcal{O}_Y$. Differential is given by the de Rham differential acting on the coefficients $c_{j,i_1\cdots i_n}$.

(3) We define a dg-category $D(\mathcal{X})$ such as follows. Objects are finite complexes of locally free $\mathcal{O}_Y$-modules of finite rank. For any two such complexes E_1 and E_2 we define the space of morphisms as

$$Hom(E_1,E_2)=\Gamma(Y,Hom_{\mathcal{O}_Y}(E_1,E_2)\hat{\otimes}_{\mathcal{O}_Y}\hat{\Omega}_*^Y),$$

where we use the completed tensor product on the RHS. Differential and grading on the spaces of morphisms are induced by those on $E_1,E_2,\hat{\Omega}_Y^*$.

According to the general philosophy of the previous section we interpret this dg-category as a noncommutative dg ind-manifold. Notice that in general we have to work with the non-Archimedean field $\mathbf{C}_\varepsilon$ rather than with $\mathbf{C}((q))$ (the latter can be used under some integrality conditions on $\mathcal{X}$).

Remark 3: *The above discussion indicates the relevance of non-Archimedean geometry to mirror symmetry. There are too many non-Archimedean aspects of Kähler geometry in general and mirror symmetry in particular to discuss them here. We refer the reader to Kontsevich and Soibelman (2000a, 2004c), and Kontsevich and Tschinkel (2004) for some of them. Foundational facts about non-Archimedean geometry and Berkovich spectra can be found in Berkovich (1990).*

V. NONCOMMUTATIVE SPACE $F(\mathcal{X})$

We will sketch main steps in the definition of the A_∞-category $F(\mathcal{X})$, assuming that the base Y of the torus fibration $p: T_Y/T_Y^{\mathbf{Z}} \to Y$ has dimension greater than one.

The total space V of the torus fibration carries canonical symplectic form ω, canonical metric g_V (it is invariant with respect to the natural torus action on V) and a complex structure J compatible with ω and g_V. Moreover, V carries a Calabi–Yau manifold structure.

Let $L \subset V$ be a Lagrangian submanifold such that $p_{|L}: L \to Y$ is an unramified covering.

(1) Objects of the A_∞-category $F(V)$ (the Fukaya category of V) are pairs (L, ρ) where L is a Lagrangian submanifold as above (let us call it admissible) and ρ is a local system on L. We will call L the support of the object (L, ρ).

(2) For two objects with transversal supports we define the space of morphisms such as follows:

$$Hom_{F(V)}((L_1,\rho_1),(L_2,\rho_2)) := (\oplus_{x \in L_1 \cap L_2} Hom(\rho_{1x}, \rho_{2x})) \otimes \mathbf{C}_\varepsilon.$$

There is a $\mathbf{Z}$-grading of the space of morphisms given in terms of Maslov index $deg: L_1 \cap L_2 \to \mathbf{Z}$.

(3) The A_∞-structure is defined by means of a collection of maps (higher compositions) of graded vector spaces

$$m_k^{F(V)}: \otimes_{0 \leqslant i \leqslant k-1} Hom_{F(V)}((L_i,\rho_i),(L_{i+1},\rho_{i+1})) \to Hom_{F(V)}((L_0,\rho_0),(L_k,\rho_k))[2-k],$$

where $k \geqslant 1$ and the sequence $(L_0, \ldots, L_k)$ corresponds to a "transversal" sequence of objects of $F(V)$.

In the case, when all local systems are trivial of rank one, the map m_k is defined such as follows. Let D be a standard disc $D = \{z \in \mathbf{C} \,|\, |z| \leqslant 1\}$. Let us fix a sequence $(L_0, \ldots, L_k)$ of supports of objects with pairwise transversal intersections, intersection points $x_i \in L_i \cap L_{i+1}, 0 \leqslant i \leqslant k-1$, $x_k \in L_0 \cap L_k$, and $\beta \in \pi_2^{free}(V, \cup_{0 \leqslant i \leqslant k} L_i)$. We denote by $\mathcal{M}(L_0, \ldots, L_k; x_0, \ldots, x_k; \beta)$ the set of collections $(y_0, \ldots, y_k; \psi)$, where $y_i, 0 \leqslant i \leqslant k$ are cyclically ordered pairwise distinct points on the boundary ∂D, and $\psi: D \to (V, J)$ a pseudo-holomorphic map such that $\psi(y_i) = x_i$, $\psi(\overline{y_i y_{i+1}}) \subset L_i, 0 \leqslant i \leqslant k, y_0 = y_k$, $[\psi] = \beta$. Here $\overline{y_i y_{i+1}}$ denotes the arc between y_i and y_{i+1}. There is a natural action of $PSL(2, \mathbf{R})$ on $\mathcal{M}(L_0, \ldots, L_k; x_0, \ldots, x_k; \beta)$ arising from the holomorphic action on D by fractional linear transformations. The action is free except for the case $k=1, x_0 = x_1, \beta = 0$, which is not relevant for our purposes.

Let $x_i \in L_i \cap L_{i+1}, 0 \leqslant i \leqslant k-1, x_k \in L_0 \cap L_k$ satisfy the condition $deg\ x_k = \Sigma_{0 \leqslant i \leqslant k-1} deg\ x_i + 2 - k$. Then the matrix element $(m_k(x_0, x_1, \ldots, x_{k-1}), x_k)$ is given by the formula $(m_k(x_0, x_1, \ldots, x_{k-1}), x_k) = \Sigma \pm q^{(\beta, [\omega])}$, where $q = \exp(-1/\varepsilon)$, and the sum is taken over all $PSL(2, \mathbf{R})$-orbits of points in $\mathcal{M}(L_0, \ldots, L_k; x_0, \ldots, x_k; \beta)$. Signs are derived from orientations of certain cycles in the moduli space

$$\mathcal{M} = \mathcal{M}(L_0, \ldots, L_k; x_0, \ldots, x_k; \beta)/PSL(2, \mathbf{R}).$$

The precise definition depends on some other choices [see Fukaya *et al.* (2000) and Kontsevich and Soibelman (2000a) for more details].

(4) The dilation of the lattice $T_Y^{\mathbf{Z}}$ by a parameter η such that $(y, v) \mapsto (y, \eta v), y \in Y, v \in T_y Y$, gives rise to a family of complex structures J_η on V (and the corresponding family of holomorphic volume forms Ω_η). In this way one obtains a family of A_∞-categories with the same objects and morphisms as $F(V)$, but with varying higher compositions $m_n^\eta, n \geqslant 1$. Moreover, one can prove that there exist limits $m_n^\infty = \lim_{\eta \to 0} m_n^\eta$ and they give rise to an A_∞-category, which we denote by $F(\mathcal{X})$ and call the *Fukaya-Oh category*. See Kontsevich and Soibelman (2000a), where its relation to the Morse theory is discussed and an important conjecture from Fukaya and Oh (1998) was proved. Furthermore, it was used in Kontsevich and Soibelman (2000a) for the proof of a version of homological mirror conjecture for Abelian varieties.

Remark 4: *In the above sketch we skip several important points. In particular, there is an*

obvious problem with identity morphisms and nontransversal Lagrangian supports of objects. Also, it is possible to have a Lagrangian submanifold $L\subset V$ and a pseudo-holomorphic disc D with the boundary $\partial D\subset L$. This creates the so-called "m_0-problem" in the definition of the Fukaya category, and requires a generalization of the notion of A_∞-category we mentioned before. We again refer the reader to Fukaya et al. (2000) and Kontsevich and Soibelman (2000a, 2004a, 2004b) for the discussion on how to overcome these (and some other) difficulties in the definition of the Fukaya category.

VI. DEFORMATION THEORY OF A_∞-CATEGORIES

Deformation theory of $F(\mathcal{X})$ and $D(\mathcal{X})$ is a special case of the deformation theory of A_∞-categories (or, more generally, noncommutative dg ind-manifolds). We are going to illustrate it in the case of the category with one object, since the general case is similar (see Kontsevich, 1994; Kontsevich and Soibelman, 2004a, 2004b).

Let A be a $\mathbf{Z}$-graded vector space over the field k of characteristic zero. We denote by $C^\bullet(A,A)=\Pi_{n\geqslant 0}\, Hom_{Vect_k^{\mathbf{Z}}}(A^{\otimes n},A)$ the graded space of *Hochschild cochains*. Shifting the grading by 1 we can introduce a graded Lie algebra structure on $C^\bullet(A,A)[1]=\Pi_{n\geqslant 0}(C^\bullet(A,A)[1])^n$. The Lie bracket is called the *Gerstenhaber bracket*. It has the following well-known geometric interpretation. Consider the formal neighborhood of zero in the noncommutative affine space $A[1]$. Then $C^\bullet(A,A)[1]$ is the graded Lie algebra of vector fields on this neighborhood. It contains the graded Lie subalgebra $C^\bullet_+(A,A)[1]$ of vector fields preserving zero. Algebraically these graded Lie algebras are interpreted as derivations of the corresponding tensor coalgebras generated by $A[1]$. To have a structure of an $\mathcal{A}_\infty$-algebra on A is the same as to have an element $m\in C^\bullet_+(A,A)[1]$ of degree +1 such that $[m,m]=0$ where $[x,y]$ denotes the Gerstenhaber bracket of x and y. To have a structure of an A_∞-category A with one object X such that $Hom_{\mathcal{A}}(X,X)=A$ means the same thing but this time $m\in C^\bullet(A,A)[1]$. In the latter case we can have a nontrivial $m_0\in Hom_{Vect_k^{\mathbf{Z}}}(k,A)$. In either case m gives rise to a structure of differential-graded Lie algebra (DGLA for short) on $C^\bullet(A,A)[1]$. In the case of the category with one object it is the structure of DGLA on $C^\bullet(A,A)[1]$, with the differential $d=d_m=[m,\bullet]$. The pair $(C^\bullet(A,A)[1],d)$ is called the *Hochschild complex* of the category (the terminology is slightly abused because we care not only about structure of a complex, but also about the Lie bracket). The cohomology of this complex is called the *Hochschild cohomology* and is denoted by $HH^\bullet(A,A)$. The pair $(C^\bullet_+(A,A)[1],d)$ is called the *truncated* Hochschild complex. The same terminology is applied to the A_∞-algebra A.

Definition 5: *The deformation functor associated with the DGLA $(C^\bullet(A,A)[1],d)$ is the functor $Def_A: Artin_k\to Sets$ from the category of Artinian local k-algebras to sets, such that for an Artinian algebra R with the maximal ideal m_R the set $Def_A(R)$ consists of classes of equivalence of solutions $\gamma\in(C(A,A)[1])^1\otimes m_R$ to the Maurer–Cartan equation*

$$d\gamma+\tfrac{1}{2}[\gamma,\gamma]=0,$$

modulo the following action of the group $\exp((C(A,A)[1])^0\otimes m_R)$:

$$\gamma\mapsto g\gamma g^{-1}-dg\cdot g^{-1}.$$

Geometrically, the deformation functor can be interpreted in the following way. Let $g=C^\bullet(A,A)[1]$ be our DGLA. Then the cocommutative cofree coalgebra $C(g[1])=\oplus_{n\geqslant 0}S^n(g[1])$ gives rise to a (commutative) ind-affine scheme (in fact, formal manifold) with the marked point zero. The differential d gives rise to a vector field $d_{g[1]}$ in the formal neighborhood of zero. Higher compositions (products) m_n are Taylor coefficients of the vector field $d_{g[1]}$ at zero. In particular, if $m_0\neq 0$, then the vector field does not vanish at zero. The Maurer–Cartan equation singles out the formal subscheme Z of zeros of the vector field [more precisely it gives R-points $Z(R)$ for every $R\in Artin_k$]. Suppose $0\in Z(R)$. Then for any local Artinian ring R we obtain an A_∞-category $\mathcal{A}(R)$ such that the set of objects $Ob(\mathcal{A}(R))$ is $Z(R)$ and the A_∞-structure defined by $m+\gamma$, where m is the

A_∞-structure on $\mathcal{A}$ and γ is a solution to the Maurer–Cartan equation. Therefore the DGLA $g = C^\bullet(A,A)[1]$ gives rise to the deformation functor describing the formal deformation theory of the A_∞-category with one object.

The ind-affine scheme Z admits a (singular) foliation: two points γ and γ' of $Z(R)$ belong to the same leaf of the foliation iff they can be joined by the curve which is tangent to the distribution $[d_{g[1]}, \bullet]$ (see Kontsevich, 1997; Kontsevich and Soibelman, 2004a, 2000b). This construction gives rise to a functor isomorphic to Def_A.

The same considerations apply to general A_∞-categories. Deformation theory of an A_∞-algebra structure on a fixed graded vector space A is controlled by the DGLA $g_+ = C^\bullet_+(A,A)[1]$.

The notion of *quasi-isomorphism* of noncommutative (or commutative) dg ind-manifolds corresponds to the notion of quasi-isomorphism of the corresponding differential-graded coalgebras. The following result explains the role of this notion.

Theorem 2 (Kontsevich, 1997; Kontsevich and Soibelman, 2004a): *Quasi-isomorphic dg ind-manifolds with marked points give rise to isomorphic deformation functors.*

In other words, the corresponding deformation theories are equivalent. If a dg ind-manifold has an affine structure at the marked point (i.e., if an explicit isomorphism of coalgebras $B \simeq S(V[1])$ is chosen), then V is called an L_∞-algebra (or homotopy Lie algebra). Often the above notion of quasi-isomorphism refers directly to V. If V is quasi-isomorphic to an L_∞-algebra with the trivial structure, then the deformation functor is especially simple (since the Maurer–Cartan equation is empty). In this case the formal moduli space is smooth (example: formal moduli space of deformations of the complex structure on a Calabi–Yau manifold).

The structure of the tangent space to the moduli space of deformations of an A_∞-category is described in the following two results (see Kontsevich and Soibelman, 2004b).

Theorem 3: *Let X be a noncommutative dg ind-manifold corresponding to an A_∞-algebra A, and $CC^\bullet(A,A) := CC^\bullet(X,X)$ be the Hochschild cochain complex. Then one has the following quasi-isomorphism of complexes*

$$CC^\bullet(X,X)[1] \simeq T_{[id_X]}(Maps(X,X)),$$

where $T_{[id_X]}$ denotes the tangent complex at the identity map.

Corollary 2: *Let $\mathcal{A}$ be an A_∞-category with finite-dimensional Hochschild cohomology. Then*

$$HH^\bullet(\mathcal{A},\mathcal{A}) \simeq Ext^\bullet(Id_{\mathcal{A}}, Id_{\mathcal{A}}),$$

where the RHS denotes the cohomology of the tangent complex at the identity functor $Id_{\mathcal{A}}$ [we consider the identity functor as the identity map $id_X \in Maps(X,X)$, where X is the noncommutative dg ind-manifold corresponding to the A_∞-category $Funct(\mathcal{A},\mathcal{A})$].

Let me demonstrate how these results can be applied to homological mirror symmetry. Under the assumption $\overline{Y} = Y$ one can compute the Hochschild cohomology of the A_∞-categories $D(\mathcal{X})$ and $F(\mathcal{X})$ in terms of the torus fibration $p: T_Y/T_Y^{\mathbf{Z}} \to Y$. The total space V of the torus fibration is a symplectic manifold. Then (see Kontsevich, 1994) $HH^\bullet(F(\mathcal{X}),F(\mathcal{X})) \simeq Ext^\bullet_{F(V\times V)}(\Delta,\Delta)$, where $\Delta \subset V \times V$ is the diagonal, considered as a Lagrangian submanifold, equipped with the trivial local system. Similarly $HH^\bullet(D(\mathcal{X}),D(\mathcal{X})) \simeq Ext^\bullet_{D(V\times V)}(\mathcal{O}_\Delta,\mathcal{O}_\Delta)$. In both cases the cohomology groups can be computed (see Kontsevich, 1994) and coincide with the total cohomology of V, graded as in the Introduction. The Fukaya category gives rise to the quantum cohomology product on $H^\bullet(X)$. The equivalence of A_∞-categories $F(\mathcal{X})$ and $D(\mathcal{X}^\vee)$ implies the existence of the mirror map between the moduli spaces of their formal deformations. More explicitly, the equivalence $F(\mathcal{X}) \simeq D(\mathcal{X}^\vee)$ is given by a combination of the Legendre transform along Y with the non-Archimedean analog of the Fourier–Mukai transform along fibers of the torus fibration (see Kontsevich and Soibelman, 2000a).

Remark 5: *The A_∞-category $F(\mathcal{X})$ is a "generic fiber" of the one-parameter deformation of the "trivial" A_∞-category $F_{triv}(\mathcal{X})$. Objects and morphisms of $F_{triv}(\mathcal{X})$ are the same as for $F(\mathcal{X})$. All compositions $m_n^{F_{triv}(X)}, n \geqslant 0$, are equal to zero. This observation follows from the fact that $F(\mathcal{X})$*

can be actually defined over the ring $\mathbf{C}_\varepsilon^+ \subset \mathbf{C}_\varepsilon$ *consisting of formal series with all non-negative* λ_i. *Moreover, all higher compositions* m_n *are given by formal series which start with* $\exp(-\lambda/\varepsilon), \lambda > 0$. *Hence they vanish modulo the ideal J consisting of such series (assuming certain integrality conditions we have a formal family over* $\mathbf{C}[[q]]$, *and all* m_n *vanish modulo* $q\mathbf{C}[[q]]$).

VII. SATURATED A_∞-CATEGORIES AND NONCOMMUTATIVE CALABI–YAU MANIFOLDS

For an A_∞-category $\mathcal{A}$ there exists its *triangulated envelope* $\mathcal{A}^{tr}$, which is a *triangulated* A_∞-category [see Appendix B and Kontsevich and Soibelman (2004b)]. The category of complexes is an A_∞-category, and it is triangulated. The A_∞-category $D(\mathcal{X}) = D(\mathcal{X})^{tr}$ is triangulated, but $F(\mathcal{X})$ is not. Replacing the latter by its triangulated envelope (called the category of twisted complexes) one can formulate the homological mirror conjecture as an equivalence $F(\mathcal{X})^{tr} \simeq D(\mathcal{X}^\vee)^{tr}$. The dg-category $D(\mathcal{X})$ is an A_∞-version of the derived category of coherent sheaves on the rigid analytic space $(Y, \mathcal{O}_Y)$ (remember that we are discussing the case $\overline{Y} = Y$). Both categories $F(\mathcal{X})^{tr}$ and $D(\mathcal{X})$ possess the Serre duality: for any two objects M and N one has a functorial isomorphism $Hom(M,N)^* \simeq Hom(M, N[2dim_{\mathbf{R}} Y])$ (see Kontsevich, 1994). Furthermore, the A_∞-category $D(\mathcal{X})$ is saturated [see Appendix B and Kontsevich and Soibelman (2004b)]. Homological mirror symmetry predicts an equivalence of triangulated A_∞-categories compatible with the dualities. The last observation can be used for the following approach to the proof of homological mirror conjecture.

(1) Construct a collection of objects $(M_i)_{i \in I}$ in $F(\mathcal{X})$ which generate $F(\mathcal{X})^{tr}$.
(2) Construct the mirror functor $\varphi: F(\mathcal{X}) \to D(\mathcal{X}^\vee)$.
(3) Prove that the minimal triangulated subcategory of $D(\mathcal{X}^\vee)$, which contains all $\varphi(M_i)$, contains also the generator of $D(\mathcal{X}^\vee)$. Then φ provides the desire equivalence.

For example, one can take as $(M_y)_{y \in Y}$ the set of Lagrangian tori which are fibers of the torus fibration $p: T_Y / T_Y^{\mathbf{Z}} \to Y$. Then $\varphi(M_y)$ is a torsion sheaf. Such sheaves generate the A_∞-category $D(\mathcal{X})$. This idea can be used even in the case of a singular torus fibration.

Motivated by all that, one can try to extend homological mirror symmetry to the world of noncommutative spaces. In particular, one needs to define a noncommutative analog of Calabi–Yau manifold. Recall [see Appendix B and Kontsevich and Soibelman (2004b)] that if $\mathcal{A}$ is a triangulated A_∞-category, then the *Serre functor* is an A_∞-autoequivalence $S: \mathcal{A} \to \mathcal{A}$ of triangulated A_∞-categories, such that for any two objects M, N one has a functorial isomorphism

$$Hom_{\mathcal{A}}(M,N)^* \simeq Hom_{\mathcal{A}}(N, S(M)).$$

It is well-known that if X is a smooth projective variety over a field k and $\mathcal{A} = D^b(X)$ is the bounded derived category of coherent sheaves (or rather $\mathcal{A}$ is the A_∞-version of $D^b(X)$, constructed via complexes of perfect sheaves), then $S(F^\bullet) = F^\bullet \otimes K_X[dim\ X]$ is a Serre functor. If X is a Calabi–Yau manifold, then the canonical sheaf K_X is trivial, and the Serre functor reduces to the shift by the dimension. This motivates the following definition.

Definition 6: *(a) A noncommutative Calabi–Yau manifold of dimension d (a.k.a. Calabi–Yau category) is a saturated* A_∞*-category* $\mathcal{A}$ *which carries a Serre functor S such that* $S \simeq [d], d \in \mathbf{Z}_+$.

(b) A fractional noncommutative Calabi–Yau manifold of dimension d is defined as in (a) with the last condition being replaced by $S^m \simeq [dm]$ *for* $d \in \mathbf{Z}_+$ *and some integer* $m \geqslant 1$.

The notion of fractional Calabi–Yau manifold can be useful even in the commutative case. Fractional Calabi–Yau manifolds can appear as derived categories of coherent sheaves on orbifolds or derived categories of representations of oriented quivers. Hopefully the homological mirror symmetry is a fact about the (properly defined) moduli space (stack) of noncommutative Calabi–Yau manifolds. The reader can think that "commutative" points of this moduli space (i.e., ordinary Calabi–Yau manifolds) are similar to the commutative algebras as points in the moduli space of all associative (or A_∞ algebras) (see Kontsevich, 1997; Kontsevich and Soibelman,

2000b). This analogy implies that the tangent space to the moduli space of A_∞-deformations of a "commutative" Calabi–Yau manifold should carry a structure of 2-algebra [Deligne's conjecture, see Kontsevich and Soibelman (2000b)].

VIII. DEFORMATION THEORY OF A_∞-CATEGORIES WITH SERRE DUALITY

Let X be a noncommutative complex dg ind-manifold corresponding to a small A_∞-category $\mathcal{A}$. The moduli space of formal deformations of $\mathcal{A}$ is a (commutative) dg ind-manifold $\mathcal{M}_X$ with the marked point $[X] \in \mathcal{M}_X$. The tangent space $T_{[X]}\mathcal{M}_X$ is isomorphic to the Hochschild cohomology (Corollary 2): $HH^\bullet(\mathcal{A},\mathcal{A}) \simeq \oplus_{i\geqslant 0} Ext^i_{Funct}(Id_\mathcal{A}, Id_\mathcal{A})$, where $Funct = Funct(\mathcal{A},\mathcal{A})$ denotes the A_∞-category of A_∞-functors. It turns out that if $\mathcal{A}$ possesses the Serre duality (in particular if X is a noncommutative Calabi–Yau manifold), then one can say more. We are going to sketch the main idea below in the case of an A_∞-algebra A with a nondegenerate trace. We skip the definition of a trace in the A_∞-case. The reader can think of A as an associative algebra. In this case the definition of a trace is obvious. Let $\mathcal{M}_{A,trace}$ denote the moduli space of deformations of A as an A_∞-algebra with a trace, while $\mathcal{M}_A$ denotes the moduli space of its deformations as an A_∞-algebra. There is natural (forgetful) morphism of dg ind-manifolds with marked points, $f: \mathcal{M}_{A,trace} \to \mathcal{M}_A$. It is easy to see that $T_{[A]}\mathcal{M}_{A,trace} \simeq HC_\bullet(A) \simeq HC^\bullet(A)$, where $HC_\bullet$ and $HC^\bullet$ denotes the cyclic homology and cohomology, respectively (they can be identified by means of the trace). It is well-known that $HC^\bullet(A)$ is a module over $HC^\bullet(\mathbf{C}) \simeq H^\bullet(\mathbf{CP}^\infty) \simeq \mathbf{C}[u]$. For the periodic cyclic cohomology $HP^\bullet(A)$ one has $HP^\bullet(A) \simeq HC^\bullet(A) \otimes_{HC^\bullet(\mathbf{C})} \mathbf{C}$. Hence we have a family of vector spaces over the line $\mathbf{C}$. The fiber over $u \neq 0$ is isomorphic to $HP^\bullet(A)$, and the fiber over $u=0$ is isomorphic to the Hochschild cohomology $HH^\bullet(A,A)$. Then for any $u \neq 0$ we have a linear map $HC^\bullet(A) = T_{[A]}\mathcal{M}_{A,trace} \to HP^\bullet(A)$, i.e., to a one-form α on $\mathcal{M}_{A,trace}$ with values in $HP^\bullet(A)$.

Conjecture 3: *The one-form α is closed.*

If the conjecture is true, then locally $\alpha = dg_u$ for some function g_u. This gives us a map $g_u: \mathcal{M}_{A,trace} \to HP^\bullet(A) \simeq HP_\bullet(A)$ which is defined up to a constant.

Conjecture 4: *This map gives rise to an embedding of $\mathcal{M}_{A,trace}$ in the affine space, with the underlying vector space being the space of sections of a vector bundle on* $\mathbf{C}$ *with the fiber over $u \neq 0$ isomorphic to $HP_\bullet(A)$.*

Corollary 3: *There is a family of dg ind-manifolds $(\mathcal{M}_A^u)_{u\in\mathbf{C}}$ such that $\mathcal{M}_A^{u=0} \simeq \mathcal{M}_A$ and $\mathcal{M}_A^{u\neq 0}$ carries an affine structure with the pole of first order at $u=0$.*

The grading on the tangent space $T_{[A]}\mathcal{M}_A \simeq HH^\bullet(A,A)$ arises as the limit of filtrations on the tangent spaces to $\mathcal{M}_A^u, u \neq 0$.

It is natural to expect that the mirror functor extends to an isomorphism of the one-parameter families of dg ind-manifolds $\mathcal{M}_A^u$, constructed for $F(\mathcal{X})$ and $D(\mathcal{X}^\vee)$. It gives not only an isomorphism of moduli spaces at $u=0$ [i.e., equivalences of A_∞-categories $F(\mathcal{X})$ and $D(\mathcal{X}^\vee)$ and the moduli spaces of their formal deformations] but also identifies the corresponding Hodge structures arising from the filtrations on the tangent space to $\mathcal{M}_A^u, u \neq 0$ (see Barannikov, 1999), Sec. V, where the "holomorphic" side of the story was considered).

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APPENDIX A: MODULI SPACE OF CONFORMAL FIELD THEORIES

It was first suggested in Kontsevich and Soibelman (2000a) that mirror symmetry should be treated in the framework of collapsing conformal field theories, thus making yet another link to noncommutative geometry. Here we recall very briefly the data of CFT.

Unitary conformal field theory (abbreviated by CFT below) is well-defined mathematically. It is described by the following data:

(1) A real number $c \geqslant 0$ called central charge.
(2) A bi-graded pre-Hilbert *space of states* $H=\oplus_{p,q\in \mathbf{R}_{\geqslant 0}} H^{p,q}, p-q\in \mathbf{Z}$ such that $dim(\oplus_{p+q\leqslant E} H^{p,q})$ is finite for every $E\in \mathbf{R}_{\geqslant 0}$. Equivalently, there is an action of the Lie group $\mathbf{C}^*$ on H, so that $z\in \mathbf{C}^*$ acts on $H^{p,q}$ as $z^p\overline{z}^q := (z\overline{z})^p \overline{z}^{q-p}$.
(3) An action of the product of Virasoro and anti-Virasoro Lie algebras $Vir\times \overline{Vir}$ (with the same central charge c) on H, so that the space $H^{p,q}$ is an eigenspace of the generator L_0 (resp. $\overline{L_0}$) with the eigenvalue p (resp. q).
(4) The space H carries some additional algebraic structures derived from the operator product expansion (OPE). The OPE is described by a linear map $H\otimes H\to H\hat{\otimes}\mathbf{C}\{z,\overline{z}\}$. Here $\mathbf{C}\{z,\overline{z}\}$ is the topological ring of formal power series $f=\Sigma_{p,q}\, c_{p,q} z^p\overline{z}^q$ where $c_{p,q}\in \mathbf{C}, p,q\to +\infty, p,q \in \mathbf{R}, p-q\in \mathbf{Z}$. The OPE satisfies a list of axioms [see Gawedzki (2000) for the details].

For a given CFT one can consider its group of symmetries (i.e., the group of automorphisms of the space $H=\oplus_{p,q} H^{p,q}$ preserving all the structures). Conjecturally the group of symmetries is a compact Lie group of dimension less than or equal to $dim\ H^{1,0}$.

Let us fix real numbers $c_0\geqslant 0$, $E_{min}>0$, and consider the moduli space $\mathcal{M}_{c\leqslant c_0}^{E_{min}}$ of all irreducible CFTs with the central charge $c\leqslant c_0$ and

$$min\{p+q>0 | H^{p,q}\neq 0\}\geqslant E_{min}.$$

It is expected that $\mathcal{M}_{c\leqslant c_0}^{E_{min}}$ is a compact real analytic stack of finite local dimension. The dimension of the base of the minimal versal deformation of a given CFT is less than or equal to $dim\ H^{1,1}$. We define $\mathcal{M}_{c\leqslant c_0}=\cup_{E_{min}>0}\mathcal{M}_{c\leqslant c_0}^{E_{min}}$. It is natural to compactify this stack by adding boundary components corresponding to certain asymptotic degenerations of the theories with $E_{min}\to 0$. Conjecturally, the compactified space is a compact stack $\overline{\mathcal{M}}_{c\leqslant c_0}$. We will loosely use the word "space" instead of the word "stack."

Remark 6: *Mirror symmetry is related to $N=2$ superconformal field theories (SCFTs). There is a version of the above data and axioms for SCFT. In that case each $H^{p,q}$ is a Hermitian super vector space. There is an action of the super extension of the product of Virasoro and anti-Virasoro algebra on H. We will not distinguish between CFTs and SCFTs, because except for some minor details, main conclusions are true in both cases. The $N=2$ analog of the compactified moduli space will be denoted by $\overline{\mathcal{M}}_{c\leqslant c_0}^{N=2}$.*

Physicists believe that to a Calabi–Yau manifold X of "large volume" one can assign an $N=2$ superconformal field theory, denoted by *SCFT(X)*. The construction assumes some other choices [like the so-called *B*-field, which can be thought of as an element of $H^2(X,\mathbf{R}/\mathbf{Z})$]. Calabi–Yau manifolds X and $X^\vee$ are called dual if $SCFT(X)$ is equivalent to $SCFT(X^\vee)$. One can think of $SCFT(X)$ as the "noncommutative extension" of X. Central charge plays a role of the dimension. Compactified moduli space $\overline{\mathcal{M}}_{c\leqslant c_0}^{N=2}$ contains the moduli space of Calabi–Yau manifolds of the fixed dimension as a boundary stratum. In other words, targets for sigma models can be thought of as "commutative degenerations at infinity" of the noncommutative spaces.

Observation that $SCFT(X)$ does not determine the underlying Calabi–Yau manifold gives a striking parallel to the fact that the derived category of coherent sheaves of a projective variety does not determine it up to an isomorphism if K_X is trivial [see Bondal and Orlov (2002) about the philosophy of replacing a projective variety by the derived category of coherent sheaves on it]. The importance of the derived categories in homological mirror symmetry was recognized by Kontsevich at the early stage of his program (see Kontsevich, 1994).

APPENDIX B: TRIANGULATED AND SATURATED A_∞-CATEGORIES

The material of this section is largely borrowed from Kontsevich and Soibelman (2004b).

First we will define pairs of A_∞-categories (in fact dg-categories) $C_1^{(i)}, C_2^{(i)}, 1 \leqslant i \leqslant 5$.

(1) The category $C_1^{(1)}$ is the empty category with no objects.

The category $C_2^{(1)}$ has one object F such that $Hom(F,F)=0$.

(2) The category $C_1^{(2)}$ is an A_∞-category with two objects E_1, E_2 such that $Hom(E_i,E_j)=0$ for $i \neq j$, and $Hom(E_i,E_i)=k$ for all i,j.

The category $C_2^{(2)}$ has three objects F_1, F_2, F such that $Hom(F_i,F_j) \simeq Hom(E_i,E_j)$ and $Hom(F,F_1)=Hom(F,F_2)=Hom(F_1,F)=Hom(F_2,F)=k, Hom(F,F)=k \oplus k$.

(3) The category $C_1^{(3)}$ has one object E_1 such that $Hom(E_1,E_1)=k$.

The category $C_2^{(3)}$ has three objects F_0, F_1, F_{-1} such that $Hom(F_i,F_j)=k[i-j]$ for all i,j.

The differentials on the morphisms are zero in all cases 1–3.

(4) The category $C_1^{(4)}$ has two objects E_1, E_2 such that $Hom(E_1,E_1)=0$ and all other spaces of morphisms are isomorphic to the ground field k.

Differentials are trivial on the spaces of morphisms.

The category $C_2^{(4)}$ has three objects F_1, F_2, F such that $Hom(F_i,F_j) \simeq Hom(E_i,E_j)$ for all i,j. We set $Hom(F_1,F)=k$ with the trivial differential, and $Hom(F_2,F)=k[1] \oplus k$. Furthermore, $Hom(F,F_1)=k \oplus k[-1], Hom(F,F_2)=k[-1], Hom(F,F)=k \oplus k \oplus k[-1]$.

Differentials on the spaces of morphisms are defined in such a way that $F=F_1[1] \oplus F_2$ with the differential corresponding to the cone of a morphism. For example, $Hom(F_2,F)=k[1] \oplus k$ carries the differential d such that $d(1_{k[1]})=1_k$.

(5) The category $C_1^{(5)}$ has one object E_1 such that $Hom(E_1,E_1)=k[p]/(p^2-p)$, where $deg\ p=0$.

The category $C_2^{(5)}$ has two objects F_1, F such that $Hom(F_1,F_1)=k[p]/(p^2-p), deg\ p=0$ and all other spaces of morphisms are equal to the ground field k.

The differentials are trivial for these categories.

Obviously there are A_∞-functors $\phi_i: C_1^{(i)} \to C_2^{(i)}, 1 \leqslant i \leqslant 5$, such that $\phi_i(E_j)=F_j$ for all j. The functors ϕ_i are faithful (i.e., induce embeddings on the zero cohomologies of the complexes of morphisms).

Definition 7: *We say that an A_∞-category $\mathcal{A}$ satisfies the Axiom i, $1 \leqslant i \leqslant 5$, if the induced A_∞-functor $\phi_i^*: Funct(C_2^{(i)}, \mathcal{A}) \to Funct(C_1^{(i)}, \mathcal{A})$ is an equivalence of A_∞-categories of functors*.

We say that the category $\mathcal{A}$ is triangulated if it satisfies Axioms 1–5.

Axioms 1–5 have special names:

Axiom 1: Existence of a zero object of the category.

Axiom 2: Existence of the direct sum of two objects.

Axiom 3: Existence of shifts of an object.

Axiom 4: Existence of a cone of a morphism.

Axiom 5: Splitting of the image of a projector.

Motivations for these names are self-evident from the definitions [for example, in the case of Axiom 5 one thinks of the object F as of $p(F_1)$].

Similarly to the conventional theory of triangulated and derived categories one can define the notion of a thick subcategory of a triangulated A_∞-category. Then one can embed an A_∞-category $\mathcal{C}$ into the A_∞-category $\hat{\mathcal{C}}=Funct(\mathcal{C}^{op}, \mathbf{K})$, where $\mathbf{K}$ is the category of complexes of k-vector spaces. The embedding A_∞-functor Yo is an A_∞-analog of the Yoneda functor. Finally, an A_∞-category $\mathcal{C}$ is triangulated iff its image $Yo(\mathcal{C})$ is a thick subcategory of $\hat{\mathcal{C}}$ [see Kontsevich and Soibelman (2004b) for the details].

Let $\mathcal{C}$ be a triangulated A_∞-category over k.

Definition 8: *We say that $\mathcal{C}$ is saturated if the following properties are satisfied*:

(1) *For any* $E,F \in Ob(\mathcal{C})$ *and one has* $\Sigma_{n\in\mathbf{Z}} dim(Hom(E,F[n])) < \infty$.
(2) *The identity functor* $Id_{\mathcal{C}}$ *belongs to the smallest triangulated category generated by the image of the natural bifunctor* $\Psi \in Bifunct((\mathcal{C}^{op},\mathcal{C}),Funct(\mathcal{C},\mathcal{C}))$ *such that* $\Psi(X,Y)(Z) = Hom_C(X,Y)\otimes Z$ *for any* $X,Y,Z \in Ob(\mathcal{C})$.

Definition 9: *The triangulated envelope of a set of objects of a triangulated* A_∞*-category is the minimal triangulated subcategory containing this set of objects*.

The triangulated envelope consists of images of projectors of finite extensions of shifts of given objects. Then we can say that the condition (2) above means that the identity functor belongs to the triangulated envelope of the set $\Psi(Ob(\mathcal{C}))$. Let us denote by S^{tr} the triangulated envelope of the set S. If $S=\{F\}$ consists of one object F, we say that F is a *generator* of the category.

Proposition 3: *If* $\mathcal{C}$ *is saturated, then it has a generator*.

Example 4: *Let* A *be an* A_∞*-algebra. The category* $A-mod$ *of* A_∞*-modules over* A *is saturated iff* A *is a perfect* A*-*A*-bimodule, i.e., as an* A_∞*-bimodule* A *is isomorphic to a direct summand of an extension of the sequence* $(A^{op}\otimes A)[n_i], n_i \in \mathbf{Z}$ *(in the category of bimodules)*.

Example 5 (Kontsevich, 1994, 1997; Seidel, 2000): Let X *be a Calabi–Yau manifold,* $f: X \to \mathbf{CP}^1$ *be a holomorphic map which has only isolated singularities. Assume that the generic fiber of* f *is a Calabi–Yau manifold* $Y, dim_{\mathbf{C}} Y > 2$. *Then the triangulated envelope of the Fukaya category* $F(Y)$ *is saturated. [Hint: it is generated by the Lagrangian spheres vanishing at the critical points. Indeed the shift functor* $E \mapsto E[2]$ *(monodromy at infinity) can be represented as a product of reflections at the vanishing spheres. It follows that the identity functor belongs to the triangulated envelope of the set of vanishing Lagrangian spheres.]*

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Integrable renormalization I: The ladder case

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In recent years a Hopf algebraic structure underlying the process of renormalization in quantum field theory was found. It led to a Birkhoff factorization for (regularized) Hopf algebra characters, i.e., for Feynman rules. In this work we would like to show that this Birkhoff factorization finds its natural formulation in terms of a classical r-matrix, coming from a Rota–Baxter structure underlying the target space of the regularized Hopf algebra characters. Working in the rooted tree Hopf algebra, the simple case of the Hopf subalgebra of ladder trees is treated in detail. The extension to the general case, i.e., the full Hopf algebra of rooted trees or Feynman graphs, is briefly outlined. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In 1960 the mathematician Glen Baxter[1] used a simple algebraic identity to solve an analytic problem in probability. Later, in 1963 Atkinson[2] gave a characterization of this relation in terms of Birkhoff's concept of a so-called subdirect (de)composition of algebras. It was Rota who investigated this identity more thoroughly and realized its importance within combinatorics and other fields in mathematics.[3–5] This identity is called the Rota–Baxter relation and will be introduced in the next section. See Refs. 6,7 for reviews and Refs. 8–12 for recent developments relating this identity to other fields in mathematics.

The same relation in its Lie algebraic version was later rediscovered under the name (operator form of the modified) classical Yang–Baxter (here the relation is named after the physicists Yang and Baxter) equation within the field of integrable systems.[13–15] See Ref. 16 for a nice review, especially with respect to double Lie algebras and factorization theorems, i.e., the Riemann–Hilbert problem.

Very recently the Rota–Baxter relation was found to be of crucial importance within the Hopf algebraic approach of Kreimer, and Connes and Kreimer to renormalization theory of perturbative quantum field theory.[17–20] It implies a Birkhoff decomposition of Hopf algebra characters with the target space being a Rota–Baxter algebra. See Ref. 21 for a first introduction.

In this work we aim at a clarification of the link between the last two subjects. We show how the Rota–Baxter relation on the target space of the Hopf algebra characters can be lifted to the Lie algebra of infinitesimal characters. Atkinson's theorem then implies an infinitesimal factorization on this space. This factorization in turn implies the Birkhoff decomposition for the Hopf algebra

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characters. We derive its twisted antipode form first found by one of us.[17] There it was introduced in a formal way mainly motivated by its ability to reproduce Zimmermann's forest formula. Dimensional regularization together with a minimal subtraction scheme furnishes one special case (distinguished by its convenience in applied particle physics) of our approach in which the target space consists of the algebra of Laurent series with finite pole part. Its Rota–Baxter structure stems from the projection onto the pole part of a Laurent series. Here, we will discuss the algebraic Birkhoff decomposition for general Rota–Baxter maps R, provided by various choices of renormalization schemes. Let us mention here that we will restrict our attention later on to the case of the Hopf subalgebra of rooted ladder trees. In this manner we can avoid lengthy formulas generated by the Baker-Campbell-Hausdorff formula, and can treat this case in full technical detail. In the end it will be outlined though how the general case, i.e., for arbitrary rooted trees or graphs, is derived. Details and also a mathematically more rigorous presentation will be given in a forthcoming paper, emphasizing the link to integrable systems.

The paper is structured as follows. In the next section we introduce the notion of a Rota–Baxter algebra and its main characterization by Atkinson's theorem. Section III contains the main results. We briefly introduce the Hopf algebra of rooted trees and the group of characters and its Lie algebra of infinitesimal characters, with target space of the Rota–Baxter type. The Birkhoff decomposition is then derived. We stress that we obtain Bogoliubov's R-bar operation from scratch, as a natural consequence of Atkinson's theorem. We end this work with a summary and an outline describing the case when the Hopf algebra is not cocommutative.

II. ROTA–BAXTER ALGEBRAS AND THE DOUBLE CONSTRUCTION

Let $\mathbb{K}$ be a field of characteristic 0. By a $\mathbb{K}$-algebra we mean an associative algebra over $\mathbb{K}$ that is not necessarily unital or commutative unless stated otherwise.

Definition 2.1: Let $\mathcal{A}$ be a $\mathbb{K}$-algebra with a $\mathbb{K}$-linear map $R:\mathcal{A}\to\mathcal{A}$. We call $\mathcal{A}$ a Rota–Baxter $\mathbb{K}$-algebra and R a Rota–Baxter map (of weight $\theta\in\mathbb{K}$) if the operator R holds the following Rota–Baxter relation of weight $\theta\in\mathbb{K}$:

$$R(x)R(y)+\theta R(xy)=R\big(R(x)y+xR(y)\big),\qquad \forall\, x,y\in\mathcal{A}. \tag{1}$$

[Some authors denote this relation in the form $R(x)R(y)=R\big(R(x)y+xR(y)+\lambda xy\big)$, so $\lambda=-\theta$.]

We note that a Rota–Baxter relation can be defined on $\mathcal{A}$ even when the multiplication on $\mathcal{A}$ is not associative, e.g., when $\mathcal{A}$ is a Lie or pre-Lie algebra. In the case $\theta=0$, the Rota–Baxter operator is somewhat degenerate (see Atkinson's theorem below). When $\theta\neq 0$, a simple transformation $R\to\theta^{-1}R$ gives the standard form of Eq. (1). For the rest of the paper we will always assume the Rota–Baxter map to be of weight $\theta=1$, i.e., to be in standard form.

Remark 2.2: (1) If R fulfills relation (1) for $\theta=1$ then $\tilde{R}:=id-R$ fulfills the same Rota–Baxter relation.

(2) The images of R and $id-R$ give subalgebras in $\mathcal{A}$.

Example 2.3: (1) An important class of Rota–Baxter maps is given by certain projectors. This is the case for the minimal subtraction map R_{MS} in renormalization theory, which is a Rota–Baxter map of weight $\theta=1$ on the algebra of Laurent series $\mathbb{C}[\![\epsilon,\epsilon^{-1}]$.[18] For $\Sigma_{k\geqslant -m}^{\infty}c_k\epsilon^k\in\mathbb{C}[\![\epsilon,\epsilon^{-1}]$,

$$R_{\mathrm{MS}}\left(\sum_{k\geqslant -m}^{\infty}c_k\epsilon^k\right):=\sum_{k\geqslant -m}^{-1}c_k\epsilon^k. \tag{2}$$

.

(2) Another nice example[10] of a Rota–Baxter map of weight $\theta\in\mathbb{K}$ is the operator $\beta:M_n^{\mathrm{up}}(\mathbb{K})\to M_n^{\mathrm{up}}(\mathbb{K})$ defined on the subalgebra of $n\times n$ upper triangular matrices $M_n^{\mathrm{up}}(\mathbb{K})\subset M_n(\mathbb{K})$, mapping an element x to the diagonal matrices $M_n^{\mathrm{up}}(\mathbb{K})\ni x\mapsto\beta(x)\in M_n^{d}(\mathbb{K})\subset M_n^{\mathrm{up}}(\mathbb{K})$:

$$(\beta(x))_{ij} := \delta_{ij}\theta\sum_{k\geqslant i}^{n} x_{ik}.$$

(3) The Riemann integral,

$$R[f](x) := \int_0^x f(y)dy,$$

provides an example for a Rota–Baxter map of weight zero; (1) for $\theta=0$ gives the rule for integration by parts.

We now introduce the modified Rota–Baxter relation. Its Lie algebraic version can be found in Refs. 13,14.

Definition 2.4: Let $\mathcal{A}$ be a Rota–Baxter algebra, R its Rota–Baxter map. Define the modified Rota–Baxter map to be the operator $B:\mathcal{A}\to\mathcal{A}, B:=id-2R$, and call the corresponding relation fulfilled by B:

$$B(x)B(y) = B(B(x)y + xB(y)) - xy, \quad \forall\, x,y \in \mathcal{A} \tag{3}$$

the modified Rota–Baxter relation.

Proposition 2.5: In the case of the Rota–Baxter algebra $\mathcal{A}$ to be either an associative or pre-Lie $\mathbb{K}$-algebra, the (modified) Rota–Baxter relation naturally extends to the Lie algebra $\mathcal{L}_{\mathcal{A}}$ with bracket $[x,y]:=xy-yx, \forall\, x,y\in\mathcal{A}$:

$$[R(x),R(y)] + R([x,y]) = R([R(x),y] + [x,R(y)]), \tag{4}$$

$$[B(x),B(y)] = B([B(x),y] + [x,B(y)]) - [x,y]. \tag{5}$$

The proof of this follows from a simple calculation. The relations (4) and (5) are well-known as the (operator form of the) classical Yang–Baxter and modified Yang-Baxter equation.

The following Proposition 2.6 and Theorem 2.9 characterize Rota–Baxter algebras.

Proposition 2.6: Let $\mathcal{A}$ be a Rota–Baxter algebra with (modified) Rota–Baxter map $R(B=id-2R)$. Equipped with the new product,

$$a*_R b := R(a)b + aR(b) - ab \tag{6}$$

$$= -\frac{1}{2}(B(a)b + aB(b)), \tag{7}$$

$\mathcal{A}$ is again a Rota–Baxter algebra of the same type, denoted by $\mathcal{A}_R$.

The proof of this proposition is immediate by the definition of $*_R$. We call this new Rota–Baxter algebra $\mathcal{A}_R$ the double of $\mathcal{A}$.

Remark 2.7: (1) It is obvious that Proposition 2.6 implies a whole hierarchy of doubles $\mathcal{A}_R^{(i)}$ (here, $*_R=*_R^{(1)}$):

$$\mathcal{A}_R^{(0)} := \mathcal{A}, \quad \mathcal{A}_R^{(1)} := (\mathcal{A},*_R),\ldots, \quad \mathcal{A}_R^{(i)} := (\mathcal{A},*_R^{(i)}),\ldots,$$

$$a*_R^{(i)}b := \left.\frac{d^i}{dt^i}\right|_{t=0} e^{(-1/2)tB}(a)e^{(-1/2)tB}(b), \quad a,b\in\mathcal{A}.$$

Let us call $\mathcal{A}_R^{(i)}$ the *i-th* double of $\mathcal{A}$ and the double of $\mathcal{A}_R^{(i-1)}$.

(2) The Rota–Baxter map becomes an algebra homomorphism between $\mathcal{A}_R^{(i)}$ and $\mathcal{A}_R^{(i-1)}, i\in\mathbb{N}$:

$$R(a*_R^{(i)}b) = R(a)*_R^{(i-1)}R(b).$$

(3) For the Rota–Baxter map $\tilde{R} := id - R$, we have

$$\tilde{R}(a *_R^{(i)} b) = -\tilde{R}(a) *_R^{(i-1)} \tilde{R}(b).$$

The last equation can be written as $\hat{R} := -\tilde{R}, \hat{R}(a *_R^{(i)} b) = \hat{R}(a) *_R^{(i-1)} \hat{R}(b)$. As a side remark we should mention that the notion of the double of $\mathcal{A}$ for associative and nonassociative algebras may be found in Ref. 14.

A relation closely related to the Rota–Baxter relation (1) is

$$N(x)N(y) + N^2(xy) = N(N(x)y + xN(y)), \quad x,y \in \mathcal{A}. \tag{8}$$

The map N might be called an associative Nijenhuis operator or just Nijenhuis map for short.[28] In this setting "associative" refers to the relation (8) to distinguish it clearly from its Lie algebraic version:[29,30]

$$[N(x),N(y)] + N^2([x,y]) = N([N(x),y] + [x,N(y)]). \tag{9}$$

As in the case of the Rota–Baxter relation, a Nijenhuis map on a $\mathbb{K}$-algebra $\mathcal{A}$ also gives a Nijenhuis map for the associated Lie algebra $\mathcal{L}_{\mathcal{A}} := (\mathcal{A}, [-,-]), [-,-]$ being the commutator. Also, similar to the case of the Rota–Baxter relation the associative Nijenhuis identity implies a hierarchy of algebra products. We will not go further into details with respect to this relation.

Proposition 2.8: Let $\mathcal{A}$ be a commutative, associative Rota–Baxter algebra. For $n \in \mathbb{N}, x \in \mathcal{A}$ we have

$$(-R(x))^n = -R\left(x^n + \sum_{k=1}^{n-1} \binom{n}{k} (-R(x))^{(n-k)} x^k\right), \tag{10}$$

$$\tilde{R}(x)^n = \tilde{R}\left(x^n + \sum_{k=1}^{n-1} \binom{n}{k} (-R(x))^{(n-k)} x^k\right). \tag{11}$$

The proof works inductively. Proposition 2.8 will lead us to the twisted antipode formula.[17–19]

We come now to the important result of Atkinson, reformulating the Rota–Baxter relation in terms of a subdirect (de)composition in the sense of Birkhoff.

Theorem 2.9 (Atkinson[2]): *For a $\mathbb{K}$-algebra $\mathcal{A}$ with a linear map $R: \mathcal{A} \to \mathcal{A}$ to be a Rota–Baxter $\mathbb{K}$-algebra, it is necessary and sufficient that $\mathcal{A}$ has a subdirect Birkhoff decomposition.*

It should be underlined here that this theorem is true quite generally, in the sense that the algebra needs not to be associative, nor commutative.

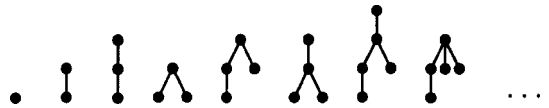
Essentially, the subdirect Birkhoff decomposition in this case means that the Cartesian product $\mathcal{D} := (R(\mathcal{A}), -\tilde{R}(\mathcal{A})) \subset \mathcal{A} \times \mathcal{A}$ is a subalgebra in $\mathcal{A} \times \mathcal{A}$ and that every element $x \in \mathcal{A}$ has a unique decomposition $x = R(x) + \tilde{R}(x)$. The double construction introduced here and Atkinson's theorem should be compared with the results in Refs. 13–16.

III. *R*-MATRIX APPROACH TO RENORMALIZATION: THE ROOTED LADDER TREE CASE

We will now briefly introduce the Connes–Kreimer Hopf algebra of rooted trees.[22–24]

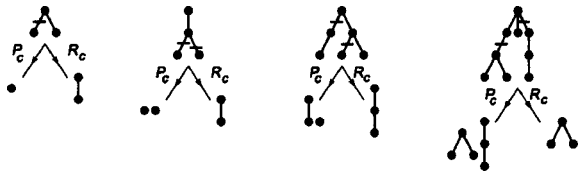
Definition 3.1: A rooted tree is a finite, connected oriented graph without loops in which every vertex has exactly one incoming edge, except one (the root) which has no incoming but only outgoing edges. We denote the set of edges and vertices of a rooted tree T by $E(T), V(T)$, respectively.

Let us denote the set of (isomorphism classes of) rooted trees by $\mathcal{T}_{\mathrm{rt}}$:



Let $\mathcal{H}_{\mathrm{rt}}$ be the commutative algebra generated by these symbols $T \in \mathcal{T}_{\mathrm{rt}}$ (one for each isomorphism class). The commutative product $m_{\mathcal{H}_{\mathrm{rt}}}: \mathcal{H}_{\mathrm{rt}} \otimes \mathcal{H}_{\mathrm{rt}} \to \mathcal{H}_{\mathrm{rt}}$ is written as concatenation $m_{\mathcal{H}_{\mathrm{rt}}}(T', T'') =: T'T''$ and the empty tree is denoted by 1 giving the unit. The algebra may be graded by the number of vertices $\#(T) = |V(T)|$ of the rooted tree T. We equip this algebra with a counit map $\epsilon: \mathcal{H}_{\mathrm{rt}} \to \mathbb{K}, \epsilon(1) := 1$ and $\epsilon(T_1 \cdots T_n) = 0$ for $T_1 \cdots T_n \neq 1$.

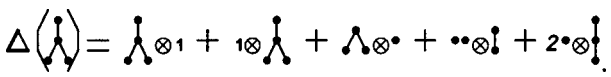
We now define the coproduct $\Delta: \mathcal{H}_{\mathrm{rt}} \to \mathcal{H}_{\mathrm{rt}} \otimes \mathcal{H}_{\mathrm{rt}}$. For this we first introduce the notion of simple cuts on rooted trees. A simple or admissible cut c_T of a tree T is a subset of its edges such that along any path from its root to one of its leaves one meets at most one element of c_T. Deleting the set $c_T \subset E(T)$ of edges in T produces one tree R_{c_T} still containing the original root and a set of pruned rooted trees P_{c_T}, the roots of which are identified with the vertex which had the cut edge in c_T as an incoming edge. The following examples may be helpful in understanding the concept of simple cuts, R_{c_T} and P_{c_T}:



The coproduct may then be defined as follows. Let C_T be the set of all admissible cuts of the rooted tree T. We exclude the empty cut $c_T^{(0)}, P_{c_T^{(0)}} = \emptyset, R_{c_T^{(0)}} = T$ and the full cut $c_T^{(1)}, P_{c_T^{(1)}} = T, R_{c_T^{(1)}} = \emptyset$:

$$\Delta(T) = T \otimes 1 + 1 \otimes T + \sum_{c_T \in C_T} P_{c_T}(T') \otimes R_{c_T}(T''). \tag{12}$$

Here T', respectively, T'' stand for the rooted trees produced when applying c_T. As an example we calculate the coproduct of the rooted tree of weight $\#(\cdot) = 4$:

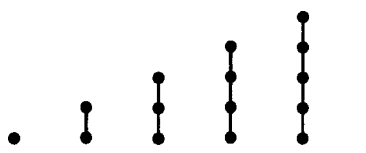


The coproduct (12) is extended by linearity, and we define it to be an algebra homomorphism $\Delta(T_1 \cdots T_n + T_{n+1} \cdots T_m) = \Pi_{i=1}^{n} \Delta(T_i) + \Pi_{i=n+1}^{m} \Delta(T_i), \Delta(1) := 1 \otimes 1$. Obviously, (12) is not cocommutative. So far we have a connected graded bialgebra, hence by general arguments a rooted tree Hopf algebra with antipode $S: \mathcal{H}_{\mathrm{rt}} \to \mathcal{H}_{\mathrm{rt}}$:

$$S(T) := -T - \sum_{c_T \in C_T} S(P_{c_T}(T')) R_{c_T}(T''). \tag{13}$$

Again we exclude the empty and full cut, i.e. $c_T^{(0)}, c_T^{(1)}$, respectively, in the above sum.

The Hopf algebra $\mathcal{H}_{\mathrm{rt}}$ contains a cocommutative Hopf subalgebra denoted by $\mathcal{H}_{l\ \mathrm{rt}}$, generated by rooted ladder graphs:



which we will denote in general by $t_n \in \mathcal{H}_{l\ \mathrm{rt}} \subset \mathcal{H}_{\mathrm{rt}}$, where $n \in \mathbb{N}$ is the number of vertices, having at most one incoming and also at most one outgoing edge. By t_0 we denote the unit, i.e. the empty tree 1. The coproduct then becomes

$$\Delta(t_n) = t_n \otimes 1 + 1 \otimes t_n + \sum_{i=1}^{n-1} t_i \otimes t_{n-i}. \tag{14}$$

The graded dual $\mathcal{H}_{\mathrm{rt}}^*$ equipped with the convolution product $f \star g := m_{\mathbb{K}} \circ f \otimes g \circ \Delta, f, g \in \mathcal{H}_{\mathrm{rt}}^*$ becomes an associative $\mathbb{K}$-algebra. We denote the pairing by brackets, $\langle f, T \rangle := f(T) \in \mathbb{K}$.

Let $\mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}} \subset \mathcal{H}_{\mathrm{rt}}^*$ be the group of characters, i.e. algebra morphisms into $\mathbb{K}$, with inverse $\phi^{-1} := \phi \circ S, \phi \in \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}$. Let $\partial\, \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}} \subset \mathcal{H}_{\mathrm{rt}}^*$ be the Lie algebra of infinitesimal characters, i.e. derivations into $\mathbb{K}$:

$$Z(T'T'') = Z(T')\epsilon(T'') + \epsilon(T')Z(T''), \quad Z \in \partial\ \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}, \tag{15}$$

with Lie bracket

$$[Z', Z''] := Z' \star Z'' - Z'' \star Z'. \tag{16}$$

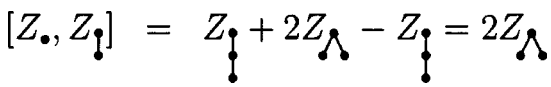
$\partial\, \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}$ is generated by the infinitesimal characters Z_T indexed by rooted trees $T \in \mathcal{T}_{\mathrm{rt}}$, and defined by

$$\langle Z_T, T' \rangle := \delta_{T,T'}. \tag{17}$$

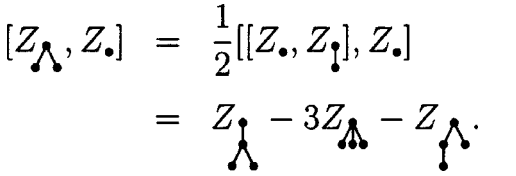
Tree monomials are excluded from the index set due to the Leibniz rule (15). The Lie bracket for these generators is given by Ref. 22:

$$[Z_{T'}, Z_{T''}] = \sum_{T \in \mathcal{T}_{\mathrm{rt}}} (n(T', T''; T) - n(T'', T'; T)) Z_T, \tag{18}$$

where the $n(T', T''; T) \in \mathbb{N}$ denote so-called section coefficients which count the number of single simple cuts, $|c_T| = 1$, such that $P_{c_T} = T'$ and $R_{c_T} = T''$:



(19)



(20)

Remark 3.2: (1) The composition $Z_{T'} \star Z_{T''} = \Sigma_{T \in \mathcal{T}_{\mathrm{rt}}} n(T', T''; T) Z_T$ defines a left pre-Lie algebra structure on $\partial\, \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}$.

(2) Antisymmetrizing this pre-Lie product gives the above Lie algebra, which lies at the heart of the combinatorics of renormalization theory in pQFT.[25,26]

The exponential map gives the bijection from $\partial\, \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}} \to \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}$:

$$\exp^{\star}(Z) := \sum_{n=0}^{\infty} \frac{Z^{\star n}}{n!} \in \mathrm{char}_{\mathbb{K}}\, \mathcal{H}_{\mathrm{rt}}. \tag{21}$$

Here Z is given as a series,

$$Z = \sum_{T \in \mathfrak{T}_{rt}} a^T Z_T = a^{\bullet} Z_{\bullet} + a^{\bullet^1} Z_{\bullet^1} + a^{\bullet^2} Z_{\bullet^2} + a^{\bullet^3} Z_{\bullet^3} + \cdots$$

The exponential map (21) is well defined since due to the Leibniz rule (15) we have $Z^{\star n}(T)=0$ for $n>\#(T)$.

Following the Hopf algebraic approach to renormalization in perturbative quantum field theory (pQFT), we introduce the notion of regularized (infinitesimal) characters, mapping $\mathcal{H}_{\mathrm{rt}}$ into a commutative, associative, unital Rota–Baxter algebra $\mathcal{A}$. [$\mathcal{A}=\mathbb{C}[\![\epsilon,\epsilon^{-1}]$ in dimensional regularization together with minimal subtraction in pQFT, where the Rota–Baxter R map is then given by Eq. (2).] We therefore extend $\mathcal{H}_{\mathrm{rt}}^{*}$ to $\mathcal{H}_{\mathrm{rt}}^{*}\otimes\mathcal{A}=L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$, consisting of $\mathbb{K}$-linear maps from $\mathcal{H}_{\mathrm{rt}}$ into the Rota–Baxter algebra $\mathcal{A}$, i.e. $\langle\phi,T\rangle\in\mathcal{A}, \phi\in L(\mathcal{H}_{\mathrm{rt}},\mathcal{A}), T\in\mathcal{H}_{\mathrm{rt}}$.

We then lift the Rota–Baxter map $R:\mathcal{A}\to\mathcal{A}$ to $L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$.

Proposition 3.3: Define the linear map $\mathcal{R}:L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})\to L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$ *by* $f\mapsto\mathcal{R}(f):=R\circ f:\mathcal{H}_{\mathrm{rt}}\to R(\mathcal{A})$. *Then* $L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$ *becomes an associative, unital Rota–Baxter algebra. The Lie algebra of infinitesimal characters* $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}\subset L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$ *with bracket (16) becomes a Lie Rota–Baxter algebra, i.e. for* $Z',Z''\in\partial\,\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$,

$$[\mathcal{R}(Z'),\mathcal{R}(Z'')]=\mathcal{R}([Z',\mathcal{R}(Z'')])+\mathcal{R}([\mathcal{R}(Z'),Z''])-\mathcal{R}([Z',Z'']). \tag{22}$$

Notice that we replaced $\mathbb{K}$ by $\mathcal{A}$ for the target space of the regularized infinitesimal characters. The proof follows from the fact that R is $\mathbb{K}$-linear and

$$\begin{aligned}
\mathcal{R}(f)\star\mathcal{R}(g)(T) &= m_{\mathcal{A}}(\mathcal{R}(f)\otimes\mathcal{R}(g))\circ\Delta(T)\\
&= m_{\mathcal{A}}(R(f(T_{(1)}))\otimes R(g(T_{(2)})))\\
&\overset{(1)}{=} -R\circ m_{\mathcal{A}}(f(T_{(1)})\otimes g(T_{(2)}))+R\circ m_{\mathcal{A}}(f(T_{(1)})\otimes R(g(T_{(2)})))\\
&\quad +R\circ m_{\mathcal{A}}(R(f(T_{(1)}))\otimes g(T_{(2)}))\\
&= -R\circ m_{\mathcal{A}}(f\otimes g)\circ\Delta(T)+R\circ m_{\mathcal{A}}(f\otimes\mathcal{R}(g))\circ\Delta(T)+R\circ m_{\mathcal{A}}(\mathcal{R}(f)\otimes g)\circ\Delta(T)\\
&= \mathcal{R}(f\star\mathcal{R}(g))(T)+\mathcal{R}(\mathcal{R}(f)\star g)(T)-\mathcal{R}(f\star g)(T),
\end{aligned} \tag{23}$$

where we used Sweedler's notation $\Delta(T)=\Sigma T_{(1)}\otimes T_{(2)}$ for the coproduct (12), omitting the summation sign above. For the second assertion, we only have to show that $\mathcal{R}:\partial\,\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}\to\partial\,\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$, but this again follows from the $\mathbb{K}$-linearity of R and $\epsilon(T)\in\mathbb{K}$.

Using the double construction and Atkinson's theorem of Sec. II we have the following.

Lemma 3.4: The Rota–Baxter algebra $L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$ *equipped with the convolution product,*

$$f\star_{\mathcal{R}}g=f\star\mathcal{R}(g)+\mathcal{R}(f)\star g-f\star g, \tag{24}$$

gives a Rota–Baxter algebra structure on the set of linear functionals into the double $\mathcal{A}_R$ *of* $\mathcal{A}$, *denoted by* $L(\mathcal{H}_{\mathrm{rt}},\mathcal{A}_R)$. *An analog for* $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}$ *exists and is denoted by* $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}\mathcal{R}}$. $\mathcal{R}$ *becomes a (Lie) algebra morphism* $(\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}\mathcal{R}}\to\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}})L(\mathcal{H}_{\mathrm{rt}},\mathcal{A}_R)\to L(\mathcal{H}_{\mathrm{rt}},\mathcal{A})$.

Remark 3.5: The above is also true for $\widetilde{R}:=id-R$, respectively $\widetilde{\mathcal{R}}$ (see Remark 2.7). We will denote $\mathcal{R}(\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}})$ by $\mathcal{L}^{-}_{\mathcal{H}_{\mathrm{rt}}^{*}}$ and $\widetilde{\mathcal{R}}(\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}})$ by $\mathcal{L}^{+}_{\mathcal{H}_{\mathrm{rt}}^{*}}$.

We now apply Atkinson's theorem to the Lie algebra $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}$ of infinitesimal characters, the generators of the group of Hopf algebra characters $\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$.

Lemma 3.6: Every infinitesimal character $Z\in\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}$ *has a unique subdirect Birkhoff decomposition* $Z=\mathcal{R}(Z)+\widetilde{\mathcal{R}}(Z)$.

Remark 3.7: (1) In the case of an idempotent Rota–Baxter map R we have a direct decomposition $\mathcal{A}=\mathcal{A}_{-}+\mathcal{A}_{+}$, respectively, $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}=\mathcal{L}^{-}_{\mathcal{H}_{\mathrm{rt}}^{*}}+\mathcal{L}^{+}_{\mathcal{H}_{\mathrm{rt}}^{*}}$.

(2) Let $Z \in \mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^*}$ be the infinitesimal character generating the character $\phi = \exp^\star(Z) \in \mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$. Using the result in Proposition 2.8, easily generalized to the noncommutative case, we then see that $\exp^\star(-\mathcal{R}(Z)) = \mathcal{R}(\exp^{\star_{\mathcal{R}}}(-Z))$.

Let us define

$$b[\phi] := \exp^{\star_{\mathcal{R}}}(-Z),$$

which is a character of $\mathcal{H}_{\mathrm{rt}} \to \mathcal{A}_R$, i.e., $b[\phi] \in \mathrm{char}_{\mathcal{A}_R}\mathcal{H}_{\mathrm{rt}}$ and which we will call Bogoliubov's recursion R-map for reasons which will become clear soon. Therefore

$$\begin{aligned}\exp^\star(-\mathcal{R}(Z))(T'T'') &= \mathcal{R}(\exp^{\star_{\mathcal{R}}}(-Z))(T'T'') = R(b[\phi](T') *_R b[\phi](T'')) \\ &= \exp^\star(-\mathcal{R}(Z))(T')\exp^\star(-\mathcal{R}(Z))(T''). \qquad (25)\end{aligned}$$

We then have the following.

Lemma 3.8: The Lie Rota–Baxter map $\mathcal{R}(\tilde{\mathcal{R}})$ becomes a Lie group (anti-) homomorphism from $\mathrm{char}_{\mathcal{A}_R}\mathcal{H}_{\mathrm{rt}}$ to $\mathrm{char}_{\mathcal{A}}^{-(+)}\mathcal{H}_{\mathrm{rt}}$, *where* $\mathrm{char}_{\mathcal{A}}^{-(+)}\mathcal{H}_{\mathrm{rt}}$ *are the Lie subgroups generated by the Lie subalgebras* $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^*}^{-(+)}$.

As we already mentioned in the Introduction, here we will only consider in detail the simple case of the cocommutative Hopf subalgebra $\mathcal{H}_{l\ \mathrm{rt}}$, respectively $L(\mathcal{H}_{l\ \mathrm{rt}}, \mathcal{A})$. The latter is generated by the $Z_{t_n} \in \partial\,\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}, n \in \mathbb{N}$ and necessarily is an Abelian Lie algebra $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}, [Z_{t_n}, Z_{t_m}] = 0, n, m \in \mathbb{N}$.

The Abelianess of $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}$ and Atkinson's result imply the following theorem [which extends to the non-Abelian case using the appropriate BCH formulas for the (multi-)commutator of $\mathcal{R}(Z)$ with $\tilde{\mathcal{R}}(Z)$].

Theorem 3.9 (Ladder case of integrable renormalization): *Let $\phi \in \mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{l\ \mathrm{rt}}$ be generated by $Z \in \mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}$, i.e.* $\exp^\star(Z) = \phi$. *We have the following factorization*:

$$\exp^\star(Z) = \phi = \exp^\star(\mathcal{R}(Z) + \tilde{\mathcal{R}}(Z)) = \exp^\star(\mathcal{R}(Z)) \star \exp^\star(\tilde{\mathcal{R}}(Z)). \qquad (26)$$

Proposition 3.10: With the same assumption as in Theorem 3.9 and the definitions $\phi_-^{-1} := \exp^\star(\mathcal{R}(Z))$ and $\phi_+ := \exp^\star(\tilde{\mathcal{R}}(Z))$, we have

$$\phi_-(t_n) = \exp^\star(-\mathcal{R}(Z))(t_n) = \mathcal{R}(\exp^{\star_{\mathcal{R}}}(-Z))(t_n) \qquad (27)$$

$$= -R\left\{\phi(t_n) + \sum_{k=1}^{n-1} \phi_-(t_k)\phi(t_{n-k})\right\}, \qquad (28)$$

$$\phi_+(t_n) = \exp^\star(\tilde{\mathcal{R}}(Z))(t_n) = -\tilde{\mathcal{R}}(\exp^{\star_{\mathcal{R}}}(-Z))(t_n) \qquad (29)$$

$$= \tilde{R}\left\{\phi(t_n) + \sum_{k=1}^{n-1} \phi_-(t_k)\phi(t_{n-k})\right\}. \qquad (30)$$

The proof of this proposition follows immediately by Proposition 2.8 and (10) and (11). It can be generalized to the non-Abelian case using the Hochschild cohomology of the Hopf algebra as in Ref. 27 and the resolution of the non-Abelian Lie algebra in terms of its lower central series.

Remark 3.11: (1) From expressions (25), (27), and (29) it is evident that $\phi_\pm$ are characters. We will see the same for the general case.

(2) For the ladder case we therefore arrive at the following result. Since $\exp^{\star}(-\mathcal{R}(Z)) = \mathcal{R}(\exp^{\star_{\mathcal{R}}}(-Z)) =: \mathcal{R}(b[\phi])$ (Remark 3.7), we have

$$b[\phi](t_n) = \exp^{\star_{\mathcal{R}}}(-Z)(t_n) = -\phi(t_n) - \sum_{k=1}^{n-1} \phi_-(t_k)\phi(t_{n-k}).$$

This justifies the name Bogoliubov's $\overline{R}$-map[19] for $b[\phi]$, which finds its natural algebraic formulation as a character $b[\phi]=\exp^{\star_{\mathcal{R}}}(-Z) \in \mathrm{char}_{\mathcal{A}_R} \mathcal{H}_{l\ \mathrm{rt}}$ and which is mapped by the Rota–Baxter operator $\mathcal{R}$ into $\mathrm{char}_{\mathcal{A}} \mathcal{H}_{l\ \mathrm{rt}}$. As mentioned before this result carries over to the general case, i.e., to the noncocommutative Hopf algebras of Feynman graphs or arbitrary decorated rooted trees. Note that formulas (28) and (30) have been established already in Ref. 17, while to express (27) and (29) in a convenient way using the necessary BCH corrections will be reserved to future work.

Also, we would like to underline the similarity with the factorization theorems in Refs. 14–16. We will dwell on this connection in greater depth in the future.

Let us summarize the result in Proposition 3.10. The (Abelian) Lie algebra $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}$ naturally extends to a Lie Rota–Baxter algebra due to the Rota–Baxter structure on its target space. Therefore it contains two Lie algebra structures with respect to the original Lie bracket and the double coming from the Rota–Baxter map $\mathcal{R}$. Due to Atkinson's theorem it decomposes into two Lie subalgebras $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}^{-(+)}$ which generate the Lie subgroups $\mathrm{char}_{\mathcal{A}}^{-(+)} \mathcal{H}_{l\ \mathrm{rt}}$. The infinitesimal decomposition on $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}$ extends in the ladder case to the global factorization on the Lie group $\mathrm{char}_{\mathcal{A}} \mathcal{H}_{l\ \mathrm{rt}}$. We have the following diagrams on the Lie algebra level, respectively, Lie group level.

Let b denote Bogoliubov's recursion formula, which is defined in terms of the exponential with respect to the double product $\star_{\mathcal{R}}$. We define $\mathcal{G}^l := \mathrm{char}_{\mathcal{A}} \mathcal{H}_{l\ \mathrm{rt}}, \mathcal{G}_{\mathcal{R}}^l := \mathrm{char}_{\mathcal{A}_R} \mathcal{H}_{l\ \mathrm{rt}}$ and $\mathcal{G}^{l\pm} := \mathrm{char}_{\mathcal{A}}^{\pm} \mathcal{H}_{l\ \mathrm{rt}}$:

$$\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^* \mathcal{R}} \overset{(\mathcal{R},\mathcal{R}-id)}{\rightarrow} (\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}^-, \mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}^+) \overset{(id,-id)}{\rightarrow} \mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^*}. \tag{31}$$

Here, $Z=\mathcal{R}(Z)-(\mathcal{R}-id)(Z)=(id,-id)\circ(\mathcal{R},\mathcal{R}-id)(Z)$ gives the infinitesimal factorization, i.e., Atkinson's theorem:

$$\mathcal{G}^l \overset{b}{\rightarrow} \mathcal{G}_{\mathcal{R}}^l \overset{(-\mathcal{R}\otimes\tilde{\mathcal{R}})}{\rightarrow} (\mathcal{G}^{l-}, \mathcal{G}^{l+}) \overset{m_{\mathcal{G}^l}}{\rightarrow} \mathcal{G}^l. \tag{32}$$

The last diagram contains the global factorization, i.e. on the level of the Lie group $\mathcal{G}^l$ coming from the Lie algebra $\mathcal{L}_{\mathcal{H}_{l\ \mathrm{rt}}^*}$.

Remark 3.12: (1) Using the idea of normal coordinates in Ref. 31, we may relate the simple rooted ladder graphs, given by Schur polynomials $P^{(n)}(t_1,\ldots,t_n)$ of order n for each rooted ladder tree t_n and the $\phi_\pm$ character in the following way. [Schur polynomial of order $n, P^{(n)}$: Taylor expansion of $\log(\Sigma_{n\geq 0} t_n x^n) = \Sigma_{n\geq 0} P^{(n)}(t_1,\ldots,t_n)x^n$.[31]] Starting with the regularized character $\phi: \mathcal{H}_{\mathrm{rt}} \rightarrow \mathcal{A}$, we define the series (we omit tensor product signs)

$$Z_\phi := \sum_{n>0} Z_{t_n} \phi(P^{(n)}(t_1,\ldots,t_n)) \in \mathrm{char}_{\mathbb{K}} \mathcal{H}_{\mathrm{rt}} \otimes \mathcal{A}.$$

It then follows from Ref. 31 that $\exp^{\star}(Z_{\phi})(t_n)=\phi(t_n)$, i.e. Z_{ϕ} is the infinitesimal character generating the Lie group element ϕ. As an example we calculate $\phi_{-}(\bullet\!\!\uparrow)$:

$$\begin{aligned} exp^{\star}(-\mathcal{R}(Z_{\phi}))(\bullet\!\!\uparrow) &= \Big\{ -Z_{\bullet\!\!\uparrow}R\big(\phi(P^{(3)}(\bullet,\bullet,\bullet\!\!\uparrow))\big) \\ &\quad +\frac{1}{2}(Z_{\bullet}\star Z_{\bullet\!\!\uparrow}+Z_{\bullet\!\!\uparrow}\star Z_{\bullet})R(\phi(\bullet))R\big(\phi(P^{(2)}(\bullet,\bullet\!\!\uparrow))\big) \\ &\quad +\frac{-1}{3!}Z_{\bullet}\star Z_{\bullet}\star Z_{\bullet}R(\phi(\bullet))^3\Big\}\Big(\bullet\!\!\uparrow\Big) \\ &= -R\Big(\phi\big(P^{(3)}(\bullet,\bullet,\bullet\!\!\uparrow)\big)-R(\phi(\bullet))R\big(\phi(P^{(2)}(\bullet,\bullet\!\!\uparrow))\big) \\ &\qquad +\frac{1}{3!}R(\phi(\bullet))^3\Big). \end{aligned}$$

(2) Let us briefly outline the approach to the general case. The full Lie algebra of infinitesimal characters $\mathcal{L}_{\mathcal{H}_{\mathrm{rt}}^{*}}$ is of course non-Abelian and therefore the factorization has to include contributions in a subtractive manner to eliminate BCH terms. This may be achieved in a systematic way using the Baker–Campbell–Hausdorff (BCH) functional,

$$\mathrm{BCH}(A,B) := \frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]-[B,[A,B]])+\cdots,$$

which starts with a commutator, i.e., is of order >1 in the number of infinitesimal characters. Recursively, order by order in the grading on $\mathcal{H}_{\mathrm{rt}}$, the correct contributions may be calculated. The first term of second order essentially takes care of the cherry tree $\curlywedge$ renormalization:

$$\chi^{(2)}=-\frac{1}{2}[\mathcal{R}(Z),Z],$$

for $\phi=\exp^{\star}(Z)\in \mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$ and which should be compared to (19). Again, the normal coordinates theorem in Ref. 31 provides a convenient way to identify terms from the BCH formula. This way we derive the implicitly given formulas for $\phi_{\pm}$ in Ref. 19, respectively give an explicit formula for them in terms of the exponential map and an element in the image of the Rota–Baxter maps $\mathcal{R}$, respectively $\widetilde{\mathcal{R}}$.

(3) The present setting resembles the loop algebra-group case of integrable systems theory. The generalization takes place by using a general Rota–Baxter algebra as the target space. In a later publication we will dwell more carefully on this point.

(4) Following the recent work by Sakakibara[32] we derive the scattering type formula for $\phi_{\pm}$. We first extend the Lie algebra $\partial\,\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$ by an element Z_0 such that $[Z_0,Z_T]=Y(Z_T):=\#(T)Z_T$ where Y is the grading operator $Y(T):=\#(T)$, i.e. a derivation on $\mathcal{H}_{\mathrm{rt}}$ (see Ref. 20 for details). This implies a one parameter group $\theta_t\in\mathrm{Aut}(\mathcal{H}_{\mathrm{rt}})$ acting on $\mathrm{char}_{\mathcal{A}}\,\mathcal{H}_{\mathrm{rt}}$ by

$$\langle\theta_t(\phi),T\rangle := \langle\phi,\theta_t(T)\rangle,$$

i.e. $\theta_t=\mathrm{Ad}_{\exp^{\star}(tZ_0)}$, and such that $(d\theta_t/dt)|_{t=0}=Y$. We then define a so-called β-function:

$$\beta(\phi) := \phi_{\pm}\star Y(\phi_{\pm}^{-1})=\phi_{\pm}\star[Z_0,\phi_{\pm}^{-1}]=\phi_{\pm}\star Z_0\star\phi_{\pm}^{-1}-Z_0,$$

such that[32]

$$\exp^{\star}(t(\beta(\phi)+Z_0))\star\exp^{\star}(-tZ_0)=\phi_{\pm}\star\theta_t(\phi_{\pm}^{-1})\overset{t\to\infty}{\longrightarrow}\phi_{\pm}.$$

This should be compared to the expression we found for $\phi_{\pm}$ in terms of the Rota–Baxter map $\mathcal{R}$.

IV. SUMMARY, CONCLUSION AND OUTLOOK

In an earlier work[19] the combinatorics of renormalization in pQFT was described in terms of a Birkhoff factorization of the regularized Hopf algebra characters. The identification of the singular part ϕ_- as a character relies on the Rota–Baxter structure on the target space of the characters. Emphasizing the latter point and restricting for pedagogical reasons to the simple case of rooted ladder trees we were able to derive the twisted antipode formula for the singular part of the Birkhoff decomposition, solely using the properties of the Rota–Baxter map lifted to the Lie algebra of infinitesimal characters.

Extending this simple exercise to the general case of a noncocommutative Hopf algebra poses no conceptual challenge but becomes technically more demanding and will be presented elsewhere.

In our view it is important to underline that it is the Lie algebra of rooted trees, or more generally the insertion-elimination Feynman Lie algebra, which completely describes the process of renormalization in pQFT. This will become even more apparent when we treat the general case, indicated in the last remark in Sec. III. These results strongly indicate that there is a deeper link between the realm of (classically) integrable systems and the RG-flows. The last point especially demands for a deeper understanding of the Lie algebra of infinitesimal characters, respectively, the Lie Group of regularized characters. We hope that this may be partly achieved by analyzing the link to the well established field of integrable systems.

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On the Fock space for nonrelativistic anyon fields and braided tensor products

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We realize the physical N-anyon Hilbert spaces, introduced previously via unitary representations of the group of diffeomorphisms of the plane, as N-fold braided-symmetric tensor products of the 1-particle Hilbert space. This perspective provides a convenient Fock space construction for nonrelativistic anyon quantum fields along the more usual lines of boson and fermion fields, but in a braided category, and clarifies how discrete (lattice) anyon fields relate to anyon fields in the continuum. We also see how essential physical information is encoded. In particular, we show how the algebraic structure of the anyonic Fock space leads to a natural anyonic exclusion principle related to intermediate occupation number statistics, and obtain the partition function for an idealized gas of fixed anyonic vortices. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1787620]

I. INTRODUCTION

Anyons are particles or excitations in two-dimensional space that obey exchange statistics interpolating those of bosons and fermions. When two identical anyons are exchanged without coincidence along a continuous path in the plane, their relative winding number m (the net number of counterclockwise exchanges) is well-defined, depending only on the homotopy class of the path implementing the exchange. The quantum-mechanical wave function then acquires a relative phase $e^{im\theta}$, where θ is a real fixed parameter between 0 and 2π. When $\theta=0$ we have bosons, and $\theta=\pi$ corresponds to fermions.

The possibility of such intermediate statistics was suggested by Leinaas and Myrheim[1] and confirmed by Goldin, Menikoff, and Sharp,[2] who derived the quantum theory rigorously from representations of local nonrelativistic current algebra and the corresponding diffeomorphism group. They obtained the anyonic shifts in angular momentum and energy spectra, and made connections with configuration space topology and the physics of charged particles circling regions of magnetic flux. The term "anyon" was subsequently introduced by Wilczek,[3] who proposed a model for such objects based on charged-particle/flux-tube composites and suggested their association with fractional spin in two dimensions. The idea found some immediate applications to surface phenomena and related areas of physics.[4,5] Reference 6 clarified that the shift in the angular momentum spectrum associated with anyons is in the kinetic (or orbital) angular momentum, not the canonical (or total) angular momentum.

In Ref. 7 the *braid group* B_N was identified as the group whose one-dimensional representations describe the anyonic wave function symmetry. A more extensive discussion of the braid group and anyon statistics followed in Ref. 8, where it was argued that only the one-dimensional

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representations of B_N should occur in quantum mechanics. However, as noted in Ref. 9, the diffeomorphism group approach allows also the possibility of quantum systems described by higher-dimensional representations of B_N (particles later termed "plektons"). An overview of that approach, which underlies the present article, may be found in Ref. 10.

The extensive development of these ideas that occurred during the 1980s and early 1990s, including their relation to Chern–Simons quantum field theories, their application in describing the integer and fractional quantum Hall effects, and their role in describing possible mechanisms for superconductivity, are reviewed in Refs. 11 and 12.

Anyonic systems can also be associated with quantum groups and q-deformations of classical Lie algebras.[13–17] In Ref. 18 it was shown that creation and annihilation fields for anyons could be constructed so as to intertwine the N-anyon representations of the group of compactly supported diffeomorphisms $\mathrm{Diff}_c(\mathbb{R}^2)$ in the Hilbert space $\mathcal{H}_N$ of N-particle states. The assumption that these fields transform consistently with the diffeomorphism group representations dictates the form they should take; and the fact that they obey q-commutation relations, where q is the anyonic phase shift, emerges as a consequence of this. In this work, the spaces $\mathcal{H}_N$ were constructed (for each N) using "topological configurations" of N points equipped with attached filaments going out to infinity in the plane.

In the present article, we show how to construct such a theory along lines more familiar from bosonic (respectively, fermionic) algebras of canonical commutation (resp. anticommutation) relations—i.e., CCR (resp. CAR) algebras—where the N-particle Fock subspaces are built up by symmetrizing or antisymmetrizing sets of 1-particle states. We shall effectively "q-symmetrize"[19] using braided category techniques coming out of quantum group theory,[20] so that

$$\mathcal{H}_N = \mathcal{H}_1 \underset{s}{\otimes} \mathcal{H}_1 \underset{s}{\otimes} \cdots \underset{s}{\otimes} \mathcal{H}_1$$

(N times), where $\otimes_s$ is the symmetrized tensor product with respect to a certain symmetry Ψ_0. A difficulty in formulating anyonic field theory this way has been the apparent need to work in a *strictly* braided category, with a braiding Ψ defined by q. The fact that the braid group is infinite would then seem to require an infinite sum of powers of q. But it turns out that the associated operator Ψ_0 obeys the condition $\Psi_0^2 = \mathrm{id}$. Thus it generates an action of the symmetric group S_N, rather than the braid group B_N. In effect, the nontrivial braid group representation and its inverse conspire with each other to give us a braided tensor category that is actually *symmetric* (up to sets of measure zero).

Moreover, in our construction the full anyonic Fock space $S_{\Psi_0}(\mathcal{H}_1)$, obtained as the direct sum of the different spaces $\mathcal{H}_1 \otimes_s \cdots \otimes_s \mathcal{H}_1$, is an algebra with product $\otimes_s$. This algebra generalizes the algebra of functions on a linear space or superspace in the Bose or Fermi cases, with its respective commutative or anticommutative product. The annihilation and creation operators in our construction then act by pointwise multiplication and (functional) differentiation on this space, exactly in conformity with the usual functional representation in field theory. The difference is that the anyonic case only makes sense in a braided category, with a braiding Ψ. In this category $S_{\Psi_0}(\mathcal{H}_1)$ is the "coordinate ring" of a braided group, with the braided coproduct $\underline{\Delta}$ expressing addition.[13,20–22] The use here of *two* Yang–Baxter operators Ψ and Ψ_0 is a general feature of the theory of such "braided linear spaces," and the strictness of the braiding Ψ is essential for this.

As an important application, we show how the structure of $S_{\Psi_0}(\mathcal{H}_1)$ as the braided version of the coordinate algebra of a linear space leads to an "anyonic exclusion principle" when q is a root of unity. Specifically, with $q^r = 1$, the creation operator $\psi^*(x)$ cannot occur in a reduced Fock state more than $r-1$ times. This important physical fact means that the relevant occupation number statistics is of the nature of Gentile statistics,[23] and has some similarities to other algebraic approaches to generalized exclusion principles such as that proposed in Ref. 24. The exclusion also applies to states obtained from the smeared field; i.e., $\psi^*(h)^r = 0$ in our Hilbert space representation for any test function h. Earlier articles have approached the fractional exclusion statistics of a one-dimensional gas, or of anyons in two space dimensions, from quite different perspectives;[25–30] see also Ref. 31.

An outline of the present article is as follows: In Sec. II we summarize the topological construction of the spaces $\mathcal{H}_N$ of N-anyon states, and write the corresponding current algebra, diffeomorphism group, and anyon creation and annihilation field representations. In Sec. III we carry out our construction using braided symmetric tensor categories, and in Sec. IV we show that this indeed leads to the same result as the earlier topological construction. In Sec. V we provide some algebraic consequences, including the anyonic exclusion principle when q is a root of unity. Throughout we consider both the physical continuum case and the discrete case, as the latter may be useful for lattice versions of the theory or for anyon fields on a finite number of points. The discrete case turns out to have a number of instructive subtleties. Finally, in Sec. VI we offer some further comments of a conceptual nature.

II. TOPOLOGICAL STATE SPACES $\mathcal{H}_N$

We begin by recalling the set-up for anyon field representations proposed in Ref. 18. For the nonrelativistic quantum theory of identical particles in n space dimensions, we are interested in representations ρ, J of the semidirect sum Lie algebra $C_c^\infty(\mathbb{R}^n) \rtimes \mathrm{vect}_c(\mathbb{R}^n)$, where ρ and J are self-adjoint operator-valued distributions describing the mass and momentum densities, respectively, i.e.,

$$\rho(f) = \int \rho(x) f(x) \mathrm{d}^n x, \quad J(v) = \int J(x) \cdot v(x) \mathrm{d}^n x,$$

where the test function $f \in C_c^\infty(\mathbb{R}^n)$ is a compactly-supported real-valued C^∞ function on $\mathbb{R}^n$, and $v \in \mathrm{vect}_c(\mathbb{R}^n)$ is a compactly-supported (tangent) vector field on $\mathbb{R}^n$. Then the well-known current algebra

$$[\rho(f), \rho(g)] = 0, \quad [\rho(f), J(v)] = i\hbar \rho(\nabla_v f), \quad [J(v), J(w)] = -i\hbar J([v,w]) \tag{1}$$

represents the bracket in the Lie algebra, where $[v,w]$ is the usual Lie bracket of vector fields. The group-level version is based on the natural semidirect product of the group of compactly-supported functions under addition, with the group of compactly-supported diffeomorphisms of $\mathbb{R}^n$ under composition: $G = C_c^\infty(\mathbb{R}^n) \rtimes \mathrm{Diff}_c(\mathbb{R}^n)$, with $(f,\phi)\cdot(g,\psi) = (f + g\circ\phi, \psi\circ\phi)$. Then in a continuous unitary representation of G, we can write the 1-parameter subgroups $U(f)$ and $V(\phi_t)$, where ϕ_t is the flow on $\mathbb{R}^n$ generated by v. Under appropriate conditions, the self-adjoint generators defined from $U(f) = e^{i\rho(f)}$ and $V(\phi_t) = e^{i(t/\hbar)J(v)}$ represent the current algebra. The idea is that different physical systems in quantum mechanics should correspond to different (unitarily inequivalent) irreducible representations of G.

In particular consider a family $\mathcal{H}_N$ of Hilbert spaces, where $N \in \mathbb{N}$, along with annihilation operators $\psi(h)$ and creation operators $\psi^*(h)$, where the test functions h belong to a domain in $\mathcal{H}_1$. Thus

$$\psi(h): \mathcal{H}_{N+1} \to \mathcal{H}_N, \quad \psi^*(h): \mathcal{H}_N \to \mathcal{H}_{N+1}.$$

Suppose we have representations U_N, V_N in $\mathcal{H}_N$ of the group $G = C_c^\infty(\mathbb{R}^n) \rtimes \mathrm{Diff}_c(\mathbb{R}^n)$, for each N, intertwined by ψ and ψ^* in such a way that

$$U_{N+1}(f)\psi^*(h) = \psi^*(U_1(f)h) U_N(f), \quad V_{N+1}(\phi)\psi^*(h) = \psi^*(V_1(\phi)h) V_N(\phi). \tag{2}$$

Then the U_N, V_N $(N = 1,2,3,\ldots)$ are interpreted as a *hierarchy* of representations of G describing systems of N particles (or quantum excitations) of the species created and annihilated by the field operators. At the level of the algebra, the corresponding requirements are

$$[\rho(f), \psi^*(h)] = \psi^*(\rho_1(f)h), \quad [J(v), \psi^*(h)] = \psi^*(J_1(v)h). \tag{3}$$

Here ψ^* is the adjoint of ψ; but we note that later, when we consider the discrete anyonic case, that will be modified.

When $n=2$, one has the possibility in this general framework of anyonic representations of G, and corresponding fields satisfying Eqs. (2) and (3). Then the representation U_N, V_N of G acts in the Hilbert space

$$\mathcal{H}_N = L^2_{B_N}(\tilde{\Delta}_N),$$

defined as follows. The configuration space Δ_N for N identical anyons is the space of (unordered) N-point subsets of $\mathbb{R}^2$; thus $\gamma \in \Delta_N$ is given by $\gamma=\{x_1,\ldots,x_N\}\subset\mathbb{R}^2$. The fundamental group $\pi_1(\Delta_N)$ is B_N, the braid group on N-strands. We denote by $\tilde{\Delta}_N$ the universal covering space of Δ_N, which has infinitely many sheets; for $\tilde{\gamma}\in\tilde{\Delta}_N$, we have the projection map $p:\tilde{\gamma}\to\gamma$. The braid group then acts on $\tilde{\Delta}_N$; writing this action as $\tilde{\gamma}\to\tilde{\gamma}\cdot b$ for $b\in B_N$, we have $p(\tilde{\gamma}\cdot b)=p(\tilde{\gamma})$. The elements of $\mathcal{H}_N$ are now wave functions $\tilde{\Phi}$ on $\tilde{\Delta}_N$, taking values in an inner product space $\mathcal{V}$ that carries a unitary representation $T(b)$ of B_N. We shall consider only the case $\mathcal{V}=\mathbb{C}$ (scalar-valued wave functions), and one-dimensional representations of B_N. Such a representation is specified by choosing a fixed phase $q=\exp i\theta$, and setting $T(b)=q$ when b is the crossing of one strand over another in a forward (left over right) direction. The wave functions are required to be *equivariant* under T, in the sense that for all $b\in B_N$,

$$\tilde{\Phi}(\tilde{\gamma}\cdot b) = T(b)\tilde{\Phi}(\tilde{\gamma}).$$

In other words, $\tilde{\Phi}\in\mathcal{H}_N$ is an equivariant section of a vector bundle over $\tilde{\Delta}_N$. When $\tilde{\Phi}_1$ and $\tilde{\Phi}_2$ satisfy the same such equivariance condition, the product $\overline{\tilde{\Phi}_1(\tilde{\gamma})}\tilde{\Phi}_2(\tilde{\gamma})$ depends only on $\gamma=p(\tilde{\gamma})$, and not on the particular choice of $\tilde{\gamma}$ within $p^{-1}(\gamma)$ at which $\tilde{\Phi}_1$ and $\tilde{\Phi}_2$ are evaluated. Thus we may write the integral of this product with respect to a (local) Lebesgue measure $dx_1\cdots dx_N$ on Δ_N. Finally, we take $\mathcal{H}_N$ to consist of the square-integrable functions, so that for any pair $\tilde{\Phi}_1$, $\tilde{\Phi}_2$,

$$\langle\tilde{\Phi}_1,\tilde{\Phi}_2\rangle = \int_{\Delta_N}\overline{\tilde{\Phi}_1(\tilde{\gamma})}\tilde{\Phi}_2(\tilde{\gamma})dx_1\cdots dx_N<\infty \tag{4}$$

defines the inner product of $\tilde{\Phi}_1$ with $\tilde{\Phi}_2$ in $\mathcal{H}_N$.

Given any diffeomorphism ϕ of $\mathbb{R}^2$, let ϕ act on Δ_N in the obvious way. This action lifts to an action on $\tilde{\Delta}_N$ compatible with the projection map, i.e., if $p(\tilde{\gamma})=\gamma$, then $p(\phi\tilde{\gamma})=\phi\gamma$. The N-anyon representation in $\mathcal{H}_N$ is then defined by

$$U_N(f)\tilde{\Phi}(\tilde{\gamma}) = e^{i\Sigma_{j=1}^N f(x_j)}\tilde{\Phi}(\tilde{\gamma}),\quad V_N(\phi)\tilde{\Phi}(\tilde{\gamma}) = \tilde{\Phi}(\phi\tilde{\gamma})\prod_{j=1}^N\sqrt{\mathcal{J}_\phi(x_j)}, \tag{5}$$

where $\mathcal{J}_\phi$ is the Jacobian of ϕ. The factor of $\Pi_{j=1}^N\sqrt{\mathcal{J}_\phi(x_j)}$ means that V_N transforms $\overline{\tilde{\Phi}_1(\tilde{\gamma})}\tilde{\Phi}_2(\tilde{\gamma})\ \Pi_{j=1}^N dx_j$ to $\overline{\tilde{\Phi}_1(\phi\tilde{\gamma})}\tilde{\Phi}_2(\phi\tilde{\gamma})\ \Pi_{j=1}^N\mathcal{J}_\phi(x_j)dx_j$, and thus does not change the value of the inner product.

One may construct these representations more explicitly as follows. We describe an element of $\tilde{\Delta}_N$ by a set of nonintersecting paths $\Gamma=\{\Gamma_1,\ldots,\Gamma_N\}$ in the plane, extending from infinity in (let us say) the negative y-direction, and terminating in the unordered set γ of N distinct points in $\mathbb{R}^2$. Then $\tilde{\Delta}_N$ is the set of homotopy classes of such Γ, with the projection map given by mapping Γ to the set of its end points. We shall call the homotopy class of Γ a "topological configuration." Moreover, we can lift any configuration $\gamma\in\Delta_N$ (with the exception of a measure zero set) to the element Γ_0^γ belonging to $\tilde{\Delta}_N$, given by taking paths that go vertically downward (in the negative y-direction) from each point in γ. This defines a sheet $\Gamma_0(\Delta_N)\subset\tilde{\Delta}_N$ that we conventionally associate with the identity element of B_N. Now diffeomorphisms in $\mathrm{Diff}_c(\mathbb{R}^2)$ act as the identity at $y=-\infty$ since they are compactly supported, and so they lift from Δ_N to act on the space of topological configurations.

Consider the subgroup $\mathrm{Diff}_c^\gamma(\mathbb{R}^2)$ of diffeomorphisms that take the set of end points γ of a fixed topological configuration Γ into itself. This is the stability subgroup for the point $\gamma \in \Delta_N$. A diffeomorphism $\phi \in \mathrm{Diff}_c^\gamma(\mathbb{R}^2)$ then determines an element of B_N by its action on Γ_0^γ, denoted by $b = h_\gamma(\phi)$. Moreover, given any topological configuration Γ with end points γ, we can obtain it by starting with Γ_0^γ (with the same end points γ), and applying a diffeomorphism $\phi \in \mathrm{Diff}_c^\gamma(\mathbb{R}^2)$, so that $\phi\Gamma_0^\gamma = \Gamma$. Then h_γ is a surjective homomorphism, from $\mathrm{Diff}_c^\gamma(\mathbb{R}^2)$ onto B_N. A topological configuration Γ with end points γ is conventionally identified with the pair (γ, b); when b is the identity element, we have Γ_0^γ. The equivariance condition in this description becomes

$$\tilde{\Phi}(\Gamma) = T(b)\tilde{\Phi}(\Gamma_0^\gamma).$$

Thus it is enough to specify $\tilde{\Phi}$ on the sheet $\Gamma_0(\Delta_N)$; the equivariance condition then defines it almost everywhere in $\tilde{\Delta}_N$.

In this explicit realization, one next defines the creation and annihilation fields intertwining the N-anyon representations (5) in accordance with Eqs. (2) or (3). Given an N-point subset $\gamma \subset \mathbb{R}^2$, and $x \in \mathbb{R}^2$, let us denote by Γ_x^γ the element of $\tilde{\Delta}_{N+1}$ that is obtained by *adjoining* to Γ_0^γ an additional path, terminating at x, that extends toward $y = -\infty$ on the *left* of all the paths in Γ_0^γ (this modifies the convention in Ref. 18). Then we set

$$(\psi(x)\tilde{\Phi})(\Gamma_0^\gamma) = \tilde{\Phi}(\Gamma_x^\gamma).$$

To write the adjoint field, let $\hat{\gamma}_j = \gamma - \{x_j\}$, where j refers to some indexing of the elements of γ. The topological configuration $\Gamma_x^{\hat{\gamma}_j}$ then defines an element of $\tilde{\Delta}_N$, with the set of terminal points $\hat{\gamma}_j \cup \{x\}$. Express $\Gamma_x^{\hat{\gamma}_j}$ as $\phi\Gamma_0^{\hat{\gamma}_j \cup \{x\}}$, and define $b_{x,j} = h_{\hat{\gamma}_j \cup \{x\}}(\phi)$. Then

$$(\psi^*(x)\tilde{\Phi})(\Gamma_0^\gamma) = \sum_{j=1}^{N} \delta(x - x_j)\tilde{\Phi}(\Gamma_0^{\hat{\gamma}_j}) T^*(b_{x,j}).$$

In this realization, one can recover the local current algebra (1) by defining

$$\rho(x) = \psi^*(x)\psi(x), \quad J(x) = \frac{\hbar}{2i}(\psi^*(x)(\nabla\psi)(x) - (\nabla\psi^*)(x)\psi(x)), \tag{6}$$

where ρ is the number density of anyons and J is the momentum density. Then also

$$[\rho(f), \psi^*(h)] = \psi^*(fh), \quad [J(v), \psi^*(h)] = \frac{\hbar}{2i}\psi^*(\nabla_v h + \nabla \cdot (vh)), \tag{7}$$

which are precisely Eqs. (3). Equations (1), (3), and (6) are the same in the anyonic case as in the usual Bose or Fermi cases. But now we have, in place of the CCR or CAR algebras, the following equal-time q-commutation relations:[18] in the half-space $x^1 < y^1$, with $[A, B]_q = AB - qBA$ (where the phase q generates the representations $T(b)$ of B_N),

$$[\psi(x), \psi(y)]_q = [\psi^*(x), \psi^*(y)]_q = 0, \quad [\psi(y), \psi^*(x)]_q = \delta(x - y). \tag{8}$$

In the complementary half-space $x^1 > y^1$, q must be replaced by $\bar{q} = q^{-1}$. The choice of a half-space, like the definition of the sheet $\Gamma_0(\Delta_N)$, is conventional and has no physical consequence.

III. ANYONIC FOCK SPACE CONSTRUCTION

For the usual bosonic or fermionic representations, we have of course a more conventional construction. Let $\mathcal{H} = \mathcal{H}_1 = L^2(\mathbb{R}^n)$ be the space of 1-particle states, and $\mathcal{H}_N = \mathcal{H}^{\otimes_s N}$ be a symmetrized or skew symmetrized tensor product. Then $\psi^*(h) = h\otimes_s$ and $\psi(h)$ is given by the interior product, yielding the usual equal-time commutation or anticommutation relations, respectively. In this section we give such a "Fock space" construction, more in line with the usual Bose or Fermi

cases but now with nontrivial q-statistics. We then show in Sec. IV that in the continuum case it is isomorphic to the topological construction of Ref. 18 described above. We shall use the machinery of braided linear spaces and braided Weyl algebras as described in Refs. 20–22, and elsewhere.

Let us start with a construction that works for any totally ordered space $(X,<)$. We shall initially take X to be discrete. Note that we do *not* assume here that ψ^* is the adjoint of ψ, although this turns out to be true in the continuum case (see Sec. VI); a more complicated relation holds between ψ and ψ^* in the discrete case. Subsequently we consider $X=\mathbb{R}^2$, with $x<y$ if $x^1<y^1$, or if $x^1=y^1$ then $x^2<y^2$.

Let $\mathcal{H}$ denote a space of functions on X, and $\{\delta_x\}$ a basis of δ-functions. We also define the functions

$$\epsilon_0(x,y)=\begin{cases}1 & \text{if } x<y,\\ 0 & x=y,\\ -1 & x>y,\end{cases}$$

$$\epsilon(x,y)=\begin{cases}1 & \text{if } x\leqslant y,\\ -1 & x>y.\end{cases}$$

These are almost, but not quite, the same. Even in the continuum case they are not quite the same, because of the existence of distributions with support on the set $x=y$. In what follows, we derive a version of the equal time q-commutation relations (8) as

$$\psi(x)\psi(y)=q^{\epsilon_0(x,y)}\psi(y)\psi(x),\quad \psi^*(x)\psi^*(y)=q^{\epsilon_0(x,y)}\psi^*(y)\psi^*(x),$$

$$\psi(x)\psi^*(y)-q^{\epsilon(y,x)}\psi^*(y)\psi(x)=\delta(x-y),\quad \forall\, x,y\in X, \tag{9}$$

where as noted ψ^* is not the same as the adjoint operator $\psi^\dagger$. Equations (9) are the refinement of Eqs. (8) that comes out of our Fock space construction, and are consistent with the representations of the fields described using the topological configurations above.

A. Discrete version

Let $(X,<)$ be a discrete totally ordered space, $\mathcal{H}$ a space of functions on X, and δ_x the function that is 1 on x and 0 elsewhere in X. We define the generalized flip (or braiding) operators Ψ, $\Psi_0:\mathcal{H}\otimes\mathcal{H}\to\mathcal{H}\otimes\mathcal{H}$ by

$$\Psi_0(\delta_x\otimes\delta_y)=q^{\epsilon_0(x,y)}\delta_y\otimes\delta_x,\quad \Psi(\delta_x\otimes\delta_y)=q^{\epsilon(x,y)}\delta_y\otimes\delta_x. \tag{10}$$

These both obey the familiar braid or Yang–Baxter relations

$$\Psi_{12}\Psi_{23}\Psi_{12}=\Psi_{23}\Psi_{12}\Psi_{23},$$

where the numerical subscripts refer to the position in $\mathcal{H}^{\otimes 3}$. They also satisfy the cross-compatibility conditions

$$(\Psi+\mathrm{id})(\Psi_0-\mathrm{id})=0,\quad (\Psi_0)_{12}\Psi_{23}\Psi_{12}=\Psi_{23}\Psi_{12}(\Psi_0)_{23},\quad \Psi_{12}\Psi_{23}(\Psi_0)_{12}=(\Psi_0)_{23}\Psi_{12}\Psi_{23}. \tag{11}$$

In addition $\Psi_0^2=\mathrm{id}$, but this fact and the braid relations for Ψ_0 are not essential here.

One can write these operators in an R-matrix form: $\Psi(\delta_x\otimes\delta_y)=\delta_b\otimes\delta_a R^{a\ b}_{\ x\ y}$ (summing over the repeated variables a, b), with $R^{a\ b}_{\ x\ y}=\delta^a_{\ x}\delta^b_{\ y}q^{\epsilon(x,y)}$; and similarly for Ψ_0, in terms of a matrix R'. Associated to any such R, R'-matrices (Ref. 20, Th. 10.2.1) is a "braided linear space" which in our case we denote $S_{\Psi_0}(\mathcal{H})$. It is defined as the quadratic algebra generated by formal products of the $\{\delta_x\}$ generators, modulo the relations

$$\delta_x \underset{s}{\otimes} \delta_y = \underset{s}{\otimes}(\Psi_0(\delta_x \otimes \delta_y)) \equiv \delta_y \underset{s}{\otimes} \delta_x q^{\epsilon_0(x,y)}, \tag{12}$$

where we denote the product in $S_{\Psi_0}(\mathcal{H})$ by $\otimes_s$. The actual braiding Ψ enters in the braided coproduct $\underline{\Delta}: S_{\Psi_0}(\mathcal{H}) \to S_{\Psi_0}(\mathcal{H}) \otimes S_{\Psi_0}(\mathcal{H})$, that makes $S_{\Psi_0}(\mathcal{H})$ a braided group or a Hopf algebra in a braided category. On generators, this is just the linear coproduct given by $\underline{\Delta}\delta_x = \delta_x \otimes 1 + 1 \otimes \delta_x$, but it extends to products under $\otimes_s$ via Ψ; thus

$$\underline{\Delta}(\delta_x \underset{s}{\otimes} \delta_y) = (\delta_x \underset{s}{\otimes} \delta_y) \otimes 1 + \delta_x \otimes \delta_y + q^{\epsilon(x,y)} \delta_y \otimes \delta_x + 1 \otimes (\delta_x \underset{s}{\otimes} \delta_y). \tag{13}$$

As explained in Ref. 20, for the theory of braided spaces one needs not one but *two* operators. One of these operators controls the "internal" noncommutativity of the algebra, and the other controls the "external" noncommutativity or braid statistics with other independent copies. In our case, the physics actually dictates the use of Ψ rather than Ψ_0 in the second role; as only this choice in Eq. (13) correctly reduces to the constant minus sign in the flip for fermions when $q=-1$.

Next, we define the operators ψ_x^* and ψ^x on $S_{\Psi_0}(\mathcal{H})$, by left multiplication and braided differentiation, respectively. Let $[N+1, \Psi] = \mathrm{id} + \Psi_{12} + \Psi_{12}\Psi_{23} + \cdots + \Psi_{12}\cdots\Psi_{N,N+1}$ be the braided integer matrix,[20,22] where, for example, Ψ_{12} denotes Ψ acting in the (1, 2) pair of copies of $\mathcal{H}$. Then,

$$\psi_x^*(\delta_{x_1} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_N}) = \delta_x \underset{s}{\otimes} \delta_{x_1} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_N}, \tag{14}$$

and

$$\begin{aligned}\psi^x(\delta_{x_1} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_{N+1}}) &= \delta_{y_2} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{y_{N+1}} [N+1, \Psi]^{x y_2 \cdots y_{N+1}}_{x_1 x_2 \cdots x_{N+1}} \\ &= \delta^x_{x_1} \delta_{x_2} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_{N+1}} + q^{\epsilon(x_1,x)} \delta^x_{x_2} \delta_{x_1} \underset{s}{\otimes} \delta_{x_3} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_{N+1}} \\ &\quad + \cdots + q^{\epsilon(x_1,x)+\cdots+\epsilon(x_N x)} \delta^x_{x_{N+1}} \delta_{x_1} \underset{s}{\otimes} \cdots \underset{s}{\otimes} \delta_{x_N}.\end{aligned} \tag{15}$$

Clearly the braided derivative ψ^x (or ∂^x in the notation of Ref. 20) is given by the evaluation or interior product pairing with $\mathcal{H}$, but extended to the whole of $S_{\Psi_0}(\mathcal{H})$ as a braided derivation. This is like a super-derivation, but using Ψ to braid ψ^x past elements of $\mathcal{H}$. These operators of braided differentiation arise as infinitesimal translations on the braided space, as expressed through the linear braided coproduct. From the braided Leibniz rule for these operators, one has easily the following relations:[20]

$$\psi_x^* \psi_y^* = \psi_b^* \psi_a^* R'^{a\ b}_{\ x\ y} = \psi_y^* \hat{\psi}_x^* q^{\epsilon_0(x,y)}, \quad \psi^x \psi^y = R'^{x\ y}_{\ a\ b} \psi^b \psi^a = q^{\epsilon_0(x,y)} \psi^y \psi^x, \tag{16}$$

and

$$\delta^x_y = \psi^x \psi^*_y - \psi^*_a R^{a\ x}_{\ y\ b} \psi^b = \psi^x \psi^*_y - q^{\epsilon(y,x)} \psi^*_y \psi^x, \tag{17}$$

just as in Eqs. (9). Notice that the ψ^x operators again obey the algebra $S_{\Psi_0}(\mathcal{H})$, as do (more obviously) the ψ_x^*, but now we have also the cross relation (17).

To sum up, the space $S_{\Psi_0}(\mathcal{H})$, which should be viewed geometrically as the algebra of Ψ_0-symmetric functions (on the dual space of $\mathcal{H}$), first decomposes as a vector space. We have $S_{\Psi_0}(\mathcal{H}) = \oplus_N \mathcal{H}^{\otimes_s N}$, where the components $\mathcal{H} \otimes_s \cdots \otimes_s \mathcal{H}$ (N copies) consist of Ψ_0-symmetric functions of degree N. We shall study these components more explicitly in the next section. Secondly, the same algebra acts by "pointwise multiplication" and "infinitesimal translation" on itself, generating a braided Weyl algebra and satisfying the relations (9) in our discrete setting. This construction generalizes both the usual CCR and CAR algebras, along with their usual realizations on symmetric or antisymmetric product algebras. All of this is an easy case of the general theory of braided spaces and braided derivatives,[22] for our particular R, R'-matrices.

Note also that although we have carefully distinguished δ_x (the basis of the space $\mathcal{H}$ generating $S_{\Psi_0}(\mathcal{H})$) from the operators ψ_x^* and ψ^x that act on $S_{\Psi_0}(\mathcal{H})$, we can also identify $\mathcal{H}$ with the space generated by the ψ_x^* acting on 1 by multiplication. Thus we can identify the whole "acted-upon" copy of $S_{\Psi_0}(\mathcal{H})$ with the copy of $S_{\Psi_0}(\mathcal{H})$ generated by the ψ_x^*. The vacuum state is $|0\rangle = 1$. From the geometrical point of view, the ψ^x act by braided differentiation. From the "Fock space" point of view, they act via the commutation relations and the condition that $\psi^x|0\rangle = 0$.

Finally, let us specialize X to a finite ordered set, writing $X = \{1, \ldots, n\}$. Then using Eqs. (15), we have the following results for $S_{\Psi_0}(\mathcal{H})$ and the corresponding braided Weyl algebra:

$$\psi_i^* \psi_j^* = q \psi_j^* \psi_i^*, \quad \psi^i \psi^j = q \psi^j \psi^i, \quad \psi^i \psi_j^* = q^{-1} \psi_j^* \psi^i, \quad \psi^j \psi_i^* = q \psi_i^* \psi^j \quad (\forall\, i < j)$$

$$\psi^i \psi_i^* - q \psi_i^* \psi^i = 1 \quad (\forall\, i), \tag{18}$$

where

$$\psi_i^* |m_1, \ldots, m_n\rangle = q^{-\Sigma_{j<i} m_j} |m_1, \ldots, m_i + 1, \ldots, m_n\rangle,$$

$$\psi^i |m_1, \ldots, m_n\rangle = q^{\Sigma_{j<1} m_j} [m_i; q] |m_1, \ldots, m_i - 1, \ldots, m_n\rangle. \tag{19}$$

Here

$$|m_1, \ldots, m_n\rangle = (\psi_1^*)^{m_1} \cdots (\psi_n^*)^{m_n} |0\rangle,$$

while

$$[m; q] = 1 + q + \cdots + q^{m-1} = (1 - q^m)/(1 - q)$$

is a "q-integer." These equations yield, for example, the "density operator" as

$$\rho_i = \psi_i^* \psi^i, \quad \rho_i |m_1, \ldots, m_n\rangle = [m_i; q] |m_1, \ldots, m_n\rangle. \tag{20}$$

We note again that the final equation of (18) implies ψ_i^* cannot be the adjoint of ψ^i unless q is real. In general the q-integers in Eq. (20) are complex, and the operator ρ_i is not self-adjoint.

Although we are taking the above "quantum-mechanical harmonic oscillator" point of view, the same mathematical structures can also be viewed as space–time position and momentum generators. Then we would denote the generators δ_i by X^i, and regard them as the coordinates of a noncommutative spacetime, with the usual "q-plane" relations, $X_i X_j = q X_j X_i$ for $i < j$. Similarly, we would write $\psi_i^* = \hat{X}_i$ for the operation of left-multiplication by X_i, and $\psi^i = \partial^i$ for the braided differentiation

$$\partial^i (X_1^{m_1} \cdots X_n^{m_n}) = q^{\Sigma_{j<i} m_j} [m_i; q] X_1^{m_1} \cdots X_i^{m_i - 1} \cdots X_n^{m_n}.$$

This is the "geometrical" point of view to which we alluded above. Here ∂^i acts on the X_i variable by q-differentiation, with an additional braiding q-factor as ∂^i moves past the X_j, $j < i$, in order to reach the X_i. Note that the q-plane is usually associated with more complicated R-matrices related to quantum groups $\mathrm{SL}_q(n)$ but this is not the case here. Indeed, many different R-matrices can give the same quantum plane.

B. Functional version

We next proceed to a functional version of the above, more suitable for the continuum case. Clearly, on general functions $h, g \in \mathcal{H}$, the braiding is given by

$$\Psi_0(h \otimes g)(x, y) = g(x) h(y) q^{-\epsilon_0(x,y)}, \tag{21}$$

where $\Psi_0(h \otimes g) = \int dx dy \Psi_0(h \otimes g)(x, y) \delta_x \otimes \delta_y$ (the integrals here and below should be interpreted as sums in the discrete case). Next, a basis for $\mathcal{H} \otimes_s \cdots \otimes_s \mathcal{H}$ is given by "normal ordering," i.e., we

choose $\{\delta_{x_1}\otimes_s\cdots\otimes_s\delta_{x_N}|x_1\leqslant x_2\leqslant\cdots\leqslant x_N\}$. We let the coefficients in this basis be partially defined functions $f(x_1,x_2,\ldots,x_N)$ so that

$$f=\int_{x_1\leqslant\cdots\leqslant x_N}dx_1\cdots dx_N f(x_1,x_2,\ldots,x_N)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_{x_N}.$$

Then, defining $\psi^*(h)=\int dx h(x)\hat{\delta}_x$, we compute

$$\begin{aligned}\psi^*(h)f=&\int_{x\leqslant x_1\leqslant\cdots\leqslant x_N}dx dx_1\cdots dx_N h(x)f(x_1,\ldots,x_N)\,\delta_x\underset{s}{\otimes}\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}x_{x_N}\\&+q^{-1}\int_{x_1<x\leqslant x_2\cdots\leqslant x_N}dx_1dx\cdots dx_N h(x)f(x_1,\ldots,x_N)\,\delta_{x_1}\underset{s}{\otimes}\delta_x\underset{s}{\otimes}\delta_{x_2}\underset{s}{\otimes}\cdots\otimes\delta_{x_N}+\cdots\\&+q^{-N}\int_{x_1\leqslant\cdots\leqslant x_N<x}dx_1\cdots dx_N dx h(x)f(x_1,\ldots,x_N)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_{x_N}\underset{s}{\otimes}\delta_x,\end{aligned}\tag{22}$$

where we have used the relations (12). After relabeling, we read off the coefficients as

$$\begin{aligned}(\psi^*(h)f)(x_1,\ldots,x_{N+1})=&\,h(x_1)f(x_2,\ldots,x_{N+1})+q^{-1}h(x_2)f(x_1,x_3,\ldots,x_{N+1})+\cdots\\&+q^{-N}h(x_{N+1})f(x_1,\ldots,x_N),\end{aligned}\tag{23}$$

for distinct "normally ordered" arguments. This is our representation of ψ^* in the continuum case.

Similarly, we linearly extend the definition (15) of ∂^x, doing in each case one of the integrals and relabeling the integration variables $x_1,\ldots,x_N$. This gives

$$\begin{aligned}\psi(x)f=&\int_{x\leqslant x_1\cdots\leqslant x_N}dx_1\cdots dx_N f(x,x_1,\ldots,x_N)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_N\\&+q\int_{x_1\leqslant x\leqslant x_2\leqslant\cdots\leqslant x_N}dx_1\cdots dx_N f(x_1,x,x_2,\ldots,x_N)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_N+\cdots\\&+q^N\int_{x_1\leqslant\cdots\leqslant x_N\leqslant x}dx_1\cdots dx_N f(x_1,\ldots,x_N,x)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_N,\end{aligned}$$

which yields

$$(\psi(x)f)(x_1,\ldots,x_N)=q^m f(x_1,\ldots,x_m,x,x_{m+1},\ldots,x_N)\quad\text{for } x_m<x<x_{m+1},\tag{24}$$

with distinct, "normally ordered" $x_1,\ldots,x_N$ (using the usual conventions for $m=0$ or $m=N$). This is our representation of ψ in the continuum case.

Finally, if the basis elements are taken in a different order, the corresponding coefficients are related through Eq. (12), e.g., we have

$$f(x_2,x_1,\ldots,x_N)=q^{\epsilon_0(x_1,x_2)}f(x_1,x_2,\ldots,x_N),$$

and so forth. In this way, any coefficient function defined on "normally ordered" arguments extends uniquely to an element of $\mathcal{H}^{\otimes N}$ obeying such relations.

Hence, proceeding now in the continuum case, we can characterize $\mathcal{H}\otimes_s\cdots\otimes_s\mathcal{H}$ as the subspace of "Ψ_0-symmetric" functions

$$\mathcal{H}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\mathcal{H}=\{f\in\mathcal{H}^{\otimes N}|f(\sigma(x_1,\ldots,x_N))=q^{\ell(\sigma)}f(x_1,\ldots,x_N),\ \ \forall\,\sigma\in S_N, x_1<\cdots<x_N\},\tag{25}$$

where $\ell(\sigma)$ is the length of the permutation σ. It suffices to impose the symmetrization condition here almost everywhere. For example,

$$\mathcal{H}\underset{s}{\otimes}\mathcal{H}=\{f|f(y,x)=qf(x,y),\ \ \forall\,x<y\},$$

and

$$\mathcal{H}\underset{s}{\otimes}\mathcal{H}\underset{s}{\otimes}\mathcal{H}=\{f|f(y,x,z)=f(x,z,y)=qf(x,y,z), f(z,x,y)=f(y,z,x)=q^2f(x,y,z),$$
$$f(z,y,x)=q^3f(x,y,z),\ \ \forall\,x<y<z\}.$$

Making use of the subspace description (25), there is a corresponding formula for the action of $\psi^*(h)$ that involves factors of q^{ϵ}. For example, letting $\psi^*(h)$ act on a function $f\in\mathcal{H}\otimes_s\mathcal{H}$, we have

$$(\psi^*(h)f)(x,y,z)=h(x)f(y,z)+q^{\epsilon(y,x)}h(y)f(x,z)+q^{\epsilon(z,x)+\epsilon(z,y)}h(z)f(x,y).\tag{26}$$

The general formula for degree N is

$$\psi^*(h)f=(\mathrm{id}+\Psi_{12}+\Psi_{23}\Psi_{12}+\cdots+\Psi_{N,N+1}\cdots\Psi_{23}\Psi_{12})(h\otimes f),\tag{27}$$

which up to a normalization is just $h\otimes f$ followed by total Ψ-symmetrization (given the assumed Ψ-symmetry of f). Similarly, the formula for $\psi(x)$ may be written in the subspace description. It comes out simply as the interior product

$$\psi(x)f=f(x,\ldots),\tag{28}$$

where we evaluate the first argument of f at x. These are the field operators when we work with N-particle wave functions as symmetrized functions in N variables, as in the usual Bose or Fermi Fock spaces.

When there are products of fields, we will typically smear at least some of the variables with test functions to make sense of the distributions. Thus the q-commutation relations can be written as

$$\psi(x)\psi(h)=\psi(\theta_{0x}h)\psi(x),\quad \psi^*(x)\psi^*(h)=\psi^*(\theta_{0x}h)\psi^*(x),$$

$$\psi(h)\psi^*(x)=\psi^*(x)\psi(\theta_x h)+h(x),\tag{29}$$

for $x\in X$ and h in a dense domain of $\mathcal{H}$, where for each fixed x we define

$$\theta_{0x}(y)=q^{\epsilon_0(x,y)},\quad \theta_x(y)=q^{\epsilon(x,y)}$$

as functions of y (having modulus 1 when q is a phase), and where $\theta_{0x}h$ and $\theta_x h$ refer to the action on $\mathcal{H}$ given by pointwise multiplication. The second equation of (29) can also be written

$$\psi(x)\psi^*(h)=\psi^*(\overline{\theta}_x h)\psi(x)+h(x),$$

where $\overline{\theta}_x(y)=q^{\epsilon(y,x)}$.

As before, essentially the same algebra $S_{\Psi_0}(\mathcal{H})$ leads both to the Hilbert space of the system with components $\mathcal{H}^{\otimes_s N}$ as above (ignoring its algebra structure), and to the generalized field algebra of the $\psi^*(h)$ together with another copy for the $\psi(h)$ as an algebra of operator-valued

distributions obeying (9) and represented according to (23) and (24). The Fock space can also be viewed as generated by the operators $\psi^*(h)$ for a sufficient set of test functions h, acting repeatedly on $|0\rangle$.

We also have a geometrical picture as at the end of the last section, with $\psi(h)$ acting now by "braided functional differentiation."

C. Unitarity considerations

Until now we have worked rather generally, and have taken q to be arbitrary. We now work specifically over $\mathbb{C}$, and take q to be a phase. Addressing first the continuum case, we consider the L^2 inner product on $\mathcal{H}$, and verify that all our operator constructions are suitably self-adjoint.

First we see that Ψ_0 is self-adjoint, since

$$(a\otimes b,\Psi_0(h\otimes g))=\int\int dxdy\overline{a}(x)\overline{b}(y)g(x)h(y)q^{-\epsilon_0(x,y)}$$

$$=\int\int dxdy\overline{\Psi_0(a\otimes b)(y,x)}h(y)g(x)=(\Psi_0(a\otimes b),h\otimes g).$$

Next we make use of the fact that the spaces $\mathcal{H}\otimes_s\cdots\otimes_s\mathcal{H}$ have L^2 inner products, when we write their elements as functions f defined on the fundamental domain of "normally ordered" coordinates. We perform the integration over this domain. Thus:

$$(g,\psi^*(h)f)=\int_{x_1\leqslant\cdots\leqslant x_{N+1}}dx_1\cdots dx_{N+1}\overline{g}(x_1,\ldots,x_{N+1})\cdot\sum_{m=0}^{N+1}q^{-m}h(x_{m+1})f(x_1,\ldots,\hat{x}_{m+1},\ldots,x_{N+1})$$

$$=\sum_{m=0}^{N}\int_{x_1\leqslant\cdots\leqslant x_N}dx_1\cdots dx_N\cdot\overline{\int_{x_m}^{x_{m+1}}dxq^m\overline{h}(x)g(x_1,\ldots,x_m,x,x_{m+1},\ldots,x_N)f(x_1,\ldots,x_N)}$$

$$=(\psi(\overline{h})g,f),\tag{30}$$

where we have used the previous results for $\psi^*(h)$ and $\psi(x)$, interpreted $\psi(\overline{h})$ as the integral of $\psi(x)$ times $\overline{h}$, and relabeled the x_i in the calculation. The cases $m=0$ and $m=N$ are understood in the obvious way (the integration is then taken to $\pm\infty$). In the summations for $\psi^*(h)f$ (see Eq. (22)) some of the inequalities in the region of integration are strict, but we are permitted to ignore this distinction in the present continuum case.

Finally, in our subspace description of $\mathcal{H}\otimes_s\cdots\otimes_s\mathcal{H}$ we would like to define the inner product in terms of that on $\mathcal{H}^{\otimes N}$. Indeed, for f, g extended to Ψ_0-symmetric elements of $\mathcal{H}^{\otimes N}$, we have

$$(g,f)_{\mathcal{H}^{\otimes N}}=\sum_{\sigma\in S_N}\int_{x_1\leqslant\cdots\leqslant x_N}dx_1\cdots dx_N\overline{g}(\sigma(x_1,\ldots,x_N))f(\sigma(x_1,\ldots,x_N))=N!\,(g,f).$$

That is, the natural inner product with respect to which ψ and ψ^* are mutually adjoint is $N!^{-1}$ times the usual tensor product inner product. Alternatively, if one wished to use the usual tensor product inner product, then one should work with $(N+1)^{-1}\psi^*(h)$. From Eq. (27) we see that this would then be a true averaging over the symmetric group, and would correspond to the usual normalization in the Bose and Fermi cases.

For the continuum case, we see that ψ^* is the adjoint of ψ as in Ref. 18. The discrete case requires us to perform summations instead of integrations, and to be careful about the domains of summation. Thus, in the second term of Eq. (22), we have $x_1<x\leqslant x_2\leqslant\cdots\leqslant x_N$; and similarly for the other terms. Then, as a correction to Eq. (30), we have the following:

$$(\psi(\overline{h})g,f) = (g,\psi^*(h)f) + \sum_{x_1\leqslant x_2\leqslant\cdots\leqslant x_N} (q^{-1}h(x_1)\overline{g}(x_1,x_1,x_2,\ldots,x_N) + \cdots$$
$$+ q^{-N}h(x_N)\overline{g}(x_1,\ldots,x_{N-1},x_N,x_N))\cdot f(x_1,\ldots,x_N). \tag{31}$$

Writing $\psi(\overline{h})^\dagger = \psi^*(h) + T_h^*$, where $\psi(\overline{h})^\dagger$ is the adjoint of $\psi(\overline{h})$, we find

$$T_h^*(\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_{x_N}) = \sum_{m=1}^{N} q^{-m}h(x_m)\,\delta_{x_1}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_{x_m}\underset{s}{\otimes}\delta_{x_m}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\delta_{x_N}$$

where δ_{x_m} is duplicated on the right-hand side, and where $x_1\leqslant\cdots\leqslant x_N$.

To proceed further, it is convenient (though not essential) to use the simplified notation for the set $X=\{1,\ldots,n\}$. We then find

$$T_i^*((\delta_1)^{m_1}\cdots(\delta_n)^{m_n}) = q^{-\Sigma_{j<i}m_j}(q^{-1}+\cdots+q^{-m_i})(\delta_1^{m_1})\cdots(\delta_i^{m_i+1})\cdots(\delta_n)^{m_n}$$

(where we have omitted the symbols $\otimes_s$ for the symmetrized tensor product). Hence

$$T_i^*|m_1,\ldots,m_n\rangle = q^{-1}q^{-\Sigma_{j<i}m_j}[m_i;q^{-1}]|m_1,\ldots,m_i+1,\ldots,m_n\rangle,$$

and

$$\psi^{i\dagger}|m_1,\ldots,m_n\rangle = (1+q^{-1}[m_i;q^{-1}])\psi_i^*|m_1,\ldots,m_n\rangle = [m_i+1;q^{-1}]\psi_i^*|m_1,\ldots,m_n\rangle.$$

Noting that $\rho_i^\dagger$ has values which are the complex conjugates of the values of the diagonal operator ρ_i in Eq. (20), we see that

$$\psi^{i\dagger} = \rho_i^\dagger\psi_i^*, \quad \psi^i = (\psi_i^*)^\dagger\rho_i. \tag{32}$$

It is worth remarking that

$$\psi^{i\dagger}\psi^i|m_1,\ldots,m_n\rangle = \rho_i^\dagger\rho_i = |[m_i;q]|^2|m_1,\ldots,m_n\rangle = \frac{1-\cos m_i\theta}{1-\cos\theta}|m_1,\ldots,m_n\rangle \tag{33}$$

if $q=e^{i\theta}$.

While the density operators ρ_i are not self-adjoint in the discrete case, they have some nice properties. For example,

$$[\rho_i,\psi_j^*] = 0 = [\rho_i,\psi^j] \quad (\forall\, i\neq j)$$

but

$$\rho_i\psi_i^* - q\psi_i^*\rho_i = \psi_i^*, \quad \psi^i\rho_i - q\rho_i\psi^i = \psi^i, \tag{34}$$

with similar relations for $\rho_i^\dagger$; also $[\rho_i,\rho_i^\dagger]=0$. The results differ from the continuum case, where we already know that Eq. (7) holds with the usual commutator, not the q-commutator of Eq. (34).

The same conclusions apply for any discrete set X. The origin of the differences from the corresponding equations in the continuum case is that in the discrete case, we have treated the δ-function in Eq. (9) as a Kronecker-δ with values 0 and 1. This makes it the "same size" as the δ-functions arising in the combinatorics of the summations. Such a treatment leads to elegant q-deformation formulas, as obtained above. For a $\mathbb{Z}^n$-lattice theory that correctly converges in the zero-spacing limit to the continuum theory, one could use $\delta_{x,y}/\Delta^n$ in the right-hand side of Eq. (9), where Δ is the lattice spacing.

IV. IDENTIFICATION WITH THE TOPOLOGICAL PICTURE

It remains to identify the Hilbert spaces $\mathcal{H}_N$ in the previous section with the braided-symmetrized tensor products we have obtained. Let the map $\pi: B_N\to S_N$ be the natural homomor-

phism defined by identifying a crossing with its inverse crossing. As in Sec. II, we describe a topological configuration $\tilde{\gamma}$ by the pair (γ,b), where $p(\tilde{\gamma})=\gamma\in\Delta_N(\mathbb{R}^2)$, and where $b\in B_N$ (the fundamental group of Δ_N). Then with $\gamma=\{x_1,\ldots,x_N\}$,

$$\mathcal{H}_N\cong\mathcal{H}\underset{s}{\otimes}\cdots\underset{s}{\otimes}\mathcal{H},\quad \tilde{\Phi}(\gamma,b)=f(\pi(b)(x_1,\ldots,x_N)),\quad \forall\, x_1<x_2\cdots<x_N.$$

While γ is unordered, we introduce the conventional lexicographic ordering in indexing its elements.

For example if $x<y<z$ in $\mathbb{R}^2$, then

$$\tilde{\Phi}(\{x,y,z\},e)=f(x,y,z),\quad \tilde{\Phi}(\{x,y,z\},b_{23})=f(x,z,y)=q\tilde{\Phi}(\{x,y,z\},e)=qf(x,y,z)$$

by equivariance, where b_{23} is the braid group generator braiding strand 2 with strand 3. In general, if $x_1<\cdots<x_N$, then

$$f(\sigma(x_1,\ldots,x_N))=\tilde{\Phi}(\{x_1,\ldots,x_N\},i(\sigma))=q^{\ell(\sigma)}\tilde{\Phi}(\{x_1,\ldots,x_N\},e)=q^{\ell(\sigma)}f(x_1,\ldots,x_N),\qquad(35)$$

where $i(\sigma)$ is the braid defined as follows: Let $\sigma=s_{j_1}\cdots s_{j_{\ell(\sigma)}}$ be a reduced expression for σ in terms of simple exchanges $s_j=(j,j+1)$. Let b_j be the braid group generator braiding strands j and $j+1$. Then $i(\sigma)=b_{j_1}\cdots b_{j_{\ell(\sigma)}}$. Note that $i(\sigma)$ does not define a group homomorphism. Equation (35) is just as required; our symmetry condition on f corresponds to the equivariance under B_N of $\tilde{\Phi}$.

Likewise, using the definitions in Sec. II and the diagrammatic notation as in Ref. 18, one obtains

$$(\psi^*(h)\tilde{\Phi})(\{x,y,z\},e)=q^{-\#(y,z<x)}h(x)\tilde{\Phi}(\{y,z\},e)+q^{-\#(x,z<y)}h(y)\tilde{\Phi}(\{x,z\},e)$$
$$+q^{-\#(x,y<z)}h(z)\tilde{\Phi}(\{x,y\},e),$$

as well as

$$(\psi(z)\tilde{\Phi})(\{x,y\},e)=q^{\#(x,y<z)}\tilde{\Phi}(\{x,y,z\},e),$$

where $\#(x,y<z)$ denotes the number of points in the set $\gamma=\{x,y\}$ to the left of z in $\mathbb{R}^2$. These actions are to be compared with (24) and (26). Similarly one proves in general that the two constructions coincide; that is, the representation of the anyon creation and annihilation fields in the spaces $\mathcal{H}_N$ of topological configurations is equivalent to their representation in the braided Fock space by $h\otimes_s$ and the interior product.

V. ROOTS OF UNITY AND THE ANYONIC EXCLUSION PRINCIPLE

In this section we specialize further to the case where $q=e^{2\pi i/r}$ is a primitive rth root of unity. Our main observation is that in the continuum case, the explicit representation (23) on Ψ_0-symmetric tensor products implies that

$$\psi(h)^r=0,\quad \psi^*(h)^r=0\quad(\forall h);\qquad(36)$$

that is, we have an *anyonic exclusion principle*. Here h is any test-function, and the smearing of ψ by h makes sense of the products of distributions. By taking "bump functions" that are increasingly localized at an arbitrary point x, we can also write informally,

$$\psi(x)^r=0,\quad \psi^*(x)^r=0\quad(\forall x),\qquad(37)$$

a condition which we shall justify directly in the discrete case. Before doing so let us note that conversely, the pointwise condition (37) in the discrete case implies (36), since

$$\psi(\lambda\delta_x+\mu\delta_y)^r=(\lambda\psi(x)+\mu\psi(y))^r=\sum_{s=0}^{s=r}\lambda^s\mu^{r-s}\psi(x)^s\psi(y)^{r-s}\begin{bmatrix} r \\ s \end{bmatrix}_{;q^{\epsilon_0(y,x)}}=\lambda^r\psi(x)^r+\mu^r\psi(y)^r, \tag{38}$$

for any constants λ,μ and $x\neq y$. In obtaining (38), we use the q-binomial theorem for q-commuting quantities, with q-binomial coefficients defined in the usual way but with q-integers in place of integers in the factorials. Since $q^r=1$ we have $[r;q^{\pm1}]=0$ and hence only $s=0$ and $s=r$ contribute. So the pointwise and smeared versions are formally equivalent, with the smeared version being more suitable in the continuum case.

To prove (36) in the continuum, we use (23) acting on the vacuum (the identity function with no arguments) to deduce that

$$\psi^*(h)^m(x_1,\ldots,x_m)=[m;q^{-1}]!\,h(x_1)\cdots h(x_m)$$

for all non-negative integers m. This follows by induction on m. It is true for $m=1$; assuming it for m, we have

$$\begin{aligned}\psi^*(h)^{m+1}(x_1,\ldots,x_{m+1})&=h(x_1)\psi^*(h)^m(x_2,\ldots,x_{m+1})+q^{-1}h(x_2)\psi^*(h)^m(x_1,x_3,\ldots,x_{m+1})+\cdots\\&\quad+q^{-m}h(x_{m+1})\psi^*(h)^m(x_1,\ldots,x_m)\\&=(1+q^{-1}+\cdots+q^{-m})[m;q^{-1}]!h(x_1)\cdots h(x_{m+1})\end{aligned}$$

as required. The exclusion principle follows when $q^r=1$, since then $[r;q^{-1}]=0$ as already noted above. Next, letting $\psi^*(h)^r$ act on any Fock state of the form $\psi^*(h_1)\cdots\psi^*(h_N)|0\rangle$, we move $\psi^*(h)^r$ to the right until it arrives to act on the vacuum. In doing so, h will be replaced by a convolution with all the $h_1,\ldots,h_N$ [see Eqs. (29)], giving us a new function h'. But we have already verified that $\psi^*(h')^r|0\rangle$ for all test functions; hence (36) holds in the representation. The result for $\psi(h)^r$ follows, as in the continuum case it is the adjoint.

In fact, in the continuum theory one can formally conclude (36) as a statement about operator-valued distributions. We exhibit the reasoning for $r=3$ (the general case is similar). We have

$$\begin{aligned}\psi^*(h)^3&=\int dxdydzh(x)h(y)h(z)\psi^*(x)\psi^*(y)\psi^*(z)\\&=\sum_{\sigma\in S_3}\int_{\sigma(x)<\sigma(y)<\sigma(z)}dxdydzh(x)h(y)h(z)q^{-\ell(\sigma)}\psi^*(\sigma(x))\psi^*(\sigma(y))\psi^*(\sigma(z))\\&=\sum_{\sigma\in S_3}q^{-\ell(\sigma)}\int_{x<y<z}dxdydz\psi^*(x)\psi^*(y)\psi^*(z)=0,\end{aligned}$$

where we have written $\sigma(x,y,z)=(\sigma(x),\sigma(y),\sigma(z))$, and where $\ell(\sigma)$ is the length of the permutation. In effect we have broken up the threefold integral into 3! permutations of the fundamental domain where $x<y<z$ (not being concerned about coincident points since these form a subset of measure zero); then we have used the q-commutation relations (9), and finally we have changed variables to give many copies of the integral over the fundamental domain. The result is zero since $\Sigma q^{-\ell(\sigma)}=[3;q^{-1}]!=0$ when $q^3=1$. The same argument holds for general r and for $\psi(h)^r=0$.

The arguments for the discrete case are more subtle, and indeed the formulas $\psi(x)^r=0$ and $\psi^*(x)^r=0$ do not hold automatically in our representation. Rather, we argue that in this case it is natural to *impose* these according to the algebraic structure. This is similar to "truncated versions" of quantum groups and other q-algebras in conformal field theory and other settings at roots of unity. Indeed we then have $\Psi^r=\mathrm{id}$ for the braiding, and we are essentially in the setting that has been called "anyonic vector spaces " in Refs. 13 and 20.

From a physical point of view, the key observation is that for q a primitive rth root of unity, the operators

$$\psi(x)^r, \quad \psi^*(x)^r$$

are in any case central. In fact, from (9) we have $\psi(x)^m\psi(y)=q^{m\epsilon_0(x,y)}\psi(y)\psi(x)^m$, and

$$\begin{aligned}\psi(x)^m\psi^*(y) &= \psi(x)^{m-1}q^{\epsilon(y,x)}\psi^*(y)\psi(x) + \psi(x)^{m-1}\delta(x-y)\\ &= q^{m\epsilon(y,x)}\psi^*(y)\psi(x)^m + \delta(x-y)\psi(x)^{m-1}[m;q^{\epsilon(y,x)}].\end{aligned}$$

Hence, when $q^r=1$, we have $[r;q^{\pm1}]=0$ and $\psi(x)^r$ is central. Note that here it is critical that we used ϵ and not ϵ_0 in the calculation involving $\psi^*(y)$. Similarly, we have that $\psi^*(x)^r$ central. Therefore, in an irreducible sector of the theory, these operators should be set to multiples of the identity.

This argument is needed only in the discrete case, but the algebraic structures apply (suitably understood) in both cases; thus we have used a notation applicable to both.

As for which value these operators should be assigned, we have already seen that (37) is suitable for the constraint to be linear (basis independent), in the sense of applying to all h. Clearly zero is the only value with this property. Another way to reach the same conclusion is in terms of the braided coproduct on $S_{\Psi_0}(\mathcal{H})$. On products it extends by Ψ, and one has

$$\underline{\Delta}\psi^*(x)^r = \sum_{s=0}^{s=r}\psi^*(x)^s\otimes\psi^*(x)^{r-s}\begin{bmatrix} r \\ s \end{bmatrix}_{;q} = \psi^*(x)^r\otimes 1 + 1\otimes\psi^*(x)^r.$$

A similar result holds for $\psi(x)^r$. Since $\underline{\Delta}1=1\otimes 1$, only (37) allows the braided coproduct to descend to the reduced algebra; no other constant will do. Moreover, since this $\underline{\Delta}$ underlies the braided-differentiation operation ∂^x in Sec. III A, our representation of ψ^* (and more obviously ψ) then descends to an action of the truncated algebra $S_{\Psi_0}(\mathcal{H})$ (in which (37) is imposed) on itself, by the same formulas as before. This is in subtle contrast to the continuum case, where (36) already holds.

Next we note that because $\psi^*(x)$ and $\psi^*(y)$ commute up to a factor $q^{\epsilon_0(x,y)}$, any state formed by a sequence of creation field operators applied to the vacuum, where r or more occurrences of $\psi^*(x)$ are included, must vanish. That is,

$$\psi^*(x)\psi^*(y)\psi^*(z)\cdots\psi^*(x)\psi^*(w)\cdots\psi^*(x)\cdots|0\rangle = 0$$

if there are r or more instances of $\psi^*(x)$. The distinct $\psi^*(y)$, $\psi^*(z)$ and so forth can equally be annihilation fields $\psi(y)$, $\psi(z)$ and so forth, since these too q-commute with $\psi^*(x)$.

More generally, a state formed from the vacuum will be zero if there are m annihilation $\psi(x)$ operators, and $r+m$ or more $\psi^*(x)$. This can be proved by induction on m, as follows. The case $m=0$ is covered above. Suppose it is true for $m-1$. Given an expression with m annihilation operators, look at the rightmost $\psi(x)$. Applying the q-commutation relation with the ψ^* to its right, we move $\psi(x)$ to the right and pick up a second term with a δ-function and with one fewer $\psi(x)$, and at most one fewer $\psi^*(x)$; by our induction hypothesis, this second term vanishes. Meanwhile, the first term has $\psi(x)$ one step to the right; repeating this eventually brings it to act directly on $|0\rangle$, giving zero. This proof makes sense in the discrete case, or with the assumption that the δ-functions are approximated by bounded functions with the limit taken only at the end (in order to treat $\delta(0)$ as a number). More precisely, in terms of annihilation operators smeared with test functions,

$$\psi^*(x)\cdots\psi(h_1)\cdots\psi^*(x)\cdots\psi(h_m)\cdots\psi^*(x)\cdots|0\rangle = 0$$

if there are m annihilation operators and at least $r+m$ creations $\psi^*(x)$ anywhere in the string. This follows from (29) and a similar proof by induction.

For general $\psi^*(h)$ we always have the exclusion principle (36). But the stronger version, in which some of the $\psi^*(h)$ are not adjacent, is more complicated. The various $\psi^*(h)$ needed are modified by the intervening creation field operators, according to (29). Thus, one has instead exclusion conditions that take the form

$$\psi^*(\theta_{0x_1}\cdots\theta_{0x_m}h)^{n_0}\psi^*(x_1)\psi^*(\theta_{0x_2}\cdots\theta_{0x_m}h)^{n_1}\cdots\psi^*(x_{m-1})\psi^*(\theta_{0x_m}h)^{n_{m-1}}\psi^*(x_m)\psi^*(h)^{n_m}|0\rangle = 0,$$

when $n_0+\cdots+n_m \geqslant r$. In the Bose or Fermi cases, the functions θ_{0x} are constant (± 1), up to a set of measure zero; but otherwise they must be taken into account. The same complication applies when there are annihilation operators present. This would appear to be a feature of the anyonic theory $(r>2)$, that is not present for fermions.

On the other hand, we do not see this complication if all our smeared fields have disjoint support. Thus, from (29) we find that

$$\psi^*(h)\psi^*(g) = \psi^*(g)\psi^*(h)\begin{cases} q & \text{if } \mathrm{supp}(h) < \mathrm{supp}(g) \\ q^{-1} & \text{if } \mathrm{supp}(h) > \mathrm{supp}(g) \end{cases}$$

$$\psi(h)\psi^*(g) = (\overline{g},h) + \psi^*(g)\psi^*(h)\begin{cases} q^{-1} & \text{if } \mathrm{supp}(h) < \mathrm{supp}(g) \\ q & \text{if } \mathrm{supp}(h) > \mathrm{supp}(g) \end{cases}$$

with a similar equation for $\psi(h)\psi(g)$. When they occur, these have a similar form to (9). Hence, as an application, one may take the $\psi^*(x)$ as given more precisely by smearing with "bump functions" of small support around the relevant point. As long as these bumps do not touch, the various smeared $\psi^*(x)$ fields behave as in the discrete case, and may be collected together by similar relations. For such states we have the full exclusion principle again, without any complications when the instances of the smeared field $\psi^*(x)$ are separated from each other in the product of field operators.

With this last observation in mind, let us give a straightforward application of the exclusion principle to a gas of noninteracting anyonic particles (e.g., vortices) localized in disjoint sets around points $x_1,\ldots,x_n$ in $\mathbb{R}^2$. Let us suppose that each particle carries a fixed unit E of energy, which does not depend on the positions; the latter will therefore be considered as fixed (or else, we must factor out the resulting degeneracy). As per the discrete version of the theory, the reduced range of states is then

$$|m_1,\ldots,m_n\rangle = \psi^*(x_1)^{m_1}\cdots\psi^*(x_n)^{m_n}|0\rangle, \quad m_i = 0,\ldots,r-1.$$

Let us decompose this reduced Hilbert space as $\oplus_N \mathcal{H}_N$ according to $N=\Sigma_{i=1}^n m_i$, which is the value of the occupation number operator

$$\mathcal{N} = \int dx\rho(x) = \int dx\psi^*(x)\psi(x).$$

The statistical partition function is then

$$Z_\beta = \mathrm{Trace}(e^{-\beta E\mathcal{N}}) = \sum_N e^{-\beta EN}\dim(\mathcal{H}_N) = \sum_{\{m_i\}} e^{-\beta E\Sigma_i m_i} = [r;e^{-\beta E}]^n. \tag{39}$$

The q-integer again appears, but now at the real value $e^{-\beta E}$. Each mode ψ_i^* may be counted separately, so that the computation here is the same as that for 1 particle, but raised to the nth power. When $r=2$ we recover the usual partition function for fermions, while for $r=\infty$ we recover the usual result for bosons

$$[2;e^{-\beta E}] = e^{-\beta E}+1; \quad [\infty;e^{-\beta E}] = \frac{1}{1-e^{-\beta E}}.$$

The general formula $[r;e^{-\beta E}]$ interpolates the two. From the partition function one may then proceed as usual to obtain the thermodynamic properties of such a gas.[32]

More generally, we may take Hamiltonians with interaction terms, including those that arise from the field theory rather than the harmonic oscillator point of view (i.e., with kinetic and current–current interaction terms). Such applications will be developed elsewhere.

VI. CONCLUDING REMARKS

We have obtained a generalized exclusion principle for anyons—an important physical result—not from analysis of the statistical mechanics of anyons, but from the explicit representation of nonrelativistic creation and annihilation fields in an appropriate braided tensor product space. As one would expect in this context, the principle holds when the anyonic phase shift is a root of unity. It applies both to smeared fields $\psi(h)$, $\psi^*(h)$ and to (unsmeared) operator-valued distributions $\psi(x)$, $\psi^*(x)$ satisfying q-commutation relations; but it takes a rather cleaner form in the latter case (a subtle distinction that disappears for bosons and fermions).

On the other hand, the discrete version in which we work directly with points (rather then with increasingly peaked bump functions) turns out to be different and algebraically more complicated; with ψ^i and ψ_i^* no longer adjoint to each other. The fact that one has a different theory from the continuum limit is an interesting feature of our analysis. We believe this subject, and its relation to Gentile statistics and to generalized harmonic oscillators, deserves some renewed attention.

Let us also mention some related conceptual aspects of interest. Our construction of $S_{\Psi_0}(\mathcal{H})$ in Sec. II is manifestly dependent on an ordering, since this enters in the braiding. This is true for quantum planes (see the remarks at the start of Sec. V), where $X=\{1,2,\ldots,n\}$ is the indexing set; and it remains true when we apply our formalism to the second quantization of nonrelativistic fields (so that X denotes physical space). The Fock space construction might then seem to be strongly dependent on the somewhat artificial lexicographical total ordering on $\mathbb{R}^2$ used in Sec. III. However the isomorphism in Sec. IV, with the spaces $\mathcal{H}_N$ described by means of topological configurations, tells us that in fact the underlying diffeomorphism invariance remains as far as the physics is concerned. The lexicographical ordering places the physical system into an algebraic form described by the symmetric tensor products $\otimes_s$, but this is for mathematical convenience only.

This suggests an answer to a certain puzzle in q-deformed physics—how to physically interpret noncommutative tensor products (as generated by noncocommutative quantum groups). That is, if A and B are two physically equivalent systems, what is the difference between $A\otimes_s B$ and $B\otimes_s A$, and which is the correct description of the joint system? In our anyonic model this is an unphysical distinction that is needed to work algebraically; just as (physically) the points $\gamma=\{x_1,\ldots,x_N\}$ in Δ_N are intrinsically unordered, but it can nevertheless be helpful (mathematically) to order them. This is the difference between diffeomorphisms of the manifold $\mathbb{R}^2$ acting on subsets of $\mathbb{R}^2$, and the coordinate description of their lifting to the universal covering space of N-identical-particle configuration space.

Another interesting feature is the way that the strictness of the braiding Ψ comes about from the structure of the singularities at coincident points (expressed here as Kronecker or Dirac δ-functions). In general one has diagonal singularities when multiplying operator fields, but in some cases (such as in conformal field theory) these can be controlled (e.g., by the operator product expansion). It would be interesting to see how braidings that arise in conformal field theory relate to diffeomorphism group ideas and to q-Fock space ideas along the lines of the present paper. In some situations, such as the Wess–Zumino–Witten model, there is also a topological path picture leading to the quantum group $U_q(su_2)$.

Finally, we note that the basic ideas described here apply also to plektons—particles associated with higher-dimensional (non-Abelian) unitary representations of the braid group. Here $T(b)$ in Sec. II is not simply a phase, but a finite-dimensional unitary operator acting on a multicomponent wave function; and we work with a multiplet of operator fields. Essentially, we then have an R-matrix for the linear braid group representation, in place of q in the formulas above; and we must also be more careful about ordering. Thus the creation and annihilation fields act no longer by multiplication by powers of q representing the number of crossings in the resulting braid, but

by matrix operation on the multiplet. In place of $q^{\epsilon(x,y)}$ and $q^{\epsilon_0(x,y)}$, we define Ψ and Ψ_0, using R or R^{-1} according to the ordering—but with the same conceptual picture that we have used in the anyonic case.

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q-conformal invariant equations and *q*-plane wave solutions

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We give new solutions of the quantum conformal deformations of the full Maxwell equations in terms of deformations of the plane wave. We study the compatibility of these solutions with the conservation of the current. We also start the study of quantum linear conformal (Weyl) gravity by writing the corresponding *q*-deformed equations. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1790049]

I. INTRODUCTION

One of the purposes of quantum deformations is to provide an alternative of the regularization procedures of quantum field theory. Applied to Minkowski space–time the quantum deformations approach is also an alternative to Connes' noncommutative geometry.[1] The first step in such an approach is to construct a noncommutative quantum deformation of Minkowski space–time. There are several possible such deformations, cf. Refs. 2–6. We shall follow the deformation of Ref. 6 which is different from the others, the most important aspect being that it is related to a deformation of the conformal group.

The first problem to tackle in a noncommutative deformed setting is to study the *q*-deformed analogues of the conformally invariant equations. Here we continue the study of hierarchies of deformed equations derived in Refs. 6–8 with the use of quantum conformal symmetry. We give now a description of our setting starting from the simplest example.

It is well known that the d'Alembert equation,

$$\Box\varphi(x) = 0, \quad \Box = \partial^{\mu}\partial_{\mu} = (\partial_0)^2 - (\vec{\partial})^2, \tag{1.1}$$

is conformally invariant, cf., e.g., Ref. 9. Here φ is a scalar field of fixed conformal weight, $x = (x_0, x_1, x_2, x_3)$ denotes the Minkowski space–time coordinates. Not known was the fact that (1.1) may be interpreted as conditionally conformally invariant equation and thus may be rederived from a subsingular vector of a Verma module of the algebra sl(4), the complexification of the conformal algebra su(2,2).[7]

The same idea was used in Ref. 7 to derive a *q*-d'Alembert equation, namely, as arising from a subsingular vector of a Verma module of the quantum algebra $U_q(\mathrm{sl}(4))$. The resulting equation is a *q*-difference equation and the solution spaces are built on the noncommutative *q*-Minkowski space–time of Ref. 6.

Besides the *q*-d'Alembert equation in Ref. 7 were derived a whole hierarchy of equations corresponding to the massless representations of the conformal group and parametrized by a

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non-negative integer r.[7] The case $r=0$ corresponds to the q-d'Alembert equation, while for each $r>0$ there are two couples of equations involving fields of conjugated Lorentz representations of dimension $r+1$. For instance, the case $r=1$ corresponds to the massless Dirac equation, one couple of equations describing the neutrino, the other couple of equations describing the antineutrino, while the case $r=2$ corresponds to the Maxwell equations.

The construction of solutions of the q-d'Alembert hierarchy was started in Ref. 10 with the q-d'Alembert equation. One of the solutions given was a deformation of the plane wave as a formal power series in the noncommutative coordinates of q-Minkowski space–time and four-momenta. This q-plane wave has some properties analogous to the classical one but is not an exponent or q-exponent. Thus, it differs conceptually from the classical plane wave and may serve as a regularization of the latter. In the same sense it differs from the q-plane wave in the paper,[11] which is not surprising, since there is used different q-Minkowski space–time (from Refs. 2–4) and different q-d'Alembert equation both based only on a (different) q-Lorentz algebra, and not on q-conformal [or $U_q(\mathrm{sl}(4))$] symmetry as in our case. In fact, it is not clear whether the q-Lorentz algebra of Refs. 2–4 used in Ref. 11 is extendable to a q-conformal algebra.

For the equations labeled by $r>0$ it turned out that one needs a second q-deformation of the plane wave in a conjugated basis.[12] The solutions of the hierarchy in terms of the two q-plane waves were given in Ref. 12 for $r=1$ and in Ref. 13 for $r>1$. Later these two q-plane waves were generalized and correspondingly more general solutions of the hierarchy were given in Ref. 14.

Another hierarchy derived in Ref. 6 is the Maxwell hierarchy. The two hierarchies have only one common member—the Maxwell equations—they are the lowest member of the Maxwell hierarchy and the $r=2$ member of the massless hierarchy. The compatibility of the solutions of the free q-Maxwell equations with the q-potential equations was studied.[15]

In the present paper we study the full q-Maxwell equations and the compatibility of their solutions with the conservation of the current. We give new solutions of the full q-Maxwell equations in two conjugated bases. The solutions of the homogeneous equations are also new (generalizing previously given solutions).

Another family contained in Ref. 8, but not explicated there, is related with the linear conformal (Weyl) gravity which we start to study in this paper. Namely, in the last section we write the quantum conformal deformations of the linear conformal (Weyl) gravity.

II. PRELIMINARIES

First we introduce new Minkowski variables,

$$x_\pm \equiv x_0 \pm x_3,\ \ v \equiv x_1 - ix_2,\ \ \overline{v} \equiv x_1 + ix_2, \tag{2.1}$$

which (unlike the x_μ), have definite group-theoretical interpretation as part of a six-dimensional coset of the conformal group SU(2, 2) (as explained in Ref. 6). In terms of these variables, e.g., the d'Alembert equation (1.1) is

$$\Box\varphi = (\partial_-\partial_+ - \partial_v\partial_{\overline{v}})\varphi = 0. \tag{2.2}$$

In the q-deformed case we use the noncommutative q-Minkowski space–time of Ref. 6 which is given by the following commutation relations (with $\lambda \equiv q - q^{-1}$):

$$x_\pm v = q^{\pm 1} v x_\pm,\ \ x_\pm \overline{v} = q^{\pm 1}\overline{v} x_\pm,\ \ x_+x_- - x_-x_+ = \lambda v\overline{v},\ \ \overline{v}v = v\overline{v}, \tag{2.3}$$

with the deformation parameter being a phase: $|q|=1$. Relations (2.3) are preserved by the anti-linear anti-involution ω:

$$\omega(x_\pm) = x_\pm,\ \ \omega(v) = \overline{v},\ \ \omega(q) = \overline{q} = q^{-1}\ \ (\omega(\lambda) = -\lambda). \tag{2.4}$$

The solution spaces consist of formal power series in the q-Minkowski coordinates (which we give in two conjugate bases):

$$\varphi = \sum_{j,n,\ell,m \in \mathbb{Z}_+} \mu_{jn\ell m} \varphi_{jn\ell m}, \quad \varphi_{jn\ell m} = \hat{\varphi}_{jn\ell m}, \widetilde{\varphi}_{jn\ell m}, \tag{2.5}$$

$$\hat{\varphi}_{jn\ell m} = v^j x_-^n x_+^\ell \overline{v}^m, \tag{2.6}$$

$$\widetilde{\varphi}_{jn\ell m} = \overline{v}^m x_+^\ell x_-^n v^j = \omega(\hat{\varphi}_{jn\ell m}). \tag{2.7}$$

The solution spaces (2.5) are representation spaces of the quantum algebra $U_q(\mathrm{sl}(4))$. For the latter we use the rational basis of Jimbo.[16] The action of $U_q(\mathrm{sl}(4))$ on $\hat{\varphi}_{jn\ell m}$ was given in Ref. 17, and on $\widetilde{\varphi}_{jn\ell m}$ in Ref. 12. Because of the conjugation ω we are actually working with the conformal quantum algebra which is a deformation of $U(\mathrm{su}(2,2))$.

Further we suppose that q is not a nontrivial root of unity.

In order to write our q-deformed equations in compact form it is necessary to introduce some additional operators. We first define the operators

$$\hat{M}_\kappa^\pm \varphi = \Sigma_{j,n,\ell,m \in \mathbb{Z}_+} \mu_{jn\ell m} \hat{M}_\kappa^\pm \varphi_{jn\ell m}, \quad \kappa = \pm, v, \overline{v}, \tag{2.8}$$

$$T_\kappa^\pm \varphi = \Sigma_{j,n,\ell,m \in \mathbb{Z}_+} \mu_{jn\ell m} T_\kappa^\pm \varphi_{jn\ell m}, \quad \kappa = \pm, v, \overline{v}, \tag{2.9}$$

and $\hat{M}_+^\pm$, $\hat{M}_-^\pm$, $\hat{M}_v^\pm$, $\hat{M}_{\overline{v}}^\pm$, respectively, act on $\varphi_{jn\ell m}$ by changing by ± 1 the value of j, n, ℓ, m, respectively, while $T_+^\pm$, $T_-^\pm$, $T_v^\pm$, $T_{\overline{v}}^\pm$, respectively, act on $\varphi_{jn\ell m}$ by multiplication of $q^{\pm j}$, $q^{\pm n}$, $q^{\pm \ell}$, $q^{\pm m}$, respectively. We shall use also the "logs" N_κ such that $T_\kappa = q^{N_\kappa}$. Now we can define the q-difference operators,

$$\hat{\mathcal{D}}_\kappa \varphi = \frac{1}{\lambda} \hat{M}_\kappa^{-1} (T_\kappa - T_\kappa^{-1}) \varphi = \frac{1}{\lambda} \hat{M}_\kappa^{-1} (q^{N_\kappa} - q^{-N_\kappa}) \varphi. \tag{2.10}$$

Note that when $q \to 1$ then $\hat{D}_\kappa \to \partial_k$. Using (2.8) and (2.10) the q-d'Alembert equation may be written as,[7,12] respectively,

$$(q \hat{\mathcal{D}}_- \hat{\mathcal{D}}_+ T_v T_{\overline{v}} - \hat{\mathcal{D}}_v \hat{\mathcal{D}}_{\overline{v}}) T_v T_- T_+ T_{\overline{v}} \hat{\varphi} = 0, \tag{2.11}$$

$$(\hat{\mathcal{D}}_- \hat{\mathcal{D}}_+ - q \hat{\mathcal{D}}_v \hat{\mathcal{D}}_{\overline{v}} T_v T_{\overline{v}}) T_- T_+ \widetilde{\varphi} = 0. \tag{2.12}$$

Note that when $q \to 1$ both Eqs. (2.11) and (2.12) go to (2.2). Note that the operators in (2.8) and (2.10)–(2.12) for different variables commute, i.e., we have passed to commuting variables. However, keeping the normal ordering it is straightforward to pass back to noncommuting variables.

Next we recall that the Maxwell's equations are part also of Maxwell's hierarchy of equations. The quantum conformal deformation of the equations of the hierarchy are[6]

$${}_q I_{nq}^+ F_n^+ = {}_q J^n, \quad {}_q I_n^- {}_q F_n^- = {}_q J^n, \tag{2.13}$$

where in the basis (2.6) the operators are

$$\begin{aligned} {}_q I_n^+ = \tfrac{1}{2}\big((q\hat{\mathcal{D}}_v + \hat{M}_{\overline{z}} \hat{\mathcal{D}}_+ (T_- T_v)^{-1} T_{\overline{v}}) T_- [n + 2 - N_z]_q - q^{-n-2} (\hat{\mathcal{D}}_- T_- + q^{-1} \hat{M}_{\overline{z}} \hat{\mathcal{D}}_{\overline{v}} \\ - \lambda \hat{M}_v \hat{M}_{\overline{z}} \hat{\mathcal{D}}_- \hat{\mathcal{D}}_+ T_{\overline{v}}) T_-^{-1} \hat{\mathcal{D}}_z) T_+ T_v T_z T_{\overline{z}}^{-1}, \end{aligned} \tag{2.14}$$

$${}_q I_n^- = \tfrac{1}{2}(\hat{\mathcal{D}}_{\overline{v}} + q \hat{M}_z \hat{\mathcal{D}}_+ T_{\overline{v}} T_- T_v^{-1} - q\lambda \hat{M}_v \hat{\mathcal{D}}_- \hat{\mathcal{D}}_+ T_{\overline{v}}) T_{\overline{v}} [n + 2 - N_{\overline{z}}]_q - \tfrac{1}{2} q^{n+3} (\hat{\mathcal{D}}_- + q \hat{M}_z \hat{\mathcal{D}}_v T_-) \hat{\mathcal{D}}_{\overline{z}} T_- T_{\overline{v}}, \tag{2.15}$$

while where in the basis (2.7) the operators are

$$
\begin{aligned}
{}_qI_n^+ = {} & \tfrac{1}{2}q(\hat{\mathcal{D}}_v + \hat{M}_{\bar{z}}\hat{\mathcal{D}}_+T_-T_{\bar{v}}^{-1}T_v)T_v[n+2-N_z]_q - \tfrac{1}{2}q^{n+3}(\hat{\mathcal{D}}_- + \hat{M}_z\hat{\mathcal{D}}_{\bar{v}}T_- \\
& + \lambda q^{-1}\hat{M}_v\hat{M}_{\bar{z}}\hat{\mathcal{D}}_-\hat{\mathcal{D}}_+T_{\bar{v}}^{-1}T_-)\hat{\mathcal{D}}_zT_-T_v,
\end{aligned} \tag{2.16}
$$

$$
\begin{aligned}
{}_qI_n^- = {} & \tfrac{1}{2}((\hat{\mathcal{D}}_{\bar{v}}T_{\bar{v}}T_- + \hat{M}_z\hat{\mathcal{D}}_+T_v + q^{-1}\lambda\hat{M}_v\hat{\mathcal{D}}_-\hat{\mathcal{D}}_+T_-)[n+2-N_{\bar{z}}]_q \\
& - q^{-n-2}(\hat{\mathcal{D}}_- + \hat{M}_z\hat{\mathcal{D}}_vT_-^{-1})\hat{\mathcal{D}}_{\bar{z}}T_{\bar{v}})T_+T_{\bar{z}}T_z^{-1}.
\end{aligned} \tag{2.17}
$$

Note that for $q=1$ (2.14) and (2.15) coincide with (2.16) and (2.17), respectively. Maxwell's equations $\partial^\mu F_{\mu\nu}=J_\nu$, $\epsilon_{\mu\nu\rho\sigma}\partial^\mu F^{\rho\sigma}=0$ are obtained from (2.13) for $n=0$, $q=1$, substituting the fixed helicity constituents $F^\pm$ by $F^+=z^2(F_1^+ + iF_2^+) - 2zF_3^+ - (F_1^+ - iF_2^+)$, $F^-=\bar{z}^2(F_1^- - iF_2^-) - 2\bar{z}F_3^- - (F_1^- + iF_2^-)$, $F_k^\pm = F_{k0} \pm (i/2)\varepsilon_{k\ell m}F_{\ell m} = E_k \pm iH_k$, $J^0 = \bar{z}z(J_0+J_3) + z(J_1+iJ_2) + \bar{z}(J_1-iJ_2) + (J_0-J_3)$, and then comparing the coefficients of the resulting first order polynomials in z and $\bar{z}$.

We shall look for solutions of the full q-Maxwell's equations in terms of deformations of the plane wave. Let us first recall these deformations from Ref. 14. The first deformation is given in the basis (2.6):

$$
\widehat{\exp}_q(k,x) = \sum_{s=0}^{\infty} \frac{1}{[s]_q!}\hat{h}_s,
$$

$$
[s]_q! \equiv [s]_q[s-1]_q \cdots [1]_q,\ [0]_q! \equiv 1,\ [n]_q \equiv \frac{q^n - q^{-n}}{q - q^{-1}}, \tag{2.18}
$$

$$
\begin{aligned}
\hat{h}_s = {} & \beta^s \sum_{a,b,n \in \mathbb{Z}_+} \frac{(-1)^{s-a-b}q^{n(s-2a-2b+2n)+a(s-a-1)+b(-s+a+b+1)}q^{P_s(a,b)}}{\Gamma_q(a-n+1)\Gamma_q(b-n+1)\Gamma_q(s-a-b+n+1)[n]_q!} \\
& \times k_v^{s-a-b+n}k_-^{b-n}k_+^{a-n}k_{\bar{v}}^n v^n x_-^{a-n}x_+^{b-n}\bar{v}^{s-a-b+n},
\end{aligned}
$$

$$
(\beta^s)^{-1} = \sum_{p=0}^{s} \frac{q^{(s-p)(p-1)+p}}{[p]_q![s-p]_q!}, \tag{2.19}
$$

where the momentum components $(k_v, k_-, k_+, k_{\bar{v}})$ are supposed to be noncommutative between themselves [obeying the same rules (2.3) as the q-Minkowski coordinates], and commutative with the coordinates. Further, Γ_q is a q-deformation of the Γ-function, of which here we use only the properties $\Gamma_q(p)=[p-1]_q!$ for $p \in \mathbb{N}$, $1/\Gamma_q(p)=0$ for $p \in \mathbb{Z}_-$; $P_s(a,b)$ is a polynomial in a, b. Note that $(\hat{h}_s)|_{q=1}=(k\cdot x)^s$ and thus $(\widehat{\exp}_q(k,x))|_{q=1}=\exp(k\cdot x)$. This q-plane wave has some properties analogous to the classical one but is not an exponent or q-exponent, cf. Ref. 18. This is enabled also by the fact (true also for $q=1$) that solving the equations may be done in terms of the components $\hat{h}_s$. This deformation of the plane wave generalizes the original one from Ref. 10 to obtain which one sets $P_s(a,b)=0$, in which case we shall use the notation f_s for the components from Ref. 10 since

$$
(\hat{h}_s)_{P_s(a,b)=0} = f_s. \tag{2.20}
$$

Each $\hat{h}_s$ satisfies the q-d'Alembert equation (2.11) on the momentum q-cone,

$$
\mathcal{L}_q^k \equiv k_-k_+ - q^{-1}k_vk_{\bar{v}} = k_+k_- - qk_vk_{\bar{v}} = 0. \tag{2.21}
$$

The second deformation is given in the basis (2.7),

$$\widetilde{\exp}_q(k,x)=\sum_{s=0}^{\infty}\frac{1}{[s]_q!}\tilde{h}_s, \tag{2.22}$$

$$\tilde{h}_s=\tilde{\beta}^s\sum_{a,b,n}\frac{(-1)^{s-a-b}q^{n(2a+2b-2n-s)+a(a-s-1)+b(s-a-b+1)}q^{Q_s(a,b)}}{\Gamma_q(a-n+1)\Gamma_q(b-n+1)\Gamma_q(s-a-b+n+1)[n]_q!}$$
$$\times k_v^n k_+^{a-n}k_-^{b-n}k_v^{s-a-b+n}\bar{v}^{s-a-b+n}x_+^{b-n}x_-^{a-n}v^n,$$

$$(\tilde{\beta}^s)^{-1}=\sum_{p=0}^{s}\frac{q^{(p-s)(p-1)+p}}{[p]_q!\,[s-p]_q!}, \tag{2.23}$$

where $Q_s(a,b)$ are arbitrary polynomials. If the latter are zero then $\widetilde{\exp}_q(k,x)$ becomes the q-plane wave deformation found in Ref. 12. The $\tilde{h}_s$ have the same properties as the $\hat{h}_s$ but the conjugated basis is used; in particular, they satisfy the q-d'Alembert equation (2.12) on the momentum q-cone (2.21).

III. SOLUTIONS OF THE *q*-MAXWELL EQUATIONS

First we shall use the basis (2.6). The solutions of (2.13) for $n=0$ in the homogeneous case ($J=0$) are

$$\hat{F}^{h\pm}\doteq({}_qF_0^{\pm})_{J=0}=\sum_{m,s=0}^{\infty}\frac{1}{[s]_q!}\hat{F}_{ms}^{h\pm}(k)f_s, \tag{3.1}$$

$$\hat{F}_{ms}^{h+}(k)=\sum_{i=0}^{m}\left(\sum_{j=0}^{m-i}\hat{p}_{ij}^{ms1}k_v^ik_-^{m-i-j}k_{\bar{v}}^j(k_v-q^{s+6}zk_-)(k_v-q^{s+3}zk_-)+\hat{p}_i^{ms2}k_v^ik_{\bar{v}}^{m-i}(k_v-q^{s+6}zk_-)(k_+-q^{s+3}zk_{\bar{v}})\right.$$
$$\left.+\sum_{j=0}^{m-i}\hat{p}_{ij}^{ms3}k_v^ik_+^{m-i-j}k_{\bar{v}}^j(k_+-q^{s+6}zk_{\bar{v}})(k_+-q^{s+3}zk_{\bar{v}})\right), \tag{3.2}$$

$$\hat{F}_{ms}^{h-}(k)=\sum_{i=0}^{m}\left(\sum_{j=0}^{m-i}\hat{r}_{ij}^{ms1}k_v^ik_-^{m-i-j}k_{\bar{v}}^j(k_{\bar{v}}-q^{-1}\bar{z}k_-)(k_{\bar{v}}-\bar{z}k_-)+\hat{r}_i^{ms2}k_v^ik_{\bar{v}}^{m-i}(k_+-q^{-1}\bar{z}k_v)(k_{\bar{v}}-\bar{z}k_-)\right.$$
$$\left.+\sum_{j=0}^{m-i}\hat{r}_{ij}^{ms3}k_v^ik_+^{m-i-j}k_{\bar{v}}^j(k_+-q^{-1}\bar{z}k_v)(k_+-\bar{z}k_v)\right), \tag{3.3}$$

where $\hat{p}_{i(j)}^{msa},\hat{r}_{i(j)}^{msa}$ are independent constants. The check that these are solutions is done for commutative Minkowski coordinates and noncommutative momenta on the q-cone. The terms with $m=0$ of the solutions (3.1)–(3.3), were obtained earlier[13] (later they were generalized using more general q-plane waves[14]). The solution (3.3) can be written in terms of the deformed plane wave if we suppose that the $\hat{r}_{i(j)}^{msa}$ for different s coincide, $\hat{r}_{i(j)}^{msa}=\hat{r}_{i(j)}^{ma}$. Then we have

$$\hat{F}^{h-}=\sum_{m=0}^{\infty}\hat{F}_m^{h-}(k)\exp_q(k,x),\quad \hat{F}_m^{h-}(k)=\hat{F}_{ms}^{h-}(k). \tag{3.4}$$

In the inhomogeneous case the solutions of (2.13) for $n=0$ are

$${}_qJ^0=\bar{z}z\hat{J}_+ + z\hat{J}_v+\bar{z}\hat{J}_{\bar{v}}+\hat{J}_-, \tag{3.5}$$

$$\hat{J}_\kappa = \sum_{m,s=o}^{\infty} \frac{1}{[s]_q!} \hat{J}_\kappa^{ms}(k) f_{s-1}, \quad \kappa = \pm, v, \bar{v}; \tag{3.6}$$

$$\hat{J}_+^{ms}(k) = -\hat{K}_m^s(k) k_-; \tag{3.7}$$

$$\hat{J}_-^{ms}(k) = -q^{-s-2} \hat{K}_m^s(k) k_+,$$

$$\hat{J}_v^{ms}(k) = \hat{K}_m^s(k) k_{\bar{v}},$$

$$\hat{J}_{\bar{v}}^{ms}(k) = q^{-s-2} \hat{K}_m^s(k) k_v,$$

$$\hat{K}_m^s(k) \doteq \hat{\gamma}_v^s k_v^{m+1} + \hat{\gamma}_-^s k_-^{m+1} + \hat{\gamma}_+^s k_+^{m+1} + \hat{\gamma}_{\bar{v}}^s k_{\bar{v}}^{m+1};$$

$${}_qF_0^{\pm} = \hat{F}^{\pm} + \hat{F}^{h\pm}; \tag{3.8}$$

$$\hat{F}^{\pm} = \sum_{m,s=0}^{\infty} \frac{1}{[s]_q!} \hat{F}_{ms}^{\pm}(k) f_s, \tag{3.9}$$

$$\hat{F}_{ms}^{+}(k) = 2d_s q^{-s}((q^{-s-5}\hat{\gamma}_-^s k_-^m + z\hat{\gamma}_v^s k_v^m)(k_v - q^{s+3} z k_-) + (q^{-s-5}\hat{\gamma}_v^s k_{\bar{v}}^m + z\hat{\gamma}_+^s k_+^m)(k_+ - q^{s+3} z k_{\bar{v}})),$$

$$\hat{F}_{ms}^{-}(k) = 2d_s q^{-2s-2}((\hat{\gamma}_-^s k_-^m + q^{-2}\bar{z}\hat{\gamma}_v^s k_{\bar{v}}^m)(k_{\bar{v}} - \bar{z} k_-) + (\hat{\gamma}_v^s k_v^m + q^{-2}\bar{z}\hat{\gamma}_+^s k_+^m)(k_+ - \bar{z} k_v)),$$

where $d_s = \beta^s / \beta^{s+1}$. As in the homogeneous case we cannot make $\hat{F}_{ms}^{+}(k)$ independent of s. We can make $\hat{F}_{ms}^{-}(k)$ independent of s by choosing $\hat{\gamma}_\kappa^s \sim q^{2s} d_s^{-1}$, but we cannot make $\hat{J}_\kappa^{ms}(k)$ independent of s.

Since we work with the full Maxwell equations we have also to check the q-deformation of the current conservation $\partial^\nu J_\nu = 0$,

$$I_{13} J = 0, \tag{3.10}$$

$$\begin{aligned} I_{13} = {} & q^3 [N_z - 1]_q T_z \hat{\mathcal{D}}_{\bar{z}} \hat{\mathcal{D}}_v T_v T_- T_+ + q \hat{\mathcal{D}}_z T_z \hat{\mathcal{D}}_{\bar{z}} \hat{\mathcal{D}}_- T_v T_+ + q [N_z - 1]_q T_z [N_{\bar{z}} - 1]_q \hat{\mathcal{D}}_+ T_+ T_{\bar{v}} \\ & + q^{-1} [N_{\bar{z}} - 1]_q \hat{\mathcal{D}}_z T_z \hat{\mathcal{D}}_{\bar{v}} T_v T_-^{-1} T_+ - \lambda \hat{M}_v [N_{\bar{z}} - 1]_q \hat{\mathcal{D}}_z T_z \hat{\mathcal{D}}_- \hat{\mathcal{D}}_+ T_v T_-^{-1} T_+ T_{\bar{v}}. \end{aligned} \tag{3.11}$$

Substituting (3.5) and (3.6) in the above we get

$$q J_+^s(k) k_+ + J_v^s(k) k_v + q^{s+2} J_{\bar{v}}^s k_{\bar{v}} + q^{s+1} J_-^s(k) k_- = 0. \tag{3.12}$$

The latter is fulfilled by the explicit expressions in (3.7), but we should note that these expressions fulfill also the following splittings of (3.12):

$$\begin{gathered} q J_+^s(k) k_+ + J_v^s(k) k_v = 0, \quad q J_{\bar{v}}^s(k) k_{\bar{v}} + J_-^s(k) k_- = 0, \\ J_+^s(k) k_+ + q^{s+1} J_{\bar{v}}^s(k) k_{\bar{v}} = 0, \quad J_v^s(k) k_v + q^{s+1} J_-^s(k) k_- = 0. \end{gathered} \tag{3.13}$$

Furthermore the expressions from (3.7) fulfill also

$$qJ^s_+(k)k_{\overline{v}} + J^s_v(k)k_- = 0, \quad qJ^s_{\overline{v}}(k)k_+ + J^s_-(k)k_v = 0,$$
$$J^s_+(k)k_v + q^{s+1}J^s_{\overline{v}}(k)k_- = 0, \quad J^s_v(k)k_+ + q^{s+1}J^s_-(k)k_{\overline{v}} = 0. \tag{3.14}$$

Now we shall use the basis (2.7). Then solutions of (2.13) for $n=0$ in the homogeneous case ($J=0$) are

$$\widetilde{F}^{h\pm} \doteq ({}_qF^{\pm}_0)_{J=0} = \sum_{m,s=0}^{\infty} \frac{1}{[s]_q!}\widetilde{F}^{h\pm}_{ms}(k)\widetilde{h}_s, \tag{3.15}$$

$$\widetilde{F}^{h+}_{ms}(k) = \sum_{i=0}^{m}\left(\sum_{j=0}^{m-i}\widetilde{p}^{ms1}_{ij}k^i_{\overline{v}}k^{m-i-j}_-k^j_v(k_v - zk_-)(k_v - qzk_-) + \widetilde{p}^{ms2}_i k^i_{\overline{v}}k^{m-i}_v(k_+ - zk_{\overline{v}})(k_v - qzk_-)\right.$$
$$\left. + \sum_{j=0}^{m-i}\widetilde{p}^{ms3}_{ij}k^i_{\overline{v}}k^{m-i-j}_+k^j_v(k_+ - zk_{\overline{v}})(k_+ - qzk_{\overline{v}})\right), \tag{3.16}$$

$$\widetilde{F}^{h-}_{ms}(k) = \sum_{i=0}^{m}\left(\sum_{j=0}^{m-i}\widetilde{r}^{ms1}_{ij}k^i_{\overline{v}}k^{m-i-j}_-k^j_v(k_{\overline{v}} - q^{s+1}\overline{z}k_-)(k_{\overline{v}} - q^{s+2}\overline{z}k_-) + \widetilde{r}^{ms2}_i k^i_v k^{m-i}_{\overline{v}}(k_{\overline{v}} - q^{s+1}\overline{z}k_-)(k_+ - q^{s+2}\overline{z}k_v)\right.$$
$$\left. + \sum_{j=0}^{m-i}\widetilde{r}^{ms3}_{ij}k^i_v k^{m-i-j}_+k^i_{\overline{v}}(k_+ - q^{s+1}\overline{z}k_v)(k_+ - q^{s+2}\overline{z}k_v)\right), \tag{3.17}$$

where $\widetilde{p}^{msa}_{i(j)}, \widetilde{r}^{msa}_{i(j)}$ are independent constants, $Q_s(a,b)=0$ in $\widetilde{h}_s$. The terms with $m=0$ of the solutions (3.15)–(3.17) were obtained earlier in Ref. 13 (and using the generalized q-plane wave in Ref. 14). The solution (3.16) can be written in terms of the deformed plane wave if we suppose that the $\widetilde{p}^{msa}_{i(j)}$ for different s coincide, $\widetilde{p}^{msa}_{i(j)} = \widetilde{p}^{ma}_{i(j)}$. Then we have

$$\widetilde{F}^{h+} = \sum_{m=0}^{\infty}\widetilde{F}^{h+}_m(k)\widetilde{\exp}_q(k,x), \quad \widetilde{F}^{h+}_m(k) = \widetilde{F}^{h+}_{ms}(k). \tag{3.18}$$

In the inhomogeneous case the solutions of (2.13) for $n=0$ are

$${}_qJ^0 = \overline{z}z\widetilde{J}_+ + z\widetilde{J}_v + \overline{z}\widetilde{J}_{\overline{v}} + \widetilde{J}_-; \tag{3.19}$$

$$\widetilde{J}_\kappa = \sum_{m,s=o}^{\infty}\frac{1}{[s]_q!}\widetilde{J}^{ms}_\kappa(k)\widetilde{h}_{s-1}, \quad \kappa = \pm, v, \overline{v}; \tag{3.20}$$

$$\widetilde{J}^{ms}_+(k) = -q^{s+1}\widetilde{K}^s_m(k)k_-, \tag{3.21}$$

$$\widetilde{J}^{ms}_-(k) = -q^{-1}\widetilde{K}^s_m(k)k_+,$$

$$\widetilde{J}^{ms}_v(k) = \widetilde{K}^s_m(k)k_{\overline{v}},$$

$$\widetilde{J}^{ms}_{\overline{v}}(k) = q^s\widetilde{K}^s_m(k)k_v,$$

$$\widetilde{K}^s_m(k) \doteq \widetilde{\gamma}^s_v k^{m+1}_v + \widetilde{\gamma}^s_- k^{m+1}_- + \widetilde{\gamma}^s_+ k^{m+1}_+ + \widetilde{\gamma}^s_{\overline{v}}k^{m+1}_{\overline{v}};$$

$$ {}_qF_0^{\pm} = \tilde{F}^{\pm} + \tilde{F}^{h\pm}; \tag{3.22} $$

$$ \tilde{F}^{\pm} = \sum_{m,s=0}^{\infty} \frac{1}{[s]_q!} \tilde{F}^{\pm}_{ms}(k)\tilde{h}_s, \tag{3.23} $$

$$ \tilde{F}^{+}_{ms}(k) = 2\tilde{d}_s q^{s-2}((\tilde{\gamma}^s_{-} k_{-}^m + q^{-1} z \tilde{\gamma}^s_{v} k_{v}^m)(k_v - qzk_{-}) + (\tilde{\gamma}^s_{v} k_{\bar{v}}^m + q^{-1} z \tilde{\gamma}^s_{+} k_{+}^m)(k_{+} - qzk_{\bar{v}})), $$

$$ \tilde{F}^{-}_{ms}(k) = 2\tilde{d}_s((q^{-s-3}\tilde{\gamma}^s_{-} k_{-}^m + q\bar{z}\tilde{\gamma}^s_{v} k_{\bar{v}}^m)(k_{\bar{v}} - q^{s+2}\bar{z}k_{-}) + (q^{-s-3}\tilde{\gamma}^s_{v} k_{v}^m + q\bar{z}\tilde{\gamma}^s_{+} k_{+}^m)(k_{+} - q^{s+2}\bar{z}k_{v})), $$

where $\tilde{d}_s = \tilde{\beta}^s / \tilde{\beta}^{s+1}$, $Q_s(a,b) = 0$ in $\tilde{h}_s$. We cannot make $\tilde{F}^{-}_{ms}(k)$ or $\tilde{J}^{ms}_{\kappa}(k)$ independent of s. We can make $\tilde{F}^{+}_{ms}(k)$ independent of s by choosing $\tilde{\gamma}^s_{\kappa} \sim q^{-s}\tilde{d}_s^{-1}$.

Also here we shall check whether the q-deformation of the current conservation (3.10) is fulfilled. The analog of (3.11) in the basis (2.7) is

$$ \begin{aligned} I_{13} = {} & [N_z - 1]_q \hat{\mathcal{D}}_{\bar{z}} T_{\bar{z}} \hat{\mathcal{D}}_v T_{\bar{v}} T_{+} T_{-}^{-1} + q \hat{\mathcal{D}}_{\bar{z}} T_{\bar{z}} \hat{\mathcal{D}}_z \hat{\mathcal{D}}_{-} T_{\bar{v}} T_{+} + q[N_{\bar{z}} - 1]_q T_{\bar{z}} [N_z - 1]_q \hat{\mathcal{D}}_{+} T_{+} T_v \\ & + q^2 [N_{\bar{z}} - 1]_q \hat{\mathcal{D}}_z T_{\bar{z}} \hat{\mathcal{D}}_{\bar{v}} T_{\bar{v}} T_{-} T_{+} - \lambda q \hat{M}_v [N_{\bar{z}} - 1]_q \hat{\mathcal{D}}_z T_{\bar{z}} \hat{\mathcal{D}}_{-} \hat{\mathcal{D}}_{+} T_{-} T_{+}. \end{aligned} \tag{3.24} $$

Then the analog of (3.12) is

$$ J^s_{+}(k)k_{+} + q^s J^s_{v}(k)k_v + J^s_{\bar{v}} k_{\bar{v}} + q^s J^s_{-}(k)k_{-} = 0. \tag{3.25} $$

The latter is fulfilled by the explicit expressions in (3.21), but we should note that these expressions fulfill also the following splittings of (3.25):

$$ \begin{gathered} J^s_{+}(k)k_{+} + q^s J^s_{v}(k)k_v = 0, \quad J^s_{\bar{v}}(k)k_{\bar{v}} + q^s J^s_{-}(k)k_{-} = 0, \\ J^s_{+}(k)k_{+} + J^s_{\bar{v}}(k)k_{\bar{v}} = 0, \quad J^s_{v}(k)k_v + J^s_{-}(k)k_{-} = 0. \end{gathered} \tag{3.26} $$

Furthermore the expressions from (3.21) fulfill also

$$ \begin{gathered} J^s_{+}(k)k_{\bar{v}} + q^s J^s_{v}(k)k_{-} = 0, \quad J^s_{\bar{v}}(k)k_{+} + q^s J^s_{-}(k)k_v = 0, \\ J^s_{+}(k)k_v + J^s_{\bar{v}}(k)k_{-} = 0, \quad J^s_{v}(k)k_{+} + J^s_{-}(k)k_{\bar{v}} = 0. \end{gathered} \tag{3.27} $$

Summarizing, we have given new solutions of the full q-Maxwell equations in two conjugated bases (2.6) and (2.7). The solutions of the homogeneous equations are also new (the old solutions are special cases). We see that the roles of the solutions F^{+} and F^{-} are exchanged in the two conjugated bases. We note also that the current components are different: $\hat{J}^{ms}_{\kappa} \neq \tilde{J}^{ms}_{\kappa}$ (for $q \neq 1$, $\kappa \neq v$), and in both cases they cannot be made independent of s. Thus, there is no advantage of choosing either of the bases (2.6) or (2.7). It may be also possible to use both in a Connes–Lott type model.[19]

IV. LINEAR CONFORMAL GRAVITY

We consider now the quantum group analogs of linear conformal gravity following the approach of Ref. 8. We start with the $q=1$ situation and we first write the Weyl gravity equations in an indexless formulation, trading the indices for two conjugate variables $z, \bar{z}$, just as for the Maxwell equations.

Weyl gravity is governed by the Weyl tensor,

$$C_{\mu\nu\sigma\tau} = R_{\mu\nu\sigma\tau} - \tfrac{1}{2}(g_{\mu\sigma}R_{\nu\tau} + g_{\nu\tau}R_{\mu\sigma} - g_{\mu\tau}R_{\nu\sigma} - g_{\nu\sigma}R_{\mu\tau}) + \tfrac{1}{6}(g_{\mu\sigma}g_{\nu\tau} - g_{\mu\tau}g_{\nu\sigma})R, \tag{4.1}$$

where $g_{\mu\nu}$ is the metric tensor. Linear conformal gravity is obtained when the metric tensor is written as $g_{\mu\nu}=\eta_{\mu\nu}+h_{\mu\nu}$, where $\eta_{\mu\nu}$ is the flat Minkowski metric, $h_{\mu\nu}$ are small so that all quadratic and higher order terms are neglected. In particular, $R_{\mu\nu\sigma\tau}=\frac{1}{2}(\partial_\mu\partial_\tau h_{\nu\sigma}+\partial_\nu\partial_\sigma h_{\mu\tau} - \partial_\mu\partial_\sigma h_{\nu\tau}-\partial_\nu\partial_\tau h_{\mu\sigma})$. The equations of linear conformal gravity are

$$\partial^\nu\partial^\tau C_{\mu\nu\sigma\tau} = T_{\mu\sigma}, \tag{4.2}$$

where $T_{\mu\nu}$ is the energy-momentum tensor. From the symmetry properties of the Weyl tensor it follows that it has 10 independent components. These may be chosen as follows (introducing notation for future use):

$$C_0 = C_{0123},\ \ C_1 = C_{2121},\ \ C_2 = C_{0202},\ \ C_3 = C_{3012},$$

$$C_4 = C_{2021},\ \ C_5 = C_{1012},\ \ C_6 = C_{2023}, \tag{4.3}$$

$$C_7 = C_{3132},\ \ C_8 = C_{2123},\ \ C_9 = C_{1213}.$$

Furthermore, the Weyl tensor transforms as the direct sum of two conjugate Lorentz irreps, which we shall denote as $C^\pm$. The tensors $T_{\mu\nu}$ and $h_{\mu\nu}$ are symmetric and traceless with nine independent components.

In order to be more precise we recall that the physically relevant representations T^χ of the four-dimensional conformal algebra su(2,2) may be labeled by $\chi=[n_1,n_2;d]$, where n_1,n_2 are non-negative integers fixing finite-dimensional irreducible representations of the Lorentz subalgebra [the dimension being $(n_1+1)(n_2+1)$], and d is the conformal dimension (or energy). [In the literature these Lorentz representations are labeled also by $(j_1,j_2)=(n_1/2,n_2/2)$.] The Weyl tensor transforms as the direct sum,

$$\begin{gathered}\chi^+ \oplus \chi^-, \\ \chi^+ = [4,0;2],\ \ \chi^- = [0,4;2],\end{gathered} \tag{4.4}$$

while the energy-momentum tensor and the metric transform as

$$\chi_T = [2,2;4],\ \ \chi_h = [2,2;0], \tag{4.5}$$

as anticipated. Indeed, $(n_1,n_2)=(2,2)$ is the nine-dimensional Lorentz representation (carried by $T_{\mu\nu}$ or $h_{\mu\nu}$), and $(n_1,n_2)=(4,0),(0,4)$ are the two conjugate five-dimensional Lorentz representations (carried by $C^\pm$), while the conformal dimensions are the canonical dimensions of a energy-momentum tensor ($d=4$), of the metric ($d=0$), and of the Weyl tensor ($d=2$). (For comparison, note that the Maxwell components F^+, F^-, used in the preceding sections, have signatures: [2, 0; 2], [0, 2; 2], respectively, while the current J has signature [1, 1; 3].) Further, we shall use again the fact that a Lorentz irrep (spin-tensor) with signature (n_1,n_2) may be represented by a polynomial $G(z,\bar z)$ in z, $\bar z$ of order n_1,n_2, respectively. More explicitly, for the irreps mentioned above we use

$$C^+(z) = z^4C_4^+ + z^3C_3^+ + z^2C_2^+ + zC_1^+ + C_0^+, \tag{4.6a}$$

$$C^-(\bar z) = \bar z^4C_4^- + \bar z^3C_3^- + \bar z^2C_2^- + \bar zC_1^- + C_0^-, \tag{4.6b}$$

$$T(z,\bar z) = z^2\bar z^2T'_{22} + z^2\bar zT'_{21} + z^2T'_{20} + z\bar z^2T'_{12} + z\bar zT'_{11} + zT'_{10} + \bar z^2T'_{02} + \bar zT'_{01} + T'_{00}, \tag{4.6c}$$

$$h(z,\overline{z}) = z^2\overline{z}^2 h'_{22} + z^2\overline{z}h'_{21} + z^2 h'_{20} + z\overline{z}^2 h'_{12} + z\overline{z}h'_{11} + zh'_{10} + \overline{z}^2 h'_{02} + \overline{z}h'_{01} + h'_{00}, \tag{4.6d}$$

where the indices on the right-hand side are not Lorentz-covariance indices, they just indicate the powers of z, $\overline{z}$. The components $C_k^{\pm}$ are given in terms of the Weyl tensor components as follows:

$$\begin{gathered}
C_0^+ = C_2 - \tfrac{1}{2}C_1 - C_6 + i(C_0 + \tfrac{1}{2}C_3 + C_7),\\
C_1^+ = 2(C_4 - C_8 + i(C_9 - C_5)),\\
C_2^+ = 3(C_1 - iC_3),\\
C_3^+ = 8(C_4 + C_8 + i(C_9 + C_5)),\\
C_4^+ = C_2 - \tfrac{1}{2}C_1 + C_6 + i(C_0 + \tfrac{1}{2}C_3 - C_7),\\
C_0^- = C_2 - \frac{C_1}{2} - C_6 - i(C_0 + \tfrac{1}{2}C_3 + C_7),\\
C_1^- = 2(C_4 - C_8 - i(C_9 - C_5)),\\
C_2^- = 3(C_1 + iC_3),\\
C_3^- = 2(C_4 + C_8 - i(C_9 + C_5)),\\
C_4^- = C_2 - \tfrac{1}{2}C_1 + C_6 - i(C_0 + \tfrac{1}{2}C_3 - C_7),
\end{gathered} \tag{4.7}$$

while the components T'_{ij} are given in terms of $T_{\mu\nu}$ as follows:

$$\begin{gathered}
T'_{22} = T_{00} + 2T_{03} + T_{33},\\
T'_{11} = T_{00} - T_{33},\\
T'_{00} = T_{00} - 2T_{03} + T_{33},\\
T'_{21} = T_{01} + iT_{02} + T_{13} + iT_{23},\\
T'_{12} = T_{01} - iT_{02} + T_{13} - iT_{23},\\
T'_{10} = T_{01} + iT_{02} - T_{13} - iT_{23},\\
T'_{01} = T_{01} - iT_{02} - T_{13} + iT_{23},\\
T'_{20} = T_{11} + 2iT_{12} - T_{22},\\
T'_{02} = T_{11} - 2iT_{12} - T_{22},
\end{gathered} \tag{4.8}$$

and similarly for h'_{ij} in terms of $h_{\mu\nu}$.

In these terms all linear conformal (Weyl) gravity equations (4.2) may be written in compact form as the following pair of equations:

$$\widetilde{I}^{+}C^{+}(z) = T(z,\overline{z}), \tag{4.9a}$$

$$\widetilde{I}^{-}C^{-}(\overline{z}) = T(z,\overline{z}), \tag{4.9b}$$

where the operators $I^{\pm}$ are given as follows:

$$\begin{aligned}\widetilde{I}^{+} = {} & (z^2\overline{z}^2\partial_+^2 + z^2\partial_v^2 + \overline{z}^2\partial_{\overline{v}}^2 + \partial_-^2 + 2z^2\overline{z}\partial_v\partial_+ + 2z\overline{z}^2\partial_+\partial_{\overline{v}} + 2z\overline{z}(\partial_-\partial_+ + \partial_v\partial_{\overline{v}}) + 2\overline{z}\partial_-\partial_{\overline{v}} + 2z\partial_v\partial_-)\partial_z^2 \\ & - 6(z\overline{z}^2\partial_+^2 + z\partial_v^2 + 2z\overline{z}\partial_v\partial_+ + \overline{z}^2\partial_+\partial_{\overline{v}} + \overline{z}(\partial_-\partial_+ + \partial_v\partial_{\overline{v}}) + \partial_v\partial_-)\partial_z 12(\overline{z}^2\partial_+^2 + \partial_v^2 + 2\overline{z}\partial_v\partial_+),\end{aligned} \tag{4.10a}$$

$$\begin{aligned}\widetilde{I}^{-} = {} & (z^2\overline{z}^2\partial_+^2 + z^2\partial_v^2 + \overline{z}^2\partial_{\overline{v}}^2 + \partial_-^2 + 2z^2\overline{z}\partial_v\partial_+ + 2z\overline{z}^2\partial_+\partial_{\overline{v}} + 2z\overline{z}(\partial_-\partial_+ + \partial_v\partial_{\overline{v}}) + 2\overline{z}\partial_-\partial_{\overline{v}} + 2z\partial_v\partial_-)\partial_z^2 \\ & - 6(z^2\overline{z}\partial_+^2 + \overline{z}\partial_{\overline{v}}^2 + 2z\overline{z}\partial_+\partial_{\overline{v}} + z^2\partial_v\partial_+ + z(\partial_-\partial_+ + \partial_v\partial_{\overline{v}}) + \partial_-\partial_{\overline{v}})\partial_z 12(z^2\partial_+^2 + \partial_{\overline{v}}^2 + 2z\partial_+\partial_{\overline{v}}).\end{aligned} \tag{4.10b}$$

To make more transparent the origin of these expressions and in the same time to derive the quantum group deformation of (4.9) and (4.10) we first introduce the following parameter-dependent operators:

$$\widetilde{I}^{+}(n) = \tfrac{1}{2}(n(n-1)I_1^2I_2^2 - 2(n^2-1)I_1I_2^2I_1 + n(n+1)I_2^2I_1^2), \tag{4.11a}$$

$$\widetilde{I}^{-}(n) = \tfrac{1}{2}(n(n-1)I_3^2I_2^2 - 2(n^2-1)I_3I_2^2I_3 + n(n+1)I_2^2I_3^2), \tag{4.11b}$$

where

$$I_1 \equiv \partial_z, \quad I_2 \equiv \overline{z}\overline{z}\partial_+ + z\partial_v + \overline{z}\partial_{\overline{v}} + \partial_-, \quad I_3 \equiv \partial_{\overline{z}}. \tag{4.12}$$

It is easy to check that we have the following relation:

$$\widetilde{I}^{\pm} = \widetilde{I}^{\pm}(4). \tag{4.13}$$

We note in passing that group theoretically the operators I_a correspond to the three simple roots of the root system of sl(4), while the operators $I_n^{\pm}$ correspond to the two nonsimple nonhighest roots.[20]

This is the form that is immediately generalizable to the q-deformed case. Using results from Ref. 8 we have

$${}_q\widetilde{I}^{+}(n) = \tfrac{1}{2}([n]_q[n-1]_{qq}I_{1q}^2I_2^2 - 2[n-1]_q[n+1]_{qq}I_{1q}I_{2q}^2I_1 + [n]_q[n+1]_{qq}I_{2q}^2I_1^2), \tag{4.14a}$$

$${}_q\widetilde{I}^{-}(n) = \tfrac{1}{2}([n]_q[n-1]_{qq}I_{3q}^2I_2^2 - 2[n-1]_q[n+1]_{qq}I_{3q}I_{2q}^2I_3 + [n]_q[n+1]_{qq}I_{2q}^2I_3^2), \tag{4.14b}$$

where the q-deformed versions ${}_qI_a$ of (4.12) in the basis (2.6) are

$${}_qI_1 = \hat{\mathcal{D}}_zT_zT_vT_+(T_-T_{\overline{v}})^{-1}, \tag{4.15a}$$

$$\begin{aligned}{}_qI_2 = {} & (q\hat{M}_z\hat{\mathcal{D}}_vT_-^2 + \hat{M}_z\hat{M}_{\overline{z}}\hat{\mathcal{D}}_+T_-T_{\overline{v}}T_v^{-1} + \hat{\mathcal{D}}_-T_- + q^{-1}\hat{M}_{\overline{z}}\hat{\mathcal{D}}_{\overline{v}} - \lambda\hat{M}_v\hat{M}_{\overline{z}}\hat{\mathcal{D}}_-\hat{\mathcal{D}}_+T_{\overline{v}})T_{\overline{v}}T_{\overline{z}}^{-1},\end{aligned} \tag{4.15b}$$

$$ {}_qI_3 = \hat{\mathcal{D}}_z T_{\bar{z}}. \tag{4.15c} $$

Then the *q*-Weyl equations are

$$ {}_q\tilde{I}^{+}(4)C^{+}(z) = T(z,\bar{z}), \tag{4.16a} $$

$$ {}_q\tilde{I}^{-}(4)C^{-}(\bar{z}) = T(z,\bar{z}). \tag{4.16b} $$

[For comparison, note that for the derivation of the *q*-Maxwell operators (2.13) were used for the following expressions: ${}_qI_n^{+}=\frac{1}{2}([n+2]_{qq}I_{1q}I_2-[n+3]_{qq}I_{2q}I_1)$, ${}_qI_n^{-}=\frac{1}{2}([n+2]_{qq}I_{3q}I_2-[n+3]_{qq}I_{2q}I_3)$.]

Finally, we write down the pair of equations which give the Weyl tensor components in terms of the metric tensor,

$$ {}_q\tilde{I}^{+}(2)h(z,\bar{z}) = C^{+}(z), \tag{4.17a} $$

$$ {}_q\tilde{I}^{-}(2)h(z,\bar{z}) = C^{-}(\bar{z}). \tag{4.17b} $$

We stress the advantage of the indexless formalism due to which two different pairs of equations, (4.16) and (4.17), may be written using the same parameter-dependent operator expressions by just specializing the values of the parameter.

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Degenerate principal series of quantum Harish–Chandra modules

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In this paper we study a quantum analog of a degenerate principal series of $U_q\mathfrak{su}_{n,n}$-modules $(0<q<1)$ related to the Shilov boundary of the quantum $n\times n$-matrix unit ball. We give necessary and sufficient conditions for the modules to be simple and unitarizable and investigate their equivalence. These results are q-analogs of known classical results on reducibility and unitarizability of $\mathrm{SU}(n,n)$-modules obtained by Johnson, Sahi, Zhang, Howe, and Tan. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1786348]

I. INTRODUCTION

In this paper we investigate a quantum analog of the degenerate principal series of representations of the algebra $U_q\mathfrak{su}_{n,n}$ related to the Shilov boundary of the quantum $n\times n$-matrix unit ball. We give necessary and sufficient conditions for the representations to be irreducible and unitary.

In this work we provide q-analogs of classical results obtained by Johnson, Sahi, Zhang, Howe, and Tan.[1–5] Another degenerate principal series is considered in the Klimyk and Pakuliak paper.[6]

We use Bargman's approach for investigating representations (see Ref. 7, where unitary strongly continuous irreducible representations of the group SU(1,1) were described). Explicit formulas for operators of $\mathfrak{su}_{1,1}$-representations were found in a weight vectors basis in Ref. 7. Results on irreducibility and unitarizability can be obtained from the formulas as corollaries.

In the general case one needs much more effort to obtain similar formulas. Important results in this direction were obtained by Howe in Ref. 1. He received certain results on irreducibility and unitarizability of modules of the simplest degenerate principal series for $\mathrm{U}(m,n)$ and some other classical groups.

The Lee paper[8] directly continues this Howe work. In Ref. 8 the degenerate principal series for $\mathrm{U}(n,n)$ related to the Shilov boundary of the $n\times n$-quantum ball is investigated and answers to the same questions are obtained.

This work generalizes results from Ref. 8 to the quantum case with $0<q<1$. Passing to the limit as $q\mapsto 1$ one can get up to notation the results of the above-mentioned paper.

This paper is organized as follows: In Sec. II we define the representations $\pi_{\alpha,\beta}$ of the degenerate principal series [see (5)]. In Sec. III we investigate the equivalence of $\pi_{\alpha,\beta}$ (see Proposition 3). In Sec. IV we discuss some auxiliary results on $\pi_{\alpha,\beta}$. These results will be used in the sequel. In Sec. V we give necessary and sufficient for $\pi_{\alpha,\beta}$ to be irreducible (see Proposition 11). For the case $\pi_{\alpha,\beta}$ is reducible, we describe all its irreducible subrepresentations. In Sec. VI we find explicit formulas for intertwining operators between $\pi_{\alpha,\beta}$ and $\pi_{-n-\beta,-n-\alpha}$ [see (17)]. In Sec. VII we investigate unitarizability of irreducible representations of the degenerate principal series. Most of the technical details of the proofs are contained in the Appendix.

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II. DEFINITION OF THE DEGENERATE PRINCIPAL SERIES OF REPRESENTATIONS

Recall some concepts on geometric realizations for certain series of representations of real semisimple Lie groups and Lie algebras.

Consider the affine algebraic group $G=\mathrm{SL}_{2n}(\mathbb{C})$ and its maximal parabolic subgroup

$$P=\left\{\begin{pmatrix} A & B \\ 0 & D \end{pmatrix} \middle| A,B,D \in Mat_{n,n}(\mathbb{C}), (\det A)(\det D)=1\right\}.$$

Then the projective variety G/P is isomorphic to the space $Gr_n(\mathbb{C}^{2n})$ of n-dimensional subspaces in $\mathbb{C}^{2n}$. The subgroup $K=S(GL_n(\mathbb{C})\times GL_n(\mathbb{C}))$ acts naturally on G/P. Denote by Ω the open K-orbit. It can be easily proved that

$$\Omega=\{L \in Gr_n(\mathbb{C}^{2n}) | \dim L \cap (\mathbb{C}^n)_1 = \dim L \cap (\mathbb{C}^n)_2 = 0\},$$

where $(\mathbb{C}^n)_1$ and $(\mathbb{C}^n)_2$ are the subspaces generated by the elements $\{\varepsilon_1,\ldots,\varepsilon_n\}$, $\{\varepsilon_{n+1},\ldots,\varepsilon_{2n}\}$ of the standard basis for $\mathbb{C}^{2n}$, respectively. It can be verified that Ω is an affine variety.

Set

$$\mathbf{t}=\begin{pmatrix} t_{11} & t_{12} & \cdots & t_{12n} \\ \cdots & \cdots & \cdots & \cdots \\ t_{n1} & t_{n2} & \cdots & t_{n2n} \end{pmatrix}, \quad \mathrm{rk}\mathbf{t}=n,$$

and $\mathbb{C}[\mathrm{Mat}_{n,2n}] \overset{\text{def}}{=} \mathbb{C}[t_{11},\ldots,t_{n2n}]$. Define

$$t_J^{\wedge n} \overset{\text{def}}{=} \sum_{s\in S_n} (-1)^{l(s)} t_{1j_{s(1)}} \cdot t_{2j_{s(2)}} \cdots t_{nj_{s(n)}},$$

where $l(s)$ is the length of permutation s, $J=\{j_1,\ldots,j_n\}$, $1\leqslant j_1<\cdots<j_n\leqslant 2n$, and t_{ij} are the matrix entries of $\mathbf{t}$. The elements $t_J^{\wedge n}$ are called Plucker projective "coordinates" on $Gr_n(\mathbb{C}^{2n})$. Denote by $\mathbb{C}[\mathrm{Pl}_{n,2n}]\subset\mathbb{C}[\mathrm{Mat}_{n,2n}]$ the subalgebra generated by all $t_J^{\wedge n}$.

Consider the algebra $\mathbb{C}[\Omega]$ of regular functions on Ω. Let us introduce some notation. Set $t \overset{\text{def}}{=} t^{\wedge n}_{\{n+1,\ldots,2n\}}$ and

$$z_a^b = t^{-1} t^{\wedge n}_{J_{ab}}, \quad a,b=1,\ldots,n, \quad \text{where } J_{ab}=\{n+1,\ldots,2n\}\setminus\{2n+1-b\}\cup\{a\};$$

$$\mathbf{z}=\begin{pmatrix} z_1^1 & \ldots & z_1^n \\ \ldots & \ldots & \ldots \\ z_n^1 & \ldots & z_n^n \end{pmatrix}, \quad \det\mathbf{z}=\det\begin{pmatrix} z_1^1 & \ldots & z_1^n \\ \ldots & \ldots & \ldots \\ z_n^1 & \ldots & z_n^n \end{pmatrix}.$$

Then the algebra $\mathbb{C}[\Omega]$ is canonically isomorphic to the localization of the algebra $\mathbb{C}[\mathrm{Mat}_n] \overset{\text{def}}{=} \mathbb{C}[z_1^1,\ldots,z_n^n]$ with respect to the multiplicative set $(\det\mathbf{z})^{\mathbb{Z}_+}$. The vector space $\mathbb{C}[\Omega]=\mathbb{C}[\mathrm{Mat}_n]_{\det\mathbf{z}}$ can be naturally equipped with the $\mathfrak{sl}_{2n}$-module structure and the K-module structure, and these structures are compatible (see Ref. 9).

Therefore the action of the universal enveloping algebra $U\mathfrak{sl}_{2n}$ in the vector space $\mathbb{C}[\mathrm{Mat}_n]_{\det\mathbf{z}}$ is well defined. Moreover, the $U\mathfrak{sl}_{2n}$-action in the localization of the algebra $\mathbb{C}[\mathrm{Pl}_{n,2n}]$ with respect to the multiplicative set $t^{\mathbb{Z}_+}$ is well defined. Hence the $U\mathfrak{sl}_{2n}$-action in the space $\mathbb{C}[\mathrm{Mat}_n]_{\det\mathbf{z}}\cdot(\det\mathbf{z})^\alpha t^\beta$ is well defined for each $\alpha,\beta\in\mathbb{Z}$ (they are spaces of sections of homogeneous vector bundles over Ω; we pass from $\alpha,\beta\in\mathbb{Z}$ to $\alpha,\beta\in\mathbb{R}$ standardly).

Now let us pass to the quantum case. Everywhere in the sequel $q\in(0,1)$, $\mathbb{C}$ is the ground field and all algebras are unital and associative.

Denote by $U_q\mathfrak{sl}_{2n}$ the algebra defined by its generators $\{E_i,F_i,K_i,K_i^{-1}\}_{i=1}^{2n-1}$ and the relations

$$K_iK_j = K_jK_i, \quad K_iK_i^{-1} = K_i^{-1}K_i = 1;$$

$$K_iE_i = q^2E_iK_i, \quad K_iF_i = q^{-2}F_iK_i;$$

$$E_iF_j - F_jE_i = \delta_{ij}(K_i - K_i^{-1})/(q - q^{-1});$$

$$K_iE_j = q^{-1}E_jK_i, \quad K_iF_j = qF_jK_i, \quad |i-j| = 1;$$

$$E_i^2E_j - (q + q^{-1})E_iE_jE_i + E_jE_i^2 = 0, \quad |i-j| = 1;$$

$$F_i^2F_j - (q + q^{-1})F_iF_jF_i + F_jF_i^2 = 0, \quad |i-j| = 1;$$

$$K_iE_j - E_jK_i = K_iF_j - F_jK_i, = E_iE_j - E_jE_i = F_iF_j - F_jF_i = 0, \quad |i-j| > 1.$$

We equip $U_q\mathfrak{sl}_{2n}$ with the standard Hopf algebra structure. The comultiplication, the counit and the antipode are defined by their actions on the generators:

$$\triangle E_j = E_j \otimes 1 + K_j \otimes E_j, \quad \varepsilon(E_j) = 0, \quad S(E_j) = -K_j^{-1}E_j,$$

$$\triangle F_j = F_j \otimes K_j^{-1} + 1 \otimes F_j, \quad \varepsilon(F_j) = 0, \quad S(F_j) = -F_jK_j,$$

$$\triangle K_j = K_j \otimes K_j, \quad \varepsilon(K_j) = 1, \quad S(K_j) = K_j^{-1}$$

for all $j = 1, \ldots, 2n-1$.

The algebra $\mathbb{C}[\mathrm{Mat}_{n,2n}]_q$ of polynomials on the quantum $n \times 2n$-matrix space is defined by its generators $\{t_{ij}\}_{i=1,\ldots,n;j=1,\ldots,2n}$ and the relations (cf. Ref. 10)

$$t_{ik}t_{jk} = qt_{jk}t_{ik}, \quad t_{ki}t_{kj} = qt_{kj}t_{ki}, \quad i < j,$$

$$t_{ij}t_{kl} = t_{kl}t_{ij}, \quad i < k \text{ and } j > l,$$

$$t_{ij}t_{kl} - t_{kl}t_{ij} = (q - q^{-1})t_{ik}t_{jl}, \quad i < k \text{ and } j < l. \tag{1}$$

Define q-minors as follows:

$$t_{IJ}^{\wedge k} \overset{\text{def}}{=} \sum_{s \in S_k} (-q)^{l(s)} t_{i_1 j_{s(1)}} \cdots t_{i_k j_{s(k)}}, \tag{2}$$

for any $I = \{i_1, \ldots, i_k\}$, $1 \leqslant i_1 < \cdots < i_k \leqslant n$, $J = \{j_1, \ldots, j_k\}$, $1 \leqslant j_1 < \cdots < j_k \leqslant 2n$; here $l(s)$ denotes the length of permutation s.

Consider the algebra $\mathbb{C}[\mathrm{Pl}_{n,2n}]_q \subset \mathbb{C}[\mathrm{Mat}_{n,2n}]_q$ generated by all q-minors $t_{\{1,\ldots,n\}J}^{\wedge n}$, card $J = n$. It is equipped with the standard $U_q\mathfrak{sl}_n^{op} \otimes U_q\mathfrak{sl}_{2n}$-module algebra structure. ($U_q\mathfrak{sl}_n^{op}$ is a Hopf algebra with the same multiplication and the opposite comultiplication.) It is easy to show that the $U_q\mathfrak{sl}_n^{op}$-structure can be reconstructed from the below equalities:

$$K_l t_{ij} = \begin{cases} q^{-1}t_{ij}, & l = i-1, \\ qt_{ij}, & l = i, \\ 0, & \text{otherwise;} \end{cases}$$

$$E_l t_{ij} = q^{-1/2} \cdot \begin{cases} t_{(i+1)j}, & l = i, \\ 0, & \text{otherwise;} \end{cases} \qquad F_l t_{ij} = q^{1/2} \cdot \begin{cases} t_{(i-1)j}, & l = i-1, \\ 0, & \text{otherwise.} \end{cases}$$

The element $t \overset{\text{def}}{=} t^{\wedge n}_{\{1,2,\ldots,n\}\{n+1,n+2,\ldots,2n\}}$ quasicommutes with t_{ij} for all $i=1,\ldots,n$, $j=1,\ldots,2n$ and is $U_q\mathfrak{sl}_n^{op}$-invariant.

Denote by $\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ the localization of the algebra $\mathbb{C}[\mathrm{Pl}_{n,2n}]_q$ with respect to the multiplicative system $t^{\mathbb{Z}_+}$. Introduce q-analogs of coordinates on Ω as follows:

$$z_a^b \overset{\text{def}}{=} t^{-1} t^{\wedge n}_{\{1,2,\ldots,n\}J_{ab}}, \tag{3}$$

where $J_{ab}=\{n+1,n+2,\ldots,2n\}\setminus\{2n+1-b\}\cup\{a\}$.

The defining relations for the subalgebra generated by the elements z_a^b are obtained in Ref. 11:

$$z_a^{b_1} z_a^{b_2} = q z_a^{b_2} z_a^{b_1}, \quad b_1 < b_2,$$

$$z_{a_1}^{b} z_{a_2}^{b} = q z_{a_2}^{b} z_{a_1}^{b}, \quad a_1 < a_2,$$

$$z_{a_1}^{b_1} z_{a_2}^{b_2} = z_{a_2}^{b_2} z_{a_1}^{b_1}, \quad b_1 < b_2 \text{ and } a_1 > a_2,$$

$$z_{a_1}^{b_1} z_{a_2}^{b_2} - z_{a_2}^{b_2} z_{a_1}^{b_1} = (q - q^{-1}) z_{a_1}^{b_2} z_{a_2}^{b_1}, \quad b_1 < b_2 \text{ and } a_1 < a_2.$$

(For the special case $n=2$ see the Noumi paper.[12])

It can be checked easily that $zt=qtz$ for any $z \in \{z_a^b \mid a,b=1,\ldots,n\}$.

It can be proved that for any $\xi \in U_q\mathfrak{sl}_{2n}$, $f \in \mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ there is a unique Laurent polynomial $p_{f,\xi}$ of the variable $u=q^k$ with coefficients in $\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ such that $p_{f,\xi}(q^k)=\xi\cdot(ft^k)t^{-k}$. This allows one to prove the existence of an extension of the $U_q\mathfrak{sl}_{2n}$-module algebra structure onto $\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ (see Ref. 13).

The subalgebra generated by z_a^b is the algebra $\mathbb{C}[\mathrm{Mat}_n]_q$ of "polynomials on the quantum $n\times n$-matrix space" [cf. (1)]. The algebra $\mathbb{C}[\mathrm{Mat}_n]_q$ is a $U_q\mathfrak{sl}_{2n}$-module subalgebra of the $U_q\mathfrak{sl}_{2n}$-module algebra $\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ (see Ref. 14).

Proposition 1 (Ref. 14): For all $a,b=1,\ldots,n$

$$K_n^{\pm 1} z_a^b = \begin{cases} q^{\pm 2} z_a^b, & a = n \text{ and } b = n \\ q^{\pm 1} z_a^b, & (a = n \text{ and } b \neq n) \text{ or } (a \neq n \text{ and } b = n) \\ z_a^b, & \text{otherwise,} \end{cases}$$

$$F_n z_a^b = q^{1/2} \cdot \begin{cases} 1, & a = n \text{ and } b = n \\ 0, & \text{otherwise,} \end{cases} \qquad E_n z_a^b = -\, q^{1/2} \cdot \begin{cases} q^{-1} z_a^n z_n^b, & a \neq n \text{ and } b \neq n \\ (z_n^n)^2, & a = n \text{ and } b = n \\ z_n^n z_a^b, & \text{otherwise} \end{cases}$$

and for all $k \neq n$ we have

$$K_k^{\pm 1} z_a^b = \begin{cases} q^{\pm 1} z_a^b, & (k < n \text{ and } a = k) \text{ or } (k > n \text{ and } b = 2n-k), \\ q^{\mp 1} z_a^b, & (k < n \text{ and } a = k+1) \text{ or } (k > n \text{ and } b = 2n-k+1), \\ z_a^b, & \text{otherwise,} \end{cases}$$

$$F_k z_a^b = q^{1/2}\cdot\begin{cases} z_{a+1}^b, & k<n \text{ and } a=k,\\ z_a^{b+1}, & k>n \text{ and } b=2n-k,\\ 0, & \text{otherwise,}\end{cases}\quad E_k z_a^b = q^{-1/2}\cdot\begin{cases} z_{a-1}^b, & k<n \text{ and } a=k+1,\\ z_a^{b-1}, & k>n \text{ and } b=2n-k+1,\\ 0, & \text{otherwise.}\end{cases}$$

□

In the sequel we use the following notation for q-minors:

$$\mathbf{z}^{\wedge k\{b_1,\dots,b_k\}}_{\{a_1,\dots,a_k\}} \overset{\text{def}}{=} \sum_{s\in S_k}(-q)^{l(s)} z^{b_{s(1)}}_{a_1}\cdots z^{b_{s(k)}}_{a_k}, \tag{4}$$

where $a_1<\cdots<a_k$, $b_1<\cdots<b_k$. It is known that the element $\det_q \mathbf{z} \overset{\text{def}}{=} \mathbf{z}^{\wedge n\{1,\dots,n\}}_{\{1,\dots,n\}}$ belongs to the center of $\mathbb{C}[\mathrm{Mat}_n]_q$ and $\mathbb{C}[\mathrm{Mat}_n]_q$ has no zero divisors.

Denote by $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$ the localization of the algebra $\mathbb{C}[\mathrm{Mat}_n]_q$ with respect to the multiplicative system $(\det_q \mathbf{z})^{\mathbb{Z}_+}$. We consider $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$ as a q-analog of the space of regular functions on the open orbit Ω. Let $\tilde{t}=t^{\wedge n}_{\{1,\dots,n\}\{1,\dots,n\}}$. Since $\det_q \mathbf{z}=t^{-1}\tilde{t}$, we see that the algebra $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$ is a $U_q\mathfrak{sl}_{2n}$-module subalgebra of the $U_q\mathfrak{sl}_{2n}$-module algebra $\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t\cdot\tilde{t}}$. (As above, to verify that the extension is well defined we use the following fact: for all $\xi\in U_q\mathfrak{sl}_{2n}$, $f\in V$ the vector valued function $\xi\cdot(f(\det_q \mathbf{z})^k)(\det_q \mathbf{z})^{-k}$ is a Laurent polynomial of the variable $u=q^k$.)

Denote by V the vector space $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$. Assume first that $\alpha,\beta\in\mathbb{Z}$. Define a representation $\pi_{\alpha,\beta}: U_q\mathfrak{sl}_{2n}\to \mathrm{End}\, V$ as follows:

$$\pi_{\alpha,\beta}(\xi)f=(\xi\cdot(f(\tilde{t})^\alpha t^\beta))t^{-\beta}(\tilde{t})^{-\alpha}=(\xi\cdot(f(\det_q \mathbf{z})^\alpha t^{\beta+\alpha}))t^{-\alpha-\beta}(\det_q \mathbf{z})^{-\alpha} \tag{5}$$

for every $\xi\in U_q\mathfrak{sl}_{2n}$, $f\in V$. For each $\lambda\in\mathbb{Z}$ we have

$$E_j t^\lambda=0,\quad F_j t^\lambda=0,\quad K_j t^\lambda=t^\lambda,\quad j=1,\dots,2n-1,\quad j\neq n,$$

$$E_n t^\lambda=q^{-3/2}\frac{1-q^{-2\lambda}}{1-q^{-2}}z_n^n t^\lambda,\quad F_n t^\lambda=0,\quad K_n^{\pm1}t^\lambda=q^{\mp\lambda}t^\lambda,$$

$$E_j(\det_q \mathbf{z})^\lambda=0,\quad F_j(\det_q \mathbf{z})^\lambda=0,\quad K_j(\det_q \mathbf{z})^\lambda=(\det_q \mathbf{z})^\lambda,\quad j=1,\dots,2n-1,\quad j\neq n,$$

$$K_n^{\pm1}((\det_q \mathbf{z})^\lambda)=q^{\pm2\lambda}(\det_q \mathbf{z})^\lambda,\quad E_n((\det_q \mathbf{z})^\lambda)=-q^{1/2}\frac{1-q^{2\lambda}}{1-q^2}z_n^n(\det_q \mathbf{z})^\lambda,$$

$$F_n((\det_q \mathbf{z})^\lambda)=q^{1/2}\frac{1-q^{-2\lambda}}{1-q^{-2}}\mathbf{z}^{\wedge n-1}_{\{1,\dots,n-1\}\{1,\dots,n-1\}}(\det_q \mathbf{z})^{\lambda-1},\quad \lambda\neq0.$$

From these equalities we see that for each $\xi\in U_q\mathfrak{sl}_{2n}$, $f\in V$ the vector valued function $p_{f,\xi}(q^\alpha,q^\beta)\overset{\text{def}}{=}\pi_{\alpha,\beta}(\xi)(f)$ is a Laurent polynomial of the variables q^α, q^β. These Laurent polynomials are defined by their values on the set $\{(q^\alpha,q^\beta)\,|\,\alpha,\beta\in\mathbb{Z}\}$ and deliver the canonical "analytic continuation" for $\pi_{\alpha,\beta}(\xi)(f)$ to $(\alpha,\beta)\in\mathbb{C}^2$.

Let $(\alpha,\beta)\in\mathbb{C}^2$. Define a representation $\pi_{\alpha,\beta}(\xi)(f)\overset{\text{def}}{=}p_{f,\xi}(q^\alpha,q^\beta)$. Indeed, to prove that the representation $\pi_{\alpha,\beta}$ is well defined for $(\alpha,\beta)\in\mathbb{C}^2$ it is sufficient to verify some identities for Laurent polynomials. These identities are correct for $\alpha,\beta\in\mathbb{Z}$.

Introduce a "deformation parameter" h by the equality $q=e^{-h/2}$. Clearly, if $\alpha_1=\alpha_2+i(2\pi/h)$ and $\beta_1=\beta_2+i(2\pi/h)$, then $\pi_{\alpha_1,\beta_1}=\pi_{\alpha_2,\beta_2}$. Then it is enough to consider $(\alpha,\beta)\in D$, where

$$D=\left\{(\alpha,\beta)\in\mathbb{C}^2|0\leqslant \operatorname{Im}\alpha<\frac{2\pi}{h},0\leqslant \operatorname{Im}\beta<\frac{2\pi}{h}\right\}.$$

Recall that a representation $\rho: U_q\mathfrak{sl}_{2n}\to \operatorname{End} W$ is called *weight* if the representation space W decomposes as follows:

$$W=\bigoplus_{\lambda} W_\lambda,\quad \text{where } \lambda=(\lambda_1,\ldots,\lambda_{2n-1})\in\mathbb{Z}^{2n-1},$$

$$W_\lambda=\left\{v\in W|\rho(K_j^{\pm})v=q^{\pm\lambda_j}v, j=1,\ldots,2n-1\right\}.$$

The subspace W_λ is called weight subspace with weight λ. In the sequel we will consider only weight representations. It is clear that $\pi_{\alpha,\beta}$ is a weight representation if and only if $q^{\alpha-\beta}\in q^{\mathbb{Z}}$.

Let W be a weight $U_q\mathfrak{sl}_{2n}$-module. Define operators H_i for $i=1,\ldots,2n-1$ by the formula $H_i|_{W_\lambda}=\lambda_i$.

III. EQUIVALENCE OF THE REPRESENTATIONS

Recall that $q=e^{-h/2}$. For any complex α,β such that $0\leqslant \operatorname{Im}\alpha<2\pi/h$, $0\leqslant \operatorname{Im}\beta<2\pi/h$, the statements $\alpha-\beta\in\mathbb{Z}$ and $q^{\alpha-\beta}\in q^{\mathbb{Z}}$ are equivalent.

Proposition 2: If $\alpha,\beta\notin\mathbb{Z}$, then the representations $\pi_{\alpha,\beta}$ and $\pi_{-n-\beta,-n-\alpha}$ are equivalent.

The proof is reduced to explicit formulas for the intertwining operators. It is given in Sec. VI.

If $\alpha,\beta\in\mathbb{Z}$, then the representations $\pi_{\alpha,\beta}$ and $\pi_{-n-\beta,-n-\alpha}$ are not equivalent. This fact follows from the statement that only one of the representations $\pi_{\alpha,\beta}$ and $\pi_{-n-\beta,-n-\alpha}$ for integral α,β has a finite dimensional subrepresentation. An explanation of this fact is given in the end of Sec. V.

The representations $\pi_{\alpha,\beta}$ and $\pi_{\alpha-1,\beta+1}$ are equivalent for all α,β. The corresponding intertwining operator $T: V\to V$ is defined as follows: for every $f\in V=\mathbb{C}[\operatorname{Mat}_n]_{q,\det_q \mathbf{z}}$ $T(f)=f(\det_q \mathbf{z})^{-1}$. Indeed, since for each $f\in V$, $\xi\in U_q\mathfrak{sl}_{2n}$;

$$\begin{aligned}\pi_{\alpha-1,\beta+1}(\xi)(f)&=(\xi\cdot(f(\det_q \mathbf{z})^{\alpha-1}t^{\beta+\alpha}))t^{-\alpha-\beta}(\det_q \mathbf{z})^{1-\alpha}\\&=(\xi\cdot(f(\det_q \mathbf{z})^{-1}(\det_q \mathbf{z})^{\alpha}t^{\beta+\alpha}))t^{-\alpha-\beta}(\det_q \mathbf{z})^{-\alpha}(\det_q \mathbf{z})=\pi_{\alpha,\beta}(\xi)(f(\det_q \mathbf{z})^{-1})\det_q \mathbf{z},\end{aligned}$$

we see that T intertwines the representations $\pi_{\alpha,\beta}$ and $\pi_{\alpha-1,\beta+1}$. Therefore without loss of generality we can assume that $\alpha,\beta\in\mathcal{D}$, where

$$\mathcal{D}=\left\{(\alpha,\beta)\in\mathbb{C}^2|\alpha-\beta\in\{0,1\},0\leqslant \operatorname{Im}\alpha<\frac{2\pi}{h},0\leqslant \operatorname{Im}\beta<\frac{2\pi}{h}\right\}. \tag{6}$$

Let us introduce an equivalence relation on $\mathcal{D}$. The equivalence class of (α,β) consists of one point for $\alpha,\beta\in\mathbb{Z}$ and from two points for $\alpha,\beta\notin\mathbb{Z}$:

$$(\alpha_1,\beta_1)\sim(\alpha_2,\beta_2),\quad \text{iff}\begin{cases}\alpha_1=-n-\beta_2,\ \beta_1=-n-\alpha_2 & \text{for } \operatorname{Im}\alpha_1=\operatorname{Im}\alpha_2=0,\\ \alpha_1=\dfrac{2\pi i}{h}-n-\beta_2,\ \beta_1=\dfrac{2\pi i}{h}-n-\alpha_2, & \text{otherwise.}\end{cases}$$

Proposition 3: The set of equivalence classes $\mathcal{D}/\sim$ is in the one-to-one correspondence $(\alpha,\beta)\mapsto\pi_{\alpha,\beta}$ with the set of equivalence classes of the representations of the degenerate principal series.

Proof: By the above, each representation of the degenerate principal series is equivalent to the representation $\pi_{\alpha,\beta}$ for some $(\alpha,\beta)\in\mathcal{D}$.

Prove that the representations π_{α_1,β_1} and π_{α_2,β_2}, with (α_1,β_1), $(\alpha_2,\beta_2)\in\mathcal{D}$, are equivalent if and only if $(\alpha_1,\beta_1)\sim(\alpha_2,\beta_2)$. For that we calculate the action of a central element $C\in U_q\mathfrak{sl}_{2n}^{\text{ext}}$ (see Ref. 15 for the definition). It can be proved that $\pi_{\alpha,\beta}(C)$ is a scalar operator for all $\alpha,\beta\in\mathcal{D}$.

From Ref. 16 it follows that there exists a unique central element C which acts on the $U_q\mathfrak{sl}_{2n}$-highest vector v^{high} with weight λ as follows:

$$C(v^{\text{high}}) = \sum_{j=0}^{2n-1} q^{-2(\mu_j,\lambda+\rho)} v^{\text{high}},$$

where $\mu_0=\varpi_1$, $\mu_j=-\varpi_j+\varpi_{j+1}$ for $j=1,\dots,2n-2$, $\mu_{2n-1}=-\varpi_{2n-1}$, ϖ_j are the fundamental weights, 2ρ is the sum of positive roots of the Lie algebra $\mathfrak{sl}_{2n}$, and we choose the invariant scalar product such that $(\alpha,\alpha)=2$ for any simple root α.

First let α,β be integers. It can be proved that

$$\pi_{\alpha,\beta}(C)(\det_q \mathbf{z})^\beta = 4 \operatorname{ch}\frac{h}{2}(\alpha+\beta+n)\left(\sum_{j=0}^{n-1}\operatorname{ch}\frac{h}{2}j\right)(\det_q \mathbf{z})^\beta.$$

Hence $\pi_{\alpha,\beta}(C)=4\operatorname{ch}(h/2)(\alpha+\beta+n)(\Sigma_{j=0}^{n-1}\operatorname{ch}(h/2)j)\cdot \mathrm{Id}$ for all $(\alpha,\beta)\in\mathcal{D}$.

Suppose that π_{α_1,β_1} and π_{α_2,β_2} are equivalent. Equivalent representations have the same weight lattice. Therefore $(\alpha_1-\beta_1)-(\alpha_2-\beta_2)\in 2\mathbb{Z}$. Since $(\alpha_1,\beta_1),(\alpha_2,\beta_2)\in\mathcal{D}$, we see that $(\alpha_1-\beta_1)-(\alpha_2-\beta_2)=0$.

Then the equivalent representations π_{α_1,β_1} and π_{α_2,β_2} have the same values of central characters, which means that

$$\left(\operatorname{ch}\frac{h}{2}(\alpha_1+\beta_1+n)-\operatorname{ch}\frac{h}{2}(\alpha_2+\beta_2+n)\right)\sum_{j=0}^{n-1}\operatorname{ch}\frac{h}{2}j=0.$$

Since $0\leqslant \operatorname{Im}\alpha_1<2\pi/h$, $0\leqslant\operatorname{Im}\beta_1<2\pi/h$, $0\leqslant\operatorname{Im}\alpha_2<2\pi/h$, $0\leqslant\operatorname{Im}\beta_2<2\pi/h$, we have that $\alpha_1+\beta_1=\alpha_2+\beta_2$, or $\alpha_1+\beta_1=-\alpha_2-\beta_2-2n$, or $\alpha_1+\beta_1=-\alpha_2-\beta_2-2n-(4\pi i/h)$. If $\alpha_1+\beta_1=\alpha_2+\beta_2$, then $\alpha_1=\alpha_2$ and $\beta_1=\beta_2$. For any fixed nonintegral α_1,β_1 there is a unique pair $(\alpha_2,\beta_2)\in\mathcal{D}$ such that either $\alpha_1+\beta_1=-\alpha_2-\beta_2-2n$ or $\alpha_1+\beta_1=-\alpha_2-\beta_2-2n-(4\pi i/h)$, and $(\alpha_1,\beta_1)\sim(\alpha_2,\beta_2)$. Although for integral parameters π_{α_1,β_1} and π_{α_2,β_2} are not equivalent, because the only one of them has a finite-dimensional subrepresentation. This can be deduced from Corollary 4. Thus each equivalence class in $\mathcal{D}$ is assigned to a unique equivalence class of the representations of the degenerate principal series $\pi_{\alpha,\beta}$. □

IV. AUXILIARY STATEMENTS ON THE $\pi_{\alpha,\beta}$-STRUCTURE

In this section we describe some necessary technical results, that will be useful in the sequel.

Everywhere in this section we assume that $n>1$. However, Propositions 4, 7, and 10 and Corollaries 1 and 2 are still sensible and correct for $n=1$.

Let $U_q\mathfrak{k}_{ss}\subset U_q\mathfrak{sl}_{2n}$ be the Hopf subalgebra generated by E_j, F_j, $K_j^{\pm1}$, $j=1,\dots,2n-1$, $j\neq n$ and $U_q\mathfrak{k}\subset U_q\mathfrak{sl}_{2n}$ be the Hopf subalgebra generated by $K_n^{\pm1}$ and $U_q\mathfrak{k}_{ss}$.

Note that $\pi_{\alpha,\beta}|_{U_q\mathfrak{k}_{ss}}$ does not depend on α,β. The following preliminary result on reducibility of $\pi_{\alpha,\beta}$ is well known in the classical case. For brevity, set

$$\mathbf{z}^{\wedge k}=\mathbf{z}^{\wedge k\{1,\cdots,k\}}_{\{1,\cdots,k\}}$$

(note that, obviously $\mathbf{z}^{\wedge n}=\det_q\mathbf{z}$). Introduce the following notation: $\hat{K}=\{\overline{\mathbf{k}}=(k_1,\dots,k_n)\in\mathbb{Z}^n \mid k_1\geqslant k_2\geqslant\cdots\geqslant k_n\}$, $\mathbf{e_j}=(0,\dots,\overset{j}{1},\dots,0)\in\mathbb{Z}^n$.

Proposition 4: The representation space V for $\pi_{\alpha,\beta}$ splits into a sum of simple pairwise nonisomorphic $U_q\mathfrak{k}$-modules as follows:

$$V=\bigoplus_{\overline{\mathbf{k}}\in\hat{K}} V_{\overline{\mathbf{k}}},\quad \text{with } V_{\overline{\mathbf{k}}}=\pi_{\alpha,\beta}(U_q\mathfrak{k})\cdot v^{\frac{h}{\mathbf{k}}}_{\overline{\mathbf{k}}} \quad\text{and}\quad v^{\frac{h}{\mathbf{k}}}_{\overline{\mathbf{k}}}=(\mathbf{z}^{\wedge1})^{k_1-k_2}\cdots(\mathbf{z}^{\wedge n-1})^{k_{n-1}-k_n}(\mathbf{z}^{\wedge n})^{k_n}.$$

Proof: Consider the filtration $V=\cup_{k=0}^{\infty}V^{(k)}$ with $V^{(k)}=\mathbb{C}[\mathrm{Mat}_n]_q\cdot(\det_q \mathbf{z})^{-k}$. It is sufficient to prove that

$$V^{(k)}=\bigoplus_{k_n\geqslant -k} V_{\mathbf{k}}^{-}.$$

Equip the vector space $V^{(k)}$ with the natural grading $V^{(k)}=\overset{\infty}{\underset{j=-nk}{\oplus}}(V^{(k)})_j$ as follows: $(V^{(k)})_j=\{v\in V^{(k)}\,|\,K_0 v=q^{2j}v\}$, with $K_0\overset{\text{def}}{=}K_1K_2^2K_3^3\cdots K_n^nK_{n+1}^{n-1}\cdots K_{2n-2}^2K_{2n-1}$. Therefore we must prove that

$$(\mathbb{C}[\mathrm{Mat}_n]_q\cdot(\det_q \mathbf{z})^{-k})_j=\bigoplus_{\substack{k_n\geqslant -k,\\ k_1+\cdots+k_n=j}} V_{\mathbf{k}}^{-}. \tag{7}$$

For $k=0$ statement (7) means that $(\mathbb{C}[\mathrm{Mat}_n]_q)_j=\bigoplus_{k_n\geqslant 0,k_1+\cdots+k_n=j} V_{\mathbf{k}}^{-}$.

First, the dimensions of homogeneous components $\mathbb{C}[\mathrm{Mat}_n]_{q,j}$ of the standardly graded algebra $\mathbb{C}[\mathrm{Mat}_n]_q$ are equal to the dimensions in the classical case,

$$\dim\,\mathbb{C}[\mathrm{Mat}_n]_{q,j}=\binom{n^2+j-1}{j}$$

(it can be easily proved via the Bergman diamond lemma,[15] Sec. 4.1.5). Second, the dimensions of the $U_q\mathfrak{k}$-modules $V_{\mathbf{k}}^{-}$ are equal to the classical ones (this follows from results of quantum groups theory,[17] Chap. 5). Third, there is the well-known Hua result on the coincidence of the dimensions $\mathbb{C}[\mathrm{Mat}_n]_j$ and $\bigoplus_{\substack{k_n\geqslant 0,\\ k_1+k_2+\cdots+k_n=j}} V_{\mathbf{k}}^{-}$ in the classical case.[18] Hence,

$$\dim\,(\mathbb{C}[\mathrm{Mat}_n]_q)_j=\sum_{\substack{k_n\geqslant 0,\\ k_1+\cdots+k_n=j}}\dim V_{\mathbf{k}}^{-},$$

and, finally,

$$(\mathbb{C}[\mathrm{Mat}_n]_q)_j=\bigoplus_{\substack{k_n\geqslant 0,\\ k_1+\cdots+k_n=j}} V_{\mathbf{k}}^{-}.$$

For $k>0$ one has

$$(\mathbb{C}[\mathrm{Mat}_n]_q\cdot(\det_q \mathbf{z})^{-k})_j=\mathbb{C}[\mathrm{Mat}_n]_{q,nk+j}\cdot(\det_q \mathbf{z})^{-k}=\bigoplus_{\substack{k_n\geqslant 0,\\ k_1+\cdots+k_n=nk+j}} V_{\mathbf{k}}^{-}\cdot(\det_q \mathbf{z})^{-k}=\bigoplus_{\substack{k_n\geqslant -k,\\ k_1+\cdots+k_n=j}} V_{\mathbf{k}}^{-}.$$

(Since there are no zero divisors in $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$, the proof of statement (7) follows from the last equality.) □

Remark: It can be easily verified that $v_{\mathbf{k}}^{h}$ is a $U_q\mathfrak{k}$-highest vector and with weight $(k_1-k_2,\ldots,k_{n-1}-k_n,2k_n+\alpha-\beta,k_{n-1}-k_n,\ldots,k_1-k_2)$. Then the highest weight of simple $U_q\mathfrak{k}$-module $V_{\mathbf{k}}^{-}$ is equal to $(k_1-k_2,\ldots,k_{n-1}-k_n,2k_n+\alpha-\beta,k_{n-1}-k_n,\ldots,k_1-k_2)$.

In the classical case $\mathfrak{sl}_{2n}=\mathfrak{p}^{-}\oplus\mathfrak{k}\oplus\mathfrak{p}^{+}$ where

$$\mathfrak{p}^{-}=\left\{\begin{pmatrix}0&0\\A&0\end{pmatrix}\middle|\,A\in\mathrm{Mat}_{n,n}(\mathbb{C})\right\},\quad \mathfrak{p}^{+}=\left\{\begin{pmatrix}0&A\\0&0\end{pmatrix}\middle|\,A\in\mathrm{Mat}_{n,n}(\mathbb{C})\right\}.$$

Therefore $U\mathfrak{sl}_{2n}\simeq U\mathfrak{p}^{-}\otimes U\mathfrak{k}\otimes U\mathfrak{p}^{+}$ as $U\mathfrak{k}$-modules ($U\mathfrak{p}^{-}$ and $U\mathfrak{p}^{-}$ are $U\mathfrak{k}$-modules under the adjoint action).

In the quantum case we have an analog of this decomposition obtained by Jakobsen in Ref. 19. A quantum analog $\mathrm{ad}_a, a \in U_q\mathfrak{sl}_{2n}$ of the adjoint action is introduced via the Hopf algebra structure of $U_q\mathfrak{sl}_{2n}$. (The operator ad_a is defined on $b \in U_q\mathfrak{sl}_{2n}$ in the following way: $\mathrm{ad}_a(b) = \Sigma S(a')ba''$, where $\Delta a = \Sigma a' \otimes a''$ is the comultiplication, S is the antipode in $U_q\mathfrak{sl}_{2n}$.) There are n^2-dimensional vector subspaces $\mathfrak{p}_q^+ = U_q\mathfrak{k} \cdot E_n$, $\mathfrak{p}_q^- = U_q\mathfrak{k} \cdot (K_n F_n)$, which are $U_q\mathfrak{k}$-invariant under the adjoint action. Instead of $U\mathfrak{p}^-$, $U\mathfrak{p}^+$, there are the subalgebras $U_q\mathfrak{p}^-$, $U_q\mathfrak{p}^+ \subset U_q\mathfrak{sl}_{2n}$ generated by $\mathfrak{p}_q^-$, $\mathfrak{p}_q^+$, respectively. The algebras $U_q\mathfrak{p}^-$ and $U_q\mathfrak{p}^+$ are $U_q\mathfrak{k}$-modules under the adjoint action. Therefore in the quantum case we get $U_q\mathfrak{sl}_{2n} \simeq U_q\mathfrak{p}^- \otimes U_q\mathfrak{k} \otimes U_q\mathfrak{p}^+$ as $U_q\mathfrak{k}$-modules (see Ref. 19). It is worthwhile to note that $U_q\mathfrak{p}^-$ and $U_q\mathfrak{p}^+$ are not Hopf subalgebras unlike the classical case.

In the last part of this section we describe how each $U_q\mathfrak{k}$-isotypic component $V_{\mathbf{k}}^-$ transforms under the action of $\mathfrak{p}_q^-$ and $\mathfrak{p}_q^+$. This allows one to understand how V transforms under the $U_q\mathfrak{sl}_{2n}$-action. Since

$$U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n) \simeq \mathbb{C}[K_0^{\pm 1}] \otimes (U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n) = \mathbb{C}[K_0^{\pm 1}] \otimes U_q\mathfrak{k}_{ss},$$

where

$$K_0 = K_1 K_2^2 K_3^3 \cdots K_n^n K_{n+1}^{n-1} \cdots K_{2n-2}^2 K_{2n-1}, \tag{8}$$

and $\pi_{\alpha,\beta}(K_0)$ acts by scalar multiplications in every isotypic component, we see that $V_{\mathbf{k}}^-$ is a simple $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-module. Hence the $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-module $V_{\mathbf{k}}^-$ decomposes into a tensor product of $U_q\mathfrak{sl}_n$-modules: $V_{\mathbf{k}}^- \simeq V_{\mathbf{k}}^{(1)} \otimes V_{\mathbf{k}}^{(2)}$ with $V_{\mathbf{k}}^{(1)} = L(k_1 - k_2, \ldots, k_{n-1} - k_n)$, $V_{\mathbf{k}}^{(2)} = L^*(k_1 - k_2, \ldots, k_{n-1} - k_n)$, where we denote by $L(k_1 - k_2, \ldots, k_{n-1} - k_n)$ and $L^*(k_1 - k_2, \ldots, k_{n-1} - k_n)$ the simple finite dimensional $U_q\mathfrak{sl}_n$-modules with highest weights $(k_1 - k_2, \ldots, k_{n-1} - k_n)$ and $(k_{n-1} - k_n, \ldots, k_1 - k_2)$, respectively.

We can equip the vector spaces $V_{\mathbf{k}}^{(1)}$ and $V_{\mathbf{k}}^{(2)}$ with the structure of $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-modules as follows:

$$(\xi \otimes \eta)(v) = \xi \cdot (\varepsilon(\eta)v), \quad (\xi \otimes \eta)(v^*) = \eta \cdot (\varepsilon(\xi)v^*),$$

for all $\xi, \eta \in U_q\mathfrak{sl}_n$, $v \in V_{\mathbf{k}}^{(1)}$, $v^* \in V_{\mathbf{k}}^{(2)}$, where ε denotes the counit of $U_q\mathfrak{sl}_n$. Note that as $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-modules

$$\mathfrak{p}_q^+ \simeq \mathbb{C}^n \otimes (\mathbb{C}^n)^*, \quad \mathfrak{p}_q^- \simeq (\mathbb{C}^n)^* \otimes \mathbb{C}^n,$$

where $\mathbb{C}^n$ is the vector representation of $U_q\mathfrak{sl}_n$. Consider the natural maps

$$m_{\mathbf{k}}^+ : \mathfrak{p}_q^+ \otimes V_{\mathbf{k}}^- \to V, \quad m_{\mathbf{k}}^- : \mathfrak{p}_q^- \otimes V_{\mathbf{k}}^- \to V.$$

Since there exist the $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-homomorphisms

$$\mathfrak{p}_q^+ \otimes V_{\mathbf{k}}^- \simeq \mathbb{C}^n \otimes (\mathbb{C}^n)^* \otimes V_{\mathbf{k}}^{(1)} \otimes V_{\mathbf{k}}^{(2)} \simeq \mathbb{C}^n \otimes V_{\mathbf{k}}^{(1)} \otimes (\mathbb{C}^n)^* \otimes V_{\mathbf{k}}^{(2)},$$

$$\mathfrak{p}_q^- \otimes V_{\mathbf{k}}^- \simeq (\mathbb{C}^n)^* \otimes \mathbb{C}^n \otimes V_{\mathbf{k}}^{(1)} \otimes V_{\mathbf{k}}^{(2)} \simeq (\mathbb{C}^n)^* \otimes V_{\mathbf{k}}^{(1)} \otimes \mathbb{C}^n \otimes V_{\mathbf{k}}^{(2)},$$

we have the well-defined morphisms

$$\mathcal{M}_{\mathbf{k}}^+ : \mathbb{C}^n \otimes V_{\mathbf{k}}^{(1)} \otimes (\mathbb{C}^n)^* \otimes V_{\mathbf{k}}^{(2)} \to V,$$

$$\mathcal{M}_{\mathbf{k}}^- : (\mathbb{C}^n)^* \otimes V_{\mathbf{k}}^{(1)} \otimes \mathbb{C}^n \otimes V_{\mathbf{k}}^{(2)} \to V.$$

For instance, if we consider a $U_q\mathfrak{sl}_n$-highest vector $v_1 \in \mathbb{C}^n \otimes V^{(1)}_{\mathbf{k}}$ and a $U_q\mathfrak{sl}_n$-highest vector $v_2 \in (\mathbb{C}^n)^* \otimes V^{(2)}_{\mathbf{k}}$, then $\mathcal{M}^+_{\mathbf{k}}(v_1 \otimes v_2)$ is a $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$-highest vector (or, equivalently, a $U_q\mathfrak{k}$-highest vector) in V.

In the sequel we are going to get explicit formulas for $U_q\mathfrak{sl}_n$-highest vectors $\zeta_j \in \mathbb{C}^n \otimes L(k_1-k_2,\dots,k_{n-1}-k_n)$, $j=1,\dots,n$ with weights $(k_1,\dots,k_j+1,\dots,k_n)$, respectively.

In the classical case auxiliary elements $F_{m,j}$ of the universal enveloping algebra $U\mathfrak{sl}_n$ are used in such formulas.

Lemma 1 (Ref. 8, lemma 3.4): Let $1 \leqslant k \leqslant n-1$ *and* $1 \leqslant m < j \leqslant n$.

(1) *If* $1 \leqslant k < m$ *or* $j < k \leqslant n$, *then* $E_k F_{m,j} = F_{m,j} E_k$;
(2) *If* $k=m$, *then* $E_m F_{m,j} \equiv F_{m+1,j}(H_m + \cdots + H_{j-1} + j - m - 1) \pmod{U\mathfrak{sl}_n \cdot E_m}$;
(3) *If* $m < k \leqslant j$, *then* $E_k F_{m,j} \equiv 0 \pmod{U\mathfrak{sl}_n \cdot E_k}$. □

Explicit formulas for the elements $F_{m,j}$ are used for the proof of lemma:

$$F_{m,j} = F_{m+1,j}F_m + \sum_{t=m+2}^{j} (-1)^{t+m+1} F_{t,j} \mathrm{ad}_{F_{t-1}} \cdots \mathrm{ad}_{F_{m+1}F_m} H(j; m+1, t-1),$$

where $H(j;p,s) = \Pi_{a=p}^{s}(H_a + \cdots + H_{j-1} + j - a)$.

We find quantum analogs of the previous lemma and the elements in $U_q\mathfrak{sl}_n$.

For $1 \leqslant m \leqslant j \leqslant n$ define $F_{m,j} \in U_q\mathfrak{sl}_n$ inductively as follows:

$$F_{j,j} = 1, \quad F_{j-1,j} = F_{j-1}K_{j-1},$$

$$F_{m,j} = F_{m+1,j}F_m K_m + \sum_{s=m+2}^{j} (-1)^{s+m+1} F_{s,j} \, \mathrm{ad}_{F_{s-1}} \cdots \mathrm{ad}_{F_{m+1}}(F_m K_m) K(j, m+1, s-1),$$

where $K(j,p,r) = \Pi_{a=p}^{r} q^{j-a} K_a \cdots K_{j-1}[H_a + \cdots + H_{j-1} + j - a]_q$.

Here and everywhere below we use the standard notation $[x]_q = (q^x - q^{-x})/(q - q^{-1})$.

Lemma 2: The following relations are satisfied:

$$(1)\ K_i F_{m,j} = F_{m,j} K_i \quad \textit{for } 1 \leqslant i < m-1 \textit{ or } j < i \leqslant n, \tag{9}$$

$$(2)\ K_j F_{m,j} = q F_{m,j} K_j, \quad K_{m-1} F_{m,j} = q F_{m,j} K_{m-1}, \tag{10}$$

$$(3)\ q K_{j-1} F_{m,j} = F_{m,j} K_{j-1}, \quad q K_m F_{m,j} = F_{m,j} K_m, \tag{11}$$

$$(4)\ E_i F_{m,j} = F_{m,j} E_i \quad \textit{for } 1 \leqslant i < m-1 \textit{ or } j < i \leqslant n, \tag{12}$$

$$(5)\ E_{m-1} F_{m,j} = q F_{m,j} E_{m-1}, \quad E_j F_{m,j} = q F_{m,j} E_j, \tag{13}$$

$$(6)\ E_i F_{m,j} \equiv 0 (\mathrm{mod}\ U_q\mathfrak{sl}_n \cdot E_i) \quad \textit{for } m < i < j, \tag{14}$$

$$(7)\ E_m F_{m,j} \equiv F_{m+1,j} q^{j-m} K_m \cdots K_{j-1} [H_m + \cdots + H_{j-1} + j - m - 1]_q \ (\mathrm{mod}\ U_q\mathfrak{sl}_n \cdot E_m). \tag{15}$$

This lemma is proved in the Appendix. □

Let $(\varepsilon_1,\dots,\varepsilon_n)$ be the standard basis for $\mathbb{C}^n$. Suppose $u \in L(k_1-k_2,\dots,k_{n-1}-k_n)$ *is a* $U_q\mathfrak{sl}_n$-highest vector with weight $(k_1-k_2,\dots,k_{n-1}-k_n)$.

Proposition 5: Define vectors $\{\zeta_j\}_{j=1}^n$ *as follows:*

$$\zeta_j = \sum_{m=1}^{j} (-q^2)^{m-1} \varepsilon_m \otimes F_{m,j} K_-(j,1,m-1)u \in \mathbb{C}^n \otimes L(k_1-k_2, \ldots, k_{n-1}-k_n),$$

where $K_-(j,p,r)=\Pi_{a=p}^{r} q^{j-a-1} K_a \cdots K_{j-1}[H_a+\cdots+H_{j-1}+j-a-1]_q$. *Then* ζ_j *is a* $U_q\mathfrak{sl}_n$*-highest vector* (i.e., $E_i\zeta_j=0$ for all $i=1,\ldots,n-1$) *with weight* $(k_1-k_2,\ldots,k_{j-1}-k_j-1,k_j+1-k_{j+1},\ldots,k_{n-1}-k_n)$ *for* $j=1,\ldots,n$.

Proof: Using Lemma 2, it is easy to prove that ζ_j are weight vectors. We claim that $E_i\zeta_j=0$ for all $1\leqslant i\leqslant n$, $1\leqslant j\leqslant n$. Indeed, by Lemma 2,

$$\begin{aligned} E_i\zeta_j &= E_i\left(\sum_{m=1}^{j} (-q^2)^{m-1}\varepsilon_m \otimes F_{m,j}K_-(j,1,m-1)u\right) \\ &= \sum_{m=1}^{j} (-q^2)^{m-1} E_i(\varepsilon_m \otimes F_{m,j}K_-(j,1,m-1)u) \\ &= (-q^2)^i \varepsilon_i \otimes F_{i+1,j}K_-(j,1,i)u + (-q^2)^{i-1}E_i(\varepsilon_i \otimes F_{i,j}K_-(j,1,i-1)u) \\ &= (-q^2)^{i-1}(-q^2\varepsilon_i \otimes F_{i+1,j}K_-(j,1,i)u + q\varepsilon_i \otimes F_{i+1,j}q^{j-i}K_i\cdots K_{j-1}[H_i+\cdots+H_{j-1}+j-i \\ &\quad -1]_q K_-(j,1,i-1)u) = 0. \end{aligned}$$

□

Similarly, we are going to get explicit formulas for $U_q\mathfrak{sl}_n$-highest vectors $\xi_j \in (\mathbb{C}^n)^* \otimes L^*(k_1-k_2,\ldots,k_{n-1}-k_n)$. For $1\leqslant r\leqslant t\leqslant n$ introduce the elements $S_{r,t}\in U_q\mathfrak{sl}_n$ as follows (classic analogs of these elements were investigated by Lee in Ref. 8):

$$S_{t,t}=1, \quad S_{t-1,t}=F_tK_t,$$

$$S_{r,t}=S_{r,t-1}F_tK_t+\sum_{s=r+1}^{t-1} S_{r,s-1}\,\mathrm{ad}_{F_s}\cdots\mathrm{ad}_{F_{t-1}}(F_tK_t)L(t,s,t-1),$$

where $L(j,p,r)=\Pi_{a=p}^{r} q^{a-j}K_{j+1}\cdots K_a[H_{j+1}\cdots+H_a+a-j]_q$.

Lemma 3: The following relations are satisfied:

(1) $K_iS_{r,t}=S_{r,t}K_i$ *for* $1\leqslant i<r$ *or* $t+1<i\leqslant n$,
(2) $K_rS_{r,t}=qK_rS_{r,t}$, $K_{t+1}S_{r,t}=qK_{t+1}S_{r,t}$,
(3) $K_{r+1}S_{r,t}=q^{-1}K_{r+1}S_{r,t}$, $K_tS_{r,t}=q^{-1}K_tS_{r,t}$,
(4) $E_iS_{r,t}=S_{r,t}E_i$ *for* $1\leqslant i<r$ *or* $t+1<i\leqslant n$,
(5) $E_rS_{r,t}=qS_{r,t}E_r$, $E_{t+1}S_{r,t}=qS_{r,t}E_{t+1}$,
(6) $E_iS_{r,t}\equiv 0 \pmod{U_q\mathfrak{sl}_n\cdot E_i}$ for $r<i<t$,
(7) $E_tS_{r,t}\equiv -S_{r,t-1}q^{t-r}K_{r+1}\cdots K_t[H_{r+1}+\cdots+H_t+t-r-1]_q \pmod{U_q\mathfrak{sl}_n\cdot E_t}$.

The proof of this lemma is completely analogous to the proof of Lemma 2.

Let $(\varepsilon_1^*,\ldots,\varepsilon_n^*)$ be the basis for $(\mathbb{C}^n)^*$ dual to the basis $(\varepsilon_1,\ldots,\varepsilon_n)$ for $\mathbb{C}^n$. Suppose that $u^*\in L^*(k_1-k_2,\ldots,k_{n-1}-k_n)$ is a $U_q\mathfrak{sl}_n$-highest vector with weight $(k_{n-1}-k_n,\ldots,k_1-k_2)$. The proof of the next statement is similar to the proof of Proposition 5.

Proposition 6: Define vectors $\{\xi_j\}_{j=1}^n$ *as follows:*

$$\xi_j=\sum_{m=j}^{n}\varepsilon_m^*\otimes S_{j,m}L_-(j,m+1,n)u^* \in (\mathbb{C}^n)^*\otimes L^*(k_1-k_2,\ldots,k_{n-1}-k_n),$$

where $L_-(j,p,r)=\Pi_{a=p}^{r} q^{a-j-1}K_{j+1}\cdots K_a[H_{j+1}+\cdots+H_a+a-j-1]_q$. *Then* ξ_j *is a* $U_q\mathfrak{sl}_n$*-highest vector with weight* $(k_{n-1}-k_n,\ldots,k_{n-j+1}+1-k_{n-j+2},k_{n-j}-k_{n-j+1}-1,\ldots,k_1-k_2)$ *for* $j=1,\ldots,n$. □

It follows from Propositions 5 and 6 that $\mathcal{M}^{+-}_{\mathbf{k}}: \mathbb{C}^n\otimes V^{(1)}_{-\mathbf{k}}\otimes(\mathbb{C}^n)^*\otimes V^{(2)}_{-\mathbf{k}}\to\oplus_{j=1}^n V_{-\mathbf{k}+\mathbf{e}_j}$. For all $j,k=1,\ldots,n$ the vectors $\mathcal{M}^{+-}_{\mathbf{k}}(\zeta_j\otimes\xi_k)$ are $U_q\mathfrak{sl}_n\otimes U_q\mathfrak{sl}_n$-highest vectors in V. By the action of

$\pi_{\alpha,\beta}(K_0)$ [see (8)], the vector $\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_k)$ is a $U_q\mathfrak{k}$-highest vector in $V_{\overline{\mathbf{k}+\mathbf{e}_j}}$ if and only if $k=n-j+1$. Since every isotypic component occurs with multiplicity one, $\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_{n-j+1}) = c_j \cdot v^h_{\overline{\mathbf{k}+\mathbf{e}_1}} = c_j \cdot (\mathbf{z}^{\wedge 1})^{k_1-k_2+1} \cdots (\mathbf{z}^{\wedge n-1})^{k_{n-1}-k_n} (\mathbf{z}^{\wedge n})^{k_n}$ for some $c_j \in \mathbb{C}$. (Here and below we suppose that if $\overline{\mathbf{m}}=(m_1,\ldots,m_n) \notin \hat{K}$, then $V_{\overline{\mathbf{m}}}=0$ and $v^h_{\overline{\mathbf{m}}}=0$.)

The proof of the next statement, reduced to computation of c_j, is given in the Appendix.

Proposition 7: For every $j=1,\ldots,n, \overline{\mathbf{k}} \in \hat{K}$,

$$\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_{n-j+1}) = c_j(\beta,k_j) v^h_{\overline{\mathbf{k}+\mathbf{e}_j}},$$

where $c_j(\beta,k_j)=q^{-\beta-n/2}[\beta-k_j+j-1]_q \omega_j(\overline{\mathbf{k}},q)$ *and* $\omega_j(\overline{\mathbf{k}},q) \neq 0$ *for all* $\overline{\mathbf{k}} \in \hat{K}$.

We deduce sufficient conditions for reducibility of $\pi_{\alpha,\beta}$ from Proposition 7.

Let α, β be fixed. For any $j=1,\ldots,n$ and $\overline{\mathbf{k}} \in \hat{K}$ if $c_j(\beta,k_j) \neq 0$, then there exist $v \in V_{\overline{\mathbf{k}}}$, $\xi \in \mathfrak{p}^+_q$ such that $\pi_{\alpha,\beta}(\xi)\cdot v \in V_{\overline{\mathbf{k}+\mathbf{e}_j}}$. That means $\pi_{\alpha,\beta}(U_q\mathfrak{sl}_{2n})\cdot V_{\overline{\mathbf{k}}} \supset V_{\overline{\mathbf{k}+\mathbf{e}_j}}$.

Let us consider in details other cases, i.e., let $c_j(\beta,k_j)=0$ for some k_j. For fixed β, by Proposition 7 and (6), the equation $c_j(\beta,k_j)=0$ is equivalent to $\beta-k_j+j-1=0$.

Corollary 1: For all $j=1,\ldots,n$, $\overline{\mathbf{k}} \in \hat{K}$, *the subspace* $V^j_{\leqslant k} \overset{\text{def}}{=} \oplus_{\{\overline{\mathbf{k}'} \in \hat{K} | k \geqslant k'_j\}} V_{\overline{\mathbf{k}'}}$ *is a* $U_q\mathfrak{sl}_{2n}$*-submodule in* V *iff* $\beta-k+j-1=0$.

Proof: Let $j=1$, the other cases are similar. The necessity easily follows from the above. Prove the sufficiency. If $\beta-k_1=0$, then $\mathcal{M}^+_{\overline{\mathbf{k}}}(\mathfrak{p}^+_q \otimes V_{\overline{\mathbf{k}}}) \subset \oplus^n_{j=2} V_{\overline{\mathbf{k}+\mathbf{e}_j}}$. Introduce the natural filtration on $U_q\mathfrak{p}^+$ (here $U_q\mathfrak{p}^+$ is the algebra generated by $\mathfrak{p}^+_q$) in the following way: $U_q\mathfrak{p}^+ = \cup_{n\geqslant 0} (U_q\mathfrak{p}^+)^{(n)}$. Then $\pi_{\alpha,\beta}((U_q\mathfrak{p}^+)^{(1)})(V_{\overline{\mathbf{k}}}) \subset V_{\overline{\mathbf{k}}} \oplus (\oplus^n_{j=2} V_{\overline{\mathbf{k}+\mathbf{e}_j}})$. In the same way, $\pi_{\alpha,\beta}((U_q\mathfrak{p}^+)^{(2)})(V_{\overline{\mathbf{k}}}) \subset \pi_{\alpha,\beta}((U_q\mathfrak{p}^+)^{(1)}) \times (V_{\overline{\mathbf{k}}} \oplus (\oplus^n_{j=2} V_{\overline{\mathbf{k}+\mathbf{e}_j}})) \subset V_{\overline{\mathbf{k}}} \oplus (\oplus^n_{j=2} V_{\overline{\mathbf{k}+\mathbf{e}_j}}) \oplus (\oplus_{n\geqslant j_1 \geqslant j_2 \geqslant 2} V_{\overline{\mathbf{k}+\mathbf{e}_{j_1}+\mathbf{e}_{j_2}}})$. Then $\pi_{\alpha,\beta}(U_q\mathfrak{p}^+)(V_{\overline{\mathbf{k}}}) \subset \oplus^\infty_{m=0} \times (\oplus_{n\geqslant j_1 \geqslant \cdots \geqslant j_m \geqslant 2} V_{\overline{\mathbf{k}+\mathbf{e}_{j_1}+\cdots+\mathbf{e}_{j_m}}})$, and $\pi_{\alpha,\beta}(U_q\mathfrak{sl}_{2n})(V_{\overline{\mathbf{k}}}) \subset \pi_{\alpha,\beta}(U_q\mathfrak{p}^-)\pi_{\alpha,\beta}(U_q\mathfrak{k}) \times (\pi_{\alpha,\beta}(U_q\mathfrak{p}^+)V_{\overline{\mathbf{k}}}) \subset \pi_{\alpha,\beta}(U_q\mathfrak{p}^-)\pi_{\alpha,\beta}(U_q\mathfrak{k})(\oplus^\infty_{m=0}(\oplus_{n\geqslant j_1 \geqslant \cdots \geqslant j_m \geqslant 2} V_{\overline{\mathbf{k}+\mathbf{e}_{j_1}+\cdots+\mathbf{e}_{j_m}}})) \subset \pi_{\alpha,\beta}(U_q\mathfrak{p}^-)(\oplus_{m\geqslant 0} \times (\oplus_{n\geqslant j_1 \geqslant \cdots \geqslant j_m \geqslant 2} V_{\overline{\mathbf{k}+\mathbf{e}_{j_1}+\cdots+\mathbf{e}_{j_m}}})) \subset V^1_{\leqslant k}$. Obviously the subspace $V^1_{\leqslant k}$ is a $U_q\mathfrak{sl}_{2n}$-submodule in V. □

By the same arguments as in Propositions 5, 6, and 7, one has the following.

Proposition 8: Define vectors $\{\xi'_j\}^n_{j=1}$ *as follows:*

$$\xi'_j = \sum_{m=j}^{n} \varepsilon^*_m \otimes S_{j,m} L_-(j,m+1,n) u \in (\mathbb{C}^n)^* \otimes L(k_1-k_2,\ldots,k_{n-1}-k_n),$$

where $L_-(j,p,r)=\Pi^r_{a=p} q^{a-j-1} K_{j+1} \cdots K_a [H_{j+1}+\cdots+H_a+a-j-1]_q$. *Then* ξ'_j *is a* $U_q\mathfrak{sl}_n$*-highest vector with weight* $(k_1-k_2,\ldots,k_{j-1}-k_j+1,k_j-1-k_{j+1},\ldots,k_{n-1}-k_n)$ *for* $j=1,\ldots,n$. □

Proposition 9: Define vectors $\{\zeta'_j\}^n_{j=1}$ *as follows:*

$$\zeta'_j = \sum_{m=1}^{j} (-q^2)^{m-1} \varepsilon_m \otimes F_{m,j} K_-(j,1,m-1) u^* \in \mathbb{C}^n \otimes L^*(k_1-k_2,\ldots,k_{n-1}-k_n),$$

where $K_-(j,p,r)=\Pi^r_{a=p} q^{j-a-1} K_a \cdots K_{j-1} [H_a+\cdots+H_{j-1}+j-a-1]_q$. *Then* ζ'_j *is a* $U_q\mathfrak{sl}_n$*-highest vector with weight* $(k_{n-1}-k_n,\ldots,k_{n-j+1}-k_{n-j}-1,k_{n-j}+1-k_{n-j-1},\ldots,k_1-k_2)$ *for* $j=1,\ldots,n$. □

The proof of the next statement, reduced as for Proposition 7 to the computation of d_j, is given in the Appendix.

Proposition 10: For every $j=1,\ldots,n$, $\overline{\mathbf{k}} \in \hat{K}$

$$\mathcal{M}^-_{\overline{\mathbf{k}}}(\xi'_j \otimes \zeta'_{n-j+1}) = d_j(\alpha,k_j) v^h_{\overline{\mathbf{k}-\mathbf{e}_j}},$$

where $d_j(\alpha,k_j)=q^{\alpha+n/2}[\alpha+k_j+n-j]_q \varpi_j(\overline{\mathbf{k}},q)$ *and* $\varpi_j(\overline{\mathbf{k}},q) \neq 0$ *for all* $\overline{\mathbf{k}} \in \hat{K}$. □

By (6) and Proposition 10, we see that the equations $d_j(\alpha,k_j)=0$ and $\alpha+k_j+n-j=0$ are equivalent.

Corollary 2: For all $j=1,\dots,n$, $\overline{\mathbf{k}}\in\hat{K}$ *the subspace* $V^j_{\geqslant k}\overset{\text{def}}{=}\oplus_{\{\overline{\mathbf{k}'}\in\hat{K}|k'_j\geqslant k\}}V_{\overline{\mathbf{k}'}}$ *is a* $U_q\mathfrak{sl}_{2n}$*-submodule in* V *iff* $\alpha+k_j+n-j=0$. □

V. REDUCIBILITY OF $\pi_{\alpha,\beta}$

Proposition 11: The representation $\pi_{\alpha,\beta}$ *is irreducible if and only if* α,β *satisfy the following equivalent conditions (since* $\alpha-\beta\in\mathbb{Z}$*, these conditions are equivalent):*

$$1.\ \alpha\notin\mathbb{Z};\ 2.\ \beta\notin\mathbb{Z}.$$

Proof: Suppose $\alpha\notin\mathbb{Z}$, $\beta\notin\mathbb{Z}$. Consider the system of equations

$$\begin{cases}\beta-k_1=0,\\ \beta-k_2+1=0,\\ \dots\\ \beta-k_n+n-1=0,\\ \alpha+k_1+n-1=0,\\ \dots\\ \alpha+k_n=0.\end{cases}$$

This system has no integral solution. Therefore $c_j(\beta,k_j)$ and $d_j(\alpha,k_j)$ do not vanish. Let W be a $U_q\mathfrak{sl}_{2n}$-submodule of V. Then $W=\oplus_{\overline{\mathbf{k}}\in I}V_{\overline{\mathbf{k}}}$ for some $I\subset\hat{K}$. Then, for all $\overline{\mathbf{k}}\in I$ and $j=1,\dots,n$, it follows that $\overline{\mathbf{k}}+\mathbf{e_j}$, $\overline{\mathbf{k}}-\mathbf{e_j}\in I$ (if the respective indexes belong to $\hat{K}$). Therefore if $I\neq\emptyset$, then $I=\hat{K}$, and the module V has no proper submodules, i.e., it is simple. Conversely, by Corollaries 1 and 2, if $\pi_{\alpha,\beta}$ is irreducible, then $\alpha\notin\mathbb{Z}$, $\beta\notin\mathbb{Z}$. □

Corollary 3: Let $\alpha,\beta\in\mathbb{Z}$*, and let* W *be the representation space of a subrepresentation of* $\pi_{\alpha,\beta}$*. Then* W *is a finite intersection of some of the* $U_q\mathfrak{sl}_{2n}$*-modules* $V^j_{\geqslant k}$, $V^j_{\leqslant k}$ *defined in Corollaries 1,2.*

The proof follows directly from the previous proof. □

Now suppose that $\alpha,\beta\in\mathbb{Z}$. We will investigate reducibility and proper subrepresentations of $\pi_{\alpha,\beta}$. We use figures as in Refs. 1 and 8 for a description.

Each $U_q\mathfrak{k}$-isotypic component $V_{\overline{\mathbf{k}}}$ is assigned to the point $(k_1,\dots,k_n)\in\mathbb{R}^n$. Thus $\hat{K}$ is assigned to the set $\mathbf{K}^+=\{(k_1,\dots,k_n)\,|\,k_1\geqslant\dots\geqslant k_n\}\subset\mathbb{R}^n$. Consider $2n$ hyperplanes:

$$\mathcal{L}^+_j:k_j=\beta+j-1;\ \ \mathcal{L}^-_j:k_j=-\alpha-n+j.$$

These hyperplanes are parallel to the coordinate axis and pass through points with integral coordinates. The distance between $\mathcal{L}^+_j$ and $\mathcal{L}^-_j$ is equal to $\alpha+\beta+n-1$.

By Corollaries 1 and 2,

$$\overline{\mathbf{k}}\in\mathcal{L}^+_j\ \text{iff}\quad U_q\mathfrak{sl}_{2n}\cdot V_{\overline{\mathbf{k}}}\supset V_{\overline{\mathbf{k}+\mathbf{e_j}}};\quad \overline{\mathbf{k}}\in\mathcal{L}^-_j\quad\text{iff } U_q\mathfrak{sl}_{2n}\cdot V_{\overline{\mathbf{k}}}\supset V_{\overline{\mathbf{k}-\mathbf{e_j}}}.$$

Investigate the example $n=2$. In this case $\mathcal{L}^\pm_j$, $j=1,2$ are just lines on the plane $\mathbb{R}^2$, parallel to the coordinate axis. Let us consider different values of $\alpha+\beta$.

Case 1: $\alpha+\beta\geqslant 0$. In this case the line $\mathcal{L}^+_1$ lies to the right of $\mathcal{L}^-_1$, $\mathcal{L}^+_2$ lies higher than $\mathcal{L}^-_2$. The lines $\mathcal{L}^\pm_1$, $\mathcal{L}^\pm_2$ are shown in Fig. 1. The intersection point of $\mathcal{L}^+_1$ and $\mathcal{L}^-_2$ has the coordinates $(\beta,-\alpha)$ and belongs to $\mathbf{K}^+$. Arrows attached to $\mathcal{L}^\pm_j$ show the direction of isotypic components "movement" under $\pi_{\alpha,\beta}$. There exists a unique simple submodule $V^s=\oplus_{\{\overline{\mathbf{k}}\in\hat{K}|k_1\leqslant\beta,k_2\geqslant-\alpha\}}V_{\overline{\mathbf{k}}}$ in V.

Case 2: $\alpha+\beta=-1$. In this case the lines $\mathcal{L}^+_1$ and $\mathcal{L}^-_1$, $\mathcal{L}^+_2$ and $\mathcal{L}^-_2$ coincide. The intersection point of the lines $\mathcal{L}^+_1$ and $\mathcal{L}^+_2$ does not belong to $\mathbf{K}^+$ (Fig. 2). There are two simple submodules in V: $V^s_1=\oplus_{\{\overline{\mathbf{k}}\in\hat{K}|k_1=-1-\alpha\}}V_{\overline{\mathbf{k}}}$ and $V^s_2=\oplus_{\{\overline{\mathbf{k}}\in\hat{K}|k_2=-\alpha\}}V_{\overline{\mathbf{k}}}$.

Case 3: $\alpha+\beta=-2$. In this case the line $\mathcal{L}^+_1$ lies to the left of $\mathcal{L}^-_1$, $\mathcal{L}^+_2$ lies lower than $\mathcal{L}^-_2$.

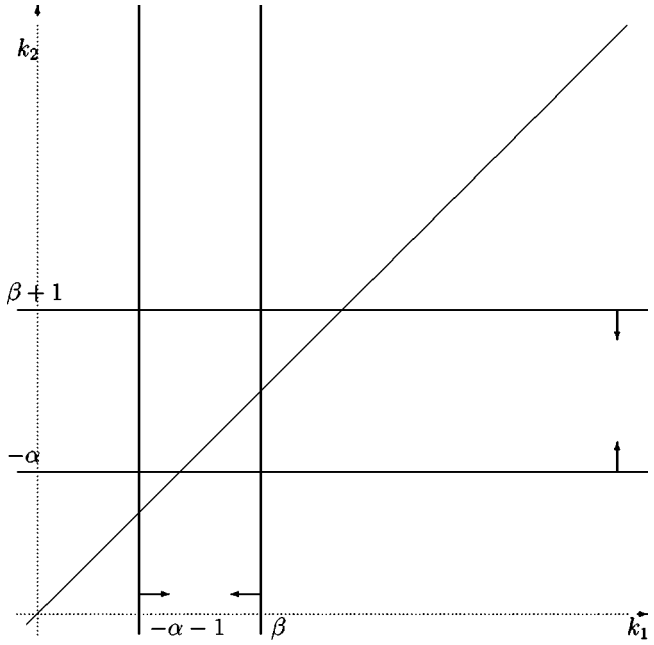

FIG. 1. Structure of $\pi_{\alpha,\beta}$ with $\alpha+\beta\geqslant 0$.

However, the lines $\mathcal{L}_1^-$ and $\mathcal{L}_2^+$ intersect in the point with coordinates $(-\alpha-1,\beta+1)$ (see Fig. 3). Besides, the distance between $\mathcal{L}_j^+$ and $\mathcal{L}_j^-$ is equal to 1. This shows that V is a direct sum of three submodules:

$$V_1^s=\bigoplus_{\{\bar{\mathbf{k}}\in\hat{K}|k_1\leqslant\beta\}} V_{\bar{\mathbf{k}}},\quad V_2^s=\bigoplus_{\{\bar{\mathbf{k}}\in\hat{K}|k_2\geqslant-\alpha\}} V_{\bar{\mathbf{k}}},\quad V_3^s=\bigoplus_{\{\bar{\mathbf{k}}\in\hat{K}|k_1\geqslant-\alpha-1,k_2\leqslant\beta+1\}} V_{\bar{\mathbf{k}}}.$$

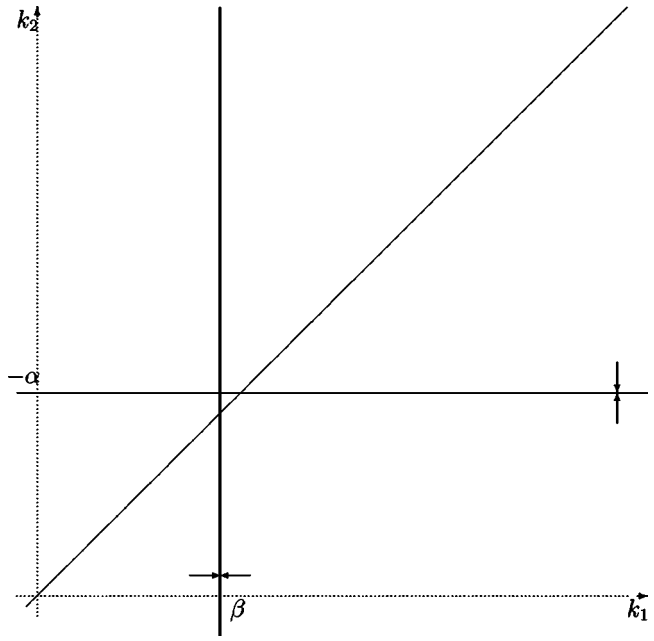

FIG. 2. Structure of $\pi_{\alpha,\beta}$ with $\alpha+\beta=-1$.

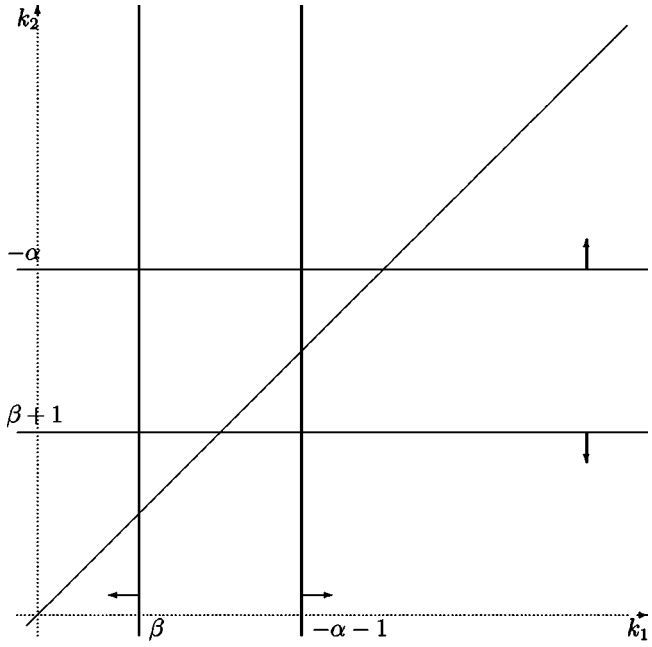

FIG. 3. Structure of $\pi_{\alpha,\beta}$ with $\alpha+\beta=-2$.

Case 4: $\alpha+\beta\leqslant -3$. In this case the intersection point of $\mathcal{L}_1^+$ and $\mathcal{L}_1^+$ belongs to $\mathbf{K}^+$ (see Fig. 4). Also, there are simple submodules V_1^s, V_2^s, V_3^s in V, but V does not decompose into their direct sum.

Turn now to the general case. Consider all possible values of $\alpha+\beta+n-1$.

Case 1: $\alpha+\beta+n-1\geqslant 1$. In this case the hyperplanes $\mathcal{L}_j^{\pm}$, $j=1,\ldots,n$ bound in $\mathbf{K}^+$ the subset that corresponds to a unique simple *finite dimensional* submodule

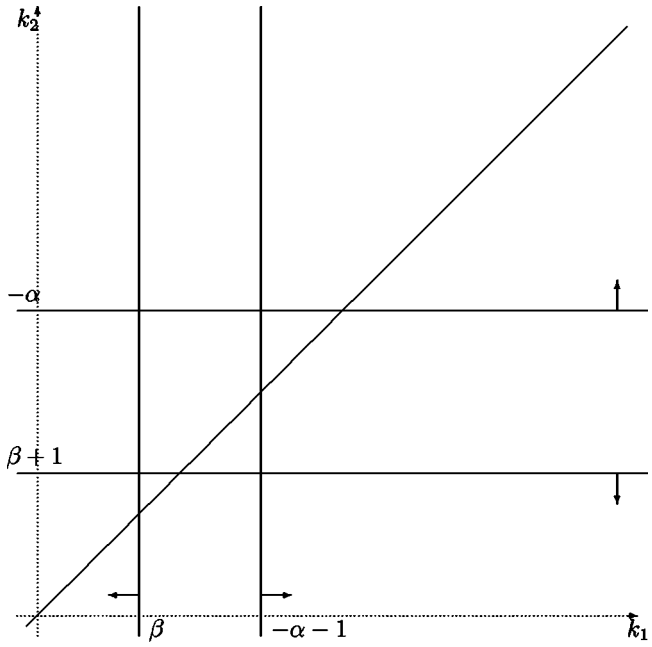

FIG. 4. Structure of $\pi_{\alpha,\beta}$ with $\alpha+\beta\leqslant -3$.

$$V^s = \bigoplus_{\{\overline{\mathbf{k}} \in \hat{K} \mid -\alpha-n+j \leqslant k_j \leqslant \beta+j-1 \text{ for all } j=1,\ldots,n\}} V_{\overline{\mathbf{k}}}^-.$$

Case 2: $\alpha+\beta+n-1=0$. In this case the hyperplanes $\mathcal{L}_j^+$ and $\mathcal{L}_j^-$ coincide. There are n simple submodules in V:

$$V_j^s = \bigoplus_{\{\overline{\mathbf{k}} \in \hat{K} \mid k_j = \beta+j-1\}} V_{\overline{\mathbf{k}}}^-, \quad j = 1, \ldots, n. \tag{16}$$

Case 3: $\alpha+\beta=-n$. Here the distance between $\mathcal{L}_j^+$ and $\mathcal{L}_j^-$ is equal to 1. This allows one to decompose the set $\hat{K}$ into a direct sum of $n+1$ subsets $\hat{K}_i$, $i=1,\ldots,n+1$, those correspond to the simple submodules: $V_i^s = \oplus_{\{\overline{\mathbf{k}} \in \overline{K}_i\}} V_{\overline{\mathbf{k}}}^- \subset V$. The subsets $\hat{K}_i$ are defined as follows:

$$\hat{K}_i = \{\overline{\mathbf{k}} \in \hat{K} \mid k_{i-1} \geqslant -\alpha - n + i - 1, \beta + i - 1 \geqslant k_i\}$$

(for $i=1$ and $i=n+1$ we put, respectively, $\hat{K}_1 = \{\overline{\mathbf{k}} \in \hat{K} \mid k_1 \leqslant \beta\}$ and $\hat{K}_{n+1} = \{\overline{\mathbf{k}} \in \hat{K} \mid k_n \geqslant -\alpha\}$).

Case 4: $\alpha+\beta+n-1 \leqslant -2$. Also, there are simple submodules corresponded to the subsets $\hat{K}_i$. However, V is not equal to their direct sum.

Thus we have proved the following:

Corollary 4: For $\alpha, \beta \in \mathbb{Z}$ *the only one from the representations* $\pi_{\alpha,\beta}$ *and* $\pi_{-n-\beta,-n-\alpha}$ *has an irreducible finite dimensional subrepresentation*. □

VI. INTERTWINING OPERATORS

In this section we construct the intertwining operators between the representations $\pi_{\alpha,\beta}$ and $\pi_{-n-\beta,-n-\alpha}$ for nonintegral α, β. This allows one to prove Proposition 2.

Let $A: V \to V$ be an intertwining operator, i.e., for all $\xi \in U_q\mathfrak{sl}_{2n}$, $v \in V$, we have $A\pi_{\alpha,\beta}(\xi)(v) = \pi_{-n-\beta,-n-\alpha}(\xi)(Av)$. The operators $\pi_{\alpha,\beta}(U_q\mathfrak{k}_{ss})$ are independent of α, β and $\pi_{\alpha,\beta}(K_n) = \pi_{-n-\beta,-n-\alpha}(K_n)$. Also, $V_{\overline{\mathbf{k}}}^-$ and $V_{\overline{\mathbf{m}}}^-$ are nonisomorphic $U_q\mathfrak{k}$-modules for $\overline{\mathbf{k}} \neq \overline{\mathbf{m}}$. Then $A(\alpha,\beta)|_{V_{\overline{\mathbf{k}}}^-} = a_{\overline{\mathbf{k}}}^-(\alpha,\beta)$, $a_{\overline{\mathbf{k}}}^-(\alpha,\beta) \in \mathbb{C}$. Let us find necessary conditions for A to be an intertwining operator in terms of $a_{\overline{\mathbf{k}}}^-(\alpha,\beta)$. By Propositions 5, 6, 8, and 9, it follows that for all $\overline{\mathbf{k}} \in \hat{K}$ there exist ϑ_j, $\eta_j \in U_q\mathfrak{sl}_{2n}$, $j=1,\ldots,n$, such that $\pi_{\alpha,\beta}(\eta_j)(v_{\overline{\mathbf{k}}}^h) = c_j(\beta,k_j)v_{\overline{\mathbf{k}+\mathbf{e_j}}}^h$ and $\pi_{\alpha,\beta}(\vartheta_j)(v_{\overline{\mathbf{k}}}^h) = d_j(\alpha,k_j)v_{\overline{\mathbf{k}-\mathbf{e_j}}}^h$. (Recall that $v_{\overline{\mathbf{k}}}^h$ is the $U_q\mathfrak{k}$-highest vector in $V_{\overline{\mathbf{k}}}^-$.) Therefore the necessary conditions look as follows: for all $j=1,\ldots,n, \overline{\mathbf{k}} \in \hat{K}$,

$$A\pi_{\alpha,\beta}(\eta_j)(v_{\overline{\mathbf{k}}}^h) = \pi_{-n-\beta,-n-\alpha}(\eta_j)(Av_{\overline{\mathbf{k}}}^h) \quad \text{and} \quad A\pi_{\alpha,\beta}(\vartheta_j)(v_{\overline{\mathbf{k}}}^h) = \pi_{-n-\beta,-n-\alpha}(\vartheta_j)(Av_{\overline{\mathbf{k}}}^h).$$

Equivalently, in terms of $a_{\overline{\mathbf{k}}}^-$,

$$a_{\overline{\mathbf{k}+\mathbf{e_j}}}^-(\alpha,\beta)c_j(\beta,k_j)v_{\overline{\mathbf{k}+\mathbf{e}_j}}^h = a_{\overline{\mathbf{k}}}^-(\alpha,\beta)c_j(-n-\alpha,k_j)v_{\overline{\mathbf{k}+\mathbf{e_j}}}^h,$$

$$a_{\overline{\mathbf{k}-\mathbf{e_j}}}^-(\alpha,\beta)d_j(\alpha,k_j)v_{\overline{\mathbf{k}-\mathbf{e_j}}}^h = a_{\overline{\mathbf{k}}}^-(\alpha,\beta)d_j(-n-\beta,k_j)v_{\overline{\mathbf{k}-\mathbf{e_j}}}^h.$$

Thus the coefficients $a_{\overline{\mathbf{k}}}^-$ of the intertwining operator A must satisfy the following conditions: for all $j=1,\ldots,n, \overline{\mathbf{k}} \in \hat{K}$,

$$\frac{a_{\overline{\mathbf{k}+\mathbf{e_j}}}^-(\alpha,\beta)}{a_{\overline{\mathbf{k}}}^-(\alpha,\beta)} = \frac{c_j(-n-\alpha,k_j)}{c_j(\beta,k_j)}, \quad \frac{a_{\overline{\mathbf{k}-\mathbf{e_j}}}^-(\alpha,\beta)}{a_{\overline{\mathbf{k}}}^-(\alpha,\beta)} = \frac{d_j(-n-\beta,k_j)}{d_j(\alpha,k_j)}.$$

We get from Propositions 7 and 10 that for all $j=1,\ldots,n, \overline{\mathbf{k}} \in \hat{K}$,

$$\frac{a^{-}_{\mathbf{k}+\mathbf{e_j}}(\alpha,\beta)}{a^{-}_{\mathbf{k}}(\alpha,\beta)} = q^{n+\alpha+\beta}\frac{[-n-\alpha-k_j+j-1]_q}{[\beta-k_j+j-1]_q}, \quad \frac{a^{-}_{\mathbf{k}-\mathbf{e_j}}(\alpha,\beta)}{a^{-}_{\mathbf{k}}(\alpha,\beta)} = q^{-n-\beta-\alpha}\frac{[-\beta+k_j-j]_q}{[\alpha+k_j+n-j]_q}.$$

As we see, the coefficients $a^{-}_{\mathbf{k}}(\alpha,\beta)$ are defined up to a scalar multiplier. By additional assumption $a^{-}_{\mathbf{0}}(\alpha,\beta)=1$, we get the explicit formulas for the coefficients $a^{-}_{\mathbf{k}}(\alpha,\beta)=A(\alpha,\beta)|_{V^{-}_{\mathbf{k}}}$ of the intertwining operator A,

$$a^{-}_{\mathbf{k}}(\alpha,\beta) = \prod_{j=1}^{n} P_j(\alpha,\beta), \tag{17}$$

where

$$P_j(\alpha,\beta) = \begin{cases} \prod\limits_{i=0}^{k_j-1} \dfrac{1-q^{2(\alpha+n+i-j+1)}}{1-q^{2(-\beta+i-j+1)}}, & \text{for } k_j > 0, \\ 1, \quad \text{for } k_j = 0, \\ \prod\limits_{i=1+k_j}^{0} \dfrac{1-q^{2(-\beta+i-j)}}{1-q^{2(\alpha+n+i-j)}}, & \text{for } k_j < 0. \end{cases}$$

For fixed $\alpha-\beta\in\mathbb{Z}$, the operator A is a meromorphic operator-function with simple poles in integral points.

VII. UNITARIZABLE REPRESENTATIONS OF THE DEGENERATE PRINCIPAL SERIES

In this section we find necessary and sufficient conditions for modules of the degenerate principal series and their simple submodules to be unitarizable.

Equip $U_q\mathfrak{sl}_{2n}$ with the involution $*$ as follows:

$$E_n^* = -K_nF_n, \quad F_n^* = -E_nK_n^{-1}, \quad K_n^* = K_n,$$

$$E_j^* = K_jF_j, \quad F_j^* = E_jK_j^{-1}, \quad K_j^* = K_j, \quad j=1,\dots,2n-1, \quad j\neq n.$$

The $*$-Hopf algebra $U_q\mathfrak{su}_{n,n} \overset{\text{def}}{=} (U_q\mathfrak{sl}_{2n},*)$ is a q-analog of $U\mathfrak{su}_{n,n}$, and its subalgebra $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n) \overset{\text{def}}{=} (U_q\mathfrak{k},*)$ is a q-analog of $U\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n)$.

Let us introduce two auxiliary $*$-algebras $\mathrm{Pol}(S(\mathbb{U}))_q$ and $\mathrm{Pol}(\widehat{S(\mathbb{U})})_q$ (a quantum analog of the Shilov boundary $S(\mathbb{U})$ of the matrix ball is introduced in Ref. 20). Equip the algebra $\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$ with the involution $*$ defined by the formula

$$(z_a^b)^* = (-q)^{a+b-2n}(\det_q \mathbf{z})^{-1}\det_q \mathbf{z}_a^b,$$

where $\det_q \mathbf{z}_a^b$ is the q-determinant of the matrix derived from $\mathbf{z}$ by deleting the line b and the column a. Put $\mathrm{Pol}(S(\mathbb{U}))_q=(\mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}},*)$ and equip it with the natural structure of a $*$-module algebra over $U_q\mathfrak{su}_{n,n}$. The involutions in $\mathrm{Pol}(S(\mathbb{U}))_q$ and $U_q\mathfrak{su}_{n,n}$ are compatible, i.e., for all $f\in\mathrm{Pol}(S(\mathbb{U}))_q$, $\xi\in U_q\mathfrak{su}_{n,n}$ we have

$$(\xi f)^* = (S(\xi))^* f^*,$$

where S is the antipode in the Hopf algebra $U_q\mathfrak{sl}_{2n}$.

The $*$-algebra $\mathrm{Pol}(\widehat{S(\mathbb{U})})_q$ is generated by z_a^b, $a,b=1,\dots,n$, $(\det_q \mathbf{z})^{-1}$, t and t^{-1}. The relations between z_a^b and $(\det_q \mathbf{z})^{-1}$ are inherited from the $*$-algebra $\mathrm{Pol}(S(\mathbb{U}))_q$, the other relations are provided by the following:

$$t^{-1}t = tt^{-1} = 1, \quad tt^* = t^*t, \quad tz_a^b = q^{-1}z_a^b t, \quad t^* z_a^b = qz_a^b t^*, \quad a,b = 1, \ldots, n.$$

Consider an embedding of $U_q\mathfrak{su}_{n,n}$-module algebras $\mathrm{Pol}(\widehat{S(\mathbb{U})})_q \hookrightarrow \mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$ which maps t to t and z_a^b to $t^{-1}t^{\wedge n}_{\{1,\ldots,n\}J_a\ b}$ [see (3)]. Using this embedding, we can extend the $U_q\mathfrak{su}_{n,n}$-module structure from $\mathrm{Pol}(S(\mathbb{U}))_q$ onto $\mathrm{Pol}(\widehat{S(\mathbb{U})})_q$.

In Ref. 20, the invariant integral over the Shilov boundary of the quantum matrix ball $f \mapsto \int_{S(\mathbb{U})_q} f d\mu$ is defined and the following statement is actually proved.

Proposition 12: The linear subspace $(t^{-n})^* \cdot \mathrm{Pol}(S(\mathbb{U}))_q \cdot t^{-n} \subset \mathrm{Pol}(\widehat{S(\mathbb{U})})_q$ *is a* $U_q\mathfrak{su}_{n,n}$*-module. The linear functional*

$$(t^{-n})^* \cdot f \cdot t^{-n} \mapsto \int_{S(\mathbb{U})_q} f d\mu$$

is a $U_q\mathfrak{su}_{n,n}$*-invariant integral.*

The precise meaning of two next propositions will be given if we continue $\mathrm{Pol}(\widehat{S(\mathbb{U})})_q$ via adding to the list of generators t^λ, $(t^*)^\lambda$, $(\det_q \mathbf{z})^\lambda$ for all $\lambda \in \mathbb{C}$. The relations between the "new" generators and the action of E_j, F_j, $K_j^{\pm 1}$, $j = 1, \ldots, 2n-1$ can be derived from the corresponding formulas for t^m, $(\det_q \mathbf{z})^m$ and $(t^*)^m$, where $m \in \mathbb{Z}$. From the previous proposition it follows

Proposition 13 (cf. Ref. 13, lemma 3.2): Let $\mathrm{Re}\,\lambda = -n$*. Then the linear subspace*

$$((\det_q \mathbf{z})^{\lambda/2} t^\lambda)^* \cdot \mathrm{Pol}(S(\mathbb{U}))_q \cdot (\det_q \mathbf{z})^{\lambda/2} t^\lambda \subset \mathrm{Pol}(\widehat{S(\mathbb{U})})_q$$

is a $U_q\mathfrak{su}_{n,n}$*-module. The linear functional*

$$((\det_q \mathbf{z})^{\lambda/2} t^\lambda)^* \cdot f \cdot (\det_q \mathbf{z})^{\lambda/2} t^\lambda \mapsto \int_{S(\mathbb{U})_q} f d\mu$$

is a $U_q\mathfrak{su}_{n,n}$*-invariant integral.*

For each α, $\beta \in \mathbb{Z}$ define an embedding $i_{\alpha,\beta}$: $V = \mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}} \hookrightarrow \mathrm{Pol}(\widehat{S(\mathbb{U})})_q$ by the formula $i_{\alpha,\beta}(f) = f \cdot (\det_q \mathbf{z})^\alpha \cdot t^{\alpha+\beta}$ for all $f \in \mathbb{C}[\mathrm{Mat}_n]_{q,\det_q \mathbf{z}}$. Using these embeddings and the commutative relations between t, t^{-1} and $\det_q \mathbf{z}$, we get the following.

Corollary 5: Let $\mathrm{Re}(\alpha+\beta) = -n$*. Then the sesquilinear form* $V \times V \to \mathbb{C}$ *defined by*

$$\langle f_1, f_2 \rangle = \int_{S(\mathbb{U})_q} f_2^* f_1 d\mu$$

satisfies the condition $(\pi_{\alpha,\beta}(\xi)u, v) = (u, \pi_{\alpha,\beta}(\xi^*)v)$ *for all* $u, v \in V$, $\xi \in U_q\mathfrak{sl}_{2n}$.

Recall the definition of unitarizable module. Let A be a $*$-Hopf algebra, W an A-module. Then an A-module W is *unitarizable* if there exists a Hermitian form (i.e., sesquilinear Hermitian-symmetric positive definite form) $(\cdot,\cdot)$, which is A-invariant, i.e.,

$$(au, v) = (u, a^* v) \quad \text{for any } u, v \in W, a \in A.$$

Therefore the representation $\pi_{\alpha,\beta}$ is unitary if $\mathrm{Re}(\alpha+\beta) = -n$. Such representations form *the principal unitary series.*

Now we are going to find all unitarizable simple modules of the degenerate principal series and their unitarizable submodules.

Weight subspaces are pairwise orthogonal with respect to every $U_q\mathfrak{su}_{n,n}$-invariant scalar product. Therefore the isotypic components $V_{\overline{\mathbf{k}}}$ are pairwise orthogonal too. From Proposition 4 and the Burnside theorem (see Ref. 21, Sec. 27), it follows that in every component $V_{\overline{\mathbf{k}}}$ there exists a unique up to a constant $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_n)$-invariant scalar product. Fix such scalar products via the integral over the Shilov boundary of the quantum matrix ball[20]

$$\langle u,v\rangle_{\mathbf{k}}^{-}=\int_{S(\mathbb{U})_q} v^{*}u d\mu \quad u,v\in V_{\mathbf{k}}^{-}.$$

Hence each invariant scalar product $(\cdot,\cdot)$: $V\times V\to\mathbb{C}$ is assigned to a set $\{c_{\mathbf{k}}^{-}\}_{\mathbf{k}\in K^{+}}^{-}\subset\mathbb{R}_{+}$ such that $(u,v)=c_{\mathbf{k}}^{-}\langle u,v\rangle_{\mathbf{k}}^{-}$ for all $u,v\in V_{\mathbf{k}}^{-}$. Conversely, each $\{c_{\mathbf{k}}^{-}\}_{\mathbf{k}\in K^{+}}^{-}\subset\mathbb{R}_{+}$ defines a unique sesquilinear Hermitian-symmetric positive definite $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n)$-invariant form in V.

Let us find explicit conditions for the coefficients $\{c_{\mathbf{k}}^{-}\}$ to define a $U_q\mathfrak{su}_{n,n}$-invariant form.

Using the decomposition $U_q\mathfrak{sl}_{2n}\simeq U_q\mathfrak{p}^{-}\otimes U_q\mathfrak{k}\otimes U_q\mathfrak{p}^{+}$ from Sec. IV and the definitions of $U_q\mathfrak{p}^{+}$ and $U_q\mathfrak{p}^{-}$, we see that it is sufficient to investigate the invariance of $(\cdot,\cdot)$ under the subspaces $\mathfrak{p}_q^{+}$ and $\mathfrak{p}_q^{-}$. Moreover, it is enough to prove $\mathfrak{p}_q^{+}$-invariance of $(\cdot,\cdot)$. We can see that if $(\cdot,\cdot)$ is $\mathfrak{p}_q^{+}$-invariant, then it is $\mathfrak{p}_q^{-}$-invariant. Indeed, for all $\eta\in\mathfrak{p}_q^{-}$, u, $v\in V$ we have $(\eta u,v)=\overline{(v,\eta u)}=\overline{(\eta^{*}v,u)}=(u,\eta^{*}v)$.

Investigate the $\mathfrak{p}_q^{+}$-invariance of the form $(\cdot,\cdot)$. From the results of Sec. IV it follows that $\pi_{\alpha,\beta}(\mathfrak{p}_q^{+})(V_{\mathbf{k}}^{-})\subset\oplus_{j=1}^{n}V_{\mathbf{k}+\mathbf{e}_j}^{-}$. Since the isotypic components $V_{\mathbf{k}}^{-}$ are pairwise orthogonal, one needs to check the invariance in "nonzero cases" only (that means for $u\in V_{\mathbf{k}}^{-}$, $v\in V_{\mathbf{k}+\mathbf{e}_j}^{-}$, $j=1,\dots,n$). In this case the invariant conditions are the following: for all $\xi\in U_q\mathfrak{sl}_{2n}$, $u\in V_{\mathbf{k}}^{-}$, $v\in V_{\mathbf{k}+\mathbf{e}_j}^{-}$, $j=1,\dots,n$,

$$(P_{\mathbf{k}+\mathbf{e}_j}^{-}(\pi_{\alpha,\beta}(\xi)u),v)\big|_{V_{\mathbf{k}+\mathbf{e}_j}^{-}}=(u,P_{\mathbf{k}}^{-}(\pi_{\alpha,\beta}(\xi^{*})v))\big|_{V_{\mathbf{k}}^{-}},$$

where $P_{\mathbf{k}}^{-}:V\to V_{\mathbf{k}}^{-}$ is an orthogonal projection onto $V_{\mathbf{k}}^{-}$. In other words,

$$c_{\mathbf{k}+\mathbf{e}_j}\langle P_{\mathbf{k}+\mathbf{e}_j}^{-}(\pi_{\alpha,\beta}(\xi)u),v\rangle_{\mathbf{k}+\mathbf{e}_j}^{-}=c_{\mathbf{k}}^{-}\langle u,P_{\mathbf{k}}^{-}(\pi_{\alpha,\beta}(\xi^{*})v)\rangle_{\mathbf{k}}^{-}.$$

First consider the case $\alpha,\ \beta\notin\mathbb{Z}$. Recall that from Propositions 5, 6, 8, and 9 it follows that in $(\mathfrak{p}_q^{-}\oplus\mathfrak{p}_q^{+})\otimes V_{\mathbf{k}}^{-}$ there exist $U_q\mathfrak{k}_{ss}$-highest vectors $\psi_{j,l}^{\pm}$, $j,\ l=1,\dots,n$ with weights $(k_1-k_2,\dots,k_{j-1}-(k_j\pm1),(k_j\pm1)-k_{j+1},\dots,k_{n-1}-k_n,2k_n+\alpha-\beta,k_{n-1}-k_n,\dots,(k_{n-l+1}\mp1)-k_{n-l+2},k_{n-1}-(k_{n-l+1}\mp1),\dots,k_1-k_2)$, respectively. Define $U_q\mathfrak{k}$-invariant maps

$$T_{\mathbf{k},j}^{\pm}:(\mathfrak{p}_q^{-}\oplus\mathfrak{p}_q^{+})\otimes V_{\mathbf{k}}^{-}\to V_{\mathbf{k}\pm\mathbf{e}_j}^{-}$$

by their values on the $U_q\mathfrak{k}_{ss}$-highest vectors as follows:

$$T_{\mathbf{k},j}^{+}(\psi_{j,l}^{+})=\begin{cases}\omega_j(\overline{\mathbf{k}},q)\cdot v_{\mathbf{k}+\mathbf{e}_j}^{h} & l=n-j+1;\\ 0 & l\neq n-j+1;\end{cases}$$

$$T_{\mathbf{k},j}^{-}(\psi_{j,l}^{-})=\begin{cases}\varpi_j(\overline{\mathbf{k}},q)\cdot v_{\mathbf{k}-\mathbf{e}_j}^{h} & l=n-j+1;\\ 0 & l\neq n-j+1.\end{cases}$$

Here $v_{\mathbf{k}}^{h}$, $\varpi_j(\overline{\mathbf{k}},q)$ and $\omega_j(\overline{\mathbf{k}},q)$ are introduced in Propositions 4, 7, and 10.

Lemma 4: For all $\xi\in\mathfrak{p}_q^{-}\oplus\mathfrak{p}_q^{+}$, $u\in V_{\mathbf{k}}^{-}$, $j=1,\dots,n$ the following holds:

$$P_{\mathbf{k}+\mathbf{e}_j}^{-}(\pi_{\alpha,\beta}(\xi)u)=q^{-\beta-n/2}[\beta-k_j+j-1]_qT_{\mathbf{k},j}^{+}(\xi\otimes u);$$

$$P_{\mathbf{k}-\mathbf{e}_j}^{-}(\pi_{\alpha,\beta}(\xi)u)=q^{\alpha+n/2}[\alpha+k_j+n-j]_qT_{\mathbf{k},j}^{-}(\xi\otimes u).$$

Proof: The proof completely repeats the proof of Lemma 9.10 of Ref. 8. □

Using the last lemma, we can rewrite the $U_q\mathfrak{su}_{n,n}$-invariance condition of the scalar product as follows: for all $\xi\in\mathfrak{p}_q^{-}\oplus\mathfrak{p}_q^{+}$, $u\in V_{\mathbf{k}}^{-}$, $v\in V_{\mathbf{k}+\mathbf{e}_j}^{-}$, $j=1,\dots,n$

$$q^{-\beta-n/2}[\beta-k_j+j-1]_qc_{\mathbf{k}+\mathbf{e}_j}^{-}\langle T_{\mathbf{k},j}^{+}(\xi\otimes u),v\rangle_{\mathbf{k}+\mathbf{e}_j}^{-}=\overline{q^{\alpha+n/2}[\alpha+(k_j+1)+n-j]_q}c_{\mathbf{k}}^{-}\langle u,T_{\mathbf{k}+\mathbf{e}_j,j}^{-}(\xi^{*}\otimes v)\rangle_{\mathbf{k}}^{-}.$$

Proposition 14: $\langle T^{+}_{\mathbf{k},j}(\xi\otimes u),v\rangle^{-}_{\mathbf{k}+\mathbf{e_j}}=-\langle u,T^{-}_{\mathbf{k}+\mathbf{e_j},j}(\xi^{*}\otimes v)\rangle^{-}_{\mathbf{k}}$ *for all* $j=1,\dots,n$.

Proof: Since the maps $T^{\pm}_{\mathbf{k},j}$ do not depend on $\alpha,\ \beta\in\mathcal{D}$, it is enough to consider only the special case $\mathrm{Re}(\alpha+\beta)=-n$. In this case the representation $\pi_{\alpha,\beta}$ is unitary, thus we can put $c^{-}_{\mathbf{k}}=1$ for all $\overline{\mathbf{k}}\in\hat{K}$. Since $\overline{q^{\alpha+n}}=q^{-\beta}$, we see that

$$q^{-\beta-n/2}\frac{q^{\beta-k_j+j-1}-q^{-\beta+k_j-j+1}}{q-q^{-1}}(\langle T^{+}_{\mathbf{k},j}(\xi\otimes u),v\rangle^{-}_{\mathbf{k}+\mathbf{e_j}}+\langle u,T^{-}_{\mathbf{k}+\mathbf{e_j},j}(\xi^{*}\otimes v)\rangle^{-}_{\mathbf{k}})=0.$$

If we consider nonintegral $\alpha,\ \beta$, then $q^{\beta-k_j+j-1}-q^{-\beta+k_j+1-j}$ does not vanish. This completes the proof. □

Recall that $\alpha,\ \beta\notin\mathbb{Z}$. Thus the $U_q\mathfrak{su}_{n,n}$-invariance condition of the scalar product can be rewritten as follows: for all $\overline{\mathbf{k}}\in\hat{K},\ j=1,\dots,n$

$$(1-q^{2(-\beta+k_j+1-j)})(\overline{1-q^{2(\alpha+(k_j+1)+n-j)}})^{-1}=+\frac{c^{-}_{\mathbf{k}}}{c^{-}_{\mathbf{k}+\mathbf{e_j}}}. \tag{18}$$

Since the scalar product must be positive definite, we have the following necessary conditions for the unitarizability of modules of the degenerate principal series (recall that $q=e^{-h/2}$): for all $\overline{\mathbf{k}}\in\hat{K},\ j=1,\dots,n$

$$\mathrm{sh}\,\frac{h}{2}(\beta-k_j+j-1)\overline{\left(\mathrm{sh}\,\frac{h}{2}(\alpha+(k_j+1)+n-j)\right)}^{-1}>0.$$

Using these inequalities, we can present the following series of simple unitary *representations of the degenerate principal series* related to the Shilov boundary.

The principal unitary series: $\mathrm{Re}(\alpha+\beta)=-n,\ \alpha,\ \beta\notin\mathbb{Z}$. In this case all representations are unitary. The invariant scalar product is provided by the $U_q\mathfrak{su}_{n,n}$-invariant integral.[20]

The complementary series: $\mathrm{Im}(\alpha+\beta)=0,\ |\mathrm{Re}\,\alpha+n|<1,\ |\mathrm{Re}\,\beta|<1,\ (\mathrm{Re}\,\alpha+n)\mathrm{Re}\,\beta<0,$ $\alpha,\beta\notin\mathbb{Z}$. In this case the representations $\pi_{\alpha,\beta}$ are unitary too. (The required invariant scalar product $(\cdot,\cdot)$ is defined by the coefficients $\{c^{-}_{\mathbf{k}}\}$ as follows: let $c^{-}_{\mathbf{0}}=1$, other coefficients are computed from recurrent relations such as (18).)

The strange series: $\mathrm{Im}\,\alpha=\pi/h$. For such values of the parameters the respective representations $\pi_{\alpha,\beta}$ are irreducible and unitary. This series of representations has no classical analog. For the first time it appears in unpublished works of Korogodsky and in Klimyk and Groza's paper (see Ref. 6).

Now let $\alpha,\beta\in\mathbb{Z}$. (Recall that in this case $\pi_{\alpha,\beta}$ is reducible.) For such α,β there might exist unitarizable simple submodules in the respective module (we will mention them below), although the module is not unitarizable. For each simple submodule the same arguments as in the "general case" on the $U_q\mathfrak{su}_{n,n}$-invariance of scalar product can be applied. In each case we have the necessary conditions like (18), however they must be satisfied only on a certain part of $\hat{K}$. Consider all possible cases:

Case 1: $\alpha+\beta\geqslant 2-n$. In this case the representation is not unitary and its unique irreducible subrepresentation is not unitary too.

Case 2: $\alpha+\beta=1-n$. In this case there exist n irreducible unitary subrepresentations of the representation $\pi_{\alpha,1-n-\alpha}$. Precisely, V^{s}_{j} (see (16)) is a simple submodule in V for any $j=1,\dots,n$. Notice that each V^{s}_{j} can be equipped with a $U_q\mathfrak{su}_{n,n}$-invariant scalar product $(\cdot,\cdot)$. Such modules are called small representations because they have "poor" decompositions into isotypic components.

Case 3: $\alpha+\beta=-n$. In this case the representations are completely reducible, their irreducible subrepresentations V^{s}_{i}, $i=1,\dots,n+1$ (see Sec. V) are unitary (actually, the required invariant scalar product is the same as for the principal unitary series).

Case 4: $\alpha+\beta\leqslant -1-n$. In this case the submodules V^{s}_{i}, $i=1,\dots,n+1$ are unitary although there exist nonunitarizable quotient modules in V.

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APPENDIX

Let us prove Lemma 2. This proof is a q-analog of the proof of Lemma 3.4 from Ref. 8.

Proof of Lemma 2: Statements (9)–(12) can be easily checked.

For example, check the equality $K_jF_{m,j}=qF_{m,j}K_j$. For $j-m=1$, i.e., $m=j-1$, we see that $K_jF_{j-1,j}=K_jF_{j-1}K_{j-1}=F_{j-1}K_{j-1}K_j=qF_{j-1,j}K_j$. Assume that for $j-m<r$ Eqs. (9)–(12) are proved. Let $j-m=r$. Then,

$$\begin{aligned}
K_jF_{m,j} &= K_j(F_{m+1,j}F_mK_m + \sum_{s=m+2}^{j}(-1)^{s+m+1}F_{s,j}\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1))\\
&= K_jF_{m+1,j}F_mK_m + \sum_{s=m+2}^{j}(-1)^{s+m+1}K_jF_{s,j}\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1)\\
&= qF_{m+1,j}K_jF_mK_m + q\sum_{s=m+2}^{j-1}(-1)^{s+m+1}F_{s,j}K_j\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1)\\
&\quad + q(-1)^{j+m+1}\,\mathrm{ad}_{F_{j-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K_j = qF_{m,j}K_j.
\end{aligned}$$

The proof is completed by induction.

Using (12), prove equality (14). Recall that $[x]_q=(q^x-q^{-x})/(q-q^{-1})$,

$$\begin{aligned}
E_mF_{m,j} &= \sum_{s=m+2}^{j}(-1)^{s+m+1}E_mF_{s,j}\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + E_mF_{m+1,j}F_mK_m\\
&\equiv \sum_{s=m+2}^{j}(-1)^{s+m+1}F_{s,j}E_m\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + qF_{m+1,j}E_mF_mK_m\\
&\equiv q\sum_{s=m+2}^{j}(-1)^{s+m}F_{s,j}\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+2}}(F_{m+1}K_{m+1})K_m^2K(j,m+1,s-1) + qF_{m+1,j}[H_m]_qK_m\\
&= \left(\sum_{s=m+2}^{j}(-1)^{s+m+2}F_{s,j}\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+2}}(F_{m+1}K_{m+1})K(j,m+2,s-1)\right)\\
&\quad \times K_m^2\cdot q^{j-m-1}\,K_{m+1}\cdots K_{j-1}[H_{m+1}+\cdots+H_{j-1}+j-m-1]_q) + qF_{m+1,j}[H_m]_qK_m\\
&= qF_{m+1,j}(q^{j-m-1}K_m^2K_{m+1}\cdots K_{j-1}[H_{m+1}+\cdots+H_{j-1}+j-m-1]_q + [H_m]_qK_m)\\
&= F_{m+1,j}q^{j-m}K_m\cdots K_{j-1}[H_m+\cdots+H_{j-1}+j-m-1]_q \ (\mathrm{mod}\ U_q\mathfrak{sl}_n\cdot E_m).
\end{aligned}$$

Prove equality (13) by induction. If $j-m=2$ and $m<i<j$, then $i=j-1$, and (13) means that $E_{j-1}F_{j-2,j}\equiv 0\ (\mathrm{mod}\ U_q\mathfrak{sl}_n\cdot E_{j-1})$. It can be proved as follows:

$$\begin{aligned}
E_{j-1}F_{j-2,j} &= E_{j-1}(F_{j-1,j}F_{j-2}K_{j-2}K(j,j-1,j-2) - \mathrm{ad}_{F_{j-1}}(F_{j-2}K_{j-2})K(j,j-1,j-1))\\
&\equiv [H_{j-1}]_qK_{j-1}F_{j-2}K_{j-2} - qF_{j-2}K_{j-2}K_{j-1}[H_{j-1}+1]_q = 0\ (\mathrm{mod}\ U_q\mathfrak{sl}_n\cdot E_{j-1}).
\end{aligned}$$

For the inductive step it is sufficient to check that for all $m<i<j$,

$$
\begin{aligned}
E_iF_{m,j} &= \sum_{s=m+2}^{j} (1-)^{s+m+1} E_iF_{s,j}\,\mathrm{ad}F_{s-1}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + E_iF_{m+1,j}F_mK_m \\
&\equiv \sum_{s=m+2}^{i-1} (-1)^{s+m+1} E_iF_{s,j}\,\mathrm{ad}_{F_{s-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + E_iF_{m+1,j}F_mK_m \\
&\quad + \sum_{s=i+1}^{j} (-1)^{s+m+1} E_iF_{s,j}\,\mathrm{ad}_{F_{s-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) \\
&\quad + (-1)^{i+m+1} E_iF_{i,j}\,\mathrm{ad}_{F_{i-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,i-1) \pmod{U_q\mathfrak{sl}_n\cdot E_i}
\end{aligned}
$$

(we use (12) and (14)). By the inductive hypothesis, for $s<i$ we have $E_iF_{s,j}\equiv 0 \pmod{U_q\mathfrak{sl}_n\cdot E_i}$, therefore for all $m<s<i$ there exists an element $X_s\in U_q\mathfrak{sl}_n$ such that $E_iF_{s,j}=X_sE_i$. From (12), $E_iF_{s,j}=F_{s,j}E_i$. From (14), $E_iF_{i,j}=qF_{i+1,j}q^{j-i-1}K_i\cdots K_{j-1}[H_i+\cdots+H_{j-1}+j-i-1]_q$. Thus,

$$
\begin{aligned}
E_iF_{m,j} &\equiv \sum_{s=m+2}^{i-1} (-1)^{s+m+1} X_sE_i\,\mathrm{ad}_{F_{s-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + X_{m+1}E_iF_mK_m \\
&\quad + \sum_{s=i+1}^{j} (-1)^{s+m+1} F_{s,j}E_i\,\mathrm{ad}_{F_{s-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,s-1) + (-1)^{i+m+1} \\
&\quad \times F_{i+1,j}q^{j-i}K_i\cdots K_{j-1}[H_i+\cdots+H_{j-1}+j-i-1]_q\,F_{i-1}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)\cdot K(j,m+1,i-1) \\
&\equiv (-1)^{i+m+1} qF_{i+1,j}\,\mathrm{ad}_{F_{i-1}}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,i) + (-1)^{i+m} \\
&\quad \times F_{i+1,j}E_i\,\mathrm{ad}_{F_i}\cdots \mathrm{ad}_{F_{m+1}}(F_mK_m)K(j,m+1,i) = 0 \pmod{U_q\mathfrak{sl}_n\cdot E_i}.
\end{aligned}
$$

□

The proof of Lemma 3 is similar.

Let us prove Proposition 7. We just have to compute the coefficients $c_j(\beta,k_j)$. Recall that there is a $U_q\mathfrak{sl}_n\otimes U_q\mathfrak{sl}_n$-isomorphism $j_1:\mathfrak{p}_q^+\simeq\mathbb{C}^n\otimes(\mathbb{C}^n)^*$, where $\mathbb{C}^n$ is the vector representation of $U_q\mathfrak{sl}_n$. The isomorphism j_1^{-1} on the elements of the standard basis for $\mathbb{C}^n\otimes(\mathbb{C}^n)^*$ is defined as follows:

$$
\begin{aligned}
&j_1^{-1}\begin{pmatrix} \varepsilon_1\otimes\varepsilon_1^* & \cdots & \varepsilon_1\otimes\varepsilon_n^* \\ \cdots & \cdots & \cdots \\ \varepsilon_{n-1}\otimes\varepsilon_1^* & \cdots & \cdots \\ \varepsilon_n\otimes\varepsilon_1^* & \cdots & \varepsilon_n\otimes\varepsilon_n^* \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{ad}_{E_1}\cdots\mathrm{ad}_{E_{n-1}}E_n & \cdots & \cdots & (-1)^{n-1}\mathrm{ad}_{E_{2n-1}}\cdots\mathrm{ad}_{E_{n+1}}\mathrm{ad}_{E_1}\cdots\mathrm{ad}_{E_{n-1}}E_n \\ \cdots & \cdots & \cdots & \cdots \\ \mathrm{ad}_{E_{n-1}}E_n & \cdots & \cdots & \cdots \\ E_n & -\mathrm{ad}_{E_{n+1}}E_n & \cdots & (-1)^{n-1}\mathrm{ad}_{E_{2n-1}}\cdots\mathrm{ad}_{E_{n+1}}E_n \end{pmatrix}.
\end{aligned}
$$

(This follows from the equalities $\mathrm{ad}_{F_j}E_n=0$, $\mathrm{ad}^2_{E_j}E_n=0$ for $j=1,\ldots,2n-1, j\neq n$, $\mathrm{ad}_{K_j}E_n=E_n$ for $j=1,\ldots,n-2,n+2,\ldots,2n-1$, $\mathrm{ad}_{K_j}E_n=q^{-1}E_n$ for $j=n-1$ or $j=n+1$.) Consider the following embeddings of vector spaces:

$$\iota_1: U_q\mathfrak{sl}_n \hookrightarrow U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n, \quad \xi \mapsto \xi \otimes 1;$$

$$\iota_2: U_q\mathfrak{sl}_n \hookrightarrow U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n, \quad \xi \mapsto 1 \otimes \xi.$$

Set $\xi^{(1)} = \iota_1(\xi)$ and $\xi^{(2)} = \iota_2(\xi)$.

From Propositions 5 and 6, we deduce that for all $j = 1, \ldots, n, \overline{\mathbf{k}} \in \hat{K}$

$$\begin{aligned}\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_{n-j+1}) &= \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j} (-q^2)^{m-1}\varepsilon_m \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \\ &\quad \otimes \sum_{m=n-j+1}^{n} \varepsilon^*_m \otimes S^{(2)}_{n-j+1,m}L^{(2)}_-(n-j+1,m+1,n)u^*\Bigg) \\ &= \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j}\sum_{l=n-j+1}^{n} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_l \otimes F_{m,j}K_-(j,1,m-1)u \\ &\quad \otimes S_{n-j+1,l}L_-(n-j+1,l+1,n)u^*\Bigg).\end{aligned}$$

Proposition 15: For all $j = 1, \ldots, n, \overline{\mathbf{k}} \in \hat{K}$

$$\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_{n-j+1}) = \lambda^-(n-j+1,n-j+2,n)\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*),$$

where

$$L^{(2)}_-(n-j+1,n-j+2,n)(v^h_{\overline{\mathbf{k}}}) = \lambda^-(n-j+1,n-j+2,n)v^h_{\overline{\mathbf{k}}}.$$

Proof: In the same way as in Ref. 8, we have

$$\begin{aligned}\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \xi_{n-j+1}) &= \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j}\sum_{l=n-j+1}^{n} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_l \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \\ &\quad \otimes S^{(2)}_{n-j+1,l}L^{(2)}_-(n-j+1,l+1,n)u^*\Bigg) \\ &= \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_{n-j+1} \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \\ &\quad \otimes L^{(2)}_-(n-j+1,n-j+2+1,n)u^*\Bigg) + \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j}\sum_{l=n-j+2}^{n} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_l \\ &\quad \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \otimes S^{(2)}_{n-j+1,l}L^{(2)}_-(n-j+1,l+1,n)u^*\Bigg) \\ &= \lambda^-(n-j+1,n-j+2,n)\mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_{n-j+1} \\ &\quad \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \otimes u^*\Bigg) + \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j}\sum_{l=n-j+2}^{n} (-q^2)^{m-1}\varepsilon_m \otimes \varepsilon^*_l \\ &\quad \otimes F^{(1)}_{m,j}K^{(1)}_-(j,1,m-1)u \otimes S^{(2)}_{n-j+1,l}L^{(2)}_-(n-j+1,l+1,n)u^*\Bigg)\end{aligned}$$

$$= \lambda^-(n-j+1,n-j+2,n)\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*)$$
$$+ \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{l=n-j+2}^{n} \sum_{m=1}^{j} (-q^2)^{m-1} \varepsilon_m \otimes (\mathrm{ad}_{E_{n-l-2}} \cdots \mathrm{ad}_{E_j})^{(2)} \varepsilon^*_{n-j+1}$$
$$\otimes F^{(1)}_{m,j} K^{(1)}_-(j,1,m-1)u \otimes S^{(2)}_{n-j+1,l} L^{(2)}_-(n-j+1,l+1,n)u^* \Bigg)$$
$$= \lambda^-(n-j+1,n-j+2,n)\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*)$$
$$+ \sum_{l=n-j+1}^{n} (\mathrm{ad}_{E_{n-l-2}} \cdots \mathrm{ad}_{E_j})^{(2)} S^{(2)}_{n-j+1,l} L^{(2)}_-(n-j+1,l+1,n)\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1}$$
$$\otimes u^*).$$

The vector $\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*) \in V_{\overline{\mathbf{k}+\mathbf{e}_j}}$ and is a $U_q\mathfrak{sl}_n \otimes 1$-highest vector. Therefore $\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*) \in V_{\overline{\mathbf{k}+\mathbf{e}_j}}$, $\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*) = c \cdot v^h_{\overline{\mathbf{k}+\mathbf{e}_j}}$ with some $c \in \mathbb{C}$. Now we conclude that in the obtained expression all summands except the first equal 0. □

To find $c_j(\beta,k_j)$ we must compute

$$\mathcal{M}^+_{\overline{\mathbf{k}}}(\zeta_j \otimes \varepsilon^*_{n-j+1} \otimes u^*) = \mathcal{M}^+_{\overline{\mathbf{k}}}\Bigg(\sum_{m=1}^{j} (-q^2)^{m-1} \varepsilon_m \otimes \varepsilon^*_{n-j+1} \otimes F^{(1)}_{m,j} K^{(1)}_-(j,1,m-1)u \otimes u^* \Bigg)$$
$$= \sum_{m=1}^{j} (-q^2)^{m-1} \pi_{\alpha,\beta}((-1)^{j-1} \mathrm{ad}_{E_{n+j-1}} \cdots \mathrm{ad}_{E_{n+1}} \mathrm{ad}_{E_m} \cdots \mathrm{ad}_{E_{n-1}} E_n) F^{(1)}_{m,j} K^{(1)}_-$$
$$\times (j,1,m-1)(v^h_k). \tag{A1}$$

We need some auxiliary lemmas. Recall that in this paper we introduce the notation for q-minors of the matrix $\mathbf{z}$ [see (4)]. Set $\mathbf{z}^{\wedge k}_{a_1,\ldots,a_k} = \mathbf{z}^{\wedge k\{1,\ldots,k\}}_{\{a_1,\ldots,a_k\}}$.

Lemma 5: For all $1 \leqslant m \leqslant k \leqslant j-2$,

$$(-q)^{j-k-1} \mathbf{z}^{\wedge j-1} \mathbf{z}^{\wedge k}_{1,\ldots,m-1,m+1,\ldots,j} - \sum_{s=k+1}^{j-2} (-q)^{s-k-1} \mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j} \mathbf{z}^{\wedge k}_{1,\ldots,m-1,m+1,\ldots,s} = \mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j} \mathbf{z}^{\wedge k}.$$

□

Lemma 6: For all $1 \leqslant m \leqslant j \leqslant n$ *we have* $F_{m,j} = q^{j-m-1} G_{m,j}$, *where*

$$G_{m,j} = F_m K_m F_{m+1,j} + \sum_{s=m+2}^{j} (-q)^{s-m-1} \mathrm{ad}_{F_{s-1}} \cdots \mathrm{ad}_{F_{m+1}} (F_m K_m) F_{s,j} K_-(j,m+1,s-1).$$

□

Lemma 7: For all $1 \leqslant m \leqslant j \leqslant n$

$$G_{m,j}(v^h_{\overline{\mathbf{k}}}) = (q^{1/2})^{j-m} \kappa_-(j,m,j-1) \mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j} \frac{v^h_{\overline{\mathbf{k}}}}{\mathbf{z}^{\wedge j-1}},$$

where

$$K_-(j,m+1,j-1)(v^h_{\overline{\mathbf{k}}}) = \kappa_-(j,m,j-1) v^h_{\overline{\mathbf{k}}}.$$

Proof: We prove this lemma by induction. For $j-m=1$ the statement is obvious, since

$$G_{m,m+1}(v_{\mathbf{k}}^{\underline{h}}) = F_m K_m((\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdots(\mathbf{z}^{\wedge n})^{k_n})$$
$$= q^{k_m-k_{m+1}}q^{1/2}[k_m-k_{m+1}]_q(\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdots(\mathbf{z}^{\wedge m-1})^{k_{m-1}-k_m}\mathbf{z}^{\wedge m}_{1,\ldots,m-1,m+1}$$
$$\times(\mathbf{z}^{\wedge m})^{k_m-k_{m+1}-1}\cdot(\mathbf{z}^{\wedge m+1})^{k_{m+1}-k_{m+2}}\cdots(\mathbf{z}^{\wedge n})^{k_n}$$
$$= q^{1/2}\kappa_-(m+1,m,m)\mathbf{z}^{\wedge m}_{1,\ldots,m-1,m+1}v_{\mathbf{k}-\mathbf{e}_m}^{\underline{h}}.$$

For the proof of the inductive step we use two previous lemmas. By Lemma 6, we have

$$G_{m,j}(v_{\mathbf{k}}^{\underline{h}}) = \sum_{s=m+2}^{j}(-q)^{s-m-1}\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)\cdot(F_{s,j}K_-(j,m+1,s-1))(v_{\mathbf{k}}^{\underline{h}}) + F_mK_mF_{m+1,j}(v_{\mathbf{k}}^{\underline{h}})$$
$$= F_mK_mF_{m+1,j}(v_{\mathbf{k}}^{\underline{h}}) + \sum_{s=m+2}^{j}(-q)^{s-m-1}\kappa_-(j,m+1,s-1)\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)F_{s,j}(v_{\mathbf{k}}^{\underline{h}}).$$

By the inductive hypothesis, for all $j-s<j-m$

$$G_{m,j}(v_{\mathbf{k}}^{\underline{h}}) = q^{1/2(j-m-1)}\kappa_-(j,m+1,j-1)F_mK_m\left(\mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j}\frac{v_{\mathbf{k}}^{\underline{h}}}{\mathbf{z}^{\wedge j-1}}\right)$$
$$+\sum_{s=m+2}^{j}(-q)^{s-m-1}\cdot q^{1/2(j-s)}\kappa_-(j,m+1,s-1)\kappa_-(j,s,j-1)\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)$$
$$\times\left(\mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j}\frac{v_{\mathbf{k}}^{\underline{h}}}{\mathbf{z}^{\wedge j-1}}\right)$$
$$= q^{1/2(j-m-1)}\kappa_-(j,m+1,j-1)\cdot(F_mK_m)\left(\mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j}\frac{v_{\mathbf{k}}^{\underline{h}}}{\mathbf{z}^{\wedge j-1}}\right)$$
$$+\sum_{s=m+2}^{j}(-q^{1/2})^{s-m-1}\,\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)\left(\mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j}\frac{v_{\mathbf{k}}^{\underline{h}}}{\mathbf{z}^{\wedge j-1}}\right).$$

Using the explicit formulas for the $U_q\mathfrak{sl}_{2n}$-action in $\mathbb{C}[\mathrm{Mat}_n]_q$ and properties of the comultiplication (see Sec. II), we obtain that

$$\mathrm{ad}_{F_{s-1}}\cdots\mathrm{ad}_{F_{m+1}}(F_mK_m)\left(\mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j}\frac{v_{\mathbf{k}}^{\underline{h}}}{\mathbf{z}^{\wedge j-1}}\right)$$
$$= (q^{1/2})^{s-m}(q^{k_m-k_{m+1}}[k_m-k_{m+1}]_q(\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge m-1})^{k_{m-1}-k_m}\mathbf{z}^{\wedge m}_{1,\ldots,m-1,m+1,\ldots,s}$$
$$\cdot(\mathbf{z}^{\wedge m})^{k_m-k_{m+1}-1}\cdots(\mathbf{z}^{\wedge s-1})^{k_{s-1}-k_s}\mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j}(\mathbf{z}^{\wedge s})^{k_s-k_{s+1}}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge n})^{k_n}$$
$$+(-q)q^{k_m-k_{m+1}+k_{m+1}-k_{m+2}}[k_{m+1}-k_{m+2}]_q(\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge m})^{k_m-k_{m+1}}$$
$$\cdot\mathbf{z}^{\wedge m+1}_{1,\ldots,m-1,m+1,\ldots,s}(\mathbf{z}^{\wedge m+1})^{k_{m+1}-k_{m+2}-1}\cdots(\mathbf{z}^{\wedge s-1})^{k_{s-1}-k_s}\mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j}\cdot(\mathbf{z}^{\wedge s})^{k_s-k_{s+1}}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge n})^{k_n}$$
$$+\ \cdots\ +(-q)^{s-2}q^{k_m-k_{m+1}+\cdots+k_{s-2}-k_{s-1}}[k_{s-2}-k_{s-1}]_q\cdot(\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge s-2})^{k_{s-2}-k_{s-1}}$$
$$\times\mathbf{z}^{\wedge s-1}_{1,\ldots,m-1,m+1,\ldots,s}\cdot(\mathbf{z}^{\wedge s-1})^{k_{s-1}-k_s-1}\mathbf{z}^{\wedge j-1}_{1,\ldots,s-1,s+1,\ldots,j}$$
$$\cdot(\mathbf{z}^{\wedge s})^{k_s-k_{s+1}}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge n})^{k_n}+(-q)^{s-1}q^{k_m-k_{m+1}+\cdots+k_{s-1}-k_s}[k_{s-1}-k_s]_q(\mathbf{z}^{\wedge 1})^{k_1-k_2}\cdot\ \cdots$$
$$\cdot(\mathbf{z}^{\wedge s-2})^{k_{s-2}-k_{s-1}}(\mathbf{z}^{\wedge s-1})^{k_{s-1}-k_s}\mathbf{z}^{\wedge j-1}_{1,\ldots,m-1,m+1,\ldots,j}(\mathbf{z}^{\wedge s})^{k_s-k_{s+1}}\cdot\ \cdots\ \cdot(\mathbf{z}^{\wedge n})^{k_n}).$$

Finally, by Lemma 5, we see that

$$G_{m,j}(v_{\mathbf{k}}^{h}) = (q^{1/2})^{j-m}\kappa_-(j,m+1,j-1)\cdot \mathbf{z}_{1,\ldots,m-1,m+1,\ldots,j}^{\wedge j-1}\frac{v_{\mathbf{k}}^{h}}{\mathbf{z}^{\wedge j-1}}\cdot\frac{q^{2(j-2+k_1-k_j)}-1}{q-q^{-1}}.$$

□

By the last lemma and (A1), we can compute the coefficients $c_j(\beta,k_j)$ introduced in Proposition 7.

Proposition 16: For all $1\leqslant j\leqslant n$,

$$\mathcal{M}^{+}_{\mathbf{k}}(\zeta_j\otimes\varepsilon^{*}_{n-j+1}\otimes u^{*}) = q^{-\beta-n/2+k_j+j}[\beta-k_j+j-1]_q\kappa_-(j,1,j-1)v_{\mathbf{k}+\mathbf{e_j}}^{h}.$$

Proof: We have

$$\begin{aligned}
&\mathcal{M}^{+}_{\mathbf{k}}(\zeta_j\otimes\varepsilon^{*}_{n-j+1}\otimes u^{*})\\
&=\sum_{m=1}^{j}(-q^2)^{m-1}\pi_{\alpha,\beta}((-1)^{j-1}\,\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_m}\cdots\mathrm{ad}_{E_{n-1}}E_n)\cdot F^{(1)}_{m,j}K^{(1)}_{-}(j,1,m-1)v_{\mathbf{k}}^{h}\\
&=\sum_{m=1}^{j}(-q^2)^{m-1}\kappa_-(j,1,m-1)\cdot\pi_{\alpha,\beta}((-1)^{j-1}\,\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_m}\cdots\mathrm{ad}_{E_{n-1}}E_n)F^{(1)}_{m,j}v_{\mathbf{k}}^{h}.
\end{aligned}$$

By Lemma 7,

$$\begin{aligned}
\mathcal{M}^{+}_{\mathbf{k}}(\zeta_j\otimes\varepsilon^{*}_{n-j+1}\otimes u^{*}) &= \sum_{m=1}^{j-1}(-q^2)^{m-1}q^{j-m-1}(q^{1/2})^{j-m}\kappa_-(j,m,j-1)\kappa_-(j,1,m-1)\cdot(-1)^{j-1}\\
&\quad\times\pi_{\alpha,\beta}(\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_m}\cdots\mathrm{ad}_{E_{n-1}}E_n)\left(\mathbf{z}_{1,\ldots,m-1,m+1,\ldots,j}^{\wedge j-1}\frac{v_{\mathbf{k}}^{h}}{\mathbf{z}^{\wedge j-1}}\right)\\
&\quad+(-q^2)^{j-1}\kappa_-(j,1,j-1)\pi_{\alpha,\beta}((-1)^{j-1}\,\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_j}\cdots\mathrm{ad}_{E_{n-1}}E_n)\\
&\quad\times(v_{\mathbf{k}}^{h})\\
&= q^{3/2j-3}\kappa_-(j,1,j-1)\sum_{m=1}^{j-1}(-1)^{j+m}q^{m/2}\\
&\quad\cdot\pi_{\alpha,\beta}(\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_m}\cdots\mathrm{ad}_{E_{n-1}}E_n)\\
&\quad\times\left(\mathbf{z}_{1,\ldots,m-1,m+1,\ldots,j}^{\wedge j-1}\frac{v_{\mathbf{k}}^{h}}{\mathbf{z}^{\wedge j-1}}\right)+q^{2j-2}\kappa_-(j,1,j-1)\\
&\quad\times\pi_{\alpha,\beta}(\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\,\mathrm{ad}_{E_j}\cdots\mathrm{ad}_{E_{n-1}}E_n)(v_{\mathbf{k}}^{h}).
\end{aligned}$$

In Sec. II the following morphism of $U_q\mathfrak{sl}_{2n}$-modules was defined:

$$\iota:\mathbb{C}[\mathrm{Mat}_n]_q\to\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t},\quad \iota(z_{\{a_1,\ldots,a_k\}}^{\wedge k\{b_1,\ldots,b_k\}}) = t^{-1}t_{\{1,\ldots,n\}J}^{\wedge n},$$

with

$$J=\{n+1,\ldots,2n\}\setminus\{2n+1-b_1,\ldots,2n+1-b_k\}\cup\{a_1,\ldots,a_k\}.$$

Therefore $\iota(\mathbf{z}^{\wedge k})=t^{-1}t_{\{1,\ldots,n\}\{1,\ldots,k,n+1,\ldots,2n-k\}}^{\wedge n}$. It follows that

$$\iota(v_{\mathbf{k}}^{h}) = q^{c}t^{-k_1}(t_{\{1,\ldots,n\}\{1,n+1,\ldots,2n-1\}}^{\wedge n})^{k_1-k_2}\cdots(t_{\{1,\ldots,n\}\{1,\ldots n\}}^{\wedge n})^{k_n},$$

where some $c\in\mathbb{C}$. Using the definition of $\pi_{\alpha,\beta}$, we obtain that for all $\xi\in U_q\mathfrak{sl}_{2n}, f\in\mathbb{C}[\mathrm{Pl}_{n,2n}]_{q,t}$

$$\pi_{\alpha,\beta}(\xi)(f) = q^{c}t^{-\beta}\xi\cdot(t^{\beta}f(t^{\wedge n}_{\{1,\ldots,n\}\{1,\ldots,n\}})^{\alpha})(t^{\wedge n}_{\{1,\ldots,n\}\{1,\ldots,n\}})^{-\alpha}.$$

For $m<j$,

$$\begin{aligned}&(\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\mathrm{ad}_{E_m}\cdots\mathrm{ad}_{E_{n-1}}E_n)(t^{\wedge n\{1,\ldots,n\}}_{\{1,\ldots,m-1,m+1,\ldots,j,n+1,\ldots,2n-j,2n-m+1\}})\\ &\quad=(-1)^{m-j}(q^{-1/2})^{j+n-m}q^{m-j-1}t^{\wedge n}_{\{1,\ldots,n\}\{1,\ldots,j,n+1,\ldots,2n-j\}},\end{aligned}$$

and for $m=j$ $(\mathrm{ad}_{E_{n+j-1}}\cdots\mathrm{ad}_{E_{n+1}}\mathrm{ad}_{E_j}\cdots\mathrm{ad}_{E_{n-1}}E_n)(t^{\wedge n}_{\{1,\ldots,n\}\{1,\ldots,j-1,n+1,\ldots,2n-j+1\}})$ $=(q^{-1/2})^{n}t^{\wedge n}_{\{1,\ldots,n\}\{1,\ldots,j,n+1,\ldots,2n-j\}}$. For other summands we use an analog of Lemma 5. Finally, we have

$$\begin{aligned}\mathcal{M}^{+}_{-\mathbf{k}}(\zeta_j\otimes\varepsilon^{*}_{n-j+1}\otimes u^{*}) &= \kappa_{-}(j,1,j-1)q^{-n/2}\cdot\left(q^{2}\sum_{m=1}^{j-1}q^{2m-2}+\frac{1-q^{-2\beta+2k_1}}{1-q^{-2}}\right.\\ &\quad\left.+\sum_{m=1}^{j-1}q^{-2\beta+2k_m}\frac{1-q^{-2k_m+2k_{m+1}}}{1-q^{-2}}\right)\cdot v^{h}_{\mathbf{k}+\mathrm{e}_j}\\ &= q^{-\beta-n/2+k_j+j}\kappa_{-}(j,1,j-1)[\beta-k_j+j-1]_q v^{h}_{\mathbf{k}+\mathrm{e}_j}.\end{aligned}$$

□

Repeat the same arguments to prove Proposition 10. First, we have the explicit formulas for the isomorphism $j_2:\mathfrak{p}^{-}_{q}\simeq(\mathbb{C}^n)^{*}\otimes\mathbb{C}^n$:

$$j_2^{-1}\begin{pmatrix}\varepsilon^{*}_1\otimes\varepsilon_1 & \cdots & \varepsilon^{*}_n\otimes\varepsilon_1\\ \cdots & \cdots & \cdots\\ \varepsilon^{*}_1\otimes\varepsilon_n & \cdots & \varepsilon^{*}_n\otimes\varepsilon_n\end{pmatrix}$$

$$=\begin{pmatrix}(-1)^{n-1}\mathrm{ad}_{F_1}\cdots\mathrm{ad}_{F_{n-1}}(K_nF_n) & \cdots & -\mathrm{ad}_{F_{n-1}}(K_nF_n) & K_nF_n\\ \cdots & \cdots & \cdots & \mathrm{ad}_{F_{n+1}}(K_nF_n)\\ \cdots & & & \\ (-1)^{n-1}\mathrm{ad}_{F_{2n-1}}\cdots\mathrm{ad}_{F_{n+1}}\mathrm{ad}_{F_1}\cdots\mathrm{ad}_{F_{n-1}}(K_nF_n) & \cdots & \cdots & \mathrm{ad}_{F_{2n-1}}\cdots\mathrm{ad}_{F_{n+1}}(K_nF_n)\end{pmatrix}.$$

For the proof of Proposition 10 we must compute the following:

$$\begin{aligned}\mathcal{M}^{-}_{-\mathbf{k}}(\xi'_j\otimes\zeta'_{n-j+1}) &= \mathcal{M}^{-}_{-\mathbf{k}}\left(\sum_{m=j}^{n}\varepsilon^{*}_m\otimes S^{(1)}_{j,m}L^{(1)}_{-}(j,m+1,n)u\right.\\ &\quad\left.\otimes\sum_{m=1}^{n-j+1}(-q^2)^{m-1}\varepsilon_m\otimes F^{(2)}_{m,n-j+1}K^{(2)}_{-}(n-j+1,1,m-1)u^{*}\right)\\ &= \mathcal{M}^{-}_{-\mathbf{k}}\left(\sum_{m=j}^{n}\sum_{l=1}^{n-j+1}(-q^2)^{l-1}\varepsilon^{*}_m\otimes\varepsilon_l\otimes S^{(1)}_{j,m}L^{(1)}_{-}(j,m+1,n)u\right.\\ &\quad\left.\otimes F^{(2)}_{l,n-j+1}K^{(2)}_{-}(n-j+1,1,l-1)u^{*}\right).\end{aligned}$$

Proposition 17: For all $1\leqslant j\leqslant n$

$$\mathcal{M}^{-}_{-\mathbf{k}}(\xi'_j\otimes\zeta'_{n-j+1}) = \lambda_{-}(j,j+1,n)\mathcal{M}^{-}_{-\mathbf{k}}(\varepsilon^{*}_j\otimes u\otimes\zeta'_{n-j+1}),$$

where

$$L_{-}^{(1)}(j,j+1,n)u = \lambda_{-}(j,j+1,n)u.$$

The proof is similar to the proof of Proposition 15.

Therefore in order to find the coefficients $d_j(\alpha,k_j)$ introduced in Proposition 10 we must only compute

$$\mathcal{M}^{-}_{\mathbf{k}}(\varepsilon_j^* \otimes u \otimes \zeta'_{n-j+1}) = \mathcal{M}^{-}_{\mathbf{k}}\left(\sum_{l=1}^{n-j+1}(-q^2)^{l-1}\varepsilon_j^* \otimes \varepsilon_l \otimes u \otimes F_{l,n-j+1}K_{-}(n-j+1,1,l-1)u^*\right)$$

$$= \sum_{l=1}^{n-j+1}(-q^2)^{l-1}\pi_{\alpha,\beta}(\mathrm{ad}_{F_j}\cdots\mathrm{ad}_{F_{n-1}}\mathrm{ad}_{F_{n-1+l}}\cdots\mathrm{ad}_{F_{n+1}}(K_nF_n))$$

$$\cdot F^{(2)}_{l,n-j+1}K^{(2)}_{-}(n-j+1,1,l-1)(v^{h}_{\mathbf{k}}).$$

These computations are analogous to the ones from the proof of Proposition 16.

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A combinatorial approach to the set-theoretic solutions of the Yang–Baxter equation

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A bijective map r: $X^2 \to X^2$, where $X=\{x_1,\ldots,x_n\}$ is a finite set, is called a *set-theoretic solution of the Yang–Baxter equation* (YBE) if the braid relation $r^{12}r^{23}r^{12}=r^{23}r^{12}r^{23}$ holds in X^3. A nondegenerate involutive solution (X,r) satisfying $r(xx)=xx$, for all $x \in X$, is called *square-free solution*. There exist close relations between the square-free set-theoretic solutions of YBE, the semigroups of I-type, the semigroups of skew polynomial type, and the Bieberbach groups, as it was first shown in a joint paper with Michel Van den Bergh. In this paper we continue the study of square-free solutions (X,r) and the associated Yang–Baxter algebraic structures—the semigroup $S(X,r)$, the group $G(X,r)$ and the k-algebra $A(k,X,r)$ over a field k, generated by X and with quadratic defining relations naturally arising and uniquely determined by r. We study the properties of the associated Yang–Baxter structures, and prove a conjecture of the present author that the three notions: a square-free solution of (set-theoretic) YBE, a semigroup of I type, and a semigroup of skew-polynomial-type, are equivalent. This implies that the Yang–Baxter algebra $A(k,X,r)$ is a Poincaré–Birkhoff–Witt-type algebra, with respect to some appropriate ordering of X. We conjecture that every square-free solution of YBE is retractable, in the sense of Etingof–Schedler–Solovyev. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1788848]

I. INTRODUCTION

The Yang–Baxter equation appeared in 1967[36] in Statistical Mechanics and turned out to be one of the basic equations in mathematical physics, and more precisely for introducing the theory of quantum groups. At present the study of quantum groups, and, in particular, the solutions of the Yang–Baxter equation attracts the attention of a broad circle of scientists and mathematicians.

Let V be a vector space over a field k. We recall that a linear automorphism R of $V \otimes V$ *is a solution of the Yang–Baxter equation*, if the equality

$$(R \otimes id_V)(id_V \otimes R)(R \otimes id_V) = (id_V \otimes R)(R \otimes id_V)(id_V \otimes R) \tag{1.1}$$

holds in the automorphism group of $V \otimes V \otimes V$. R is a solution of the *quantum Yang–Baxter equation* (QYBE) if

$$R^{12}R^{13}R^{23} = R^{23}R^{13}R^{12}, \tag{1.2}$$

where R^{ij} means R acting on the ith and jth component.

Finding all solutions of the Yang–Baxter equation is a difficult task far from being resolved. Nevertheless many solutions of these equations have been found during the last 20 years and the related algebraic structures (Hopf algebras) have been studied (for example, see Ref. 20). Most of these solutions were "deformations" of the identity solution. In 1990 Drinfeld[5] posed the problem

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of studying a class of solutions that are obtained in a different way—the so-called *set-theoretic solutions*.

Definition 1.1: Let X be a nonempty set. Let $r: X\times X\to X\times X$ be a bijection of the Cartesian product $X\times X$ onto itself. The map r is called *a set-theoretic solution of the Yang–Baxter equation*, if

$$(r\times id_X)(id_X\times r)(r\times id_X)=(id_X\times r)(r\times id_X)(id_X\times r).$$

Each set-theoretic solution r of the Yang–Baxter equation induces an operator R on $V\otimes V$ for the vector space V spanned by X, which is, clearly, a solution of (1.1). Various works dealing with set-theoretic solutions appeared during the last decade, cf. Refs. 35, 18, 15, 6, 7, 33, 23, 26, and 30.

The purpose of this paper is first to present some recent conjectures on the set-theoretic solutions of the Yang–Baxter equation, and to give an account of the research in this area, and, second to continue the study of the general algebraic and homological properties of the algebraic structures related to the so-called square-free solutions. Our approach is combinatorial. To each solution (X,r) we associate a semigroup $S=S(X,r)$, a group $G=G(X,r)$ (the group was also studied in Ref. 6), and a quadratic algebra over a field k, $A(k,X,r)\simeq kS$, each of them with a set of n generators X and with quadratic defining relations $\mathfrak{R}(X,r)$ naturally arising and uniquely determined by r. We study the "behavior" of these relations, and use the obtained information for establishing structural and homological properties of the associated algebraic objects. This approach is natural, for usual linear solutions one has similar ideas for instance in Manin's work.[25] In the case of set-theoretic solutions to YBE it was initiated in the joint paper with Michel Van den Bergh,[15] and applied to the study of the close relations between different mathematical objects such as set-theoretic solutions of the Yang–Baxter equation, semigroups of I-type (which appeared in the study of Sklyanin algebras) and the semigroups S_0 associated with the class of skew-polynomial rings with binomial relations, introduced and studied in Refs. 8 and 9. The semigroups S_0, called *semigroups of skew-polynomial type* are standard finitely presented, more precisely, they are defined in terms of a finite number of generators and quadratic square-free relations, which form a Groebner basis (or equivalently, the algebra $A=kS$ is a PBW algebra) cf. 2.19. It is proven in Ref. 15 that each skew-polynomial semigroup S_0 defines a nondegenerate set-theoretic solution $r=r(S_0)$ of the Yang–Baxter equation. In connection with this result the present author made the conjecture that under the restriction that X is finite and r is *square-free*, i.e., $r(x,x)=(x,x)$ for each $x\in X$, all nondegenerate involutive solutions can be obtained in this way, cf. 2.18. The Main theorem 2.26 proves this conjecture, and shows that there exists an ordering on X, $X=\{x_1<x_2<\cdots<x_n\}$, such that the Yang–Baxter algebra $\mathcal{A}=\mathcal{A}(k,X,r)$ is a Poincaré–Birkhoff–Witt-type algebra, with a k-basis—the set of ordered monomials $\{x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}\,|\,\alpha_i\geqslant 0, 1\leqslant i\leqslant n\}$. This result is used to show that each *binomial solution* of the Yang–Baxter equation is obtained from a *binomial skew-polynomial ring*, see 9.7. We show that the Yang–Baxter semigroup $S=S(X,r)$ is a distributive lattice. Finally we study generalized twisted unions of solutions and multipermutation solutions. We make a stronger conjecture, 2.28, that every square-free solution (X,r) is retractable, furthermore it is a multipermutation solution of level $m<n$.

In this work we will not be in a position to develop specific physical applications but already we can say that several of the structures we introduce are highly relevant for physics. For example, the groups $G(X,r)$ act on each other to form a matched pair of groups and are hence a natural source of quantum groups of bicrossproduct type. More details are to appear in our sequel.[16] Bicrossproduct quantum groups themselves are increasing importance in noncommutative geometry as for example the Connes–Kreimer quantum groups associated to renormalization, the κ-Poincaré quantum groups related to deformed spacetime, and the original "Planck-scale" quantum group; see Ref. 24 for this background.

II. BASIC NOTIONS AND RESULTS

In this section we first recall some basic notions, definitions, and results, from Refs. 6 and 15. They are related to both quantum group theory and noncommutative algebra, so we recall them for convenience of readers with various mathematical background. Next we formulate the main results of the paper and a conjecture about set-theoretic solutions of YBE.

We fix a finite nonempty set X with n elements. We shall often identify the sets $X\times X$ and X^2, the set of all monomials of length two in the free semigroup $\langle X\rangle$.

Definition 2.1 (Ref. 6): Let $r:X\times X\to X\times X$ be a bijective map, we shall refer to it as (X,r). The components of r are the maps $\mathcal{L}:X\times X\to X$ and $\mathcal{R}:X\times X\to X$ defined by the equality

$$r(x,y)=(\mathcal{L}_x(y),\mathcal{R}_y(x)).$$

(i) (X,r) is *left nondegenerate* if for each x the map $\mathcal{L}_x(y)$ is a bijective function of y; (X,r) is *right nondegenerate* if for each y the map $\mathcal{R}_y(x)$ is a bijective function of x; (X,r) is *nondegenerate* if it is left and right nondegenerate.

(ii) (X,r) is involutive if

$$r^2=id_{X\times X}. \tag{2.1}$$

(iii) (X,r) is *a braided set* if r satisfies the braid relation

$$r^{12}r^{23}r^{12}=r^{23}r^{12}r^{23}, \tag{2.2}$$

where $r^{12}=r\times id_X$ and $r^{23}=id_X\times r$.

(iv) (X,r) is *symmetric* if it is braided and involutive.

(v) If (X,r) is a braided, involutive and nondegenerate set we shall call it simply *a solution*.

Clearly, every braided set presents a set-theoretic solution of the Yang–Baxter equation. A general study of nondegenerate symmetric sets was given in Ref. 6.

In Ref. 15 was found a special class of solutions, here we call them *square-free solutions* (cf. 2.2), which are defined via the semigroups of skew-polynomial type. These semigroups were introduced and studied first in Ref. 8. The study continued in Refs. 9, 10, 15, and 19, cf. also Ref. 17.

Definition 2.2: A map $r:X^2\to X^2$ is *square-free* if it acts trivially on $\mathrm{diag}(X^2)$ i.e., $r(xx)=xx$, for all $x\in X$.

Example 2.3: Let X be a nonempty set and let $r(xy)=yx$. Then (X,r) is a square-free solution, which is called *the trivial solution*.

Example 2.4 (Permutational solution, Lyubashenko, Ref. 5): Let X be a nonempty set, let f,g be maps $X\to X$ and let $r(xy)=g(y)f(x)$. Then (a) (X,r) is nondegenerate if and only if f and g are bijective; (b) (X,r) is braided if and only if $fg=gf$; (c) (X,r) is involutive if and only if $f=g^{-1}$.

Remark 2.5: Note that for any permutation f of X, the map r defined as $r(xy)=f(y)f^{-1}(x)$, is a solution, but in general r is not square-free. In fact, a permutational involutive solution r is square-free if and only if $f=id_X$, i.e., $r=id_{X^2}$. Nevertheless, we prove in 3.7 that each square-free solution behaves "locally" as a permutational solution.

Clearly, when the order $|X|=2$, the only square-free solution (X,r) is the trivial one. The lowest order of X which allows a nontrivial, square-free solution is 3, as shown in the following:

Example 2.6: Let $X=\{x_1,x_2,x_3\}$. Up to renumerating of the set X there exists a unique nontrivial square-free solution (X,r), namely,

$$r(x_3x_1)=x_2x_3,\quad r(x_2x_3)=x_3x_1,$$

$$r(x_3x_2)=x_1x_3,\quad r(x_1x_3)=x_3x_2,$$

$$r(x_2x_1)=x_1x_2,\quad r(x_1x_2)=x_2x_1,\quad r(x_ix_i)=x_ix_i,\quad i=1,2,3.$$

Up to isomorphism of solutions, there exist 5 square-free solutions (X,r) with $|X|=4$. The one with the greatest number nontrivial relations is given in the following example.

Example 2.7: Let $X=\{x_1,x_2,x_3,x_4\}$ and let r be defined as

$$r(x_1x_3)=x_4x_2,\quad r(x_4x_2)=x_1x_3,\quad r(x_1x_4)=x_3x_2,\quad r(x_3x_2)=x_1x_4,$$

$$r(x_2x_3)=x_4x_1,\quad r(x_4x_1)=x_2x_3,\quad r(x_2x_4)=x_3x_1,\quad r(x_3x_1)=x_2x_4,$$

$$r(x_1x_2)=x_2x_1,\quad r(x_2x_1)=x_1x_2,\quad r(x_3x_4)=x_4x_3,\quad r(x_4x_3)=x_3x_4,$$

$$r(x_ix_i)=x_ix_i,\quad i=1,\ldots,4.$$

Then (X,r) is a square-free solution. Consider the permutation $\sigma=(12)(34)$. For x,y which belong to different orbits of σ one has $r(xy)=\sigma(y)\sigma^{-1}(x)$, and when x and y belong to the same orbit, then $r(xy)=\sigma^2(y)\sigma^{-2}(x)=yx$.

Definition 2.8: The braid group B_n is the group generated by n generators $b_1,\ldots,b_n$ and defining relations

$$b_ib_j=b_jb_i,|i-j|>1; \tag{2.3}$$

$$b_ib_{i+1}b_i=b_{i+1}b_ib_{i+1}. \tag{2.4}$$

Recall that the symmetric group S_n is isomorphic to the quotient of B_n by the relations $b_i^2=1$.

The following remark is obvious, see for example Ref. 6.

Remark 2.9: Let $m\geqslant 3$ be an integer. (i) The assignment $b_i\to r^{ii+1}$, $1\leqslant i\leqslant m-1$, extends to an action of B_m on X^m if and only if (X,r) is a braided set. (ii) The assignment $b_i\to r^{ii+1}$, $1\leqslant i\leqslant m-1$, extends to an action of S_m on X^m if and only if (X,r) is a symmetric set. (Here, as usual, $r^{ii+1}=id_{X^{(i-1)}}\times r\times id_{X^{(m-i-1)}}$.)

The next well-known fact (see Ref. 6), gives the relation between the braided sets (i.e., the set-theoretic solutions of the Yang–Baxter equation) and the set-theoretic solutions of the quantum Yang–Baxter equation.

Fact 2.10: Let $r:X^2\to X^2$ be a bijection, $\sigma:X^2\to X^2$ be the flip $\sigma(xy)=yx$, for all $x,y\in X$. Let $R=\sigma\circ r$ (i.e., R is the so called R-matrix *corresponding to r). Then r satisfies the set-theoretic Yang–Baxter equation if and only if R satisfies the quantum Yang–Baxter equation:*

$$R^{12}R^{13}R^{23}=R^{23}R^{13}R^{12}. \tag{2.5}$$

Furthermore, r is involutive if and only if R satisfies (2.5) and the unitarity condition

$$R^{21}R=1. \tag{2.6}$$

In the spirit of a recent trend called a *combinatorial approach in algebra*, to each bijective map $r:X^2\to X^2$ we associate canonically finitely presented algebraic objects (see precise definition in 2.12) generated by X and with quadratic defining relations $\mathfrak{R}$ naturally determined as

$$\mathfrak{R}=\mathfrak{R}(r)=\{(u=r(u))|u\in X^2,u\neq r(u)\text{ as words in }X^2\}. \tag{2.7}$$

We study the close relations between the combinatorial properties of the defining relations, e.g., of the map r, and the structural properties of the associated algebraic objects.

Notation 2.11: For a nonempty set X, as usual, we denote by $\langle X\rangle$ the free semigroup generated by X, and by $k\langle X\rangle$—the free associative k-algebra generated by X, where k is an arbitrary field. For a set $F\subseteq k\langle X\rangle$, (F) denotes the two sided ideal of $k\langle X\rangle$, generated by F.

Definition 2.12: Assume that $r:X^2\to X^2$ is an involutive, bijective map.

(i) The semigroup

$$S = S(X,r) = \langle X; \mathfrak{R}(r) \rangle,$$

with a set of generators X and a set of defining relations $\mathfrak{R}(r)$ is called *the semigroup associated with* (X,r).

(ii) *The group* $G=G(X,r)$ *associated with* (X,r) is defined as

$$G = G(X,r) = {}_{gr}\langle X; \mathfrak{R}(r) \rangle.$$

(iii) For arbitrary fixed field k, *the k-algebra associated with* (X,r) is defined as

$$\mathcal{A} = \mathcal{A}(k,X,r) = k\langle X \rangle / (\mathfrak{R}(r)). \tag{2.8}$$

Clearly $\mathcal{A}$ is a quadratic algebra, generated by X and with defining relations $\mathfrak{R}(r)$. Furthermore, $\mathcal{A}$ is isomorphic to the semigroup algebra $kS(X,r)$.

Manin[25] introduced the notion of a *Yang–Baxter algebra*. He calls *a Yang–Baxter algebra* a quadratic algebra A with defining relation determined via arbitrary fixed Yang–Baxter operator. In this spirit we give the following definition.

Definition 2.13: Assume (X,r) is a solution. Then $S(X,r)$, $G(X,r)$, and $\mathcal{A}(k,X,r)$ are called, respectively, *the Yang–Baxter semigroup, the Yang–Baxter group*, and *the Yang–Baxter k-algebra, associated with* (X,r). We shall also use the abbreviation "YB" for "Yang–Baxter."

In the case when (X,r) is a solution, $G(X,r)$ is also called *the structure group of* (X,r), see Ref. 6.

Example 2.14: Let (X,r) be the trivial solution, i.e., $r(xy)=yx$, for all $x,y \in X$, then clearly, $S(X,r)=[x_1,\ldots,x_n]$, is the free Abelian semigroup generated by X, $G(X,r)=Z^X$, is the free Abelian group generated by X, and $\mathcal{A}(k,X,r)=k[x_1,\ldots,x_n]$ is the commutative polynomial ring over k.

Definition 2.15: Let $S=\langle X;\mathfrak{R}\rangle$ be a semigroup with a set of generators X and a set of quadratic binomial defining relations

$$\mathfrak{R} = \{xy = y'x' | x,y,x',y' \in X\}.$$

We assume that each monomial $u \in X^2$, occurs in at most one relation in $\mathfrak{R}$. Define the map $r = r(S): X^2 \to X^2$ as follows:

(i) $r(xy)=xy$, if xy is a monomial of length 2 which does not occur in any relation in $\mathfrak{R}$; and
(ii) if $(xy=y'x') \in \mathfrak{R}$, then we set $r(xy)=y'x'$ and $r(y'x')=xy$. We call $r(S)$ *the map associated with the semigroup S*.

Note that if r is the map defined by the set of relations of a YB-semigroup $S=\langle X;\mathfrak{R}\rangle$, then the set $(X;r)$ is always symmetric, since clearly, $r^2=id_{X^2}$.

We give now an example of a Yang–Baxter semigroup S with 11 generators. In fact, S belongs to the class of semigroups of skew-polynomial type, 2.19, and the map $r(S)$ is a square-free solution.

Example 2.16: Let $S=\langle X;\mathfrak{R}\rangle$, where the set of generators is $X=\{1,2,\ldots,8,a,b,c\}$ and the defining relations are

$$1a = a2, \quad 2a = a1, \quad 2b = b3, \quad 3b = b2, \quad 3a = a4, \quad 4a = a3, \quad 4c = c1, \quad 1c = c4,$$

$$5a = a6, \quad 6a = a5, \quad 6b = b7, \quad 7b = b6, \quad 7a = a8, \quad 8a = a7, \quad 8c = c5, \quad 5c = c8,$$

$$1b = b5, \quad 5b = b1, \quad 2c = c6, \quad 6c = c2, \quad 3c = c7, \quad 7c = c3, \quad 4b = b8, \quad 8b = b4,$$

$$ab = ca, \quad ac = ba, \quad bc = cb, \quad ij = ji, \quad 1 \leqslant i,j \leqslant 8.$$

Remark 2.17: Let S_0 be a semigroup of skew-polynomial type (see 2.19). Let $r=r(S_0)$ be the map defined by the relations of S_0. Then (X,r) is a square-free solution (cf Ref. 15, Theorem 1.2,

also Theorem 2.26). Furthermore, S_0 is a cancelative semigroup, and has a group of quotients $\mathrm{gr}(S_0)$, which is a central localization of S_0, see Ref. 19. It is clear, that the groups $\mathrm{gr}(S_0)$ and the associated group $G(X,r)$ are isomorphic. Moreover, the set X is embedded in $G(X,r)$.

The semigroups of skew-polynomial type were discovered while the author was searching for a new class of Artin–Schelter regular rings. It turned out that *the skew-polynomial rings with binomial relations*, or shortly *binomial skew-polynomial rings* introduced and studied in Refs. 8–10, provide a class of Artin–Schelter regular rings of arbitrary global dimension, cf. Refs. 10, 14, and 15. Furthermore, with each ring $\mathcal{A}_0$ of this type we associate (uniquely) a semigroup $\mathcal{S}_0$ which defines (via its relations) a nondegenerate set-theoretic solution $r(\mathcal{S}_0)$ of the Yang–Baxter equation, cf. Ref. 15. It is easy to generalize this result by showing that each skew-polynomial ring with binomial relations defines a solution of the classical Yang–Baxter equation, see Theorem 9.7. The semigroup $\mathcal{S}_0$ is called a semigroup of skew-polynomial type. The results in Ref. 15 and further study of the combinatorial properties of the solutions inspired the following Conjecture, which we reported first in a talk at the International Conference in Ring Theory, Miskolc, 1996, see also Refs. 11 and 12.

Main Conjecture 2.18 (Ref. 13): Let (X,r) be a square-free (nondegenerate, involutive) solution of the Yang–Baxter equation. Then the set X can be ordered so, that the associated semigroup is of skew-polynomial type.

Definition 2.19: We say that the semigroup S_0 is *a semigroup of skew-polynomial type* (or shortly, *a skew-polynomial semigroup*) if it has a standard finite presentation as $S_0=\langle X;\mathfrak{R}_0\rangle$, where the set of generators X is ordered: $x_1<x_2<\cdots<x_n$, and the set

$$\mathfrak{R}_0=\{\, x_jx_i=x_{i'}x_{j'}\,|\,1\leqslant i<j\leqslant n,1\leqslant i'<j'\leqslant n\},$$

contains precisely $n(n-1)/2$ quadratic square-free binomial defining relations, each of them satisfying the following conditions:

(i) each monomial $xy\in X^2$, with $x\neq y$, occurs in exactly one relation in $\mathfrak{R}_0$; a monomial of the type xx does not occur in any relation in $\mathcal{R}_0$;
(ii) if $(x_jx_i=x_{i'}x_{j'})\in\mathcal{R}_0$, with $1\leqslant i<j\leqslant n$, then $i'<j'$, and $j>i'$ (further studies show that this also implies $i<j'$, see Ref. 9);
(iii) the monomials $x_kx_jx_i$ with $k>j>i,1\leqslant i,j,k,\leqslant n$ do not give rise to new relations in S_0, or equivalently, cf. Ref. 4, $\mathfrak{R}_0$ is a Groebner basis with respect to the degree-lexicographic ordering of the free semigroup $\langle X\rangle$.

Remark 2.20: Suppose S_0 is a semigroup of skew-polynomial type. It follows from the Diamond Lemma[4] that, each element w of S can be presented uniquely as an ordered monomial

$$w=x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n},$$

where $\alpha_i\geqslant 0,1\leqslant i\leqslant n$. This presentation is called *the normal form of w* and denoted as $\mathrm{Nor}(w)$. It follows from the Diamond lemma, that two monomials w_1,w_2 in the free semigroup $\langle X\rangle$ are equal in S if and only if their normal forms coincide, $\mathrm{Nor}(w_1)=\mathrm{Nor}(w_2)$. Thus S_0 can be identified as a set with the set of ordered monomials

$$\mathcal{N}_0=\{x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}|\alpha_i\geqslant 0,1\leqslant i\leqslant n\}. \tag{2.9}$$

Furthermore, for an arbitrary field k, the set $\mathcal{N}_0$ is a k-basis of the quadratic algebra

$$A_0=k\langle X\rangle/(\mathfrak{R}_0)\simeq kS_0.$$

Clearly, A_0 is a Poincaré–Birkhoff–Witt-algebra in the sense of Priddy[27] with $\mathcal{N}_0$ as a PBW-basis.

Remark 2.21: In Ref. 19 the skew-polynomial semigroups S_0 are called *binomial semigroups*.

We now recall the definition of the semigroups of *I*-type, see Ref. 15, which are closely related to both—the semigroups of skew-polynomial type and the set-theoretic solutions of Yang–Baxter equation. The rings of *I*-type were introduced and studied by Tate and Van den Bergh in their work on the homological properties of Sklyanin Algebras.[34]

Notation 2.22: Until the end of the paper we shall denote by

$$\mathcal{U} = [u_1, \ldots, u_n], \tag{2.10}$$

the free commutative multiplicative semigroup generated by $u_1, \ldots, u_n$.

Definition 2.23 (Ref. 15): A semigroup S generated by $\{x_1, \ldots, x_n\}$ is said to be of *(left) I-type* if there exists a bijection $v: \mathcal{U} \to S$ called *(a left) I-structure*, such that $v(1)=1$, and such that for each $a \in \mathcal{U}$ there is an equality of sets $\{v(u_1a), v(u_2a), \ldots, v(u_na)\} = \{x_1v(a), x_2v(a), \ldots, x_nv(a)\}$. Analogously one defines *a right I-structure* $v_1: \mathcal{U} \to S$.

Remark 2.24: It can be extracted from Ref. 15, see also (4.1), that if (X,r) is a square-free solution, and $S=S(X,r)$ is the associated YB semigroup, then

(a) There exists a unique left *I*-structure $v: \mathcal{U} \to S$, such that $v(u_i)=x_i$, for $1 \leqslant i \leqslant n$.
(b) There exists a unique right *I*-structure $v_1: \mathcal{U} \to S$, such that $v_1(u_i)=x_i$ for $1 \leqslant i \leqslant n$.

In Sec. IV, Proposition 4.16, we show that a semigroup of *I*-type is a distributive lattice with respect to the order induced from "one-sided" divisibility, defined below.

Definition 2.25: For every pair $a, b \in S$ we set

(i) $a|_l b$, if and only if there exists a monomial $c \in S$, such that $b=ca$. We call this relation *divisibility with respect to the left multiplication.*
(ii) $a|_r b$, if and only if there exists a monomial $c \in S$, such that $b=ac$. This relation is called *divisibility with respect to the right multiplication.*

The following theorem proved in Sec. VI verifies the Main Conjecture 2.18.

Main Theorem 2.26: *Assume that X is a finite set of order $n \geqslant 1$, and $r: X \times X \to X \times X$ is a square-free involutive bijection. Let $S=S(X,r)$ be the semigroup associated with (X,r) and let $\mathcal{A}=\mathcal{A}(k,X,r)$ be the quadratic k-algebra associated with (X,r), where k is an arbitrary field. Then the following conditions are equivalent:*

(1) *(X,r) is a nondegenerate solution of the set-theoretic Yang–Baxter equation.*
(2) *$S=S(X,r)$ is a semigroup of I-type.*
(3) *There exists an ordering on X, $X=\{x_1 < x_2 < \cdots < x_n\}$, such that $S=S(X,r)$ is a semigroup of skew-polynomial type.*
(4) *There exists an ordering on X, $X=\{x_1 < x_2 < \cdots < x_n\}$ such that for every field k the quadratic k-algebra $\mathcal{A}=\mathcal{A}(k,X,r)$ is a Poincaré–Birkhoff–Witt algebra, with a k-basis—the set of ordered monomials $\mathcal{N}_0$.*

Moreover, each of these conditions implies that the solution (X,r) is decomposable, i.e., X a disjoint union of two nonempty r-invariant subsets.

Corollary 2.27: Let (X,r) be a square-free solution, with associated semigroup $S=S(X,r)$. Then $(S, |_l)$ is a distributive lattice. Furthermore the left I-structure $v: \mathcal{U} \to S$ is an isomorphism of lattices.

Condition 2.26.2 implies, cf. Refs. 14 and 15, various nice algebraic and homological properties of the algebra $\mathcal{A}=\mathcal{A}(k,X,r)$, like being a Noetherian domain, Koszul, Cohen–Macaulay, Artin–Schelter regular, etc. In particular the semigroup S is cancelative. Hence it is naturally embedded in its group of quotients $\mathrm{gr}(S)=G(X,r)$. We recall these results in Theorem 6.1.

My student, Garcia Roman shows in Ref. 29 that for an explicitly given solution (X,r), condition 2.26.3 is equivalent to a standard problem from Linear Programming.

In Ref. 16 is presented a matched pairs approach to the set-theoretic solutions of the Yang–Baxter equation. One of the main results in Ref. 16, given here as Theorem 5.6 covers all known constructions of solutions (X,r), restricted to the case of square-free solutions, with X a finite set.

In Sec. VIII we study retractability of solutions, generalized twisted unions of solutions, and multipermutation solutions.

Section IX gives an application of the Main Theorem to a particular class of solutions of the classical Yang–Baxter equation called *binomial solutions of YBE*. We show that each binomial solution of the classical Yang–Baxter equation is obtained from binomial skew polynomial rings. Therefore the associated Yang–Baxter algebra has a PBW type k-basis, and the nice algebraic and homological properties of binomial skew-polynomial rings. The study of these algebras continues in Ref. 14.

We close this section with the following conjecture:

Strong Conjecture 2.28: (I) Every square-free solution (X,r), where X is a finite set of order $n\geqslant 2$, is retractable, see 8.5. Furthermore (X,r) is a multipermutation solution of level $m<n$.

(II) Every multipermutation square-free solution of level m is a generalized twisted union of multipermutation solutions of levels $\leqslant m-1$.

III. THE CYCLIC CONDITION AND COMBINATORICS IN $S(X,r)$

In this section we introduce a combinatorial technique for non-degenerate square-free solutions (X,r), which associates cycles in $\mathrm{Sym}(X)$ to each pair of elements y,x in X. We call the corresponding property of r *cyclic condition*. The cyclic condition is the base for all combinatorial techniques in this paper. We use it here to deduce more precise pictures of the left and right actions of the group $G(X,r)$ on X, and to show that each involutive square-free solution acts "locally" as a permutational solution. Lemma 3.9 gives more precise information about the relations $\mathfrak{R}(r)$, which is used throughout the paper. We use the lengths of the cycles occurring in $S(X,r)$ to deduce some important relations of higher degrees in $S(X,r)$, and to introduce an invariant integer $M=M(X,r)$ called *the cyclic degree of* (X,r).

Definition 3.1: Let $r:X\times X\to X\times X$ be a bijection.

(1) We say that (X,r) satisfies *the weak cyclic condition*, if for every pair $y,x\in X$, there exist two disjoint cycles $\mathcal{L}_y^x=(x_1,\ldots,x_m)$ and $\mathcal{R}_x^y=(y_k,\ldots,y_1)$ in the symmetric group $\mathrm{Sym}(X)$, such that $x=x_1,y=y_1$, and for all $1\leqslant i\leqslant m$, $1\leqslant j\leqslant k$ there are equalities:

$$r(y_jx_i)=\mathcal{L}_y^x(x_i)\mathcal{R}_x^y(y_j)=x_{i+1}y_{j-1}, \tag{3.1}$$

where $x_{m+1}:=x_1$, and $y_0:=y_k$.

In particular, $r(yx)=\mathcal{L}_y^x(x)\mathcal{R}_x^y(y)=x_2y_k$.

In this case we also say that the semigroup $S(X,r)$ satisfies *the weak cyclic condition*.

(2) (X,r) satisfies *the cyclic condition*, if for every pair $y,x\in X$, there exist two disjoint cycles $\mathcal{L}_y^x=(x_1,\ldots,x_m)$ and $\mathcal{L}_x^y=(y_1,\ldots,y_k)$ in $\mathrm{Sym}(X)$, such that $x=x_1,y=y_1$, and for all $1\leqslant i\leqslant m$, $1\leqslant j\leqslant k$ there are equalities:

$$r(x_iy_j)=y_{j+1}x_{i-1} \text{ and } r(y_jx_i)=x_{i+1}y_{j-1}, \tag{3.2}$$

where $x_0=x_m,x_{m+1}:=x_1$, and $y_0:=y_k,y_{k+1}=y_1$.

In particular, for every pair $(y,x)\in X\times X$, the disjoint cycles $\mathcal{L}_y^x$ and $\mathcal{L}_x^y$ satisfy

$$r(y,x)=\mathcal{L}_y^x(x)(\mathcal{L}_x^y)^{-1}(y), \text{ and } r(x,y)=\mathcal{L}_x^y(y)(\mathcal{L}_y^x)^{-1}(x). \tag{3.3}$$

We call $\mathcal{L}_x^y$ and $\mathcal{L}_y^x$ *the pair of cycles associated with* (y,x).

If this is the case for (X,r) we also say that the semigroup $S(X,r)$ satisfies *the cyclic condition*.

Remark 3:2: Clearly, the (strong) cyclic condition implies that r is involutive. We will show that every involutive square-free solution (X,r) satisfies the cyclic condition and use this to study the left (and the right) action of $G(X,r)$ on X. Note that if the cyclic condition holds, and we set

$$\sigma=\sigma_{y,x}=\sigma_{x,y}=(x_1,\ldots,x_m)(y_1,\ldots,y_k)\in\mathrm{Sym}(X),$$

the map r is expressible "locally" as a permutational solution

$$r(y_jx_i)=\sigma(x_i)\sigma^{-1}(y_j) \quad \text{and} \quad r(x_iy_j)=\sigma(y_j)\sigma^{-1}(x_i).$$

If we do not assume involutiveness for r, then, in general, only the weak cyclic condition is satisfied. We give an example, see 3.3, of a noninvolutive solution in which the cyclic condition does not hold.

Example 3.3: Let $X=\{x_1,x_2,x_3,x_4,x_5,x_6\}$ and suppose the map $r:X^2\to X^2$ is defined as

$$x_1x_2\leftrightarrow x_2,x_1; \quad x_3x_4\leftrightarrow x_4x_3;$$

$$x_3x_5\leftrightarrow x_5x_3; \quad x_3x_6\leftrightarrow x_6x_3;$$

$$x_4x_5\leftrightarrow x_5x_4; \quad x_4x_6\leftrightarrow x_6x_4; \quad xx\leftrightarrow xx, \text{ for all } x\in X;$$

$$x_1x_3\to x_4x_2\to x_1x_5\to x_6x_2\to x_1x_3;$$

$$x_1x_4\to x_3x_2\to x_1x_6\to x_5x_2\to x_1x_4;$$

$$x_2x_3\to x_4x_1\to x_2x_5\to x_6x_1\to x_2x_3;$$

$$x_2x_4\to x_3x_1\to x_2x_6\to x_5x_1\to x_2x_4.$$

Then (X,r) is a noninvolutive solution, with $r^4=id_{X^2}$. Furthermore

$$\mathcal{L}_{x_1}=(x_3x_4)(x_5x_6), \quad \mathcal{R}_{x_1}=(x_3x_6)(x_4x_5), \quad \text{and } \mathcal{R}_{x_1}\neq(\mathcal{L}_{x_1})^{-1}.$$

Recall first a well known fact from Ref. 6.

Fact 3.4 (Ref. 6): Let (X,r) be nondegenerate, $G=G(X,r)$. Then (X,r) is a braided set if and only if the following three conditions are satisfied:

(1) *The assignment $x\to\mathcal{L}_x$ induces a left action of G on X;*
(2) *The assignment $x\to\mathcal{R}_x$ induces a right action of G on X;*
(3) *The following equality holds for any $x, y, z\in X$:*

$$\mathcal{L}_{\mathcal{R}_{\mathcal{L}_y(z)}(x)}(\mathcal{R}_z(y))=\mathcal{R}_{\mathcal{L}_{\mathcal{R}_y(x)}(z)}(\mathcal{L}_x(y)). \tag{3.4}$$

Notation 3.5: We shall denote by $O_G(x)$ the orbit of x, $x\in X$, under the left action of G on X.

Lemma 3.6: Let $r:X\times X\to X\times X$ be a bijection. Then in the notation of 3.1 the following holds:

(I) *Conditions (1), (2), and (3) are equivalent.* (II) *Conditions (4), (5), and (6) are equivalent. Each of them implies (1), (2), and (3).*

(1) *(X,r) satisfies the weak cyclic condition.*
(2) *For every $x,y\in X, x\neq y$, there are equalities*

$$\mathcal{L}_{\mathcal{R}_x(y)}(x)=\mathcal{L}_y(x) \quad \textit{and } \mathcal{R}_{\mathcal{L}_y(x)}(y)=\mathcal{R}_x(y). \tag{3.5}$$

(3) *For all $i,j, 1\leqslant i\leqslant m$, $1\leqslant j\leqslant k$, there are equalities*

$$\mathcal{L}^{x_i}_{y_j}=\mathcal{L}^x_y=(x_1,\ldots,x_m), \quad \textit{and } \mathcal{R}^{y_j}_{x_i}=\mathcal{R}^y_x=(y_1,\ldots,y_k). \tag{3.6}$$

(4) *(X,r) satisfies the cyclic condition.*
(5) *For all $x,y\in X$ there are equalities:*

$$\mathcal{R}_x(y)=\mathcal{L}_x^{-1}(y), \quad \text{and } \mathcal{L}_{\mathcal{R}_x(y)}(x)=\mathcal{L}_y(x). \tag{3.7}$$

(6) *For all $i,j, 1\leqslant i\leqslant m$, $1\leqslant j\leqslant k$, there are equalities*

$$\mathcal{L}_{y_j}^{x_i} = (\mathcal{R}_{y_j}^{x_i})^{-1} = \mathcal{L}_y^x = (x_1, \ldots, x_m), \tag{3.8}$$

and

$$\mathcal{L}_{x_i}^{y_j} = (\mathcal{R}_{x_i}^{y_j})^{-1} = \mathcal{L}_x^y = (y_1, \ldots, y_k). \tag{3.9}$$

The following theorem gives an account of various conditions on the bijective maps $r: X^2 \to X^2$ and the corresponding semigroup $S(X,r)$. For some of them we assume neither that r is necessarily a solution of the Yang–Baxter equation, nor we assume that r is involutivene.

Theorem 3.7: *Let $r: X^2 \to X^2$ be a bijective map, denoted by (X,r). Let $S = S(X,r)$ be the semigroup associated to (X,r). Let $\mathcal{L}_x$ and $\mathcal{R}_x$ be the left and right components of r, introduced in 2.1. Consider the following conditions:*

(1) *(a) (X,r) is left nondegenerate; (b) (X,r) is right nondegenerate.*
(2) *(a) (Right Ore condition) For every pair $a,b \in X$, there exists a unique pair $x,y \in X$, such that $ax = by$; (b) (Left Ore condition) For every pair $a,b \in X$ there exists a unique pair $z,t \in X$, such that $za = tb$.*
(3) *(X,r) is square-free and nondegenerate.*
(4) *$\mathcal{L}_x$ is a bijection and $\mathcal{L}_x(y) \neq x$, for each $y \neq x$; $\mathcal{R}_y$ is a bijection and $\mathcal{R}_y(x) \neq y$, for each $y \neq x$.*

Then the following is true:

(A) *The conditions 1(a) and 2(a) are equivalent; the conditions 1(b) and 2(b) are equivalent;*
(B) *The conditions 3 and 4 are equivalent.*
(C) *If (X,r) is a nondegenerate square-free solution of the Yang–Baxter equation (not necessarily involutive) then the weak cyclic condition 3.1.1 holds.*
(D) *If (X,r) is a nondegenerate involutive square-free solution of the Yang–Baxter equation, then the cyclic condition 3.1.2 holds.*

Proof: (A) $(1.a) \Rightarrow (2.a)$ Let $a,b \in X$. By our assumption the function $\mathcal{L}_a$ is a bijection of X onto itself, so there exists a unique y such that $\mathcal{L}_a(y) = b$, hence the equality $r(ay) = \mathcal{L}_a(y)\mathcal{R}_y(a)$ gives $r(ay) = bz$, for some $z \in X$. But r is a bijective map on X^2 onto itself, so z is also determined uniquely. The implication $(1.b) \Rightarrow (2.b)$ is analogous.

The implications $(2.a) \Rightarrow (1.a)$ and $(2.b) \Rightarrow (1.b)$ are obvious.

(B) $3 \Rightarrow 4$. Let $x,y \in X$, $x \neq y$. By assumption $r(xx) = xx$, so $\mathcal{L}_x(x) = x \neq \mathcal{L}_x(y)$. $4 \Rightarrow 3$. Let $x \in X$, clearly there is an equality of sets

$$\{\mathcal{L}_x(y) | y \in X, y \neq x\} = X \setminus \{x\}$$

so $\mathcal{L}_x(x) = x$. Similarly $\mathcal{R}_x(x) = x$, thus $r(xx) = xx$.

For the following lemmas we assume the hypothesis of the theorem.

Lemma 3.8: If (X,r) is nondegenerate and square-free, then $r(xy) \neq xy$ if and only if $x \neq y$.

Proof: The statement of the lemma follows immediately from B and from the equation $r(xy) = \mathcal{L}_x(y)\mathcal{R}_y(x)$. □

Lemma 3.9 gives important and explicit information about the relations $\mathfrak{R}(r)$. In fact relations (3.10) and (3.11) are used in almost every computation throughout the paper.

Lemma 3.9: If (X,r) is a nondegenerate and square-free solution of the Yang–Baxter equation (not necessarily involutive), then the following conditions hold in S:

$$[yx = x'y', x \neq y] \Rightarrow [yx' = x''y', y'x = x'y''], \tag{3.10}$$

for some $x'', y'' \in X$.

Furthermore, there are equalities:

$$yxx = x'x'y'', \quad \text{and } yyx = x''y'y'. \tag{3.11}$$

Proof: Let $x \neq y$ and let $yx = x'y'$, or equivalently, $r(yx) = x'y'$. It follows from (3.8) that $yx \neq x'y'$, as monomials in the free semigroup $\langle X \rangle$. Assume that

$$r(yx') = x''y''. \tag{3.12}$$

Now consider the "Yang–Baxter diagram"

$$\begin{array}{ccc} yyx & \overset{r\times id_X}{\longrightarrow} & yyx \\ id_X \times r \downarrow & & \downarrow id_X \times r \\ yx'y' & & yx'y' \\ r \times id_X \downarrow & & \downarrow r \times id_X \\ x''y''y' & \overset{id_X\times r}{\longrightarrow} & x''y''y' \end{array} . \tag{3.13}$$

It follows then that $r(y''y') = y''y'$, which, since r is square-free, is possible only if $y'' = y'$. We have shown that

$$(yx = x'y') \Rightarrow (yx' = x''y') \tag{3.14}$$

($y' = y$ is possible). Note that $x'' \neq y, y'$.

Similarly, we prove that

$$(yx = x'y') \Rightarrow (y'x = x'y'') \tag{3.15}$$

for some appropriate $y'' \in X$.

The equality $yyx = x''y'y'$ in S also follows from the diagram (3.13). □

The validity of conditions C and D can be deduced from the following lemma. Note that in the hypothesis of the lemma we do not assume that (X, r) is a solution.

Lemma 3.10: (i) (X, r) *satisfies the weak cyclic condition 3.1.1 if and only if r is nondegenerate and satisfies condition* (3.10).

(ii) Suppose (X, r) *satisfies the weak cyclic condition. Then r is involutive if and only if for every pair* $y, x \in X$ *one has* $\mathcal{L}_y^x = (\mathcal{R}_y^x)^{-1}$.

Proof: Clearly, the weak cyclic condition 3.1.1 implies (3.10) and r nondegenerate. Assume now that r is nondegenerate and condition (3.10) holds.

Suppose $y, x \in X$, $y \neq x$, and $r(yx) = x'y'$ ($x' = x$, or $y' = y$ are possible). We denote $x_1 = x$, $x_2 = x'$, and apply (3.10) successively to obtain a sequence of pairwise distinct elements $x_1, \ldots, x_m \in X$, such that

$$r(yx_i) = x_{i+1}y', \quad \text{for } 1 \leqslant i \leqslant m-1, \quad \text{and } r(yx_m) = x_1y'. \tag{3.16}$$

Similarly (after an appropriate re-numeration) we obtain $y_1 = y, y_2, \ldots, y_k = y' \in X$, such that

$$r(y_jx_1) = x_2y_{j-1}, \quad \text{for } 2 \leqslant j \leqslant k, \quad \text{and } r(y_1x_1) = x_2y_m. \tag{3.17}$$

We claim that

$$r(y_jx_i) = x_{i+1}y_{j-1}, \quad \text{for } 1 \leqslant i \leqslant m, \quad 1 \leqslant j \leqslant k, \tag{3.18}$$

where $x_{m+1} := x_1$, $y_0 := y_m$. We prove (3.18) by induction on j.

Step 1: $j = 1$. Clearly (3.16), with $y_k = y'$, give the base for the induction. Assume (3.18) is satisfied for all $j, 1 \leqslant j \leqslant j_0 - 1$. We shall prove (3.18) for $j = j_0$, $1 \leqslant i \leqslant m-1$, using induction on i. The base of the induction,

$$r(y_{j_0}x_1) = x_2y_{j_0-1}, \tag{3.19}$$

follows from (3.17). Assume now (3.18) is true for all $i < i_0$. In particular,

$$r(y_{j_0}x_{i_0-1}) = x_{i_0}y_{j_0-1}. \tag{3.20}$$

Then by (3.10) one has

$$r(y_{j_0}x_{i_0}) = ty_{j_0-1}, \quad \text{for some } t \in X, \tag{3.21}$$

we apply (3.10) again and obtain

$$r(y_{j_0-1}x_{i_0}) = tz, \tag{3.22}$$

for some $z \in X$. It follows from the inductive assumption that

$$r(y_{j_0-1}x_{i_0}) = x_{i_0+1} + y_{j_0-2}, \tag{3.23}$$

which together with (3.22) gives $t = x_{i_0+1}$ thus $r(y_{j_0}x_{i_0}) = x_{i_0+1}y_{j_0-1}$. We have proven that (3.18) holds for all i, $1 \leqslant i \leqslant m$, and $j = j_0$, which verifies (3.18). This proves (i).

We set $\mathcal{L}_y^x = (x_1, \ldots, x_m) \in \mathrm{Sym}(X)$, and $(\mathcal{R}_x^y)^{-1} = (y_1, \ldots, y_k) \in \mathrm{Sym}(X)$. Consider the permutation

$$\sigma_{y,x} = (x_1, \ldots, x_m)(y_1, \ldots, y_k).$$

Clearly,

$$r(y_jx_i) = \sigma_{y,x}(x_i)\sigma_{y,x}^{-1}(y_j). \tag{3.24}$$

Assume now that r is involutive, and apply r to (3.18) to obtain $r(x_{i+1}y_{j-1}) = y_jx_i$. This implies for $1 \leqslant i \leqslant m$ and $1 \leqslant j \leqslant k$:

$$\mathcal{L}_x^y = \mathcal{L}_{x_i}^y = (y_1, \ldots, y_k) = (\mathcal{R}_x^y)^{-1} = (\mathcal{R}_{x_i}^y)^{-1}, \tag{3.25}$$

$$\mathcal{L}_y^x = \mathcal{L}_{y_j}^x = (x_1, \ldots, x_m) = (\mathcal{R}_y^x)^{-1} = (\mathcal{R}_{y_j}^x)^{-1}. \tag{3.26}$$

Conversely, (3.25) and (3.26) imply that $\sigma_{y,x} = \sigma_{x,y}$ therefore r is involutive. This proves the lemma, and completes the proof of the theorem. □

Remark 3.11: Let (X, r) be an arbitrary square-free nondegenerate solution (not necessarily involutive). Consider the left and the right actions of G on X, see (3.4), extending the assignment $y \to \mathcal{L}_y$, respectively, $x \to \mathcal{R}_x$, where $\mathcal{L}_y$, $\mathcal{R}_x \in \mathrm{Sym}(X)$ are the permutations defined via $r(yx) = \mathcal{L}_y(x)\mathcal{R}_x(y)$. Since each permutation has a presentation as a product of disjoint cycles in $\mathrm{Sym}(X)$ (unique up to commutation of multiples) we obtain that the cycle $\mathcal{L}_y^x = (x_1, \ldots, x_m)$, $(x_1 = x)$ occurs as a multiple in such a presentation of $\mathcal{L}_y$ and the cycle $\mathcal{R}_x^y = (y_1, \ldots, y_k)$ is a multiple of the corresponding presentation for $\mathcal{R}_x$. The surprising part is that each pair y_i, x_i with $1 \leqslant j \leqslant k$ and $1 \leqslant i \leqslant m$, produces the same pair of cycles: $\mathcal{L}_{y_j}^{x_i} = \mathcal{L}_y^x = (x_1, \ldots, x_m)$, and $\mathcal{R}_{x_i}^{y_j} = \mathcal{R}_x^y = (y_1, \ldots, y_k)$. Therefore although in general $\mathcal{L}_{y_j} \neq \mathcal{L}_y$, each permutation $\mathcal{L}_{y_j}$, $1 \leqslant j \leqslant k$ contains the same cycle $(x_1, \ldots, x_m)$ in its presentation as products of disjoint cycles in $\mathrm{Sym}(X)$. Analogously, the cycle $(y_1, \ldots, y_k)$ participates in the presentation of each $\mathcal{R}_{x_i}$, $1 \leqslant i \leqslant m$, as a product of disjoint cycles. We do not know how the cycles L_y^x and R_y^x, are related to each other, in the general (noninvolutive) case of square-free nondegenerate solutions, besides the obvious property, that each of them contains x, see example 3.3. In the case of involutive solutions (X, r) there is a "symmetry" $\mathcal{L}_y^x = (\mathcal{R}_y^x)^{-1} = (x_1, \ldots, x_m)$ for each pair $y \neq x, y, x \in X$.

Notation 3.12: To avoid complicated expressions, sometimes we shall use also the notation ${}^xy = \mathcal{L}_x(y)$ and $y^x = \mathcal{R}_x(y)$.

The following corollary is a "translation" of the cyclic condition in the new notation. It can be extracted from a more general result in Ref. 16.

Corollary 3.13: Let $r: X \times X \to X \times X$ be a nondegenerate involutive bijection. Consider the following conditions:

(1) ${}^{x}x=x$ *for every* $x\in X$.
(2) $r(x,x)=(x,x)$ *for every* $x\in X$.
(3) (X,r) *satisfies the cyclic condition.*
(4) *For every* $x,y\in X$ *there are equalities:*

$$ {}^{({}^{x}y)}x = {}^{y}x; \quad ({}^{y}x)^{y} = {}^{y}(x^{y}) = x. \tag{3.27}$$

Then the following is true:

(a) *Conditions 1 and 2 are equivalent.*
(b) *Conditions 3 and 4 are equivalent.*

Convention 3.14: In the rest of the paper we shall consider only involutive nondegenerate square-free solutions (X,r) of the Yang–Baxter equation; they will be briefly called *square-free solutions*.

Let $x\in X$. Clearly, for $t\in X$ the cycle $\mathcal{L}_x^t$ is of length one if and only if $xt=tx'$.

Notation 3.15: We denote by $\mathcal{G}_L=\mathcal{G}_L(X,r)$ the image of $G(X,r)$ under the group homomorphism $\mathcal{L}:G\to\mathrm{Sym}(X)$, which extends the assignment $x\to\mathcal{L}_x$. $\mathcal{G}_R=\mathcal{G}_R(X,r)$ denotes the image of $G(X,r)$ under the group homomorphism $\mathcal{R}:G\to\mathrm{Sym}(X)$, which extends the assignment $x\to\mathcal{R}_x$.

Lemma 3.16: Let (X,r) *be a square-free solution,* $\mathcal{L}_x$*, and* $\mathcal{R}_x$ *be the left and right components of r, which are extended to a left, respectively right action of* $G(X,r)$ *on X. Then*

(1) *The permutation* $\mathcal{L}_x$ *is presented as a product of disjoint cycles in* $\mathrm{Sym}(X)$ *via the equality*

$$\mathcal{L}_x = \mathcal{L}_x^{t_1}\mathcal{L}_x^{t_2}\cdots\mathcal{L}_x^{t_s}, \tag{3.28}$$

where $t_1,\ldots,t_s$ *are representatives of all disjoint orbits of* $\mathcal{L}_x$ *in X.*

(2) *The permutations* $\mathcal{L}_x$ *and* $\mathcal{R}_x$ *satisfy the equality*

$$\mathcal{R}_x = (\mathcal{L}_x)^{-1}. \tag{3.29}$$

Furthermore, the two permutation groups determined by the left and right action of $G(X,r)$ *on X coincide:*

$$\mathcal{G}_R = \mathcal{G}_L.$$

(3) *The assignment* $x\to\mathcal{L}_x$, $x\in X$, *determines the solution r uniquely, via the formula*

$$r(x,y) = \mathcal{L}_x(y)(\mathcal{L}_y)^{-1}(x).$$

To each solution we associate an invariant integer number $M=M(X,r)$ defined as follows.

Definition 3.17: (1) For every $x\in X$ we denote by M_x the order of the permutation $\mathcal{L}_x$ in $\mathrm{Sym}(X)$, i.e. (in the notation of 3.16) the least common multiple of the lengths of the cycles $\mathcal{L}_x^{t_i}$, $1\leqslant i\leqslant s$.

(2) By $M=M(X,r)$ we denote the least common multiple of all M_x, where $x\in X$, and call M the *cyclic degree* of the solution (X,r).

Lemma 3.18: Suppose $ax=ya'$, *for some* $x,y,a,a'\in X$. *Then* $M_x=M_y$.

Proof: It will be enough to show that the length k of each cycle $\mathcal{L}_x^{\xi}$ occurring in $\mathcal{L}_x$ divides M_y. □

Proposition 3.19: Assume $x,y\in X$, *and* $O_G(x)=O_G(y)$. *Then* $M_y=M_x$.

Corollary 3.20: Suppose $M_x\neq M_y$, *for some* $x,y\in X$. *Then G acts nontransitively on X, and X is decomposable into a disjoint union of two r-invariant subsets.*

The following proposition follows easily from the cyclic condition, and 3.17.

Proposition 3.21: Let (X,r) *be a square-free solution of cyclic degree M. Let p, and q be arbitrary natural numbers. Suppose* $y,x\in X$, $y\neq x$, *and let k, m be the natural numbers defined in 3.1. Let* M_x *denote the order of* $\mathcal{L}_x$. *Then the following equalities hold:*

$$y^m x = x y_k^m, \tag{3.30}$$

$$y^p x^q = (x')^q (y')^p, \quad \text{where } x' = (\mathcal{L}_y)^p(x), \quad \text{and } y' = (\mathcal{L}_x)^{-q}(y), \tag{3.31}$$

$$x^{M_x} y = y (x_m)^{M_x}, \tag{3.32}$$

$$x^M y^M = y^M x^M. \tag{3.33}$$

The next corollary follows immediately from (3.33).

Corollary 3.22: Let (X,r) be a square-free solution, then the center of the Yang–Baxter algebra $\mathcal{A}(k,X,r)$ contains all symmetric functions in $x_1^M, x_2^M, \ldots, x_n^M$.

Corollary 3.23: Let (X,r) be a square-free solution. Then the group $A = gr[x_1^M, \ldots x_n^M]$ is a free Abelian subgroup of $G(X,r)$ of index M^n.

IV. THE LATTICE STRUCTURE OF $S(X,r)$

In this section we show that for a semigroup $\mathcal{S}$ of left I-type, the relation $|_l$ of left divisibility, defined in 2.25, and the left I-structure $v:\mathcal{U}\to S$, see 2.23, are compatible, and prove that $(S,|_l)$ is a distributive lattice. Analogous results are true for semigroups with right I-structure $v_1:\mathcal{U}\to S$. As a corollary we obtain that the Yang–Baxter semigroup $S=S(X,r)$ has a structure of distributive lattice, induced by its left I-structure v. We keep the notation from the previous sections. In particular,

$$\mathcal{U} = [u_1, \ldots, u_n] \tag{4.1}$$

is the free commutative multiplicative semigroup generated by $u_1, \ldots, u_n$, and $\langle X\rangle$ denotes the free semigroup generated by X. The definition of an I-structure is given in 2.23.

The following result can be extracted from Ref. 15, Theorem 1.3.

Theorem 4.1: *Let (X,r) be a square-free solution and $S=S(X,r)$ be the associated Yang–Baxter semigroup. Then*

(A) *There exists a unique left I-structure $v:\mathcal{U}\to S$, which is inductively defined by the following conditions:*

(1) $v_1(1)=1$, $v(u_i)=x_i$, *for* $1\leqslant i\leqslant n$.

(2) *For every* $b\in\mathcal{U}$ *and every* i, $1\leqslant i\leqslant n$, *there exists an* $x_{b,i}\in X$, *such that* $v(u_i b) = x_{b,i} v(b)$. *Moreover, there is an equality of sets*

$$\{x_{b,i} | 1 \leqslant i \leqslant n\} = \{x_1, \ldots, x_n\}. \tag{4.2}$$

(3) *For every* $b\in\mathcal{U}$, *and* $1\leqslant i,j\leqslant n$, *there is a relation in S*:

$$x_{u_j b,i} x_{b,j} = x_{u_i b,j} x_{b,i}. \tag{4.3}$$

(B) *There exists a unique right I-structure $v_1:\mathcal{U}\to S$, which satisfies the following conditions:*

(1) $v_1(1)=1$, $v_1(u_i)=x_i$, *for* $1\leqslant i\leqslant n$.

(2) *For every* $b\in\mathcal{U}$ *and every* i, $1\leqslant i\leqslant n$, *there exists an* $x_{i,b}\in X$, *such that* $v(b u_i) = v(b) x_{i,b}$. *Furthermore, there is an equality of sets*

$$\{x_{i,b} | 1 \leqslant i \leqslant n\} = \{x_1, \ldots, x_n\}. \tag{4.4}$$

(3) *For every* $b\in\mathcal{U}$, *and* $1\leqslant i,\ j\leqslant n$, *there is a relation in S*:

$$x_{i,b u_j} x_{j,b} = x_{j,b u_i} x_{i,b}. \tag{4.5}$$

Remark 4.2: Suppose $\mathcal{S}$, is a semigroup of (left) I-type generated by $x_1, \ldots, x_n$, with a left

I-structure $v:\mathcal{U}\to\mathcal{S}$. Then in general, v satisfies a modified version on condition A where condition 1 is modified to

$$v(u_j)=x_{i_j},\quad 1\leqslant j\leqslant n, \tag{4.6}$$

where $i_1,\ldots,i_n$ is a permutation of $1,\ldots,n$ and conditions 2 and 3 are unchanged. Moreover (4.6) determines the bijection v uniquely. Analogous statement is true for right I-structures. Without loss of generality we can consider only the special I-structure v and v_1 defined in theorem 4.1.

Notation 4.3: Throughout this section $\mathcal{S}$ will denote a semigroup of I-type generated by $x_1,\ldots,x_n$ with a left I-structure v and a right I-structure v_1. We assume that v and v_1 satisfy conditions 4.1(A) and 4.1(B), respectively.

Remark 4.4: Note that given $a\in\mathcal{U}$, in finitely many steps one can find effectively the monomials $v(a)$ and $v_1(a)$. In particular, it is easy to see that for any i, $1\leqslant i\leqslant n$, and any positive integer k there are equalities $v(u_i^k)=v_1(u_i^k)=x_i^k$. In general, for a monomial $u\in\mathcal{U}$ there might be inequality $v(u)\neq v_1(u)$ (as elements of $\mathcal{S}$), see 4.11.

We study first the properties of the relations "$|_l$"-*divisibility with respect to left multiplication* or shortly-*left divisibility* and "$|_r$"-*right divisibility* on $\mathcal{S}$, defined as

$$a|_l b,\quad \text{if there exists a } c\in\mathcal{S}, \text{ such that } b=ca, \tag{4.7}$$

$$a|_r b,\quad \text{if there exists a } d\in\mathcal{S}, \text{ such that } b=ad. \tag{4.8}$$

The following lemma shows that the left I-structure v is compatible with the left divisibility.

Lemma 4.5: $|_l$ is a partial order on $\mathcal{S}$, compatible with the left multiplication. Furthermore, this order is compatible with the left I-structure v. More precisely, the following two conditions hold:

(a) *If $a|b\in\mathcal{U}$ (i.e. $b=ca$ is an equality in $\mathcal{U}$) then $v(a)|_l v(b)$;*
(b) *Conversely, let $a,b,c\in\mathcal{S}$ satisfy $b=ca$. Let a_0, b_0 be the unique elements of $\mathcal{U}$ which satisfy $v(a_0)=a$ and $v(b_0)=b$. Then $b_0=c_0a_0$, for some $c_0\in\mathcal{U}$.*

Proof: First we show that $|_l$ is an ordering on $\mathcal{S}$ as a set. Clearly, $a|_l a$ for every $a\in S$. It is known that each semigroup $\mathcal{S}$ of I-type is with cancellation low, see Ref. 15. It follows then that $a|_l b$ and $b|_l a$ imply $a=b$. The transitiveness follows at once from the definition of $|_l$.

Next we prove (a). Assume $b=ca$, for $a,b,c\in\mathcal{U}$. We use induction on the length $|c|$ of c to find a monomial $c'\in\mathcal{S}$, such that $v(b)=c'v(a)$. If $c=u_i$, then by the definition of v we have $v(b)=v(u_ia)=x_{a,i}v(a)$. Assume that the statement of the proposition is true for all c of length $\leqslant m$. Let $b=ca$, where $|c|=m+1$. Then $c=u_id$, where $1\leqslant i\leqslant n$, and $|d|=m$. We have $v(b)=v(u_ida)=x_{da,i}v(da)$. By the inductive assumption $v(da)=d'v(a)$, so $v(b)=x_{da,i}d'v(a)$, which proves (a). Assume now that $a,b\in\mathcal{S}$ and $b=ca$, for a $c\in\mathcal{S}$. By definition, v is a bijection, so there are unique a_0 and b_0 in $\mathcal{U}$, such that $v(a_0)=a$, and $v(b_0)=b$. We have to find a $c_0\in\mathcal{U}$, such that $b_0=c_0a_0$. We show this again by induction on the length $|c|$ of c. If $|c|=1$, then $c=x_i\in X$. It follows from 4.1 that there is an equality of sets

$$\{v(u_1a_0),\ldots,v(u_na_0)\}=\{x_1v(a_0),\ldots,x_nv(a_0)\}. \tag{4.9}$$

Clearly, then there exists a j, such that $v(u_ja_0)=x_iv(a_0)=x_ia=b$. This gives $b_0=u_ja_0$. Assume (b) is true for all $c\in\mathcal{S}$ with length $|c|\leqslant k$. Let $b=ca$, where $|c|=k+1$. Then $c=xd$, for some $x\in X$ and $|d|=k$. It follows from the inductive assumption that there is a $d_0\in\mathcal{U}$, such that

$$v(d_0a_0)=dv(a). \tag{4.10}$$

In addition an equality of sets similar to (4.9) shows that there exists a u_j, such that $v(u_jd_0a_0)=xv(d_0a_0)$. The last equality together with (4.10) gives $v(u_jd_0a_0)=xv(d_0a_0)=xda=ca$, so $c_0=u_jd_0$ satisfies the desired equality $b_0=c_0a_0$. □

An analogous statement is true for the right I-structure v_1.

Lemma 4.6: Let $a,b\in\mathcal{S}$. (a) There exists a uniquely determined least common multiple of a and b, with respect to $|_l$, that is a monomial w of minimal length, such that $w=w_1a=w_2b$, for some $w_1, w_2\in S$. (b) There exists a uniquely determined least common multiple, of a and b, with respect to $|_r$, that is a monomial w' of minimal length, such that $w'=aw_1'=bw_2'$, for some $w_1', w_2'\in S$.

Proof: The map v is bijective, so $a=v(a_0)$, and $b=v(b_0)$, for some uniquely determined a_0 and b_0 in $\mathcal{U}$. Let w_0 be the least common multiple $a_0\sqcup b_0$ of a_0 and b_0 in $\mathcal{U}$. It follows from (4.5) that $v(w_0)=\xi v(a_0)=\eta v(b_0)$. Thus $w=v(w_0)$ satisfies

$$w=\xi a=\eta b, \tag{4.11}$$

is a common multiple of a and b (with respect to $|_l$). That w is of minimal possible length among the monomials satisfying (4.11) follows from (4.5). This proves (a). An analogous argument proves (b). □

Notation 4.7: By $a\sqcup b$ we denote the least common multiple of a and b with respect to $|_l$. $a\vee b$ denotes the least common multiple of a and b with respect to $|_r$.

Lemma 4.8: Let v, v_1 be the left and the right I-structures on $\mathcal{S}$, defined in 4.3. Then (a) v is a lattice isomorphism for $(\mathcal{U},|)$ and $(\mathcal{S},|_l)$; (b) v_1 is a lattice isomorphism for $(\mathcal{U},|)$ and $(\mathcal{S},|_r)$.

Definition 4.9: Let $u\in\mathcal{S}$. We say that $h\in X$ is a *head* of u (as an element of $\mathcal{S}$), if u can be presented as $u=hu'$, for some $u'\in\mathcal{S}$. The element $t\in X$ is called *a tail* of u (in $\mathcal{S}$) if $u=u''t$ is an equality in $\mathcal{S}$, for some $u''\in\mathcal{S}$.

Note that a monomial u has exactly one head (respectively: u has exactly one tail) if and only if it is of the shape $u=x^m$, for some $x\in X$, $m\geqslant 1$.

Example 4.10: The relation $(xy=y'x')\in\mathfrak{R}$ implies that the heads of xy are x and y', and its tails are y and x'. Furthermore, $xy=x\vee y'=y\sqcup x'$.

Example 4.11: Consider the YB semigroup $S=\langle X;\mathfrak{R}\rangle$, where $X=\{x_1,x_2,x_3,x_4\}$ and the set of relations is

$$x_4x_1=x_2x_3,\quad x_4x_2=x_1x_3,\quad x_3x_1=x_2x_4,\quad x_3x_2=x_1x_4,\quad x_1x_2=x_2x_1,\quad x_3x_4=x_4x_3.$$

Then

$$v(u_2u_4)=x_1x_4=x_3x_2=v_1(u_1u_3),\quad v_1(u_2u_4)=x_4x_1=x_2x_3=v(u_1u_3),$$

$$v(u_2^2u_4)=x_3x_2^2=x_1x_4x_2=x_1^2x_4=v_1(u_1^2u_3),$$

$$v_1(u_2^2u_4)=x_2^2x_4=x_2x_3x_1=x_4x_1^2.$$

Clearly, $v(u_2^2u_4)\neq v_1(u_2^2u_4)$ as elements of S. In fact, $v(u_2^2u_4)=v_1(u_1^2u_3)$. For $w=x_1^2x_4$ there are equalities in S

$$w=x_2^2\sqcup x_4=x_1^2\vee x_4.$$

Lemma 4.12: Let $w_0\in\mathcal{U}$. Suppose $w_0=u_{i_1}^{\alpha_1}u_{i_2}^{\alpha_2}\cdots u_{i_k}^{\alpha_k}$, where $1\leqslant i_1<i_2<\cdots i_k\leqslant n$, and all α_j are positive integers. Then,

(a) $v(w_0)=x_{i_1}^{\alpha_1}\sqcup x_{i_2}^{\alpha_2}\sqcup\cdots\sqcup x_{i_k}^{\alpha_k}$;
(b) $v_1(w_0)=x_{i_1}^{\alpha_1}\vee x_{i_2}^{\alpha_2}\vee\cdots\vee x_{i_k}^{\alpha_k}$.

Remark 4.13: In general, for $w\in\mathcal{U}$ there might be an inequality $v(w)\neq v_1(w)$ and it is not true that $a\sqcup b=a\vee b$, cf. (4.11). Still for the special monomial

$$W_0=u_1u_2\cdots u_n \tag{4.12}$$

one has

$$v(W_0)=v_1(W_0)=x_1\sqcup x_2\sqcup\cdots\sqcup x_n=x_1\vee x_2\vee\cdots\vee x_n. \tag{4.13}$$

Definition 4.14: The monomial $W=v(u_1u_2\cdots u_n)$ is called *the principal monomial of* $\mathcal{S}$.

Remark 4.15: The principal monomial W "encodes" important information about $\mathcal{S}$ and the solution (X,r). In particular, if (X,r) is a solution and $A=A(k,X,r)$, is the associated Yang–Baxter algebra, then the Koszul dual algebra $A^!$ is Frobenius and W projects to a basis of the socle of $A^!$. In Ref. 14 we study various properties of the principal monomial W, and their implication to the properties of A.

Proposition 4.16: Let $\mathcal{S}$ be a semigroup of I-type, let v and v_1 be the left and right structures on $\mathcal{S}$ as in 4.3. Then following conditions hold:

(1) *$(\mathcal{S},|_l)$ is a distributive lattice. More precisely, any monomial $w\in\mathcal{S}$ has a unique presentation as $w=x_1^{\alpha_1}\sqcup x_2^{\alpha_2}\sqcup\cdots\sqcup x_n^{\alpha_n}$, where α_i is a uniquely determined non-negative integer for each i, $1\leqslant i\leqslant n$. In particular, for each i, with $\alpha_i\geqslant 1$, there is an equality $w=w_ix_i^{\alpha_i}$, where $w_i\in\mathcal{S}$, and x_i does not occur as a tail of w_i.*

(2) *The properties of the lattice $(\mathcal{S},|_r)$ are analogous. In particular, every element $w\in\mathcal{S}$ has a unique presentation as $w=x_1^{\beta_1}\vee x_2^{\beta_2}\vee\cdots\vee x_n^{\beta_n}$, where all β_i are non-negative integers.*

(3) *The following are equalities in $\mathcal{S}$:*

$$W_0=v_1(u_1u_2\cdots u_n)=x_1\vee x_2\vee\cdots\vee x_n=x_1\sqcup x_2\sqcup\cdots\sqcup x_n=v(u_1u_2\cdots u_n).$$

Proof: It is well known that $\mathcal{U}$ is a distributive lattice with respect to the order of divisibility, $a|b$. In particular, every element $a\in\mathcal{U}$ has a unique presentation $a=u_1^{k_1}u_2^{k_2}\cdots u_n^{k_n}$, where $k_1,\ldots,k_n$ are non-negative integers, and $a=u_1^{k_1}\sqcup u_2^{k_2}\sqcup\cdots\sqcup u_n^{k_n}$ ($v\sqcup w$ denotes the least common multiple of v, w in $\mathcal{U}$). Lemma 4.8 implies condition (1). One can show using induction on k that a monomial of the shape $u_{i_1}u_{i_2}\cdots u_{i_k}$, where all u_{i_j} are pairwise distinct, has exactly k different heads and k distinct tails. Therefore the monomial $W_0=v(u_1u_2\cdots u_n)$ has exactly n distinct heads (respectively, n distinct tails) so the set of heads for W_0 coincides with X. □

V. UNIONS OF SOLUTIONS AND MATCHED PAIRS OF GROUPS

In this section we briefly recall some definitions and properties of unions of solutions. We also state a recent result from Ref. 16, in which matched pairs approach is used to describe extensions of solutions.

Definition 5.1 (Ref. 6): Let (X,r) be a solution. A subset $Y\subseteq X$ is *r-invariant*, if r restricts to a bijection $r_Y: Y\times Y\to Y\times Y$. (X,r) is *decomposable* if it can be presented as a union of two nonempty disjoint r-invariant subsets. A solution (Z,r) is *a union* of the solutions (X,r_X) and (Y,r_Y), if $X\cap Y=\emptyset$, $Z=X\cup Y$, as a set, and the bijection r extends r_X, and r_Y.

Clearly, (Z,r) is a union of two nonempty r-invariant subsets, if and only if it is decomposable.

Remark 5.2 (Ref. 6): Suppose the solution (Z,r) is a union of (X,r_X) and (Y,r_Y). Then the map r induces bijections

$$X\times Y\to Y\times X, \text{ and } Y\times X\to X\times Y.$$

Note that a (disjoint) union (Z,r) of two square-free solutions (X,r_X), and (Y,r_Y) is also a square-free solution. The cyclic condition implies then that for every $z\in Z$, there is an equality $\mathcal{R}_z=\mathcal{L}_z^{-1}$. Therefore the equality $r(x,y)=(\mathcal{L}_{x|Y}(y),\mathcal{L}_{y|X}^{-1}(x))$ defines a left action of the groups $G(X,r_X)$ on the set Y and a left action of the group $G(Y,r_Y)$ on the set X. Furthermore for every $z\in Z$ there is an equality of permutations in $\mathrm{Sym}(Z)$: $\mathcal{L}_z=\mathcal{L}_{z|X}\mathcal{L}_{z|Y}$. The following lemma is straightforward.

Lemma 5.3: Let (X,r) be a solution. Suppose $X_1,X_2,\ldots,X_k$ are all disjoint orbits of the left action of $G(X,r)$ on X. Then r induces solutions (X_i,r_i), $1\leqslant i\leqslant k$, where each r_i is the restriction of r on $X_i\times X_i$. Furthermore, X is a disjoint union of (X_i,r_i), $1\leqslant i\leqslant k$.

Clearly, (X,r) is decomposable if and only if $G(X,r)$ acts nontransitively on X.

Remark 5.4: Rump[30] proved that every square-free solution (X,r) is decomposable.

Therefore to understand the structure of a solution and also for constructing solutions it is essential to study extensions of solutions.

Definition 5.5 (Ref. 6): Suppose (X,r_X) and (Y,r_Y) are (disjoint) solutions. The set of *extensions of X by Y*, denoted by $\mathrm{Ext}(X,Y)$, is defined as the set of all decomposable solutions Z which are unions of X and Y.

It is shown in Ref. 6, that given (X,r_X), and (Y,r_Y), an element Z of $\mathrm{Ext}(X,Y)$ is uniquely determined by the function: $r_{X,Y}: X\times Y \to Y\times X$.

The fact that every square-free solution (Z,r) can be presented as a union of two disjoint solutions (X,r_X) and (Y,r_Y), where the bijective map $r: Z\times Z \to Z\times Z$ extends the maps r_X, and r_Y, implies that the following theorem covers all known constructions of solutions restricted to the square-free case.

Theorem 5.6 (Ref. 16): *Let (X,r_X) and (Y,r_Y) be disjoint solutions, $G_X=G(X,r_X)$, $G_Y=G(Y,r_Y)$ be the groups associated with (X,r_X), and (Y,r_Y), respectively. Suppose that $Z=X\cup Y$ and the bijective map $r: Z\times Z\to Z\times Z$ is an extension of the maps r_X and r_Y. Then (Z,r) is a solution if and only if (G_X,G_Y) is a matched pair of groups, in the sense of Majid.*[24] *Moreover (Z,r) is square-free if and only if (X,r_X) and (Y,r_Y) are square-free solutions.*

VI. THE EQUIVALENCE OF THE NOTIONS SQUARE-FREE SET-THEORETIC SOLUTION OF THE YANG–BAXTER EQUATION, SEMIGROUP OF I TYPE, AND SEMIGROUP OF SKEW-POLYNOMIAL-TYPE

We keep all notation and conventions from the previous sections. As usual (X,r) is a square-free solution, where $X=\{x_1,\ldots,x_n\}$ is a finite set with n elements, $S=S(X,r)$, $G=G(X,r)$, and $\mathcal{A}(k,X,r)$ are the associated Yang–Baxter semigroup, group and algebra over a field k, defined in 2.12. In this section we prove Theorem 2.26.

For convenience of the reader, we first recall some basic algebraic and homological properties of $S=S(X,r)$ and $\mathcal{A}(k,X,r)$.

Theorem 6.1 (**Ref. 15**): *Let X be a finite set of n elements, (X,r) be a square-free solution. Let $S=S(X,r)$, $G(X,r)$, and $\mathcal{A}=k\langle X;\mathfrak{R}(r)\rangle$ be the associated Yang–Baxter semigroup, group, and algebra over a field k, respectively. Then the following conditions hold:*

(1) *The semigroup S is of I-type*;
(2) *S is a semigroup with cancellation and $G(X,r)$ is its group of quotients*;
(3) *S is Noetherian*;
(4) *The algebra $\mathcal{A}$ is a Noetherian domain*;
(5) *The Hilbert series of $\mathcal{A}$ is $H_{\mathcal{A}}(t)=1/(1-t)^n$, the same as the Hilbert series of the commutative polynomial rings in n variables over k*;
(6) (Ref. 14) *$\mathcal{A}$ is Koszul*;
(7) *$\mathcal{A}$ satisfies the Auslander condition*;
(8) *$\mathcal{A}$ is Cohen–Macaulay*;
(9) *$\mathcal{A}$ is Artin–Schelter regular ring of global dimension n*;
(10) *The Koszul dual $\mathcal{A}^!$ of A is a Frobenius algebra*;
(11) (Ref. 17) *$\mathcal{A}$ satisfies a polynomial identity. Moreover, S satisfies a semigroup identity*;
(12) *$\mathcal{A}$ is catenary*.

Sketch of the proof: For the definition of "Cohen–Macaulay" and the "Auslander condition" see Ref. 22. Artin–Schelter regular rings are defined in Ref. 3. Conditions 6.1.1–6.1.9 can be extracted from Ref. 15 (cf. Ref. 15, Theorems 1.3, 1.4).

Condition 6.1.11 follows from a more general result in Ref. 17. It is proven (cf. Ref. 17, Theorem 3.1 and Corollary 3.2) that if a semigroup S has homogeneous defining relations, and the semigroup algebra $k[S]$ is right Noetherian and has finite Gelfand–Kirillov dimension, then $k[S]$ satisfies a polynomial identity, and S satisfies a semigroup identity.

Condition 6.1.12 follows from Ref. 31. A The Koszul dual algebra $A^!$ for arbitrary quadratic graded algebra A was introduced in Ref. 25. In Ref. 14 we give the precise defining relations for $A^!$ and a direct combinatorial proof that $A^!$ is Frobenius (in fact, we prove more: that $A^!$ is a

quantum Grassmanian algebra). Condition 6.1.10 follows also from the fact that a Koszul algebra A of finite global dimension is Gorenstein if and only if $A^!$ is Frobenius, see Ref. 32, Proposition 5.10.

The following theorem proves Conjecture 2.18.

Theorem 6.2: *Let (X,r) be a square-free solution, where X is a finite set with n elements, $n\geqslant 2$. Then there exists an ordering of $X=\{x_1<x_2<\cdots<x_n\}$, such that the Yang–Baxter semigroup $S(X,r)$ is of skew-polynomial type (with respect to this ordering), and the Yang–Baxter algebra $A(k,X,r)$, over an arbitrary field k is a PBW algebra with a k-basis the set of ordered monomials:*

$$\mathcal{N}_0=\{x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}|\alpha_i\geqslant 0, 1\leqslant i\leqslant n\}.$$

Under the hypothesis of the theorem we first prove some lemmas.

Lemma 6.3: There exists an ordering on X, $X=\{x_1<x_2<\cdots<x_n\}$, such that for any pair $x,t\in X$ the following holds:

$$(tx=x't')\in\mathfrak{R}(X,r),\quad \text{and } (t>x)\Rightarrow(x'<t'). \tag{6.1}$$

Proof: We use induction on $n=|X|$. Assume that the statement of the lemma is true for all solutions (X,r), with $|X|\leqslant n-1$. It follows from a theorem of Rump,[30] that every square-free solution (X,r), where X is a finite set, is decomposable into a disjoint union $X=Y\cup Z$ of two nonempty r-invariant subsets Y,Z. Suppose $|Y|=k$, $|Z|=m$, $k+m=n$. Let r_Y and r_Z be the restrictions on r on Y^2 and Z^2, respectively. It follows from the inductive assumption that there exist orderings $Y=\{y_1<\cdots<y_k\}$, and $Z=\{z_1<\cdots<z_m\}$, which satisfy condition 6.1. We set $y_1<\cdots<y_k<z_1<\cdots<z_m$ and verify that this is an ordering on X, which satisfies 6.1. Assume

$$tx=x't'\in\mathfrak{R}(X,r),\ \text{and } t>x. \tag{6.2}$$

We have to show that $x'<t'$. Clearly if $t,x\in Y$, or $t,x\in Z$, then by the inductive assumption and by the choice of the ordering $<$, condition 6.1 is satisfied. Assume now $x\in Y$, and $t\in Z$. (Note that the case $t\in Y$, $x\in Z$ is impossible since we assume $t>x$.) The sets Y, and Z, are r-invariant, therefore by 5.2 r induces a map $Z\times Y\to Y\times Z$. In particular $tx=x't'\in\mathfrak{R}(X,r)$, and $t\in Z$, $x\in Y$, imply that $x'\in Y$, $t'\in Z$. Hence, by the choice of $<$, there is an inequality $x'<t'$, which proves 6.1. □

Lemma 6.4: Suppose condition 6.1 holds. Let x, $t\in X$, and let $\mathcal{L}_t^x=(x_1,\ldots,x_k)$, $\mathcal{L}_x^t=(t_1,\ldots,t_m)$ be their associated disjoint cycles, see 3.1. Then $t_1>x_1$ implies $t_j>x_i$, for all i, j, $1\leqslant i\leqslant k$, $1\leqslant j\leqslant m$.

Proof: Using induction on i, we first show that

$$t_1>x_i,\quad 1\leqslant i\leqslant k. \tag{6.3}$$

By hypothesis $t_1>x_1$, which gives the base for the induction. Assume

$$t_1>x_s,\quad \text{for } 1\leqslant s\leqslant i-1. \tag{6.4}$$

We claim $t_1>x_i$. Assume the contrary,

$$t_1<x_i. \tag{6.5}$$

Note that $t_1=x_i$ is impossible, since the cycles $\mathcal{L}_t^x$ and $\mathcal{L}_x^t$ are disjoint. By the cyclic condition, 3.1 one has

$$t_1x_{i-1}=x_it_m, \tag{6.6}$$

and

$$t_1 x_i = \begin{cases} x_{i+1} t_m & \text{if } i < k \\ x_1 t_m & \text{if } i = k. \end{cases} \tag{6.7}$$

In the case when $i=k$, we obtain immediately a contradiction with (6.1), since

$$t_1 x_k = x_1 t_m, \quad \text{and } x_1 < t_1 < x_k < t_m. \tag{6.8}$$

Assume now $i<k$. Then (6.1) and (6.7), and the assumption (6.5), imply

$$x_{i+1} > t_m. \tag{6.9}$$

At the same time, the equalities (6.6) and (6.4) give

$$t_m > x_i. \tag{6.10}$$

We have obtained

$$x_{i+1} > t_m > x_i > t_1 > x_1. \tag{6.11}$$

Induction on j and analogous argument show, that for $1 \leqslant j \leqslant k-i$, the following inequalities hold:

$$x_{i+j} > t_m > x_i > t_1 > x_1. \tag{6.12}$$

In particular,

$$x_k > t_m > x_i > t_1 > x_1. \tag{6.13}$$

Now the equality $t_1 x_k = x_1 t_m$ together with (6.13) give a contradiction with (6.1). We have shown that

$$t_1 > x_i, \quad \text{for all } i, \quad 1 \leqslant i \leqslant k. \tag{6.14}$$

Induction on j and analogous argument show that

$$t_j > x_i, \quad \text{for all } i, \quad 1 \leqslant i \leqslant k. \tag{6.15}$$

This proves the lemma. □

Lemma 6.5: Let (X,r) be a square-free solution, with an ordering $<$ on X which satisfies (6.1), $S=S(X,r)$ be the associated Yang–Baxter semigroup. Then the following two conditions are satisfied:

(1)

$$(tx = x't') \in \mathfrak{R}(X,r) \quad \text{and } (t > x) \Rightarrow (x' < t') \text{ and } (t > x'). \tag{6.16}$$

(2) *The relations $\mathfrak{R}(X,r)$ form a Groebner basis, with respect to the degree-lexicographic ordering in the free semigroup $\langle X \rangle$, induced by $<$, or equivalently the monomials txu, where $t,x,u \in X$ and $t>x>u$ do not give rise to new relations in $S(X,r)$.*

Proof: Condition (6.16) follows immediately from Lemma 6.4. Therefore the set of defining relations $\mathfrak{R}=\mathfrak{R}(X,r)$ for the Yang–Baxter semigroup $S(X,r)$ satisfies the following:

$$(x_j x_i = x_{i'} x_{j'}) \in \mathfrak{R} \quad \text{and } (j > i) \Rightarrow (i' < j'), \quad \text{and } (j > i'). \tag{6.17}$$

We have to show that $\mathfrak{R}$ is Groebner basis. It follows from the theory of Groebner bases, that each monomial $u \in \langle X \rangle$ has a unique normal form, denoted by $\mathrm{Nor}(u)$, with respect to the so called *reduced Groebner basis*, $\mathfrak{R}_0$, which is uniquely determined by the set $\mathfrak{R}$ and, $\mathfrak{R} \subseteq \mathfrak{R}_0$. As a set S can be identified with the set of normal monomials

$$\mathcal{N}(S) = \{\mathrm{Nor}(u) | u \in \langle X \rangle\}. \tag{6.18}$$

Knowing the normal monomials one can uniquely restore the set of obstructions, i.e., the set of highest monomials in the reduced Groebner basis, $\mathfrak{R}_0$. To verify the equality $\mathfrak{R}=\mathfrak{R}_0$, therefore $\mathfrak{R}$ is a Groebner basis, it will be enough to show that the "ambiguities" $x_k x_j x_i$, where $n \geqslant k > j > i \geqslant 1$, do not give rise to new relations in $S(X,r)$, or equivalently, that each monomial of the shape $x_i x_j x_k$, with $1 \leqslant i \leqslant j \leqslant k \leqslant n$ is normal, with respect to $\mathfrak{R}_0$. This will follow immediately from a stronger statement:

Lemma 6.6: Each ordered monomial $u = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$, where $\alpha_i \geqslant 0$, $1 \leqslant i \leqslant n$ is in normal form with respect to the reduced Groebner basis $\mathfrak{R}_0$ in $\langle X \rangle$.

Proof: Each relation in $\mathfrak{R}$ satisfies (6.17), so its highest monomial is $x_j x_i$, with $j > i$, therefore the normal form $\mathrm{Nor}(u)$ of each $u \in \langle X \rangle$ does not contain $x_j x_i, j > i$ as a sub word. This shows that

$$S = \mathcal{N}(S) \subseteq \mathcal{N}_0, \tag{6.19}$$

where $\mathcal{N}_0$ is the set of ordered monomials $\mathcal{N}_0 = \{x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n} | \alpha_i \geqslant 0, 1 \leqslant i \leqslant n\}$.

The existence of the I-structure v on $S(X,r)$ (by definition $v: \mathcal{U} \to S$ is a bijection) implies the equality $\mathcal{N}(S) = \mathcal{N}_0$. □

We have proved 6.5. □

Proof of the theorem: The theorem follows from Lemma 6.5. Note that the Diamond Lemma 2.2 implies that the Yang–Baxter algebra $\mathcal{A} = \mathcal{A}(k,X,r)$ is PBW in the sense of Priddy,[27] and the set of ordered monomials $\mathcal{N}_0$ projects to a k-basis of $\mathcal{A}$ (as a k-vector space).

Proof of theorem A: The equivalence of 2.26.1 and 2.26.2 follow from Ref. 15, Theorem 1.4. The implications 2.26.1 $\Rightarrow$ 2.26.3, and 2.26.1 $\Rightarrow$ 2.26.4 follow from theorem 6.2. Clearly, the theory of Groebner basis implies the equivalence of conditions 2.26.3 and 2.26.4. Theorem 1.2 (Ref. 15), proves the implication 2.26.3 $\Rightarrow$ 2.26.1.

VII. MORE ABOUT $S(X,r)$ AND $G(X,r)$

In this section, as usual (X,r) denotes a square-free solution, where X is a finite set of n elements. We show that $G = G(X,r)$ acts by conjugation on the set $X^M = \{x_1^M, \ldots, x_n^M\}$, where $M = M(X,r)$ is the cyclic degree of (X,r) defined in 3.17. We compare this action with the left action of $G(X,r)$ on the set X. Next we prove that $G(X,r)$ contains a free Abelian subgroup A of index M^n, and prove that the quotient group $\overline{G} = G/A$ can be presented as a product of its Sylow subgroups (cf. 7.10). This implies a presentation of the group $\mathcal{G}_L(X,r)$ as a product of its Sylow subgroups. As a corollary we obtain a result of Etingof–Schedler–Solovyev,[6] that the group $G(X,r)$ is solvable.

Notation 7.1: For any positive integer k we set $X^{(k)} = \{x_1^k, \ldots, x_n^k\}$. By $S^k = \langle X^{(k)} \rangle$ we denote the submonoid of $S = S(X,r)$ generated by $X^{(k)}$. If $A, B \subset S$, then as usual, AB denotes the set of all elements u of the form $u = ab$, with $a \in A$, $b \in B$.

Proposition 7.2: Let k be a positive integer, $X^{(k)}$ and S^k as in 7.1. Then the following conditions hold:

(1) *The map r induces a map $r_k: X^{(k)} \times X^{(k)} \to X^{(k)} \times X^{(k)}$ such that $(X^{(k)}, r_k)$ is a square-free solution;*
(2) *S^k is of I-type;*
(3) *$S^k S^j = S^j S^k$ is an equality of sets in S, for every two positive integers k and j.*

It follows from 3.21 that for any pair $x, y \in X$ and $M = M(X,r)$ being the cyclic degree of the solution, there is an equality in S,

$$yx^M = x_2^M y, \text{ where } \mathcal{L}_y(x) = x_2.$$

This implies that G acts by conjugation on the set $X^{(M)}$. The following corollary follows easily from the existence of the I-structure v, and 3.21.

Corollary 7.3: Suppose (X,r) is a square-free solution. Then,

(1) *$S(X,r)$ contains the free Abelian semigroup $[x_1^M,\dots,x_n^M]=S^M$;*
(2) *$S(X,r)$ is left and right Noetherian*;
(3) *The group $A=gr[x_1^M,\dots,x_n^M]$ is a free Abelian normal subgroup of G of index M^n*;
(4) *The group $G=G(X,r)$ acts by conjugation on the set $X^{(M)}$. Moreover the action of A on $X^{(M)}$ is trivial, thus the quotient group $\overline{G}=G/A$ acts on $X^{(M)}$ by conjugation. Clearly, $\overline{G}$ is a finite group of order M^n*;
(5) *The group A is contained in the kernel* $\ker\mathcal{L}$ *of the homomorphism $\mathcal{L}:G\to Sym(X)$. Therefore there exists an epimorphism $\overline{\mathcal{L}}:\overline{G}\to\mathcal{G}_L$, induced by $\mathcal{L}$, satisfying the equality: $\mathcal{L}=\overline{\mathcal{L}}\circ\nu$, where ν is the natural epimorphism $\nu:G\to\overline{G}$*;
(6) *The order of $\mathcal{G}_L$ divides M^n.*

Notation 7.4: For every $y\in X$ we denote by $O(y^M)$ the orbit of y^M under the action if G on $X^{(M)}$. For $x, y\in X$ we define an equivalence on X by setting $x\approx y$ iff $O(x^M)=O(y^M)$. By $X(y)$ we denote the equivalence class of y, $y\in X$.

The lemma below follows straightforward from the definition of the actions of G on the sets X and X^M, and from Proposition 3.21.

Lemma 7.5: The following conditions hold:

(1) *There exists a one-to-one correspondence between the G-orbits of X^M and the G-orbits of X. More precisely for every $\xi\in X$, there are equalities $O_G(\xi)=X(\xi)=\{x\in X\,|\,x^M\in O(\xi^M)\}$. Furthermore, the orbits $O_G(\xi)$ can be obtained simply by acting with the "semigroup" elements of G,* i.e., *$y\in O_G(x)$ if and only if, there exist monomials $a,b\in S$, $a=a_1\cdots a_k$, and $b=b_1\cdots b_k$ $(a_i,b_i\in X)$ and elements $y_1,\dots,y_k\in X$, such that there are equalities:*

$$a_kx=y_kb_k,\quad a_{k-1}y_k=y_{k-1}b_{k-1},\quad\dots,\quad a_1y_1=yb_1. \tag{7.1}$$

(2) *If $x\in X(a)$, and $y\in X(b)$, for some $a, b\in X$ (not necessarily $a\neq b$) then there is an equality $xy=y'x'$, with $y'\in X(b)$, $x'\in X(a)$.*
(3) *Each orbit $O_G(\xi)$, $\xi\in X$ is r-invariant.*
(4) *X is r-decomposable if and only if $\overline{G}$ does not act transitively on X^M. More precisely, if $O_{\overline{G}}(\xi_i^M)$, $1\leqslant i\leqslant k$ are all disjoint orbits of this action then X splits into a disjoint union of k nonempty r-invariant subsets: $X_1=O_G(\xi_1),\dots,X_k=O_G(\xi_k)$.*

Remark 7.6: It is a routine fact, that the order of each orbit $O(x^M)$, $x\in X$ is a divisor of the order M^n of $\overline{G}$, see for example Ref. 2, 6.1.

A sufficient condition for r-decomposability of X follows immediately from 7.6. As a corollary we obtain a result from Ref. 6, that every solution (X,r), where X is of prime order p is decomposable.

Corollary 7.7: If M is not divisible by some prime divisor p of n, then the action of $\overline{G}$ (and of G) on $X^{(M)}$ is not transitive and X is a disjoint union of k r-invariant subsets, where $k\geqslant 2$ is the number of orbits in $X^{(M)}$.

Corollary 7.8 (Ref. 6): If $n=p$ is a prime number, then X is a disjoint union of two nonempty r-invariant subsets.

Next we study the relations between the cyclic degree $M=M(X,r)$, the Sylow subgroups of $\overline{G}$, and the cyclic properties of the semigroup $S(X,r)$. Note that

Notation 7.9: Let $M=M(X,r)$ be the cyclic degree of the solution (X,r) defined in 3.17. Suppose $M=p_1^{\alpha_1}p_2^{\alpha_2}\cdots p_k^{\alpha_k}$, where $p_1,\dots,p_k$ are distinct prime numbers, and $\alpha_1\cdots\alpha_k$ are positive integers. For $i=1,\dots,k$, we set

$$q_i=M/p_i^{\alpha_i},$$

$$S^{q_i} = \langle x_1^{q_i}, \ldots, x_n^{q_i} \rangle,$$

the submonoid of S generated by $x_1^{q_i}, \ldots, x_n^{q_i}$, $1 \leqslant i \leqslant k$. We denote by $\overline{S^{q_i}}$ the natural image of S^{q_i} in the quotient group $\overline{G}$, and by $\mathcal{L}(S^{q_i})$ the image of S^{q_i} under the homomorphism $\mathcal{L}: G \to \mathcal{G}_L \subset \mathrm{Sym}(X)$, defined by the left action of G on X.

Clearly, the integers $q_1, \ldots, q_k$ are pairwise coprime, and $\overline{S^{q_i}}$ are submonoids of $\overline{G}$.

The next theorem gives a presentation of $\overline{G}$ as a product of its Sylow subgroups. Surprisingly it also allows one to consider each element of $\overline{G}$ as an element of the monoid $\overline{S}$.

Theorem 7.10: *The following conditions hold:*

(1) *For every i, $1 \leqslant i \leqslant r$, the submonoid $\overline{S^{q_i}}$ is a subgroup of order $p_i^{n\alpha_i}$ in $\overline{G}$. In particular, it is a Sylow p_i-subgroup of $\overline{G}$.*
(2) *For every pair q_i, q_j, $1 \leqslant i, j \leqslant r$, there is an equality $\overline{S^{q_i}}.\overline{S^{q_j}} = \overline{S^{q_j}}.\overline{S^{q_i}}$.*
(3) *The group $\overline{G}$ is a product of its Sylow subgroups: $\overline{G} = \overline{S^{q_1}} \cdots \overline{S^{q_k}}$. In particular, $\overline{G} = \overline{S}$.*
(4) *For each i, $1 \leqslant i \leqslant k$, such that $\mathcal{L}(S^{q_i}) \neq id_X$, $\mathcal{L}(S^{q_i})$ is a p_i-Sylow subgroup of $\mathcal{G}_L$.*
(5) *Let $1 \leqslant i_1, \ldots, i_s \leqslant k$ be all indices, for which $\mathcal{L}(S^{q_{i_j}}) \neq \{id_X\}$, $1 \leqslant j \leqslant s$. Then the group $\mathcal{G}_L = \mathcal{G}_L(X, r)$ is a product of its Sylow subgroups:*

$$\mathcal{G}_L = \mathcal{L}(S^{q_{i_1}}) \cdots \mathcal{L}(S^{q_{i_s}}).$$

In particular, $\mathcal{G}_L = \mathcal{L}(S)$.
(6) *The groups $\mathcal{G}_L$, $\overline{G}$, and G are solvable.*

Proof: Consider $\overline{S^{q_i}}$, where $1 \leqslant i \leqslant k$. Note first that as a finite submonoid of the group $\overline{G}$, $\overline{S^{q_i}}$ is a subgroup of $\overline{G}$. We claim that the order of $\overline{S^{q_i}}$ is exactly $p_i^{n\alpha_i}$. The equalities 3.31 imply that every element w of $\overline{S^{q_i}}$ can be presented as

$$w = \overline{v((u_1^{q_i})^{\beta_1} \cdots (u_n^{q_i})^{\beta_n})}, \tag{7.2}$$

where $0 \leqslant \beta_s \leqslant p_i^{\alpha_i}$ for all $s, 1 \leqslant s \leqslant n$. We set $\beta = (\beta_1, \beta_2, \ldots, \beta_n)$, and $w = w(\beta)$, for the monomial w determined by (7.2). It follows from the properties of the I-structure v on S and from 3.31 that each inequality $\beta' \neq \beta''$ implies an inequality in $\overline{S}$,

$$w(\beta') \neq w(\beta''). \tag{7.3}$$

This implies that $\overline{S^{q_i}}$ is a group of order $(p_i^{\alpha_i})^n$ thus a Sylow p_i subgroup of $\overline{G}$, which proves 1.

Next we recall that for every pair of integers $i, j, 1 \leqslant i, j \leqslant k$, and for every pair $x, y \in X$ there exist $z, t \in X$, such that the equality

$$x^{q_i} y^{q_j} = z^{q_j} t^{q_i} \tag{7.4}$$

holds in S. This implies that $\overline{S^{q_i} S^{q_j}} = \overline{S^{q_j} S^{q_i}}$ for all i, j, which verifies 2. Let $S' = \langle S^{q_1}, \ldots, S^{q_k} \rangle$ be the submonoid of S, generated by $S^{q_1}, \ldots, S^{q_k}$. It follows from 7.4 that there is an equality

$$S' = S^{q_1} \cdots S^{q_k}. \tag{7.5}$$

Hence

$$\overline{S'} = \overline{S^{q_1}} \cdots \overline{S^{q_k}} \tag{7.6}$$

is a presentation of $\overline{S'}$ as a product of subgroups with pairwise co-prime orders: $p_1^{n\alpha_1}, \ldots, p_k^{n\alpha_k}$, respectively. It follows then that the order of $\overline{S'}$ is exactly $p_1^{n\alpha_1} \cdots p_k^{n\alpha_k} = M^n$, thus $\overline{G} = \overline{S^{q_1}} \cdots \overline{S^{q_k}}$. This proves 3. The proof of 4, and 5 is routine. □

Note that, in general the Sylow subgroups $\overline{S^{q_i}}$ might not be normal subgroups of $\overline{G}$, as shows the following example.

Example 7.11: Let $S=\langle X;\Re\rangle$, where $X=\{x_i|1\leqslant i\leqslant 6\}\cup\{y_j|1\leqslant j\leqslant 4\}$ and the relations $\Re$ are defined by the permutation

$$\sigma=(x_1x_2x_3x_4x_5x_6)(y_1y_2y_3y_4) \tag{7.7}$$

as follows:

$$y_jx_i=\sigma(x_i)\sigma^{-1}(y_j),\quad \text{and } x_iy_j=\sigma_1(y_j)\sigma^{-1}(x_i)\quad \text{for } 1\leqslant i\leqslant 6,\ 1\leqslant j\leqslant 4; \tag{7.8}$$

$$x_ix_k=\sigma^3(x_k)\sigma^{-3}(x_i),\quad \text{for all } i\neq k(\text{mod }3),\ 1\leqslant i,k\leqslant 6; \tag{7.9}$$

$$x_ix_k=x_kx_i,\quad \text{for all } i=k(\text{mod }3),\ 1\leqslant i,k\leqslant 6; \tag{7.10}$$

$$y_jy_k=\sigma^2(y_k)\sigma^{-2}(y_j),\quad \text{for all } j\neq k(\text{mod }2),\ 1\leqslant j,k\leqslant 4; \tag{7.11}$$

$$y_jy_k=y_ky_j,\quad \text{for all } j=k(\text{mod }2),\ 1\leqslant j,k\leqslant 4. \tag{7.12}$$

It is easy to verify that the set of relations $\Re$ defines naturally a square-free solution, r, thus S is a YB semigroup. The set of all lengths of cycles is 6, 4, 2, so $M=12=2^2.3$, and (in the notation 7.9), $q_1=3$, and $q_2=4$. Thus, by Theorem 7.10, $\overline{G}=\overline{S^3}\,\overline{S^4}$. Note that none of the subgroups $\overline{S^3}$, $\overline{S^4}$ is normal in $\overline{G}$.

One can use Theorem 7.10 to give a straightforward proof of the r-decomposability of (X,r) in all cases when the cycles are not enough "dense" on X. More precisely, the following corollary is true.

Corollary 7.12: Suppose that there exists a prime divisor p of n, and an $x\in X$, such that x does not belong to a cycle of length divisible by p. Then the action of $\overline{G}$ on X is nontransitive, therefore (X,r) is decomposable.

VIII. MULTIPERMUTATION SOLUTIONS AND GENERALIZED TWISTED UNIONS

We give a description of the generalized twisted unions of solutions $Z=X\cup Y$, showing that the group $G_Y=G(Y,r_Y)$ acts as automorphisms on X, and all the elements ξ of an orbit $O(x)=O_{G_Y}(x)$ have the same action on Y see 8.3. Lemma 8.10 generalizes the cyclic condition. We give a conjecture that every multipermutation solution of level m is a generalized twisted union of multipermutation solutions of level $\leqslant m-1$. We keep the notation and conventions from the previous sections. In particular, as before we shall use both notation ${}^xy=\mathcal{L}_x(y)$ and $y^x=\mathcal{R}_x(y)$.

Definition 8.1 (Ref. 6): Let (Z,r), be a disjoint union of the solutions (X,r_X), and (Y,r_Y).

(1) (Z,r) is called *a twisted union* of X and Y if the maps $r_{XY}:X\times Y\to Y\times X$ and $r_{YX}:Y\times X\to X\times Y$ are defined as

$$r_{XY}(x,y)=(g(y),f^{-1}(x)) \tag{8.1}$$

and

$$r_{YX}(y,x)=(f(x),g^{-1}(y)), \tag{8.2}$$

where $f\in\text{Sym}(X)$, and $g\in\text{Sym}(Y)$ are fixed.

(2) (Z,r) is *a generalized twisted union* of X and Y if the map r is determined by the formula

$$r_{XY}(x,y) = (\mathcal{L}_{x|Y}(y), \mathcal{R}_{y|X}(x)), \tag{8.3}$$

where the permutations $\mathcal{L}_{x|Y} \in \mathrm{Sym}(Y)$, and $\mathcal{R}_{y|X} \in \mathrm{Sym}(X)$ satisfy the following condition:

For every $y \in Y$ the permutation $\mathcal{L}_{x^y|Y}: Y \to Y$ is independent of y, and for every $x \in X$, the permutation $\mathcal{R}_{x_y|X}: X \to X$ is independent of x.

Notation 8.2: When the element $\xi \in Z$ is specified we shall simply write, as usual, $\mathcal{L}_x(\xi)$, or ${}^x\xi$ instead of $\mathcal{L}_{x|Y}(\xi)$, respectively, $\mathcal{L}_y(\xi)$, ${}^y\xi$ instead of $\mathcal{L}_{y|X}(\xi)$.

Proposition 8.3: Let (Z,r) be union of the disjoint solutions (X,r_X) and (Y,r_Y). Then (Z,r) is a generalized twisted union of X and Y if and only if for every pair x,y, $x \in X$, $y \in Y$ the following equalities hold:

$$\mathcal{L}_{x^y|Y} = \mathcal{L}_{x|Y} = \mathcal{L}_{y_x|Y}; \tag{8.4}$$

$$\mathcal{L}_{x_y|X} = \mathcal{L}_{y|X} = \mathcal{L}_{y^x|X}. \tag{8.5}$$

Proof: Note first that the equalities (8.4) and (8.5) imply that (Z,r) is a generalized twisted union of X and Y.

Assume now that (Z,r) is a generalized twisted union of X and Y. Let $x \in X$, $y \in Y$. We have to show that for every $z \in Y$ there is an equality

$$\mathcal{L}_{x^y}(z) = \mathcal{L}_x(z). \tag{8.6}$$

By definition 8.1 the map $\mathcal{L}_{x^y|Y}: Y \to Y$ is independent of $y \in Y$. Hence for every pair $y,z \in Y$ there is an equality

$$\mathcal{L}_{x^y}(z) = \mathcal{L}_{x^z}(z). \tag{8.7}$$

By the cyclic condition in (Z,r), see (3.27), one has

$$\mathcal{L}_{x^z}(z) = \mathcal{L}_x(z). \tag{8.8}$$

Now the Eqs. (8.7) and (8.8) imply

$$\mathcal{L}_{x^y}(z) = \mathcal{L}_x(z) \tag{8.9}$$

for every $z \in Y$. We have shown that

$$\mathcal{L}_{x^y|Y} = \mathcal{L}_{x|Y} \tag{8.10}$$

for arbitrary $x \in X$ and $y \in Y$. We apply this to the pair ${}^yx \in X$ and $y \in Y$ and obtain

$$\mathcal{L}_{({}^yx)^y|Y} = \mathcal{L}_{y_x|Y}. \tag{8.11}$$

By (3.27) there is an equality,

$$({}^yx)^y = x, \tag{8.12}$$

which together with (8.11) and (8.10) implies $\mathcal{L}_{y_x|Y} = \mathcal{L}_{x|Y} = \mathcal{L}_{x^y|Y}$.

This completes the proof of (8.4). Analogous argument proves (8.5). □

Theorem 8.4: *Let (Z,r) be a generalized twisted union of the solutions (X,r_X) and (Y,r_Y), and let $G_X = G(X,r_X)$, $G_Y = G(Y,r_Y)$ be the associated Yang–Baxter groups. Suppose $O_{G_Y}(\xi_1),\ldots, O_{G_Y}(\xi_p)$ are the (distinct) orbits of the action of the group G_Y on X, and $O_{G_X}(\eta_1),\ldots, O_{G_X}(\eta_q)$ are the (distinct) orbits of the action of G_X on Y. Then the following conditions are satisfied.*

(1) *The assignment*

$$x \to \mathcal{L}_{x|Y}, \quad \textit{for all } x \in X$$

extends to a group homomorphism

$$L_X : G(X, r_X) \to Aut(Y, r_Y).$$

(2) *Let H_X denote the kernel Ker L_X. Then each orbit $O_{G_Y}(\xi_i)$, is contained in the left coset $\xi_i H_X$, i.e., $O_{G_Y}(\xi_i) \subseteq \xi_i H_X$. In particular, for every $x \in O_{G_Y}(\xi_i)$, $1 \leqslant i \leqslant p$ there is an equality*

$$\mathcal{L}_{x|Y} = \mathcal{L}_{\xi_i|Y}. \tag{8.13}$$

(3) *The assignment*

$$y \to \mathcal{L}_{y|X}, \quad \textit{for all } y \in Y$$

extends to a group homomorphism

$$L_Y : G(Y, r_Y) \to Aut(X, r_X).$$

(4) *Let H_Y denote the kernel Ker L_Y. Then $O_{G_X}(\eta_j) \subseteq \eta_j H_Y$, for $1 \leqslant j \leqslant q$. In particular, for every $y \in O_{G_X}(\eta_j)$, there is an equality*

$$\mathcal{L}_{y|X} = \mathcal{L}_{\eta_j|X}. \tag{8.14}$$

Definition 8.5 (Ref. 6): Let (X, r) be a square-free solution. Define an equivalence relation on X as $x \sim y$ if and only if $\mathcal{L}_x = \mathcal{L}_y$.

Clearly, since $\mathcal{R}_x = \mathcal{L}_x^{-1}$, one has also $x \sim y$ iff $\mathcal{R}_x = \mathcal{R}_y$. Let $X^\sim = X/\sim$. It is known, see Ref. 6, that the solution $r : X \times X \to X \times X$ induces a bijection $r^\sim : X^\sim \times X^\sim \to X^\sim \times X^\sim$, so that $(X^\sim, r^\sim)$ is a solution. It is not difficult to see that this solution is also square-free. The solution $(X^\sim, r^\sim)$ is called the *retraction of* (X, r) and is denoted by $\mathrm{Ret}(X, r)$. The solution is *retractable* if $\sim$ is a nontrivial equivalence relation, or equivalently $\mathrm{Ret}(X, r) \neq (X, r)$. In the case when $\sim$ is the trivial equivalence on X, the solution (X, r) is called *irretractable*.

Lemma 8.6: For any $x, y \in X$ the equivalence $x \sim y$ implies $xy = yx$.

Definition 8.7: Inductively, for $1 < k$ we define the retractions of higher level as $\mathrm{Ret}^k(X, r) = \mathrm{Ret}(\mathrm{Ret}^{k-1}(X, r))$.

We denote by $x^{(k)}$ the image of x in $\mathrm{Ret}^k(X, r)$. The set

$$[x^{(k)}] := \{\xi \in X \mid \xi^{(k)} = x^{(k)}\} \tag{8.15}$$

is called *the k*th *retract orbit* of x.

Definition 8.8 (Ref. 6): A solution (X, r) is called *multipermutation solution of level m* if m is the minimal nonnegative integer, such that $\mathrm{Ret}^m(X, r)$ is finite of order 1.

*Lemma 8.9: For any positive integer k, and any $x \in X$ the k*th *retract orbit $[x^{(k)}]$ is r-invariant. Furthermore, if we denote by $\mathbf{r}_{x,k}$ the corresponding solution induced by r, then $([x^{(k)}], \mathbf{r}_{x,k})$ is a multipermutation solution of level k.*

Lemma 8.10: Let (X, r) be a square-free solution. Then the following conditions hold:

(1) *For every $x, y, t \in X$, and k a positive integer,*

$$y^{(k)} = t^{(k)} \Rightarrow \left({}^y x\right)^{(k-1)} = \left({}^t x\right)^{(k-1)}. \tag{8.16}$$

(2) *For every $x, y, t \in X$*

$$y^{(2)} = t^{(2)} \Rightarrow {}^y x \sim {}^t x, \quad \textit{in particular, } {}^y t \sim t, \textit{ and } {}^t y \sim y. \tag{8.17}$$

Proof: We first prove 1. By hypothesis, $y^{(k)} = t^{(k)}$, or equivalently

$$y^{(k-1)} \sim t^{(k-1)}. \tag{8.18}$$

Let $x \in X$. Clearly,

$$yx = \xi y_1, \quad tx = \xi_1 t_1, \quad \text{for some } \xi, \xi_1, y_1, t_1 \in X. \tag{8.19}$$

This implies the following equalities in $\mathrm{Ret}^{k-1}(X,r)$;

$$y^{(k-1)}x^{(k-1)} = \xi^{(k-1)}y_1^{(k-1)}, \tag{8.20}$$

and

$$t^{(k-1)}x^{(k-1)} = \xi_1^{(k-1)}t_1^{(k-1)}.$$

It follows then from (8.18) that

$$\xi^{(k-1)} = \xi_1^{(k-1)}, \quad \text{or equivalently, } \xi^{(k-2)} \sim \xi_1^{(k-2)}. \tag{8.21}$$

By (8.19), one has $\xi = {}^{y}x$, and $\xi_1 = {}^{t}x$, which proves 1. Condition 2 follows straightforward from 1, with $k=2$, and the cyclic condition. □

Corollary 8.11: Let (X,r) be a multipermutation solution of level m, $G_X = G(X,r)$ be the associated Yang–Baxter group. Then for every $y \in X$ one has

$$O_{G_X}(y) \subseteq [y^{(m-1)}],$$

*where $O_{G_X}(y)$ is the G_X orbit of y in X, and $[y^{(m-1)}]$ is the $(m-1)$*th *retract orbit of y. In particular, $O_{G_X}(y)$ is a multipermutation solution of level at most $m-1$.*

The cyclic condition, ${}^{({}^{y}x)}(y) = {}^{x}y$ is "extended" to the class $[y^{(2)}]$ by the following lemma.

Lemma 8.12: Let (X,r) be a solution. Then the following conditions hold.

(1) *For every $x \in X$, and $z \in [y^{(2)}]$ there is an equality*

$${}^{({}^{y}x)}(z) = {}^{x}z \tag{8.22}$$

and

$$\mathcal{L}_{y_{x|[y^{(2)}]}} = \mathcal{L}_{x|[y^{(2)}]}. \tag{8.23}$$

(2) *Suppose that $[x^{(2)}] \neq [y^{(2)}]$, and the set $[y^{(2)}]$ is invariant under the left action of $G([x^{(2)}], \mathbf{r}_{x,2})$, respectively, $[x^{(2)}]$ is invariant under the left action of $G([y^{(2)}], \mathbf{r}_{y,2})$. Then the disjoint union $Z = [x^{(2)}] \cup [y^{(2)}]$ is a generalized twisted union of $[x^{(2)}]$ and $[y^{(2)}]$. Moreover, (Z, r_Z) is a multipermutation solution of level 3, where r_Z is the restriction of r on $Z \times Z$.*

Proof: Let $x \in X$, and let $z \in y^{(2)}$. We will show that (8.22) holds. It follows from (8.17) that

$${}^{y}x \sim {}^{z}x. \tag{8.24}$$

So, by the definition of $\sim$, and by the cyclic condition,

$${}^{({}^{y}x)}(z) = {}^{({}^{z}x)}(z) = {}^{x}z. \tag{8.25}$$

We have shown (8.22). Clearly, (8.22) implies (8.23). Condition 2 follows easily from 1. □

Corollary 8.13: Let (X,r) be a multipermutation solution of level 3. Then (X,r) is a generalized twisted union of multipermutation solutions of level $\leqslant 2$.

Example 8.14: Let $X = \{x, x_1, \xi, \xi_1, t, t_1, \eta, \eta_1, y, y_1\}$ and let r be determined via

$$\mathcal{L}_x = \mathcal{L}_{x_1} = (tt_1)(\eta\eta_1)(yy_1); \tag{8.26}$$

$$\mathcal{L}_{\xi} = \mathcal{L}_{\xi_1} = (t\eta)(t_1\eta_1)(yy_1); \tag{8.27}$$

$$\mathcal{L}_{t} = \mathcal{L}_{t_1} = \mathcal{L}_{\eta} = \mathcal{L}_{\eta_1} = id_X; \tag{8.28}$$

$$\mathcal{L}_{y} = \mathcal{L}_{y_1} = (x\xi)(x_1\xi_1). \tag{8.29}$$

Then $\mathrm{Ret}(X,r)=(X^{\sim},r^{\sim})$, where $X^{\sim}=\{x^{\sim},\xi^{\sim},t^{\sim},y^{\sim}\}$, and $r^{\sim}$ is determined by $\mathcal{L}y^{\sim}=(x^{\sim}\xi^{\sim})$, $\mathcal{L}_{x^{\sim}}=\mathcal{L}_{\xi^{\sim}}=\mathcal{L}_{t^{\sim}}=id_{X^{\sim}}$. Clearly, $X^{(2)}=\{y^{(2)},x^{(2)}\}$, and $\mathrm{Ret}^2(X,r)$ is the trivial solution, therefore $\mathrm{Ret}^3(X,r)=1$. In this case (X,r) is a multipermutation solution of level 3.

IX. BINOMIAL SOLUTIONS OF THE CLASSICAL YANG–BAXTER EQUATION

In this section we study a particular class of solutions of the classical Yang–Baxter equation, we call them *binomial solutions*. We show that there is a close relation between the binomial solutions of the classical Yang–Baxter equation and the *binomial skew-polynomial rings*, a class of PBW algebras, which are Artin–Schelter regular domains. These rings were introduced in Ref. 8, and studied in Refs. 9, 10, 15, 14, 21, and 19.

Definition 9.1: Let V be a finite dimensional vector space over a field k with a k-basis $X=\{x_1,\ldots,x_n\}$. Suppose the linear automorphism $R: V\otimes V\to V\otimes V$ is a solution of the Yang–Baxter equation. We say that R is *a binomial solution of the (classical) Yang–Baxter equation* or shortly *binomial solution* if the following conditions hold:

(1) For every pair $i\neq j$, $1\leqslant i,\ j\leqslant n$,

$$R(x_j\otimes x_i)=c_{ij}x_{i'}\otimes x_{j'},\quad R(x_{i'}\otimes x_{j'})=\frac{1}{c_{ij}}x_j\otimes x_i, \tag{9.1}$$

where $c_{ij}\in k\backslash\{0\}$, $i'\neq j'$.

(2) For all i, $1\leqslant i\leqslant n$

$$R(x_i\otimes x_i)=x_i\otimes x_i. \tag{9.2}$$

(3) R is *nondegenerate*, that is *the associated set-theoretic solution* $(X,r(R))$ is nondegenerate, where $r=r(R): X\times X\to X\times X$ is defined as

$$r(x_j,x_i)=(x_{i'},x_{j'})\quad \text{if } R(x_j\otimes x_i)=c_{ij}x_{i'}\otimes x_{j'}. \tag{9.3}$$

Note that definition 9.1 implies that for each binomial solution R of the Yang–Baxter equation the associated set-theoretic solution $(X,r(R))$ is square-free.

Notation 9.2: By (k,X,R) we shall denote a binomial solution of the classical Yang–Baxter equation.

Each binomial solution (k,X,R) defines a quadratic algebra $\mathcal{A}_R=\mathcal{A}(k,X,R)$, namely *the associated Yang–Baxter algebra*, in the sense of Manin.[25] The algebra $\mathcal{A}(k,X,R)$ is generated by X and has quadratic defining relations, $\mathfrak{R}(R)$ determined by R similarly to (2.7):

$$\mathfrak{R}(R)=\{(x_jx_i-c_{ij}x_{i'}x_{j'})\,|\,R(x_j\otimes x_i)=c_{ij}x_{i'}\otimes x_{j'}\}_{1\leqslant i\neq j\leqslant n}. \tag{9.4}$$

Sometimes it is more convenient to work with the free associative algebra $k\langle X\rangle$, instead of working with the tensor algebra, generated by V. Similarly to the identification of $X\times X$ and the set of X^2, we identify the vector spaces $V^{\otimes m}$ and $\mathrm{Span}_k X^m$, $m\geqslant 1$.

Theorem 9.7 gives the close relation between the binomial solutions of the classical Yang–Baxter equation and the *binomial skew-polynomial rings*. It is an analog of Theorem 2.26.

Now we recall the definition of a binomial skew-polynomial ring.

Definition 9.3 (Ref. 8): Let $\mathcal{A}_0=\mathcal{A}_0(k,X,\mathfrak{R}_0)=k\langle X\rangle/(\mathfrak{R}_0)$ be a finitely presented quadratic algebra.

(a) We say that $\mathcal{A}_0(k,X,\mathfrak{R}_0)$ is *an algebra with binomial relations of skew-polynomial type,* if the set of generators X is ordered: $X=\{x_1<x_2<\cdots<x_n\}$, and the set of defining relations

$$\mathfrak{R}_0=\{x_jx_i=c_{ij}x_{i'}x_{j'}|1\leqslant i<j\leqslant n,\},$$

contains precisely $n(n-1)/2$ quadratic square-free binomial relations such that the following three conditions hold:

(1) Each monomial xy, with $x\neq y$, $x, y\in X$ occurs in exactly one relation in $\mathfrak{R}_0$; a monomial of the type xx does not occur in any relation in $\mathfrak{R}_0$;
(2) $c_{ij}\neq 0$, for all i,j with $1\leqslant i<j\leqslant n$;
(3) For every pair, i,j with $1\leqslant i<j\leqslant n$, there are inequalities: $j>i'$, $i'<j'$.

(b) An algebra $\mathcal{A}_0=\mathcal{A}_0(k,X,\mathfrak{R}_0)$ with binomial relations of skew-polynomial type is called *a binomial skew-polynomial ring* (we refer to it also as *a skew-polynomial ring with binomial relations*, see Ref. 8) if

(4) $\mathfrak{R}_0$ is a Groebner basis of the ideal $I=(\mathfrak{R}_0)$ in the free associative algebra $k\langle X\rangle$, with respect to the degree-lexicographic ordering of the free semigroup $\langle X\rangle$.

Remark 9.4: It follows from the Diamond Lemma, cf. Ref. 4, that condition 9.3.4 is equivalent to each of the conditions (4′) and (4″) below.

(4′) The set of ordered monomials,

$$\mathcal{N}_0=\{x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}|\alpha_i\geqslant 0,1\leqslant i\leqslant n\}$$

is a k-basis of $\mathcal{A}_0$, as a k-vector space.

(4″) The monomials $x_kx_jx_i$, with $k>j>i$ do not give rise to new relations in $\mathcal{A}_0$.

Note that given the relations $\mathfrak{R}_0$, condition (4″) is recognizable.

Definition 9.5: Let $\mathcal{A}_0=\mathcal{A}_0(k,X,\mathfrak{R}_0)$ be an algebra with binomial relations of skew-polynomial-type.

Let V be the k-vector space with a basis $x_1,\ldots,x_n$. Consider the linear automorphism $R=R(\mathfrak{R}_0)$ of $V\otimes V$ defined as follows:

(a) for each pair i, j, $1\leqslant i<j\leqslant n$, we set

$$R(x_j\otimes x_i)=c_{ij}x_{i'}\otimes x_{j'},\quad 1\leqslant i<j\leqslant n,$$

$$R(x_{i'}\otimes x_{j'})=\frac{1}{c_{ij}}x_j\otimes x_i,\quad 1\leqslant i<j\leqslant n;$$

(b) for each i, $1\leqslant i\leqslant n$

$$R(x_i\otimes x_i)=x_i\otimes x_i.$$

We say that R is *the automorphism* associated with the relations $\mathfrak{R}_0$, and denote it by $R(\mathfrak{R}_0)$. We also define the bijection $r=r(\mathfrak{R}_0)$ of X^2 onto itself, as

$$r(x_jx_i)=x_{i'}x_{j'},\quad r(x_{i'}x_{j'})=x_jx_i,\quad \text{whenever } x_jx_i=c_{ij}x_{i'}x_{j'}\in\mathfrak{R}_0, \tag{9.5}$$

and

$$r(xx)=xx,\quad \text{for all } x\in X. \tag{9.6}$$

Lemma 9.6: Assume that $\mathcal{A}_0(k,X,\mathfrak{R}_0)=k\langle X\rangle/(\mathfrak{R}_0)$ is an algebra with binomial relations of skew-polynomial type, and let $R=R(\mathfrak{R}_0)$ be the automorphism of $V\otimes V$ associated with the rela-

tions $\mathfrak{R}_0$. Then R is a solution of the classical Yang–Baxter equation if and only if $\mathfrak{R}_0$ is Groebner basis.

Proof: Assume that $R=R(\mathfrak{R}_0)$ is a solution of the Yang–Baxter equation. We will prove that $\mathfrak{R}_0$ is a Groebner basis. It will be enough to show that each monomial $x_kx_jx_i$, with $k>j>i$, can be reduced by means of reductions defined via $\mathfrak{R}_0$ to a unique element of the shape $\alpha_{ijk}x_{i'}x_{j'}x_{k'}$, where $1\leqslant i'<j'<k'\leqslant n$, and α_{ijk} is a uniquely determined coefficient, $0\neq\alpha_{ijk}\in k$. Let $(X,r(R))$ be the associated set-theoretic solution, see (9.3). Denote $r^{12}=r\times id_X$, $r^{23}=id_X\times r$. Then the group ${}_{\mathrm{gr}}\langle r^{12},r^{23}\rangle$, which is isomorphic to the symmetric group S_3, acts on the set X^3. Consider the orbit $\mathcal{O}_0$ of $w=x_kx_jx_i$ under this action. It is not difficult to see that it has precisely 6 elements. By Lemma 6.5, the relations $\mathfrak{R}(r)$ form a Groebner basis, therefore the orbit $\mathcal{O}_0$ contains exactly one ordered monomial, namely some $w_0=x_{i'}x_{j'}x_{k'}$, such that $1\leqslant i'<j'<k'\leqslant n$.

Clearly, the orbit $\mathcal{O}$ of $x_kx_jx_i$ under the action of ${}_{\mathrm{gr}}\langle R^{12},R^{23}\rangle$ on kX^3 contains the same monomials of X^3 as $\mathcal{O}_0$, but, in general, they occur with nonzero coefficients which might be different from 1. In particular, $\mathcal{O}$ contains exactly one element in *normal form modulo* $\mathfrak{R}_0$, namely $\alpha x_{i'}x_{j'}x_{k'}$ where $\alpha\in k$, $\alpha\neq 0$. It is also clear that each sequence of reductions (in the sense of Ref. 4) reduces the monomial $x_kx_jx_i$ to some element of the orbit $\mathcal{O}$. It follows then, that the ambiguity $x_kx_jx_i$, $k>j>i$ is solvable, therefore $\mathfrak{R}_0$ is Groebner basis.

Conversely, let $\mathfrak{R}_0$ be a Groebner basis. Consider the associated linear automorphism $R(\mathfrak{R}_0)$ and the associated bijective map $r=r(R(\mathfrak{R}_0)):X^2\to X^2$. By Ref. 15, Theorem 1.4, r is a solution of the set-theoretic Yang–Baxter equation. Now one can easily deduce that $R(\mathfrak{R}_0)$ is a solution of the classical Yang–Baxter equation. □

Theorem 9.7: *Let V be finite-dimensional vector space over a field k, with a k-basis X. Suppose R is a linear automorphism of $V\otimes V$. Then the following conditions are equivalent:*

(1) *(k,X,R) is a binomial solution of the classical Yang–Baxter equation.*
(2) *There exists an ordering of X, $X=\{x_1<x_2<\cdots<x_n\}$, such that the associated quadratic algebra $\mathcal{A}=\mathcal{A}(k,X,R)=k\langle X\rangle/(\mathfrak{R}(R))$ is a binomial skew-polynomial ring.*

Furthermore, each of the above conditions implies that $\mathcal{A}$ is a Yang–Baxter algebra which satisfies conditions 4–11 of Theorem 6.1. In particular, $\mathcal{A}$ is PBW, a Noetherian domain, and an Artin–Schelter regular ring of global dimension n.[1,28]

Proof: (1)⇒(2). Assume (k,X,R) is a binomial solution of the classical Yang–Baxter equation. Consider the associated set-theoretic solution $(X,r(R))$. It follows from 2.26 that there exists an ordering $X=\{x_1<\cdots<x_n\}$ such that the relations $\mathfrak{R}(r(R))$ are of skew-polynomial type. Then the relations $\mathfrak{R}(R)$ of the Yang–Baxter algebra $\mathcal{A}$ associated to (k,X,R) are also of skew-polynomial-type. Now Lemma 9.6 implies that $\mathfrak{R}(R)$ is a Groebner basis, therefore $\mathcal{A}(k,X,R)$ is a skew-polynomial ring. The implication (1)⇒(2) follows from Lemma 9.6.

The remaining part of the theorem presents properties of the skew-polynomial rings with binomial relations, $\mathcal{A}_0$, which can be extracted from our previous works. The Noetherian properties were proven in Ref. 9, a combinatorial proof of the Artin–Schelter regularity of $\mathcal{A}_0$ was first given in Ref. 10. Conditions 4–11 of Theorem 6.1, have been deduced in Ref. 15 from algebraic and homological properties of the semigroups S of I-type and the associated semigroup algebras kS. □

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Recoupling Lie algebra and universal ω-algebra

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We formulate the algebraic version of recoupling theory suitable for commutation quantization over any gradation. This gives a generalization of graded Lie algebra. Underlying this is the new notion of an ω-algebra defined in this paper. ω-algebra is a generalization of algebra that goes beyond nonassociativity. We construct the universal enveloping ω-algebra of recoupling Lie algebras and prove a generalized Poincaré–Birkhoff–Witt theorem. As an example we consider the algebras over an arbitrary recoupling of $\mathbb{Z}_n$ graded Heisenberg Lie algebra. Finally we uncover the usual coalgebra structure of a universal envelope and substantiate its Hopf structure. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1789281]

I. INTRODUCTION

Graded Lie algebra[1–3] is of fundamental importance in quantum theory. It is the algebraic structure necessary to introduce a commutator (for bosons) and anticommutator (for fermions) to achieve quantization of a physical system. The universal enveloping algebra provides creation and annihilation operators which generate ensembles of particles. These particles must form representations of symmetries present in the physical system and as such must satisfy an appropriate recoupling theory. In Joyce[4] from broad physical requirements the most general form of a recoupling theory was deduced. This leads to a complete representation theory[5–9] generalizing the Racah–Wigner calculus.[10–14] The process of recoupling could at best introduce recoupling phases for associativity, commutativity, and identity graded according to some Abelian group. For example, this Abelian group is $\mathbb{Z}_n$ for SU(n). Usually the identity and associativity are implicity taken to be unity. However, Joyce[4,15] demonstrated that for SU(3) color this restriction admitted no Bose–Fermi recoupling. Moreover, it was shown that nonassociative recoupling phases breaking the pentagon condition were crucial.

In the associative case the commutativity phase factors are precisely the color (or commutation) factors of color algebra.[16–21] The general case is a nontrivial extension which is necessary in order to accommodate SU(3) color. This paper reviews the recoupling phases and defines the extension of graded Lie algebra (or color algebra) embodying the general recoupling situation, called *recoupling Lie algebra*.

There is no acceptable notion of universal enveloping algebra. For example, Isaac *et al.*[22] investigated SU(3) color. Although an apparent confinement mechanism[23] analogous to the octonion confinement principle of Günaydin and Gürsey[24] applies the envelope itself is finite. For example, the Bose–Fermi deformativity phase for two mesons is $\xi_{1,2,1,2}=-1$ prohibiting the existence of such a composite. This would run contrary to the existence of boundless multiple mesonic (and baryonic) states observed in nature. The difficulty arises because any universal envelope based on the pentagon constraint, such as an algebra, is too restrictive. The solution is to be found in the new notion of an ω-algebra. This is an extension of algebra where such statements as $(ab)(cd)$, ambiguous in the sense that there is no unique order in which to evaluate, are avoided. In ω-algebra this example would be either $(ab)_1(cd)_2$ or $(ac)_2(cd)_1$. The first (respectively, second)

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evaluates *ab* after (respectively, before) *cd*. Using this notion we construct a universal enveloping ω-algebra and prove the corresponding ω-Poincaré–Birkhoff–Witt theorem under suitable conditions. Note that the proof does not utilize the notion of an ω-module which would parallel the standard proof. (See, for example, Knapp.[25]) We uncover the usual coalgebra structure of the universal enveloping ω-algebra and describe its Hopf structure.

Given the natural extension of algebra given by ω-algebra it is natural to consider in general omegafied structures. Particularly, ω-coalgebra, ω-bialgebra, Hopf ω-algebra, ω-modules, ω-comodules, and ω-tensor product. The last leading to a notion of ω-Fock space. All these require a general theory of ω-monoidal category theory.[26]

The last 20 years or so has seen the intense development of braided structures[27–29] in mathematics and physics. We suggest that any equally intense focus should be given to generalizations of nonassociative structures. Let us not forget the important role that nonassociative structures already play in physics. The most notable example being Lie alegbra.[25] For a survey of nonassociative structures in physics see Lõhmus *et al.*[30]

II. SYMMETRIC UNITAL PSEUDOMONOIDAL RECOUPLING

We begin with the constraints on the recoupling phase factors of a unital symmetric premonoidal recoupling as derived in Joyce.[4] This is a special case of the full premonoidal theory[31,32] and admits nonassociative recouplings. Given an Abelian group $\mathbb{A}$ then a recoupling is determined by its phase factors, compactly written as the maps

$$\xi:\mathbb{A}^4 \to S^1,\ \ (m,n,p,q) \mapsto \xi_{m,n,p,q}, \tag{1}$$

$$\alpha:\mathbb{A}^3 \to S^1,\ \ (m,n,p) \mapsto \alpha_{m,n,p}, \tag{2}$$

$$\gamma:\mathbb{A}^2 \to S^1,\ \ (m,n) \mapsto \gamma_{m,n}, \tag{3}$$

$$\lambda:\mathbb{A} \to S^1,\ \ m \mapsto \lambda_m, \tag{4}$$

$$\rho:\mathbb{A} \to S^1,\ \ m \mapsto \rho_m \tag{5}$$

for all $m,n,p,q \in \mathbb{A}$ where $S^1 \subset \mathbb{C}\backslash\{0\}$ is the unit circle. Note that the restriction to S^1 could be generalized to the invertible elements of any field. These phases define, respectively, recouplings for deformativity, associativity, commutativity, and left and right identity. It turns out to be useful to define a further phase map

$$\beta:\mathbb{A}^3 \to S^1,\ \ (n,m,p) \mapsto \beta_{n,m,p} = \frac{\alpha_{m,n,p}\alpha_{n,p,m}}{\alpha_{n,m,p}} \tag{6}$$

for all $m,n,p \in \mathbb{A}$. The phases are constrained by

$$\xi_{m,n,p,q} = \frac{\alpha_{m,n,p}\alpha_{m,n+p,q}\alpha_{n,p,q}}{\alpha_{m+n,p,q}\alpha_{m,n,p+q}}, \tag{7}$$

$$\xi_{m,n,p,q} = \xi_{n,m,p,q}, \tag{8}$$

$$\xi_{p,q,m,n} = \frac{1}{\xi_{m,n,p,q}}, \tag{9}$$

$$\gamma_{m,n+p} = \frac{\gamma_{m,n}\gamma_{m,p}}{\beta_{n,m,p}}, \tag{10}$$

$$\gamma_{n,m} = \frac{1}{\gamma_{m,n}}, \tag{11}$$

$$\lambda_{m+n} = \frac{\lambda_m}{\alpha_{0,m,n}}, \tag{12}$$

$$\rho_m = \alpha_{m,0,n}\lambda_n, \tag{13}$$

$$\rho_{m+n} = \alpha_{m,n,0}\rho_n \tag{14}$$

for all $m,n,p,q,r \in \mathbb{A}$. Note that (7) provides a formula for $\xi_{m,n,p,q}$ and (13) provides a formula for ρ_m. Thus ξ and ρ are entirely redundant, as of course is β. Finally we denote the $\mathbb{A}$ graded recoupling by the triplet (α,γ,λ). The set of recouplings for a given Abelian group $\mathbb{A}$ is denoted $R_{\mathbb{A}}$. This is itself an Abelian group with addition given by pointwise multiplication $(\alpha_1,\gamma_1,\lambda_1)+(\alpha_2,\gamma_2,\lambda_2)=(\alpha_1\cdot\alpha_2,\gamma_1\cdot\gamma_2,\lambda_1\cdot\lambda_2)$. Clearly the identity is the recoupling with all phases one and the inverse is given by $-(\alpha,\gamma,\lambda)=(1/\alpha,1/\gamma,1/\lambda)$.

We make the following observations. Due to (10) we have

$$\beta_{p,m,n} = \beta_{n,m,p}. \tag{15}$$

The constraints (8) and (9) imply the condition

$$\xi_{m,n,p,q} = \xi_{m,n,q,p}. \tag{16}$$

Taking $n=0$ in (12) gives

$$\alpha_{0,m,0} = 1. \tag{17}$$

Hence (13) with $m=n=0$ shows $\lambda_0=\rho_0$. Thus (12) with $m=0$ provides us with a formula for λ_m, and (13) with $n=0$ a formula for ρ_m, in terms of λ_0, $\alpha_{m,0,0}$, and $\alpha_{0,0,m}$,

$$\lambda_m = \frac{\lambda_0}{\alpha_{0,0,m}}, \tag{18}$$

$$\rho_m = \alpha_{m,0,0}\lambda_0. \tag{19}$$

Substituting these formulas back into (12), (13), and (14) gives formulas for α when one index is 0,

$$\alpha_{m,n,0} = \frac{\alpha_{m+n,0,0}}{\alpha_{n,0,0}}, \tag{20}$$

$$\alpha_{m,0,n} = \alpha_{m,0,0}\alpha_{0,0,n}, \tag{21}$$

$$\alpha_{0,m,n} = \frac{\alpha_{0,0,m+n}}{\alpha_{0,0,m}}, \tag{22}$$

for all m, $n \in \mathbb{A}$. Taking $n=p=0$ in (10) gives

$$\gamma_{m,0} = \alpha_{m,0,0}\alpha_{0,0,m}. \tag{23}$$

In particular $\gamma_{0,0}=1$. Substituting into (7) using (20), (21), and (22) gives

$$\xi_{m,n,p,q} = 1, \tag{24}$$

whenever $m=0$, $n=0$, $p=0$ or $q=0$. Thus we have the following two choices of independent phases given by λ_0, λ_m, and ρ_m where $m \in \mathbb{A}\backslash\{0\}$ or λ_0, $\alpha_{m,0,0}$, and $\alpha_{0,0,m}$ where $m \in \mathbb{A}\backslash\{0\}$.

Let **Rcp** be the category of recouplings whose objects are recouplings $(\alpha, \gamma, \lambda)$ and whose morphisms $(\alpha, \gamma, \lambda) \to (\alpha', \gamma', \lambda')$ are group homomorphisms $\phi: \mathbb{A}' \to \mathbb{A}$ satisfying

$$\alpha(\phi \times \phi \times \phi) = \alpha', \tag{25}$$

$$\gamma(\phi \times \phi) = \gamma', \tag{26}$$

$$\lambda\phi = \lambda'. \tag{27}$$

A recoupling $(\alpha, \gamma, \lambda)$ is called reducible if there is a group $\mathbb{A}'$ of lower cardinality than $\mathbb{A}$ and an epimorphism $\phi: (\alpha', \gamma', \lambda') \to (\alpha, \gamma, \lambda)$. (That is, $\phi: \mathbb{A} \to \mathbb{A}'$ is onto.) Whenever such a morphism exists the recoupling is constant on each fiber $\phi^{-1}(a')$. This gives an isomorphism between the typical fiber $\mathrm{Ker}\,\phi = \phi^{-1}(0)$ direct product the base space $\mathrm{coKer}\,\phi = \mathbb{A}'$ and $\mathbb{A}$. Equivalently, $\mathbb{A}/\mathrm{Ker}\,\phi \cong \mathbb{A}'$.

Example 1: Let $\mathbb{A}' \subset \mathbb{A}$ then we may extended any recoupling $(\alpha', \gamma', \lambda')$ on $\mathbb{A}'$ to a recoupling $(\alpha, \gamma, \lambda)$ on $\mathbb{A}$ as follows. Let $\phi: \mathbb{A}/\mathbb{A}' \to \mathbb{A}$ be a mapping satisfying $\phi(m+\mathbb{A}') \in m+\mathbb{A}'$, that is a choice function. Given $m \in \mathbb{A}$ there is a unique $\hat{m} \in \mathbb{A}'$ such that $m = \hat{m} + \phi(m+\mathbb{A}')$. Thus we define the reducible recoupling on $\mathbb{A}$ (reducible to $\mathbb{A}'$) by $\alpha_{m,n,p} = \alpha'_{\hat{m},\hat{n},\hat{p}}$, $\gamma_{m,n} = \gamma'_{\hat{m},\hat{n}}$, and $\lambda_m = \lambda'_{\hat{m}}$.

III. ALGEBRAIC RECOUPLING THEORY

We develop an extension of graded Lie algebra[1–3] utilizing the recoupling phase theory summerized in the preceding section. In this paper we let $\mathbb{N}_+ = \{1, 2, 3, \ldots\}$ be the multiplicative monoid of natural numbers, and $\mathbb{N} = \{0\} \cup \mathbb{N}_+ = \{0, 1, 2, \ldots\}$ the additive monoid of natural numbers.

Definition 1: A recoupling Lie algebra for a symmetric unital recoupling $(\alpha, \gamma, \lambda)$ over an Abelain group $\mathbb{A}$ is an $\mathbb{A}$ graded vector space

$$\mathcal{L} = \bigoplus_{m \in \mathbb{A}} \mathcal{L}_m, \tag{28}$$

and an $\mathbb{A}$ graded bilinear map $[\_, \_]: \mathcal{L} \otimes \mathcal{L} \to \mathcal{L}$ called the commutator taking $a \otimes b \mapsto [a, b]$ satisfying

(i) *Recoupling skew-symmetry,*

$$[a, b] = -\gamma_{m,n}[b, a] \tag{29}$$

for all $a \in \langle\mathcal{L}\rangle_m$ and $b \in \langle\mathcal{L}\rangle_n$.

(ii) *Recoupling Jacobi identity,*

$$\alpha_{m,p,n}[[a, b], c] - \alpha_{m,n,p}\gamma_{n,p}[[a, c], b] - \alpha_{m,n,p}\alpha_{m,p,n}[a, [b, c]] = 0 \tag{30}$$

for all $a \in \langle\mathcal{L}\rangle_m$, $b \in \langle\mathcal{L}\rangle_n$, and $c \in \langle\mathcal{L}\rangle_p$.

The commutator is a multiplication for $\mathcal{L}$ making it an algebra. The grade zero component $\langle\mathcal{L}\rangle_0$ is a Lie subalgebra of $\mathcal{L}$ and has the adjoint action on $\mathcal{L}$.

Given two recoupling Lie algebras $\mathcal{L}$ and $\mathcal{L}'$ over the same recoupling we can form the direct sum recoupling Lie algebra $\mathcal{L} \oplus \mathcal{L}'$ which is the direct sum of the underlying vector spaces with the bracket defined by

$$[a \oplus a', b \oplus b'] = [a,b] \oplus 0 + 0 \oplus [a',b'], \tag{31}$$

where a, b, a', $b' \in \mathcal{L}$. It is easy to see that the recoupling skew-symmetry and Jacobi identities hold.

If $\mathbb{A}=\mathbb{Z}_1$ there is only the trivial choice of recoupling and hence $\mathcal{L}$ (with the commutator) is a Lie algebra. For $\mathbb{Z}_2$ one can take all phases one except $\gamma_{1,1}=\pm 1$. If $\gamma_{1,1}=1$ then $\mathcal{L}$ is a Lie algebra, otherwise $\gamma_{1,1}=-1$ and $\mathcal{L}$ is a super Lie algebra. For $\mathbb{A}=\mathbb{Z}_N$ with α and λ trivial we obtain $\gamma_{m,n}=\gamma_{1,1}^{mn}$. If $\gamma_{1,1}=1$ we have a Lie algebra, otherwise $\gamma_{1,1}=-1$ and N is even giving the $\mathbb{Z}_N$ graded Lie algebras of Green.[16] Moreover, these recouplings are reducible to the $\mathbb{Z}_2$ recoupling with $\gamma_{1,1}=-1$.

IV. ω-ALGEBRA

Nonassociative recoupling requires a generalization of the notion of an algebra. This will allow us to define universal envelopes, prove a corresponding Poincaré–Birkhoff–Witt theorem and deduce a generalized Hopf structure.

Definition 2: A weak ω-algebra consists of a vector space $\mathcal{A}$, a family of symmetric subspaces $\mathcal{D}_n$ of $\mathcal{A}\otimes\mathcal{A}$ for all $n\in\mathbb{N}_+$ such that $\mathcal{D}_m\subset\mathcal{D}_n$ whenever $m<n$, and a family of linear maps $\mu_m:\mathcal{D}_m\to\mathcal{A}$ for all $m\in\mathbb{N}_+$.

To simplify notation we write $\mu_m(a\otimes b)$ as $(ab)_m$. Recall that symmetry of $\mathcal{D}_m$ means $a\otimes b \in \mathcal{D}_m$ if and only if $b\otimes a\in\mathcal{D}_m$.

An enhanced coupling tree is a rooted planar binary tree t whose set of nodes is a finite subset of $\mathbb{N}$ such that the root node is 0 and every sequence of nodes from the root node to a leaf node is an increasing sequence. Let $|t|$ represent the number of its leaves, $\{t\}_E\subset\mathbb{N}$ the set of nodes and $\{t\}\subset\{t\}_E$ the nodes of t that are not leaves nor the root. Let T_E denote the set of enhanced coupling trees. We define two useful families of cutting operations on T_E. Let $m\in\mathbb{N}$ then we define, respectively, the upper and lower cut operations $\vee_m$, $\wedge_m: T_E\to T_E$ as follows. Given $t\in T_E$ cut the edge joining m to its immediate descendent. The tree containing m is taken to be $\vee_m t$ (the empty tree if $m\notin\{t\}_E$) and $\wedge_m t$ the portion remaining. Two enhanced coupling trees s and t are equivalent, written $s\sim t$, if the trees with the leaf and root edges and nodes removed are identical. Each equivalence class is called a coupling tree. The set of coupling trees is denoted $T=T_E/\sim$.

Let $t\in T$ then we define $\mathcal{D}_t$ inductively to be the linear span of all $a_1\otimes\cdots\otimes a_{|t|}\in\mathcal{A}^{\otimes|t|}$ such that $a_j\otimes a_k\in\mathcal{D}_m$ for all $l\leqslant j<k\leqslant|t|$ and

$$a_1\otimes\cdots\otimes a_{i-1}\otimes\mu_m(a_i\otimes a_{i+1})\otimes a_{i+2}\otimes\cdots\otimes a_{|t|}\in\mathcal{D}_{\wedge_m t}, \tag{32}$$

where $m=\sup\{t\}$ and m was attached to the ith leaf of $\wedge_m t$. If t is the tree with two leaves and the single internal node m then $\mathcal{D}_t=\mathcal{D}_m$. If $t=|$ is the unique tree consisting of a single edge then $\mathcal{D}_t=\mathcal{A}$ or the empty tree $t=\emptyset$ then $\mathcal{D}_t=\{0\}$. Now we can define the product map $\mu_t:\mathcal{D}_t\to\mathcal{A}$ of $|t|$ factors given by t. Inductively this is defined by

$$\mu_t(a_1\otimes\cdots\otimes a_{|t|})=\mu_{\wedge_m t}(1^{\otimes i-1}\otimes\mu_m\otimes 1^{\otimes|t|-i-1}), \tag{33}$$

where $m=\sup\{t\}$ and m was attached to the ith leaf of $\wedge_m t$.

With this notation we can easily define the important notion of a (strong) ω-algebra.

Definition 3: A (strong) ω-algebra $\mathcal{A}$ is a weak ω-algebra such that given $s,t\in T$ and $m\in\mathbb{N}_+$ then whenever $\{s\}\cap\{t\}=\emptyset$ and $\inf\{s\}$, $\inf\{t\}>m$ we have $\mu_s(\mathcal{D}'_s)\otimes\mu_t(\mathcal{D}'_t)\subset\mathcal{D}_m$ whenever $\mathcal{D}'_s\otimes\mathcal{D}'_t\subset\mathcal{D}_{(st)_m}$. *The ω-algebra is called strict if whenever s,t are such that $\{s\}\cap\{t\}\neq\emptyset$ or* $\inf\{s\}$, $\inf\{t\}>m$ *then we have that the intersection of the span of $\{\mu_s(\mathcal{D}'_s)\otimes\mu_t(\mathcal{D}'_t):\mathcal{D}'_s\otimes\mathcal{D}'_t\subset\mathcal{D}_{(st)_m}\}$* with $\mathcal{D}_m$ is empty.

Define $\mathcal{A}_m=\{a\in\mathcal{A}:$ there is $b\in\mathcal{A}$ with $a\otimes b\in\mathcal{D}_m\}$. Thus $\mathcal{A}_n\subset\mathcal{A}_m$ whenever $m<n$ and $\mu_{m+1}(\mathcal{D}_{m+1})\subset\mathcal{A}_m$. An ω-algebra is called unital if there is $1\in\mathcal{A}_1$ such that $1\otimes a\in\mathcal{D}_m$ for all $a\in\mathcal{A}_m$ and

$$\mu_m(1 \otimes a) = \mu_m(a \otimes 1) = a \tag{34}$$

for all $a \in \mathcal{A}_m$ and $m \in \mathbb{N}_+$. We write this as $(1a)_m = a = (a1)_m$. Note that a unital ω-algebra cannot be strict. An ω-algebra is called associative if

$$\mu_m(\mu_n(a \otimes b) \otimes c) = \mu_m(a \otimes \mu_n(b \otimes c)), \tag{35}$$

for all $a \otimes b,\ b \otimes c \in \mathcal{D}_n$ and $m < n$. This may be written in the compact form $((ab)_n c)_m = (a(bc)_n)_m$. And commutative if

$$\mu_m(a \otimes b) = \mu_m(b \otimes a) \tag{36}$$

for all $a \otimes b \in \mathcal{D}_m$ and $m \in \mathbb{N}_+$.

Every algebra is an ω-algebra with $\mathcal{D}_m = \mathcal{A} \otimes \mathcal{A}$ and $\mu_m = \mu$ for all $m \in \mathbb{N}_+$. Given an algebra $\mathcal{A}$ then one may construct the ω-algebra $\omega[\mathcal{A}]$ over $\mathcal{A}$ as follows. Consider the vector space $\mathcal{A}\{\mathcal{P}(\mathbb{N}_+)\}$ built from the finite power Abelian monoid $\mathcal{P}(\mathbb{N}_+)$ of finite subsets of $\mathbb{N}_+$. A typical element is a finite formal sum $a = \Sigma_{P \in \mathcal{P}(\mathbb{N}_+)} a^P P$ with $a^P \in \mathcal{A}$. That is, only a finite number of the coefficients are nonzero. A multiplication is given by

$$ab = \sum_{P,Q \in \mathcal{P}(\mathbb{N}_+)} a^P b^Q P \cup Q. \tag{37}$$

Take $\omega[\mathcal{A}]$ to be the vector space $\mathcal{A}\{\mathcal{P}(\mathbb{N}_+)\}$. Let $\mathcal{D}_n$ be the linear span of $\{a \otimes b \in \omega[\mathcal{A}] \otimes \omega[\mathcal{A}] : a^P, b^Q \neq 0$ implies $P \cap Q = \varnothing$ and $(P \cup Q) \cap \{1, \ldots, n\} = \varnothing$ for all $P, Q \in \mathcal{P}(\mathbb{N}_+)\}$ then $\mathcal{A}_m = \{a \in \omega[\mathcal{A}] : a^P \neq 0$ implies $P \cap \{1, \ldots, m\} = \varnothing$ for all $P \in \mathcal{P}(\mathbb{N}_+)\}$. We define the bilinear maps $\mu_m : \mathcal{D}_m \to \omega[\mathcal{A}]$ by

$$(ab)_m = \sum_{P,Q \in \mathcal{P}(\mathbb{N}_+)\setminus\{\varnothing\}} a^P b^Q P \cup Q \cup \{m\} + \sum_{P \in \mathcal{P}(\mathbb{N}_+)\setminus\{\varnothing\}} (a^P b^\varnothing + a^\varnothing b^P) P + a^\varnothing b^\varnothing \varnothing \tag{38}$$

for all $a \otimes b \in \mathcal{D}_m$. If $\mathcal{A}$ is unital then so is $\omega[\mathcal{A}]$ with unit $\varnothing$. If $\mathcal{A}$ is associative (respectively, commutative) then so is $\omega[\mathcal{A}]$.

An important construction is the free ω-algebra over coupling trees. Let $\mathbb{C}\{T\}$ the vector space freely generated by T. Let $\mathcal{D}_m$ be the subspace spanned by the coupling trees $s \otimes t \in \mathbb{C}\{T\} \otimes \mathbb{C}\{T\}$ where s, t have no labels in common and all labels greater than m. We define $\mu_m : \mathcal{D}_m \to \mathbb{C}\{T\}$ to be given by joining the roots of the coupling trees s, t to the node m. Thus m is the root of the joined tree $(st)_m$. The unit is the tree with no leaves.

One may form the tensor product of two ω-algebras $\mathcal{A}$ and $\mathcal{A}'$ as follows. Let $\mathcal{A} \otimes \mathcal{A}'$ be the usual tensored vector space. Define the trivial symmetric braid $R : \mathcal{A}' \otimes \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}'$ by $R(a' \otimes a) = a \otimes a'$ for all $a \in \mathcal{A}$ and $a' \in \mathcal{A}'$. The bilinear products $\mu'' : \mathcal{D}''_m \to \mathcal{A} \otimes \mathcal{A}'$ are given by $\mu''_m = (\mu_m \otimes \mu'_m)(1 \otimes R \otimes 1)$ and

$$\mathcal{D}''_m = \{f \otimes g \otimes h \otimes k \in (\mathcal{A} \otimes \mathcal{A}')^{\otimes 2} : f \otimes h \in \mathcal{D}_m \text{ and } g \otimes k \in D'_m\}. \tag{39}$$

In particular we have

$$\mu''_m(f \otimes g \otimes h \otimes k) = \mu_m(f \otimes h) \otimes \mu'_m(g \otimes k) \tag{40}$$

for all $g \in \mathcal{A}'$, $h \in \mathcal{A}$, and $m \in \mathbb{N}_+$. It is straightforward to check that this does indeed define an ω-algebra. If $\mathcal{A}$ and $\mathcal{A}'$ are unital then so is $\mathcal{A} \otimes \mathcal{A}'$ with unit $1 \otimes 1'$. If $\mathcal{A}$ and $\mathcal{A}'$ are associative (respectively, commutative) then $\mathcal{A} \otimes \mathcal{A}'$ is associative (respectively, commutative).

A morphism of ω-algebras is a linear map $\phi : \mathcal{A} \to \mathcal{A}'$ satisfying

$$(\phi \otimes \phi)\mathcal{D}_m \subset \mathcal{D}'_m, \tag{41}$$

$$\phi\mu_m = \mu'_m(\phi \otimes \phi) \tag{42}$$

for all $m \in \mathbb{N}_+$. It follows that $\phi\mathcal{A}_m \subset \mathcal{A}'_m$.

An ω-algebra $\mathcal{A}$ is called a derived ω-algebra $\mathcal{A}'$ if there is an isomorphism $\phi: \mathcal{A} \to \omega[\mathcal{A}']$. Moreover, this isomorphism is weakly universal from $\mathcal{A}$ to $\omega[\mathcal{A}']$. Hence given another algebra $\mathcal{B}$ such that $\mathcal{A} \cong \omega[\mathcal{B}]$ then $\mathcal{A}' \cong \mathcal{B}$. Similarly we can conclude that $\omega[\mathcal{A}' \otimes \mathcal{A}''] \subset \omega[\mathcal{A}'] \otimes \omega[\mathcal{A}'']$ for all algebras $\mathcal{A}'$ and $\mathcal{A}''$ by considering the subset $\mathcal{A}''\emptyset$ of $\omega[\mathcal{A}'']$.

An ω-algebra $\mathcal{A}$ is $\mathbb{A}$ graded if the underlying vector space and bilinear products are all $\mathbb{A}$ graded. In detail, if

$$\mathcal{A} = \bigoplus_{p \in \mathbb{A}} \mathcal{A}_p \tag{43}$$

then define $\langle \mathcal{D}_m \rangle_{p,q} = \{d \in \langle \mathcal{A} \rangle_p \otimes \langle \mathcal{A} \rangle_q : d \in \mathcal{D}_m\}$ for all $p, q \in \mathbb{A}$ and $m \in \mathbb{N}_+$, then we have that

$$\mathcal{D}_m = \bigoplus_{(p,q) \in \mathbb{A}^2} \langle \mathcal{D}_m \rangle_{p,q}. \tag{44}$$

The bilinear product is $\mathbb{A}$ graded if $\mu_m \langle \mathcal{D}_m \rangle_{p,q} \subset \langle \mathcal{A} \rangle_{p+q}$. In particular the free algebra $\mathbb{C}[T]$ over coupling trees is $\mathbb{Z}$ graded because the monoid T is $\mathbb{Z}$ graded by leaf number.

An $\mathbb{A}$ graded ω-algebra $\mathcal{A}$ is called a recoupling ω-algebra if there is a recoupling $(\alpha, \gamma, \lambda)$ and $\hbar \in \langle \mathcal{A}_1 \rangle_0$ over $\mathbb{A}$ such that

$$((ab)_n c)_m = \alpha_{k,l,p}(a(bc)_n)_m, \tag{45}$$

$$(ab)_m = \gamma_{k,l}(ba)_m, \tag{46}$$

$$(\hbar a)_m = \lambda_k a, \tag{47}$$

$$(a\hbar)_m = \rho_k a \tag{48}$$

for all $a \in \langle \mathcal{A} \rangle_k$, $b \in \langle \mathcal{A} \rangle_l$, $c \in \langle \mathcal{A} \rangle_p$, and $m, n \in \mathbb{N}_+$ such that $m < n$. No recoupling ω-algebra is strict.

V. UNIVERSAL ENVELOPING ω-ALGEBRA

In order to give the construction of universal enveloping ω-algebra we need some preliminary structures. Let $T^* \supset T$ be the set of coupling trees with nodules attached to some leaves. Given a set X, let $T^*(X)$ be the ω-monoid of (noduled) coupling trees over X. That is the set of coupling trees whose leaves are labeled by elements of $X \amalg \{\circ\}$ where $\circ$ denotes the nodule. Thus $(t, \mathbf{x}) \in T^* \times X^n$, where n is the number of leaves of t less the number of attached nodules, is composed of a coupling tree t whose nodule-free leaves are labeled (in order) by the n-tuple $\mathbf{x}$. $T^*(X)$ inherits the ω-multiplication from T^* given by

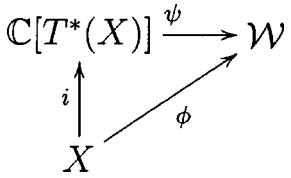
$$((s, \mathbf{x})(t, \mathbf{y}))_m = ((st)_m, \mathbf{xy}), \tag{49}$$

where $\mathbf{xy}$ is the concatenate of the tuples $\mathbf{x}$ and $\mathbf{y}$. The unit is the tree with no leaves. This ω-monoid is $\mathbb{Z} \times \mathbb{Z}$ graded by leaf and nodule number. In order to construct the free ω-algebra over $T^*(X)$ we need the notion of an ω-ideal.

Definition 4: Given an ω-algebra $\mathcal{A}$, a left (*respectively, right*) *ω-ideal $\mathcal{J}$ is a subspace of $\mathcal{A}$ such that for all $m \in \mathbb{N}_+$, $a \in \mathcal{A}$ and $b \in \mathcal{J}$ such that $a \otimes b \in \mathcal{D}_m$ we have $(ab)_m \in \mathcal{J}$* [*respectively, $(ba)_m \in \mathcal{J}$*]. *An ω-ideal is both a left and right ω-ideal.*

Let $\mathbb{C}[T^*(X)]$ be the vector space freely generated by $T^*(X)$. An ω-multiplication is given by $\mu_m(\Sigma_k a^k(s_k, \mathbf{x}_k), \Sigma_l b^l(t_l, \mathbf{y}_l)) = \Sigma_{k,l} a^k b^l((s_k t_l)_m, \mathbf{x}_k \mathbf{y}_l)$ where $a^k b^l \in \mathbb{C}$, $s_k \otimes t_l \in \mathcal{D}_m$, $\mathbf{x}_k \in X^{|s_k|}$ and $\mathbf{y}_l \in X^{|t_l|}$. Clearly $\mathbb{C}[T^*(X)]$ is a unital ω-algebra. We call it the free ω-algebra over X. Moreover, it

has the following universal property. Let $i:X\to\mathbb{C}[T^*(X)]$ be the insertion map $x\mapsto(|,x)$ where $|$ is the unique coupling tree with one leaf. Given any unital ω-algebra $\mathcal{W}$ and mapping $\phi:X\to\mathcal{W}$ there is a unique $\psi:\mathbb{C}[T^*(X)]\to\mathcal{W}$ such that



commutes. If $X=\oplus_{m\in A}\langle X\rangle_m$ is $\mathbb{A}$-graded then so is $T^*(X)$ and hence $\mathbb{C}[T^*(X)]$. Each coupling tree $t\in T^*$ defines a canonical map $t:X\to T^*(X)$ given by $t\mathbf{x}=(t,\mathbf{x})$. Given a coupling tree t with n leaves and $\mathbf{x}\in X^n$ where each x_k is of grade m_k then $t\mathbf{x}$ has grade $m_1+\cdots+m_n$.

Given a recoupling Lie algebra $\mathcal{L}$ let X be an $\mathbb{A}$-graded basis for $\mathcal{L}$. We write $X=X_+\amalg X_-$ where the grade m of any member of $X_\pm$ satisfies $\gamma_{m,m}=\pm1$, respectively. The universal enveloping algebra of $\mathcal{L}$ is defined to be

$$\mathcal{U}(\mathcal{L})=\mathbb{C}[T^*(X)]/\mathcal{J}, \tag{50}$$

where $\mathcal{J}$ is the ideal with generators

$$((r\mathbf{x}s\mathbf{y})_l t\mathbf{z})_k-\alpha_{m,n,p}(r\mathbf{x}(s\mathbf{y}t\mathbf{z})_l)_k, \tag{51}$$

$$(xy)_k-\gamma_{m,n}(yx)_k-[x,y], \tag{52}$$

$$(\circ r\mathbf{x})_k-\lambda_m r\mathbf{x}, \tag{53}$$

$$(r\mathbf{x}\circ)_k-\rho_m r\mathbf{x}, \tag{54}$$

where $r,s,t\in T^*(X)$ have, respectively, u, v, and w leaves, $\mathbf{x}\in X^u$, $\mathbf{y}\in X^v$, and $\mathbf{z}\in X^w$ are of grades m, n, and p, respectively, $x\in\langle X\rangle_m$, $y\in\langle X\rangle_n$, and $k<l$. The symbol $\circ$ represents the unique tree with a single leaf that has a nodule attached. The universal enveloping algebra $\mathcal{U}(\mathcal{L})$ has the following universal property.

Proposition 1: Given an ω-algebra $\mathcal{W}$ and linear map $\phi:\mathcal{L}\to\mathcal{W}$ satisfying

$$((r\phi^u(\mathbf{a})s\phi^v(\mathbf{b}))_l t\phi^w(\mathbf{c}))_k-\alpha_{m,n,p}(r\phi^u(\mathbf{a})(s\phi^v(\mathbf{b})t\phi^w(\mathbf{c}))_l)_k, \tag{55}$$

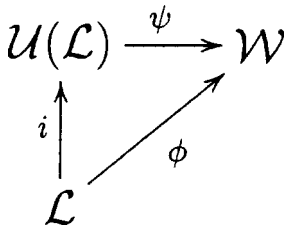
$$(\circ r\phi^u(\mathbf{a}))_k=\lambda_m r\phi^u(\mathbf{a}), \tag{56}$$

$$(r\phi^u(\mathbf{a})\circ)_k=\rho_m r\phi^u(\mathbf{a}) \tag{57}$$

for all $r,s,t\in T^*$ with, respectively, u, v, and w leaves, $\mathbf{a}\in\langle\mathcal{L}^u\rangle_m$, $\mathbf{b}\in\langle\mathcal{L}^v\rangle_n$, $\mathbf{c}\in\langle\mathcal{L}^w\rangle_p$ and $k<l$, and satisfying

$$\phi([a,b])=(\phi(a)\phi(b))_k-\gamma_{m,n}(\phi(b)\phi(a))_k \tag{58}$$

for all $a\in\langle\mathcal{L}\rangle_m$, $b\in\langle\mathcal{L}\rangle_n$ and $k\in\mathbb{N}_+$, then there is a unique morphism $\psi:\mathcal{U}(\mathcal{L})\to\mathcal{W}$ such that



commutes.

The universal $\mathcal{U}(\mathcal{L})$ is of course defined up to isomorphism. The universal envelope $\mathcal{U}(\mathcal{L})$ inherits an $\mathbb{A}\times\mathbb{Z}$ grading from the free ω-algebra $\mathbb{C}[T^*(X)]$ or equivalently the ω-monoid $T^*(X)$. The $\mathbb{Z}$ grading corrresponding to nodule number is lost because of (53) or (54). We write

$$\mathcal{U}(\mathcal{L}) = \bigoplus_{m\in Z} \mathcal{U}(\mathcal{L})_m, \tag{59}$$

where $\mathcal{U}(\mathcal{L})_m$ is generated by trees with m nodule free leaves.

VI. THE GROUPOID OF UNIVERSAL ω-ALGEBRA

In this section we reveal the combinatorics underlying universal ω-algebra. These results are fundamental to the proof of the ω-Poincaré–Birkhoff–Witt theorem in the next section. The ω-monoidal groupoid of interest is built from the ω-monoidal groupoid of noduled coupling trees **CpTr** and the exploded symmetric ω-monoidal groupoid **xS** of the symmetric groups. These groupoids are based on **NCpTree** and the exploded Artin braid groupoid **xB** defined in Joyce.[32]

The ω-monoidal groupoid **CpTr** is defined to have objects T^* with a unique arrow between $s,t\in T^*$ provided they have the same number of nodule free leaves. Thus

$$\mathbf{CpTr} = \coprod_{n\in\mathbb{N}} \mathbf{CpTr}_n, \tag{60}$$

where the objects of the full subcategory $\mathbf{CpTr}_n$ are T^*_n, the coupling trees with n nodule free leaves. Note that $\mathbf{NCpTree}_n$ is finite where as $\mathbf{CpTr}_n$ is infinite. Furthermore, there is a forgetful functor $U:\mathbf{CpTr}\to\mathbf{NCpTree}$ given by renaming the nodes of t by $1,\ldots,|\{t\}|$ in the unique way preserving order. The resultant tree Ut underlies premonoidal categories.

In addition to the upper and lower cutting operations defined earlier we define the left and right cutting operations. Given $t\in T^*$ the left (respectively, right) cut Lt (respectively, Rt) is the maximal subtree formed from the left (respectively, right) descedents of the root. Finally we note that a tree t is left (respectively, right) justified if $R\vee_m t$ (respectively, $L\vee_m t$) is a singleton set for every $m\in\{t\}$.

If we forget the ordering of nodes then we arrive at the groupoid of bracketing trees with nodules **NBrTree** and the evident forgetful functor $V:\mathbf{NCpTree}\to\mathbf{NBrTree}$. The groupoid of bracketing trees with nodules admits the functor $\otimes:\mathbf{NBrTree}\times\mathbf{NBrTree}\to\mathbf{NBrTree}$ given by joining roots. Thus two trees with m and n leaves join to give a tree with $m+n$ leaves. The identity object is the empty tree. Thus **NBrTree** is a strict monoidal category. Since **CpTr** is an ω-monoid then given $(s,t)\in\mathcal{D}_m$ we have $VU(st)_m=(VUs)\otimes(VUt)$. See Joyce[26] for the full theory of ω-monoidal category theory.

The exploded symmetric ω-monoidal groupoid **xS** has as objects all permutations. There is defined to be an arrow between two permutations π and σ whenever they have the same length. Moreover, this arrow is unique and given by $\sigma\pi^{-1}:\pi\to\sigma$. Thus

$$\mathbf{xS} = \coprod_{n\in\mathbb{N}} \mathbf{xS}_n, \tag{61}$$

where the objects of the full subcategory $\mathbf{xS}_n$ are S_n.

The ω-monoidal groupoid of universal ω-algebra is

$$\mathcal{U} = \coprod_{n\in\mathbb{N}} \mathbf{CpTr}_n \times \mathbf{xS}_n. \tag{62}$$

The set of *elementary* arrows spanning the category are given as follows.

(i) Arrows $(s,1)\to(t,1)$ that prune (or graft in opposite direction) a nodule. That is there is $m\in\{s\}$ such that $\wedge_m s=t$ with $L\vee_m s=\circ$ or $R\vee_m s=\circ$.
(ii) Arrows $(s,\pi)\to(s,(i\,i+1)\pi)$ that interchange two adjacent leafs and the i and $i+1$ leaves have the same descendants.
(iii) Arrows $(s,\pi)\to(t,\pi)$ which swing a single edge between two nodes with immediate descendant m. That is, for a left to right swing $\wedge_m s=\wedge_m t$ and $LL\vee_m s=L\vee_n t$, $RL\vee_m s=LR\vee_m t$, $R\vee_m s=RR\vee_m t$.

These arrows play a crucial role in the next section whereby each is associated with either left and right identitivity, commutativity or associativity, respectively.

VII. ω-POINCARÉ–BIRKHOFF–WITT THEOREM

The ω-Poincaré–Birkhoff–Witt theorem provides a basis for the universal envelope $\mathcal{U}(\mathcal{L})$ just constructed. We suppose that $\mathbb{A}$ is ordered by $<$. Given a recoupling Lie algebra $\mathcal{L}$ an important subalgebra is the commutator subalgebra $[\mathcal{L},\mathcal{L}]$. Let X_0 be an $\mathbb{A}$-graded basis for $[\mathcal{L},\mathcal{L}]$ then for each $x\in X_0$ there is $m,n\in\mathbb{A}$ such that $m\leqslant n$ and $x\in[\langle\mathcal{L}\rangle_m,\langle\mathcal{L}\rangle_n]$. We impose an order $<$ on X_0 satisfying $x<x'$ implies $m\leqslant m'$ where $x\in\langle\mathcal{L}\rangle_m$ and $x'\in\langle\mathcal{L}\rangle_{m'}$. We extend X_0 to an $\mathbb{A}$-graded basis X for $\mathcal{L}$. Let $X_1=X\backslash X_0$ then $X=X_0\amalg X_1$. We extend the order $<$ ensuring that $x<y$ whenever $x\in X_0$ and $y\in X_1$. The order on X_1 is required to satisfy $y<y'$ implies $n\leqslant n'$ where $y\in\langle\mathcal{L}\rangle_n$ and $y'\in\langle\mathcal{L}\rangle_{n'}$.

Next we characterize admissible tuples of X. A tuple $\mathbf{x}\in X_0^M$ is *admissible* if and only if $x_1<\cdots<x_M$ and for all $a\in\langle\mathcal{L}\rangle_m$, $b\in\langle\mathcal{L}\rangle_n$, $c\in\langle\mathcal{L}\rangle_p$, and $d\in\langle L\rangle_q$ with $[a,b]=x_i$ and $[c,d]=x_j$ $(1\leqslant i\neq j\leqslant M)$ we have $\xi_{m,n,p,q}=1$. A tuple $\mathbf{x}\in X^M$ is *admissible* if and only if $x_1<\cdots<x_M$, every subtuple $\mathbf{x}_0$ with components in X_0 is admissible and for all $1\leqslant i,j,k\leqslant N$ distinct, $a\in\langle\mathcal{L}\rangle_m$ and $b\in\langle\mathcal{L}\rangle_n$ with $[a,b]=x_i$ we have $\xi_{m,n,p,q}=1$ where $x_j\in\langle\mathcal{L}\rangle_p$ and $x_k\in\langle\mathcal{L}\rangle_q$. We denote the collection of admissible ordered tuples of X by $\mathrm{Adm}(X)$. This set is $\mathbb{A}$-graded given by adding grades of individual components and is the disjoint union of two important subsets

$$\mathrm{Adm}(X)=\mathrm{Adm}(X)_0\amalg\mathrm{Adm}(X)_1, \tag{63}$$

where $\mathrm{Adm}(X)_0$ is the set of tuples with at least three components one of which is in X_0. $\mathrm{Adm}(X)_1$ is the complement in $\mathrm{Adm}(X)$. Note that $\mathrm{Adm}(X)_1$ contains the empty tuple which has no components.

If we append a nodule to the basis X we extend the order $<$ on $X\amalg\{\circ\}$ by $\circ<x$ for all $x\in X$. Let $\mathcal{I}=\{x\in X^n:\text{for some } n\in\mathbb{N} \text{ such that } x_i\leqslant x_{i+1} \text{ for all } i=1,\ldots,n-1\}$. This set contains $\mathrm{Adm}(X)$. We partition $\mathcal{I}$ into $\mathcal{I}_+\amalg\mathcal{I}_-$ where $\mathcal{I}_-=\{x\in\mathcal{I}:\text{there exists } i \text{ such that } x_i=x_{i+1}\in X_-\}$ and clearly $\mathcal{I}_+=\mathcal{I}\backslash\mathcal{I}_-$. Consequently $\mathrm{Adm}(X)$ inherits this partition. The set of vectors in the theorem is $\mathrm{Adm}(X)_+$.

Theorem 1 (ω–Poincaré–Birkhoff–Witt): Let $\mathcal{L}$ be a recoupling Lie algebra. Let X be a basis for $\mathcal{L}$ constructed previously. A basis for the universal enveloping algebra $\mathcal{U}(\mathcal{L})$ is given by

$$(\cdots((x_1x_2)_{N-1}x_3)_{N-2}\cdots x_N)_1, \tag{64}$$

where $(x_1,\ldots,x_N)\in\mathrm{Adm}(X)_{+0}$, *and*

$$(\cdots((x_1x_2)_{k_1}x_3)_{k_2}\cdots x_N)_{k_{N-1}}, \tag{65}$$

where $(x_1,\ldots,x_N)\in Adm(X)_{+1}$ *and* $k_1>k_2>\cdots>k_{N-1}$.

The ideal $\mathcal{J}$ used in the construction of $\mathcal{U}(\mathcal{L})$ is given by

$$\mathcal{J} = \text{span}_{I \in I} \mathcal{J}_I, \tag{66}$$

where $\mathcal{J}_I$ is the subideal generated by (51)–(53) restricted to coupling trees of $n=|I|$ nodule free leaves that are a rearrangement of I. To prove spanning we require the next lemma. Let $L^* \subset T^*$ be the set of left-justified coupling trees. That is if $t \in L^*$ with nodes $n_1, \ldots, n_N$ (from left to right) then $n_1 > \cdots > n_N$. The set of labeled left-justified coupling trees is denoted $L^*(X)$. For each $n \in \mathbb{N}$ let $\tau_n \in L^*$ be the unique left-justified coupling tree with n leaves and no nodules.

Lemma 1: Let $I \in \mathcal{I}$, t a coupling tree with N leaves and $n=|I|$ nodule free leaves, and $\pi \in S_n$.

(i) *We have that*

$$t(\pi I) + \mathcal{J}_I = b_{t,I,\pi} \tau_n I + \mathbf{x}_{t,I,\pi} + \mathcal{J}_I \tag{67}$$

for some $b_{t,\pi,I} \in S^1$ and

$$\mathbf{x}_{t,\pi,I} \in \left(\bigoplus_{\substack{m<n \\ p \leqslant N-n}} \mathbb{C}[T^*(X)]_{m,p} \right) \oplus \left(\bigoplus_{p<N-n} \mathbb{C}[T^*(X)]_{n,p} \right). \tag{68}$$

(ii) *Moreover, if $I \in \mathcal{I}_-$ then*

$$t(\pi I) + \mathcal{J}_I = \mathbf{y}_{t,I,\pi} + \mathcal{J}_I \tag{69}$$

for some

$$\mathbf{y}_{t,I,\pi} \in \left(\bigoplus_{\substack{m<n \\ p \leqslant N-n}} \mathbb{C}[T^*(X)]_{m,p} \right) \oplus \left(\bigoplus_{p<N-n} \mathbb{C}[T^*(X)]_{n,p} \right). \tag{70}$$

(iii) *If $I \in \mathcal{I} \backslash Adm(X)$ then $t(\pi I) \in \mathcal{J}_I$.*

Proof: Let $\mathcal{E}$ be the set of elementary arrows in **CpTr**. Define the evaluation map $\text{eval}: \mathcal{E} \times \mathcal{I} \to \mathbb{C}[T^*(X)]$ given by mapping each elementary arrow $E:(s,\sigma) \to (s',\sigma')$ under $I \in \mathcal{I}$ to the generating function between $s(\sigma I)$ and $s'(\sigma' I)$ given by (51), (52), (53), and (54).

To prove (i) we note that there exists a composable sequence of elementary arrows $E_1, \ldots, E_N$ in **CpTr** from (t,π) to $(\tau_n, 1)$. Let the source of E_k be denoted (t_k, π_k) and the target (t_{k+1}, π_{k+1}) then $t_1 = t$, $\pi_1 = \pi$, $t_{N+1} = \tau_n$, and $\pi_{N+1} = 1$. We find that $t_k(\pi_k I) - \text{eval}(E_k, I) = b_k t_{k+1}(\pi_{k+1} I) + \mathbf{x}_k$ for some $b_k \in S^1$ and $\mathbf{x}_k$ in (68). Since $\text{eval}(E_k, I) \in \mathcal{J}_I$ then we have that

$$t_k(\pi_k I) + \mathcal{J}_I = b_k t_{k+1}(\pi_{k+1} I) + \mathbf{x}_k + \mathcal{J}_I \tag{71}$$

for $k = 1, \ldots, N$. Hence (67) holds with $b_{t,\pi,I} = \Pi_{k=1}^N b_k$ and

$$\mathbf{x}_{t,\pi,I} = \sum_{k=1}^{N} \left(\prod_{l=1}^{k-1} b_l \right) \mathbf{x}_k. \tag{72}$$

To prove (ii) let $\sigma \in S_n$ such that the first two entries of σI are in X_-. Then by (i) the evaluation of the arrow $(t,\sigma) \to (t,(12)\sigma)$ at I gives $t(\sigma I) + \mathcal{J}_I = -t((12)\sigma I) + \mathbf{x} + \mathcal{J}_I$ for some $\mathbf{x}$ in (68). Thus we have that

$$t(\sigma I) + \mathcal{J}_I = \tfrac{1}{2}\mathbf{x} + \mathcal{J}_I. \tag{73}$$

Also by (i) we can find a, $b \in S^1$ and $\mathbf{y}$, $\mathbf{z}$ in (68) satisfying

$$t(\pi I) + \mathcal{J}_I = a \tau_n I + \mathbf{y} + \mathcal{J}_I, \tag{74}$$

$$t(\sigma I) + \mathcal{J}_I = b \tau_n I + \mathbf{z} + \mathcal{J}_I. \tag{75}$$

A simple calculation substituting (75) then (73) into (74) yields

$$t(\pi I) + \mathcal{J}_I = \frac{a}{2b}\mathbf{x} + \mathbf{y} - \frac{a}{b}\mathbf{z} + \mathcal{J}_I. \tag{76}$$

The result follows with $\mathbf{y}_{t,\pi,I}=(a/2b)\mathbf{x}+\mathbf{y}-(a/b)\mathbf{z}$.

Finally to prove (iii) suppose $I \notin \mathrm{Adm}(X)$. Either there is $a \in \langle\mathcal{L}\rangle_m$, $b \in \langle\mathcal{L}\rangle_n$, $c \in \langle\mathcal{L}\rangle_p$, $d \in \langle\mathcal{L}\rangle_q$, and $i \neq j$ with $[a,b]=I_i$ and $[c,d]=I_j$ such that $\xi_{m,n,p,q} \neq 1$; or there is $a \in \langle\mathcal{L}\rangle_m$, $b \in \langle\mathcal{L}\rangle_n$, $I_j \in \langle\mathcal{L}\rangle_p$, $I_k \in \langle\mathcal{L}\rangle_q$ and $i \neq j \neq k \neq i$ with $[a,b]=I_i$ such that $\xi_{m,n,p,q} \neq 1$. In the first case we choose $s \in L$ and $\pi \in S_{|I|}$ such that there is an arrow $(s,\pi) \to (t,\pi)$ and $(\sigma\pi^{-1}I)_1=I_i$ and $(\sigma\pi^{-1}I)_2=I_j$. Thus it follows from Proposition 2 (this proposition, proved later, does not depend on this result) and (85) that

$$\vee_{\sup\{s\}} s(I_i,I_j) = \xi_{m,n,p,q} \vee_{\sup\{s\}} s(I_i,I_j). \tag{77}$$

Since $\xi_{m,n,p,q} \neq 1$ we have that $\vee_{\sup\{s\}} s(I_i,I_j) \in \mathcal{J}_{(a,b,c,d)} \subset \mathcal{J}$. Thus $(s,\sigma)I \in \mathcal{J}$ from which it follows that $(t,\pi)I \in \mathcal{J}$. In the second case we choose $s \in L$ and $\pi \in S_{|I|}$ such that there is an arrow $(s,\pi) \to (t,\pi)$ and $(\sigma\pi^{-1}I)_1=I_i$, $(\sigma\pi^{-1}I)_2=I_j$ and $(\sigma\pi^{-1}I)_3=I_k$. Thus it follows from Proposition 2 and (83) that

$$\vee_{\sup\{s\}\setminus\{\sup\{s\}\}} s(I_i,I_j,I_k) = \xi_{m,n,p,q} \vee_{\sup\{s\}\setminus\{\sup\{s\}\}} s(I_i,I_j,I_k). \tag{78}$$

Since $\xi_{m,n,p,q} \neq 1$ we have that $\vee_{\sup\{s\}\setminus\{\sup\{s\}\}} s(I_i,I_j,I_k) \in \mathcal{J}_{(a,b,c,d)} \subset \mathcal{J}$. Thus $(s,\sigma)I \in \mathcal{J}$ from it follows that $(t,\pi)I \in \mathcal{J}$. This completes the proof.

To prove that $\mathrm{Adm}(X)_+$ spans $\mathcal{U}(\mathcal{L})$ we use induction on $\oplus_{m<n}\mathcal{U}(\mathcal{L})_m$. Clearly it holds for $m=1$. Now suppose it holds for n and that $x \in \oplus_{m<n+1}\mathcal{U}(\mathcal{L})_m$ then we may decompose x as

$$x = \sum_{t,\pi,I} a^{t,\pi,I} t(\pi I), \tag{79}$$

where all but finitely many $a^{t,\pi,I}$ are zero. Thus we have by the lemma

$$x + \mathcal{J} = \sum_{t,\pi,I} a^{t,\pi,I} b^{t,\pi,I} \tau_n I + \sum_{t,\pi,I} a^{t,\pi,I} \mathbf{x}_{t,\pi,I} + \mathcal{J} \tag{80}$$

$$= \left(\sum_{t,\pi,I \in \mathrm{Adm}(X)_+} a^{t,\pi,I} b^{t,\pi,I} \tau_n I + \mathcal{J} \right) + \left(\sum_{t,\pi,I \in I} a^{t,\pi,I} b^{t,\pi,I} \mathbf{y}_{t,\pi,I} + \sum_{t,\pi,I} a^{t,\pi,I} \mathbf{x}_{t,\pi,I} + \mathcal{J} \right) \tag{81}$$

The first line by (i) and the second line by (ii) and (iii) of the lemma. The first term is in the span by definition, while the second term is in the span by the induction step. Hence $\mathrm{Adm}(X)_+$ spans $\mathcal{U}(\mathcal{L})$.

The other half of the theorem is to prove that $\mathrm{Adm}(X)_+$ is a linearly independent set in $\mathcal{U}(\mathcal{L})$. To this end we prove the next theorem below. We define the groupoid of noduled coupling trees labeled by X to be

$$\mathcal{U}(X) = \coprod_{n \in \mathbb{N}} \mathcal{U}_n \times X^n. \tag{82}$$

We also introduce the ω-monoid $\mathcal{J}_{00}$ defined by the generating relations

$$(|(||)_k)_h([a,b],c,d) - \xi_{m,n,p,q}(|(||)_l)_h([a,b],c,d), \tag{83}$$

$$((||)_k|)_h(a,b,[c,d]) - \xi_{m,n,p,q}((||)_l|)_h(a,b,[c,d]), \tag{84}$$

$$(||)_h([a,b],[c,d]) - \xi_{m,n,p,q}(||)_h([a,b],[c,d]) \tag{85}$$

for all a, b, c, $d \in X$ of grades m, n, p, q, respectively, and $h<k$, l. By construction one observes that $\mathbb{C}[T^*(X)]/\mathcal{J}_{00}$ is spanned by $\mathrm{Adm}(X)$.

Now we can state a Mac Lane coherence between $\mathcal{U}(X)$ and the one object category $\mathbb{C}[T^*(X)]$ with composition given by addition.

Theorem 2: *There is a functor*

$$F:\mathcal{U}(X) \to \mathbb{C}[T^*(X)]/\mathcal{J}_{00} \tag{86}$$

taking primitive arrows to their corresponding generating relations.

Proof: Premonoidal Mac Lane coherence implies F restricted to **CpTr**(X) is a functor. In remains to incorporate commutivity. Given a transposition $\sigma: s\mathbf{x} \to t((kk+1)\mathbf{x})$ where $i \leqslant k \leqslant |\mathbf{x}| - 1$, we can find arrows $f: s(\mathbf{x}) \to r(\mathbf{x})$ and $g: r((kk+1)\mathbf{x}) \to t((kk+1)\mathbf{x})$ in **CpTr** where $r \in T$ with k and $k+1$ siblings, such that $\sigma = g\sigma_{r,k} f$ where $\sigma_k: r\mathbf{x} \to r((kk+1)\mathbf{x})$. We define $F(\sigma) = F(g)F(\sigma_{r,k})F(f)$. This definition is independent of f, g, and r provided the squares

$$\begin{array}{ccc}
((||)_k(||)_l)_h\mathbf{x} & \longrightarrow & ((||)_k(||)_l)_h((12)\mathbf{x}) \\
\downarrow & & \downarrow \\
((||)_l(||)_k)_h\mathbf{x} & \longrightarrow & ((||)_l(||)_k)_h((12)\mathbf{x})
\end{array}$$

$$\begin{array}{ccc}
((||)_k(||)_l)_h\mathbf{x} & \longrightarrow & ((||)_k(||)_l)_h((34)\mathbf{x}) \\
\downarrow & & \downarrow \\
((||)_l(||)_k)_h\mathbf{x} & \longrightarrow & ((||)_l(||)_k)_h((34)\mathbf{x})
\end{array}$$

commute for all $h < k < l$ and $\mathbf{x} \in X^4$ under F. This may be seen from the proof of theorems 9 and 20 in Joyce.[32] A short calculation shows that these are the generating conditions (83) and (84) and so belong to $\mathcal{J}_{00}$. The proof is completed by showing symmetric braid conditions hold under F. That is,

$$F(\sigma_k)F(\sigma_k) = 1, \tag{87}$$

$$F(\sigma_k)F(\sigma_l) = F(\sigma_l)F(\sigma_k) \text{ whenever } |k-l| > 1, \tag{88}$$

$$F(\sigma_{k+1})F(\sigma_k)F(\sigma_{k+1}) = F(\sigma_k)F(\sigma_{k+1})F(\sigma_k) \text{ provided } k < |\mathbf{x}| \tag{89}$$

for all k, $l = 1, 2, \ldots, |\mathbf{x}|$. The first holds by the recoupling symmetry. The second by choosing $r \in T$ with k and $k+1$ siblings and l and $l+1$ siblings. The last condition follows by taking $r \in T$ such that k and $k+1$ are siblings and their parent node has sibling $k+2$. Thus the condition holds provided

$$\begin{array}{ccccc}
((||)_k|)_l(a,b,c) & \longrightarrow & ((||)_k|)_l(b,a,c) & \longrightarrow & ((||)_k|)_l(b,c,a) \\
\downarrow & & & & \downarrow \\
((||)_k|)_l(a,c,b) & \longrightarrow & ((||)_k|)_l(c,a,b) & \longrightarrow & ((||)_k|)_l(c,b,a)
\end{array}$$

commutes for all $k < l$ and a, b, $c \in X$ under F. Suppose a, b, and c are of grades m, n, and p, respectively, then the diagonal dashed arrow is well-defined if and only if

$$(||)_l([a,b],c) + \alpha_{n,m,p}\gamma_{m,n}(||)_l(b,[c,a]) + \frac{\alpha_{n,m,p}}{\alpha_{n,p,m}}\gamma_{m,n}\gamma_{m,p}(||)_l([b,c],a)$$

$$= \alpha_{m,n,p}(||)_l(a,[b,c]) + \frac{\alpha_{m,n,p}}{\alpha_{m,p,n}}\gamma_{n,p}(||)_l([a,c],b) + \frac{\alpha_{m,n,p}\alpha_{p,m,n}}{\alpha_{m,p,n}}\gamma_{n,p}\gamma_{m,p}(||)_l(c,[a,b]). \quad (90)$$

Substituting $(\|)_l([a,b],c)=\gamma_{m+n,p}(\|)_l(c,[a,b])+[[a,b],c]$ and similarly for $(\|)_l(b,[c,a])$ and $(\|)_l([b,c],a)$ reduces this condition to the recoupling Jacobi identity. Hence it vanishes.

This result has the obvious corollary.

Corollary 1: There is a unique extension of F to the ω-algebra morphism

$$\widetilde{F}:\mathbb{C}[\mathcal{U}(X)] \to \mathbb{C}[T^*(X)]/\mathcal{J}_{00}. \quad (91)$$

We have the following expected embedding.

Proposition 2: We have that $\mathcal{J}_{00} \subset \mathcal{J}$.

Proof: We must show that (83), (84), and (85) are a consequence of the generating relations for $\mathcal{J}$. As a direct result of these we have the square

$$\begin{array}{ccc} ((||)_k(||)_l)_h(a,b,c,d) & \longrightarrow & ((||)_k(||)_l)_h(b,a,c,d) \\ \downarrow & & \downarrow \\ ((||)_l(||)_k)_h(a,b,c,d) & \longrightarrow & ((||)_l(||)_k)_h(b,a,c,d) \end{array}$$

in $\mathcal{J}$ for all $a \in \langle\mathcal{L}\rangle_m$, $b \in \langle\mathcal{L}\rangle_n$, $c \in \langle\mathcal{L}\rangle_p$, $d \in \langle\mathcal{L}\rangle_q$ and $m, n, p, q \in \mathbb{A}$. This loop evaluates under F to give (83). Similarly we may obtain (84). Finally we have

$$(1-\xi_{m,n,p,q})(|(||)_k)_l([a,b],c,d) = (1-\xi_{m,n,p,q})\gamma_{p,q}(|(||)_k)_l([a,b],d,c) + (1-\xi_{m,n,p,q})(||)_l([a,b],[c,d]). \quad (92)$$

Since the first two terms are in $\mathcal{J}$ then the last must be also. Hence (85) is in $\mathcal{J}$.

A simple corollary is as follows.

Corollary 2: The subspace spanned by $Adm(X)_{0+}$ *is an algebra.*

Let $I \in \mathrm{Adm}(X)_+$ and $\mathcal{U}(X)_I$ the coupling trees with $|I|$ nodule free leaves labeled by I. We have that

$$\widetilde{F}(\mathbb{C}[\mathcal{U}(X)_I]) = \mathcal{J}_I. \quad (93)$$

Lemma 2: Let $I \in Adm(X)_+$ *and* $j \in \mathcal{J}_I$ *then whenever*

$$j \in \mathrm{span}_{I' \in I\setminus\{I\}, |I'| \leqslant |I|}\mathcal{J}_{I'} \quad (94)$$

we have that $j=0$.

Proof: Suppose $I \in \mathrm{Adm}(X)_{+1}$. The other case when $I \in \mathrm{Adm}(X)_{+0}$ will follow by a similar agrument using rooted planar binary trees. Let $(t,\pi) \to (t,\pi')$ be an arrow such that $I_{\pi i}=I_{\pi' i}$ for all $i=1,2,\ldots,|I|$. The tuple I is partitionable into constant maximal subtuples. Choose $s \in T$ such that the leaves corresponding to subtuples of length at least two are the descendents of a unique node. We have the diagram

$$\begin{array}{ccc} (t,\pi) & \longrightarrow & (t,\pi') \\ \downarrow & & \downarrow \\ (s,1) & \longrightarrow & (s,\pi'\pi^{-1}) \end{array}$$

in $\mathcal{U}$. If we evaluate this diagram at I and apply F then the side arrows are equal and if the bottom arrow is zero the top arrow is zero. Indeed the bottom arrow evaluates as zero because constant subtuples of I of at least length two are bosonic. That is the commutator vanishes and the phase is unity. Given $\pi, \sigma \in S_{|I|}$ we say they are equivalent applied to I if $I_{\pi i} - I_{\sigma i}$ for all $i = 1, \ldots, |I|$. The set of equivalence classes we denote S_I/I. Let r be the nodule free left-justified tree with $|I$ leaves then a spanning set for $\mathcal{J}_I$ is given by the arrows $rI \to r(\pi I)$ where $\pi \in S_{|I|}/I$ under F. That is, each element is of the form

$$rI - \phi_\pi r(\pi I) + b_\pi \tag{95}$$

for some $\phi_\pi \in S^1$ and

$$b_\pi \in \text{span}_{I' \in \mathcal{I}, |I'| < |I|} \mathcal{J}_{I'} \tag{96}$$

for all $\pi \in S_{|I|}/I$. This is clearly a basis since $rI - \phi_\pi r(\pi I)$ where $\pi \in S_{|I|}/I$ is a basis. This completes the proof of the lemma. Let $I_1, \ldots, I_N \in \text{Adm}(X)_+$ be any finite distinct collection with I_k of length n_k, and $a_1, \ldots, a_N \in \mathbb{C}\backslash\{0\}$ such that

$$\sum_{k=1}^{N} a_k \tau_{n_k} I_k = 0, \tag{97}$$

Choose I_m such that $n_k \leqslant n_m$ for all $k = 1, \ldots, N$. We have that

$$a_m \tau_{n_m} I_m = - \sum_{\substack{k=1 \\ k \neq m}}^{N} a_k \tau_{n_k} I_k \in \text{span}_{I' \in \mathcal{I}\backslash\{I_m\}, |I'| \leqslant |I_m|} \mathcal{J}_{I'} \tag{98}$$

Hence by the lemma $a_m = 0$ giving a contradiction. Thus $\text{Adm}(X)_+$ is a linearly independent set. This completes the proof of the ω-Poincaré–Birkhoff–Witt theorem.

VIII. $\mathbb{Z}_N$-GRADED HEISENBERG RECOUPLING LIE ALGEBRA

We consider in detail a generalized version of the Heisenberg algebra $\mathcal{H}$ for any $\mathbb{Z}_N$ graded recoupling. The recoupling Lie algebra is spanned by a grade 0 element h, grade 1 elements a_μ and grade $N-1$ elements $a_\mu^\dagger$ for all $\mu \in \mathcal{I}$ satisfying

$$[a_\mu, a_\nu] = 0, \quad [a_\mu, h] = 0,$$

$$[a_\mu^\dagger, a_\nu^\dagger] = 0, \quad [a_\mu^\dagger, h] = 0,$$

$$[a_\mu, a_\nu^\dagger] = \delta_{\mu,\nu} h, \quad [h, h] = 0$$

for all $\mu, \nu \in \mathcal{I}$. For simplicity suppose $\mathcal{I}$ is finite. We see that $\text{Adm}(\mathcal{H}) = \mathcal{H}$. Moreover, we usually identify the element h with $\hbar\circ$. Thus we work in the factored universal ω-algebra $\mathcal{U}(H)/h - \hbar\circ$.

The grade 0 component $\langle \mathcal{H} \rangle_0$ is a Lie algebra. Define $h_{\mu\nu} = a_\mu a_\nu^\dagger$ then a straight forward calculation in the universal enveloping algebra $\mathcal{U}(\mathcal{H})/h - \hbar\circ$ shows that

$$\begin{aligned}[h_{\mu\nu}, h_{\mu'\nu'}] = \hbar \frac{\alpha_{1,N-1,0}\lambda_0}{\alpha_{N-1,1,N-1}\alpha_{0,0,N-1}} \gamma_{N-1,1} \left(\delta_{\mu\nu'} h_{\mu'\nu} - \frac{\alpha_{0,0,1}}{\alpha_{1,0,0}} \gamma_{1,1}\gamma_{N-1,N-1} \delta_{\mu'\nu} h_{\mu\nu'} \right) \\ + (1 - \gamma_{1,1}\gamma_{N-1,N-1}) h_{\mu\nu} h_{\mu'\nu'}\end{aligned} \tag{99}$$

Closure requires $\gamma_{1,1}\gamma_{N-1,N-1} = 1$ and $\alpha_{1,0,0} = \alpha_{0,0,1}$ giving the Lie algebra $u(1) \oplus su(|\mathcal{I}|)$.

Two straightforward calculations in the universal enveloping algebra $\mathcal{U}(\mathcal{H})/h - \hbar\circ$ demonstrate

$$[h_{\mu\nu},a_\lambda]=-\hbar\alpha_{1,0,0}\lambda_0\gamma_{0,1}\gamma_{1,1}\delta_{\nu,\lambda}a_\mu+\left(1-\frac{\gamma_{0,1}\gamma_{1,1}\gamma_{1,N-1}}{\alpha_{1,N-1,1}}\right)h_{\mu\nu}a_\lambda, \tag{100}$$

$$[h_{\mu\nu},a_\lambda^\dagger]=\hbar\frac{\gamma_{0,N-1}\gamma_{N-1,1}\lambda_0}{\alpha_{N-1,1,N-1}\alpha_{0,0,N-1}}\delta_{\mu\lambda}a_\nu^\dagger+\left(1-\frac{\gamma_{0,N-1}\gamma_{N-1,1}\gamma_{N-1,N-1}}{\alpha_{N-1,1,N-1}}\right)h_{\mu\nu}a_\lambda^\dagger. \tag{101}$$

Closure requires the term of each to vanish. Furthermore, if a_μ and $a_\mu^\dagger$ are to be a pair of lowering and raising elements then $\gamma_{0,1}=\gamma_{0,N-1}=1$. The adjoint action on the space spanned by a_μ gives the fundamental representation, while on the space spanned by $a_\mu^\dagger$ gives the dual fundamental representation. We define the (standard) Bose–Fermi $\mathbb{A}$ graded recoupling as the following irreducible recoupling. We take $\lambda_m=\rho_m=1$ and

$$\gamma_{m,n}=\begin{cases}1, & m=0 \text{ or } n=0\\ -1, & \text{otherwise},\end{cases} \tag{102}$$

$$\alpha_{m,n,p}=\begin{cases}1, & m=0,n=0,p=0 \text{ or } m+n=0\\ -1, & \text{otherwise}.\end{cases} \tag{103}$$

The $m+n=0$ in the definition of $\alpha_{m,n,p}$ may equally well be replaced by $n+p=0$. These determine the deformativity phases to be

$$\xi_{m,n,p,q}=\begin{cases}1, & m=0,n=0,p=0,q=0,m+n=0 \text{ or } p+q=0,\\ -1, & \text{otherwise}.\end{cases} \tag{104}$$

Algebraic formulas for α,ξ, and γ utilizing Kronecker deltas are given in the Appendix. For this recoupling the Heisenberg algebra reduces to

$$[h_{\mu\nu},h_{\mu'\nu'}]=\hbar\delta_{\mu'\nu}h_{\mu\nu'}-\hbar\delta_{\mu\nu'}h_{\mu'\nu}, \tag{105}$$

$$[h_{\mu\nu},a_\lambda]=\hbar\delta_{\nu,\lambda}a_\mu, \tag{106}$$

$$[h_{\mu\nu},a_\lambda^\dagger]=\hbar\delta_{\mu\lambda}a_\nu^\dagger, \tag{107}$$

where $\mu,\nu,\mu',\nu',\lambda\in\mathcal{I}$. For SU(3) color with a $\mathbb{Z}_3$ graded Bose–Fermi recoupling Heisenberg Lie algebra the universal envelope is an ω-algebra satisfying the Pauli exclusion principle and avoiding the confinement outlined in Joyce.[4,15]

IX. HOPF STRUCTURE OF THE UNIVERSAL ENVELOPING ω-ALGEBRA

The universal ω-algebra of a recoupling Lie algebra possesses coalgebra and Hopf algebralike structures. Let $\mathcal{U}^0(\mathcal{L})$ be the maximal ω-subalgebra of $\mathcal{U}(\mathcal{L})$ excluding the unit.

Proposition 3: The universal ω-algebra $\mathcal{U}(\mathcal{L})$ is a coalgebra.

A comultiplication $\Delta:\mathcal{U}(\mathcal{L})\to\mathcal{U}(\mathcal{L})^{\otimes 2}$ is given by

$$\Delta(a)=1\otimes a+a\otimes 1, \tag{108}$$

$$\Delta(1)=1\otimes 1, \tag{109}$$

whenever $a\in\mathcal{U}^0(\mathcal{L})$. The corresponding counit $\epsilon:\mathcal{U}(\mathcal{L})\to\mathbb{C}$ is given by

$$\epsilon(a)=0, \tag{110}$$

$$\epsilon(1) = 1, \tag{111}$$

whenever $a \in \mathcal{U}^0(\mathcal{L})$.

Using the symmetric unital braid R we can construct a coalgebra structure for $\mathcal{U}(\mathcal{L})$. Comultiplication and counit are given by

$$\Delta(a \otimes b) = (\Delta \otimes \Delta)(a \otimes R(b \otimes a) \otimes b), \tag{112}$$

$$\epsilon(a \otimes b) = \epsilon(a) \otimes \epsilon(b), \tag{113}$$

for all $a, b \in \mathcal{U}(\mathcal{L})$. We say that the coalgebra and ω-algebra are compatible if $\mu_m : \mathcal{D}_m \to \mathcal{A}$ are coalgebra morphisms on the restricted domain $\mathcal{D}_m$ for each $m \in \mathbb{N}_+$. Equivalently, the comultiplication is a morphim between the ω-algebras $\mathcal{U}(\mathcal{L})$ and $\mathcal{U}(\mathcal{L})^{\otimes 2}$. Algebraically these conditions are

$$\Delta\mu_m(a \otimes b) = (\mu_m \otimes \mu_m)(1 \otimes R \otimes 1)(\Delta(a) \otimes \Delta(b)), \tag{114}$$

$$\epsilon\mu_m(a \otimes b) = \epsilon(a) \otimes \epsilon(b), \tag{115}$$

$$\Delta(1) = 1 \otimes 1 \tag{116}$$

whenever $a \otimes b \in \mathcal{D}_m$, for all $m \in \mathbb{N}_+$. One can easily check that these all hold.

Definition 5: A Hopf ω-algebra is a unital ω-algebra $\mathcal{A}$ with a compatible coalgebra structure and an antipode S. The antipode is a contravariant morphism $S : \mathcal{A} \to \mathcal{A}$ satisfying

$$\mu_m(S \otimes 1)\Delta(a) = \eta(a)\epsilon(a) = \mu_m(1 \otimes S)\Delta(a) \tag{117}$$

for all $a \in \mathcal{U}(\mathcal{L})$ such that $(S \otimes 1)\Delta(a) \in \mathcal{D}_m$, for all $m \in \mathbb{N}_+$.

One can easily check that an antipode for $\mathcal{U}(\mathcal{L})$ is the unique linear map given by $S(a) = -a$ whenever $a \in \mathcal{U}^0(\mathcal{L})$ and $S(1) = 1$.

X. CONCLUSION

We have extended the notion of a graded Lie algebra to include the recoupling phases of Joyce[4] necessary in the description of SU(3) color. In order to construct the appropriate notion of a universal envelope we required the new notion of an ω-algebra. One may think of this as a generalization of algebra where the order in which brackets are evaluated is unique, avoiding ambiguous statements such as $(ab)(cd)$. We constructed the universal enveloping ω-algebra and proved the corresponding ω-Poincaré–Birkhoff–Witt theorem. Finally we recovered the usual coalgebra structure and uncovered the Hopf structure of the universal enveloping ω-algebra.

The results of this paper provide motivation for the omegafication of a number of structures requiring the development of a general theory of ω-monoidal categories.[26] Of particular interest is an ω-tensor product (and ω-Fock space) which should be the appropriate setting for the representation theory of ω-algebra. This requires notions of ω-coalgebra, ω-bialgebra, and Hopf ω-algebra.

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APPENDIX

Algebraic formulas for the (standard) Bose-Fermi recoupling phases are given by

$$\lambda_m = 1, \tag{A1}$$

$$\gamma_{m,n} = -1 + 2\delta_{m,0} + 2\delta_{n,0} - 2\delta_{m,0}\delta_{n,0}, \tag{A2}$$

$$\begin{aligned}\alpha_{m,n,p} = &-1 + 2\delta_{m,0} + \delta_{n,0} + \delta_{m+n,0} + \delta_{p,0} - 2\delta_{m,0}\delta_{n,0} - 2\delta_{m,0}\delta_{m+n,0} - 2\delta_{n,0}\delta_{m+n,0} - 2\delta_{m,0}\delta_{p,0}\\ &- 2\delta_{n,0}\delta_{p,0} - 2\delta_{m+n,0}\delta_{p,0} + 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0} + 2\delta_{m,0}\delta_{n,0}\delta_{p,0} + 2\delta_{m,0}\delta_{m+n,0}\delta_{p,0} + 2\delta_{n,0}\delta_{m+n,0}\delta_{p,0}\\ &- 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p,0},\end{aligned} \tag{A3}$$

$$\begin{aligned}\xi_{m,n,p,q} = &-1 + 2\delta_{m,0} + 2\delta_{n,0} + 2\delta_{m+n,0} + 2\delta_{p,0} + 2\delta_{q,0} + 2\delta_{p+q,0} - 2\delta_{m,0}\delta_{n,0} - 2\delta_{m,0}\delta_{m+n,0}\\ &- 2\delta_{n,0}\delta_{m+n,0} - 2\delta_{m,0}\delta_{p,0} - 2\delta_{m,0}\delta_{q,0} - 2\delta_{m,0}\delta_{p+q,0} - 2\delta_{n,0}\delta_{p,0} - 2\delta_{n,0}\delta_{q,0} - 2\delta_{n,0}\delta_{p+q,0}\\ &- 2\delta_{m+n,0}\delta_{p,0} - 2\delta_{m+n,0}\delta_{q,0} - 2\delta_{m+n,0}\delta_{p+q,0} - 2\delta_{p,0}\delta_{q,0} - 2\delta_{p,0}\delta_{p+q,0} - 2\delta_{q,0}\delta_{p+q,0}\\ &+ 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0} + 2\delta_{m,0}\delta_{n,0}\delta_{p,0} + 2\delta_{m,0}\delta_{n,0}\delta_{q,0} + 2\delta_{m,0}\delta_{n,0}\delta_{p+q,0} + 2\delta_{m,0}\delta_{m+n,0}\delta_{p,0}\\ &+ 2\delta_{m,0}\delta_{m+n,0}\delta_{q,0} + 2\delta_{m,0}\delta_{m+n,0}\delta_{p+q,0} + 2\delta_{n,0}\delta_{m+n,0}\delta_{p,0} + 2\delta_{n,0}\delta_{m+n,0}\delta_{q,0} + 2\delta_{n,0}\delta_{m+n,0}\delta_{p+q,0}\\ &+ 2\delta_{m,0}\delta_{p,0}\delta_{q,0} + 2\delta_{m,0}\delta_{p,0}\delta_{p+q,0} + 2\delta_{m,0}\delta_{q,0}\delta_{p+q,0} + 2\delta_{n,0}\delta_{p,0}\delta_{q,0} + 2\delta_{n,0}\delta_{p,0}\delta_{p+q,0}\\ &+ 2\delta_{n,0}\delta_{q,0}\delta_{p+q,0} + 2\delta_{m+n,0}\delta_{p,0}\delta_{q,0} + 2\delta_{m+n,0}\delta_{p,0}\delta_{p+q,0} + 2\delta_{m+n,0}\delta_{q,0}\delta_{p+q,0} + 2\delta_{p,0}\delta_{q,0}\delta_{p+q,0}\\ &- 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p,0} - 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{q,0} - 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p+q,0} - 2\delta_{m,0}\delta_{n,0}\delta_{p,0}\delta_{q,0}\\ &- 2\delta_{m,0}\delta_{n,0}\delta_{p,0}\delta_{p+q,0} - 2\delta_{m,0}\delta_{n,0}\delta_{q,0}\delta_{p+q,0} - 2\delta_{m,0}\delta_{m+n,0}\delta_{p,0}\delta_{q,0} - 2\delta_{m,0}\delta_{m+n,0}\delta_{p,0}\delta_{p+q,0}\\ &- 2\delta_{m,0}\delta_{m+n,0}\delta_{q,0}\delta_{p+q,0} - 2\delta_{n,0}\delta_{m+n,0}\delta_{p,0}\delta_{q,0} - 2\delta_{n,0}\delta_{m+n,0}\delta_{p,0}\delta_{p+q,0} - 2\delta_{n,0}\delta_{m+n,0}\delta_{q,0}\delta_{p+q,0}\\ &- 2\delta_{m,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0} - 2\delta_{n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0} - 2\delta_{m+n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0} + 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p,q,0}\\ &+ 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p,0}\delta_{p+q,0} + 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{q,0}\delta_{p+q,0} + 2\delta_{m,0}\delta_{n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0}\\ &+ 2\delta_{m,0}\delta_{m+n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0} + \delta_{n,0}\delta_{m+n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0} - 2\delta_{m,0}\delta_{n,0}\delta_{m+n,0}\delta_{p,0}\delta_{q,0}\delta_{p+q,0}\end{aligned} \tag{A4}$$

for all $m, n, p, q \in \mathbb{A}$.

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Division algebras: Family replication

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The known link of the division algebras to 10-dimensional spacetime and one leptoquark family is extended to encompass three leptoquark families. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1786682]

I. INTRODUCTION

No volume devoted to noncommutative mathematical structures of any sort would be complete without some attention paid to the quaternions (**H**) and octonions (**O**). These, together with the commutative algebras **R** (real numbers) and **C** (complex numbers), are the four real normed division algebras, linked to much that is elegant, noteworthy and exceptional in mathematics. The obviously central role of **R** and **C** in physics has also led many to believe that **H** and **O** should have an equally central role in fundamental physics as they do in mathematics. In this article we further develop the idea that in fact all of these algebras tensored together should play a role in constructing the Standard Model. Our observations are also relevant to recent developments in string theory, where the octonions are becoming increasingly of interest. We direct the reader to John Baez's excellent review for a broader discussion of quaternions and octonions.[1]

This article is an extension of work begun in Ref. 2, which builds on Ref. 3. There it is assumed that none of the three hypercomplex division algebras (**C**, **H** and **O**) is to be distinguished over any other, and all should play a role. Thus it was proposed to consider

$$\mathbf{T}=\mathbf{C}\otimes\mathbf{H}\otimes\mathbf{O}$$

as a starting point for a particle physics model. Here **T** is nothing more than the complexification of the quaternionization of the octonions. More precisely, we considered $\mathbf{T}^2=\mathbf{T}\oplus\mathbf{T}$ as follows.

Each of these algebras, **C**, **H**, **O**, the tensor product, **T** and $\mathbf{T}^2$, is a spinor space (see Ref. 2). A Dirac algebra spinor of a fundamental fermion like the electron is conventionally represented as an element of $\mathbf{C}^4$, and so is 8-dimensional over the reals. **T** is 64-dimensional, and $\mathbf{T}^2$, a complexified $\mathbf{R}^{1,9}$ spinor, is 128-dimensional. Since $128=(8+8)\times 8$, and associated with the first family of leptons and quarks there are 8 fermions and 8 antifermions (neutrinos treated as Dirac throughout), one might hope that $\mathbf{T}^2$ is the correct object to account for 16 Dirac spinors. This turns out to be a good point of view as shown in detail in Refs. 2 and 3, and elsewhere; many of the mathematical features of the Standard Model of quarks and leptons indeed fall naturally out of a theory based mathematically on this spinor space $\mathbf{T}^2$.

One feature that has, however, been missing, is how to account for the higher leptoquark families two and three in this picture. We propose a solution now.

II. PRELIMINARIES

Let PSO_k be a projective special orthogonal group. In Ref. 4 the following is noted.

(1) The existence of **C** implies that PSO_2 is commutative.
(2) The existence of **H** implies $PSO_4\cong PSO_3\times PSO_3$.
(3) The existence of **O** implies that PSO_8 has a triality automorphism of order 3.

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We also have natural actions of the special orthogonal groups on the division algebras as spinor spaces.

(1) The special orthogonal group SO_2 acting on 2^1-dimensional **C** can be represented by multiplication by a single complex unit, $u+iv$, where $u^2+v^2=1$.
(2) Any element of the group SO_4 acting on the 2^2-dimensional **H** requires at most 16 quaternion doublets, (u,v), summing actions of the form

$$x \to u_L v_R[x] = uxv.$$

This becomes somewhat obvious when we realize that SO_4 is generated by the six elements q_{Li} and q_{Ri}, where q_i, $i=1,2,3$, are the three imaginary quaternion units, and q_{Li} and q_{Ri} are the maps

$$X \to q_i X, \quad X \to X q_i,$$

for X in **H**. A general element of SO_4 takes the form $u+v^i q_{Li}+r^j q_{Rj}+s^{ij} q_{Li} q_{Rj}$ $(1+3+3+9=16)$, with suitable conditions placed on the coefficients.
(3) Any element of the group SO_8 acting on the 2^3-dimensional **O** requires at most 64 octonion triples, (u,v,w), summing actions of the form

$$X \to u_L v_L w_L[X] = u(v(wX)).$$

This becomes somewhat obvious when we realize that SO_8 is generated by the 28 elements e_{La} and e_{Lab}, where e_a, $a=1,\ldots,7$, are the imaginary octonion units, and e_{La} and e_{Lab} (and e_{Labc}) are the maps

$$X \to e_a X, \quad X \to e_a(e_b X), \quad X \to e_a(e_b(e_c X)),$$

for X in **O** (no right multiplication is needed: see Ref. 2). A general element of SO_8 takes the form $u+v^a e_{La}+r^{ab} e_{Lab}+s^{abc} e_{Labc}$ $(1+7+21+35=64)$, with suitable conditions placed on the coefficients.

Finally, we make a key observation from p. 12 of the Conway and Sloane book on sphere packings (Ref. 5), where three laminated lattices are singled out for their density and simplicity. These are (1) $\Lambda_2=A_2$, which can be represented in $\mathbf{C^1}$; (2) $\Lambda_8=E_8$, which can be represented in $\mathbf{H^2}$ (and $\mathbf{O^1}$); (3) Λ_{24} (Leech lattice), which can be represented in $\mathbf{O^3}$.

In each case the representations are intimately related to certain integral elements over the underlying division algebras (Refs. 4 and 5).

We will also need some notations:

(i) $\mathbf{K}_L, \mathbf{K}_R$—the algebras of left and right actions of an algebra **K** on itself;
(ii) $\mathbf{K}_A$—the algebra of the combined left and right actions of an algebra **K** on itself;
(iii) $M_n(\mathbf{K})$—$n \times n$ matrices over the algebra **K**;
(iv) $\mathbf{K}^n$—and the $n \times 1$ column over **K**;
(v) $\mathcal{CL}(p,q)$—the Clifford algebra of the real spacetime with signature $(p+,q-)$.

III. THREE LEPTOQUARK FAMILES

One thing to note from the mathematical preliminaries is that $\mathbf{C^1}$, $\mathbf{H^2}$ and $\mathbf{O^3}$ are each associated to exceptional structures. Motivated particularly by the list of lattice representations, we therefore propose to consider as the spinor space for the Standard Model,

$$\mathbf{T^6} = \mathbf{C^1} \otimes \mathbf{H^2} \otimes \mathbf{O^3}.$$

Clearly, if $\mathbf{T^2}$ accounts for one full family and its antifamily, then $\mathbf{T^6}$ should account for three, which is the accepted number.

First of all, let $\mathbf{P}=\mathbf{C}\otimes\mathbf{H}$; then $\mathbf{P}_L$ is isomorphic to the Pauli algebra, so $M_2(\mathbf{P}_L)$ is isomorphic to the Dirac algebra, and $\mathbf{H}_R$, which commutes with $M_2(\mathbf{P}_L)$ (which acts on $\mathbf{H^2}$), provides an internal $SU(2)$ degree of freedom.

One can do much the same thing[2] with $\mathbf{T}$. $\mathbf{T}_L$ is a Pauli-like algebra, and $M_2(\mathbf{T}_L)$ is the Dirac algebra of 1,9-spacetime. Again there remains the internal $\mathbf{H}_R$ commuting with $M_2(\mathbf{T}_L)$, providing an isospin $SU(2)$. The associated spinor space ($\mathbf{T}^2$) transforms with respect to the standard symmetry as the direct sum of a leptoquark family and antifamily of 1,3-Dirac spinors.

We would like to proceed similarly with $\mathbf{T}^6$. However, in Ref. 2 the algebra $M_2(\mathbf{T}_L)$, which acts on $\mathbf{T}^2$, is isomorphic to a Clifford algebra [the complexification of $\mathcal{CL}(1,9)$], which is relevant to our interpretation above. But since all Clifford algebras are 2^k-dimensional, the $3^2 2^{13}$-dimensional $M_6(\mathbf{T}_A)$ (which is the full algebra of actions associated with $\mathbf{T}^6$) is not a Clifford algebra.

Let us plow ahead anyway, and first look at the 2^{15}-dimensional $M_4(\mathbf{T}_A)$, isomorphic to the complexification of $\mathcal{CL}(1,13)$. This acts on $\mathbf{T}^4$, which is a pair of leptoquark families (and their antifamilies). We let

$$\epsilon=\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad \alpha=\begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad \beta=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \gamma=\begin{bmatrix}0&1\\-1&0\end{bmatrix}.$$

We define, for example, the following 4×4 real matrix:

$$[\beta\otimes\alpha]=\begin{bmatrix}0&\alpha\\\alpha&0\end{bmatrix}.$$

We will use the $\mathcal{CL}(1,13)$ 1-vector basis [let $\mathcal{CL}_k(p,q)$ be the $\boldsymbol{k}$-vector basis of $\mathcal{CL}(p,q)$]:

$$[\epsilon\otimes\beta](iq_{R3}),\quad [\epsilon\otimes\gamma]q_{Lk}e_{L7}(iq_{R3}),\quad k=1,2,3,\quad [\epsilon\otimes\gamma]ie_{Lp}(iq_{R3}),\quad p=1,\ldots,6,$$

$$[\beta\otimes\epsilon]q_{R1},\quad [\beta\otimes\epsilon]q_{R2},\quad [\beta\otimes\alpha]q_{R3},\quad [\gamma\otimes\alpha].$$

The first line contains 10 elements which generate a $\mathcal{CL}(1,9)$ subalgebra of $\mathcal{CL}(1,13)$. This is essentially the $\mathcal{CL}(1,9)$ that appeared in Ref. 2. The second line contains 4 elements which generate a $\mathcal{CL}(0,4)$ subalgebra. Under the commutator product the associated 2-vectors are a basis for $so(4)\sim su(2)\times su(2)$. The six generators are

$$\frac{1}{2}(1\pm[\alpha\otimes\epsilon])\{[\epsilon\otimes\alpha]q_{R1},[\epsilon\otimes\alpha]q_{R2},[\epsilon\otimes\epsilon]q_{R3}\}.$$

The 4×4 real matrix $[\alpha\otimes\epsilon]$ is the product of the last four 1-vectors above; hence it commutes with the $\mathcal{CL}(1,9)$ 1-vectors, but anticommutes with the $\mathcal{CL}(0,4)$ 1-vectors. Therefore it can be used to reduce the 1,13-spacetime to 1,9-spacetime. In particular, at the 1-vector level,

$$\frac{1}{2}(1\pm[\alpha\otimes\epsilon])\mathcal{CL}_1(1,13)\frac{1}{2}(1\pm[\alpha\otimes\epsilon])=\mathcal{CL}_1(1,9)\frac{1}{2}(1\pm[\alpha\otimes\epsilon]).$$

At the 2-vector level,

$$\frac{1}{2}(1\pm[\alpha\otimes\epsilon])so(1,13)\frac{1}{2}(1\pm[\alpha\otimes\epsilon])=(so(1,9)\times su(2))\frac{1}{2}(1\pm[\alpha\otimes\epsilon]),$$

each projector $\frac{1}{2}(1\pm[\alpha\otimes\epsilon])$ picking out a $su(2)$ half of $so(4)$, and projecting from the spinor space, $\mathbf{T}^4$, a $\mathbf{T}^2$ subspace. Hence this reduction results in exactly the scenario developed in Ref. 2, except doubled. Projection operators, $\rho_{L\pm}=\frac{1}{2}(1\pm ie_{L7})$ and $\rho_{R\pm}=\frac{1}{2}(1\pm ie_{R7})$, further reduce the $\mathcal{CL}_1(1,9)$ to $\mathcal{CL}_1(1,3)$, and yielding a total Lie algebra reduction:

$$so(1,13) \mapsto so(1,9) \times su(2) \mapsto so(1,3) \times u(1) \times su(2) \times su(3).$$

The associated $\mathbf{T}^2$ subspace is the direct sum of a family and antifamily of leptons and quarks, transforming appropriately with respect to $u(1) \times su(2) \times su(3)$.

With a Clifford algebra and spinors we can form a Dirac operator and Lagrangian. If there were 2^k families then $\mathbf{T}^{2k}$ would be the appropriate hyperspinor space, acted on by a conventional Clifford algebra. But it is believed there are exactly 3 families, and we will have to get a little creative in constructing a Dirac-like Lagrangian for this case.

A Dirac operator for the $\mathcal{CL}(1,13)$ 2-family model developed above would be

$$\begin{bmatrix} \partial\!\!\!/_{1,9} & \partial\!\!\!/^{+}_{0,4} \\ \partial\!\!\!/^{-}_{0,4} & \partial\!\!\!/_{1,9} \end{bmatrix},$$

built from the original set of 14 1-vectors. (As noted in Ref. 6, this leads to interfamily mixing, including neutrinos.) For the 3-family case, one suggestion is to incorporate 3 of these 2-family Dirac operators into something new, motivated by the form of matrices in the exceptional Jordan algebra. In particular, consider a Lagrangian term like

$$\bar{\Psi} D \Psi = [\bar{\psi}_1 \quad \bar{\psi}_2 \quad \bar{\psi}_3] \begin{bmatrix} \partial\!\!\!/_{1,9} & \partial\!\!\!/^{+}_{0,4} & \partial\!\!\!/^{-}_{0,4} \\ \partial\!\!\!/^{-}_{0,4} & \partial\!\!\!/_{1,9} & \partial\!\!\!/^{+}_{0,4} \\ \partial\!\!\!/^{+}_{0,4} & \partial\!\!\!/^{-}_{0,4} & \partial\!\!\!/_{1,9} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \bar{\psi}_1 \partial\!\!\!/_{1,9} \psi_1 + \bar{\psi}_1 \partial\!\!\!/^{+}_{0,4} \psi_2 + \cdots .$$

Each of the $\psi_k, k=1,2,3$, is a complete leptoquark family plus antifamily residing in a copy of $\mathbf{T}^2$. There are three terms like $\bar{\psi}_1 \partial\!\!\!/_{1,9} \psi_1$, from which we derive single family interactions (Refs. 2 and 3), and six of the form $\bar{\psi}_1 \partial\!\!\!/^{+}_{0,4} \psi_2$, which mixes two different families—on the assumption $\partial\!\!\!/^{+}_{0,4} \psi_2 \neq 0$ (see Ref. 6).

If this approach is valid there is much that needs to be done to complete the picture. In particular, there is no single conventional pseudo-orthogonal space associated with the operator $\mathcal{D}$. Should the three $\partial\!\!\!/_{1,9}$ on the diagonal, and three $\partial\!\!\!/^{+}_{0,4}$ off-diagonal, be distinct? How does one obtain bivectors leading to Lie group actions and internal symmetries?

There are other 3×3 structures that may be relevant in this context, including a kind of Fermionic Clifford algebra related to supersymmetry (Ref. 3, p. 25). This has not been pursued to this point.

APPENDIX

We list for completeness the explicit generators of the special orthogonal groups realized on the division algebras, as used above:

$$so_2 : i.$$

$$so_8 : \left\{ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \right\} \{q_{Li}, q_{Rj}\},$$

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \{1, q_{Li} q_{Rj}\}.$$

$$so_{24} : \left\{ \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \right\} \{e_{La}, e_{Lab}\},$$

$$\left\{\begin{bmatrix}1&0&0\\0&1&0\\0&0&0\end{bmatrix},\begin{bmatrix}1&0&0\\0&0&0\\0&0&1\end{bmatrix},\begin{bmatrix}0&0&0\\0&1&0\\0&0&1\end{bmatrix}\right\}\{e_{La},e_{Lab}\},$$

$$\left\{\begin{bmatrix}0&1&0\\-1&0&0\\0&0&0\end{bmatrix},\begin{bmatrix}0&0&-1\\0&0&0\\1&0&0\end{bmatrix},\begin{bmatrix}0&0&0\\0&0&1\\0&-1&0\end{bmatrix}\right\}\{1,e_{Labc}\}.$$

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Braided cyclic cocycles and nonassociative geometry

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We use monoidal category methods to study the noncommutative geometry of nonassociative algebras obtained by a Drinfeld-type cochain twist. These are the so-called quasialgebras and include the octonions as braided-commutative but nonassociative coordinate rings, as well as quasialgebra versions $\mathcal{C}_q(G)$ of the standard q-deformation quantum groups. We introduce the notion of ribbon algebras in the category, which are algebras equipped with a suitable generalized automorphism σ, and obtain the required generalization of cyclic cohomology. We show that this *braided cyclic cohomology* is invariant under a cochain twist. We also extend to our generalization the relation between cyclic cohomology and differential calculus on the ribbon quasialgebra. The paper includes differential calculus and cyclic cocycles on the octonions as a finite nonassociative geometry, as well as the algebraic noncommutative torus as an associative example. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1787621]

I. INTRODUCTION

In the influential work,[1] Drinfeld extended quantum groups or Hopf algebras to a more general notion of quasi-Hopf algebras stable under conjugation of the coproduct by a "twist." In a dual form the cotwist element F is a cochain and modifies the product of the coquasi-Hopf algebra. In Ref. 2 this construction was formulated as a monoidal equivalence between the comodule category of the coquasi-Hopf algebra H and that of the cotwisted coquasi-Hopf algebra H^F. The differential geometry of quantum groups H^F from this point of view and assuming F was a cocycle (so that we stay in the associative setting) was studied in Ref. 3. The more general coquasi-Hopf setting was used recently in Ref. 4 and applied to the standard quantum groups $\mathbb{C}_q(G)$. This work proved that there is no associative differential algebra on the standard quantum groups with classical dimensions (i.e., deforming the classical case in a strict sense) but that this is possible as a supercoquasi-Hopf algebra $\Omega(\mathbb{C}_q(G))$. This could be considered a first hint that nonassociative geometry is necessary for a full understanding even of ordinary quantum groups. It also suggests that one should take seriously nonassociative coordinate algebras themselves (not just their exterior algebras) and moreover in much greater generality than just (coquasi-)Hopf algebras alone.

We do this in the present paper for algebras A in monoidal Abelian categories. The idea is that the nicest nonassociative algebras, which we call *quasialgebras*, should be ones which are nonassociative but which may be viewed as associative by deforming the tensor product to a monoidal category with nontrivial associator $\Phi_{U,V,W}: U\otimes(V\otimes W)\to(U\otimes V)\otimes W$ for the rebracketing of tensor products of objects U,V,W. This complements the established idea of using braided categories to view certain noncommutative algebras as "commutative" with respect to a nontrivial braiding $\Psi_{V,W}: V\otimes W\to W\otimes V$ for objects V,W, see Ref. 5. Similarly, building on work of Drinfeld[1] we will find quasialgebra versions $\mathcal{C}_q(G)$ of the standard quantum groups which are nonassociative but more commutative (i.e., one can trade one feature for the other).

In general terms, we study several key constructions borrowed from noncommutative geometry[6,7] but now in the setting of quasialgebras, i.e., of algebras in monoidal categories with nontrivial associator. The idea is to think of the quasialgebra geometrically as by definition the coordinates of a "quasiassociative" space, which may also be noncommutative (for example, commutative with respect to a nontrivial braiding) and hence a "quantum quasispace." Thus, in Sec. III we will associate a cocyclic module (see Ref. 6) to any algebra in a braided monoidal *Ab*-category. We show that the morphism

$$\lambda = (\sigma \otimes \mathrm{id})\Psi$$

provides for us a cyclicity morphism in this category and hence a "braided cyclic cohomology" theory. Here $\Psi: A^{\otimes(n+1)} \otimes A \to A \otimes A^{\otimes(n+1)}$ is the braiding isomorphism and $\sigma: A \to A$ is a "generalized algebra automorphism." For reasons which will become clear, we call it a *ribbon automophism* on the algebra A and call (A, σ) a *ribbon (quasi)algebra*. In the associative trivially braided case σ becomes an automorphism in the usual sense and our braided cyclic cohomology reduces to the "twisted" cohomology in Ref. 7 which has been successfully applied to quantum groups such as $\mathbb{C}_q(SL_2)$. We also study how braided cyclic cocycles relate to differential calculus in the monoidal category.

The other key goal of the paper concerns the provision of examples. Indeed, the need for some kind of nonassociative geometry is hinted at from several directions in mathematical physics including string theory. Its need is also indicated from Poisson geometry, where the idea of a generalized Poisson bracket violating the usual Jacobi identity is proposed.[8] It turns out that an adequate class that appears to cover such examples is based on the use of Drinfeld-type cotwists, but not for (coquasi-)Hopf algebras H as above. Rather, we consider an algebra A in the monoidal category of H-comodules. After applying the monoidal equivalence one has an algebra A_F in the category of H^F-comodules. Indeed, all algebras and algebraic constructions "gauge transform" in this way. The A_F construction was introduced in Ref. 9 (in a module version) and for our purposes takes the form[5]

$$A_F = A, \quad \text{with the new product } a \cdot_F b = F(a_{(1)}, b_{(1)}) a_{(2)} b_{(2)},$$

where $a_{(1)} \otimes a_{(2)}$ denotes the (left) coaction. It turns out that a great many noncommutative algebras of interest fit into this cotwist framework for suitable H and F. Indeed, switching on F is a useful formulation of quantization as an extension of the Moyal product: Even if A is commutative, A_F in general becomes noncommutative when F is not symmetric since

$$a \cdot_F b = F(a_{(1)}, b_{(1)}) F^{-1}(b_{(2)}, a_{(2)}) b_{(3)} \cdot_F a_{(3)}.$$

More relevant for us, even if A is associative, A_F in general becomes nonassociative unless F obeys a 2-cocycle condition.[5] Recent applications include Refs. 10–12 in the associative case and Ref. 13, in the nonassociative case.

Section IV contains theorems about how braided cyclic cohomology and differential geometry respond under such cotwists. Thus, suppose for the sake of discussion that A possesses a left covariant differential calculus, $\Omega = \oplus_{k=0}^{n} \Omega_k$ which is supercommutative, i.e., two homogeneous differential forms ω and ω' commute up to a sign $(-1)^{|\omega||\omega'|}$. Thus in particular functions (0-forms) and n-forms commute. Therefore if $\int: \Omega_n \to \mathbb{C}$ is a closed graded trace in the sense of Connes then its character is a cyclic cocycle.[6] Now if we cotwist the superalgebra of differential forms with the same cocycle from one side as above, we obtain a calculus Ω_F for A_F but now functions and n-forms no longer commute. The noncommutativity is controlled by

$$\omega\omega' = (-1)^{|\omega||\omega'|} F(\omega_{(1)}, \omega'_{(1)}) F^{-1}(\omega'_{(2)}, \omega_{(2)}) \omega'_{(3)} \omega_{(3)},$$

where the product is the cotwisted $\cdot_F$ one. Consequently the character $\varphi(a^0, \ldots, a^n) = \int a^0 da^1 \cdots da^n$ after cotwisting is no longer a cyclic cocycle but obeys

$$\sum_{i=0}^{n}(-1)^i\varphi(a^0,\ldots,a^ia^{i+1},\ldots,a^{n+1})$$
$$+(-1)^{n+1}F(a^0_{(1)}\cdots a^n_{(1)},a^{n+1}_{(1)})F^{-1}(a^{n+1}_{(2)},a^0_{(2)}\cdots a^n_{(2)})\varphi(a^{n+1}_{(3)}a^0_{(3)},a^1_{(3)},\ldots,a^n_{(3)})=0.$$

The corresponding formula in the case where F is just a cochain not a cocycle, is much more involved and contains the associator in its formula (see Sec. IV A). We obtain, rather, a braided cyclic cocycle in the "gauge equivalent" category of H^F-comodules. Section IV A also contains rather concrete formulas when the background Hopf algebra H is coquasitriangular. Section IV B specializes the theory to the important case where in fact H is the group algebra of an Abelian group, which is the setting needed for many examples including the octonions.

Finally, Sec. V presents a collection of key examples demonstrating the theory in our paper. We explicitly give the differential calculus and a cyclic cocycle on the octonions as a finite nonassociative geometry, as well as the usual (algebraic) noncommutative torus. Section V C also outlines the theory applied to formal deformation theory, where we obtain the quasialgebras $\mathcal{C}_q(G)$ as mentioned above, using Drinfeld's associator obtained from solving the Knizhnik–Zamalochikov equations. We can also in principle use cotwising to deformation-quantize the quasi-Poisson manifold structure on a G-manifold M proposed in Ref. 8 (which was not achieved before), which we do as a quasialgebra $\mathcal{C}_q(M)$. We also construct the differential calculus and braided cyclic cocycles on all these quasialgebras. Further details of these potential examples will be presented elsewhere.

On the technical side, we start in the preliminary Sec. II, by explicitly embedding, in a canonical way, any general (relaxed) braided monoidal *Ab*-category in a strict braided monoidal *Ab*-category. This underlies Mac Lane's coherence theorem[14] and ensures that one can work with a relaxed category like a strict one. We also recall the Drinfeld's "gauge transformation" (in a dual cotwist sense) at the level of braided monoidal *Ab*-categories as in Ref. 2.

We conclude the Introduction with the geometric motivation behind our theory. In what follows we will consider "branched ribbon tangles," a modification of the usual notion of ribbon tangles (see Ref. 15, and the references there). We are not going to give a precise meaning of a branched ribbon tangle, but limit ourselves to an informal discussion. Thus let us define d_i, $0\leqslant i\leqslant n$ and d_{n+1} to be the isotopy type of the branched ribbon tangles in the strip $\mathbb{R}^2\times[0,1]$ in Figs. 1(a) and 1(b), respectively. Here by isotopy we mean isotopy in $\mathbb{R}^2\times[0,1]$ constant in boundary intervals on the lines $z=0$ and $z=1$ in the plane $x=0$. Then intuitively we have the isotopies in Fig. 1 parts (c), (d), (e), and (f). In part (d) we used the isotopy in part (g). All these isotopies should be clear except (f) which may need more explanation; in fact ignoring vertical bands indexed from 1 to $n+1$ in part (f), the left-hand side of (f) is isotopic with the left-hand side of (h). Now considering the last diagram in (h), rotate the upper branch in this diagram by 360° to give the right-hand side of (f). Now as in Ref. 15 or 5 we define the composition of two branched ribbon tangles by putting one on top of the other one and compressing the resulting diagram to the strand $\mathbb{R}^2\times[0,1]$. Then parts (c), (d), (e), and (f) of Fig. 1 mean

$$d_id_j=d_{j-1}d_i.$$

These relations are the main content of the notion of a simplicial object in the category. Note that one can work essentially in the category of ribbon tangles as in Ref. 15, where roughly speaking, a morphism is just an isotopy type of a ribbon tangle. This would need, however, some geometric considerations whereas we prefer to work in a purely algebraic manner. Thus in Sec. III we axiomatize the precise assumptions which will lead us to above relations in the context of a general braided monoidal category. In this case, for braided categories we use the usual graphical calculus, which should not be confused with the above isotopy argument on actual ribbon graphs which are embedded surfaces in space. We recall that any braided category is the image of the

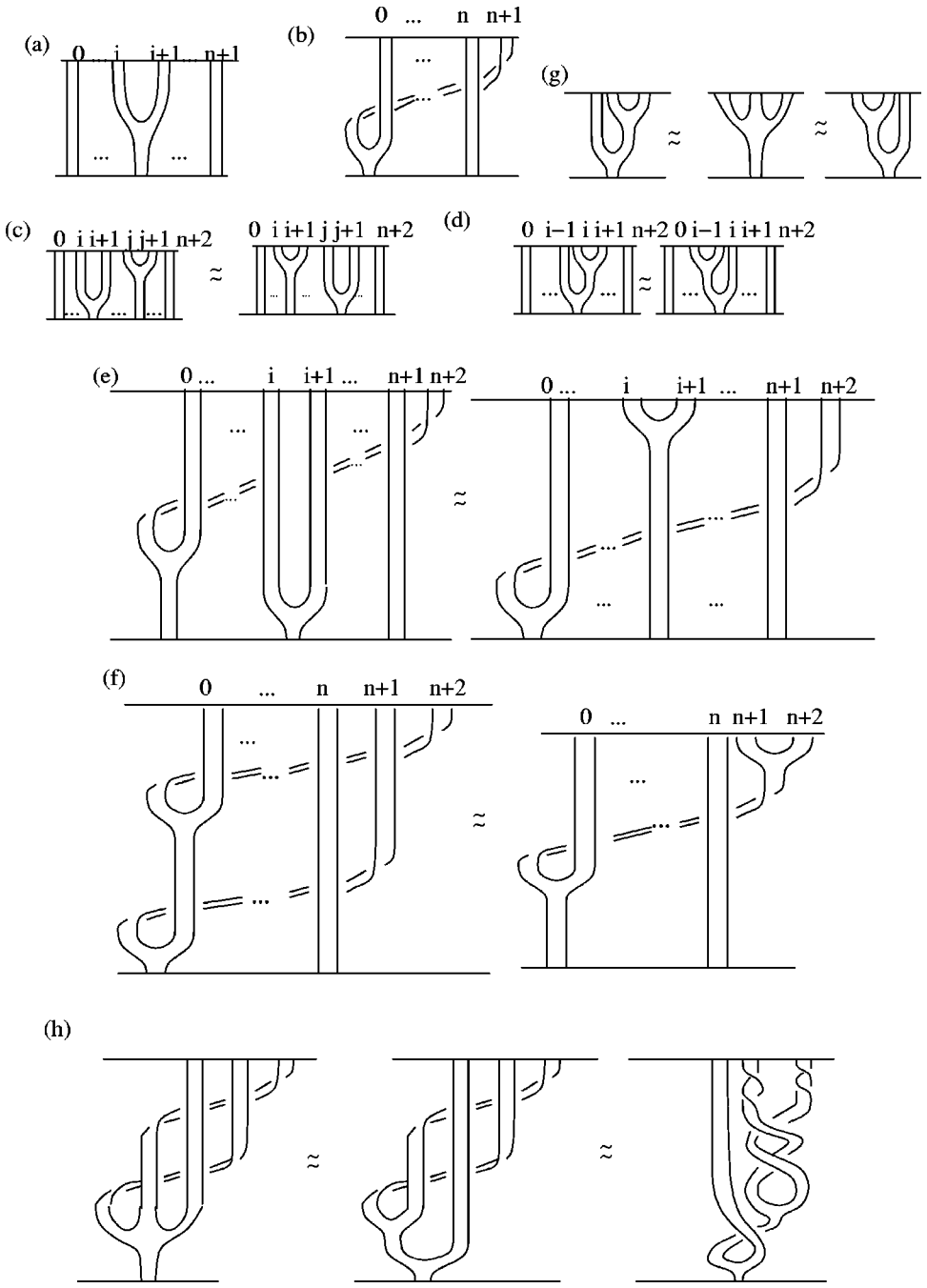

FIG. 1. Branched ribbon tangles, with (a), $0 \leqslant i \leqslant n$. (c), $0 \leqslant i < j-1 \leqslant n$. (d), $1 \leqslant j \leqslant n+1$. (e), $0 \leqslant i \leqslant n$.

category of braids which allows for the representation of the axiomatic properties of $\otimes, \Psi$ by strands and their braiding in the graphical notation (see the Preliminaries). In the same way, one can define a functor from the category of branched ribbon graphs (see Ref. 15) to our category in Sec. III such that two isotopic branched ribbon tangles have the same image under this functor, and the image of branched ribbon tangles under this functor can be considered as graphical symbols.

II. PRELIMINARIES: MONOIDAL CATEGORIES, COHERENCE, AND "GAUGE" EQUIVALENCE

Here we establish the basic notations and methods needed in the paper. In order to be able to work effectively with the nonassociativity, we need in particular to fix some conventions on bracketing and explain related issues. Then we recall the notion of monoidal equivalence used in the construction of our examples.

Let $(\mathcal{C},\otimes,\Phi,\Psi)$ be a braided monoidal Ab-category, where Φ is the associator and Ψ is the braiding. We refer to Refs. 15 and 5 for the axioms, but briefly $\otimes:\mathcal{C}\times\mathcal{C}\to\mathcal{C}$ is a functor and $\Phi\in\mathrm{Nat}(\otimes(\otimes),(\otimes)\otimes)$ and $\Psi\in\mathrm{Nat}(\otimes,\otimes^{\mathrm{op}})$ are natural isomorphisms obeying respectively the pentagon and two hexagon identities with regard to composite objects. The pentagon identifies two ways to go from $U\otimes(V\otimes(W\otimes Z))\to((U\otimes V)\otimes W)\otimes Z$ using two and three applications of Φ, respectively. The hexagons identify $(V\otimes W)\otimes Z\to Z\otimes(V\otimes W)$ in two ways and $V\otimes(W\otimes Z)\to(W\otimes Z)\otimes V$ in two ways, using Ψ,Φ. The coherence theorem of Mac Lane in the symmetric case (when $\Psi^2=\mathrm{id}$ is assumed) and of Joyal and Street[16] in the general braided case, ensures that once these are assumed, one may (a) drop brackets entirely, inserting Φ as needed for any composition to make sense, and (b) represent Ψ,Ψ^{-1} by braid crossings $\times$ and inverse braid crossings $\times$; if two braid compositions are equal then so are the compositions of Ψ,Ψ^{-1}. We assume the monoidal category is unital and denote the unit object by $\mathbf{1}$, where for simplicity we will assume that $U\otimes\mathbf{1}=\mathbf{1}\otimes U=U$, $\forall U\in\mathcal{C}$ and $\Phi_{U,V,W}=\mathrm{id}$ whenever at least one of the objects U,V or W is $\mathbf{1}$. Similarly for the braiding when present. By Ab-monoidal category we mean that for each pair of objects U and V the set $\mathrm{Hom}(U,V)$ is an additive Abelian group such that the composition and tensor product of morphisms are bilinear. Then one can easily show that $K:=\mathrm{Hom}(\mathbf{1},\mathbf{1})$ is a commutative ring with unit.

Next, in order to be completely explicit, we canonically extend any braided monoidal Ab-category $\mathcal{C}$ into a strict braided monoidal Ab-category. First of all, using induction on n we define a family Λ_n of sets as follows. Let for $n>0$, $\mathcal{C}^n$ be the n times Cartesian product of $\mathcal{C}$ with itself. Let Λ_1 be the single set whose element is the identity functor on $\mathcal{C}$ and let Λ_2 be the single set whose element is the functor $\otimes:\mathcal{C}\times\mathcal{C}\to\mathcal{C}$. Now suppose that $\Lambda_k, k<n$ has been defined already such that for each $\alpha\in\Lambda_k$ there is an associated functor $\overline{\alpha}:\mathcal{C}^k\to\mathcal{C}$, then we define Λ_n for $n>2$ to be the set of all pairs (α,β), $\alpha\in\Lambda_k$, $\beta\in\Lambda_l$, $k<n$, $l<n$, $k+l=n$ and we associate to the pair (α,β) the functor $\otimes(\overline{\alpha}\times\overline{\beta}):\mathcal{C}^n\to\mathcal{C}$. For $U_i\in\mathcal{C}$, $1\leqslant i\leqslant n$ and $\alpha\in\Lambda_n$ the symbol $(U_1\otimes\cdots\otimes U_n;\alpha)$ or $U_1\otimes_\alpha\cdots\otimes_\alpha U_n$ will denote the object $\overline{\alpha}(U_1,\ldots,U_n)$.

Now let $\overline{\mathcal{C}}$ be the category whose objects are symbols $U_1\otimes\cdots\otimes U_n$, $n=1,2,\ldots,U_i\in\mathcal{C}$ such that if $n>1$ then $U_i\neq\mathbf{1},\forall i$. The object $\mathbf{1}$ of $\overline{\mathcal{C}}$ is called the degree zero object and the objects $U_1\otimes\cdots\otimes U_n$, $n=1,2,\ldots,\mathbf{1}\neq U_i\in\mathcal{C}$ are called of degree n. To define morphisms in this category we recall that by Mac Lane's coherence theorem there exists a unique family of isomorphisms $I^\alpha_\beta=I^\alpha_\beta(U_1,\ldots,U_m):(U_1\otimes\cdots\otimes U_m;\alpha)\to(U_1\otimes\cdots\otimes U_m;\beta)$, $\alpha,\beta\in\Lambda_m,\mathbf{1}\neq U_i\in\mathcal{C}$, induced by the associator satisfying $I^\alpha_\beta=\mathrm{id}$ for $m=1,2$ and

$$I^\beta_\gamma I^\alpha_\beta=I^\alpha_\gamma,\qquad\forall\,\alpha,\ \beta,\ \gamma\in\Lambda_m, \tag{2.1}$$

$$I^{\alpha_1}_{\alpha_2}(U_1,\ldots,U_k)\otimes I^{\beta_1}_{\beta_2}(U_{k+1},\ldots,U_m)=I^{(\alpha_1,\beta_1)}_{(\alpha_2,\beta_2)}(U_1,\ldots,U_m),\quad\alpha_1,\alpha_2\in\Lambda_k,\ \beta_1,\ \beta_2\in\Lambda_{m-k}, \tag{2.2}$$

$$I^{(\mathrm{id},\otimes)}_{(\otimes,\mathrm{id})}(U_1,U_2,U_3)=\Phi_{U_1,U_2,U_3}. \tag{2.3}$$

We call these isomorphisms, the *higher degree associators* of $\mathcal{C}$.

Next we define an equivalence relation among the morphisms in $\cup_{\alpha\in\Lambda_m,\beta\in\Lambda_n}\mathrm{Hom}_{\mathcal{C}}((U_1\otimes\cdots\otimes U_m;\alpha),(V_1\otimes\cdots\otimes V_n;\beta))$ by

$$f_1 \sim f_2 \Leftrightarrow f_2 = I^{\beta_1}_{\beta_2}(V_1, \ldots, V_n) f_1 I^{\alpha_2}_{\alpha_1}(U_1, \ldots, U_m) \tag{2.4}$$

for $f_i:(U_1\otimes\cdots\otimes U_m;\alpha_i)\to(V_1\otimes\cdots\otimes V_n;\beta_i)$, $\alpha_i\in\Lambda_m,\beta_i\in\Lambda_n,i=1,2$. One can easily show that the above relation is an equivalence relation and each equivalence class contains one and only one representative in each set $\mathrm{Hom}_{\mathcal{C}}((U_1\otimes\cdots\otimes U_m;\alpha),(V_1\otimes\cdots\otimes V_n;\beta))$. We now define $\mathrm{Hom}_{\overline{\mathcal{C}}}(U_1\otimes\cdots\otimes U_m, V_1\otimes\cdots\otimes V_n)$ to be the equivalence classes of all morphisms in the set $\cup_{\alpha\in\Lambda_m,\beta\in\Lambda_n}\mathrm{Hom}_{\mathcal{C}}((U_1\otimes\cdots\otimes U_m;\alpha),(V_1\otimes\cdots\otimes V_n;\beta))$. We denote the equivalence classes by notation $[f]$.

For morphisms $f:U_1\otimes\cdots\otimes U_l\to V_1\otimes\cdots\otimes V_m$ and $g:V_1\otimes\cdots\otimes V_m\to W_1\otimes\cdots\otimes W_n$ in $\overline{\mathcal{C}}$ we define composition gf to be the class of morphism $g^{\beta}_{\gamma}f^{\alpha}_{\beta}$. Here f^{α}_{β} and g^{β}_{γ} are the representatives of f and g in $\mathrm{Hom}_{\mathcal{C}}((U_1\otimes\cdots\otimes U_l;\alpha),(V_1\otimes\cdots\otimes V_m;\beta))$ and $\mathrm{Hom}_{\mathcal{C}}((V_1\otimes\cdots\otimes V_m;\beta),(W_1\otimes\cdots\otimes W_n;\gamma))$ respectively, for arbitrary $\alpha\in\Lambda_l,\beta\in\Lambda_m,\gamma\in\Lambda_n$. One can easily show that this composition is well-defined and is associative, and that the classes of identity morphisms in $\mathcal{C}$ are identity morphisms in $\overline{\mathcal{C}}$.

To define a monoidal structure on $\overline{\mathcal{C}}$ we define $\mathbf{1}\otimes\mathbf{1}:=\mathbf{1}$ and $\mathbf{1}\otimes(U_1\otimes\cdots\otimes U_m):=U_1\otimes\cdots\otimes U_m=:(U_1\otimes\cdots\otimes U_m)\otimes\mathbf{1}$ and $(U_1\otimes\cdots\otimes U_m)\otimes(V_1\otimes\cdots\otimes V_n):=U_1\otimes\cdots\otimes U_m\otimes V_1\otimes\cdots\otimes V_n$ for $\mathbf{1}\neq U_i,V_i$. And for $f:U_1\otimes\cdots\otimes U_m\to V_1\otimes\cdots\otimes V_n$ and $f':U'_1\otimes\cdots\otimes U'_{m'}\to V'_1\otimes\cdots\otimes V'_{n'}$ we define $f\otimes f'$ to be the equivalence class of the morphism $f^{\alpha}_{\beta}\otimes f'^{\alpha'}_{\beta'}:(U_1\otimes\cdots\otimes U_m\otimes U'_1\otimes\cdots\otimes U'_{m'};(\alpha,\alpha'))\to(V_1\otimes\cdots\otimes V_n\otimes V'_1\otimes\cdots\otimes V'_{n'};(\beta,\beta'))$, $\alpha\in\Lambda_m,\alpha'\in\Lambda_{m'},\beta\in\Lambda_n,\beta\in\Lambda_{n'}$. Again one can show this is well-defined by using (2.2). From naturality of the associator, it is obvious that this tensor product is associative and the unit object of $\mathcal{C}$ is also unit object of this product. Therefore $\overline{\mathcal{C}}$ is a strict monoidal category. Similarly the addition of two morphisms $f,g:U_1\otimes\cdots\otimes U_m\to V_1\otimes\cdots\otimes V_n$ is defined to be the equivalence class of the morphism $f^{\alpha}_{\beta}+g^{\alpha}_{\beta}$, $\alpha\in\Lambda_m,\beta\in\Lambda_n$, and it is straightforward to show this is well-defined and $\overline{\mathcal{C}}$ is a strict monoidal *Ab*-category.

Finally, when $\mathcal{C}$ is braided, we define braid isomorphisms $\overline{\Psi}_{U_1\otimes\cdots\otimes U_m,V_1\otimes\cdots\otimes V_n}$ to be the equivalence class of morphism $\Psi_{(U_1\otimes\cdots\otimes U_m;\alpha),(V_1\otimes\cdots\otimes V_n;\beta)}$. It is easy to show that $\overline{\mathcal{C}}$ equipped with this isomorphisms becomes a strict braided monoidal *Ab*-category.

Note that the strict braided monoidal category $\overline{\mathcal{C}}$ is an extension of $\mathcal{C}$ as an *Ab*-category but not as a braided monoidal one. Nevertheless, the braided monoidal structure of $\mathcal{C}$ is used in building $\overline{\mathcal{C}}$ and allows us to replace any nonstrict $\mathcal{C}$ by the strict $\overline{\mathcal{C}}$ by regarding its objects and morphisms in $\overline{\mathcal{C}}$. Note that $\mathcal{C}$ does not inherit an associative tensor product from $\overline{\mathcal{C}}$ because if we regard two objects U and V in $\mathcal{C}$ as first degree objects of $\overline{\mathcal{C}}$ then their tensor product $U\otimes V$ in $\overline{\mathcal{C}}$ is a second degree object of $\overline{\mathcal{C}}$ and therefore it is not in $\mathcal{C}$ which is the set of objects of degree less than two in $\overline{\mathcal{C}}$. For example we know that an algebra in a strict monoidal category is defined to be an object A equipped with a morphism $m:A\otimes A\to A$ such that $m(\mathrm{id}\otimes m)=m(m\otimes\mathrm{id})$ as a morphism from $A\otimes A\otimes A$ to A. Now let $\mathcal{C}$ be a nonstrict monoidal category, but view it in $\overline{\mathcal{C}}$. We define similarly, an algebra A to be an object in $\mathcal{C}$ (a first degree object in $\overline{\mathcal{C}}$) equipped with a morphism $m:A\otimes A\to A$ (a morphism from a second degree object to a first degree object in $\overline{\mathcal{C}}$) such that $m(\mathrm{id}\otimes m)=m(m\otimes\mathrm{id})$ as an equality between morphisms from $A\otimes A\otimes A$ (a third degree object in $\overline{\mathcal{C}}$) to A (a first degree object in $\overline{\mathcal{C}}$). If in addition there exists a morphism $\eta:\mathbf{1}\to A$ such that $m(\mathrm{id}\otimes\eta)=m(\eta\otimes\mathrm{id})=\mathrm{id}$ then we call (A,m,η) a unital algebra in $\mathcal{C}$.

The above construction of the family $\{\Lambda_n\}_n$ can be done for any set equipped with a binary action on it. Explicitly let A be a set with a binary action $.:A\times A\to A$, then similarly, using induction, for each n we have a set of n-fold actions $A\times\cdots\times A\to A$. We denote this set again by $\{\Lambda_n\}_n$ and for $\alpha\in\Lambda_n$ and $a^i\in A$, $1\leqslant i\leqslant n$ we use the notation $a^1{}_{._\alpha}\cdots{}_{._\alpha}a^n$ for $\alpha(a^1,\ldots,a^n)$.

We also want to recall quite explicitly the notion of a tensor functor between braided monoidal categories. It is known[2] that equivalence by such tensor functors is the correct notion of "gauge transformation" relevant to the Drinfeld cotwist. At the moment, we give the general categorical

setting for this. Thus, let $(\mathcal{C},\otimes,\Phi,\Psi)$ and $(\mathcal{C}',\otimes',\Phi',\Psi')$ be two braided unital monoidal *Ab*-categories and let $T:\mathcal{C}\to\mathcal{C}'$ be an additive functor such that $T(\mathbf{1})=\mathbf{1}'$ and suppose that there exists a natural isomorphism $\mathcal{F}$ between the functors $\otimes'(T\times T), T\otimes:\mathcal{C}\times\mathcal{C}\to\mathcal{C}'$, i.e., there exists a family of isomorphisms $\mathcal{F}_{U,V}:T(U)\otimes' T(V)\to T(U\otimes V)$ in $\mathcal{C}'$, $\forall U,V\in\mathcal{C}$, such that $\mathcal{F}_{U,\mathbf{1}}=\mathcal{F}_{\mathbf{1},U}=\mathrm{id}_{T(U)}$ and for all objects U_i,V_i, $i=1,2$ and morphisms $f:U_1\to U_2, g:V_1\to V_2$ in $\mathcal{C}$ we have

$$T(f\otimes g)\mathcal{F}_{U_1,V_1}=\mathcal{F}_{U_2,V_2}(T(f)\otimes' T(g)). \tag{2.5}$$

Now suppose that

$$T(\Phi_{U,V,W})\mathcal{F}_{U,V\otimes W}(\mathrm{id}_{T(U)}\otimes'\mathcal{F}_{V,W})=\mathcal{F}_{U\otimes V,W}(\mathcal{F}_{U,V}\otimes\mathrm{id}_{T(W)})\Phi'_{T(U),T(V),T(W)} \tag{2.6}$$

and

$$T(\Psi_{U,V})\mathcal{F}_{U,V}=\mathcal{F}_{V,U}\Psi'_{T(U),T(V)} \tag{2.7}$$

$\forall U,V,W\in\mathcal{C}$.

Definition 1: A tensor functor between two braided monoidal Ab-categories $(\mathcal{C},\otimes,\Phi,\Psi)$ *and* $(\mathcal{C}',\otimes',\Phi',\Psi')$ *is a pair* $(T,\mathcal{F})$ *as above. A "gauge transformation" between braided monoidal Ab-categories is an invertible tensor functor, in which case we say that the categories are "gauge equivalent."*

Indeed, if T is an invertible functor, we set

$$\mathcal{F}'_{U',V'}:=T^{-1}(\mathcal{F}^{-1}_{T^{-1}(U'),T^{-1}(V')}),\quad \forall U',V'\in\mathcal{C}'.$$

Then $(T^{-1},\mathcal{F}')$ is a tensor functor from $(\mathcal{C}',\otimes',\Phi',\Psi')$ to $(\mathcal{C},\otimes,\Phi,\Psi)$. To prove this let U'_i, V'_i, U', V' and W' be objects in $\mathcal{C}'$, where $i=1,2$, and let $f':U'_1\to U'_2, g':V'_1\to V'_2$ be morphisms in $\mathcal{C}'$, then we set $U_i:=T^{-1}(U'_i)$, $V_i:=T^{-1}(V'_i)$, $i=1,2$, $f:=T^{-1}(f')$ and $g:=T^{-1}(g')$. Then from (2.5) we get $\mathcal{F}^{-1}_{U_2,V_2}T(f\otimes g)=(f'\otimes' g')\mathcal{F}^{-1}_{U_1,V_1}$. Thus applying T^{-1} to this relation we get

$$T^{-1}(f'\otimes' g')\mathcal{F}'_{U'_1,V'_1}=\mathcal{F}'_{U'_2,V'_2}(T^{-1}(f')\otimes' T^{-1}(g')) \tag{2.8}$$

which is the counterpart of (2.5) for pair $(T^{-1},\mathcal{F}')$. The counterpart of (2.7) for the pair $(T^{-1},\mathcal{F}')$ can be proved similarly. Let us prove (2.6) for $(T^{-1},\mathcal{F}')$. At first note that if we apply (2.8) for $f'=\mathrm{id}_{U'}, g'=\mathcal{F}^{-1}_{V,W}$ then we get $T^{-1}(\mathrm{id}_{U'}\otimes'\mathcal{F}^{-1}_{V,W})\mathcal{F}'_{U',T(V\otimes W)}=\mathcal{F}'_{U',V'\otimes W'}(\mathrm{id}_{T^{-1}(U')}\otimes' T^{-1}(\mathcal{F}^{-1}_{V,W}))=\mathcal{F}'_{U',V'\otimes W'}(\mathrm{id}_{T^{-1}(U')}\otimes'\mathcal{F}'_{V',W'})$, and similarly applying (2.8) for $f'=\mathcal{F}^{-1}_{U,V}, g'=\mathrm{id}_{W'}$ we get $T^{-1}(\mathcal{F}^{-1}_{U,V}\otimes'\mathrm{id}_{W'})\mathcal{F}'_{T(U\otimes V),W'}=\mathcal{F}'_{U'\otimes V',W'}(T^{-1}(\mathcal{F}^{-1}_{U,V})\otimes'\mathrm{id}_{T^{-1}(W')})=\mathcal{F}'_{U'\otimes V',W'}(\mathcal{F}'_{U',V'}\otimes'\mathrm{id}_{T^{-1}(W')})$. We call these two relations auxiliary relations. Now from (2.6) we deduce $\Phi'_{U',V',W'}(\mathrm{id}_{U'}\otimes'\mathcal{F}^{-1}_{V,W})\mathcal{F}^{-1}_{U,V\otimes W}=(\mathcal{F}^{-1}_{U,V}\otimes\mathrm{id}_{W'})\mathcal{F}^{-1}_{U\otimes V,W}T(\Phi_{U,V,W})$ and if we apply T^{-1} to this relation and use the auxiliary relations then we get the counterpart of (2.6).

We need to check how the above notions of tensor functor and gauge equivalence extend to $\overline{\mathcal{C}}$. Thus, given $(T,\mathcal{F})$, we construct a family of isomorphisms $S_\alpha=S_\alpha(U_1,\ldots,U_m):(T(U_1)\otimes'\cdots\otimes' T(U_m);\alpha)\to T(U_1\otimes\cdots\otimes U_m;\alpha)$, $\forall\alpha\in\Lambda_m$, $U_i\in\mathcal{C}$, by induction on m; for $m=1$ we set $S_\alpha(U)=\mathrm{id}_{T(U)}$ and for $m=2$ we set $S_\alpha(U_1,U_2)=\mathcal{F}_{U_1,U_2}$. Now let S_α have been defined already for $\alpha\in\Lambda_k$, $k<m$ and let $\gamma\in\Lambda_m$. Then by definition of the set Λ_m there exist unique integers k, $l<m$ and unique $\alpha\in\Lambda_k$, $\beta\in\Lambda_l$ such that $k+l=m$ and $\gamma=(\alpha,\beta)$. Then we set

$$S_{(\alpha,\beta)}(U_1,\ldots,U_m):=\mathcal{F}_{(U_1\otimes\cdots\otimes U_k;\alpha),(U_{k+1}\otimes\cdots\otimes U_m;\beta)}(S_\alpha(U_1,\ldots,U_k)\otimes' S_\beta(U_{k+1},\ldots,U_m)). \tag{2.9}$$

Now let I'^{α}_{β} denote the corresponding higher degree associators for $\mathcal{C}'$, then we claim that

$$S^{-1}_\beta T(I^\alpha_\beta(U_1,\ldots,U_m))S_\alpha=I'^{\alpha}_{\beta}(U'_1,\ldots,U'_m), \tag{2.10}$$

where $U'_i=T(U_i)$. To prove this, let us denote the left-hand side of the above relation by $J^\alpha_\beta(U'_1,\ldots,U'_m)$. We check that the relations (2.1)–(2.3) hold for this family and therefore by

uniqueness of higher degree associators the claim will be proven. We have

$$J^{\beta}_{\gamma}J^{\alpha}_{\beta}=S^{-1}_{\gamma}T(I^{\beta}_{\gamma})S_{\beta}S^{-1}_{\beta}T(I^{\alpha}_{\beta})S_{\alpha}=S^{-1}_{\gamma}T(I^{\beta}_{\gamma}I^{\alpha}_{\beta})S_{\alpha}=S^{-1}_{\gamma}T(I^{\alpha}_{\gamma})S_{\alpha}=J^{\alpha}_{\gamma}$$

and

$$\begin{aligned}J^{\alpha_1}_{\alpha_2}\otimes' J^{\beta_1}_{\beta_2}&=S^{-1}_{\alpha_2}T(I^{\alpha_1}_{\alpha_2})S_{\alpha_1}\otimes' S^{-1}_{\beta_2}T(I^{\beta_1}_{\beta_2})S_{\beta_1}=(S^{-1}_{\alpha_2}\otimes' S^{-1}_{\beta_2})(T(I^{\alpha_1}_{\alpha_2})\otimes' T(I^{\beta_1}_{\beta_2}))(S_{\alpha_1}\otimes' S_{\beta_1})\\&=S^{-1}_{(\alpha_2,\beta_2)}\mathcal{F}_{X_2,Y_2}(T(I^{\alpha_1}_{\alpha_2})\otimes' T(I^{\beta_1}_{\beta_2}))\mathcal{F}^{-1}_{X_1,Y_1}S_{(\alpha_1,\beta_1)}=S^{-1}_{(\alpha_2,\beta_2)}T(I^{\alpha_1}_{\alpha_2}\otimes I^{\beta_1}_{\beta_2})S_{(\alpha_1,\beta_1)}\\&=S^{-1}_{(\alpha_2,\beta_2)}T(I^{(\alpha_1,\beta_1)}_{(\alpha_2,\beta_2)})S_{(\alpha_1,\beta_1)}=J^{(\alpha_1,\beta_1)}_{(\alpha_2,\beta_2)},\end{aligned}$$

where for simplicity we wrote $X_i=(U_1\otimes\cdots\otimes U_k;\alpha_i)$, $Y_i=(U_{k+1}\otimes\cdots\otimes U_m;\beta_i)$, and we have

$$\begin{aligned}J^{(\mathrm{id},\otimes')}_{(\otimes',\mathrm{id})}(U'_1,U'_2,U'_3)&=S^{-1}_{(\otimes',\mathrm{id})}T(I^{(\mathrm{id},\otimes)}_{(\otimes,\mathrm{id})}(U_1,U_2,U_3))S_{(\mathrm{id},\otimes')}\\&=(\mathcal{F}^{-1}_{U_1,U_2}\otimes\mathrm{id}_{T(U_3)})\mathcal{F}^{-1}_{U_1\otimes U_2,U_3}T(\Phi_{U_1,U_2,U_3})\mathcal{F}_{U_1,U_2\otimes U_3}(\mathrm{id}_{T(U_1)}\otimes\mathcal{F}_{U_2,U_3})\\&=\Phi'_{U'_1,U'_2,U'_3},\end{aligned}$$

where we used $S_{(\mathrm{id},\otimes')}(U_1,U_2,U_3)=\mathcal{F}_{U_1,U_2\otimes U_3}(\mathrm{id}_{T(U_1)}\otimes\mathcal{F}_{U_2,U_3})$ which comes from (2.9), and similarly for $S_{(\otimes',\mathrm{id})}$.

Now let $\overline{\mathcal{C}}$ and $\overline{\mathcal{C}'}$ be the canonical extensions of $\mathcal{C}$ and $\mathcal{C}'$ to strict braided monoidal *Ab*-categories respectively. We define a functor $\overline{T}:\overline{\mathcal{C}}\to\overline{\mathcal{C}'}$ by $\overline{T}(U_1\otimes\cdots\otimes U_m):=T(U_1)\otimes'\cdots\otimes' T(U_m)$ and for morphism $f:U_1\otimes\cdots\otimes U_m\to V_1\otimes\cdots\otimes V_n$ in $\overline{\mathcal{C}}$ we define $\overline{T}(f)$ as follows: let $f^{\alpha}_{\beta}:(U_1\otimes\cdots\otimes U_m;\alpha)\to(V_1\otimes\cdots\otimes V_n;\beta)$ be the representative of f for any $\alpha\in\Lambda_m$, $\beta\in\Lambda_n$. We define $\overline{T}(f)$ be the equivalence class of the morphism $S^{-1}_{\beta}T(f^{\alpha}_{\beta})S_{\alpha}:(T(U_1)\otimes'\cdots\otimes' T(U_m);\alpha)\to(T(V_1)\otimes'\cdots\otimes' T(V_n);\beta)$. We must show that this definition does not depend to the choice of the representative. Thus let $f^{\alpha_i}_{\beta_i}$, $i=1,2$ be two representatives of f then we have

$$I'^{\beta_1}_{\beta_2}S^{-1}_{\beta_1}T(f^{\alpha_1}_{\beta_1})S_{\alpha_1}I'^{\alpha_2}_{\alpha_1}=S^{-1}_{\beta_2}T(I^{\beta_1}_{\beta_2})S_{\beta_1}S^{-1}_{\beta_1}T(f^{\alpha_1}_{\beta_1})S_{\alpha_1}S^{-1}_{\alpha_1}T(I^{\alpha_2}_{\alpha_1})S_{\alpha_2}=S^{-1}_{\beta_2}T(I^{\beta_1}_{\beta_2}f^{\alpha_1}_{\beta_1}I^{\alpha_2}_{\alpha_1})S_{\alpha_2}=S^{-1}_{\beta_2}T(f^{\alpha_2}_{\beta_2})S_{\alpha_2}.$$

Thus $\overline{T}(f)$ is well-defined.

Next, for composable morphisms f and g in $\overline{\mathcal{C}}$ we have

$$\overline{T}(gf)=[S^{-1}_{\gamma}T(g^{\beta}_{\gamma}f^{\alpha}_{\beta})S_{\alpha}]=[S^{-1}_{\gamma}T(g^{\beta}_{\gamma})S_{\beta}S^{-1}_{\beta}T(f^{\alpha}_{\beta})S_{\alpha}]=\overline{T}(g)\overline{T}(f)$$

and for addable morphisms f and g in $\overline{\mathcal{C}}$ we have $\overline{T}(f+g)=[S^{-1}_{\beta}T(f^{\alpha}_{\beta}+g^{\alpha}_{\beta})S_{\alpha}]=\overline{T}(f)+\overline{T}(g)$. Clearly for all objects $X=U_1\otimes\cdots\otimes U_m$, $Y=V_1\otimes\cdots\otimes V_n$ in $\mathcal{C}$ we have $T(X\otimes Y)=T(X)\otimes'T(Y)$ and if $X'=U'_1\otimes\cdots\otimes U'_{m'}$, $Y'=V'_1\otimes\cdots\otimes V'_{n'}$ are other objects in $\overline{\mathcal{C}}$ and $f:X\to Y$, $g:X'\to Y'$ are morphisms in $\overline{\mathcal{C}}$ we have

$$\begin{aligned}\overline{T}(f\otimes g)=[S^{-1}_{(\beta,\beta')}T(f^{\alpha}_{\beta}\otimes g^{\alpha'}_{\beta'})S_{(\alpha,\alpha')}]&=[(S^{-1}_{\beta}\otimes' S^{-1}_{\beta'})\mathcal{F}^{-1}_{Y_{\beta},Y'_{\beta'}}T(f^{\alpha}_{\beta}\otimes g^{\alpha'}_{\beta'})\mathcal{F}^{-1}_{X_{\alpha},X'_{\alpha'}}(S_{\alpha}\otimes' S_{\alpha'})]\\&=[(S^{-1}_{\beta}\otimes' S^{-1}_{\beta'})(T(f^{\alpha}_{\beta})\otimes' T(g^{\alpha'}_{\beta'}))(S_{\alpha}\otimes' S_{\alpha'})]\\&=[S^{-1}_{\beta}T(f^{\alpha}_{\beta})S_{\alpha}\otimes' S^{-1}_{\beta'}T(g^{\alpha'}_{\beta'})S_{\alpha'}]=\overline{T}(f)\otimes'\overline{T}(g),\end{aligned}$$

where $X_{\alpha}=(U_1\otimes\cdots\otimes U_m;\alpha)$, $X'_{\alpha'}=(U'_1\otimes\cdots\otimes U'_m;\alpha')$, $Y_{\beta}=(V_1\otimes\cdots\otimes V_n;\beta)$, $Y'_{\beta'}=(V'_1\otimes\cdots\otimes V'_n;\beta')$.

Now, with the above notation for X,Y,X_{α}, and Y_{β}, we show that

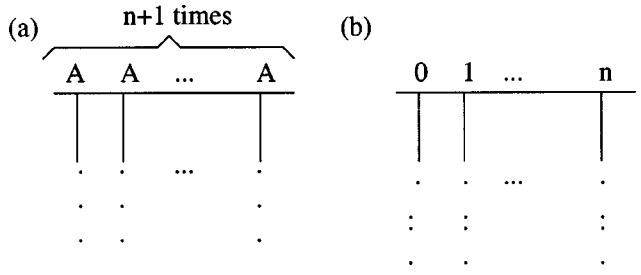

FIG. 2. Notation for multiple $\otimes$ products.

$$\overline{T}(\overline{\Psi}_{X,Y}) = \overline{\Psi}'_{\overline{T}(X),\overline{T}(Y)}. \tag{2.11}$$

Let us denote $\overline{\Psi}_{X,Y}$ by f for brevity. Then by definition for $\alpha \in \Lambda_m$, $\beta \in \Lambda_n$ we have $f^{(\alpha,\beta)}_{(\beta,\alpha)} = \Psi_{X_\alpha, Y_\beta}$. Thus,

$$\begin{aligned}\overline{T}(\overline{\Psi}_{X,Y}) &= [S^{-1}_{(\beta,\alpha)} T(f^{(\alpha,\beta)}_{(\beta,\alpha)}) S_{(\alpha,\beta)}] = [(S^{-1}_\beta \otimes' S^{-1}_\alpha)\mathcal{F}^{-1}_{Y_\beta, X_\alpha} T(\Psi_{X_\alpha, Y_\beta})\mathcal{F}^{-1}_{X_\alpha, Y_\beta}(S_\alpha \otimes' S_\beta)] \\ &= [(S^{-1}_\beta \otimes' S^{-1}_\alpha)\Psi'_{T(X_\alpha),T(Y_\beta)}(S_\alpha \otimes' S_\beta)] \\ &= [\Psi'_{\overline{T}(X)_\alpha, \overline{T}(Y)_\beta}] = \overline{\Psi}'_{\overline{T}(X),\overline{T}(Y)},\end{aligned}$$

where by $\overline{T}(X)_\alpha$ we mean $(T(U_1)\otimes' \cdots \otimes' T(U_m); \alpha)$ and by $\overline{T}(Y)_\beta$ we mean $(T(V_1)\otimes' \cdots \otimes' T(V_n); \beta)$ and in the fourth equality we used naturality of the braiding in $\mathcal{C}'$.

Summarizing the above argument, we have

Proposition 2: Any tensor functor $(T, \mathcal{F})$ from $(\mathcal{C}, \otimes, \Phi, \Psi)$ to $(\mathcal{C}', \otimes', \Phi', \Psi')$ induces a canonical additive functor $\overline{T}: \overline{\mathcal{C}} \to \overline{\mathcal{C}'}$ obeying

(i) $\overline{T}(X \otimes Y) = \overline{T}(X) \otimes' \overline{T}(Y)$, *for all objects X, Y in* $\overline{\mathcal{C}}$;

(ii) $\overline{T}(f \otimes g) = \overline{T}(f) \otimes' \overline{T}(g)$, *for all morphisms f, g in* $\overline{\mathcal{C}}$;

(iii) $\overline{T}(\overline{\Psi}_{X,Y}) = \Psi'_{\overline{T}(X),\overline{T}(Y)}$, *for all objects X, Y in* $\overline{\mathcal{C}}$.

III. BRAIDED HOCHSCHILD AND CYCLIC COHOMOLOGY

Before starting this section let us agree that if in a diagram all the bands are labeled by an object A, we label the bands by integers $0, 1, 2, 3, \ldots$. For examples we use the diagram (b) instead of diagram (a) in Fig. 2. We let $\mathcal{C}$ be a braided unital monoidal *Ab*-category.

Definition 3: A ribbon algebra in $\mathcal{C}$ is an algebra (A, m, η) (see the previous section) equipped with an isomorphism $\sigma: A \to A$ such that

$$m(\sigma \otimes \sigma)\Psi^2 = \sigma m, \quad \sigma\eta = \eta,$$

where $\Psi = \Psi_{A,A}$ is the braiding $A \otimes A \to A \otimes A$.

If the category $\mathcal{C}$ is the category of vector spaces over a field with trivial braiding i.e., the flip, then these relations mean that σ is just an algebra automorphism preserving the unit. In fact this Definition 3 is a combination of the axioms of an algebra homomorphism and the axiom for the relation between the braiding and the ribbon structure in a ribbon category. In particular, any algebra A in a ribbon category $\mathcal{C}$ is automatically ribbon with $\sigma = \nu_A$ where ν is the ribbon isomorphism. We recall that a ribbon category is a braided monoidal category equipped with natural isomorphisms ν_X for any object X such that

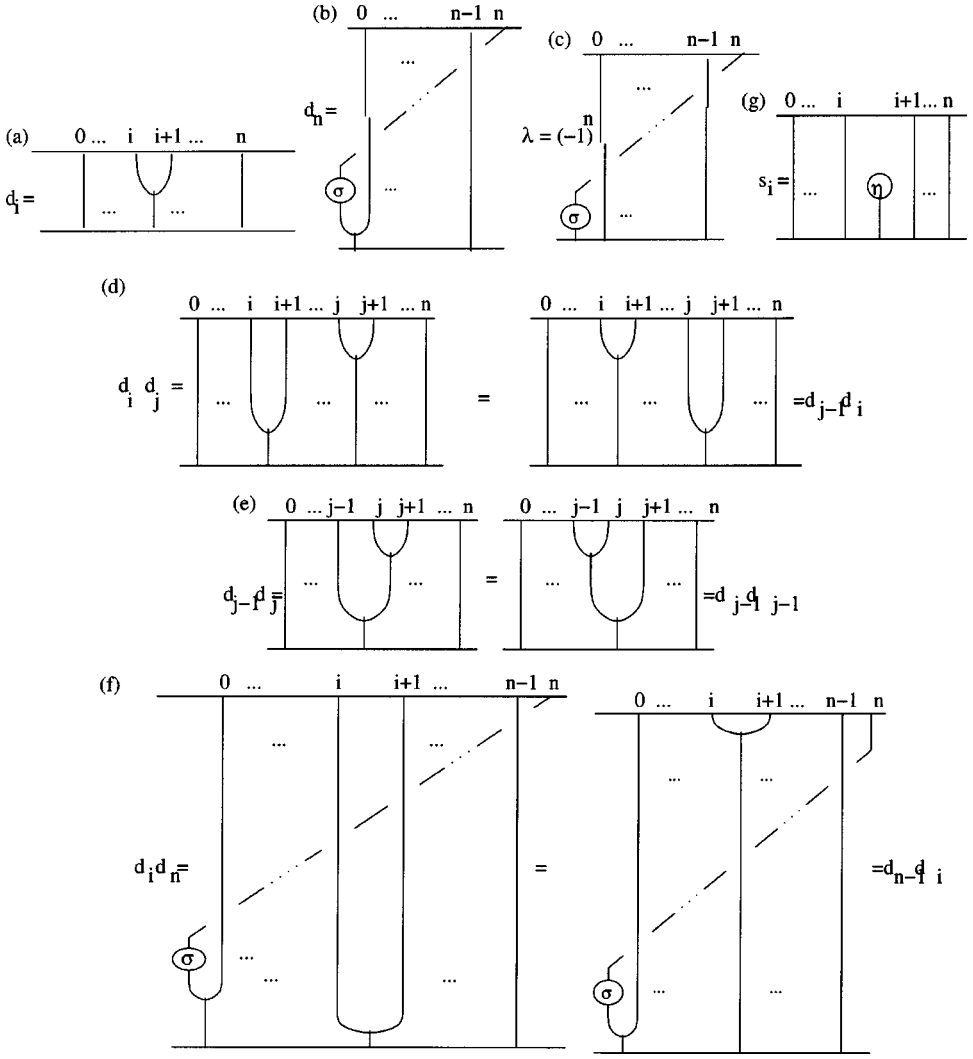

FIG. 3. Structure of C_n.

$$\nu_{X\otimes Y}=(\nu_X\otimes\nu_Y)\circ\Psi_{Y,X}\circ\Psi_{X,Y}$$

for all X, Y. Since the product of A is a morphism, we conclude by functoriality that $\nu_A\circ m=m\circ\nu_{A\otimes A}=m\circ(\nu_A\otimes\nu_A)\circ\Psi^2$ as required. There are also plenty of examples where $\mathcal{C}$ does not need to be a ribbon category. For example, if A is a braided group or Hopf algebra in a braided category $\mathcal{C}$, then its antipode $S:A\to A$ is known[5] to be braided-antimultiplicative with the result that $\sigma=S^2$ makes A into a ribbon algebra in the sense above.

This definition will be rather essential for us in the construction of braided Hochschild and cyclic cohomology. We call σ a *ribbon automorphism* for the algebra A. As mentioned in the previous section, we will work via the strict extension $\overline{\mathcal{C}}$ of $\mathcal{C}$.

We set $C_n=A^{\otimes(n+1)}$, $n\geqslant 0$ as an object of $\overline{\mathcal{C}}$ of degree $n+1$ and define morphisms

$$d_i=d_i^{(n)}:C_n\to C_{n-1},\quad s_i=s_i^{(n)}:C_n\to C_{n+1},\quad 0\leqslant i\leqslant n,\quad \lambda=\lambda_n:C_n\to C_n \tag{3.1}$$

in $\overline{\mathcal{C}}$ by diagrams (a), (b), (c), and (g) in Fig. 3, where all bands in all diagrams in Fig. 3 are labeled by object A in $\mathcal{C}$. We use a diagrammatic notation for morphisms as explained in the Preliminaries.

Theorem 4: *On C_n we have*

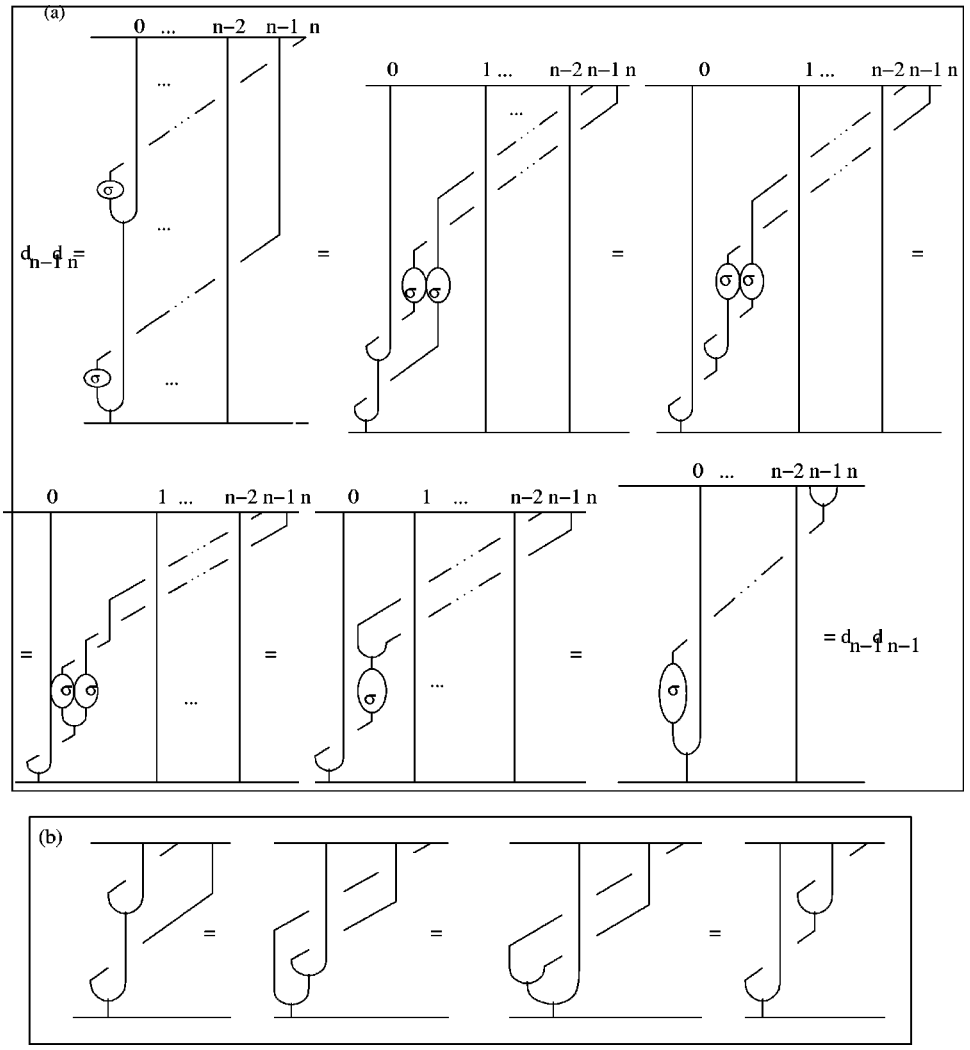

FIG. 4. Further diagrams in the structure of C_n.

$$(i)\ d_i d_j = d_{j-1} d_i, \quad 0 \leqslant i < j \leqslant n, \quad (ii)\ s_i s_j = s_{j+1} s_i, \quad 0 \leqslant i \leqslant j \leqslant n,$$

$$(iii)\ d_i s_j = \begin{cases} s_{j-1} d_i, & i < j \\ \mathrm{id}, & i = j \text{ or } i = j+1 \\ s_j d_{i-1}, & i > j+1, \end{cases}$$

$$(iv)\ d_i \lambda = -\lambda d_{i-1}, \quad 1 \leqslant i \leqslant n, \quad d_0 \lambda = (-1)^n d_n,$$

$$(v)\ s_i \lambda = -\lambda s_{i-1}, \quad 1 \leqslant i \leqslant n, \quad s_0 \lambda = (-1)^n \lambda^2 s_n,$$

$$(vi)\ d_i \lambda^{n+1} = \lambda^n d_i, \quad (vii)\ s_i \lambda^{n+1} = \lambda^{n+2} s_i, \quad 0 \leqslant i \leqslant n.$$

Proof: (i) The proof by means of graphical calculus is in Fig. 3 parts (d) (for $j<n, i<j-1$), (e) (for $j<n, i=j-1$), (f) (for $j=n, i<n-1$) and Fig. 4 part (a) (for $j=n, i=n-1$). Note that in the third equality of Fig. 4(a) we used the identity in Fig. 4(b) and in the fifth equality we used Definition 3.

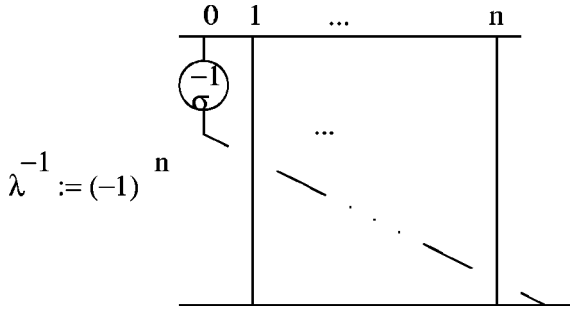

FIG. 5. Inverse of λ on C_n.

The proofs of parts (ii)–(v) are very straightforward and we leave them to the reader. (vi) At first note that λ is invertible with inverse given in Fig. 5. Now from the recursive relations in first part of (iv) it is easy to compute all the d_i in terms of d_n and λ and then using the last part of (iv) we compute d_i in terms of d_0 and λ as $d_i=(-1)^i\lambda^{-n+i}d_0\lambda^{n-i+1}$, $0\leqslant i\leqslant n$. In particular $d_0=\lambda^{-n}d_0\lambda^{n+1}$. Thus $d_i=(-1)^i\lambda^i d_0\lambda^{-i}$, $\forall i$. Hence we have

$$d_i\lambda^{n+1}=(-1)^i\lambda^i d_0\lambda^{n+1-i}=(-1)^i\lambda^i\lambda^n d_0\lambda^{-i}=(-1)^i\lambda^n\lambda^i d_0\lambda^{-i}=\lambda^n d_i.$$

Part (vii) is similar to (iv). ■

Following the strategy in Ref. 7, we now define

$$C^n(\mathcal{C};A,\sigma)=\{\varphi\in \mathrm{Hom}_{\overline{C}}(A^{\otimes(n+1)},\mathbf{1})\,|\,\varphi\lambda^{n+1}=\varphi\}. \tag{3.2}$$

By the above Theorem 4 the morphisms d_i, λ and s_i induce morphisms

$$d_i:C^{n-1}\to C^n,\quad \lambda:C^n\to C^n,\quad s_i:C^{n+1}\to C^n,\quad 0\leqslant i\leqslant n, \tag{3.3}$$

respectively, where we use same symbols. Hence for example $d_i(\varphi):=\varphi d_i$, $\varphi\in C^{n-1}$. Then we obtain a cocyclic module $\{C^n\}_{n\geqslant 0}$ with the above linear maps as face, cyclicity and degeneracy maps respectively. Namely we have

$$On\ C^{n-1};\quad d_jd_i=d_id_{j-1},\quad 0\leqslant i<j\leqslant n,$$

$$On\ C^{n+1};\quad s_js_i=s_is_{j+1},\quad 0\leqslant i\leqslant j\leqslant n,$$

$$On\ C^n;\quad s_jd_i=\begin{cases} d_is_{j-1}, & i<j\\ \mathrm{id}, & i=j\ or\ i=j+1\\ d_{i-1}s_j, & i>j+1,\end{cases}$$

$$On\ C^{n-1};\quad \lambda d_i=-d_{i-1}\lambda,\quad 1\leqslant i\leqslant n,\quad \lambda d_0=(-1)^n d_n,$$

$$On\ C^{n+1};\quad \lambda s_i=-s_{i-1}\lambda,\quad 1\leqslant i\leqslant n,\quad \lambda s_0=(-1)^n s_n\lambda^2,$$

$$On\ C^n;\quad \lambda^{n+1}=\mathrm{id}.$$

Therefore the general theory of Hochschild and cyclic cohomology[6] gives us a cochain complex (C^*,d), $d:=\Sigma_{i=0}^n(-1)^i d_i$ and we call the cohomology of this complex the *braided Hochschild cohomology* of the ribbon algebra (A,σ) in the category $\mathcal{C}$ and denote it by $HH^*(\mathcal{C};A,\sigma)$. We also have a subcomplex of the above complex defined as usual by

$$C^n_\lambda(\mathcal{C};A,\sigma)=\{\varphi\in \mathrm{Hom}_{\overline{C}}(A^{\otimes(n+1)},\mathbf{1})\,|\,\lambda(\varphi)=\varphi\}$$

and we call its cohomology the *braided cyclic cohomology* of the ribbon algebra (A,σ) in the category $\mathcal{C}$ and denote it by $HC^*(\mathcal{C};A,\sigma)$.

Now we suppose that the ring $K=\mathrm{Hom}(\mathbf{1},\mathbf{1})$ is a field containing $\mathbb{Q}$, the rational numbers. Then again the general theory of Hochschild and cyclic cohomology gives the SIB-long exact sequence

$$\cdots \to HC^{n-1} \overset{\mathcal{S}}{\to} HC^{n+1} \overset{\mathcal{I}}{\to} HH^{n+1} \overset{\mathcal{B}}{\to} HC^n \to \cdots,$$

where $\mathcal{I}$ is induced from the inclusion map $C^*_\lambda \hookrightarrow C^*$ and $\mathcal{B}$ is implemented by the Connes's boundary map $\mathcal{B}:C^{n+1}\to C^n$ defined by $\mathcal{B}=(-1)^n N(s_{-1}+s_n)$, where $N=\Sigma_{i=0}^n \lambda^i$ and $s_{-1}=(-1)^n s_0 \lambda^{-1}$ is the extra degeneracy map. Finally, $\mathcal{S}$ is the periodicity map which [see, for example Ref. 17, formula (10.15)], is given explicitly by

$$\mathcal{S}(\varphi) = \frac{-1}{n(n+1)} \sum_{1\leqslant i\leqslant j\leqslant n} (-1)^{i+j} d_{i-1}(d_{j-1}(\varphi)). \tag{3.4}$$

Let us now extend the notion of an ordinary "differential calculus" (DC) over an ordinary algebra (i.e., a DC over an algebra in the category of vector spaces) to an algebra A inside a monoidal *Ab*-category. Until now we have seen only the universal calculus treated in such generality,[18] using diagrammatic methods. In fact the axioms are the same as usual, namely part of a differential graded algebra[6] including A in degree zero; but this time all objects and morphisms must be inside the category. Thus, a *differential calculus of degree* $1\leqslant n\leqslant\infty$ *over algebra* (A,m,η), *in* $\mathcal{C}$ is a sequence of objects $\Omega=\{\Omega_i\}_{i=0}^n$ in $\mathcal{C}$ together with morphisms $\{m_{i,j}:\Omega_i\otimes\Omega_j \to \Omega_{i+j}\}_{i,j=0}^n$, called multiplication and morphisms $d=\{d_i:\Omega_i\to\Omega_{i+1}\}_{i=0}^n$, called exterior differentials, such that $\Omega_0=A$, $m_{0,0}=m$, all with the well-known axioms for an ordinary DC when viewed in the category $\overline{\mathcal{C}}$. For instance, the diagram of the Leibniz rule is in Fig. 6(c), where by labels i and j we mean Ω_i and Ω_j. We do need to say some words about the following axiom of an ordinary DC, where one usually requires that every k-form is a sum of k-forms of the form $a^0 da^1\cdots da^k$ for some $a^i\in A$. We translate this axiom for a DC in a category by requiring that for each k the morphisms

$$m(\mathrm{id}\otimes d):A\otimes\Omega_{k-1}\to\Omega_k \tag{3.5}$$

be epimorphisms. One can easily conclude by using induction on k, that the morphisms

$$m(\mathrm{id}_A\otimes d^{\otimes k}):A^{\otimes(k+1)}\to\Omega_k$$

are epimorphisms of $\overline{\mathcal{C}}$ (the converse is also true but we do not need it). We recall that a morphism $f:U\to V$ in a category is called an *epimorphism* if for each pair of morphisms $g,h:V\to W$ the equality $gf=hf$ implies $g=h$. We suppose in what follows that the tensor product of two epimorphisms in $\mathcal{C}$ is also an epimorphism.

Definition 5: A ribbon DC over a ribbon algebra (A,σ) *is a DC,* Ω, *together with a sequence of automorphisms* $\{\sigma_i:\Omega_i\to\Omega_i\}_{i=0}^n$ *such that* $\sigma_0=\sigma$ *and*

$$m_{i,j}(\sigma_i\otimes\sigma_j)\Psi_{j,i}\Psi_{i,j}=\sigma_{i+j}m_{i,j}, \quad d_i\sigma_i=\sigma_{i+1}d_i \tag{3.6}$$

for all i, j, where by $\Psi_{i,j}$ *we mean* Ψ_{Ω_i,Ω_j}.

This has been presented in Fig. 6(b). It means that σ extends to a ribbon structure on Ω in a manner compatible with d.

Definition 6: A ribbon graded trace *(r.g.t.) on a degree n ribbon DC is a morphism* $\int:\Omega_n \to \mathbf{1}$ *such that if* $i+j=n$, *then*

$$\int m_{i,j} = (-1)^{ij} \int m_{j,i}(\sigma_j\otimes \mathrm{id}_{\Omega_i})\Psi_{i,j}. \tag{3.7}$$

It is called closed *if* $\int d=0$.

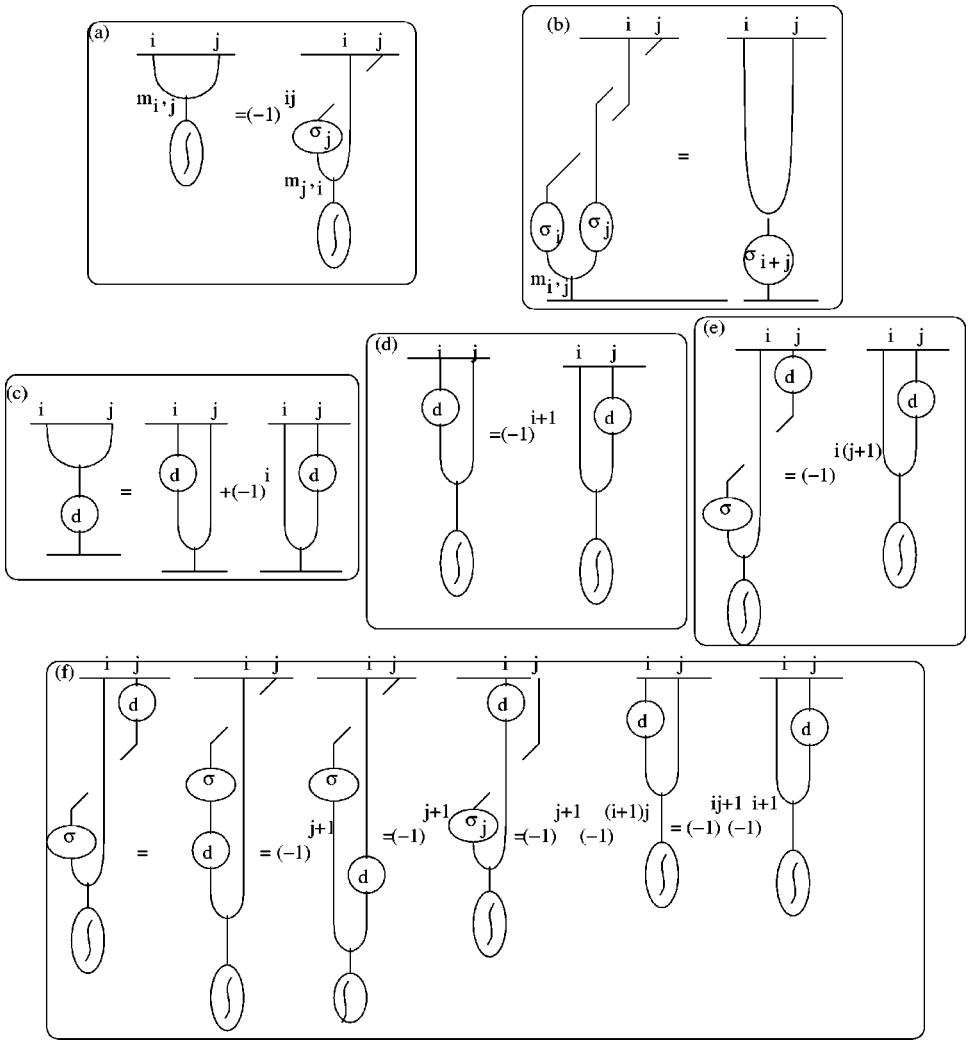

FIG. 6. Ribbon differential calculi and ribbon graded traces.

This has been presented in Fig. 6(a). If $\int$ satisfies (3.7) at least for $i=n$, $j=0$ on a (not necessarily ribbon) DC on a ribbon algebra in $\mathcal{C}$ then we call it a *weak ribbon graded trace* (w.r.g.t.). Following the strategy in Ref. 7 we have

Proposition 7: On a ribbon DC, any w.r.g.t. is also a r.g.t.

Proof: We use induction on j. Let (3.7) be true for j; we prove it for $j+1$. We have the identity in Fig. 6(e) as proven in part (f). In part (f) we used part (d) which is an immediate consequence of the Leibniz rule [represented by the diagrams in part (c)] and closedness of $\int$. In the fourth equality of part (f) we used the induction hypothesis. Now we have the identity in Fig. 7(a) as proven in part (b), where i means Ω_i, j means Ω_j and 0 means $\Omega_0=A$. Here in the third equality we used the equality in Fig. 6(e) and in the sixth equality we used (3.7). Now since the morphism $m(\mathrm{id}\otimes d):A\otimes\Omega_j\to\Omega_{j+1}$ is an epimorphism, then by our assumption, $\mathrm{id}\otimes(m(\mathrm{id}\otimes d)):\Omega_i\otimes A\otimes\Omega_j\to\Omega_i\otimes\Omega_{j+1}$, is also an epimorphism. Thus from the equality in Fig. 7(a) we conclude that the induction hypothesis holds for $j+1$. ■

Theorem 8: *Let Ω be a (not necessarily ribbon) DC of degree $0\leqslant n\leqslant\infty$ on the ribbon algebra (A,σ) in $\mathcal{C}$, and $\int$ a closed w.r.g.t. on Ω. Define the morphism in $\overline{\mathcal{C}}$*

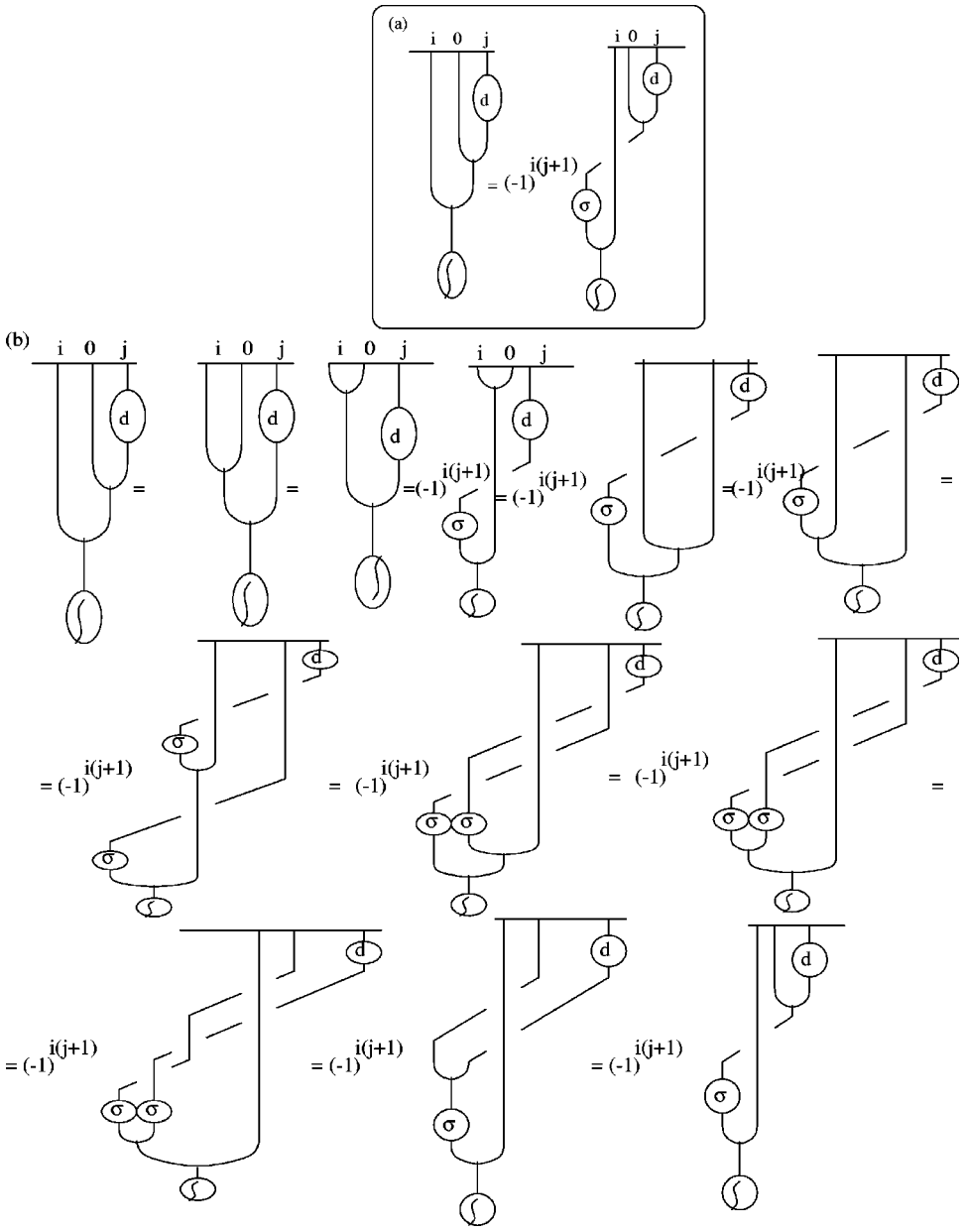

FIG. 7. Further diagrams in the construction of ribbon graded traces.

$$\varphi: A^{\otimes(n+1)} \to \mathbf{1}, \quad \varphi = \int m(id \otimes d^{\otimes n}) \tag{3.8}$$

[the diagram of φ is in Fig. 9(c)]. Then φ is a braided cyclic cocycle, i.e., $\varphi \in Z^n_\lambda(\mathcal{C}; A, \sigma)$. Here m is the morphism $A \otimes \Omega_1^{\otimes n} \to \Omega_n$ induced by the multiplication morphisms m_i (using associativity).

Proof: Let us denote the morphism $md^{\otimes k}$ by f_k. Then clearly we have $f_k = m(d \otimes f_{k-1}) = m(f_{k-1} \otimes d)$ and $df_k = 0$ and by definition we have $\varphi = \int m(\mathrm{id} \otimes f_n)$. Then the proof that $\lambda(\varphi) = \varphi$ is in Fig. 8, where the left-hand side diagram is by definition $\lambda(\varphi) = \varphi$ and by $[k]$ we mean $A^{\otimes k}$.

To prove that φ is cocycle we first note the identity in Fig. 9(a) as proven in part (b). Now

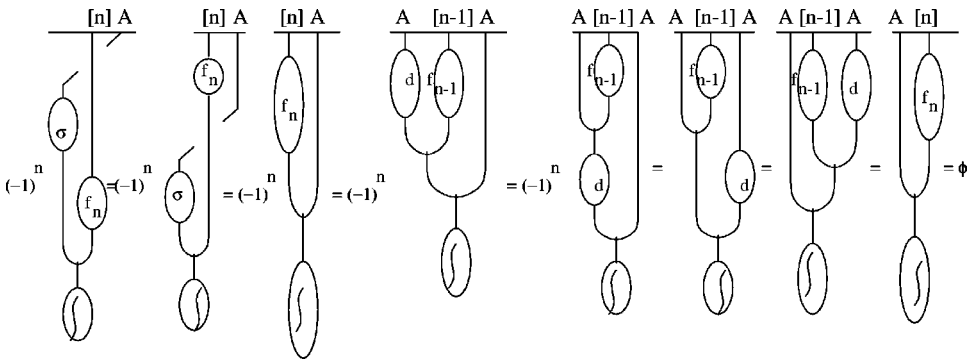

FIG. 8. Construction of a braided cyclic cocycle.

applying $\int$ to both sides of this identity and using the definition of φ, we just need to prove that the left-hand side is $d_n(\varphi)$, which is in part (d). ■

Finally, we study the behavior of braided cyclic cohomology with respect to gauge transformation between braided monoidal *Ab*-categories, using the definitions from the previous section.

Theorem 9: *Let* $(T,\mathcal{F})$ *be a tensor functor between braided monoidal Ab-categories* $(\mathcal{C}, \otimes, \Phi, \Psi)$ *and* $(\mathcal{C}', \otimes', \Phi', \Psi')$, *and let* (A, m, η, σ) *be a ribbon algebra in* $\mathcal{C}$. *Then* $A' := T(A)$ *is a ribbon algebra in* $\mathcal{C}'$ *with product* $m' := T(m)$, *unit* $\eta' := T(\eta)$ *and ribbon structure* $\sigma' := T(\sigma)$. *Moreover, there exists a morphism of cocyclic modules*

$$\overline{T}: C^n(\mathcal{C}; A, \sigma) \to C^n(\mathcal{C}'; A', \sigma').$$

If in addition $\mathcal{C}$ *and* $\mathcal{C}'$ *are gauge equivalent then the above morphism is a cocyclic module isomorphism and therefore induces an isomorphism between Hochschild and cyclic cohomologies of A and A′ in* $\mathcal{C}$ *and* $\mathcal{C}'$, *respectively*.

Proof: At first suppose $\mathcal{C}$, $\mathcal{C}'$ are strict categories and $\mathcal{F}$ is trivial i.e., $T(U \otimes V) = T(U) \otimes' T(V)$ and $\mathcal{F}_{U,V} = \mathrm{id}$ for all objects U, V in $\mathcal{C}$. Then from (2.5) and (2.7) we get $T(f \otimes g) = T(f) \otimes' T(g)$ for all morphisms f, g in $\mathcal{C}$, and $T(\Psi_{U,V}) = \Psi'_{T(U),T(V)}$. In this case it is obvious that (A', m', η', σ') is a ribbon algebra in $\mathcal{C}'$. Now if d_i, s_i, λ_i and d_i', s_i', λ_i' are the face, degeneracy and cyclicity maps for A and A', respectively, then since these maps are constructed by composition, addition or tensor product of the product of A, identity, braiding or ribbon morphisms and since T preserves composition, addition and tensor product of morphisms, we deduce easily that $d_i' = T(d_i)$, $s_i' = T(s_i)$, and $\lambda_i' = T(\lambda_i)$. Thus the theorem is proved in this case. Now since braided Hochschild and cyclic cohomology is defined inside the extended strict category $\overline{\mathcal{C}}$, the general nonstrict case follows using Proposition 2. ■

IV. BRAIDED CYCLIC COHOMOLOGY OF QUASIALGEBRAS OVER COQUASITRIANGULAR COQUASIBIALGEBRAS

In this section we use "gauge transformation" to construct nontrivial quasialgebras following the methods in Ref. 13, and see how the differential calculi and the braided cyclic cohomology behave in this case. We start with the general theory before specializing to the group algebra case of particular interest. Concrete examples then follow in Sec. V.

A. General construction by Drinfeld cotwists

We recall Refs. 2 and 5, cf. Ref. 1;

Definition 10: A coquasitriangular coquasibialgebra is a coalgebra (H, Δ, ϵ) *equipped with a linear map* $.: H \otimes H \to H$, *called product, an associated unit element, a convolution invertible "unital 3-cocycle," in the sense of a linear map* $\phi: H^{\otimes 3} \to \mathbb{C}$ *satisfying*

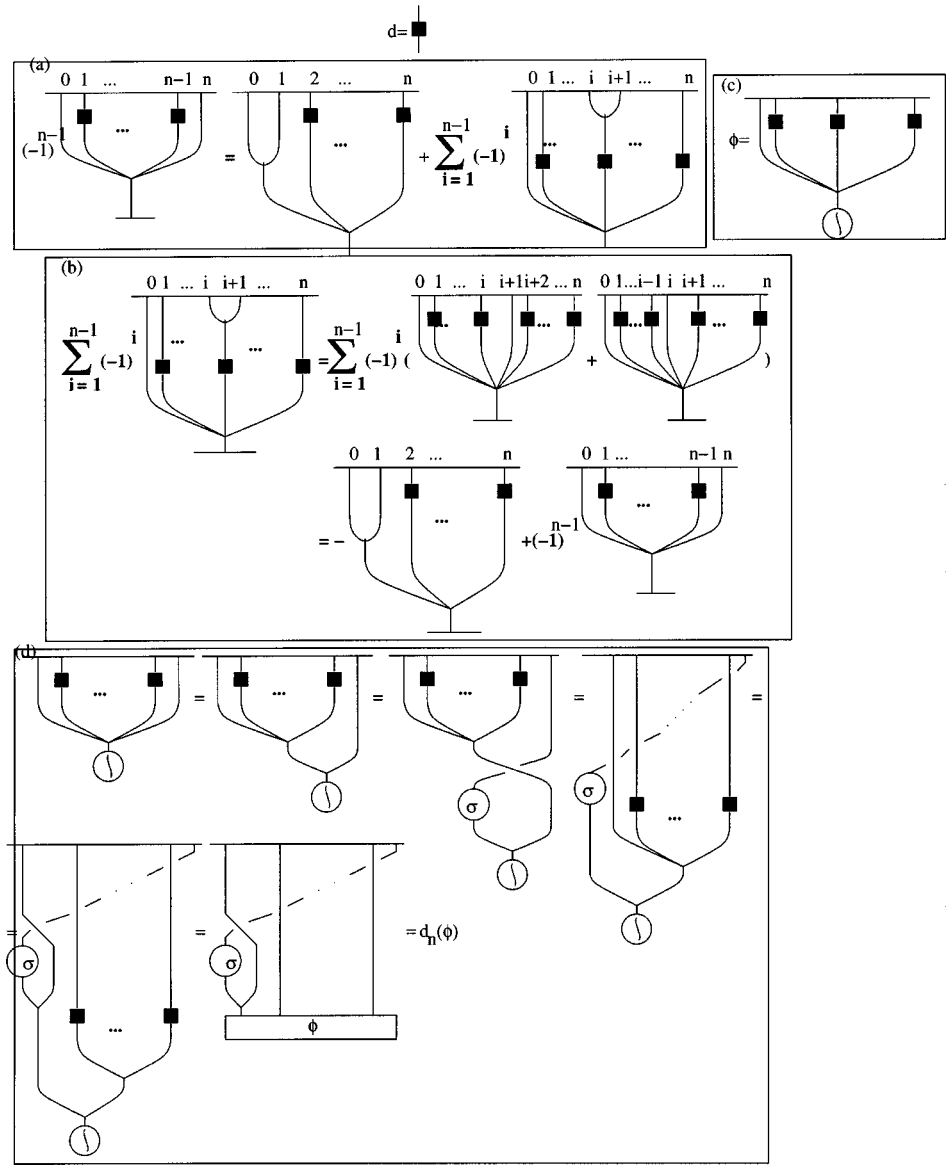

FIG. 9. Further diagrams in the construction of a braided cyclic cocycle.

$$\phi(b_{(1)},c_{(1)},d_{(1)})\phi(a_{(1)},b_{(2)}\,.\,c_{(2)},d_{(2)})\phi(a_{(2)},b_{(3)},c_{(3)}) = \phi(a_{(1)},b_{(1)},c_{(1)}\,.\,d_{(1)})\phi(a_{(2)}\,.\,b_{(2)},c_{(2)},d_{(2)}),$$

$$\phi(a,1,b) = \epsilon(a)\epsilon(b),$$

such that Δ,ϵ *are multiplicative and*

$$a_{(1)}\,.\,(b_{(1)}\,.\,c_{(1)})\phi(a_{(2)},b_{(2)},c_{(2)}) = \phi(a_{(1)},b_{(1)},c_{(1)})(a_{(2)}\,.\,b_{(2)})\,.\,c_{(2)},$$

$\forall a,b,c,d \in H$, *and finally a convolution invertible linear map* $\mathcal{R}:H\otimes H\to\mathbb{C}$, *satisfying*

$$\mathcal{R}(a\,.\,b,c) = \phi(c_{(1)},a_{(1)},b_{(1)})\mathcal{R}(a_{(2)},c_{(2)})\phi^{-1}(a_{(3)},c_{(3)},b_{(2)})\mathcal{R}(b_{(3)},c_{(4)})\phi(a_{(4)},b_{(4)},c_{(5)}),$$

$$\mathcal{R}(a,b\,.\,c) = \phi^{-1}(b_{(1)},c_{(1)},a_{(1)})\mathcal{R}(a_{(2)},c_{(2)})\phi(b_{(2)},a_{(3)},c_{(3)})\mathcal{R}(a_{(4)},b_{(3)})\phi^{-1}(a_{(5)},b_{(4)},c_{(4)}),$$

$$b_{(1)} \,.\, a_{(1)}\mathcal{R}(a_{(2)},c_{(2)}) = \mathcal{R}(a_{(1)},b_{(1)})a_{(2)} \,.\, b_{(2)}.$$

Also we recall that the category of (left) H-comodules (abbreviated as H-Com) is a braided monoidal Ab-category with

$$\Phi_{U,V,W}: U \otimes (V \otimes W) \to (U \otimes V) \otimes W, \quad u \otimes v \otimes w \mapsto \phi(u_{(1)},v_{(1)},w_{(1)})u_{(2)} \otimes v_{(2)} \otimes w_{(2)},$$

$$\Psi_{U,V}: U \otimes V \to V \otimes U, \quad u \otimes v \mapsto \mathcal{R}(v_{(1)},u_{(1)})v_{(2)} \otimes u_{(2)}$$

$\forall U,V,W \in H$-Com. An algebra A in this category is called a *left quantum quasispace* (or left H-comodule quasialgebra[13]). This means that we have a left H-comodule structure, $A \to H \otimes A$, $a \mapsto a_{(1)} \otimes a_{(2)}$, a linear map $.: A \otimes A \to A$, called product, which is unital, associative in the category and equivariant under the coaction of H. Specifically,

$$a \,.\, (b \,.\, c) = \phi(a_{(1)},b_{(1)},c_{(1)})(a_{(2)} \,.\, b_{(2)}) \,.\, c_{(2)}, \quad (a \,.\, b)_{(1)} \otimes (a \,.\, b)_{(2)} = a_{(1)} \,.\, b_{(1)} \otimes a_{(2)} \,.\, b_{(2)}, \quad a,b \in A.$$

Finally, a ribbon structure for A in the sense of Sec. III means a H-comodule isomorphism $\sigma: A \to A$ such that

$$\sigma(a \,.\, b) = \mathcal{R}(b_{(1)},a_{(1)})\mathcal{R}(a_{(2)},b_{(2)})\sigma(a_{(3)}) \,.\, \sigma(b_{(3)}). \tag{4.1}$$

Now let us describe explicitly a braided cyclic cocycle in this category. First of all by the argument in Sec. II, for H-comodules U_i, $1 \leqslant i \leqslant n$, a morphism $U_1 \otimes \cdots \otimes U_n \to \mathbb{C}$ in the category of H-Com, is an equivalence class of H-comodule intertwiners $U_1 \otimes_\alpha \cdots \otimes_\alpha U_n \to \mathbb{C}$ for all $\alpha \in \Lambda_n$. Here a H-comodule intertwiner $U_1 \otimes_\alpha \cdots \otimes_\alpha U_n \to \mathbb{C}$ means a linear map $f: U_1 \otimes \cdots \otimes U_n \to \mathbb{C}$ satisfying

$$f(u^1 \otimes \cdots \otimes u^n)1 = u^1_{(1)\cdot_\alpha} \cdots {}_{\cdot_\alpha} u^n_{(1)} f(u^1_{(2)} \otimes \cdots \otimes u^n_{(2)}), \quad \forall\, u_i \in U_i, \tag{4.2}$$

where we have used $U_1 \otimes \cdots \otimes U_n$ for the usual vector space tensor product, $u^1 \otimes \cdots \otimes u^n$ meaning an element of the vector space $U_1 \otimes \cdots \otimes U_n$ and the notation $u^1{}_{._\alpha} \cdots u^n$ as defined in Sec. II. Similarly, a morphism $U_1 \otimes \cdots \otimes U_m \to V_1 \otimes \cdots \otimes V_n$ is an equivalence class of H-comodule intertwiners $U_1 \otimes_\alpha \cdots \otimes_\alpha U_m \to V_1 \otimes_\beta \cdots \otimes_\beta V_n$, $\alpha \in \Lambda_m, \beta \in \Lambda_n$.

Now let us describe the morphisms $d_i: C_n = A^{\otimes(n+1)} \to C_{n-1} = A^{\otimes n}$, $0 \leqslant i \leqslant n-1$ in our particular category. These are represented by morphisms

$$A \otimes_\alpha \cdots \otimes_\alpha (A \otimes A) \otimes_\alpha \cdots \otimes_\alpha A \to A \otimes_\alpha \cdots \otimes_\alpha A,$$

$$(a^0 \otimes \cdots \otimes a^n) \mapsto (a^0 \otimes \cdots \otimes a^i \,.\, a^{i+1} \otimes \cdots \otimes a^n), \quad a^i \in A, \alpha \in \Lambda_n$$

while d_n by definition is $(m_A \otimes \mathrm{id}_{n-1})(\sigma_A \otimes \mathrm{id}_n)\Psi_{n,1}$, where $\Psi_{n,1} := \Psi_{A^{\otimes n},A}$ and $\mathrm{id}_k := \mathrm{id}_{A^{\otimes k}}$. Let us write for simplicity X for $A^{\otimes^{n-1}_\alpha}$, $\alpha \in \Lambda_{n-1}$. Then the representative of d_n from $(A \otimes X) \otimes A$ to $A \otimes X$ is $(m_A \otimes \mathrm{id}_X)\phi_{A,A,X}(\sigma \otimes \mathrm{id}_{A\otimes X})\Psi_{A\otimes X,A}$ which has value on $a^0 \otimes \cdots \otimes a^n$ equal to

$$\begin{aligned}
&\mathcal{R}(a^n_{(1)},a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(1)}))(m_A \otimes \mathrm{id}_X)\phi_{A,A,X}(\sigma \otimes \mathrm{id}_{A\otimes X})(a^n_{(2)} \otimes (a^0_{(2)} \otimes (a^1_{(2)} \otimes_\alpha \cdots \otimes_\alpha a^{n-1}_{(2)})))\\
&= \mathcal{R}(a^n_{(1)},a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(1)}))(m_A \otimes \mathrm{id}_X)\phi_{A,A,X}(\sigma(a^n_{(2)}) \otimes (a^0_{(2)} \otimes (a^1_{(2)} \otimes_\alpha \cdots \otimes_\alpha a^{n-1}_{(2)})))\\
&= \mathcal{R}(a^n_{(1)},a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(1)}))\phi(a^n_{(2)},a^0_{(2)},a^1_{(2)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(2)})(m_A \otimes \mathrm{id}_X)((\sigma(a^n_{(3)}) \otimes a^0_{(3)}) \otimes (a^1_{(3)}\\
&\quad \otimes_\alpha \cdots \otimes_\alpha a^{n-1}_{(3)}))\\
&= \mathcal{R}(a^n_{(1)},a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(1)}))\phi(a^n_{(2)},a^0_{(2)},a^1_{(2)\cdot_\alpha} \cdots {}_{\cdot_\alpha} a^{n-1}_{(2)})\sigma(a^n_{(3)}) \,.\, a^0_{(3)} \otimes a^1_{(3)} \otimes \cdots \otimes a^{n-1}_{(3)}.
\end{aligned}$$

Therefore the representative of d_n from $(A \otimes (A^{\otimes^{n-1}_\alpha})) \otimes A$ to $A \otimes (A^{\otimes^{n-1}_\alpha})$ is

$$d_n(a^0 \otimes \cdots \otimes a^n) = \mathcal{R}(a^n_{(1)}, a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots \cdot_\alpha a^{n-1}_{(1)}))\phi(a^n_{(2)}, a^0_{(2)}, a^1_{(2)\cdot_\alpha} \cdots \cdot_\alpha a^{n-1}_{(2)})\sigma(a^n_{(3)}) \,.\, a^0_{(3)} \otimes a^1_{(3)} \otimes \cdots \otimes a^{n-1}_{(3)}, \tag{4.3}$$

where $\alpha \in \Lambda_{n-1}$.

We can similarly represent λ with the representative $(A \otimes (A^{\otimes_\alpha^{n-1}})) \otimes A \to A \otimes (A \otimes (A^{\otimes_\alpha^{n-1}}))$ by

$$\lambda(a^0 \otimes \cdots \otimes a^n) = (-1)^n \mathcal{R}(a^n_{(1)}, a^0_{(1)} \,.\, (a^1_{(1)\cdot_\alpha} \cdots \cdot_\alpha a^{n-1}_{(1)}))\sigma(a^n_{(2)}) \otimes a^0_{(2)} \otimes \cdots \otimes a^{n-1}_{(2)}, \tag{4.4}$$

where $\alpha \in \Lambda_{n-2}$.

Next a DC, $\Omega(A) = \oplus_{i=0}^n \Omega_i(A)$, on A in this category is just a left H-covariant DC as in Ref. 19, except that the product of forms are associative up to the associator, namely,

$$\omega \,.\, (\omega' \,.\, \omega'') = \phi(\omega_{(1)}, \omega'_{(1)}, \omega''_{(1)})(\omega_{(2)} \,.\, \omega'_{(2)}) \,.\, \omega''_{(2)}, \quad \forall\, \omega, \omega', \omega'' \in \Omega.$$

A w.r.g.t. on $\Omega(A)$ is a left H-invariant functional $\Omega_n \to \mathbb{C}$ satisfying

$$\int \omega \,.\, a = \mathcal{R}(a_{(1)}, \omega_{(1)}) \int \sigma(a_{(2)}) \,.\, \omega_{(2)}. \tag{4.5}$$

Now we recall briefly the so-called Drinfeld cotwist and associated "gauge transformation." For this discussion we will denote the product of two elements a and b in H or A, just by ab and we keep the notation $a*b$ or $a \,.\, b$, respectively, for the new products defined as follows. Thus for $(H, \Phi, \mathcal{R})$ as above and any convolution invertible linear map $F: H \otimes H \to \mathbb{C}$ obeying $F(a,1) = F(1,a) = \epsilon(a)$, $\forall\, a \in H$ (a 2-cochain), we define a coquasitriangular coquasibialgebra H^F as follows; H^F as a coalgebra is, by definition, (H, Δ, ϵ) itself and the product for H^F is defined by[1]

$$a * b := F(a_{(1)}, b_{(1)}) a_{(2)} b_{(2)} F^{-1}(a_{(3)}, b_{(3)}), \tag{4.6}$$

the unital 3-cocycle for H^F is defined by

$$\phi_F(a,b,c) := F(b_{(1)}, c_{(1)}) F(a_{(1)}, b_{(2)} c_{(2)}) \phi(a_{(2)}, b_{(3)}, c_{(3)}) F^{-1}(a_{(3)} b_{(4)}, c_{(4)}) F^{-1}(a_{(4)}, b_{(5)}) \tag{4.7}$$

and the coquasitriangular structure for H^F is defined by

$$\mathcal{R}_F(a,b) := F(b_{(1)}, a_{(1)}) \mathcal{R}(a_{(2)}, b_{(2)}) F^{-1}(a_{(3)}, b_{(3)}) \tag{4.8}$$

$\forall\, a, b \in H$. This is the dual version of the Drinfeld twist (see Ref. 5). Then, as above, we have a braided monoidal Ab-category, namely H^F-Com, which is nothing other than H-Com, as an Ab-category but with new monoidal and braided structures. We denote the tensor product, the associator and the braiding of this category by $\otimes_F, \Phi_F, \psi_F$ respectively.

If A is a quantum quasispace over H then there is a gauge transformed copy of it in H^F-Com, namely we cotwist the product of A as[13]

$$a \,.\, b := F(a_{(1)}, b_{(1)}) a_{(2)} b_{(2)}, \quad \forall\, a, b \in A,$$

then A_F is by definition A as a left H-comodule equipped with the above product. It is easy to see that A_F is a (left) quantum quasispace over H^F, see Ref. 13.

Now let us show that if σ is a ribbon structure for A in H-Com, then σ is still a ribbon structure for A_F in the category of left H^F-Com. Indeed,

$$\begin{aligned}
&\mathcal{R}_F\,(b_{(1)},a_{(1)})\mathcal{R}_F(a_{(2)},b_{(2)})\sigma(a_{(3)})\,.\,\sigma(b_{(3)})\\
&\quad=F(a_{(1)},b_{(1)})\mathcal{R}(b_{(2)},a_{(2)})F^{-1}(b_{(3)},a_{(3)})F(b_{(4)},a_{(4)})\mathcal{R}(a_{(5)},b_{(5)})F^{-1}(a_{(6)},b_{(6)})\\
&\qquad\times F(a_{(7)},b_{(7)})\sigma(a_{(8)})\sigma(b_{(8)})\\
&\quad=F(a_{(1)},b_{(1)})\mathcal{R}(b_{(2)},a_{(2)})\mathcal{R}(a_{(3)},b_{(3)})\sigma(a_{(4)})\sigma(b_{(4)})\\
&\quad=F(a_{(1)},b_{(1)})\sigma(a_{(2)}b_{(2)})\\
&\quad=\sigma(a\,.\,b)
\end{aligned}$$

as required.

Next it is known that the cotwisted comodule algebra $\Omega(A_F):=\Omega(A)_F$ is a DC over the algebra A_F in the category of H^F-Com (see Ref. 12). We recall that differential forms in $\Omega(A_F)$ are the same as differential forms in $\Omega(A)$ with the same coaction of H on them and the differential operator, d, remaining unchanged, but the product of forms has been cotwisted to

$$\omega\,.\,\omega':=F(\omega_{(1)},\omega'_{(1)})\omega_{(1)}\omega'_{(2)}.$$

Therefore for left invariant forms this product does not change, i.e., we have

$$\omega\,.\,\omega'=\omega\omega',\quad a\,.\,\omega=a\omega,\quad \omega\,.\,a=\omega a,\quad \forall\,\omega\in\Omega^{inv},\ a\in A,$$

where Ω^{inv} denote the space of left invariant forms.

Let us show now that if $\int$ is a w.r.g.t. on $\Omega(A)$ then it is also a w.r.g.t. on $\Omega(A_F)$. Indeed,

$$\begin{aligned}
\mathcal{R}_F(a_{(1)},\omega_{(1)})\int\sigma(a_{(2)})\,.\,\omega_{(2)}&=F(\omega_{(1)},a_{(1)})\mathcal{R}(a_{(2)},\omega_{(2)})F^{-1}(a_{(3)},\omega_{(3)})F(a_{(4)},\omega_{(4)})\int\sigma(a_{(5)})\omega_{(5)}\\
&=\int F(\omega_{(1)},a_{(1)})\omega_{(2)}a_{(2)}=\int\omega\,.\,a
\end{aligned}$$

as required.

Remark: Observe that even if the associator and coquasitriangular structure are trivial before gauge transformation, they are typically no longer trivial after gauge transformation. Even if F is a Hopf algebra 2-cocycle,[5] the associator after gauge transformation becomes trivial but the coquasitriangular structure is not typically trivial but is cotriangular. Also note that the F needed for gauge transformation of classical semisimple Lie groups to their quantum counterpart are not Hopf algebra 2-cocycles but are 2-cochains, thus these observations imply that we do need to consider the class of braided cyclic cocycles during such transformations.

As for any monoidal category $\mathcal{C}$ the functor $\mathcal{C}^n\to\mathcal{C}$, $(U_1,\ldots,U_n)\mapsto(\cdots((U_1\otimes U_2)\otimes U_3)\otimes\cdots)\otimes U_n$ is called the *left-to-right arranger*. We can use this to give explicit left-to-right representatives of all formulas. Finally, the categories $(H\text{-Com},\otimes,\Phi,\Psi)$ and $(H^F\text{-Com},\otimes_F,\Phi_F,\psi_F)$ are gauge equivalent, which is the categorical meaning of the Drinfeld cotwist, see Ref. 2. We choose $T=\mathrm{id}$ and $\mathcal{F}_{U,V}(u\otimes v):=F(u_{(1)},v_{(1)})u_{(2)}\otimes v_{(2)}$. Here $\mathcal{F}_{U,V}$ is a morphism in H^F-Com since

$$\begin{aligned}
(u\otimes v)_{(1)}\otimes\mathcal{F}_{U,V}(u\otimes v)_{(2)}&=u_{(1)}*v_{(1)}\otimes F(u_{(2)},v_{(2)})u_{(3)}\otimes v_{(3)}\\
&=F(u_{(1)},v_{(1)})u_{(2)}v_{(2)}F^{-1}(u_{(3)},v_{(3)})\otimes F(u_{(4)},v_{(4)})u_{(5)}\otimes v_{(5)}\\
&=F(u_{(1)},v_{(1)})u_{(2)}v_{(2)}\otimes u_{(3)}\otimes v_{(3)}=(\mathcal{F}_{U,V}(u\otimes v))_{(1)}\otimes(\mathcal{F}_{U,V}(u\otimes v))_{(2)}.
\end{aligned}$$

Similarly, $\mathcal{F}^{-1}_{U,V}(u\otimes v)=F^{-1}(u_{(1)},v_{(1)})u_{(2)}\otimes v_{(2)}$ is a morphism in H^F-Com. Moreover, (2.5) is a consequence of the definition of a morphism in the category of H-Com and (2.6) and (2.7) are consequences of (4.7) and (4.8). Therefore by Theorem 9 we have:

Theorem 11: *There is an isomorphism of cocyclic modules*

$$\overline{\mathrm{id}}: C^k(H\text{-Com}; A, \sigma) \to C^k(H^F\text{-Com}; A_F, \sigma), \quad \varphi \mapsto \varphi_F.$$

For instance if φ^{lr} be the left-to-right representative of φ then the left-to-right representative of φ_F, which we denote by φ_F^{lr} is

$$\varphi_F^{lr}(a^0, \ldots, a^k) = F(a^0_{(1)}, a^1_{(1)}) F(a^0_{(2)} a^1_{(2)}, a^2_{(1)}) F((a^0_{(3)} a^1_{(3)}) a^2_{(2)}, a^3_{(1)}) \cdots \times F((\cdots((a^0_{(k)} a^1_{(k)}) a^2_{(k-1)}) \cdots) a^{k-1}_{(2)}, a^k_{(1)}) \varphi^{lr}(a^0_{(k+1)}, a^1_{(k+1)}, a^2_{(k)} \ldots, a^k_{(2)}). \quad (4.9)$$

Proof: This is Theorem 9 in our present case. In (4.9) we just used the definition of S_α (see Sec. II). ■

B. Braided cyclic cocycles on group algebras and *G*-graded quasialgebras

Let G be a group and $H = \mathbb{C}G$ the group algebra on G. This is a Hopf algebra with

$$\Delta g = g \otimes g, \quad \varepsilon(g) = 1, \quad S(g) = g^{-1}, \quad \forall\, g \in G$$

we recall that a unital 3-cocycle for $H = \mathbb{C}G$ is just the linear extension of a group cocycle $\phi: G^3 \to \mathcal{C} - \{0\}$ in the sense of a function $\phi: G^3 \to \mathbb{C} - \{0\}$ obeying

$$\phi(g_1, g_2, g_3)\phi(g_0, g_1 g_2, g_3)\phi(g_0, g_1, g_2) = \phi(g_0, g_1, g_2 g_3)\phi(g_0 g_1, g_2, g_3), \quad \phi(g_0, e, g_1) = 1, \quad \forall\, g_i \in G.$$

Of interest is the case when G is Abelian. Since H is cocommutative and associative, we can consider $\mathbb{C}G$ as a coquasibialgebra with any ϕ, including to start with the trivial $\phi \equiv 1$. Then in this standard case, since we assume G is Abelian, a coquasitriangular structure is just a group bicharacter $\mathcal{R}: G^2 \to \mathbb{C} - \{0\}$ in the sense of a function obeying

$$\mathcal{R}(g_0 g_1, g_2) = \mathcal{R}(g_0, g_2)\mathcal{R}(g_1, g_2), \quad \mathcal{R}(g_0, g_1 g_2) = \mathcal{R}(g_0, g_1)\mathcal{R}(g_0, g_2), \quad \forall\, g_i \in G.$$

Again to start with we can choose the trivial $\mathcal{R} \equiv 1$, so that $\mathbb{C}G$ is considered as a coquasitriangular coquasibialgebra with trivial associator and trivial coquasitriangular structure.

Next a left $\mathbb{C}G$-comodule means precisely a G-graded vector space V with coaction of $\mathbb{C}G$ on it given by $\alpha(v) = |v| \otimes v$, where $|v| \in G$ denotes the degree of a homogeneous vector $v \in V$.[5] An algebra A in the category of $\mathbb{C}G$-comodules is just a G-graded algebra (recall that we have chosen trivial associator for $\mathbb{C}G$). Now since for every bialgebra H (that is a coquasibialgebra with trivial associator), $A = H$ is an H-comodule algebra with the coproduct of H taken as coaction of H on A, we can consider the algebra $A = \mathbb{C}G$ in the category of $\mathbb{C}G$-comodules. Since we have chosen the trivial coquasitriangular structure for $H = \mathbb{C}G$, a ribbon structure $\sigma: A = \mathbb{C}G \to A = \mathbb{C}G$ is just a group homomorphism $\sigma: G \to G$ extended by linearity to $\mathbb{C}G$.

Finally, let $\{\chi_i: G \to \mathbb{C} - \{0\}\}_{i=1}^n$ be a finite set of group characters. We extend each χ_i on $\mathbb{C}G$ by linearity and denote the extended map still by χ_i. Clearly we have $\chi_i(ab) = \chi_i(a)\chi_i(b)$ $\forall a, b \in A$, $\forall i$. It is well-known that if Λ is an n-dimensional vector space with basis $\{\omega_i\}_{i=1}^n$ then there exists a unique left covariant FODC, Γ, on $A = \mathbb{C}G$ such that $\forall g \in G$, $\forall i$

$$\omega_i g = \chi_i(g) g \omega_i, \quad dg = \sum_{i=1}^n (\chi_i(g) - 1) g \omega_i. \quad (4.10)$$

In fact these calculi are bicovariant and the space of right invariant forms $\Gamma^{r.\mathrm{inv}}$, coincides with the space of left invariant forms, $\Gamma^{l.\mathrm{inv}} = \Lambda$. Thus the Woronowicz braiding $\Psi: \Gamma \otimes_A \Gamma \to \Gamma \otimes_A \Gamma$ is just the map, $\Psi(a\omega \otimes_A \omega') = a\omega' \otimes_A \omega$, $\forall \omega, \omega' \in \Gamma^{l.\mathrm{inv}}$. Hence the relations among basis 1-forms ω_i in the DC, $\Omega := T(\Gamma)/\ker(\Psi - id)$, are $\omega_i^2 = 0$, $\omega_i \omega_j = -\omega_j \omega_i$, $\forall i, j$, where $T(\Gamma)$ is the tensor algebra over Γ. Therefore we have a top form $\theta := \omega_1 \cdots \omega_n$ for the space of left invariant n-forms, i.e., the space of left invariant n-forms is one dimensional. Now let us define $\pi: \Omega_n \to A$ and $\rho: A \to A$ as follows; since $\{\theta\}$ is a free A-basis for Ω_n, for each $\omega \in \Omega_n$ and $a \in A$ there exist unique elements of A, $\pi(\omega)$ and $\rho(a)$ such that $\omega = \pi(\omega)\theta$ and $\theta a = \rho(a)\theta$. One can easily verify that both π and ρ are morphisms in the category of H-comodules, and ρ is an algebra automorphism and by very

definition we have $\pi(a\omega)=a\pi(\omega)$, $\pi(\omega a)=\pi(\omega)\rho(a)$. In our case of $A=\mathbb{C}G$ by (4.10) we have

$$\rho(g)=\chi_1(g)\cdots\chi_n(g)g.$$

Next there exists a unique left and right invariant functional on $\mathbb{C}G$ defined by

$$h(g)=0, \quad \forall\, g\neq e, \quad h(e)=1 \tag{4.11}$$

which defines a canonical left invariant functional

$$\int:\Omega_n\to\mathbb{C}, \quad \int\omega := h(\pi(\omega)). \tag{4.12}$$

Since $\omega a=\pi(\omega)\theta a=\pi(\omega)\rho(a)\theta=\rho(a)\pi(\omega)\theta=\rho(a)\omega$, we have $\int\omega a=\int\rho(a)\omega$. Thus $\int$ is a w.r.g.t. with ribbon morphism $\sigma(g)=\chi_1(g)\cdots\chi_n(g)g$. Let us show that it is closed. Since $\int$ is left covariant we have $(\int dg_1\cdots dg_n)e=g_1\cdots g_n\int dg_1\cdots dg_n$, $\forall g_i\in G$ thus if $g_1\cdots g_n\neq e$, then $\int dg_1\cdots dg_n=0$, and if $g_1\cdots g_n=e$ then we have

Proposition 12: If for $g_0,\ldots,g_k\in G$ we have $g_0\cdots g_k=e$, then $dg_0\cdots dg_k=0$.

Proof: We have $g^{-1}dg=\Sigma_{i=1}^n(\chi_i(g)-1)\omega_i$ and $(dg^{-1})g=\Sigma_{i=1}^n(\chi_i(g^{-1})-1)g^{-1}\omega_i g=\Sigma_{i=1}^n(\chi_i(g^{-1})-1)\chi_i(g)\omega_i=-\Sigma_{i=1}^n(\chi_i(g)-1)\omega_i$. Thus $dg^{-1}dg=(dg^{-1})gg^{-1}dg=-\Sigma_{i=1}^n(\chi_i(g)-1)(\chi_j(g)-1)\omega_i\omega_j=0$. Thus $dg^{-1}dg=0$ and $d\omega(g)=d(g^{-1}dg)=dg^{-1}dg=0$. Since every left invariant form $\omega\in\Omega_{\text{inv}}$ is generated by left invariant 1-forms, we deduce that $d\omega=0$, $\forall\,\omega\in\Omega_{\text{inv}}$. Now we show by induction on k that for arbitrary $g_1,\ldots,g_k\in G$ we have $(g_1\cdots g_k)^{-1}dg_1\cdots dg_k\in\Omega^k_{\text{inv}}$; for $k=1$ it is clear, and since for every $g\in G$ by (4.10) we have $g\Omega_{\text{inv}}=\Omega_{\text{inv}}g$ we conclude by using the induction hypothesis that $(g_1\cdots g_k)^{-1}dg_1\cdots dg_k=g_k^{-1}((g_1\cdots g_{k-1})^{-1}dg_1\cdots dg_{k-1})dg_k\in\Omega^k_{\text{inv}}$. Now since $g_0=(g_1\cdots g_k)^{-1}$ we see that $dg_0\cdots dg_k=d((g_1\cdots g_k)^{-1}dg_1\cdots dg_k)=0$. ■

Hence the character $\varphi(g_0,\ldots,g_n)=\int g_0dg_1\cdots dg_n$ is a trivially braided cyclic cocycle. Now we calculate φ explicitly. First of all, using (4.10) one has

$$dg_1\cdots dg_n=\sum_{i_1,\ldots,i_n=1}^{n}(\chi_{i_1}(g_1)-1)\cdots(\chi_{i_n}(g_n)-1)$$
$$\times\chi_{i_1}(g_2)\cdots\chi_{i_1}(g_n)\chi_{i_2}(g_3)\cdots\chi_{i_2}(g_n)\cdots\chi_{i_{n-1}}(g_n)g_1\cdots g_n\omega_{i_1}\cdots\omega_{i_n}.$$

Now for any permutation $\tau\in S_n$ we have $\omega_{\tau(1)}\cdots\omega_{\tau(n)}=\text{sgn}(\tau)\omega_1\cdots\omega_n$. Therefore $\varphi(g_0,\ldots,g_n)=0$, if $g_0\cdots g_n\neq e$ and if $g_0\cdots g_n=e$, then

$$\varphi(g_0,\ldots,g_n)=\sum_{\tau\in S_n}\text{sgn}(\tau)(\chi_{\tau(1)}(g_1)-1)\cdots(\chi_{\tau(n)}(g_n)-1)\chi_{\tau(1)}(g_2)\cdots\chi_{\tau(1)}(g_n)\chi_{\tau(2)}(g_3)$$
$$\cdots\chi_{\tau(2)}(g_n)\cdots\chi_{\tau(n-1)}(g_n).$$

Using the fact that χ_i are group characters we conclude that

$$\varphi(g_0,\ldots,g_n)=\sum_{\tau\in S_n}\text{sgn}(\tau)(\chi_{\tau(1)}(g_1\cdots g_n)-\chi_{\tau(1)}(g_2\cdots g_n))$$
$$(\chi_{\tau(2)}(g_2\cdots g_n)-\chi_{\tau(2)}(g_3\cdots g_n))\cdots(\chi_{\tau(n)}(g_n)-1). \tag{4.13}$$

Hence we have a braided monoidal *Ab*-category, namely the category of G-graded vector spaces with trivial braiding and trivial associator, and we have an algebra A in it, i.e., $A=\mathbb{C}G$ itself but with a nontrivial ribbon structure $\sigma:G\to G$, a group homomorphism given by $\sigma(g)=\chi_1(g)\cdots\chi_n(g)g$. Moreover, we have a DC on A and a closed w.r.g.t. and therefore the corresponding cyclic cocycle. This is therefore an example of the theory in Ref. 7.

Moreover, since we are working with a strict category we can suppress the subscript α in the expression $U_1\otimes_\alpha\cdots\otimes_\alpha U_n$ and $a^0\cdot_\alpha\cdots\cdot_\alpha a^n$. Therefore the maps d_i and λ become as usual. Let us

describe them in this case more explicitly. First of all a morphism $\varphi: A^{\otimes(k+1)} \to \mathbb{C}$ in this category is determined by a function $\varphi: G^{k+1} \to \mathbb{C}$ such that $\varphi(g_0, \dots, g_k)e = g_0 \cdots g_k \varphi(g_0, \dots, g_k)$, but since G is a vector space basis for $\mathbb{C}G$, we conclude

$$\mathrm{Hom}_{G\text{-Vec}}((\mathbb{C}G)^{\otimes(k+1)}, \mathbb{C}) = \{\varphi: G^{k+1} \to \mathbb{C} | \varphi(g_0, \dots, g_k) = 0, \text{ if } g_0 \cdots g_k \neq e\} \tag{4.14}$$

and

$$(b\varphi)(g_0, \dots, g_{k+1}) = \sum_{i=0}^{k} (-1)^i \varphi(g_0, \dots, g_i g_{i+1}, \dots, g_{k+1}) + (-1)^{k+1} \chi(g_{k+1}) \varphi(g_{k+1} g_0, \dots, g_k), \tag{4.15}$$

$$(\lambda\varphi)(g_0, \dots, g_k) = (-1)^k \chi(g_k) \varphi(g_k, g_0, \dots, g_{k-1}), \tag{4.16}$$

where $\chi = \chi_1 \cdots \chi_n$. Note that since $(\lambda^{k+1}\varphi)(g_0, \dots, g_k) = (-1)^{k(k+1)} \chi(g_0 \cdots g_k) \varphi(g_0, \dots, g_k)$ we conclude that

$$C^k(G - \mathrm{Vec}; \mathbb{C}G, \overline{\chi}) = \mathrm{Hom}_{G\text{-Vec}}((\mathbb{C}G)^{\otimes(k+1)}, \mathbb{C}) = \{\phi: G^{k+1} \to \mathbb{C} | \phi(g_0, \dots, g_k) = 0, \text{ if } g_0 \dots g_k \neq e\},$$

where $\overline{\chi}(g) := \chi_1(g) \cdots \chi_n(g) g$.

Now we are ready to cotwist all of the above to obtain a braided cyclic cocycle. Thus, let $F: G^2 \to \mathbb{C} - \{0\}$ be a function such that $F(g,e) = F(e,g) = 1$, $\forall g \in G$ and $H = \mathbb{C}G$ as above. Then after cotwisting, H^F has the same product as H, because

$$g_1 \,.\, g_2 = F(g_1, g_2) g_1 g_2 F(g_1, g_2)^{-1} = g_1 g_2, \quad \forall\, g \in G.$$

But we have nontrivial 3-cocycle

$$\phi_F(g_1, g_2, g_3) = F(g_2, g_3) F(g_1, g_2 g_3) F(g_1, g_2)^{-1} F(g_1 g_2, g_3)^{-1} \tag{4.17}$$

and nontrivial cotriangular structure

$$\mathcal{R}_F(g_1, g_2) = F(g_2, g_1) F(g_1, g_2)^{-1}. \tag{4.18}$$

Therefore we have a cotriangular coquasibialgebra which we denote by $\mathbb{C}^F G$ and an algebra in the category of $\mathbb{C}^F G$-comodules is called a *G-graded quasialgebra*[13] i.e., a G-graded algebra $A = \oplus_{g \in G} A_g$ such that

$$a(bc) = \phi_F(|a|, |b|, |c|)(ab)c \tag{4.19}$$

on homogeneous elements. Recall that we chose $A = \mathbb{C}G$ as an algebra in the category of G-graded vector spaces which cotwists to a G-graded quasialgebra $A_F = \mathbb{C}_F G$ with the product

$$g_1 \,.\, g_2 = F(g_1, g_2) g_1 g_2. \tag{4.20}$$

We also have

$$\int \omega \,.\, g = F(g, \omega_{(1)}) F(\omega_{(1)}, g)^{-1} \chi_1(g) \cdots \chi_n(g) \int g \,.\, \omega_{(2)}, \tag{4.21}$$

while the isomorphism of Theorem 12 becomes

$$\varphi_F(g_0, \dots, g_k) = F(g_0, g_1) F(g_0 g_1, g_2) \cdots F(g_0 \cdots g_{k-1}, g_k) \varphi(g_0, \dots, g_k). \tag{4.22}$$

V. EXAMPLES

In this section we collect examples that demonstrate key aspects of the theory above. They are all constructed using cotwisting on coquasitriangular Hopf algebras in Sec. IV. The first two are based on Abelian groups as in Sec. IV B.

A. Octonions

Let $G=\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$. Thus $\mathbb{C}G$ is an associative algebra with generators $\{1,u,v.w\}$ and relations

$$u^2=1,\quad v^2=1,\quad w^2=1,\quad uv=vu,\quad uw=wu,\quad vw=wv.$$

For simplicity we will use the notation $\mathbf{i}=u^{i_1}v^{i_2}w^{i_3}$ and $\mathbf{i}+\mathbf{j}=u^{i_1+j_1}v^{i_2+j_2}w^{i_3+j_3}$ as well. In fact this notation is statement of the group $\mathbb{Z}_2^3$ as an additive group. Each $\mathbb{Z}_2$ has a unique nonzero differential calculus (the universal one) and it is natural to equip G with the "direct product" of three copies of this. To do this, we choose three characters

$$\chi_1(u^iv^jw^k)=(-1)^i,\quad \chi_2(u^iv^jw^k)=(-1)^j,\quad \chi_3(u^iv^jw^k)=(-1)^k,\quad i,j,k=0,1.$$

Then by (4.10) we have

$$\omega_1u=-u\omega_1,\quad \omega_2u=u\omega_2,\quad \omega_3u=u\omega_3,$$

$$\omega_1v=v\omega_1,\quad \omega_2v=-v\omega_2,\quad \omega_3v=v\omega_3,$$

$$\omega_1w=w\omega_1,\quad \omega_2w=w\omega_2,\quad \omega_3w=-w\omega_3,$$

and again by (4.10) we have

$$du=-2u\omega_1,\quad dv=-2v\omega_2,\quad dw=-2w\omega_3,$$

and

$$(du)u=-udu,\quad (dv)u=udv,\quad (dw)u=udw,$$

$$(du)v=vdu,\quad (dv)v=-vdv,\quad (dw)v=vdw,$$

$$(du)w=wdu,\quad (dv)w=wdv,\quad (dw)w=-wdw,$$

and therefore

$$(du)^2=(dv)^2=(dw)^2=0,$$

$$dudv=-dvdu,\quad dudw=-dwdu,\quad dvdw=-dwdv.$$

Now using the Leibniz rule and the above relations we have $d(uv)=-2uv(\omega_1+\omega_2)$, $d(uw)=-2uw(\omega_1+\omega_3)$, and $d(vw)=-2vw(\omega_2+\omega_3)$ and thus we have $d(uvw)=(du)vw+u(dvw)=-2uvw(\omega_1+\omega_2+\omega_3)$. Therefore, generally, we have

$$d(u^{i_1}v^{i_2}w^{i_3})=-2u^{i_1}v^{i_2}w^{i_3}(i_1\omega_1+i_2\omega_2+i_3\omega_3),\quad i_k=0,1,\quad k=1,2,3$$

or in additive notation

$$d\mathbf{i}=-2\mathbf{i}(i_1\omega_1+i_2\omega_2+i_3\omega_3).$$

Using this formula and the above commutation relations we obtain

$$\begin{aligned}\pi(\mathbf{i}d\mathbf{j}d\mathbf{k}d\mathbf{l})=&-8(\mathbf{i}+\mathbf{j}+\mathbf{k}+\mathbf{l})[(-1)^{l_2+l_3}l_1((-1)^{k_2}j_2k_3-(-1)^{k_3}j_3k_2)\\&+(-1)^{l_1+l_3}l_2((-1)^{k_3}j_3k_1-(-1)^{k_1}j_1k_3)+(-1)^{l_1+l_2}l_3((-1)^{k_1}j_1k_2-(-1)^{k_2}j_2k_1)].\end{aligned}$$

Thus we calculate the character of the trivially braided ribbon graded trace defined by (4.12) as

$$\varphi(\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}) = -8[(-1)^{l_2+l_3}l_1((-1)^{k_2}j_2k_3 - (-1)^{k_3}j_3k_2) + (-1)^{l_1+l_3}l_2((-1)^{k_3}j_3k_1 - (-1)^{k_1}j_1k_3) + (-1)^{l_1+l_2}l_3((-1)^{k_1}j_1k_2 - (-1)^{k_2}j_2k_1)] \tag{5.1}$$

if $\mathbf{i}+\mathbf{j}+\mathbf{k}+\mathbf{l}=0$, and zero otherwise. One can compute this from the general formula (4.13) as well.

Now we study cotwisting of $G=\mathbb{Z}_2^3$ to the octonions. The complex numbers, the quaternions, the octonions and the higher Cayley algebras can be constructed by the Cayley–Dixon process. On the other hand it has been shown in Ref. 13 that these algebras are G-graded quasialgebras of the form $\mathbb{C}_F G$ for G a power of $\mathbb{Z}_2$ and for a suitable F.

For octonions we take[13] $G=\mathbb{Z}_2^3$ and

$$F(\mathbf{i},\mathbf{j}) = (-1)^{i_1(j_1+j_2+j_3)+i_2(j_2+j_3)+i_3j_3+j_1i_2i_3+i_1j_2i_3+i_1i_2j_3} \tag{5.2}$$

which has coboundary

$$\phi_F(\mathbf{i},\mathbf{j},\mathbf{k}) = (-1)^{|\mathbf{ijk}|}, \tag{5.3}$$

where $|\mathbf{i}\ \mathbf{j}\ \mathbf{k}|$ is a short notation for determinant of the matrix whose columns are the vectors $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$, respectively.

We denote the cotwisted product by $x.y=F(x,y)xy$, $\forall x,y\in\mathbb{C}G$. Then we have the following relations:

$$u\,.\,u=-1,\quad v\,.\,v=-1,\quad w\,.\,w=-1,\quad u\,.\,v=-v\,.\,u,\quad u\,.\,w=-w\,.\,u,$$

$$v\,.\,w=-w\,.\,v,\quad u\,.\,(v\,.\,w)=-(u\,.\,v)\,.\,w$$

and the relations between 0-forms and left invariant forms remain unchanged after twisting the above DC on $G=\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$. But we have

$$du\,.\,u=-u\,.\,du,\quad dv\,.\,u=-u\,.\,dv,\quad dw\,.\,u=-u\,.\,dw,$$

$$du\,.\,v=-v\,.\,du,\quad dv\,.\,v=-v\,.\,dv,\quad dwv=-v\,.\,dw,$$

$$du\,.\,w=-w\,.\,du,\quad dv\,.\,w=-w\,.\,dv,\quad dw\,.\,w=-w\,.\,dw,$$

and

$$du\,.\,du=dv\,.\,dv=dw\,.\,dw=0,$$

$$du\,.\,dv=dv\,.\,du,\quad du\,.\,dw=dw\,.\,du,\quad dv\,.\,dw=dw\,.\,dv.$$

This is our natural differential calculus or "exterior algebra" for the octonions as obtained by cotwisting. Like the octonions themselves, it is a nonassociative quasialgebra. We see that now the function algebra generators and their differentials uniformly anticommute, while the latter mutually commute.

From the above, we have $d(u.v)=du.v+u.dv=-2u.\omega_1.v-2u.v.\omega_2=-2u.v.(\omega_1+\omega_2)$ and similarly we have $d(u.w)=-2u.w.(\omega_1+\omega_3)$ and $d(v.w)=-2v.w.(\omega_2+\omega_3)$ and $d((u.v).w)=d(u.v).w+(u.v).dw=-2(u.v.(\omega_1+\omega_2)).w-2(u.v).w.\omega_3=-2(u.v).w.(\omega_1+\omega_2)-2(u.v).w.\omega_3=-2(u.v).w.(\omega_1+\omega_2+\omega_3)$. Therefore, generally, we have

$$d((u^i\,.\,v^j)\,.\,w^k)=-2(u^i\,.\,v^j)\,.\,w^k(i\omega_1+j\omega_2+k\omega_3),\quad i,j,k=0,1.$$

Using formula (4.22) we can then calculate

$$\varphi_F(\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}) = F(\mathbf{i},\mathbf{j})F(\mathbf{i}+\mathbf{j},\mathbf{k})F(\mathbf{i}+\mathbf{j}+\mathbf{k},\mathbf{l})\varphi(\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l})$$

as the left-to-right representative of the character.

Let us remark that the octonions presented in the above way can be viewed as a "nonassociative quantization" of $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$ as follows. Indeed, it is well-known that the Weyl algebra of canonical quantization in quantum mechanics can be formally presented as a "Moyal product" modifying the original algebra $A=C^\infty(\mathbb{R}^n)$ to a new algebra A_F with product

$$a\,.\,b = e^{\hbar\Sigma_{i,j}B_{ij}\partial_i\otimes\partial_j}(a\otimes b),$$

where $\hbar$ is a deformation parameter and B an antisymmetric tensor. The product in the original A is understood on the right. The F for the octonions similarly has a quadratic term in its exponent; cotwisting by this gives the Clifford algebra on $\mathbb{R}^3$ so this is like a "free field" quantization of $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$. The further cubic term in the F for the octonions is a bit like a "Chern–Simmons" interaction term and it is this which make $\phi_F=\partial F$ nontrivial. If we accept this analogy then we have the following proposal for physics: one might try to build cubic and higher interactions in quantum mechanics or quantum field theory by means of *nonassociative quantization* of the form

$$a\,.\,b = e^{\hbar\mathcal{L}_0+\hbar V}(a\otimes b),$$

where $\mathcal{L}_0$ is a bidifferential operator (as above) corresponding to a free particle and V is an additional term of joint degree three or higher to encode interactions. Another possibility is to take for F simply a phase factor $e^{\hbar S_0(a,b)+\hbar V(a,b)}$, where S_0 is the bilinear functional in the free field action and V is cubic or higher. The general idea, to be pursued elsewhere, is be to build such interaction terms into the algebra where their effect is a mild quasiassociativity; the system would still be equivalent to the the free case in the sense of being strictly related by cotwisting, allowing the theory to be solved as easily as the free case.

B. Noncommutative algebraic torus

Let $G=\mathbb{Z}\times\mathbb{Z}$. Thus $\mathbb{C}G$ is an associative algebra with free invertible commuting generators u,v. The standard calculus on algebra $\mathbb{C}G$, i.e., the two-dimensional bicovariant DC can be written with basis $\{\omega_1,\omega_2\}$ for left invariant 1-forms and relations

$$\omega_k a = a\omega_k,\quad d(u^iv^j) = u^iv^j(i\omega_1+j\omega_2),\quad \omega_k^2=0,\quad \omega_1\omega_2=-\omega_2\omega_1,$$

$\forall a\in\mathbb{C}G$, $\forall i,\ j\in\mathbb{Z}$. This is obtained from characters as in the finite group case via a limiting procedure.[12]

Then we have $\pi(u^{i_1}v^{i_2}d(u^{j_1}v^{j_2})d(u^{k_1}v^{k_2}))=(j_1k_2-j_2k_1)u^{i_1+j_1+k_1}v^{i_2+j_2+k_2}$ and hence

$$\varphi(u^{i_1}v^{i_2},u^{j_1}v^{j_2},u^{k_1}v^{k_2}) = j_1k_2-j_2k_1 \tag{5.4}$$

if $i_1+j_1+k_1=i_2+j_2+k_2=0$, and zero otherwise.

Next, as in Ref. 12 we chose the cocycle $F(u^{i_1}v^{i_2},u^{j_1}v^{j_2})=e^{\imath\theta i_2j_1}$ to gauge transform the category of $\mathbb{Z}\times\mathbb{Z}$-graded vector spaces. Then the algebra $\mathbb{C}_FG$ after cotwisting of the product has the relations $v\,.\,u=e^{\imath\theta}u\,.\,v$, which we call *algebraic noncommutative torus*. This observation itself is well-known already for the full noncommutative torus C^*-algebra in a more explicit (noncategorical) context.[20] From our point of view the algebra is associative since above F is a cocycle, but it still gives a nontrivial example of the theory of Sec. IV.

Now using (4.22) we compute the character of the above DC after gauge transformation as

$$\begin{aligned}\varphi_F(u^{i_1}v^{i_2},u^{j_1}v^{j_2},u^{k_1}v^{k_2}) &= F(u^{i_1}v^{i_2},u^{j_1}v^{j_2})F(u^{i_1}v^{i_2}u^{j_1}v^{j_2},u^{k_1}v^{k_2})\varphi(u^{i_1}v^{i_2},u^{j_1}v^{j_2},u^{k_1}v^{k_2})\\ &= e^{\imath\theta(i_2j_1+(i_2+j_2)k_1)}(j_1k_2-j_2k_1).\end{aligned} \tag{5.5}$$

Since, by the very definition of F, we have $u^{\cdot i}v^{\cdot j}=u^iv^j$, $\forall i,j\in\mathbb{Z}$, we conclude that

$$\varphi_F(u^{\cdot i_1}v^{\cdot i_2},u^{\cdot j_1}v^{\cdot j_2},u^{\cdot k_1}v^{\cdot k_2}) = e^{\imath\theta(i_2j_1+(i_2+j_2)k_1)}(j_1k_2-j_2k_1). \tag{5.6}$$

We remark that we have $v^{\cdot j}u^{\cdot i}=e^{\imath\theta ij}u^iv^j$, $\forall i,j\in\mathbb{Z}$. Note that σ is trivial in this example.

C. Quantum quasimanifolds covariant under quantum groups $\mathbb{C}_q(G)$

Here we take the initial Hopf algebra to be $H=\mathbb{C}(G)$, the algebraic version of a classical Lie group of complex simple Lie algebra g. More precisely, we need to work in a deformation-theoretic setting where $H=\mathbb{C}(G)[[\hbar]]$ is extended over this ring $\mathbb{C}[[\hbar]]$ of formal power series in a deformation parameter $\hbar$, rather than working over $\mathbb{C}$ itself. With this proviso, we are able to use the theory in Sec. IV A with F a cochain with values in $\mathbb{C}[[\hbar]]$. By essentially dualizing the theory in Ref. 1, one knows that there exists an F such that

$$\mathbb{C}_q(G) \cong (\mathbb{C}(G)[[\hbar]])^F,$$

i.e., such that after cotwisting one obtains the (formal power-series version of the) standard quantum group $\mathbb{C}_q(G)$. Here $q=e^{\hbar/2}$. Note that although the required F is not a cocycle so that the cotwist on the right-hand side here is in theory a coquasi-Hopf algebra, its coboundary $\phi_{\mathrm{KZ}}=\partial F$ [which is obtained by solving the Knizhnik–Zamolochikov (KZ) equations] happens to be central in the sense

$$abc = \phi_{\mathrm{KZ}}(a_{(1)},b_{(1)},c_{(1)})a_{(2)}b_{(2)}c_{(2)}\phi_{\mathrm{KZ}}^{-1}(a_{(3)},b_{(3)},c_{(3)})$$

so that the coquasi-Hopf algebra on the right-hand side happens to remain associative as indeed is $\mathbb{C}_q(G)$ on the left-hand side (since it is a usual Hopf algebra). This point of view has been expounded recently in Ref. 4. Let us note only that it is not exactly the one of Drinfeld even before dualization. For that one should start with $\mathbb{C}(G)[[\hbar]]$ as a nontrivial coquasi-Hopf algebra with a nontrivial initial coquasitriangular structure $\mathcal{R}_0$ built from the Killing form and a certain ϕ_0 as the initial associator, which is the object actually obtained by Drinfeld by solving the KZ-equations. Here ϕ_0 is closely related to ϕ_{KZ} above as its "inverse" in the sense that cotwisting it by F gives ε (the trivial associator). In this way, Drinfeld's theory in the cotwist form would cotwist a certain coquasi-Hopf algebra $(\mathbb{C}(G)[[\hbar]],\mathcal{R}_0,\phi_0)$ into the ordinary Hopf algebra $\mathbb{C}_q(G)$ with its usual quasitriangular structure and trivial associator. By contrast in Ref. 4 one starts with $\mathbb{C}(G)[[\hbar]]$ as completely classical with trivial coquasitriangular structure and trivial associator, and obtains after cotwisting $(\mathbb{C}_q(G),\mathcal{R}_F,\phi_{\mathrm{KZ}})$ as a cotriangular coquasi-Hopf algebra. Like in our examples based on Abelian groups, this happens to be an ordinary Hopf algebra in its algebra and coalgebra. Here $\mathcal{R}_F$ is given by (4.8) and ϕ_{KZ} by (4.7). This cotriangular coquasi-Hopf algebra $(\mathbb{C}_q(G),\mathcal{R}_F,\phi_{\mathrm{KZ}})$ is the object under which our examples of quantum quasispaces below are covariant. As an algebra and coalgebra it coincides with the usual quantum group $\mathbb{C}_q(G)$.

Thus, in Ref. 4 this $(\mathbb{C}_q(G),\mathcal{R}_F,\phi_{\mathrm{KZ}})$ construction was used to obtain a quantum differential calculus on $\mathbb{C}_q(G)$ as a supercoquasi-Hopf algebra $\Omega(\mathbb{C}(G))^F$. We extend this setting now to any manifold M on which the classical Lie group G acts. More precisely, we assume that there are algebraic versions $\mathbb{C}(M)$ for the coordinate algebra and for a coaction $\mathbb{C}(M)\to\mathbb{C}(G)\otimes\mathbb{C}(M)$. Thus $\mathbb{C}(M)$ is given as an algebra in our initial category of $\mathbb{C}(G)$-comodules. Moreover, we extend all this data to the formal power series setting (we adjoin $\hbar$).

Theorem 13: *Let M be a classical G-manifold in the sense above. Then there is a quasialgebra $\mathcal{C}_q(M)=(\mathbb{C}(M)[[\hbar]])_F$ in the category of $\mathbb{C}_q(G)$-comodules, where $\mathbb{C}_q(G)$ is the standard quantum group associated to G viewed as a cotriangular coquasi-Hopf algebra. Moreover, $\mathcal{C}_q(M)$ has a quasiassociative differential calculus $\Omega(\mathbb{C}(M))_F$.*

Proof: We apply the theory of Sec. IV A with $H=\mathbb{C}(G)[[\hbar]]$, F the cochain above and $A=\mathbb{C}(M)[[\hbar]]$. ■

Similarly, any classical data on M such as a cyclic cocycle twists to a braided cyclic one on the symmetric but nontrivially monoidal category of $\mathbb{C}_q(G)$-comodules.

Let us note also that when all of our data are obtained from exponentiating infinitesimal data, we can look at the structure of $\mathcal{C}_q(M)$ to lowest order. Then one finds

$$\{\{a,b\},c\}+\{\{b,c\},a\}+\{\{c,a\},b\}=2\tilde{n}(a\otimes b\otimes c),$$

where $n\propto[r_{+12},r_{+23}]\in g\otimes g\otimes g$ is the leading order part of ϕ_{KZ} as explained in Ref. 4. Here r_+ is the symmetric part of the standard classical r-matrix of g and is a multiple of the Killing form. In this case the left-invariant trivector field $\tilde{n}$ given by the action of n is some multiple of the canonical "Cartan tensor" that exists for any manifold M acted upon by a semisimple Lie algebra. We see that $\mathcal{C}_q(M)$ is not the quantization of a usual Poisson manifold but of a "quasi-Poisson" manifold. Such a weaker concept was proposed recently in Ref. 8 and we see that we have succeed in quantizing it using cotwisting. We see, moreover, that the quantum quasispace $\mathbb{C}_q(M)$ remains covariant but under the quantum group $\mathbb{C}_q(G)$ (viewed as a cotriangular coquasi Hopf algebra). Let us note, however, one technical difference from Ref. 8; our quasi-Poisson manifold is associated with an action of G not to a Poisson action of G (these are not quite the same thing).

Finally, we can apply all of this theory to $M=G$, i.e., to $A=\mathbb{C}(G)[[\hbar]]$, where G acts on itself by translation, i.e., $A=H$ and the coaction is via the coproduct. This is the same idea as for our examples with finite groups, but now with G a Lie group of a simple Lie algebra.

Corollary 14: The standard quantum groups $\mathbb{C}_q(G)$ *have quasialgebra versions* $\mathcal{C}_q(G)$ as algebras in the category of $\mathbb{C}_q(G)$*-comodules as a symmetric monoidal category*.

Proof: Here $\mathcal{C}_q(G)=(\mathbb{C}(G)[[\hbar]])_F$, where we use the one-sided cotwist, in contrast to the Drinfeld cotwist which gives $(\mathbb{C}_q(G),\mathcal{R}_F,\phi_{\mathrm{KZ}})$ as explained above. The former lives in the category of comodules of the latter. ■

If one wants to be concrete, let $\{t^i{}_j\}$ be the matrix of generators of the classical Lie group G. These generate the classical $\mathbb{C}(G)$ with the usual "matrix" coproduct. If we know F then we know in particular the tensors

$$F^{i\ j}_{k\ l}=F(t^i{}_k,t^j{}_l),\quad (\Delta_2F)^{i\ j\ k}_{l\ m\ n}=F(t^i{}_l,t^j{}_m t^k{}_n),\quad (\Delta_1F)^{i\ j\ k}_{l\ m\ n}=F(t^i{}_l t^j{}_m,t^k{}_n),$$

and so forth, where the product is in the classical $\mathbb{C}(G)[[\hbar]]$. Next, we denote the generators of $\mathcal{C}_q(G)$ by $\{x^i{}_j\}$ say. They are the same as the $t^i{}_j$ but with a new product which then enjoys the deformed relations

$$x_1x_2=FF_{21}^{-1}x_2x_1.$$

We use here the standard notation in quantum group theory, where the numerical indices refer to the position in a tensor product. These relations have to be combined with the nonassociativity relations

$$x_1(x_2x_3)=F_{23}(\Delta_2F)(\Delta_1F)^{-1}F_{12}^{-1}(x_1x_2)x_3.$$

The commutation relations reflect that the quasispace is braided-commutative with respect to the cotriangular structure $\mathcal{R}_F$, while the nonassociativity relations reflect the associator ϕ_{KZ} obtained from F.

We also have a calculus, cocycle etc. on $\mathcal{C}_q(G)$, with $\Omega(\mathcal{C}_q(G))=\Omega(\mathbb{C}(G)[[\hbar]])_F$. Choosing a matrix of invariant classical differential forms as generators of the classical calculus, one has similar "F-matrix" formulas for the relations in the deformed calculus on $\mathcal{C}_q(G)$, and so forth. Further details will be given elsewhere.

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Quasi-Hopf algebras and representations of octonions and other quasialgebras

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Modules over a quasialgebra (here, by quasialgebra we mean a left H-module algebra, where H is a quasi-Hopf algebra), as defined by Albuquerque and Majid, coincide with modules over a certain associative algebra, a quasi-Hopf smash product. As a consequence of this, we get that the category of modules over the octonions is isomorphic to the category of modules over the algebra of 8×8 real matrices. We provide a new approach to the endomorphism quasialgebra associated to a left H-module, which in the finite dimensional case yields the same results as the one of Albuquerque and Majid. We discuss possible definitions as endomorphism quasialgebras for Heisenberg doubles of a finite dimensional quasi-Hopf algebra. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1789280]

I. INTRODUCTION

The starting point of this paper was the following question we asked ourselves: What could be a module over the octonions? The usual approach to octonions (we refer to Ref. 2 for a recent survey of the existing theory for the octonions) does not provide an answer. However, it turned out that such an answer is possible using the recent Hopf-algebraic approach to octonions proposed by Albuquerque and Majid in Ref. 1. Namely, they first introduced the concept of a "quasialgebra," as being an algebra in a tensor category (in this paper we restrict the term to algebras in the tensor category of modules over a quasi-Hopf algebra) and then proved that the (nonassociative) algebra of octonions is such a quasialgebra; they defined also a module over a quasialgebra A as being an A-module in the same tensor category where A lives as an algebra and hence a suitable definition of modules over the octonions may be derived from this.

If H is a quasi-Hopf algebra and M is a *finite dimensional* left H-module, Albuquerque and Majid constructed the so-called "endomorphism quasialgebra" of M—which is built on the vector space $\mathrm{End}(M)$ and will be denoted below by $\mathrm{end}(M)$—using "tensor-categorical" techniques, that is by introducing first a quasialgebra structure on $M\otimes M^*$ and then transfering it to $\mathrm{End}(M)$ via the linear isomorphism $\mathrm{End}(M)\simeq M\otimes M^*$. Also, if A is an algebra in the category of left H-modules, they proved that setting a structure of an A-module on M is equivalent to giving a quasialgebra map $A\to \mathrm{end}(M)$.

There is an obvious analogy with what happens for other classes of algebras (associative or Lie), where setting a module structure on a vector space is equivalent to giving an algebra map from the algebra to a certain "endomorphism algebra" constructed out of the vector space, but in those cases one can construct the "endomorphism algebra" of any object (not necessarily finite dimensional), so it is natural to see whether this is possible also for the class of quasialgebras.

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In order to explain our contribution to this subject, let us first recall some results from Ref. 6. First, if H is a quasi-Hopf algebra, B an associative algebra and $v:H\to B$ an algebra map, then on B one can introduce a structure of an algebra in the tensor category of left H-modules (a left H-module algebra structure, in the terminology of Ref. 6), denoted by B^v. Second, if A is a left H-module algebra, an associative algebra, denoted by $A\#H$ and called the smash product, has been introduced in Ref. 6 and the left $A\#H$-modules were described. These turned out to coincide with the A-modules in the category of left H-modules (called left A, H-modules in Ref. 6).

The first aim of this paper is to point out that the modules over a quasialgebra, as defined by Albuquerque and Majid, coincide with modules over an associative algebra, namely, a quasi-Hopf smash product. As a consequence, we obtain that the category of modules over a twisted group quasialgebra kG_F is isomorphic to the category of modules over the algebra of $|G|$ by $|G|$ matrices over k (where $|G|$ is the order of the group G), and in particular that the category of modules over the octonions is isomorphic to the category of modules over the algebra of 8×8 real matrices.

The second aim is to provide a different approach to the endomorphism quasialgebra associated to an object, which works also in the *infinite dimensional case*. Namely, if H is a quasi-Hopf algebra, A a left H-module algebra and M a left H-module, we have the algebra map $v:H\to \mathrm{End}(M)$, $v(h)(m)=h\cdot m$, so we can consider the left H-module algebra $\mathrm{End}(M)^v$ (this will be the endomorphism quasialgebra associated to M); then we prove that setting a structure of a left A, H-module on M is equivalent to giving a morphism of left H-module algebras $\varphi:A\to \mathrm{End}(M)^v$ (the proof relies on the use of the smash product $A\#H$). Also, we prove that if M is a finite dimensional left H-module, then $\mathrm{End}(M)^v$ coincides with $\mathrm{end}(M)$ defined in Ref. 1 as left H-module algebras, and that if M is moreover a left A, H-module, then the map φ coincides with the similar map $A\to \mathrm{end}(M)$ defined by Albuquerque and Majid.

As an immediate consequence of the identification $\mathrm{End}(M)^v\equiv \mathrm{end}(M)$ and of results in Ref. 4, we obtain that if M is a finite dimensional Yetter–Drinfeld H-module, then $\mathrm{End}(M)^v$ is a Yetter–Drinfeld H-module algebra.

The analogy with the classes of associative or Lie algebras mentioned before can be pushed forward. Namely, the concepts of a *bimodule* over an associative or Lie algebra are a manifestation of a single concept, that of a bimodule over an algebra with respect to a class of algebras (see Ref. 18). We prove that if H is a quasi-bialgebra and A is a left H-module algebra, then an A-bimodule with respect to the class of left H-module algebras, in the sense of Ref. 18, is the same as an A-bimodule in the tensor category of left H-modules.

In the final section we discuss possible definitions as endomorphism quasialgebras for Heisenberg doubles of a finite dimensional quasi-Hopf algebra.

II. PRELIMINARIES

We work over a commutative field k. All algebras, linear spaces, etc., will be over k; unadorned $\otimes$ means $\otimes_k$. Following Drinfeld,[9] a quasi-bialgebra is a fourtuple $(H,\Delta,\varepsilon,\Phi)$, where H is an associative algebra with unit, Φ is an invertible element in $H\otimes H\otimes H$, and $\Delta:H\to H\otimes H$ and $\varepsilon:H\to k$ are algebra homomorphisms satisfying the identities

$$(\mathrm{id}\otimes\Delta)(\Delta(h))=\Phi(\Delta\otimes\mathrm{id})(\Delta(h))\Phi^{-1}, \tag{2.1}$$

$$(\mathrm{id}\otimes\varepsilon)(\Delta(h))=h\otimes 1,\quad (\varepsilon\otimes\mathrm{id})(\Delta(h))=1\otimes h, \tag{2.2}$$

for all $h\in H$, and Φ has to be a normalized 3-cocycle, in the sense that

$$(1\otimes\Phi)(\mathrm{id}\otimes\Delta\otimes\mathrm{id})(\Phi)(\Phi\otimes 1)=(\mathrm{id}\otimes\mathrm{id}\otimes\Delta)(\Phi)(\Delta\otimes\mathrm{id}\otimes\mathrm{id})(\Phi), \tag{2.3}$$

$$(\mathrm{id}\otimes\varepsilon\otimes\mathrm{id})(\Phi)=1\otimes 1\otimes 1. \tag{2.4}$$

The map Δ is called the coproduct or the comultiplication, ε the counit and Φ the reassociator. As for Hopf algebras[19] we denote $\Delta(h)=\Sigma h_1\otimes h_2$, but since Δ is only quasi-coassociative we adopt the further convention

$$(\Delta\otimes\mathrm{id})(\Delta(h))=\sum h_{(1,1)}\otimes h_{(1,2)}\otimes h_2,\ \ (\mathrm{id}\otimes\Delta)(\Delta(h))=\sum h_1\otimes h_{(2,1)}\otimes h_{(2,2)},$$

for all $h\in H$. We will denote the tensor components of Φ by capital letters, and those of Φ^{-1} by small letters, namely,

$$\Phi=\sum X^1\otimes X^2\otimes X^3=\sum T^1\otimes T^2\otimes T^3=\sum V^1\otimes V^2\otimes V^3=\cdots,$$

$$\Phi^{-1}=\sum x^1\otimes x^2\otimes x^3=\sum t^1\otimes t^2\otimes t^3=\sum v^1\otimes v^2\otimes v^3=\cdots.$$

The quasi-bialgebra H is called a quasi-Hopf algebra if there exists an antiautomorphism S of the algebra H and elements $\alpha,\beta\in H$ such that, for all $h\in H$, we have

$$\sum S(h_1)\alpha h_2=\varepsilon(h)\alpha\ \text{ and }\ \sum h_1\beta S(h_2)=\varepsilon(h)\beta, \tag{2.5}$$

$$\sum X^1\beta S(X^2)\alpha X^3=1\ \text{ and }\ \sum S(x^1)\alpha x^2\beta S(x^3)=1. \tag{2.6}$$

For a quasi-Hopf algebra the antipode is determined uniquely up to a transformation $\alpha\mapsto U\alpha$, $\beta\mapsto\beta U^{-1}$, $S(h)\mapsto US(h)U^{-1}$, where $U\in H$ is invertible. The axioms for a quasi-Hopf algebra imply that $\varepsilon(\alpha)\varepsilon(\beta)=1$, so, by rescaling α and β, we may assume without loss of generality that $\varepsilon(\alpha)=\varepsilon(\beta)=1$ and $\varepsilon\circ S=\varepsilon$. The identities (2.2)–(2.4) also imply that

$$(\varepsilon\otimes\mathrm{id}\otimes\mathrm{id})(\Phi)=(\mathrm{id}\otimes\mathrm{id}\otimes\varepsilon)(\Phi)=1\otimes 1\otimes 1. \tag{2.7}$$

Together with a quasi-bialgebra or a quasi-Hopf algebra $H=(H,\Delta,\varepsilon,\Phi,S,\alpha,\beta)$ we also have H^{op}, H^{cop} and $H^{\mathrm{op,cop}}$ as quasi-bialgebras (respectively, quasi-Hopf algebras), where "op" means opposite multiplication and "cop" means opposite comultiplication. The structures are obtained by setting $\Phi_{\mathrm{op}}=\Phi^{-1}$, $\Phi_{\mathrm{cop}}=(\Phi^{-1})^{321}$, $\Phi_{\mathrm{op,cop}}=\Phi^{321}$, $S_{\mathrm{op}}=S_{\mathrm{cop}}=(S_{\mathrm{op,cop}})^{-1}=S^{-1}$, $\alpha_{\mathrm{op}}=S^{-1}(\beta)$, $\beta_{\mathrm{op}}=S^{-1}(\alpha)$, $\alpha_{\mathrm{cop}}=S^{-1}(\alpha)$, $\beta_{\mathrm{cop}}=S^{-1}(\beta)$, $\alpha_{\mathrm{op,cop}}=\beta$, and $\beta_{\mathrm{op,cop}}=\alpha$.

Next we recall that the definition of a quasi-bialgebra or quasi-Hopf algebra is "twist covariant" in the following sense. An invertible element $F\in H\otimes H$ is called a *gauge transformation* or *twist* if $(\varepsilon\otimes\mathrm{id})(F)=(\mathrm{id}\otimes\varepsilon)(F)=1$. If H is a quasi-bialgebra or a quasi-Hopf algebra and $F=\Sigma F^1\otimes F^2\in H\otimes H$ is a gauge transformation with inverse $F^{-1}=\Sigma G^1\otimes G^2$, then we can define a new quasi-bialgebra (respectively, quasi-Hopf algebra) H_F by keeping the multiplication, unit, counit (and antipode in the case of a quasi-Hopf algebra) of H and replacing the comultiplication, reassociator and the elements α and β by

$$\Delta_F(h)=F\Delta(h)F^{-1}, \tag{2.8}$$

$$\Phi_F=(1\otimes F)(\mathrm{id}\otimes\Delta)(F)\Phi(\Delta\otimes\mathrm{id})(F^{-1})(F^{-1}\otimes 1), \tag{2.9}$$

$$\alpha_F=\sum S(G^1)\alpha G^2,\ \ \beta_F=\sum F^1\beta S(F^2). \tag{2.10}$$

It is well known that the antipode of a Hopf algebra is an anti-coalgebra morphism. For a quasi-Hopf algebra, we have the following statement: there exists a gauge transformation $f\in H\otimes H$ such that

$$f\Delta(S(h))f^{-1} = \sum (S \otimes S)(\Delta^{\mathrm{cop}}(h)) \quad \text{for all } h \in H. \tag{2.11}$$

The element f can be computed explicitly. First set

$$\sum A^1 \otimes A^2 \otimes A^3 \otimes A^4 = (\Phi \otimes 1)(\Delta \otimes \mathrm{id} \otimes \mathrm{id})(\Phi^{-1}), \tag{2.12}$$

$$\sum B^1 \otimes B^2 \otimes B^3 \otimes B^4 = (\Delta \otimes \mathrm{id} \otimes \mathrm{id})(\Phi)(\Phi^{-1} \otimes 1), \tag{2.13}$$

and then define $\gamma, \delta \in H \otimes H$ by

$$\gamma = \sum S(A^2)\alpha A^3 \otimes S(A^1)\alpha A^4 \text{ and } \delta = \sum B^1 \beta S(B^4) \otimes B^2 \beta S(B^3). \tag{2.14}$$

Then f and f^{-1} are given by the formulas

$$f = \sum (S \otimes S)(\Delta^{\mathrm{cop}}(x^1))\gamma\Delta(x^2\beta S(x^3)), \tag{2.15}$$

$$f^{-1} = \sum \Delta(S(x^1)\alpha x^2)\delta(S \otimes S)(\Delta^{\mathrm{cop}}(x^3)). \tag{2.16}$$

If H is a quasi-Hopf algebra, following Refs. 10 and 11 we may define the elements

$$p_R = \sum p^1 \otimes p^2 = \sum x^1 \otimes x^2 \beta S(x^3), \quad q_R = \sum q^1 \otimes q^2 = \sum X^1 \otimes S^{-1}(\alpha X^3)X^2, \tag{2.17}$$

$$p_L = \sum \tilde{p}^1 \otimes \tilde{p}^2 = \sum X^2 S^{-1}(X^1 \beta) \otimes X^3, \quad q_L = \sum \tilde{q}^1 \otimes \tilde{q}^2 = \sum S(x^1)\alpha x^2 \otimes x^3 \tag{2.18}$$

satisfying the relations (for all $h \in H$):

$$\sum q_1^1 p^1 \otimes q_2^1 p^2 S(q^2) = 1 \otimes 1, \quad \sum q^1 p_1^1 \otimes S^{-1}(p^2) q^2 p_2^1 = 1 \otimes 1, \tag{2.19}$$

$$\sum S(\tilde{p}^1)\tilde{q}^1\tilde{p}_1^2 \otimes \tilde{q}^2\tilde{p}_2^2 = 1 \otimes 1, \quad \sum \tilde{q}_1^2\tilde{p}^1 S^{-1}(\tilde{q}^1) \otimes \tilde{q}_2^2\tilde{p}^2 = 1 \otimes 1, \tag{2.20}$$

$$\sum \Delta(h_1)p_R[1 \otimes S(h_2)] = p_R[h \otimes 1], \quad \sum [1 \otimes S^{-1}(h_2)]q_R\Delta(h_1) = [h \otimes 1]q_R, \tag{2.21}$$

$$\sum \Delta(h_2)p_L[S^{-1}(h_1) \otimes 1] = p_L[1 \otimes h], \quad \sum [S(h_1) \otimes 1]q_L\Delta(h_2) = [1 \otimes h]q_L. \tag{2.22}$$

Suppose that $(H, \Delta, \varepsilon, \Phi)$ is a quasi-bialgebra. If U, V, W are left (right) H-modules, define $a_{U,V,W}$, $\mathbf{a}_{U,V,W}: (U \otimes V) \otimes W \to U \otimes (V \otimes W)$ by

$$a_{U,V,W}((u \otimes v) \otimes w) = \mathbf{\Phi} \cdot (u \otimes (v \otimes w)),$$

$$\mathbf{a}_{U,V,W}((u \otimes v) \otimes w) = (u \otimes (v \otimes w)) \cdot \mathbf{\Phi}^{-1}.$$

The category ${}_H\mathcal{M}$ ($\mathcal{M}_H$) of left (right) H-modules becomes a monoidal category (see Refs. 12 and 14 for the terminology) with tensor product $\otimes$ given via Δ, associativity constraints $a_{U,V,W}$ ($\mathbf{a}_{U,V,W}$), unit k as a trivial H-module and the usual left and right unit constraints.

Now, let H be a quasi-bialgebra. We say that a k-vector space A is a left H-module algebra if it is an algebra in the monoidal category ${}_H\mathcal{M}$, that is A has a multiplication and a usual unit 1_A satisfying the following conditions:

$$(aa')a'' = \sum (X^1 \cdot a)[(X^2 \cdot a')(X^3 \cdot a'')], \tag{2.23}$$

$$h \cdot (aa') = \sum (h_1 \cdot a)(h_2 \cdot a'), \tag{2.24}$$

$$h \cdot 1_A = \varepsilon(h)1_A, \tag{2.25}$$

for all $a, a', a'' \in A$ and $h \in H$, where $h \otimes a \to h \cdot a$ is the left H-module structure of A. Following Ref. 6 we define the smash product $A\#H$ as follows: as vector space $A\#H$ is $A \otimes H$ (elements $a \otimes h$ will be written $a\#h$) with multiplication given by

$$(a \# h)(a' \# h') = \sum (x^1 \cdot a)(x^2 h_1 \cdot a') \# x^3 h_2 h', \tag{2.26}$$

for all $a, a' \in A$, $h, h' \in H$. Then $A\#H$ is an associative algebra with unit $1_A\#1$.

If A' is another left H-module algebra, a map $f: A \to A'$ is a morphism of left H-module algebras if it is multiplicative, unital and a morphism of left H-modules.

For further use we need also the notion of right H-module algebra. Let H be a quasi-bialgebra. We say that a k-linear space C is a right H-module algebra if C is an algebra in the monoidal category $\mathcal{M}_H$, i.e., C has a multiplication and a usual unit 1_C satisfying the following conditions:

$$(cc')c'' = \sum (c \cdot x^1)[(c' \cdot x^2)(c'' \cdot x^3)], \tag{2.27}$$

$$(cc') \cdot h = \sum (c \cdot h_1)(c' \cdot h_2), \tag{2.28}$$

$$1_C \cdot h = \varepsilon(h)1_C, \tag{2.29}$$

for all $c, c', c'' \in C$ and $h \in H$, where $c \otimes h \to c \cdot h$ is the right H-module structure of C.

Let H be a quasi-bialgebra, $F \in H \otimes H$ a gauge transformation and A a left H-module algebra. Then, following Refs. 6 and 5, we can define a new multiplication on A, by

$$a \diamond b = \sum (G^1 \cdot a)(G^2 \cdot b), \quad \forall\, a, b \in A, \tag{2.30}$$

where $F^{-1} = \Sigma G^1 \otimes G^2$. If we denote by $A_{F^{-1}}$ the resulting structure, then $A_{F^{-1}}$ becomes a left H_F-module algebra, with the same unit and H-action as for A, and moreover the map

$$\lambda: A \# H \to A_{F^{-1}} \# H_F, \ \lambda(a \# h) = \sum F^1 \cdot a \# F^2 h,$$

is an algebra isomorphism.

If H is a quasi-Hopf algebra, B an associative algebra and $v: H \to B$ an algebra map, then, following Ref. 6, we can introduce on the vector space B a left H-module algebra structure, denoted by B^v in what follows, for which the multiplication, unit and left H-action are

$$b \star b' = \sum v(X^1) b v(S(x^1 X^2) \alpha x^2 X_1^3) b' v(S(x^3 X_2^3)), \quad \forall\, b, b' \in B, \tag{2.31}$$

$$1_{B^v} = v(\beta), \tag{2.32}$$

$$h \triangleright_v b = \sum v(h_1) b v(S(h_2)), \quad \forall\, h \in H, b \in B. \tag{2.33}$$

If H is a quasi-Hopf algebra and A is a left H-module algebra, define the following maps:

$$j: H \to A \# H, \ j(h) = 1 \# h, \quad \forall\, h \in H, \tag{2.34}$$

$$i_0: A \to A \# H, \quad i_0(a) = \sum x^1 \cdot a \# x^2 \beta S(x^3), \quad \forall\, a \in A. \tag{2.35}$$

Then, by Ref. 6, j is an algebra map and i_0 is a morphism of left H-module algebras from A to $(A\#H)^j$. Moreover, the following universal property of the smash product $A\#H$ holds (see Ref. 6, Proposition 2.9): if B is an associative algebra, $v: H \to B$ is an algebra map and $\varphi: A \to B^v$ is a morphism of left H-module algebras, then there exists a unique algebra map $\varphi \# v: A\#H \to B$ such that $(\varphi \# v) \circ i_0 = \varphi$ and $(\varphi \# v) \circ j = v$; this map may be described explicitly as follows:

$$(\varphi \# v)(a \# h) = \sum v(X^1)\varphi(a)v(S(X^2)\alpha X^3 h), \quad \forall\, a \in A, \ h \in H. \tag{2.36}$$

Now recall from Ref. 6 the following concept.

Definition 2.1: Let H be a quasi-bialgebra and A a left H-module algebra. We say that M, a k-linear space, is a left A, H-module if

(i) M is a left H-module with action denoted by $h \otimes m \mapsto h \cdot m$.
(ii) A acts weakly on M to the left, i.e., there exists a k-linear map $A \otimes M \to M$, denoted by $a \otimes m \mapsto a \triangleright m$, such that $1_A \triangleright m = m$ for all $m \in M$.
(iii) The following compatibility relations hold:

$$a \triangleright (b \triangleright m) = \sum [(x^1 \cdot a)(x^2 \cdot b)] \triangleright (x^3 \cdot m), \tag{2.37}$$

$$h \cdot (a \triangleright m) = \sum (h_1 \cdot a) \triangleright (h_2 \cdot m), \tag{2.38}$$

for all $h \in H$, a, $b \in A$ and $m \in M$ (these conditions may be expressed equivalently by saying that M is a left A-module in the tensor category ${}_H\mathcal{M}$).

The category of all left A, H-modules, morphisms being the maps that are H-linear and preserve the A-action, will be denoted by ${}_{A,H}\mathcal{M}$.

Let $A\#H$-mod be the category of left $A\#H$-modules; we have the following result (see Ref. 6).

Proposition 2.2: Let H be a quasi-bialgebra and A a left H-module algebra. Then the categories ${}_{A,H}\mathcal{M}$ and $A\#H$-mod are isomorphic.

The isomorphism is given as follows. If $M \in A\#H$-mod with $A\#H$-module structure given by $(a\#h) \otimes m \mapsto (a\#h) \cdot m$, then $M \in {}_{A,H}\mathcal{M}$ with A-action given by $a \triangleright m = (a\#1) \cdot m$ and H-action given by $h \cdot m = (1\#h) \cdot m$. Conversely, if $M \in {}_{A,H}\mathcal{M}$, then M becomes a left $A\#H$-module with action $(a\#h) \cdot m = a \triangleright (h \cdot m)$.

III. OCTONIONS AND OTHER TWISTED GROUP QUASIALGEBRAS

Let G be a finite group, kG its group algebra and $k(G)$ the dual Hopf algebra of kG. We recall first the setting in Ref. 1, but in a quasi-Hopf framework (not dual quasi-Hopf as in Ref. 1). Let $T: G \times G \to k^*$ be an invertible map, with inverse $F: G \times G \to k^*$, such that $T(1,x) = T(x,1) = 1$ for all $x \in G$, and regard T and F as extended to $kG \otimes kG$, so we can regard them as elements in $k(G) \otimes k(G)$, where they become gauge transformations. So, we have the Hopf algebra $k(G)$, T a gauge transformation on it, and we have the left $k(G)$-module algebra kG [with the left regular action of $k(G)$ on kG, that is $p \rightharpoonup x = p(x)x$ for all $p \in k(G)$ and $x \in G$]. From the preliminaries, we know that we can consider the left $k(G)_T$-module algebra kG_F, and also that we have an algebra isomorphism,

$$kG_F \# k(G)_T \simeq kG \# k(G).$$

Let us mention that the multiplication in kG_F (denoted in Ref. 1 by $k_F G$), which is given by

$$x \cdot_F y = F(x,y)xy, \quad \forall\ x,y \in G,$$

is in general nonassociative, and that $k(G)_T$, though is a Hopf algebra (being commutative), is regarded here as a quasi-Hopf algebra, with reassociator obtained by extending the map $\phi: G \times G \times G \to k^*$ given by

$$\phi(x,y,z) = \frac{T(x,yz)T(y,z)}{T(xy,z)T(x,y)} = \frac{F(x,y)F(xy,z)}{F(y,z)F(x,yz)},$$

so in general kG_F is a $k(G)_T$-module algebra *only* in the quasi-Hopf sense (*not* in the Hopf sense).

Now, it is well known (see Ref. 16) that $kG\#k(G)$, which is the Heisenberg double of kG, is isomorphic as an algebra to the matrix algebra $M_{|G|}(k)$, where $|G|$ is the order of G. Since left kG_F, $k(G)_T$-modules coincide to left $kG_F\#k(G)_T$-modules, we get the following result.

Proposition 3.1: *The category of left kG_F, $k(G)_T$-modules is isomorphic to the category of left $M_{|G|}(k)$-modules.*

In particular, as proved in Ref. 1, the algebra $\mathcal{O}$ of octonions is of the form kG_F, for $G = Z_2 \times Z_2 \times Z_2$ (where Z_2 is the group with two elements) and a certain map F, so we get the following as a consequence.

Corollary 3.2: The category of modules over the octonions is isomorphic to the category of modules over the algebra of 8×8 real matrices.

IV. THE ENDOMORPHISM QUASIALGEBRA ASSOCIATED TO A MODULE

Lemma 4.1: Let H be a quasi-Hopf algebra, B, C associative algebras, $\eta: B \to C$, $j: H \to B$, $v: H \to C$ algebra maps such that $\eta \circ j = v$. Then the map $\eta: B^j \to C^v$ is a morphism of left H-module algebras.

Proof: Follows by a direct computation, using the formulas (2.31)–(2.33). □

Let H be a quasi-Hopf algebra and M a left H-module, with action denoted by $h \otimes m \mapsto h \cdot m$. Consider the (usual) associative algebra $\mathrm{End}(M)$ (with composition) and define $v: H \to \mathrm{End}(M)$, $v(h)(m) = h \cdot m$, which is an algebra map, so we can consider the left H-module algebra $\mathrm{End}(M)^v$, whose multiplication, unit and H-action are given as follows [using the formulas (2.31)–(2.33)]:

$$(u \star u')(m) = \sum X^1 \cdot u(S(x^1X^2)\alpha x^2 X_1^3 \cdot u'(S(x^3X_2^3) \cdot m)), \tag{4.1}$$

$$1_{\mathrm{End}(M)^v}(m) = v(\beta)(m) = \beta \cdot m, \tag{4.2}$$

$$(h \triangleright_v u)(m) = \sum h_1 \cdot u(S(h_2) \cdot m), \tag{4.3}$$

for all $h \in H$, $u, u' \in \mathrm{End}(M)^v$, $m \in M$.

Suppose now that we have also a left H-module algebra A, with notation $h \otimes a \mapsto h \cdot a$ and $a \otimes a' \mapsto aa'$. Our first aim is to prove the following result.

Theorem 4.2: *Setting a structure of a left A, H-module on M is equivalent to giving a morphism of left H-module algebras $\varphi: A \to End(M)^v$. The correspondence is given as follows: if M is a left A, H-module (with A-action denoted by $a \otimes m \mapsto a \triangleright m$) then the map $\varphi: A \to End(M)^v$ is given by*

$$\varphi(a)(m) = \sum (p^1 \cdot a) \triangleright (p^2 \cdot m), \quad \forall\ a \in A,\ m \in M, \tag{4.4}$$

where $p_R = \Sigma p^1 \otimes p^2 = \Sigma x^1 \otimes x^2 \beta S(x^3)$. Conversely, if $\varphi: A \to End(M)^v$ is a morphism of left H-module algebras, then M becomes a left A, H-module, with A-action given by

$$a \triangleright m = \sum q^1 \cdot \varphi(a)(S(q^2) \cdot m), \quad \forall\ a \in A,\ m \in M, \tag{4.5}$$

where $q_R=\Sigma q^1\otimes q^2=\Sigma X^1\otimes S^{-1}(\alpha X^3)X^2$, *and the H-action being the original H-module structure of M*.

Proof: Suppose first that M is a left A, H-module, with A-action $a\otimes m\mapsto a\triangleright m$. As we know, this is equivalent to M being a left $A\#H$-module, with structure

$$(a\#h)\cdot m=a\triangleright(h\cdot m),\quad \forall\, a\in A,\ h\in H,\ m\in M.$$

So, considering the usual associative algebra $\mathrm{End}(M)$, we obtain an algebra map $\eta:A\#H\to\mathrm{End}(M)$, $\eta(a\#h)(m)=(a\#h)\cdot m$. We also have the canonical algebra map $j:H\to A\#H$, $j(h)=1\#h$; since we obviously have that $\eta\circ j=v$, we may apply the previous lemma and obtain that the map $\eta:(A\#H)^j\to\mathrm{End}(M)^v$ is a morphism of left H-module algebras. It follows from the preliminaries that the map $i_0:A\to(A\#H)^j$, $i_0(a)=\Sigma p^1\cdot a\#p^2$, where $p_R=\Sigma p^1\otimes p^2=\Sigma x^1\otimes x^2\beta S(x^3)$, is a morphism of left H-module algebras, so the composition

$$\varphi=\eta\circ i_0:A\to\mathrm{End}(M)^v$$

is also a morphism of left H-module algebras, and one can easily check that it is given by

$$\varphi(a)(m)=\sum(p^1\cdot a)\triangleright(p^2\cdot m),\quad \forall\, a\in A,\ m\in M.$$

Conversely, let $\varphi:A\to\mathrm{End}(M)^v$ be a morphism of left H-module algebras; by applying the universal property of the smash product $A\#H$ (see Sec. II) for $B=\mathrm{End}(M)$, we obtain the algebra map $\varphi\#v:A\#H\to\mathrm{End}(M)$, which [using the formula (2.36)] may be expressed as follows:

$$(\varphi\#v)(a\#h)(m)=\sum q^1\cdot\varphi(a)(S(q^2)h\cdot m),\quad \forall\, a\in A,\ h\in H,\ m\in M.$$

Hence, M becomes a left $A\#H$-module (i.e., a left A, H-module) with action

$$(a\#h)\cdot m=\sum q^1\cdot\varphi(a)(S(q^2)h\cdot m),\quad \forall\, a\in A,\ h\in H,\ m\in M.$$

In particular, the A-action is given by

$$a\triangleright m=(a\#1)\cdot m=\sum q^1\cdot\varphi(a)(S(q^2)\cdot m),\quad \forall\, a\in A,\ m\in M,$$

and, using the fact that $\Sigma q^1\beta S(q^2)=1$ [which follows from the relation (2.6)], we obtain that the H-action is given by

$$(1\#h)\cdot m=\sum q^1\beta S(q^2)h\cdot m=h\cdot m,\quad \forall\, h\in H,\ m\in M.$$

Now the only thing left to prove is that the two correspondences are inverse to each other.

If M is an A, H-module with A-action denoted by $\triangleright$, if φ is the associated map $\varphi:A\to\mathrm{End}(M)^v$ and we denote by $\triangleright'$ the A-action associated to φ, we have (for all $a\in A$ and $m\in M$):

$$a\triangleright' m=\sum q^1\cdot((p^1\cdot a)\triangleright(p^2S(q^2)\cdot m))$$

$$(2.38)=\sum(q_1^1p^1\cdot a)\triangleright(q_2^1p^2S(q^2)\cdot m)$$

$$(2.19)=a\triangleright m.$$

Conversely, if $\varphi:A\to\mathrm{End}(M)^v$ is a left H-module algebra map, if $\triangleright$ is the A-action obtained from φ and φ' is the map obtained from this A, H-module structure on M, we have (for all $a\in A$ and $m\in M$)

$$\begin{aligned}\varphi'(a)(m) &= \sum (p^1 \cdot a) \triangleright (p^2 \cdot m)\\ &= \sum q^1 \cdot \varphi(p^1 \cdot a)(S(q^2)p^2 \cdot m)\\ &= \sum q^1 \cdot ((p^1 \triangleright_v \varphi(a))(S(q^2)p^2 \cdot m))\end{aligned}$$

$$\begin{aligned}(4.3) &= \sum q^1 \cdot (p_1^1 \cdot \varphi(a)(S(p_2^1)S(q^2)p^2 \cdot m))\\ &= \sum q^1 p_1^1 \cdot \varphi(a)(S(S^{-1}(p^2)q^2 p_2^1) \cdot m)\end{aligned}$$

$$(2.19) = \varphi(a)(m),$$

and the proof is complete. □

By taking in the Theorem $A = \mathrm{End}(M)^v$ and $\varphi = \mathrm{id}$, we obtain the following consequence:

Corollary 4.3: If H is a quasi-Hopf algebra and M is a left H-module, then M becomes a left $\mathrm{End}(M)^v$*, H-module [i.e., a left* $\mathrm{End}(M)^v \# H$*-module], with* $\mathrm{End}(M)^v$*-action given by*

$$u \triangleright m = \sum q^1 \cdot u(S(q^2) \cdot m), \tag{4.6}$$

for all $u \in \mathrm{End}(M)^v$, $m \in M$.

We study now the behavior of the construction $\mathrm{End}(M)^v$ under twisting. Namely, let H be a quasi-Hopf algebra, $F \in H \otimes H$ a gauge transformation and M a left H-module. Then M is also a left H_F-module, with the same H-action. Denote by $v: H \to \mathrm{End}(M)$ and $v_F: H_F \to \mathrm{End}(M)$ the corresponding algebra maps, and consider the H-module algebra $\mathrm{End}(M)^v$ and the H_F-module algebra $\mathrm{End}(M)^{v_F}$; we also consider the H_F-module algebra $\mathrm{End}(M)^v_{F^{-1}}$. In view of similar results concerning invariance under twisting, one might expect to have $\mathrm{End}(M)^{v_F} \equiv \mathrm{End}(M)^v_{F^{-1}}$, but in general this is not true. Nevertheless, we will prove that they are isomorphic as left H_F-module algebras.

Actually, we will prove something more general. Let H be a quasi-Hopf algebra, $F \in H \otimes H$ a gauge transformation, B an associative algebra, $v: H \to B$ an algebra map, which will be denoted by v_F when considered as a map from H_F to B.

Proposition 4.4: The map

$$\psi: B^v_{F^{-1}} \to B^{v_F}, \quad \psi(b) = \sum v(F^1) b v(S(F^2)), \quad \forall\, b \in B,$$

is an isomorphism of left H_F*-module algebras*.

Proof: The map ψ is obviously bijective, with inverse given by $\psi^{-1}(b) = \Sigma v(G^1) b v(S(G^2))$, for all $b \in B$, where $F^{-1} = \Sigma G^1 \otimes G^2$. Then one checks by a direct computation that ψ is a morphism of left H_F-module algebras, using the formulas for Δ_F, Φ_F, α_F, β_F and for the multiplications, units and actions in B^{v_F} and $B^v_{F^{-1}}$. □

By taking $B = \mathrm{End}(M)$, we obtain the following.

Corollary 4.5: $\mathrm{End}(M)^{v_F}$ *and* $\mathrm{End}(M)^v_{F^{-1}}$ *are isomorphic as left* H_F*-module algebras*.

If H is a quasi-Hopf algebra, the left H-module algebra H^{id_H} was denoted in Ref. 6 by H_0; its multiplication is given by

$$g \star h = \sum X^1 g S(x^1 X^2) \alpha x^2 X_1^3 h S(x^3 X_2^3), \quad \forall\, g, h \in H,$$

the unit is β and the left H-action is $h \triangleright h' = \Sigma h_1 h' S(h_2)$, for all h, $h' \in H$. Then, from the above proposition, we get also the following consequence (by taking $B = H$, $v = \mathrm{id}_H$ in the proposition):

Corollary 4.6: $(H_0)_{F^{-1}} \simeq (H_F)_0$ *as left* H_F*-module algebras, with an isomorphism given by* $\psi: (H_0)_{F^{-1}} \to (H_F)_0$, $\psi(h) = \Sigma F^1 h S(F^2)$ *for all* $h \in H$, *where* $F = \Sigma F^1 \otimes F^2$ *is a gauge transformation on H*.

For completeness' sake and further use, we also treat the case of right A-modules in ${}_H\mathcal{M}$.

Let H be a quasi-bialgebra and A a left H-module algebra. If we let A^{op} be A with opposite multiplication, then it is easy to see that A^{op} becomes a left H^{cop}-module algebra, with the same unit and H-action as for A.

If H is a quasi-Hopf algebra, B an associative algebra and $v:H\to B$ an algebra map, consider v as algebra map from H^{cop} to B and denote it by v_{cop}; then we have the left H^{cop}-module algebra $B^{v_{\mathrm{cop}}}$, and by the above $(B^{v_{\mathrm{cop}}})^{\mathrm{op}}$ becomes a left H-module algebra, which will be denoted by B_v. Its multiplication, unit and H-action are

$$b\cdot b'=\sum v(x^3)b'v(S^{-1}(\alpha X^3x^2)X^2x_2^1)bv(S^{-1}(X^1x_1^1)),\quad \forall\, b,b'\in B, \tag{4.7}$$

$$1_{B_v}=v(S^{-1}(\beta)), \tag{4.8}$$

$$h\to b=\sum v(h_2)bv(S^{-1}(h_1)),\quad \forall\, h\in H,\ b\in B. \tag{4.9}$$

Consequently, if M is a left H-module and $v:H\to\mathrm{End}(M)$ is the algebra map as before, we can consider the left H-module algebra $\mathrm{End}(M)_v$, whose structure is

$$(u\cdot u')(m)=\sum x^3\cdot u'(S^{-1}(\alpha X^3x^2)X^2x_2^1\cdot u(S^{-1}(X^1x_1^1)\cdot m)), \tag{4.10}$$

$$1_{\mathrm{End}(M)_v}(m)=S^{-1}(\beta)\cdot m, \tag{4.11}$$

$$(h\to u)(m)=\sum h_2\cdot u(S^{-1}(h_1)\cdot m), \tag{4.12}$$

for all $u,\ u'\in\mathrm{End}(M)_v$, $m\in M$, $h\in H$.

Now, if H is a quasi-bialgebra and A is a left H-module algebra, we can define a right A, H-module M as being a right A-module in ${}_H\mathcal{M}$. That is, M must be a left H-module, together with a right A-action $M\otimes A\to M$, $m\otimes a\mapsto m\triangleleft a$, with $m\triangleleft 1=m$ for all $m\in M$, such that

$$(m\triangleleft a)\triangleleft b=\sum (X^1\cdot m)\triangleleft[(X^2\cdot a)(X^3\cdot b)], \tag{4.13}$$

$$h\cdot(m\triangleleft a)=\sum (h_1\cdot m)\triangleleft(h_2\cdot a), \tag{4.14}$$

for all $h\in H$, $m\in M$, $ab\in A$.

It is easy to see that M being a right A, H-module is equivalent to M being a left A^{op}, H^{cop}-module (i.e., a left $A^{\mathrm{op}}\#H^{\mathrm{cop}}$-module). Then, if H is moreover a quasi-Hopf algebra and using also the fact that the elements p_R and q_R for H^{cop} may be expressed as $p_R^{\mathrm{cop}}=p_L^{21}$ and $q_R^{\mathrm{cop}}=q_L^{21}$, where p_L and q_L are the ones for H, by applying the theorem for A^{op}, H^{cop}, M, $\mathrm{End}(M)^{v_{\mathrm{cop}}}$, we obtain the following result.

Proposition 4.7: Let H be a quasi-Hopf algebra, A a left H-module algebra and M a left H-module. Then setting a structure of a right A, H-module on M is equivalent to giving a morphism of left H-module algebras $\eta:A\to End(M)_v$. The correspondence is given as follows: if M is a right A, H-module (with A-action denoted by $m\otimes a\mapsto m\triangleleft a$) then the map $\eta:A\to End(M)_v$ is given by

$$\eta(a)(m)=\sum(\tilde{p}^1\cdot m)\triangleleft(\tilde{p}^2\cdot a),\quad \forall\, a\in A,\ m\in M, \tag{4.15}$$

where $p_L=\Sigma\tilde{p}^1\otimes\tilde{p}^2=\Sigma X^2S^{-1}(X^1\beta)\otimes X^3$. Conversely, if $\eta:A\to End(M)_v$ is a morphism of left H-module algebras, then M becomes a right A,H-module, with A-action given by

$$m\triangleleft a=\sum\tilde{q}^2\cdot\eta(a)(S^{-1}(\tilde{q}^1)\cdot m),\quad \forall\, a\in A,\ m\in M, \tag{4.16}$$

where $q_L=\Sigma\tilde{q}^1\otimes\tilde{q}^2=\Sigma S(x^1)\alpha x^2\otimes x^3$, *and the H-action being the original H-module structure of* M.

As we have seen, the construction of $\mathrm{End}(M)_v$ was obtained from the one of $\mathrm{End}(M)^v$ by taking opposites and co-opposites. However, there is also another relation between the two constructions. Namely, if M is a left H-module, it is well known that on the linear dual of M we can introduce two left H-module structures, denoted by M^* and ${}^*M$, with H-actions $(h\cdot m^*)(m)=m^*(S(h)\cdot m)$, for all $h\in H$, $m\in M$, $m^*\in M^*$, respectively, $(h\cdot {}^*m)(m)={}^*m(S^{-1}(h)\cdot m)$ for all $h\in H$, $m\in M$, ${}^*m\in {}^*M$ [the corresponding algebra maps $H\to\mathrm{End}(M^*)$ and $H\to\mathrm{End}({}^*M)$ are denoted by v^*, respectively, ${}^*v$].

If $u:M\to M$ is a linear map, we denote by u^* its transpose given by $u^*(\xi)=\xi\circ u$ for all $\xi\in M^*$.

We have then the following result, which generalizes a part of Proposition 4.7 in Ref. 8.

Proposition 4.8: Let H be a quasi-Hopf algebra and M a left H-module. Then the map $u\mapsto u^*$ *gives H-module algebra morphisms* $End(M)^v\to End(M^*)_{v^*}$ *and* $End(M)_v\to End({}^*M)^{{}^*v}$, *which are isomorphisms if M is finite dimensional.*

Proof: Follows by a direct computation, using the formulas for the structures of the H-module algebras $\mathrm{End}(M)_v$, $\mathrm{End}(M^*)_{v^*}$, etc. □

Let again H be a quasi-bialgebra and A a left H-module algebra. We introduce now the concept of an A, H-bimodule, as being an A-bimodule in ${}_H\mathcal{M}$. That is, M must be a left H-module which is a left and a right A, H-module (with A-actions denoted by $\triangleright$ and $\triangleleft$) and such that

$$(a\triangleright m)\triangleleft b=\sum (X^1\cdot a)\triangleright[(X^2\cdot m)\triangleleft(X^3\cdot b)],\quad \forall\, a,b\in A,\ m\in M. \tag{4.17}$$

Recall now from Ref. 18 the following concept. Let $\mathcal{C}$ be a class of (not necessarily associative) algebras, $A\in\mathcal{C}$ and M a linear space with two linear actions $a\otimes m\mapsto a\triangleright m$ and $m\otimes a\mapsto m\triangleleft a$ of A on M. Then on the direct sum $A\oplus M$ one can introduce an algebra structure (called the *semidirect sum or split null extension*) by defining a multiplication in $A\oplus M$ by

$$(a+m)(a'+m')=aa'+(m\triangleleft a'+a\triangleright m'), \tag{4.18}$$

for all a, $a'\in A$ and m, $m'\in M$. Then, if $A\oplus M$ with this algebra structure is in $\mathcal{C}$, we say that M is an A-bimodule with respect to $\mathcal{C}$. If $\mathcal{C}$ is the class of all associative algebras or of all Lie algebras, we obtain the usual concepts of bimodule for these types of algebras. We have then the following result.

Proposition 4.9: Let H be a quasi-bialgebra, A a left H-module algebra and M a k-linear space. Then M is an A-bimodule with respect to the class of left H-module algebras (that is, $A\oplus M$ *is a left H-module algebra) if and only if M is an A, H-bimodule.*

Proof: If M is an A, H-bimodule, one can prove by a direct computation that $A\oplus M$ becomes a left H-module algebra. Conversely, if $A\oplus M$ is a left H-module algebra, then first M becomes a left H-module with structure induced from the one of $A\oplus M$. Then, if the unit of $A\oplus M$ is an element of the form a_0+m_0, writing down the unit condition we obtain first that a_0 should be 1_A, then that $1_A\triangleright m=m\triangleleft 1_A=m$ for all $m\in M$ and finally that $m_0=0$. Similarly, writing down the conditions for $A\oplus M$ to be a left H-module algebra, by taking properly particular values of the elements involved we obtain finally the conditions expressing the fact that M is an A, H-bimodule. □

V. THE FINITE DIMENSIONAL CASE

Let H be a quasi-Hopf algebra, A a left H-module algebra and M a *finite dimensional* left H-module. Then, by using the identification $\mathrm{End}(M)\simeq M\otimes M^*$, Albuquerque and Majid introduced in Ref. 1 a left H-module algebra structure on $\mathrm{End}(M)$, and, if M is also a left A, H-module, a morphism of left H-module algebras $A\to\mathrm{End}(M)$. Our aim now is to prove that they actually coincide with $\mathrm{End}(M)^v$ and $\varphi:A\to\mathrm{End}(M)^v$, respectively (notation as in the preceding section).

Let us recall some well-known facts, cf. Refs. 12 and 14. If H is a quasi-Hopf algebra and M is a left H-module, we consider the two left H-modules M^* (the left dual) and ${}^*M$ (the right dual) as before. If M is moreover finite dimensional and we fix $\{e_1,\dots,e_n\}$ a basis in M with $\{e^1,\dots,e^n\}$ its dual basis in M^*, then we have the k-linear maps,

$$ev_M: M^* \otimes M \to k,\quad coev_M: k \to M \otimes M^*, \tag{5.1}$$

$$ev_M(e^i \otimes e_j) = e^i(\alpha \cdot e_j),\quad coev_M(1) = \sum_{i=1}^{n} \beta \cdot e_i \otimes e^i, \tag{5.2}$$

$$ev'_M: M \otimes {}^*M \to k,\quad coev'_M: k \to {}^*M \otimes M, \tag{5.3}$$

$$ev'_M(e_i \otimes e^j) = e^j(S^{-1}(\alpha) \cdot e_i),\quad coev'_M(1) = \sum_{i=1}^{n} e^i \otimes S^{-1}(\beta) \cdot e_i \tag{5.4}$$

(the evaluation and coevaluation maps), which are H-linear and make M a *rigid* object in ${}_H\mathcal{M}$.

With this notation, let us recall from Ref. 1 that $M \otimes M^*$ becomes a left H-module algebra, as follows: the left H-module structure is the tensor product of M and M^*, and the multiplication is given by the formula

$$(\mathrm{id}_M \otimes (ev_M \otimes \mathrm{id}_{M^*})) \circ (\mathrm{id}_M \otimes a^{-1}_{M^*,M,M^*}) \circ a_{M,M^*,M\otimes M^*} \tag{5.5}$$

[as a map $(M \otimes M^*) \otimes (M \otimes M^*) \to M \otimes M^*$]. On the other hand, the map

$$\lambda: \mathrm{End}(M) \to M \otimes M^*,\quad \lambda(u) = \sum_{i=1}^{n} u(e_i) \otimes e^i,\quad \forall\, u \in \mathrm{End}(M)$$

is a linear isomorphism, with inverse

$$\lambda^{-1}: M \otimes M^* \to \mathrm{End}(M),\quad \lambda^{-1}(m \otimes \xi)(m') = \xi(m')m,\quad \forall\, m,m' \in M,\ \xi \in M^*,$$

so we can transfer the H-module algebra structure of $M \otimes M^*$ to $\mathrm{End}(M)$ via λ; let us denote by $\mathrm{end}(M)$ this H-module algebra structure on $\mathrm{End}(M)$ (this is the one appearing, with different notation, in Ref. 1).

Proposition 5.1: With notation as above, $\mathrm{end}(M)$ *and* $\mathrm{End}(M)^v$ *coincide as left H-module algebras.*

Proof: The fact that $\mathrm{end}(M) = \mathrm{End}(M)^v$ as left H-modules follows from the fact, proved in Ref. 7, that the map λ given above, considered as a map $\lambda: \mathrm{End}(M)^v \to M \otimes M^*$, is H-linear. So, we only have to prove that the multiplications of $\mathrm{end}(M)$ and $\mathrm{End}(M)^v$ coincide. Let us compute the multiplication in $\mathrm{end}(M)$. By using the identification $\mathrm{end}(M) \simeq M \otimes M^*$ via λ and by considering the multiplication as a map $\mathrm{end}(M) \otimes \mathrm{end}(M) \to M \otimes M^*$, the sequence of compositions in formula (5.5) looks as follows [for $u\ u' \in \mathrm{end}(M)$]:

$$\begin{aligned}
u \otimes u' &\mapsto \sum (u(e_i) \otimes e^i) \otimes (u'(e_j) \otimes e^j) \\
&\mapsto \sum X^1 \cdot u(e_i) \otimes (X^2 \cdot e^i \otimes (X^3_1 \cdot u'(e_j) \otimes X^3_2 \cdot e^j)) \\
&\mapsto \sum X^1 \cdot u(e_i) \otimes ((x^1X^2 \cdot e^i \otimes x^2X^3_1 \cdot u'(e_j)) \otimes x^3X^3_2 \cdot e^j) \\
&\mapsto \sum (x^1X^2 \cdot e^i)(\alpha x^2X^3_1 \cdot u'(e_j))X^1 \cdot u(e_i) \otimes x^3X^3_2 \cdot e^j \\
&= \sum e^i(S(x^1X^2)\alpha x^2X^3_1 \cdot u'(e_j))X^1 \cdot u(e_i) \otimes x^3X^3_2 \cdot e^j
\end{aligned}$$

$$= \sum X^1 \cdot u(S(x^1X^2)\alpha x^2X_1^3 \cdot u'(e_j)) \otimes x^3X_2^3 \cdot e^j,$$

so, if $m \in M$, the multiplication of end(M) is

$$\begin{aligned}(u \cdot u')(m) &= \sum (x^3X_2^3 \cdot e^j)(m)X^1 \cdot u(S(x^1X^2)\alpha x^2X_1^3 \cdot u'(e_j)) \\ &= \sum e^j(S(x^3X_2^3) \cdot m)X^1 \cdot u(S(x^1X^2)\alpha x^2X_1^3 \cdot u'(e_j)) \\ &= \sum X^1 \cdot u(S(x^1X^2)\alpha x^2X_1^3 \cdot u'(S(x^3X_2^3) \cdot m)),\end{aligned}$$

and one can see that this is exactly the multiplication of $\mathrm{End}(M)^v$. Moreover, the unit of $\mathrm{End}(M)^v$ coincides with $coev_M(1)$ after the identification $\mathrm{End}(M)^v \equiv M \otimes M^*$ via λ. □

Suppose now that M is not only a left H-module, but also a left A, H-module, where A is a left H-module algebra. Then Albuquerque and Majid constructed in Ref. 1 a map $\rho: A \to \mathrm{end}(M)$, which is a morphism of left H-module algebras, and which is given as follows:

$$\rho = \lambda^{-1} \circ (\triangleright \otimes \mathrm{id}_{M^*}) \circ a^{-1}_{A,M,M^*} \circ (\mathrm{id} \otimes coev_M). \tag{5.6}$$

Proposition 5.2: The left H-module algebra maps $\varphi: A \to \mathrm{End}(M)^v$ and $\rho: A \to \mathrm{end}(M)$ *coincide*.

Proof: Let us describe the map ρ explicitly. For $a \in A$, we have

$$\begin{aligned}\rho(a) &= \lambda^{-1} \circ (\triangleright \otimes \mathrm{id}_{M^*}) \circ a^{-1}_{A,M,M^*}\Big(a \otimes \Big(\sum \beta \cdot e_i \otimes e^i\Big)\Big) \\ &= \sum \lambda^{-1} \circ (\triangleright \otimes \mathrm{id}_{M^*})((x^1 \cdot a \otimes x^2\beta \cdot e_i) \otimes x^3 \cdot e^i) \\ &= \sum \lambda^{-1}((x^1 \cdot a) \triangleright (x^2\beta \cdot e_i) \otimes x^3 \cdot e^i),\end{aligned}$$

so, for $m \in M$, we obtain

$$\begin{aligned}\rho(a)(m) &= \sum (x^3 \cdot e^i)(m)(x^1 \cdot a) \triangleright (x^2\beta \cdot e_i) \\ &= \sum e^i(S(x^3) \cdot m)(x^1 \cdot a) \triangleright (x^2\beta \cdot e_i) \\ &= \sum (x^1 \cdot a) \triangleright (x^2\beta S(x^3) \cdot m) = \sum (p^1 \cdot a) \triangleright (p^2 \cdot m),\end{aligned}$$

and this is exactly the formula for $\varphi(a)(m)$, hence we have $\rho = \varphi$. □

Moreover, Albuquerque and Majid proved that if H is a quasi-Hopf algebra and M is a finite dimensional left H-module, then we have an action of end(M) on M, which, using the identification $\mathrm{end}(M) \simeq M \otimes M^*$ via λ, is given by the map

$$(\mathrm{id}_M \otimes ev_M) \circ a_{M,M^*,M}: (M \otimes M^*) \otimes M \to M. \tag{5.7}$$

Then, using the formulas for λ, ev_M and $a_{M,M^*,M}$, one can verify that this action coincides with the one given by the formula (4.6).

Suppose again that H is a quasi-Hopf algebra and M is a finite dimensional left H-module. Then, similarly to the definition of end(M), we can define another left H-module algebra structure on $\mathrm{End}(M)$, by first introducing one on $^*M \otimes M$ by the formula

$$((\mathrm{id}_{^*M} \otimes ev'_M) \otimes \mathrm{id}_M) \circ (a_{^*M,M,^*M} \otimes \mathrm{id}_M) \circ a^{-1}_{^*M \otimes M,^*M,M}$$

for the multiplication and $coev'_M(1)$ for the unit, and then transfering it to $\mathrm{End}(M)$ via the canonical linear isomorphism $\mathrm{End}(M) \simeq {}^*M \otimes M$. Then a similar computation yields the following result.

Proposition 5.3: The H*-module algebra structure induced on* $\mathrm{End}(M)$ *by the one of* $^*M \otimes M$ *coincides with* $\mathrm{End}(M)_v$.

We give now an application of the identification $\mathrm{End}(M)^v \equiv \mathrm{end}(M)$. Let us first recall from Ref. 15 that a (left) Yetter–Drinfeld module over H is a left H-module M, together with a left H-coaction on M and some compatibility conditions between the two structures, ensuring that if we take the category of Yetter–Drinfeld modules, it is just the center of the monoidal category of left H-modules (we refer to Ref. 15 for detail).

Suppose now that H is a quasi-Hopf algebra and M is a finite dimensional Yetter–Drinfeld module. The following result generalizes the corresponding one for Hopf algebras proved in Ref. 8.

Proposition 5.4: *End*$(M)^v$ *and End*$(M)_v$ *are algebras in the category of Yetter–Drinfeld modules over* H.

Proof: We give the proof only for $\mathrm{End}(M)^v$, it is similar for $\mathrm{End}(M)_v$. It was proved in Ref. 4 that M^*, the left dual of M, becomes also a Yetter–Drinfeld module, so $M \otimes M^*$ is a Yetter–Drinfeld module too; by the identification $\mathrm{End}(M)^v \equiv M \otimes M^*$ via λ we obtain that $\mathrm{End}(M)^v$ is also a Yetter–Drinfeld module. Since we already know that $\mathrm{End}(M)^v$ is an algebra in ${}_H\mathcal{M}$, the only thing left to prove would be that the multiplication and unit of $\mathrm{End}(M)^v$ intertwine the corresponding H-coaction on $\mathrm{End}(M)^v$; a direct proof of these facts would be quite technical and difficult (even for the unit). However, we can give an immediate proof using the identification $\mathrm{End}(M)^v \equiv \mathrm{end}(M)$. Namely, it was proved in Ref. 4 that ev_M and $coev_M$ are morphisms not only in ${}_H\mathcal{M}$, but also in the Yetter–Drinfeld category, so the multiplication (5.5) of $\mathrm{end}(M)$ is a morphism in the Yetter–Drinfeld category, and similarly for the unit of $\mathrm{end}(M)$, which is exactly $coev_M$, and we are done. Alternatively, we can obtain the result as a particular case of general results on braided tensor categories in Ref. 20. □

VI. SOME EXAMPLES OF ENDOMORPHISM QUASIALGEBRAS: HEISENBERG DOUBLES

We start this section by giving an example taken from Ref. 3, which will turn out to be of the type $\mathrm{End}(M)^v$. If H is a finite dimensional quasi-Hopf algebra, in Ref. 3 was constructed the so-called *quasi-smash product* $H\overline{\#}H^*$, which is a left H-module algebra structure built on $H \otimes H^*$, with multiplication, unit and H-action given, for all $h, h' \in H$ and $\xi, \xi' \in H^*$, by

$$(h\overline{\#}\xi)(h'\overline{\#}\xi') = \sum hh'_1x^1\overline{\#}(\xi \leftharpoonup h'_2x^2)(\xi' \leftharpoonup x^3), \tag{6.1}$$

$$1_{H\overline{\#}H^*} = 1_H\overline{\#}\varepsilon, \tag{6.2}$$

$$h \cdot (h'\overline{\#}\xi) = h'\overline{\#}h \rightharpoonup \xi, \tag{6.3}$$

where $\rightharpoonup$ and $\leftharpoonup$ are the left and right regular actions of H on H^* given by

$$(h \rightharpoonup \xi)(h') = \xi(h'h), \quad (\xi \leftharpoonup h)(h') = \xi(hh'). \tag{6.4}$$

Then, in Ref. 3 was constructed a linear isomorphism,

$$\mu: H\overline{\#}H^* \simeq \mathrm{End}(H), \quad \mu(h\overline{\#}\xi)(h') = \sum \xi(h'_2\tilde{p}^2)hh'_1\tilde{p}^1, \tag{6.5}$$

for all $h, h' \in H$ and $\xi \in H^*$, where $p_L = \Sigma\tilde{p}^1 \otimes \tilde{p}^2 = \Sigma X^2S^{-1}(X^1\beta) \otimes X^3$, with inverse

$$\mu^{-1}: \mathrm{End}(H) \to H\overline{\#}H^*, \quad \mu^{-1}(u) = \sum u(\tilde{q}^2(e_i)_2)S^{-1}(\tilde{q}^1(e_i)_1)\overline{\#}e^i, \tag{6.6}$$

for all $u \in \mathrm{End}(H)$, where $\{e_i\}$ and $\{e^i\}$ are dual bases in H and H^*, and $q_L = \Sigma\tilde{q}^1 \otimes \tilde{q}^2 = \Sigma S(x^1)\alpha x^2 \otimes x^3$. Then, the H-module algebra structure of $H\overline{\#}H^*$ was transfered to $\mathrm{End}(H)$ via μ, where it looks as follows (the multiplication, unit and H-action):

$$(u \underline{\circ} u')(h) = \sum u(u'(hx^3X_2^3)S^{-1}(S(x^1X^2)\alpha x^2X_1^3))S^{-1}(X^1), \tag{6.7}$$

$$1_{\mathrm{End}(H)} = S^{-1}(\beta) \rightharpoonup \mathrm{id}_H, \quad (h \cdot u)(h') = u(h'h_2)S^{-1}(h_1), \tag{6.8}$$

for all $u, u' \in \mathrm{End}(H)$ and $h, h' \in H$. Then one can easily check that this H-module algebra structure on $\mathrm{End}(H)$ is exactly $\mathrm{End}(M)^v$, where M is H regarded as a left H-module with action $h \cdot m = mS^{-1}(h)$ for all $m, h \in H$. The quasismash product $H\overline{\#}H^*$ was called the Heisenberg double of H (its multiplication generalizes the one in the usual Heisenberg double of a Hopf algebra), cf. Ref. 3. For reasons to be discussed below, we call it the *first* Heisenberg double of H and denote it by $\mathcal{H}_1(H)$.

To motivate this terminology, we discuss the case of the Heisenberg double $\mathcal{H}(H)$ of a finite dimensional Hopf algebra H. It is built on $H \otimes H^*$ and has the following tensor-categorical properties: it is a left $D(H)$-module algebra and a right $D(H)^{\mathrm{cop}}$-module algebra [and hence a $D(H)$, $D(H)^{\mathrm{cop}}$-bimodule algebra], where $D(H)$ is the Drinfeld double of H and the actions of $D(H)$ on $\mathcal{H}(H)$ are the left and right regular actions if we regard $\mathcal{H}(H) \equiv D(H)^*$ as linear spaces, see Refs. 13 and 17 for all these. In particular, $\mathcal{H}(H)$ is a left H-module algebra [with action $h \cdot (h' \# \xi) = h' \# h \rightharpoonup \xi$] and a right H^{cop}-module algebra.

Now, if one tries to define a quasi-Hopf analogue of the Heisenberg double, one should obtain the same tensor-categorical properties as in the Hopf case. But since the three tensor-categorical properties of the Heisenberg double normally cannot be satisfied simultaneously in the quasi-Hopf case, it follows that one might be looking for (at least) *three* Heisenberg doubles of a finite dimensional quasi-Hopf algebra. The first one then should be $\mathcal{H}_1(H) = H\overline{\#}H^*$ defined in Ref. 3, which is a left H-module algebra, and a construction for the third was proposed in Ref. 17, providing a $D(H)$, $D(H)^{\mathrm{cop}}$-bimodule algebra. Now we propose a definition for the second one, which will be a right H^{cop}-module algebra and will be realized also as an endomorphism quasialgebra.

Again we start with a general construction. If H is a quasi-bialgebra and A is a left H-module algebra with action $h \otimes a \mapsto h \cdot a$, then one can prove that A^{op} becomes a right $H^{\mathrm{op\ cop}}$-module algebra, with action $a \cdot h = h \cdot a$. Then we have the following result.

Proposition 6.1: Let H be a quasi-Hopf algebra, B an associative algebra and $v: H \to B$ an algebra map. Define a new multiplication on B by

$$b \odot b' = \sum v(S^{-1}(x_2^3X^3))bv(x_1^3X^2S^{-1}(x^2X^1\beta))b'v(x^1), \quad \forall\, b, b' \in B, \tag{6.9}$$

and denote by ${}^vB$ this structure. Then ${}^vB$ becomes a right H^{cop}-module algebra, with unit $v(S^{-1}(\alpha))$ and right H-action on ${}^vB$ given by

$$b_v \triangleleft h = \sum v(S^{-1}(h_2))bv(h_1), \tag{6.10}$$

for all $h \in H$ and $b \in {}^vB$, where $\Delta(h) = \Sigma h_1 \otimes h_2$ is the comultiplication of H.

Proof: Since v is an algebra map, $v: H^{\mathrm{op}} \to B^{\mathrm{op}}$ is also an algebra map, which will be denoted by v^{op}. Then we can consider $(B^{\mathrm{op}})^{v^{\mathrm{op}}}$, which is a left H^{op}-module algebra, hence, by the above remark, we get that $((B^{\mathrm{op}})^{v^{\mathrm{op}}})^{\mathrm{op}}$ becomes a right $(H^{\mathrm{op}})^{\mathrm{op\ cop}} = H^{\mathrm{cop}}$-module algebra, and one can easily see that ${}^vB$ is exactly this $((B^{\mathrm{op}})^{v^{\mathrm{op}}})^{\mathrm{op}}$. □

In particular we may take $B = H$, $v = \mathrm{id}_H$, and obtain a right H^{cop}-module algebra structure on H, or we may take M to be a left H-module and the map $v: H \to \mathrm{End}(M)$ as before, and we get a right H^{cop}-module algebra ${}^v\mathrm{End}(M)$.

We are now interested in the case when $M = H$ with the left regular action on itself, so we have the algebra map $v: H \to \mathrm{End}(H)$, $v(h)(h') = hh'$, and we can consider the right H^{cop}-module algebra ${}^v\mathrm{End}(H)$. Let us record that the right H-action on ${}^v\mathrm{End}(H)$ is given by $(u_v \triangleleft h)(h') = \Sigma S^{-1}(h_2)u(h_1h')$, for all $h, h' \in H$ and $u \in {}^v\mathrm{End}(H)$, where $\Delta(h) = \Sigma h_1 \otimes h_2$ is the comultiplication

of H. We propose this ${}^v\mathrm{End}(H)$ as the *second* Heisenberg double of H and denote it by $\mathcal{H}_2(H)$. This proposal will be supported by the next results.

Suppose now that H is moreover finite dimensional. Then, besides the isomorphism μ introduced in Ref. 3, we can construct another linear isomorphism between $H\otimes H^*$ and $\mathrm{End}(H)$, namely,

$$\nu: H\otimes H^* \to \mathrm{End}(H),\quad \nu(h\otimes\xi)(h') = \sum \xi(X^2 h'_2 \tilde{p}^2) S^{-1}(X^3) h X^1 h'_1 \tilde{p}^1,$$

for all $h,h'\in H$ and $\xi\in H^*$; one can prove as in Ref. 3 that its inverse is given by

$$\nu^{-1}: \mathrm{End}(H) \to H\otimes H^*,\quad \nu^{-1}(u) = \sum S^{-1}(x^3) u(\tilde{q}^2 (e_i)_2) S^{-1}(\tilde{q}^1 (e_i)_1) x^1 \otimes e^i \leftharpoonup x^2,$$

for all $u\in\mathrm{End}(H)$.

Now, we consider on $\mathrm{End}(H)$ the right H^{cop}-module algebra structure ${}^v\mathrm{End}(H)$, and we can transfer it to $H\otimes H^*$ via the isomorphisms μ or ν, thus obtaining two (isomorphic) right H^{cop}-module algebra structures on $H\otimes H^*$.

Proposition 6.2: If we denote by $\leftharpoonup$, *respectively* $\leftharpoondown$, *the right H-module structures of* $H\otimes H^*$ *obtained by transfer via* μ, *respectively* ν, *then* $\leftharpoonup$ *and* $\leftharpoondown$ *look as follows*:

$$(h'\otimes\xi)\leftharpoonup h = \sum S^{-1}(h_2) h' h_{(1,1)} \otimes \xi \leftharpoonup h_{(1,2)}, \tag{6.11}$$

$$(h'\otimes\xi)\leftharpoondown h = \sum S^{-1}(h_{(2,2)}) h' h_1 \otimes \xi \leftharpoonup h_{(2,1)}, \tag{6.12}$$

for all $h,h'\in H$ *and* $\xi\in H^*$, *where* $\Delta(h)=\Sigma h_1\otimes h_2$ *is the comultiplication of H*.

Proof: We give the proof only for $\leftharpoonup$, the one for $\leftharpoondown$ is similar. We compute $(h'\otimes\xi)\leftharpoonup h \in H\otimes H^*$ by applying it to an element $g\in H$ on the second component. We have

$$\begin{aligned}((h'\otimes\xi)\leftharpoonup h)(g) &= \mu^{-1}(\mu(h'\otimes\xi)_v \triangleleft h)(g)\\ &= \sum (\mu(h'\otimes\xi)_v \triangleleft h)(\tilde{q}^2 g_2) S^{-1}(\tilde{q}^1 g_1)\\ &= \sum (v(S^{-1}(h_2))\mu(h'\otimes\xi) v(h_1))(\tilde{q}^2 g_2) S^{-1}(\tilde{q}^1 g_1)\\ &= \sum S^{-1}(h_2)\mu(h'\otimes\xi)(h_1\tilde{q}^2 g_2) S^{-1}(\tilde{q}^1 g_1)\\ &= \sum S^{-1}(h_2)\xi(h_{(1,2)}\tilde{q}^2_2 g_{(2,2)}\tilde{p}^2) h' h_{(1,1)}\tilde{q}^2_1 g_{(2,1)}\tilde{p}^1 S^{-1}(g_1) S^{-1}(\tilde{q}^1)\\ (2.22) &= \sum \xi(h_{(1,2)}\tilde{q}^2_2\tilde{p}^2 g) S^{-1}(h_2) h' h_{(1,1)}\tilde{q}^2_1\tilde{p}^1 S^{-1}(\tilde{q}^1)\\ (2.20) &= \sum \xi(h_{(1,2)} g) S^{-1}(h_2) h' h_{(1,1)} = \sum (S^{-1}(h_2) h' h_{(1,1)} \otimes \xi \leftharpoonup h_{(1,2)})(g),\end{aligned}$$

and the proof is finished. □

Now, let H be a finite dimensional quasi-Hopf algebra. We recall from Refs. 10 and 11 the two realizations of the quantum double of H built on $H^*\otimes H$, hereafter denoted by $D_1(H)$ and $D_2(H)$, whose multiplications are, respectively, given, for all $\xi,\xi'\in H^*$ and $h,h'\in H$, by

$$(\xi\otimes h)(\xi'\otimes h') = \sum (\Omega^1 \rightharpoonup \xi \leftharpoonup \Omega^5)(\Omega^2 h_{(1,1)} \rightharpoonup \xi' \leftharpoonup S^{-1}(h_2)\Omega^4) \otimes \Omega^3 h_{(1,2)} h',$$

$$(\xi\otimes h)(\xi'\otimes h') = \sum (\omega^1 \rightharpoondown \xi \leftharpoondown \omega^5)(\omega^2 h_1 \rightharpoondown \xi' \leftharpoondown S^{-1}(h_{(2,2)})\omega^4) \otimes \omega^3 h_{(2,1)} h',$$

where $\Omega=\Sigma\Omega^1\otimes\cdots\otimes\Omega^5$, $\omega=\Sigma\omega^1\otimes\cdots\otimes\omega^5\in H^{\otimes 5}$ are given by

$$\Omega = \sum X^1_{(1,1)} x^1 y^1 \otimes X^1_{(1,2)} x^2 y^2_1 \otimes X^1_2 x^3 y^2_2 \otimes S^{-1}(f^1 X^2 y^3) \otimes S^{-1}(f^2 X^3), \tag{6.13}$$

$$\omega = \sum x^1 \otimes x^2 Y^1 \otimes x_1^3 X^1 Y_1^2 \otimes S^{-1}(f^1 x_{(2,1)}^3 X^2 Y_2^2) \otimes S^{-1}(f^2 x_{(2,2)}^3 X^3 Y^3), \tag{6.14}$$

and where $f=\Sigma f^1 \otimes f^2$ is the twist defined in (2.15).

Using these formulas, one can prove that the comultiplications of $D_1(H)^*$ and $D_2(H)^*$ (both identified with $H \otimes H^*$ as linear spaces), dual to the above multiplications, are given by

$$\Delta_{D_1(H)^*}(h \otimes \xi) = \sum (\Omega^5 h_1 \Omega^1 \otimes [e^i(\xi_1 \leftharpoonup \Omega^3)]e^j) \otimes (S^{-1}(e_j)\Omega^4 h_2 \Omega^2 e_i \otimes \xi_2), \tag{6.15}$$

$$\Delta_{D_2(H)^*}(h \otimes \xi) = \sum (\omega^5 h_1 \omega^1 \otimes e^i[(\xi_1 \leftharpoonup \omega^3)e^j]) \otimes (S^{-1}(e_j)\omega^4 h_2 \omega^2 e_i \otimes \xi_2), \tag{6.16}$$

for all $h \in H$ and $\xi \in H^*$, where $\Delta(\xi)=\Sigma \xi_1 \otimes \xi_2$ is the comultiplication of H^* and $\{e_i\}$ and $\{e^i\}$ are dual bases in H and H^*. Using these formulas, one can prove that the right regular actions of $D_1(H)$ on $D_1(H)^*$ and of $D_2(H)$ on $D_2(H)^*$, respectively, look as follows:

$$(h' \otimes \xi) \leftharpoonup (\xi' \otimes h) = \sum \xi'(\Omega^5 h_1' \Omega^1) S^{-1}(h_2) \Omega^4 h_2' \Omega^2 h_{(1,1)} \otimes \xi \leftharpoonup \Omega^3 h_{(1,2)},$$

$$(h' \otimes \xi) \leftharpoonup (\xi' \otimes h) = \sum \xi'(\omega^5 h_1' \omega^1) S^{-1}(h_{(2,2)}) \omega^4 h_2' \omega^2 h_1 \otimes \xi \leftharpoonup \omega^3 h_{(2,1)},$$

for all $h, h' \in H$ and $\xi, \xi' \in H^*$. By taking $\xi' = \varepsilon$ in these formulas, we get two right H-module structures on $H \otimes H^*$, and one can easily see that they are exactly (6.11) and (6.12).

Let us mention that, if the proposed definitions of $\mathcal{H}_1(H)$ and $\mathcal{H}_2(H)$ are natural, they should be not only left H and, respectively, right H^{cop}-module algebras, but also left $D(H)$ and, respectively, right $D(H)^{\mathrm{cop}}$-module algebras, but so far we have not been able to prove this (direct computations are very cumbersome).

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Frobenius monads and pseudomonoids

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Six equivalent definitions of Frobenius algebra in a monoidal category are provided. In a monoidal bicategory, a pseudoalgebra is Frobenius if and only if it is star autonomous. Autonomous pseudoalgebras are also Frobenius. What it means for a morphism of a bicategory to be a projective equivalence is defined; this concept is related to "strongly separable" Frobenius algebras and "weak monoidal Morita equivalence." Wreath products of Frobenius algebras are discussed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1788852]

I. INTRODUCTION

Over the last two decades, the relevance of categories to physics has become widely acknowledged in at least two particular areas: quantum group theory (QGT) [see Joyal and Street (1991), Kassel (1995), Majid (1995)] and topological quantum field theory (TQFT) [see Kock (2003) and Kerler and Volodymyr (2001)]. Quantum groups arise from the Yang–Baxter equation of statistical mechanics, while each quantum group has a monoidal (or "tensor") category of representations. A two-dimensional TQFT can be regarded as a tensor-preserving functor from a monoidal category of 2-cobordisms to the category of vector spaces. Monoidal categories can be used to construct the known three-dimensional TQFTs while some four-dimensional TQFTs can be constructed using monoidal bicategories (see Baez). Both QGT and TQFT feature categories whose morphisms come from low-dimensional topology (braids, links, tangles, surfaces, and so on). Mainly for the benefit of readers from mathematical physics, in this introduction and the next section, we will warm up to the categorical notions just mentioned and a few others we require.

Of course, the use in physics of (classical) groups and their representations goes back many score years. A lot of information about a group G is contained in its characters. Characters are group morphisms from G into the multiplicative monoid of an appropriate field k. In other words, we find a category (in this case the category of monoids) where G and k both live as objects so that it makes sense to look at morphisms between these objects.

Representations reveal even more about G than characters yet can be introduced using the same philosophy. The group G can be regarded as a category ΣG having only one object and every morphism invertible. Although this could be taken as the definition of group, it is often helpful to maintain a notational distinction between the group and the one-object category (after all, groups can be defined in alternative categorical terms as discrete closed monoidal categories). We think of ΣG as a kind of suspension of G, where the morphisms of ΣG are the elements of G. Since we have put G into the category Cat of categories, we can look at morphisms from ΣG into other categories such as the category Vect_k of vector spaces over k. These are precisely linear representations of the group G: a morphism of categories $F:\Sigma G \to \mathrm{Vect}_k$ (functor) takes the one object of ΣG to the vector space underlying the representation and the morphisms of ΣG to action by those group elements.

This paper is concerned with the identification of mathematical structure on objects of interest. The structure of particular interest is an abstraction of Frobenius algebra; we will soon recall the

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basic concept. The connection between TQFT and Frobenius algebras is pointed out in Kock (2003) and we proceed to outline how that works. Some connection between quantum groups and Frobenius algebras is already apparent from the fact that quantum groups are Hopf algebras and finite-dimensional Hopf algebras are Frobenius [Larson and Sweedler (1969)]. We intend to deepen the connection between Frobenius algebras and quantum group theory.

A k-algebra A is called *Frobenius* when it is equipped with an exact pairing

$$\sigma: A \otimes A \to k$$

satisfying the condition

$$\sigma((ab) \otimes c) = \sigma(a \otimes (bc))$$

for all elements a, b and c of A. (The exact bilinear pairing in the sense of monoidal category theory here means that A is finite dimensional as a vector space and the pairing provides an isomorphism between A and its linear dual.) In fact, σ is determined by a linear function $\varepsilon: A \to k$ via the formulas $\varepsilon(a) = \sigma(1, a)$ and $\sigma(a, b) = \varepsilon(ab)$. The group algebra kG of any finite group G is Frobenius when equipped with the form σ that has $\sigma(x, y) = 1$ if and only if $xy = 1$.

We shall recall in Sec. II how each Frobenius algebra becomes a coalgebra. However, in the case where the Frobenius algebra comes from a finite-dimensional Hopf algebra, this coalgebra is not the same as the coalgebra underlying the Hopf algebra. For one thing, a morphism of Frobenius algebras (preserving the algebra and coalgebra structure) is invertible [see Kock (2003); Sec. III D], whereas Hopf algebra morphisms between group algebras are in bijection with group morphisms.

Each commutative Frobenius algebra determines (uniquely up to isomorphism) a two-dimensional TQFT; that is, a tensor-preserving functor from the monoidal category 2-Cob of two-dimensional cobordisms to Vect_k. More precisely, the category of commutative Frobenius k-algebras is equivalent to the category of symmetric strong-monoidal functors from 2-Cob to Vect_k [see Kock (2003), Theorem 3.3.2]. Both of these categories are actually groupoids: every morphism is invertible. We already mentioned this fact for Frobenius algebras, while the monoidal category 2-Cob is *autonomous* (that is, its objects all have both left and right duals) and this already implies that every morphism between 2D TQFTs is invertible.

A category $\mathcal{V}$ is *monoidal* when it is equipped with a functor $\otimes: \mathcal{V} \times \mathcal{V} \to \mathcal{V}$ (called the *tensor product*), an object I of V (called the *tensor unit*), and three natural families of isomorphisms

$$(A \otimes B) \otimes C \cong A \otimes (B \otimes C), \quad I \otimes A \cong A \cong A \otimes I$$

in $\mathcal{V}$ (called *associativity* and *unital constraints*), such that the pentagon, involving the five ways of bracketing four objects, commutes, and the associativity constraint with $B = I$ is compatible with the unit constraints. Call $\mathcal{V}$ *braided* when it is equipped with a natural family of isomorphisms

$$c_{A,B}: A \otimes B \cong B \otimes A$$

(called the *braiding*) satisfying two conditions (one expressing $c_{A \otimes B,C}$ in terms of associativity constraints, $1_A \otimes c_{B,C}$ and $c_{C,A} \otimes 1_B$, and a similar one for $c_{A,B \otimes C}$). A braiding is a *symmetry* when $c_{B,A} \circ c_{A,B} = 1_{A \otimes B}$. A monoidal category is called *strict* when the associativity and unital constraints are identities.

Monoids can be defined in any monoidal category $\mathcal{V}$. A *monoid* in $\mathcal{V}$ is an object A equipped with a multiplication $\mu: A \otimes A \to A$ and a unit $\eta: I \to A$ satisfying unital and associativity conditions. A monoid in the category Set of sets, where the tensor product is cartesian product, is a monoid in the usual sense. If we use the coproduct (disjoint union) in Set as tensor product, every set has a unique monoid structure. A monoid in Vect_k, with the usual tensor product of vector spaces, is precisely a k-algebra; monoids in monoidal k-linear categories are also sometimes called algebras. A monoid in the category Cat of categories (where the morphisms are functors and the tensor product is a Cartesian product) is a strict monoidal category. For any category $\mathcal{A}$, the category $[\mathcal{A}, \mathcal{A}]$ of endofunctors on A becomes strict monoidal by taking composition as the

tensor product: a monoid in $[\mathcal{A},\mathcal{A}]$ is called a *monad* on $\mathcal{A}$ [see MacLane (1971) for the theory of monads and their algebras].

Frobenius structure on a monoid makes sense in any monoidal category. We recall this in Sec. II, where we assemble some facts about Frobenius monoids. Many of the facts are scattered throughout the literature. To begin with, for a concrete case that denies us the luxury of symmetry, we express the results in terms of monads on categories; but clearly the results carry over to monoids in general monoidal categories.

In a symmetric (or even braided) monoidal category we can define commutative monoids. In fact, what is shown in Kock (2003) is that 2-Cob possesses a distinguished commutative Frobenius monoid and that every commutative Frobenius monoid in every symmetric monoidal category is the image, under an essentially unique symmetric monoidal functor, of the distinguished one.

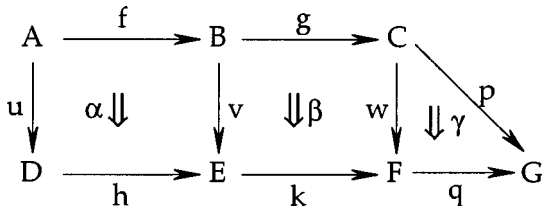
Notice from the above discussion that it is the strict monoidal categories, and not the general ones, that are genuinely examples of monoids in Cat. The reason nonstrictness arises is that Cat is a 2-category: natural transformations between the functors provide Cat with the two-dimensional structure of *2-morphisms* or *2-cells* and their compositions. Cartesian product is compatible with the 2-cells and so Cat is actually a *monoidal 2-category*.

Composition of functors is strictly associative so Cat itself is stricter than it might be in the two-dimensional setting. This leads to a weaker version of 2-category due to Bénabou (1967). A *bicategory* $\mathcal{B}$ has *objects*, and, for objects A and B, we have a category $\mathcal{B}(A,B)$ (called a *hom-category*) whose objects are called *morphisms* $f:A\to B$ of $\mathcal{B}$, whose morphisms are called *2-cells* $\theta:f\Rightarrow g:A\to B$ of $\mathcal{B}$, and whose composition is called *vertical composition* in B; there are functors

$$-\circ-:\mathcal{B}(B,C)\times\mathcal{B}(A,B)\to\mathcal{B}(A,C)$$

(called *horizontal composition*) and morphisms $1_A:A\to A$ (called *identity morphisms*). Horizontal composition is associative with units the identity morphisms: but only up to invertible 2-cells that are just like the associativity and unital constraints of a monoidal category. In fact, for each object A, the category $\mathcal{B}(A,A)$ becomes monoidal by using the horizontal composition as tensor product; this is the two-dimensional version of the fact that endomorphism sets in any category are monoids. An object A together with a monoid t, η, μ in the monoidal category $\mathcal{B}(A,A)$ is called a *monad* in $\mathcal{B}$. Each monoidal category $\mathcal{V}$ can be regarded as a bicategory $\Sigma\mathcal{V}$ with one object; the endohom of that object is $\mathcal{V}$ and the horizontal composition is the tensor product of $\mathcal{V}$.

In a bicategory, Bénabou introduced the operation of *pasting* which is applied to diagrams such as

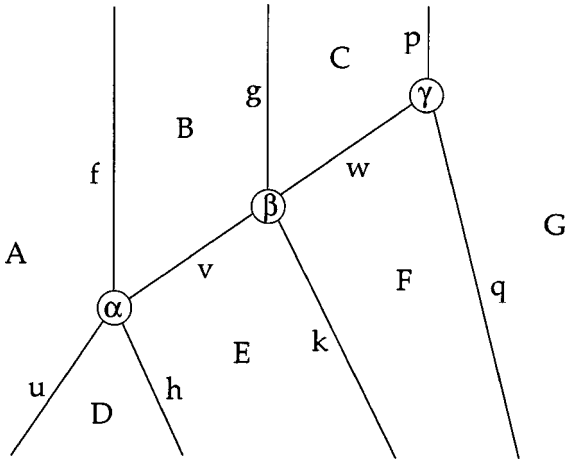


in which the left square depicts a 2-cell $\alpha:v\circ f\Rightarrow h\circ u$, the middle square depicts a 2-cell $\beta:w\circ g\Rightarrow k\circ v$ and the right triangle depicts a 2-cell $\gamma:p\Rightarrow q\circ w$. Once a bracketing is chosen for the upper path $p\circ g\circ f$ yielding a morphism $s:A\to G$ and a bracketing is chosen for the lower path $q\circ k\circ h\circ u$ yielding a morphism $t:A\to G$, there is a unique 2-cell $\sigma:s\Rightarrow t$ determined by the diagram using the compositions and constraints of the bicategory; we call σ the *pasting composite* of the diagram. In the exemplary diagram, taking $s=p\circ(g\circ f)$ and $t=q\circ(k\circ(h\circ u))$, we obtain σ as the composite

$$p\circ(g\circ f)\overset{\alpha\circ(g\circ f)}{\to}(q\circ w)\circ(g\circ f)\cong q\circ((w\circ g)\circ f)\overset{q\circ(\beta\circ f)}{\to}q\circ((k\circ v)\circ f)$$

$$\cong q\circ(k\circ(v\circ f))\overset{q\circ(k\circ\alpha)}{\to}q\circ(k\circ(h\circ u))$$

in the category $\mathcal{B}(A,G)$. For simplicity we sometimes ignore the brackets and constraints in describing such composites (that is, we act as if we were in a 2-category). String diagrams can also be used: suffice it to say here that the string diagram corresponding to our pasting diagram is as follows where the 2-cells label vertices, the morphisms label edges, and the objects label faces.



Each bicategory $\mathcal{B}$ has *duals* $\mathcal{B}^{\mathrm{op}}$, $\mathcal{B}^{\mathrm{co}}$, and $\mathcal{B}^{\mathrm{coop}}$: the first has morphisms reversed, the second has 2-cells reversed, while the third has both morphisms and 2-cells reversed.

In any bicategory B, we can define *adjoint morphisms*: we say $u:A\to B$ is right adjoint to $f:B\to A$ when there are 2-cells

$$\varepsilon:f\circ u\Rightarrow 1_A:A\to A \quad\text{and}\quad \eta:1_B\Rightarrow u\circ f:B\to B$$

(called the *counit* and *unit*) satisfying the following 2-cell equations: $(\varepsilon\circ f)(f\circ\eta)=1_f$ and $(u\circ\varepsilon)(\eta\circ u)=1_u$ (the reader might like to draw the pasting and string diagrams as an exercise). We say u is an *equivalence* when it is right adjoint to an f with invertible counit and unit (actually, in this case we do not need to have the 2-cell equations; the unit can always be rechosen so that they hold). If u is right adjoint to f, then B together with $t=u\circ f$ form a monad in B with unit η and multiplication $u\circ\varepsilon\circ f$.

For any morphism $f:X\to Y$ in the bicategory, we write $f^*:Y\to X$ for a right adjoint should there be one.

An object U of a monoidal category $\mathcal{V}$ is said to be *right dual* to an object V when the morphism U is right adjoint to V in the bicategory $\Sigma\mathcal{V}$. For example, a vector space U is a right dual in Vect_k if and only if U is finite dimensional; in this case, U is right dual to the space $\mathrm{Vect}_k(U,k)$ of linear functions from U to k. A monoidal category is called *right autonomous* when every object has a right dual; it is called *autonomous* when every object has both a left and right dual. If V is symmetric then every right dual is also a left dual.

There is a weaker kind of monoidal duality that was conceived by Barr [see Barr (1979, 1995, 1996)] based on examples in topological algebra yet the notion has received a lot of attention by computer scientists interested in Girard's "linear logic." A monoidal category $\mathcal{V}$ is said to be **-autonomous* when there is an equivalence of categories $S:\mathcal{V}\to\mathcal{V}^{\mathrm{op}}$ and a natural family of isomorphisms

$$\mathcal{V}(U \otimes V, I) \cong \mathcal{V}(V, SU).$$

Each autonomous monoidal $\mathcal{V}$ is *-autonomous with SU a right dual for U; the existence of left duals is needed for this S to be an equivalence.

If $\mathcal{B}$ and $\mathcal{D}$ are bicategories, a *lax functor* (or "morphism") $F: \mathcal{B} \to \mathcal{D}$ consists of a function between the sets of objects together with functors

$$F_{A,B}: \mathcal{B}(A,B) \to \mathcal{D}(FA, FB)$$

and 2-cells $F_{B,C}(g) \circ F_{A,B}(f) \Rightarrow F_{A,C}(g \circ f)$, natural in f and g, and $1_{FA} \Rightarrow F(1_A)$; these 2-cells satisfy three conditions very much like associativity and unital conditions for a monoid. When these structural 2-cells are all invertible the lax functor is called a *pseudofunctor* (or "homomorphism"). A *biequivalence* is a pseudofunctor F for which each $F_{A,B}$ is an equivalence of categories and, for each object D of $\mathcal{D}$, there is an object A of B and an equivalence $FA \xrightarrow{\sim} D$. Every bicategory is biequivalent to a 2-category (giving some justification for leaving out constraints when writing equations).

Between pseudofunctors there are *pseudonatural transformations*: these are a two-dimensional version of natural transformation in which the naturality equations are "broken" by asking them to hold only up to extra invertible 2-cells that satisfy some further conditions [see Kelly and Street (1974), for example]. There is a bicategory $\mathrm{Hom}(\mathcal{B}, \mathcal{D})$ whose objects are the pseudofunctors from $\mathcal{B}$ to $\mathcal{D}$, whose morphisms are the pseudonatural transformations, and whose 2-cells are called *modifications*. We shall only have need of modifications in one place in this paper (in defining "scalars") and there we shall spell out exactly what we mean.

A 2-category can be defined to be a strict bicategory: one in which the associativity and unital constraints are identities. So Cat is special among bicategories; it is strict. Cartesian product is also special among monoidal structures on bicategories; it is stricter in many ways than required of a general monoidal bicategory. A bicategory B is *monoidal* when it is equipped with a pseudofunctor $\otimes: \mathcal{B} \times \mathcal{B} \to \mathcal{B}$ and an object I together with associativity and unital constraints much like a monoidal category except that they need only be equivalences rather than isomorphisms and they need only satisfy the conditions up to further selected isomorphisms that themselves satisfy conditions. Monoidal bicategories are not all monoidally biequivalent to monoidal 2-categories but some degree of strictness can be attained. We do not need more detail than this; however, the interested reader can consult Day and Street (1997) and McCrudden (1999).

In any monoidal bicategory it is possible to define *pseudomonoids*; these are like monoids except that the associativity and unital conditions only hold up to invertible 2-cells that are called *associativity and unit constraints*; they are required to satisfy conditions that are said to express *coherence*; again, a reference is Day and Street (1997). In particular, a pseudomonoid in Cat is precisely a monoidal category. Hence a pseudomonoid is also called a "monoidal object" of the monoidal bicategory.

In Sec. III we continue this review of categorical structures highlighting enriched categories.

In Sec. IV we define what it means for a pseudomonoid in any monoidal bicategory to be Frobenius. It is an easy corollary of results of Day *et al.* (2003) that every autonomous pseudomonoid (whose unit has a right adjoint) is Frobenius. As we have mentioned, finite dimensional Hopf algebras are known to be Frobenius, yet our corollary provides a setting in which even the more general quasi-Hopf algebras of Drinfeld are Frobenius irrespective of dimension. Another example is any autonomous monoidal $\mathcal{V}$-category. In Day and Street (2004), we showed how quantum groups (and more generally "quantum groupoids") and star-autonomous monoidal categories are instances of the same mathematical structure. Although the term Frobenius was not used in Day and Street (2004), the star-autonomy defined there is precisely the higher-dimensional version of Frobenius structure.

Section V is largely inspired by the discussion of "weak monoidal Morita equivalence" in Müger (2003a, 2003b) where it is shown that monoidal categories that are equivalent in this weak sense still give rise to the same state sum invariants of closed oriented 3-manifolds [see Barrett and Westbury (1996, 1999)]. We define a notion of projective equivalence between objects in any

bicategory. In the same general setting, we define what it means for a Frobenius monad to be strongly separable and relate this to projective equivalence. Both concepts require the abstract notion of "scalar" determined by the bicategory. In the bicategory of k-linear categories for a commutative ring k, the scalars are in bijection with elements of k. Section VI says a little about Morita equivalence.

Finally, in Sec. VII, we discuss wreath products of Frobenius algebras. This is done at the level of generalized distributive laws between monads as developed in Lack and Street (2002).

II. FROBENIUS MONADS

Let $\mathbf{T}=(T,\eta,\mu)$ be a monad on a category $\mathcal{X}$. We write $\mathcal{X}^{\mathbf{T}}$ for the category of $\mathbf{T}$-algebras in the sense of Eilenberg and Moore (1965) (although those authors called monads "triples"). We write $U^{\mathbf{T}}:\mathcal{X}^{\mathbf{T}}\to\mathcal{X}$ for the forgetful functor and $F^{\mathbf{T}}:\mathcal{X}\to\mathcal{X}^{\mathbf{T}}$ for its left adjoint. Similarly, for a comonad $\mathbf{G}=(G,\varepsilon,\delta)$, we write $\mathcal{X}^{\mathbf{G}}$ for the category of $\mathbf{G}$-coalgebras, we write $V^{\mathbf{G}}:\mathcal{X}^{\mathbf{G}}\to\mathcal{X}$ for the forgetful functor, and we write $C^{\mathbf{G}}:\mathcal{X}\to\mathcal{X}^{\mathbf{G}}$ for the right adjoint of $V^{\mathbf{G}}$.

Before defining Frobenius monads and finding several equivalent definitions, we shall recall the results in Sec. 3 of Eilenberg and Moore (1965) on adjoint monads. Let $\mathbf{T}=(T,\eta,\mu)$ be a monad on a category $\mathcal{X}$ such that the endofunctor T has a right adjoint: our notation is $T\dashv G$ with counit $\sigma:TG\to 1$ and unit $\rho:1\to GT$. Eilenberg and Moore showed that:

AM1: $\mathbf{G}=(G,\varepsilon,\delta)$ is a comonad where ε and δ are the mates [in the sense of Kelly and Street (1974)] of η and μ under adjunction, with the explicit formulas being

$$\varepsilon=\sigma\circ\eta G \quad\text{and}\quad \delta=G^2\sigma\circ G^2\mu G\circ G\rho TG\circ\rho G,$$

and the comonad $\mathbf{G}$ is said to be *right adjoint* to the monad $\mathbf{T}$;

AM2: mateship under adjunction of action and coaction defines an isomorphism of categories $\mathcal{X}^{\mathbf{T}}\cong\mathcal{X}^{\mathbf{G}}$ that commutes with the forgetful functors $U^{\mathbf{G}}$ and $V^{\mathbf{G}}$ into $\mathcal{X}$;

AM3: each of the forgetful functors $U^{\mathbf{T}}$ and $V^{\mathbf{G}}$ has both left and right adjoints; and,

AM4: if $F\dashv U\dashv C$, then the comonad generated by $U\dashv C$ is right adjoint to the monad generated by $F\dashv U$.

We can add the following extra observation on adjoint monads; it is a trivial consequence of Beck's monadicity theorem [Beck (2003)].

AM5: if $F\dashv U\dashv C$ and U is conservative (that is, reflects invertibility of morphisms) then the comparison functor, into the category of Eilenberg–Moore algebras for the monad generated by $F\dashv U$, is an equivalence;

If $\mathbf{T}=(T,\eta,\mu)$ is a monad on a category $\mathcal{X}$ such that the endofunctor T has a left adjoint H, we can apply the duality explained in Street (1972) to obtain five corresponding results. In particular, there is a comonad $\mathbf{H}=(H,\varepsilon,\delta)$ for which there is an isomorphism $\mathcal{X}_{\mathbf{T}}\cong\mathcal{X}_{\mathbf{H}}$ where $\mathcal{X}_{\mathbf{T}}$ and $\mathcal{X}_{\mathbf{H}}$ are the Kleisli categories of the monad $\mathbf{T}$ and the comonad $\mathbf{H}$, respectively. Also, if a functor $F:\mathcal{X}\to\mathcal{K}$ has a left adjoint, a right adjoint, and is essentially surjective on objects, then $\mathcal{K}$ is equivalent to the Kleisli categories for the appropriately generated monad and comonad on $\mathcal{X}$.

Definition 1.1: A monad $\mathbf{T}=(T,\eta,\mu)$ is called *Frobenius* when it is equipped with a natural transformation $\varepsilon:T\to 1$ such that there exists a natural transformation $\rho:1\to T^2$ satisfying the equations

$$T\mu\circ\rho T=\mu T\circ T\rho \quad\text{and}\quad T\varepsilon\circ\rho=\eta=\varepsilon T\circ\rho.$$

Lemma 1.2: *For a Frobenius monad* $\mathbf{T}$, *put* $\delta:=T\mu\circ\rho T=\mu T\circ T\rho$. *Then*

(a) $T\mu\circ\delta T=\delta\circ\mu=\mu T\circ T\delta$,
(b) $T\varepsilon\circ\delta=1_T=\varepsilon T\circ\delta$,
(c) $\rho=\delta\circ\eta$.

Proof:

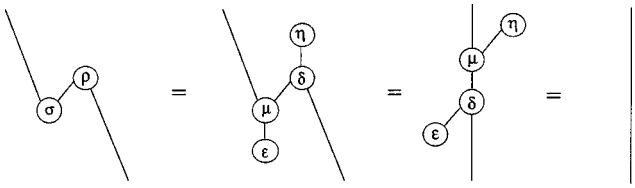
(a) $T\mu\circ\delta T = T\mu\circ T\mu T\circ\rho T^2 = T\mu\circ T^2\mu\circ\rho T^2 = T\mu\circ\rho T\circ\mu = \delta\circ\mu$
$\mu T\circ T\delta = \mu T\circ T\mu T\circ T^2\rho = \mu T\circ\mu T^2\circ T^2\rho = \mu T\circ T\rho\circ\mu = \delta\circ\mu$
(b) $T\varepsilon\circ\delta = T\varepsilon\circ\mu T\circ T\rho = \mu\circ T^2\varepsilon\circ T\rho = \mu\circ T\eta = 1_T$
$\varepsilon T\circ\delta = \varepsilon T\circ T\mu\circ\rho T = \mu\circ\varepsilon T^2\circ\rho T = \mu\circ\eta T = 1_T$
(c) $\delta\circ\eta = T\mu\circ\rho T\circ\eta = T\mu\circ T^2\eta\circ\rho = \rho.$ Q.E.D.

Remark: Condition (a) of Lemma 1.2 has occurred in the work of Carboni and Walters [see Carboni and Walters (1987) and Carboni (1991)] and of Boyer and Joyal [unfortunately Boyer and Joyal (1994) is unpublished, but see Street (1995) for some details]. The condition relates to separability of algebras and discreteness. Condition (b) expesses that ε is a counit for the comultiplication δ. Condition (c) suggests dually introducing $\sigma = \varepsilon\circ\mu$ as we shall now do.

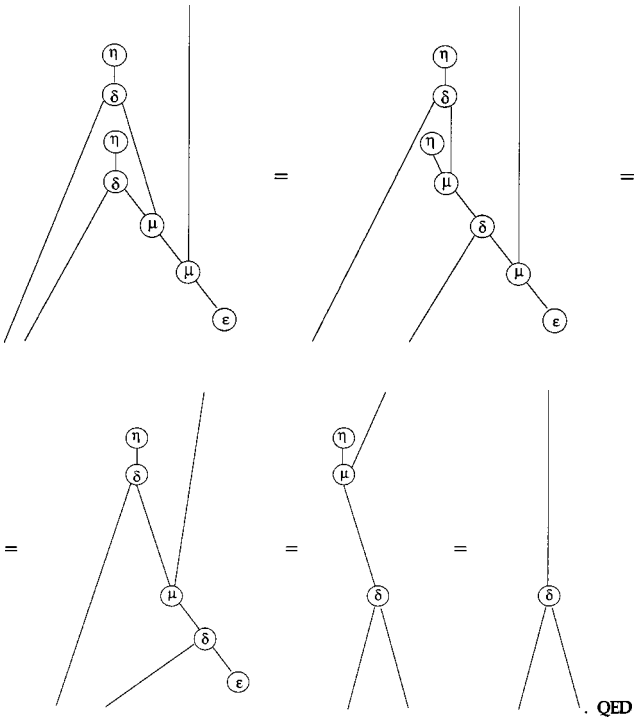
Lemma 1.3: *For a Frobenius monad* $\mathbf{T}$, *there is an adjunction* $T\dashv T$ *with counit* $\sigma = \varepsilon\circ\mu : T^2 \to 1$ *and unit* $\rho : 1 \to T^2$. *Moreover,* $\mathbf{G} = (T, \varepsilon, \delta)$ *is a right adjoint comonad for the monad* $\mathbf{T}$.

Proof: We shall do this using the string calculus [as justified by Joyal and Street (1991)]. We use Lemma 1.2.

One of the counit/unit identities is proved by the following calculation; look in a mirror for the proof of the other.



For the second sentence we need to show that $\delta = T^2\sigma\circ T^2\mu G\circ T\rho T^2\circ\rho T$ and $\varepsilon = \sigma\circ\eta T$. The latter is easy since $\sigma\circ\eta T = \varepsilon\circ\mu\circ\eta T = \varepsilon$. For the former we have



Q.E.D.

Remark: (a) It follows from the first sentence of Lemma 1.3 that ρ is uniquely determined by the monad $\mathbf{T} = (T, \eta, \mu)$ and ε. This is because the counit σ is determined by μ and ε, and the counit of any adjunction uniquely determines the unit.

(b) It is implicit (using AM1) in the second sentence of Lemma 1.3 that δ is coassociative.

Proposition 1.4: *For a Frobenius monad* $\mathbf{T}$, *the left adjoint* $F^{\mathbf{T}}:\mathcal{X}\to\mathcal{X}^{\mathbf{T}}$ *to the forgetful functor* $U^{\mathbf{T}}:\mathcal{X}^{\mathbf{T}}\to\mathcal{X}$ *is also a right adjoint to* $U^{\mathbf{T}}$ *with counit* ε.

Proof: By AM2 we know that there is an isomorphism of categories $K:\mathcal{X}^{\mathbf{T}}\cong\mathcal{X}^{\mathbf{G}}$ such that $V^{\mathbf{G}}K=U^{\mathbf{T}}$. The left adjoint $F^{\mathbf{T}}$ to $U^{\mathbf{T}}$ is given by $F^{\mathbf{T}}X=(\mathbf{T}^2X\xrightarrow{\mu_X}TX)$ and the right adjoint $C^{\mathbf{G}}$ to $V^{\mathbf{G}}$ is given by $C^{\mathbf{G}}X=(TX\xrightarrow{\delta_X}T^2X)$. Since $T\mu\cdot\rho T=\delta$, we see that μ and δ are mates as required to prove that $KF^{\mathbf{T}}=C^{\mathbf{G}}$. Since $V^{\mathbf{G}}\dashv C^{\mathbf{G}}$ with counit ε, we have $V^{\mathbf{G}}K\dashv K^{-1}C^{\mathbf{G}}$ with counit ε; that is, $U^{\mathbf{T}}\dashv F^{\mathbf{T}}$ with counit ε. Q.E.D.

Proposition 1.5: *Suppose* $F\dashv U\dashv F$ (written $F\vdash\!\dashv U$). *Then the monad* $\mathbf{T}$ *generated by the adjunction* $F\dashv U$ *together with the counit for* $U\dashv F$ is Frobenius.

Proof: Let $\lambda:FU\to 1$ be the counit and $\eta:1\to UF$ be the unit for $F\dashv U$. Let $\varepsilon:UF\to 1$ be the counit and $\kappa:1\to FU$ be the unit for $U\dashv F$. The multiplication for $\mathbf{T}$ is $\mu=U\lambda F$. Take $\rho=U\kappa F\circ\eta:1\to T^2$. Then $\mathbf{T}$ with ε is Frobenius since

$$T\mu\circ\rho T=UFU\lambda F\circ U\kappa FUF\circ\eta UF=U\kappa F\circ U\lambda F\circ\eta UF=U\kappa F=U\kappa F\circ U\lambda F\circ UF\eta$$
$$=U\lambda FUF\circ UFU\kappa F\circ UF\eta=\mu T\circ T\rho,$$

$$T\varepsilon\circ\rho=UF\varepsilon\circ U\kappa F\circ\eta=\eta,\quad\text{and}\quad\varepsilon T\circ\rho=\varepsilon UF\circ U\kappa F\circ\eta=\eta.$$

Q.E.D.

See Freyd *et al.* (1999) for a discussion of $F\vdash\!\dashv U$ in the special case where *inter alia* U is fully faithful.

Theorem 1.6: *Suppose* $\mathbf{T}=(T,\eta,\mu)$ *is a monad on a category* $\mathcal{X}$ *and suppose* $\varepsilon:T\to 1$ *is a natural transformation. Then the following conditions are equivalent*:

(a) *equipped with* ε, *the monad* $\mathbf{T}$ *is Frobenius*;
(b) *there exists a natural transformation* $\delta:T\to TT$ *such that*

$$T\mu\circ\delta T=\delta\circ\mu=\mu T\circ T\delta\quad\text{and}\quad T\varepsilon\circ\delta=1_T=\varepsilon T\circ\delta;$$

(c) *there exists a comonad* $\mathbf{G}=(T,\varepsilon,\delta)$ *such that*

$$T\mu\circ\delta T=\delta\circ\mu=\mu T\circ T\delta;$$

(d) *there exists a counit* $\sigma:T^2\to 1$ *for an adjunction* $T\dashv T$ *satisfying the equation*

$$\sigma\circ T\mu=\sigma\circ\mu T,$$

where $\varepsilon=\sigma\circ\mu T$;
(e) *the natural transformation* $\sigma=\varepsilon\circ\mu:T^2\to 1$ *is a counit for an adjunction* $T\dashv T$;
(f) *the functor* $F^{\mathbf{T}}:\mathcal{X}\to\mathcal{X}^{\mathbf{T}}$ is right adjoint to $U^{\mathbf{T}}:\mathcal{X}^{\mathbf{T}}\to\mathcal{X}$ with counit ε.

Proof: Equivalence of (a), (b), and (c).

We have proved that (a) implies (b) and (c). Clearly (c) implies (b). To see that (b) implies (a), put $\rho=\delta\circ\eta$. Then,

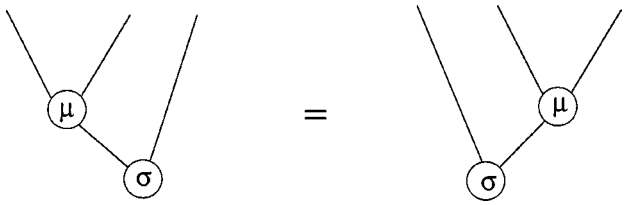
$$T\mu\circ\rho T=T\mu\circ\delta T\circ\eta T=\delta\circ\mu\circ\eta T=\delta=\delta\circ\mu\circ T\eta=\mu T\circ T\delta\circ T\eta=\mu T\circ T\rho\ \text{and}$$

$$T\varepsilon\circ\rho=T\varepsilon\circ\delta\circ\eta=\eta=\varepsilon T\circ\delta\circ\eta=\varepsilon T\circ\rho.$$

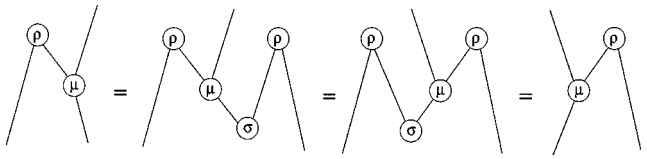
Equivalence of (a) and (d).

Assuming (a), we know that $\sigma=\varepsilon\circ\mu:T^2\to 1$ is a counit for $T\dashv T$ by (b). But then $\sigma\circ T\mu=\sigma\circ\mu T$ is obvious by associativity of μ.

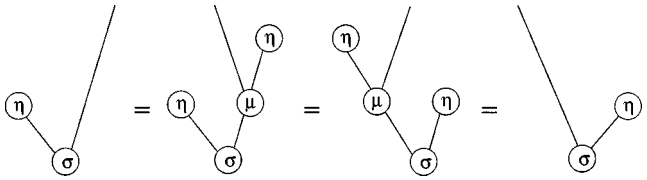
Assume (d) and note that $\sigma\circ T\mu=\sigma\circ\mu T$, in string notation, becomes



Let ρ be the unit corresponding to the counit σ. The following proves $T\mu\circ\rho T=\mu T\circ T\rho$.



Now notice that $\sigma\circ\eta T=\sigma\circ T\eta$ by the following calculation.



So put $\varepsilon=\sigma\circ\eta T=\sigma\circ T\eta$ and notice that

$$T\varepsilon\circ\rho=T\sigma\circ T^2\eta\circ\rho=T\sigma\circ\rho T\circ\eta=\eta=\sigma T\circ T\rho\circ\eta=\sigma T\circ\eta T^2\circ\rho=\varepsilon T\circ\rho.$$

So (a) holds.

Equivalence of (a) and (e).

Lemma 1.3 provides one direction. Conversely, if (e) holds then (d) holds since $\sigma\circ T\mu=\sigma\circ\mu T$ by associativity of μ. So (a) holds.

Equivalence of (a) and (f).

This is an immediate consequence of Propositions 1.4 and 1.5. Q.E.D.

It is clear from Theorem 1.6 that our definition agrees with Lawvere's definition of Frobenius monad [see Lawvere (1969), pp. 151 and 152]. Using the "algebra" terminology, it also agrees for example with Chap. 5 of Carmody (1995), Sec. 6 of Bichon and Street (2003) and Definition 3.1 of Müger (2003a, 2003b).

It follows also that the notion of Frobenius monad is self-dual in the sense that it is the same as a comonad $\mathbf{G}=(G,\varepsilon,\delta)$ with a natural transformation $\eta:1_X\to G$ such that $\delta\circ\eta$ is a unit for $G\dashv G$.

III. REVIEW OF ENRICHED CATEGORIES

References for enriched categories are Kelly (1982) and Lawvere (1974). Let $\mathcal{V}$ denote a particularly familiar symmetric monoidal category. The reader really only needs to keep in mind the category Set of sets with Cartesian product as tensor product and the category Vect_k of k-linear spaces with usual tensor product. There are other nice examples such as Cat with Cartesian product or the category DGVect_k of chain complexes of (that is, differential graded) vector spaces.

We call $\mathcal{V}$ our *base* monoidal category. A *category $\mathcal{A}$ enriched in the base $\mathcal{V}$*, also called a *$\mathcal{V}$-category*, consists of:

(i) a set $\mathrm{ob}\,\mathcal{A}$ whose elements are called *objects*;
(ii) for each pair of objects A and B of $\mathcal{A}$, an object $\mathcal{A}(A,B)$ of $\mathcal{V}$ (that some people write as $\mathrm{Hom}_{\mathcal{A}}(A,B)$);
(iii) morphisms $\mathcal{A}(B,C)\otimes\mathcal{A}(A,B)\to\mathcal{A}(A,C)$ in $\mathcal{V}$ called *composition*; and
(iv) morphisms $I\to\mathcal{A}(A,A)$ in $\mathcal{V}$ called *identity morphisms of $\mathcal{A}$*;

subject to associativity and unital conditions. There is an underlying ordinary category whose objects are the same as those of $\mathcal{A}$ and whose morphisms $f:A\to B$ (we call them *morphisms of* $\mathcal{A}$) are morphisms $f:I\to\mathcal{A}(A,B)$ in $\mathcal{V}$. Each object A of $\mathcal{A}$ determines a monoid $\mathcal{A}(A,A)$ in $\mathcal{V}$. Each monoid M in $\mathcal{V}$ determines a $\mathcal{V}$-category ΣM with one object whose endohom is M. Taking the other view, we can think of $\mathcal{V}$-categories as "monoids in $\mathcal{V}$ with several objects."

When $\mathcal{V}=\mathrm{Set}$, a $\mathcal{V}$-category is a category. When $\mathcal{V}=\mathrm{Vect}_k$, a $\mathcal{V}$-category is a k-linear category (this is simply an ordinary category whose homs are k-vector spaces and whose composition is bilinear). Each k-algebra E determines a Vect_k-category ΣE with one object. A 2-category is a Cat-category!

The nice bases $\mathcal{V}$ we have in mind are *closed*: for each pair of objects X and Y of $\mathcal{V}$ there is an object $[X,Y]$ (called the *internal hom* of X and Y) and a natural bijection

$$\mathcal{V}(W\otimes X,Y)\cong\mathcal{V}(W,[X,Y]).$$

In this case $\mathcal{V}$ itself becomes a $\mathcal{V}$-category; so sometimes we write $\mathcal{V}(X,Y)$ for the object $[X,Y]$ rather than merely its underlying set. In a nonsymmetric monoidal category $\mathcal{V}$ this $[X,Y]$ would be called a *left internal hom*. A *right internal hom* $[X,Y]_r$ satisfies

$$\mathcal{V}(X\otimes W,Y)\cong\mathcal{V}(W,[X,Y]_r).$$

In any monoidal category $\mathcal{V}$ then, if U is right dual to V, then there is a right internal hom of V and any Y given by $[V,Y]_r=U\otimes Y$.

The *opposite* $\mathcal{A}^{\mathrm{op}}$ of a $\mathcal{V}$-category $\mathcal{A}$ is the $\mathcal{V}$-category with the same objects as $\mathcal{A}$ and with $\mathcal{A}^{\mathrm{op}}(A,B)=\mathcal{A}(B,A)$; the composition uses that of $\mathcal{A}$ but "in the reverse order" as allowed by the symmetry of $\mathcal{V}$. We will see that, in the appropriate context, $\mathcal{A}^{\mathrm{op}}$ is a dual of $\mathcal{A}$ in the same way that for finite-dimensional vector spaces V, the space V^* of linear functionals is a dual of V.

The definition of $\mathcal{V}$-*functor* $T:\mathcal{A}\to\mathcal{B}$ between $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ is made in the obvious way: it consists of a function $T:\mathrm{ob}\,\mathcal{A}\to\mathrm{ob}\,\mathcal{B}$ and morphisms

$$T=T_{A,B}:\mathcal{A}(A,B)\to\mathcal{B}(TA,TB)$$

in $\mathcal{V}$ (called *the effect of T on homs*) compatible with composition and identities. The definition of $\mathcal{V}$-*natural transformation* $\theta:T\Rightarrow T':\mathcal{A}\to\mathcal{B}$ needs a little more care in general, however, for the cases $\mathcal{V}=\mathrm{Set}$ and $\mathcal{V}=\mathrm{Vect}_k$, it amounts to an ordinary natural transformation.

With compositions that are straightforward (especially in the examples), we obtain a 2-category $\mathcal{V}$-Cat whose objects are (small) $\mathcal{V}$-categories, whose morphisms are $\mathcal{V}$-functors and whose 2-cells are $\mathcal{V}$-natural transformations. As a technical point concerning size, we allow ourselves to write $\mathcal{V}$-Cat $(\mathcal{A},\mathcal{B})$ for the category of $\mathcal{V}$-functors from $\mathcal{A}$ to $\mathcal{B}$ even when $\mathcal{A}$ and $\mathcal{B}$ are not small.

There is a *tensor product* $\mathcal{A}\otimes\mathcal{B}$ of $\mathcal{V}$-categories with $\mathrm{ob}(\mathcal{A}\otimes\mathcal{B})=\mathrm{ob}\,\mathcal{A}\times\mathrm{ob}\,\mathcal{B}$ and

$$(\mathcal{A}\otimes\mathcal{B})((A,B),(A',B'))=\mathcal{A}(A,A')\otimes\mathcal{B}(B,B');$$

the composition uses the compositions of $\mathcal{A}$ and $\mathcal{B}$ and the symmetry of $\mathcal{V}$. The unit for this tensor product is the $\mathcal{V}$-category $\mathcal{I}$ with one object, denoted by $\cdot$, and with $\mathcal{I}(\cdot,\cdot)=I$. Equipped with this, $\mathcal{V}$-Cat becomes a symmetric monoidal 2-category. Actually it is also closed; we now describe the internal hom.

For $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$, there is a $\mathcal{V}$-*functor category* $[\mathcal{A},\mathcal{B}]$: it is the $\mathcal{V}$-category whose objects are $\mathcal{V}$-functors from $\mathcal{A}$ to $\mathcal{B}$ and whose homs are given by the ends

$$[\mathcal{A},\mathcal{B}](T,T') = \int_A \mathcal{B}(TA,T'A)$$

[see MacLane (1971) for Yoneda–Day–Kelly integral notation]. In the examples of bases of interest here, it is clear that the $\mathcal{V}$-natural transformations from T to T' form an object of $\mathcal{V}$. There is a canonical isomorphism of categories

$$V\text{-Cat}(\mathcal{C},[\mathcal{A},\mathcal{B}]) \cong \mathcal{V}\text{-Cat}(\mathcal{C}\otimes\mathcal{A},\mathcal{B}).$$

There is another monoidal bicategory $\mathcal{V}$-Mod whose objects are also the (small) $\mathcal{V}$-categories; in this case however, the hom-categories are defined by

$$\mathcal{V}\text{-Mod}(\mathcal{A},\mathcal{B}) = \mathcal{V}\text{-Cat}(\mathcal{B}^{\mathrm{op}}\otimes\mathcal{A},\mathcal{V}).$$

In other words, the morphisms of $\mathcal{V}$-Mod are $\mathcal{V}$-functors $M:\mathcal{B}^{\mathrm{op}}\otimes\mathcal{A}\to\mathcal{V}$ and the 2-cells are $\mathcal{V}$-natural transformations. These objects M of $\mathcal{V}$-Mod $(\mathcal{A},\mathcal{B})$ are called *modules* from $\mathcal{A}$ to $\mathcal{B}$ (or "left $\mathcal{A}$-, right $\mathcal{B}$-bimodules") because of the actions (albeit a "several object version" of action)

$$\mathcal{A}(A,A')\otimes M(B,A)\otimes\mathcal{B}(B',B)\to M(B',A')$$

that correspond to the effect of M on homs. The composite of modules $M:\mathcal{A}\to\mathcal{B}$ and $N:\mathcal{B}\to\mathcal{C}$ is defined by the coend

$$(N\circ M)(C,A) = \int^B M(B,A)\otimes N(C,B);$$

this colimit can be constructed by taking a sum (coproduct) in $\mathcal{V}$ over all objects B and factoring out the left action of $\mathcal{B}$ on N and the right action of $\mathcal{B}$ on M (instead of a composition we can think of it as a tensor product over $\mathcal{B}$: in that spirit we can write $N\circ M = M\underset{\mathcal{B}}{\otimes} N$. This composition (like tensor product) is only associative up to isomorphism (which is allowed in a bicategory). The identity module of $\mathcal{A}$ is the module $1_{\mathcal{A}}$ defined by $1_{\mathcal{A}}(A,A') = \mathcal{A}(A,A')$.

Each $\mathcal{V}$-functor $T:\mathcal{A}\to\mathcal{B}$ yields modules $T_*:\mathcal{A}\to\mathcal{B}$ and $T^*:\mathcal{B}\to\mathcal{A}$ defined by $T_*(B,A) = \mathcal{B}(B,TA)$ and $T^*(A,B) = \mathcal{B}(TA,B)$. In fact, T^* is right adjoint to T_* in the bicategory $\mathcal{V}$-Mod: the unit $1_{\mathcal{A}}\to T^*\circ T_*$ has components

$$\mathcal{A}(A,A')\to\int^B \mathcal{B}(TA,B)\otimes\mathcal{B}(B,TA') = \mathcal{B}(TA,TA')$$

given by the effect of T on homs. We obtain an "inclusion" pseudofunctor

$$\mathcal{V}\text{-Cat}\to\mathcal{V}\text{-Mod}$$

that takes each $\mathcal{V}$-category to itself, takes each $\mathcal{V}$-functor T to T_*, and is bijective on 2-cells; so we sometimes write T for the module T_*.

So we can think of $\mathcal{V}$-Mod as an expansion of $\mathcal{V}$-Cat designed to provide the morphisms in $\mathcal{V}$-Cat with right adjoints. Not only adjoints but equivalences in $\mathcal{V}$-Mod are also of interest.

Equivalence in $\mathcal{V}$-Mod is called *Cauchy equivalence of $\mathcal{V}$-categories*. In the particular case where $\mathcal{V}$ is the monoidal category of Abelian groups with the usual tensor product, we obtain the notion of Cauchy equivalence for additive categories. Rings R can be regarded as additive categories ΣR with a single object; in this way, Cauchy equivalence is none other than ordinary Morita equivalence of rings.

Each $\mathcal{V}$-category $\mathcal{A}$ has a *Cauchy completion* $Q\mathcal{A}$: it is the smallest full sub-$\mathcal{V}$-category of the $\mathcal{V}$-functor $\mathcal{V}$-category $P\mathcal{A}=[\mathcal{A}^{\mathrm{op}},\mathcal{V}]$ that contains the representable $\mathcal{V}$-functors $\mathcal{A}(-,A)$ and is closed under absolute $\mathcal{V}$-colimits. [Absolute $\mathcal{V}$-colimits are those preserved by all $\mathcal{V}$-functors; see Street (1983).] For example, if $\mathcal{V}=\mathrm{Set}$ then $Q\mathcal{A}$ is the completion of the category $\mathcal{A}$ under splitting of idempotents; and if $\mathcal{V}=\mathrm{Vect}_k$, then $Q\mathcal{A}$ is the completion of the additive category $\mathcal{A}$ under

direct sums and splitting of idempotents. For reasonable $\mathcal{V}$, if $\mathcal{A}$ is small, so is $Q\mathcal{A}$ [see Johnson (1989b)].

It is easy to see that $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are Cauchy equivalent if and only if $P\mathcal{A}$ and $P\mathcal{B}$ are equivalent $\mathcal{V}$-categories (that is, equivalent in the 2-category $\mathcal{V}$-Cat). It is well known [see Street (1983) for a proof in a very general context] that $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are Cauchy equivalent if and only if $Q\mathcal{A}$ and $Q\mathcal{B}$ are equivalent $\mathcal{V}$-categories. The inclusion of $Q\mathcal{A}$ in $QQ\mathcal{A}$ is an equivalence, so $\mathcal{A}$ is Cauchy equivalent to $Q\mathcal{A}$. We say $\mathcal{A}$ is *Cauchy complete* when it admits all absolute $\mathcal{V}$-colimits; that is, when the inclusion of $\mathcal{A}$ in $Q\mathcal{A}$ is an equivalence.

Tensor product of $\mathcal{V}$-categories extends to $\mathcal{V}$-Mod making $\mathcal{V}$-Mod a symmetric monoidal bicategory and the inclusion of $\mathcal{V}$-Cat in $\mathcal{V}$-Mod strict monoidal. We have seen that $\mathcal{V}$-Cat is closed. However, there is a much stronger structure possessed by $\mathcal{V}$-Mod; it is "autonomous" like the category of finite-dimensional vector spaces, and we shall now make this precise.

We work in a monoidal bicategory $\mathcal{B}$. A morphism $e:A\otimes B\to I$ is called a *biexact pairing* when the functor

$$\mathcal{B}(C,B\otimes D)\to\mathcal{B}(A\otimes C,D),$$

taking $C\xrightarrow{f}B\otimes D$ to $A\otimes C\xrightarrow{A\otimes f}A\otimes B\otimes D\xrightarrow{e\otimes D}D$, is an equivalence of categories for all objects C and D. In this case, there is a unique (up to isomorphism) morphism $n:I\to B\otimes A$ such that the composite $A\xrightarrow{A\otimes n}A\otimes B\otimes A\xrightarrow{e\otimes A}A$ is isomorphic to the identity of A. We say that B is a *right bidual* for A with *counit* e and *unit* n. Of course, A is called a *left bidual* for B.

The monoidal bicategory $\mathcal{B}$ is called *autonomous* when each object has both a left and a right bidual. A choice of right bidual of an object A is denoted by A°: with unit $n:I\to A^\circ\otimes A$ and counit $e:A\otimes A^\circ\to I$.

In the case of $\mathcal{V}$-Mod, a right bidual for the $\mathcal{V}$-category $\mathcal{A}$ is provided by $\mathcal{A}^{\mathrm{op}}$ since

$$\mathcal{V}\text{-Mod}(\mathcal{A}\otimes\mathcal{B},\mathcal{C})\cong\mathcal{V}\text{-Cat}(\mathcal{C}^{\mathrm{op}}\otimes\mathcal{A}\otimes\mathcal{B},\mathcal{V})\cong\mathcal{V}\text{-Mod}(\mathcal{B},\mathcal{A}^{\mathrm{op}}\otimes\mathcal{C}).$$

The counit $e:\mathcal{A}\otimes\mathcal{A}^{\mathrm{op}}\to I$ is the module defined by $e(\cdot,A,A')=\mathcal{A}(A',A)$. Since $\mathcal{V}$-Mod is symmetric, it is autonomous.

IV. FROBENIUS PSEUDOMONOIDS

We consider a pseudomonoid (or monoidal object) A in a monoidal bicategory $\mathcal{B}$: the underlying object is also denoted by A, the unit is $j:I\to A$, the multiplication is $p:A\otimes A\to A$, and there are invertible coherent associativity and unital constraints. When the unit constraints are identities, the pseudomonoid is said to be *normalized*. When the unit and associativity constraints are identities, the pseudomonoid is said to be *strict*; it is then just a monoid.

Motivated by Theorem 1.6(e) we make a natural higher-dimensional extension of the Frobenius notion.

Definition 3.1: A pseudomonoid A is *Frobenius* when it is equipped with a morphism $l:A\to I$ such that the composite

$$A\otimes A\xrightarrow{p}A\xrightarrow{l}I$$

is a biexact pairing.

Proposition 1.1 of Day *et al.* (2003) states that the pseudomonoid A is *left autonomous* with dualization $d:A^\circ\to A$ if and only if

$$p^*\cong(p\otimes A)\circ(A\otimes d\otimes A)\circ(A\otimes n),$$

and this holds if and only if

$$(p \circ (d \otimes A))^* \cong (A^\circ \otimes p) \circ (n \otimes A).$$

Proposition 1.2 of Day *et al.* (2003) gives the formula

$$d \cong (A \otimes e) \circ (p^* \otimes A^\circ) \circ (j \otimes A^\circ).$$

Furthermore, in the case where j has a right adjoint, Proposition 1.4 of Day *et al.* (2003) states that A is also right autonomous, and then simply called autonomous, if and only if d is an equivalence. Then the right adjoint d^* of d is an inverse equivalence and [Proposition 1.2 of Day *et al.* (2003)] is given by the formula

$$d^* \cong (A^\circ \otimes j^*) \circ (A^\circ \otimes p) \circ (n \otimes A).$$

Proposition 3.1: *Every autonomous pseudomonoid* (A, j, p), *for which* j *has a right adjoint, is Frobenius with* $l = j^*$.

Proof: In an autonomous monoidal bicategory, the composite $\sigma: A \otimes A \xrightarrow{p} A \xrightarrow{l} I$ is a biexact pairing if and only if the corresponding morphism

$$\hat{\sigma}: A \xrightarrow{n \otimes A} A^\circ \otimes A \otimes A \xrightarrow{A^\circ \otimes \sigma} A^\circ$$

is an equivalence. So, with $l = j^*$, we have

$$\hat{\sigma} = (A^\circ \otimes j^*) \circ (A^\circ \otimes p) \circ (n \otimes A) \cong d^*,$$

an equivalence. Q.E.D.

A pseudocomonoidal structure on A in Proposition 3.1 is provided by j^* and p^*; compare Theorem 1.6(c). We also note that there are isomorphisms

$$p^* \cong (d \otimes A) \circ (A^\circ \otimes p) \circ (n \otimes A) \cong (A \otimes p) \circ (\rho \otimes A) \cong (p \otimes A) \circ (A \otimes \rho),$$

where $\rho = (I \xrightarrow{j} A \xrightarrow{p^*} A \otimes A)$.

Example: *Quasi-Hopf algebras*

A *quasibialgebra* (over a field k) is a k-algebra H equipped with algebra morphisms

$$\Delta: H \to H \otimes H \quad \text{and} \quad E: H \to k,$$

and with an invertible element $\phi \in H \otimes H \otimes H$, such that

$$(E \otimes 1_H)(\Delta(a)) = a = (1_H \otimes E)(\Delta(a)) \quad \text{and} \quad \phi(\Delta \otimes 1_H)(\Delta(a)) = (1_H \otimes \Delta)(\Delta(a))\phi$$

for all $a \in H$; furthermore, ϕ satisfies the *pentagon condition*

$$(1 \otimes 1 \otimes \Delta)(\phi) \cdot (\Delta \otimes 1 \otimes 1)(\phi) = (1 \otimes \phi) \cdot (1 \otimes \Delta \otimes 1)(\phi) \cdot (\phi \otimes 1).$$

(A quasibialgebra reduces to an ordinary bialgebra when ϕ is the identity element $1 \otimes 1 \otimes 1$.) We can make $H \otimes H$ into a left $H \otimes H$-, right H-bimodule by means of the actions

$$(a \otimes b) \cdot (x \otimes y) \cdot c = \sum_i axc_i^1 \otimes byc_i^2,$$

where $\Delta(c) = \sum_i c_i^1 \otimes c_i^2$; for the time being, let us call this bimodule M. Given an algebra antimorphism $S: H \to H$, there is another left $H \otimes H$-, right H-bimodule structure defined on $H \otimes H$ by the actions

$$(a \otimes b) \cdot (x \otimes y) \cdot c = \sum_j axS(b_j^1) \otimes b_j^2 yc,$$

where $\Delta(b) = \sum_j b_j^1 \otimes b_j^2$; for the time being, let us call this bimodule N. A *quasi-Hopf algebra* is a

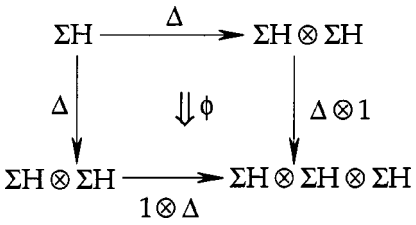
quasibialgebra H together with an algebra antimorphism $S:H\to H$ (called the *antipode*) and a bimodule isomorphism $\pi:M\cong N$. This is equivalent to the original definition of Drinfel'd (1990) that, instead of the isomorphism π, involved two elements α and β of H satisfying the equations

$$E(c)\alpha=\sum_i S(c_i^1)\alpha c_i^2,\quad E(c)\beta=\sum_i c_i^1\beta S(c_i^2),$$

$$\sum_i \phi_i^1\beta S(\phi_i^2)\alpha\phi_i^3=1,\quad \text{and}\quad \sum_i S(\phi_i^{-1})\alpha\phi_i^{-2}\beta S(\phi_i^{-3})=1$$

[see Sec. 2.4 of Majid (1995)]. We shall say a bit more about the equivalence of the definitions soon.

Take $\mathcal{V}=\mathrm{Vect}_k$ and recall that a k-algebra A is a one-object V-category ΣA. It is obvious that an algebra morphism $f:A\to B$ is the same as a $\mathcal{V}$-functor $f:\Sigma A\to\Sigma B$. So what is a $\mathcal{V}$-natural transformation $\sigma:f\Rightarrow g$ in terms of the algebra morphisms f and g from A to B ? It is nothing other than an element α of B such that $\alpha f(a)=g(a)\alpha$ for all elements a of A. Therefore we see that ϕ belongs in the square



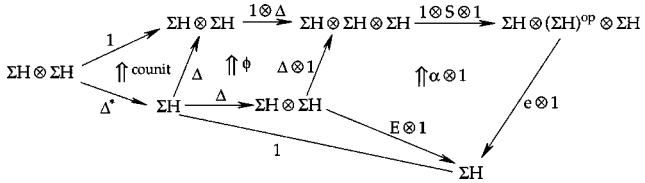
in $\mathcal{V}$-Cat. From this it follows easily that: *a quasibialgebra structure on an algebra H is precisely a normalized pseudomonoid structure on* ΣH *in* $(\mathcal{V}\text{-Cat})^{\mathrm{coop}}$.

Now we move from $(\mathcal{V}\text{-Cat})^{\mathrm{coop}}$ to $(\mathcal{V}\text{-Mod})^{\mathrm{coop}}$ where $\mathcal{V}$-functors have right adjoints and the object ΣH^{op} is a bidual for ΣH. Here we can observe that the right adjoint $\Delta^*:\Sigma H\otimes\Sigma H\to\Sigma H$ of Δ is the bimodule M above and the composite module

$$\Sigma H\otimes\Sigma H\xrightarrow{\Sigma H\otimes\Delta}\Sigma H\otimes\Sigma H\otimes\Sigma H\xrightarrow{\Sigma H\otimes S\otimes\Sigma H}\Sigma H\otimes\Sigma H^{\mathrm{op}}\otimes\Sigma H\xrightarrow{e\otimes\Sigma H}\Sigma H$$

is N. It follows that: *a quasi-Hopf structure on the quasialgebra H is precisely a left autonomous structure on the normalized pseudomonoid* ΣH *in* $(\mathcal{V}\text{-Mod})^{\mathrm{coop}}$. Therefore Proposition 3.1 applies to yield a Frobenius structure on ΣH in $(\mathcal{V}\text{-Mod})^{\mathrm{coop}}$ using E^*. This means that ΣH becomes a pseudomonoid in $\mathcal{V}$-Mod using E^* and Δ^*; of course, this is not the original algebra structure on H.

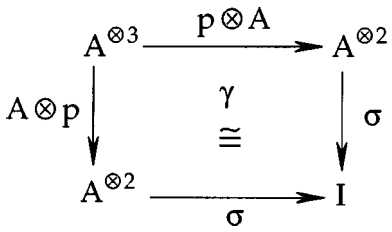
Finally in this example, we can say something about the equivalent definitions of quasi-Hopf algebra: specifically about how π is obtained from α and ϕ. The above-mentioned equation satisfied by the element α of H says precisely that it is a (bi)module morphism from E to $e\circ(1\otimes S)\circ\Delta$ (note that E is k and $e\circ(1\otimes S)\circ\Delta$ is H with appropriate actions). Then π is the pasting composite of the following diagram.



Similarly, β is used to define a 2-cell in the opposite direction; the further conditions on α, β, and ϕ say that this really is the inverse of π. Further details can be found in the general results of Day *et al.* (2003). This ends our example.

In Sec. 9 of Day and Street (2004) a *form* for a pseudomonoid A in a monoidal bicategory $\mathcal{B}$

is defined to be a morphism $\sigma: A \otimes A \to I$ together with an invertible 2-cell γ as below.



Then the authors define the pseudomonoid to be $*$-*autonomous* when σ is a biexact pairing. **(**There was an extra condition in [Day and Street (2004)] requiring σ to be "representable"; however, this is automatic under a mild completeness condition on the pseudomonoid.**)**

Proposition 3.2: A pseudomonoid is $*$-autonomous if and only if it is Frobenius.

Proof: Suppose σ and γ is a form on the pseudomonoid A with σ a biexact pairing. Put $l = (A \xrightarrow{j \otimes A} A \otimes A \xrightarrow{\sigma} I)$ so that

$$\sigma \cong \sigma \circ (p \otimes A) \circ (j \otimes A) \cong \sigma \circ (A \otimes p) \circ (j \otimes A) \cong \sigma \circ (j \otimes A) \circ p \cong l \circ p,$$

where the second isomorphism involves γ. So A equipped with l is Frobenius. Conversely, put $\sigma = l \circ p$ which is a biexact pairing by definition of Frobenius; the isomorphism γ is obtained by composing the associativity constraint

$$p \circ (p \otimes A) \cong p \circ (A \otimes p)$$

on the left with l. Q.E.D.

Corollary 3.3: For any object X of $\mathcal{B}$ and any equivalence $v: X \to X^{\circ\circ}$, the pseudomonoid $X^{\circ} \otimes X$ is Frobenius when equipped with $l: X^{\circ} \otimes X \xrightarrow{1 \otimes v} X^{\circ} \otimes X^{\circ\circ} \xrightarrow{e} I$.

Example: Star-autonomous monoidal enriched categories

A $\mathcal{V}$-category $\mathcal{A}$ is *monoidal* when it is equipped with the structure of pseudomonoid in $\mathcal{V}$-Cat; we write $\#: \mathcal{A} \otimes \mathcal{A} \to \mathcal{A}$ for the "multiplication" $\mathcal{V}$-functor (to distinguish it from the tensor product $\otimes$ of $\mathcal{V}$) and J for the unit object. We say that $\mathcal{A}$ is $*$-*autonomous* when it is equipped with an equivalence of $\mathcal{V}$-categories $S: \mathcal{A} \to \mathcal{A}^{\mathrm{op}}$ and a $\mathcal{V}$-natural family of isomorphisms

$$\mathcal{A}(A \# B, J) \cong \mathcal{A}(B, SA).$$

This is a straightforward enrichment of the concept due to Barr (1996) and considered more generally in Day and Street (2004) in connection with quantum groupoids. Here we want to emphasize the Frobenius aspect. In order to obtain an autonomous monoidal bicategory, we need to move from $\mathcal{V}$-Cat to $\mathcal{V}$-Mod. Because of the way we have defined $\mathcal{V}$-Mod, it is better to consider $\mathcal{A}^{\mathrm{op}}$ rather than $\mathcal{A}$; to say one is monoidal is the same as saying the other is. For simplicity, we also suppose $\mathcal{A}$ is Cauchy complete (see Sec. VI); then any equivalence $\mathcal{A} \to \mathcal{A}^{\mathrm{op}}$ in $\mathcal{V}$-Mod is automatically of the form S_* for an equivalence $S: \mathcal{A} \to \mathcal{A}^{\mathrm{op}}$ in $\mathcal{V}$-Cat. As a consequence of Proposition 3.2 we have that: *the monoidal $\mathcal{V}$-category $\mathcal{A}$ is $*$-autonomous if and only if $\mathcal{A}^{\mathrm{op}}$ is Frobenius in* $\mathcal{V}$-Mod. If we write $\check{S}: \mathcal{A}^{\mathrm{op}} \otimes \mathcal{A}^{\mathrm{op}} \to \mathcal{I}$ for the module defined by $\check{S}(A,B) = \mathcal{A}(B, SA)$, we see that the isomorphism defining $*$-autonomy is precisely $J^* \circ \#_* \cong \check{S}$. Corollary 3.3 implies a result of Day and Street (2004) that, for any $\mathcal{V}$-category $\mathcal{X}$, the monoidal $\mathcal{V}$-category $\mathcal{X}^{\mathrm{op}} \otimes \mathcal{X}$ is $*$-autonomous.

V. PROJECTIVE EQUIVALENCES

This section was inspired to a large extent by the discussion of "weak monoidal Morita equivalence" in Müger (2003a, 2003b).

It is well known what it means for a morphism to be an equivalence in any bicategory and that every equivalence can be made an adjoint equivalence. We wish to discuss a more general notion of equivalence. For this we need to clarify a concept of scalar.

A *scalar* for a bicategory $\mathcal{D}$ is a modification

$$\omega: 1_{1_{\mathcal{D}}} \to 1_{1_{\mathcal{D}}}: 1_{\mathcal{D}} \to 1_{\mathcal{D}}: \mathcal{D} \to \mathcal{D}.$$

That is, ω assigns to each object A of $\mathcal{D}$ a 2-cell $\omega_A: 1_A \to 1_A$ such that, for all morphisms $f: A \to B$,

$$f\omega_A = \omega_B f.$$

Scalars form a commutative monoid under composition. By abuse of language, 2-cell $\theta: f \Rightarrow f: X \to Y$ will be called a *scalar* when there exists an actual scalar ω such that

$$\theta = f\omega_X;$$

we say θ is an *invertible scalar* when ω is invertible.

Take the example of enriched categories; that is, in the case where $\mathcal{D} = \mathcal{V}$-Mod. It is easy to see that the commutative monoid of scalars is isomorphic to the endomorphism monoid $\mathcal{V}(I, I)$ of the unit object I. In particular, when $\mathcal{V}$ is the category of sets, the monoid is trivial (consisting only of the identity). More interestingly, if $\mathcal{V}$ is the monoidal category of modules over a commutative ring k then the scalars for $\mathcal{V}$-Mod are precisely the elements of k.

Remark: The braided monoidal category $\mathrm{Hom}(\mathcal{D}, \mathcal{D})(1_{\mathcal{D}}, 1_{\mathcal{D}})$ whose objects are pseudonatural transformations of the identity of $\mathcal{D}$, whose morphisms are modifications, and whose tensor product is either of the two compositions, is called the *center* of the bicategory $\mathcal{D}$. So scalars are endomorphisms of the unit of the centre. If $\mathcal{D}$ is the one-object bicategory $\Sigma\mathcal{C}$ with hom monoidal category $\mathcal{C}$ then $\mathrm{Hom}(\mathcal{D}, \mathcal{D})(1_{\mathcal{D}}, 1_{\mathcal{D}})$ is the center $Z\mathcal{C}$ of $\mathcal{C}$ in the sense of Joyal and Street (1991).

Definition 4.1: A morphism $u: A \to X$ in a bicategory $\mathcal{D}$ is called a *projective equivalence* when there is a morphism $f: X \to A$ adjoint to u on both sides (that is, $f \dashv u$) and there are invertible scalars ω and ϖ such that the composites

$$1_X \overset{\eta}{\to} uf \overset{\varepsilon}{\to} 1_X \quad \text{and} \quad 1_A \overset{\kappa}{\to} fu \overset{\lambda}{\to} 1_A$$

are equal to ω_X and ϖ_A, respectively, where η, λ and κ, ε are the unit-counit pairs for the adjunctions.

In any projective equivalence, by suitable rescaling of units and counits, we can ensure that either ω or ϖ is an identity. Equivalences are precisely the projective equivalences in which both ω and ϖ can be chosen to be identities.

Proposition 4.1: A composite of projective equivalences is a projective equivalence.

Proof: Suppose $f \dashv u$ with $u: A \to X$ and $f' \dashv u'$ with $u': X \to K$ where η, λ and κ, ε are the unit-counit pairs for the adjunctions $f \dashv u$ and those for $f' \dashv u'$ are similar except that they have primes. The counit for $u'u \dashv ff'$ is

$$u'uff' \overset{u'\varepsilon f'}{\to} u'f' \overset{\varepsilon'}{\to} 1_K$$

while the unit for $ff' \dashv u'u$ is

$$1_K \overset{\eta'}{\to} u'f' \overset{u'\eta f'}{\to} u'uff'.$$

But $\varepsilon \circ \eta = \omega_X$ and $\varepsilon' \circ \eta' = \omega'_K$. So,

$$\varepsilon' \circ (u'\varepsilon f') \circ (u'\eta f') \circ \eta' = \varepsilon' \circ (u'(\varepsilon \circ \eta)f') \circ \eta' = \varepsilon' \circ (u'\omega_X f') \circ \eta' = \varepsilon' \circ (\omega_K u'f') \circ \eta'$$
$$= \varepsilon' \circ \eta' \circ \omega_K = \omega'_K \circ \omega_K = (\omega' \circ \omega)_K.$$

A similar argument applies for the other composite. Q.E.D.

Definition 4.2: A Frobenius monad $\mathbf{t} = (t, \eta, \mu, \varepsilon, \delta)$ on an object X of $\mathcal{D}$ is *strongly separable* when there exist invertible scalars ω and ϖ such that the composites

$$1_X \overset{\eta}{\longrightarrow} t \overset{\varepsilon}{\longrightarrow} 1_X \quad \text{and} \quad t \overset{\delta}{\longrightarrow} tt \overset{\mu}{\longrightarrow} t$$

are equal to ω_X and $\varpi_X t$, respectively.

Proposition 4.2: A morphism in $\mathcal{D}$ is a projective equivalence if and only if it is monadic via a strongly separable Frobenius monad.

Proof: A projective equivalence $u: A \to X$ is conservative since the counit λ for its left adjoint is a retraction (split epimorphism). Since u also has a right adjoint, it is monadic. The composites $\varepsilon \circ \eta$ and $\mu \circ \delta = u\lambda f \circ u\kappa f = u(\lambda \circ \kappa)f$ are invertible scalars from Definition 4.1. So u generates a strongly separable Frobenius monad on X.

Conversely, suppose we have a strongly separable Frobenius monad $\mathbf{t} = (t, \eta, \mu, \varepsilon, \delta)$ on X and $u: A \to X$ together with action $\xi: tu \to u$ provide an Eilenberg–Moore construction for $\mathbf{t}$. So there exists $f \dashv u$, where uf is isomorphic to t and ξf transports to μ. We can replace t by uf so that $\xi f = \mu$. Then η is the unit for $f \dashv u$ and ε is the counit for $u \dashv f$. So we have that $\varepsilon \circ \eta$ is an invertible scalar. The counit κ for $f \dashv u$ is determined by $u\kappa = \xi$ and unit λ for $u \dashv f$ is determined by

$$u\lambda = t\xi \circ \delta u \circ \eta u.$$

So,

$$u(\kappa \circ \lambda) = \xi \circ t\xi \circ \delta u \circ \eta u = \xi \circ \mu u \circ \delta u \circ \eta u = \xi \circ \varpi_X u \circ \eta u = \varpi_X u \circ \xi \circ \eta u = \varpi_X u = u\varpi_A,$$

which implies that $\kappa \circ \lambda = \varpi_A$. Therefore u is a projective equivalence. Q.E.D.

VI. VARIATIONS ON MORITA EQUIVALENCE

Suppose $\mathcal{A}$ is a monoidal $\mathcal{V}$-category (that is, a pseudomonoid in $\mathcal{V}$-Cat). Then $P\mathcal{A}$ becomes a cocomplete monoidal $\mathcal{V}$-category via the convolution tensor product

$$(M * N)(A) = \int^{XY} \mathcal{A}(A, X \otimes Y) \otimes MX \otimes NY$$

of Day (1970). Monoidal $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are defined to be *Cauchy equivalent* when $P\mathcal{A}$ and $P\mathcal{B}$ are equivalent monoidal $\mathcal{V}$-categories (that is, equivalent in the 2-category of monoidal $\mathcal{V}$-categories and monoidal $\mathcal{V}$-functors). Johnson (1989a) showed that the convolution tensor product on $P\mathcal{A}$ restricts to $Q\mathcal{A}$ and that monoidal $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are Cauchy equivalent if and only if $Q\mathcal{A}$ and $Q\mathcal{B}$ are equivalent monoidal $\mathcal{V}$-categories. Moreover $\mathcal{A}$ is Cauchy equivalent to $Q\mathcal{A}$ as monoidal $\mathcal{V}$-categories.

From this we see in particular that Cauchy equivalence, monoidal or not, is a special case of equivalence once we find the appropriate ambient bicategory. Having in Sec. IV weakened the notion of equivalence to projective equivalence, we can now contemplate projective Cauchy equivalence. Two $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are *projectively Cauchy equivalent* when $P\mathcal{A}$ and $P\mathcal{B}$ are projectively equivalent $\mathcal{V}$-categories. For $\mathcal{V}$ equal to the category of sets or the category of Abelian groups, this concept is the same as Cauchy equivalence. However, if $\mathcal{V}$ is the category of vector spaces over a field, for example, we do obtain a weaker kind of equivalence; in particular, this applies to associative unital algebras over the field. In general, $\mathcal{A}$ and $\mathcal{B}$ are projectively Cauchy equivalent if and only if $Q\mathcal{A}$ and $Q\mathcal{B}$ are projectively equivalent $\mathcal{V}$-categories.

Similarly, two monoidal $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are *projectively Cauchy equivalent* when $P\mathcal{A}$ and $P\mathcal{B}$ are projectively equivalent monoidal $\mathcal{V}$-categories. If $\mathcal{V}$ is the category of vector spaces over a field k, we do obtain a weaker kind of Cauchy equivalence for monoidal k-linear categories. In general, monoidal $\mathcal{V}$-categories $\mathcal{A}$ and $\mathcal{B}$ are projectively Cauchy equivalent if and only if $Q\mathcal{A}$ and $Q\mathcal{B}$ are projectively equivalent monoidal $\mathcal{V}$-categories.

VII. WREATH PRODUCTS OF FROBENIUS ALGEBRAS

As in Sec. II, we express our results in terms of monads rather than algebras.

We shall begin by recalling some notions from Lack and Street (2002). Given a 2-category $\mathcal{K}$, there is a 2-category $\mathrm{EM}(\mathcal{K})$ which turns out to be the free completion of $\mathcal{K}$ with respect to the Eilenberg–Moore construction on monads. Explicitly, an object of $\mathrm{EM}(\mathcal{K})$ is a pair (A,t) where A is an object of $\mathcal{K}$ and t is a monad on A in $\mathcal{K}$. A morphism $(f,\phi):(A,t)\to(B,s)$ consists of a morphism $f:A\to B$ and 2-cell $\phi:s\circ f\Rightarrow f\circ t$ in $\mathcal{K}$ satisfying two compatibility conditions with the units η and multiplications μ of the monads t and s. A 2-cell $\rho:(f,\phi)\Rightarrow(g,\psi)$ is a 2-cell $\rho:f\Rightarrow g\circ t$ in $\mathcal{K}$ such that

$$(g\circ\mu)(\rho\circ t)\phi=(g\circ\mu)(\psi\circ t)(s\circ\rho).$$

Composition in the category $\mathrm{EM}(\mathcal{K})((A,t),(B,s))$ involves using the multiplication μ of t. Horizontal composition is straightforward.

A *wreath* in $\mathcal{K}$ is defined in Lack and Street (2002) to be a monad in $\mathrm{EM}(\mathcal{K})$. Explicitly, a wreath consists of an object A of $\mathcal{K}$, monad t on A, a morphism $s:A\to A$, and 2-cells $\lambda:t\circ s\Rightarrow s\circ t$, $\iota:1_A\Rightarrow s\circ t$, and $\nu:s\circ s\Rightarrow s\circ t$ satisfying seven conditions (on top of those that say t is a monad). Notice that s need not itself be a monad, but it could be while ι and ν could be obtained from the unit and multiplication: in this case λ is called a *distributive law* between the monads t and s.

For any wreath, we obtain a monad structure on the composite endomorphism $s\circ t$. The unit is ι and the multiplication is the composite

$$s\circ t\circ s\circ t\xrightarrow{s\circ\lambda\circ t}s\circ s\circ t\circ t\xrightarrow{\nu\circ\mu}s\circ t\circ t\xrightarrow{s\circ\mu}s\circ t.$$

This composite monad is the *wreath product*.

A wreath is called *Frobenius* when the monad (s,λ) on (A,t) in $\mathrm{EM}(\mathcal{K})$ is equipped with a Frobenius structure. We leave this to the reader to make more explicit [Johnson (1989b)].

Proposition 6.1: *The wreath product of a Frobenius wreath on a Frobenius monad* (A,t) *is Frobenius*.

Proof: Without loss of generality we may suppose $\mathcal{K}$ admits the Eilenberg–Moore construction. We use Theorem 1.6(f). Since (A,t) is Frobenius, the left adjoint f^t to $u^t:A^t\to A$ is also right adjoint. The Eilenberg–Moore construction on the wreath, as a monad in $\mathrm{EM}(\mathcal{K})$, is the wreath product. So the left adjoint of the underlying $(A,s\circ t)\to(A,t)$ is also a right adjoint. Since all 2-functors preserve adjunctions, the 2-functor $\mathrm{EM}(\mathcal{K})\to\mathcal{K}$ assigning to each monad its Eilenberg–Moore construction, assigns to $(A,s\circ t)\to(A,t)$, a morphism $A^{s\circ t}\to A^t$ whose left adjoint is also its right adjoint. The underlying $A^{s\circ t}\to A$ is the composite of the underlyings $A^{s\circ t}\to A^t\to A$, and so has a two-sided adjoint. It follows then that $s\circ t$ is Frobenius. Q.E.D.

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Higher gauge theory—differential versus integral formulation

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The term higher gauge theory refers to the generalization of gauge theory to a theory of connections at two levels, essentially given by 1- and 2-forms. So far, there have been two approaches to this subject. The differential picture uses non-Abelian 1- and 2-forms in order to generalize the connection 1-form of a conventional gauge theory to the next level. The integral picture makes use of curves and surfaces labeled with elements of non-Abelian groups and generalizes the formulation of gauge theory in terms of parallel transports. We recall how to circumvent the classic no-go theorems in order to define non-Abelian surface ordered products in the integral picture. We then derive the differential picture from the integral formulation under the assumption that the curve and surface labels depend smoothly on the position of the curves and surfaces. We show that some aspects of the no-go theorems are still present in the differential (but not in the integral) picture. This implies a substantial structural difference between nonperturbative and perturbative approaches to higher gauge theory. We finally demonstrate that higher gauge theory provides a geometrical explanation for the extended topological symmetry of *BF*-theory in both pictures. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1790048]

I. INTRODUCTION

Gauge theory can be formulated in two ways which we term the differential and the integral picture. As an illustration, recall, for example, Maxwell's equations which can be formulated either in terms of integral equations relating electric and magnetic fluxes through surfaces and currents through solenoids (this is actually the form which corresponds to experimental setups and in which the laws of electrodynamics were originally discovered) (integral picture) or alternatively in terms of the familiar differential equations (differential picture).

Similarly, any gauge theory can be formulated in two ways. Let M be some space–time manifold and the gauge group G be a Lie group with Lie algebra $\mathfrak{g}$. In the differential formulation of gauge theory, one considers a connection of some principal G-bundle $P \to M$. In local coordinates, i.e., using a local trivialization of the bundle, the connection is given by a $\mathfrak{g}$-valued connection 1-form A which transforms under changes of the coordinates as

$$A \mapsto A' = g^{-1}Ag + g^{-1}\,\mathrm{d}g, \tag{1.1}$$

where $g: U_1 \cap U_2 \to G$ denotes a transition function on the overlap of the coordinate patches $U_1, U_2 \subseteq M$.

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The connection is usually taken to be the basic field of the theory, i.e., the variation in the action principle is with respect to A, and in a path integral quantum theory, one must integrate over all possible connections. The Lagrangian and the action of the theory depend on the curvature,

$$F = \mathrm{d}A + \tfrac{1}{2}[A,A], \tag{1.2}$$

which is a $\mathfrak{g}$-valued 2-form. It transforms under coordinate changes in a gauge covariant way,

$$F \mapsto F' = g^{-1}Fg. \tag{1.3}$$

As an alternative to this differential picture, there exists the integral formulation. In this formulation, one uses the group valued parallel transports,

$$U_\gamma = P\exp\left(\int_\gamma A\right) \in G, \tag{1.4}$$

along curves $\gamma:[0,1]\to M, \tau\mapsto\gamma(\tau)$ as the basic variables. Locally, the parallel transport always exists, and it is uniquely determined as the solution of the first order matrix differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}U_\gamma(t) = [A_\mu(\gamma(t))\,\dot\gamma^\mu(t)]U_\gamma(t), \tag{1.5}$$

where we have written

$$U_\gamma(t) = P\exp\left(\int_0^t A_\mu(\gamma(\tau))\,\dot\gamma^\mu(\tau)\mathrm{d}\tau\right), \tag{1.6}$$

for the parallel transport along γ from $\tau=0$ to $\tau=t$. The initial condition is $U_\gamma(0)=1\in G$.

The curvature can then be calculated from the holonomy U_γ of a closed loop γ in the limit in which the loop shrinks to infinitesimal size. This integral picture of gauge theory closely resembles what is done in lattice gauge theory, but without the restriction that the curves must live on some fixed lattice. Note that in the integral formulation, the parallel transports satisfy various relations.

Now let us illustrate the basic idea of higher gauge theory. Suppose first that the gauge group in conventional gauge theory is Abelian, say $G=\mathrm{U}(1)$. Then the connection 1-form A is imaginary and the transition functions are of the form $g(x)=e^{\varphi(x)}$, where $\varphi:\mathrm{U}\to i\mathbb{R}$ is a suitable imaginary valued function, and (1.1) becomes

$$A \mapsto A' = A + \mathrm{d}\varphi, \tag{1.7}$$

so that the curvature 2-form (1.2) is just the exterior derivative,

$$F = \mathrm{d}A. \tag{1.8}$$

Abelian gauge theory with (1.7) and (1.8) now admits the following higher level generalization. Let A be some (imaginary valued) p-form which becomes the basic field of the theory. The Lagrangian and the action depend only on the curvature $(p+1)$-form $F=\mathrm{d}A$. The theory therefore enjoys a local gauge symmetry with the transformation law (1.7) for some $(p-1)$-form φ. This is a consequence of the Poincaré lemma because locally any closed p-form $A-A'$ is of the form $\mathrm{d}\varphi$. The Abelian theory at level p is therefore completely governed by the de Rham cohomology of M.

The Abelian theory at level $p=2$ is known in the physics literature as Kalb–Ramond fields,[1] and at generic level p as p-form electrodynamics.[2] Both refer to the differential picture of the theory. The corresponding integral picture makes use of p-dimensional surfaces labeled with elements of the Abelian group U(1). If the p-surfaces were restricted to a fixed hypercubic lattice, we would have at level $p=0$ the xy model of statistical mechanics, at $p=1$, U(1)-lattice gauge theory, and at higher p the models of Ref. 3.

We refer to these higher level theories as *higher gauge theory*. Does there exist a non-Abelian higher gauge theory, at least at level $p=2$? Many authors[4–8] have attempted to construct such models, but the necessity to find an underlying geometrical picture by suitably generalizing fiber bundles seems to impose serious constraints. To our knowledge, the most thoroughly studied model was the Freedman–Townsend model[4] which, however, has only an Abelian local symmetry and lacks a geometrical understanding of why this must be Abelian.

What precisely are the geometrical conditions involved in higher gauge theory? The coboundary condition $d\circ d=0$ of the Abelian case is, of course, no longer useful as the curvature F is in general no longer just dA, but rather given by (1.2). Assume we have some non-Abelian connection 2-form and wish to define its curvature 3-form. Geometrically, the 2-form would be associated with surfaces labeled by elements of some non-Abelian group H, and the curvature 3-form should be some group element associated with a closed surface, composed from several constituent surfaces that are all labeled with elements of H. Since the group H is non-Abelian and there is no canonical surface order available, we simply do not know how to compose the various non-Abelian labels.

Recall that the points of a curve have a natural order, and the definition of the parallel transport along a given curve indeed makes use of this order. For higher dimensional submanifolds, however, such a canonical order is not available. This lack of natural order has led Teitelboim[9] to the formulation of a no-go theorem ruling out the existence of non-Abelian gauge theories for extended objects. This applies essentially to any gauge theory whose connection is a non-Abelian p-form, $p\geqslant 2$.

With the introduction of 2-categories in mathematics, it recently became possible to sidestep this no-go theorem at $p=2$. On the mathematical side, there is the construction of non-Abelian gerbes generalizing fiber bundles, see, for example, Ref. 10. It is expected that gerbes provide the desired generalization of fiber bundles. They are, for example, conjectured to play a role in theories on coincident 5-branes is string theory, see for example, Refs. 11 and 12. In the present paper, we prefer a slightly different approach based on the definition of Lie 2-groups by Baez[13] which generalize ordinary Lie groups to a higher level and which include the symmetries of gerbes at least in the case of strict categories. This will allow us to explicitly solve the surface ordering problem, thereby providing a rigorous basis for Chepelev's conjectures,[7] and to see in detail how Teitelboim's no-go theorem is avoided. Our results finally provide the geometrical background to most of the traditional approaches to non-Abelian 2-forms, at least as long as strict categories are sufficient, and explain geometrically why there are some restrictions that become effective only if one requires smooth 1- and 2-forms, but not necessarily in a nonperturbative approach. It comes as a surprise that *BF*-theory which is usually not mentioned in the context of non-Abelian 2-forms, does form a nontrivial example of higher gauge theory.

Let us now briefly outline our approach. Starting from the notion of Lie 2-groups, Baez has defined Lie 2-algebras and started to generalize the differential picture of gauge theory to a theory involving non-Abelian connection 1- and 2-forms.[13] Open questions in this approach are the precise form of the local gauge transformations and of the gauge invariant expressions which are required in order to define Lagrangians and actions in physics.

Also starting from the notion of Lie 2-groups, we have generalized the integral picture of gauge theory to a theory involving curves and surfaces labeled with elements of non-Abelian groups.[14] This formulation has the advantage that the theory of 2-categories dictates the form of the local gauge transformations and the expressions for the gauge invariant quantities. The no-go theorems can be avoided because the underlying 2-categorical structure leads to a nontrivial interplay of the curve and surface labels.

An important question is how the differential[13] and the integral approach[14] are related. In this paper, we start from the integral picture of Ref. 14 and systematically derive the corresponding differential expressions by studying the non-Abelian curve and surface labels of the theory in the infinitesimal limit, assuming that the labels depend smoothly on the curves and surfaces. In the smooth case, we find an additional flatness condition at level 1 which has not yet appeared in the

literature. It implies in particular that the non-Abelian part of the connection 2-form agrees with the curvature of the connection 1-form, that the curvature 2-form vanishes and that the curvature 3-form is Abelian.

We show that an interesting example of higher gauge theory is given by *BF*-theory with non-Abelian gauge group[15] in which the level-1 flatness is a key feature of the theory, in fact encoded in the field equations. The theory of 2-categories then provides the explanation for the extended local (topological) symmetry. Otherwise, the resulting conditions show that the classic no-go theorems reappear only in the differential picture in which they rule out the naive generalization of the Yang–Mills action. The algebraic structure of the integral picture, however, still allows us to have nontrivial central group elements that characterize the 2-curvature associated with closed labeled surfaces which we call 2-holonomies. If the center of the gauge group is discrete such as, for example, for SU(N), the differential picture would require these central elements to be trivial, but in the integral picture and in any nonperturbative quantum theory based on it, no such restriction applies. The integral picture is therefore more general than the differential one and is in some sense essentially nonperturbative.

Since the nontrivial central elements can be interpreted as the presence of singularities of codimension 2, one can say that the integral picture of higher gauge theory rather predicts the existence of topological defects in the differential formulation.

The present paper is structured as follows. In Sec. II, we recall the construction of higher gauge theory in the integral formulation as it was developed in Ref. 14. Our presentation is self-contained. We emphasize the calculational aspects and try to hide as much as possible of the 2-category theory in our notation. In Sec. III, we then derive the differential formulation of higher gauge theory starting from the integral picture and compare the result with Ref. 13. We conclude in Sec. IV with comments on interesting questions for further investigations.

II. THE INTEGRAL FORMULATION

In this section, we review the integral picture of higher gauge theory following Ref. 14. We call the higher level model a 2-*gauge theory* whereas we refer to conventional gauge theory as a 1-*gauge theory* in view of the hierarchy of models sketched in Ref. 14. The theory is formulated at the integral level, i.e., it describes curves and surfaces which are labeled with data from some algebraic structure, supplementing the parallel transports of conventional 1-gauge theory by additional group elements which are used to label surfaces.

A. Lie 2-groups

The algebraic structure required to describe a 1-gauge theory is just some gauge group G, usually taken to be a Lie group. The geometric objects that are labeled with algebraic data, are the curves giving rise to the parallel transports of the theory. The group structure ensures that we can consistently compose (multiply) parallel transports and also reverse their direction (inversion).

The algebraic structure for a 2-gauge theory is a so-called 2-group.[13,16] This is a pair G, H of groups with two maps. (We define here a *crossed module*, a structure from which we can construct a strict 2-group.[13,16]) The first map is a group homomorphism $t: H \to G$, i.e.,

$$t(h_1 \cdot h_2) = t(h_1) \cdot t(h_2), \tag{2.1}$$

$$t(1) = 1, \tag{2.2}$$

for all $h_1, h_2 \in H$. The second map is an action of G on H by automorphisms. This is an operation $g \triangleright h$ taking values in H, which is a group action, i.e.,

$$(g_1 \cdot g_2) \triangleright h = g_1 \triangleright (g_2 \triangleright h), \tag{2.3}$$

$$1 \triangleright h = h, \tag{2.4}$$

for all $g_1, g_2 \in G$ and $h \in H$, such that $h \mapsto g \triangleright h$ is a homomorphism for each $g \in G$, i.e.,

$$g \triangleright (h_1 \cdot h_2) = (g \triangleright h_1) \cdot (g \triangleright h_2), \tag{2.5}$$

$$g \triangleright 1 = 1, \tag{2.6}$$

for all $h_1, h_2 \in H$. These maps are required to satisfy the following two compatibility conditions:

$$t(g \triangleright h) = g \cdot t(h) \cdot g^{-1}, \tag{2.7}$$

$$t(h) \triangleright h' = h \cdot h' \cdot h^{-1}, \tag{2.8}$$

for all $g \in G, h, h' \in H$. A Lie 2-group is a 2-group in which G and H are Lie groups and both maps t and $\triangleright$ are smooth.

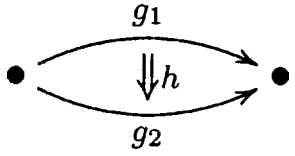
Plenty of examples of Lie 2-groups are known.[13,14] Here we mention the following cases.

(1) The *Euclidean* and *Poincaré 2-groups*. Here $H = \mathbb{R}^n$ is Euclidean or Minkowski space and $G = \mathrm{SO}(n)$ or $\mathrm{SO}(n-1,1)$. The map t is trivial, i.e., $t(h) = 1$ for all $h \in H$, and $\triangleright$ is the obvious action by rotation.
(2) More generally, one can choose H to be any vector space on which the Lie group G is represented. The map t is trivial in this case, and $\triangleright$ and is the action of G on its representation H. In this way, one defines, for example, the *adjoint* and the *co-adjoint* 2*-groups* in which $H = \mathfrak{g}$ or $H = \mathfrak{g}^*$ where $\mathfrak{g}$ denotes the Lie algebra of G.
(3) The *automorphism* 2*-groups*. Let H be any Lie group and G its group of automorphisms. The action $g \triangleright h$ is the application of the particular automorphism, and $t: H \to G$ associates with each element h the corresponding *inner automorphism* $h' \mapsto hh'h^{-1}$. This example is related to non-Abelian gerbes.[13] For example, if $H = \mathrm{SU}(2)$, we have $G = \mathrm{SU}(2)/\mathbb{Z}_2 \cong \mathrm{SO}(3)$ where $\mathbb{Z}_2$ is the centre of SU(2). In general, $\ker t \subseteq Z(H)$ is always contained in the center of H.

B. 2-gauge theory

In a 2-gauge theory, we have to label geometric objects at two levels. Curves are labeled by elements of G. Their composition and orientation reversal is defined as in conventional gauge theory.

In addition, surfaces are labeled with elements of H. For each surface (the elementary surfaces are chosen to have the topology of a disk), we choose two reference points on the boundary (full dots in the diagram below, we are going to suppress them later on) and split the boundary into two curves with labels $g_1 \in G$ (*source*) and $g_2 \in G$ (*target*) as follows:



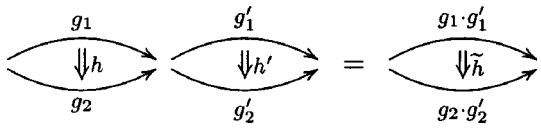
(2.9)

The label h of the surface is required to satisfy

$$t(h) = = g_2 \cdot g_1^{-1}, \tag{2.10}$$

i.e., $t(h)$ is the (inverse) holonomy along the boundary curve. This condition appears when we use the Lie crossed module in order to construct a Lie 2-group.[13,14,16] The first reference point is the base point of this holonomy and therefore plays a role in (2.10) whereas the second reference point does not enter this condition.

We can now compose surfaces in two different ways. First, we can join them *horizontally* in one common reference point,

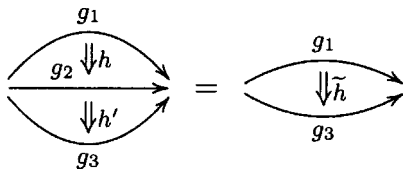


(2.11)

where the label of the composition is given by

$$\tilde{h} = h \cdot (g_1 \triangleright h'). \tag{2.12}$$

Note the asymmetry: the source of the first surface acts on the label of the second one. [The pairs (h, g_1) of surface label and source curve label form the semidirect product $H \rtimes G$ under horizontal composition.] As required, it follows that $t(\tilde{h}) = (g_2 g_2')(g_1 g_1')^{-1}$. Alternatively, we can glue the surfaces *vertically* along a common curve,



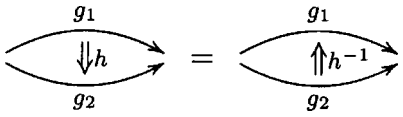
(2.13)

where the composition is simply given by

$$\tilde{h} = h' \cdot h. \tag{2.14}$$

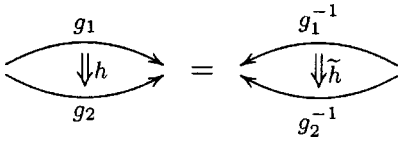
Observe that $t(\tilde{h}) = g_3 g_1^{-1}$ as expected.

The orientation of a surface can be reversed if it is labeled by the inverse element h^{-1} instead,



(2.15)

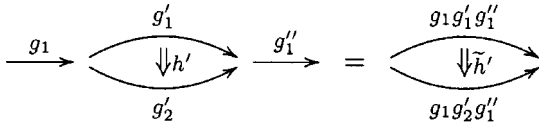
Both source and target curve of some surface can be reversed,



(2.16)

if the surface label is replaced by $\tilde{h} = g_1^{-1} \triangleright h^{-1}$. Observe that $t(\tilde{h}) = g_2^{-1}(g_1^{-1})^{-1}$ as required.

An important operation is known as *whiskering*. By attaching whiskers to a surface h, for example, attaching whiskers g_1 and g_1'' to some surface h' with source g_1' and target g_2',



(2.17)

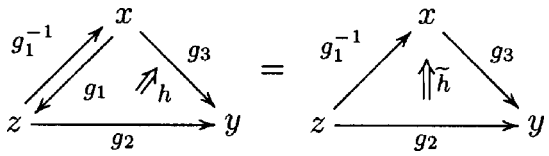
we can construct a surface with source $g_1 g_1' g_1''$ and target $g_1 g_2' g_1''$, carrying the label

$$\tilde{h}' = g_1 \triangleright h'. \tag{2.18}$$

The attachment of the left whisker can be understood as a special case of the horizontal composition (2.11) in which $g_1 = g_2$ and $h = 1$ so that the left surface collapses to a line. A similar

argument is available for the right whisker. The asymmetry in the expression (2.18) originates from the asymmetry of the horizontal composition (2.12).

Whiskering allows us to change the reference points of a surface. For example, starting from a surface h with reference points x and y, i.e., source $g_1 \cdot g_2$ and target g_3,



(2.19)

we can whisker from the left by g_1^{-1} and obtain the surface $\tilde{h}=g_1^{-1}\triangleright h$ with reference points z and y, i.e., source g_2 and target $g_1^{-1}\cdot g_3$.

Given any collection of curves and surfaces, a *configuration* of 2-gauge theory is an assignment of elements of G to the curves and of elements of H to the surfaces so that the following conditions hold. Compositions of curves are labeled by the product of elements in G, curves of opposite orientation are labeled by the inverse group element. For each surface labeled by $h \in H$, we have $t(h)=g_2\cdot g_1^{-1}$ where g_1 and g_2 are the source and target curve, respectively. Finally, compositions of surfaces, and surfaces whose reference points have been changed, are labeled as described above in this section. The configurations thus defined can be viewed as the classical configurations of 2-gauge theory or, in a path integral quantum theory, these are the configurations over which we sum in the path integral. The path integral was given in detail in Ref. 14.

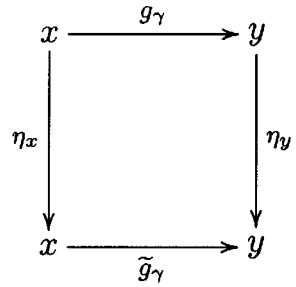
C. Local 2-gauge transformations

The 2-gauge theory defined in the preceding section enjoys an extended local gauge symmetry which we call a *local* 2*-gauge symmetry*.

First recall the conventional local 1-gauge symmetry in a formulation of gauge theory in the language of parallel transports. A local gauge transformation is given by a *generating function* assigning group elements $\eta_x, \eta_y \in G$ to the points. For each curve γ from point x to point y with label $g_\gamma \in G$, the transformed parallel transport is then calculated by

$$\tilde{g}_\gamma = \eta_x^{-1} g_\gamma \eta_y, \tag{2.20}$$

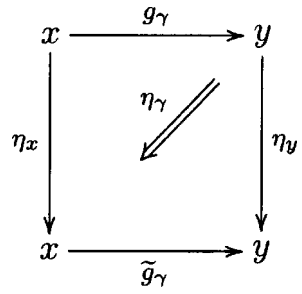
which we visualize by the following diagram:



(2.21)

We say that the diagram *commutes*, i.e., it does not matter which way a round we go from one corner to another. If we view all four labeled curves g_γ, $\tilde{g}_\gamma$, η_x, and η_y as a gauge connection, then this connection is *flat*, i.e., the parallel transport is path independent.

In 2-gauge theory, the local gauge transformation (2.20) is weakened by extending the generating function to the next level. The 2*-generating function* not only assigns group elements $\eta_x, \eta_y \in G$ to the points, but there is the additional freedom of choosing elements $\eta_\gamma \in H$ for the curves. (These curve labels are in general path dependent.) Diagram (2.21) is generalized to



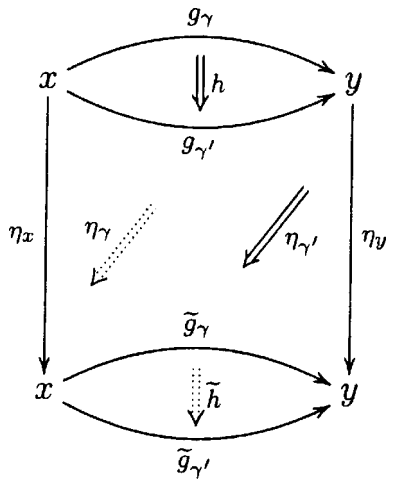
(2.22)

where we require $t(\eta_\gamma)=(\eta_x\tilde{g}_\gamma)(g_\gamma\eta_y)^{-1}$. The full diagram involving g_γ, $\tilde{g}_\gamma$, η_x, η_y, and η_γ can therefore be viewed as a configuration of 2-gauge theory in which the surface labeled with η_γ has the source $g_\gamma\cdot\eta_y$ and the target $\eta_x\cdot\tilde{g}_\gamma$. We can thus calculate the gauge transformed parallel transport by

$$\tilde{g}_\gamma = \eta_x^{-1}t(\eta_\gamma)g_\gamma\eta_y, \tag{2.23}$$

which generalizes the conventional local gauge transformation (2.20).

This is the prescription of how to transform the curve labels. In 2-gauge theory, we must specify in addition how to transform the surface labels. Therefore we write down the surface analogue of the diagram (2.21) and require that for each surface labeled $h\in H$ with source and target curves γ, γ' labeled by g_γ and $g_{\gamma'}$, the following "tin can" diagram:



(2.24)

2-*commutes*. This means that it does not matter which way round we compose the labeled surfaces, i.e., the configuration of 2-gauge theory shown in diagram (2.24) is 2-*flat*. The top of this "tin can" is the old configuration and the bottom the new one with curve labels $\tilde{g}_\gamma$, $\tilde{g}_{\gamma'}$ and surface label $\tilde{h}$. The transformed surface label is thus given by

$$\tilde{h} = \eta_x^{-1}\triangleright(\eta_{\gamma'}h\eta_\gamma^{-1}). \tag{2.25}$$

We can summarize this paragraph as follows. The local 2-gauge transformations are given by 2-generating functions which assign elements of G to the points and elements of H to the curves. The transformed curve and surface labels are then determined by (2.23) and (2.25). Although, at first sight, these transformation rules look quite artificial, they follow immediately from the underlying 2-categorical structure.[14]

D. Pure 2-gauge and 2-flatness

In conventional 1-gauge theory, we say that a configuration is *pure gauge* if it is gauge equivalent to the trivial connection in which all curves are assigned the group unit. A configuration

is therefore pure gauge if there exists a generating function associating group elements $\eta_j \in G$ with all points so that the parallel transports are given by

$$g_{12} = \eta_1^{-1}\eta_2, \tag{2.26}$$

for any curve from 1 to 2, cf. (2.20). Observe that any configuration which is pure gauge, is also *flat*, i.e., its parallel transports are path independent.

In complete analogy, we say that a configuration of 2-gauge theory is *pure* 2-*gauge* if it is 2-gauge equivalent to the trivial configuration in which all curves are labeled by the group unit of G and all surfaces by the group unit of H. A configuration with curve labels $g_\gamma, g_{\gamma'} \in G$ and surface labels $h \in H$ is therefore pure 2-gauge if there exists a 2-generating function that assigns elements $\eta_x, \eta_y \in G$ to the points and $\eta_\gamma, \eta_{\gamma'} \in H$ to the curves such that for any curve γ from x to y,

$$g_\gamma = \eta_x^{-1} t(\eta_\gamma)\eta_y, \tag{2.27}$$

and for any surface with source curve g_γ and target curve $g_{\gamma'}$,

$$h = \eta_x^{-1} \triangleright (\eta_{\gamma'}\eta_\gamma^{-1}), \tag{2.28}$$

cf. (2.23) and (2.25).

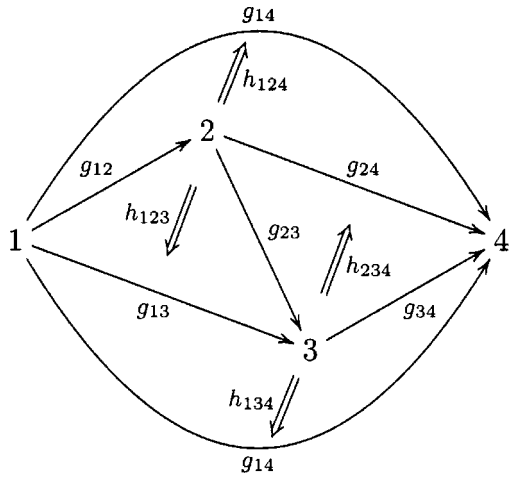
A configuration of 2-gauge theory is called 2-*flat* if the surface label on any surface of topology S^2 which is the boundary of a 3-ball, is just the group unit $1 \in H$. As a consequence, in 2-flat configurations, the surface label of any disk shaped surface depends only on the boundary (source and target) curve labels in G. Note also that being pure 2-gauge implies 2-flatness.

E. Composition of labeled surfaces

In this section, we describe how the language of 2-gauge theory can be used in order to define compositions of labeled surfaces. We will make use of this surface composition in Sec. II F in order to construct gauge invariant quantities that are associated with closed surfaces, and in Sec. III in order to derive the differential formulation.

In Sec. II B, we have introduced a number of operations by which we can modify and combine labeled surfaces: vertical and horizontal composition, two types of orientation reversal and the change of reference point by whiskering. These rules can be employed in order to calculate the composition of elementary surfaces to arbitrarily large ones.

We illustrate this procedure for the boundary surface of a tetrahedron,



(2.29)

We have numbered the vertices by 1, 2, 3, 4. The edges (j,k), $j<k$, are labeled by group elements $g_{jk} \in G$ and the triangles (j,k,ℓ), $j<k<\ell$, by elements $h_{jk\ell} \in H$. We have oriented the triangles

(j,k,ℓ) so that they have the source $g_{jk}\cdot g_{k\ell}$ and the target $g_{j\ell}$, i.e., $t(h_{jk\ell})=g_{j\ell}(g_{jk}g_{k\ell})^{-1}$.

We choose reference points, here 1 and 4, and cut the tetrahedron surface along the edge (14). This *base edge* forms both the source and the target curve of the surface. Imagine that a curve starting from the source sweeps out the entire surface until it reaches the target. This determines the ordering of the vertical composition of the constituent surfaces. We just have to make sure that all surfaces are composable, i.e., they have the suitable reference points and the correct orientation in order to compose them vertically by (2.13).

Consider the diagram (2.29). We first move the curve from g_{14} to $g_{12}g_{24}$ via h_{124}^{-1}. At this stage we cannot compose the result with the triangle (123) because source and target would not match, but we can use the orientation reversed triangle (234), whiskered from the left by g_{12}. This moves our curve to $g_{12}g_{23}g_{34}$ using the label $g_{12}\triangleright h_{234}^{-1}$ of the whiskered and reversed surface. In the next step, we can use the triangle (123), whiskered from the right by g_{34} which does not change the label h_{123}. Finally, we move our curve from $g_{13}g_{34}$ to g_{14} along h_{134}.

The label associated to the boundary surface of the tetrahedron is therefore the vertical composition, cf. (2.13),

$$\tilde{h}=h_{134}h_{123}(g_{12}\triangleright h_{234}^{-1})h_{124}^{-1}. \tag{2.30}$$

This is a useful notation for the automorphism 2-group in which typically both G and H are non-Abelian. In the case of the Euclidean and the Poincaré 2-groups, it is preferable to write the group structure of H additively, i.e.,

$$\tilde{h}=h_{134}+h_{123}-g_{12}\triangleright h_{234}-h_{124}. \tag{2.31}$$

The following geometrical picture illustrates the surface composition. Imagine the surface labels $h_{jk\ell}$ are interpreted in a local coordinate system associated with their first reference point j, the common starting point of their source and target curves. If we vertically compose surfaces that are based at the same reference point, i.e., whose labels are given in the same coordinate system, the composition is just the group product in H, cf. (2.14). If the reference points and therefore the coordinate systems are different, however, then we must parallel transport before we can compare and multiply their surface labels. In the example (2.30), this is relevant for the surface h_{234}, the only surface that is not based at point 1 but rather at 2. We have to whisker h_{234}^{-1} from the left by g_{12} in order to obtain a surface $g_{12}\triangleright h_{234}^{-1}$ with reference point 1.

For a closed surface of topology S^2, i.e., of genus zero, source and target curve agree so that $t(\tilde{h})=1$. Recall that $\ker t\subseteq Z(H)$ is always contained in the center $Z(H)$ of H and therefore Abelian. We call the labels $h\in\ker t$ of closed surfaces the 2-*holonomies* of the theory.

F. Gauge invariant expressions

For all the assignments of algebraic data to geometric objects, we should understand how they depend on the choices made. Consider, for example, the holonomy along a closed loop (*Wilson loop*) in conventional gauge theory. It still depends on the base point of the loop. It does so, however, in a well-understood way. Changing the base point leads to the conjugation of the holonomy with the parallel transport from the old to the new base point. Any group character applied to the holonomy yields an invariant. Observe that the independence of the base point and the invariance under local gauge transformations are both implemented by the same operation, namely by calculating the character. Due to its gauge invariance, the character can then serve as the Lagrangian or as the action of a physical theory.

An analogous result can be shown for the integral picture of 2-gauge theory.[14] Consider a closed surface of topology S^2, for example, the surface of the tetrahedron (2.29). We must choose a *base edge* at which we start and finish the surface composition. In our tetrahedron example this was the edge (14). When we change the base edge, holding its two end points fixed, then the 2-holonomy h' of such a closed surface (*Wilson surface*) is conjugated,

$$h' \mapsto hh'h^{-1}, \tag{2.32}$$

by the label $h \in H$ associated with the surface enclosed between the old and the new base edge. If we change the reference point of a closed surface (the starting point of its base edge) by whiskering with $g \in G$, then the 2-holonomy is acted upon by the corresponding parallel transport,

$$h' \mapsto g \triangleright h'. \tag{2.33}$$

We have seen that the 2-holonomies, i.e., the labels h' associated with closed surfaces, are contained in $\ker t$. The functions s: $\ker t \to \mathbb{R}$ that are independent of the base edge and of the reference points, i.e., that satisfy for all $g \in G$, $h \in H$, and $h' \in \ker t$,

$$\begin{aligned} s(hh'h^{-1}) &= s(h'), \\ s(g \triangleright h') &= s(h'), \end{aligned} \tag{2.34}$$

are called *2-actions*. We have shown in Ref. 14 that these are precisely the functions of the 2-holonomy that are invariant under the local 2-gauge transformations (2.23) and (2.25), hence the name. They form the generalization of the Wilson action to 2-gauge theory.

For the Euclidean and Poincaré 2-groups, the 2-actions are the maps $s: H \to \mathbb{R}$ that are constant on the orbits of G on $H = \mathbb{R}^n$, i.e., they are functions of the invariant Euclidean or Minkowski norm, $s(v) = f(\eta(v,v))$ where $f: \mathbb{R} \to \mathbb{R}$ is any function, $v \in \mathbb{R}^n$, and η denotes the Euclidean or Minkowski scalar product. For the automorphism 2-group, any map $s: Z(H) \to \mathbb{R}$ gives rise to an acceptable 2-action.

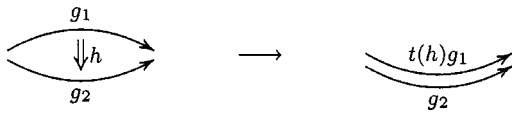
Even though there exists no canonical surface ordering, we have shown, using ideas from the theory of 2-categories, that the interplay of curves and surfaces not only circumvents the no-go theorems, but also provides us with an unambiguous and gauge covariant composition of labeled surfaces.

Whereas in conventional gauge theory, the gauge invariant expressions are associated with closed loops, we have seen that in 2-gauge theory, we can form 2-gauge invariant expressions for closed surfaces. Is there a also a 2-gauge invariant expression associated with loops, i.e., a direct generalization of the Wilson loop to 2-gauge theory?

Recall that in a 1-gauge theory, we would just calculate the (real part of a unitary) character,

$$\chi(g_2^{-1} g_1), \tag{2.35}$$

of the holonomy $g_2^{-1} g_1 \in G$ in order to obtain a locally 1-gauge invariant expression. If we take into account a possibly nontrivial transport of curves along surfaces, then we cannot directly compare the two curve labels g_1 and g_2, but rather we must surface transport one curve onto the other,



(2.36)

Rather than the usual holonomy $g_2^{-1} g_1$, we should therefore consider the expression,

$$\mathcal{F} = g_2^{-1} t(h) g_1, \tag{2.37}$$

which takes the surface transport into account. Due to condition (2.10), however, this expression always gives the group unit of G, $\mathcal{F} = 1$.

There is therefore no loop based gauge invariant expression in 2-gauge theory which would generalize the Wilson loop of 1-gauge theory, but only the surface based construction with the invariance (2.34).

III. THE DIFFERENTIAL FORMULATION

In this section, we derive the differential formulation of 2-gauge theory which corresponds to the integral picture of the preceding section. We therefore study the integral formulation of 2-gauge theory on squares, cubes, and hypercubes, assume that the labels depend smoothly on the positions of the curves and surfaces and consider the limit in which these shrink to infinitesimal size.

The theory we derive uses the same connection 1- and 2-forms as Baez[13] which have also been found independently by Hofman,[8] but with a flatness condition at level 1 which has not yet appeared in the literature. As a bonus, we can also derive the local gauge transformations.

A. Lie 2-algebras

Just as the differential picture of conventional gauge theory involves the Lie algebra $\mathfrak{g}$ of the gauge group G, we need here the appropriate generalized notion of a Lie algebra associated with the gauge 2-group.

A *Lie 2-algebra* consists of two Lie algebras $\mathfrak{g}$ and $\mathfrak{h}$ with two maps. (We describe here a differential crossed module, a structure from which we can construct a strict Lie 2-algebra.[13,17]) The first map, $\tau:\mathfrak{h}\to\mathfrak{g}$, is a homomorphism of Lie algebras, i.e., a linear map that satisfies

$$\tau([Y_1,Y_2])=[\tau(Y_1),\tau(Y_2)], \tag{3.1}$$

for all $Y_1,Y_2\in\mathfrak{h}$. The second map is an action of $\mathfrak{g}$ on $\mathfrak{h}$ by derivations, i.e., a bilinear operation $X\triangleright Y$ for $X\in\mathfrak{g}$, $Y\in\mathfrak{h}$, taking values in $\mathfrak{h}$, such that it is an action, i.e.,

$$[X_1,X_2]\triangleright Y=X_1\triangleright(X_2\triangleright Y)-X_2\triangleright(X_1\triangleright Y), \tag{3.2}$$

for all $X_1,X_2\in\mathfrak{g}$ and $Y\in\mathfrak{h}$, and such that for any $X\in\mathfrak{g}$, the map $Y\mapsto X\triangleright Y$ is a derivation on $\mathfrak{h}$, i.e., linear and,

$$X\triangleright[Y_1,Y_2]=[X\triangleright Y_1,Y_2]+[Y_1,X\triangleright Y_2], \tag{3.3}$$

for all $Y_1,Y_2\in\mathfrak{h}$. These maps are required to satisfy the following two compatibility conditions:

$$\tau(X\triangleright Y)=[X,\tau(Y)], \tag{3.4}$$

$$\tau(Y)\triangleright Y'=[Y,Y'], \tag{3.5}$$

for all $X\in\mathfrak{g}$, $Y,Y'\in\mathfrak{h}$.

Given some Lie 2-group in terms of the Lie groups G, H and the maps t and $\triangleright$ (Sec. II A), one can construct its Lie 2-algebra as follows.[17] The Lie algebras $\mathfrak{g}$ and $\mathfrak{h}$ are the Lie algebras of the Lie groups G and H. The map $\tau:\mathfrak{h}\to\mathfrak{g}$ is the derivative $\tau=\mathrm{d}t$ of the map $t:H\to G$. Finally, let the map,

$$\alpha:G\to \mathrm{Aut}\,H,\quad \alpha(g)[h]:=g\triangleright h, \tag{3.6}$$

associate an automorphism $\alpha(g)$ of H with each element $g\in G$. Then the derivative of α,

$$\mathrm{d}\alpha:\mathfrak{g}\to \mathrm{Der}\ \mathfrak{h},\quad X\mapsto \mathrm{d}\alpha(X), \tag{3.7}$$

associates with each element $X\in\mathfrak{g}$ a derivation $\mathrm{d}\alpha(X)$ of $\mathfrak{h}$. The operation $\triangleright$ in the definition of the Lie 2-algebra is chosen to be $X\triangleright Y:=\mathrm{d}\alpha(X)[Y]$.

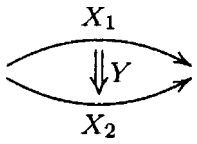
Consider first the Lie 2-algebra of the Euclidean and Poincaré 2-groups. In this case, $\mathfrak{g}=\mathfrak{so}(n)$ or $\mathfrak{g}=\mathfrak{so}(n-1,1)$, and $\mathfrak{h}=\mathbb{R}^n$. The action of $\mathfrak{g}$ on $\mathfrak{h}$ is in the defining representation of $\mathfrak{g}$, and the map $\tau:\mathfrak{h}\to\mathfrak{g}$ is the null map.

For the automorphism 2-group of $H=\mathrm{SU}(2)$, we have $G=\mathrm{SU}(2)/\mathbb{Z}_2$. In this case, both Lie algebras agree, $\mathfrak{g}=\mathfrak{h}$, and we have $t(Y)=Y$ for all $Y\in\mathfrak{h}$. Finally, the action of $\mathfrak{g}$ on $\mathfrak{h}=\mathfrak{g}$ is the adjoint action, $X\triangleright Y=[X,Y]$.

Let us conclude this section with a remark on the category theory underlying the construction of Lie 2-algebras. When we construct a Lie 2-algebra from the differential crossed module, there is the condition [analogous to (2.10)],

$$\tau(Y) = X_2 - X_1, \tag{3.8}$$

for each 2-cell,



(3.9)

$X_i \in \mathfrak{g}$, $Y \in \mathfrak{h}$, of the 2-category which is defined by the Lie 2-algebra. In the gauge theory language, this would correspond to an infinitesimally small surface. The condition (3.8) is in fact already present in the 2-vector spaces of Ref. 17.

B. Notation

For the discussion of the differential picture of higher gauge theory, we restrict ourselves to trivial bundles and present the theory in the language of the $\mathfrak{g}$- and $\mathfrak{h}$-valued connection 1- and 2-forms. As we will see in the following section, the basic fields of the differential picture are a $\mathfrak{g}$-valued connection 1-form A and an $\mathfrak{h}$-valued connection 2-form B.

We denote by d_A the exterior covariant derivative for the connection A which acts on $\mathfrak{g}$-valued p-forms φ by

$$\mathrm{d}_A(\varphi) = \mathrm{d}\varphi + [A, \varphi]. \tag{3.10}$$

Here the bracket of a 1-form A with a p-form φ, both taking values in $\mathfrak{g}$, is defined by

$$[A, \varphi] := A^a \wedge \varphi^b [T_a, T_b], \tag{3.11}$$

where we have chosen a basis (T_a) of $\mathfrak{g}$ and written $A = A^a T_a$, $\varphi = \varphi^b T_b$ with coefficient forms A^a and φ^b. Summation over repeated indices is understood. Similarly, we define the action of d_A on $\mathfrak{h}$-valued p-forms ψ, using the action of $\mathfrak{g}$ on $\mathfrak{h}$ via the operation $\triangleright$,

$$\mathrm{d}_A(\psi) = \mathrm{d}\psi + A \triangleright \psi, \tag{3.12}$$

where the $\triangleright$ of a $\mathfrak{g}$-valued 1-form with an $\mathfrak{h}$-valued p-form is defined by

$$A \triangleright \psi := A^a \wedge \psi^b (T_a \triangleright T'_b), \tag{3.13}$$

where (T_a) denotes a basis of $\mathfrak{g}$ and (T'_b) a basis of $\mathfrak{h}$. We calculate for $\mathfrak{g}$-valued p-forms φ,

$$(\mathrm{d}_A \circ \mathrm{d}_A)(\varphi) = [F, \varphi], \tag{3.14}$$

and for $\mathfrak{h}$-valued p-forms ψ,

$$(\mathrm{d}_A \circ \mathrm{d}_A)(\psi) = F \triangleright \psi. \tag{3.15}$$

C. Configuration variables and their curvature

We shall first identify the basic fields and their associated curvature. We then compute their respective transformations under the local 2-gauge transformations.

We assume that all labels depend smoothly on the curves and surfaces. The key idea for the derivation of the differential picture is to write down the integral formulation on squares and cubes

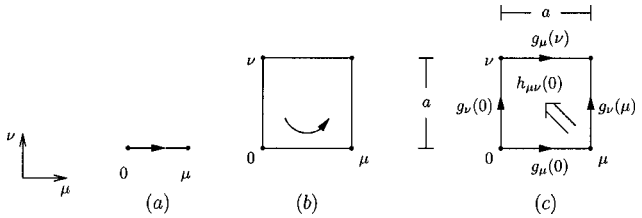


FIG. 1. Conventions for the integral formulation of 2-gauge theory on the squares, in particular (c) the generalized holonomy (3.22).

and then to study the limit in which these shrink to infinitesimal size. We write the labels $g \in G$, $h \in H$ as exponentiated curve and surface integrals over approximately constant differential forms,

$$g_\mu(0) = e^{\int_\gamma A} \sim e^{aA_\mu},$$
$$h_{\mu\nu}(0) = e^{\int_S B} \sim e^{a^2 B_{\mu\nu}}. \tag{3.16}$$

Here γ denotes a curve of length a from $x=0$ to $x=\mu$ and S a square of area a^2 in the $(\mu\nu)$-plane. We abbreviate the coordinates by $x=\mu := ae_\mu$ where e_μ is a vector of unit length. All A_μ, etc., without argument are at $x=0$.

The basic fields in the differential picture are the $\mathfrak{g}$-valued connection 1-form $A=A_\mu\,\mathrm{d}x^\mu$ and the $\mathfrak{h}$-valued connection 2-form $B=\frac{1}{2}B_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu$. Note that $h_{\mu\nu}=h_{\nu\mu}^{-1}$.

We will make use of the usual Taylor expansion,

$$g_\mu(\alpha) \sim e^{aA_\mu + a^2\partial_\alpha A_\mu}, \tag{3.17}$$

$$h_{\mu\nu}(\alpha) \sim e^{a^2 B_{\mu\nu} + a^3 \partial_\alpha B_{\mu\nu}}. \tag{3.18}$$

When we have a product of Lie group elements, the Baker–Hausdorff formula allows us to get the corresponding operation at the Lie algebra level,

$$e^x e^y = e^{x+y+(1/2)[x,y]+\cdots}. \tag{3.19}$$

The action $\mathrm{d}\alpha$ of $\mathfrak{g}$ on $\mathfrak{h}$ is the infinitesimal version of the action of G over H,

$$g_\beta(0) \triangleright h_{\mu\nu}(\beta) \sim e^{a^2 B_{\mu\nu} + a^3 \partial_\beta B_{\mu\nu} + a^3\, \mathrm{d}\alpha(A_\beta)(B_{\mu\nu})}. \tag{3.20}$$

The map $\tau:\mathfrak{h}\to\mathfrak{g}$ is the infinitesimal version of the map $t:H\to G$,

$$t(h_{\mu\nu}) \sim e^{a^2 \tau(B_{\mu\nu})}. \tag{3.21}$$

As mentioned earlier, they satisfy the compatibility conditions (3.5) and (3.4). The approximations (3.16)–(3.20) together with (3.4) and (3.5) are all we need in order to derive the differential picture.

So far we have identified as the basic fields the generalized connection (A,B) in agreement with Ref. 13. Let us now calculate a curvature 2-form, using the holonomy around an infinitesimal square, and a curvature 3-form, using the 2-holonomy around an infinitesimal cube.

In 1-gauge theory, the curvature 2-form is given by an infinitesimal Wilson loop. In the context of 2-gauge theory, it depends also on the B-field because of (2.37). The expression $\mathcal{F}$ of (2.37) reads for the square of Fig. 1(c),

$$e^{a^2\tilde{F}_{\mu\nu}} \sim \mathcal{F}_{\mu\nu} = g_\mu^{-1}(\nu) g_\nu(0)^{-1} t(h_{\mu\nu}(0)) g_\mu(0) g_\nu(\mu). \tag{3.22}$$

Using the approximations (3.16)–(3.19) and dropping all terms of order a^3 in the exponent, we obtain the curvature 2-form $\tilde{F}_{\mu\nu}=\frac{1}{2}\tilde{F}_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu$ as follows:

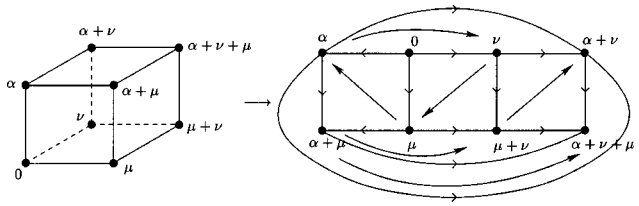


FIG. 2. A flattend cube in order to read off the 2-holonomy (3.26)

$$\tilde{F}_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] + \tau(B_{\mu\nu}) = F_{\mu\nu} + \tau(B_{\mu\nu}), \tag{3.23}$$

where F denotes the conventional curvature of A. This agrees with Baez's expression[13] (up to a sign which is matter of convention),

$$\tilde{F} = \mathrm{d}A + \frac{1}{2}[A,A] + \tau(B) = F + \tau(B). \tag{3.24}$$

We have therefore found a geometrical interpretation for the generalized curvature $\tilde{F}$ from the surface transport of the curve (2.36).

It is important here to remember that in the definition of a strict Lie 2-group, we have $\mathcal{F} = 1 \in H$ in (2.37) and therefore at the differential level,

$$\tau(B) = -F. \tag{3.25}$$

This condition is the alter ego of the equations (2.10) and (3.8) and has some drastic consequences: it means that the curvature 2-form $\tilde{F}$ is always zero.

Let us now compute the curvature 3-form $G = \frac{1}{6} G_{\alpha\mu\nu}\, \mathrm{d}x^\alpha \wedge \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu$ associated with A and B. It is the differential counterpart of the 2-holonomy around a cube (Fig. 2).

To calculate it, we use the same technique as for the tetrahedron in (2.29) and (2.30). We obtain

$$e^{a^3 G_{\alpha\mu\nu}} \sim \mathcal{G}_{\alpha\mu\nu} = [g_\alpha(0) \triangleright h_{\mu\nu}(\alpha)] h_{\mu\alpha}(0) [g_\mu(0) \triangleright h_{\nu\alpha}(\mu)] h_{\nu\mu}(0) [g_\nu(0) \triangleright h_{\alpha\mu}(\nu)] h_{\alpha\nu}(0). \tag{3.26}$$

Let us use once again the approximations (3.16)–(3.19) and drop all terms of order a^4 in the exponent, so that we get

$$G_{\alpha\mu\nu} = \partial_\alpha B_{\mu\nu} + \mathrm{d}\alpha(A_\alpha)(B_{\mu\nu}) + \partial_\nu B_{\alpha\mu} + \mathrm{d}\alpha(A_\nu)(B_{\alpha\mu}) + \partial_\mu B_{\nu\alpha} + \mathrm{d}\alpha(A_\mu)(B_{\nu\alpha}), \tag{3.27}$$

and using the simplified notation,

$$G = \mathrm{d}B + A \triangleright B = \mathrm{d}_A(B). \tag{3.28}$$

This coincides with Baez's definition of the curvature 3-form.[13]

D. Differential gauge transformations

In order to derive the differential form of the local 2-gauge transformations (2.23) and (2.25), we draw the analogous diagrams for a square and a cube, respectively, cf. Figs. 1 and 2. Here the old configuration corresponds to the bottom of the diagram, the new one to the top. We parametrize differential gauge transformations by the height ε of these diagrams, i.e., the 2-generating function,

$$\eta_\alpha(0) \sim e^{\varepsilon X}, \tag{3.29}$$

$$\eta_{\mu\alpha}(0) \sim e^{\varepsilon a Y_\mu}, \tag{3.30}$$

is parametrized by a $\mathfrak{g}$-valued function X and by an $\mathfrak{h}$-valued 1-form $Y = Y_\mu \, \mathrm{d}x^\mu$. Similarly to Sec. III C, we use the Taylor expansion,

$$\eta_\alpha(\mu) \sim e^{\varepsilon(X + a\partial_\mu X)}, \tag{3.31}$$

$$\eta_{\mu\alpha}(\nu) \sim e^{\varepsilon(aY_\mu + a^2 \partial_\nu Y_\mu)}, \tag{3.32}$$

the convention $\eta_{\mu\alpha} = \eta^{-1}_{\alpha\mu}$, the derivative $\tau = \mathrm{d}t$,

$$t(\eta_{\mu\alpha}(0)) \sim e^{a\varepsilon\tau(Y_\mu)}, \tag{3.33}$$

and the group actions,

$$g_\nu(0) \triangleright \eta_{\mu\alpha}(\nu) \sim e^{\varepsilon(aY_\mu + a^2\partial_\nu Y_\mu + a^2 \, \mathrm{d}\alpha(A_\nu)(Y_\mu))}, \tag{3.34}$$

$$\eta_\alpha(0) \triangleright h_{\mu\nu}(0) \sim e^{a^2(B_{\mu\nu} + \varepsilon \, \mathrm{d}\alpha(X)(B_{\mu\nu}))}. \tag{3.35}$$

The gauge transformation for the connection 1-form A is read off from the square of Fig. 1 and the formula (2.20),

$$e^{aA_\mu + a\varepsilon\delta A_\mu} \sim \tilde{g}_\mu(\alpha) = \eta_\alpha^{-1}(0) t(\eta_{\mu\alpha}(0)) g_\mu(0) \, \eta_\alpha(\mu). \tag{3.36}$$

Using the approximations (3.16)–(3.19) and dropping terms of order ε^2 and a^2 in the exponent, we get the gauge transformation,

$$A_\mu \mapsto A_\mu + \varepsilon \, \delta A_\mu, \quad \delta A_\mu = \partial_\mu X + [A_\mu, X] + \tau(Y_\mu), \tag{3.37}$$

that is

$$\delta A = \mathrm{d}_A(X) + \tau(Y). \tag{3.38}$$

The 2-gauge transformations of the B-field can be deduced from the flattened cube (Fig. 2) whose height in α-direction is ε for the gauge transformation,

$$e^{a^2 B_{\mu\nu} + a^2\varepsilon\delta B_{\mu\nu}} \sim \tilde{h}_{\mu\nu}(\beta) = \eta_\alpha(0)^{-1} \triangleright \{\eta_{\nu\alpha}(0)[g_\nu(0) \triangleright \eta_{\mu\alpha}(\nu)] h_{\mu\nu}(0) [g_\mu(0) \triangleright \eta^{-1}_{\nu\alpha}(\mu)] \eta^{-1}_{\mu\alpha}(0)\}. \tag{3.39}$$

The infinitesimal transformation is calculated as usual with the help of (3.16)–(3.19), dropping terms of order ε^2 and a^3 in the exponent, and we get

$$B_{\mu\nu} \mapsto B_{\mu\nu} + \varepsilon \, \delta B_{\mu\nu},$$

$$\delta B_{\mu\nu} = -\partial_\mu Y_\nu + \partial_\nu Y_\mu - \mathrm{d}\alpha(A_\mu)(Y_\nu) + \mathrm{d}\alpha(A_\nu)(Y_\mu) - \mathrm{d}\alpha(X)(B_{\mu\nu}). \tag{3.40}$$

So by using the shorthand notation, we have

$$\delta B = -\mathrm{d}Y - A \triangleright Y - X \triangleright B = -\mathrm{d}_A(Y) - X \triangleright B. \tag{3.41}$$

From the gauge transformations (3.37) and (3.40) for A and B, we can deduce the transformation of the curvature 2-form,

$$\tilde{F} \mapsto \tilde{F} + \varepsilon \, \delta\tilde{F}, \quad \delta\tilde{F} = [\tilde{F}, X], \tag{3.42}$$

up to terms of order ε^2. This means that $\tilde{F}$ transforms covariantly even without the assumption $\tilde{F} = 0$, and on the other hand, that the transformation preserves the condition $\tilde{F} = 0$.

For the curvature 3-form G, we obtain after a rather lengthy calculation,

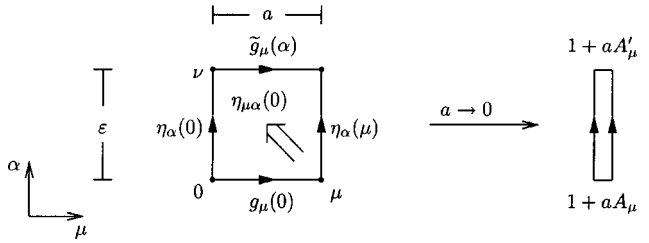


FIG. 3. The local gauge transformation of the edge labels in the integral picture, cf. (3.50). The bottom layer is the old configuration, the top layer the new one. In order to pass to the differential picture, we shrink the rectangle to infinitesimal width, $a \to 0$, but keep its height ε fixed.

$$G \mapsto G + \varepsilon \delta G, \quad \delta G = -\tilde{F} \triangleright Y - X \triangleright G, \tag{3.43}$$

up to terms of order ε^2. This transformation shows that G transforms covariantly if and only if $\tilde{F} = 0$. However, if we are considering the case of a strict Lie 2-algebra, then this flatness condition is naturally present, and G transforms covariantly, moreover it sees only the level 1 of the generating function,

$$\delta G = -X \triangleright G. \tag{3.44}$$

E. Large gauge transformations

In the preceding section, we have derived the differential gauge transformations in the differential picture. What can we conclude from their existence?

Recall first the role of large and differential gauge transformations in conventional non-Abelian gauge theory with gauge group G. A large gauge transformation is a bundle automorphism of the principal bundle $P \to M$. In a local trivialization on $U \subseteq M$, it is given by a G-valued generating function $g: U \to G$. The connection 1-form and the curvature 2-form transform as

$$A \mapsto g^{-1} A g + g^{-1}\, \mathrm{d}g, \tag{3.45}$$

$$F \mapsto g^{-1} F g. \tag{3.46}$$

It is often convenient to consider only the tangents to the above transformations which means to parametrize g in terms of the Lie algebra,

$$g = e^{\varepsilon X}, \tag{3.47}$$

where $X: U \to \mathfrak{g}$ is a Lie algebra valued function. If G is compact and connected, then the exponential map is surjective, see for example, Ref. 18, and any generating function is of this form. If G is noncompact or not connected, this is in general no longer true. Usually, one considers the parametrization (3.47) only for small ε and finds

$$A \mapsto A + \varepsilon(\mathrm{d}X + [A, X]) = A + \varepsilon \mathrm{d}_A(X), \tag{3.48}$$

$$F \mapsto F + \varepsilon[F, X], \tag{3.49}$$

dropping terms of order ε^2. Since we know that we can always integrate these differential gauge transformations, we can recover the large transformations as long as the exponential map is surjective.

Let us now try to derive the large counterparts of the differential 2-gauge transformations of Sec. III D. Therefore, we again consider the integral formulation on squares and cubes, but this time we keep the height ε fixed and consider only the limit $a \to 0$, see Fig. 3.

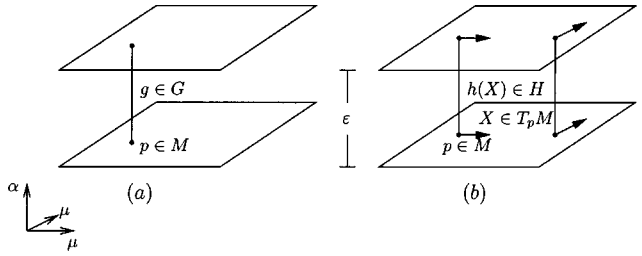


FIG. 4. (a) After shrinking the square of Fig. 3 to infinitesimal width $a \to 0$, its vertical edges carry a group label $g(p) = \eta_\alpha(p) \in G$ at each point $p \in M$. (b) The vertical surface label $\eta_{\mu\alpha}(p)$ would ideally yield an H-valued 1-form $h_\mu(p)\mathrm{d}x^\mu = \eta_{\mu\alpha}(p)\mathrm{d}x^\mu$ which associates with each vector $X \in T_pM$ an element $h(X) \in H$. The linear structure of T_pM here imposes a serious constraint as we explain in the text.

First we restrict ourselves to the case in which the curve labels of the gauge generating transformation are trivial, i.e., the surface in Fig. 3 has the trivial label $\eta_{\mu\alpha}(0) = 1 \in H$. Rather than (3.36), we now write $e^{aA_\mu} \sim g_\mu(0)$ and $e^{aA'_\mu} \sim \tilde{g}_\mu(\alpha)$ and obtain

$$(1 + aA'_\mu) \sim e^{aA'_\mu} \sim \eta_\alpha(0)^{-1} e^{aA_\mu} \eta_\alpha(\mu) \sim \eta_\alpha(0)^{-1}(1 + aA_\mu)(\eta_\alpha(0) + a\partial_\mu \eta_\alpha(0)). \tag{3.50}$$

Dropping terms of order a^2, this gives the familiar transformation rule (3.45) for the G-valued function $g(p) = \eta_\alpha(p)$, $p \in U$. The index α was just used in order to denote the vertical gauge direction in our figure.

All the data required in order to describe the gauge transformation are associated with vertical curves or surfaces which link the bottom with the top layer of Fig. 3. If the surface label is trivial, i.e., if the gauge generating transformation assigns the group unit $1 \in H$ to each curve, we have to deal only with vertical lines labeled by elements,

$$\eta_\alpha(p) = g(p) \in G, \tag{3.51}$$

at each point $p \in U$, Fig. 4(a). Indeed, the gauge generating function,

$$g{:}\mathrm{U} \to G, \tag{3.52}$$

can be visualized by a bunch of such vertical lines between the old configuration (bottom) and the new one (top). It poses no problem that the labels are in the group G. The transformation is just a change of coordinates.

Let us now consider the case in which the curve labels of the 2-generating function are nontrivial, i.e., the square in Fig. 3 has a nontrivial label $\eta_{\mu\alpha}(0) \in H$. The index α just indicates that the surface is vertical, but the index μ has indeed a geometrical meaning. In order to derive the differential gauge transformations we have expanded (3.30) in terms of both a and ε in order to obtain a 1-form $Y_\mu \, \mathrm{d}x^\mu$ as the differential expression.

If we expand only in terms of a, but keep ε fixed, we run into the following geometrical obstruction as depicted in Fig. 4(b). By expansion in terms of a, we wish to obtain a 1-form, say $h_\mu \, \mathrm{d}x^\mu$, from the vertical surface. For any tangent vector $X \in T_pM$ at some point $p \in U$, we should therefore be able to evaluate $h(X) = h_\mu X^\mu$. On the other hand, from the surface label, $\eta_{\mu\alpha}(0) \in H$, there remains for each choice of μ a group element in H. We are tempted to write,

$$\eta_{\mu\alpha}(p) = h_\mu(p) \in H. \tag{3.53}$$

Since T_pM is a linear space, however, this is possible only if h_μ gives rise to a linear map,

$$h{:}TM \to H. \tag{3.54}$$

This condition is stronger than that in (3.51) and (3.52).

The construction of the large gauge transformations in the differential picture is therefore possible only if $H=\mathbb{R}^n$ for some n. In this case, the action $\triangleright$ of G on H is actually a representation of the Lie group G and induces a representation $\triangleright$ of the Lie algebra $\mathfrak{g}$ on H.

We parametrize the large gauge transformations by $h_\mu(p) \in H$, $p \in M$, i.e.,

$$\eta_{\mu\alpha}(p) = a h_\mu(p), \tag{3.55}$$

identifying H with its Lie algebra and indicating that h_μ is already a quantity of order a. Rather than (3.36), we obtain for the transformation of the connection 1-form,

$$A \mapsto A' = g^{-1}Ag + g^{-1}\,\mathrm{d}g + \tau(h). \tag{3.56}$$

In order to derive the large gauge transformations for the connection 2-form $B_{\mu\nu}$, we replace (3.39) by

$$e^{a^2 B'_{\mu\nu}} \sim \eta_\alpha^{-1}(0) \triangleright [\eta_{\nu\alpha}(0)(e^{aA_\nu} \triangleright \eta_{\mu\alpha}(\nu)) e^{a^2 B_{\mu\nu}} (e^{aA_\mu} \triangleright \eta_{\nu\alpha}^{-1}(\mu))\, \eta_{\mu\alpha}^{-1}(0)]. \tag{3.57}$$

Expanding everything up to order a^2, using $\eta_\alpha(0)=g(0)$, (3.55), and $h_\mu(\nu)=h_\mu(0)+a\partial_\nu h_\mu(0)$, we obtain the transformation

$$B \mapsto B' = g^{-1} \triangleright B - \mathrm{d}_A(h). \tag{3.58}$$

From the large gauge transformations (3.56) and (3.58) one can recover the differential transformations (3.38) and (3.41) using the parametrizations (3.47) and (3.55).

We conclude that we have a full extended local gauge symmetry only if $H \cong \mathbb{R}^n$. In general, it is not possible to integrate the differential gauge transformations and to obtain proper (large) transformations. The large transformations are given by (3.56) and (3.58), and

$$G \mapsto G' = g^{-1} \triangleright G. \tag{3.59}$$

F. Pure 2-gauge and 2-flatness

For the case $H \cong \mathbb{R}^n$, we can now express the condition of being pure 2-gauge (Sec. II D) in the differential language. A generalized connection (A,B) is pure gauge if there exists (locally) a G-valued function $g: \mathrm{U} \to G$ and an H-valued 1-form $h: T^*M|_U \to H$ such that,

$$A = g^{-1}\,\mathrm{d}g + \tau(h), \tag{3.60}$$

$$B = -\,\mathrm{d}h. \tag{3.61}$$

It is straightforward to show that these configurations are also 2-flat.

G. Flatness at level 1

The level-1 flatness condition $\tilde{F}=0$, cf (3.25), has the following effect on the curvature 3-form. The definition $G=\mathrm{d}_A(B)$ implies $\tau(G)=\mathrm{d}_A(\tau(B))=-\mathrm{d}_A(F)=0$ by the Bianchi identity for the conventional curvature F of A. This implies that G takes values in $\ker\tau \lhd \mathfrak{h}$ which is an Abelian ideal of $\mathfrak{h}$. This is the differential counterpart of the result[14] that the 2-holonomy of an S^2 surface in the integral picture takes values in the Abelian normal subgroup $\ker t \lhd H$ (Sec. II F).

We can always decompose the $\mathfrak{h}$-valued connection 2-form $B = z \oplus B'$ where $z \in \ker\tau$ and $\mathfrak{h} = \ker\tau \oplus \mathfrak{h}'$ is split into a direct sum of vector spaces. The non-Abelian part of B is therefore contained in $B' \in \mathfrak{h}'$ and related to the conventional curvature F of A by $F=-\tau(B')$ due to (3.25). The only contribution to B unrelated to the curvature of A is contained in some Abelian subalgebra of $\mathfrak{h}$.

H. Higher Bianchi identities

As a generalization of the Bianchi identity $d_A(F)=0$ of conventional 1-gauge theory, we have in 2-gauge theory,

$$d_A(\tilde{F}) = d_A(F) + \tau(d_A(B)) = \tau(G) = 0, \tag{3.62}$$

where we have used the condition (3.25) only in the last step, and

$$d_A(G) = F \triangleright B = -\tau(B) \triangleright B = -[B,B] = 0, \tag{3.63}$$

where we have used (3.25) in the second step. They can be derived from the integral picture by drawing the square and cube from the definition of the curvature 2- and 3-form and by parallel transporting the entire diagram in an independent direction.

I. Examples

BF-theory: Consider first the special example in which we use the adjoint 2-group of some Lie group G, i.e., $H=\mathfrak{g}$ is the Lie algebra, G acts on $H=\mathfrak{g}$ by the adjoint action, and the map $t:H\to G$ is $t(h)=1$ for all $h\in H$. The corresponding Lie 2-algebra is given by the Lie algebras $\mathfrak{g}=\mathfrak{h}$, the adjoint action of $\mathfrak{g}$ on $\mathfrak{h}$ and the null map $\tau=dt=0$.

In this case, the differential forms A, B, F, $\tilde{F}$, and G are all $\mathfrak{g}$-valued. In four dimensions, one can therefore consider the Lagrangian of BF-theory,[15]

$$\mathcal{L} = \mathrm{tr}_{\mathfrak{g}}(B \wedge F). \tag{3.64}$$

The local 2-gauge transformations are generated by a $\mathfrak{g}$-valued function X and a $\mathfrak{g}$-valued 1-form Y,

$$\delta A = d_A(X), \tag{3.65}$$

$$\delta B = d_A(Y) - [X,B], \tag{3.66}$$

$$\delta F = -[X,F], \tag{3.67}$$

$$\delta G = -[X,G]. \tag{3.68}$$

They encompass both the ordinary local gauge symmetry (generated by X) and the extended, so-called topological, local symmetry which is a special feature of BF-theory (generated by Y). Both are unified in the local 2-gauge symmetry. We have therefore discovered the actual geometrical reason for the topological symmetry of BF-theory. Notice that the level-1 flatness condition (3.25) reads in this case $F=0$ which is actually one of the field equations of BF-theory.

Notice that in the case of BF-theory, the Abelian ideal is $\ker t=\mathfrak{g}$ which is an Abelian group using the addition of elements of $\mathfrak{g}$, even though $\mathfrak{g}$ as a Lie algebra can be non-Abelian if the gauge group G is non-Abelian.

Yang–Mills theory: Let us now try to construct a higher level analogue of the Yang–Mills action. In conventional gauge theory, the Yang–Mills Lagrangian reads

$$\mathcal{L} = \mathrm{tr}_g(F \wedge {*F}), \tag{3.69}$$

where $\mathrm{tr}_{\mathfrak{g}}$ denotes the Cartan–Killing form of $\mathfrak{g}$. A candidate for a Lagrangian density in higher gauge theory is therefore given by the expression

$$\mathcal{L} = \mathrm{tr}_{\mathfrak{h}}(G \wedge {*G}). \tag{3.70}$$

We could have tried $\mathrm{tr}_{\mathfrak{g}}(\tilde{F} \wedge {*\tilde{F}})$ which, however, vanishes because of (3.25) in the case of strict Lie 2-groups. We have seen that the curvature 3-form G is always Abelian.

If we choose the Euclidean or Poincaré 2-group, we have $\mathfrak{g}=\mathfrak{so}(n)$ or $\mathfrak{so}(n-1,1)$, $\mathfrak{h}=\mathbb{R}^n$ and $\tau:\mathfrak{h}\to\mathfrak{g}$ the null map. This implies in particular that $\tilde{F}=F$, and the condition (3.25) furthermore states that the connection A is flat. In addition, we have a connection 2-form B taking values in $\mathfrak{h}=\mathbb{R}^n$ with a curvature 3-form $G=\mathrm{d}_A(B)$. Locally, the flatness of A implies that it is pure gauge, i.e., gauge equivalent to $A=0$, so that locally G is just the exterior derivative, $G=\mathrm{d}B$. The Yang–Mills Lagrangian (3.70) therefore agrees locally with that of Abelian 2-form electrodynamics.

A similar result can be shown for all 2-groups in which $H=V$ is a vector space on which G is represented. The connection 1-form A is locally pure gauge and the Yang–Mills Lagrangian (3.70) reduces to that of Abelian 2-form electrodynamics.

Consider finally the automorphism 2-group of $H=\mathrm{SU}(2)$, i.e., $\mathfrak{g}=\mathfrak{h}=\mathfrak{su}(2)$, τ is the identity map, and $\mathfrak{g}$ acts on $\mathfrak{h}=\mathfrak{g}$ by the adjoint action. In this case, the condition (3.25) implies that $B=-F$ is just (minus) the ordinary curvature 2-form of A. The Yang–Mills Lagrangian (3.70) therefore vanishes because of the conventional Bianchi identity $G=\mathrm{d}_A(B)=-\mathrm{d}_A(F)=0$.

With the known Lie 2-groups alone, it is therefore not possible to find a nontrivial generalization of the Yang–Mills action. This is in outright contrast to the integral picture for which we have shown[14] that nontrivial generalizations exist. This result points towards a genuine discrepancy between perturbative and nonperturbative formulations of higher gauge theory on which we comment in the conclusion.

IV. CONCLUSION AND OUTLOOK

In this paper, we have reviewed both the integral and the differential picture of higher gauge theory. One main result is the appearance of the condition (3.25) at the differential level as soon as the curve and surface labels depend smoothly on the positions of the curves and surfaces.

Another main result is that we are able to construct large (as opposed to differential) 2-gauge transformations in the differential picture only in the case in which $H\cong\mathbb{R}^n$ as an Abelian group. This seriously restricts the applications of the differential formulation and prevents us from obtaining an interesting level-2 generalization of Yang–Mills theory. *BF*-theory, however, forms an interesting example of a 2-gauge theory. The local 2-gauge transformations unify the two types of local symmetries of *BF*-theory and thereby provide a structural explanation for the existence of the topological symmetry of *BF*-theory.

We have chosen the language of 2-groups[13] in order to study higher gauge theory. The categorical structure of 2-groups leads directly to the integral picture[14] and as a consequence to the differential formulation as derived in the present paper. Alternatively it would be possible to use the language of gerbes and to start with a differential formulation of higher gauge theory. One can then ask under which conditions it is possible to integrate the connection 1-form along curves and the connection 2-form along surfaces in a consistent way. The result of the present article suggests the conjecture that (3.25) is the required integrability condition.

How serious are the restrictions we have found, in particular the Abelianness of the curvature 3-form?

First note that all the Lie 2-groups and Lie 2-algebras used in the present paper are *strict*. They form only the simplest examples of these structures which can be constructed in a general 2-categorical framework, but there exist the more general notions of *weak* and *coherent* 2-groups and their Lie 2-algebras. For 2-groups, see, for example, Refs. 19 and 20 and for Lie 2-algebras.[17] One can hope that the differential picture becomes less restrictive once we generalize from strict Lie 2-groups and 2-algebras to weak ones. Since the origin of the level-1 flatness is the very basic condition (2.10), a fully successful weakening should therefore allow for a non-Abelian kernel of the map $t:H\to G$.

We also observe that the nontrivial 2-holonomies are ruled out in the differential picture only if one requires the connection 1- and 2-forms to be both smooth and well defined everywhere in space–time. In particular, in the integral picture with the automorphism 2-group of SU(2), we can have $\mathbb{Z}_2$-valued 2-holonomies associated with surfaces of topology S^2. If we assume that a smooth

deformation of the surface changes the 2-holonomy only smoothly, then the nontrivial $\mathbb{Z}_2$-element indicates that the S^2 is not smoothly contractible. This can be interpreted as an indication that there are singularities of codimension 2 in the theory which are actually *predicted* by the algebraic structure. Solitonlike solutions of some classical field equations come to mind. In fact, the integral picture for the inner automorphism group of SU(3) is related to the symmetries of center vortices in QCD as sketched in Ref. 14.

The difference of the differential and the integral picture is much deeper, though. As an illustration, we refer to a result in the context of the path integral quantization of conventional gauge theory. For simplicity, assume that we work in the Euclidean setting (i.e., with imaginary time) on some Riemannian manifold M.

The obvious naive choice is to consider the set $\mathcal{A}$ of all smooth connections A on M which form an affine space, and then to divide out the action of the gauge transformations. This step, however, destroys the linear structure so that the standard techniques fail to construct a useful path integral measure on the quotient $\mathcal{A}/\mathcal{G}$. This failure to implement the gauge symmetry correctly can be seen as a main reason why perturbative QCD does not predict confinement as observed in nature.

A nonperturbative approach, see, for example, Ref. 21, is to consider the collection of all graphs embedded in M, to study gauge theory in the integral picture on these graphs, i.e., all connections that are given by group labels attached to the edges of the graph, and finally to make use of a refinement relation on the class of all graphs which facilitates the construction of a projective continuum limit for the set of connections. Not only does this set of generalized connections form a compact Hausdorff space, it is also possible to fully divide out the gauge symmetry. This set of generalized connections modulo gauge transformations is a huge space that includes not only smooth or continuous connections, but rather mainly distributional ones. In order to appreciate the physical significance of this space of generalized connections it is useful to recall the most basic example of a field theory which admits a rigorous Euclidean path integral quantization, the free relativistic scalar field. Its path integral measure[22] is supported mainly on nonsmooth scalar fields. In fact, the subsets of smooth fields form sets of measure zero.

This is a strong indication that a restriction to smooth fields does not yield an adequate description of the corresponding quantum theory and that we should take the integral formulation seriously. In a proper continuum limit, constructed from a suitable refinement of the integral formulation of higher gauge theory, the above-mentioned codimension-2 singularities will not only be allowed, they may actually be abundant in the path integral.

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Homological mirror symmetry, deformation quantization and noncommutative geometry

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We discuss the possible relationship of homological mirror symmetry with deformation quantization. We speculate that after certain nonlinear "twist" the Fukaya category becomes equivalent to the category of holonomic modules over a quantized algebra of functions. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The mathematical foundation of mirror symmetry belongs both to geometry (the Strominger-Yau-Zaslow conjecture; see Strominger *et al.*, 1996) and algebra (Kontsevich's homological mirror symmetry program; see Kontsevich, 1994). In the present paper we deal with some aspects of the latter. Our methods and conjectures have an algebraic (categorical) nature. On the other hand, based on the ideas of Kontsevich (1994) and Kontsevich and Soibelman (2000, in press), we stress the role of *noncommutative* geometry of mirror symmetry, making an attempt to connect it with deformation quantization. The latter is a generalization of the theory of (pseudo)-differential operators (or D-modules) to arbitrary symplectic manifolds.

In homological mirror symmetry and in the theory of D-modules one meets similar objects. They are pairs (L,ρ) where L is a Lagrangian manifold, and ρ is a flat bundle on L (local system). In the framework of homological mirror symmetry such pairs are objects of the so-called Fukaya category, which is the principal mathematical structure of the genus zero part of the A-model. In the framework of D-modules they are holonomic D-modules (in the C^∞ category). It is natural to compare the categories themselves. This comparison is the main theme of the present paper.

One can object any relationship between mirror symmetry and deformation quantization. Indeed we have the following.

(a) Theory of D-modules works well in an algebraic or complex analytic framework, while the Fukaya category (and in general Floer theory) exists in the C^∞-category only.
(b) In mirror symmetry one considers a series in an exponentially small (with respect to the symplectic structure) parameter, while in deformation quantization the parameter "is of the size" of the symplectic structure.

From our point of view these are rather research problems than objections.

In regard to point (a) we remark that the finding of a complex analog of the Floer theory is an interesting problem. At this time we can only speculate in this direction.

Our aim in the present paper is to summarize our present understanding of the topic and make some conjectures. Our main conjecture can be briefly formulated such as follows.

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(i) There is a category of holonomic modules over the quantized algebra of smooth functions on a symplectic manifold.
(ii) It is possible to change morphisms in this category by a kind of integral transformation, so that it becomes equivalent (at least locally) to the Fukaya category of the same symplectic manifold.

Let us mention two possible applications of this idea. First, it can help in the construction of an algebraic model of the Fukaya category (analogy: de Rham complex is an algebraic model of Morse complex). Second, it might help to resolve some difficulties in the definition of the Fukaya category (nontransversality of supports, nonexistence of identity morphisms, etc.). In our opinion the current situation is not completely satisfactory despite the recent progress (cf., for example, Fukaya *et al.*, 2000). Third, one can go beyond Lagrangian submanifolds by considering coisotropic submanifolds or even nonsmooth varieties (cf. Kapustin and Orlov, 2001). Finally, one hopes to achieve a deeper understanding of the relationship at the level of chiral algebras (see Beilinson and Drinfeld, 1999; Malikov *et al.*, 1998; Kapranov and Vasserot, 2001). Hence the subject of this paper is just the first approximation to the full picture.

The paper is organized as follows. In Sec. II we briefly recall basics on the deformation theory and A_∞-categories. Our purpose in this section is to fix the language. Details of the formalism will be explained in Kontsevich and Soibelman (in press).

In Sec. III we recall the main facts about the Fukaya category, which is one of the main structures of homological mirror symmetry. Section IV is a reminder on the deformation quantization of symplectic manifolds. Section V is devoted to the comparison of the Fukaya category with the category of holonomic modules over the quantized algebra of functions.

The main idea of Sec. III goes back to the pioneering paper (Kontsevich, 1994). As explained in loc. cit., homological mirror symmetry is not a statement about individual categories, but rather about families of A_∞-categories over $\mathbf{Z}$-graded formal schemes. Geometrically this structure is modeled by a "family of noncommutative differential-graded manifolds over a commutative differential-graded base." The framework in which the latter phrase has a precise meaning will be explained in Kontsevich and Soibelman (in press). The reader can keep in mind the example of the deformation theory of an associative algebra. In this case one has a family of associative algebras parametrized by the formal moduli space $\mathcal{M}_A$ of deformations of a given algebra A. The moduli space $\mathcal{M}_A$ is a formal pointed differential-graded manifold (dg-manifold for short) (see, for example, Kontsevich, 1997 and Kontsevich and Soibelman, 2000). By definition $\mathcal{M}_A$ is a base of a family of associative algebras A_γ, $\gamma \in \mathcal{M}_A$. Each algebra gives rise to a "noncommutative scheme" $\mathrm{Spec}(A_\gamma)$, hence one has the desired structure.

II. REMINDER ON A_∞-CATEGORIES AND DEFORMATION THEORY

In this section we recall some facts about the homological algebra of mirror symmetry. Full details including the necessary language of noncommutative geometry will appear in Kontsevich and Soibelman (in press). Some of the material can be found in the existing literature, for example, in Kontsevich (1994). We are not going to discuss in detail motivations for all of the definitions and notions below. The main purpose of this section is to fix the language.

Let A be a free $\mathbf{Z}$-graded k-module over a unital commutative ring k of characteristic zero (the main applications deal with the case when k is a field).

Definition 1: *An A_∞-algebra A over k is given by the following data*.

(a) *A $\mathbf{Z}$-graded free k-module A.*
(b) *A codifferential d on the cofree coalgebra $T(A[1]) = \oplus_{n \geqslant 1} A[1]^{\otimes n}$, where $A[1]$ denotes the graded free k-module such that $A[1]^i = A^{i+1}$ (A with shifted grading).*

(We recall that a codifferential means a derivation d of the coalgebra satisfying the condition $d^2 = 0$).

Since d is uniquely defined on generators, it gives rise to "higher multiplications" $m_n: A^{\otimes n} \to A, n \geqslant 1$ of degrees $2-n$ satisfying a system of quadratic equations which follows from the equation $d^2=0$.

Definition 2: *An L_∞-algebra on A is given by the following data*.

(a) *A* **Z***-graded vector space A.*
(b) *A codifferential on the cofree cocommutative coalgebra $C(A[1])=\oplus_{n\geqslant 1} S^n(A[1])$, where $S^n(V)$ denotes the nth symmetric power in the symmetric monoidal category of* **Z***-graded k-modules*.

The codifferential d defines a sequence of "higher Lie brackets" $m_n: A^{\otimes n} \to A, n \geqslant 1$ of degrees $2-n$ satisfying a system of quadratic equations which follows from the equality $d^2=0$.

It is useful to have in mind a geometric picture for both algebraic structures defined above. We start with L_∞-algebras.

An L_∞-algebra gives rise to a *formal pointed* **Z***-graded manifold X*, which carries a vector field d_X of degree +1 such that d_X vanishes at the marked point, and satisfies the condition $[d_X, d_X]=0$. This structure is called *formal pointed differential-graded manifold* in Kontsevich (1997) and Kontsevich and Soibelman (in press, 2000) (it was introduced by Schwarz under the name of the Q-manifold). The algebra of formal functions of X is isomorphic to the graded dual to the coalgebra $C(A[1])$. Thus we can write $X=Spf((C[1])^*)$, where Spf stands for the formal spectrum.

Remark 1: (a) One should remember that formal **Z***-graded manifolds have only nilpotent points*.

(b) It is useful to interpret maps m_n as a Taylor coefficient of the vector field d_X at the marked point.

Let us consider two examples.

Example 1: *Let A be an associative algebra. Then its truncated Hochschild complex $C^\bullet_+(A,A)[1]=\oplus_{n\geqslant 1}\mathrm{Hom}_k(A^{\otimes n},A)[1]$ carries a structure of differential-graded Lie algebra, hence defines a formal pointed dg-manifold (see Kontsevich, 1997)*.

One can interpret the DGLA from the example as a DGLA of derivations of the tensor coalgebra generated by $A[1]$. Equivalently, it is the DGLA of vector fields on the formal pointed graded manifold X vanishing at the marked point. Then the DGLA structure is the natural one on vector fields.

One also has the notion of a *formal differential-graded manifold*, where the condition of vanishing at the marked point is dropped. Algebraically this means that we allow the condition $m_0 \neq 0$.

Example 2: *In the previous example we consider the full Hochschild complex $C^\bullet(A,A)[1]=\oplus_{n\geqslant 0}\mathrm{Hom}_k(A^{\otimes n},A)[1]$. It gives rise to a formal dg-manifold*.

The importance of L_∞-algebras and formal dg-manifolds in deformation theory is based on the fact that they define deformation functors (see, for example Kontsevich, 1997, and Kontsevich and Soibelman, 2000). Let us briefly recall the construction. If $g=\oplus_{n\geqslant 0} g^n$ is an L_∞-algebra (g^n is the nth graded component) then one has the deformation functor from commutative nilpotent algebras (possibly graded) to groupoids. Namely to a commutative nilpotent ring R one assigns the groupoid $\mathrm{Def}_g(R)$ consisting of $\gamma \in g^1 \otimes R$ which satisfy the Maurer-Cartan equation,

$$m_1(\gamma) + m_2(\gamma,\gamma)/2\,! + \cdots + m_n(\gamma,\ldots,\gamma)/n\,! + \cdots = 0,$$

where m_n are the higher Lie brackets.

Formal deformations of many algebraic and geometric structures give rise to formal pointed dg-manifolds. Formal dg-manifolds without marked points arise, for example, when one deforms categories (i.e., when objects of a category are deformed). In Example 2 the corresponding dg-manifold controls deformations of the category with one object X such that $\mathrm{Hom}(X,X)=A$.

One can develop a similar geometric language for A_∞-algebras. Namely, an A_∞-algebra gives rise to a *noncommutative formal pointed dg-manifold*. It is modeled by the cofree coalgebra $T(A[1])$ which carries a codifferential d_X. One also has the notion of a *noncommutative formal dg-manifold* (no marked point is specified). In this case one can have a nonzero map $m_0: k \to A$.

Geometrically this structure corresponds to a vector field d_X of degree +1 such that $[d_X, d_X]=0$, without any condition at the marked point. The corresponding algebraic structure is defined in the following way.

Definition 3: *We say that a codifferential on the coalgebra* $k \oplus T(A[1])$ *defines a structure of generalized* A_∞*-algebra on* A.

The notion of a small A_∞-category is a natural generalization of the notion of A_∞-algebra. Traditionally, such a category is defined by a set of objects $Ob(\mathcal{C})$, **Z**-graded free k-modules of morphisms $\mathrm{Hom}(X,Y)$, and structures of A_∞-algebras on the spaces $\oplus_{0\leqslant i,j\leqslant n}\mathrm{Hom}(X_i,X_j)$ for any collection of objects $X_0,\ldots,X_n, n\geqslant 1$. These structures are given by the higher compositions,

$$m_n: \otimes_{0\leqslant i\leqslant n}\mathrm{Hom}(X_i,X_{i+1}) \to \mathrm{Hom}(X_0,X_n),$$

which are maps of **Z**-graded free k-modules of degrees $2-n$ satisfying quadratic relations similar to those for A_∞-algebras. The structures of A_∞-algebras are compatible with inclusions of collections of objects.

One can think of an A_∞-category $\mathcal{C}$ as of the large A_∞-algebra $\mathrm{End}(\oplus_{X\in Ob(\mathcal{C})}X)$ (compare with the relation between additive categories and associative algebras). The Hochschild complex and Hochschild cohomology of an A_∞-category can be defined in terms of this A_∞-algebra.

For any object X the k-module $\mathrm{End}(X)=\mathrm{Hom}(X,X)$ is an A_∞-algebra. Its truncated Hochschild complex gives rise to a formal pointed dg-manifold $\mathcal{M}_X$. Then the formal dg-manifold $\mathcal{M}=\sqcup_{X\in Ob(C)}\mathcal{M}_X$ "controls" A_∞-deformations of the category $\mathcal{C}$ with the fixed set of objects.

Replacing in the above discussion the truncated Hochschild complex by the full Hochschild complex one obtains a new structure called *generalized* A_∞*-category*. Generalized A_∞-categories do not have a fixed set of objects. This is due to the fact that now for the A_∞-algebra $\mathrm{End}(X)$ one can have $m_0\neq 0$. As before, one can derive the formal dg-manifold $\mathcal{M}$ [now using the generalized A_∞-algebras $\mathrm{End}(X)$]. For a commutative nilpotent k-algebra R one can consider k-points $\mathcal{M}(R)$. If $\mathcal{M}_0\subset\mathcal{M}$ is the subset of zeros of the odd vector field $d_{\mathcal{M}}$ then one can speak about objects of some A_∞-category. The objects are parametrized by $\mathcal{M}_0$. We omit here the description which can be given in terms of R-points of $\mathcal{M}_0$ and $\mathcal{M}$.

We will keep the name of the generalized A_∞-category for a slightly more general structure. The point is that we allow the higher compositions m_n be defined not for all collections of objects, but only for some of them (transversal collections). The Fukaya category discussed in the next section will be this kind of generalized A_∞-category.

We summarize without details the data defining a generalized A_∞-category in the following way.

(a) We are given a formal dg-manifold $Ob(\mathcal{C})=\mathcal{M}$.
(b) For any $n\geqslant 1$ we are given a formal dg-submanifold $\mathcal{M}^n_{\mathrm{tr}}\subset\mathcal{M}^n$ called the space of transversal n-families. It is assumed that $\mathcal{M}^1_{\mathrm{tr}}\subset\mathcal{M}$ (i.e., every object is transversal to itself).
(c) For a point $(X,Y)\in\mathcal{M}^2_{\mathrm{tr}}$ we are given a **Z**-graded free k-module $\mathrm{Hom}_{\mathcal{C}}(X,Y)$ called a space of morphisms between X and Y. These k-modules are organized in a formal dg-bundle $\mathrm{Hom}^{\mathcal{C}}\to\mathcal{M}^2_{\mathrm{tr}}$.
(d) For $n\geqslant 1$ and any $(X_0,\ldots,X_n)\in\mathcal{M}^n_{\mathrm{tr}}$ we are given a higher composition map $m_n^{(X_0,\ldots,X_n)}$ which gives rise to a morphism of the obvious pullbacks of $\mathrm{Hom}^{\mathcal{C}}$ to $\mathcal{M}^n_{\mathrm{tr}}$. The composition maps give rise to a structure of generalized A_∞-algebra $A(X_0,\ldots,X_n)$, or, equivalently to a noncommutative formal dg-manifold $\mathcal{M}(X_0,\ldots,X_n)$.
(e) Let $\mathcal{M}(\mathcal{C})$ be the inductive limit of $\mathcal{M}(X_0,\ldots,X_n)$ taken over increasing collections of transversal objects. This is a noncommutative formal dg-ind-scheme (it can be properly defined as an inductive limit in the appropriate category).
(f) Finally $\mathcal{M}(\mathcal{C})$ is a noncommutative formal dg-manifold over the commutative scheme $\mathrm{Spec}(k)$.

The structure defined in (a)–(e) is called the generalized A_∞-category. It gives rise to the usual

k-linear A_∞-category, which we will call associated to $\mathcal{C}$. The latter is defined by a noncommutative formal dg-ind-subscheme $\mathcal{M}(\mathcal{C})_0 \subset \mathcal{M}(\mathcal{C})$ of zeros of the odd vector field $d_{\mathcal{M}(\mathcal{C})}$.

Remark 2:(a) One can define the Hochschild complex of a generalized A_∞-category. It gives rise to a formal dg-manifold. The corresponding deformation functor describes the formal deformation theory of the generalized A_∞-category in the class of generalized A_∞-categories. If the category has one object X we have the full Hochschild complex of the corresponding generalized A_∞-algebra $\mathrm{End}(X)$.

(b) We do not discuss the delicate problem of unital A_∞-algebras (more generally, A_∞-categories with identity morphisms). It is an interesting question because in practice identity morphisms may be defined up to a homotopy only. All this can be formulated in the language of noncommutative geometry.

There is a notion of an A_∞-functor between two generalized A_∞-categories. A_∞-functors form themselves a generalized A_∞-category. Using A_∞-functors one defines the notion of equivalence of A_∞-categories (see Kontsevich and Soibelman, 2000).

Let us illustrate the notion of equivalence in the case when both categories have only one object. Then we are dealing with generalized A_∞-algebras, say A and B. Assume in addition that $m_0^A=0$ and $m_0^B=0$ (i.e., we have ordinary A_∞-algebras). If A is equivalent to B then the complexes (A,m_1^A) and (B,m_1^B) are quasi-isomorphic. Geometrically this means that the tangent spaces at marked points of equivalent noncommutative formal pointed dg-manifolds are quasi-isomorphic. The converse is also true (this is the A_∞-version of the inverse function theorem). A generalized A_∞-algebra with $m_0 \neq 0$ is equivalent to one which has $m_0 \neq 0$, and $m_{n\geqslant 1}=0$ (cf. the vector field which is nontrivial at a point is locally equivalent to a constant one). The latter observation explains why generalized A_∞-categories should be studied in families rather than individually. Indeed generalized A_∞-categories with $m_0 \neq 0$ are trivial in the sense that all higher compositions can be killed by an appropriate equivalence functor.

Similarly to the case of formal pointed dg-manifolds there is a theory of minimal models of noncommutative formal pointed dg-manifolds. For such a theory one needs to assume that the ground ring k is a field of characteristic zero (there is more complicated theory for nonpointed dg-manifolds).

If two A_∞-categories are equivalent then the formal pointed dg-manifolds of their deformations are quasi-isomorphic (i.e., tangent complexes at the marked points are quasi-isomorphic).

Finally, there is a theory of generalized A_∞-categories over a formal dg-base. In the above discussion we discussed the case when the base was an ordinary scheme $\mathrm{Spec}(k)$. We can also assume that the base is a formal scheme. As we will see in the next section the latter case is important in symplectic geometry.

III. FUKAYA CATEGORY

A. Fukaya category and noncommutative geometry

The Fukaya category $F(X)$ of a smooth symplectic manifold X is a generalized A_∞-category over a base. It can be constructed as an A_∞-deformation of the following trivial $\mathbf{C}$-linear category $F_0(X)$. Objects of $F_0(X)$ are pairs (L,ρ), where L is a Lagrangian submanifold of X and ρ is a local system on L. Transversal collections of objects correspond to transversal collections of Lagrangian submanifolds [in fact we need a more sophisticated transversality condition; see Kontsevich and Soibelman (2000)]. We set $\mathrm{Hom}_{F_0(X)}((L_0,\rho_0),(L_1,\rho_1)) = \oplus_{x\in L_0\cap L_1}\mathrm{Hom}(\rho_{0x},\rho_{1x})$ and $\mathrm{Hom}_{F_0(X)}((L,\rho),(L,\rho)) = \Omega^\bullet(L,\mathrm{End}(\rho))$. All compositions $m_n, n\geqslant 1$ are trivial for collections of different objects. Otherwise $m_{n\geqslant 3}=0$, and m_2 is the natural product on the differential-graded algebra $\Omega^\bullet(L,\mathrm{End}(\rho))$.

To a pair (L,ρ) one can associate a generalized A_∞-algebra $A(L,\rho)$. Let us assume for simplicity that ρ is a trivial rank one local system. Then the corresponding generalized A_∞-algebra $A(L)$ is generated by geometric cycles in L. Higher multiplications $m_n(C_1,\ldots,C_n)$ between generic cycles C_i are given by a kind of quantum cohomology construction. Namely, one counts with some weight pseudo-holomorphic maps $f:(D^2,\partial D^2)\to(X,L)$ with marked points $x_1,\ldots,x_n \in \partial D^2$.

Here $D^2 \subset \mathbf{C}$ is the standard disk. It is required that the point x_i is mapped to C_i. The weight is $\exp(-1/\epsilon \int_{D^2} f^*(\omega))$, where ω is the symplectic form on X, and ϵ is a parameter. The idea of this construction of $A(L)$ was suggested by Kontsevich. Difficult analytic details have been worked out in Fukaya, Oh, Ohta, and Ono (2000). In what follows we will assume the conditions on the data imposed in Fukaya, Oh, Ohta, and Ono (2000). The resulting generalized A_∞-algebra $A(L)$ is defined over the valuation ring $\mathbf{C}_\epsilon^{\geqslant 0} = \{f = \Sigma_{i \geqslant 1} a_i e^{-\lambda_i/\epsilon}\}$, where $a_i \in \mathbf{C}, a_1 \neq 0$, and $\lambda_i \geqslant 0$ is a monotonically increasing sequence of real numbers such that $\lim_{i \to +\infty} \lambda_i = +\infty$. The valuation map is given by $v(f) = \lambda_1$. The corresponding valuation field $\mathbf{C}_\epsilon$ consists of series f as above, with $\lambda_i \in \mathbf{R}$. It is useful to notice that $\mathbf{C}_\epsilon^{\geqslant 0}$ contains the maximal ideal $\mathbf{C}_\epsilon^{>0}$ consisting of series with all $\lambda_i > 0$. One observes that the composition $m_0 = 0$ modulo $\mathbf{C}_\epsilon^{>0}$, but in general $m_0 \neq 0$.

It can be proved that the disjoint union of noncommutative dg-manifolds associated with generalized A_∞-algebras $A(L, \rho)$ gives rise to a generalized A_∞-category $F_\epsilon(X)$ over the formal spectrum of the ring $\mathbf{C}_\epsilon^{\geqslant 0}$. Its reduction modulo the ideal $\mathbf{C}_\epsilon^{>0}$ is equivalent to $F_0(X)$. If the symplectic form ω satisfies certain rationality conditions then one can introduce a new parameter $q = \exp(-1/\epsilon)$, thus replacing the ring $\mathbf{C}_\epsilon^{\geqslant 0}$ by the ring of formal series $\mathbf{C}[[q]]$. Then the maximal ideal is just $q\mathbf{C}[[q]]$, and the field $\mathbf{C}_\epsilon$ coincides with the field of Laurent series $\mathbf{C}((q))$.

The Fukaya category $F(X)$ is defined as an A_∞-category obtained from $F_\epsilon(X)$ by restriction to zeros of the odd vector field. In particular, for an object A of $F(X)$ the composition m_0 vanishes: $m_0^A = 0$. The condition $m_0^A = 0$ defines a "subvariety" of the noncommutative moduli space $M^{\mathrm{NC}}_{\mathrm{Ob}(F_\epsilon(X))}$. Objects of the Fukaya category exist only along this "subvariety." This geometric picture explains why it is too naive to work with the Fukaya category for fixed ϵ, even if one can prove convergence of the series defining m_n (the latter is still an open problem).

Let us assume for simplicity the above-mentioned rationality conditions of ω. Then the Fukaya category is defined over the formal spectrum $Spf(\mathbf{C}[[q]])$. In fact one can extend the definition so that the base will be $Spf(\mathbf{C}[[q]] \otimes (\otimes_{i \neq 2} \mathbf{C}[t_{i,\mu}]))$, where q has degree zero, and $t_{i,\mu}$ are parameters of degrees $2-i$ corresponding to some basis in the graded vector space of cohomology $H^i(X, \mathbf{C})$. We introduce new parameters z, t of degree zero by setting $z = qe^t$. Then, inverting z we obtain a family of A_∞-categories over the field $\mathbf{C}((z))$ parametrized by $Spf(\mathbf{C}[[t]] \otimes (\otimes_{i \neq 2} \mathbf{C}[t_{i,\mu}]))$. This family should be thought of as the formal deformation of a certain A_∞-category over $\mathbf{C}((z))$. The tangent space to the moduli space of the formal deformations of this category is isomorphic to the cohomology $H^\bullet(X, \mathbf{C}((z)))$. The latter cohomology group is isomorphic to $\oplus_{i \geqslant 0} \mathrm{Ext}^i(\mathrm{Id}, \mathrm{Id})$, where Id is the identity functor, and the extensions are taken in the properly defined A_∞-category of endofunctors. This description is useful for the purposes of quantum cohomology (the Yoneda product on functors gives rise to the quantum product on the cohomology group).

B. Conventional approach to the Fukaya category

Below we briefly recall the "naive" definition of the Fukaya category, when the composition m_0 is ignored. It is useful in some questions, for example, in mirror symmetry for Abelian varieties (see Kontsevich and Soibelman, 2000). As we will discuss below, this "naive" Fukaya category is related to deformation quantization.

Objects of $F^{\mathrm{naive}}(X)$ are pairs (L, ρ), where $L \subset X$ is a Lagrangian submanifold and ρ is a local system on L. Morphisms between (L_0, ρ_0) and (L_1, ρ_1) are defined only if L_0 and L_1 intersect transversally. In this case $\mathrm{Hom}((L_0, \rho_0), (L_1, \rho_1)) = \oplus_{x \in L_0 \cap L_1} \mathrm{Hom}(\rho_{0x}, \rho_{1x}) \otimes \mathbf{C}_\epsilon$. The space of morphisms is $\mathbf{Z}$-graded by means of the Maslov index. Thus we are dealing with graded Lagrangian manifolds (cf. Seidel, 2000). There are higher compositions $m_n, n \geqslant 1$, which are linear maps of degrees $2-n$:

$$m_n : \otimes_{0 \leqslant i \leqslant n} \mathrm{Hom}((L_i, \rho_i), (L_{i+1}, \rho_{i+1})) \to \mathrm{Hom}((L_0, \rho_0), (L_n, \rho_n)).$$

They are defined by means of the Floer-type construction associated with the "transversal" collection of Lagrangian submanifolds $L_i, 0 \leqslant i \leqslant n$. It is usually said that the maps m_n give rise to an A_∞-structure on $F^{\mathrm{naive}}(X)$. We refer the reader to Kontsevich and Soibelman (2000) about the

details of this definition, and to Fukaya, Oh, Ohta, and Ono (2000) about definitions of the related moduli spaces.

There are several problems with the naive definition of the Fukaya category. One of the most essential is the presence of pseudo-holomorphic disks with the boundary mapped to a Lagrangian submanifold. This amounts to nontrivial maps $m_0: \mathbf{C}_\epsilon \to \mathrm{Hom}(X,X)$. As a result, the axioms of the A_∞-category are not satisfied, and one has to work with generalized A_∞-categories. It was explained in the preceeding sections [for all details see Kontsevich and Soibelman (2000)] how a consistent theory of such can be developed in the framework of noncommutative formal geometry. One can still work with $F^{\mathrm{naive}}(X)$ with understanding that it is only a part of the "true" Fukaya category $F(X)$.

IV. REMINDER ON DEFORMATION QUANTIZATION

We recall that a symplectic 2n-dimensional manifold (X,ω) gives rise to an Abelian category $C(X)$ of modules over a noncommutative algebra $A(X)$ (deformation quantization of the algebra $C^\infty(X)$ of smooth functions on X). Such a deformation quantization is nonunique. We will use the one which has the characteristic class $[\omega]/t$ [see Deligne (1995)]. The algebra $A(X)$ is a topological algebra over the ring of formal series $\mathbf{C}[[t]]$. As a $\mathbf{C}[[t]]$-module it is isomorphic to the algebra of formal series $C^\infty(X)[[t]]$. The algebra $A(X)$ consists of global sections of a sheaf of noncommutative algebras A_X, such that locally A_X is isomorphic to the sheaf of t-pseudo-differential operators on $\mathbf{R}^n$ [the latter are locally series $P=\Sigma_{|I|\geqslant 0} a_I(x)(t\partial_x)^I$]. The Poisson structure induced on $C^\infty_X \simeq A_X/tA_X$ coincides with the one given by the symplectic form.

One has a category of $A(X)$-modules M such that M is t-adically complete, flat as a $\mathbf{C}[[t]]$-module, and M/tM is the space of sections of a sheaf of modules over the sheaf of smooth functions C^∞_X. The category of A_X-modules will be denoted by $\mathcal{C}(X)$. Morphisms are defined as $\mathbf{C}[[t]]$-linear homomorphisms of topological modules. We will keep the same notation for the related category defined over the field $\mathbf{C}((t))$. It is obtained from $\mathcal{C}(X)$, respectively, $\mathcal{C}_X$ by adding t^{-1}, so that modules V and tV become equivalent.

Let $\mathrm{hol}(X)$ be a full subcategory of $\mathcal{C}(X)$ which consists of modules M such that the support $\mathrm{Supp}(M/tM)$ is a Lagrangian submanifold.

We will call objects of $\mathrm{hol}(X)$ *holonomic*. The Lagrangian support $\mathrm{Supp}(M)$ of a holonomic module will be sometimes called its *characteristic variety* of M and denoted by $Ch(M)$. The category $\mathrm{hol}(X)$ contains objects $V_{(L,\rho)}$ which correspond to pairs (L,ρ) where $L\subset X$ is a Lagrangian submanifold and ρ is a local system on L. In what follows only such objects will be considered.

Remark 3: In [Karasev and Maslov (1983)] the authors constructed (for every Lagrangian submanifold L satisfying some topological conditions) an A_X-module V_L such that $Ch(V_L)=L$. One can easily generalize their construction including local systems on L. We will call the corresponding objects Karasev–Maslov modules.

We will need symplectic manifolds $X^n, n\geqslant 2$. The corresponding symplectic forms are given by $(\omega,-\omega,-\omega,\ldots,-\omega)$.

The identity functor $\mathrm{Id}_{A_X-\mathrm{mod}}$ is represented by the $A_{X\times X}$-module K_Δ supported on the diagonal $\Delta\subset X\times X$. It can be identified with the sheaf A_X. Deformations of $A_X-\mathrm{mod}$ as an A_∞-category has the tangent complex quasi-isomorphic (after a shift) to the tangent complex to the deformations of the identity functor $\mathrm{Id}_{A_X-\mathrm{mod}}$. The latter deformations are described by the deformations of K_Δ as an object of $\mathrm{A}_{X\times X}-\mathrm{mod}$. The tangent space at K_Δ to the moduli space of its deformations is isomorphic to $\oplus_{i\geqslant 0}\mathrm{Ext}^i_{A_{X\times X}-\mathrm{mod}}(K_\Delta,K_\Delta)$. After changing scalars to $\mathbf{C}((t))$ the latter sum can be identified with $H^\bullet(X,\mathbf{C}((t)))$. We can restrict the deformation functor to the subcategory $\mathrm{hol}(X)$. It is not difficult to see that the support of a holonomic module remains Lagrangian. These observations lead to the following result.

Proposition 1:

(a) *The Hochschild cohomology of the category $A_X-\mathrm{mod}$ is isomorphic to $H^\bullet(X,\mathbf{C}((t)))$. (Here*

we consider $A_X-\mathrm{mod}$ *as an* A_∞*-category with* $m_{n\neq 2}=0$ *and* m_2 *given by the usual composition of morphisms).*

(b) *The tangent space to the deformations of an object* $(L,\rho)\in \mathrm{hol}(X)$ is isomorphic to $H^\bullet(L,\mathrm{End}(\rho))\otimes \mathbf{C}((t))$.

We also mention the following proposition [see Soibelman (2001)]. It should be compared with the definition of Hom's in the Fukaya category.

Proposition 2: *Let* $V_{(L,\rho)}$ *denotes the object of* hol_X *corresponding to the pair* (L,ρ). *If* L_0 *is transversal to* L_1 *then*

(a) $\mathrm{Ext}^i(V_{(L_0,\rho_0)},V_{(L_1,\rho_1)})$ *is trivial if* $i\neq n$, *where* $n=1/2\ \dim X$;

(b) $\mathrm{Ext}^n(V_{(L_0,\rho_0)},V_{(L_1,\rho_1)})\simeq \oplus_{x\in L_0\cap L_1}\mathrm{Hom}(\rho_{0x},\rho_{1x})\otimes \mathbf{C}((t))$;

(c) *the algebra* $\mathrm{Ext}^\bullet(V_{(L,\rho)},V_{(L,\rho)})$ *is isomorphic to the cohomology* $H^\bullet(L,\mathrm{End}(\rho))\otimes \mathbf{C}((t))$ *[cf. part (b)] of the previous Proposition).*

Let $D^b_\infty(\mathrm{hol}(X))$ be the A_∞-category associated with the category $\mathrm{hol}(X)$. It is in fact a dg-category. In order to construct it one chooses injective resolutions of A_X-modules I_M and I_N of two holonomic modules M and N. Then one defines $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(M,N)=\mathrm{Hom}^\bullet(I_M,I_N)$. In this way one obtains an A_∞-model for the derived category of the category of holonomic modules.

The discussion above shows a certain similarity between $D^b_\infty(\mathrm{hol}(X))$ and $F^{\mathrm{naive}}(X)$. At the same time their deformation theories induce different products on the cohomology of X. In case of the Fukaya category it is the quantum product, while in case of $\mathrm{hol}(X)$ it is the usual cup product. The reader will also notice that the Maslov index is not visible in the case of $\mathrm{hol}(X)$.

On the other hand we will explain in the next section that

(a) The algebras $\mathrm{End}_{D^b_\infty(\mathrm{hol}(X))}((L,\rho))$ and $\mathrm{End}_{F^{\mathrm{naive}}(X)}((L,\rho))$ are A_∞-equivalent.

(b) If L and L' are Hamiltonian isotopic, then we can "twist" the space $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}((L,\rho),(L',\rho'))$ in such a way that it becomes quasi-isomorphic to the corresponding complex of morphisms in $F^{\mathrm{naive}}(X)$.

V. COMPARISON OF THE CATEGORIES

Let (L,ρ) be a pair as before, i.e., L is a Lagrangian submanifold of X and ρ is a local system on L. Let us denote by $E_{(L,\rho)}$ the corresponding object of $F(X)$, and by $V_{(L,\rho)}$ the corresponding object of $\mathrm{hol}(X)$. We assume that $m_0=0$ in the A_∞-algebra $A(L,\rho)$. This means that in fact we are dealing with the category $F^{\mathrm{naive}}(X)$. We also assume the conditions imposed on L in Fukaya, Oh, Ohta, and Ono (2000). This allows us to make necessary choices without further explanations. In particular L is relatively spin in the sense of Fukaya, Oh, Ohta, and Ono (2000), so the moduli spaces of pseudo-holomorphic discs are orientable. Taking the Hochschild complex of $A(L,\rho)$ we can construct the formal pointed dg-manifold $\mathcal{M}_{E_{(L,\rho)}}$ of deformations of $E_{(L,\rho)}$. Similarly, we can start with the Lie algebra $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(V_{(L,\rho)},V_{(L,\rho)})$ and construct the formal pointed dg-manifold $\mathcal{M}_{V_{(L,\rho)}}$ of deformations of $V_{(L,\rho)}$.

Let us imagine that both $F^{\mathrm{naive}}(X)$ and $D^b_\infty(\mathrm{hol}(X))$ are "sheaves of A_∞-categories" on the "moduli space of objects". Let us also imagine that there is a well-defined moduli space $Lagr_X$ of Lagrangian submanifolds of X. Then we should have a natural projection $\pi:\mathcal{M}_X\to \mathrm{Lagr}_X$. If L is a Lagrangian submanifold, and $[L]\in \mathrm{Lagr}_X$, the corresponding point of the moduli space then the fiber $\pi^{-1}([L])$ consists of local systems supported on L (or on any Lagrangian submanifold representing the same equivalence class in the moduli space). We would like to compare $F^{\mathrm{naive}}(X)$ and $\mathrm{hol}(X)$ in a "small neighborhood of $[(L,\rho)]$". From the categorical point of view we have two A_∞-categories $\mathcal{A}$ and $\mathcal{B}$ with the same "space" of objects, and such that for any object X the A_∞-algebras $\mathrm{End}_{\mathcal{A}}(X)$ and $\mathrm{End}_{\mathcal{B}}(X)$ are equivalent. We would like to find a functor $\Phi:\mathcal{A}\to\mathcal{A}$ such that changing morphisms in $\mathcal{A}$ to $\mathrm{Hom}^{\mathrm{new}}_{\mathcal{A}}(X,Y)=\mathrm{Hom}_{\mathcal{A}}(X,\Phi(Y))$ one gets a new A_∞-category equivalent to $\mathcal{B}$.

A. Main conjecture

We will denote by $\mathrm{hol}(L)$ the full subcategory of $\mathrm{hol}(X)$ consisting of holonomic modules with the given support L. For simplicity we will assume the rationality condition imposed on the symplectic form ω. Hence the Fukaya category is defined over $\mathbf{C}((q))$ (this is not a serious restriction because one can consider deformation quantization over any pro-nilpotent algebra, in particular $\mathbf{C}_\varepsilon$).

Our main idea can be explained such as follows. Having in mind the intuitive picture of the previous subsection we consider both $F^{\mathrm{naive}}(X)$ and $D^b_\infty(\mathrm{hol}(X))$ in a small neighborhood of a given $[L]\in \mathrm{Lagr}_X$. For a pair L_1, L_2 sufficiently close to L we would like to find a functor $\Phi_{L_1,L_2}: D^b_\infty(\mathrm{hol}(L_2)) \to D^b_\infty(\mathrm{hol}(L_1))$, such that $\mathrm{Hom}(\rho_1, \Phi_{L_1,L_2}(\rho_2))$ [morphism as objects of $D^b_\infty(\mathrm{hol}(L_1))$] is quasi-isomorphic to $\mathrm{Hom}_{F^{\mathrm{naive}}(X)}((L_1,\rho_1),(L_2,\rho_2))$. Such a functor should be represented by a bimodule. Let us describe all this more precisely.

Let $M_i = V_{(L_i,\rho_i)} \in \mathrm{hol}(L_i), i=1,2$. We expect that there exists a Lagrangian submanifold $\Lambda_{12} = \Lambda(L_1,L_2) \subset X\times X$ and $K(L_1,L_2) = K_{\Lambda_{12}} \in \mathrm{hol}(X\times X)$ such that the following occurs.

(1) If L_1 and L_2 have a nonempty intersection then $\Lambda_{12}\circ L_1 = L_2$. Here $\Lambda\circ L = \pi_2(\pi_1^{-1}(L)\cap\Lambda)$, where $\pi_i: X\times X\to X, i=1,2$ are the natural projections. In particular we assume that the restrictions of $\pi_i, i=1,2$ to Λ are coverings.

(2) $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(M_1, K(L_1,L_2)\circ M_2) \simeq \mathrm{Hom}_{F^{\mathrm{naive}}(X)}((L_1,\rho_1),(L_2,\rho_2))$, where $\simeq$ means a quasi-isomorphism of complexes, and we consider both categories over the field $\mathbf{C}((q))$ [i.e., $q=t$ in the case of $\mathrm{hol}(X)$]. The composition $\circ$ for modules is given by the formula $K\circ M = \pi_{2*}[K\otimes \pi_1^*(M)]$.We denote by $\mathrm{Hom}^{\mathrm{new}}(M_1,M_2)$ the left hand side of (2).

(3) For a generic sequence of Lagrangian submanifolds $L_1, L_2, \ldots, L_n, n\geqslant 2$ and holonomic modules $M_1,\ldots,M_n$ such that $M_i = V_{(L_i,\rho_i)}$ for all i, we expect to have an isomorphism of A_{X^n}-modules:

$$K(L_1,L_2)\circ K(L_2,L_3)\circ\cdots\circ K(L_{n-1},L_n)\to K(L_1,L_n).$$

Such an isomorphism defines a linear map,

$$m_n^{\mathrm{new}}: \otimes_{1\leqslant i\leqslant n-1}\mathrm{Hom}^{\mathrm{new}}(M_i,M_{i+1}) \to \mathrm{Hom}^{\mathrm{new}}(M_1,M_n).$$

We expect the above data to satisfy the following.

Conjecture 1: (i) Higher compositions $m_n^{\mathrm{new}}, n\geqslant 1$ give rise to a structure of an A_∞ -category on $D^b_\infty(\mathrm{hol}(X))$.

(ii) This category is A_∞-equivalent to $F^{\mathrm{naive}}(X,\omega)$ (with $q=t$).

B. The conjecture in the case of cotangent bundle

Let us fix a Lagrangian submanifold $L\subset X$, and consider only those L' which are "very close" to L. More precisely we assume that they are not only close to L but also Hamiltonian isotopic to L. We want to "restrict" $F^{\mathrm{naive}}(X)$ to this "neighborhood of L." This means that we consider an A_∞-subcategory with the objects taken from the above-mentioned subset, and morphisms the same as in $F^{\mathrm{naive}}(X)$. We do the same thing with $\mathrm{hol}(X)$ and $D^b_\infty(\mathrm{hol}(X))$. We would like to compare these categories in the case when $X=T^*Y$ is the cotangent bundle with the standard symplectic structure (notice that a neighborhood of a Lagrangian submanifold L can be identified by a symplectomorphism with a neighborhood of the zero section in T^*L). We are going to consider Lagrangian submanifolds of the type $L_i = \{(x, df_i(x)) | x\in Y\}$. Let ρ_i be local systems on L_i.

For a pair of such Lagrangian submanifolds we have a symplectomorphism $\phi: X\to X$ such that $(x,\xi)\mapsto (x, \xi + df_2(x) - df_1(x))$. Clearly it maps isomorphically L_1 into L_2.

Let us define $\Lambda = \Lambda_{12}$ as $\mathrm{graph}(\phi)\subset X\times X$. The corresponding bimodule K_Λ is the quotient of $A_X \boxtimes A_X^{op}$ by the left ideal generated by the relation $a\otimes 1 = 1\otimes e^{(1/t)ad(f_2-f_1)}(a)$, $a\in A_X$. Here $ad(a)\times(b) = ab-ba$ (clearly A_X contains C^∞_Y as a subalgebra, so the ideal is well-defined).

Notice that $\exp 1/t(ad(f_2-f_1))\exp 1/t(ad(f_3-f_2))\cdots\exp 1/t(ad(f_n-f_{n-1}))=\exp 1/t(ad(f_n-f_1))$. Hence we have an isomorphism $K(L_1,L_2)\circ K(L_2,L_3)\circ\cdots\circ K(L_{n-1},L_n)\to K(L_1,L_n)$.

In order to check the conjecture we may assume that $f_1=0$. Then we observe that

$$\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(\rho_1,K(L_1,L_2)\circ\rho_2)=\Omega^\cdot(Y,\rho_1^*\otimes\rho_2),$$

where the rhs is the complex of de Rham forms with values in the local system. Let $\nabla_i, i=1,2$ denote the flat connection on $\rho_i, i=1,2$. Then the differential is given by $\nabla_1^*\otimes 1+1\otimes\nabla_2+df_2\wedge(\cdot)$. The latter complex is equivalent to the standard de Rham complex (without df_2) if one twists the sections by $\exp((1/t)f_2)$, i.e., $s\mapsto s\exp((1/t)f_2)$. Then according to Kontsevich and Soibelman (2000), in Sec. IV the resulting complex is quasi-isomorphic to $\mathrm{Hom}_{F^{\mathrm{naive}}(X)}((L_1,\rho_1),(L_2,\rho_2))$. We remark that in the notation of Kontsevich and Soibelman (2000), one has $q=\exp(-1/\varepsilon)$.

Remark 4:. *The case of a general symplectic manifold does not follow automatically from the results of this section. Indeed, in order to define morphisms in the Fukaya category for Lagrangian submanifolds in a small neighborhood of a given L one has to consider pseudo-holomorphic disks which do not belong entirely to the neighborhood (we are restricted by the boundary conditions only). Nevertheless, if our main conjecture is true, one can find a family of kernels $K(L_1,L_2)$ which takes care of such disks.*

C. Complex structure on the moduli space of holonomic modules

We observe that the tangent space to the moduli space of deformations of a module $M\in\mathrm{hol}(X),\mathrm{supp}(M)=L$ is isomorphic to $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(M,M)$ [derived deformations of $\mathrm{Hom}_{\mathrm{hol}(X)\times(\mathrm{Id}_X,\mathrm{Id}_X)}$]. There is a natural embedding $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(L))}(M,M)\to\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(M,M)$, corresponding to the deformations with the fixed support L. On the other hand there is a natural projection $\mathrm{Hom}_{D^b_\infty(\mathrm{hol}(X))}(M,M)\to\Omega^\cdot(L)$, where $\Omega^\cdot(L)$ denotes the de Rham complex of L. Indeed, a deformation of the module M induces the deformation of the support of M. The latter are controlled by differential forms on the support. We can perform computations in the derived categories. Then we have an exact sequence of the tangent spaces to the formal moduli spaces of deformations:

$$\mathrm{Ext}^\cdot_{\mathrm{hol}(L)}(M,M)\to\mathrm{Ext}^\cdot_{\mathrm{hol}(X)}(M,M)\to H^\cdot_{DR}(L).$$

Suppose that M is a simple module. Then

$$R\,\mathrm{Hom}_{\mathrm{hol}(L)}(M,M)\simeq R\Gamma(L,R\underline{\mathrm{Hom}}(M,M))\simeq R\Gamma(L,\mathbf{C}_L)\simeq\Omega^\cdot(L).$$

Taking the first cohomology (this corresponds to "classical" tangent space) we obtain in this case an exact sequence,

$$H^1_{DR}(L)\to\mathrm{Ext}^1_{\mathrm{hol}(X)}(M,M)\to H^1_{DR}(L).$$

This means that the tangent space to the "classical" deformations of M inside of $\mathrm{hol}(X)$ is twice as big as the tangent space to the "classical" deformations of L inside of Lagr_X. If X is a Calabi–Yau manifold then one hopes to obtain a complex structure on the moduli space of formal deformations of a simple holonomic module M. We expect that it is isomorphic to a subvariety in the dual Calabi-Yau manifold. In order to describe the complex structure explicitly we need to identify the tangent space $T_L(\mathrm{Lagr}_X)$ with the tangent space $T_M(\mathrm{hol}(L))$. It is sufficient to describe the lifting of paths from Lagr_X to $\mathrm{hol}(L)$. Given a path $L(t)\subset\mathrm{Lagr}_X$ such that $L(0)=L$, we define a path $M(t)\subset\mathrm{hol}(L),M(0)=M$ in the following way: $M(t)=M\otimes\rho(t)$. Here $\rho(t)$ is the restriction to $L(t)$ of the unitary bundle over X with a connection ∇ such that $\mathrm{curv}(\nabla)=\omega_X$ (it is often called the pre-quantum line bundle). The restriction of ∇ to $L(t)$ is a flat connection.

VI. CONCLUSION

We have suggested the way to compare the Fukaya category with the category of holonomic modules over the quantized algebra of smooth functions. The idea is for a pair of Lagrangian submanifolds L_1, L_2 to find a kernel $K(L_1, L_2)$ which transforms local systems (or more general A_X-modules) supported on L_2 to local systems supported on L_1. We have conjectured that it is possible to make these choices in such a way that the counting of instantons (i.e., higher compositions in the Fukaya category) can be replaced by pure algebraic operation of taking homomorphisms between local systems having the same Lagrangian support. We have checked the conjecture in the simplest case. It would be interesting to check it in other cases as well as "globalize" this picture, finding kernels $K(L_1, L_2)$ for Lagrangian submanifolds which are not close to each other.

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Deformation quantization in singular spaces

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We present a method of quantizing analytic spaces X immersed in an arbitrary smooth ambient manifold M. Remarkably our approach can be applied to singular spaces. We begin by quantizing the cotangent bundle of the manifold M. Using a supermanifold framework we modify the Fedosov construction in a way such that the $\star$-product of the functions lifted from the base manifold turns out to be the usual commutative product of smooth functions on M. This condition allows us to lift the ideals associated to the analytic spaces on the base manifold to form left (or right) ideals on $(\mathcal{O}_{\Omega^1 M}[[\hbar]],\star_\hbar)$ in a way independent of the choice of generators and leading to a finite set of PDEs defining the functions in the quantum algebra associated with X. Some examples are included. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1788847]

I. INTRODUCTION

Deformation quantization is mathematically speaking a way of defining noncommutative associative products on a Poisson manifold, called $\star$-products, in a way such that the noncommutativity is controlled by a deformation parameter. The usual pointwise product is recovered as a limit case when this deformation parameter is negligible and the Poisson structure is found to be in the same fashion a limit case of the $\star$-commutator in accordance with the quantum correspondence principle.

Formally speaking, consider a smooth manifold N. A star product on $\mathcal{O}_N[[\hbar]]$ is an associative $\mathbb{R}[[\hbar]]$-linear product

$$f\star_\hbar g := \sum_{k=0}^{\infty} \left(-\frac{i\hbar}{2}\right)^k m_k(f,g),$$

where any m_k is a bidifferential operator of finite total order and $m_0(f,g)=fg$. It then can be shown that the operation on $\mathcal{O}_N[[\hbar]]$ defined by $\{f,g\}=\lim_{\hbar\to 0}(1/i\hbar)[f,g]$ is indeed a Poisson structure on M. (For a review from the mathematical perspective see Ref. 1.)

From the physics point of view deformation quantization is a new autonomous reformulation of quantum mechanics. Although still in development nowadays it is capable of reproducing numerous examples from the ordinary operator formulation and has been found to be closely related to the path integral formulation. (For a review from the physics perspective, see Refs. 2 and 3.)

One of the most powerful trends of work in mathematical physics during the last century was the generalization of the formulation of physical theories from the Euclidean case to the manifold framework. In this way classical mechanics was formulated in terms of a Poisson structure generalizing the classical notion of the Poisson bracket. Another example of this has been the gener-

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alization of the operator formulation of quantum mechanics to the nonflat case. Different answers have been found e.g., geometric quantization, group theoretic quantization. (For an extended discussion, see Ref. 4.)

Deformation quantization has followed a similar way going from the first $\star$-product found by Moyal following physical ideas and then generalized by Fedosov, who gave an explicit construction of a $\star$-product in an arbitrary symplectic manifold.[5,6]

The quantization of singular spaces has been somewhat rejected until very recently. This is one of the new possibilities provided by deformation quantization, since the traditional approaches breakdown in this case. Merkulov proposed in Ref. 7 a way of quantizing algebraic varieties immersed in some $\mathbb{R}^n$. This included the possibility of a nonempty set of singular points.

In this work we provide a general construction to quantize arbitrary analytic spaces (including the singular case), immersed in any smooth analytic real manifold. (A different approach can be found in Ref. 8.) We summarize the general context of this work in the following:

	Euclidean	Manifold framework
Classical mechanics	Poisson bracket	Poisson structure
Quantum mechanics	Heisenberg's formulation	e.g., group quantization
Deformation quantization	Moyal $\star$-product	Fedosov construction
Deformation quantization of singular spaces	Merkulov's work	This article

II. QUANTIZATION OF ANALYTIC SPACES

Consider a smooth analytic manifold M and $\mathcal{O}_M[[\hbar]]$, the ring of formal power series with global analytic functions as coefficients equipped with the usual commutative product. Classically an analytic space $(X,\mathcal{O}_X[[\hbar]])$ immersed on M is defined by choosing a finitely generated vanishing ideal I. Then the subspace X, which in general is not a smooth submanifold, corresponds to the set of solutions of the system of equations $\phi_i=0$, for any set $\phi_1,\ldots,\phi_n$ of generators of I. The associated ring of functions is defined then as $\mathcal{O}_X[[\hbar]]=\mathcal{O}_M[[\hbar]]/I$. (For a detailed exposition see, for example, Ref. 9.)

Now consider the cotangent bundle $\pi:\Omega^1M\to M$. The ideal I can be lifted via $\pi^{-1}(I)$ and in this way an analytic space $(X,\mathcal{O}_X[[\hbar]])$ can be defined. This time $\mathcal{O}_X[[\hbar]]=\mathcal{O}_{\Omega^1M}[[\hbar]]/\pi^{-1}(I)$ and $X\subset\Omega^1M$. In physical terms this would describe a system with a set of constrictions in the configuration space. Our goal is to define a quantum version of this structure capable of dealing with singular spaces.

Note that if one tries to replace naively the pointwise product of functions by the star product on Ω^1M (which can be found via the standard Fedosov construction for symplectic manifolds), one finds two possible scenarios. If one fixes a set of generators of the vanishing ideal $\pi^{-1}(I)$ before quantizing, the construction will depend on this choice since the star product depends on the smoothness around the vanishing points of the possible choices of generators. On the other hand, if one avoids this choice and defines a left (or right) ideal and proceeds to determine the normalizer, one finds an infinite number of equations.

In our approach, we modify the Fedosov construction[5,6] in a way that allows us to find a quantum algebra independently of the choice of generators and corresponding to the solutions of a finite set of partial differential equations.

The quantization procedure goes as follows:

Step 1. Initial data: The necessary data to begin the construction are

(1) *A smooth manifold M*;
(2) *A torsion free affine connection ∂ defined on M*;
(3) *The vanishing ideal I associated to the classical analytic space*.

Step 2. Quantization of $\Omega^1 M$: Before discussing the details we give in rough terms an overview of this step (for a related material on the deformation quantization of cotangent bundles with a different approach, see Ref. 10). The goal is to construct a star product on the ring of functions $\mathcal{O}_{\Omega^1 M}[[\hbar]]$ which coincides with the pointwise multiplication when restricted to functions lifted from the base, which is not the case in general for the standard Fedosov construction. The main tool is an auxiliary algebra $\mathcal{W}$ where a star product $\star_\hbar$ can be defined in a straightforward manner. Then a subalgebra $\mathcal{W}_D \subset \mathcal{W}$ with a one to one correspondence that we will denote as $\phi: \mathcal{O}_{\Omega^1 M}[[\hbar]] \to \mathcal{W}_D$ is found. The star product $\star'_\hbar$ for $\mathcal{O}_{\Omega^1 M}[[\hbar]]$ is defined as the one making the following diagram commute:

$$\begin{array}{ccc} \mathcal{O}_{\Omega^1 M}[[\hbar]] \otimes \mathcal{O}_{\Omega^1 M}[[\hbar]] & \overset{\star'_\hbar}{\rightarrow} & \mathcal{O}_{\Omega^1 M}[[\hbar]] \\ \phi \otimes \phi \downarrow & & \downarrow \phi \\ \mathcal{W}_D \otimes \mathcal{W}_D & \underset{\star_\hbar}{\rightarrow} & \mathcal{W}_D \end{array}$$

Then the key point in this step is to find the subalgebra $\mathcal{W}_D$, which turns out to be the set of flat sections of a connection, and the correspondent map ϕ.

Now we proceed with the exposition in detail. We shall use the language of supermanifolds which makes it more simple and makes the nature of the objects used more transparent.

Consider a $(3n|n)$-dimensional supermanifold $\mathcal{M} := \Omega^1 M \times_M TM \times_M \Pi(TM)$ (where we have used the parity change operator Π). For a coordinate system in $\Omega^1 M$ of the form $(x^1 \ldots x^n, p_1 \ldots p_n)$ we have an associated coordinate system on $\mathcal{M}$ of the form

$$(x^1 \cdots x^n, p_1 \cdots p_n, y^1 \cdots y^n, \psi^1 \cdots \psi^n).$$

Definition 2.1: The Weyl algebra $\mathcal{W}$ *on the supermanifold* $\mathcal{M}$ *is the usual supercommutative algebra* $\mathcal{O}_{\mathcal{M}}[[\hbar]]$*, and a typical element of* $\mathcal{W}$ *has locally the form*

$$a(x,p,y,\psi) = \sum_{k,p,r=0}^{\infty} \hbar^k a^{k_1 \cdots k_r}_{k,i_1 \cdots i_p, j_1 \cdots j_q}(x) y^{i_1} \cdots y^{i_p} p_{k_1} \cdots p_{k_r} \psi^{j_1} \cdots \psi^{j_q}, \tag{1}$$

where the tensor $a^{k_1 \cdots k_r}_{k,i_1 \cdots i_p, j_1 \cdots j_q}$ *is symmetric in the* $i_1 \cdots i_p$ *and* $k_1 \cdots k_r$ *indices and antisymmetric in the* $j_1 \cdots j_r$ *indices.*

There is a natural $\star$-product defined on $\mathcal{W}$ given as follows:

$$f \star_\hbar g = \exp\left(-\frac{i\hbar}{2} \left(\frac{\partial^2}{\partial y^a \partial \tilde{p}_a} - \frac{\partial^2}{\partial \tilde{y}^a \partial p_a} \right) \right) f(x,p,y,\psi) g(x,\tilde{p},\tilde{y},\psi)\big|_{p=\tilde{p}, y=\tilde{y}},$$

where $f, g \in \mathcal{W}$. This product is manifestly covariant and is easy to check it is associative. Note also that $f \star_\hbar g = g \star_{-\hbar} f$.

Then some auxiliary vector fields on $\mathcal{M}$ are defined:

$$\text{(i)} \quad \delta := \psi^a \frac{\partial}{\partial y^a},$$

$$\text{(ii)} \quad \delta^\star := y^a \frac{\partial}{\partial \psi^a},$$

$$\text{(iii)} \quad d := \psi^a \frac{\partial}{\partial x^a},$$

$$\text{(iv)}\ \ \delta^{-1}a := \frac{\delta^*}{p+q}a,$$

$$\text{(v)}\ \ \partial a := \psi^j \partial_i a,$$

where $a \in \mathcal{W}$ is a homogeneous element of order p in the variable y^a and of order q in the anticommutative variable ψ^a.

Lemma 2.2: Let $a \in \mathcal{W}$ be a homogeneous element as in the last paragraph and define $a_{00} := a(x,p,0,0)$, then

$$\text{(i)}\ \ \delta^2 a = 0,$$

$$\text{(ii)}\ \ \delta^{*2} a = 0,$$

$$\text{(iii)}\ \ \delta a = -\frac{i}{\hbar}[p_j\psi^j, a]_*,$$

$$\text{(iv)}\ \ a = a_{00} + \frac{1}{p+q}(\delta\delta^* a + \delta^* \delta a).$$

Proof is done by direct calculation, to illustrate we show the check for (iii) which goes as follows:

$$\begin{aligned}-\frac{i}{\hbar}[p_i\psi^i, a]_* &= -\frac{i}{\hbar}\left(p_i\psi^i a + \left(\frac{-i\hbar}{2}\right)\left(\frac{\partial^2}{\partial y^a \partial \tilde{p}_a} - \frac{\partial^2}{\partial \tilde{y}^a \partial p_a}\right) p_i\psi^i a(x,\tilde{y},\tilde{p},\psi) - (-1)^{\tilde{a}}\left(a p_i\psi^i + \left(\frac{-i\hbar}{2}\right)\right.\right.\\ &\quad \left.\left.\times\left(\frac{\partial^2}{\partial y^a \partial \tilde{p}_a} - \frac{\partial^2}{\partial \tilde{y}^a \partial p_a}\right) a(x,y,p,\psi)\tilde{p}_i\psi^i\right)\right)\\ &= -\frac{i}{\hbar}\left(\frac{-i\hbar}{2}\right)\left(-\psi^i\frac{\partial a}{\partial y^i} - (-1)^{\tilde{a}}\frac{\partial a}{\partial y^i}\psi^i\right) = \psi^i\frac{\partial a}{\partial y^i} = \delta a.\end{aligned}$$

□

Note that property (iv) implies that for all $a \in \mathcal{W}$ there is a decomposition

$$a = \delta\delta^{-1}a + \delta^{-1}\delta a + a_{00}. \tag{2}$$

The local expression of ∂ is

$$\partial a = \psi^a\left(\frac{\partial}{\partial x^a} + \Gamma^c_{ab}p_c\frac{\partial}{\partial p_b} - \Gamma^c_{ab}y^b\frac{\partial}{\partial y_c}\right)a. \tag{3}$$

Lemma 2.3: It is possible to express ∂a as

$$\partial a = da + \frac{i}{\hbar}[\Gamma, a]_*$$

for some $\Gamma \in \mathcal{W}$ of odd parity.

Proof: This can be shown as follows. Consider, for some constant α, the expression

$$da + [\alpha\Gamma, a]_* = da + i\hbar\alpha\left(-\frac{\partial\Gamma}{\partial y^b}\frac{\partial a}{\partial p_b} + \frac{\partial\Gamma}{\partial p_c}\frac{\partial a}{\partial y^c}\right) + O(\hbar^2).$$

Comparing this equation with Eq. (3) leads us to the equations

$$\psi^a\Gamma^c_{ab}p_c = -i\hbar\frac{\partial\alpha\Gamma}{\partial y^b}, \quad -\psi^a\Gamma^c_{ab}y^b = i\hbar\frac{\partial\alpha\Gamma}{\partial p_c}.$$

This implies that we must take $\Gamma=\Gamma^c_{ab}y^bp_c\psi^a$ and $\alpha=i/\hbar$ and the result follows. □

The auxiliary algebra is defined as the set $\mathcal{W}_D:=\{a\in\mathcal{W}:Da=0\}$, for some connection $D=\psi^aD_a$ that must satisfy the integrability condition $D^2=0$. It turns out that taking $D=\partial$ is not a good choice as the following proposition shows.

Proposition 2.4: The integrability condition for the connection ∂ can be expressed as

$$\partial^2 a = \frac{i}{\hbar}[R,a]_* \tag{4}$$

where $R:=\frac{1}{2}\psi^b\psi^cR^d_{abc}p_dy^a$.

Proof:

$$\begin{aligned}\frac{1}{2}[\partial,\partial]_*a &= \frac{1}{2}\left[\psi^a\left(\frac{\partial}{\partial x^a}+\Gamma^c_{ab}p_c\frac{\partial}{\partial p_b}-\Gamma^c_{ab}y^b\frac{\partial}{\partial y^c}\right),\psi^d\left(\frac{\partial}{\partial x^d}+\Gamma^f_{de}p_f\frac{\partial}{\partial p_e}-\Gamma^f_{de}y^e\frac{\partial}{\partial y^f}\right)\right]_{*a}\\ &= \frac{1}{2}\psi^a\psi^d\left(\left(\frac{\partial\Gamma^f_{de}}{\partial x^a}-\frac{\partial\Gamma^f_{ae}}{\partial x^d}\right)p_f\frac{\partial}{\partial p_e}+\left(\frac{\partial\Gamma^f_{ae}}{\partial x^d}-\frac{\partial\Gamma^f_{de}}{\partial x^a}\right)y^e\frac{\partial}{\partial y^f}+(\Gamma^f_{am}\Gamma^m_{de}-\Gamma^m_{ae}\Gamma^f_{dm})p_f\frac{\partial}{\partial p_e}\right.\\ &\quad\left.+(\Gamma^m_{ae}\Gamma^f_{dm}-\Gamma^m_{de}\Gamma^f_{am})y^e\frac{\partial}{\partial y^f}\right)a.\end{aligned}$$

And since

$$R^i_{jkl}=\frac{\partial\Gamma^i_{jl}}{\partial x^k}-\frac{\partial\Gamma^i_{jk}}{\partial x^l}+\Gamma^i_{mk}\Gamma^m_{jl}-\Gamma^i_{ml}\Gamma^m_{jk},$$

we have that

$$\partial^2=\frac{1}{2}\psi^b\psi^c\left(R^d_{abc}p_d\frac{\partial}{\partial p_a}-R^d_{abc}y^a\frac{\partial}{\partial y^d}\right)$$

and, on the other hand, we have

$$\frac{i}{\hbar}[R,a]_*=\frac{\partial R}{\partial y^a}\frac{\partial a}{\partial p_a}-\frac{\partial R}{\partial p_d}\frac{\partial a}{\partial y^d}.$$

This implies that we must take

$$R=\tfrac{1}{2}\psi^b\psi^cR^d_{abc}p_dy^a,$$

in order to have $\partial^2=(i/\hbar)[R,\cdot]_*$. This completes the proof. □

In other words the connection ∂ should be flat to fulfill the condition, which is far too restrictive. The way out is to define a new generalized connection of the form

$$Da=da+\frac{i}{\hbar}[-\psi^ap_a+\Gamma+\gamma,a]_*=\partial a+\frac{i}{\hbar}[-\psi^ap_a+\gamma,a]_*,$$

where γ is

$$\gamma=\sum_{n=3}^{\infty}\Gamma^a_{i_1\cdots i_n,b}y^{i_1}\cdots y^{i_n}p_a\psi^b, \tag{5}$$

to be determined to fulfill the integrability condition. Further calculation shows

$$D^2a=\frac{i}{\hbar}[R,a]_*+\frac{i}{\hbar}\partial[-\psi^\mu p_a+\gamma,a]_*+\frac{i}{\hbar}[-\psi^\mu p_a+\gamma,\partial a]_*+\left(\frac{i}{\hbar}\right)^2[-\psi^\mu p_a+\gamma,[-\psi^\mu p_a+\gamma,a]_*]_*$$
$$=\frac{i}{\hbar}[R,a]_*+\frac{i}{\hbar}[\partial\gamma,a]_*+\left(\frac{i}{\hbar}\right)^2\frac{1}{2}[[\psi^\mu p_a+\gamma,-\psi^\mu p_a+\gamma]_*,a]_*=\frac{i}{\hbar}\left[R+\partial\gamma-\delta\gamma+\frac{i}{\hbar}\gamma\star_\hbar\gamma,a\right]_*.$$

Then the equivalent condition for having $D^2=0$ is

$$\delta\gamma=R+\partial\gamma+\frac{i}{\hbar}\gamma^2. \tag{6}$$

Proposition 2.5: γ is a solution of Eq. (6) if and only if

$$\gamma=\delta^{-1}R+\delta^{-1}\left(\partial\gamma+\frac{i}{\hbar}\gamma^2\right) \tag{7}$$

and the condition $\delta^{-1}\gamma=0$ is fulfilled.

Fedosov's proof[6] can be applied here so we shall not include it.

Substitution of the general form of γ given in (5) into Eq. (7) leads to an iterative process with initial condition $\delta^{-1}R$. The first terms of the solution are

$$\gamma=\tfrac{1}{3}R^d_{abc}y^ay^b\psi^cp_d+\tfrac{1}{12}\partial_lR^d_{abc}y^ly^ay^b\psi^cp_d+\cdots.$$

The subalgebra $\mathcal{W}_D$ is defined by the condition $Da=0$, i.e.,

$$\delta a=\partial a+\frac{i}{\hbar}[\gamma,a]_*. \tag{8}$$

Proposition 2.6: There is a one to one correspondence $\phi:\mathcal{O}_{\Omega^1M}[[\hbar]]\to\mathcal{W}_D$.

Proof: This can be shown as follows. Condition (8) is equivalent to

$$a=a_{00}+\delta^{-1}\left(\partial a+\left[\frac{i}{\hbar}\gamma,a\right]_*\right). \tag{9}$$

The equivalence of these two equations is proved as in the Fedosov construction. Indeed, since $D^2a=0$

$$\delta Da=\partial Da+\left[\frac{i}{\hbar}\gamma,Da\right]_*. \tag{10}$$

On the other hand, using (9) $\delta^{-1}Da=0$ and so

$$Da=\delta^{-1}\left(\partial Da+\left[\frac{i}{\hbar}\gamma,Da\right]_*\right).$$

Solution of this equation by an iterative process implies that $Da=0$. The converse assertion is trivial.

These are the first few terms of the solution for Eq. (9)

$$a=a_{00}+\partial_ia_{00}y^i+\frac{1}{2}\partial_i\partial_ja_{00}y^iy^j+\frac{1}{6}\partial_i\partial_j\partial_ka_{00}y^iy^jy^k-\frac{1}{12}R^d_{abc}y^ay^bp_d\frac{\partial a_{00}}{\partial p_c}+\cdots$$

giving the one to one map $a_{00}\mapsto\phi(a_{00}):=a$. □

The star product for $f_{00},g_{00}\in\mathcal{O}_{\Omega^1M}[[\hbar]]$ is finally defined as

$$f_{00}\star'_\hbar g_{00} = \phi^{-1}(f\star_\hbar g),$$

where $\phi^{-1}(f\star_\hbar g)=f\star_\hbar g(x,p,y,0)_{|y=0}$. The star product $\star'_\hbar$ inherits from $\star_\hbar$ the natural shift from left to right multiplication $f_{00}\star_\hbar g_{00}=g_{00}\star_{-\hbar}f_{00}$, implying that our construction will not depend on our choice to use left ideals instead of right ideals.

We find our key result for this step

Theorem 2.7: *Let* $f_{00},g_{00}\in\pi^*(\mathcal{O}_M[[\hbar]])$, then

$$f_{00}\star'_\hbar g_{00} = f_{00}g_{00}.$$

Proof: Suppose that in Eq. (9) the starting condition $a_{00}(x,p)$ does not depend on p, therefore the commutator $[\gamma,a_{00}]$ vanishes and one can check that this happens for every step in the iterative solution. We are left then with the equation

$$a = a_{00}(x,p) + \delta^{-1}(\psi^i\partial_i a).$$

Solutions of this equation are

$$a = a_{00} + \sum_{i=1}^{n}\frac{1}{n!}\partial_{i_1}\cdots\partial_{i_n}a_{00}y^{i_1}\cdots y^{i_n}.$$

Star products of functions of this type are clearly just the usual commutative product. Now let f_{00},g_{00} be two functions not depending on p then

$$f_{00}(x)\star'_\hbar g_{00}(x) = \phi^{-1}(f\star_\hbar g) = \phi^{-1}(fg) = f_{00}(x)g_{00}(x).$$

□

From this point we denote the star product on Ω^1M simply as $\star_\hbar$.

Step 3. Define the left ideal $\mathcal{J}_l$ *and compute the normalizer* $\mathcal{N}_l$: With the natural projection $\pi:\Omega^1M\to M$ the ideal $I\subset\mathcal{O}_M[[\hbar]]$ can be lifted to Ω^1M giving a set $\pi^*(I)\subset\mathcal{O}_{\Omega^1M}$ which defines a left ideal

$$\mathcal{J}_l = \{\mathcal{O}_{\Omega^1M}[[\hbar]]\star_\hbar\pi^*(I)\}.$$

Consider now the normalizer $\mathcal{N}_l\subset A_{\mathcal{M}}$ for the left ideal $\mathcal{J}_l$,

$$\mathcal{N}_l = \{h\in\mathcal{O}_{\Omega^1M}[[\hbar]]:\pi^*(I)\star_\hbar h\subset\mathcal{J}_l\}.$$

Clearly $\mathcal{J}_l\subset\mathcal{N}_l$ and moreover $\mathcal{J}_l$ is a double sided ideal of $\mathcal{N}_l$, this is

$$f\star_\hbar s\in\mathcal{J}_l,\quad s\star_\hbar f\in\mathcal{J}_l,$$

for all $f\in\mathcal{N}_l$, $s\in\mathcal{J}_l$.

Step 4. Take the quotient $\mathcal{Q}_X:=\mathcal{N}_l/\mathcal{J}_l$: *The result is a well defined noncommutative associative algebra which we call the quantum algebra of observables of X.*

Computing the normalizer of a one-sided ideal and taking the quotient to find a noncommutative ring is a rather common procedure which in general leads to conditions difficult to solve, but in our case, remarkably we have

Theorem 2.8: *The algebra* $\mathcal{Q}_X$ *corresponds to the quotient solution space of a finite number of partial differential equations and it does not depend on the choice of generators of the ideal I.*

Proof: The key point of the proof is given by theorem 2.7. This implies that for any $g\in\mathcal{O}_{\Omega^1M}$ the condition to be in the normalizer

$$\pi^{-1}(I)\star_\hbar g = 0 \bmod \mathcal{J}_l$$

is equivalent to

$$\left(\sum_{i=1}^{n}\alpha_i\phi_i\right)\star_\hbar g=\sum_{i=1}^{n}\alpha_i\star_\hbar(\phi_i\star_\hbar g)=0 \bmod \mathcal{J}_l. \tag{11}$$

In other words to the condition that $\phi_i\star_\hbar g=0 \bmod \mathcal{J}_l$ for the n generators ϕ_i of $\pi^{-1}(I)$. Each equation being in fact a partial differential equation for functions in $\mathcal{O}_{\Omega^1 M}[[\hbar]]$. The independence of the choice of generators of the ideal follows trivially from the fact that any new set of generators $\tilde{\phi}_i$ can be rewritten as a combination of the original ones leading again to Eq. (11). □

III. EXAMPLES

We shall develop next several examples of the explained technique when the ambient configuration space is $\mathbb{R}^2$. The natural choice of star product is the Moyal product on $\Omega^1\mathbb{R}^2$, given by

$$f*_\lambda g=e^{\lambda\Sigma_{i=1}^{2}(\partial/\partial_{x_i}\,\partial/\partial_{\tilde{p}_i}-\partial/\partial_{\tilde{x}_i}\,\partial/\partial_{p_i})}f(x_1,x_2,p_1,p_2)g(\tilde{x}_1,\tilde{x}_2,\tilde{p}_1,\tilde{p}_2)_{|\tilde{x}=x,\tilde{p}=p}$$

with $f,g\in\mathcal{O}_{\Omega^1\mathbb{R}^2}[[\lambda]]$. Clearly the Moyal product of functions not depending on the momentum variables coincides with the pointwise product. We shall be using the following:

Lemma 3.1: Every analytic function $f(x_1,x_2,p_1,p_2)\in\Omega^1\mathbb{R}^2$ can be uniquely decomposed as

$$f(x_1,x_2,p_1,p_2)=\sum_{i,j=0}^{\infty}f_{ij}(p_1,p_2)*_\lambda x_1^i *_\lambda x_2^j. \tag{12}$$

Proof: It is sufficient to note that

$$h(p_1,p_2)x_1^M x_2^N=h(p_1,p_2)*_\lambda x_1^M x_2^N-\sum_{n=1}^{M}\sum_{k=0}^{\min(N,n)}\frac{(-\lambda)^n}{(n-k)!\,k!}\frac{M!\,N!}{(M-n+k)!\,(N-k)!}x_1^{M-n+k}x_2^{N-k}\frac{\partial^n h}{\partial p_1^{(n-k)}\partial p_2^k}$$

implying that the Taylor expansion can be re-expressed in terms of the Moyal product. □

A. The cross

Consider now the analytic variety of the cross defined by the equation $x_1x_2=0$. Any function on the quantum algebra $\mathcal{Q}=\mathcal{N}_l/\mathcal{J}_l$ can be expressed as

$$h(x_1,x_2,p_1,p_2)=h_0(p_1,p_2)+h_1(x_1,p_1,p_2)*_\lambda x_1+h_2(x_2,p_1,p_2)*_\lambda x_2.$$

The left ideal is

$$\mathcal{J}_l=\{f*_\lambda x_1x_2 : f\in\mathcal{O}_{\Omega^1\mathbb{R}^2}\}.$$

The condition for the function h to be in the normalizer $\mathcal{N}_l$ is $x_1x_2*_\lambda h\in\mathcal{J}_l$, i.e.,

$$\begin{aligned}0 \bmod \mathcal{J}_l &= x_1x_2*_\lambda h_0+x_1x_2*_\lambda h_1*_\lambda x_1+x_1x_2*_\lambda h_2*_\lambda x_2\\ &=[x_1x_2,h_0]+[x_1x_2,h_1]*_\lambda x_1+[x_1x_2,h_2]*_\lambda x_2\\ &=2\lambda\frac{\partial^2 h_0}{\partial p_1\partial p_2}+\left(\frac{\partial h_0}{\partial p_2}+\lambda\frac{\partial^2 h_1}{\partial p_1\partial p_2}+x_1\frac{\partial h_1}{\partial p_2}\right)*_\lambda x_1+\left(\frac{\partial h_0}{\partial p_1}+\lambda\frac{\partial^2 h_2}{\partial p_1\partial p_2}+x_2\frac{\partial h_2}{\partial p_1}\right)*_\lambda x_2.\end{aligned}$$

Solutions have the form

$$h_1(x_1,p_1,p_2)=-\frac{h_0^2(p_2)}{x_1}+\xi(x_1,p_2)e^{-x_1p_1/\lambda}+a(x_1,p_1),$$

$$h_2(x_2,p_1,p_2) = -\frac{h_0^1(p_1)}{x_2} + \zeta(x_2,p_1)e^{-x_2p_2/\lambda} + b(x_2,p_2),$$

where $h_0^1(p_1), h_0^2(p_2)$ are arbitrary functions. The solutions of the form $h_0^2(p_2)/x_1, h_0^1(p_1)/x_2$ are not defined on the cross, therefore we do not consider them, similarly the terms $\xi(x_1,p_2)e^{-x_1p_1/\lambda}$ and $\zeta(x_2,p_1)e^{-x_2p_2/\lambda}$ must be rejected as they are not meromorphic in λ. (However such solutions may have a physical interpretation which we hope to elucidate later.)

We have then a family of functions for the quantum algebra of the cross given by

$$\mathcal{Q}_C := \{h \in \mathcal{O}_{\Omega^1\mathbb{R}^2}[[\lambda]]: h(x_1,x_2,p_1,p_2) = a(x_1,p_1)*_\lambda x_1 + b(x_2,p_2)*_\lambda x_2\}.$$

Computing the Moyal product of two elements h, $\tilde{h} \in \mathcal{Q}_C$ and eliminating terms with the factor x_1x_2 we find

$$h*_\lambda\tilde{h} = (a*_\lambda x_1 + b*_\lambda x_2)*_\lambda(\tilde{a}*_\lambda x_1 + \tilde{b}*_\lambda x_2) = a*_\lambda x_1*_\lambda\tilde{a} + b*_\lambda x_2*_\lambda\tilde{b}.$$

In other words the quantum algebra of the cross has then elements of the form

$$h = (a(x_1,p_1), b(x_2,p_2)),$$

where a, b are arbitrary functions and the noncommutative product is

$$h\star_C\tilde{h} = (a*_\lambda x_1*_\lambda\tilde{a}, b*_\lambda x_2*_\lambda\tilde{b}).$$

B. The double line

Consider now the analytic space of the double line defined by the equation $x_2^2=0$. Functions of the quantum algebra $\mathcal{N}_l/\mathcal{J}_l$ can be represented as

$$h(x_1,x_2,p_1,p_2) = h_0(x_1,p_1,p_2) + h_1(x_1,p_1,p_2)*_\lambda x_2.$$

The condition for h to be in the normalizer of the left ideal $\mathcal{J}_l=\{f*_\lambda x_2^2; f \in \mathcal{O}_{\Omega^1\mathbb{R}^2}\}$ is

$$0 \bmod \mathcal{J}_l = [x_2^2,h_0] + [x_2^2,h_1]*_\lambda x_2.$$

Leading to the differential equation

$$x_2\frac{\partial h_0}{\partial p_2} + \lambda x_2\frac{\partial^2 h}{\partial p_2^2} + \lambda^2\frac{\partial^3 h}{\partial p_2^3} = 0$$

whose general solution is

$$h(x_1,x_2,p_1,p_2) = a(x_1,p_1) + b(x_1,p_1)p_2 + \left(c(x_1,p_1) + d(x_1,p_1)p_2 - \frac{b(x_1,p_1)}{2\lambda}p_2^2\right)*_\lambda x_2.$$

The product of two of these functions can be represented as a matrix star product denoted as $\star$, in the following way:

$$\phi(h) := \begin{pmatrix} a+2\lambda d & b \\ 2\lambda c & a \end{pmatrix} \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}.$$

Then

$$\phi(h)\star\phi(\tilde{h})) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}*_\lambda\begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} = \begin{pmatrix} A*_\lambda\tilde{A} + B*_\lambda\tilde{C} & A*_\lambda\tilde{B} + B*_\lambda\tilde{D} \\ C*_\lambda\tilde{A} + D*_\lambda\tilde{C} & C*_\lambda\tilde{B} + D*_\lambda\tilde{D} \end{pmatrix}$$

is equal to $\phi(h*_\lambda\tilde{h})$.

C. Line with a double point

We shall proceed now with the quantization of the line with a double point defined as the quotient of the quantum algebra of the double line quotient by the ideal generated by $x_1x_2=0$ which has the form

$$\phi(h*_\lambda x_1x_2)=\phi(h)\star\phi(x_1x_2)=\begin{pmatrix}A & B\\ C & D\end{pmatrix}*_\lambda\begin{pmatrix}0 & 0\\ x_1 & 0\end{pmatrix}=\begin{pmatrix}B*_\lambda x_1 & 0\\ D*_\lambda x_1 & 0\end{pmatrix},$$

where B, D are arbitrary functions depending on x_1, p_1. The corresponding normalizer will be the set of solutions of the equation

$$\begin{pmatrix}0 & 0\\ x_1 & 0\end{pmatrix}*_\lambda\begin{pmatrix}a & b\\ c & d\end{pmatrix}=0 \bmod \mathcal{J}_l, \tag{13}$$

where a, b, c, d are a different set of arbitrary functions depending on x_1, p_1. This implies in turn that $b=0$ since the only solutions of the differential equation $x_1b+\lambda\partial_{p_1}b=0$ are not in the space of acceptable formal functions. Then $a(x_1,p_1)$ must be a solution of the equation

$$x_1*_\lambda a=0(\bmod D*_\lambda x_1).$$

Decomposing $a=\Sigma_{i=0}^{\infty}a_i(p_1)*_\lambda x_1^i$ and factoring out we can rewrite this as

$$x_1*_\lambda a_0(p_1)=0(\bmod D*_\lambda x_1).$$

Lemma 3.2:

$$A(x,p)*_\lambda B(p)=\sum_{n=0}^{\infty}(2\lambda)^nA_n(p)B^{(n)}(p)(\bmod D*_\lambda x),$$

where $A(x,p)=\Sigma A_n(p)*_\lambda x^n$ *and* $B^{(n)}$ *is the nth derivative of* B.

Proof:

$$\sum_{i=0}^{\infty}A_i(p)*_\lambda x^{i-1}*_\lambda x*_\lambda B(p)=\sum_{i=0}^{\infty}A_i(p)*_\lambda x^{i-1}*_\lambda 2\lambda B^{(1)}(\bmod D*_\lambda x)=\sum_{i=0}^{\infty}(2\lambda)^iA_i(p)*_\lambda B^{(i)}(p).$$

□

In particular this implies that the second equation means that $a=k$ for some constant. Then the normalizer has the form

$$\begin{pmatrix}k & 0\\ c(x_1,p_1) & d(x_1,p_1)\end{pmatrix}.$$

The last step is to factor out the members of the left ideal from this normalizer. This means to take

$$c(x_1,p_1)\bmod D*_\lambda x_1.$$

The resulting quantum algebra for the line with a double point is the set of matrices of the form

$$\begin{pmatrix}k & 0\\ c(p_1) & d(x_1,p_1)\end{pmatrix}$$

with multiplication law

$$\begin{pmatrix} k & 0 \\ c(p_1) & d(x_1,p_1) \end{pmatrix} \star' \begin{pmatrix} \tilde{k} & 0 \\ \tilde{c}(p_1) & \tilde{d}(x_1,p_1) \end{pmatrix}$$
$$= \begin{pmatrix} k\tilde{k} & 0 \\ \tilde{k}c(p_1) + \sum_{n=0}^{\infty} (2\lambda)^n d_n(p_1)\tilde{c}^{(n)}(p_1) & d(x_1,p_1) *_\lambda \tilde{d}(x_1,p_1) \end{pmatrix},$$

where we have used Lemma 3.2.

D. The doubly fattened circle

Let us consider now the space associated to the ideal generated by $x_1^2+x_2^2$, that we refer to as the "doubly fattened" circle. Although the zero set of this polynomial is just the origin the resulting quantum algebra, as we shall show, is nontrivial. Any function in this quantum algebra can be represented as

$$h(x_1,x_2,p_1,p_2) = h_0(x_1,p_1,p_2) + h_1(x_1,p_1,p_2) *_\lambda x_2.$$

The left ideal is

$$\mathcal{J}_l = \{f *_\lambda (x_1^2 + x_2^2) : f \in \mathcal{O}_{\Omega^1\mathbb{R}^2}[[\lambda]]\}.$$

The condition for a function $h(x_1,x_2,p_1,p_2)$ to be in the normalizer is

$$0 \bmod \mathcal{J}_l = (x_1^2 + x_2^2) *_\lambda h = -\frac{\partial h_1}{\partial p_2} x_1^2 + 2\lambda x_1 \frac{\partial^2 h_1}{\partial p_1 \partial p_2} - \lambda^2 \frac{\partial^3 h_1}{\partial p_1^2 \partial p_2} + \lambda \frac{\partial^2 h_0}{\partial p_2^2} + x_1 \frac{\partial h_0}{\partial p_1} + \left(\frac{\partial h_0}{\partial p_2} + \lambda \frac{\partial^2 h_1}{\partial p_2^2} + x_1 \frac{\partial h_1}{\partial p_1} \right) *_\lambda x_2.$$

Manipulations in the last equation lead to the condition

$$x_1^2(\Delta h_1) - \lambda^2 \frac{\partial^2}{\partial p_2^2}(\Delta h_1) = 0,$$

where $\Delta = \partial_{p_1}^2 + \partial_{p_2}^2$, is the Laplacian operator. Therefore the two-dimensional spherical harmonics give a family of solutions h_1.

E. Conclusion

We have shown a way to define noncommutative associative products to analytic spaces immersed in analytic manifolds. The procedure works for smooth spaces and more remarkably it works for singular spaces. This opens new possibilities in the field of deformation quantization and leaves many open questions. One such question is how the singularity affects the resulting algebra, or more generally how the singularity type affects it. Questions like these can be studied through the introduction of parameters deforming the analytic spaces which will enter the partial differential equations defining the associated algebras. These equations turn out to be complex in most cases. New techniques need to be developed to find the representation of the algebras to make possible the study of such questions.

Another interesting possibility is to develop a comparative study of the different quantization programs. The common goal of all such programs is to give a quantized version of classical physical systems. Naturally for any given classical system there should be a unique physical quantum version, thus one would expect the different approaches to be equivalent in some sense. Having an affirmative answer to this would give a hint of some deep mathematical relations between the different approaches.

Another important line of work is to develop proper physical applications of the program. A rather interesting question to be studied is to find out how the singularity affects the physics of the space.

We expect to elucidate these and other questions in the future.

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Classification of extensions of principal bundles and transitive Lie groupoids with prescribed kernel and cokernel

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The equivalence of principal bundles with transitive Lie groupoids due to Ehresmann is a well-known result. A remarkable generalization of this equivalence, given by Mackenzie, is the equivalence of principal bundle extensions with those transitive Lie groupoids over the total space of a principal bundle, which also admit an action of the structure group by automorphisms. In this paper the existence of suitably equivariant transition functions is proved for such groupoids, generalizing consequently the classification of principal bundles by means of their transition functions, to extensions of principal bundles by an equivariant form of Čech cohomology. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1786349]

INTRODUCTION

Lie groupoids are categories where every arrow has an inverse, plus a smooth structure. They generalize at the same time the notion of a manifold and a group, and are widely understood to be part of the general context of noncommutative geometry. First, because groupoids are inherently noncommutative objects, to a greater extent than are groups. Second, Lie groupoids provide a modern context for the understanding of the geometry of symplectic and Poisson manifolds, which are equipped with noncommutative structures. Following a result of Mackenzie, it was shown in Ref. 1, that the prequantization problem for a symplectic manifold amounts to the existence of a suitable transitive Lie groupoid. Furthermore, given a Poisson manifold, the existence of a (nontransitive) symplectic groupoid provides a way to quantize it.

A rough and descriptive definition of a Lie groupoid is a pair of manifolds Ω and M such that the elements of Ω are arrows between points of M. The functions $\alpha,\beta:\Omega\to M$ mapping every arrow to its source and target points in M are differentiable. Moreover there is a differentiable way to multiply suitable arrows (such that the source of one is exactly the target of the other), and the inversion of arrows is also differentiable. In this setting, for $x,y\in M$ we denote Ω_x the set of arrows in Ω with source x, Ω^y the arrows with target y and Ω_x^y the arrows with source x and target y. In particular, Ω_x^x is a Lie group called the *orbit* of Ω at x. A Lie groupoid is denoted by $\Omega\rightrightarrows M$.

The simplest example of a Lie groupoid is the product $M\times M\rightrightarrows M$ of a manifold M, with the obvious groupoid structure. This is called the "pair" groupoid. If Ω and Ξ are Lie groupoids over the same base manifold M, then a smooth map $\varphi:\Omega\to\Xi$ is a *morphism* of Lie groupoids if $\alpha\circ\varphi=\alpha$, $\beta\circ\varphi=\beta$ and $\varphi(\eta\cdot\xi)=\varphi(\eta)\cdot\varphi(\xi)$ for any pair of composable arrows in Ω. For example, given any Lie groupoid $\Omega\rightrightarrows M$, the map $(\beta,\alpha):\Omega\to M\times M$ is a morphism of Lie groupoids. This particular morphism is called the *anchor*.

The most well-known classification of Lie groupoids is the one of the transitive case. Transitive Lie groupoids are the ones whose anchor is a surjective submersion, in other words there is an arrow between any two points in M. The choice of a basepoint $x\in M$ for a transitive Lie groupoid $\Omega\rightrightarrows M$ gives rise to the principal bundle $\Omega_x(M,\Omega_x^x,\beta_x)$. The principal bundles arising

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from different choices of elements in M are isomorphic. Given a principal bundle $P(M,G,\pi)$ on the other hand, the associated transitive Lie groupoid is the quotient $(P\times P)/G \rightrightarrows M$. The groupoid structure here is as follows: For an element $\langle u_2,u_1\rangle$, the source is $\pi(u_1)$ and the target $\pi(u_2)$. Suitable arrows $\langle u_2,u_1\rangle$ and $\langle u_2',u_1'\rangle$ such that there exists a $g\in G$ with $u_1=u_2'g$ can be multiplied by

$$\langle u_2,u_1\rangle\langle u_2',u_1'\rangle=\langle u_2,u_1'g\rangle.$$

The inverse of $\langle u_2,u_1\rangle$ is $\langle u_1,u_2\rangle$ and the unit element over an $x\in M$ is $\langle u,u\rangle$ for any $u\in P$ such that $\pi(u)=x$. It is shown in Ref. 8, Vol. II, Sec. I that the two processes are mutually inverse.

So transitive Lie groupoids are classified by the well-known classification of principal bundles by Čech cohomology.

A different classification of the transitive case was given by Mackenzie in Ref. 9. It was shown that if we shift the point of view from the prescription of Ω_x^x (for any given basepoint) to the prescription of the Lie group bundle $I\Omega$ over M, of orbits, then transitive Lie groupoids are classified by Čech cohomology with Abelian coefficients. This classification is always possible to calculate in contrast with the often non-Abelian classification of principal bundles. To achieve this classification, a transitive Lie groupoid is considered as an extension,

$$I\Omega \rightarrowtail \overset{(\beta,\alpha)}{\Omega} \twoheadrightarrow M\times M,$$

of the Lie groupoid $M\times M\rightrightarrows \mathrm{M}$ (with the obvious groupoid structure) by the Lie group bundle $I\Omega$, instead of the principal bundle $\Omega_x(M,\Omega_x^x,\beta_x)$. For example, the groupoid extension associated to a principal bundle $P(M,G)$ is

$$\frac{P\times G}{G} \rightarrowtail \frac{P\times P}{G} \twoheadrightarrow M\times M, \tag{1}$$

where $(P\times G)/G\to M$ is the well-known gauge group bundle of $P(M,G)$ (where the G-action on itself implied is the adjoint). The usual classification of principal bundles by $\check{H}^1(M,G)$ is the answer to the problem "given a Lie group G and a manifold M, classify all principal bundles $P(M,G)$." Mackenzie's results imply that if we shift the problem to "given a Lie group bundle $F\to M$ classify all groupoid extensions of $M\times M$ by this bundle," then we get a classification by Čech cohomology with coefficients in an Abelian group which is always computable, instead of $\check{H}^1(M,G)$.

Another classification appeared recently by Moerdijk. In Ref. 11 regular Lie groupoids are classified, i.e., those whose orbits have a constant dimension. Many Lie groupoids are regular, for example those arising from regular Poisson manifolds; moreover all transitive Lie groupoids are regular. Extensions appear in this classification as well. Namely, it is shown that regular Lie groupoids are extensions of foliation groupoids by bundles of connected Lie groups, and they are classified as such. In the case of transitive Lie groupoids, the results in Ref. 9 are a variation of the results of Moerdijk in Ref. 11.

The main result of the present paper is the classification of extensions of transitive Lie groupoids by bundles of Lie groups. Denote such an extension,

$$F \rightarrowtail \Omega \twoheadrightarrow \Xi, \tag{2}$$

where F is a bundle of Lie groups and Ω,Ξ are Lie groupoids, all of them over the same connected manifold M. Due to the equivalence of transitive Lie groupoids with principal bundles, such extensions are equivalent to extensions of principal bundles,

$$N \rightarrowtail Q(M,H) \twoheadrightarrow P(M,G). \tag{3}$$

Here N is a Lie group and the notation implies the existence of an extension of Lie groups,

$$N \rightarrowtail H \twoheadrightarrow G.$$

On the other hand, an extension of principal bundles (3) gives rise to the extension of transitive Lie groupoids over M,

$$\frac{Q \times N}{H} \rightarrowtail \frac{Q \times Q}{H} \twoheadrightarrow \frac{P \times P}{G}.$$

Here the quotient $(Q \times N)/H \rightarrow M$ is the bundle of Lie groups associated to the principal bundle $Q(M,H)$ through the action of H on N by (the restrictions of) inner automorphisms. It is shown in Ref. 7 that the two processes are mutually inverse.

From this point of view, the importance of such a classification is more than the generalization of the classification of transitive Lie groupoids to extensions. The central problem it deals with is the classification of the covering bundles of a given principal bundle $P(M,G)$ with connected base manifold M. Less abstract uses of such a classification arise from an abundance of paradigms of extensions of principal bundles (see for example Ref. 6).

The classification of extensions (2) is made possible using a result of Mackenzie.[7] It was proved that such extensions are equivalent to a special kind of transitive Lie groupoids, the so-called PBG-groupoids. These are transitive Lie groupoids over the total space of a principal bundle which admit an action of the Lie group of the bundle by Lie groupoid isomorphisms. A description of this equivalence is given in Sec. II of this paper. Roughly speaking, the PBG-groupoid that corresponds to (2) is a Lie groupoid over the principal bundle $P(M,G)$, together with a G-action by (Lie groupoid) automorphisms. Thinking in terms of the extension of principal bundles (3) corresponding to (2), this is a remarkable result; because although the Lie group G does not always act on the kernel N (unless N is Abelian), due to Mackenzie's result there always exists a Lie groupoid which admits an action of G.

Once this result is well understood, the problem shifts to the classification of PBG-groupoids. The classification we give here is similar to the one given for general transitive Lie groupoids. In that case, the equivalence with principal bundles ensures the existence of transition functions for Lie groupoids, which suffice to classify them by the usual Čech cohomology. In the case of PBG-groupoids though, it is necessary to encode the group action as well, and the existence of transition functions which keep track of the action is not established.

In this paper it is shown that there exist transition functions for PBG-groupoids which are equivariant in a certain sense. This is a nonstandard notion of equivariance which we call *isometablicity*. In turn, a nonstandard form of equivariance in Čech cohomology arises. The first isometablic Čech cohomology then classifies PBG-groupoids.

Furthermore, a rather old problem is answered. Lie algebroids are the infinitesimal objects that arise from Lie groupoids, remotely related to them like Lie algebras are related to Lie groups. Mackenzie in Ref. 8 gave a classification of transitive Lie algebroids, but it is not clear how this classification integrates to the groupoid level. A reformulation of the isometablic transition functions is given here, which clearly differentiates to the equivariant analog of the classification given in Ref. 8.

This paper is structured in the following way: Section I is an account of PBG-groupoids and their relation with extensions of Lie groupoids and principal bundles. In Sec. II the relevant connection theory is described, emphasizing on the material that is of use for the scope of this paper. In Sec. III we prove the existence of transition functions which keep track of the group action, and clarify the notion of isometablicity. In Sec. IV we give the classification of PBG-Lie group bundles. A remarkable result yielding from this is that the local G-actions which give rise to the notion of isometablicity are local expressions of the action of G on the Lie group bundle $I\Omega$ of a given PBG-groupoid $\Omega \rightrightarrows P(M,G)$. Section V contains the proof of the fact that isometablic transition functions indeed classify PBG-groupoids. In Sec. VI we provide the reformulation of iosmetablic transition functions to a form that differentiates to the equivariant analog of the classification of Lie algebroids given in Ref. 8. Finally, the formulation of the suitable cohomology groups where the cocycles of isometablic transition functions live is given in Sec. VII.

I. LIE GROUPOID EXTENSIONS AND PBG-GROUPOIDS

In this section we recall in short the material from Ref. 7 on the correspondence of extensions of transitive Lie groupoids to PBG-groupoids.

Definition 1.1: A PBG-groupoid *is a Lie groupoid* $\Omega \rightrightarrows P$ *whose base is the total space of a principal bundle* $P(M,G)$ *together with a right action of* G *on the manifold* Ω *such that for all* $(\xi,\eta)\in\Omega*\Omega$ *and* $g\in G$ *we have*

(i) $\beta(\xi\cdot g)=\beta(\xi)\cdot g$ and $\alpha(\xi\cdot g)=\alpha(\xi)\cdot g$;
(ii) $1_{u\cdot g}=1_u\cdot g$;
(iii) $(\xi\eta)\cdot g=(\xi\cdot g)(\eta\cdot g)$;
(iv) $(\xi\cdot g)^{-1}=\xi^{-1}\cdot g$.

The notation $\Omega*\Omega$ stands for the pairs $(\xi,\eta)\in\Omega\times\Omega$ such that $\alpha(\xi)=\beta(\eta)$. We denote a PBG-groupoid Ω over the principal bundle $P(M,G)$ by $\Omega\rightrightarrows P(M,G)$ and the right-translation in Ω coming from the G-action by $\widetilde{R}_g$ for any $g\in G$. The right-translation in P will be denoted by R_g. The previous definition implies that $\widetilde{R}_g$ is an automorphism of the Lie groupoid Ω over the diffeomorphism R_g for all $g\in G$. A morphism φ of Lie groupoids between two PBG-groupoids Ω and Ω' over the same principal bundle is called a morphism of PBG-groupoids if it preserves the group actions, namely if $\varphi\circ\widetilde{R}_g=\widetilde{R}'_g\circ\varphi$ for all $g\in G$. In the same fashion, a PBG-Lie group bundle (PBG-LGB) is a Lie group bundle F over the total space P of a principal bundle $P(M,G)$ such that the group G acts on F by Lie group bundle automorphisms. We denote a PBG-LGB by $F\to P(M,G)$. It is easy to see that the gauge Lie group bundle $I\Omega\to P$ associated with a PBG-groupoid $\Omega\rightrightarrows P(M,G)$ is a PBG-LGB.

Numerous examples of transitive PBG-groupoids and their corresponding extensions can be found in Ref. 6. In Ref. 2 nontransitive examples are given as well. Transitive PBG-groupoids are the concern of this paper, due to their equivalence with extensions of transitive Lie groupoids (or, equivalently, extensions of principal bundles[7]). Let us give an outline of this equivalence.

Given an extension of Lie groupoids (2), the choice of a basepoint gives rise to its corresponding principal bundle extension (3) as was discussed in the Introduction. With the notation of (3), the Lie group N acts on the manifold Q by the restriction of the H-action on Q to the embedding of N in H. It is immediate that $Q(P,N,\pi)$ is a principal bundle. Here the projection $\pi:Q\twoheadrightarrow P$ is the surjective submersion given with the extension (3). In Ref. 7 this was called the *transverse bundle*.

Denote Ω the (transitive) Lie groupoid $(Q\times Q)/N\rightrightarrows P$ associated to the transverse bundle, and define a right action of the Lie group G on Ω by

$$\langle q_2,q_1\rangle g=\langle q_2h,q_1h\rangle,$$

where $h\in H$ is any element which projects to g. It is trivial to see that this action is well defined and makes Ω a transitive PBG-groupoid over the principal bundle $P(M,G)$.

It is shown in Ref. 7, Sec. 1.3 that the Lie group bundle $I\Omega\to P$ of the orbits of Ω is isomorphic to the pullback bundle $\pi*((Q\times N)/H)$. Therefore the PBG-groupoid $\Omega\rightrightarrows P(M,G)$ can be presented canonically in the following form:

$$\pi*\left(\frac{Q\times N}{H}\right)\rightarrowtail\Omega\twoheadrightarrow P\times P.$$

Here the injection is

$$(p,\langle q,n\rangle)\mapsto\langle qnh^{-1},qh^{-1}\rangle,$$

where the element $h\in H$ is chosen so that $\pi(q)=p\pi(h)$. Moreover, it is shown in Ref. 7, Sec. 1.6, that $I\Omega$ is a PBG-Lie group bundle over $P(M,G)$, the action of G defined as

$$(p,\langle q,n\rangle)_g = (pg,\langle q,n\rangle).$$

Conversely, consider given a transitive PBG-groupoid $\Upsilon \rightrightarrows P(M,G)$. It follows easily from (i) of Definition 1.1 that the action of G is free. In Ref. 7, Sec. 2.2 it is shown that the criterion of Godement (see Ref. 4, Sec. 16.10.3) applies, therefore the quotient manifold Υ/G exists and the projection $\sharp:\Upsilon\to\Upsilon/G$ is a surjective submersion.

This manifold has a natural Lie groupoid structure with base M defined as follows: Since the source and target projections of Υ are G-equivariant, they induce maps $\alpha',\beta':\Upsilon/G\to M$, which are surjective submersions because the projection $\sharp$, the projection of the principal bundle $P(M,G)$, as well as the source and target maps of Υ are submersions as well. Take $u_1,u_2\in\Upsilon$ such that $\alpha'(\langle u_1\rangle)=\beta'(\langle u_2\rangle)$. Then there exists $g\in G$ such that $\alpha(u_1)=\beta(u_2)g$, so it is meaningful to define

$$\langle u_1\rangle\langle u_2\rangle = \langle u_1u_2g\rangle.$$

Finally, the map $(\beta,\alpha):\Upsilon\to P\times P$ is equivariant, so it induces a smooth submersion $\pi:\Upsilon/G \to (P\times P)/G$. It is clear that this is a groupoid morphism over M, and its kernel is $I\Upsilon/G$. Therefore

$$\frac{I\Upsilon}{G} \rightarrowtail \frac{\Upsilon}{G} \overset{\pi}{\twoheadrightarrow} \frac{P\times P}{G}$$

is an extension of Lie groupoids over M. Finally, it is easy to see that the two processes are mutually inverse. In Ref. 7 the following theorem is proven.

Theorem 1.2: *The category of transitive Lie groupoid extensions is equivalent to the category of transitive PBG-groupoids.*

II. CONNECTIONS OF PBG-GROUPOIDS

An alternative formulation of the connection theory of principal bundles is by using the Atiyah sequence. Given a principal bundle $P(M,G,p)$, it follows from the fact that the bundle projection p is G-invariant, that the vector bundle morphism $Tp:TP\to TM$ quotients to a map $p*:TP/G \to TM$ which, like Tp, is a fiberwise surjective vector bundle morphism, therefore a surjective submersion. The kernel of this map is of course T^pP/G, where T^pP is the vertical subbundle of TP, i.e., the kernel of Tp. Now the map $j:(P\times\mathfrak{g})/G\to T^pP/G$, induced by

$$P\times\mathfrak{g}\to TP,(u,X)\mapsto T_1(m_u)(X)$$

(where $m_u:G\to P$ is $g\mapsto ug$), is a vector bundle isomorphism (see Ref. 8, Appendix A, Sec. 3.2). Note that the G-action on $\mathfrak{g}$ implied here is the adjoint. Therefore the principal bundle $P(M,G,p)$ gives rise to the extension of vector bundles,

$$\frac{P\times\mathfrak{g}}{G} \overset{j}{\rightarrowtail} \frac{TP}{G} \overset{p^*}{\twoheadrightarrow} TM, \tag{4}$$

which is known as the *Atiyah sequence*.

The properties of a connection 1-form $\tilde{\gamma}:TP\to M\times\mathfrak{g}$ allow it to quotient to a left-splitting $\overline{\gamma}:TP/G\to(P\times\mathfrak{g})/G$ of (4). In turn, the rule

$$j\circ\overline{\gamma}+\gamma\circ p^* = 0$$

corresponds $\overline{\gamma}$ to a right-splitting $\gamma:TM\to TP/G$ of (4). This way the connection forms of a principal bundle correspond to the right-splittings of its Atiyah sequence. Respectfully, the curvature of the connection 1-form $\tilde{\gamma}$ corresponds to the 2-form $R_\gamma:TM\times TM\to(P\times\mathfrak{g})/G$ defined by $C_\gamma(X,Y)=\gamma[X,Y]-[\gamma(X),\gamma(Y)]$.

The module of sections of the vector bundle $TP/G \to M$ can be identified with the G-invariant vector fields of P (see Ref. 8, Appendix A), thus inheriting a Lie bracket which, together with p^*, satisfy the properties of the following definition.

Definition 2.1: A Lie algebroid *is a vector bundle A on base M together with a vector bundle map $\sharp: A \to TM$, called the* anchor *of A, and a bracket $[,]: \Gamma A \times \Gamma A \to \Gamma A$ which is $\mathbb{R}$-bilinear, alternating, satisfies the Jacobi identity, and is such that we have the following:*

(i) $\sharp([X,Y]) = [\sharp X, \sharp Y]$;
(ii) $[X, fY] = f[X,Y] + (\sharp X)(f)Y$;

for all $X, Y \in \Gamma A$ and $f \in C^\infty(M)$.

Basic material on Lie algebroids can be found in Refs. 8 and 5. The notion of a Lie algebroid generalizes that of the tangent bundle TM of a given manifold M, which can be thought of as a Lie algebroid with the well-known Lie bracket of vector fields and the identity as the anchor map. Moreover, any bundle of Lie algebras is a Lie algebroid with zero as the anchor map.

If A and A' are Lie algebroids over the same base M, then a morphism of Lie algebroids $\varphi: A \to A'$ over M is a vector bundle morphism such that $\sharp' \circ \varphi = \sharp$ and $\varphi([X,Y]) = [\varphi(X), \varphi(Y)]$ for $X, Y \in \Gamma A$. A Lie algebroid is called *transitive* if its anchor map is a surjective submersion. In this case the kernel of the anchor map is a bundle of Lie algebras, called the *adjoint bundle*, and the Lie algebroid can be presented as an extension of vector bundles,

$$L \rightarrowtail A \overset{\sharp}{\twoheadrightarrow} TM, \tag{5}$$

where the injection of L into A and the anchor map are morphisms of Lie algebroids.

Definition 2.2: Let A, A' be Lie algebroids over the manifold M and $L \to M$. An extension of vector bundles,

$$K \rightarrowtail A \twoheadrightarrow A',$$

is called an extension of Lie algebroids *if the injection and surjection maps are morphisms of Lie algebroids*.

Extensions such as (5) are the simplest form of Lie algebroid extensions, in fact, they are just an alternative way to present a transitive Lie algebroid A over a manifold M. In this setting, the connection theory of principal bundles gives rise to the following notions.

Definition 2.3: Let $L \rightarrowtail A \overset{\sharp}{\twoheadrightarrow} TM$ be a transitive Lie algebroid.

(i) *A connection of A is a vector bundle morphism $\gamma: TM \to A$ such that $\sharp \circ \gamma = 0$.*
(ii) *The* curvature *of a connection γ is the 2-form $C_\gamma: TM \times TM \to L$ defined by*

$$C_\gamma(X,Y) = \gamma[X,Y] - [\gamma(X), \gamma(Y)],$$

for all $X, Y \in \Gamma A$.

A connection γ is called flat *if $C_\gamma = 0$.*

Note that a flat connection is evidently a morphism of Lie algebroids $\gamma: TM \to A$.

All Lie groupoids differentiate to Lie algebroids. A full account of this process can be found in Ref. 8, Vol. III, Sec. 3. The reader can get a rough idea by comparing the extension (1) to the Atiyah sequence (4). Lie III does not apply for groupoids and algebroids though. The integrability of Lie algebroids has a cohomological obstruction in the transitive case, which was given by Mackenzie in Ref. 8, Vol. V. In the nontransitive case, integrability of Lie algebroids is a problem of different order which was tackled by Crainic and Fernandes in Ref. 3. In general, a Lie algebroid that integrates to a Lie groupoid $\Xi \rightrightarrows M$ is denoted by $A\Xi$. Note that the tangent bundle TM of a manifold M integrates to the "pair" groupoid $M \times M \rightrightarrows M$.

Analogously with the reformulation of principal bundle connections as right-splittings of the Atiyah sequence, it is legitimate to regard the *connections* of a transitive Lie groupoid $\Xi \rightrightarrows M$ as

the connections of the Lie algebroid $A\Xi$ it differentiates to, and the same is valid for the curvature 2-forms. This terminology will be used in the remainder of this paper.

Once again though, the concern of this paper is extensions of transitive Lie groupoids, so let us make a fresh start by giving the notion of a PBG-algebroid.

Definition 2.4: A PBG-algebroid *over the principal bundle $P(M,G)$ is a Lie algebroid A over P together with a right action of G on A denoted by $(X,g)\mapsto \hat{R}_g(X)$ for all $X\in A, g\in G$ such that each $\hat{R}_g: A\to A$ is a Lie algebroid automorphism over the right translation R_g in P.*

We denote a PBG-algebroid A over $P(M,G)$ by $A\Rightarrow P(M,G)$. The G-action on A induces an action of G on the module ΓA of sections of the vector bundle $A\to M$, namely

$$X\cdot g=\hat{R}_g\circ X\circ R_{g^{-1}}.$$

The right-translation with respect to this action is denoted by $\hat{R}^{\Gamma}_g:\Gamma A\to\Gamma A$ for all $g\in G$. With this notation Definition 2.4 implies that

$$\hat{R}^{\Gamma}_g([X,Y])=[\hat{R}^{\Gamma}_g(X),\hat{R}^{\Gamma}_g(Y)].$$

Given a *transitive* PBG-algebroid $A\Rightarrow P(M,G,p)$, its adjoint bundle $L\to P$ inherits a G-action by automorphisms, thus making

$$L\rightarrowtail A\overset{\sharp}{\twoheadrightarrow} TP$$

an extension of PBG-algebroids. That is to say it is an extension of Lie algebroids such that the injection and surjection maps are moreover equivariant. It is shown in Ref. 2, Sec. 3.4 that the Godement criterion applies, so the quotient manifold A/G exists. Therefore the previous extension quotients to a vector bundle extension,

$$\frac{L}{G}\rightarrowtail\frac{A}{G}\overset{\sharp^{/G}}{\twoheadrightarrow}\frac{TP}{G},\tag{6}$$

of the (integrable) Lie algebroid TP/G by the quotient Lie algebra bundle L/G. Observe that since the quotient manifold A/G exists, the vector bundle structure of A quotients to $A/G\to M$. Moreover, the natural projection $\natural^A:A\to A/G$ is a pullback over $p:P\to M$.

The vector bundle A/G has the following Lie algebroid structure: The anchor is the composition of vector bundle morphisms $p_*\circ\sharp^{/G}$. Moreover, the sections of A/G are isomorphic to the G-invariant sections of A, therefore $\Gamma(A/G)$ inherits the Lie bracket from $\Gamma^G A$. The verification that this bracket together with the anchor map $p_*\circ\sharp^G$ satisfy the properties of a Lie algebroid can be found in Ref. 7, Sec. 3.2. It is immediate that A/G is transitive. A more elaborate presentation of the extension 6 is given in Fig. 1, which helps to keep track of all the structures related to the Lie algebroid extension. Note that the adjoint bundle K of A/G is an extension of $(P\times g)/G$ by L/G. This diagram makes it clear that the cokernel of the extension (6) is in fact the Atiyah sequence of the bundle $P(M,G,p)$.

On the other hand, pulling back (6) by the map $Tp:TP\to TM$ we recover the given PBG-algebroid (see Ref. 7, Sec. 4). This consists of the proof of the following theorem.

Theorem 2.5: *The category of transitive PBG-algebroids over a manifold M is equivalent to the category of Lie algebroid extensions,*

$$K\rightarrowtail A\twoheadrightarrow A\Xi,\tag{7}$$

of an integrable transitive Lie algebroid by a Lie algebra bundle (over M).

Now extensions of Lie groupoids differentiate to extensions (7). The connection theory of Lie groupoid extensions (2) is encoded by the right-splittings of extensions (7). These in turn correspond to the following notion of connection for the equivalent PBG-algebroid (see Refs. 6 and 7).

Definition 2.6: Let $A\Rightarrow P(M,G,p)$ be a transitive PBG-algebroid. A connection $\gamma:TP\to A$ is

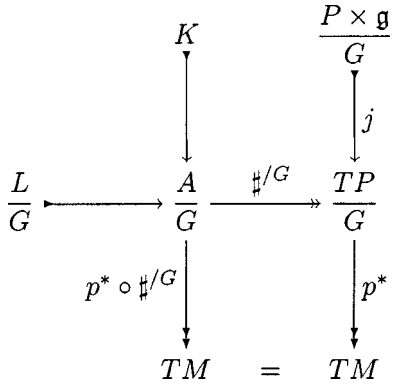

FIG. 1. The extension of Lie algebroids induced by a PBG-algebroid.

called isometablic, *if it satisfies*

$$\gamma \circ TR_g = \hat{R}_g \circ \gamma. \tag{8}$$

An account of isometablic connections and their holonomy is given in Ref. 2, however in this paper we are interested in a different problem. The groupoid extensions that we intend to classify have a prescribed kernel and cokernel. In other words, *given* a transitive Lie groupoid $\Xi \rightrightarrows M$ and a Lie algebra bundle $F \to M$, we classify all transitive Lie groupoids $\Phi \to M$ which fit into a Lie groupoid extension,

$$F \rightarrowtail \Phi \twoheadrightarrow \Xi.$$

In this sense, we are interested in the connections of Φ rather than the splittings of the extension of the Lie algebroid extension $AF \rightarrowtail A\Phi \twoheadrightarrow A\Xi$. The following theorem clarifies exactly what these connections correspond to in the relevant PBG-algebroid.

Theorem 2.7: *Suppose we are given a transitive PBG-algebroid* $A \Rightarrow P(M,G,p)$ *and consider its corresponding extension of Lie algebroids (6) over* M. *The connections of the (transitive) Lie algebroid* $A/G \to M$ *are equivalent to the isometablic connections of* A *which vanish on the kernel* T^pP *of* $Tp: TP \to TM$.

Proof: Consider an isometablic connection $\gamma: TP \to A$ such that $\gamma(X) = 0$ if $X \in T^pP$. This quotients to a splitting $\gamma^{/G}: TP/G \to A/G$. Given a connection $\delta: TM \to TP/G$ of the principal bundle $P(M,G)$, define

$$\widetilde{\gamma} = \gamma^{/G} \circ \delta: TM \to \frac{A}{G}.$$

The assumption that γ vanishes on the kernel of Tp makes the definition of $\tilde{\gamma}$ independent from the choice of δ. It follows immediately from the assumption that δ is a connection of $P(M,G)$ and $\gamma^{/G}$ is a splitting of (6) that this is a connection of the Lie algebroid A/G.

Conversely, given a connection $\theta: TM \to A/G$ of the Lie algebroid A/G, compose it with the anchor map $p^*: TP/G \twoheadrightarrow TM$ of the Atiyah sequence corresponding to the bundle $P(M,G,p)$ [see (4)] to the vector bundle morphism,

$$\overline{\theta} = \theta \circ p^*: \frac{TP}{G} \to \frac{A}{G}.$$

Denote $\natural: TP \to TP/G$ and $\natural^A: A \to A/G$ the natural projections. Since $\natural^A$ is a pullback over $p: P \to M$, there is a unique vector bundle morphism $\gamma: TP \to A$ such that

$$\natural^A \circ \gamma = \overline{\theta} \circ \natural .$$

Due to the G-invariance of $\natural$ and $\natural^A$ the morphism of vector bundles $\hat{R}_{g^{-1}} \circ \gamma \circ TR_g$ also satisfies the previous equation for every $g \in G$; therefore it follows from the uniqueness argument that γ is isometablic. It is an immediate consequence of the previous equation that γ vanishes at T^pP.

To see that it is indeed a connection of A, let us recall the fact that θ is a connection of A/G. This gives $p^* \circ \sharp^{/G} \circ \theta = \mathrm{id}_{TM}$. Now $\sharp^{/G} = \natural \circ \sharp$ and by definition we have $p^* \circ \natural = Tp$, therefore $Tp \circ \sharp \circ \theta = \mathrm{id}_{TM}$. Now take an element $X \in TP$. Then $Tp(X) \in TM$, and it follows from this equation that there exists an element $g \in G$ such that

$$(\sharp \circ \theta)(Tp(X)) = X \cdot g.$$

Multiplying this by g^{-1} and using the G-invariance of Tp we get

$$\sharp \circ (\theta \circ Tp) = \mathrm{id}_{TP}.$$

Finally, from the properties of the pullback, it follows immediately that γ is the map $(\pi, \overline{\theta} \circ \natural)$, where $\pi : TP \to P$ is the natural projection of the tangent bundle. It is straightforward to check that this reformulates to $(\pi, \theta \circ Tp)$, and this proves that γ is a connection. ■

Definition 2.8: The isometablic connections of a PBG-algebroid $A \Rightarrow P(M,G,p)$ which vanish at the kernel T^pP of p^* are called basic connections.

It is therefore necessary to focus on basic connections of PBG-groupoids for the purpose of this paper. The following result follows from Proof 2.7.

Corollary 2.9: Let $A \Rightarrow P(M,G)$ be a transitive PBG-algebroid. A flat connection of the Lie algebroid $A/G \to M$ gives rise to a unique flat basic connection of A.

Note that the Proof 2.7 does not give force to the converse of this result. That is because the connection of A/G corresponding to a given flat basic connection of A arises by composition with an arbitrary connection of TP/G, which is not necessarily a flat one, unless the bundle $P(M,G)$ is flat.

III. TRANSITION FUNCTIONS FOR TRANSITIVE PBG-GROUPOIDS

This section is concerned with the study of those transition functions of transitive PBG-groupoids which encode the group action.

Let us start with a principal bundle $P(M,G)$ and a simple open cover $\mathcal{U} = \{U_i\}_{i \in I}$ of M. This is an open cover such that each U_i is contractible, and the intersection of two as well as three open sets is also contractible. Then a cover $\mathcal{P} = \{P_i\}_{i \in I}$ of P by principal bundle charts such that $P_i \cong U_i \times G$ exists.

Consider now a PBG-groupoid $\Omega \rightrightarrows P(M,G)$ over this bundle and its corresponding Lie algebroid $A\Omega \Rightarrow P(M,G)$ with adjoint bundle $L\Omega$. The extension of Lie algebroids corresponding to that is

$$\frac{L\Omega}{G} \rightarrowtail \frac{A\Omega}{G} \twoheadrightarrow \frac{TP}{G}.$$

It follows from Ref. 8, Vol. IV, Sec. 4 that the Lie algebroid $A\Omega/G$ (over M) has local flat connections $\tilde{\theta}_i^* : TU_i \to (A\Omega/G)_{U_i}$. Due to 2.9 these give rise to flat *basic* connections $\theta_i^* : TP_i \to A\Omega_{P_i}$.

Since the connections $\tilde{\theta}_i^*$ are flat, they can be regarded as morphisms of Lie algebroids. Now consider the following theorem from Ref. 10.

Theorem 3.1: *Let Ω, Ξ be Lie groupoids over the same manifold M and $\mu : A\Omega \to A\Xi$ a Lie algebroid morphism. If Ω is α-simply connected, then there exists a unique morphism of Lie groupoids $\varphi : \Omega \to \Xi$ which differentiates to μ,* i.e., *$\varphi^* = \mu$.*

With the assumption that every U_i is contractible, and by force of the previous result, it follows that the $\tilde{\theta}_i^*$'s integrate uniquely to morphisms of Lie groupoids $\tilde{\theta}_i : U_i \times U_i \to \Omega_{U_i}^{U_i}/G$. It was

shown in Proof 2.7 that the basic flat connections θ_i^* corresponding to the $\widetilde{\theta}_i^*$'s are in essence the maps $\widetilde{\theta}_i^* \circ T_p$, therefore they also integrate uniquely to morphisms of Lie groupoids,

$$\theta_i : P_i \times P_i \to \Omega_{P_i}^{P_i}.$$

Proposition 3.2: The θ_i's are morphisms of PBG-groupoids.

Proof: It suffices to prove the equivariance of the θ_i's. For every $g \in G$, the map θ_i^g: $P_i \times P_i \to \Omega_{P_i}^{P_i}$ defined by

$$\theta_i^g(u,v) = \theta_i(ug, vg)g^{-1}$$

is clearly a morphism of Lie groupoids and it differentiates to θ_i^*. It therefore follows from the uniqueness of θ_i that $\theta_i^g = \theta_i$ for all $g \in G$; consequently θ_i is equivariant. ■

For every $i \in I$ choose an element $u_i \in P_i$ and define $\overline{\sigma_i}$: $P_i \to \Omega_{P_i}$ by $\overline{\sigma_i}(u) = \theta_i(u, u_i)$. We call these maps *schisms*. Note that $\overline{\sigma_i}(u_i) = 1_{u_i}$. The following proposition clarifies the behavior of the schisms with respect to the G-action. We call this notion of equivariance *isometablicity* because it follows directly from the isometablicity property of the local flat connections of the PBG-groupoid we discussed above.

Proposition 3.3: The schisms $\overline{\sigma_i}$ are isometablic *in the sense that*

$$\overline{\sigma_i}(ug) = (\overline{\sigma_i}(u)g) \cdot \overline{\sigma_i}(u_i g),$$

for all $u \in P_i$ and $g \in G$.

Proof: From the definition of the $\overline{\sigma_i}$'s and the equivariance of the morphisms θ_i we get $(\overline{\sigma_i}(u)g) \cdot \overline{\sigma_i}(u_i g) = (\theta_i(u, u_i)g) \cdot \theta_i(u_i g, u_i) = \theta_i(ug, u_i g) \cdot \theta_i(u_i g, u_i) = \theta_i(ug, u_i) = \overline{\sigma_i}(ug)$. ■

For every choice of a $u_i \in P_i$, consider the Lie group $H_i = \Omega_{u_i}^{u_i}$. In order to refer to a unique Lie group independent to the index $i \in I$, we need to fix a $u_0 \in P$ and define $H = \Omega_{u_0}^{u_0}$. Then, for every $i \in I$ choose a $\xi_i \in \Omega_{u_0}^{u_i}$ and consider the maps τ_i: $H_i \to H$ defined by $\tau_i(\eta) = \xi^{-1} \cdot \eta \cdot \xi$. These are isomorphisms of Lie groups. Now define σ_i: $P_i \to \Omega_{u_0}$ by

$$\sigma = \overline{\sigma_i} \cdot \xi_i.$$

These are sections of the Lie groupoid Ω. Note that $\sigma_i(u_i) = \xi_i$. The isometablicity of these sections is described in the following proposition:

Proposition 3.4: The sections σ_i are isometablic *in the sense that*

$$\sigma_i(ug) = [\sigma_i(u)g] \cdot (\xi_i^{-1} g) \cdot \sigma_i(u_i g),$$

for all $i \in I$, $u \in P_i$ and $g \in G$.

The proof is a straightforward calculation.

Now we look at the isometablicity of the transition functions. We denote $\{\overline{s_{ij}} : P_{ij} \to \Omega_{u_j}^{u_i}\}_{i,j \in I}$ the transition functions of the schisms $\{\overline{\sigma_i}\}_{i \in I}$ and $\{s_{ij} : P_{ij} \to \Omega_{u_0}^{u_0}\}_{i,j \in I}$ the transition functions of the sections $\{\sigma_i\}_{i \in I}$. The following proposition is an immediate consequence of the isometablicity of the schisms and the sections.

Proposition 3.5: For every $i, j \in I$ such that $P_{ij} \neq \emptyset$, $u \in P_{ij}$ and $g \in G$ we have the following.

(i) $\overline{s_{ij}}(ug) = \overline{\sigma_i}(u_i g)^{-1} \cdot (\overline{s_{ij}}(u)g) \cdot \overline{\sigma_j}(u_j g)$.
(ii) $s_{ij}(ug) = \sigma_i(u_i g)^{-1} \cdot (\xi_i g) \cdot (s_{ij}(u)g) \cdot (\xi_j g)^{-1} \cdot \sigma_j(u_j g)$.

This gives rise to the following formulation of G-actions:

Definition 3.6: Denote $\Omega_{u_i}^{u_i} = H_i$ and $\Omega_{u_0}^{u_0} = H$. The following formulas:

(i) $\overline{\rho_{ij}} : G \times H_i \to H_i$, $\overline{\rho_{ij}}(g^{-1})(h_i) = \overline{\sigma_i}(u_i g)^{-1} \cdot (h_i g) \cdot \overline{\sigma_j}(u_j g)$, *and*
(ii) $\rho_{ij} : G \times H \to H$, $\rho_{ij}(g^{-1})(h) = \sigma_i(u_i g)^{-1} \cdot (\xi_i g) \cdot (hg) \cdot (\xi_j g)^{-1} \cdot \sigma_j(u_j g)$, *define families of G-actions on H_i and H, respectively.*

With this notation, it is legitimate to reformulate the isometablicity equations of 3.5 to

$$\overline{s_{ij}}(ug) = \overline{\rho_{ij}}(g^{-1})(\overline{s_{ij}}(u))$$

and

$$s_{ij}(ug) = \rho_{ij}(g^{-1})(s_{ij}(u)).$$

Let us now examine the properties of the G-actions $\overline{\rho_{ij}}$ and ρ_{ij}. The proof of the following proposition is, again, straightforward.

Proposition 3.7: Let $\Omega \rightrightarrows P(M,G)$ be a PBG-groupoid. Then the families of G-actions $\{\overline{\rho_{ij}}\}_{i,j\in I}$ and $\{\rho_{ij}\}_{i,j\in I}$ satisfy the following identities:

$$\rho_{ij}(g^{-1})(h_1h_2) = \rho_{ik}(g^{-1})(h_1)\rho_{kj}(g^{-1})(h_2), \tag{9}$$

for all $i,j,k \in I$ such that $P_{ijk} \neq \emptyset$ and $h_1, h_2 \in H$:

$$\begin{aligned}\rho_{ij}(g^{-1})(h) &= \rho_{ii}(g^{-1})(h) \cdot \sigma_i(u_ig)^{-1} \cdot (\xi_ig) \cdot (\xi_jg)^{-1} \cdot \sigma_j(u_jg) \\ &= \sigma_i(u_ig)^{-1} \cdot (\xi_ig) \cdot (\xi_jg)^{-1} \cdot \sigma_j(u_jg) \cdot \rho_{jj}(g^{-1})(h),\end{aligned} \tag{10}$$

$$\tau_i(\overline{\rho_{ii}}(g^{-1})(h_i)) = \rho_{ii}(g^{-1})(\tau_i(h_i)), \tag{11}$$

for all $h_i \in H_i$.

Due to (10), it is possible to say that the family of actions $\{\rho_{ij}\}_{i,j\in I}$ is fully determined by the subset of those actions with $i=j$. Now (11) shows that for all $i \in I$ the isomorphism $\tau_i: H_i \to H$ maps every G-action $\overline{\rho_{ii}}$ on H_i exactly to the G-action ρ_{ii} on H.

Last, notice that (9) is a nonstandard property. From this it follows immediately that $\rho_{ii}(g^{-1})(e_H) = e_H$ for all $i \in I$. These two properties almost make the ρ_{ij}'s representations in a certain sense. We single out (9) by giving the following definition.

Definition 3.8: Let G and H be Lie groups. If a family $\{\rho_{ij}\}_{i,j\in I}$ of G-actions on H satisfy

$$\rho_{ij}(g^{-1})(h_1h_2) = \rho_{ik}(g^{-1})(h_1)\rho_{kj}(g^{-1})(h_2),$$

for all $g \in G$, $h_1, h_2 \in H$ and $i,j,k \in I$, then G is said to be acting on H by cocycle morphisms.

A. Equivalence of transition functions

So far we have demonstrated that PBG-groupoids have sections which are suitably equivariant. These sections arise naturally from the local flat basic connections that exist on the algebroid level. But what happens if we start with a different family of local flat basic connections?

Let us start with two families $\{\theta_i^*\}_{i\in I}$ and $\{\theta'^*_i\}_{i\in I}$ of flat basic connections over the same cover $\mathcal{P} = \{P_i\}_{i\in I}$ of P by principal bundle charts. Then there exist maps $\ell_i^*: TP_i \to P_i \times \mathfrak{h}_i$ such that

$$\theta'^*_i = \theta_i^* + \ell_i^*,$$

for every $i \in I$. Here $\mathfrak{g}_i$ denotes the Lie algebra of the Lie group H_i. Therefore every ℓ_i^* must also be isometablic, that is to say

$$\ell_i^*(Xg) = \ell_i^*(X)g,$$

for all $X \in TP_i$ and $g \in G$. Moreover, the ℓ_i^*'s integrate to PBG-groupoid morphisms $\ell_i: P_i \times P_i \to H_i$ such that $\theta'_i = \theta_i \cdot \ell_i$. As far as the isometablicity of the ℓ_i's is concerned, it follows that

$$\ell_i(ug, vg) = \overline{\rho_{ii}}(g^{-1})(\ell_i(u,v)). \tag{12}$$

Now define $\overline{r_i}: P_i \to H_i$ by

$$\overline{r_i}(u) = \ell_i(u, u_i),$$

and $r_i : P_i \to H$ by $r_i = \tau_i \circ \overline{r_i}$. That is to say,

$$r_i(u) = \xi_i^{-1} \cdot \overline{r_i}(u) \cdot \xi_i,$$

for all $u \in P_i$. We call the $\overline{r_i}$'s and the r_i's *conjugation* maps. The proof of the following proposition is a simple calculation.

Proposition 3.9: The schisms, sections and the respective transition data induced by $\{\theta_i^*\}_{i\in I}$ *and* $\{\theta'^*_i\}_{i\in I}$ *are related by the following:*

(i) $\overline{\sigma'}_i = \overline{\sigma_i} \cdot \overline{r_i}$,
(ii) $\overline{s'}_{ij} = \overline{r_i}^{-1} \cdot \overline{s_{ij}} \cdot \overline{r_j}$,
(iii) $\sigma'_i = \sigma_i \cdot r_i$,
(iv) $s'_{ij} = r_i^{-1} \cdot s_{ij} \cdot r_j$.

Corollary 3.10: The families of G-actions $\rho = \{\rho_{ij}\}_{i,j\in I}$ *and* $\rho' = \{\rho'_{ij}\}_{i,j\in I}$ *arising from the connections* θ_i^* *and* $\theta_i'^*$*, respectively, are related by*

$$\rho'_{ij}(g^{-1})(h) = r_i(u_i g)^{-1} \cdot \rho_{ij}(g^{-1})(h) \cdot r_j(u_j g),$$

for all $h \in H$ *and* $g \in G$.

Now let us examine the isometablicity of the conjugation maps.

Proposition 3.11: The conjugation maps satisfy the following:

(i) $\overline{r_i}(ug) = \overline{\rho_{ii}}(g^{-1})\big(\overline{r_i}(u)\big) \cdot \overline{r_i}(u_i g)$,
(ii) $r_i(ug) = \rho_{ii}(g^{-1})\big(r_i(u)\big) \cdot r_i(u_i g)$,

for all $u \in P_i$ *and* $g \in G$.

Proof: Note that (ii) follows by applying the isomorphisms τ_i to (i) and taking into account (11). For (i) we have

$$\overline{r_i}(ug) = \ell_i(ug, u_i) = \ell_i(ug, u_i g) \cdot \ell(u_i g, u_i).$$

Because of (12) the last part of the above equation becomes $\overline{\rho_{ii}}(g^{-1})\big(\ell(u, u_i)\big) \cdot \ell(u_i g, u_i)$, and the result follows. ■

IV. THE CLASSIFICATION OF PBG-LIE GROUP BUNDLES

Consider the adjoint bundle $I\Omega \to P(M, G)$ associated with a given PBG-groupoid $\Omega \rightrightarrows P(M, G)$. This section is concerned with the isometablic transition data that classifies this bundle. Apart from this classification, another result given here is that the G-actions ρ_{ij} given in the previous section are local expressions of the action of G on the Lie group bundle $I\Omega$.

Proposition 4.1: Let $\{U_i\}_{i\in I}$ *be a simple open cover of* M *and* $P_i \cong U_i \times G$ *charts of the principal bundle* $P(M, G)$*. The maps* $\psi_i : P_i \times H \to I\Omega_{P_i}$ *defined by*

$$\psi_i(u, h) = \sigma_i(u) \cdot h \cdot \sigma_i(u)^{-1}$$

are local charts for the Lie group bundle $I\Omega$*. They are isometablic in the sense that*

$$\psi_i\big(ug, \rho_{ii}(g^{-1})(h)\big) = \psi_i(u, h) \cdot g.$$

Proof: The fact that ψ_i is a bijection and $\psi_{i,u} : H \to \Omega_u^u$ is a morphism of Lie groups for all $u \in P_i$ are simple calculations. For the isometablicity we have

$$\begin{aligned}\psi_i\big(ug, \rho_{ii}(g^{-1})(h)\big) &= \sigma_i(ug) \cdot \rho_{ii}(g^{-1})(h) \cdot \sigma_i(ug)^{-1} \\ &= \big(\sigma_i(u)g\big) \cdot (\xi_i^{-1} g) \cdot \sigma_i(u_i g) \cdot \sigma_i(u_i g)^{-1} \cdot (\xi_i g) \cdot (hg) \cdot (\xi_i^{-1} g) \\ &\quad \cdot \sigma_i(u_i g) \cdot \sigma_i(u_i g)^{-1} \cdot (\xi_i g) \cdot \big(\sigma_i(u)^{-1} g\big)\end{aligned}$$

$$= (\sigma_i(u)g) \cdot (\xi_i g) \cdot (\sigma_i(u)^{-1}g) = \psi_i(u,g) \cdot g.$$

■

The transition functions of these charts are $\alpha_{ij}: P_{ij} \to \mathrm{Aut}(H)$ defined by

$$\alpha_{ij}(u)(h) = s_{ij}(u) \cdot h \cdot s_{ij}(u)^{-1}.$$

As far as the isometablicity of the respective transition functions is concerned, the following proposition is a straightforward calculation.

Proposition 4.2: The transition functions α_{ij} are isometablic in the sense that

$$\alpha_{ij}(ug)(\rho_{jj}(g^{-1})(h)) = \rho_{ii}(g^{-1})(\alpha_{ij}(u)(h)). \tag{13}$$

Theorem 4.3: *Let $P(M,G)$ be a principal bundle, $\mathcal{P}=\{P_i\}_{i\in I}$ be an open cover of P by principal bundle charts and H a Lie group. Let $\rho=\{\rho_i\}_{i\in I}$ be a family of actions of G on H. Given a cocycle $\alpha=\{\alpha_{ij}: P_{ij} \to \mathrm{Aut}(H)\}_{i,j\in I}$ which satisfies* (13)*, there exists a PBG-Lie group bundle over $P(M,G)$ with transition functions the given ones.*

Proof: Let $F_i = U_i \times H$ and on the union of the F_i define the following equivalence relation:

$$(i,(u_1,h_1)) \sim (j,(u_2,h_2)) \Leftrightarrow u_1 = u_2 = u \text{ and } h_2 = \alpha_{ij}(u)(h_1).$$

This is an equivalence relation because we assumed that the α_{ij}'s form a cocycle. Denote the quotient set by F and equivalence classes $\langle i,(u,h)\rangle$. Define a map $\pi: F \to P$ by $\pi\langle i,(u,h)\rangle = u$ and a G-action by

$$\langle i,(u,h)\rangle \cdot g = \langle i,(ug, \rho_i(g^{-1})(h))\rangle.$$

It is easy to see that the map $\psi_i: P_i \times H \to \pi^{-1}(P_i)$ defined by $(u,h) \mapsto \langle i,(u,h)\rangle$ is an equivariant bijection. Give F the smooth structure induced from the manifolds $P_i \times H$ via the ψ_i's. Clearly $F \to P(M,G)$ is a PBG-Lie algebra bundle, and its transition functions are

$$\psi_{i,u}^{-1}(\psi_{j,u}(h)) = \psi_{i,u}^{-1}(\langle j,(u,h)\rangle) = \psi_{i,u}^{-1}(\langle i,(u,\alpha_{ij}(u)(h))\rangle) = \alpha_{ij}(u)(h).$$

■

It will be shown in Sec. VI that the construction of a PBG-LGB given in Theorem 4.3 is well defined. The family of G-actions $\{\rho_{ij}\}_{i,j\in I}$ arises naturally from the local flat basic connections that every PBG-groupoid has. A remarkable result, which is presented here, is that these actions are really only local expressions of the G-action on the groupoid. We prove this for the subset of the ρ_{ij}s for which $i=j$. This is enough, as it was shown in (10) that these actions determine the whole family. To this end, it is necessary to establish the notion of an action groupoid.

Definition 4.4: Given a manifold M together with a right action of a Lie group G on M, the action groupoid $M \rtimes G \rightrightarrows M$ associated with this action is the product manifold $M \times G$, together with the following groupoid structure:

(i) *The source map is $\alpha(x,g)=x$, and the target map $\beta(x,g)=xg$.*
(ii) *Multiplication is defined by $(xg,h)\cdot(x,g)=(x,gh)$.*
(iii) *The unit element over any $x \in M$ is $1_x=(x,e_G)$.*
(iv) *The inverse of an element $(x,g) \in M \rtimes G$ is (xg,g^{-1}).*

Note that the action groupoid is transitive if and only if the G-action on M is transitive.

Now suppose given a PBG-groupoid $\Omega \rightrightarrows P(M,G)$ and a cover $\mathcal{P}=\{P_i\}_{i\in I}$ of P by principal bundle charts. For every $i \in I$, consider the action groupoid $P_i \rtimes G \rightrightarrows P_i(U_i,G)$ and define a map $\tilde{\rho}_i: P_i \rtimes G * I\Omega_{P_i} \to I\Omega_{P_i}$ by

$$\tilde{\rho}_i((u,g), \eta \in \Omega_u^u) = \psi_i(ug, \rho_{ii}(g^{-1})(\psi_{i,u}^{-1}(\eta))).$$

Obviously, $\pi(\tilde{\rho}_i((u,g),\eta)) = ug = \beta(u,g)$ and $\tilde{\rho}_i((u,e_G),\eta) = \eta$. It is easily verified that

$$\widetilde{\rho}_i((ug_1,g_2)\cdot(u,g_1),\eta)=\widetilde{\rho}_i((ug_1,g_2),\widetilde{\rho}_i(u,g_1),\eta).$$

Also, each $\widetilde{\rho}_i(u,g)$ is an automorphism of Ω^u_u; therefore it is a representation of the Lie groupoid $P_i\twoheadrightarrow G$ on the Lie group bundle $I\Omega_{P_i}$, in the sense of Ref. 9. The following proposition allows us to "glue" the $\widetilde{\rho}_i$'s together to a global map.

Proposition 4.5: For all $i,j\in I$ such that $P_{ij}\neq\emptyset$, $u\in P_{ij}$, $g\in G$ and $\eta\in\Omega^u_u$ we have

$$\widetilde{\rho}_i((u,g),\eta)=\widetilde{\rho}_j((u,g),\eta).$$

Proof: The isometablicity of the α_{ij}'s gives

$$\begin{aligned}\widetilde{\rho}_i((u,g),\eta)&=\psi_i(ug,\rho_{ii}(g^{-1})(\psi^{-1}_{i,u}(\eta)))=\psi_i(ug,\rho_{ii}(g^{-1})(\alpha_{ij}(u)(\psi^{-1}_{j,u}(\eta))))\\&=\psi_i(ug,\alpha_{ij}(ug)(\rho_{jj}(g^{-1})(\psi^{-1}_{i,u}(\eta))))\\&=\psi_j(ug,\rho_{jj}(g^{-1})(\psi^{-1}_{i,u}(\eta)))=\widetilde{\rho}_j((u,g),\eta).\end{aligned}$$

■

Now we can define $\rho:(P\twoheadrightarrow G)*I\Omega\to I\Omega$ by $\rho((u,g),\eta\in\Omega^u_u)=\widetilde{\rho}_i((u,g),\eta)$, if $u\in P_i$. The previous proposition shows that it is well defined. More than that, it is a representation because each $\widetilde{\rho}_i$ is. As a matter of fact, ρ is a lot simpler than it seems. Since the charts $\{\psi_i\}_{i\in I}$ are isometablic we have

$$\rho((u,g),\eta)=\psi_i(ug,\rho_{ii}(g^{-1})(\psi^{-1}_{i,u}(\eta)))=\psi_i(u,\psi^{-1}_{i,u}(\eta))\cdot g=\eta\cdot g.$$

So ρ is, in fact, just the PBG structure of $I\Omega$.

Conversely, it is possible to retrieve the local representations $\{\rho_{ii}\}_{i\in I}$ from the PBG structure of $I\Omega$. Suppose $\{\sigma_i:P_i\to\Omega_{u_0}\}_{i\in I}$ is a family of sections of Ω. Consider the charts $\psi_i:P_i\times H\to I\Omega_{P_i}$ defined as $\psi_{i,u}(h)=I_{\sigma_i(u)}(h)$ and define $\widetilde{\rho}_i:P_i\twoheadrightarrow G\to\mathrm{Aut}(H)$ by

$$\widetilde{\rho}_i(u,g)(h)=\psi^{-1}_{i,ug}(\psi_{i,u}(h)\cdot g),$$

for all $g\in G$, $h\in H$ and $u\in P_i$. This is a morphism of Lie groupoids over $P_i\to\cdot$. For every $i\in I$ choose $u_i\in P_i$ and define

$$\rho_{ii}(g^{-1})(h)=\widetilde{\rho}_i(u_i,g)(h)=\psi^{-1}_{i,u_ig}(\psi_{i,u}(h)\cdot g).$$

Then

$$\rho_{ii}(g^{-1})(h)=I_{\sigma_i(u_ig)^{-1}}(I_{\sigma_i(u_i)}(h)\cdot g)=\sigma_i(u_ig)^{-1}\cdot(\sigma_i(u_i)g)\cdot(hg)\cdot(\sigma_i(u_i)^{-1}g)\cdot\sigma_i(u_ig).$$

The latter is exactly the original definition of the ρ_{ii}'s. Since the ρ_{ii}'s determine the ρ_{ij}'s, the previous considerations are the proof of the following theorem.

Theorem 4.6: *Given a PBG-groupoid $\Omega\rightrightarrows P(M,G)$, the representations $\{\rho_{ij}\}_{i\in I}$ are local expressions of the PBG structure of $I\Omega$.*

V. THE CLASSIFICATION OF TRANSITIVE PBG-GROUPOIDS

In this section we deal with a single result: It is shown that the isometablic transition functions classify transitive PBG-groupoids.

Theorem 5.1: *Let $P(M,G)$ be a principal bundle and $\mathcal{P}=\{P_i\}_{i\in I}$ an open cover of P by principal bundle charts. Consider a Lie group H and a family of actions $\rho=\{\rho_{ij}\}_{i,j\in I}$ of G on H which has the property of the cocycle morphism. Given a ρ-isometablic cocycle $\{s_{ij}:P_{ij}\to H\}_{i,j\in I}$ there is a PBG-groupoid Ω over $P(M,G)$ whose PBG-Lie group bundle $I\Omega$ of orbits is the one produced by $\{\alpha_{ij}=I_{s_{ij}}\}_{i,j\in I}$.*

Proof: For every $i,j\in I$ consider the sets $\Sigma^j_i=P_i\times H\times P_j$ and let $\Sigma=\cup_{i,j\in I}\Sigma^j_i$. Consider the equivalence relation

$$(i,u,h,v,j) \sim (i',u',h',v',j') \Leftrightarrow u = u', v = v' \text{ and } h' = s_{i'i}(u) \cdot h \cdot s_{jj'}(v).$$

Then it is shown in Ref. 8, Vol.II, Sec. 2.19 that the following defines a groupoid structure on the quotient $\Omega = \Sigma/\sim$: The source and target projections are $\langle i,u,h,v,j\rangle = v$, $\langle i,u,h,v,j\rangle = u$, the object inclusion map is $1: u \mapsto 1_u = \langle i,u,e_H,u,i\rangle$ (any $i \in I$ such that $u \in P_i$), and the multiplication is

$$\langle i,u,h_1,v,j_1\rangle \cdot \langle j_2,v,h_2,w,k\rangle = \langle i,u,h_1 \cdot s_{j_1j_2}(v) \cdot h_2,w,k\rangle.$$

The inversion is $\langle i,u,h,v,j\rangle^{-1} = \langle j,v,h^{-1},u,i\rangle$. This groupoid becomes a PBG-groupoid with action

$$\langle i,u,h,v,j\rangle \cdot g = \langle i,ug,\rho_{ij}(g^{-1})(h),vg,j\rangle.$$

This is well defined because if $\langle i,u,h,v,j\rangle = \langle i',u,h',v',j'\rangle$; then $h' = s_{i'i}(u) \cdot h \cdot s_{jj'}(v)$. The cocycle morphism condition then gives

$$\rho_{i'j'}(g^{-1})(h') = \rho_{i'i}(g^{-1})(s_{i'i}(u)) \cdot \rho_{ij}(g^{-1})(h) \cdot \rho_{jj'}(g^{-1})(s_{jj'}(u)) = s_{i'i}(ug) \cdot \rho_{ij}(g^{-1})(h) \cdot s_{jj'}(ug).$$

So, $\langle i,u,h,v,j\rangle \cdot g = \langle i',u,h',v,j'\rangle \cdot g$. It is straightforward that this action makes Ω a PBG-groupoid. For instance, we prove here that this action preserves the multiplication. Again, because of the cocycle morphism property, we have

$$\begin{aligned}
(\langle i,u,h_1,v,j_1\rangle \cdot \langle j_2,v,h_2,w,k\rangle) \cdot g &= \langle i,u,h_1 \cdot s_{j_1j_2} \cdot h_2,w,k\rangle \cdot g \\
&= \langle i,ug,\rho_{ik}(g^{-1})(h_1 \cdot s_{j_1j_2} \cdot h_2),w,k\rangle \\
&= \langle i,ug,\rho_{ij_1}(g^{-1})(h_1) \cdot \rho_{j_1j_2}(g^{-1})(s_{j_1j_2}(v)) \cdot \rho_{j_2k}(g^{-1})(h_2),wg,k\rangle \\
&= \langle i,ug,\rho_{ij_1}(g^{-1})(h_1) \cdot s_{j_1j_2}(vg) \cdot \rho_{j_2k}(g^{-1})(h_2),wg,k\rangle \\
&= (\langle i,u,h_1,v,j_1\rangle \cdot g) \cdot (\langle j_2,v,h_2,w,k\rangle \cdot g).
\end{aligned}$$

Proposition 5.2: Let $P(M,G)$ be a principal bundle, $\{P_i\}_{i\in I}$ an open cover of P by principal bundle charts, H a Lie group and ρ', ρ be two families of actions of G on H by cocycle morphisms which are conjugate under a family of maps $r = \{r_i: P_i \to H\}_{i\in I}$ such that $r_i(ug) = \rho_{ii}(g^{-1})(r_i(u)) \cdot r_i(u_ig)$ for all $u \in P_i$, $g \in G$ and $i \in I$. Let $\{s_{ij}\}_{i,j\in I}$ and $\{s'_{ij}\}_{i,j\in I}$ be ρ'-isometablic and ρ-isometablic systems of transition data over $\{P_i\}_{i\in I}$ with values in H, respectively, which are equivalent under the family of maps r. Let Ω' and Ω be the PBG-groupoids constructed from $\{s_{ij}\}_{i,j\in I}$ and $\{s'_{ij}\}_{i,j\in I}$, respectively. Then the map $\varphi: \Omega' \to \Omega$ defined by

$$\langle i,u,v,h\rangle \mapsto \langle i,u,r_i(u) \cdot h \cdot r_j(v)^{-1},v,j\rangle$$

is an isomorphism of PBG-groupoids over $P(M,G)$.

Proof: It is shown in Ref. 8, Vol. II, Sec. 2.19 that φ is an isomorphism of Lie groupoids. To show that it is an isomorphism of PBG-groupoids, take any $g \in G$. Then

$$\begin{aligned}
\varphi(\langle i,u,h,v,j\rangle \cdot g) &= \varphi(\langle i,ug,\rho'_{ij}(g^{-1})(h),vg,j\rangle) \\
&= \langle i,ug,r_i(ug) \cdot ri(u_ig)^{-1}\rho_{ij}(g^{-1})(h) \cdot r_j(u_jg) \cdot r_j(vg)^{-1},vg,j\rangle \\
&= \langle i,ug,\rho_{ii}(g^{-1})(r_i(u)) \cdot r_i(u_ig) \cdot r_i(u_ig)^{-1}\rho_{ij}(g^{-1})(h) \cdot r_j(u_jg) \cdot r_j(u_jg)^{-1}\rho_{jj}(g^{-1}) \\
&\quad \times (r_j(v)^{-1}),vg,j\rangle \\
&= \langle i,ug,\rho_{ij}(g^{-1})(r_i(u) \cdot h \cdot r_j(v)^{-1}),vg,j\rangle = \varphi(\langle i,u,h,v,j\rangle) \cdot g.
\end{aligned}$$

■

VI. ISOMETABLIC TRANSITION DATA

Let us move to the Lie algebroid level for a while. In Ref. 8, Vol. IV, Sec. 4, it is shown that a transitive Lie algebroid $L \rightarrowtail A \twoheadrightarrow TM$ is locally described by the following data: If $\mathfrak{h}$ denotes the fiber type of L, then for a simple open cover $\{U_i\}_{i\in I}$ of M there exists a family of differential-2-forms $\chi=\{\chi_{ij}: TU_{ij}\times TU_{ij}\to U_{ij}\times\mathfrak{h}\}_{i,j\in I}$ and a cocycle $\alpha=\{\alpha_{ij}: U_{ij}\to \mathrm{Aut}(\mathfrak{h})\}_{i,j\in I}$ such that we have the following:

(i) The χ_{ij}s are Maurer-Cartan forms, i.e., $\delta\chi_{ij}+[\chi_{ij},\chi_{ij}]=0$, whenever $U_{ij}\neq\emptyset$;
(ii) $\chi_{ik}=\chi_{ij}+\alpha_{ij}(\chi_{jk})$, whenever $U_{ijk}\neq\emptyset$;
(iii) $\Delta(\alpha_{ij})=\mathrm{ad}\circ\chi_{ij}$, whenever $U_{ij}\neq\emptyset$.

The α_{ij}'s here are the transition functions of the Lie algebra bundle L. The notation Δ stands for the Darboux derivative. More than that, it is shown that this data classifies transitive Lie algebroids.

Since transitive Lie groupoids differentiate to transitive Lie algebroids, it is reasonable to expect that so does the respective classification data. Mackenzie in Ref. 8, Vol. III, Sec. 5 gives a full account of this process, however it is expected that the transition functions that classify a transitive Lie groupoid can be reformulated in a fashion which makes their correspondence to the pair (χ,α) on the algebroid level immediate.

In this section we give this reformulation for transitive PBG-groupoids. For any PBG-groupoid $\Omega\to P(M,G)$ such that the fiber bundle of the associated PBG-Lie group bundle $I\Omega$ is H, we have the following definition.

Definition 6.1: The Lie groupoid morphisms χ_{ij}: $P_{ij}\times P_{ij}\to H$ *defined by*

$$\chi_{ij}(u,v)=s_{ij}(u)\cdot s_{ji}(v)$$

(*over the map* $P_{ij}\to\cdot$) *are called transition morphisms.*

Let us see now how the transition morphisms intertwine with the transition functions α_{ij}.

Proposition 6.2: The transition morphisms χ_{ij} *and the transition functions* α_{ij} *satisfy the following:*

(i) $\chi_{ik}(u,v)=\chi_{ij}(u,v)\cdot\alpha_{ij}(v)\big(\chi_{jk}(u,v)\big)$.
(ii) *For a choice of* $u_{ij}\in P_{ij}$,

$$\alpha_{ij}(u)=I_{\chi_{ij}(u,u_{ij})}\circ I_{s_{ij}(u_{ij})}.$$

(iii) $\rho_{ii}(g^{-1})\big(\chi_{ij}(u,v)\big)=\chi_{ij}(ug,vg)$.

Again, the proof is straightforward. Note that these conditions differentiate to the respective ones on the Lie algebroid level.

Definition 6.3: Let $P(M,G)$ *be a principal bundle,* $\mathcal{P}=\{P_i\}_{i\in I}$ *a cover of* P *by principal bundle charts,* H *a Lie group and* $\rho=\{\rho_i\}_{i\in I}$ *a family of* G*-actions on* H. *Let* $\chi=\{\chi_{ij}: P_{ij}\times P_{ij}\to H\}_{i,j\in I}$ *be a family of Lie groupoid morphisms and* $\alpha=\{\alpha_{ij}: P_{ij}\to \mathrm{Aut}(H)\}_{i,j\in I}$ *a cocycle, such that we have the following:*

(i) $\rho_{ii}(g^{-1})\big(\chi_{ij}(u,v)\big)=\chi_{ij}(ug,vg)$;
(ii) $\alpha_{ij}(ug)\big(\rho_{jj}(g^{-1})(h)\big)=\rho_{ii}(g^{-1})\big(\alpha_{ij}(u)(h)\big)$;
(iii) $\chi_{ik}(u,v)=\chi_{ij}(u,v)\cdot\alpha_{ij}(v)\big(\chi_{jk}(u,v)\big)$;
(iv) *For a choice of* $u_{ij}\in P_{ij}$,

$$\alpha_{ij}(u)=I_{\chi_{ij}(u,u_{ij})}\circ I_{s_{ij}(u_{ij})}.$$

Then the pair (χ,α) *is called a* ρ-isometablic system of transition data over $P(M,G)$ with values in H.

Let us now examine the relation of systems of transition data when we start with different

families of flat isometablic basic connections. Denote (χ,α) and (χ',α') the respective systems of isometablic transition data. Again, the proof of the following proposition is just a matter of calculations.

Proposition 6.4: Two ρ-isometablic and ρ'-isometablic systems of transition data (χ,α) and (χ',α'), respectively, are related by

$$\chi'_{ij}(u,v) = r_i(u)^{-1}[\chi_{ij}(u,v)\cdot\alpha_{ij}(v)(r_i(u)\cdot r_j(v)^{-1})]\cdot r_i(v) \tag{14}$$

and

$$\alpha'_{ij}(u) = I_{r_i(u)^{-1}}\circ\alpha_{ij}(u)\circ I_{r_j(u)}. \tag{15}$$

Definition 6.5: Two isometablic systems of transition data which satisfy (14) and (15) are called equivalent.

Finally we prove that the PBG-Lie group bundles induced by equivalent transition functions are isomorphic, thus showing that the classification of PBG-Lie group bundles we gave in 4.3 is well defined.

Theorem 6.6: *Let $P(M,G)$ be a principal bundle, $\mathcal{P}=\{P_i\}_{i\in I}$ a cover of P by principal bundle charts and H a Lie group. Let $\rho=\{\rho_i\}_{i\in I}$ and $\rho'=\{\rho'_i\}_{i\in I}$ be two families of actions of G on H such that we have the following:*

(i) $\rho_i(g^{-1})(h_1h_2)=\rho_i(g^{-1})(h_1)\cdot\rho_i(g^{-1})(h_2)$

(ii) *There exists a family of maps $\{r_i:P_i\to H\}_{i\in I}$ which are ρ-isometablic [i.e. $r_i(ug)=\rho_i(g^{-1})(r_i(u))\cdot r_i(u_ig)$] such that*

$$\rho'_i(g^{-1})(h) = r_i(u_ig)^{-1}\cdot\rho_i(g^{-1})(h)\cdot r_i(u_ig).$$

If α and α' are cocycles which satisfy (15) which give rise to the PBG-Lie group bundles F and F', respectively, then the map $\varphi:F\to F'$,

$$\langle i,(u,h)\rangle \mapsto \langle i,(u,r_i(u)^{-1}\cdot h\cdot r_i(u))\rangle$$

is an isomorphism of PBG-Lie algebra bundles.

The proof of this is analogous to the one given in 5.2.

VII. ISOMETABLIC COHOMOLOGY

In this section we give a formulation of the cohomology that classifies PBG-groupoids. In general, consider a principal bundle $P(M,G)$, a cover $\mathcal{P}=\{P_i\}_{i\in I}$ of P by principal bundle charts and a Lie group H. We also suppose given a family $\rho=\{\rho_{ij}\}_{i,j\in I}$ of G-actions on H with the property of the cocycle morphism.

For $n\geqslant 3$ we denote by $\check{C}^n_G(P,H)$ the set of differentiable maps $e_{i_0,\ldots,i_n}:P_{i_0,\ldots,i_n}\to H$ such that for every $u\in P_{i_0,\ldots,i_n}$ and $g\in G$ we have the following:

(i) $e_{i_0,\ldots,i_n}(ug)=\rho_{i_{n-1},i_{n-2}}(g^{-1})(e_{i_0,\ldots,i_n}(u))$, if n is odd, and

(ii) $e_{i_0,\ldots,i_n}(ug)=\rho_{i_{n-1},i_{n-3}}(g^{-1})(e_{i_0,\ldots,i_n}(u))$, if n is even.

For $n=0$ define $\check{C}^0_G(P,H)$ to be the set of $e_i:P_i\to H$ such that $e_i(ug)=\rho_{ii}(g^{-1})(e_i(u))$. For $n=1$ define $\check{C}^1_G(P,H)$ to be the set of $e_{ij}:P_{ij}\to H$ such that $e_{ij}(ug)=\rho_{ij}(g^{-1})(e_{ij}(u))$. Finally, define $\check{C}^2_G(P,H)$ to be the set of e_{ijk}'s such that $e_{ijk}(ug)=\rho_{jj}(g^{-1})(e_{ijk}(u))$ and identify $\check{C}^{-1}_G(P,H)$ with H.

Then the usual Čech differential $\delta:\check{C}^n(P,H)\to\check{C}^{n+1}(P,H)$, defined by

$$\delta(e)_{i_0,\ldots,i_n} = \prod_{k=0}^{n}[e_{i_0,\ldots,\hat{i_k},\ldots,i_n}]^{(-1)^{k+1}},$$

is *isometablic* in the sense that

(i) $\delta(e)_{i_0,\ldots,i_n}(ug)=\rho_{i_{n-1}i_{n-2}}(g^{-1})(\delta(e)_{i_0,\ldots,i_n}(u))$ if n is odd, and
(ii) $\delta(e)_{i_0,\ldots,i_n}(ug)=\rho_{i_{n-1}i_{n-3}}(g^{-1})(\delta(e)_{i_0,\ldots,i_n}(u))$ if n is even.

Definition 7.1: The cohomology of the complex,

$$\ldots\xrightarrow{\delta}\check{C}^n_G(P,H)\xrightarrow{\delta}\check{C}^{n+1}_G(P,H)\xrightarrow{\delta}\ldots,$$

is called an isometablic Čech *cohomology and is denoted by* $\check{H}^n_G(P,H)$.

The next theorem follows immediately from 5.1.

Theorem 7.2: *With the notation above, PBG-groupoids are classified by* $\check{H}^1_G(P,H)$.

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Hopf maps as static solutions of the complex eikonal equation

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We demonstrate that a class of torus-shaped Hopf maps with arbitrary linking number obeys the static complex eikonal equation. Further, we explore the geometric structure behind these solutions, explaining thereby the reason for their existence. As this equation shows up as an integrability condition in certain nonlinear field theories, the existence of such solutions is of some interest. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1792931]

I. INTRODUCTION

In this article we want to report on a class of Hopf maps with arbitrary linking number, which are, at the same time, static solutions to the complex eikonal equation. Further, we want to explore the geometric structure which is behind these solutions and explains, in fact, their existence.

The eikonal equation reads

$$(\partial^\mu \chi)(\partial_\mu \chi) = 0, \tag{1}$$

and describes, for a real scalar function χ, the propagation of wave fronts (field discontinuities) in Minkowski space. Its generalization to complex χ has some applications in optics and quantum mechanics, as well as in general relativity (see Ref. 1 and the literature cited there). In Ref. 1 an algebraic procedure (based on twistor methods) for the construction of complex solutions to Eq. (1) was developed, and some examples of singular solutions were provided. The complex eikonal equation admits even static solutions, i.e., solutions to the equation

$$(\nabla \chi) \cdot (\nabla \chi) = 0, \tag{2}$$

in contrast to the case of real χ.

The complex eikonal equation (1) has also appeared, in quite a different context, as an integrability condition in some nonlinear field theories. In the last few years there has been rising interest in integrable field theories in higher (i.e., more than two) dimensions, where solitonic solutions are, in many cases, provided by certain Hopf maps, see, e.g., Refs. 2–5. In addition, some nonlinear field theories which are, in general, not integrable, contain *integrable subsectors* where certain integrability conditions are satisfied. Specifically, the complex eikonal equation (1) defines integrable subsectors in the Skyrme and Skyrme–Faddeev models.[6,7] For static, solitonic solutions, this condition reduces to the static complex eikonal equation (2). Finite energy solitons in these integrable subsectors correspond to static solutions defined on one-point compactified $\mathbb{R}^3$ and may, therefore, be identified with functions on S^3 via stereographic projection. Further, the target space of the fields χ in the integrable subsectors can be identified with the Riemann sphere S^2 (i.e., χ is a holomorphic variable on $\mathbb{C}$). Therefore, the fields χ in the integrable subsectors of these models are Hopf maps $S^3 \to S^2$, and can be classified by the Hopf index (the homotopy group $\pi_3(S^2) = \mathbb{Z}$). Consequently, solutions of the complex, static eikonal equation which are, at the same time, Hopf maps, are of some interest for these nonlinear field theories, because they provide finite energy field configurations in their integrable subsectors.

In addition, the static complex eikonal equation (2) has appeared as an integrability condition for the existence of multiple zero modes of the static, Abelian Dirac operator.[8–10] In this case, solutions χ to Eq. (2) are again required to be Hopf maps. The Hopf maps described below will indeed give rise to the construction of new classes of zero modes with new and interesting properties, but this issue shall be discussed elsewhere.

In Sec. II we show that certain toroidal Hopf maps $\chi^{(m,n)}$ obey the static eikonal equation for arbitrary integer m and n (here m and n count the number of times the level curves of χ wrap around the two circular directions of a certain torus). Further, we briefly discuss the symmetries of the static eikonal equation, which enables us to construct new solutions from the ones just mentioned.

In Sec. III we explain the geometric structure which lies behind the existence of these solutions. It turns out that the solutions of Sec. II may be understood as pullbacks of trivial solutions of the complex eikonal equation in two dimensions which preserve some metric properties, providing thereby nontrivial three-dimensional solutions. Further, we give a sufficient condition for the existence of solutions of the geometric type discussed in this paper.

II. THE SOLUTIONS

In the sequel, we will express Hopf maps as complex-valued functions which depend on three variables like, e.g., (x,y,z). Here, the space spanned by these variables may be interpreted either as one-point compactified $\mathbb{R}^3$ or as the three-sphere S^3, where a stereographic projection has been performed. The solutions to the static eikonal equation described below do not depend on this interpretation, i.e., they may be interpreted as solutions on $\mathbb{R}^3$ or on S^3. This result is related to the fact that the metrics on $\mathbb{R}^3$ and S^3 are conformally equivalent (i.e., equal up to a local, space-dependent scale transformation), as will become clear in the next section.

The simplest Hopf map is

$$\chi^{(1,1)} = i\frac{2(x+iy)}{2z+i(r^2-1)} \tag{3}$$

[the meaning of the superscript $(1,1)$ is explained below in Eq. (10)]. Further, $r^2 \equiv x^2+y^2+z^2$, and the irrelevant pre-factor i has been chosen for later convenience. The simplest Hopf map is well-known to obey the static eikonal equation (2), see, e.g., Ref. 8. Before demonstrating this fact, we want to introduce toroidal coordinates (η,ξ,φ) via

$$x = q^{-1}\sinh\,\eta\cos\,\varphi, \quad y = q^{-1}\sinh\,\eta\sin\,\varphi,$$

$$z = q^{-1}\sin\,\xi; \quad q = \cosh\,\eta - \cos\,\xi. \tag{4}$$

Further, we need the gradient in terms of the toroidal coordinates,

$$\nabla = (\nabla\eta)\partial_\eta + (\nabla\xi)\partial_\xi + (\nabla\varphi)\partial_\varphi = q\left(\hat{e}_\eta\partial_\eta + \hat{e}_\xi\partial_\xi + \frac{1}{\sinh\,\eta}\hat{e}_\varphi\partial_\varphi\right), \tag{5}$$

where $(\hat{e}_\eta,\hat{e}_\xi,\hat{e}_\varphi)$ form an orthonormal frame in $\mathbb{R}^3$. In terms of toroidal coordinates, the simplest Hopf map reads

$$\chi^{(1,1)} = \sinh\,\eta\, e^{i\varphi+i\xi}. \tag{6}$$

Here, surfaces of $\eta=$const are tori in $\mathbb{R}^3$. These tori are rotation symmetric around the z axis, and all of them enclose the circle $C=\{\vec{x}\in\mathbb{R}^3 : z=0\wedge r^2=1\}$. The coordinates φ and ξ are angular coordinates along the two circular directions on each torus. Each level curve of $\chi^{(1,1)}$ (i.e., each curve $\chi^{(1,1)}=$const) is located on one torus. It is, in fact, a circle that winds once around each circular direction of the torus. Further, any two different level curves are linked with linking number one, and this linking number is the geometric definition of the Hopf index [which is equal to one for the simplest Hopf map (3)].

For a simple demonstration of the fact that the Hopf map (6) really obeys the eikonal equation it is useful to re-express a general Hopf map χ in terms of two real functions (modulus S and phase σ) like

$$\chi = S\, e^{i\sigma}. \tag{7}$$

In terms of these real functions, the static eikonal equation (2) leads to the conditions

$$(\nabla S)\cdot(\nabla \sigma) = 0, \qquad (\nabla S)^2 = S^2(\nabla \sigma)^2. \tag{8}$$

For the simplest Hopf map (6) we find, with $S=\sinh\,\eta$, $\sigma=\xi+\varphi$,

$$\nabla S = q\,\cosh\,\eta\,\hat{e}_\eta, \qquad \nabla\,\sigma = q\left(\hat{e}_\xi + \frac{1}{\sinh\,\eta}\hat{e}_\varphi\right), \tag{9}$$

which indeed obey Eqs. (8). The important point here is that the equations (8) are expressed only in terms of the target space coordinates S and σ, making the problem essentially two-dimensional. This is precisely what happens for the simplest Hopf map. The factor q, which is present in (9) and cannot be expressed in terms of the target space coordinates, cancels in the relations (8).

A simple generalization to higher Hopf maps is provided by the functions

$$\chi^{(m,n)} = f(\eta)\, e^{in\varphi+im\xi}, \quad m,n \in \mathbb{Z}, \tag{10}$$

which are true Hopf maps if the real function f obeys certain regularity conditions like, e.g., $f(0)=0$ and $f(\infty)=\infty$ (what we assume in the sequel). The level curves of these Hopf maps still lie on the same tori as above, but now they wind n times around the φ direction and m times around the ξ direction. Further, the Hopf index N_{H} (i.e., the linking number of any two different level curves) is $N_{\mathrm{H}}=nm$.

We find for the gradient

$$\nabla\chi^{(m,n)} = q\, e^{im\xi+in\varphi}\left(f'\hat{e}_\eta + imf\hat{e}_\xi + \frac{in}{\sinh\,\eta}f\hat{e}_\varphi\right), \tag{11}$$

where $f'\equiv\partial_\eta f$, and Eq. (2) leads to the simple differential equation

$$\frac{f'}{f} = \left(m^2 + \frac{n^2}{\sinh^2\,\eta}\right)^{1/2} \tag{12}$$

with the solution

$$f = \sinh^{|n|}\,\eta\frac{(|m|\cosh\,\eta + \sqrt{n^2+m^2\,\sinh^2\,\eta})^{|m|}}{(|n|\cosh\,\eta + \sqrt{n^2+m^2\,\sinh^2\,\eta})^{|n|}}. \tag{13}$$

These solutions are genuine Hopf maps for all nonzero, integer m,n, because f obeys $f(0)=0$, $f(\infty)=\infty$.

At this point it is of interest to briefly consider the symmetries of the complex static eikonal equation (2). This will lead to some further understanding of these solutions and allow to construct more solutions from the ones obtained so far. The symmetry group of Eq. (2) is a direct product of base space and target space symmetries, where the group of base space symmetries is the conformal group in three-dimensional Euclidean space. The group of target space symmetries is given locally by the maps $\chi\to F(\chi)$, where F is an arbitrary complex function of χ, but not of its complex conjugate $\overline{\chi}$. The requirement that the solutions $\chi'=F(\chi)$ are single-valued again restricts the allowed functions $F(\cdot)$ to the set of holomorphic functions on $\mathbb{C}$.

The presence of the conformal symmetry on base space implies that the ansatz (10) is an "educated guess" for a solution to Eq. (2) in the sense of the Lie theory of symmetry. That is to say, if we choose a rotation about the z axis and a certain combination of proper conformal transformation along the z axis and translation along the z axis as a maximal set of two commuting

base space transformations, then the corresponding infinitesimal symmetry generators (vectors $\mathbf{v}^i$) are precisely given by the tangent vectors along φ and ξ, $\mathbf{v}^1=\partial_\varphi$, and $\mathbf{v}^2=\partial_\xi$. The ansatz (10) is invariant under a combination of these base space transformations and phase transformations of the target space variable χ, i.e., under the action of the vector fields $\tilde{\mathbf{v}}^1=\partial_\varphi - in\chi\partial_\chi$ and $\tilde{\mathbf{v}}^2=\partial_\xi - im\chi\partial_\chi$, which provides precisely the educated guess according to Lie. A concise discussion of these points can be found in Ref. 4, where the symmetries of an integrable model with infinitely many Hopf solitons are discussed in detail.

Further, we may use the target space symmetries to construct more solutions from the ones given in (13). In fact, each field $\chi'=F(\chi)$ is a solution, where χ is a solution and F is a holomorphic function on $\mathbb{C}$.

III. GEOMETRIC BACKGROUND

Here we want to explain the geometric structure behind the solutions (13), which will, in fact, allow to understand the reason why they exist. For this purpose, let us first observe that there exist trivial solutions to the complex eikonal equation in $\mathbb{R}^2$ or, equivalently, in $\mathbb{C}$. Indeed, for real, cartesian coordinates $(u,v)\in\mathbb{R}^2$ with $w=u+iv$ and gradient

$$\nabla^{(2)} \equiv \hat{e}_u\partial_u + \hat{e}_v\partial_v, \tag{14}$$

the complex eikonal equation $(\nabla^{(2)}f(w))^2=0$ is equivalent to the Cauchy–Riemann equations, which are obeyed by arbitrary holomorphic functions $f(w)$. So, obviously, the complex coordinate $w=u+iv$ itself obeys the eikonal equation,

$$(\nabla^{(2)}w)^2 = 0. \tag{15}$$

By introducing the modulus ρ and phase ϕ of w,

$$w = \rho e^{i\phi}, \tag{16}$$

this equation leads to the conditions

$$(\nabla^{(2)}\rho)\cdot(\nabla^{(2)}\phi) = 0, \qquad (\nabla^{(2)}\rho)^2 = \rho^2(\nabla^{(2)}\phi)^2. \tag{17}$$

It holds in fact also that

$$(\nabla^{(2)}\rho)^2 = \rho^2(\nabla^{(2)}\phi)^2 = 1. \tag{18}$$

Conditions (17) are completely analogous to the conditions (8) in three dimensions. This leads to the natural assumption that the conditions (8) in three dimensions are just the pullbacks under the Hopf map χ of the two-dimensional conditions (17). In the sequel we want to show that this is true in a specific sense.

For this purpose, we want to re-express the above remarks in a more geometric fashion, where we introduce the metrics of the spaces under consideration and replace the gradients by exterior derivatives.

The metric on the space $\mathbb{R}^2$ is

$$g^{(2)} = d\rho\otimes d\rho + \rho^2 d\phi\otimes d\phi, \tag{19}$$

and the dual metric is

$$G^{(2)} = \partial_\rho\otimes\partial_\rho + \frac{1}{\rho^2}\partial_\phi\otimes\partial_\phi. \tag{20}$$

The conditions (17) translate into

$$G^{(2)}(d\rho,d\phi) = 0, \quad G^{(2)}(d\rho,d\rho) = \rho^2 G^{(2)}(d\phi,d\phi) = 1, \tag{21}$$

and are obviously true.

The metric in $\mathbb{R}^3$ is

$$g = q^{-2}(d\eta \otimes d\eta + d\xi \otimes d\xi + \sinh^2 \eta\, d\varphi \otimes d\varphi)$$
$$= \frac{q^{-2}}{1+t^2}[dt \otimes dt + (1+t^2)d\xi \otimes d\xi + t^2(1+t^2)d\varphi \otimes d\varphi], \tag{22}$$

where (η, ξ, φ) are the toroidal coordinates [see (4)] and the coordinate

$$t = \sinh \eta \tag{23}$$

was introduced for later convenience. The dual metric is

$$G = (1+t^2)q^2\left(\partial_t \otimes \partial_t + \frac{1}{1+t^2}\partial_\xi \otimes \partial_\xi + \frac{1}{t^2(1+t^2)}\partial_\varphi \otimes \partial_\varphi\right). \tag{24}$$

As a next step we need the observation that a Hopf map χ introduces a fiber-bundle structure on one-point compactified $\mathbb{R}^3$ (or, equivalently, on S^3). Here, the fibers are the level curves of the Hopf map. The fiber has the topology of the circle S^1, and the base space has the topology of the sphere S^2 for all Hopf maps, but the induced metric properties depend on the specific Hopf map.

Further, the Hopf map allows for a decomposition of the tangent bundle TM of the fiber bundle $M=\mathbb{R}^3$ (or S^3) into vertical and horizontal directions at each point of M. Thereby two subbundles of the full tangent bundle TM are induced, which are called the vertical distribution V and the horizontal distribution H. The vertical direction at each point points along the fiber and is spanned (in our case) by one vertor field e_3 which is pushed forward to zero under the Hopf map, $\chi_* e_3 = 0$. The horizontal directions are spanned (in our case) by two vector fields e_1, e_2, which are perpendicular to the vertical vector e_3. Obviously, the vertical direction only depends on the Hopf map, whereas the horizontal directions depend on the bundle metric, as well. Further, we will choose all three vectors e_i to have unit length (this condition depends, of course, on the metric). This decomposition leads to an analogous decomposition at each point $p \in M$ of the cotangent space T_p^*M into a vertical direction spanned by ω_3 and horizontal directions spanned by ω_1 and ω_2, where the ω_i are defined via

$$(\omega_i, e_j) = \delta_{ij}, \tag{25}$$

and $(\cdot,\cdot)$ denotes the canonical inner product.

Finally, the decomposition of the tangent space (and the cotangent space) into vertical and horizontal directions allows for a corresponding decomposition of the metric and its dual into a vertical and a horizontal component, $g = g_\mathrm{v} + g_\mathrm{h}$. They may be expressed like

$$g_\mathrm{h} = \omega_1 \otimes \omega_1 + \omega_2 \otimes \omega_2, \quad g_\mathrm{v} = \omega_3 \otimes \omega_3, \tag{26}$$

$$G_\mathrm{h} = e_1 \otimes e_1 + e_2 \otimes e_2, \quad G_\mathrm{v} = e_3 \otimes e_3, \tag{27}$$

in terms of the above vector fields and one-forms (observe that this notation just expresses the metric in terms of vielbeins in a coordinate-independent way).

Now we are in a position, eventually, to formulate sufficient conditions for the existence of solutions to the conditions (8).

One sufficient condition is like follows: Obviously, the push-forward χ_* of the Hopf map defines an isomorphism from vectors in the horizontal distribution H of TM at points $\vec{x}$ to vectors in TN at points $\chi(\vec{x})$ (here N is the target space manifold, i.e., $\mathbb{C}$ or S^2, and M is the fiber bundle). Now assume that this isomorphism is, at the same time, an isometry, i.e., the length $|\chi_* v|$ of a pushed-forward vector field $\chi_* v$ in TN w.r.t. the metric $g^{(2)}$ on N at points $\chi(\vec{x})$ is equal to the length $|v|$ of an arbitrary horizontal vector field v in H with respect to the horizontal metric g_h at points $\vec{x}$. Then, obviously, the lengths of one-forms remain invariant under the pull-back χ^*. For a Hopf map $w = \chi(\vec{x})$, which reads, in terms of real coordinates, like

$$\rho = S(\vec{x}), \quad \phi = \sigma(\vec{x}), \tag{28}$$

this means that the lengths should pull back like

$$|d\rho| = |dS|, \quad |d\phi| = |d\sigma|, \tag{29}$$

and the target space metric $g^{(2)}$ expressed in coordinates ρ, ϕ should be identical to the horizontal metric $g_{\rm h}$ expressed in coordinates S, σ. Obviously, length relations are now conserved under the pull-back, as well,

$$|d\rho|^2 = \rho^2 |d\phi|^2 \quad \Rightarrow \quad |dS|^2 = S^2 |d\sigma|^2, \tag{30}$$

$$G^{(2)}(d\rho, d\phi) = 0 \quad \Rightarrow G_{\rm h}(dS, d\sigma) = 0, \tag{31}$$

which is precisely what we need in order to have solutions to the conditions (8). (Maps χ such that the push-forward $\chi_*: H \to TN$ is an isometry are called Riemannian submersions and are described at length, e.g., in Ref. 11.)

It turns out that the condition on the Hopf map χ to be a Riemannian submersion is too strong for our purposes. But there is a simple generalization which does just what we want. Suppose that the lengths of horizontal vector fields are multiplied by a *common* factor at each point under the push-forward, instead of being invariant. Then the lengths of one-forms will be multiplied by a common factor under the pull-back, and this is sufficient for the conservation of the length relations (30) and (31) under the pull-back. For the horizontal metric $g_{\rm h}$ and the target space metric $g^{(2)}$ this implies that they should be conformally equivalent, i.e., equal up to a local scale factor. This is precisely what happens for our solutions, as we want to demonstrate now explicitly.

First, we want to demonstrate it for the simplest Hopf map (6). We re-display the metric in $\mathbb{R}^3$,

$$g = [dt \otimes dt + (1+t^2) d\xi \otimes d\xi + t^2 (1+t^2) d\varphi \otimes d\varphi], \tag{32}$$

where we already ignored an irrelevant local scale factor, see (22). For the Hopf map $\chi = Se^{i\sigma}$ with $S = t$, $\sigma = \xi + \varphi$, the vertical unit vector field e_3 is

$$e_3 = \frac{1}{1+t^2}(\partial_\xi - \partial_\varphi) \tag{33}$$

(remember that $e_3(\sigma) = e_3(S) = 0$). The horizontal unit vector fields may be chosen as

$$e_1 = \partial_t, \quad e_2 = \frac{t}{1+t^2}(\partial_\xi + t^{-2}\partial_\varphi). \tag{34}$$

The corresponding vertical and horizontal one-forms are

$$\omega_1 = dt, \quad \omega_2 = t(d\xi + d\varphi), \tag{35}$$

$$\omega_3 = d\xi - t^2 d\varphi, \tag{36}$$

and the horizontal metric is

$$g_{\rm h} = \omega_1 \otimes \omega_1 + \omega_2 \otimes \omega_2 = dt \otimes dt + t^2 (d\xi + d\varphi) \otimes (d\xi + d\varphi). \tag{37}$$

Obviously, this is identical to the target space metric (19) once the identification $\rho \to t$, $\phi \to \sigma = \xi + \varphi$ is made.

Now we repeat this procedure for the class of Hopf maps $S = t$, $\sigma = m\xi + n\varphi$ which are genuine Hopf maps with toroidal symmetry, but not yet the solutions (13). We find for the horizontal and vertical unit vector fields

$$e_1 = \partial_t, \quad e_2 = \frac{t}{\sqrt{(n^2 + m^2t^2)(1 + t^2)}}(m\partial_\xi + nt^{-2}\partial_\varphi), \tag{38}$$

$$e_3 = \frac{1}{\sqrt{(n^2 + m^2t^2)(1 + t^2)}}(n\partial_\xi - m\partial_\varphi), \tag{39}$$

and for the corresponding one-forms

$$\omega_1 = dt, \quad \omega_2 = t\sqrt{\frac{1 + t^2}{n^2 + m^2t^2}}(md\xi + nd\varphi), \tag{40}$$

$$\omega_3 = \sqrt{\frac{1 + t^2}{n^2 + m^2t^2}}(nd\xi - mt^2d\varphi). \tag{41}$$

The horizontal metric now is

$$g_{\mathrm{h}} = dt \otimes dt + t^2\frac{1 + t^2}{n^2 + m^2t^2}(md\xi + nd\varphi) \otimes (md\xi + nd\varphi), \tag{42}$$

and is not yet manifestly conformally equivalent to the target space metric. However, the horizontal metric only depends on the "horizontal" coordinates $S=t$ and $\sigma=m\xi+n\varphi$ and, therefore, certainly *is* conformally equivalent to the target space metric, because it is a well-known fact that two different metrics on a two-dimensional surface with a given topology are always conformally equivalent (see, e.g., Theorem 13.1.1 in Ref. 12). All we have to do is to find the coordinate transformation from the horizontal coordinates (S, σ) to some new coordinates $(\tilde{S}, \tilde{\sigma})$ such that the conformal equivalence becomes manifest. This shows that the initial problem must have a solution, i.e., higher Hopf maps, related to the Hopf maps (10), which solve the static eikonal equation, *must* exist.

Explicitly, a transformation $(t, \sigma) \to (\tilde{t}(t), \sigma)$ is sufficient such that

$$g_{\mathrm{h}} = \frac{t^2}{\tilde{t}^2}\frac{1 + t^2}{n^2 + m^2t^2}[d\tilde{t} \otimes d\tilde{t} + \tilde{t}^2(md\xi + nd\varphi) \otimes (md\xi + nd\varphi)]. \tag{43}$$

Therefore, $\tilde{t}$ has to obey

$$(dt)^2 = \frac{(1 + t^2)t^2}{(n^2 + m^2t^2)\tilde{t}^2}(d\tilde{t})^2 \quad \Rightarrow \quad \frac{1}{\tilde{t}}\frac{d\tilde{t}}{dt} = \frac{1}{t}\sqrt{\frac{n^2 + m^2t^2}{1 + t^2}}. \tag{44}$$

Re-introducing the variable η and using $\tilde{t}(t)=\tilde{t}(\sinh\ \eta) \equiv f(\eta)$, Eq. (44) leads to Eq. (12) with the solution (13).

We want to close with two remarks. Firstly, the geometric setting developed above easily leads to more Hopf maps which solve the static eikonal equation. Obviously, the sufficient condition for the existence of a solution related to a given Hopf map is that the induced horizontal metric should be expressible—up to a local scale factor—in terms of the horizontal coordinates (S, σ) (where the Hopf map is $\chi=Se^{i\sigma}$). Once this condition is met, the solution can be found by transforming to new horizontal coordinates $(\tilde{S}, \tilde{\sigma})$ such that the horizontal metric is manifestly conformally equivalent to the target space metric. This transformation is always possible for genuine Hopf maps. The simplest example of this type for the generation of new solutions is the composition of existing solutions with maps $S^2 \to S^2$, i.e., the choice of new complex-valued functions $\chi' = F(\chi)$, where $F(\cdot)$ is a holomorphic function (e.g., a rational map), and χ is a solution. However, we already found these solutions from the symmetries of the static eikonal equation in Sec. II.

Second, we want to remark that the above Hopf maps (10) do, in fact, provide genuine Riemannian submersions from the three-sphere S^3 to some two-dimensional target spaces with the

topology of the two-sphere but, in general, metrics different from the two-sphere (except for the simplest case $m=n=1$, which provides a Riemannian submersion from S^3 to S^2, see, e.g., Refs. 10 and 11). This may be understood from what we said above by noting that the local scale factor q^{-2}, which is present in the metric on $\mathbb{R}^3$ (see (22)), and which cannot be expressed in terms of the horizontal coordinates alone, is absent for the metric on S^3.

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On *P*-adic λ-model on the Cayley tree

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We consider a nearest-neighbor p-adic λ-model with spin values ±1 on the Cayley tree of order $k \geqslant 1$. We prove that a p-adic Gibbs measure is unique for $p \geqslant 3$. If $p=2$ then we find a condition which guarantees uniqueness of p-adic Gibbs measure. Besides, the results are applied to the p-adic Ising model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1792932]

I. INTRODUCTION

The p-adic numbers were first introduced by the German mathematician K. Hensel. For about a century after the discovery of p-adic numbers, they were mainly considered objects of pure mathematics. However, numerous applications of these numbers to theoretical physics have been proposed in papers.[1,2,6,7,13,18] It is known[7] that number of p-adic models in physics cannot be described using ordinary probability theory based on the Kolmogorov axioms.[12] New probability models- p-adic probability models were investigated in Refs. 7 and 8. This is non-Kolmogorovean model, since probabilities take values in fields of p-adic numbers.

In Refs. 9 and 10 the theory of stochastic processes with values in p-adic and more general non-Archimedean fields having probability distributions with non-Archimedean values, has been developed. The non-Archimedean analog of the Kolmogorov theorem that gives the possibility to construct wide classes of stochastic processes by using finite dimensional probability distributions, was proved.

It is known that the theory of statistical mechanics lies in the base of the theory of probability and stochastic processes. Since the theory of probabilities and stochastic processes in a non-Archimedean setting has been introduced, it is natural to begin the study and initiate further the development of the problems of statistical mechanics in the context of the p-adic theory of probability.

One of the central problems in the theory of Gibbs measures is to describe infinite-volume Gibbs measures corresponding to a given Hamiltonian. However, a complete analysis of the set of Gibbs measures for a specific Hamiltonian is often a difficult problem. If for a given Hamiltonian there are at least two Gibbs measures then it is said that a *phase transition* occurs for the model.

The existence of a phase transition for the Ising model (real case) on the Cayley tree of order $k \geqslant 2$ was established by Katsura and Takisawa.[5] The analysis of the Cayley tree Ising model can be extended in several directions (see Refs. 14, 15, and 4).

In this paper we develop the p-adic probability theory approaches to the study of some statistical mechanics models on a Cayley tree in the field of p-adic numbers. In Ref. 3 we have proved the existence of the phase transition for the homogeneous p-adic Potts model with $q \geqslant 2$

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spin variables on the set of integers $\mathbb{Z}$. The present paper deals with a nonhomogeneous p-adic λ-model on the Cayley tree of order k, $k \geqslant 1$. The aim of this paper is to show the uniqueness of Gibbs measures for the considered model.

II. DEFINITIONS AND PRELIMINARY RESULTS

A. *p*-adic numbers and measures

Let $\mathbb{Q}$ be the field of rational numbers. Every rational number $x \neq 0$ can be represented in the form $x = p^r(n/m)$, where $r, n \in \mathbb{Z}$, m is a positive integer, $(p,n)=1$, $(p,m)=1$ and p is a fixed prime number. The p-adic norm of x is given by

$$|x|_p = \begin{cases} p^{-r} & \text{for } x \neq 0 \\ 0 & \text{for } x = 0. \end{cases}$$

It satisfies the following properties:

1) $|xy|_p = |x|_p |y|_p$,
2) the strong triangle inequality

$$|x+y|_p \leqslant \max\{|x|_p, |y|_p\},$$

this is a non-Archimedean norm.

The completion of $\mathbb{Q}$ with respect to p-adic norm is called p-adic field which is denoted by $\mathbb{Q}_p$.

The well-known Ostrovsky's theorem asserts that norms $|x|_\infty = |x|$ and $|x|_p$, $p = 2,3,5,\ldots$ exhaust all nonequivalent norms on $\mathbb{Q}$ (see Ref. 11). Any p-adic number $x \neq 0$ can be uniquely represented in the canonical series:

$$x = p^{\gamma(x)}(x_0 + x_1 p + x_2 p^2 + \cdots),$$

where $\gamma = \gamma(x) \in \mathbb{Z}$ and x_j are integers, $0 \leqslant x_j \leqslant p-1$, $x_0 > 0$, $j = 0,1,2,\ldots$ (for more details see Refs. 11 and 17). In this case $|x|_p = p^{-\gamma(x)}$.

Let $B(a,r) = \{x \in \mathbb{Q}_p : |x-a|_p \leqslant r\}$, where $a \in \mathbb{Q}_p$, $r > 0$. The p-adic logarithm is defined by series

$$\log_p(x) = \log_p(1 + (x-1)) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{(x-1)^n}{n},$$

which converges for $x \in B(1,1)$. And p-adic exponential is defined by

$$\exp_p(x) = \sum_{n=1}^{\infty} \frac{x^n}{n!},$$

which converges for $x \in B(0, p^{-1/(p-1)})$.

Lemma 2.1:[11,17] *Let $x \in B(0, p^{-1/(p-1)})$ then we have*

$$|\exp_p(x)|_p = 1, \quad |\exp_p(x) - 1|_p = |x|_p < 1, \quad |\log_p(1+x)|_p = |x|_p < p^{-1/(p-1)}$$

and

$$\log_p(\exp_p(x)) = x, \quad \exp_p(\log_p(1+x)) = 1 + x.$$

Let $(X, \mathcal{B})$ be a measurable space, where $\mathcal{B}$ is an algebra of subsets X. A function $\mu : \mathcal{B} \to \mathbb{Q}_p$ is said to be a p-adic measure if for any $A_1, \ldots, A_n \subset \mathcal{B}$ such that $A_i \cap A_j = \varnothing$ $(i \neq j)$ the equality holds

$$\mu\left(\bigcup_{j=1}^{n} A_j\right) = \sum_{j=1}^{n} \mu(A_j).$$

A p-adic measure is called a probability measure if $\mu(X)=1$.

For more detailed information about p-adic measures please refer to Refs. 7 and 8.

B. The Cayley tree

The Cayley tree Γ^k of order $k \geqslant 1$ is an infinite tree, i.e., a graph without cycles, such that each vertex of which lies on $k+1$ edges. Let $\Gamma^k=(V,\Lambda)$, where V is the set of vertices of Γ^k, Λ is the set of edges of Γ^k. The vertices x and y are called *nearest neighbors*, which is denoted by $l=\langle x,y\rangle$ if there exists an edge connecting them. A collection of the pairs $\langle x,x_1\rangle,\ldots,\langle x_{d-1},y\rangle$ is called *path* from the point x to the point y. The distance $d(x,y), x,y \in V$, on the Cayley tree, is the length of the shortest path from x to y.

We set

$$W_n=\{x \in V | d(x,x^0)=n\},$$

$$V_n=\bigcup_{m=1}^{n} W_m=\{x \in V | d(x,x^0) \leqslant n\},$$

$$L_n=\{l=\langle x,y\rangle \in L | x,y \in V_n\},$$

for an arbitrary point $x^0 \in V$.

Denote

$$S(x)=\{y \in W_{n+1} : d(x,y)=1\} \quad x \in W_n,$$

this set is called the set *direct successors* of x. Observe that any vertex $x \neq x^0$ has k direct successors and x^0 has $k+1$.

C. The *p*-adic λ-model

We consider a p-adic λ-model, where the spin takes values in the set $\Phi=\{-1,1\}\subset\mathbb{Q}_p$ and is assigned to the vertices of the tree. A configuration σ on V is then defined as a function $x \in V \to \sigma(x) \in \Phi$; in a similar fashion one defines a configuration σ_n and $\sigma^{(n)}$ on V_n and W_n, respectively. The set of all configurations on V (resp. V_n, W_n) coincides with $\Omega=\Phi^V$ (resp. $\Omega_{V_n}=\Phi^{V_n}, \Omega_{W_n}=\Phi^{W_n}$). One can see that $\Omega_{V_n}=\Omega_{V_{n-1}}\times\Omega_{W_n}$. Using this, for given configurations $\sigma_{n-1} \in \Omega_{V_{n-1}}$ and $\sigma^{(n)} \in \Omega_{W_n}$ we define their concatenations by the formula

$$\sigma_{n-1}\vee\sigma^{(n)}=\{\{\sigma_n(x),x \in V_{n-1}\},\{\sigma^{(n)}(y),y \in W_n\}\}.$$

It is clear that $\sigma_{n-1}\vee\sigma^{(n)} \in \Omega_{V_n}$. Let functions $\lambda_{x,y}:(u,v) \in \Phi\times\Phi \to \lambda_{x,y}(u,v) \in \mathbb{Q}_p$. be given for each pairs of neighboring vertices x,y. The Hamiltonian $H_n:\Omega_{V_n}\to\mathbb{Q}_p$ of the p-adic inhomogeneous λ-model has the form

$$H_n(\sigma_n)=\sum_{\langle x,y\rangle \in L_n}\lambda_{x,y}(\sigma_n(x),\sigma_n(y)), \quad n \in \mathbb{N}, \tag{2.1}$$

where the sum is taken over all pairs of neighboring vertices $\langle x,y\rangle$ and $\sigma_n \in \Omega_{V_n}$.

We say that (2.1) is *homogeneous* λ-*model* if all functions $\lambda_{xy}(u,v)$ do not depend on x,y and in this case we put $\lambda(u,v):=\lambda_{x,y}(u,v), \forall\langle x,y\rangle \in L$.

We note that λ-model of this type were firstly considered in Ref. 15.

III. CONSTRUCTION OF GIBBS MEASURES

In this subsection we give a construction of a special class of Gibbs measures for p-adic λ-model on the Cayley tree.

To define Gibbs measure we need in the following

Lemma 3.1: Let $h_x, x \in V$ be a $\mathbb{Q}_p$-valued function such that $h_x \in B(0, p^{-1/(p-1)})$ for all $x \in V$ and $|\lambda_{x,y}(u,v)|_p < p^{-1/(p-1)}$ for all $u, v \in \Phi$. Then the relation

$$H_n(\sigma) + \sum_{x \in W_n} h_x \sigma(x) \in B(0, p^{-1/(p-1)}),$$

is valid for any $n \in \mathbb{N}$.

The proof easily follows from the strong triangle inequality for the norm $|\cdot|_p$.

Let $h: x \in V \to h_x \in \mathbb{Q}_p$ be a function of $x \in V$ such that $|h_x|_p < p^{-1/(p-1)}$ for all $x \in V$. Given $n = 1, 2, \ldots$ consider a p-adic probability measure $\mu^{(n)}$ on Φ^{V_n} defined by

$$\mu_h^{(n)}(\sigma_n) = Z_n^{-1} \exp_p \left\{ H_n(\sigma_n) + \sum_{x \in W_n} h_x \sigma(x) \right\}. \tag{3.1}$$

Here, as before, $\sigma_n: x \in V_n \to \sigma_n(x)$ and Z_n is the corresponding partition function:

$$Z_n = \sum_{\tilde{\sigma}_n \in \Omega_{V_n}} \exp_p \left\{ H(\tilde{\sigma}_n) + \sum_{x \in W_n} h_x \tilde{\sigma}(x) \right\}.$$

Note that according to Lemma 3.1 the measures $\mu^{(n)}$ exist.

The compatibility conditions for $\mu_h^{(n)}(\sigma_n), n \geqslant 1$ are given by the equality

$$\sum_{\sigma^{(n)} \in \Omega_{W_n}} \mu_h^{(n)}(\sigma_{n-1} \vee \sigma^{(n)}) = \mu_h^{(n-1)}(\sigma_{n-1}), \tag{3.2}$$

where $\sigma_{n-1} \in \Omega_{V_{n-1}}$.

We note that an analog of the Kolmogorov extension theorem for distributions can be proved for p-adic distributions given by (3.1) (see Ref. 10). Then according to the Kolmogorov theorem there exists a unique p-adic measure μ_h on $\Omega = \Phi^V$ such that for every $n = 1, 2, \ldots$ and $\sigma_n \in \Phi^{V_n}$ the equality holds

$$\mu_h(\{\sigma|_{V_n} = \sigma_n\}) = \mu_h^{(n)}(\sigma_n),$$

which will be called *p-adic Gibbs measure* for the considered λ-model. It is clear that the measure μ_h depends on the function h_x. By $\mathcal{S}_\lambda$ we denote the set of all p-adic Gibbs measures associated with functions $h = (h_x, x \in V)$. If $|\mathcal{S}_\lambda| \geqslant 2$, then we can say that, for this model, there exists *a phase transition*, otherwise, we say there is *no phase transition* (here $|A|$ means the cardinality of a set A). In other words, the phase transition means that there are two different functions $h = (h_x, x \in V)$ and $s = (s_x, x \in V)$ for which there exists two μ_h and μ_s p-adic Gibbs measures on Ω, respectively.

The following statement describes conditions on h_x guaranteeing the compatibility condition of measures $\mu^{(n)}(\sigma_n)$.

Theorem 3.2: *The measures $\mu^{(n)}(\sigma_n), n = 1, 2, \ldots$ satisfy the compatibility condition (3.2) if and only if for any $x \in V$ the following equation holds:*

$$h_x = \sum_{y \in S(x)} F_{x,y}(h_y; \lambda) \tag{3.3}$$

where $S(x)$ is the set of all direct successors of $x \in V$ and

$$F_{x,y}(h, \lambda) = \frac{1}{2} \log_p \left(\frac{\exp_p(\lambda_{x,y}(1,1)) \exp_p(2h) + \exp_p(\lambda_{x,y}(1,-1))}{\exp_p(\lambda_{x,y}(-1,1)) \exp_p(2h) + \exp_p(\lambda_{x,y}(-1,-1))} \right).$$

Proof: *Necessity*. According to the compatibility condition (3.2) we have

$$Z_n^{-1}\sum_{\sigma^{(n)}}\exp_p\left[\sum_{\langle x,y\rangle\in L_n}\lambda_{x,y}(\sigma(x),\sigma(y))+\sum_{x\in W_n}h_x\sigma(x)\right]$$
$$=Z_{n-1}^{-1}\exp_p\left[\sum_{\langle x,y\rangle\in L_{n-1}}\lambda_{x,y}(\sigma(x),\sigma(y))+\sum_{x\in W_{n-1}}h_x\sigma(x)\right]. \quad (3.4)$$

It yields

$$\frac{Z_{n-1}}{Z_n}\sum_{\sigma(n)}\exp_p\left[\sum_{x\in W_{n-1}}\sum_{y\in S(x)}\lambda_{x,y}(\sigma(x),\sigma(y))+\sum_{x\in W_{n-1}}\sum_{y\in S(x)}h_y\sigma(y)\right]=\prod_{x\in W_{n-1}}\exp_p(h_x\sigma(x)). \quad (3.5)$$

From this equality we find

$$\frac{Z_{n-1}}{Z_n}\prod_{x\in W_{n-1}}\prod_{y\in S(x)}\sum_{\sigma(y)\in\Phi}\exp_p(\lambda_{x,y}(\sigma(x),\sigma(y))+h_y\sigma(y))=\prod_{x\in W_{n-1}}\exp_p(h_x\sigma(x)). \quad (3.6)$$

Now fix $x\in W_{n-1}$ and dividing the equalities (3.6) with $\sigma(x)=1$ and $\sigma(x)=-1$ we obtain

$$\prod_{y\in S(x)}\frac{\sum_{\sigma(y)\in\Phi}\exp_p(\lambda_{x,y}(1,\sigma(y))+h_y\sigma(y))}{\sum_{\sigma(y)\in\Phi}\exp_p(\lambda_{x,y}(-1,\sigma(y))+h_y\sigma(y))}=\exp_p(2h_x), \quad (3.7)$$

hence we get

$$\prod_{y\in S(x)}\frac{\exp_p(\lambda_{x,y}(1,1))\exp_p(2h_y)+\exp_p(\lambda_{x,y}(1,-1))}{\exp_p(\lambda_{x,y}(-1,1))\exp_p(2h_y)+\exp_p(\lambda_{x,y}(-1,-1))}=\exp_p(2h_x), \quad (3.8)$$

which implies (3.3).

Sufficiency: Now assume that (3.3) is valid, then it implies (3.8), and hence (3.7). From (3.7) we obtain the following equality:

$$a(x)\exp_p(h_x\sigma)=\prod_{y\in S(x)}\sum_{\tilde\sigma(y)\in\Phi}\exp_p(\lambda_{x,y}(\sigma,\tilde\sigma(y))+h_y\tilde\sigma(y)),\quad \sigma\in\{-1,1\};$$

this equality implies

$$\prod_{x\in W_{n-1}}a(x)\exp_p(h_x\sigma(x))=\prod_{x\in W_{n-1}}\prod_{y\in S(x)}\sum_{\tilde\sigma(y)\in\Phi}\exp_p(\lambda_{x,y}(\sigma(x),\tilde\sigma(y))+h_y\tilde\sigma(y)), \quad (3.9)$$

where

$$\sigma(z)=\begin{cases}\sigma, & z=x\\ \sigma(z), & z\neq x\end{cases}\qquad \sigma\in\{-1,1\}.$$

Denoting $A_n(x)=\Pi_{x\in W_n}a(x)$ from (3.9) and (3.2) we find

$$Z_{n-1}A_{n-1}\mu_h^{(n-1)}(\sigma_{n-1})=Z_n\sum_{\tilde\sigma^{(n)}}\mu_h^{(n)}(\sigma_{n-1}\vee\tilde\sigma^{(n)}).$$

Since each $\mu_h^{(n)}$, $n\geqslant 1$ measure is a *p*-adic probability measure, so we should have

$$\sum_{\sigma_{n-1}}\sum_{\tilde\sigma^{(n)}}\mu_h^{(n)}(\sigma_{n-1}\vee\tilde\sigma^{(n)})=1,\quad \sum_{\sigma_{n-1}}\mu_h^{(n-1)}(\sigma_{n-1})=1.$$

Therefore, from these equalities we find $Z_{n-1}A_{n-1}=Z_n$ which means that (3.2) is valid.

Observe that according to this Theorem the problem of describing of *p*-adic Gibbs measures is reduced to the description of solutions of functional equation (3.3).

IV. THE UNIQUENESS OF GIBBS MEASURE FOR THE *p*-ADIC λ-MODEL

In this section we will show that the phase transition does not occur for the p-adic λ-model. Put

$$\Xi = \{h = (h_x, x \in V) : h_x \text{ satisfies the equation (3.3)}\}.$$

According to Theorem 3.2 the description of Gibbs measures is reduced to the description of elements of the set Ξ.

A. Nonhomogeneous case

In this subsection we will consider nonhomogeneous λ-model. We claim that the function $\lambda_{x,y}$ satisfies the following condition: for all nearest-neighbor vertices $x, y \in V$ the equality

$$\exp_p(\lambda_{x,y}(1,1)) + \exp_p(\lambda_{x,y}(1,-1)) = \exp_p(\lambda_{x,y}(-1,1)) + \exp_p(\lambda_{x,y}(-1,-1)), \tag{4.1}$$

is valid.

This condition implies that the function $h_x = 0, \forall x \in V$ is a solution of (3.3).

Let $S(x) = \{x_1, \ldots, x_k\}$, here as before $S(x)$ is the set of direct successors of x. Then the equation (3.3) can be rewritten as follows:

$$z_x = \prod_{i=1}^{k} \alpha_{x,i}, \tag{4.2}$$

where $z_x = \exp_p(h_x)$, $z_{x_i} = \exp_p(h_{x_i})$,

$$\alpha_{x,i} = \frac{a_{x,x_i} z_{x_i} + b_{x,x_i}}{c_{x,x_i} z_{x_i} + d_{x,x_i}},$$

$$\begin{aligned} a_{x,x_i} &= \exp_p(\lambda_{x,x_i}(1,1)), \quad & b_{x,x_i} &= \exp_p(\lambda_{x,x_i}(1,-1)), \\ c_{x,x_i} &= \exp_p(\lambda_{x,x_i}(-1,1)), \quad & d_{x,x_i} &= \exp_p(\lambda_{x,x_i}(-1,-1)) \end{aligned} \tag{4.3}$$

for every $i = 1, \ldots, k$, here as before $|h_x|_p \leqslant 1/p$ for all $x \in V$.

Lemma 4.2: If $|a_i - 1|_p \leqslant M$ *and* $|a_i|_p = 1$, $i = 1, \ldots, n$, *then*

$$\left| \prod_{i=1}^{n} a_i - 1 \right|_p \leqslant M. \tag{4.4}$$

Proof: We prove by induction on n. The case $n = 1$ is the condition of lemma. Suppose that (4.4) is valid at $n = m$. Now let $n = m + 1$. Then we have

$$\left| \prod_{i=1}^{m+1} a_i - 1 \right|_p = \left| \prod_{i=1}^{m+1} a_i - \prod_{i=1}^{m} a_i + \prod_{i=1}^{m} a_i - 1 \right|_p \leqslant \max\left\{ \left| \prod_{i=1}^{n} a_i (a_{n+1} - 1) \right|_p, \left| \prod_{i=1}^{n} a_i - 1 \right|_p \right\} \leqslant M.$$

This completes the proof.

Lemma 4.3: For every $x \in V$ *the following inequality holds*

$$|h_x|_p \leqslant \frac{1}{p} \max_{1 \leqslant i \leqslant k} \{|h_{x_i}|_p\}.$$

Proof: For every $m \in \{1, 2, \ldots, k\}$ we have

$$|\alpha_{x,m}-1|_p=\left|\frac{(a_{x,x_m}-c_{x,x_m})(z_{x_m}-1)}{c_{x,x_m}z_{x_m}+d_{x,x_m}}\right|_p\leqslant\frac{1}{p}|h_{x_m}|_p.$$

Here we have used (4.1) and the following relations: for $p\geqslant 3$

$$|a_{x,x_m}-c_{x,x_m}|_p\leqslant\frac{1}{p},\quad |c_{x,x_m}z_{x_m}+d_{x,x_m}|_p=1,$$

for $p=2$

$$|a_{x,x_m}-c_{x,x_m}|_p\leqslant\frac{1}{2^2},\quad |c_{x,x_m}z_{x_m}+d_{x,x_m}|_p=\frac{1}{2},$$

which follow from (4.3) and the equality $|\exp_p(x)-1|_p=|x|_p$ (see Lemma 2.1). Then according to Lemma 4.2 and (4.2) we obtain

$$|h_x|_p=|z_x-1|_p\leqslant\frac{1}{p}\max_{1\leqslant i\leqslant k}\{|h_{x_i}|_p\}.$$

Lemma is proved.

Theorem 4.4: *Let* $k\geqslant 1$, $|\lambda_{x,y}(u,v)|_p\leqslant 1/p$ *for all* $<x,y>\in L$, $u,v\in\Phi$ *and (4.1) be satisfied. Then for the p-adic nonhomogeneous* λ*-model (2.1) on the Cayley tree of order k there is no phase transition for any prime p.*

Proof: To obtain the proof it is enough to show that $\Xi=\{h_x\equiv 0\}$. In order to do so it is enough to show that for arbitrary $\varepsilon>0$ and every $x\in V$ the inequality $\|h_x\|_p<\varepsilon$ is valid. Let $n_0\in\mathbb{N}$ be such that $1/p^{n_0}<\varepsilon$. According to Lemma 4.3 we have

$$|h_x|_p\leqslant\frac{1}{p}|h_{x_{i_0}}|_p\leqslant\frac{1}{p^2}|h_{x_{i_0,i_1}}|_p\leqslant\cdots\leqslant\frac{1}{p^{n_0-1}}|h_{x_{i_0,\ldots,i_{n_0-2}}}|_p\leqslant\frac{1}{p^{n_0}}<\varepsilon,$$

here $x_{i_0,\ldots,i_n,j}$, $j=\overline{1,k}$ are direct successors of $x_{i_0,\ldots,i_n}$, where

$$|h_{x_{i_0,\ldots,i_m}}|_p=\max_{1\leqslant j\leqslant k}\{|h_{x_{i_0,\ldots,i_{m-1},j}}|_p\}.$$

This completes the proof.

B. Homogeneous case

In this subsection we will consider the homogeneous λ-model, i.e., $\lambda_{xy}(u,v)=\lambda(u,v)$, $\forall\langle x,y\rangle\in L$.

In this subsection at first we restrict ourselves to the description of translation-invariant ($h_x=h\in\mathbb{Q}_p$, $\forall x\in V$) elements of Ξ.

Let $h_x=h$ for all $x\in V$. Then (3.3) implies

$$\left(\frac{\exp_p(\lambda(1,1))\exp_p(2h)+\exp_p(\lambda(1,-1))}{\exp_p(\lambda(-1,1))\exp_p(2h)+\exp_p(\lambda(-1,-1))}\right)^k=\exp_p(2h).\tag{4.5}$$

Denoting

$$\begin{gathered}z=\exp_p(2h),\quad a=\exp_p(\lambda(1,1)),\quad b=\exp_p(\lambda(1,-1)),\\ c=\exp_p(\lambda(-1,1)),\quad d=\exp_p(\lambda(-1,-1)),\end{gathered}\tag{4.6}$$

from (4.5) we obtain

$$\left(\frac{az+b}{cz+d}\right)^k = z. \tag{4.7}$$

Denote

$$f(x) = \left(\frac{ax+b}{cx+d}\right)^k.$$

Let $S_1=\{x \in \mathbb{Q}_p : |x|_p=1\}$. Then it is clear that $f(S_1) \subset S_1$. Using this fact for every $x \in S_1$ we find

$$|f(x)-1|_p = \left|\frac{(a-c)x+b-d}{cx+d}\right|_p \left|\sum_{m=0} k-1\left(\frac{ax+b}{cx+d}\right)^m\right|_p \leqslant \frac{1}{p}, \tag{4.8}$$

here we have used (4.6) and Lemma 2.1.

Let $x,y \in S_1$, then

$$|f(x)-f(y)|_p = \left|\frac{ax+b}{cx+d}-\frac{ay+b}{cy+d}\right|_p \left|\sum_{m=0}^{k-1}\left(\frac{ay+b}{cy+d}\right)^m\left(\frac{ax+b}{cx+d}\right)^{k-m-1}\right|_p \leqslant \frac{|ad-bc|_p|x-y|_p}{|cx+d|_p|cy+d|_p}. \tag{4.9}$$

Now consider two different cases with respect to p.

Let us assume that $p \geqslant 3$. In this case we have

$$|ad-bc|_p \leqslant \frac{1}{p}, \quad |cx+d|_p = 1, \quad |cy+d|_p = 1,$$

which are obtained from (4.6) and Lemma 2.1. Using these equalities from (4.9) it can be found

$$|f(x)-f(y)|_p \leqslant \frac{1}{p}|x-y|_p. \tag{4.10}$$

Now suppose $p=2$. Then

$$|ad-bc|_p \leqslant \frac{1}{2^2}, \quad |cx+d|_p = \frac{1}{2}, \quad |cy+d|_p = \frac{1}{2}.$$

We claim that $|ad-bc|_p \leqslant 1/2^3$ is satisfied. It follows from (4.9) that

$$|f(x)-f(y)|_2 \leqslant \frac{1}{2}|x-y|_2. \tag{4.11}$$

Thus the equalities (4.10) and (4.11) imply that f is a contraction of S_1, hence f has a unique fixed point $\zeta \in S_1$ such that $|\zeta-1|_p \leqslant 1/p$ (see (4.8)). So we have proved the following

Proposition 4.5: (i) Let $p \geqslant 3$ and $|\lambda(u,v)|_p \leqslant 1/p$ for all $\langle x,y\rangle \in L$, $u,v \in \Phi$. Then for the p-adic homogeneous λ-model (2.1) on the Cayley tree of order k $(k \geqslant 1)$ the Eq. (4.5) has a unique solution.

(ii) Let $p=2$, $|\lambda(u,v)|_2 \leqslant 1/2^2$ for all $\langle x,y\rangle \in L$, $u,v \in \Phi$ and the following condition be satisfied:

$$|\exp_p(\lambda(1,1))\exp_p(\lambda(-1,-1)) - \exp_p(\lambda(-1,1))\exp_p(\lambda(1,-1))|_2 \leqslant \frac{1}{2^3}. \tag{4.12}$$

Then for the 2-adic homogeneous λ-model (2.1) on the Cayley tree of order k $(k \geqslant 1)$ the Eq. (4.5) has a unique solution.

Theorem 4.6: *Let the condition of the previous Proposition be satisfied. Then for the p-adic*

homogeneous λ*-model (2.1) on the Cayley tree of order k there is no phase transition for any prime p*.

Proof: In the homogeneous model (4.2) is written as

$$z_x = \prod_{i=1}^{k} \alpha_{x,i}, \tag{4.13}$$

here

$$\alpha_{x,i} = \frac{az_{x_i}+b}{cz_{x_i}+d},$$

where as before $z_x = \exp_p(h_x), z_{x_i} = \exp_p(h_{x_i})$, and the coefficients a,b,c,d are defined by (4.6).

Let ζ be a solution of (4.7). Then using (4.13) we have

$$\begin{aligned}
|z_x-\zeta|_p &= \left|\prod_{i=1}^{k}\left(\frac{az_{x_i}+b}{cz_{x_i}+d}\right)-\left(\frac{a\zeta+b}{c\zeta+d}\right)^k\right|_p \\
&= \left|\prod_{i=1}^{k}\left(\frac{az_{x_i}+b}{cz_{x_i}+d}\right)-\left(\frac{az_{x_k}+b}{cz_{x_k}+d}\right)\left(\frac{a\zeta+b}{c\zeta+d}\right)^{k-1}+\left(\frac{az_{x_k}+b}{cz_{x_k}+d}\right)\left(\frac{a\zeta+b}{c\zeta+d}\right)^{k-1}-\left(\frac{a\zeta+b}{c\zeta+d}\right)^k\right|_p \\
&\leqslant \max\left\{\left|\frac{az_{x_k}+b}{cz_{x_k}+d}\right|_p\left|\prod_{i=1}^{k-1}\left(\frac{az_{x_i}+b}{cz_{x_i}+d}\right)-\left(\frac{a\zeta+b}{c\zeta+d}\right)^{k-1}\right|_p, \left|\frac{a\zeta+b}{c\zeta+d}\right|_p^{k-1}\left|\frac{az_{x_k}+b}{cz_{x_k}+d}-\frac{a\zeta+b}{c\zeta+d}\right|_p\right\} \\
&= \max\left\{\left|\frac{az_{x_k}+b}{cz_{x_k}+d}\right|_p\left|\prod_{i=1}^{k-1}\left(\frac{az_{x_i}+b}{cz_{x_i}+d}\right)-\left(\frac{a\zeta+b}{c\zeta+d}\right)^{k-1}\right|_p, \frac{|z_{x_k}-\zeta|_p|ad-bc|_p}{|cz_{x_k}+d|_p|c\zeta+d|_p}\right\} \\
&\leqslant \cdots \leqslant \max\left\{\frac{|z_{x_k}-\zeta|_p|ad-bc|_p}{|cz_{x_k}+d|_p|c\zeta+d|_p}\right\} \leqslant \frac{1}{p}\max_{1\leqslant m\leqslant k}\{|z_{x_m}-\zeta|_p\}.
\end{aligned}$$

Now repeating the argument of the proof of Theorem 4.4 we obtain $z_x=\zeta$ for all $x\in V$. This completes the proof.

V. APPLICATIONS TO *p*-ADIC ISING MODEL

In this section we will show that the phase transition does not occur for the *p*-adic Ising model.

Recall the *p*-adic Ising model. This model is a particular case of λ-model, namely it corresponds to the function:

$$\lambda_{x,y}(u,v) = J_{x,y}uv + \eta(u+v), \tag{5.1}$$

here $|J_{x,y}|\leqslant p^{-1/(p-1)}$, $|\eta|_p \leqslant p^{-1/(p-1)}$ and $\langle x,y\rangle \in L$, $u,v\in\{-1,1\}$.

First consider the case $\eta=0$, this corresponds to the inhomogeneous *p*-adic Ising model without external field. For the considered model it is easy to see that the condition (4.1) is satisfied. So according to Theorem 4.4 we infer that the following

Theorem 5.1: *Let* $k\geqslant 1$, $|J_{x,y}|_p \leqslant p^{-1/(p-1)}$ *for all* $\langle x,y\rangle \in L$. *Then for the p-adic inhomogeneous Ising model on the Cayley tree of order k there is no phase transition for any prime p*.

Now consider a case $J_{x,y}=J$ for all $\langle x,y\rangle\in L$ and $\eta\neq 0$. This corresponds to the homogeneous *p*-adic Ising model with an external field.

Let $p=2$, then the condition (4.12) can be written as follows:

$$|\exp_p(J+2\eta)\exp_p(J-2\eta)-\exp_p(-J)\exp_p(-J)|_2=|\exp_p(4J)-1|_2=|4J|_2\leqslant\frac{1}{2^4},$$

here we have used Lemma 2.1. Hence (4.12) is satisfied. So we can formulate the following.

Theorem 5.2: *Let* $k\geqslant 1$, $|\eta|_p\leqslant p^{-1/(p-1)}$ *and* $|J|_p\leqslant p^{-1/(p-1)}$ *for all* $\langle x,y\rangle\in L$. *Then for the p-adic homogeneous Ising model on the Cayley tree of order k there is no phase transition for any prime p*.

Remark: It is known[5,16] that for the Ising model on the Cayley tree of order $k\geqslant 2$ over $\mathbb{R}$ on some condition upon parameter $J_{x,y}$ there is a phase transition. Theorems 5.1 and 5.2 show the difference between the real Ising model and the considered *p*-adic one.

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On extremal quantum states of composite systems with fixed marginals

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We study the convex set $\mathcal{C}(\rho_1,\rho_2)$ of all bipartite quantum states with fixed marginal states ρ_1 and ρ_2. The extremal states in this set have recently been characterized by Parthasarathy [Ann. Henri Poincaré (to appear), quant-ph/0307182]. Here we present an alternative necessary and sufficient condition for a state in $\mathcal{C}(\rho_1,\rho_2)$ to be extremal. Our approach is based on a canonical duality between bipartite states and a certain class of completely positive maps and has the advantage that it is easier to check and to construct explicit examples of extremal states. In dimension 2×2 we give a simple new proof for the fact that all extremal states in $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$ are precisely the projectors onto maximally entangled wave functions. We also prove that in higher dimension this does not hold and construct an explicit example of an extremal state in $\mathcal{C}(\frac{1}{3}\mathbb{1},\frac{1}{3}\mathbb{1})$ that is not maximally entangled. Generalizations of this result to higher dimensions are also discussed. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1776642]

I. INTRODUCTION

In the paradigmatic situation encountered in quantum information processing, two or more (often spatially separated) parties share the different parts of a composite quantum system. The parties are able to perform arbitrary operations on their respective parts "locally" and to communicate classically among each other to orchestrate their actions. The fundamental realization in quantum information theory is that sharing the parts of a composite quantum system can enable the parties to perform certain communication or information processing tasks more efficiently than classically (see Ref. 1 for an introduction). Mathematically this setting raises a number of new and interesting structural questions. Among them the study of quantum channels and the characterization of quantum entanglement play a central role.[2–4] The present work is devoted to the characterization of the set of quantum states with fixed marginal states. This problem was recently posed and studied in detail by Parthasarathy.[5] Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two finite dimensional complex Hilbert spaces, corresponding to two finite level quantum systems S_1 and S_2. Without loss of generality we assume that $d:=\dim(\mathcal{H}_1)=\dim(\mathcal{H}_2)$. (Otherwise we embed the lower dimensional Hilbert space into the larger one.) The states for S_i are given by the positive operators on $\mathcal{H}_i$ with trace one. We denote the set of all states on $\mathcal{H}_i$ by $\mathsf{S}(\mathcal{H}_i)$. The composite quantum system S_{12} of S_1 and S_2 is described by the tensor product $\mathcal{H}_1\otimes\mathcal{H}_2$. A *state* for S_{12} is a positive operator on $\mathcal{H}_1\otimes\mathcal{H}_2$ with trace one. The space of all states is denoted by $\mathsf{S}(\mathcal{H}_1\otimes\mathcal{H}_2)$. Consider $\rho\in\mathsf{S}(\mathcal{H}_1\otimes\mathcal{H}_2)$. The *reductions* or *marginal states* of ρ are given by $\rho_1:=\mathrm{tr}_2(\rho)\in\mathsf{S}(\mathcal{H}_1)$ and $\rho_2:=\mathrm{tr}_1(\rho)\in\mathsf{S}(\mathcal{H}_2)$. Here tr_1 and tr_2 denote the partial traces over $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Now fix $\rho_1\in\mathsf{S}(\mathcal{H}_1)$ and $\rho_2\in\mathsf{S}(\mathcal{H}_2)$. We denote by $\mathcal{C}(\rho_1,\rho_2)$ the convex set of all states $\rho\in\mathsf{S}(\mathcal{H}_1\otimes\mathcal{H}_2)$ whose marginal states are equal to ρ_1 and ρ_2, respectively. The set of extreme points of $\mathcal{C}(\rho_1,\rho_2)$ will be denoted by $\mathcal{E}(\rho_1,\rho_2)$. Throughout this paper we will denote the set of all operators on a Hilbert space $\mathcal{H}$ by $\mathsf{L}(\mathcal{H})$. The identity in $\mathsf{L}(\mathcal{H})$ is denoted by $\mathbb{1}$, or, when $\mathcal{H}$ is d-dimensional, by $\mathbb{1}_d$. Slightly abusing the notation we will also denote the identity map from $\mathsf{L}(\mathcal{H})$ into itself by $\mathbb{1}$.

In his work[5] Parthasarathy presented a necessary and sufficient condition for an element $\rho\in\mathcal{C}(\rho_1,\rho_2)$ to be an extreme point. This was then used to derive an upper bound on the rank of such an extremal state. In the special case $\mathcal{H}_1=\mathcal{H}_2=\mathbb{C}^2$ and $\rho_1=\rho_2=\frac{1}{2}\mathbb{1}_2$, Parthasarathy found that

a state $\rho \in \mathcal{C}(\frac{1}{2}\mathbb{1}_2, \frac{1}{2}\mathbb{1}_2)$ is extremal if and only if it is a projector onto the subspace spanned by a maximally entangled wave function. A wave function in $\mathbb{C}^2 \otimes \mathbb{C}^2$ is called maximally entangled if it is of the form $|\psi_+\rangle = (1/\sqrt{2})(|0\rangle|\phi_0\rangle + |1\rangle|\phi_1\rangle)$ where $\{|0\rangle, |1\rangle\}$ denotes the canonical basis of $\mathbb{C}^2$ and where $\{|\phi_0\rangle, |\phi_1\rangle\}$ is any other orthonormal basis of $\mathbb{C}^2$. For higher dimensions the question of whether or not there are extremal states with maximally mixed marginals—i.e., states in $\mathcal{E}(\frac{1}{d}\mathbb{1}, \frac{1}{d}\mathbb{1})$—that are not projectors onto maximally entangled wave functions was left open in Ref. 5.

In the present work we present an alternative approach to the characterization of $\mathcal{E}(\rho_1, \rho_2)$ that transforms the problem into that of finding the extreme points of a certain convex set of completely positive maps that satisfy an additional requirement. This will allow us to derive an alternative necessary and sufficient condition for a state $\rho \in \mathcal{C}(\rho_1, \rho_2)$ to be extremal. We will then study the special case of states with maximally mixed marginals, i.e., when $\rho_1 = \rho_2 = (1/d)\mathbb{1}$. For $d = 2$ we will give a simple proof for Parthasarathy's result that the extremal states are exactly the projectors onto maximally entangled wave functions. For $d > 2$ our results imply that there are extremal states in $\mathcal{E}(\mathbb{1}/d, \mathbb{1}/d)$ that are not projectors onto maximally entangled pure states. We give an explicit example for an extremal state on $\mathbb{C}^3 \otimes \mathbb{C}^3$ with maximally mixed marginals that is not equal to a projector onto a maximally entangled wave function. Finally, we discuss generalizations of this result to higher dimensions.

II. DUALITY BETWEEN BIPARTITE STATES AND COMPLETELY POSITIVE MAPS

The approach in the present paper relies upon a duality between bipartite quantum states on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and completely positive maps $\Lambda : \mathsf{L}(\mathcal{H}_2) \to \mathsf{L}(\mathcal{H}_1)$ that preserve the trace of the completely mixed state, i.e., that satisfy $\mathrm{tr}(\Lambda((1/d)\mathbb{1})) = 1$ (this is very often called the *Jamiołkowski isomorphism*, see Ref. 6 and, for a related duality, Ref. 2). A map $\Lambda : \mathsf{L}(\mathcal{H}_2) \to \mathsf{L}(\mathcal{H}_1)$ is called completely positive if $\Lambda \otimes \mathbb{1} : \mathsf{L}(\mathcal{H}_2 \otimes \mathcal{K}) \to \mathsf{L}(\mathcal{H}_1 \otimes \mathcal{K})$ is positive for any finite dimensional ancilla Hilbert space $\mathcal{K}$.

We make the identification $\mathcal{H}_1 \simeq \mathbb{C}^d$ and $\mathcal{H}_2 \simeq \mathbb{C}^d$. In other words, we pick orthonormal bases in $\mathcal{H}_1$ and $\mathcal{H}_2$ and identify them with the canonical real basis in $\mathbb{C}^d$ and $\mathbb{C}^d$, respectively. We denote these bases by $\{|i\rangle_1\}_{i=1}^d$ and $\{|i\rangle_2\}_{i=1}^d$, respectively. Finally, we introduce the maximally entangled pure wave function

$$|\psi_+\rangle := \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle_2 |i\rangle_2 \in \mathcal{H}_2 \otimes \mathcal{H}_2.$$

The duality between bipartite state and completely positive maps depends explicitly on this choice for the canonical bases. Let $\Lambda : \mathsf{L}(\mathcal{H}_2) \to \mathsf{L}(\mathcal{H}_1)$ be a completely positive map with $\mathrm{tr}(\Lambda((1/d)\mathbb{1})) = 1$. Then

$$\rho_\Lambda := \Lambda \otimes \mathbb{1}(|\psi_+\rangle\langle\psi_+|) \tag{1a}$$

defines a bipartite state on $\mathcal{H}_1 \otimes \mathcal{H}_2$. The complete positivity of Λ ensures that $\rho \geqslant 0$ while the condition $\mathrm{tr}(\Lambda((1/d)\mathbb{1})) = 1$ ensures that $\mathrm{tr}(\rho_\Lambda) = 1$.

Conversely, let ρ be a bipartite state on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Then

$$\Lambda_\rho(\sigma) := d\,\mathrm{tr}_2[(\mathbb{1} \otimes \sigma^{\mathsf{T}}\rho)] \tag{1b}$$

defines a completely positive map $\Lambda_\rho : \mathsf{L}(\mathcal{H}_2) \to \mathsf{L}(\mathcal{H}_1)$ that satisfies $\mathrm{tr}(\Lambda_\rho((1/d)\mathbb{1})) = 1$. Here $^{\mathsf{T}}$ denotes the transposition with respect to the canonical real basis. By explicit calculation one checks that for a given Λ we have $\Lambda_{\rho_\Lambda} = \Lambda$ and for a given ρ we have $\rho_{\Lambda_\rho} = \rho$. Thus the correspondence $\Lambda \leftrightarrow \rho$ described by Eqs. (1a) and (1b) is bijective.[6]

III. JOINT LINEAR INDEPENDENCE

To formulate the main result in this paper it is useful to introduce the concept of *joint linear independence* of two families of vectors. In the following definition $X^{\times r}$ denotes the r-fold Cartesian product of the set X by itself.

Definition 1: *Let V and W be complex vector spaces. Then two ordered r-tuples $(v_i)_{i=1}^r \in V^{\times r}$ and $(w_i)_{i=1}^r \in W^{\times r}$ are called* jointly linearly independent *if the family $\{v_i \oplus w_i\}_{i=1}^r$ in the direct sum $V \oplus W$ is a linearly independent family*.

Notice that this definition depends on the order of the r-tuples. The following is an immediate consequence of the definition.

Lemma 1: *Let V and W be complex vector spaces and let $(v_i)_{i=1}^r \in V^{\times r}$ and $(w_i)_{i=1}^r \in W^{\times r}$ be two ordered r-tuples of vectors. If $\{v_i\}_{i=1}^r$ is linearly independent in V or if $\{w_i\}_{i=1}^r$ is linearly independent in W, then $(v_i)_{i=1}^r$ and $(w_i)_{i=1}^r$ are jointly linearly independent.*

Notice that the converse implication does not hold in general. If $\{v_i\}_{i=1}^r$ is linearly dependent in V and if $\{w_i\}_{i=1}^r$ is linearly dependent in W, then $\{v_i \oplus w_i\}_{i=1}^r$ is not necessarily linearly dependent in $V \oplus W$.

Lemma 2: *Let V be a complex *-algebra and let $(v_j)_{j=1}^r \in V^{\times r}$ be an ordered r-tuple of elements. If $\{v_j\}_j$ is linearly dependent, then the r^2-tuples $(v_i^* v_j)_{ij}$ and $(v_j v_i^*)_{ij}$ cannot be jointly linearly independent.*

Proof: Since $\{v_j\}_j$ is linearly dependent, there exist $(\lambda_j)_j \in \mathbb{C}^r$ such that $\lambda_{j_0} \neq 0$ for some j_0 and $\Sigma_{j=1}^r \lambda_j v_j = 0$. Therefore also $\Sigma_{ij} \delta_{ii_0} \lambda_j (v_i^* v_j, v_j v_i^*) = 0$ for all i_0. □

IV. EXTREMAL STATES IN $\mathcal{C}(\rho_1, \rho_2)$

Let $\rho \in \mathcal{C}(\rho_1, \rho_2)$. In $\mathcal{H}_2$ consider an orthonormal basis of eigenvectors of ρ_2, i.e., $\rho_2 = \Sigma_i r_i |r_i\rangle\langle r_i|$. We identify the basis $\{|r_i\rangle\}_{i=1}^d$ of eigenvectors of ρ_2 with the canonical real basis of $\mathcal{H}_2 \simeq \mathbb{C}^d$. Further, we write

$$|\psi_+\rangle := \frac{1}{\sqrt{d}} \sum_i |r_i\rangle \otimes |r_i\rangle. \tag{2}$$

In the sequel it is always understood that the bijection between states and completely positive maps from Sec. II is with respect to this choice of the canonical basis and that the maximally entangled state in Eq. (1a) is the state from Eq. (2). To every state $\rho \in \mathcal{C}(\rho_1, \rho_2)$ Eq. (1b) gives a unique completely positive map Λ_ρ that satisfies

$$\Lambda_\rho(\mathbb{1}) = d\rho_1, \tag{3a}$$

$$\Lambda'_\rho(\mathbb{1}) = d\rho_2. \tag{3b}$$

Here Λ'_ρ denotes the canonical dualization of Λ_ρ defined by $\mathrm{tr}(\Lambda'_\rho(x)y) = \mathrm{tr}(x\Lambda_\rho(y))$ for all y. In terms of the Kraus representation of $\Lambda_\rho(x) = \Sigma_j V_j^\dagger x V_j$ the conditions (3a) and (3b) can be expressed as

$$\sum_j V_j^\dagger V_j = d\rho_1, \tag{4a}$$

$$\sum_j V_j V_j^\dagger = d\rho_2. \tag{4b}$$

We denote the set of all completely positive maps $\Lambda : \mathsf{L}(\mathcal{H}_2) \to \mathsf{L}(\mathcal{H}_1)$ satisfying the conditions (3a) and (3b) by $\mathrm{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$. It is clear that $\mathrm{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ is a convex set. The bijection described in (1a) and (1b) obviously respects the convex structure. In particular it establishes a bijection between $\mathcal{E}(\rho_1, \rho_2)$ and the extreme points of $\mathrm{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$.

We are now ready to state our main result.

Theorem 1: *Let* $\Lambda:\mathsf{L}(\mathcal{H}_2)\to\mathsf{L}(\mathcal{H}_1)$ *be a completely positive map in* $\mathrm{CP}(\mathcal{H}_2,\mathcal{H}_1,\rho_1,\rho_2)$. *Then* Λ *is extreme in* $\mathrm{CP}(\mathcal{H}_2,\mathcal{H}_1,\rho_1,\rho_2)$ *if and only if* Λ *admits an expression* $\Lambda(x)=\Sigma_j V_j^\dagger x V_j$ *for all* $x\in\mathsf{L}(\mathcal{H}_2)$, *where* V_i *are* $d\times d$ *matrices, satisfying the following conditions*:

(i) $\Sigma_j V_j^\dagger V_j = d\rho_1$,
(ii) $\Sigma_j V_j V_j^\dagger = d\rho_2$, *and*
(iii) $(V_i^\dagger V_j)_{ij}$ *and* $(V_j V_i^\dagger)_{ij}$ *are jointly linearly independent.*

For the proof of Theorem 1 we need the following lemma. For a proof see Remark 4 in Ref. 7.

Lemma 3: Let Λ *be a completely positive map with Kraus representation* $\Lambda(x)=\Sigma_j V_j^\dagger x V_j$ *with* $\{V_j\}_j^\ell$ *linearly independent. Let* $\{W_p\}_p^{\ell'}$ *be a class of* $d\times d$ *matrices, then* Λ *has the expression* $\Lambda(x)=\Sigma_p^{\ell'} W_p^\dagger x W_p$ *if and only if there exists an isometric* $\ell'\times\ell$ *matrix* $(\mu_{pi})_{pi}$, *such that* $W_p=\Sigma_i\mu_{pi}V_i$ *for all* p.

Proof of Theorem 1: The proof is an only slight modification and generalization of the proof of Theorem 5 in Ref. 7. We include it for the convenience of the reader. First assume that Λ is extremal in $\mathrm{CP}(\mathcal{H}_2,\mathcal{H}_1,\rho_1,\rho_2)$. We express Λ in Kraus form $\Lambda(x)=\Sigma_j V_j^\dagger x V_j$. Without loss of generality we can assume that $\{V_j\}_j$ is linearly independent.[7] Now suppose that $\Sigma\lambda_{ij}V_i^\dagger V_j=0$ and $\Sigma_{ij}\lambda_{ij}V_jV_i^\dagger=0$. We need to show that $\lambda_{ij}=0$. Without loss of generality we can assume that $(\lambda_{ij})_{ij}$ is a Hermitian matrix and $-\mathbb{1}\leqslant(\lambda_{ij})_{ij}\leqslant\mathbb{1}$ (for details see Ref. 7).

Define $\Phi_\pm:\mathsf{L}(\mathcal{H}_2)\to\mathsf{L}(\mathcal{H}_1)$ by $\Phi_\pm(x):=\Sigma_j V_j^\dagger x V_j\pm\Sigma_{ij}\lambda_{ij}V_i^\dagger x V_j$. Hence $\Phi_\pm(\mathbb{1})=d\rho_1$ and $\Phi'_\pm(\mathbb{1})=d\rho_2$ We set $\mathbb{1}+(\lambda_{ij})_{ij}=(\alpha_{ij})_{ij}^\dagger(\alpha_{ij})_{ij}\geqslant 0$ and $W_i:=\Sigma_j\alpha_{ij}V_j$ By direct computation, $\Phi_+(x)=\Sigma_i W_i^\dagger x W_i$. Hence Φ_+ is completely positive. Similarly it can be shown that Φ_- is completely positive. Since Λ is extremal, we find that $\Lambda=\Phi_+$. Therefore by Lemma 3 $(\alpha_{ij})_{ij}$ is an isometry and $\mathbb{1}+(\lambda_{ij})_{ij}=\mathbb{1}$. This implies $(\lambda_{ij})_{ij}=0$.

Now assume that Λ admits a representation of the form $\Lambda(x)=\Sigma_j V_j^\dagger x V_j$ for all $x\in\mathsf{L}(\mathcal{H}_2)$ where $\Sigma_j V_j^\dagger V_j=d\rho_1$, $\Sigma_j V_j V_j^\dagger=d\rho_2$, and $(V_i^\dagger V_j)_{ij}$ and $(V_jV_i^\dagger)_{ij}$ are jointly linearly independent. By Lemma 2 also $\{V_j\}_j$ is linearly independent. Now suppose $\Lambda=\frac{1}{2}(\Phi_1+\Phi_2)$ with $\Phi_1(x)=\Sigma_p W_p^\dagger x W_p$, $\Phi_2(x)=\Sigma_q Z_q^\dagger x Z_q$, and $\Sigma_p W_p^\dagger W_p=\Sigma_q Z_q^\dagger Z_q=d\rho_1$, $\Sigma_p W_p W_p^\dagger=\Sigma_q Z_q Z_q^\dagger=d\rho_2$ Since $\Lambda(x)=\frac{1}{2}\Sigma_p W_p^\dagger x W_p+\frac{1}{2}\Sigma_q Z_q^\dagger x Z_q$, it follows by Lemma 3 that W_p and Z_q can be expressed as a linear combination of the V_j. Let $W_p=\Sigma_i\mu_{pi}V_i$ for all p. Then $\Sigma_j V_j^\dagger V_j=\Sigma_p W_p^\dagger W_p=\Sigma_{pij}\mu_{pi}^*\mu_{pj}V_i^\dagger V_j$ and $\Sigma_j V_jV_j^\dagger=\Sigma_p W_pW_p^\dagger=\Sigma_{pij}\mu_{pi}^*\mu_{pj}V_jV_i^\dagger$. The joint linear independence of $(V_i^\dagger V_j)_{ij}$ and $(V_jV_i^\dagger)_{ij}$ implies $\Sigma_p\mu_{pi}^*\mu_{pj}=\delta_{ij}$. In other words $(\mu_{pi})_{pi}$ is an isometry. By Lemma 3, we conclude that $\Lambda=\Phi_1$ Thus Λ is extremal in $\mathrm{CP}(\mathcal{H}_2,\mathcal{H}_1,\rho_1,\rho_2)$. □

Corollary 1: Let $\rho\in\mathcal{C}(\rho_1,\rho_2)$. *Write the spectral decomposition of* ρ_2 *as* $\rho_2=\Sigma_i r_i|r_i\rangle\langle r_i|$. *Then* $\rho\in\mathcal{E}(\rho_1,\rho_2)$ *if and only if there exists a family of* $d\times d$ *matrices* $\{V_j\}$ *such that* ρ *can be expressed as*

$$\rho=\frac{1}{d}\sum_{ijk}V_j^\dagger|r_i\rangle\langle r_k|V_j\otimes|r_i\rangle\langle r_k|,$$

where $\{V_j\}_j$ *satisfy the following conditions:*

(i) $\Sigma_j V_j^\dagger V_j=d\rho_1$,
(ii) $\Sigma_j V_j V_j^\dagger=d\rho_2$, *and*
(iii) $(V_i^\dagger V_j)_{ij}$ *and* $(V_jV_i^\dagger)_{ij}$ *are jointly linearly independent.*

Remark 1: Suppose $\Lambda:\mathsf{L}(\mathcal{H}_2)\to\mathsf{L}(\mathcal{H}_1)$ *is completely positive. Then we can write* $\Lambda(x)=\Sigma_j V_j^\dagger x V_j$ *where* $\{V_j\}_{i=1}^\ell$ *is a class of linearly independent* $d\times d$ *matrices. Therefore* $\ell\leqslant d^2$. *If* Λ *is extremal in* $\mathrm{CP}(\mathcal{H}_2,\mathcal{H}_1,\rho_1,\rho_2)$, *we can conclude that* $\ell\leqslant\sqrt{2}d$. *Indeed,* $(V_i^\dagger V_j)_{ij}$ *and* $(V_jV_i^\dagger)_{ij}$ *are jointly linearly independent only if the cardinal number of* $\{V_i^\dagger V_j\oplus V_jV_i^\dagger\}_{ij}$ *is smaller than* $\dim(\mathsf{L}(\mathcal{H}_2))+\dim(\mathsf{L}(\mathcal{H}_1))$. *In other words,* $\ell^2\leqslant 2d^2$, i.e., $\ell\leqslant\sqrt{2}d$. *Parthasarathy found a slightly stronger bound in* Ref. 5. $\ell\leqslant\sqrt{2d^2-1}$ *It is not known whether this bound is tight.*

Remark 2: The bound $\ell\leqslant\sqrt{2}d$ *also implies that for any* $\rho\in\mathcal{E}(\rho_1,\rho_2)$ *we have* $\mathrm{rank}(\rho)\leqslant\sqrt{2}d$. *In all dimensions* $d\geqslant 2$ *this implies that any* $\rho\in\mathcal{E}(\rho_1,\rho_2)$ *is singular.*

V. EXAMPLES

A. A two dimensional example

Consider $\mathbb{C}^2\otimes\mathbb{C}^2$ and the convex set $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$ of states on $\mathbb{C}^2\otimes\mathbb{C}^2$ with maximally mixed marginals. This is a physically interesting example. It was previously studied in Ref. 5.

Assume that $\rho\in\mathcal{E}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$, i.e., that ρ is extremal in $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$. By Corollary 1 there is a linearly independent family of 2×2 matrices $\{V_i\}_{i=1}^{\ell}$ such that

$$\rho=\frac{1}{2}\sum_{ijk} V_j^\dagger|r_i\rangle\langle r_k|V_j\otimes|r_i\rangle\langle r_k|,$$

where $\{V_j\}$ satisfy the following conditions:

$$\sum_j V_j^\dagger V_j=\mathbb{1}_2, \tag{5a}$$

$$\sum_j V_j V_j^\dagger=\mathbb{1}_2, \tag{5b}$$

and where $(V_i^\dagger V_j)_{ij}$ and $(V_jV_i^\dagger)_{ij}$ are jointly linearly independent.

By Remark 1 either $\ell=1$ or $\ell=2$. In the case $\ell=1$, the matrix V_1 is unitary and it follows from Corollary 1 that ρ is equal to the projector onto the subspace spanned by a maximally entangled wave function.

Now consider the case $\ell=2$. Consider the singular value decompositions of V_1 and V_2, respectively, i.e., $V_1=\Sigma_{s=1}^2\sqrt{\nu_s(1)}|\varphi_s\rangle\langle\psi_s|$ and $V_2=\Sigma_{s=1}^2\sqrt{\nu_s(2)}|\varphi_s'\rangle\langle\psi_s'|$, where $\nu_s(i)$ are non-negative coefficients and where $\{|\psi_s\rangle\}_{s=1}^2$, $\{|\psi_s'\rangle\}_{s=1}^2$, $\{|\varphi_s\rangle\}_{s=1}^2$ and $\{|\varphi_s'\rangle\}_{s=1}^2$ are four orthonormal bases of $\mathbb{C}^2$. Then $V_1^\dagger V_1=\Sigma_{s=1}^2\nu_s(1)|\psi_s\rangle\langle\psi_s|$, $V_2^\dagger V_2=\Sigma_{s=1}^2\nu_s(2)|\psi_s'\rangle\langle\psi_s'|$, $V_1V_1^\dagger=\Sigma_{s=1}^2\nu_s(1)|\varphi_s\rangle\langle\varphi_s|$ and $V_2V_2^\dagger=\Sigma_{s=1}^2\nu_s(2)|\varphi_s'\rangle\langle\varphi_s'|$.

First consider the case of degenerate singular values, i.e., assume $\nu_1(1)=\nu_2(1)$. Then $V_1^\dagger V_1=V_1V_1^\dagger=\nu_1(1)\mathbb{1}$ and $V_2^\dagger V_2=V_2V_2^\dagger=\nu_1(2)\mathbb{1}$. Moreover, (5a) and (5b) imply that $\nu_1(1)=1-\nu_1(2)$. However, this implies that $(V_i^\dagger V_j)_{ij}$ and $(V_jV_i^\dagger)_{ij}$ are not jointly linearly independent. By Corollary 1 ρ is not extremal in $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$. This is a contradiction.

Second, consider the case of nondegenerate singular values, i.e., $\nu_1(1)\neq\nu_2(1)$. In this case Eqs. (5a) and (5b) imply that $\nu_s(1)=1-\nu_s(2)$, $|\varphi_s\rangle=|\varphi_s'\rangle$ and $|\psi_s\rangle=|\psi_s'\rangle$ for $s=1$, 2. By direct computation it is easily verfied that $V_1^\dagger V_2=V_2^\dagger V_1$ and $V_1V_2^\dagger=V_2V_1^\dagger$. This implies that $(V_i^\dagger V_j)_{ij}$ and $(V_jV_i^\dagger)_{ij}$ are not jointly linearly independent. Again by Corollary 1 ρ is not extremal in $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$. A contradiction.

We summarize our results in the following proposition.

Proposition 1: In dimension 2×2 the extremal states in $\mathcal{C}(\frac{1}{2}\mathbb{1},\frac{1}{2}\mathbb{1})$ are precisely the projectors onto the subspaces spanned by maximally entangled pure wave functions.

Proposition 1 has previously been found, using different methods, by Parthasarathy in Ref. 5.

B. A three dimensional example

From the preceding example it is clear that also in higher dimensions all projectors onto the subspaces spanned by maximally entangled wave functions are extremal elements in $\mathcal{C}((1/d)\mathbb{1},(1/d)\mathbb{1})$. However, in the present section we show that the extension of Proposition 1 to higher dimensions does not hold. In other words the set of extremal states in $\mathcal{C}((1/d)\mathbb{1},(1/d)\mathbb{1})$ is not exhausted by the projectors onto maximally entangled pure states. Here we use our characterization of extremal states in $\mathcal{C}((1/d)\mathbb{1},(1/d)\mathbb{1})$ to construct an explicit counterexample in dimension 3×3.

Denote by $\{|i\rangle\}_{i=1}^3$ the canonical real orthonormal basis of $\mathbb{C}^3$. Define the following operators:

$$V_1 = \frac{1}{\sqrt{2}}(|1\rangle\langle 1| + |2\rangle\langle 3|), \tag{6a}$$

$$V_2 = \frac{1}{\sqrt{2}}(|2\rangle\langle 2| + |3\rangle\langle 1|), \tag{6b}$$

$$V_3 = \frac{1}{\sqrt{2}}(|3\rangle\langle 3| + |1\rangle\langle 2|). \tag{6c}$$

By explicit calculation one checks that $\Sigma_{j=1}^3 V_j^\dagger V_j = \Sigma_j^3 V_j V_j^\dagger = \mathbb{1}$. Moreover,

$$V_1^\dagger V_2 = V_3 V_1^\dagger = \tfrac{1}{2}|3\rangle\langle 2|, \tag{7a}$$

$$V_1^\dagger V_3 = V_3 V_2^\dagger = \tfrac{1}{2}|1\rangle\langle 2|, \tag{7b}$$

$$V_2^\dagger V_3 = V_1 V_2^\dagger = \tfrac{1}{2}|1\rangle\langle 3|, \tag{7c}$$

$$V_2^\dagger V_1 = V_1 V_3^\dagger = \tfrac{1}{2}|2\rangle\langle 3|, \tag{7d}$$

$$V_3^\dagger V_1 = V_2 V_3^\dagger = \tfrac{1}{2}|2\rangle\langle 1|, \tag{7e}$$

$$V_2^\dagger V_2 = V_2 V_3^\dagger = \tfrac{1}{2}|3\rangle\langle 1|. \tag{7f}$$

Hence $\{V_i^\dagger V_j\}_{ij}$ and $\{V_j V_i^\dagger\}_{ij}$ are both linearly independent and thus by Lemma 1 jointly linearly independent. By Corollary 1 the state

$$\rho := \frac{1}{3}\sum_{ijk=1}^{3} V_j^\dagger |i\rangle\langle k| V_j \otimes |i\rangle\langle k| \tag{8}$$

is extremal in $\mathcal{C}(\frac{1}{3}\mathbb{1}, \frac{1}{3}\mathbb{1})$. An explicit calculation gives the following matrix representation of ρ in the canonical product basis in lexicographic order:

$$\rho = \frac{1}{6}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

This state is entangled but not maximally entangled and an extremal element of $\mathcal{C}(\frac{1}{3}\mathbb{1}, \frac{1}{3}\mathbb{1})$.

C. Higher dimensions

It is possible to construct counterexamples to Proposition 1 also in higher dimensions. For instance, consider $\mathbb{C}^2 \otimes \mathbb{C}^2$. We denote the canonical basis of $\mathbb{C}^4$ as usual by $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$. The three dimensional example above can be generalized to dimension 4×4 by letting

$$V_1 = \frac{1}{\sqrt{3}}(|1\rangle\langle 1| + |2\rangle\langle 4| + |3\rangle\langle 2|),$$

$$V_2 = \frac{1}{\sqrt{3}}(|2\rangle\langle 2| + |3\rangle\langle 1| + |4\rangle\langle 3|),$$

$$V_3 = \frac{1}{\sqrt{3}}(|3\rangle\langle 3| + |4\rangle\langle 2| + |1\rangle\langle 4|),$$

$$V_4 = \frac{1}{\sqrt{3}}(|4\rangle\langle 4| + |1\rangle\langle 3| + |2\rangle\langle 1|).$$

It is straightforward to show that both $(V_i^\dagger V_j)_{ij}$ and $(V_j V_i^\dagger)_{ij}$ are linearly independent families. Thus an analysis similar to the one given above shows that

$$\rho := \frac{1}{4}\sum_{ijk=1}^{4} V_j^\dagger |i\rangle\langle k| V_j \otimes |i\rangle\langle k| \tag{10}$$

is extremal in $\mathcal{C}(\frac{1}{4}\mathbb{1}, \frac{1}{4}\mathbb{1})$ but is not a maximally entangled pure state. It is easy to construct similar counterexamples also in higher dimensions. It seems therefore likely that there are counterexamples to Proposition 1 in all dimensions greater than 2.

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The Newtonian limit of the relativistic Boltzmann equation

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The relativistic Boltzmann equation for a constant differential cross section and with periodic boundary conditions is considered. The speed of light appears as a parameter $c > c_0$ for a properly large and positive c_0. A local existence and uniqueness theorem is proved in an interval of time independent of $c > c_0$ and conditions are given such that in the limit $c \to +\infty$ the solutions converge, in a suitable norm, to the solutions of the nonrelativistic Boltzmann equation for hard spheres. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1793328]

I. INTRODUCTION

Our purpose in this paper is to show that solutions of the relativistic Boltzmann equation are well-approximated by solutions of the classical (nonrelativistic) Boltzmann equation. A more precise statement will be given later in the Introduction.

The relativistic Boltzmann equation can be written in the form

$$\partial_t f + \hat{p} \cdot \nabla_x f = Q_{\mathrm{rel}}(f,f), \tag{1.1}$$

where the various symbols have the following meaning. $f = f(t,x,p)$ is the distribution function in phase-space of a single nondegenerate relativistic gas. $\hat{p} = cp/p_0$ is the relativistic velocity, with c denoting the speed of light and $y_0 = \sqrt{c^2 + |y|^2}$. The molecular rest-mass is set to unity and the convention for the signature of Minkowski's metric is $(+---)$, so that $p_0 = p^0$. Finally, Q_{rel} is the relativistic collision operator defined by

$$Q_{\mathrm{rel}}(f,g) = \int_{\mathbb{R}^3} \int_{S^2} \mathcal{K}_c(p,q,\omega)[f(p')g(q') - f(p)g(q)]\mathrm{d}\omega\, \mathrm{d}q. \tag{1.2}$$

In the previous definition, p', q' are the momenta after the elastic collision of two particles with pre-collisional momenta p, q. These quantities are subjected to the conservation of momentum and energy, which read as

$$p + q = p' + q', \quad \mathcal{E}_c(p) + \mathcal{E}_c(q) = \mathcal{E}_c(p') + \mathcal{E}_c(q'), \quad \mathcal{E}_c(y) = cy_0. \tag{1.3}$$

A solution of (1.3) can be represented as

$$p' = p - a(p,q,\omega)\omega, \quad q' = q + a(p,q,\omega)\omega, \tag{1.4}$$

where

$$a(p,q,\omega) = \frac{2(p_0 + q_0)[c^{-1}\omega \cdot (\hat{p} - \hat{q})]p_0 q_0}{(p_0 + q_0)^2 - [\omega \cdot (p + q)]^2}.$$

Using this representation, the relativistic collision kernel $\mathcal{K}_c$ takes the form

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$$\mathcal{K}_c(p,q,\omega) = 16\sigma(c^2+\mathfrak{g}^2)\frac{(p_0+q_0)^2|\omega\cdot(\hat{p}-\hat{q})|}{[(p_0+q_0)^2-(\omega\cdot(p+q))^2]^2}, \tag{1.5}$$

$$\mathfrak{g} = \frac{1}{\sqrt{2}}(p_0q_0 - p\cdot q - c^2)^{1/2}. \tag{1.6}$$

Here $\mathfrak{g}$ is a Lorentz invariant defined so that $-2\mathfrak{g}$ is the relative momentum in the center of mass system and σ denotes the differential cross section. In general σ is a function of $\mathfrak{g}$ and of a second Lorentz invariant quantity which in the center of mass system reduces to the cosine of the scattering angle of the collision. In this article the differential cross section is assumed to be constant. As usual, the local dependence on (t,x) in (1.2) is omitted. This formulation of the relativistic Boltzmann equation for $c=1$ is derived for instance in Refs. 6,7. We refer to Refs. 1,3,5,10 for more background on the subject.

In this paper, the solutions of (1.1) will be directly compared to the solutions of the classical Boltzmann equation for hard spheres, which is

$$\partial_t f_\infty + p\cdot\nabla_x f_\infty = Q_{\mathrm{cl}}(f_\infty, f_\infty), \tag{1.7}$$

where

$$Q_{\mathrm{cl}}(f,g) = d\int_{\mathbb{R}^3}\int_{S^2}|\omega\cdot(p-q)|[f(\overline{p})g(\overline{q}) - f(p)g(q)]\mathrm{d}\omega\,\mathrm{d}q. \tag{1.8}$$

The meaning of the various symbols in (1.7) is the same as in the relativistic case. The post-collisional momenta are now denoted by $\overline{p},\overline{q}$, the conservation of momentum and energy take the form $p+q=\overline{p}+\overline{q}$ and $\frac{1}{2}|p|^2+\frac{1}{2}|q|^2=\frac{1}{2}|\overline{p}|^2+\frac{1}{2}|\overline{q}|^2$, respectively, while the analog of (1.4) in the classical case is

$$\overline{p} = p - \omega\cdot(p-q)\omega, \quad \overline{q} = q + \omega\cdot(p-q)\omega. \tag{1.9}$$

The factor d in (1.8) is the differential cross section for hard spheres interaction, which is a constant with the same dimensions as σ, namely $[length]^2$. A standard mathematical reference for the classical Boltzmann equation is Ref. 4.

In this paper it is shown that there is a class of solutions to the relativistic Boltzmann equation which have a Newtonian limit, i.e., which tend to solutions of the classical Boltzmann equation (in the corresponding class) as the speed of light goes to infinity. For this purpose, the speed of light will be treated as a parameter $c>c_0$—where c_0 is a fixed and properly large positive constant—and the difference between the classical and the relativistic solution will be estimated as $c\to+\infty$. (No loss of generality arises in letting $c>c_0$, since only the limit behavior as $c\to+\infty$ is of interest here.) In order to obtain the correct Newtonian limit it is also necessary to relate the constants d and σ in a proper way. From (1.5) it follows that $\mathcal{K}_c(p,q,\omega)\to 4\sigma|\omega\cdot(p-q)|$ as $c\to+\infty$. This leads to *postulate* the relation $4\sigma=d$. By further choosing units such that $d=1$, the classical collision kernel reduces to $|\omega\cdot(p-q)|$, while the relativistic collision kernel becomes

$$\mathcal{K}_c(p,q,\omega) = 2(p_0q_0 - p\cdot q + c^2)\frac{(p_0+q_0)^2|\omega\cdot(\hat{p}-\hat{q})|}{[(p_0+q_0)^2-(\omega\cdot(p+q))^2]^2}. \tag{1.10}$$

The precise formulation of the result will be now given. The conditions on the distribution functions mentioned in the theorem are introduced thereafter. The symbol $\mathbb{T}^3$ denotes the three-torus and the norm $\|\ \|_{0,1}$ is defined as follows:

$$\|g(t)\|_{0,1} = \int_{\mathbb{R}^3}|g(t,p)|_0\mathrm{d}p, \quad |g(t,p)|_0 = \sup_{x\in\mathbb{T}^3}|g(t,x,p)|.$$

Theorem 1: *Let $f_\infty(t)$ be a solution of* (1.7) *which satisfies the properties (C1), (C2) and with initial datum $f_\infty^{\mathrm{in}} \in C^1$ such that $|\nabla_p f_\infty^{\mathrm{in}}|_0 \in L^1(\mathbb{R}^3)$. Let $f_c(t)$ be a solution of* (1.1), *depending on $c > c_0$, which satisfies the properties (R1)–(R3) and with the c-dependent initial datum f_c^{in}. Assume $\|f_\infty^{\mathrm{in}} - f_c^{\mathrm{in}}\|_{0,1} = O(c^{-1})$ as $c \to +\infty$. Then*

$$\lim_{c \to +\infty} \|f_\infty(t) - f_c(t)\|_{0,1} = 0, \quad t \in [0,T].$$

The following notation will be used. Given two functions g and h on $\mathbb{R}^n$ we write $g \lesssim h$ if the estimate $g \leqslant Dh$ holds for a positive constant D independent of $c > c_0$. The constant D may also depend on the length of some time interval $[0,T]$, in which case we write $g \lesssim h$ for $t \in [0,T]$. Whenever necessary or convenient, the constant D will be recovered in the computations.

The classes of solutions of the Boltzmann equations to be considered are defined by the following properties. In the classical case it is required that, in some interval $[0,T_1]$:

$$\text{(C1)}\ f_\infty \in C([0,T_1] \times \mathbb{T}^3 \times \mathbb{R}^3),$$

$$\text{(C2)}\ \exists\, \alpha_0 > 0 : f_\infty(t,x,p) \lesssim \exp(-\alpha_0 |p|^2), \quad t \in [0,T_1], \quad x \in \mathbb{T}^3, \quad p \in \mathbb{R}^3.$$

In the relativistic case let f_c denote a (one parameter family of) solution(s) of (1.1) and require that, for all $c > c_0$ and in some interval $[0,T_c]$,

$$\text{(R1)}\ f_c \in C([0,T_c] \times \mathbb{T}^3 \times \mathbb{R}^3),$$

$$\text{(R2)}\ \exists\, \beta_0 > 0 : f_c(t,x,p) \lesssim \exp[-\beta_0(\mathcal{E}_c(p) - c^2)], \quad t \in [0,T_c], \quad x \in \mathbb{T}^3, \quad p \in \mathbb{R}^3,$$

$$\text{(R3)}\ T_2 := \inf_{c > c_0} T_c > 0.$$

Let us briefly comment on the above conditions. The existence of solutions to the classical Boltzmann equation satisfying the properties (C1), (C2) is proved in Ref. 9—see also Refs. 2,8 for questions concerning the global existence of such solutions. A similar argument applies to the relativistic Boltzmann equation to prove the local existence and uniqueness of solutions satisfying (R1)—(R3). A short sketch of the proof is given in Sec. III to show that the property (R3) is satisfied. The latter is necessary for studying the Newtonian limit, since it assures that the existence interval of a solution of the relativistic Boltzmann equation does not shrink to zero as $c \to +\infty$. The time T in Theorem 1 is defined as the minimum between T_1 and T_2.

Note also that the assumption $x \in \mathbb{T}^3$ allows one to neglect technical difficulties not related to the problem under discussion, such us the choice of boundary or fall-off conditions. The generalization of the result when x lies in a region of $\mathbb{R}^3$ with a smooth boundary—or simply $x \in \mathbb{R}^3$—is not attempted here but it should not be too difficult.

II. PROOF OF THE MAIN THEOREM

The following lemma collects some estimates which are required in the proof of the main theorem.

Lemma 1: The following estimates hold:

$$\text{(a)}\ |q' - \overline{q}| + |p' - \overline{p}| \lesssim \frac{(|q| + |p|)^3}{c^2},$$

$$\text{(b)}\ |\mathcal{K}_c(p,q,\omega) - |\omega \cdot (p-q)|| \lesssim \frac{(1 + |p| + |q|)^9}{c^2},$$

$$\text{(c)} \quad \iint \mathcal{K}_c(p,q,\omega)\exp\left[-\beta_0(\mathcal{E}_c(q)-c^2)\right]\mathrm{d}\omega\,\mathrm{d}q \lesssim (1+|p|).$$

Proof: From (1.4) and (1.9) we have

$$|q'-\overline{q}| = |p'-\overline{p}| = |\omega\cdot(p-q)-a|,$$

and a computation shows that

$$\omega\cdot(p-q)-a = \frac{\omega\cdot(p+q)(|p|^2-|q|^2+(\omega\cdot p)^2-(\omega\cdot q)^2)}{(p_0+q_0)^2-[\omega\cdot(p+q)]^2} = \frac{\text{Num}}{\text{Den}}.$$

Moreover,

$$\begin{aligned}\text{Den} &= 2c^2+|p|^2+|q|^2+2\sqrt{c^2+|p|^2}\sqrt{c^2+|q|^2}-(\omega\cdot p)^2-(\omega\cdot q)^2-2(\omega\cdot p)(\omega\cdot q)\\ &\geqslant 2c^2+2\sqrt{c^2+|p|^2}\sqrt{c^2+|q|^2}-2|p||q| \geqslant 2c^2+\frac{c^2(c^2+|p|^2+|q|^2)}{\sqrt{c^2+|p|^2}\sqrt{c^2+|q|^2}}. \qquad (2.11)\end{aligned}$$

In particular $\text{Den} > 2c^2$ and since $\text{Num} \lesssim (|p|+|q|)^3$, the estimate (a) is proved. Next, from (1.10) we have

$$\begin{aligned}|\mathcal{K}_c(p,q,\omega)-|\omega\cdot(p-q)|| &\lesssim \left|\frac{2(p_0q_0-p\cdot q+c^2)(p_0+q_0)^2(\omega\cdot\hat{p}-\omega\cdot\hat{q})}{[(p_0+q_0)^2-(\omega\cdot(p+q))^2]^2}-\omega\cdot(p-q)\right|\\ &\lesssim |\omega\cdot p|\left|\frac{2c(p_0q_0-p\cdot q+c^2)(p_0+q_0)^2}{p_0[(p_0+q_0)^2-(\omega\cdot(p+q))^2]^2}-1\right|+(q\leftrightarrow p), \qquad (2.12)\end{aligned}$$

where $(q\leftrightarrow p)$ denotes the expression obtained by exchanging p and q in the first term. Recall the definition of "Den" in (2.11). The first term in (2.12) is estimated as

$$\begin{aligned}&\frac{|p|}{p_0(\text{Den})^2}|2c(p_0q_0+c^2)(p_0+q_0)^2-2cp\cdot q(p_0+q_0)^2-p_0(p_0+q_0)^4-p_0[\omega\cdot(p+q)]^4\\ &\quad+2p_0(p_0+q_0)^2[\omega\cdot(p+q)]^2|\\ &\lesssim \frac{|p|}{p_0(\text{Den})^2}|(p_0+q_0)^2(2cp_0q_0+2c^3-p_0^3-p_0q_0^2-2p_0^2q_0)+c^3(1+|p|+|q|)^5|.\end{aligned}$$

Here $p_0(\text{Den})^2 \geqslant 4c^5$ and so to prove (b) one needs to estimate only the expression containing the fifth order powers of c, which is given by

$$\mathcal{P}(p,q) = (p_0+q_0)^2[2cp_0q_0+2c^3-p_0^3-p_0q_0^2-2p_0^2q_0].$$

We have

$$\frac{|\mathcal{P}(p,q)|}{p_0(\text{Den})^2} \lesssim \frac{(1+|p|+|q|)^2}{c^3}|2cp_0q_0+2c^3-p_0^3-p_0q_0^2-2p_0^2q_0|.$$

Using that

$$2cp_0q_0-2p_0^2q_0 = \frac{2p_0q_0}{c+p_0}(c^2-p_0^2) \leqslant 2c|p|^2(1+|q|),$$

$$c^3-p_0q_0^2 = c^2(c-p_0)-c|q|^2(1+|p|) \leqslant \frac{c^2(c^2-p_0^2)}{c+p_0}+c|q|^2(1+|p|) \leqslant c(|p|^2+|q|^2)(1+|p|),$$

$$c^3 - p_0^3 = c^3\left(1 - \left(1 + \frac{|p|^2}{c^2}\right)^{3/2}\right) \leqslant c(1+|p|)^6,$$

and repeating the argument for the second term in (2.12) concludes the proof of (b). To prove (c) consider the following pointwise estimate on $\mathcal{K}_c$:

$$\begin{aligned}\mathcal{K}_c &\lesssim \frac{cp_0q_0}{(\mathrm{Den})^2}(p_0^2+q_0^2+2p_0q_0)(|p|/p_0+|q|/q_0)\\ &\lesssim \frac{c}{(\mathrm{Den})^2}[|p|p_0^2q_0+|p|q_0^3+2|p|p_0q_0^2+p_0^3|q|+p_0|q|q_0^2+2p_0^2q_0|q|]\\ &\lesssim \frac{c^4}{(\mathrm{Den})^2}(1+|p|)(1+|q|^2)^{3/2}\left(1+\frac{|p|^2}{c^2}\right).\end{aligned}$$

From (2.11) it follows that

$$\mathrm{Den} \geqslant c^2\frac{\sqrt{1+|p|^2/c^2}}{\sqrt{1+|q|^2/c^2}}.$$

Moreover, since $\sqrt{c^4+c^2|q|^2}-c^2 \geqslant \frac{1}{2}(\sqrt{1+|q|^2}-1)$, then

$$\exp[-\beta_0(\mathcal{E}_c(q)-c^2)] \lesssim \exp\left[-\frac{\beta_0}{2}\sqrt{1+|q|^2}\right], \tag{2.13}$$

and so

$$\iint \mathcal{K}_c(p,q,\omega)e^{-\beta_0(\mathcal{E}_c(q)-c^2)}\,\mathrm{d}\omega\,\mathrm{d}q \lesssim (1+|p|)\int (1+|q|^2)^{5/2}e^{(-\beta_0/2)\sqrt{1+|q|^2}}\mathrm{d}q,$$

by which the claim follows. □

Remark 1: The simple estimate (2.13) will be often used in the sequel for the same purpose as in Lemma 1, i.e., to obtain an estimate independent of $c > c_0$ of the integrals containing the factor $\exp[-\beta_0(\mathcal{E}_c(q)-c^2)]$.

In the class of solutions that we are considering, the distribution functions satisfy the Boltzmann equations in the mild form

$$f_c(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t Q_{\mathrm{rel}}(s,x+\hat{p}(s-t),p)\mathrm{d}s, \tag{2.14}$$

$$f_\infty(t,x,p) = f_\infty^{\mathrm{in}}(x-pt,p) + \int_0^t Q_{\mathrm{cl}}(s,x+p(s-t),p)\mathrm{d}s. \tag{2.15}$$

We use this representation to estimate the following quantity:

$$F_\eta[f_\infty] = \int \sup_{|h|<\eta}|f_\infty(p+h)-f_\infty(p)|_0\mathrm{d}p, \quad \eta > 0.$$

Lemma 2: For all $\eta_0, T > 0$, $\eta \in [0,\eta_0]$ *and* $t \in [0,T]$, *there exists a positive constant* $C = C(T,\eta_0,\alpha_0)$ *such that*

$$F_\eta[f_\infty] \leqslant C\sqrt{F_\eta[f_\infty^{\mathrm{in}}]}.$$

Proof: By (1.8),

$$Q_{\mathrm{cl}}(f_\infty,f_\infty)(p+h)=\iint |\omega\cdot(p-q)|[f_\infty(\overline{p}+h)f_\infty(\overline{q}+h)-f_\infty(p+h)f_\infty(q+h)]\mathrm{d}\omega\,\mathrm{d}q.$$

Therefore by (2.15),

$$\begin{aligned}|f_\infty(p+h)-f_\infty(p)|_0 \le |f_\infty^{\mathrm{in}}(p+h)-f_\infty^{\mathrm{in}}(p)|_0 &+\int_0^t\iint |\omega\cdot(p-q)||f_\infty(q)|_0|f_\infty(p+h)\\ &-f_\infty(p)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}s+\int_0^t\iint |\omega\cdot(p-q)||f_\infty(\overline{q})|_0|f_\infty(\overline{p}+h)\\ &-f_\infty(\overline{p})|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}s+\int_0^t\iint |\omega\cdot(p-q)||f_\infty(p+h)|_0|f_\infty(q+h)\\ &-f_\infty(q)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}s+\int_0^t\iint |\omega\cdot(p-q)||f_\infty(\overline{p}+h)|_0|f_\infty(\overline{q}+h)\\ &-f_\infty(\overline{q})|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}s.\end{aligned}$$

Hence changing to the post-collisional variables,

$$\begin{aligned}F_\eta[f_\infty] &\le F_\eta[f_\infty^{\mathrm{in}}]+\int_0^t\iiint |\omega\cdot(p-q)|e^{-\alpha_0|q|^2}\sup_{|h|<\eta}|f_\infty(p+h)-f_\infty(p)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}s\\ &\quad+\int_0^t\sup_{|h|<\eta}\iiint |\omega\cdot(p-h-q)|e^{-\alpha_0|p|^2}|f_\infty(q+h)-f_\infty(q)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}s\\ &= F_\eta[f_\infty^{\mathrm{in}}]+\mathrm{A}+\mathrm{B}.\end{aligned}$$

For $R>0$ we write

$$\begin{aligned}\mathrm{A} &\le \int_0^t\int_{|p|\le R}(1+|p|)\sup_{|h|<\eta}|f_\infty(p+h)-f_\infty(p)|_0\,\mathrm{d}p\,\mathrm{d}s+\int_0^t\int_{|p|>R}(1+|p|)\\ &\quad\times\exp[-\alpha_0(|p|^2-2\eta|p|)]\mathrm{d}p\,\mathrm{d}s\le (1+R)\int_0^t F_\eta[f_\infty](s)\mathrm{d}s+Ce^{-\alpha_0R^2/2}.\end{aligned}$$

The estimate for B is obtained in the same way,

$$\mathrm{B}\le[1+(R+\eta_0)]\int_0^t F_\eta[f_\infty](s)\mathrm{d}s+Ce^{-\alpha_0R^2/2}.$$

Hence, finally,

$$F_\eta[f_\infty](t)\le F_\eta[f_\infty^{\mathrm{in}}]+Ce^{-\alpha_0R^2/2}+[1+(R+\eta_0)]\int_0^t F_\eta[f_\infty](s)\mathrm{d}s.$$

Choose R such that $e^{-\alpha_0R^2/2}=(1+F_{\eta_0}[f_\infty^{\mathrm{in}}])^{-1}F_\eta[f_\infty^{\mathrm{in}}]$, so that

$$F_\eta[f_\infty](t)\le Ce^{-\alpha_0R^2/2}+[1+(R+\eta_0)]\int_0^t F_\eta[f_\infty](s)\mathrm{d}s.$$

Hence, by the Grönwall Lemma,

$$F_\eta[f_\infty](t) \lesssim C\exp\left[-\frac{\alpha_0 R^2}{2}+(R+\eta_0)t\right] \lesssim C\exp\left(-\frac{\alpha_0 R^2}{4}\right)\sup_{R>0}\exp\left[-\frac{\alpha_0 R^2}{4}+(R+\eta_0)T\right]$$
$$\lesssim C\exp\left(-\frac{\alpha_0 R^2}{4}\right)=C\sqrt{F_\eta[f_\infty^{\mathrm{in}}]}.$$

□

Note also that for an initial datum as given in Theorem 2 the estimate $F_\eta[f_\infty^{\mathrm{in}}]\lesssim\eta$ holds. Then Lemma 2 implies

$$F_\eta[f_\infty]\lesssim\sqrt{\eta}. \tag{2.16}$$

The next goal is to estimate the difference $Q_{\mathrm{rel}}-Q_{\mathrm{cl}}$ in the norm $\|\ \|_{0,1}$.

Lemma 3: The following estimate holds:

$$\|Q_{\mathrm{rel}}(t)-Q_{\mathrm{cl}}(t)\|_{0,1}\lesssim c^{-1}(\log c)^{5/4}+\exp[-\beta_0(\sqrt{c^4+c^2\log c}-c^2)]+\exp[-\alpha_0\log c]$$
$$+\sqrt{\log c}\|f_\infty(t)-f_c(t)\|_{0,1}.$$

Proof: From (1.2) and (1.8),

$$\|Q_{\mathrm{rel}}(t)-Q_{\mathrm{cl}}(t)\|_{0,1}\lesssim\iiint|\mathcal{K}_c(p,q,\omega)[f(p')f(q')-f(p)f(q)]-|\omega\cdot(p-q)|[f_\infty(\overline{p})f_\infty(\overline{q})$$
$$-f_\infty(p)f_\infty(q)]|_0\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p=\iiint_{|p|+|q|\le\sqrt{\log c}}\cdots+\iiint_{|p|+|q|>\sqrt{\log c}}\cdots.$$

Observing the conservation of energy and using (c) of Lemma 1, the integral in the exterior region is dominated by

$$\iiint_{|p|+|q|>\sqrt{\log c}}\mathcal{K}_c(p,q,\omega)\exp[-\beta_0(\mathcal{E}_c(p)+\mathcal{E}_c(q)-2c^2)]\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p+\int\int\int_{|p|+|q|>\sqrt{\log c}}|\omega\cdot(p-q)|$$
$$\times\exp[-\alpha_0(|p|^2+|q|^2)\mathrm{d}p\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p\lesssim\exp[-\beta_0(\sqrt{c^4+c^2\log c}-c^2)]+\exp(-\alpha_0\log c).$$

For the integral over the interior part consider the splitting,

$$\iiint_{|p|+|q|\le\sqrt{\log c}}\cdots\lesssim\mathrm{I}+\mathrm{II}+\cdots+\mathrm{VIII},$$

where

$$\mathrm{I}=\iiint_{|p|+|q|\le\sqrt{\log c}}|f_c(p)|_0|f_c(q)|_0||\omega\cdot(p-q)|-\mathcal{K}_c|\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{II}=\iiint_{|p|+|q|\le\sqrt{\log c}}|f_\infty(\overline{p})|_0|f_\infty(\overline{q})|_0||\omega\cdot(p-q)|-\mathcal{K}_c|\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{III}=\iiint_{|p|+|q|\le\sqrt{\log c}}|\omega\cdot(p-q)||f_\infty(p)|_0|f_\infty(q)-f_c(q)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{IV}=\iiint_{|p|+|q|\le\sqrt{\log c}}|\omega\cdot(p-q)||f_c(q)|_0|f_\infty(p)-f_c(p)|_0\,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{V} = \iiint_{|p|+|q|\leqslant\sqrt{\log c}} \mathcal{K}_c |f_c(p')|_0 |f_c(q') - f_\infty(q')|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{VI} = \iiint_{|p|+|q|\leqslant\sqrt{\log c}} \mathcal{K}_c |f_c(p')|_0 |f_\infty(q') - f_\infty(\overline{q})|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{VII} = \iiint_{|p|+|q|\leqslant\sqrt{\log c}} \mathcal{K}_c |f_\infty(\overline{q})|_0 |f_c(p') - f_\infty(p')|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p,$$

$$\mathrm{VIII} = \iiint_{|p|+|q|\leqslant\sqrt{\log c}} \mathcal{K}_c |f_\infty(\overline{q})|_0 |f_\infty(p') - f_\infty(\overline{p})|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p.$$

It follows directly from the estimate (b) of Lemma 1 that

$$\mathrm{I} + \mathrm{II} \lesssim c^{-2}.$$

The integrals III and IV satisfy the estimate

$$\mathrm{III} + \mathrm{IV} \lesssim \int_{|q|\leqslant\sqrt{\log c}} (1 + |q|)|f_\infty(q) - f_c(q)|_0 \,\mathrm{d}q \lesssim (1 + \sqrt{\log c})\|f_\infty(t) - f_c(t)\|_{0,1}.$$

In the integral V we change to the post-collisional variables. Since $\mathcal{K}_c(p,q,\omega)\mathrm{d}q\,\mathrm{d}p = \mathcal{K}_c(p',q',\omega)\mathrm{d}q'\,\mathrm{d}p'$ and, by (1.3), $|p'|+|q'| \leqslant 4\sqrt{\log c}$ for $|p|+|q| \leqslant \sqrt{\log c}$, then

$$\mathrm{V} \lesssim \iiint_{|p|+|q|\leqslant 4\sqrt{\log c}} \mathcal{K}_c(p,q,\omega)|f_c(p)|_0 |f_c(q) - f_\infty(q)|_0 \mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p \lesssim \sqrt{\log c}\|f_\infty(t) - f(t)\|_{0,1}.$$

For the integral VI we have, by the estimate (a) of Lemma 1, Lemma 2, and (2.16),

$$\begin{aligned}
\mathrm{VI} &\lesssim \iiint_{|p|+|q|\leqslant\sqrt{\log c}} \mathcal{K}_c |f_c(p')|_0 \sup_{|h|\leqslant(\log c)^{3/2}/c^2} |f_\infty(q'+h) - f_\infty(q')|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p \\
&\lesssim \iiint_{|p|+|q|\leqslant 4\sqrt{\log c}} \mathcal{K}_c e^{-\beta_0(\mathcal{E}(p)-c^2)} \sup_{|h|\leqslant(\log c)^{3/2}/c^2} |f_\infty(q+h) - f_\infty(q)|_0 \,\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}p \\
&\lesssim \int_{|q|\leqslant 4\sqrt{\log c}} (1 + |q|) \sup_{|h|\leqslant(\log c)^{3/2}/c^2} |f_\infty(q+h) - f_\infty(q)|_0 \\
&\lesssim \sqrt{\log c} F_{(\log c)^{3/2}/c^2}[f_\infty] \lesssim c^{-1}(\log c)^{5/4}.
\end{aligned}$$

It is now straightforward to estimate VII and VIII; therefore we merely state the result

$$\mathrm{VII} + \mathrm{VIII} \lesssim c^{-1}(\log c)^{5/4} + \sqrt{\log c}\|f_\infty(t) - f(t)\|_{0,1}.$$

Collecting the various bounds, the claim follows. □

The proof of Theorem 1 is now almost complete. From (2.14) and (2.15) we have

$$\|f_c(t) - f_\infty(t)\|_{0,1} \leqslant \|f_c^{\mathrm{in}} - f_\infty^{\mathrm{in}}\|_{0,1} + \int_0^t \|Q_{\mathrm{rel}}(s) - Q_{\mathrm{cl}}(s)\|_{0,1}.$$

Using Lemma 3 and applying Grönwall's inequality one obtains, for $t \in [0,T]$,

$$\|f_c(t)-f_\infty(t)\|_{0,1} \lesssim \|f_c^{\mathrm{in}}-f_\infty^{\mathrm{in}}\|_{0,1} e^{D\sqrt{\log c}} + c^{-1}(\log c)^{5/4} e^{D\sqrt{\log c}} + \exp[-\beta_0\sqrt{c^4+c^2\log c}+\beta_0 c^2 + D\sqrt{\log c}] + \exp[-\alpha_0 \log c + D\sqrt{\log c}].$$

The expression on the right hand side tends to zero as $c\to\infty$ and this concludes the proof of Theorem 1.

III. EXISTENCE IN A UNIFORM SHORT TIME INTERVAL

The equation to be studied reads explicitly as

$$f_c(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t [Q_{\mathrm{rel}}^+(f_c,f_c) - Q_{\mathrm{rel}}^-(f_c,f_c)](s,x-\hat{p}(t-s),p)\mathrm{d}s, \tag{3.17}$$

where Q_{rel}^+ and Q_{rel}^- refer to the gain and loss part of the relativistic collision operator (1.2), respectively. Given two functions $u_0(t)$ and $l_0(t)$, the approximation sequences $\{u_n\}_{n\geqslant 0}$, $\{l_n\}_{n\geqslant 0}$ are defined recursively by

$$l_{n+1}(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t [Q_{\mathrm{rel}}^+(l_n,l_n) - Q_{\mathrm{rel}}^-(l_{n+1},u_n)](s,x-\hat{p}(t-s),p)\mathrm{d}s,$$

$$u_{n+1}(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t [Q_{\mathrm{rel}}^+(u_n,u_n) - Q_{\mathrm{rel}}^-(u_{n+1},l_n)](s,x-\hat{p}(t-s),p)\mathrm{d}s,$$

and as in Lemma 5.1 in Ref. 9 one can prove the following.

Proposition 1: Assume the beginning condition is satisfied:

$$0 \leqslant l_0(t) \leqslant l_1(t) \leqslant u_1(t) \leqslant u_0(t); \tag{3.18}$$

then $0\leqslant l_n(t)\leqslant l_{n+1}(t)\leqslant u_{n+1}(t)\leqslant u_n(t)$ *for all* $n\geqslant 0$.

Next assume that $u_0 \lesssim \exp[-\beta_0(\mathcal{E}_c(p)-c^2)]$; it follows by the previous proposition that u_n, l_n are also dominated by $\exp[-\beta_0(\mathcal{E}_c(p)-c^2)]$. Moreover $l_n(t)\uparrow l(t), u_n(t)\downarrow u(t)$, and $|u(t)|, |l(t)| \lesssim \exp[-\beta_0(\mathcal{E}_c(p)-c^2)]$. All these preliminary facts are valid for any collision kernel. When the latter is given by (1.10) one can also prove that (i) $u(t)=l(t)$ and (ii) the limit is a continuous solution of (3.17). The second statement is an obvious consequence of the first one, so only the proof of (i) will be given. By the dominated convergence theorem, $u(t), l(t)$ satisfy

$$l(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t [Q_{\mathrm{rel}}^+(l,l) - Q_{\mathrm{rel}}^-(l,u)](s,x-\hat{p}(t-s),p)\mathrm{d}s,$$

$$u(t,x,p) = f_c^{\mathrm{in}}(x-\hat{p}t,p) + \int_0^t [Q_{\mathrm{rel}}^+(u,u) - Q_{\mathrm{rel}}^-(u,l)](s,x-\hat{p}(t-s),p)\mathrm{d}s.$$

Estimating the difference $u(t)-l(t)$ in the norm $\|\ \|_{0,1}$ and using (c) of Lemma 1 we get

$$\begin{aligned}\|u(t)-l(t)\|_{0,1} &\lesssim \int_0^t \int (1+|p|)|u(s,p)-l(s,p)|_0\,\mathrm{d}p\,\mathrm{d}s \\ &\lesssim \int_0^t \int_{|p|\leqslant R} (1+|p|)|u(s,p)-l(s,p)|_0\,\mathrm{d}p\,\mathrm{d}s \\ &\quad + \int_0^t \int_{|p|>R} (1+|p|)\exp[-\beta_0(\sqrt{c^4+c^2|p|^2}-c^2)]\mathrm{d}p\,\mathrm{d}s\end{aligned}$$

$$\lesssim (1+R)\int_0^t \|u(s)-l(s)\|_{0,1} + te^{(-\beta_0/2)(\sqrt{c^4+c^2R^2}-c^2)}.$$

Hence by the Grönwall inequality

$$\|u(t)-l(t)\|_{0,1} \lesssim te^t \exp\left[DtR - \frac{\beta_0}{2}\sqrt{c^4+R^2c^2} + \frac{\beta_0}{2}c^2\right],$$

for some constant D independent of the speed of light. For $t\in[0,T]$ and $c>\sqrt{48}DT/\beta_0 := c_0$, this implies

$$\|u(t)-l(t)\|_{0,1} \lesssim e^{(-DTR)}, \quad \text{for } R > \frac{12DT}{\beta_0},$$

and so the claim $u(t)=l(t)$, for $t\in[0,T]$ and $c>c_0$ follows by letting $R\to+\infty$.

It remains to show that the beginning condition (3.18) is attained in some interval $[0,T_c]$ satisfying the property (R3) (indeed it will be shown that T_c is independent of $c>1$). Following Ref. 9 we choose $l_0\equiv 0$ and $u_0(t)$ of the form

$$u_0(t) = \omega(t)e^{-\beta(t)[\mathcal{E}_c(p)-c^2]},$$

where β and ω are positive functions and $\beta(0)=\beta_0$. We also set $\omega_0=\omega(0)$. Then u_1 are l_1 are given by

$$l_1(t,x,p) = f_c^{\text{in}}(x-\hat{p}t,p)\exp\left[-\omega(t)\iint \mathcal{K}_c(q,p,\omega)e^{-\beta(t)[\mathcal{E}_c(q)-c^2]}\mathrm{d}\omega\,\mathrm{d}q\right],$$

$$u_1(t,x,p) = f_c^{\text{in}}(x-\hat{p}t,p) + \int_0^t \omega(s)^2 \iint \mathcal{K}_c(q,p,\omega)e^{-\beta(s)[\mathcal{E}_c(p)+\mathcal{E}_c(q)-2c^2]}\mathrm{d}\omega\,\mathrm{d}q\,\mathrm{d}s.$$

Hence $0\leqslant l_1(t)\leqslant u_1(t)$. Moreover,

$$u_1(0)-u_0(0) = f_c^{\text{in}} - \omega_0 e^{-\beta_0[\mathcal{E}_c(p)-c^2]} \lesssim e^{-\beta_0[\mathcal{E}_c(p)-c^2]} - \omega_0 e^{-\beta_0[\mathcal{E}_c(p)-c^2]} \leqslant 0,$$

for ω_0 large enough and

$$\frac{d}{dt}[u_1(t,x+\hat{p}t,p)-u_0(t,x+\hat{p}t,p)] \leqslant [D(1+|p|)\omega^2 - \dot{\omega} + \omega\dot{\beta}(\sqrt{c^4+c^2|p|^2}-c^2)] \times \exp[-\beta(t)(\mathcal{E}_c(p)-c^2)],$$

where an upper dot has been used to denote differentiation in time. Hence the proof of (3.18) is complete if one can choose ω,β such that

$$D(1+|p|)\omega^2 - \dot{\omega} + \omega\dot{\beta}(\sqrt{c^4+c^2|p|^2}-c^2) \leqslant 0. \tag{3.19}$$

Let

$$\omega(t) = \frac{\omega_0}{1-3D\omega_0 t}, \quad \beta(t) = \beta_0 + \tfrac{2}{3}\log(1-3D\omega_0 t),$$

so that $\dot{\omega}=3D\omega^2$ and $\dot{\beta}=-2D\omega$. Here $t\in[0,T]$, where $T=(6D\omega_0)^{-1}(1-e^{-(3/2)\beta_0})$ so that ω and β are well-defined positive functions in $[0,T]$. In this way, the left hand side of (3.19) is dominated by $-D\omega^2\leqslant 0$ and this concludes the proof of the following

Theorem 2: *Let $f_c^{\text{in}}\in C(\mathbb{T}^3\times\mathbb{R}^3)$ such that $f_c^{\text{in}}\lesssim\exp[-\beta_0(\mathcal{E}_c(p)-c^2)]$. There exist $c_0,T>0$ such that for all $c>c_0$, the relativistic Boltzmann equation, Eq. (1.1) with $\mathcal{K}_c(p,q,\omega)$ given by*

(1.5) and initial datum f_c^{in}*, has a unique solution* $f \in C([0,T]\times\mathbb{T}^3\times\mathbb{R}^3)$ *which also satisfies* $f \lesssim \exp[-\beta_0(\mathcal{E}_c(p)-c^2)]$*; in particular the class of solutions satisfying (R1)–(R3) is not empty.*

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Exact series solution to the two flavor neutrino oscillation problem in matter

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In this paper, we present a real nonlinear differential equation for the two flavor neutrino oscillation problem in matter with an arbitrary density profile. We also present an exact series solution to this nonlinear differential equation. In addition, we investigate numerically the convergence of this solution for different matter density profiles such as constant and linear profiles as well as the Preliminary Reference Earth Model describing the Earth's matter density profile. Finally, we discuss other methods used for solving the neutrino flavor evolution problem. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1793330]

I. INTRODUCTION

In general, there are several phenomena and processes in physics, but also in other fields of science such as chemistry, that can be described in terms of a system with two (quantum mechanical) states and a time-dependent Hamiltonian, i.e., so-called two-level systems—neutrino oscillations with two flavors being one such system. Other representatives of such systems are, for example, a spin $1/2$ particle in a time-dependent electromagnetic field having the states "spin up" and "spin down," K^0-$\overline{K}^0$ mixing, a Josephson device, nuclear magnetic resonance used for encoding bits of information (i.e., quantum bits for a quantum computer), the left and right chirality states of molecules in chemistry, etc. The problem of neutrino oscillations in matter, which we are concerned with in this paper, is mathematically equivalent to a spin $1/2$ particle in a magnetic field that is constant in one direction, zero in another direction, and time-dependent in the last direction.[1]

Neutrino oscillations have recently been extensively studied in the literature[2–6] and they act as the most plausible description of both the solar[2] and atmospheric[3] neutrino problems. At an early stage, neutrino oscillations were mainly investigated with two flavors and without including matter effects. Nowadays, we know that there are at least three neutrino flavors and that matter effects are important. For example, in matter, the so-called Mikheyev–Smirnov–Wolfenstein (MSW) effect[7,8] can take place, which is an amplifying resonant effect due to the presence of matter. However, in most situations, neutrino oscillations can be effectively investigated with two flavors, since the leptonic mixing in the 1–3 sector is indeed small,[4,5] leading to the fact that the full three flavor scenario can be decoupled into two effective two flavor scenarios, each of which can be studied separately.

In this paper, we present an exact analytic solution to the two flavor neutrino oscillation problem in matter. Since there are many similar two-level systems, as discussed above, our solution will also be interesting and applicable to this kind of system. However, before we proceed to present our solution, we will give a brief overview of what has previously been done in this field. Note that this overview is not presented in chronological order. First, in Refs. 9,10, the neutrino flavor evolution has been investigated by a discretization of the effective potential.

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Second, exact solutions exist for a number of specific effective potentials.[7,11–13] Third, in Refs. 14,15, the evolution was studied by using an adiabatic approximation. Fourth, approximate solutions valid for small effective potentials have recently been studied in detail.[16] Finally, there have also been other attempts to write the evolution in terms of a second order nonlinear ordinary differential equation.[17] However, this has been done for the neutrino oscillation probability amplitudes and not for the neutrino oscillation probabilities. The advantage of working with a nonlinear differential equation for the oscillation probability rather than a linear system of differential equations for the probability amplitudes is that we only have one real variable instead of two complex variables. The disadvantage is that the resulting differential equation is nonlinear.

This paper is organized as follows. In Sec. II, the neutrino flavor evolution in matter with two flavors is studied and a second order nonlinear ordinary differential equation for the neutrino oscillation probability is derived. Then, in Sec. III, we perform series expansions of both the neutrino oscillation probability and the effective potential in order to solve the differential equation presented in Sec. II. Next, in Sec. IV, we continue by studying the numerical convergence of the solution for a number of different effective potentials and baselines. In Sec. V, we present a brief summary of other methods for solving the neutrino evolution in matter. Finally, in Sec. VI, we summarize our results and give our conclusions.

II. NEUTRINO FLAVOR EVOLUTION IN MATTER

When neutrinos propagate in matter, neutrino flavors are affected differently by coherent forward scattering against the matter constituents. Assuming that there are no sterile neutrinos, the effect of matter is to add an effective potential to ν_e; this effective potential is given by $V(t) = \sqrt{2}G_F N_e(t)$, where G_F is the Fermi coupling constant and $N_e(t)$ is the electron number density.

In the two flavor case, the time evolution of a neutrino state $|\nu(t)\rangle = (|\nu_e(t)\rangle |\nu_x(t)\rangle)^T$ is given by

$$\mathrm{i}\frac{\mathrm{d}|\nu(t)\rangle}{\mathrm{d}t} = (H_{\mathrm{vac}} + H_{\mathrm{mat}}(t))|\nu(t)\rangle, \tag{1}$$

where $H_{\mathrm{vac}} = U\,\mathrm{diag}(m_1^2, m_2^2)U^\dagger/2E$ is the free Hamiltonian in vacuum, $H_{\mathrm{mat}}(t) = \mathrm{diag}(V(t), 0)$ is the addition to the free Hamiltonian due to matter effects, and

$$U = \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \tag{2}$$

is the leptonic mixing matrix in vacuum. Here $c \equiv \cos\theta, s \equiv \sin\theta$, and θ is the leptonic mixing angle. Adding or subtracting terms proportional to the unity operator to the total Hamiltonian $H(t) = H_{\mathrm{vac}} + H_{\mathrm{mat}}(t)$ will only contribute with an overall phase to the neutrino state $|\nu(t)\rangle$, and thus, does not affect the neutrino oscillation probabilities. Using this fact, the total Hamiltonian may be written as

$$H(t) = \frac{1}{2}\begin{pmatrix} V(t) - \dfrac{\Delta m^2}{2E}\cos 2\theta & \dfrac{\Delta m^2}{2E}\sin 2\theta \\ \dfrac{\Delta m^2}{2E}\sin 2\theta & \dfrac{\Delta m^2}{2E}\cos 2\theta - V(t) \end{pmatrix} = \frac{1}{2}\left[\sigma_1 \frac{\Delta m^2}{2E}\sin 2\theta + \sigma_3\left(V(t) - \frac{\Delta m^2}{2E}\cos 2\theta\right)\right], \tag{3}$$

where the σ_i's ($i = 1, 2, 3$) are the Pauli matrices and $\Delta m^2 \equiv m_2^2 - m_1^2$ is the mass squared difference between the two mass eigenstates in vacuum.

The density matrix $\rho(t) = |\nu(t)\rangle\langle\nu(t)|$ can be parametrized as $\rho(t) = (\mathbf{1} + \mathbf{S}(t)\cdot\boldsymbol{\sigma})/2$, where $\mathbf{1}$ is the unity matrix, $\boldsymbol{\sigma} = (\sigma_1\ \sigma_2\ \sigma_3)^T$ is the vector of Pauli matrices, and $\mathbf{S}(t)$ is a vector such that $\mathbf{S}(t)^2 = 1$. Differentiating the density matrix ρ with respect to time t, the equation of motion for $\mathbf{S}(t)$ becomes

$$\dot{\mathbf{S}}(t) = \mathbf{S}(t) \times \mathbf{B}(t), \tag{4}$$

where $\mathbf{B}(t) \equiv g\mathbf{e}_1 + f(t)\mathbf{e}_3$ and we have defined $g \equiv -\sin(2\theta)\Delta m^2/2E$ and $f(t) \equiv \cos(2\theta)\Delta m^2/2E - V(t)$. Note that g is independent of time t. The probability of neutrinos produced as ν_e to oscillate into ν_x (where ν_x is some linear combination of ν_μ and ν_τ) is now given by $P(\nu_e \to \nu_x) \equiv P_{ex} = (1 - S_3(t))/2$. With the parametrization

$$\mathbf{S}(t) \equiv \begin{pmatrix} \sin\alpha\cos\beta \\ \sin\alpha\sin\beta \\ \cos\alpha \end{pmatrix}, \tag{5}$$

where $\alpha = \alpha(t)$ and $\beta = \beta(t)$, we obtain the following nonlinear system of ordinary differential equations:

$$\dot{\beta} = g\cot\alpha\cos\beta - f, \tag{6}$$

$$\dot{\alpha} = g\sin\beta. \tag{7}$$

Eliminating β from the above expressions, we obtain the differential equation

$$[\ddot{\alpha} + \cot\alpha(\dot{\alpha}^2 - G)]^2 = F(t)(G - \dot{\alpha}^2), \tag{8}$$

where $F(t) \equiv f(t)^2$ and $G \equiv g^2$.

Now, we make the substitution $p = S_3(t) = \cos\alpha$ after which Eq. (8) becomes

$$(\ddot{p} + Gp)^2 = F(t)[G(1 - p^2) - \dot{p}^2]. \tag{9}$$

Note that $F = 0$ corresponds to the so-called MSW resonance condition $\cos(2\theta)\Delta m^2/2E = V$. In this case, Eq. (9) takes the simple form

$$\ddot{p} + Gp = 0, \tag{10}$$

with the trivial solutions $p = A\cos(gt) + B\sin(gt)$ just as expected.

In general, the expression for P_{ex} is known for constant matter density and is given by[7]

$$P_{ex} = \sin^2(2\tilde{\theta})\sin^2\left(\frac{\Delta\tilde{m}^2}{4E}t\right) = \frac{G}{F+G}\sin^2\left(\frac{\sqrt{F+G}}{2}t\right), \tag{11}$$

where $\tilde{\theta}$ is the effective leptonic mixing angle in matter and $\Delta\tilde{m}^2$ is the effective mass squared difference in matter. Using that $p = 1 - 2P_{ex}$, it is a matter of trivial computation to show that this is the solution to Eq. (9) with constant F, which corresponds to any constant matter density.

In the three (n) flavor case, the density matrix can be parametrized by four $[2(n-1)]$ real parameters. If we would adopt our approach to the three (n) flavor case, then we would end up with a system of seven $[2(n-1)]$ nonlinear ordinary differential equations, which, in principle, can be solved in a manner analogous to the one described above for the two flavor case.

III. SERIES EXPANSION OF THE SOLUTION

In order to solve the propagation of neutrinos in matter with arbitrary density profiles, we adopt the method of series expansion. We suppose that neutrinos are produced as ν_e and then propagate through a given effective potential $V(t)$; this gives the initial values $p(0) = 1$ and $\dot{p}(0) = 0$. Series expanding the effective potential $V(t)$ and the quantity $p(t)$, we obtain the following expressions:

$$V(t) = \sum_{n=0}^{\infty} V_n t^n, \tag{12}$$

$$p(t) = \sum_{n=0}^{\infty} p_n t^n, \tag{13}$$

where the coefficients V_n $(n=0,1,\ldots)$ define the effective potential and where we wish to compute the coefficients p_n $(n=0,1,\ldots)$. By using the relation between f and V, we obtain

$$f(t) = \sum_{n=0}^{\infty} f_n t^n, \quad f_n = \delta_{n0}\frac{\Delta m^2}{2E}\cos(2\theta) - V_n, \tag{14}$$

$$F(t) = \sum_{n=0}^{\infty} F_n t^n, \quad F_n = \sum_{k=0}^{n} f_k f_{n-k}. \tag{15}$$

Inserting the above expressions into Eq. (9) and identifying terms of the same order in t gives the relation

$$F_n G = \sum_{s=0}^{n} (s+2)(s+1)(n-s+2)(n-s+1)p_{s+2}p_{n-s+2} + \sum_{s=0}^{n} [2G(s+2)(s+1)p_{s+2}p_{n-s} + G^2 p_s p_{n-s}] + \sum_{s=0}^{n} F_{n-s}\sum_{k=0}^{s} G p_k p_{s-k} + (k+1)(s-k+1)p_{k+1}p_{s-k+1}. \tag{16}$$

For $n=0$ with the given initial conditions, Eq. (16) is a second order equation in p_2 with $p_2 = -G/2$ as a double root. This corresponds well to the fact that at $t=0$, the right-hand side of Eq. (9) vanishes for the given initial conditions and we are left with the equation $\ddot{p}(0) = -Gp(0)$. For $n=1$, Eq. (16) is trivially fulfilled (given the assumed initial conditions, terms with p_{n+2} will appear with the prefactor $Gp_0 + 2p_2$ only), while the solution to the equation for $n=2$ is simply $p_3 = 0$.

Also the solution for $n=3$ is now trivially fulfilled, since the terms including p_{n+1} also cancel for $n \geqslant 3$. For $n=4$, the equation is a second order equation in p_4 with the solutions

$$p_4 = \frac{G^2}{24} \text{ and } p_4 = \frac{G(G+F_0)}{24}. \tag{17}$$

Of these two solutions, only the latter will be a solution to our problem; this is easily checked by inserting the known solution in the case of constant effective potential from Eq. (11).

For $n \geqslant 5$, Eq. (16) is now linear in p_n. For $n \geqslant 6$, we obtain a solution for p_n in terms of lower order p_k, G, and F_s, where $k < n$ and $s \leqslant n-4$. This expression is the following recurrence relation:

$$p_n = -\frac{1}{G(n^2-3n+2)F_0}\Bigg[F_1\sum_{s=1}^{n-2}(s+1)(n-s)p_{s+1}p_{n-s} + G(G+F_0)\sum_{s=2}^{n-2}p_s p_{n-s} + F_0\sum_{s=3}^{n-3}(s+1)(n-s+1)p_{s+1}p_{n-s+1} + 2G\sum_{s=2}^{n-4}(s+2)(s+1)p_{n-s}p_{s+2} + G\sum_{s=4}^{n-1}F_{n-s}\sum_{k=0}^{s}p_k p_{s-k} + \sum_{s=4}^{n-2}F_{n-s}\sum_{k=0}^{s}(k+1)(s-k+1)p_{k+1}p_{s-k+1} + \sum_{s=3}^{n-3}(n-s+2)(n-s+1)(s+2)(s+1)p_{n-s+2}p_{s+2}\Bigg]. \tag{18}$$

For the first few coefficients we obtain

$$p_0 = 1,$$

$$p_1 = 0,$$

$$p_2 = -\frac{G}{2},$$

$$p_3 = 0,$$

$$p_4 = \frac{G}{24}(G + F_0),$$

$$p_5 = \frac{GF_1}{48},$$

$$p_6 = -\frac{G(4G^2F_0 + 8GF_0^2 + 4F_0^3 + F_1^2 - 36F_0F_2)}{2880F_0},$$

$$p_7 = -\frac{G(8GF_0^2F_1 + 8F_0^3F_1 - F_1^3 + 4F_0F_1F_2 - 48F_0^2F_3)}{5760F_0^2},$$

$$p_8 = \frac{G}{645120F_0^3}\{48GF_0^5 + 16F_0^6 - 63F_1^4 + 16F_0^4(3G^2 - 34F_2) + 312F_0F_1^2F_2 + 8F_0(GF_1^2 - 30F_2^2 - 48F_1F_3) + 4F_0^3[4(G^3 - 34GF_2 + 240F_4) - 53F_1]\}. \quad (19)$$

As can be observed by setting $F_k = 0$, the solution for $F = 0$, i.e., at the MSW resonance, is just the series expansion for $p = \cos(gt)$, which is clearly as expected.

IV. CONVERGENCE OF THE SOLUTION

In order to test our solution, we perform a number of numerical tests. First of all, we give an overview of how we approximate the electron number density (i.e., in principle, the effective potential) by a polynomial. Then, we proceed by confirming that our solution really converges nicely towards the simple trigonometric function that is the exact solution for a constant electron number density. In this case, we also study the convergence of the energy dependence of the neutrino oscillation probability $P_{ex}(L)$ for a baseline of $L = 3000$ km. After the constant electron number density case, we investigate the case of a linear effective potential, and finally, we study the case of the Preliminary Reference Earth Model (PREM).[18]

In the numerical calculations, we have used the mixing angle $\theta = 13°$ and the mass squared difference $\Delta m^2 = 2 \times 10^{-3}$ eV^2.[19] The value of θ approximately corresponds to the upper limit on the leptonic mixing angle θ_{13} from the CHOOZ experiment with $\Delta m^2 = 2 \times 10^{-3}$ eV^2.[5] The reason to use this particular choice of parameters is that θ_{13} and the large mass squared difference give the main effects to neutrino oscillations from ν_e into other flavors for the baselines and energies we have studied (for $L = 3000$ km and $E = 1$ GeV, the neutrino oscillations governed by the small mass squared difference contribute with an approximate addition of 0.05 to the neutrino oscillation probability P_{ex}, for shorter baselines and higher energies, this effect decreases); see, for example, Ref. 20. The reason for using the upper bound value for the mixing angle θ and not some smaller value is that we wish to study the behavior of our solution rather than to make any precise predictions about the neutrino oscillation probabilities.

A. Series expansion of the effective potential

In order to use the series solution, which was obtained in the previous section, we will need the coefficients V_n. In general, for a given baseline length L, the effective potential $V(t)$ can be expanded in terms of Legendre polynomials, i.e.,

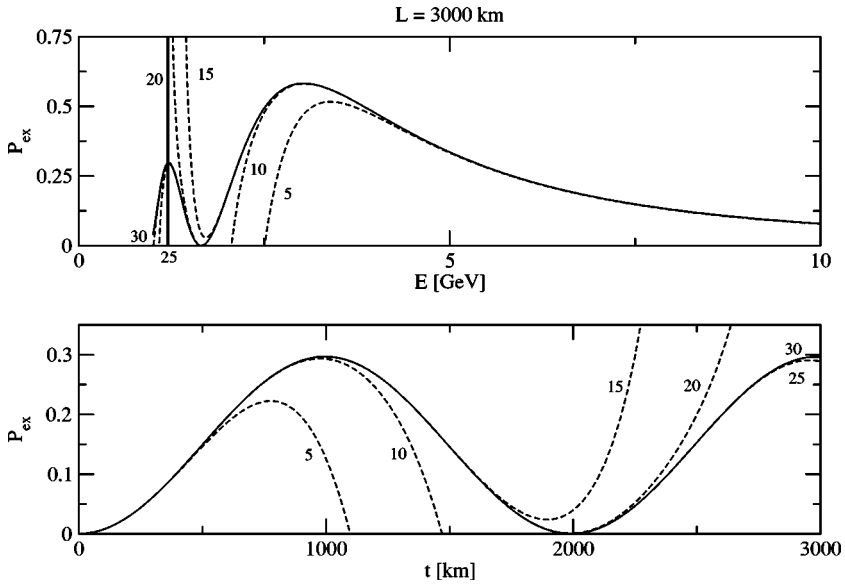

FIG. 1. The neutrino oscillation probability P_{ex} as a function of energy and time, respectively. Upper panel: The convergence of the energy spectrum given by our series expansion for a constant electron number density profile with $N_e = N_{e,\mathrm{core}}/3$. Lower panel: The convergence of the series expansion for $E = 1.2$ GeV, corresponding to the bold line in the energy spectrum. The solid curves correspond to the exact solutions and the dashed curves correspond to the series expansion. The numbers correspond to the number of terms used in the series expansion. The solid vertical line in the upper panel corresponds to the energy used for the lower panel.

$$V(x) = \sum_{n=0}^{\infty} c_n P_n(x), \quad P_n(x) = \frac{1}{n!\,2^n}\frac{\mathrm{d}^n}{\mathrm{d}x^n}[(x^2-1)^n], \quad c_n = \frac{2n+1}{2}\int_{-1}^{1} V(x)P_n(x)\mathrm{d}x, \tag{20}$$

where $x \equiv 2t/L - 1$. For numerical treatments, we cannot use the entire expansion in Legendre polynomials because of finite computer memory and finite computer time. However, if we assume that the coefficients c_n are negligible for $n > N$, where N is some integer, then we have a polynomial approximation,

$$V(x) \simeq \sum_{n=0}^{N} c_n P_n(x), \tag{21}$$

of the effective potential. Clearly, given any polynomial $V(t)$, it is a trivial matter to extract the coefficients V_n. This approach turns out to be quite handy in the case of the PREM profile, which is discussed below.

B. Constant matter density

The first case we study numerically is the case of a constant effective potential. We use the baseline length $L = 3000$ km and the electron number density $N_e = N_{e,\mathrm{core}}/3$, where $V_{\mathrm{core}} = \sqrt{2}G_{\mathrm{F}}N_{e,\mathrm{core}} \simeq 5.6 \times 10^{-19}$ MeV corresponds to a matter density of about 13 g/cm^3, which is the maximum matter density in the Earth's core.[18] In this case, the coefficients V_n are easily obtained as $V_0 = V(t)$ and $V_n = 0$ for $n > 0$. Since the exact solution to this problem is known,[7] we focus on the convergence of our solution for P_{ex}, both in the energy spectrum and the time evolution. The numerical results are shown in Fig. 1. In this figure, we can observe that approximately 20 terms are needed to reconstruct one period of oscillation and that the convergence is indeed the same as for a simple trigonometric function.

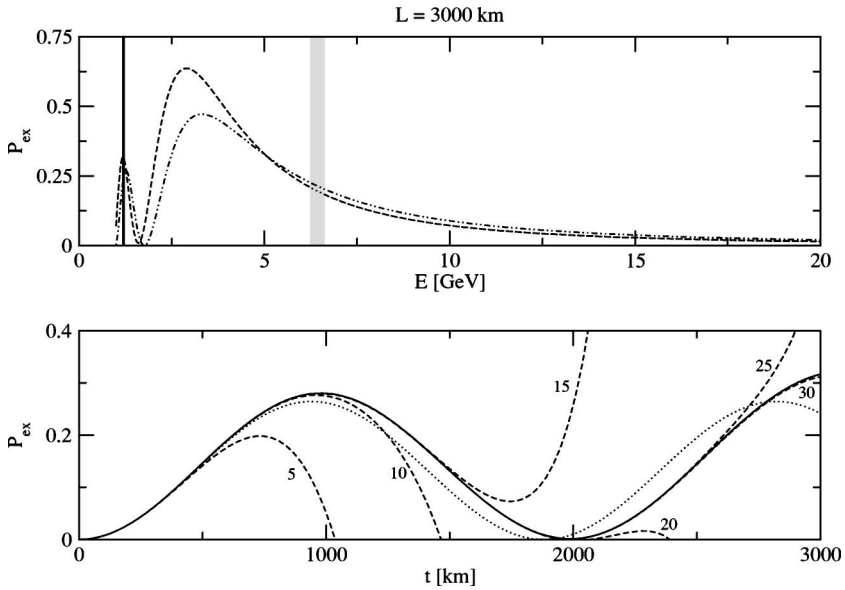

FIG. 2. The energy spectrum of the neutrino oscillation probability P_{ex} for a linear profile (upper panel) with $N_e = N_{e,\mathrm{core}}(1+t/L)/4$ along with the convergence of the solution for $E=1.2$ GeV (lower panel). In the energy spectra, the dotted curve corresponds to the numerical solution for the given profile, the dashed curve corresponds to our series solution, where we have included the first 35 terms, and the dash–dotted curve corresponds to an approximation of constant matter density. The solid vertical line corresponds to the energy used in the lower panel and the series solution is not plotted in the shaded region where it breaks down numerically. In the time evolution plot, the solid curve corresponds to the numerical solution, the dotted curve corresponds to the approximation of constant matter density, the dashed curves correspond to our series solution for different numbers of included terms, and the numbers correspond to the number of terms used for each of these curves.

C. Linearly varying matter density

Now, we turn our interest towards the case of a linearly varying effective potential. In particular, we study a baseline of $L=3000$ km, where the electron number density is given by $N_e(t)=N_{e,\mathrm{core}}(t/L+1)/4$. As in the case of constant effective potential, it is again easy to obtain the coefficients V_n from our equation for $V(t)$. Performing the numerical calculations results in Fig. 2. In this figure, we have excluded the plot for our solution in the shaded region, which roughly corresponds to an energy equal to the resonance energy of the effective potential $V=V_0$, where the solution breaks down numerically. The reason for this breakdown can be found in Eq. (18), where we repeatedly divide by F_0. For the resonance energy corresponding to $V=V_0$, we have $F_0 \sim 0$, which leads to large absolute values of numbers that should add up to a number between zero and one. Due to finite machine precision, we have numerical errors as a result.

Apart from neutrino energies near the resonance energy, we can observe that we again obtain a nice convergence of both the energy spectrum and the time evolution, where we reproduce one full oscillation by approximately 20 terms of our series expansion. It should be pointed out that this case of linearly varying matter density has no known application to experiments and only serves as an illustrative example.

D. PREM profile

For the PREM electron number density profile, which is the interesting profile in, for example, long-baseline neutrino oscillation experiments, we use the expansion in Legendre polynomials and truncate the series using $N=2$ for definiteness. In effect, this corresponds to projecting the function $V(t)$, which is an element in the vector space of real functions on the interval $[0,L]$, onto the subspace of second order polynomial functions on $[0,L]$, using the inner product

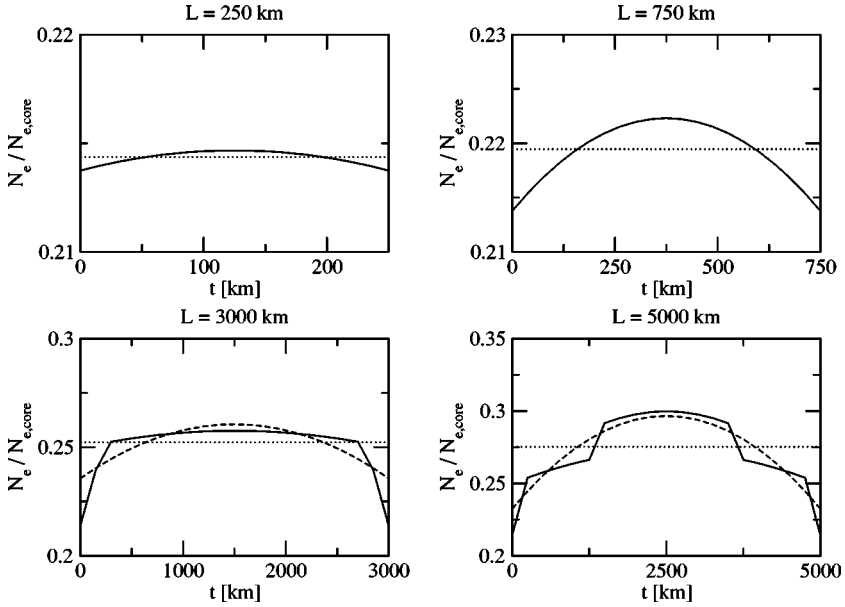

FIG. 3. The matter density profiles for different baseline lengths L according to the PREM. The solid curves are the exact profiles, the dashed curves are profiles approximated by a second order polynomial, and the dotted lines are the average matter densities, i.e., the matter density of approximations using constant electron number density. For $L=250$ km and 750 km the exact profiles and the approximations using a second order polynomial are practically the same and as a result they are not distinguishable in the figure.

$$\langle f,g\rangle = \int_0^L f(x)g(x)\mathrm{d}x. \tag{22}$$

In Fig. 3, we plot the electron number density profiles for the baseline lengths $L=250$ km, 750 km, 3000 km, and 5000 km along with the second order polynomial approximations and the constant approximations. In Fig. 4, we plot the energy spectra and time evolution at $E=1.2$ GeV for a baseline of $L=3000$ km for the PREM profile. Again, our solution is not plotted in the shaded region in which it breaks down numerically for the same reasons as discussed previously. In this case, it is apparent that if the number of terms used in the series expansion is large enough, our solution is a significant improvement from the constant matter density approximation.

Clearly, the approximation of using a second order polynomial for the electron number density gives a very good reproduction of the numerical solution (which uses the profiles obtained from the PREM). As can be seen in the time evolution plot, the error made is barely noticeable until approximately one and a half oscillations, i.e., for lower neutrino energies if the baseline length L is kept fixed. This is in good agreement with the results obtained in Ref. 21, where the effective potential is expanded in a Fourier series, as well as Ref. 22, which shows that details of the effective potential that are smaller than the oscillation length cannot be resolved by neutrino oscillations. As noticed in both of the earlier cases, about 20 terms are needed in the series expansion in order to reproduce one full oscillation.

For the PREM profile, we are also interested in a number of other baseline lengths. In particular, in Fig. 5, we plot the energy spectra for the baseline lengths $L=250$ km, 750 km, 3000 km, and 5000 km. For the baseline lengths $L=250$ km and 750 km, there is no noticeable difference between the numerical solution, our exact solution, and the approximation using constant electron number density. This is to be expected as the electron number density does not vary significantly for these baseline lengths (see Fig. 3). However, for both $L=3000$ km and 5000 km, we do observe a difference between the constant electron number density approximations and the other two solutions. Again, we can conclude that the approximation with a second order polyno-

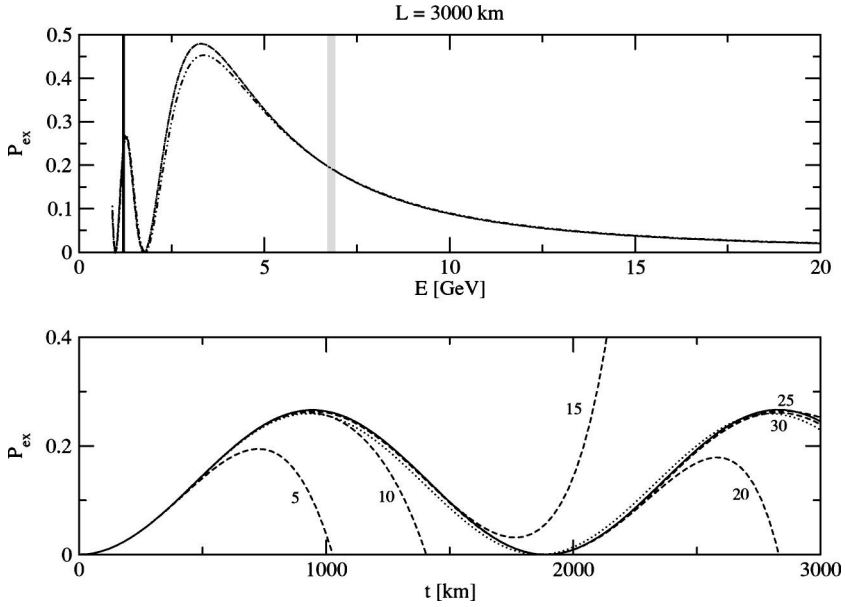

FIG. 4. The energy spectrum for the neutrino oscillation probability P_{ex} using 35 terms of our series solution (upper panel) and the convergence of the time evolution for $E=1.2$ GeV (lower panel). Here we assume a baseline of $L=3000$ km and using the PREM profile for the electron number density. In the energy spectrum, the dashed curve corresponds to the numerical solution using the PREM profile, the dotted curve corresponds to our series solution, and the dash-dotted curve corresponds to the approximation using constant matter density. The solid vertical line corresponds to the energy used in the lower panel and the series solution is not plotted in the shaded region where it breaks down numerically. In the time evolution plot, the solid curve corresponds to the numerical solution, the dotted curve to the solution for the constant matter density approximation, the dashed curves correspond to our series solution using different numbers of terms, and the numbers correspond to the number of terms used for each of these curves.

mial for the electron number density agrees remarkably well with the numerical calculation using the profile obtained directly from the PREM. Note that the comparison of the energy spectra for different matter density profiles and baselines has been studied before.[23]

For baselines longer than $L=5000$ km, the region near the resonance for $V=V_0$ tends to expand and ruin the numerical convergence of our solution. Also, this region expands if we include more terms of the series expansion. For the baseline lengths below $L=5000$ km, this can be somewhat compensated by using fewer terms of the series expansion for high energies to avoid the numerical cancellation effects and more terms for lower energies to obtain a nice convergence.

V. OTHER METHODS OF SOLVING THE NEUTRINO FLAVOR EVOLUTION

In general, there have been numerous methods on how to solve the problem of neutrino flavor evolution in matter.[7,9–17] First of all, there is the obvious formal solution using a time-ordered exponential, i.e.,

$$|\nu(t)\rangle = T\left[\exp\left(-\mathrm{i}\int_0^t H(\tau)\mathrm{d}\tau\right)\right]|\nu(0)\rangle. \tag{23}$$

This solution is exact, but it is not very helpful in actual calculations due to the nature of the time-ordered exponential. A way of solving this problem is to use a discretization of the effective potential.[9,24] The effective potential is then divided into a finite number of layers with constant effective potentials (i.e., constant electron number density), which approximate a given effective potential. Clearly, when the number of layers goes to infinity, one regains the time-ordered exponential.

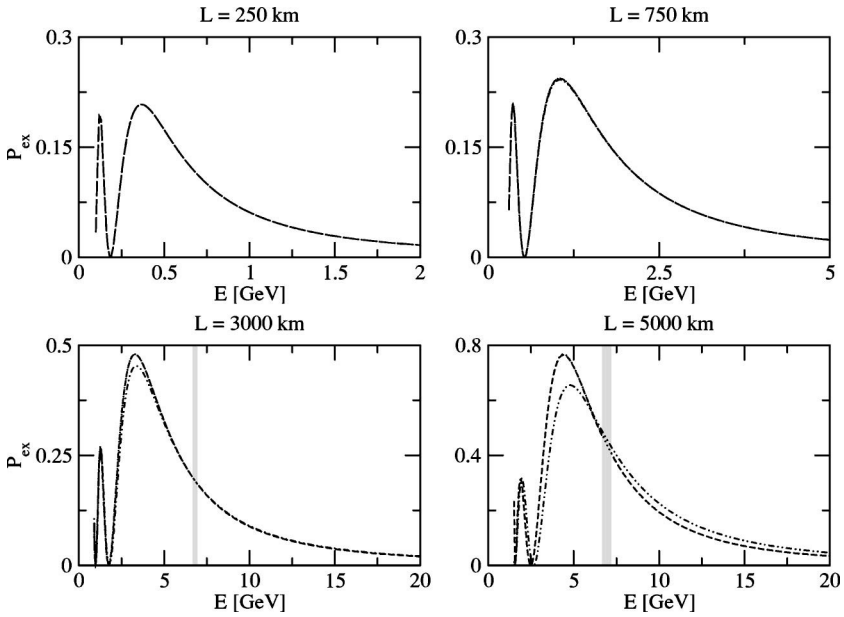

FIG. 5. The energy spectra of the neutrino oscillation probability P_{ex} for different baselines using the PREM profile for the electron number density. Again, we have used 35 terms from our series solution for each of these energy spectra and the dashed curves correspond to the numerical solutions, the dotted curves correspond to our series solution, and the dash-dotted curves correspond to the constant density approximations. The series solution is not plotted in the shaded regions where it breaks down numerically.

There is also the pure numerical approach to the problem, where the neutrino flavor evolution is easily solved numerically for any effective potential. While this gives the possibility of actually calculating numerical values for the neutrino oscillation probabilities, it does not offer any insight into how these probabilities vary with different parameters.

In addition, the neutrino flavor evolution can be analytically solved for some specific effective potentials. Examples are the constant (two flavors[7] and three flavors[11]), linearly[12] and exponentially[13] varying effective potentials.

Moreover, a widely used solution is the adiabatic solution,[14,15] where the effective potential is assumed to change slowly, so that there are no transitions between different matter eigenstates of the full Hamiltonian. This approximation can be derived by, for example, using the Wentzel–Kramers–Brillouin (WKB) method,[15] where also higher order corrections due to nonadiabatic transitions can be calculated.

There have also been earlier efforts to write the neutrino evolution equations as ordinary nonlinear differential equations; see, for example, Ref. 17. However, such equations have generally been complex differential equations for the probability amplitudes and not, as in the present case, real differential equations for the probabilities. Also, the solutions in such cases have been made for special cases of the effective potential and not as series solutions valid for all effective potentials.

Lately, approximate solutions, valid when the effective potential $V \ll \Delta m^2/(2E)$, have been presented[16] and applied to oscillations of solar neutrinos and the solar neutrino day–night effect. However, these solutions are not valid for the baseline lengths and neutrino energies which we have treated numerically.

VI. SUMMARY AND CONCLUSIONS

We have shown that solving the general problem of two flavor neutrino oscillations with an arbitrary effective potential is equivalent with solving the nonlinear ordinary differential equation,

$$(\ddot{p} + Gp)^2 = F(t)[G(1 - p^2) - \dot{p}^2], \tag{24}$$

where $G \equiv [\Delta m^2/(2E)]^2 \sin^2(2\theta), F(t) \equiv [\Delta m^2 \cos(2\theta)/(2E) - V(t)]^2$, and the neutrino oscillation probability P_{ex} is given by

$$P_{ex} = \frac{1}{2}(1 - p). \tag{25}$$

We have presented an exact solution [see Eqs. (18) and (19)] to this equation by adopting the method of series expansion of both the solution and the effective potential $V(t)$ and demonstrated the numerical convergence of this solution for a number of different effective potentials. In all cases investigated, about 20 terms in the series expansion are required to reproduce one period of oscillation. We have also seen that for the neutrino energies and baselines considered, the energy spectra of the neutrino oscillation probability is well reproduced by approximating the effective potential by a second order polynomial.

ACKNOWLEDGMENTS

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The asymptotic behavior of the stochastic Ginzburg–Landau equation with multiplicative noise

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The asymptotic behavior of the stochastic Ginzburg–Landau equation is studied. We obtain the stochastic Ginzburg–Landau equation as a finite-dimensional random attractor. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1794365]

I. INTRODUCTION

Let us consider the following stochastic Ginzburg–Landau equation perturbed by a multiplicative white noise of Itô form:

$$du = (\lambda + i\alpha)\Delta u\, dt + \nu u\, dt - (k + i\beta)|u|^2 u\, dt + \sigma u\, dW(t). \tag{1}$$

As one of the nonlinear Schrodinger equation, it can be found in many areas of physics and chemistry (Ref. 9). The white noise described by a Wiener process $W(t)$ results from the fact that small irregularity has to be taken account in some circumstances. Due to the special linear multiplicative noise, the equation (1) can be reduced to an equation with random coefficients and thus solved pathwise. As the solution of the stochastic Ginzburg–Landau equation exists globally, a natural problem is the qualitative analysis of the solution, and from which, to understand the noise effect on the deterministic differential system.

As it is well known, the equation (1) can be rewritten as the Stratonovich form (Ref. 8)

$$du = (\lambda + i\alpha)\Delta u\, dt + \left(\nu - \frac{\sigma^2}{2}\right)u\, dt - (k + i\beta)|u|^2 u\, dt + \sigma u \circ dW. \tag{2}$$

We find, if $\nu \leqslant \lambda\lambda_1 + \sigma^2/2$, the trivial solution is stable with probability one. For an unperturbed system, the stationary solution is stable if $\nu \leqslant \lambda\lambda_1$. The similar fact can also be found in the stochastic reaction-diffusion equation (Ref. 2). If $\nu > \lambda\lambda_1 + \sigma^2/2$, we need the random attractor to study the long-time behavior of our problem. The notion of an attractor of the semigroup for the associated deterministically differential system is well known to be a compact invariant set in the phase space which attracts all bounded sets of the initial state. Recently, the corresponding generalization of this concept to the stochastic case was introduced by Crauel and Flandoli (Ref. 4) and Schmalfuss (Ref. 6) independently. Since a stochastic differential equation is driven by a Wiener process, the equation is nonautonomous and the trajectory of the solution cannot be attracted by some bounded set. They exploited successfully a random attractor to tackle these difficulties by introducing a cocycle and redefining the absorption concept. It is shown that the random attractor is a proper extension and some important information on the asymptotic behavior of the stochastic system can be obtained (Ref. 3). Their framework is suitable for our problem. First, the linear multiplicative noise makes us construct a random dynamical system modeling our stochastic differential equation. By assuming that $|\beta| < k$, we verify the compactness of the absorbing set. Finally, we obtain the existence of the random attractor for the stochastic Ginzburg–Landau equation.

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Another important problem is the Hausdorff dimension of the random attractor. A finite dimension of the attractor characterize the number of degrees of freedom present in the long term dynamics of the system. Since the random attractor is not uniformly bounded, some relative restrictive assumptions must be imposed to guarantee the generalization of the theory of deterministic system to the stochastic case (Refs. 5,6). Applying the approach developed by Debussche in Ref. 5 to the stochastic Ginzburg–Landau equation, we prove that the random attractor has a finite Hausdorff dimension. The key is to prove that the cocycle associated with the stochastic equation is uniformly differentiable. It needs the bound of the solution in L^p for $\forall p \in Z^+$, which is not easy to obtain for the stochastic Ginzburg–Landau equation. We have to assume that $|\alpha| < \lambda$ to obtain the bound of the solution in L^p for $1 \leqslant p \leqslant 8$, and then to choose proper parameters to prove the differentiability.

This paper is arranged as follows. In Sec. II, we will present some preliminaries and the stability conclusion for the unperturbed system. The stability of the stationary solution for the stochastic system will be included in Sec. III. In Sec. IV, we introduce the framework of the theory of a random dynamical system and random attractor and prove the existence of the random attractor for the stochastic Ginzburg–Landau equation. In the end, we prove that the random attractor has a finite Hausdorff dimension.

II. PRELIMINARIES

Let $D \subset R^n$ $(n=1,2)$ be an open bounded set with a boundary ∂D sufficiently regular. We consider the following the stochastic Ginzburg–Landau equation in D perturbed by a multiplicative white noise:

$$du = (\lambda + i\alpha)\Delta u dt + \nu u dt - (k + i\beta)|u|^2 u dt + \sigma u dW(t), \quad \text{in} \quad D;$$

$$u(t) = 0, \quad \text{on} \quad D;$$

$$u(0) = u_0; \tag{3}$$

where $\lambda, \alpha, \nu, k, \beta, \sigma \in R, \lambda > |\alpha|, k > |\beta|, \sigma > 0$, and $W(t): \Omega \to R$ is a two-sided standard Wiener process. The unknown function u is a complex valued function defined on $D \times R^+$. We now introduce the following complex Sobolev space. Denoted by $\mathbb{X}$ with the norm $|\cdot|_{\mathbb{X}}$, the complexified space of a functional space X with the norm $|\cdot|_X$, by $(\cdot,\cdot)$ and $|\cdot|$ the inner product and the norm in $\mathbb{L}^2(D)$, respectively, by $\mathbf{((\cdot))}$ and $\|\cdot\| + |\cdot|$, the inner product and the norm in $\mathbb{H}_0^1(D)$, respectively, where

$$(u,v) = \mathrm{Re} \int_D u(x)\overline{v}(x)dx$$

for $u, v \in \mathbb{L}^2(D)$ and for $u, v \in \mathbb{H}_0^1(D)$,

$$((u,v)) = \mathrm{Re} \sum_{i=1}^{n} \int_D D_i u D_i \overline{v}\, dx, \quad \|u\| = (((u,u)))^{1/2}.$$

We always write $H = \mathbb{L}^2(D), V = \mathbb{H}_0^1(D)$, $Au = -\Delta u$, and $f(u) = |u|^2 u$. The operator A is an isomorphism from $D(A) = V \cap \mathbb{H}^2(D)$ onto H. Let $\{e_n\}$ be the orthonormal basis in H of its eigenvectors with the corresponding eigenvalues $\lambda_n, \lambda_n > 0, \lambda_n \nearrow \infty$. For the first eigenvalue, we have the inequality $\lambda_1 |u|^2 \leqslant \|u\|^2$. The stochastic Ginzburg–Landau equation (3) can be rewritten as follows in the abstract form:

$$du + (\lambda + i\alpha)Au\, dt - \nu u\, dt + (k + i\beta)f(u)dt = \sigma u\, dW(t),$$

$$u(0) = u_0. \tag{4}$$

For the unperturbed system (i.e., $\sigma=0$), the stabilization of the trivial solution and the existence of the global attractor is well known (Ref. 9). For convenience, we will give a concise statement. First the Ginzburg–Landau equation has a unique solution,

$$u \in C([0,T];H) \cap L^2(0,T;V), \quad \forall\, T<\infty \quad \text{for} \quad u_0 \in H$$

and

$$u \in C([0,T];V) \cap L^2(0,T;D(A)), \quad \forall\, T<\infty \quad \text{for} \quad u_0 \in V.$$

The energy equation can be given as

$$\frac{1}{2}\frac{d}{dt}|u|^2 + \lambda\|u\|^2 - \nu|u|^2 + k|u|_{L^4}^4 = 0. \tag{5}$$

If $\nu<\lambda\lambda_1$, (5) leads to

$$|u(t)| \leqslant |u_0|\exp\{(\nu-\lambda\lambda_1)t\},$$

which follows the stationary solution $u=0$ is exponentially stable.

If $\nu=\lambda\lambda_1$, we have from (5),

$$|u(t)| \leqslant Ct^{1/2},$$

for some constant C dependent on the initial u_0, k, and the domain D. So the stationary solution $u=0$ is asymptotically stable.

If $\nu>\lambda\lambda_1$, the dynamical system associated with the Ginzburg–Landau possesses a finite-dimensional global attractor.

The analysis above shows that, if $\nu\leqslant\lambda\lambda_1$, all the trajectories converge to 0 as $t\to\infty$. Hence, the global attractor is reduced to the stationary solution $\{0\}$.

III. STABILITY

In this section, we continue to consider the asymptotic behavior of the deterministic Ginzburg–Landau equation perturbed by a multiplicative white noise in the Itô sense. First, due to special linear multiplicative noise, the stochastic Ginzburg–Landau equation can be reduced to an equation with random coefficients by a suitable change of variable. Then the same method as the deterministic theory leads to the existence and uniqueness of the solution to (4). Consider the process

$$z(t) = e^{-\sigma W(t)},$$

which satisfies the stochastic differential equation

$$dz(t) = \frac{1}{2}\sigma^2 z\, dt - \sigma z\, dW(t).$$

The process $v(t)=z(t)u(t)$ follows the random differential equation,

$$dv(t) + (\lambda + i\alpha)Av\, dt - \left(\nu - \frac{\sigma^2}{2}\right)v\, dt + (k+i\beta)zf(u)dt = 0.$$

Since $z(t)$ is a real-valued process, the equation above can be rewritten as a more explicit form,

$$dv(t) + (\lambda + i\alpha)Av\, dt - \left(\nu - \frac{\sigma^2}{2}\right)v\, dt + (k+i\beta)z^{-2}f(v)dt = 0, \tag{6}$$

this equation can be solved pathwise. Exploiting the Galerkin approximation and *a priori* esti-

mates, the same conclusion as Theorem 5.1 in Temam[9] can be derived as folllows. For P-almost every $\omega \in \Omega$, the equation (6) possesses a unique strong solution,

$$v \in C([s,t];H) \cap L^2(s,t;V), \quad \forall\, s < t \quad \text{for } v(s) \in H$$

and

$$v \in C([s,t];V) \cap L^2(s,t;D(A)), \quad \forall\, s < t \quad \text{for } v(s) \in V.$$

Then $u(t)=Z(t)v(t)$ with $Z(t)=e^{\sigma W(t)}$ is a solution to the equation (4). We now state the stability conclusion.

Theorem 1: *Assume* $\nu < \lambda\lambda_1 + \frac{1}{2}\sigma^2$. *Then there is a P-full set* Ω_1 *such that for all* $\omega \in \Omega_1$,

$$|u(t,\omega,u_0)| \leqslant |u_0| e^{(1/2)[\nu - \lambda\lambda_1 - (1/2)\sigma^2]t}, \tag{7}$$

holds for each $u_0 \in H$, *and* $t \geqslant T(\omega)$ *for some* $T(\omega) > 0$.

Proof: Applying the Itô formula to $|u(t)|^2$, we have

$$|u(t)|^2 = |u_0|^2 + 2\int_0^t \left(-\lambda \|u(s)\|^2 + \left(\nu + \frac{\sigma^2}{2}\right)|u(s)|^2 - k|u(s)|_{L^4}^4 \right) ds + 2\int_0^t \sigma |u(s)|^2\, dW(s).$$

Let us apply once again the Itô formula to the function $\log|u(t)|^2$. It follows that

$$\begin{aligned} \log|u(t)|^2 &= \log|u_0|^2 - 2\int_0^t \frac{1}{|u(s)|^2}(\lambda\|u(s)\|^2 + k|u(s)|_{L^4}^4) ds + (2\nu - \sigma^2)t + 2\sigma W(t) \\ &\leqslant \log|u_0|^2 + (2\nu - \lambda\lambda_2 - \sigma^2)t + 2\sigma W(t). \end{aligned} \tag{8}$$

As $\lim_{t\to\infty}(W(t)/t)=0$, P-a.s., there exists a P-full set Ω_1 such that for $\omega \in \Omega_1$ there exists $T(\omega) > 0$ such that

$$\frac{2\sigma W(t)}{t} \leqslant \left(\lambda\lambda_1 + \frac{\sigma^2}{2} - \nu\right) \quad \text{for} \quad t \geqslant T(\omega),$$

holds. It leads to

$$\log|u(t)|^2 \leqslant \log|u_0|^2 + \left(\nu - \lambda\lambda_2 - \frac{1}{2}\sigma^2\right)t, \tag{9}$$

which completes the proof. □

We have proved that the trivial solution is asymptotically exponentially stable with probability one. The stability interval on ν is extended from $(-\infty, \lambda\lambda_1]$ in the unperturbed system to $(-\infty, \lambda\lambda_1 + \sigma^2/2]$ in the system perturbed by the Itô noise. Note that it is the extra term appearing in the Itô formula that leads to the longer part $[\lambda\lambda_1, \lambda\lambda_1 + \sigma^2/2]$. In fact, Stratonovich noise is the correct one in the usual idealization from smooth perturbations to rough ones, while Itô noise is artificial. Considering the Itô equation is equivalent to adding two terms: a multiplicative noise and a deterministic damping; the resulting stabilization is a trivial consequence of the addition of damping, not of the noise. Similar to the deterministic case, as $\nu > \lambda\lambda_1 + \sigma^2/2$, we will exploit the random attractor to study the long-term behavior of the stochastic Ginzburg–Landau equation.

IV. EXISTENCE OF RANDOM ATTRACTORS

Let us begin with the definitions of a random dynamical system (RDS) and a random attractor developed by Arnold (Ref. 1), Crauel and Flandoli (Ref. 4) and Schmalfuss (Ref. 6), and then prove the existence of the random attractor for the stochastic Ginzburg–Landau equation.

Let $(\Omega,\mathcal{F},P)$ be a probability space and $\{\theta_t:\Omega\to\Omega, t\in R\}$ a family of measure-preserving transformations such that $\theta_0=id_\Omega$, and $\theta_{t+s}=\theta_t\circ\theta_s$, for all $t,s\in R$. We say $\{\theta_t\}$ is a metric dynamical system on $(\Omega,\mathcal{F},P)$. We assume that θ is ergodic under P.

Definition 2: Let (X,d) be a Polish space. A measurable map,

$$\varphi:R^+\times\Omega\times X\to X,(t,\omega,x)\to\varphi(t,\omega)x,$$

is called a random dynamical system (RDS) if φ satisfies the cocycle property: $\varphi(0,\omega)=id_X$, $\varphi(t+s,\omega)=\varphi(t,\theta_s\omega)\varphi(s,\omega)$, for all $t,s\in R^+$ and P-a.s. $\omega\in\Omega$.

A RDS is continuous if $\varphi(t,\omega):X\to X$ is continuous. In order to define the random attractor, some crucial notions are needed.

Definition 3: A set-valued map $K:\Omega\to 2^X$, the set of all subsets of X, is called a random compact set if $K(\omega)$ is a compact P-almost surely and if $\omega\to d(x,K(\omega))$ is measurable for each $x\in X$, where $d(x,M):=\inf_{y\in M}d(x,y)$.

Definition 4: Let $A(\omega)$ and $B(\omega)$ be two random sets. We say the following.

(1) *$A(\omega)$ attracts $B(\omega)$ if*

$$\lim_{t\to\infty}\operatorname{dist}(\varphi(t,\theta_{-t}\omega)B(\theta_{-t}\omega),A(\omega))=0,\quad P\text{-a.s.}$$

where $\operatorname{dist}(\cdot,\cdot)$ *denotes the Hausdorff semidistance in X.*

(2) *$A(\omega)$ absorbs $B(\omega)$ if there exists $t_B(\omega)$ such that for all $t\geqslant t_B(\omega)$,*

$$\phi(t,\theta_{-t}\omega)B(\theta_{-t}\omega)\subset A(\omega),\quad P\text{-a.s.}$$

Definition 5: A random set $\mathcal{A}(\omega)$ is said to be a random attractor for the RDS φ if P-a.s.

(1) *$\mathcal{A}(\omega)$ is a random compact set.*
(2) *$\mathcal{A}(\omega)$ is invariant, that is, $\varphi(t,\omega)\mathcal{A}(\omega)=\mathcal{A}(\theta_t\omega)$, for $\forall t\geqslant 0$.*
(3) *$\mathcal{A}(\omega)$ attracts all deterministic bounded sets $B\in X$.*

Similar to the deterministic theory, the existence result of random attractors can be stated as follows (Refs. 4 and 6).

Theorem 6: *If there exists a random compact set absorbing every bounded nonrandom set $B\subset X$, the RDS φ possesses a random attractor $\mathcal{A}(\omega)$,*

$$\mathcal{A}(\omega)=\overline{\bigcup_{B\subset X}\Lambda_B(\omega)},$$

where $\Lambda_B(\omega):=\cap_{s\geqslant 0}\overline{\cup_{t\geqslant s}\varphi(t,\theta_{-t}\omega)B}$ is the omega-limit set of B.

Remark 7: (1) The random attractor in Definition 5 is in fact a global random set attractor. It is unique (Ref. 4).

(2) $\varphi(t,\theta_{-t})x$ can be interpreted as the position at $t=0$ of the trajectory which was at x at time $-t$, that is, while time t is moving, the trajectory $\varphi(t,\theta_{-t}\omega)x$ is always at the position at time zero. Therefore, the random attractor in Definition 5 is also called the "pullback attractor."

Now we construct a RDS modeling the stochastic Ginzburg–Landau equation. For example, consider the set of continuous functions with value 0 at 0,

$$\Omega=\{\omega\in C(R,R):\omega(0)=0\}.$$

Let $\mathcal{F}$ be the Borel sigma-algebra induced by the compact-open topology of Ω, and let P be a Wiener measure on $(\Omega,\mathcal{F})$. Writing $W(t,\omega)=\omega(t)$, we define

$$\theta_t\omega(s)=\omega(t+s)-\omega(t),\tag{10}$$

which satisfies $\theta_t\circ\theta_s=\theta_{t+s}$. Then $(\Omega,\mathcal{F},P,(\theta_t)_{t\in R})$ is an ergodic metric dynamical system which models white noise. We set

$$u(t,\omega) = \psi(t,s;\omega)u_s, v(t,\omega) = \phi(t,s;\omega)v_s,$$

where $u(t)$ is a solution to the equation (4) with the initial value $u(s)=u_s$ and $v(t)$ satisfies (6) with $v(s)=v_s$. Obviously, for $s\leqslant r\leqslant t$, we have

$$\psi(t,s;\omega) = \psi(t,r;\omega)\psi(r,s;\omega).$$

Thanks to (10), for any $s,t\in R^+, u_0\in H$, we have P-a.s.,

$$\psi(t+s,0;\omega)u_0 = \psi(t,0;\theta_s\omega)\psi(s,0;\omega)u_0.$$

Therefore, the process $\varphi: R^+\times\Omega\times H\to H$, defined by

$$\varphi(t,\omega)u_0 = \psi(t,0;\omega)u_0, \tag{11}$$

is a cocycle. It is a continuous RDS on H over $(\Omega,\mathcal{F},P,(\theta_t)_{t\in R})$ and models the dynamical system associated with the stochastic equation (4).

In order to prove the existence of a compact absorbing set, we give first the following estimates:

Lemma 8: Given any ball of $H, B(0,\rho)$ centered at 0 of radius ρ, there exists random variables $r_t(\omega)$ and $t(\omega,\rho)\leqslant -1$ such that for any $s\leqslant t(\omega,\rho), u_s\in B(0,\rho), v_s=z(s)u_s$ and $-1\leqslant t\leqslant 0$,

$$|\phi(t,s;\omega)v_s| \leqslant r_t(\omega), \quad P\text{-a.s.}, \tag{12}$$

holds. Hence, we have

$$|\psi(0,s;\omega)u_s| \leqslant r_0(\omega).$$

Proof: Let $v(t)=v(t,s,v_s;\omega)$ be the solution of (6) with the initial value v_s. We have

$$\frac{d}{dt}|v|^2 + \lambda\|v\|^2 = -\lambda\|v\|^2 + (2\nu-\sigma^2)|v|^2 - 2kz^{-2}|v|_{\mathbb{L}^4}^4 \leqslant -(\lambda\lambda_1+\sigma^2)|v|^2 + 2\nu|v|^2 - 2kz^{-2}|v|_{\mathbb{L}^4}^4. \tag{13}$$

Taking into account that $|v|\leqslant|D|^{1/4}|v|_{\mathbb{L}^4}$, we get

$$\begin{aligned}\frac{d}{dt}|v|^2 + \lambda\|v\|^2 &\leqslant -(\lambda\lambda_1+\sigma^2)|v|^2 + 2\nu|D|^{1/2}|v|_{\mathbb{L}^4}^2 - 2kz^{-2}|v|_{\mathbb{L}^4}^4\\ &\leqslant -(\lambda\lambda_1+\sigma^2)|v|^2 + \nu^2|D|k^{-1}z^2 - kz^{-2}|v|_{\mathbb{L}^4}^4\\ &\leqslant -(\lambda\lambda_1+\sigma^2)|v|^2 + \nu^2|D|k^{-1}z^2.\end{aligned} \tag{14}$$

It follows that, for $t\geqslant s$,

$$\begin{aligned}|v(t)|^2 &\leqslant |v(s)|^2 e^{-(\lambda\lambda_1+\sigma^2)(t-s)} + \nu^2|D|k^{-1}\int_s^t e^{-(\lambda\lambda_1+\sigma^2)(t-\tau)}z^2(\tau)d\tau\\ &\leqslant e^{-(\lambda\lambda_1+\sigma^2)t}\left(e^{(\lambda\lambda_1+\sigma^2)s}z^2(s)|u_s|^2 + \nu^2|D|k^{-1}\int_s^t e^{(\lambda\lambda_1+\sigma^2)\tau}z^2(\tau)d\tau\right).\end{aligned} \tag{15}$$

Since $e^{(\lambda\lambda_1+\sigma^2)s}z^2(s) = e^{(\lambda\lambda_1+\sigma^2)s-2\sigma W(s)}\to 0, P$-a.s. as $s\to-\infty$, we can find, for $u_s\in B(0,\rho)\subset H$, a time $t(\omega,\rho)\leqslant -1$ such that

$$e^{(\lambda\lambda_1+\sigma^2)s}z^2(s)\rho^2 \leqslant 1,$$

holds P-a.s. for $s\leqslant t(\omega,\rho)$. Hence, choosing the positive variable $r_t(\omega)$,

$$r_t^2(\omega) = e^{-(\lambda\lambda_1+\sigma^2)t}\left(1 + \nu^2|D|k^{-1}\int_{-\infty}^{t} e^{(\lambda\lambda_1+\sigma^2)\tau}z^2(\tau)d\tau\right),$$

we obtain P-a.s.$|v(t)| \leqslant r_t(\omega)$. □

Note that if $\nu < \lambda\lambda_1 + \sigma^2/2$, from (13), we obtain

$$|v(t)| \leqslant |v(0)|e^{(\nu-\lambda\lambda_1-\sigma^2/2)t}.$$

It follows that

$$|u(t,\omega)| \leqslant |u_0|e^{(\nu-\lambda\lambda_1-\sigma^2/2+\sigma[W(t)/t])t}.$$

Since $\lim_{t\to\infty}[W(t)/t]=0, P$-a.s., there exits $t(\omega)$ such that for all $t \geqslant t(\omega)$,

$$\sigma\frac{W(t)}{t} \leqslant \frac{1}{2}\left(\lambda\lambda_1 + \frac{\sigma^2}{2} - \nu\right).$$

It leads to the same result as Theorem 1. From the view of the attractor, since for $s \leqslant 0$,

$$|u(0)| \leqslant |u_s|e^{-(\nu-\lambda\lambda_1-\sigma^2/2)s-\sigma W(s)},$$

we have $|u(0)| \to 0, P$-a.s. as $s \to -\infty$. Hence the global random attractor is reduced to $\{0\}$. From now on, we will assume that $\nu \geqslant \lambda\lambda_1 + \sigma^2/2$.

Lemma 8 shows there exists an absorbing set $B(0, r_0(\omega))$ in H. In order to obtain the existence of the absorbing set in V, we need the assumption $|\beta| \leqslant k$.

First, integrating (14) between -1 and 0, we have

$$\int_{-1}^{0}\|v\|^2\,ds \leqslant \frac{1}{\lambda}\left(|v(-1)|^2 + \nu^2|D|k^{-1}\int_{-1}^{0} z^2(s)ds\right).$$

Multiplying (6) by $-\Delta\overline{v}$, integrating over D, and taking the real part, we obtain

$$\frac{1}{2}\frac{d}{dt}\|v\|^2 + \lambda|\Delta v|^2 - \left(\nu - \frac{1}{2}\sigma^2\right)\|v\|^2 = z^{-2}\,\mathrm{Re}(k+i\beta)\int f(v)\Delta\overline{v}\,dx. \tag{16}$$

Using $|\beta| \leqslant k$, the right of (16) is nonpositive,

$$\begin{aligned}\mathrm{Re}(k+i\beta)\int f(v)\Delta\overline{v}\,dx &= -\,\mathrm{Re}(k+i\beta)\int (|v|^2|\nabla v|^2 + v\,\nabla\overline{v}\nabla|v|^2)dx\\ &= -k\int |v|^2|\nabla v|^2\,dx - \frac{k}{2}\int(\nabla|v|^2)^2\,dx + \beta\,\mathrm{Im}\int v^2(\nabla\overline{v})^2\,dx\\ &\leqslant (|\beta|-k)\int |v|^2|\nabla v|^2\,dx \leqslant 0.\end{aligned}$$

So (16) can be rewritten as

$$\frac{d}{dt}\|v\|^2 \leqslant -2\lambda|\Delta v|^2 + 2\left(\nu - \frac{\sigma^2}{2}\right)\|v\|^2 \leqslant 2\left(\nu - \lambda\lambda_1 - \frac{\sigma^2}{2}\right)\|v\|^2.$$

For any $s \in [-1,0]$, we have

$$\|v(0)\|^2 \leqslant \|v(s)\|^2 + 2\left(\nu - \lambda\lambda_1 - \frac{\sigma^2}{2}\right)\int_s^0 \|v(\tau)\|^2\,d\tau.$$

Integrating again in $[-1,0]$,

$$\|v(0)\|^2 \leqslant 2\left(\frac{1}{2}+\nu-\lambda\lambda_1-\frac{\sigma^2}{2}\right)\int_{-1}^{0}\|v(s)\|^2\,ds$$
$$\leqslant \frac{2}{\lambda}\left(\frac{1}{2}+\nu-\lambda\lambda_1-\frac{\sigma^2}{2}\right)\left(|v(-1)|^2+\nu^2|D|k^{-1}\int_{-1}^{0}z^2(s)ds\right). \tag{17}$$

Therefore, given $\rho>0$, there exists $T(\omega)\leqslant -1$ such that for $s\leqslant T(\omega)$ and $u_s\in B(0,\rho)\subset H$,

$$\|u(0)\|^2=\|v(0)\|^2\leqslant R_0^2(\omega), \tag{18}$$

holds P-a.s., where

$$R_0^2=\frac{2}{\lambda}\left(\frac{1}{2}+\nu-\lambda\lambda_1-\frac{\sigma^2}{2}\right)(e^{\lambda\lambda_1+\sigma^2}+\nu^2|D|k^{-1})\left(1+\int_{-\infty}^{0}e^{(\lambda\lambda_1+\sigma^2)\tau}z^2(\tau)d\tau+\int_{-1}^{0}z^2(s)ds\right).$$

In the end, applying Theorem 6, we conclude the following.

Theorem 9: *Under the assumption $|\beta|\leqslant k$, the random dynamical system associated with the stochastic Ginzburg–Landau equation possesses a global random attractor $\mathcal{A}(\omega)$. If $\nu<\lambda\lambda_1+\sigma^2/2$, the attractor $\mathcal{A}(\omega)$ is reduced to $\{0\}$.*

Although we have obtained a compact absorbing set which guarantees the existence of the random attractor, the union in ω of $\mathcal{A}(\omega)$ is not compact in general. However, as $\sigma\to 0$, the $\mathcal{A}(\omega)$ may converge to the corresponding deterministic attractor with probability one (Ref. 3).

Since P is invariant under θ_t, the asymptotic behavior with an attraction property from 0 to ∞ can be obtained in a weaker convergence in probability, that is,

$$\lim_{t\to\infty}P(\mathrm{dist}(\varphi(t,\omega)B,\mathcal{A}(\theta_t\omega))<\varepsilon)=1,$$

holds for all $\varepsilon>0$ and all deterministic bounded set $B\subset H$. Especially, if $\nu<\lambda\lambda_1+\sigma^2/2$, the attraction as $t\to\infty$ holds not only in probability and not also ω-wise.

V. HAUSDORFF DIMENSION OF THE RANDOM ATTRACTOR

Although the random attractor is not uniformly bounded, it is expected that the theory on the Hausdorff dimension of a global attractor of a deterministic system can be generalized to the stochastic case under some assumption (Refs. 5,7). The following conclusion is due to Debussche (Ref. 5).

Theorem 10: *Let $\mathcal{A}(\omega)$ be a compact measurable set which is invariant under a random map $S(\omega),\omega\in\Omega$, for some ergodic metric dynamical system $(\Omega,\mathcal{F},P,(\theta_t)_{t\in R})$. Assume the following.*

(1) *$S(\omega)$ is almost surely uniformly differentiable on $\mathcal{A}(\omega)$, that is, for every $u,u+h\in\mathcal{A}(\omega)$ there exists $D(S(\omega,u))$ in $\mathcal{L}(\mathcal{H})$, the space of the bounded linear operator from H to H, such that*

$$|S(\omega)(u+h)-S(\omega)u-DS(\omega,u)h|\leqslant\overline{k}(\omega)|h|^{1+\mu},$$

where $\mu>0$, $\overline{k}(\omega)$ is a random variable satisfying $\overline{k}(\omega)\geqslant 1, E(\log\overline{k})<\infty$.

(2) *$\omega_d(DS(\omega,u))\leqslant\overline{\omega}_d(\omega)$ for $u\in\mathcal{A}(\omega)$ and some random variable $\overline{\omega}_d(\omega)$ satisfying $E(\log(\overline{\omega}_d))<0$, where*

$$\omega_d(L)=\alpha_1(L)\cdots\alpha_d(L),\alpha_i(L)=\sup_{\substack{F\subset H\\ \dim F\leqslant n-1}}\inf_{\varphi\in F}|L\varphi| \quad \text{for } L\in\mathcal{L}(\mathcal{H}).$$

(3) *$\alpha_1(DS(\omega,u))\leqslant\overline{\alpha}_1(\omega)$, for $u\in\mathcal{A}(\omega)$ and a random variable $\overline{\alpha}_1(\omega)\geqslant 1$ with $E(\log\overline{\alpha}_1)<\infty$.*

Then the Hausdorff dimension $d_H(\mathcal{A}(\omega))$ of $\mathcal{A}(\omega)$ is less than d almost surely.

According to this theorem, in fact, the main task is to verify that the cocycle defined by (11) has the uniform differentiability. We set

$$S(\omega) = \varphi(1,\omega), \quad T(\omega)v_0 = \phi(1,0,v_0;\omega); \tag{19}$$

then the random attractor $\mathcal{A}(\omega)$ is a compact measurable set invariant by S. Since $S(\omega) = e^{\sigma W(1)}T(\omega)$, it is easy to see that if $T(\omega)$ is almost surely uniformly differentiable with the Fréchet derivative DT, then $S(\omega)$ is also almost surely uniformly differentiable with the Fréchet derivative $DS = e^{\sigma W(1)}DT$. Consequently, we turn to prove the following.

Lemma 11: $T(\omega)$ is almost surely uniformly differentiable on $\mathcal{A}(\omega)$: for $v, v+h \in \mathcal{A}(\omega)$, there exists $DT(\omega,v) \in \mathcal{L}(\mathcal{H})$ such that

$$|T(\omega)(v+h) - T(\omega)v - DT(\omega,v)h| \leqslant \overline{k}(\omega)|h|^{1+\mu},$$

holds P-a.s., *where* $\mu > 0, \overline{k}(\omega) \geqslant 1, E(\log \overline{k}(\omega)) < \infty$ *and* $DT(\omega,v_0)h = V(1), V(t)$ *solves the first variation equation for (6),*

$$\frac{dV}{dt} = L(t,v)V,$$

$$V(0) = h, \tag{20}$$

where $v(t) = \phi(t,0,v_0;\omega), L(t,v) = -(\lambda + i\alpha)A + (\nu - \sigma^2/2) - (k + i\beta)z^{-2}f'(v)$.

The proof will be given in the Appendix.

From Eq. (20), we have

$$\frac{1}{2}\frac{d}{dt}|V|^2 = -\lambda\|V\|^2 + \left(\nu - \frac{\sigma^2}{2}\right)|V|^2 - \mathrm{Re}(k + i\beta)z^{-2}\int_D (|v|^2|V|^2 + 2v\overline{V}\,\mathrm{Re}(\overline{v}V))dx.$$

The third term of the right is nonpositive,

$$\begin{aligned} &-\mathrm{Re}(k + i\beta)\int (|v|^2|V|^2 + 2v\overline{V}\,\mathrm{Re}(\overline{v}V))dx \\ &\quad \leqslant -k\int |v|^2|V|^2\,dx - 2\int \mathrm{Re}(\overline{v}V)\{k\,\mathrm{Re}(v\overline{V}) - \beta\,\mathrm{Im}(v\overline{V})\}dx \\ &\quad \leqslant -k\int |v|^2|V|^2\,dx + 2\beta\int \mathrm{Im}(v\overline{V})\mathrm{Re}(v\overline{V})dx \leqslant (|\beta| - k)\int |v|^2|V|^2\,dx \leqslant 0. \end{aligned}$$

Hence $|V(t)| \leqslant |V(0)|e^{(\nu - \lambda\lambda_1 - \sigma^2/2)t}$. Since $\alpha_1(DT(\omega,v))$ is equal to the norm of $DT(\omega,v) \in \mathcal{L}(\mathcal{H})$, it is not difficult, choosing $\overline{\alpha_1}(\omega) = \max\{e^{\sigma W(1) + \nu - \lambda\lambda_1 - \sigma^2/2}, 1\}$, to get

$$\alpha_1(DS(\omega,u)) \leqslant \overline{\alpha_1}(\omega),$$

and $E(\log \overline{\alpha_1}) < \infty$.

Note that we can write

$$DT(\omega,v) = \exp\left\{\int_0^1 L(s,v(s))ds\right\}$$

and

$$DS(\omega,u)=\exp\left\{\sigma W(1)+\int_0^1 L(s,v(s))ds\right\}.$$

Following Ref. 9, we have

$$\omega_d(DS(\omega,u))=\sup_{\substack{|\xi_i|\in H\\ |\xi_i|\leqslant 1,i=1,\cdot,d}}\exp\left\{\sigma W(1)+\int_0^1 \mathrm{Tr}(L(s,v(s))\circ Q_d(s))ds\right\},$$

where $Q_d(s)$ is the orthogonal projector in H onto the space spanned by $V_1(s),\ldots,V_d(s)$, and $V_i(s)$ is the solution of (20) with $V(0)=\xi_i$.

Let $\varphi_i(s), i\in N$ be an orthonormal basis of H such that $Q_d(s)H=\mathrm{Span}[\varphi_1(s),\ldots,\varphi_d(s)]$; then

$$\begin{aligned}\mathrm{Tr}(L(s,v(s))\circ Q_d(s))&=\textstyle\sum_{i=1}^d (L(s,v(s))\varphi_i(s),\varphi_i(s))\\ &\leqslant -\lambda\textstyle\sum_{i=1}^d\|\varphi_i\|^2+\left(\nu-\frac{\sigma^2}{2}\right)d\leqslant -\lambda\sum_{i=1}^d\lambda_i^2+\left(\nu-\frac{\sigma^2}{2}\right)d.\end{aligned}$$

Denoting $\overline{\omega}_d(\omega)=\exp\{\sigma W(1)-\lambda\Sigma_{i=1}^d\lambda_i^2+[\nu-(\sigma^2/2)]d\}$ and choosing d such that

$$\nu-\frac{\sigma^2}{2}<\frac{\lambda}{d}\sum_{i=1}^d\lambda_i^2,$$

then we have $\omega_d(DS)\leqslant\overline{\omega}_d(\omega)$ and $E(\log(\overline{\omega}_d))<0$.

In conclusion, we have the following result.

Theorem 12: *If there exists d such that $\nu\leqslant(\sigma^2/2)+\frac{\lambda}{d}\Sigma_{i=1}^d\lambda_i$ then P-*a.s. *$d_H(\mathcal{A}(\omega))<d$.*

Note that if $\nu<\lambda\lambda_1+(\sigma^2/2)$, the random attractor $\mathcal{A}(\omega)$ consists of one point which may be a random point.

APPENDIX: PROOF OF LEMMA 11

In this appendix, we prove the differentiability of $T(\omega)$. The proof will be divided into three steps.

Step 1. Bound in $\mathbb{L}^p, p\in Z^+,\ 1\leqslant p\leqslant 8$.

Lemma 13: Assume that $\lambda\geqslant|\alpha|$ and let $v(t)$ be the solution of (6); then for $p\in Z^+, 1\leqslant p\leqslant 4$, there exists a random variable $I_{2p}(\omega)$ such that

$$\int_0^1|v(s)|_{\mathbb{L}^{2p}}^{2p}\,ds\leqslant I_{2p}(\omega),\tag{A1}$$

where we use the notation $|\cdot|_{\mathbb{L}^p}=|\cdot|_p$, and for $\forall m\geqslant 0$,

$$E(I_{2p}^m)<\infty.$$

Proof: Due to the invariance of the random attractor $\mathcal{A}(\omega)$, for $v_0\in\mathcal{A}(\omega)$, there exists the solution $v(t)$ of (6) with $v(0)=v_0$ such that $v(t)\in\mathcal{A}(\theta_t\omega)$ for $\forall t\in R$. In order to obtain (A1), we show first that for $p\in Z^+, 1\leqslant p\leqslant 3$ and $r>0$,

$$\int_{t-r}^t|v(s)|_{2p+2}^{2p+2}\,ds\leqslant C\sup_{t-r\leqslant s\leqslant t}e^{-2\sigma W(s)}\int_{t-r-1}^t|v(s)|_{2p}^{2p}\,ds,\tag{A2}$$

where C is a deterministic constant which may be changed from one line to another; sometimes we denote by $C(\omega)$ a random constant dependent on $\omega\in\Omega$. Taking the scalar product of (6) with $\overline{v}|v|^{2p-2}(p\geqslant 1)$, and using the estimate

$$\mathrm{Re}(\lambda + i\alpha)\int_D \Delta v\overline{v}|v|^{2p-2}\,dx = -\lambda p\int_D |\nabla v|^2|v|^{2p-2}\,dx - (p-1)\mathrm{Re}(\lambda + i\alpha)\int_D (\overline{v}\nabla v)^2|v|^{2p-4}\,dx$$

$$\leqslant -\lambda(p - \sqrt{2}p + \sqrt{2})\int_D |\nabla v|^2|v|^{2p-2}\,dx \leqslant 0,$$

we obtain

$$\frac{1}{2p}\frac{d}{dt}|v|_{2p}^{2p} + e^{2\sigma W(t)}|v|_{2p+2}^{2p+2} \leqslant \left(\nu - \frac{\sigma^2}{2}\right)|v|_{2p}^{2p}. \tag{A3}$$

Integrating (A3) between s and t, we have

$$\frac{1}{2p}|v(t)|_{2p}^{2p} \leqslant \frac{1}{2p}|v(s)|_{2p}^{2p} + \left(\nu - \frac{\sigma^2}{2}\right)\int_s^t |v(\tau)|_{2p}^{2p}\,d\tau.$$

Let us integrate on s once again between $t-1$ and t to give

$$|v(t)|_{2p}^{2p} \leqslant \int_{t-1}^t |v(s)|_{2p}^{2p}\,ds + 2p\left(\nu - \frac{\sigma^2}{2}\right)\int_{t-1}^t |v(s)|_{2p}^{2p}\,ds. \tag{A4}$$

Using (A4), we then integrate (A3) between $t-r$ and t to give

$$\begin{aligned}\int_{t-r}^t e^{2\sigma W(s)}|v(s)|_{2p+2}^{2p+2}\,ds, &\leqslant \frac{1}{2p}|v(t-r)|_{2p}^{2p} + \left(\nu - \frac{\sigma^2}{2}\right)\int_{t-r}^t |v(s)|_{2p}^{2p}\,ds\\ &\leqslant \frac{1}{2p}\int_{t-r-1}^{t-r} |v(s)|_{2p}^{2p}\,ds + \left(\nu - \frac{\sigma^2}{2}\right)\int_{t-r-1}^{t-r} |v(s)|_{2p}^{2p}\,ds\\ &\quad + \left(\nu - \frac{\sigma^2}{2}\right)\int_{t-r}^t |v(s)|_{2p}^{2p}\,ds \leqslant (1 + 2\nu - \sigma^2)\int_{t-r-1}^t |v(s)|_{2p}^{2p}\,ds.\end{aligned}$$

It leads to

$$\int_{t-r}^t |v(s)|_{2p+2}^{2p+2}\,ds \leqslant (1 + 2\nu - \sigma^2)\sup_{t-r\leqslant s\leqslant t} e^{-2\sigma W(s)}\int_{t-r-1}^t |v(s)|_{2p}^{2p}\,ds.$$

Writing $S_i = \sup_{1-i\leqslant s\leqslant 1} e^{-2\sigma W(s)}$, we have

$$\begin{aligned}\int_0^1 |v(s)|_{2p+2}^{2p+2}\,ds &\leqslant (1 + 2\nu - \sigma^2)S_1\int_{-1}^1 |v(s)|_{2p}^{2p}\,ds \leqslant (1 + 2\nu - \sigma^2)^2 S_1 S_2\int_{-2}^1 |v(s)|_{2p-2}^{2p-2}\,ds\\ &\leqslant (1 + 2\nu - \sigma^2)^p S_1 S_2 S_p\int_{-p}^1 |v(s)|^2\,ds.\end{aligned}$$

Since $v(-3) \in \mathcal{A}(\theta_{-3}\omega)$, we have

$$|v(-3)| \leqslant r_{-3}(\theta_{-3}\omega)$$

Finally, using (15), we obtain the bound in H of $v(t)$ for $-3 \leqslant t \leqslant 1$, and hence complete the proof. □

Step 2. Lipschitz property for the solution. Let $v_i(t)$ $(i=1,2)$ be two solution of (6) with $v_i(0) = v_i^0$ and denote $g(t) = v_1(t) - v_2(t)$. Then $g(t)$ solves

$$\frac{dg}{dt} + (\lambda + i\alpha)Ag - \left(\nu - \frac{\sigma^2}{2}\right)g + (k + i\beta)z^{-2}(f(v_1) - f(v_2)) = 0.$$

Taking the scalar product of the equation with g, we get

$$\frac{1}{2}\frac{d}{dt}|g|^2 + \lambda\|g\|^2 - \left(\nu - \frac{\sigma^2}{2}\right)|g|^2 = -\operatorname{Re}(k + i\beta)z^{-2}\int_D (f(v_1) - f(v_2))(\overline{v_1} - \overline{v_2})dx. \tag{A5}$$

Note that the right side of Eq. (A5) is bounded by

$$Cz^{-2}(|v_1|_6^3 + |v_2|_6^3)|g|^2.$$

Hence we obtain

$$|g(t)|^2 \leqslant |g(0)|^2 \exp\left\{\left(\nu - \lambda\lambda_1 - \frac{\sigma^2}{2}\right)t + C\int_0^t z^{-2}(s)(|v_1(s)|_6^3 + |v_2(s)|_6^3)ds\right\}. \tag{A6}$$

From (A1), it leads to

$$|g(1)|^2 \leqslant |g(0)|^2 \exp\left\{\nu - \lambda\lambda_1 - \frac{\sigma^2}{2} + C\sup_{0\leqslant s\leqslant 1} z^{-2}(s)I_6(\omega)\right\}.$$

Finally, we get

$$|v_1(1) - v_2(1)| \leqslant C(\omega)|v_1^0 - v_2^0|,$$

with $E(C(\omega)) < \infty$. □

Step 3. Differentiability of $T(\omega)$.

Let $r(t) = v_1(t) - v_2(t) - V(t)$, where $v_i(t)(i = 1, 2)$ be two solutions of (6) with $v_i(0) = v_i^0$ and $V(t)$ satisfies the linear equation (20) with $L(t, v_2)$ and $h = v_1^0 - v_2^0$. Then $r(t)$ satisfies the equation

$$\frac{dr}{dt} + (\lambda + i\alpha)Av - \left(\nu - \frac{\sigma^2}{2}\right)r = -(k + i\beta)z^{-2}(f(v_1) - f(v_2) - f'(v_2)(v_1 - v_2 - r)).$$

Taking the scalar product this equation with r, we get

$$\frac{1}{2}\frac{d}{dt}|r|^2 + \lambda\|r\|^2 \leqslant \left(\nu - \frac{\sigma^2}{2}\right)|r|^2 - \operatorname{Re}(k + i\beta)z^{-2}\int_D f'(v_2)|r|^2\,dx - \operatorname{Re}(k + i\beta)z^{-2}\int_D (f(v_1) - f(v_2) - f'(v_2)(v_1 - v_2))\overline{r}\,dx. \tag{A7}$$

The second term of the right side is nonpositive,

$$\begin{aligned} -\operatorname{Re}(k + i\beta)z^{-2}\int_D f'(v_2)|r|^2\,dx &= -\operatorname{Re}(k + i\beta)\int (|v_2|^2|r|^2 + 2v_2\overline{r}\operatorname{Re}(v_2\overline{r}))dx \\ &= -k\int (|v_2|^2|r|^2\,dx - 2k\int (\operatorname{Re}(v_2\overline{r}))^2\,dx + 2\beta\int \operatorname{Re}(v_2\overline{r}) \\ &\quad \times (\operatorname{Im}(v_2\overline{r}))dx \leqslant (|\beta| - k)\int |v_2|^2|r|^2\,dx \leqslant 0. \end{aligned}$$

We continue to estimate the third of (A7). First, the nonlinearity f satisfies the estimate

$$|f(v_1) - f(v_2) - f'(v_2)(v_1 - v_2)| \leqslant C(|v_1|^2 + |v_2|^2)|v_1 - v_2|.$$

By the Hölder estimate and the Sobelev embedding theorems, we have

$$-\mathrm{Re}(k+i\beta)z^{-2}\int_D (f(v_1)-f(v_2)-f'(v_2)(v_1-v_2))\bar{r}\,dx$$
$$\leqslant Cz^{-2}|(|v_1|^2+|v_2|^2)(v_1-v_2)|_s|r|_{s^*}\leqslant Cz^{-4}|(|v_1|^2+|v_2|^2)(v_1-v_2)|_s^2+\varepsilon\|r\|^2,$$

where $\varepsilon>0, s>1$ and s^* is the conjugate exponent of s. Let

$$0<\delta<\frac{2}{3},\quad 1<s<\frac{8}{6+3\delta}.$$

It follows easily that

$$1<s<\frac{2}{1+\delta},\quad s_1:=\frac{2s(2-\delta)}{2-s(1+\delta)}<8.$$

Therefore, we have

$$|(|v_1|^2+|v_2|^2)(v_1-v_2)|_s^s\leqslant C\int_D (|v_1|+|v_2|)^{3s-s(1+\delta)}|v_1-v_2|^{s(1+\delta)}\,dx$$
$$\leqslant C(|v_1|_{s_1}^{s(2-\delta)}+|v_2|_{s_1}^{s(2-\delta)})|v_1-v_2|^{s(1+\delta)}.$$

Returning to (A7), for ε small enough, we get

$$\frac{1}{2}\frac{d}{dt}|r|^2\leqslant\left(\nu-\frac{\sigma^2}{2}\right)|r|^2+Cz^{-4}(|v_1|_{s_1}^{2(2-\delta)}+|v_2|_{s_1}^{2(2-\delta)})|v_1-v_2|^{2(1+\delta)}.$$

This yields

$$|r(1)|^2\leqslant C(\omega)\int_0^1 z^{-4}(s)(|v_1(s)|_{s_1}^{2(2-\delta)}+|v_2(s)|_{s_1}^{2(2-\delta)})ds\,h^{2(1+\delta)}.$$

Writing

$$\overline{k_1^2}(\omega)=C(\omega)\sup_{0\leqslant t\leqslant 1} z^{-4}(t)\int_0^1 (|v_1(s)|_{s_1}^{2(2-\delta)}+|v_2(s)|_{s_1}^{2(2-\delta)})ds,$$

and choosing $\overline{k}(\omega)=\max\{k_1(\omega),1\}$, which satisfies $E(\log\overline{k}(\omega))<\infty$, we conclude the proof of Lemma 11.

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Umbral calculus, difference equations and the discrete Schrödinger equation

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In this paper, we discuss umbral calculus as a method of systematically discretizing linear differential equations while preserving their point symmetries as well as generalized symmetries. The method is then applied to the Schrödinger equation in order to obtain a realization of nonrelativistic quantum mechanics in discrete space–time. In this approach a quantum system on a lattice has a symmetry algebra isomorphic to that of the continuous case. Moreover, systems that are integrable, superintegrable or exactly solvable preserve these properties in the discrete case. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1780612]

I. INTRODUCTION

A sizable literature exists on discrete quantum mechanics, that is on quantum mechanics in discrete space–time. We refer to a recent review for motivation and for an extensive list of references.[20] There are many reasons for considering quantum systems in discrete space–time. One is that physical space–time may indeed be discrete, involving an elementary length related to the Planck length and some minimal time interval. Then continuous theories would only be approximations to the real world. This is the scenario proposed, for instance, in loop quantum gravity. In its recent formulation, a fundamentally discrete evolution law has been derived.[59,1,6] Further conditions must be imposed in order to provide a consistent quantum theory.[7] Another reason is the usual one: on a lattice one can avoid some of the divergence problems occuring in quantum field theories. On the other hand, some properties of quantum systems are lost in any discretization. The aim of this paper is to discuss a discretization of space–time in which the Schrödinger equation is replaced by a difference equation. This is done in such a manner that many of the essential properties of the continuous system are preserved. In particular, we preserve the Lie algebraic and integrability properties of the Schrödinger equation. This is true for the time dependent, as well as the stationary equation. The free equations, as well as those with potentials, after discretization have symmetry algebras, isomorphic to those of the continuous case. Lie point symmetries, after discretization, may however act at several points of the lattice. An application of

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our approach is to preserve Lorentz and Galilei invariance in a classical or even quantum field theory on a lattice, via a suitable discretization of the infinitesimal operators generating these symmetries.[35]

Another property that we wish to preserve is that of integrability, and also superintegrability. By integrability, for an n dimensional quantum system, we mean the existence of n well defined algebraically independent Hermitian operators $\{X_1, \ldots, X_n\}$ (including the Hamiltonian H) commuting pairwise. Superintegrability means that there exist further independent operators, $\{Y_1, \ldots, Y_k\}$, $1 \leqslant k \leqslant n-1$, commuting with the Hamiltonian H, but not necessarily with the other operators X_i, nor Y_i.[19,64,43,56,58,51,23,48,30]

Finally, we wish to preserve exact solvability in the discretization, i.e., the fact that for certain systems (like the harmonic oscillator, or hydrogen atom) it is possible to calculate all energy levels algebraically.

A mathematical tool that we shall use for the study of symmetries and exact solutions of linear equations is the so-called "umbral calculus." This calculus, which originated in 19th century with the work of Sylvester, Cayley, and others, was used for a long time as a useful tool to derive combinatorial identities (see, for instance, Ref. 50). Nevertheless, it was only with Rota *et al.*[55,54,53,52] that this calculus was set on an axiomatic basis using the language of linear algebra of operators. In Ref. 9, the interested reader can find an up to date survey concerning the origins of umbral calculus and its many applications in several branches of mathematics, like combinatorics, functional analysis, algebraic topology, theory of special functions and orthogonal polynomials, etc.

Umbral calculus has recently been used explicitly,[11] or implicitly,[22,60,57,10] to provide discrete representations of canonical commutation relations, specially in the context of exactly solvable and quasiexactly solvable quantum systems.[61–63] Linear differential equations have been discretized in a symmetry preserving manner using commuting difference operators.[17,44,18] An alternative approach[38] to symmetries of linear difference equations makes use of a discretized version of the prolongation theory of evolutionary vector fields. Finally, umbral calculus was used in an implicit manner, to obtain several different symmetry preserving discretizations of the linear heat equation.[32]

Symmetries of difference equations, mainly nonlinear ones, have recently received a lot of attention (see, e.g., Refs. 17, 44, 18, 38, 32, 41, 39, 24, 36, 37, 40, and 12–15, and references therein). What has emerged for purely difference equations is that in order to capture the essential features and usefulness of symmetries of differential equations it is necessary to make serious adjustments. Either one must go beyond point transformations to generalized ones,[25,24] or one must use symmetry adapted and transforming lattices (as proposed initially by Dorodnitsyn).[36,37,40,12–15]

In this paper we follow the first approach. We consider a fixed lattice and use umbral calculus to obtain symmetries acting simultaneously on more than one point of the lattice. We apply this approach to quantum mechanics. In Sec. II we provide a very short summary of umbral calculus. In addition to standard definitions and known facts, we obtain some new results on the relation between umbral calculus, linear difference operators and solutions of linear difference equations. Section III is devoted to an "umbral" discretization of the Schrödinger equation in a manner that preserves the algebraic features of all point symmetries. In particular, for the free Schrödinger equation we construct a realization of the Schrödinger Lie algebra in terms of difference operators. Sections IV and V are devoted to discrete analogs of quantum superintegrable systems, their spectral properties and exact solvability are discussed. Some conclusions are drawn in the final Sec. VI. In the Appendix we consider a discrete relativistic wave equation in two dimensions. We use the discrete version of Lorentz invariance to obtain solutions of the discrete wave equations and discuss their convergence properties.

II. UMBRAL CALCULUS

To make this paper self-contained let us sum up in Sec. II A some known definitions and also some results proven as theorems by Rota,[54] Roman,[52] and Dimakis *et al.*.[11]

We shall actually need umbral calculus on spaces of many variables in order to study multidimensional difference equations. However, for simplicity of exposition and notation we shall in this section restrict to the case of one variable x.

Sections II B and II C contain results that are, to our knowledge, new.

A. General theory

Let $\mathfrak{J}$ be the algebra of formal power series in a variable x, and $\mathcal{P}$ the algebra of polynomials in the same variable. The algebras will be considered over a field $\mathbb{F}$ of characteristic zero. This field in the subsequent considerations will be identified with $\mathbb{R}$ or $\mathbb{C}$. An element of $\mathfrak{J}$ is of the form

$$\sum_k a_k x^k \equiv f(x). \tag{2.1}$$

The operations defined in $\mathfrak{J}$ are the addition of series

$$\sum_{k=0}^{\infty} a_k x^k + \sum_{k=0}^{\infty} b_k x^k = \sum_{k=0}^{\infty} (a_k + b_k) x^k, \tag{2.2}$$

and the multiplication

$$\left(\sum_{k=0}^{\infty} a_k x^k\right)\left(\sum_{l=0}^{\infty} b_l x^l\right) = \sum_{m=0}^{\infty} \left(\sum_{j=0}^{m} a_j b_{m-j}\right) x^m. \tag{2.3}$$

The algebra $\mathfrak{J}$ is also called the *umbral algebra.*[52]

A polynomial sequence $p_n(x) \in \mathcal{P}$ is a sequence whose nth element is a polynomial of degree n. We will denote by $\mathcal{L}$ the algebra of linear operators acting on $\mathfrak{J}$ or $\mathcal{P}$.

Definition 2.1: A shift operator $T \in \mathcal{L}$ is a linear operator such that

$$Tp(x) = p(x + \sigma), \tag{2.4}$$

where $p(x)$ is a polynomial and $\sigma \in \mathbb{F}$.

Definition 2.2: An operator $F \in \mathcal{L}$ is said to be shift invariant if it commutes with all shift operators (i.e., with T for all values of σ).

Definition 2.3: An operator U is said to be a delta operator if it is shift invariant and

$$Ux = c \neq 0, \tag{2.5}$$

where $c \in \mathbb{F}$.

Using Definition 2.1 and the linearity of shift-invariant operators one can prove the following result. If U is a delta operator, for every $c \in \mathbb{F}$ we have

$$Uc = 0. \tag{2.6}$$

Definition 2.4: A polynomial sequence $p_n(x)$, $n = 0, 1, 2, \ldots$, is called a sequence of basic polynomials for the delta operator U if

$$p_0(x) = 1, \quad p_n(0) = 0 \quad \forall n > 0, \tag{2.7}$$

and

$$Up_n(x) = np_{n-1}(x). \tag{2.8}$$

It is easy to show that every delta operator has a unique sequence of basic polynomials. We will denote by $\mathfrak{I}$ the one-to-one correspondence between basic sequences and delta operators.

Let $\mathcal{A}$ be the algebra of shift-invariant operators, endowed with the usual operations of sum of two operators, product of a scalar with an operator, and product of two operators. We introduce a multiplication operation $*: \mathcal{A} \times \mathcal{L} \to \mathcal{L}$, defined by

$$F * O = [F,O] = FO - OF, \tag{2.9}$$

where F is a shift-invariant operator and $O \in \mathcal{L}$. In particular, if x denotes the multiplication operator $x: p(x) \to xp(x)$, then $F * x$ corresponds to what in the umbral literature is known as the Pincherle derivative of F. In this case we will write

$$F' = F * x = [F,x]. \tag{2.10}$$

Using the $*$ multiplication the Leibnitz rule becomes

$$F * (fg) = (F * f)g + f(F * g) \tag{2.11}$$

and the Jacobi identity is expressed by

$$F * G * H + G * H * F + H * F * G = 0. \tag{2.12}$$

Let us now consider a pair of shift-invariant operators: a *delta* operator $U \in \mathcal{L}$ and its conjugate operator $\beta \in \mathcal{L}$, defined in such a way that the *Heisenberg–Weyl algebra* is satisfied,

$$[U,x\beta] = 1. \tag{2.13}$$

If U is a delta operator, then the inverse of U' exists (Ref. 54, p. 18). Therefore, the operator β is determined by the relation

$$\beta = (U')^{-1}. \tag{2.14}$$

To prove this it suffices to notice that

$$1 = [U,x\beta] = [U,x]\beta = U'\beta,$$

where the property $[U,\beta]=0$ has been exploited. Equation (2.14) follows.

Let us present some specific examples of realizations of the conjugate operators U and β in terms of derivatives and shifts, respectively.

Example 2.1: The continuous case. We have

$$U = \partial_x, \quad \beta = 1. \tag{2.15}$$

Example 2.2: The discrete case. The variable x is defined over an equally spaced lattice, with spacing σ. Two of the most common choices for the discrete derivative are as follows:

(a) The right discrete derivative,

$$U = \Delta^+ = \frac{T-1}{\sigma}, \quad \beta = T^{-1}. \tag{2.16}$$

(b) The left discrete derivative,

$$U = \Delta^- = \frac{1-T^{-1}}{\sigma}, \quad \beta = T. \tag{2.17}$$

Other cases will be considered below.

Using the $*$ multiplication of Eq. (2.9) it is easy to construct the basic sequence for the operator U. Let us introduce the polynomial sequence of operators

$$P_n = (x\beta)^n, \quad n \in \mathbb{N}. \tag{2.18}$$

The delta operator U satisfies the relation

$$[U,(x\beta)^n]=n(x\beta)^{n-1},\ \ n\in N. \tag{2.19}$$

This is an immediate consequence of the definition (2.13) and of the Leibnitz rule (2.11). A proof is obtained by induction. From (2.19) we immediately obtain

$$U*P_n=nP_{n-1},\ \ n\in\mathbb{N}. \tag{2.20}$$

This shows that $\{(x\beta)^n\}_{n\in\mathbb{N}}$ is the basic sequence for the operator U, under the $*$ multiplication.

Definition 2.5: An umbral correspondence is a map $\mathcal{R}:\mathcal{L}\to\mathcal{L}$ defined by

$$(x\beta_1)^n\overset{\mathcal{R}}{\to}(x\beta_2)^n, \tag{2.21}$$

where $P_n^1=\{(x\beta_1)^n\}$ and $P_n^2=\{(x\beta_2)^n\}$ are basic sequences of operators for two delta operators U_1 and U_2, respectively.

The umbral correspondence (2.21) naturally induces a correspondence between the two operators U_1 and U_2, according to the following scheme:

$$\begin{array}{ccc}(x\beta_1)^n & \overset{\mathcal{R}}{\leftrightarrow} & (x\beta_2)^n\\ \Im\updownarrow & & \Im\updownarrow\\ U_1 & \overset{R}{\leftrightarrow} & U_2.\end{array} \tag{2.22}$$

We shall also denote the induced correspondence between delta operators by the symbol $\mathcal{R}$.

Systems of equations connected by the umbral map (2.21) share many algebraic properties. A particular case of the umbral correspondence is when U_1 is the standard derivative ∂_x, and U_2 is a discrete derivative Δ. Then according to the scheme (2.22) we have

$$\begin{array}{ccc}x^n & \overset{\mathcal{R}}{\leftrightarrow} & (x\beta)^n\\ \Im\updownarrow & & \Im\updownarrow\\ \partial_x & \overset{\mathcal{R}}{\leftrightarrow} & \Delta.\end{array} \tag{2.23, 2.24}$$

Let us observe that Definition (2.5) generalizes the notion of an umbral operator introduced in Ref. 54: an umbral operator $R:\mathcal{P}\to\mathcal{P}$ is an operator (in general not necessarily shift-invariant) which maps some basic sequence of polynomials $p_n(x)$ into another basic sequence $q_n(x)$:

$$p_n(x)\overset{R}{\leftrightarrow}q_n(x). \tag{2.25}$$

Indeed, we observe that, since β is a function of shifts and any constant is invariant under the action of a shift operator, an umbral operator R is deduced from the action of $\mathcal{R}$ simply applying the sequence of operators $(x\beta)^n$ onto 1:

$$(x\beta_1)^n\cdot 1\overset{R}{\leftrightarrow}(x\beta_2)^n\cdot 1. \tag{2.26}$$

From (2.19) we also get

$$U_i(x\beta_i)^n\cdot 1=n(x\beta_i)^{n-1}\cdot 1,\ \ i=1,2. \tag{2.27}$$

An important consequence is that the umbral correspondence (2.22) preserves commutation relations between operators in $\mathcal{L}$. In particular, it preserves Lie algebras.

Indeed, let A_1 be a m-dimensional Lie algebra, generated by vector fields $\{\mathbf{v}_i\}_{i=1,\ldots,m}$ of the form

$$\mathbf{v}_i = \sum_j a_j(x_1, \ldots, x_p)\partial_{x_j}. \tag{2.28}$$

The umbral correspondence (2.22) maps A_1 isomorphically into an algebra A_2, generated by the vector fields $\{\mathbf{v}_i^U\}_{i=1,\ldots,m}$, with

$$\mathbf{v}_i^U = \sum_j a_j(x_1\beta_{x_1}, \ldots, x_p\beta_{x_p})\Delta_{x_j}. \tag{2.29}$$

This follows from the fact that the umbral correspondence (2.22) preserves the Heisenberg–Weyl algebra.

B. Umbral calculus and linear difference operators

The umbral approach reveals its power in the study of linear difference operators.

For our purposes, namely the study of difference equations and their continuous limits, we shall need only two types of delta operators. The first is simply the derivative $U=\partial_x$, with $\beta=1$. The second is a general difference operator that has ∂_x as its continuous limit. We set

$$U \equiv \Delta = \frac{1}{\sigma}\sum_{k=l}^{m} a_k T_\sigma^k, \quad l,m \in \mathbb{Z}, \quad l < m, \tag{2.30}$$

where a_k and σ are constants and $T_\sigma \equiv T$ is the shift operator of Eq. (2.4). In order for Δ in (2.30) to be a delta operator, it must satisfy Eq. (2.5). For any function $f(x) \in \mathfrak{F}$ Eq. (2.30) implies

$$\Delta f(x) = \frac{1}{\sigma}\sum_{k=l}^{m} a_k T^k f(x) = \frac{1}{\sigma}\sum_{k=l}^{m} a_k f(x + k\sigma). \tag{2.31}$$

Using a Taylor expansion around $\sigma=0$ we get

$$\Delta f(x) = \frac{1}{\sigma}\sum_{q=0}^{\infty} \frac{f^{(q)}(x)}{q!}\sigma^q \sum_{k=l}^{m} a_k k^q. \tag{2.32}$$

Choosing $f(x)=x$ we immediately see that Eq. (2.5) implies

$$\sum_{k=l}^{m} a_k = 0, \tag{2.33}$$

and $\Sigma_{k=l}^m a_k k = c$. We require that in the continuous limit Δ be the derivative ∂_x; this implies $c=1$, i.e.

$$\sum_{k=l}^{m} a_k k = 1. \tag{2.34}$$

Equation (2.30) involves $m-l+1$ constants a_k, subject to two conditions (2.33) and (2.34). To fix all constants a_k we must impose $m-l-1$ further conditions, for instance,

$$\gamma_q \equiv \sum_{k=l}^{m} a_k k^q = 0, \quad q = 2,3, \ldots, m-l. \tag{2.35}$$

Conditions (2.33) and (2.34) are necessary and sufficient for $U=\Delta$ to be a delta operator which has the derivative ∂_x as its continuous limit.

Definition 2.6: A difference operator of order $p=m-l$ is a delta operator of the form (2.30) satisfying Eqs. (2.33) and (2.34).

Theorem 2.1: *If the difference operator Δ of order $(m-l)\geqslant 2$ satisfies the supplementary conditions (2.35) it provides an approximation of order σ^{m-l} of the derivative ∂_x.*

Proof: We immediately have from Eq. (2.32) and Eqs. (2.33)–(2.35),

$$\Delta f \underset{\sigma\to 0}{\sim} f'(x) + \frac{\sigma^{m-l}}{(m-l+1)!} f^{(m-l-1)}(x) \sum_{k=l}^{m} a_k q^{m-l-1}. \tag{2.36}$$

Q.E.D.

Remark: Formula (2.30) defines U as an operator parametrized by σ, where $\sigma\in\mathbb{F}$. It may happen that for specific values of σ the operator U could involve less than p points, and consequently its order would be less than p. Once a representation of U as a difference operator is chosen, these points can be easily determined by solving a linear system of algebraic equations.

By way of an example, let us consider the following equation:[31]

$$\Delta^3 f(x) + 3\Delta^2 f(x) + \Delta f(x) - f(x) = 0. \tag{2.37}$$

If $\Delta=(T-1)/\sigma$, for $\sigma=1$ Eq. (2.37) becomes

$$f(x+3) - f(x+1) = 0,$$

which is of second order, in an appropriate domain.

In the following, U will be assumed to be an operator of order p parametrically depending on σ, and we shall omit the simple analysis of the specific cases in which the order could be less than maximal.

Theorem 2.2: *If Δ is a difference operator of order p, then $\widetilde{\Delta}=T^j\Delta$, $j\in\mathbb{Z}$ is a difference operator of the same order.*

Proof: Let us first prove the result for $j=1$. We have

$$T\Delta = \frac{1}{\sigma}\sum_{k=l}^{m} a_k T^{k+1} = \frac{1}{\sigma}\sum_{k=l-1}^{m+1} \widetilde{a}_k T^k, \quad \widetilde{a}_k = a_{k-1}.$$

Hence

$$\sum_{k=l+1}^{m+1} \widetilde{a}_k = \sum_{k=l}^{m} a_k = 0,$$

$$\sum_{k=l+1}^{m+1} k\widetilde{a}_k = \sum_{k=l}^{m} (k+1)a_k = \sum_{k=l}^{m} k a_k = 1.$$

Thus, conditions (2.31) and (2.33) are satisfied for $\widetilde{U}$ and that is all that is needed. The proof for $j=-1$ is analogous and for j arbitrary the result follows by induction. Q.E.D.

Conditions (2.35) are not shift invariant. However, once m and l are chosen, Eqs. (2.35) can always be imposed. Their solution depends on m and l, not only on the shift invariant difference $m-l$.

Theorem 2.3: *The operator β conjugate to the difference operator Δ of Eq. (2.30) is*

$$\beta = \left(\sum_{k=l}^{m} a_k k T^k\right)^{-1}. \tag{2.38}$$

Proof: Using Eq. (2.14) we have

$$\beta = (\Delta')^{-1} = [\Delta, x]^{-1}.$$

Moreover

$$[\Delta, x] = \frac{1}{\sigma}\left(\sum_{k=l}^{m} a_k(x + k\sigma)T^k - x\sum_{k=l}^{m} a_k T^k\right) = \sum_{k=l}^{m} a_k k T^k$$

and (2.38) follows. Q.E.D.

Examples of difference operators and the corresponding operators β are Δ^+ and Δ^- of Eqs. (2.16) and (2.17). Both are of order 1. Higher order examples are

$$\Delta^s = \frac{T - T^{-1}}{2\sigma}, \quad \beta = \left(\frac{T + T^{-1}}{2}\right)^{-1}, \tag{2.39}$$

$$\Delta^{(\mathrm{III})} = -\frac{1}{6\sigma}(T^2 - 6T + 3 + 2T^{-1}), \quad \beta = \left(-\frac{T^2 - 3T - T^{-1}}{3}\right)^{-1}, \tag{2.40}$$

$$\Delta^{(\mathrm{IV})} = -\frac{1}{12\sigma}(T^2 - 8T + 8T^{-1} - T^{-2}), \quad \beta = \left(-\frac{T^2 - 4T - 4T^{-1} + T^{-2}}{6}\right)^{-1}. \tag{2.41}$$

The operators Δ^s, $\Delta^{(\mathrm{III})}$, and $\Delta^{(\mathrm{IV})}$ approximate the derivative to order σ^2, σ^3, and σ^4, respectively.

Theorem 2.4: *The expression*

$$P_n(x) \equiv (x\beta)^n \cdot 1 \tag{2.42}$$

is a well-defined polynomial in x of order n with finite coefficients depending on a finite number of nonnegative powers of the shifts σ for any difference operator Δ. The expression for P_n is

$$P_n(x) = \sum_{k=1}^{n} A_k \sigma^{n-k} x^k, \quad A_n = 1, \tag{2.43}$$

where all coefficients A_k are finite and depend only on the coefficients a_k in the definition of Δ [see Eq. (2.30)]. In particular, they do not depend on σ.

Proof: Let us consider the difference operator Δ of Eq. (2.30) and define the quantities

$$\gamma_j = \sum_{k=l}^{m} a_k k^j, \quad \gamma_0 = 0, \quad \gamma_1 = 1, \quad j = 0, 1, 2, \ldots . \tag{2.44}$$

Let us now prove Eq. (2.43) by induction. Let P_n be a basic sequence of polynomials for any Δ, as given by Eq. (2.27). Thus we set

$$P_{n+1}(x) = \sum_{a=1}^{n+1} B_a x^a, \tag{2.45}$$

and must prove that the coefficients B_a are finite and depend on σ in the proper way (i.e., $B_a = \tilde{B}_a \sigma^{n+1-a}$, where $\tilde{B}_a$ is finite and does not depend on σ).

We rewrite Eq. (2.8) (with n substituted by $n+1$) as

$$\Delta P_{n+1} = (n + 1)P_n. \tag{2.46}$$

The left-hand side is

$$\Delta P_{n+1} = \frac{1}{\sigma}\sum_{b=l}^{m} a_b \sum_{a=1}^{n+1} B_a (x+b\sigma)^a = \sum_{a=1}^{n+1} B_a \sum_{k=0}^{a} \binom{a}{k} x^k \sigma^{a-k-1}\gamma_{a-k} = \sum_{k=0}^{n+1}\sum_{a=k}^{n+1} B_a \binom{a}{k} x^k \sigma^{a-k-1}\gamma_{a-k}.$$

Comparing powers on the left- and right-hand side of Eq. (2.46), we obtain a system of linear algebraic equations for the coefficient B_k,

$$\sum_{a=k}^{n+1} B_a \binom{a}{k} \sigma^{a-k-1}\gamma_{a-k} = (n+1)A_k \sigma^{n-k}. \tag{2.47}$$

The system (2.47) has a triangular structure. For $k=n+1$, we get the identity $0=0$. For $k=n$, only one term is present on the left and we get $B_{n+1}=1$ (since we have $\gamma_0=0$ and $A_n=1$). The value $k=n-1$ gives

$$B_n = \sigma\frac{n+1}{n}\left(A_{n-1} - \frac{n}{2}\right).$$

In general, the system (2.47) implies

$$B_{n-j} = \sigma^{j+1} \sum_{k=n-j-1}^{n} \mu_k A_k, \tag{2.48}$$

where the coefficients μ_k are easy to calculate, but are cumbersome (and of little interest), so we do not spell them out. Q.E.D.

Let us present the first few basic polynomials $P_k(x)=(x\beta)^k 1$ for arbitrary Δ as given by Eq. (2.30) with γ_j defined in terms of a_k by Eq. (2.44). We obtain

$$P_0 = (x\beta)^0 \cdot 1 = 1,$$

$$P_1 = (x\beta)^1 \cdot 1 = x,$$

$$P_2 = (x\beta)^2 \cdot 1 = x^2 - \sigma\gamma_2 x, \tag{2.49}$$

$$P_3 = (x\beta)^3 \cdot 1 = x^3 - 3\sigma\gamma_2 x^2 - \sigma^2(\gamma_3 - 3\gamma_2^2)x,$$

$$P_4 = (x\beta)^4 \cdot 1 = x^4 - 6\sigma\gamma_2 x^3 + \sigma^2(-4\gamma_3 + 15\gamma_2^2)x^2 + \sigma^3(-\gamma_4 + 10\gamma_2\gamma_3 - 15\gamma_2^3)x.$$

For $\sigma\to 0$, we obviously reobtain the basic series (sequence) for $\Delta=\partial_x$.

For $\Delta^+=(T-1)/\sigma$ we have only two values of a_j, namely $a_1=1$, $a_0=-1$, hence $\gamma_j=1$, $j=2,3,\ldots$. The polynomials (2.49) in this case reduce to the well-known factorial powers $P_n = x(x-\sigma)(x-2\sigma)\cdots(x-(n-1)\sigma)$.

C. Linear difference equations and umbral equations

Let us introduce the notation $\hat{f}=f(x\beta)$, i.e., to each function $f(x)\in\mathfrak{F}$ we associate an operator $\hat{f}\in\mathfrak{L}$. We shall consider an operator equation of the form

$$\sum_{k=0}^{n} \hat{A}_k U^k \hat{f} = \hat{g}, \tag{2.50}$$

where U is a delta operator and β is its conjugate operator defined in Eqs. (2.13) and (2.14). We assume that the operators $\hat{A}_k$ and $\hat{g}$ can be expanded into formal power series in $(x\beta)$.

Definition 2.7: An umbral equation of order n is an operator equation of the form (2.50) in which the operators $\hat{A}_k$ and $\hat{g}$ are given. The unknown is the operator $\hat{f}$.

If U is specified to be $U=\partial_x$, then $\beta=1$ and Eq. (2.50) reduces to a differential equation of order n. If U is a difference operator, (2.50) is still an operator equation. Projecting both sides onto a space of functions, i.e., applying them to a constant, we obtain a difference equation. The order of the difference equations obtained projecting Eq. (2.50) may vary depending on the structure of the operator $\hat{A}_k$ (since it acts on the operator $\hat{f}$) and on the choice of the operator Δ (and consequently of β) in terms of shift operators.

Let us first take $U=\partial_x$, $\beta=1$ in Eq. (2.50). The obtained linear ODE will have n linearly independent solutions $f_i(x)$. We can expand them into formal power series about any point x_0, where x_0 is not a singular point of the equation. Now let $U=\Delta$ be a difference operator and β the corresponding conjugate operator. Then $f_i(x\beta)\cdot 1$ viewed as a formal power series, will be a solution of the corresponding difference equation.

Definition 2.8: We shall call $\hat{f}\cdot 1$ *an* "umbral solution" *of the difference equation*

$$\sum_{k=0}^{n} \hat{A}_k U^k \hat{f}\cdot 1 = \hat{g}\cdot 1 \tag{2.51}$$

if the real valued function $f(x)$ *is a solution of the differential equation*

$$\sum_{k=0}^{n} A_k \partial_x^k f(x) = g(x). \tag{2.52}$$

Thus each solution of the ODE (2.52) provides a formal power solution of the difference equation (2.51) [and of the umbral equation (2.50)]. However, Eq. (2.51) and (2.50) may have other solutions. Indeed, for a linear difference equation with constant coefficients we have the following theorem.

Theorem 2.5: *Let U be a difference operator of order p and let us assume that the operators* $\hat{A}_k$ *in Eq. (2.50) are constant. Equation (2.51) will then have np linearly independent solutions, n of them umbral ones.*

Proof: Equation (2.51) in this case is a difference equation involving $np+1$ different points. Hence to obtain a solution in a new point we must specify initial conditions in np points. This provides np linearly independent solutions, uniquely defined in the lattice points $x_n=x_0+n\sigma$.[16,31] Now, let us consider the continuous limit of Eq. (2.51). It is a linear partial differential equation of order n, possessing analytic solutions which can be expanded around any nonsingular point. Applying the umbral correspondence to the series expansion of these solutions, we obtain n solutions of Eq. (2.51) which are expressed as formal power series in $(x\beta)^k$, and therefore are elements of the algebra $\mathfrak{F}$. These are the umbral solutions admitted by Eq. (2.51). The remaining $(n-1)p$ do not belong to $\mathfrak{F}$. Q.E.D.

When $\hat{A}_k$ are polynomials in $(x\beta)$, then additional shifts may appear in the explicit form of the equations coming from the umbral equation (2.50) via projection and their order may be different than np.

As an example, let us consider the "umbral Airy equation,"

$$[\Delta^2 + ax\beta]\hat{\Psi} = 0, \quad a = \text{const}. \tag{2.53}$$

For $\Delta^+=(T-1)/\sigma$, $\beta=T^{-1}$, and $\tilde{\Psi}(x)=\hat{\Psi}\cdot 1$ we have

$$\frac{1}{\sigma^2}[\tilde{\Psi}(x+2\sigma) - 2\tilde{\Psi}(x+\sigma) + \tilde{\Psi}(x)] + ax\tilde{\Psi}(x-\sigma) = 0.$$

This is a third order difference equation since it involves the function $\tilde{\Psi}(x)$ at the points $x+2\sigma$, $x+\sigma$, x and $x-\sigma$. For $\Delta=\Delta^s$ Eq. (2.53) would seem to involve infinitely many points,

$$\frac{1}{4\sigma^2}[\tilde{\Psi}(x+2\sigma)-2\tilde{\Psi}(x)+\tilde{\Psi}(x-2\sigma)]+ax\left(\frac{T+T^{-1}}{2}\right)^{-1}\tilde{\Psi}(x)=0. \tag{2.54}$$

However, multiplying Eq. (2.54) by β^{-1} we obtain

$$\frac{1}{4\sigma^2}[\tilde{\Psi}(x+3\sigma)-\tilde{\Psi}(x+\sigma)-\tilde{\Psi}(x-\sigma)+\tilde{\Psi}(x-3\sigma)]+ax\tilde{\Psi}(x)=0. \tag{2.55}$$

This equation is a sixth order difference equation.

As a simple example of umbral and nonumbral solutions, let us consider a first order homogeneous umbral equation with constant coefficients,

$$U\hat{f}=a\hat{f},\quad a\neq 0. \tag{2.56}$$

For $U=\partial_x$, the solution is

$$f(x)=Ae^{ax}. \tag{2.57}$$

Now, let us consider the first order difference operator Δ^+. Equation (2.56) reduces to

$$f(x+\sigma)-f(x)=a\sigma f(x). \tag{2.58}$$

We look for a solution in the form $f(x)=\lambda^x$ and find

$$\lambda=(1+a\sigma)^{1/\sigma}. \tag{2.59}$$

Thus we obtain a single solution

$$f_1(x)=A(1+a\sigma)^{x/\sigma} \tag{2.60}$$

and of course we have

$$\lim_{\sigma\to 0} f(x)=Ae^{ax}. \tag{2.61}$$

The umbral correspondence provides the solution

$$f_u(x)=Ae^{axT^{-1}}\cdot 1. \tag{2.62}$$

Expanding (2.60) and (2.62) in formal power series in a, we find that the two series coincide, i.e., $f_1=f_u$.

For comparison, let us consider the second order difference operator Δ^s. Equation (2.56) in this case yields

$$f(x+\sigma)-f(x-\sigma)=2\sigma a f(x). \tag{2.63}$$

Setting $f(x)=\lambda^x$ we obtain two values of λ and the general solution of Eq. (2.63) in this case is

$$f=A_1(\sqrt{1+a^2\sigma^2}+a\sigma)^{x/\sigma}+A_2(-1)^{x/\sigma}(\sqrt{1+a^2\sigma^2}-a\sigma)^{x/\sigma}=A_1f_1+A_2f_2. \tag{2.64}$$

The first solution has e^{ax} as its continuous limit. The second one does not have a limit for $\sigma\to 0$. The umbral correspondence provides the solution

$$f_u(x)=Ae^{ax[T+T^{-1}/2]^{-1}}\cdot 1 \tag{2.65}$$

[see Eq. (2.39)]. Expanding into formal power series in a we find $f_u=f_1$ and f_2 is nonumbral.

The question arises whether an expression of the type

$$\hat{f} = e^{ax\beta} \tag{2.66}$$

is meaningful, at least in the sense of a formal power series. The problem is that for a general difference operator Δ, the expression for β, given in Eq. (2.38), is quite complicated. If we expand β into a power series in T, it will for $m-l \geqslant 3$ involve infinitely many shifts. Convergence problems may arise. Luckily, it is not Eq. (2.66) itself that provides the umbral solution of a difference equation. Rather, it is the projection of the operator $\hat{f}$ onto a space of functions, or formal power series. The expressions that appear in the corresponding expansions are $P_n(x) = (x\beta)^n \cdot 1$ and these are finite polynomials in x, and in the shifts σ, with well-defined finite coefficients (see Theorem 2.4). As a matter of fact these are the basic polynomials for the difference operator Δ defined in Eq. (2.30).

It follows that if we know a solution of the umbral equation (2.50) for $U=\partial_x$, and have

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n,$$

then for $U=\Delta$ as in (2.30) the corresponding umbral solution will be

$$\hat{f} \cdot 1 = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} P_n(x).$$

The matter of convergence is a separate issue.

Umbral calculus and especially the umbral correspondence also provide us with a powerful tool with which to handle symmetries of linear difference equations, both ordinary and partial ones. On the one hand, we can discretize a linear differential equation, in particular the linear Schrödinger equation, via the (multidimensional) umbral substitutions

$$\partial_{x_i} \overset{\mathcal{R}}{\longrightarrow} \Delta_{x_i}, \quad x_i \overset{\mathcal{R}}{\longrightarrow} x_i \beta_{x_i}, \quad \partial_t \overset{\mathcal{R}}{\longrightarrow} \Delta_t, \quad t \overset{\mathcal{R}}{\longrightarrow} t\beta_t.$$

Lie symmetries, both point and generalized ones, of linear differential equations can be expressed in terms of commuting operators. Since the umbral correspondence preserves commutation relations, it will also preserve symmetries. On the other hand, we may have more symmetries than in the continuous case due to the nonumbral solutions of the determining equations.

III. DISCRETIZATION OF THE TIME-DEPENDENT SCHRÖDINGER EQUATION PRESERVING ALL POINT SYMMETRIES

Before considering discrete space–time, let us first give a detailed and rigorous analysis of the point symmetries of the time-dependent Schrödinger equation in continuous space–time. The results will be presented in a form well suited for the discretization.

A. Point symmetries and commuting operators in continuous space–time

We write the Schrödinger equation in $\mathbb{R}^{n+1}$ as

$$L\psi = 0, \qquad L = i\partial_t - H, \quad H = -\frac{1}{2}\sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2} + \mathrm{V}(\vec{x},t). \tag{3.1}$$

A local Lie point symmetry transformation is generated by a vector field that we write in evolutionary form[47] as

$$\mathbf{v}^E = Q\partial_\psi + Q^* \partial_{\psi^*}, \tag{3.2}$$

$$Q = \eta - \tau\frac{\partial\psi}{\partial t} - \xi_k\frac{\partial\psi}{\partial x_k}. \tag{3.3}$$

The functions η, τ, and ξ_κ depend on t, $\vec{x}$, ψ, and ψ^* where the star denotes complex conjugation. These functions are determined from the requirement

$$pr^{(2)}\mathbf{v}^E(L\psi)|_{L\psi=L^*\psi^*=0} = 0, \quad pr^{(2)}\mathbf{v}^E(L^*\psi^*)|_{L\psi=L^*\psi^*=0} = 0. \tag{3.4}$$

The following theorem will provide a basis for studying the symmetries of a nonrelativistic quantum system.

Theorem 3.1: *All Lie point symmetries of the time-dependent Schrödinger equation (3.1) are generated by evolutionary vector fields of the form (3.2) with*

$$Q = \chi(\vec{x},t) + iX\psi, \tag{3.5}$$

$$X = i(\tau(t)\partial_t + \xi_k(\vec{x},t)\partial_{x_k} - i\phi(\vec{x},t)), \tag{3.6}$$

$$\xi_k(\vec{x},t) = \tfrac{1}{2}x_k\tau' - A_{kl}x_l + f_k(t), \tag{3.7}$$

$$\phi(\vec{x},t) = \frac{1}{4}\tau''r^2 + x_k f_k' + g(t) + i\left[\frac{n}{4}\tau' - B\right], \tag{3.8}$$

where the prime denotes a derivative. The function $\chi(\vec{x},t)$ satisfies the Schrödinger equation (3.1), $A_{kl}=-A_{lk}$ and B are real constants. The real functions $\tau(t)$, $f_k(t)$, $g(t)$ and the constants A_{kl} depend on the potential and satisfy the equation

$$\tau(t)\mathrm{V}_t + \xi_k(\vec{x},t)\mathrm{V}_{x_k} + \tau'\mathrm{V} + \tfrac{1}{4}\tau'''r^2 + x_k f_k'' + g' = 0, \tag{3.9}$$

with $r^2=\Sigma_{k=1}^n x_k^2$. Moreover, the linear operator X commutes with L on the solutions of the Schrödinger equation

$$[L,X]\psi|_{L\psi=0} = 0. \tag{3.10}$$

Proof: Equation (3.4) implies a system of determining equations. Those among them that come from terms involving derivatives of ψ, e.g., $\psi_x\psi_{xx}$, ψ_{xx}, ψ_x^k, $k\geqslant 1$ do not depend on the potential $\mathrm{V}(\vec{x},t)$. From them we obtain the fact that the corresponding transformations are fiber preserving and linear (inhomogeneous). That is, Q has the form (3.3) with τ and ξ_k independent of ψ and ψ^*. From the same equations we find that τ depends only on t and that $\xi_k(\vec{x},t)$ are linear in $\vec{x}$. Thus ξ_k and ϕ have the form (3.7) and (3.8), respectively.

Once these conditions are satisfied, only one determining equation remains, namely Eq. (3.9), involving the potential in a crucial manner.

To prove the commutativity relation (3.10) we use the compatibility of the two flows,

$$i\frac{\partial\psi}{\partial t} = H\psi, \quad \frac{\partial\psi}{\partial\lambda} = Q, \tag{3.11}$$

where λ is a group parameter and Q is the characteristic of the vector field [see Eqs. (3.5)–(3.8)]. Equating the cross derivatives $\psi_{t\lambda}=\psi_{\lambda t}$ and using the equation $L\chi(\vec{x},t)=0$, we obtain

$$[H,X]\psi = -iX_t\psi, \tag{3.12}$$

where ψ is any solution of the Schrödinger equation. This is equivalent to Eq. (3.10). Simply stated, finding point symmetries of the Schrödinger equation is equivalent to finding linear self-adjoint operators X commuting with L on the solution set of L. Q.E.D.

Comments:

(1) For any potential $V_k(\vec{x},t)$, the function $\chi(\vec{x},t)$, the constant B, and a constant $g=g_0$ are solutions of Eq. (3.9). Hence we always have a "trivial" symmetry algebra

$$S(\chi)=\chi(\vec{x},t)\partial_\psi+\chi^*(\vec{x},t)\partial_{\psi^*},\ L\chi=0,$$

$$N=\psi\partial_\psi+\psi^*\partial_{\psi^*}, \tag{3.13}$$

$$E=i(\psi\partial_\psi-\psi^*\partial_{\psi^*}),$$

due to the linearity of the Schrödinger equation.

(2) Each symmetry generator $\mathbf{v}^E$ provides us with a flow that is by construction compatible with the time flow (3.1), that is, we can simultaneously solve the equations (3.11). The fixed point $\partial\psi/\partial\lambda=0$ corresponds to group invariant solutions.

(3) While the result presented in Theorem 3.1 is quite simple and natural, we have not found it explicitly in the literature, so we have sketched a proof. For other results on point symmetries of linear differential equations, see, e.g., Refs. 5, 42, and 8.

Let us consider the implications of Theorem 3.1 for special cases of the potential $V(\vec{x},t)$. We shall omit the operators (3.13) that are present for any potential $V(\vec{x},t)$.

Let us first consider the free Schrödinger equation (for further discussions, see also Ref. 49). For $V(\vec{x},t)=0$ in $\mathbb{R}^{3+1}$ the so-called "Schrödinger group" was first obtained by Niederer.[45] For n arbitrary we obtain its generalization, i.e., the group Sch (n). Its Lie algebra can be written as

$$P_0=\partial_t,\ D=2t\partial_t+x_k\partial_{x_k}-\tfrac{1}{2}(\psi\partial_\psi+\psi^*\partial_{\psi^*}),$$

$$C=t^2\partial_t+tx_k\partial_{x_k}-\frac{1}{2}t(\psi\partial_\psi+\psi^*\partial_{\psi^*})+\frac{in}{4}r^2(\psi\partial_\psi-\psi^*\partial_{\psi^*}),$$

$$L_{ik}=x_i\partial_{x_k}-x_k\partial_{x_i},\ P_k=\partial_{x_k}, \tag{3.14}$$

$$B_k=t\partial_{x_k}+\frac{i}{2}x_k(\psi\partial_\psi-\psi^*\partial_{\psi^*}),$$

$$E=i(\psi\partial_\psi-\psi^*\partial_{\psi^*}).$$

The Levi decomposition[28] of this algebra for $n\geqslant 3$ is

$$\mathfrak{L}\sim[\mathrm{sl}(2,\mathbb{R})\oplus \mathrm{O}(n)]\rhd H_n, \tag{3.15}$$

where the radical H_n is the n-dimensional Heisenberg algebra. Explicitly we have

$$\mathrm{sl}(2,\mathbb{R})\sim\{P_0,D,C\},\ \mathrm{O}(n)\sim\{L_{ik}\},\ H_n\sim\{P_k,B_k,E\}. \tag{3.16}$$

We included the central element E explicitly in (3.14) since it appears in the derived algebra of the Schrödinger algebra [it is also present in (3.13)].

Equation (3.9) implies that for a general time-independent potential $V(\vec{x})$ we have only one additional symmetry generator to the set given by Eqs. (3.13), namely time translations $P_0=\partial_t$.

For a central potential $V=V(r)$, the additional elements are time translations and rotations

$$P_0=\partial_t,\ L_{ik}=x_i\partial_{x_k}-x_k\partial_{x_i},\ 1\leqslant i\leqslant k\leqslant n. \tag{3.17}$$

In the case of a translationally invariant potential $V=V(x_n)$, the additional symmetry elements are

$$P_0 = \partial_t, P_j = \partial_{x_j}, B_j = t\partial_{x_j} - ix_j(\psi\partial_\psi - \psi^* \partial_{\psi^*}),\ \ 1 \leqslant j \leqslant n-1,$$
$$L_{ik} = x_i\partial_{x_k} - x_k\partial_{x_i},\ \ 1 \leqslant i \leqslant k \leqslant n-1. \tag{3.18}$$

B. Symmetries of the discrete time-dependent Schrödinger equation

The umbral correspondence, together with Theorem 3.1 provide the tools necessary for a symmetry preserving discretization of quantum mechanics.

Indeed, let us consider a discrete space–time, more precisely an $n+1$ dimensional orthogonal and equally spaced lattice with time step σ_t and space steps σ_k, $1 \leqslant k \leqslant n$. In this space we write a "Schrödinger difference equation"

$$L_D\psi = 0,\ \ L_D = i\Delta_t - H_D,$$
$$H_D = -\frac{1}{2}\sum_{k=1}^{n} \Delta_{x_k x_k} + V(x_1\beta_1, \ldots, x_n\beta_n, t\beta_t), \tag{3.19}$$

where we have

$$[\Delta_{x_k}, x_k\beta_k] = 1,\ \ [\Delta_t, t\beta_t] = 1. \tag{3.20}$$

Each Δ_{x_k}, Δ_t is some chosen difference operator and β_k, β_t are the corresponding conjugate operators satisfying the Heisenberg commutation relations (3.20).

The continuous limit of Eq. (3.19) is Eq. (3.1), obtained by taking $\sigma_k \to 0$, $\sigma_t \to 0$, i.e.,

$$\Delta_{x_k x_k} \to \frac{\partial^2}{\partial x_k^2},\ \ \Delta_t \to \partial_t,\ \ \beta_i \to 1,\ \ \beta_t \to 1. \tag{3.21}$$

Let us assume that in the continuous limit the obtained Schrödinger equation (3.1) is invariant under some Lie point symmetry group generated by some evolutionary vector field (3.2). Symmetries of linear difference equations on fixed lattices can also be expressed in terms of evolutionary vector fields.[38,40] For Eq. (3.19) we set

$$\mathbf{v}_D^E = Q_D\partial_\psi + Q_D^*\partial_{\psi^*},$$
$$Q_D = \eta_D - \tau_D\Delta_t\psi - \xi_{k_D}\Delta_{x_k}\psi, \tag{3.22}$$

where η_D, τ_D, and ξ_{k_D} are functions of $x_i\beta_i$, $t\beta_t$, ψ, and ψ^*. The functions ψ and ψ^* are to be evaluated at the points $x_i\beta_i$, $t\beta_t$.

The prolongation of the vector field (3.22) must act on the dependent variables ψ and ψ^* and on their discrete derivatives $\Delta_t\psi$, $\Delta_{x_k x_k}\psi$. As in the continuous case, we require that an infinitesimal transformation

$$\tilde{x}_k\tilde{\beta}_k = x_k\beta_k,\ \ \tilde{t}\tilde{\beta}_t = t\beta_t,$$
$$\tilde{\psi}(\tilde{x}_k\tilde{\beta}_k, \tilde{t}\tilde{\beta}_t) = \psi(x_k\beta_k, t\beta_t) + \lambda Q_D,\ \ \lambda \ll 1 \tag{3.23}$$

should take a solution ψ into a solution $\tilde{\psi}$ of the same equation. First of all, we have

$$\tilde{\beta}_k = \beta_k,\ \ \tilde{\beta}_t = \beta_t, \tag{3.24}$$

since β_k and β_t are expressed in terms of shifts operators and we are considering equations on a fixed (not transforming) lattice. Equation (3.23) is an infinitesimal transformation in the evolu-

tionary formalism, hence only the dependent variables transform. The transformation of the discrete derivatives is given by

$$\Delta_t\tilde{\psi} = \Delta_t\psi + \lambda\Delta_t Q_D,$$
$$\Delta_{x_k x_k}\tilde{\psi} = \Delta_{x_k x_k}\psi + \lambda\Delta_{x_k x_k} Q_D, \tag{3.25}$$

where Δ_t, Δ_{x_k}, etc., are discrete total derivatives. One can of course also introduce discrete partial derivatives,[40] but we shall not need them here.

In terms of the vector fields $\mathbf{v}_D^E$of Eq. (3.22) the prolongation of $\mathbf{v}_D^E$ is

$$pr\mathbf{v}_D^E = Q_D\partial_\psi + Q_D^t\partial_{\Delta_t\psi} + Q_D^{x_k x_k}\partial_{\Delta_{x_k x_k}\psi} + \cdots + \text{c.c.}, \tag{3.26}$$

where c.c. denotes the complex conjugate terms and we have

$$Q_D^t = \Delta_t Q_D, \quad Q_D^{x_k x_k} = \Delta_{x_k x_k} Q_D. \tag{3.27}$$

The determining equations for the characteristic Q_D are obtained as in the continuous case, i.e., from the invariance condition

$$pr\mathbf{v}_D^E(L_D\psi)|_{L_D\psi=L_D^*\psi^*=0} = 0, \quad pr\mathbf{v}_D^E(L_D^*\psi^*)|_{L_D\psi=L_D^*\psi^*=0} = 0. \tag{3.28}$$

From this we conclude that the following theorem holds.

Theorem 3.2: *The discrete time-dependent Schrödinger equation (3.19) allows a Lie algebra of "umbral symmetries" isomorphic to that of its continuous limit (3.1). This Lie algebra is realized by vector fields (3.22) with*

$$Q_D = \chi(x_k\beta_k, t\beta_t) + iX_D\psi, \tag{3.29}$$

$$X_D = i\left[\tau(t\beta_t)\Delta_t + \sum_k \xi_k\Delta_{x_k} - i\phi\right], \tag{3.30}$$

$$\xi_k = \frac{1}{2}x_k\beta_k\Delta_t\tau - \sum_{l=1}^n A_{kl}x_l\beta_l + f_k(t\beta_t), \tag{3.31}$$

$$\phi = \left[\frac{1}{4}\Delta_{tt}\tau\sum_{k=1}^n (x_k\beta_k)^2 + \sum_{k=1}^n x_k\beta_k\Delta_t f_k + g(t\beta_t)\right] + i\left[\frac{n}{4}(\Delta_t\tau) - B\right]. \tag{3.32}$$

The function χ satisfies the discrete Schrödinger equation (3.19), $A_{kl}=-A_{lk}$ and B are real constants. The real functions τ, f_k and g all depend only on $t\beta_t$ and the potential $\mathrm{V}(x_k\beta_k, t\beta_t)$ satisfies

$$\tau\Delta_t\mathrm{V} + \sum_{k=1}^n \xi_k\Delta_{x_k}\mathrm{V} + (\Delta_t\tau)\mathrm{V} + \frac{1}{4}(\Delta_{ttt}\tau)\sum_{k=1}^n (x_k\beta_k)^2 + \sum_{k=1}^n x_k\beta_k\Delta_{tt}f_k + \Delta_t g = 0. \tag{3.33}$$

Finally, the difference operator X_D commutes with L_D on the solutions of the discrete Schrödinger equation (3.19):

$$[L_D, X_D]\psi|_{L_D\psi=0} = 0. \tag{3.34}$$

Proof: The proof of Theorem 3.2 is quite analogous to that of Theorem 3.1 in the continuous case. To see the similarities and differences, let us restrict ourselves to the case $n=2$.

The invariance condition (3.28) implies the following determining equations:

$$\xi_{k,\psi} = \xi_{k,\psi^*} = \tau_\psi = \tau_{\psi^*} = 0, \quad \Delta_{x_i}\tau = 0, \quad \phi_{\psi^*} = 0, \quad \phi_{\psi\psi} = 0, \tag{3.35}$$

$$\Delta_{x_1}\xi_2 + \Delta_{x_2}\xi_1 = 0, \tag{3.36}$$

$$\Delta_t\tau - 2\Delta_{x_1}\xi_1 = 0, \quad \Delta_t\tau - 2\Delta_{x_2}\xi_2 = 0, \tag{3.37}$$

$$\begin{aligned} 2i\Delta_t\xi_1 + 2\Delta_{x_1}\phi_{1\psi} + \Delta_{x_1x_1}\xi_1 + \Delta_{x_2x_2}\xi_1 = 0, \\ 2i\Delta_t\xi_2 + 2\Delta_{x_2}\phi_{1\psi} + \Delta_{x_1x_1}\xi_2 + \Delta_{x_2x_2}\xi_2 = 0, \end{aligned} \tag{3.38}$$

$$2\psi\{\tau\Delta_t V + \xi_1\Delta_{x_1}V + \xi_2\Delta_{x_2}V + V\Delta_t\tau + V\phi_\psi\} - 2V\phi + 2i\Delta_t\phi + \Delta_{x_1x_1}\phi + \Delta_{x_2x_2}\phi = 0. \tag{3.39}$$

It is now obvious that Eq. (3.30)–(3.32) (for $n=2$) provide a solution to Eq. (3.35),…, (3.38) and that (3.39) reduces to Eq. (3.33), once (3.35),…, (3.38) are solved. Equation (3.34) then follows in exactly the same manner as in the continuous case. Q.E.D.

Comment:

There is an important difference between the continuous and the discrete case. In Theorem 3.1 we presented the most general solution of the determining equations. In Theorem 3.2 we presented a solution and added the requirement that the solution should have the correct continuous limit. Take for instance the function τ. Equations (3.35) for any Δ_t, Δ_x allow the solution $\tau(t,\beta_t)$, i.e., an arbitrary function of time t and the "shift" operator β_t independently. For first order operators $\Delta^{\pm}$ (see Sec. II), the function τ will depend only on $(t\beta_t)$. This follows from the determining equations, and agrees with the result of umbral correspondence. Moreover, the result will have the correct continuous limit. Thus the discretization and the continuous equation have isomorphic symmetry algebras. For other choices of the discrete derivatives we may get more general solutions. For instance, let us consider the case of a "symmetric" derivative,

$$\Delta_x^s\tau = \frac{T_x - T_x^{-1}}{2\sigma}\tau = \frac{\tau(x+\sigma) - \tau(x-\sigma)}{2\sigma} = 0. \tag{3.40}$$

Equation (3.40) has the general solution

$$\tau = \tau_0(t) + \tau_1(t)e^{i\pi x/\sigma}, \tag{3.41}$$

$$x = x_n = x_0 + n\sigma. \tag{3.42}$$

We see that Eq. (3.40) actually allows an x-dependence in τ. However, the second term in (3.42) does not have a continuous limit (for $\sigma = x_{n+1} - x_n \to 0$). See Ref. 37 for further discussions.

C. Examples

As in the continuous case, for any discrete potential we have the "trivial" symmetries (3.13) (with $\vec{x}$, t, replaced by $x_k\beta_k$, $t\beta_t$).

Let us consider the case $V=0$, i.e., a free quantum particle in discrete space–time of dimension $n+1$. Operators commuting with the operator L_D of Eq. (3.19) are obtained from (3.14) by the umbral correspondence. We obtain the "discrete" Schrödinger algebra

$$P_0 = \Delta_t, \quad D = 2(t\beta_t)\Delta_t + \sum_{k=1}^{n}(x_k\beta_k)\Delta_{x_k} - \frac{1}{2}(\psi\partial_\psi + \psi^*\partial_{\psi^*}),$$

$$C=(t\beta_t)^2\Delta_t+\sum_{k=1}^{n}(t\beta_t)(x_k\beta_k)\Delta_{x_k}-\frac{1}{2}(t\beta_t)(\psi\partial_\psi+\psi^*\partial_{\psi^*})+\frac{in}{4}\sum_{k=1}^{n}(x_k\beta_k)^2(\psi\partial_\psi-\psi^*\partial_{\psi^*}),$$

$$L_{ik}=(x_i\beta_i)\Delta_{x_k}-(x_k\beta_k)\Delta_{x_i},\quad P_k=\Delta_{x_k},\tag{3.43}$$

$$B_k=(t\beta_t)\Delta_{x_k}+\frac{i}{2}(x_k\beta_k)(\psi\partial_\psi-\psi^*\partial_{\psi^*}),$$

$$E=i(\psi\partial_\psi-\psi^*\partial_{\psi^*}).$$

For a general time-independent potential $V(x_i\beta_i)$ we have only one additional [to (3.13)]. symmetry generator, namely time translations $P_0=\Delta_t$.

For a time-independent central potential $V=V(\Sigma_i(x_i\beta_i)^2)$ the additional symmetries are expressed by the operators

$$P_0=\Delta_t,\ L_{ik}=x_i\beta_i\Delta_{x_k}-x_k\beta_k\Delta_{x_i},\ 1\leqslant i\leqslant k\leqslant n.\tag{3.44}$$

For a translationally invariant potential $V=V(x_n\beta_n)$ the additional symmetry operators are

$$P_0=\Delta_t,$$

$$P_j=\Delta_{x_j},\quad B_j=t\beta_t\Delta_{x_j}-ix_j\beta_j(\psi\Delta_\psi-\psi^*\Delta_{\psi^*}),\quad 1\leqslant j\leqslant n-1,\tag{3.45}$$

$$L_{ik}=x_i\beta_i\Delta_{x_k}-x_k\beta_k\Delta_{x_i},\quad 1\leqslant i\leqslant k\leqslant n-1.$$

IV. DISCRETE SUPERINTEGRABLE SYSTEMS

The umbral calculus provides a systematic method for transfering results from standard quantum mechanics to quantum mechanics in a discrete space–time. This is particularly simple if the results are formulated in terms of commuting differential operators. It has been shown elsewhere[56] that there is a direct relation between generalized symmetries in quantum mechanics and higher order differential operators, commuting with the Hamiltonian. Here we shall briefly sum up the results and then adapt them to the discrete case.

A. Generalized symmetries in quantum mechanics

Let us consider the stationary Schrödinger equation in real two-dimensional Euclidean space,

$$H\psi=E\psi,\quad H=-\tfrac{1}{2}\Delta+V(x,y),\tag{4.1}$$

and look for second order generalized symmetries in their evolutionary form $\mathbf{v}^E$ (3.2) with characteristic Q satisfying

$$Q=Q(x,y,\psi,\psi_x,\psi_y,\psi_{xx},\psi_{xy},\psi_{yy}).\tag{4.2}$$

We require that the second prolongation of the vector field $\mathbf{v}^E$ should annihilate Eq. (4.1) on its solution space, i.e.,

$$pr^{(2)}\mathbf{v}^E\,(H-E)\psi\big|_{\substack{H\psi=E\psi\\ H\psi^*=E\psi^*}}=0,\quad pr^{(2)}\mathbf{v}^E\,(H-E)\psi\big|_{\substack{H\psi=E\psi\\ H\psi^*=E\psi^*}}=0.\tag{4.3}$$

If we also require that Q be energy independent, we obtain the following result.

Theorem 4.1: *The characteristic Q of the evolutionary vector field $\mathbf{v}^E=Q\partial_\psi+Q^*\partial_{\psi^*}$, corresponding to a second order generalized symmetry of the Schrödinger equation (4.1) has the form*

$$Q = X\psi + \chi(x,y), \tag{4.4}$$

$$X = aL_3^2 + b(L_3P_1 + P_1L_3) + c(L_3P_2 + P_2L_3) + d(P_1^2 - P_2^2) + 2eP_1P_2 + \alpha L_3 + \beta P_1 + \gamma P_2 + \phi(x,y). \tag{4.5}$$

The function $\chi(x,y)$ satisfies the Schrödinger equation (4.1). The operator X commutes with the Hamiltonian H,

$$[H,X] = 0. \tag{4.6}$$

The quantities $a,\ldots,e,\alpha,\beta,\gamma$ are constants and

$$P_1 = \partial_x,\ \ P_2 = \partial_y,\ \ L_3 = y\partial_x - x\partial_y \tag{4.7}$$

are generators of the Euclidean group E_2.

For a proof of Theorem 4.1, see Ref. 56.

The commutativity relation (4.6) is equivalent to the following linear partial differential equations satisfied by the potential $V(x,y)$ and the function $\phi(x,y)$,

$$[\alpha(y\partial_x - x\partial_y) + \beta\partial_x + \gamma\partial_y]V(x,y) = 0, \tag{4.8}$$

$$\begin{aligned}(-axy - bx + cy + e)(V_{xx} - V_{yy}) + [a(x^2 - y^2) - 2by - 2cx - 2d]V_{xy}\\ - 3(ay + b)V_x + 3(ax - c)V_y = 0,\end{aligned} \tag{4.9}$$

$$\phi_x = -2(ay^2 + 2by + d)V_x + 2(axy + bx - cy - e)V_y, \tag{4.10}$$

$$\phi_y = 2(axy + bx - cy - e)V_x + 2(-ax^2 + 2cx + d)V_y. \tag{4.11}$$

Here Eq. (4.9) is the compatibility condition for the two equations (4.10) and (4.11). Equation (4.8) is easily solved.

For $\alpha \neq 0$ we can translate x and y to transform $\beta \to 0,\ \gamma \to 0$. Then the potential is rotationally invariant, $V = V(r)$.

For $\alpha = 0,\ \beta^2 + \gamma^2 \neq 0$ we can rotate to obtain $\beta \to 0$. Then the potential is translationally invariant, $V = V(x)$.

To avoid the geometric symmetries (4.7) we solve Eq. (4.8) trivially by imposing $\alpha = \beta = \gamma = 0$. We then simplify the second order operator X of Eq. (4.5) by rotations, translations, and linear combinations with the Hamiltonian H.

These transformations leave two expressions in the space of the coefficients $a,\ldots,e$ invariant, namely

$$I_1 = a,\ \ I_2 = [(2ad - b^2 + c^2)^2 + 4(ae - bc)^2]. \tag{4.12}$$

In the nongeneric case when $I_1 = I_2 = 0$, a third invariant exists, namely

$$I_3 = d^2 + e^2. \tag{4.13}$$

Using these invariants, one obtains four equivalence classes of operators X and correspondingly, four classes of potentials allowing for the existence of an operator X, commuting with the Hamiltonian.[64,56] The existence of one second order operator X, satisfying (4.6) makes the system integrable. Moreover, the corresponding Schrödinger equation will allow separation of variables in Cartesian, polar, parabolic or elliptic coordinates. Which is the separable system depends on the values of the invariants (4.12) and (4.13).

We are interested in the case of superintegrable Hamiltonians, when two operators X_1 and X_2 exist, satisfying

$$[H,X_1]=[H,X_2]=0,\ \ [X_1,X_2]\neq 0. \tag{4.14}$$

Four classes of such potentials exist, each allowing the separation of variables in at least two coordinate systems. The Hamiltonians and corresponding integrals of motion are

(1)

$$\begin{aligned} H_{\mathrm{I}} &= -\frac{1}{2}(\partial_x^2+\partial_y^2)+\frac{\omega^2}{2}(x^2+y^2)+\frac{a}{2x^2}+\frac{b}{2y^2},\\ \hat{X}_1 &= P_1^2-P_2^2-\left[\omega^2(x^2-y^2)+\frac{a}{x^2}-\frac{b}{y^2}\right],\\ \hat{X}_2 &= L_3^2-\left(\frac{a}{\cos^2\phi}+\frac{b}{\sin^2\phi}\right),\\ x &= r\cos\phi,\ \ y=r\sin\phi. \end{aligned} \tag{4.15}$$

(2)

$$\begin{aligned} H_{\mathrm{II}} &= -\frac{1}{2}\left(\partial_x^2+\partial_y^2\right)+\omega^2\left(2x^2+\frac{y^2}{2}\right)+\frac{a}{2y^2}+bx,\\ \hat{X}_1 &= P_1^2-P_2^2-\left[\omega^2(4x^2-y^2)+bx-\frac{a}{y^2}\right],\\ \hat{X}_2 &= L_3P_2+P_2L_3-2\omega^2xy^2+\frac{2ax}{y^2}-by^2. \end{aligned} \tag{4.16}$$

The remaining two systems are best written in parabolic coordinates,

$$x=\tfrac{1}{2}(\xi^2-\eta^2),y=\xi\eta. \tag{4.17}$$

(3)

$$\begin{aligned} H_{\mathrm{III}} &= -\frac{1}{2}\frac{1}{\xi^2+\eta^2}(\partial_\xi^2+\partial_\eta^2)+\frac{1}{\xi^2+\eta^2}\left(2a+\frac{b}{\xi^2}+\frac{c}{\eta^2}\right),\\ X_1 &= L_3^2-2(\xi^2+\eta^2)\left(\frac{b}{\xi^2}+\frac{c}{\eta^2}\right),\\ X_2 &= L_3P_2+P_2L_3+\frac{2}{\xi^2+\eta^2}\left(a(\xi^2-\eta^2)-b\frac{\eta^2}{\xi^2}+c\frac{\xi^2}{\eta^2}\right). \end{aligned} \tag{4.18}$$

(For $b=c=0$, $a\neq 0$ this is the Coulomb atom.) The system allows separation of variables in polar and parabolic coordinates (and also in elliptic coordinates).

(4)

$$\begin{aligned} H_{\mathrm{IV}} &= -\frac{1}{2}\frac{1}{\xi^2+\eta^2}(\partial_\xi^2+\partial_\eta^2)+\frac{2a+b\xi+c\eta}{\xi^2+\eta^2},\\ \hat{X}_1 &= L_3P_1+P_1L_3+\frac{b\eta(\eta^2-\xi^2)+c\xi(\xi^2-\eta^2)-4a\eta\xi}{(\xi^2+\eta^2)}, \end{aligned} \tag{4.19}$$

$$\hat{X}_2 = L_3P_2 + P_2L_3 + 2\frac{a(\xi^2 - \eta^2) + \eta\xi(c\xi - b\eta)}{(\xi^2 + \eta^2)}.$$

The equation separates in two mutually orthogonal parabolic coordinate systems, namely (4.17) and a similar system with x and y interchanged. For $a \neq 0$, $b=c=0$ we again obtain the Coulomb atom.

We shall call the systems H_{I} and H_{II} the *generalized isotropic* and *generalized nonisotropic harmonic oscillators*, respectively. Similarly, H_{III} and H_{IV} can both be called *generalized Coulomb systems.*

The Schrödinger equations for H_{III} and H_{IV} can be rewritten as

$$\left\{-\frac{1}{2}(\partial_\xi^2 + \partial_\eta^2) - E(\xi^2 + \eta^2) + \frac{b}{2\xi^2} + \frac{c}{2\eta^2}\right\}\psi = -a\psi, \tag{4.20}$$

$$\left\{-\frac{1}{2}(\partial_\xi^2 + \partial_\eta^2) - E\left[\left(\xi - \frac{b}{2E}\right)^2 + \left(\eta - \frac{c}{2E}\right)^2\right]\right\}\psi = \left(-2a - \frac{b^2 + c^2}{4E^2}\right)\psi, \tag{4.21}$$

respectively. Thus, the system H_{III} is reduced to H_{I} with the energy $(-E)$ and coupling constant ω^2 interchanged. The system H_{IV} is reduced to a "shifted" harmonic oscillator. This interchange of the energy and a coupling constant has been called "metamorphosis of the coupling constant."[26]

B. Discrete generalized harmonic oscillators

The umbral correspondence immediately provides us with discrete versions of these systems. Let us first consider the potential V_{I} of Eq. (4.15). The discrete version of this system is

$$H_{\mathrm{I}}^D = -\frac{1}{2}(\Delta_x^2 + \Delta_y^2) + \frac{\omega^2}{2}[(x\beta_x)^2 + (y\beta_y)^2] + \frac{a}{2}(x\beta_x)^{-2} + \frac{b}{2}(y\beta_y)^{-2} \tag{4.22}$$

with the integrals of motion

$$X_1 = [-\tfrac{1}{2}\Delta_x^2 + \omega^2(x\beta_x)^2 + a(x\beta_x)^{-2}] - [-\tfrac{1}{2}\Delta_y^2 + \omega^2(y\beta_y)^2 + b(y\beta_y)^{-2}] \tag{4.23}$$

and

$$X_2 = (x\beta_x\Delta_y - y\beta_y\Delta_x)^2 - [a(1 + (x\beta_x)^{-2}(y\beta_y)^2) + b(1 + (x\beta_x)^2(y\beta_y)^{-2})]. \tag{4.24}$$

Similarly, the discrete version of the system with potential V_{II} is

$$H_{\mathrm{II}}^D = -\frac{1}{2}(\Delta_x^2 + \Delta_y^2) + \omega^2\left[2(x\beta_x)^2 + \frac{1}{2}(y\beta_y)^2\right] + \frac{a}{2}(y\beta_y)^{-2} + bx\beta_x. \tag{4.25}$$

The second order operators commuting with the Hamiltonian (4.25) are

$$X_1 = \Delta_x^2 - \Delta_y^2 - [\omega^2(4(x\beta_x)^2 - (y\beta_y)^2) + b(x\beta_x) - a(y\beta_y)^{-2}] \tag{4.26}$$

and

$$X_2 = [(y\beta_y)\Delta_x - (x\beta_x)\Delta_y]\Delta_y + \Delta_y[(y\beta_y)\Delta_x - (x\beta_x)\Delta_y] - 2\omega^2(x\beta_x)(y\beta_y)^2 + 2a(x\beta_x)(y\beta_y)^{-2} - b(y\beta_y)^2. \tag{4.27}$$

The model (4.15) has also been discretized in Ref. 62 using the formalism of raising and lowering operators.

C. Discrete generalized Coulomb potentials

To discretize the systems H_{III} and H_{IV} we again use the umbral correspondence, this time using parabolic coordinates. Thus, we replace

$$\partial_\xi \to \Delta_\xi,\ \partial_\eta \to \Delta_\eta,\ \xi \to \xi\beta_\xi,\ \eta \to \eta\beta_\eta. \tag{4.28}$$

With these replacements it is a simple matter to write the discrete versions of the systems corresponding to the potentials V_{III} and V_{IV}. Indeed, we have

$$H_{\mathrm{III}} = -\tfrac{1}{2}[(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2]^{-1}[\Delta_\xi^2 + \Delta_\eta^2 - 4a - 2b(\xi\beta_\xi)^{-2} - 2c(\eta\beta_\eta)^{-2}], \tag{4.29}$$

$$X_1 = [(\xi\beta_\xi)\Delta_\eta - (\eta\beta_\eta)\Delta_\xi]^2 - 2[(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2][b(\xi\beta_\xi)^{-2} + c(\eta\beta_\eta)^{-2}], \tag{4.30}$$

$$\begin{aligned} X_2 = {} & [(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2]^{-1}\{(\eta\beta_\eta)^2\Delta_\xi^2 - (\xi\beta_\xi)^2\Delta_\eta^2 + 2a[(\xi\beta_\xi)^2 - (\eta\beta_\eta)^2] - 2b(\eta\beta_\eta)^2(\xi\beta_\xi)^{-2} \\ & + 2c(\xi\beta_\xi)^2(\eta\beta_\eta)^{-2}\}, \end{aligned} \tag{4.31}$$

and

$$H_{\mathrm{IV}} = -\tfrac{1}{2}[(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2]^{-1}[\Delta_\xi^2 + \Delta_\eta^2 - 4a - 2b(\xi\beta_\xi) - 2c(\eta\beta_\eta)], \tag{4.32}$$

$$\begin{aligned} X_1 = {} & [(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2]^{-1}\{(\xi\beta_\xi)(\eta\beta_\eta)(\Delta_\xi^2 + \Delta_\eta^2) + [-b(\eta\beta_\eta) + c(\xi\beta_\xi)][(\xi\beta_\xi)^2 - (\eta\beta_\eta)^2] \\ & - 4a(\xi\beta_\xi)(\eta\beta_\eta)\} - \Delta_{\xi\eta}^2, \end{aligned} \tag{4.33}$$

$$\begin{aligned} X_2 = {} & \tfrac{1}{2}[(\xi\beta_\xi)^2 + (\eta\beta_\eta)^2]^{-1}\{(\eta\beta_\eta)^2\Delta_\xi^2 - (\xi\beta_\xi)^2\Delta_\eta^2 + 2a[(\xi\beta_\xi)^2 - (\eta\beta_\eta)^2] \\ & + 2(\xi\beta_\xi)(\eta\beta_\eta)[c(\xi\beta_\xi) - b(\eta\beta_\eta)]\}. \end{aligned} \tag{4.34}$$

V. EXACT SOLVABILITY AND SPECTRAL PROPERTIES OF DISCRETE SUPERINTEGRABLE SYSTEMS

We have shown that certain important properties of the Schrödinger equation, such as point and generalized symmetries, and hence also integrability, are preserved when we pass from continuous to discrete space–time via an umbral correspondence.

Another important property of some quantum systems is their "exact solvability." This means that their Hamiltonian can be transformed into a block diagonal form with finite-dimensional blocks. In other words, their complete energy spectrum can be calculated algebraically. In more mathematical terms, we give the following definition.

Definition 5.1: A quantum mechanical system with Hamiltonian H is called exactly solvable if its Hilbert space S of bound states consists of a flag of finite-dimensional subspaces,

$$S_0 \subset S_1 \subset S_2 \subset \cdots \subset S_n \subset \cdots \tag{5.1}$$

preserved by the Hamiltonian

$$HS_i \subseteq S_i. \tag{5.2}$$

All known exactly solvable systems also have the following properties.

(1) In appropriate coordinates and in an appropriate gauge, the bound state wave functions $\Psi_N(\vec{x})$ are polynomials,

$$\Psi_N(\vec{x}) = g(\vec{x})P_N(\vec{s}),\ \ s_i = s_i(\vec{x}). \tag{5.3}$$

The gauge factor $g(\vec{x})$ is *a priori* defined and can be energy dependent. The function $P_N(\vec{s})$

are polynomials of order N in the variables s_i. The integer N labels the subspaces S_i in the flag.

(2) In the same gauge g and same variables s_i the Hamiltonian H can be written as

$$H = ghg^{-1}, \quad hP_N = E_N P_N \tag{5.4}$$

with

$$h = a_{ik}^{\alpha} T_{ik}^{\alpha} + a_{ik,lm}^{\alpha\beta} T_{ik}^{\alpha} T_{lm}^{\beta}, \tag{5.5}$$

where a_{ik}^{α} and $a_{ik,lm}^{\alpha\beta}$ are constants (subject to some further conditions[21]) and

$$T_{ik}^{\alpha} = s_i^{\alpha} \partial_{s_k}, \quad \alpha = 0,1, \quad i,k = 1, \ldots, n. \tag{5.6}$$

In other words, the gauge rotated Hamiltonian h is an element of the enveloping algebra of an affine Lie algebra aff$(n,\mathbb{R})$ (or one of its subalgebras). It is clear that (5.5) guarantees that the Hamiltonian H will preserve, or decrease the order of the polynomials P_N. This is a concrete realization of the flag condition (5.2).

We mention that all known quadratically superintegrable systems are exactly solvable, in particular those of Sec. IV.[58] For the generalized harmonic oscillators the gauge factor g is equal to the ground state wave function and is energy independent. The generalized Coulomb systems have been reduced to the harmonic oscillator ones [see (4.20) and (4.21)]. However, due to the interchange of the energy and the coupling constant, the gauge factor g will be energy dependent.

The aim of this section is to show how exact solvability manifests itself in discrete space–time. First of all, let us consider an arbitrary one-dimensional linear spectral problem

$$L(\partial_x, x)\psi(x) = \lambda\psi(x). \tag{5.7}$$

Let $x=0$ be a regular point of this equation. Then any solution can be expanded into a Taylor series

$$\psi(x) = \sum_{k=0}^{\infty} a_k x^k. \tag{5.8}$$

Using the umbral correspondence we write the umbral equation

$$L(\Delta, x\beta)\psi(x\beta) = \lambda\psi(x\beta) \tag{5.9}$$

with the same eigenvalue λ as in the ODE (5.7). Viewed as a difference equation, Eq. (5.9) will have a formal power series solution,

$$\psi(x\beta)1 = \sum_{k=0}^{\infty} a_k^k (x\beta)^k \cdot 1. \tag{5.10}$$

In particular, if (5.8) is a polynomial solution, then Eq. (5.10) will also be a finite sum of terms involving the basic polynomials of the operator Δ. Thus, (5.10) will also be a polynomial and all convergence problems disappear.

Now let us turn to the specific case of the generalized harmonic oscillator system with Hamiltonian H_{I} [see Eq. (4.15)] and its discretization (4.22). The gauge factor g of Eq. (5.3) and (5.4) is

$$g = x^{p_1} y^{p_2} \exp\left[-\frac{\omega(x^2+y^2)}{2} \right], \quad a = p_1(p_1-1), \quad b = p_2(p_2-1). \tag{5.11}$$

We set $\omega x^2 = s_1$, $\omega y^2 = s_2$ and in these variables the aff$(2,\mathbb{R})$ operators of Eq. (5.6) reduce to

$$J_1 = \partial_{s_1}, \quad J_2 = \partial_{s_2}, \quad J_3 = s_1\partial_{s_1}, \quad J_4 = s_2\partial_{s_2},$$

$$J_5 = s_2\partial_{s_1},\ \ J_6 = s_1\partial_{s_2}. \tag{5.12}$$

The gauge rotated Hamiltonian h and gauge rotated integrals of motion $\hat{x_1}=g\hat{X}_1g^{-1}$, $\hat{x_2}=g\hat{X}_2g^{-1}$ can now be written as[58]

$$h = -2J_3J_1 - 2J_4J_2 + 2J_3 + 2J_4 - (2p_1+1)J_1 - (2p_2+1)J_2,$$

$$\hat{x_1} = 2J_3J_1 - 2J_4J_2 - 2J_3 + 2J_4 + (2p_1+1)J_1 - (2p_2+1)J_2, \tag{5.13}$$

$$\hat{x_2} = 4J_3J_5 + 4J_4J_6 - 8J_3J_4 + 2(2p_1+1)J_5 - 2(2p_2+1)J_3 - 2(2p_1+1)J_4 + 2(2p_2+1)J_6.$$

By construction, all three of these operators will conserve the flag of polynomials

$$P_n(s_1,s_2) = \langle (s_1)^{N_1}(s_2)^{N_2} | 0 \leqslant N_1 + N_2 \leqslant n \rangle \tag{5.14}$$

and this is the reason why the superintegrable system with Hamiltonian H_{I} is exactly solvable. The actual solutions of Eq. (5.4) are Laguerre polynomials,

$$\begin{gathered} HP_{nm} = E_{nm}P_{nm},\ \ E_{mn} = n+m, \\ P_{nm}(x,y) = L_n^{(-1/2+p_1)}(\omega x^2)L_m^{(-1/2+p_2)}(\omega y^2). \end{gathered} \tag{5.15}$$

The umbral discretization will preserve the above properties and will give umbral Laguerre polynomial expressed in terms of $x\beta_x$ and $y\beta_y$. The algebra aff$(2,\mathbb{R})$ is represented by difference operators,

$$\begin{gathered} \tilde{J}_1 = \Delta_{s_1},\ \ \tilde{J}_2 = \Delta_{s_2},\ \ \tilde{J}_3 = (s_1\beta_1)\Delta_{s_1},\ \ \tilde{J}_4 = (s_2\beta_2)\Delta_{s_2}, \\ \tilde{J}_5 = (s_2\beta_2)\Delta_{s_1},\ \ \tilde{J}_6 = (s_1\beta_1)\Delta_{s_2}. \end{gathered} \tag{5.16}$$

The formulas (5.13) remain the same (with $J_i \to \widetilde{J_i}$) and all commutation relations are preserved, as are polynomial solutions. For similar results formulated in terms of operators acting in Fock spaces and the notion of isospectral discretization see Turbiner *et al.* (Refs. 60–63, 57, and 10), and Ref. 11 for further discussions.

We mention here that other discretizations of superintegrable systems, especially the harmonic oscillator, exist in the literature.[2–4,27] They are either related to quantum groups, or the discretization is based on noncommuting coordinates in configuration space.

VI. CONCLUSIONS

Much, if not all of nonrelativistic quantum mechanics can be viewed as the "theory of the enveloping algebra of the Heisenberg algebra."

Indeed, let us define the Heisenberg algebra H_n by the relations

$$[X_j, Y_k] = \delta_{jk}C,\ \ j,k = 1,\ldots,n, \tag{6.1}$$

and then set

$$X_j = x_j,\ Y_k = -i\hbar\partial_{x_k},\ C = i\hbar. \tag{6.2}$$

We can say that all quantum mechanical operators lie in the enveloping algebra of H_n, or in an extension of the enveloping algebra obtained by adding all formal power series in $x_1,\ldots,x_n$, $p_1,\ldots,p_n$.

If we replace the coordinates x_j and the momenta p_j by some other quantities satisfying the relations (6.1) then all polynomials and all power series in these objects will commute in the same way as the corresponding quantum mechanical quantities.

Indeed, the umbral correspondence $x_i \to x_i \beta_i$, $\partial_{x_i} \to \Delta_{x_i}$ preserves the commutation relations (6.1) between quantum mechanical operators. Thus, the umbral correspondence allows us to consider quantum mechanics on a lattice and to preserve all properties of quantum mechanics in continuous space and time that are expressed in terms of the commutation properties of physical quantities (quantum mechanical operators). In particular, infinitesimal point symmetries and generalized symmetries are preserved, as shown in Secs. III and IV, respectively. Exact solvability is reduced to an algebraic property and then discretized in Sec. V (and also in Refs. 57, 62, and 63).

Some nonalgebraic properties are lost in the discretization. For instance, the "umbral vector fields" (2.29), obtained by the umbral correspondence, do not generate global transformations (like rotations, or dilations). The solutions of umbral equations (obtained by the umbral correspondence) are often formal, i.e., they may diverge.

The physical content of this paper is based on the results contained in Sec. II, where we presented and proved several theorems that, to our knowledge, extend the previously known umbral formalism to linear difference equations. In particular we associate with a linear differential equation an abstract operator equation, written in terms of delta operators, using the umbral correspondence (2.23). Any representation of Δ and β in terms of shift-invariant operators provides a difference equation, whose analytic solutions can be obtained from the solutions $\hat{f}$ of the operator equation (2.50) via the projection $\hat{f} \cdot 1 = f(x\beta) \cdot 1$. These are the umbral solutions admitted by a given difference equation. The other possible solutions do not have a continuous limit and are not provided by the umbral approach.

Many of the results presented here can be considered also in the case of q-difference operators.[34] The delta operator U in this case is defined in terms of a q-shift operator satisfying

$$T_q f(x) = f(qx). \tag{6.3}$$

In the simplest case, the q-difference operator reads

$$\Delta_q = \frac{1}{(q-1)x}(T_q - 1), \quad \lim_{q \to 1} \Delta_q f = f_x \tag{6.4}$$

and its conjugate operator, obtained imposing the Heisenberg commutation relation,

$$[\Delta_q, x\beta_q] = 1, \tag{6.5}$$

is written in terms of a q shift and differential operators as

$$\beta_q = (q-1)(qT - 1)^{-1} x \partial_x. \tag{6.6}$$

In this case we can still consider the umbral correspondence, but the Δ_q operator is not a shift invariant operator, as $[\Delta_q, T_q] \neq 0$.

Among open questions, presently under consideration, we mention the following.

(i) This paper deals with the Lie-algebraic aspects of the discretization of the Schrödinger equation. The analytic aspects, like the self-adjointness properties of the discrete Hamiltonians, and the convergence properties of the formal power series remain to be investigated.

(ii) The umbral correspondence has lead us to various linear umbral equations and difference equations. It would be of considerable interest to study their solutions directly and in the case of polynomial solutions, establish their relation to orthogonal polynomials of discrete variables, known in the literature.[50,46]

(iii) Although many of the results presented in this paper can also be carried out in the q-difference case,[34,29,33] a reformulation of the umbral theory in this case is necessary.

(iv) The connection between umbral calculus, delay equations and functional analysis should be studied.

(v) The simultaneous diagonalization of commuting sets of second order differential operators is intimately related to the separation of variables in the Schrödinger equation. It would be important to further investigate common solutions of commuting sets of difference operators from this point of view. An example of such a study is given in the Appendix, where we present solutions of an "umbral Klein–Gordon equation."

(vi) A related problem is that of establishing a connection between umbral formalisms introduced in different coordinate systems, e.g., the Cartesian quantities Δ_x, Δ_y, β_x, β_y and the corresponding polar ones, or parabolic ones Δ_ξ, Δ_η, β_ξ, β_η introduced in Secs. IV and V.

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APPENDIX: DISCRETIZATION OF A RELATIVISTIC WAVE EQUATION

Let us consider a relativistic wave equation in two dimensions,

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial z^2}\right)\phi = k\phi. \tag{A1}$$

In light-cone coordinates

$$x = \frac{z+t}{2},\ y = \frac{z-t}{2},$$

we write this equation as

$$R\phi = \frac{\partial^2}{\partial x \partial y}\phi(x,y) = -k\phi. \tag{A2}$$

Equation (A2) is invariant under the Poincaré group of two-dimensional Minkowski space. Its symmetry algebra is given by

$$P_0 = \partial_x,\ P_1 = \partial_y,\ M = x\partial_x - y\partial_y. \tag{A3}$$

Since the operators R and M commute, we can construct common eigenfunctions satisfying

$$M\phi = \lambda\phi, \tag{A4}$$

in addition to Eq. (A2). The solution of Eq. (A4) can be written as monomials $x^{n+\lambda}y^n$, or more generally

$$\phi_\lambda(x,y) = \sum_{n=0}^{\infty} a_n x^{n+\lambda} y^n \tag{A5}$$

(we choose not to follow the standard procedure of separating variables). Substituting (A5) into Eq. (A2) we obtain the recursion relation

$$a_{n+1}(n+\lambda+1)(n+1) = -ka_n, \tag{A6}$$

i.e.,

$$a_n = (-k)^n a_0 \frac{\Gamma(\lambda+1)}{\Gamma(\lambda+n+1)n!}. \tag{A7}$$

With a_n as in Eq. (A7) we write the (unnormalized) solution (A5) as

$$\phi_{\lambda k} = x^\lambda \sum_{n=0}^{\infty} (-k)^n \frac{1}{\Gamma(\lambda+n+1)n!}(xy)^n. \tag{A8}$$

This can be rewritten as

$$\phi_{\lambda k}(x,y) = \frac{1}{(k)^{\lambda/2}}\left(\frac{x}{y}\right)^{\lambda/2} J_\lambda(2\sqrt{kxy}), \tag{A9}$$

where $J_\nu(z)$ is a cylindrical function. The umbral version of the system (A2) and (A4) is

$$\Delta_x \Delta_y \psi = -k\psi, \tag{A10}$$

$$(x\beta_x \Delta_x - y\beta_y \Delta_y)\psi = \lambda\psi. \tag{A11}$$

Since Eq. (A5) is a power series we can immediately write the corresponding solution of Eq. (A1) as

$$\psi_\lambda(x,y) = \sum_{n=0}^{\infty} a_n (x\beta_x)^{n+\lambda}(y\beta_y)^n \cdot 1. \tag{A12}$$

Setting $\psi_\lambda(x,y)$ into Eq. (A10), we reobtain the two-term recursion relation (A6) with the solution (A7). The solution of the umbral system (A10) and (A11), is hence

$$\psi_\lambda(x,y) = (x\beta_x)^\lambda \sum_{n=0}^{\infty} \frac{(-k)^n}{\Gamma(\lambda+n+1)n!}(x\beta_x)^n(y\beta_y)^n \cdot 1. \tag{A13}$$

Equation (A13) provides a formal power series solution for any choice of the difference operators Δ_x, Δ_y and the corresponding conjugate operators β_x, β_y. If the series converges, then Eq. (A13) is a solution of the system (A10) and (A11).

Let us fix the values of x and y and apply the ratio test of convergence to the series (A13). The ratio of two consecutive terms is

$$\frac{a_{n+1}}{a_n} = -k \frac{1}{(\lambda+n+1)(n+1)} \frac{(x\beta_x)^{n+1}}{(x\beta_x)^n} \frac{(y\beta_y)^{n+1}\cdot 1}{(y\beta_y)^n \cdot 1}.$$

The value of this limit depends on our choice of Δ_x and Δ_y, and hence of β_x and β_y.

For the right and left derivatives Δ^+ and Δ^-, we have $\beta = T^{-1}$ and T, respectively, and hence

$$\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right| = |k| \lim_{n\to\infty}\left|\frac{(x \mp n\sigma_x)(y \mp n\sigma_y)}{(\lambda+n+1)(n+1)}\right| = |k\sigma_x\sigma_y|. \tag{A14}$$

We see that the series (A13) converges (absolutely) for any finite values of x and y, provided we have

$$|k\sigma_x\sigma_y| < 1. \tag{A15}$$

It is interesting to compare the two series expansions (A8) and (A13). In the continuous case we can introduce "polar" coordinates (ρ, α)

$$x = \frac{\rho}{2}e^{\alpha}, \quad y = \frac{\rho}{2}e^{-\alpha}, \tag{A16}$$

and Eq. (A8) then corresponds to the separation of variables

$$\phi_{\lambda k}(x,y) = e^{\lambda\alpha}\sum_{n=0}^{\infty}(-k)^n \frac{1}{n!\Gamma(\lambda+n+1)}\left(\frac{\rho}{2}\right)^{2n+\lambda} = e^{\lambda\alpha}k^{-\lambda/2}J_{\lambda}(\sqrt{k\rho}). \tag{A17}$$

In the discrete case we obtain a solution of the difference scheme by applying ψ_λ of Eq. (A13) to a constant. This is however not a separated solution, since $[(x\beta_x)(y\beta_y)]^n$ is not a function of xy alone. For example, for $\beta_i = T_i^{-1}$ and $n=2$ we have

$$[(xT_x^{-1})(yT_y^{-1})]^2 = x(x-\sigma_x)y(y-\sigma_y)T_x^{-2}T_y^{-2}.$$

Thus, separation of variables techniques in the discrete case lead to very specific "umbral" solutions like (A13). They only separate in the continuum limit. See also Refs. 17, 18, and 44 on simultaneous eigenfunctions of commuting difference operators.

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Stability of spot and ring solutions of the diblock copolymer equation

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The Γ-convergence theory shows that under certain conditions the diblock copolymer equation has spot and ring solutions. We determine the asymptotic properties of the critical eigenvalues of these solutions in order to understand their stability. In two dimensions a threshold exists for the stability of the spot solution. It is stable if the sample size is small and unstable if the sample size is large. The stability of the ring solutions is reduced to a family of finite dimensional eigenvalue problems. In one study no two-interface ring solutions are found by the Γ-convergence method if the sample is small. A stable two-interface ring solution exists if the sample size is increased. It becomes unstable if the sample size is increased further. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1782280]

I. INTRODUCTION

A diblock copolymer is a soft material, characterized by fluidlike disorder on the molecular scale and a high degree of order at longer length scales. A molecule in a diblock copolymer is a linear subchain of *A* monomers grafted covalently to another subchain of *B* monomers. Because of the repulsion between the unlike monomers, the different type subchains tend to segregate, but as they are chemically bonded in chain molecules, segregation of subchains cannot lead to a macroscopic phase separation. Only a local microphase separation occurs: microdomains rich in *A* and *B* emerge. These microdomains form morphology patterns/phases in a larger scale.

The Ohta–Kawasaki[21] free energy of an incompressible diblock copolymer melt is a functional of the *A* monomer density field. Let $u(x)$ be the relative *A* monomer number density at point x in the sample D. When there is high *A* monomer concentration at x, $u(x)$ is close to 1; when there is high concentration of *B* monomers at x, $u(x)$ is close to 0. A value of $u(x)$ between 0 and 1 means that a mixture of *A* and *B* monomers occupies x. The re-scaled, dimensionless free energy of the system is

$$I(u) = \int_D \left\{ \frac{\epsilon^2}{2} |\nabla u|^2 + \frac{\epsilon\gamma}{2} |(-\Delta)^{-1/2}(u-a)|^2 + W(u) \right\} dx, \tag{1.1}$$

which is defined in the admissible set

$$X_a = \{u \in W^{1,2}(D) : \overline{u} = a\}, \tag{1.2}$$

where $\overline{u} = (1/|D|)\int_D u\, dx$ is the average of u in D. a is a fixed constant in (0,1). It is the ratio of the number of the *A* monomers to the number of all the monomers in a chain molecule.

In (1.1) ϵ is a small positive parameter and γ is a fixed positive constant, i.e.,

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$$\epsilon \to 0, \quad \gamma \sim 1. \tag{1.3}$$

The term $W(u)$ is the internal energy field. Originally in Choksi and Ren[8] it is taken to be

$$W(u) = \begin{cases} u - u^2 & \text{if } u \in [0,1] \\ \infty & \text{otherwise.} \end{cases} \tag{1.4}$$

Here we change it to a smooth function so that W is a double well potential of equal depth. It has global minimum value 0 achieved at 0 and 1. We assume for simplicity that W is smooth, grows at least quadratically at $\pm\infty$, and symmetric about 1/2: $W(u)=W(1-u)$. 0 and 1 are nondegenerate: $W''(0)=W''(1)>0$. An example of W is $W(u)=\frac{1}{4}(u^2-u)^2$.

The other two terms in (1.1) give the entropy of the system. The peculiar nonlocal term is due to the fact that molecules in a diblock copolymer are connected long cains. It models a type of nonlocal interaction known as the Coulomb interaction (Muratov[17]). Mathematically we view $(-\Delta)^{-1}$ as a bounded positive operation from $\{\zeta \in L^2(D): \overline{\zeta}=0\}$ to $\{\xi \in W^{2,2}(D): \overline{\xi}=0\}: \xi=(-\Delta)^{-1}\zeta$ if

$$-\Delta\xi = \zeta \text{ in } D, \quad \partial_v \xi = 0 \text{ on } \partial D, \quad \overline{\xi} = 0.$$

Then $(-\Delta)^{-1/2}$ is the positive square root of $(-\Delta)^{-1}$.

To understand the parameter range (1.3) we recall the physical parameters in a diblock copolymer system (cf. Ref. 8).

(1) The polymerization index N that is the number of all the monomers in a chain molecule. We consider the ideal situation where this N is the same in all molecules;
(2) The Kuhn statistical length l measuring the average distance between two adjacent monomers in a chain molecule, which is the same regardless the monomer types;
(3) The Flory–Huggins parameter χ that measures the repulsion between unlike monomers and is inversely proportional to the absolute temperature;
(4) Relative A monomer ratio a mentioned earlier;
(5) The volume V of the sample.

They are related to the mathematical dimensionless parameters ϵ and γ by

$$\epsilon^2 = \frac{\pi^{2/3} l^2}{12a(1-a)\chi V^{2/3}}, \quad \gamma = \frac{18\sqrt{3}V}{\pi a^{3/2}(1-a)^{3/2}\chi^{1/2}N^2 l^3}. \tag{1.5}$$

Among the physical parameters a and χ are dimensionless and order 1. So we focus on l, V, and N. N is necessarily large in a polymer system. By taking ϵ small we have assumed that the sample is large compared to l. On the other hand having $\gamma \sim 1$ means that $V \sim l^3 N^2$. After we find spot and ring solutions of a finite number of microdomains separated by interfaces whose width is of order ϵ in the parameter range (1.3), we conclude that the size of a microdomain is of order l^3N^2 and the thickness of the interfaces is of order l, facts very well matched by experiments.[21]

Another choice of γ was used in Müller,[16] Nishiura and Ohnishi,[19] and Ren and Wei:[26] $\gamma \sim \epsilon^{-1}$, i.e., $V \sim l^3 N^3$. In this larger sample one finds that the number of the microdomains is of order ϵ^{-1}. Then again the size of a microdomain is of order l^3N^2.

The diblock copolymer equation

$$-\epsilon^2 \Delta u + f(u) + \epsilon\gamma(-\Delta)^{-1}(u-a) = \eta \text{ in } D, \quad \partial_\nu u = 0 \text{ on } \partial D, \quad \overline{u} = a \tag{1.6}$$

is the Euler–Lagrange equation of (1.1), where $f=W'$. For the example of W, $f(u)=u(u-1/2)(u-1)$. The unknown constant η is a Lagrange multiplier due to the constraint $\overline{u}=a$. If we integrate (1.6) over D, then

$$\eta = \overline{f(u)}. \tag{1.7}$$

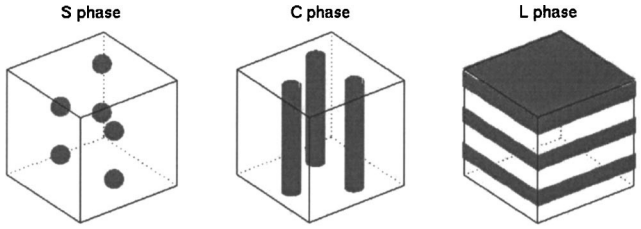

FIG. 1. The spherical, cylindrical, and lamellar morphology phases commonly observed in diblock copolymer melts. The white color indicates the concentration of type *A* monomer, and the dark color indicates the concentration of type *B* monomer.

Many morphology patterns are observed in diblock copolymers. See Bates and Fredrickson,[4] Hamley,[11] and the references therein. The most popular ones are the spherical, cylindrical, and lamellar phases, Fig. 1. The existence of the lamellar phase was shown in Ren and Wei,[24] and its stability in three dimensions was studied in Ren and Wei.[27] Surprisingly we found that the lamellar phase is only *marginally* stable. Physicists believe that defects should appear commonly in the lamellar phases, Tsori *et al.*, Refs. 36 and 17.

One type of defect is the wriggled lamellar pattern studied in Ren and Wei,[33] where interfaces separating microdomains oscillate like the sinusoidal curve. Here we study another type of defect: spot and ringlike microdomains, Fig. 2. We consider (1.6) in the unit disk $D=\{x\in R^2:|x|<1\}$. Let $v=(-\Delta)^{-1}(u-a)$. If u and v are radially symmetric, then (1.6) may be written in the radial coordinates, $r=|x|$, as

$$\begin{cases} -\epsilon^2 u_{rr}-\dfrac{\epsilon^2}{r}u_r+f(u)+\epsilon\gamma v=\eta, \\ -v_{rr}-\dfrac{1}{r}v_r=u-a, \\ u_r(0)=u_r(1)=v_r(0)=v_r(1)=0, \\ \overline{u}-a=\overline{v}=0. \end{cases} \tag{1.8}$$

The average now becomes $\overline{u}=2\int_0^1 u(r)rdr$. We are interested in radial solutions of (1.6) that show the phenomenon of microphase separation. They are close to 0 or 1 in most of D but change between 0 and 1 in small regions. These small transition regions are called the interfaces. For a radial solution u an interface may be identified by a number r_j, where $u(r_j)=1/2$. The following theorem was proved in Ren and Wei[25] using the Γ-convergence theory (cf. De Giorgi,[9] Modica,[15] and Kohn and Sternberg[14]).

Theorem 1.1 (Ren and Wei[25]): *For any $\gamma>0$, there exist two radial solutions of (1.6) on the unit disk with one circular interface when ϵ is small. If $K\geqslant 2$ and γ is large enough there exist two radial solutions with K circular interfaces when ϵ is small.*

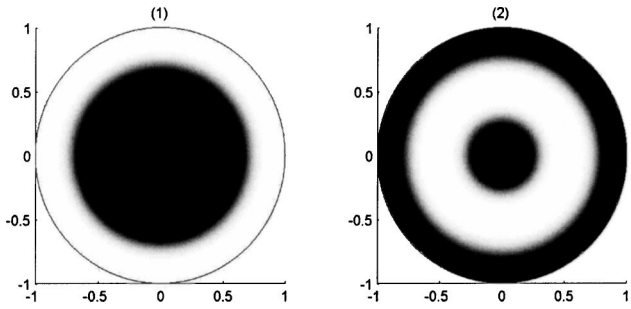

FIG. 2. (1) A spot solution. (2) A $K=2$ ring solution. In both cases $a=1/2$ and $\gamma=25$.

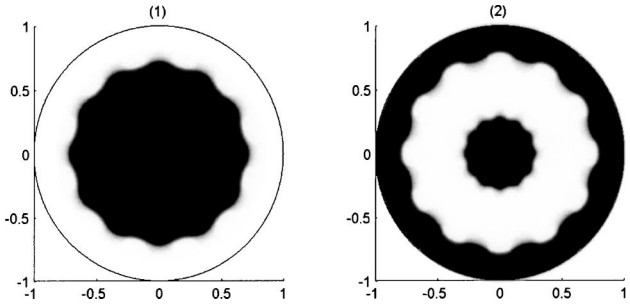

FIG. 3. Bifurcation solutions for $K=1$ and $K=2$.

For each K one of the solutions, which we simply denote by u, in Theorem 1.1 is close to 0 near the origin and the other one is close to 1 near the origin, which we denote by $\tilde{u}$. However the two solutions are related. If we change a to $1-a$ in (1.1) and (1.2), then $1-\tilde{u}$ is a solution of the new problem which is close to 0 near the origin, and $1-u$ is a solution of the new problem which is close to 1 near the origin. So it suffices to study u. u is a spot solution if $K=1$, and a ring solution if $K\geqslant 2$, Fig. 2. Throughout this paper $v=(-\Delta)^{-1}(u-a)$.

The spot solution is also useful in the study of the cylindrical phase, Fig. 1(2). A cross section of the cylindrical phase has a pattern of many spots. It is believed that these spots pack in a hexagonal way.[4] A good understanding of a single spot is essential before one can mathematically prove the existence of the cylindrical phase.

In this paper we derive a criterion for the stability of the spot and ring solutions by obtaining detailed information on the eigenvalues and eigenfunctions of the linearized problem,

$$L\varphi:=-\epsilon^2\Delta\varphi+f'(u)\varphi-\overline{f'(u)\varphi}+\epsilon\gamma(-\Delta)^{-1}\varphi=\lambda\phi \text{ in } D,\quad \partial_\nu\varphi=0 \text{ on } \partial D,\quad \overline{\phi}=0. \quad (1.9)$$

It is easy to see, Lemma 2.4, that $\lim\inf_{\epsilon\to 0}\lambda\geqslant 0$. To determine the stability we need to study the λ's that tend to 0 as $\epsilon\to 0$. These λ's are called the critical eigenvalues. They are found in Theorems 3.1 and 4.1. Consequently we show in Theorem 5.1 that the spot solution is stable if γ is small and unstable if γ is large. The threshold of γ is denoted by $\hat{\gamma}$. It is calculated numerically for various a.

To better appreciate this theorem let us recall the stationary Cahn–Hilliard equation,[5] which is (1.6) with $\gamma=0$, the local counterpart. It is known that the Cahn–Hilliard equation on the unit disk has an unstable spot solution. Once the nonlocal term with a small γ, which encourages oscillation, is added, the spot solution becomes stable. The abrupt change of stability here is discussed after the proof of Theorem 5.1. If γ is further increased, more oscillation is required and the spot solution, which only has one interface, becomes unstable.

The second change of stability has a simple physical explanation. According to (1.5) γ is proportional to the size of the sample. When the sample is sufficiently large, one big spot is unstable in two dimensions. It should break into multiple spots to form a cylindrical phase, Fig. 1(2). The value V corresponding to $\hat{\gamma}$ in $(1.5)_2$ suggests a scale for a cell with one spot in a multispot cylindrical phase.

For the ring solution ($K\geqslant 2$), we will use Theorems 3.1 and 4.1 to numerically study a case of $K=2$. When γ is small, we cannot find a ring solution by the Γ-convergence method. When γ is increased, there exists a ring solution that is stable in two dimensions. When γ is further increased over $\hat{\gamma}$, a ring solution exists but is no longer stable.

This change of stability of the ring solution and the second change of stability of the spot solution lead to a bifurcation phenomenon near $\hat{\gamma}$. Following Ref. 33 one should be able to find bifurcation solutions. They are depicted in Fig. 3. Based on our experience in Ref. 33 we suspect that most of them are stable.

More information on the model (1.1) and its extension to triblock copolymers may be found in Nakazawa and Ohta,[18] and Ren and Wei.[29] The mathematical study of stable domain structures

with multiple sharp interfaces started rather recently. On the block copolymer problem the literature includes Ohnishi *et al.*,[20] Ren and Wei,[30] Choksi,[7] Fife and Hilhorst,[10] Henry,[13] and Teramoto and Nishiura.[35] Elsewhere Ren and Truskinovsky[23] study the phenomenon in elastic bars, Ren and Wei[32,28,31] in the Seul–Andelman membrane, charged monolayers, and smectic liquid crystal films, respectively. Taniguchi[34] and Chen and Taniguchi[6] study spot and ring patterns in a free boundary problem.

The paper is organized as follows: In Sec. II we review the construction of the spot and ring solutions u, give some properties of u, and explain the classification into λ_m where $m=0,1,2,3,\ldots$ of the eigenvalues of the linearized operator at u. The properties of λ_m are given in Theorems 3.1 and 4.1 in Sec. III and IV, respectively. In Sec. V we show the stability property of the spot solution, calculate the second threshold $\hat{\gamma}$, and use Theorems 3.1 and 4.1 to study a $K=2$ ring solution. This section also includes some remarks. The Appendix contains the proof of a technical lemma.

II. PRELIMINARIES

To make the paper more readable a quantity's dependence on ϵ is usually not reflected in its notation but implied in the context. On the other hand, a quantity's independence of ϵ is often emphasized with a superscript 0. For instance the spot or ring solution u is not denoted by u_ϵ, while the $L^2(D)$-limit of u as $\epsilon\to 0$ is denoted by u^0.

Throughout the paper, the L^∞ norm of a function is denoted simply by $\|\cdot\|$. Other norms are more explicitly written, like $\|\cdot\|_2$.

We define some frequently used quantities. H is the heteroclinic solution of

$$-H''+f(H)=0,\quad H(-\infty)=0,\quad H(\infty)=1,\quad H(0)=1/2. \tag{2.1}$$

Our assumption that $W(u)=W(1-u)$ implies that $H(t)=1-H(-t)$. The interface tension τ is a constant defined by

$$\tau := \int_R (H'(t))^2\,dt. \tag{2.2}$$

In the special case $W(u)=\frac{1}{4}(u^2-u)^2$, $\tau=\sqrt{2}/12$.

Theorem 1.1 was proven in Ref. 25 by locally minimizing I in the radial class

$$X_a^R=\{u\in W^{1,2}(D): u(x)=u(|x|), \overline{u}=a\}. \tag{2.3}$$

To do so we used the Γ-convergence theory in the perturbation variational analysis. $(\epsilon\pi)^{-1}I$ converges in a particular sense to a singular limit J. J is defined in the class $\mathcal{A}$ which may be decomposed to

$$\mathcal{A}=\bigcup_{K=1}^{\infty}(\mathcal{A}_K\cup\tilde{\mathcal{A}}_K). \tag{2.4}$$

A function $\mathcal{U}$ is in $\mathcal{A}_K$ if $\overline{\mathcal{U}}=a$ and there exist $q_1,q_2,\ldots,q_K$, satisfying $0<q_1<q_2<\cdots<q_K<1$, such that $\mathcal{U}(r)=0$ if $r\in(0,q_1)$, $=1$ if $r\in(q_1,q_2)$, $=0$ if $r\in(q_2,q_3)\ldots$. Similarly a function $\tilde{\mathcal{U}}\in\tilde{\mathcal{A}}_K$ if $\overline{\tilde{\mathcal{U}}}=a$ and there exist $q_1,q_2,\ldots,q_K$, satisfying $0<q_1<q_2<\cdots<q_K<1$, such that $\tilde{\mathcal{U}}(r)=1$ if $r\in(0,q_1)$, $=0$ if $r\in(q_1,q_2)$, $=1$ if $r\in(q_2,q_3),\ldots$. By the remark after Theorem 1.1 we will not consider J in $\tilde{\mathcal{A}}$. In each $\mathcal{A}_K$ the function J depends on $\mathbf{q}=(q_1,q_2,\ldots,q_K)$ only

$$J(\mathbf{q})=2\tau(q_1+q_2+\cdots+q_K)+\gamma\int_0^1 \mathcal{V}'(r)^2 r\,dr. \tag{2.5}$$

In (2.5) $\mathbf{q}$ determines $\mathcal{U}\in\mathcal{A}_K$. We emphasize that $\mathcal{U}$ depends on all q_j. We sometimes use the notation $\mathcal{U}=\mathcal{U}(r;\mathbf{q})$. Let $\mathcal{V}$ be the solution of

$$-\mathcal{V}''-\frac{\mathcal{V}'}{r}=\mathcal{U}-a,\quad \mathcal{V}'(1)=0,\quad \overline{\mathcal{V}}=0. \tag{2.6}$$

We define G_0 to be the solution operator of (2.6) so that $\mathcal{V}=G_0[\mathcal{U}-a]$. Again we may write $\mathcal{V}=\mathcal{V}(r;\mathbf{q})$. The constraint $\overline{\mathcal{U}}=a$ becomes a constraint on $\mathbf{q}$,

$$S(\mathbf{q}):=-q_1^2+q_2^2-q_3^2+\cdots+(-1)^K q_K^2+\frac{1-(-1)^K}{2}=a. \tag{2.7}$$

To incorporate the constraint (2.7) we define $F:=J+\nu S$, where ν is the Lagrange multiplier in accordance to the constraint.

Using ideas from Refs. 15 and 14 the following result is obtained in Ref. 25.

Lemma 2.1: *If J has a strict local minimizer $\mathcal{U}(\cdot;\mathbf{r}^0)\in\mathcal{A}_K$, then there exists $\hat{\epsilon}>0$ such that for all $\epsilon\in(0,\hat{\epsilon})$,* (1.6) *has a solution u with the properties* $\lim_{\epsilon\to 0}\|u-\mathcal{U}(\cdot;\mathbf{r}^0)\|_2=0$ *and* $\lim_{\epsilon\to 0}(\epsilon\pi)^{-1}I(u)=J(\mathcal{U}(\cdot;\mathbf{r}^0))$.

Lemma 2.1 reduces I to J which is finite dimensional in each $\mathcal{A}_K$ and $\tilde{\mathcal{A}}_K$. To study J we define from the operator G_0 the Green function

$$G_0(r,s)=G_0[\delta(\cdot-s)-2s](r), \tag{2.8}$$

where $2s$ is the average of $\delta(\cdot-s)$. More explicitly

$$G_0(r,s)=\begin{cases}\dfrac{sr^2}{2}-\dfrac{3s-2s^3}{4}-s\log s & \text{if } r<s\\[2ex] \dfrac{sr^2}{2}-s\log r-\dfrac{3s-2s^3}{4} & \text{if } r\geqslant s.\end{cases} \tag{2.9}$$

Note that $G_0(r,s)$ is not symmetric in r and s, although $rG_0(r,s)$ is. Also note $\overline{\delta(\cdot-s)}=2s$. Then we may write

$$\mathcal{V}(r)=\int_0^1 G_0(r,s)(\mathcal{U}(s)-a)ds=\int_0^1 G_0(r,s)\mathcal{U}(s)ds.$$

We calculate the derivatives of J and F. J may be rewritten as

$$J(\mathbf{q})=2\tau\sum_{j=1}^{k}q_j+\gamma\int_0^1\mathcal{U}(r)\mathcal{V}(r)r\,dr.$$

Then

$$\begin{aligned}\frac{\partial J}{\partial q_j}&=2\tau+\gamma\frac{\partial}{\partial q_j}\left[\int_{q_1}^{q_2}\mathcal{V}(r)r\,dr+\int_{q_3}^{q_4}\mathcal{V}(r)r\,dr+\cdots\right]\\&=2\tau+(-1)^j\gamma q_j\mathcal{V}(q_j)+\gamma\int_0^1\mathcal{U}(r)\frac{\partial}{\partial q_j}\mathcal{V}(r)r\,dr.\end{aligned}$$

Note that

$$\frac{\partial}{\partial q_j}\mathcal{V}(r)=\frac{\partial}{\partial q_j}\left[\int_{q_1}^{q_2}G_0(r,s)ds+\int_{q_3}^{q_4}G_0(r,s)ds+\cdots\right]=(-1)^jG_0(r,q_j).$$

Hence

$$\frac{\partial J}{\partial q_j} = 2\tau + 2(-1)^j \gamma q_j \mathcal{V}(q_j),$$

and

$$\frac{\partial F}{\partial q_j} = 2\tau + 2(-1)^j \gamma q_j \mathcal{V}(q_j) + 2\nu(-1)^j q_j.$$

Let $\mathbf{r}^0=(r_1^0, r_2^0, \ldots, r_K^0)$ be a solution of $\partial F/\partial q_j=0$, $j=1,2,\ldots,K$, i.e.,

$$2\tau + 2(-1)^j \gamma r_j^0 \mathcal{V}(r_j^0) + 2\nu(-1)^j r_j^0 = 0, \quad j=1,2,\ldots,K. \tag{2.10}$$

The second derivatives of J are

$$\frac{\partial^2 J}{\partial q_j \partial q_k} = 2(-1)^{j+k} \gamma q_j G_0(q_j, q_k), \quad \text{if } j \neq k,$$

$$\begin{aligned}\frac{\partial^2 J}{\partial q_j^2} &= 2(-1)^j \gamma \mathcal{V}(q_j) + 2(-1)^j \gamma q_j ((-1)^j G_0(q_j, q_j) + \mathcal{V}'(q_j)) \\ &= 2\gamma q_j G_0(q_j, q_j) + 2(-1)^j \gamma (\mathcal{V}(q_j) + q_j \mathcal{V}'(q_j)).\end{aligned}$$

Hence

$$\frac{\partial^2 F}{\partial q_j \partial q_k} = \begin{cases} 2\gamma q_j G_0(q_j, q_j) + 2(-1)^j \gamma (\mathcal{V}(q_j) + q_j \mathcal{V}'(q_j)) + 2\nu(-1)^j & \text{if } j=k \\ 2(-1)^{j+k} \gamma q_j G_0(q_j, q_k) & \text{if } j \neq k. \end{cases} \tag{2.11}$$

At $\mathbf{r}^0$, because of (2.10), we have

$$\frac{\partial^2 F}{\partial q_j \partial q_k}(\mathbf{r}^0) = \begin{cases} 2\gamma r_j^0 G_0(r_j^0, r_j^0) + 2(-1)^j \gamma r_j^0 \mathcal{V}'(r_j^0) - \dfrac{2\tau}{r_j^0} & \text{if } j=k \\ 2(-1)^{j+k} \gamma r_j^0 G_0(r_j^0, r_k^0) & \text{if } j \neq k. \end{cases} \tag{2.12}$$

We emphasize that the function $\mathcal{V}$ in (2.12) is associated with $\mathbf{r}^0$, i.e., $\mathcal{V}=\mathcal{V}(\cdot;\mathbf{r}^0)$.

Whether a critical point $\mathbf{r}^0$ is a local minumum is determined by the matrix (2.12) in the subspace

$$T = \{\mathbf{b} = (b_1, b_2, \ldots, b_K)^T \in R^K : \sum_{j=1}^{K} (-1)^j b_j r_j^0 = 0\}. \tag{2.13}$$

T is the tangent space of the domain of J at $\mathbf{r}^0$. When (2.12) is positive definite in T, i.e.,

$$\sum_{j,k=1}^{K} \frac{\partial^2 F}{\partial q_j \partial q_k}(\mathbf{r}^0) b_j b_k > 0, \quad \text{if } \mathbf{b} \in T \text{ and } \mathbf{b} \neq 0, \tag{2.14}$$

the critical point $\mathbf{r}^0$ is a strict local minimum.

The condition (2.14) may be rephrased as follows. Define a K by K matrix $\mathbf{M}^0$ whose kj entry is

$$M_{kj}^0 = \delta_{kj}\left(-\frac{\tau}{(r_k^0)^2} + \gamma(-1)^k \mathcal{V}'(r_k^0)\right) + \gamma(-1)^{k+j} G_0(r_k^0, r_j^0), \tag{2.15}$$

where $\delta_{kj}=1$ if $k=j$ and 0 otherwise. M_{kj}^0 is not symmetric in j and k but $r_k^0 M_{kj}^0$ is. Let g^0 be a non-standard inner product on R^K defined by

$$g^0(\mathbf{A},\mathbf{B}) = \sum_{j=1}^{K} A_j B_j r_j^0, \quad \mathbf{A} = (A_1, A_2, \ldots, A_K)^T, \quad \mathbf{B} = (B_1, B_2, \ldots, B_K)^T. \tag{2.16}$$

With respect to g^0, the matrix $\mathbf{M}^0$ represents a symmetric linear operator on R^K. Also with respect by g^0 we choose an orthonormal basis $\mathbf{e}_1^0, \mathbf{e}_2^0, \ldots, \mathbf{e}_K^0$ with

$$\mathbf{e}_1^0 = \frac{1}{\sqrt{r_1^0 + r_2^0 + \cdots + r_K^0}}(-1, 1, -1, 1, \cdots, (-1)^K)^T. \tag{2.17}$$

Since

$$\frac{1}{2}\sum_{j,k=1}^{K} \frac{\partial F}{\partial q_j \partial q_k}(\mathbf{r}^0) b_j b_k = \sum_{j,k=1}^{K} M_{kj}^0 b_j b_k r_k^0 = g^0(\mathbf{M}^0\mathbf{b}, \mathbf{b}),$$

(2.14) is equivalent to the condition that $\mathbf{M}^0$ is positive definite in the $K-1$ dimensional subspace perpendicular to $\mathbf{e}_1^0$ with respect to g^0. This form of (2.14) is closer to the contents of Sec. III.

Lemma (2.1) now implies the following theorem:

Theorem 2.2: *If J has a critical point $\mathbf{r}^0$ at which* (2.12) *is positive definite in T, then there exists $\hat{\epsilon} > 0$ such that for all $\epsilon \in (0, \hat{\epsilon})$ there is a solution u of* (1.6) *with the properties* $\lim_{\epsilon\to 0}\|u - \mathcal{U}(\cdot;\mathbf{r}^0)\|_2 = 0$ *and* $\lim_{\epsilon\to 0}(\epsilon\pi)^{-1} I(u) = J(\mathcal{U}(\cdot;\mathbf{r}^0))$.

Only when $K=1$, $\mathbf{r}^0 = (r_1^0)$ alsways exists and equals $\sqrt{1-a}$. It is regarded trivially as a strict local minimizer of J. Hence when ϵ is small, a spot solution of (1.6) exists unconditionally.

When $K \geqslant 2$, J may not have a strict local minimizer. Another perturbation argument can be used. Note that when γ is large, J may be viewed as a perturbation of

$$J^*(\mathbf{q}) = \gamma \int_0^1 (\mathcal{V}'(r))^2 r dr. \tag{2.18}$$

It was proved in Ref. 25 that J^* has a unique critical point $\mathbf{r}^* = (r_1^*, r_2^*, \ldots, r_k^*)$. When γ is large, (2.12) is dominated by

$$\begin{cases} 2\gamma r_j^* G(r_j^*, r_j^*) + 2(-1)^j \gamma r_j^* \mathcal{V}'(r_j^*) & \text{if} \quad j = k \\ 2(-1)^{j+k} \gamma r_j^* G(r_j^*, r_K^*) & \text{if} \quad j \neq k. \end{cases} \tag{2.19}$$

It was shown in Ref. 25 that (2.19) is positive definite in T. For large γ $\mathbf{r}^*$ perturbs to $\mathbf{r}^0$, a strict local minimizer of J. Theorem 1.1 hence is a consequence of Theorem 2.2. In this paper we assume that the condition (2.14) is satisfied and hence u exists.

We denote the function $\mathcal{U}(\cdot;\mathbf{r}^0)$ by u^0 and set $v^0 = G_0[u^0 - \overline{u^0}]$. u^0 takes values 0 and 1, and it jumps between these two values at $r_1^0, r_2^0, \ldots, r_k^0$. The Γ-convergence theory asserts that u converges to u^0 in $L^2(D)$. Then there exist $r_1, r_2, \ldots, r_k$ such that $u(r_j) = 1/2, j = 1, 2, \ldots, K$, and $\mathbf{r} = (r_1, r_2, \ldots, r_K)^T \to \mathbf{r}_0$ as $\epsilon \to 0$. These r_j's are called the interfaces of u. We will see that they are the only interfaces.

We also need to know the asymptotic behavior of u. First we construct an *inner* expansion. Around each r_j we introduce the scaled variable $r = r_j + \epsilon t$ so to expand

$$u(r) = u(r_j + \epsilon t) = H_j(t) + \epsilon P_j(t) + \epsilon^2 Q_j(t) + \cdots. \tag{2.20}$$

Correspondingly

$$v(r) = v(r_j) + \epsilon t v'(r_j) + \cdots. \tag{2.21}$$

As we insert (2.20) and (2.21) into (1.8) we find the leading term

$$H_j(t) = H(t) \quad \text{if } j \text{ is odd}, \quad H_j(t) = H(-t) \quad \text{if } j \text{ is even}. \tag{2.22}$$

The next term is $P_j(t)$ defined to be the solution of

$$-P'' + f'(H_j)P - \frac{H_j'}{r_j} + \xi_j = 0, \quad P(0) = 0. \tag{2.23}$$

P_j is even. The constant ξ_j is chosen so that $(H_j'/r_j) + \xi_j$ is perpendicular to H_j' for solvability. Therefore

$$\xi_j = \frac{(-1)^{j+1}}{r_j} \int_R (H'(t))^2 \, dt = \frac{(-1)^{j+1}\tau}{r_j}. \tag{2.24}$$

In our rigorous setting of asymptotic expansions P_j depends on ϵ because r_j and ξ_j do so. This way we avoid expanding r_j. The third term in the inner expansion is $Q_j(t)$ which is the solution of

$$-Q'' + f'(H_j)Q - \frac{P_j'}{r_j} + \frac{tH_j'}{r_j^2} + \frac{f''(H_j)P_j^2}{2} + \gamma v'(r_j)t = 0, \quad Q(0) = 0. \tag{2.25}$$

Q_j is odd. Again Q_j depends on ϵ, via r_j and $v'(r_j)$. We set the inner approximation of u near r_j to be

$$z_j(r) = H_j\left(\frac{r - r_j}{\epsilon}\right) + \epsilon P_j\left(\frac{r - r_j}{\epsilon}\right) + \epsilon^2 Q_j\left(\frac{r - r_j}{\epsilon}\right). \tag{2.26}$$

The outer approximation is done in one step. It is denoted by z and defined for all r not equal to $r_1, r_2, \ldots, r_K$ by the equation

$$f(z) + \epsilon\gamma v(r) - \eta = 0. \tag{2.27}$$

Since $\eta = O(\epsilon)$ and $v = O(1)$, facts proved in the Appendix, z is chosen to be close to 0 or 1 on each (r_j, r_{j+1}) nonambiguously, in agreement with the shape of u, i.e., z is close to 0 on $(0, r_1)$, close to 1 on (r_1, r_2), close to 0 on (r_2, r_3), etc.

The inner approximation is used in each $(r_j - \epsilon^\alpha, r_j + \epsilon^\alpha)$ where $\alpha \in (1/2, 1)$. The outer approximation is used in $(0,1) \setminus (\cup_{j=1}^K (r_j - 2\epsilon^\alpha, r_j + 2\epsilon^\alpha))$. The inner approximation is matched to the outer approximation in the matching intervals $(r_j - 2\epsilon^\alpha, \ r_j - \epsilon^\alpha)$ and $(r_j + \epsilon^\alpha, r_j + 2\epsilon^\alpha)$, $j = 1, 2, \ldots, K$. Let χ_j be smooth cut-off functions so that

$$\chi_j(r) = \begin{cases} 0 & \text{if } r \notin (r_j - 2\epsilon^\alpha, r_j + 2\epsilon^\alpha) \\ 1 & \text{if } r \in (r_j - \epsilon^\alpha, r_j + \epsilon^\alpha), \end{cases}$$

and moreover $(\chi_j)_r = O(\epsilon^{-\alpha})$ $(\chi_j)_{rr} = O(\epsilon^{-2\alpha})$ in $(r_j - 2\epsilon^\alpha, r_j - \epsilon^\alpha)$ and $(r_j + \epsilon^\alpha, r_j + 2\epsilon^\alpha)$.

We then glue the two approximations to form a uniform approximation

$$w(r) = \sum_{j=1}^K \chi_j z_j + \left(1 - \sum_{j=1}^K \chi_j\right) z. \tag{2.28}$$

Lemma 2.3: $w - u = o(\epsilon^2)$.

According to this lemma, whose proof is left to the appendix, the uniform approximation w is accurate up to order ϵ^2. This lemma also implies that the r_j's are the only interfaces of u.

To understand the stability of a spot or a ring solution in two dimensions we need to find the spectrum, which only contains eigenvalues, of the linearized operator L defined in (1.9). We separate variables in the polar coordinates to let

$$\varphi(x) = \varphi(r\cos\theta, r\sin\theta) = \sum_{m=0}^{\infty} \phi_m(r)(A_m \cos(m\theta) + B_m \sin(m\theta)). \tag{2.29}$$

After substituting (2.29) into (1.9), we deduce that $\varphi(x)$ is a linear combination of $\phi_m(r)\cos(m\theta)$ and $\phi_m(r)\sin(m\theta)$ for some non-negative integer m. The corresponding eigenvalue λ is thus

classified into $\lambda=\lambda_m, m=0,1,2,\ldots$. The pair (λ_m,ϕ_m) satisfies the following equations:

(1) If $m=0$,

$$L_0\phi_0 := -\epsilon^2\phi_0'' - \frac{\epsilon^2}{r}\phi_0' + f'(u)\phi_0 - \overline{f'(u)\phi_0} + \epsilon\gamma G_0[\phi_0] = \lambda_0\phi_0, \quad \phi'(0)=\phi'(1)=0, \quad \overline{\phi_0} = 0; \tag{2.30}$$

(2) if $m\geq 1$,

$$L_m\phi_m := -\epsilon^2\phi_m'' - \frac{\epsilon^2}{r}\phi_m' + \frac{\epsilon^2 m^2}{r^2}\phi_m + f'(u)\phi_m + \epsilon\gamma G_m[\phi_m] = \lambda_m\phi_m, \quad \phi_m(0)=\phi_m'(1)=0. \tag{2.31}$$

The operator G_0 is defined in (2.6), and when $m\geq 1$, G_m is the inverse of the differential operator $-(d^2/dr^2)-(1/r)(d/dr)+(m^2/r^2)$ with the Neumann boundary condition at $r=1$ and the Dirichlet boundary condition at $r=0$.

Lemma 2.4: Let λ *be an eigenvalue of L. Then* $\liminf_{\epsilon\to 0}\lambda\geq 0$.

Proof: Suppose that the lemma is false. We may assume that $\lim_{\epsilon\to 0}\lambda=\lambda^0<0$. Since λ is classified in to λ_m, $m=0,1,2,\ldots$, we consider the case that λ is one of λ_0. The case $m\geq 1$ may be handled similarly and we omit the proof.

Let ϕ be an eigenfunction of (2.30) associated with λ. Without the loss of generality we assume that $\|\phi\|=\phi(r_*)=1$. First we claim that there is a r_j whose distance to r_* is of order $O(\epsilon)$. Otherwise $-\epsilon^2\phi''(r_*)\geq 1$ since r_* is a maximum; $(\epsilon^2/r)\phi'(r_*)=0$ whether or not r_* is on the boundary; $f'(u(r_*))\phi(r_*)>0$ since $f'(u(r_*))>0$ outside any ϵ-neighborhood of r_j; $\overline{f'(u)\phi} = \overline{(f'(u)-f'(0))\phi} = O(\epsilon)$ by the uniform estimate of u in Lemma 2.3; $\epsilon\gamma G_0[\phi](r_*)=O(\epsilon)$, and $\lambda\phi(r_*)=\lambda<0$. Then

$$-\epsilon^2\phi''(r_*) - \frac{\epsilon^2}{r}\phi'(r_*) + f'(u(r_*))\phi(r_*) - \overline{f'(u)\phi} + \epsilon\gamma G_0[\phi](r_*) > \lambda\phi(r_*),$$

and (2.30) is not satisfied at r_*.

If r_* is in a size $O(\epsilon)$ neighborhood of r_j, then $\phi(r_j+\epsilon t)\to\Phi\not\equiv 0$ in $C^2_{\mathrm{loc}}(R)$, and Φ satisfies $-\Phi''+f'(H_j)\Phi=\lambda^0\Phi$. However this equation has no nonzero, bounded solution when $\lambda^0<0$, since H_j is a minimizer of $E(U):=\int_R\left(\frac{1}{2}(U')^2+W(U)\right)dt$. Here U is in the class $W^{1,2}_{\mathrm{loc}}(R)$ and $\lim_{t\to\pm\infty}(U(t)-H_j(t))=0$. □

Hence to understand the stability of u we must analyze all the eigenvalues that tend to 0 as $\epsilon\to 0$. They are called the critical eigenvalues.

III. THE CRITICAL EIGENVALUES λ_0

Recall $\mathbf{M}^0$ and g^0 defined in (2.15) and (2.16), respectively, and $\mathbf{e}_j^0$ with $\mathbf{e}_1^0$ defined in (2.17).

Theorem 3.1: *When* ϵ *is sufficiently small, there exist exactly K eigenpairs* (λ_0,ϕ_0), *of* (2.30) *with* $\lambda_0=o(1)$. *One* λ_0 *is positive and of order* ϵ. *This* λ_0 *and its eigenfunction expand like*

$$\lambda_0 = \frac{2f'(0)\sum_{k=1}^{K} r_k^0}{\tau}\epsilon + o(\epsilon), \quad \phi_0 = \sum_{j=1}^{K} c_j(H_j' - \overline{H_j'}) + O(\epsilon|\mathbf{c}|).$$

where $\mathbf{c}=(c_1,c_2,\ldots c_K)^T\to\mathbf{c}^0$, *as* ϵ *tends to* 0. $\mathbf{c}^0$ *is a nonzero scaler multiple of* $\mathbf{e}_1^0$.

The remaining $K-1$ λ_0's *are positive and of order* ϵ^2. *Each of them and its corresponding eigenfunction expand like*

$$\lambda_0 = \mu_0^0 \epsilon^2 + o(\epsilon^2), \quad \phi_0 = \sum_{j=1}^{K} c_j (H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) + O(\epsilon^2 |\mathbf{c}|).$$

Let $\mathbf{c}^0 = \lim_{\epsilon \to 0} \mathbf{c}$. *Then* $\mathbf{c}^0 = \Sigma_{n=2}^{K} \tilde{c}_n^0 \mathbf{e}_n^0$, *and* μ_0^0 *and* $(\tilde{c}_2^0, \tilde{c}_3^0, \ldots, \tilde{c}_K^0)^T$ *form an eigenpair of the* $K-1$ *dimensional eigenvalue problem*

$$\sum_{m=2}^{K} \tilde{c}_m^0 g^0(\mathbf{M}^0 \mathbf{e}_m^0, \mathbf{e}_n^0) = \mu_0^0 r \tilde{c}_n^0, \quad n = 2, 3, \ldots, K.$$

We expect that the eigenfunctions associated with small eigenvalues may be approximated by combinations of

$$H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}). \tag{3.1}$$

Here H_j' is the derivative of $H_j = H_j(t)$ with respect to t evaluated at $t = (r - r_j)/\epsilon$. In this section we write (λ, ϕ) for an eigenpair (λ_0, ϕ_0). We decompose

$$\phi = \sum_{j=1}^{K} c_j (H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) + \phi^{\perp} \tag{3.2}$$

in the $L^2(D)$ space where $H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}) \perp \phi^{\perp}$ for $j = 1, 2, \ldots, K$. First we estimate

$$L_0(H_j' - \overline{H_j'}) = -\epsilon^2 (H_j')_{rr} - \frac{\epsilon^2}{r}(H_j')_r + f'(u)(H_j' - \overline{H_j'}) - \overline{f'(u)(H_j' - \overline{H_j'})} + \epsilon \gamma G_0[H_j' - \overline{H_j'}],$$

in which

$$\begin{aligned} \overline{f'(u) H_j'} &= 2 \int_0^1 (f'(H_j) + \epsilon P_j f''(H_j)) H_j' r \, dr + O(\epsilon^3) \\ &= 2\epsilon \int_R [f'(H_j) H_j' r_j + \epsilon t f'(H_j) H_j' + \epsilon P_j f''(H_j) H_j' r_j] dt + O(\epsilon^3) = O(\epsilon^3) \end{aligned} \tag{3.3}$$

since $\int_R f'(H_j) H_j' dt = \int_R t f'(H_j) H_j' dt = \int_R P_j f''(H_j) H_j' dt = 0$ ($t f'(H_j) H_j'$ and $P_j f''(H_j) H_j'$ are odd). Then

$$\begin{aligned} L_0(H_j' - \overline{H_j'}) &= (f'(u) - f'(H_j)) H_j' - \frac{\epsilon}{r} H_j'' + (\overline{f'(u)} - f'(u)) \overline{H_j'} + \epsilon^2 \gamma (-1)^{j+1} G_0(r, r_j) + O(\epsilon^3) \\ &= \epsilon f''(H_j) P_j H_j' + \epsilon^2 \left(f''(H_j) Q_j + \frac{f'''(H_j) P_j^2}{2} \right) H_j' - \frac{\epsilon}{r} H_j'' \\ &\quad + \epsilon^2 \gamma (-1)^{j+1} G_0(r, r_j) + (\overline{f'(u)} - f'(u)) \overline{H_j'} + O(\epsilon^3). \end{aligned}$$

By differentiating (2.23) we have

$$-P_j''' + f'(H_j) P_j' + f''(H_j) H_j' P_j - \frac{H_j''}{r_j} = 0.$$

Then

$$L_0(P_j' - \overline{P_j'}) = -\epsilon^2 (P_j')_{rr} - \frac{\epsilon^2}{r}(P_j')_r + f'(u)(P_j' - \overline{P_j'}) - \overline{f'(u)(P_j' - \overline{P_j'})} + \epsilon\gamma G_0[P_j' - \overline{P_j'}]$$

$$= (f'(u) - f'(H_j))P_j' - f''(H_j)H_j'P_j + \frac{H_j''}{r_j} - \frac{\epsilon}{r}P_j'' + (\overline{f'(u)} - f'(u))\overline{P_j'} + O(\epsilon^2)$$

$$= \epsilon f''(H_j)P_jP_j' - f''(H_j)H_j'P_j + \frac{H_j''}{r_j} - \frac{\epsilon}{r}P_j'' + (\overline{f'(u)} - f'(u))\overline{P_j'} + O(\epsilon^2),$$

where we have used the fact

$$\overline{f'(u)P_j'} = 2\int_0^1 f'(u)P_j' r\, dr = 2\epsilon \int_R f'(H_j)P_j' r_j dt + O(\epsilon^2) = O(\epsilon^2) \tag{3.4}$$

since $f'(H_j)P_j'$ is odd. Therefore

$$L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) = \epsilon^2 \Bigg[\left(f''(H_j)Q_j + \frac{f'''(H_j)P_j^2}{2} \right) H_j' + f''(H_j)P_jP_j' + \left(\frac{1}{\epsilon r_j} - \frac{1}{\epsilon r} \right) H_j'' - \frac{P_j''}{r} + \gamma($$
$$- 1)^{j+1} G_0(r, r_j) \Bigg] + (\overline{f'(u)} - f'(u))\overline{H_j' + \epsilon P_j'} + O(\epsilon^3).$$

On the other hand,

$$\overline{H_j'} = 2\int_0^1 H_j' r\, dr = 2\epsilon \int_R H_j'(t)(r_j + \epsilon t)dt = 2\epsilon r_j \int_R H_j'(t)dt + 2\epsilon^2 \int_R H_j'(t)t dt = 2\epsilon(-1)^{j+1} r_j$$

since $H_j'(t)t$ is odd, and

$$\overline{P_j'} = 2\int_0^1 P_j' r\, dr = 2\epsilon r_j \int_R P_j' dt + O(\epsilon^2) = O(\epsilon^2)$$

since P_j' is odd. We find

$$\overline{H_j' + \epsilon P_j'} = 2\epsilon(-1)^{j+1} r_j + O(\epsilon^3). \tag{3.5}$$

Hence we deduce that

$$L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) = \epsilon^2 \Bigg[\left(f''(H_j)Q_j + \frac{f'''(H_j)P_j^2}{2} \right) H_j' + f''(H_j)P_jP_j' + \left(\frac{1}{\epsilon r_j} - \frac{1}{\epsilon r} \right) H_j'' - \frac{P_j''}{r}$$
$$+ \gamma(-1)^{j+1} G_0(r, r_j) \Bigg] + 2\epsilon(-1)^{j+1} r_j (\overline{f'(u)} - f'(u)) + O(\epsilon^3). \tag{3.6}$$

Note that in (3.6)

$$\left(\frac{1}{\epsilon r_j} - \frac{1}{\epsilon r} \right) H_j'' = \frac{tH''(t)}{r_j r} = O(1).$$

Rewrite the equation $L_0\phi = \lambda\phi$ as

$$\sum_{j=1}^{K} c_j L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) + L_0\phi^\perp = \lambda \left(\sum_{j=1}^{K} c_j (H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})) + \phi^\perp \right). \tag{3.7}$$

Then $\phi^\perp$ satisfies

$$L_0\phi^\perp = O\left(\epsilon|\sum_{j=1}^{K}(-1)^j r_j c_j|\right) + O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)(|\mathbf{c}| + \|\phi^\perp\|). \tag{3.8}$$

Here $\|\phi^\perp\|$ is the L^∞ norm of $\phi^\perp$ on (0,1). The following lemma estimates $\phi^\perp$.

Lemma 3.2: *There exists $C>0$ independent of ϵ such that for all ψ in the domain of L_0 and $\psi \perp H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})$, $j=1,2,\cdots,K$, $\|\psi\| \leqslant C\|L_0\psi\|$.*

Proof: Suppose that the lemma is false. There exist ψ and some r_* such that $\|\psi\| = \psi(r_*) = 1$, $\psi \perp H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})$, $j=1,2,\cdots,K$, and $L_0\psi = o(1)$. Then r_* must lie in a neighborhood of r_j for some j. The size of this neighborhood must be of order ϵ. Otherwise we argue as in the proof of Lemma 2.4: $-\epsilon^2\psi''(r_*) \geqslant 0$; $(-\epsilon^2/r)\psi'(r_*) = 0$; $\epsilon\gamma G_m[\psi](r_*) = O(\epsilon)$; $\overline{f'(u)\psi} = (\overline{f'(u) - f'(0)})\psi = O(\epsilon)$; and $f'(u)\psi(r_*)$ is positive and bounded away from 0 independent of ϵ. Then the equation $L_0\psi = o(1)$ is not satisfied at r_*.

So let us assume that r_* is in a neighborhood, of size ϵ, of r_j. Then $\psi(r_j + \epsilon t) \to \Psi_0(t)$ in $C^2_{\text{loc}}(R)$ as ϵ tends to 0. Ψ_0 satisfies $-\Psi_0'' + f'(H_j)\Psi_0 = 0$. Therefore $\Psi_0 = cH_j'$ for some constant $c \neq 0$. On the other hand if we denote the inner product in $L^2(D)$ by $\langle \cdot, \cdot \rangle$, then $\psi \perp H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})$ implies

$$0 = \langle \psi, H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}) \rangle = 2\pi\epsilon c r_j \int_R (H')^2 dt + o(\epsilon),$$

which is possible only if $c = 0$. □

We obtain by Lemma 3.2 that

$$\phi^\perp = O(\epsilon|\sum_{j=1}^{K}(-1)^j r_j c_j|) + O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)(|\mathbf{c}| + \|\phi^\perp\|)$$

which implies, since $\lambda = o(1)$,

$$\phi^\perp = O(\epsilon|\sum_{j=1}^{K}(-1)^j r_j c_j|) + O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)|\mathbf{c}|. \tag{3.9}$$

We multiply (3.7) by $H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})$ and integrate with respect to $2\pi r\, dr$ over (0, 1) to find the equations

$$\sum_{j=1}^{K} \langle c_j L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'}) \rangle + \langle \phi^\perp, L_0(H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})) \rangle$$
$$= \lambda \sum_{j=1}^{K} c_j \langle H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'}) \rangle.$$

In these equations

$$\langle \phi^\perp, L_0(H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})) \rangle = O(\|\phi^\perp\| \cdot \|L_0(H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'}))\|_1),$$

where $\|\cdot\|_1$ denotes the $L^1(D)$ norm. By (3.6) we find

$$\|L_0(H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'}))\|_1 = O(\epsilon^2).$$

Then by (3.9) we deduce the equations

$$\sum_{j=1}^{K} c_j\langle L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})\rangle + O\left(\epsilon^3\Big|\sum_{j=1}^{K}(-1)^j r_j c_j\Big|\right) + O(\epsilon^4)|\mathbf{c}|$$
$$+ O(\epsilon^2|\lambda|)|\mathbf{c}| = \lambda\sum_{j=1}^{K} c_j\langle H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})\rangle, \tag{3.10}$$

for $k=1,2,\ldots,K$. The inner products in (3.10) are given in the next lemma.

Lemma 3.3: In Eq. (3.10):

(1) $\langle H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'}), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})\rangle = 2\pi\epsilon r_k \tau\delta_{jk} + O(\epsilon^2)$;

(2) $\langle L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})\rangle$
$$= 4\pi\epsilon^2(-1)^{k+j} r_j r_k \overline{f'(u)} + 2\pi\epsilon^3 r_k\left\{\delta_{jk}\left[-\frac{\tau}{r_k^2} + (-1)^k\gamma v'(r_k)\right] + \gamma(-1)^{k+j}G_0(r_k,r_j)\right\} + O(\epsilon^4).$$

Proof: (1) is obvious. To prove (2) we note that P' decays exponentially fast. Then (3.6) implies that

$$\begin{aligned}
&\langle L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})), H_k' - \overline{H_k'} + \epsilon(P_k' - \overline{P_k'})\rangle \\
&= \langle L_0(H_j' - \overline{H_j'} + \epsilon(P_j' - \overline{P_j'})), H_k' - \overline{H_k'} + \epsilon P_k'\rangle \\
&= \epsilon^2\left\langle\left(f''(H_j)Q_j + \frac{f'''(H_j)P_j^2}{2}\right)H_j' + f''(H_j)P_jP_j' + \frac{tH_j''}{r_j r} - \frac{P_j''}{r} + \gamma(-1)^{j+1}G_0(r,r_j), H_k' + \epsilon P_k'\right\rangle \\
&\quad + 2\epsilon(-1)^{j+1} r_j\langle\overline{f'(u)} - f'(u), H_k' + \epsilon P_k'\rangle + O(\epsilon^4) \\
&= \epsilon^2\left\langle\left(f''(H_j)Q_j + \frac{f'''(H_j)P_j^2}{2}\right)H_j' + f''(H)P_jP_j' + \frac{t}{r_j r}H_j'' - \frac{P_j''}{r} + \gamma(-1)^{j+1}G_0(r,r_j), H_k'\right\rangle \\
&\quad + 2\epsilon\pi(-1)^{j+1} r_j\overline{f'(u)}\,\overline{H_k' + \epsilon P_k'} + O(\epsilon^4)
\end{aligned} \tag{3.11}$$

$$\begin{aligned}
&= 2\pi\epsilon^3 r_k\left\{\delta_{jk}\int_R\left[\left(f''(H_k)Q_k + \frac{f'''(H_k)P_k^2}{2}\right)H_k' + f''(H_k)P_kP_k' + \frac{tH_k''}{r_k^2} - \frac{P_k''}{r_k}\right]H_k' dt\right. \\
&\quad \left. + \gamma(-1)^{k+1}G_0(r_k,r_j)\right\} + 4\epsilon^2\pi(-1)^{k+j} r_j r_k\overline{f'(u)} + O(\epsilon^4).
\end{aligned} \tag{3.12}$$

Note that we have again used (3.3) and (3.4) to reach (3.11), and used (3.5) to reach (3.12). To find the integral in (3.12), we differentiate (2.25) to obtain

$$-Q_k''' + f'(H_k)Q_k' + f''(H_k)H_kQ_k - \frac{P_k''}{r_k} + \frac{H_k' + tH_k''}{r_k^2} + \frac{f'''(H_k)H_k'P_k^2}{2} + f''(H_k)P_kP_k' + \gamma v'(r_k) = 0.$$

Multiplying by H_k' and integrating over $(-\infty,\infty)$ yield

$$\int_R\left[f''(H_k)Q_k(H_k')^2 - \frac{P_k''H_k'}{r_k} + \frac{(H_k')^2 + tH_k''H_k'}{r_k^2} + \frac{f'''(H_k)P_k^2(H_k')^2}{2} + f''(H_k)P_kP_k'H_k'\right]dt$$
$$+ (-1)^{k+1}\gamma v'(r_k) = 0.$$

The integral in (3.12) now becomes

$$-\frac{1}{r_k^2}\int_R (H')^2 dt + (-1)^k \gamma v'(r_k).$$

□

With Lemma 3.3 we will write (3.10) in the vector form. We view $\mathbf{c}=(c_1,c_2,\cdots,c_K)^T$ as a column vector in R^K. Let $\mathbf{R}$ be a K by K rank one matrix:

$$\mathbf{R} = 2\overline{f'(u)}\begin{bmatrix} r_1 & -r_2 & r_3 & -r_4 & \cdots & (-1)^{1+k}r_K \\ -r_1 & r_2 & -r_3 & r_4 & \cdots & (-1)^{2+k}r_K \\ r_1 & -r_2 & r_3 & -r_4 & \cdots & (-1)^{3+k}r_K \\ (-1)^{K+1}r_1 & (-1)^{K+2}r_2 & (-1)^{K+3}r_3 & (-1)^{K+4}r_4 & \cdots & r_K \end{bmatrix}, \tag{3.13}$$

and $\mathbf{M}$ be a K by K matrix whose kj entry is

$$M_{kj} = \delta_{jk}\left(-\frac{\tau}{r_k^2} + (-1)^k \gamma v'(r_k)\right) + \gamma(-1)^{k+j} G_0(r_k,r_j).$$

In R^K we define a nonstandard inner product g by

$$g(\mathbf{A},\mathbf{B}) = \sum_{j=1}^{K} A_j B_j r_j, \quad \mathbf{A} = (A_1,A_2,\ldots,A_K)^T, \quad \mathbf{B} = (B_1,B_2,\ldots,B_K)^T. \tag{3.14}$$

The matrices $\mathbf{R}$ and $\mathbf{M}$ represent symmetric linear operators on R^K with respect to this inner product. The symmetry of $\mathbf{M}$ under g is a consequence of the fact that $r_k G_0(r_k,r_j)=r_j G_0(r_j,r_k)$. Let $\{\mathbf{e}_n\}$ be an orthonormal basis under g in which

$$\mathbf{e}_1 = \sqrt{r_1+r_2+\cdots+r_K}(-1,1,-1,1\cdots,(-1)^K)^T. \tag{3.15}$$

$\mathbf{e}_1$ is an eigenvector vector of $\mathbf{R}$ with eigenvalue $2\overline{f'(u)}(r_1+r_2+\cdots+r_K)$. $\mathbf{e}_2,\mathbf{e}_3,\cdots,\mathbf{e}_K$ span the eigenspace of the eigenvalue 0, which has multiplicity $K-1$.

Now we rewrite (3.10) as

$$\epsilon^2\mathbf{R}\mathbf{c} + \epsilon^3\mathbf{M}\mathbf{c} + O(\epsilon^3|g(\mathbf{c},\mathbf{e}_1)|) + O(\epsilon^4|\mathbf{c}|) + O(\epsilon^2|\lambda||\mathbf{c}|) = \epsilon\tau\lambda\mathbf{c}. \tag{3.16}$$

In (3.16) $|\mathbf{c}|$, the norm of $\mathbf{c}$, may be understood as either the norm under the standard inner product or the norm under g, because the two norms are equivalent uniformly in ϵ.

We must consider two cases:

$$(1)\ g\left(\frac{\mathbf{c}}{|\mathbf{c}|},\mathbf{e}_1\right) \nrightarrow 0; \quad (2)\ g\left(\frac{\mathbf{c}}{|\mathbf{c}|},\mathbf{e}_1\right) = o(1).$$

Of course when $K=1$, the second case does not occur.

In the first case we use a rough form of (3.16):

$$\epsilon^2\mathbf{R}\mathbf{c} + O(\epsilon^3|\mathbf{c}|) + O(\epsilon^2|\lambda||\mathbf{c}|) = \epsilon\tau\lambda\mathbf{c}. \tag{3.17}$$

Take the g-inner product of (3.17) and $\mathbf{e}_1$:

$$2\epsilon^2\overline{f'(u)}\left(\sum_{j=1}^{K} r_j\right) g(\mathbf{c},\mathbf{e}_1) + O(\epsilon^3|\mathbf{c}|) + O(\epsilon^2|\lambda||\mathbf{c}|) = \epsilon\tau\lambda g(\mathbf{c},\mathbf{e}_1). \tag{3.18}$$

Since $g(\mathbf{c}/|\mathbf{c}|,\mathbf{e}_1) \nrightarrow 0$, (3.18) implies that

$$\lambda = \frac{\epsilon}{\tau}\left(\sum_{k=1}^{K} 2r_k\overline{f'(u)}\right) + O(\epsilon^2). \tag{3.19}$$

This eigenvalue is positive for small ϵ and of order ϵ. Consequently (3.9) implies that

$$\phi^{\perp} = O(\epsilon|\mathbf{c}|). \tag{3.20}$$

If we take the g-inner product of (3.17) and $\mathbf{e}_n$, $n \geqslant 2$, then

$$g(\mathbf{c},\mathbf{e}_n) = O(\epsilon|\mathbf{c}|), \quad n \geqslant 2. \tag{3.21}$$

The asymptotic properties of λ and ϕ in the first case follows from (3.19)–(3.21).

In the second case we take the g-inner product of (3.16) and $\mathbf{e}_n$, $n \geqslant 2$, to deduce

$$\epsilon^3 g(\mathbf{Mc},\mathbf{e}_n) + O(\epsilon^3|g(\mathbf{c},\mathbf{e}_1)|) + O(\epsilon^4|\mathbf{c}|) + O(\epsilon^2|\lambda||\mathbf{c}|) = \epsilon\tau\lambda g(\mathbf{c},\mathbf{e}_n), \quad n = 2,3,\ldots,K. \tag{3.22}$$

Note that $g(\mathbf{c}/|\mathbf{c}|,\mathbf{e}_1) = o(1)$ and (3.22) imply that $\lambda = O(\epsilon^2)$.

Then we take the g-inner product of (3.16) and $\mathbf{e}_1$:

$$2\epsilon^2\overline{f'(u)}\left(\sum_{j=1}^{K} r_j\right)g(\mathbf{c},\mathbf{e}_1) + O(\epsilon^3|\mathbf{c}|) + O(\epsilon^3|g(\mathbf{c},\mathbf{e}_1)|) + O(\epsilon^2|\lambda||\mathbf{c}|) = \epsilon\tau\lambda g(\mathbf{c},\mathbf{e}_1). \tag{3.23}$$

(3.23) and $\lambda = O(\epsilon^2)$ imply that

$$g(\mathbf{c},\mathbf{e}_1) = O(\epsilon|\mathbf{c}|), \tag{3.24}$$

which turns (3.9) to

$$\phi^{\perp} = O(\epsilon^2|\mathbf{c}|), \tag{3.25}$$

and (3.22) is simplified to

$$\epsilon^3 g(\mathbf{Mc},\mathbf{e}_n) + O(\epsilon^4|\mathbf{c}|) = \epsilon\tau\lambda g(\mathbf{c},\mathbf{e}_n), \quad n = 2,3,\ldots,K. \tag{3.26}$$

We pass limit in (3.26) and (3.24). Let $\mathbf{M}^0 = \lim_{\epsilon\to 0}\mathbf{M}$, $\mathbf{R}^0 = \lim_{\epsilon\to 0}\mathbf{R}$, $g^0 = \lim_{\epsilon\to 0} g$, $\mathbf{e}_j^0 = \lim_{\epsilon\to 0}\mathbf{e}_j$, and $\mu_0^0 = \lim_{\epsilon\to 0}\lambda/\epsilon^2$, and $\mathbf{c}^0 = \lim_{\epsilon\to 0}\mathbf{c}$, where $|\mathbf{c}^0| \neq 0$. Then

$$g^0(\mathbf{M}^0\mathbf{c}^0,\mathbf{e}_n^0) = \mu_0^0\tau g^0(\mathbf{c}^0,\mathbf{e}_n^0), \quad (n = 2,3\ldots,K), \quad g^0(\mathbf{c}^0,\mathbf{e}_1^0) = 0. \tag{3.27}$$

The second equation implies that we can decompose $\mathbf{c}^0$ as

$$\mathbf{c}^0 = \sum_{n=2}^{K} \tilde{c}_n^0\mathbf{e}_n^0. \tag{3.28}$$

The first equation in (3.27) becomes

$$\sum_{m=2}^{K} \tilde{c}_m^0 g^0(\mathbf{M}^0\mathbf{e}_m^0,\mathbf{e}_n^0) = \mu_0^0\tau\tilde{c}_n^0, \quad n = 2,3,\ldots,K. \tag{3.29}$$

Here (3.29) is a $K-1$ dimensional eigenvalue problem from which we find $K-1$ pairs of μ_0^0 and $(\tilde{c}_2^0,\tilde{c}_3^0,\ldots,\tilde{c}_K^0)$. This proves the asymptotic properties of λ and ϕ in the second case.

As we have explained in Sec. II that the construction of u via the Γ-convergence theory assumes that (2.12) is positive definite in T. The paragraph after (2.12) shows that this condition, (2.14), is equivalent to the condition that μ_0^0 in (3.29) are all positive. Hence λ_0 are all positive when ϵ is sufficiently small.

In summary, we have proven that if (λ_0,ϕ_0) is an eigenpair of (2.30) with the property $\lambda_0 = o(1)$ then λ_0 and ϕ_0 must possess the asymtotic properties described in Theorem 3.1. We still need to show that there indeed exist exactly K eigenparis of (2.30) with the properties. The proof

of this fact uses some ideas from the linear perturbation theory. Not to prolong this section we omit the proof. Instead we will give a full proof in the next section for the $m \geqslant 1$ case, which is similar to the one for the $m=0$ case.

IV. THE CRITICAL EIGENVALUES λ_m

Theorem 4.1: *When ϵ is sufficiently small, there exist exactly K eigenparis (λ_m, ϕ_m) of* (2.31) *with $\lambda_m = o(1)$. Each λ_m and ϕ_m have the asymptotic expansion*

$$\lambda_m = \epsilon^2 \mu_m^0 + o(\epsilon^2), \phi_m = \sum_{j=1}^{K} c_j (H_J' + \epsilon P_j') + O(\epsilon^2 |\mathbf{c}|).$$

μ_m^0 and the limit $\mathbf{c}^0 = \lim_{\epsilon \to 0}(c_1, c_2, \ldots, c_K)$ form an eigenpair of the K-dimensional eigenvalue problem

$$\left\{ \frac{(m^2-1)\tau}{(r_k^0)^2} + (-1)^k \gamma (v^0)'(r_k^0) \right\} c_k^0 + \gamma \sum_{j=1}^{K} (-1)^{k+j} G_m(r_k^0, r_j^0) c_j^0 = \mu_m^0 \tau c_k^0, \quad k = 1,2, \ldots, K.$$

G_m is defined after (2.31): $G_m(r,s) = G_m[\delta(\cdot - s)](r)$. More explicitly

$$G_m(r,s) = \begin{cases} \left(\dfrac{s^{1-m}}{2m} + \dfrac{s^{1+m}}{2m} \right) r^m & \text{if } r < s \\ \dfrac{s^{1+m}}{2m} (r^m + r^{-m}) & \text{if } r \geqslant s. \end{cases} \tag{4.1}$$

Note that $G_m(r,s)$ is not symmetric in r and s, although $rG_m(r,s)$ is. So with respect to g^0 the matrix in the K dimensional eigenvalue problem represents a symmetric operator.

In the proof of Theorem 4.1 we write (λ, ϕ) for (λ_m, ϕ_m) for simplicity. We decompose in $L^2(D)$

$$\phi(r) = \sum_{j=1}^{K} c_j (H_j' + \epsilon P_j') + \phi^{\perp}, \quad \text{where } \phi^{\perp} \perp H_j' + \epsilon P_j' \quad (j = 1,2, \ldots, K). \tag{4.2}$$

First we compute

$$\begin{aligned} L_m H_j' &= -\epsilon^2 (H_j')_{rr} - \frac{\epsilon^2}{r} (H_j')r + \frac{\epsilon^2 m^2}{r^2} H_j' + f'(u) H_j' + \epsilon \gamma G_m[H_j'] \\ &= (f'(u) - f'(H_j)) H_j' - \frac{\epsilon}{r} H_j'' + \frac{\epsilon^2 m^2}{r^2} H_j' + \epsilon^2 \gamma (-1)^{j+1} G_m(r, r_j) + O(\epsilon^3) \\ &= \epsilon f''(H_j) P_j H_j' + \epsilon^2 \left(f''(H_j) Q_j + \frac{f'''(H_j) P_j^2}{2} \right) H_j' - \frac{\epsilon}{r} H_j'' + \frac{\epsilon^2 m^2}{r^2} H_j' + \epsilon^2 \gamma (-1)^{j+1} G_m(r, r_j) \\ &\quad + O(\epsilon^3). \end{aligned}$$

By differentiating (2.23) we have

$$-P_j''' + f'(H_j) P_j' + f''(H_j) H_j' P_j - \frac{H_j''}{r_j} = 0.$$

Then

$$L_m P_j' = -\epsilon^2 (P_j')rr - \frac{\epsilon^2}{r}(P_j')_r + \frac{\epsilon^2 m^2}{r^2} P_j' + f'(u)P_j' + \epsilon\gamma G_m[P_j']$$

$$= (f'(u) - f'(H_j))P_j' - f''(H_j)H_j' P_j + \frac{H_j''}{r_j} - \frac{\epsilon}{r}P_j'' + O(\epsilon^2)$$

$$= \epsilon f''(H_j)P_j P_j' - f''(H_j)H_j' P_j + \frac{H_j''}{r_j} - \frac{\epsilon}{r}P_j'' + O(\epsilon^2).$$

Therefore,

$$L_m(H_j' + \epsilon P_j') = \epsilon^2 \left[\left(f''(H_j)Q_j + \frac{f'''(H_j)P_j^2}{2} \right) H_j' + f''(H_j)P_j P_j' + \frac{tH_j''}{r_j r} + \frac{m^2 H_j'}{r^2} - \frac{P_j''}{r} + \gamma(-1)^{j+1} G_m(r, r_j) \right] + O(\epsilon^3). \tag{4.3}$$

In particular,

$$L_m(H_j' + \epsilon P_j') = O(\epsilon^2). \tag{4.4}$$

Rewrite the equation $L_m\phi = \lambda\phi$ as

$$\sum_{j=1}^{K} c_j L_m(H_j' + \epsilon P_j') + L_m\phi^\perp = \lambda\left(\sum_{j=1}^{K} c_j(H_j' + \epsilon P_j') + \phi^\perp \right). \tag{4.5}$$

Then $\phi^\perp$ satisfies

$$L_m\phi^\perp = O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)(|\mathbf{c}| + \|\phi^\perp\|).$$

Lemma 4.2: There exists $C>0$ independent of ϵ such that for all $\psi \perp H_j' + \epsilon P_j'$, $j = 1, 2, \ldots, K$, $\|\psi\| \leqslant C\|L_m\psi\|$.

The proof of this lemma is similar to that of Lemma 3.2, so we omit it. We obtain by Lemma 4.2 that

$$\phi^\perp = O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)(|\mathbf{c}| + \|\phi^\perp\|),$$

which implies, since $\lambda = o(1)$, that

$$\phi^\perp = O(\epsilon^2)|\mathbf{c}| + O(|\lambda|)|\mathbf{c}|. \tag{4.6}$$

We multiply (4.5) by $H_k' + \epsilon P_k'$ and integrate with respect to $2\pi r\, dr$ over $(0,1)$. Then

$$\sum_{j=1}^{K} \langle c_j L_m(H_j' + \epsilon P_j'), H_k' + \epsilon P_k' \rangle + \langle \phi^\perp, L_m(H_k' + \epsilon P_k') \rangle = \lambda \sum_{j=1}^{K} c_j \langle H_j' + \epsilon P_j', H_k' + \epsilon P_k' \rangle,$$

which, by (4.6) and (4.4), may be written as

$$\sum_{j=1}^{K} c_j \langle L_m(H_j' + \epsilon P_j'), H_k' + \epsilon P_k' \rangle + O(\epsilon^4)|\mathbf{c}| + O(\epsilon^2|\lambda|)|\mathbf{c}| = \lambda \sum_{j=1}^{K} c_j \langle H_j' + \epsilon P_j', H_k' + \epsilon P_k' \rangle \tag{4.7}$$

for $k = 1, 2 \ldots, K$.

Lemma 4.3: In Eq. (4.7):

(1) $\langle H_j' + \epsilon P_j', H_k' + \epsilon P_k' \rangle = 2\pi\epsilon r_k \tau \delta_{jk} + O(\epsilon^2)$,

(2) $\langle L_m(H_j' + \epsilon P_j'), H_k' + \epsilon P_k' \rangle = 2\pi\epsilon^3 r_k \{ \delta_{jk}[(m^2 - 1)\tau / r_k^2 + (-1)^k \gamma v'(r_k)] + \gamma(-1)^{k+j} G_m(r_k, r_j) \} + O(\epsilon^4)$.

Proof: (1) is obvious. To prove (2) we note that P' decays exponentially fast. Then (4.3) implies that

$$\begin{aligned}\langle L_m(H_j'+\epsilon P_j'),H_k'+\epsilon P_k'\rangle &= \langle L_m(H_j'+\epsilon P_j'),H_k'\rangle + O(\epsilon^4)\\ &= 2\pi\epsilon^3 r_k\Bigg\{\delta_{jk}\int_R\Bigg[\left(f''(H_k)Q_k+\frac{f'''(H_k)P_k^2}{2}\right)H_k'+f''(H_k)P_kP_k'+\frac{tH_k''}{r_k^2}\\ &\quad+\frac{m^2H_k'}{r_k^2}-\frac{P_k''}{r_k}\Bigg]H_k'dt+\gamma(-1)^{k+j}G_m(r_k,r_j)\Bigg\}+O(\epsilon^4).\end{aligned}$$

To find the integral in the last line we follow the argument used in the proof of Lemma 3.3. □

This lemma simplifies (4.7) to

$$\left(\frac{(m^2-1)\tau}{r_k^2}+(-1)^k\gamma v'(r_k)\right)c_k+\gamma\sum_{j=1}^{K}(-1)^{k+j}G_m(r_k,r_j)c_j+O(\epsilon|\mathbf{c}|)+O\left(\frac{|\lambda||\mathbf{c}|}{\epsilon}\right)=\frac{\tau\lambda c_k}{\epsilon^2}. \tag{4.8}$$

Hence λ is of order ϵ^2. (4.6) now becomes

$$\phi^{\perp}=O(\epsilon^2|\mathbf{c}|). \tag{4.9}$$

After passing limit in (4.8) we deduce the asymptotic properties in Theorem 4.1 for λ and ϕ.

We have proved that if (λ_m,ϕ_m) is an eigenpair associated with m with $\lambda=o(1)$, then it must have the asymptotic behavior described in Theorem 4.1. To complete the proof of the theorem we proceed to show that there exist exactly K simple eigenpairs of (2.31) with the properties.

Let F be the linear subspace spanned by critical eigenfunctions. It is defined unambiguously by $F=\mathrm{span}\{\phi\in L^2(0,1):L_m(\phi)=\lambda\phi,|\lambda|<\epsilon^{1/2}\}$. Since the critical eigenvalues of L_m are of order ϵ^2, F includes all the critical eigenfunctions.

First dim F, the dimension of F, is at most K. Suppose that this is not the case. There exist two distinct eigenpairs (λ,ϕ) and (λ',ϕ') with the same asymptotic behavior. That is

$$\lambda=\epsilon^2\eta+o(\epsilon^2),\quad \lambda'=\epsilon^2\eta+o(\epsilon^2),\quad \phi=\sum_j c_j(H_j'+\epsilon P_j')+\psi,$$

$$\phi'=\sum_j c_j'(H_j'+\epsilon P_j')+\psi',\quad \lim_{\epsilon\to 0}c_j=\lim_{\epsilon\to 0}c_j'=c_j^0.$$

But the two eigenfunctions must be orthogonal, so

$$0=\langle\phi,\phi'\rangle=2\epsilon\pi g^0(\mathbf{c}^0,\mathbf{c}^0)\int_{-\infty}^{\infty}(H'(t))^2dt+o(\epsilon)|\mathbf{c}^0|^2.$$

This is obviously impossible when ϵ is sufficiently small.

Next dim F is at least K. Suppose otherwise that dim $F<K$. Define a subspace of $L^2(0,1)$: $S=\mathrm{span}\{\Sigma_j c_j^0(H_j'+\epsilon P_j')\}$, where c_j^0 are the K eigenvectors of the K-dimensional eigenvalue problem in the statement of the theorem. We use a perturbation argument. The asymmetric distance between the closed subspaces S and F is

$$d(S,F)=\sup\{d(\varphi,F):\varphi\in S,\|\varphi\|_2=1\},$$

where $d(x,F)=\inf\{\|x-y\|_2:y\in F\}$. Since dim $F<$ dim S, there exists $\Sigma_j b_j^0(H_j'+\epsilon P_j')\in S$ such that for every eigenvector in F which may be written as $\Sigma_j c_j(H_j'+\epsilon P_j')+\psi$ with $\|\psi\|=O(\epsilon^2|\mathbf{c}|)$, $g^0(\mathbf{c}/|\mathbf{c}|,\mathbf{b}^0/|\mathbf{b}^0|)=o(1)$. Then straight calculations show that

$$\left\langle \frac{\sum_j c_j(H_j'+\epsilon P_j')+\psi}{\left\|\sum_j c_j(H_j'+\epsilon P_j')+\psi\right\|_2}, \frac{\sum_j b_j^0(H_j'+\epsilon P_j')}{\left\|\sum_j b_j^0(H_j'+\epsilon P_j')\right\|_2} \right\rangle = o(1).$$

So if we use $\varphi=\Sigma_j b_j^0(H_j'+\epsilon P_j')/\|\Sigma_j b_j^0(H_j'+\epsilon P_j')\|_2$, $d(\varphi,F)=1-o(1)$ and $d(S,F)=1-o(1)$. The following lemma due to Helffer and Sjöstrand[12] will give us a contradiction.

Lemma 4.4: Let L be a self-adjoint operator on a Hilbert space H, Q a compact interval in $(-\infty,\infty)$ *and* $e_1,e_2,\ldots,e_K$ *normalized linearly independent elements in the domain of L. Assume that the following are true.*

(1) $L(e_k)=p_k e_k+r_k, \|r_k\|_H \leqslant \epsilon'$ *and* $p_k \in Q, k=1,2,\ldots,K$.
(2) *There is* $\omega>0$ *so that Q is* ω*-isolated in the spectrum of L,* i.e., $(\sigma(L)\backslash Q)\cap(Q+(-\omega,\omega))=\emptyset$.

Then $d(S,F)\leqslant K^{1/2}\epsilon'/(\omega\kappa^{1/2})$, *where* $S=span\{e_1,\ldots,e_K\}$ $F=$ *the closed subspace associated to* $\sigma(L)\cap Q$, *and* $\kappa=$ *the smallest eigenvalue of the matrix* $[\langle e_j,e_k\rangle]$.

Here we take $L=L_m$, each e_k is normalized and proportional to $\Sigma_j c_j^0(H_j'+\epsilon P_j')$ for each one of the K vectors $\mathbf{c}^0$, and S, F as before. ω and κ are positive and bounded away from 0 as $\epsilon\to 0$. Set $p_k=\eta\epsilon^2$ and $Q=[-\epsilon^{1/2},\epsilon^{1/2}]$. From (4.3) we find

$$L_m\left(\sum_j c_j^0(H_j'+\epsilon P_j')\right)-p_k\sum_j c_j^0(H_j'+\epsilon P_j')=O(\epsilon^2|\mathbf{c}^0|),$$

and on the other hand $\|\Sigma_j c_j^0(H_j'+\epsilon P_j')\|_2\sim\epsilon^{1/2}|\mathbf{c}^0|$. Therefore $\|r_k\|_2=O(\epsilon^{3/2})$, Consequently $d(S,F)=o(1)$, a contradiction.

V. THE CASES OF $K=1$ AND $K=2$

We know from Theorem 1.1 that the spot solution ($K=1$) exists for all γ. However the stability of the solution in two dimensions depends on γ. For small ϵ, the spot solution is stable if γ is small and unstable if γ is large. More precisely we have

Theorem 5.1: *Let* $K=1$. *There exists* $\hat\gamma>0$ *such that when* $\gamma\in(0,\hat\gamma)$ *there exists* $\hat\epsilon$ *such that for every* $\epsilon\in(0,\hat\epsilon)$ *all* $\lambda_m>0$, i.e., *the spot solution u is stable. On the other hand if* $\gamma>\hat\gamma$, *there exist* $\tilde\epsilon>0$ *and* $m\geqslant 2$ *such that for all* $\epsilon\in(0,\tilde\epsilon)$, $\lambda_m<0$, i.e., *u is unstable.*

Proof: Theorem 3.1 shows that when $K=1$, there is only one λ_0 with the property $\lambda=o(1)$. This λ_0 is positive and of order ϵ for all γ if ϵ is sufficiently small.

When $m=1$, in Theorem 4.1:

$$\gamma\{-(v^0)'(r_1^0)+G_1(r_1^0,r_1^0)\}=\mu_1^0\tau. \tag{5.1}$$

According to (4.1), $G_1(r_1^0,r_1^0)=((r_1^0)^3+r_1^0)/2$. When $K=1$, $a=1-(r_1^0)^2$ by (2.7) and $(v^0)'(r_1^0)=(r_1^0-(r_1^0)^3)/2$ by solving the equation

$$-(v^0)''-\frac{1}{r}(v^0)'=u^0-a,\quad (v^0)'(0)=(v^0)'(1)=0.$$

Therefore $\mu_1^0=\gamma(r_1^0)^3/\tau>0$ and $\lambda_1>0$.

When $m\geqslant 2$, let $K=1$ in Theorem 4.1:

$$\frac{(m^2-1)\tau}{(r_1^0)^2}+\gamma\left\{\frac{(r_1^0)^3-r_1^0}{2}+\frac{(r_1^0)^{2m+1}+r_1^0}{2m}\right\}=\mu_m^0\tau. \tag{5.2}$$

Clearly when γ is small, the first term on the left side dominates and μ_m^0 is positive for all $m\geqslant 2$. On the other hand we find that the quantity in the braces is negative if m is sufficiently large. Fixing such m and taking γ large enough, we find that the entire left-hand side of (5.2) becomes negative. □

The borderline value $\hat\gamma$ for γ can be calculated easily from (5.2) in two steps.

TABLE I. The value of $\hat{\gamma}$ for various a and the corresponding mode $\hat{m}$ of the principal eigenvalue $\lambda_{\hat{m}}$ which varnishes up to order ϵ^2. Here $\tau=\sqrt{2}/12$.

a	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$\hat{m}$	19	9	6	4	3, 4	3	2	2	2
$\hat{\gamma}$	2468.56	356.23	123.86	64.69	42.67	30.38	27.76	28.23	56.61

(1) For each integer $m\geqslant 2$ find $\hat{\gamma}_m$ by setting the right-hand side of (5.2) to be 0 and solving the equation for γ. If the resulting $\hat{\gamma}_m$ is less than or equal to 0, this mode m does not yield a zero eigenvalue. Discard such $\hat{\gamma}_m$.
(2) Minimize the $\hat{\gamma}_m$'s from the last step with respect to $m\geqslant 2$. The minimum is $\hat{\gamma}$, achieved at $m=\hat{m}$ where $\lambda_{\hat{m}}$, the principal eigenvalue, vanishes up to order ϵ^2.

The values $\hat{\gamma}$ for several a are reported in Table I. Curiously when $a=1/2$ the borderline $\hat{\gamma}$ occurs at two modes $\hat{m}=3$ and $\hat{m}=4$. In this case if $\gamma=\hat{\gamma}$ both λ_3 and λ_4 are of order $o(\epsilon^2)$ while the other λ_m's$(m\geqslant 2)$ are positive and $\sim\epsilon^2$.

One gains more insight into the diblock copolymer equation by comparing with the Cahn–Hilliard equation, which is (1.6) with $\gamma=0$. The Cahn–Hilliard equation also has a spot solution. Its critical eigenvalues are again classified into λ_m for non-negative integers m. If we formally set $\gamma=0$ in Theorem 3.1 and (5.2) it appears that for the Cahn–Hilliard equation λ_0 is positive and of order ϵ, and λ_m with $m\geqslant 2$ is also positive and of order ϵ^2. From (5.1) with $\gamma=0$, one thinks that up to order ϵ^2, λ_1 vanishes. These statements are actually all correct, although the exact value of λ_1 is negative, and the spot solution is unstable in the Cahn–Hilliard problem. Therefore Theorem 5.1 does not cover the Cahn–Hilliard equation. Nevertheless the distance between λ_1 and 0 is exponentially small there and is not visible in (5.1). The smallness of λ_1 is related to the phenomenon of the slow motion of a bubble profile in a general domain (see Alikakos and Fusco,[2,3] Ward,[37] and Alikakos, Bronsard and Fusco[1]). One may feel uneasy about the abrupt change from negative λ_1 to positive λ_1 as we add a nonlocal term with a small γ. This is a result of our setting of fixing γ while taking ϵ small. To find the threshold where $\lambda_1=0$ one must take γ to vary with ϵ. We suspect that a borderline lies where γ is exponentially small compared to ϵ.

When we further increase γ, we reach the second threshold where one of λ_m with $m\geqslant 2$ becomes 0. Beyond this critical γ value the spot solution is unstable. It no longer has enough oscillation demanded by the stronger nonlocal term now. Note that the first stability threshold occurs because of λ_1 which is related to the translation of the spot, while the second threshold occurs because of some λ_m with $m\geqslant 2$ which is related to the oscillation of the boundary of the spot.

The situation is more complex when $K\geqslant 2$, because the existence of u is conditional. According to Theorem 2.2, we have u if (2.12) is positive definite in T. This condition requires two things. First (2.10) must have a solution $\mathbf{r}^0$. From this $\mathbf{r}^0$ we construct $\mathcal{U}(\cdot;\mathbf{r}^0)$, $\mathcal{V}(\cdot;\mathbf{r}^0)$, g^0, $\mathbf{e}_j^0$, and finally the matrix $\mathbf{M}^0$. The second requirement is that the eigenvalues of the $K-1$ by $K-1$ matrix $g^0(\mathbf{M}^0\mathbf{e}_n^0,\mathbf{e}_m^0),n,m=2,3,\ldots,K$, in Theorem 3.1 must all be positive. When these two requirements are met, u exists and its stability in two dimensions is determined by the eigenvalues λ_m, $m\geqslant 1$. Their leading order approximations μ_m^0 are calculated from the K by K matrix in Theorem 4.1.

The determination of $\mathbf{r}^0$ and the analysis of the matrices have to be done numerically. As an example we consider $K=2$. Let $a=1/2$, $\tau=\sqrt{2}/12$, and try various values of γ. Instead of considering q_1 and q_2 under the constraint $-q_1^2+q_2^2=a$, we let $y=q_1^2$ and $q_2=\sqrt{y+a}$. Then as done in Ref. 25, J may be treated as a function, of y without constraint, $J(y)=J(q_1(y),q_2(y))$.

According to Sec. II for given y we find q_1 and q_2, $\mathcal{U}(\cdot;q_1,q_2)$, $\mathcal{V}(\cdot;q_1,q_2)$, and $J(y)$. When γ is small, e.g., $\gamma=1$, J is increasing in y, Fig. 4(1), and (2.10) has no solution.

When γ is increased to 25, J has a critical point at $y=0.0802$, Fig. 4(2), i.e., (2.10) has a solution $\mathbf{r}^0=(0.2832,0.7616)$. We calculate $g^0(\mathbf{M}^0\mathbf{e}_2^0,\mathbf{e}_2^0)$ which turns out to be positive. Hence μ_0^0

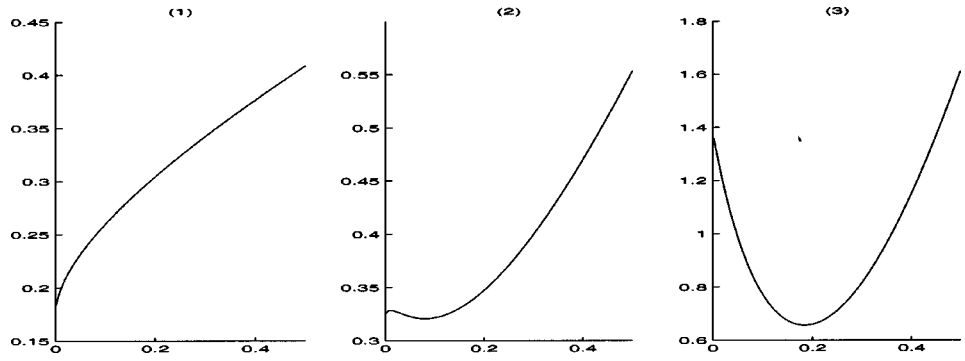

FIG. 4. (1) When $\gamma=1$, $J(y)$ is increasing in y. No $\mathbf{r}^0$ exists. (2) When $\gamma=25$, a local minimum of $J(y)$ appears and $\mathbf{r}^0$ exists. The $K=2$ ring solution is stable. (3) When $\gamma=200$, $\mathbf{r}^0$ still exists, but the $K=2$ ring solution is unstable. In all three cases $a=1/2$ and $\tau=\sqrt{2}/12$.

is positive, $y=0.0802$ is a local minimum of J, and a solution u exists. Then we compute the eigenvalues μ_m^0 of the matrix in Theorem 4.1. They are all positive, Table II. So u is a stable solution in two dimensions.

When γ is further increased to 200, J has a critical point at $y=0.1841$, Fig. 4(3), corresponding to $\mathbf{r}^0=(0.4290,0.8271)$, $g^0(\mathbf{M}^0\mathbf{e}_2^0,\mathbf{e}_2^0)$ is positive, so a solution u exists. However some $\mu_m^0(m\geqslant 1)$ are negative, Table III. Hence u is unstable in two dimensions.

There is something interesting in Fig. 4(2) and (3). If we blow them up near $y=0$, Fig. 5, then in each case we find a local *maximum* near $y=0$. This is because that $J(y)$ is increasing in y near $y=0$ and near $y=1-a$. So whenever there is a local minimum, there must be a local maximum before the local minimum. This local maximum gives rise to a solution $\hat{\mathbf{r}}^0$ of (2.10). However we cannot use the Γ-convergence theory to find a solution of (1.6) near $\mathcal{U}(\cdot;\hat{\mathbf{r}}^0)$. We conjecture that such a solution exists.

When the critical eigenvalues of a spot or a ring solution, determined from Theorems 3.1 and 4.1, are nonzero, we may expect to have a similar solution of (1.6) on a slightly perturbed domain. However finding solutions of (1.6) on a general domain $\Omega\subset R^N$ is rather difficult. It was noted in Ref. 19 that (1.6) has a singular limit as $\epsilon\to 0$. One looks for a function $u^0\in BV(\Omega)$ defined such that for a.e. $x\in\Omega$, $u^0(x)=0$ or $u^0(x)=1$ and $\overline{u^0}=a$. Let S be the union of the hypersurfaces that separate the regions $u^0=0$ from the regions $u^0=1$, and $v^0=(-\Delta)^{-1}(u^0-a)$. Then one requires that at every $x\in S$,

$$\tau\kappa(x)+\gamma v^0(x)=\eta, \tag{5.3}$$

where $\kappa(x)$ is the mean curvature of S at x viewed from the $u^0=1$ side, and η is a Lagrange multiplier to be determined. If the free boundary problem (5.3) admits an isolated stable solution u^0, then near u^0, in the $L^2(\Omega)$ sense, there exists a local minimizer solution u of (1.6) by the Γ-convergence theory. However (5.3) is a challenging nonlocal geometric problem. Even though Fig. 1(2) and (3) suggest we look for solutions with multiple spots, (5.3) implies that for such a solution the curvature of the boundary of a spot is in general not constant (there is the impact of v^0), i.e., the spots are not exactly round, unless we deal with the one spot or the ring solutions in a disk as in this paper. Nevertheless if we consider the situation where a is close to 0 (or 1), then

TABLE II. μ_m^0 when $\gamma=25$. Here $\mathbf{r}^0=(0.2832,0.7616)$.

μ_0^0	μ_1^0	μ_2^0	μ_3^0	μ_4^0	μ_5^0	μ_6^0	μ_7^0	μ_8^0	μ_9^0	μ_{10}^0
14.90	8.15	27.80	16.73	19.11	29.36	45.07	65.30	89.59	117.70	149.52
	107.71	39.65	94.79	179.58	290.33	426.53	587.96	774.51	986.13	1222.77

TABLE III. μ_m^0 when $\gamma=200$. Here $\mathbf{r}^0=(0.4290,0.8271)$.

μ_0^0	μ_1^0	μ_2^0	μ_3^0	μ_4^0	μ_5^0	μ_6^0	μ_7^0	μ_8^0	μ_9^0	μ_{10}^0
135.39	48.34	−5.03	−21.81	−10.89	19.86	18.00	15.40	21.97	35.43	54.42
	1220.57	384.95	163.82	75.22	35.73	68.85	130.74	205.72	293.01	392.18

v^0 is near constant throughout Ω and hence κ becomes close to a constant and the spots are approximately round. The cylindrical and spherical phases in Fig. 1 are thus heuristically explained. Note that in the singular limit of the Cahn–Hilliard equation, which is (5.3) without the $\gamma v^0(x)$ term, κ is constant.

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APPENDIX: PROOF OF LEMMA 2.3

Since $\eta=\overline{f(u)}$, we obtain a rough estimate for η,

$$|\eta| = |\overline{f(u)}| \leqslant C\left(\int_D W(u)dx\right)^{1/2} = O(\epsilon^{1/2}), \tag{A1}$$

since $I(u)=O(\epsilon)$. $||u||_2=O(1)$ implies that $||v||_{2,2}=O(1)$ and in particular $v=O(1)$. A maximum principle argument shows that

$$-O(\epsilon^{1/2}) = -(O(\epsilon)+O(|\eta|)) \leqslant u \leqslant 1+O(\epsilon)+O(|\eta|) = 1+O(\epsilon^{1/2}). \tag{A2}$$

In the Γ-convergence theory u satisfies $u\to u^0$ in $L^2(D)$ and $(\epsilon\pi)^{-1}I(u)\to J(u^0)$.[25] The fact $u\to u^0$ in $L^2(D)$ implies the existence of r_j where $u(r_j)=1/2$ and that $r_j\to r_j^0$ for $j=1,2,\ldots,K$. We construct a preliminary approximation h of u,

$$h(r) = H\left(\frac{r-r_1}{\epsilon}\right) + \left[H\left(-\frac{r-r_2}{\epsilon}\right)-1\right] + H\left(\frac{r-r_3}{\epsilon}\right) + \left[H\left(-\frac{r-r_4}{\epsilon}\right)-1\right] + \cdots, r\in(r_1,1),$$

and let $d=u-h$.

If we consider h on $(r_1,1)$, the argument in Proposition 8.2 (Ref. 26) shows that $d=o(1)$ on $[r_1,1]$. Next we improve (A1) to

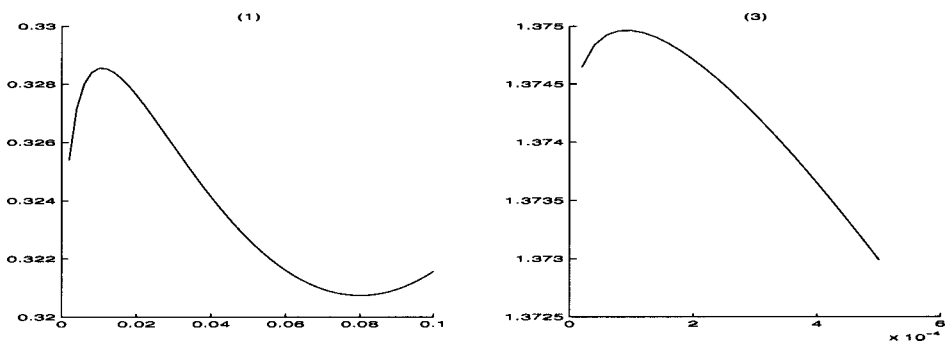

FIG. 5. (1) The enlarged Fig. 4(2) near $y=0$. (2) The enlarged Fig. 4(3) near $y=0$.

$$\eta = O(\epsilon), \tag{A3}$$

and show that

$$d = O(\epsilon) \text{ in } [r_1, 1]. \tag{A4}$$

Note that $d = u - h$ satisfies the equation

$$-\epsilon^2 d_{rr} + f'(h)d + O(||d||^2) + O(\epsilon) = \eta, \quad d(r_j) = 0 \quad (j = 1,2,\ldots,K), \quad d'(1) = 0$$

on $(r_1, 1)$. Then $d = O(\epsilon + |\eta|)$ in $[r_1, 1]$. Now we use an idea of Pohozaev.[22] Multiply the first equation of (1.8) by $r^2 u_r$ and integrate with respect to dr on (0, 1). Then

$$\int_0^1 [-\epsilon^2 (ru_r)_r (ru_r) + r^2 f(u) u_r + \epsilon\gamma r^2 v u_r] dr = \eta \int_0^1 r^2 u_r dr.$$

The first term on the left-hand side becomes 0 after integration. Applying integration by parts to the second and third terms on the left-hand side and the right-hand side shows that

$$r^2 W(u)|_{r=0}^{r=1} - 2\int_0^1 W(u) r\, dr + \epsilon\gamma r^2 v u|_{r=0}^{r=1} - \epsilon\gamma \int_0^1 u (r^2 v)_r dr = \eta(r^2 u|_{r=0}^{r=1} - 2\int_0^1 u\, r dr),$$

which is simplified to

$$W(u(1)) - \frac{1}{\pi}\int_D W(u) dx + O(\epsilon) = \eta(u(1) - a)$$

since $\epsilon\gamma v(1) u(1) = O(\epsilon)$ and $\epsilon\gamma \int_0^1 u (r^2 v)_r dr = O(\epsilon)$. The integral in the last equation is of order $O(\epsilon)$ since it is a part of $I(u)$ and $I(u) = O(\epsilon)$ by $(\epsilon\pi)^{-1} I(u) \to J(u^0)$. Moreover $u(1) \to 0$ or 1 to which a is not equal, so the last equation reads

$$\eta = O(\epsilon) + O(W(u(1))).$$

However $d = O(\epsilon + |\eta|)$ on $[r_1, 1]$ proved earlier implies that $u(1) = O(\epsilon + |\eta|)$ or $u(1) = 1 + O(\epsilon + |\eta|)$. Then $W(u(1)) = W(O(\epsilon + |\eta|)) = O((\epsilon + |\eta|)^2)$, or $W(u(1)) = W(1 + O(\epsilon + |\eta|)) = O((\epsilon + |\eta|)^2)$. Hence we derive

$$\eta = O(\epsilon) + O((\epsilon + |\eta|)^2), \quad \text{i.e., } \eta = O(\epsilon).$$

Consequently $d = O(\epsilon)$ in $[r_1, 1]$.

Now we consider u, h, and d on $(0, r_1)$. We proceed to show that $d = o(1)$ on $(0, r_1)$. Suppose that this is false. Then there exist a small $\delta > 0$, independent of ϵ, and $r_* \in [0, r_1)$ such that $|d(r_*)| = \delta$ and $|d(r)| < \delta$ if $r \in (r_*, r_1)$. δ is so small that 0 is the only critical point of W in $(-\delta, \delta)$. Since $u(\epsilon t + r_1) \to H(t)$ in $C^2_{\text{loc}}(R)$, $(r_1 - r_*)/\epsilon \to \infty$. Moreover the argument in Proposition 8.2 Ref. 26 shows that $r_* = o(1)$. There are two cases left: (1) $r_*/\epsilon \to \infty$ and $r_* = o(1)$, and (2) $r_* = O(\epsilon)$.

In the first case we multiply the first equation of (1.8) by u_r and integrate with respect to dr:

$$-\int_0^1 \frac{\epsilon^2}{r} u_r^2\, dr + W(u(1)) - W(u(0)) + \epsilon\gamma \int_0^1 v u_r\, dr = \eta(u(1) - u(0)).$$

Here $W(u(1))$ is of order $O(\epsilon^2)$ by (A4). The right-hand side is of order $O(\epsilon)$ by (A3). $\epsilon\gamma \int_0^1 v u_r\, dr$ is of order $O(\epsilon)$ after integration by parts. Hence

$$\int_0^1 \frac{\epsilon^2}{r} u_r^2 \, dr + W(u(0)) = O(\epsilon).$$

Since $W(u(0)) \geqslant 0$,

$$\int_0^1 \frac{\epsilon^2}{r} u_r^2 \, dr = O(\epsilon). \tag{A5}$$

On the other hand if we scale u at r_* so that $U(t) := u(r_* + \epsilon t) \to H(t)$ locally in C^2, then

$$\int_0^1 \frac{\epsilon^2}{r} u_r^2 \, dr = \frac{\epsilon}{r_*} \int_{-r_*/\epsilon}^{(1-r_*)/\epsilon} \frac{1}{1 + (\epsilon t + r_*)} (U')^2 \, dt \geqslant \frac{\epsilon}{r_*} \left(\int_R (H')^2 \, dt + o(1) \right). \tag{A6}$$

However (A5) and (A6) are inconsistent if $r_* = o(1)$.

In the second case we scale u so that $U(t) := u(\epsilon t) \to U^0(t)$ locally in C^2 and

$$-U^0_{tt} - \frac{U^0_t}{t} + f(U^0) = 0 \text{ in } R, \quad U^0(\infty) = 1, \quad ||U^0|| \leqslant 1.$$

Moreover $U(r_*/\epsilon) \to \delta$. We multiply the equation for U^0 by U^0_t and integrate with respect to dt over $(0, \infty)$. Then

$$-W(U^0(0)) - \int_0^\infty \frac{(U^0_t)^2}{t} dt = 0,$$

which implies that $U^0 \equiv 0$ or $U^0 \equiv 1$. Neither case is consistent with $U(r_*/\epsilon) \to \delta \in (0,1)$.

We have shown that $d = u - h = o(1)$ on (0,1). In particular we know that there are exactly K interfaces $r_1, r_2, \ldots, r_K$. Now we consider the more accurate approximation w of u defined in Sec. II. We call $(r_j - \epsilon^\alpha, r_j + \epsilon^\alpha)$ an inner region, $(0,1) \setminus (U_{j=1}^K (r_j - 2\epsilon^\alpha, r_j + 2\epsilon^\alpha))$ the outer region, and $(r_j - 2\epsilon^\alpha, r_j - \epsilon^\alpha)$ and $(r_j + \epsilon^\alpha, r_j + 2\epsilon^\alpha)$ matching regions. Recall that $\alpha \in (1/2, 1)$.

In the inner and matching regions, using (2.22), (2.23), and (2.25) we find that

$$\begin{aligned}
-\epsilon^2 \Delta z_j + f(z_j) &= -\epsilon^2 \Delta (H_j + \epsilon P_j + \epsilon^2 Q_j) + f(H_j + \epsilon P_j + \epsilon^2 Q_j) \\
&= -\left[f(H_j) + \epsilon \left(\frac{H_j'}{r} + f'(H_j) P_j - \frac{H_j'}{r_j} + \xi_j \right) + \epsilon^2 \left(\frac{P_j'}{r} + f'(H_j) Q_j - \frac{P_j'}{r_j} + \frac{t H_j'}{r_j^2} \right.\right. \\
&\quad \left.\left. + \frac{f''(H_j) P_j^2}{2} + \gamma v'(r_j) t \right) \right] + f(H_j) + \epsilon f'(H_j) P_j + \epsilon^2 \left(\frac{f''(H_j) P_j^2}{2} + f'(H_j) Q_j \right) + O(\epsilon^3) \\
&= \epsilon \xi_j - \epsilon^2 \gamma v'(r_j) t + \frac{\epsilon^2 t}{r_j} \left(\frac{1}{r} - \frac{1}{r_j} \right) H_j' + \epsilon^3 \frac{t P_j'}{r_j r} + O(\epsilon^3) = \epsilon \xi_j - \epsilon^2 \gamma v'(r_j) t + O(\epsilon^3).
\end{aligned}$$

Therefore

$$-\epsilon^2 \Delta z_j + f(z_j) + \epsilon \gamma v - \eta = \epsilon \xi_j + \epsilon \gamma v(r_j) - \eta + O(\epsilon^3 t^2) + O(\epsilon^3) = \sigma_j + O(\epsilon^{1+2\alpha}), \tag{A7}$$

where we have defined

$$\sigma_j = \epsilon \xi_j + \epsilon \gamma v(r_j) - \eta. \tag{A8}$$

By (A3) implicit differentiation of (2.27) and $v'' = O(1)$ yield that

$$-\epsilon^2 \Delta z + f(z) + \epsilon \gamma v - \eta = -\epsilon^2 \Delta z = O(\epsilon^3), \tag{A9}$$

which is valid on $(0.1) \setminus \{r_1, r_2, \ldots, r_K\}$.

We now estimate the difference of z_j and z on a matching region. First using (2.23) and (2.25) we find

$$\epsilon^2 \Delta z_j = O(\epsilon^3).$$

Then (A7) implies that

$$f(z_j) + \epsilon\gamma v - \eta = \sigma_j + O(\epsilon^{1+2\alpha}).$$

Comparing this to (2.27) we deduce that

$$z_j - z = O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) \tag{A10}$$

on the matching regions $(r_j - 2\epsilon^\alpha, r_j - \epsilon^\alpha)$ and $(r_j + \epsilon^\alpha, r_j + 2\epsilon^\alpha)$. Then we consider w in the matching region. Here by (A10)

$$\begin{aligned} -\epsilon^2 \Delta w + f(w) + \epsilon\gamma v - \eta &= -\epsilon^2 \Delta w + f(z) + \epsilon\gamma v - \eta + O(\|z_j - z\|) \\ &= -\epsilon^2 \Delta w + O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) \\ &= -\epsilon^2 \Delta z - \epsilon^2 \Delta(\chi_j(z_j - z)) + O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) \\ &= -\epsilon^2((\chi_j)_{rr}(z_j - z) + 2(\chi_j)_r(z_j - z)_r + \chi_j(z_j - z)_{rr}) \\ &\quad - \frac{\epsilon^2}{r}((\chi_j)_r(z_j - z) + \chi_j(z_j - z)_r) + O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) \\ &= O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) + O(\epsilon^{3-\alpha}). \end{aligned} \tag{A11}$$

If we let $g = u - w$, then (A7), (A9), and (A11) imply that

$$-\epsilon^2 \Delta g + f'(w)g + O(\|g\|^2) = \begin{cases} -\sigma_j + O(\epsilon^{1+2\alpha}) & \text{in an inner region} \\ O(|\sigma|) + O(\epsilon^{1+2\alpha}) + O(\epsilon^{3-\alpha}) & \text{in a matching region} \\ O(\epsilon^3) & \text{in the outer region.} \end{cases} \tag{A12}$$

We deduce from (A12) and $g(r_j) = 0$ that

$$g = O(|\sigma_j|) + O(\epsilon^{1+2\alpha}) + O(\epsilon^{3-\alpha}). \tag{A13}$$

On the other hand, if we multiply (A12) by H_j' and integrate with respect to $r\,dr$ on (0,1), then

$$\int_0^1 [-\epsilon^2 (r g_r)_r H_j' + f'(w) g H_j' r] dr + O(\epsilon \|g\|^2) = (-1)^j \epsilon \sigma_j r_j + O(\epsilon^2 |\sigma_j|) + O(\epsilon^{2+2\alpha}).$$

But the integral on the left-hand side after integration by parts becomes

$$\int_0^1 [-\epsilon g H_j'' + (f'(w) - f'(H_j)) g H_j' r] dr = O(\epsilon^2 \|g\|),$$

from which we conclude that

$$\sigma_j = O(\epsilon \|g\|) + O(\|g\|^2) + O(\epsilon^{1+2\alpha}). \tag{A14}$$

Inserting (A14) into (A13) we find that

$$g = O(\epsilon^{1+2\alpha}) + O(\epsilon^{3-\alpha}); \tag{A15}$$

substituting(A15) into (A14) we deduce that

$$\sigma_j = O(\epsilon^{1+2\alpha}). \tag{A16}$$

Since $\alpha \in (1/2, 1)$, (A15) implies that $g = o(\epsilon^2)$.

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The Avez–Seifert theorem for the relativistic Lorentz force equation

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In this paper we prove an extension of the Avez–Seifert theorem to the relativistic Lorentz force equation. Let (M,g) be a globally hyperbolic space–time, F an exact 2-form on M representing the electromagnetic field, $\hat{F}$ the Lorentz force associated to F, and q a charge for a test particle. Let p_0 and p_1 be two chronologically related points on M, then there exists a future-pointing timelike solution of the Lorentz force equation $D_s\dot{z}=q\hat{F}(z)[\dot{z}]$, connecting p_0 and p_1. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1782673]

I. INTRODUCTION

The Avez and Seifert theorem is the first classical result in Global Lorentzian Geometry; see Refs. 1, 2, and 7. It can be considered as the extension to globally hyperbolic space–times of the Hopf–Rinow Theorem in Riemannian Geometry, stating that any couple of points in a complete Riemannian manifold are joined by a minimizing geodesic. It states that on a globally hyperbolic space–time (M,g), any two causally related points p_0 and p_1 on M are connected by (at least) one future-pointing causal maximizing geodesic. In particular, if p_0 and p_1 are chronologically related then there exists a timelike future-pointing geodesic connecting p_0 and p_1.

This result has a clear geometric meaning but its importance comes from General Relativity. Indeed lightlike and timelike geodesics on a space–time represent, respectively, the trajectories of light rays and of freely falling particles (i.e., particles subjected only to the gravitational field).

Our aim in this paper is to extend the above result to the trajectories of charged particles under the action of gravitational and electromagnetic fields.

Let (M,g) be a space–time, let $\Lambda^k(M)$, $k\in\{1,2,3,4\}$, be the fiber bundle of k-forms and consider the *differential operator* $d:\Lambda^k(M)\to\Lambda^{k+1}(M)$ and the Hodge operator $*:\Lambda^k(M)\to\Lambda^{4-k}(M)$ acting on differential forms on the manifold M. An *electromagnetic field* F on the space–time (M,g), is a smooth 2-form on M satisfying the Maxwell equations of the electromagnetism; see, for instance, Refs. 4 and 6,

$$\mathrm{d}F=0,$$

$$\mathrm{d}(F^*)=4\pi J^*,$$

where J is a smooth 1-form on M called the *charge-current density*. In particular the first Maxwell equation means that the 2-form F is closed.

The *Lorentz force* associated to the electromagnetic field is the map $\hat{F}$ on TM defined for any $z\in M$ as $\hat{F}(z):T_zM\to T_zM$ and

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$$g(z)[v,\hat{F}(z)[w]] = F(z)[v,w]. \tag{1}$$

Thus for every $z \in M$, $\hat{F}(z)$ is a linear map on T_zM and, in local coordinates, the components of $\hat{F}$ are given by $\hat{F}^i_j = g^{ik}F_{kj}$, where g^{ik} is the inverse matrix of the metric tensor g_{ij}.

The Lorentz force equation governing the motion of a particle with charge q is (cf. Ref. 6)

$$D_s\dot{z} = q\hat{F}(z)[\dot{z}], \tag{2}$$

where $D_s\dot{z}$ is the covariant derivative of $\dot{z}$ along $z(s)$ associated to the Levi–Civita connection.

We will assume that F is exact and we will denote by ω a *potential form* for F, that is $d\omega = F$. Since the electromagnetic field F is exact, Eq. (2) is the Euler–Lagrange equation of the functional

$$\frac{1}{2}\int (g(z)[\dot{z},\dot{z}] + q\omega(z)[\dot{z}])ds, \tag{3}$$

where ω is a potential form of the electromagnetic field F.

Before stating our main result, we shortly recall some basic notions about causality (for details see Ref. 2).

The *causality relations* on M are defined as follows. Let $p_0\ p_1 \in M$; we call p_0 and p_1 *chronologically related* and we write $p_0 \ll p_1$, if there is a smooth future-pointing timelike curve from p_0 to p_1. Furthermore, we say p_0 and p_1 are *causally related* and we write $p_0 \leqslant p_1$, if either $p_0 = p_1$ or there is a future-pointing (hence nowhere vanishing) causal curve from p_0 to p_1.

Let $\gamma :]\!]a,b[\![\to M$ be a curve on M. A point $p \in M$ is said to be the *end point of* γ corresponding to $s=b$ if $\lim_{s\to b^-}\gamma(s) = p$. If γ is a future-pointing (respectively, past-pointing) causal curve with end point p corresponding to $s=b$, the point p is called a *future* (respectively, *past*) *end point* of γ. A causal curve is said to be *future inextendible* (respectively, *past inextendible, inextendible*) if it has no future (respectively, past, nor future neither past) end point.

A *Cauchy surface* S is a subset of M such that every inextendible causal curve meets S exactly once. A Lorentzian manifold M is said to be *globally hyperbolic* if M admits a Cauchy surface. The main result of this paper is stated in the following theorem.

Theorem 1: Let (M,g) *be a globally hyperbolic space–time, endowed with an exact* 2*-form* F, p_0, p_1 *two points on* M, $p_0 \ll p_1$. *Then for any* $q \in \mathbb{R}$ *there exists a timelike future-pointing solution of Eq. (2), connecting* p_0 *and* p_1.

The theorem will be proved by using a five-dimensional (5-D) Kaluza–Klein framework. Kaluza–Klein theories have been developed in the last century as attempts to build up a unified approach to the fundamental interactions. They are based on a higher-dimensional geometry than the 4-D geometry of Einstein relativistic gravity theory (see Ref. 5 for a survey about Kaluza–Klein theories).

According to the Kaluza–Klein framework, we will consider the 5-D manifold $\boldsymbol{M} = M \times \mathbb{R}$, endowed with the Lorentzian metric,

$$\boldsymbol{k} = g + (dy + \omega)^2, \tag{4}$$

where y is the canonical coordinate on $\mathbb{R}$. It is well known (see, for instance, Ref. 3) that the projection on M of any timelike geodesic $\boldsymbol{\gamma}$ of $(\boldsymbol{M},\boldsymbol{k})$ represents a trajectory for test particles subjected to the action of the external field ω.

The charge q_0 of the particle is determined by the constant of the motion (coming from the fact that the vector field ∂_y on $\boldsymbol{M}$ is a Killing field for the metric $\boldsymbol{k}$):

$$\boldsymbol{k}(\boldsymbol{\gamma})[\dot{\boldsymbol{\gamma}},\partial_y] = \text{const} \equiv q_0. \tag{5}$$

On any Lorentzian manifold (N,h), the timelike geodesics $\gamma = \gamma(s)$ connecting two points p_0 and p_1 on N can be characterized as the critical points of the *energy functional*,

$$\frac{1}{2}\int h(\gamma)[\dot\gamma,\dot\gamma]\mathrm{d}s,$$

on the set of the piecewise smooth timelike curves joining p_0 and p_1. In the case of the Kaluza–Klein metric (4), the Euler–Lagrange equations of the energy functional (i.e., the geodesic equations) are

$$D_s\dot z = (\dot y + \omega(z)[\dot z])\hat F(z)[\dot z],$$

$$\dot y + \omega(z)[\dot z] = \text{const}. \tag{6}$$

From (2) and (6), we see that $\dot y+\omega(z)[\dot z]$ plays effectively the role of the charge of the particle moving along the trajectory $z=z(s)$.

Thus in order to establish the existence of timelike connecting trajectories for charged particles on M, we may study the existence of the timelike connecting geodesic on $\boldsymbol{M}$.

In Sec. II we will show that if (M,g) is globally hyperbolic then $(\boldsymbol{M},\boldsymbol{k})$ is as well. The Avez and Seifert Theorem provides the existence of a timelike geodesic $\boldsymbol{z}$ for the 5-D Kaluza–Klein manifold, connecting two chronologically related points on $\boldsymbol{M}$. Thus we gain the existence of a timelike connecting trajectory $z=\pi_M(\boldsymbol{z})$ (π_M is the canonical projection on M) for a particle carrying a charge q_0, which depends on the 5-D timelike geodesic $\boldsymbol{z}$. If $q_0\neq 0$ we can reparametrize the curve z, considering the new map $c(s)=z\boldsymbol{(}(q/q_0)s\boldsymbol{)}$, where q is the fixed test charge. The map c solves Eq. (2), in fact,

$$D_{\dot c(s)}\dot c(s) = \left(\frac{q}{q_0}\right)^2 D_{\dot z((q/q_0)s)}\dot z\left(\frac{q}{q_0}s\right) = \left(\frac{q}{q_0}\right)^2 q_0\hat F\left(z\left(\frac{q}{q_0}s\right)\right)\left[\dot z\left(\frac{q}{q_0}s\right)\right] = q\hat F(c(s))[\dot c(s)].$$

Finally an analysis based on the relations between causality on the 4-D space-time (M,g) and the 5-D space-time $(\boldsymbol{M},\boldsymbol{k})$, allows us to prove the existence of a 5-D future-pointing timelike connecting geodesic having a constant of the motion $q_0\neq 0$ (in other words a 5-D future-pointing timelike geodesic $\boldsymbol{z}$, such that its projection on M is not a 4-D geodesic).

II. KALUZA–KLEIN METRICS

Let (M,g) be a space–time [i.e., (M,g) is a smooth time-oriented Lorentzian manifold] and ω a smooth 1-form on M. The Kaluza-Klein metric $\boldsymbol{k}$ associated to (M,g,ω) is defined on $\boldsymbol{M}=M\times\mathbb{R}$ as follows:

$$\boldsymbol{k}(\boldsymbol{z})[(\zeta,\eta),(\zeta',\eta')] = g(z)[\zeta,\zeta'] + (\eta+\omega(z)[\zeta])(\eta'+\omega(z)[\zeta']), \tag{7}$$

for all $\mathbf{z}\equiv(z,y)\in\boldsymbol{M}$, and for all $(\zeta,\eta),(\zeta',\eta')\in T_{\mathbf{z}}\boldsymbol{M}\equiv T_zM\times\mathbb{R}$ (throughout the paper bold symbols will refer to 5-D manifold $\boldsymbol{M}$).

Consider the canonical projections maps $\pi_M:\boldsymbol{M}\to M$, $\pi_{\mathbb{R}}:\boldsymbol{M}\to\mathbb{R}$ and denote by π_M^* and $\pi_{\mathbb{R}}^*$ the corresponding pullback maps. From (7) we see that $\boldsymbol{k}$ is given by

$$\boldsymbol{k} = \pi_M^*(g) + [\pi_{\mathbb{R}}^*(\mathrm{d}y) + \pi_M^*(\omega)]\otimes[\pi_{\mathbb{R}}^*(\mathrm{d}y) + \pi_M^*(\omega)]. \tag{8}$$

Proposition 2: $\boldsymbol{k}$ is a symmetric nondegenerate bilinear form.

Proof: $\boldsymbol{k}$ is clearly symmetric and bilinear. In order to prove that $\boldsymbol{k}(\mathbf{z})$ is nondegenerate, for any $\mathbf{z}$ in $\boldsymbol{M}$, let $\boldsymbol{\zeta}\equiv(\zeta,\eta)\in T_{\mathbf{z}}\boldsymbol{M}$ be such that for any $\boldsymbol{\zeta}'\equiv(\zeta',\eta')\in T_{\mathbf{z}}\boldsymbol{M}$:

$$\boldsymbol{k}(\mathbf{z})[\boldsymbol{\zeta},\boldsymbol{\zeta}'] = g(z)[\zeta,\zeta'] + (\eta+\omega(z)[\zeta])(\eta'+\omega(z)[\zeta']) = 0.$$

Choosing $\boldsymbol{\zeta}'\equiv(0,1)$, we obtain

$$0 = \boldsymbol{k}(\mathbf{z})[(\zeta,\eta),(0,1)] = (\eta+\omega(z)[\zeta]). \tag{9}$$

On the other hand, for any $\zeta'\in T_zM$:

$$0 = \boldsymbol{k}(\mathbf{z})[(\zeta,\eta),(\zeta',0)] = g(z)[\zeta,\zeta'] + (\eta + \omega(z)[\zeta])\omega(z)[\zeta']. \tag{10}$$

From (9) and (10) we deduce that $g(z)[\zeta,\zeta']=0$, for any $\zeta' \in T_zM$. Thus it results $\zeta=0$ and, from (9), $\eta=0$ too. □

Proposition 3: $\boldsymbol{k}$ is a Lorentzian metric.

Proof: We will show that for any $\mathbf{z} \in \boldsymbol{M}$, $\boldsymbol{k}(\mathbf{z})$ has index 1. Indeed $\boldsymbol{k}$ is positive definite on any subspace $F \subset T_{\mathbf{z}}\boldsymbol{M}$ of the form $F=F_0 \times \{0\}$, with F_0 spacelike with respect to g. On the subspace spanned by the vector $(0,1) \in T_{\mathbf{z}}\boldsymbol{M}$, it results that

$$\boldsymbol{k}(\mathbf{z})[(0,\lambda),(0,\lambda)] = \lambda^2 > 0.$$

Now let $\zeta \in T_zM$ be a timelike vector with respect to g and for any $\lambda \in \mathbb{R}$ consider the vector $\boldsymbol{\zeta} = (\zeta,\lambda) \in T_{\mathbf{z}}\boldsymbol{M}$. It results that

$$\boldsymbol{k}(\mathbf{z})[(\zeta,\lambda),(\zeta,\lambda)] = g(z)[\zeta,\zeta'] + (\lambda + \omega(z)[\zeta])^2 = \lambda^2 + 2\omega(z)[\zeta]\lambda + g(z)[\zeta,\zeta] + (\omega(z)[\zeta])^2. \tag{11}$$

From (11) we see that there exist two real numbers λ_1 and λ_2 such that, for any $\lambda \in]\!]\lambda_1,\lambda_2[\![$, $\boldsymbol{k}(\mathbf{z})[(\zeta,\lambda),(\zeta,\lambda)]<0$, that is the vector (ζ,λ) is timelike and $\boldsymbol{k}(\mathbf{z})$ has index 1. □

Let V be a timelike vector field on M which gives a time-orientation to M (i.e., V is continuous and timelike). Then consider the vector field $\boldsymbol{V}=(V,-\omega[V])$ on $\boldsymbol{M}$. Clearly $\boldsymbol{V}$ is continuous and timelike with respect to $\boldsymbol{k}$. Thus we can state the following.

Proposition 4: $(\boldsymbol{M},\boldsymbol{k})$ is time-oriented.

It is natural to consider if causality conditions satisfied by (M,g) are preserved by $(\boldsymbol{M},\boldsymbol{k})$.

Proposition 5: Assume that $\mathbf{z}=\mathbf{z}(s)$ is a smooth timelike (causal) future-pointing curve on $\boldsymbol{M}$. Then $z(s)=\pi_M(\mathbf{z}(s))$ is a smooth timelike (causal) future-pointing curve on M.

Proof: Clearly z is a smooth curve on M. Let $y=y(s)$ be the function $y(s)=\pi_{\mathbb{R}}(\mathbf{z}(s))$. From

$$0 > \boldsymbol{k}(\mathbf{z})[\dot{\boldsymbol{z}},\dot{\boldsymbol{z}}] = g(z)[\dot{z},\dot{z}] + (\dot{y} + \omega(z)[\dot{z}])^2,$$

we have that $g(z)[\dot{z},\dot{z}]<0$, that is z is timelike. Since

$$\boldsymbol{k}(\mathbf{z})[\dot{\boldsymbol{z}},\boldsymbol{V}(\mathbf{z})] = g(z)[\dot{z},V(z)],$$

and $\boldsymbol{k}(\mathbf{z})[\dot{\boldsymbol{z}},\boldsymbol{V}(\mathbf{z})]<0$, z is future-pointing. □

Another result about causality is the following.

Proposition 6: If (M,g) is globally hyperbolic, then $(\boldsymbol{M},\boldsymbol{k})$ is globally hyperbolic.

Proof: Let S be a Cauchy surface for M. We will prove that $\boldsymbol{S}=S\times\mathbb{R}$ is a Cauchy surface for $\boldsymbol{M}=M\times\mathbb{R}$. By contradiction assume that there exists an inextendible smooth future-pointing causal curve $\mathbf{z}:]\!]a,b[\![\to\boldsymbol{M}$ $(-\infty\leqslant a<b\leqslant+\infty)$, which does not intersect $\boldsymbol{S}$. Consider $z(s)=\pi_M(\mathbf{z}(s))$. Clearly z does not intersect S otherwise $\mathbf{z}$ would meet $\boldsymbol{S}$. By Proposition 5, z is a smooth future-pointing causal curve on M and, being S a Cauchy surface for M, we deduce that z must be extendible. So let p be a future end point for z corresponding to $s=b$. Now since $\mathbf{z}$ is causal we deduce that

$$|\dot{y} + \omega(z)[\dot{z}]| \leqslant \sqrt{-g(z)[\dot{z},\dot{z}]},$$

and, integrating from $c>a$ to $d<b$, we get

$$\int_c^d |\dot{y} + \omega(z)[\dot{z}]|\mathrm{d}s \leqslant \int_c^d \sqrt{-g(z)[\dot{z},\dot{z}]}\mathrm{d}s. \tag{12}$$

Now consider the Lorentzian distance function d on M associated to the metric g. Since M is globally hyperbolic and z is causal, the right-hand side of (12) is less than $d(z(c),z(d))<+\infty$. As z has future end point p corresponding to $s=b$, it results that $d(z(c),p)<+\infty$. So there exists the limit as $d\to b^-$ of the right-hand side of (12). Therefore the left-hand side of (12) has a finite limit

as $d \to b^-$. Now consider the term $\int_c^d \omega(z)[\dot{z}]\mathrm{d}s$. It is well known that, for any $q \in M$ there exists a neighborhood $U_q \subset M$ of q and a coordinate system $\varphi=(x_1,x_2,x_3,t)$ on U_q such that $V=\partial_t$ and $U_q=\Sigma \times]\!]a_1,b_1[\![$, where Σ is a spacelike hypersurface parametrized by x_1,x_2,x_3. Moreover in the coordinate system $x=(x_1,x_2,x_3) \in \Sigma$ and $t \in]\!]a_1,b_1[\![$ the metric g is given by

$$g(x,t)[(\xi,\tau),(\xi,\tau)] = \langle \alpha(x,t)\xi,\xi\rangle + 2\langle \delta(x,t),\xi\rangle\tau - \beta(x,t)\tau^2,$$

where $(\xi,\tau) \in T_x\Sigma \times \mathbb{R}$, $\langle\cdot,\cdot\rangle$ is the restriction of g to Σ, α is a smooth, symmetric positive definite operator, δ is a smooth vector field on U_q and β is a smooth, positive real function on U_q. Pick a coordinate system (U_p,φ) as above for the future end point p. Without loss of generality we can assume that $z(c) \in U_p$ and $z(d) \in U_p$, for any $c<d\leqslant b$. Denote $z(s)$ by $(x(s),t(s))$ for any $s \in]\!]c,b]\!]$. Since z is causal, we have

$$\langle \alpha(x,t)\dot{x},\dot{x}\rangle + 2\langle \delta(x,t),\dot{x}\rangle\dot{t} \leqslant \beta(x,t)\dot{t}^2. \tag{13}$$

Moreover as z is future-pointing, $\dot{t}(s) \neq 0$ on $]\!]c,b[\![$, thus $t(s)$ is strictly monotone on $]\!]c,b[\![$. Since $\omega(z(s))$ is a linear form on $T_{z(s)}M$, it results that

$$|\omega(z(s))[\dot{z}(s)]| \leqslant C(z(s))\sqrt{\langle \alpha(x(s),t(s))\dot{x}(s),\dot{x}(s)\rangle + \beta(x(s),t(s))\dot{t}(s)^2},$$

for any $s \in]\!]c,b]\!]$. But the field $\omega(z(s))$ is continuous on $]\!]c,b]\!]$, so the positive function $C(z(s))$ is uniformly bounded on $]\!]c,b]\!]$. Thus, by (13), we have

$$\int_c^d |\omega(z)[\dot{z}]|\mathrm{d}s \leqslant C_1\int_c^d \sqrt{\langle \alpha(x,t)\dot{x},\dot{x}\rangle + \beta(x,t)\dot{t}^2}\mathrm{d}s \leqslant C_2\int_c^d |\dot{t}|\mathrm{d}s = \pm C(t(d)-t(c)).$$

Passing to the limit as $d \to b^-$, we conclude that $|\omega(z)[\dot{z}]|$ is integrable on $]\!]c,b]\!]$. As

$$\lim_{d\to b^-}\int_c^d (\dot{y} - \omega(z)[\dot{z}])\mathrm{d}s \in \mathbb{R},$$

we conclude that

$$\lim_{d\to b^-} y(d) - y(c) = \lim_{d\to b^-}\int_c^d \dot{y}\mathrm{d}s \in \mathbb{R}.$$

Let $\overline{y}=\lim_{d\to b^-} y(d)$. Clearly the point $(p,\overline{y}) \in \boldsymbol{M}$ is a future end point for $\boldsymbol{z}$ corresponding to $s=b$. This fact yields the desired contradiction. Now assume that an inextendible smooth future-pointing causal curve $\boldsymbol{z}$ meets $\boldsymbol{S}$ at least twice. So the maximal causal future-pointing extension of $z(s)=\pi_M(\boldsymbol{z}(s))$ meets S at least two times. This contradiction concludes the proof. □

III. PROOF OF THEOREM 1

Let us consider the set $\mathcal{T}_{p_0,p_1}$ of the smooth future-pointing timelike curves $z:]\!]0,1]\!] \to M$ on (M,g), such that $z(0)=p_0$ and $z(1)=p_1$.

Lemma 7: Let (M,g) be globally hyperbolic and $p_0 \leqslant p_1$. Then

$$\sup_{z\in\mathcal{T}_{p_0,p_1}}\int_0^1 |\omega(z)[\dot{z}]|\mathrm{d}s < +\infty. \tag{14}$$

Proof: Denote by D the quantity $\sup_{z\in\mathcal{T}_{p_0,p_1}}\int_0^1|\omega(z)[\dot{z}]|\mathrm{d}s$ and let $\{z_n\}_{n\in\mathbb{N}} \subset \mathcal{T}_{p_0,p_1}$ be a sequence such that

$$\int_0^1 |\omega(z_n)[\dot{z}_n]|\mathrm{d}s \to D.$$

Since (M,g) is globally hyperbolic, we can extract a subsequence, denoted by z_n too, such that z_n converges to a continuous curve $z:[\![0,1]\!]\to M$ in the C^0 topology of curves (see Ref. 2, Corollary 3.32 and Proposition 3.34). Cover z by a finite number of coordinate neighborhoods $\{U_k\}_{1\leqslant k\leqslant m}$ of the same type as in the proof of Proposition 6. So $U_k=\Sigma_k\times]\!]a_k,b_k[\![$. Let $\Delta=\max_{1\leqslant k\leqslant m}(b_k-a_k)$. In the coordinate system $x_k=(x_{1k},x_{2k},x_{3k})\in\Sigma_k$ and $t_k\in]\!]a_k,b_k[\![$, the metric g is given by

$$g(x_k,t_k)[(\xi,\tau),(\xi,\tau)]=\langle\alpha_k(x_k,t_k)\xi,\xi\rangle_k+2\langle\delta_k(x_k,t_k),\xi\rangle_k\tau-\beta_k(x_k,t_k)\tau^2,$$

for any $(\xi,\tau)\in T_{x_k}\Sigma_k\times\mathbb{R}$. Consider a partition $\{[\![s_{k-1},s_k]\!]\}_{1\leqslant k\leqslant m}$, $s_0=0<s_1<\cdots<s_m=1$, of the interval $[\![0,1]\!]$, such that $z([\![s_{k-1},s_k]\!])\subset U_k$. As z_n converges to z in the C^0 topology of curves, it results definitively, up to reparametrize the curves z_n, $z_n([\![s_{k-1},s_k]\!])\subset U_k$. Now arguing as in Proposition 6, we have

$$\langle\alpha_k(x_{nk},t_{nk})\dot{x}_{nk},\dot{x}_{nk}\rangle_k+2\langle\delta_k(x_{nk},t_{nk}),\dot{x}_{nk}\rangle_k\dot{t}_{nk}<\beta_k(x_{nk},t_{nk})\dot{t}_{nk}^2;$$

furthermore $\dot{t}_{nk}(s)\neq 0$ on $[\![s_{k-1},s_k]\!]$ and

$$\begin{aligned}\int_0^1|\omega(z_n(s))[\dot{z}_n(s)]|\mathrm{d}s&=\sum_{k=1}^m\int_{s_{k-1}}^{s_k}|\omega(z_{nk}(s))[\dot{z}_{nk}(s)]|\mathrm{d}s\\&\leqslant C\sum_{k=1}^m\int_{s_{k-1}}^{s_k}\sqrt{\langle\alpha_k(x_{nk},t_{nk})\dot{x}_{nk},\dot{x}_{nk}\rangle_k+\beta_k(x_{nk},t_{nk})\dot{t}_2^{nk}}\mathrm{d}s\\&\leqslant C\sum_{k=1}^m\int_{s_{k-1}}^{s_k}|\dot{t}_{nk}|\mathrm{d}s\leqslant Cm\Delta.\end{aligned}$$

Passing to the limit on n, we conclude. □

Proof of Theorem 1: We begin by considering the case $q>0$. Since $p_0\ll p_1$, there exists a smooth future-pointing timelike curve $z:[\![0,1]\!]\to M$ on (M,g), such that $z(0)=p_0$ and $z(1)=p_1$. So consider the curve $\boldsymbol{z}:[\![0,1]\!]\to\boldsymbol{M}$ defined as $\boldsymbol{z}(s)=(z(s),-\int_0^s\omega(z)[\dot{z}]\mathrm{d}s)$. Clearly $\boldsymbol{z}(0)=(p_0,0)$, $\boldsymbol{z}(1)=(p_1,-\int_0^1\omega(z)[\dot{z}]\mathrm{d}s)$, $\boldsymbol{z}$ is a future-pointing timelike curve on $(\boldsymbol{M},\boldsymbol{k})$, and the points $(p_0,0)$ and $(p_1,-\int_0^1\omega(z)[\dot{z}]\mathrm{d}s)$ are chronologically related on $(\boldsymbol{M},\boldsymbol{k})$. Thus set

$$\upsilon_1=\sup_{z\in\mathcal{T}_{p_0,p_1}}\left(-\int_0^1\omega(z)[\dot{z}]\mathrm{d}s\right).$$

Let $\varepsilon>0$ and consider the points $(p_0,-\varepsilon)$ $(p_1,\upsilon_1-\varepsilon/2)$. Since the relation $\ll$ is open, $(p_0,-\varepsilon)\ll(p_1,\upsilon_1-\varepsilon/2)$ for ε small enough. Hence there exists a 5-D future-pointing timelike geodesic $\boldsymbol{\gamma_1}$ connecting $(p_0,-\varepsilon)$ and $(p_1,\upsilon_1-\varepsilon/2)$. Let $q_1=\boldsymbol{k}(\boldsymbol{\gamma_1})[\dot{\boldsymbol{\gamma}}_{\boldsymbol{1}},\partial_y]$. It results that $q_1=\dot{y}_1+\omega(\gamma_1)[\dot{\gamma}_1]$, with $y_1=\pi_{\mathbb{R}}(\boldsymbol{\gamma_1})$ and $\gamma_1=\pi_{\boldsymbol{M}}(\boldsymbol{\gamma_1})\in\mathcal{T}_{p_0,p_1}$. Therefore

$$q_1=y_1(1)-y_1(0)+\int_0^1\omega(\gamma_1)[\dot{\gamma}_1]\mathrm{d}s=\upsilon_1-\frac{\varepsilon}{2}+\varepsilon+\int_0^1\omega(\gamma_1)[\dot{\gamma}_1]\mathrm{d}s\geqslant\frac{\varepsilon}{2}>0.$$

As $q_1=\dot{y}_1+\omega(\gamma_1)[\dot{\gamma}_1]>0$, we can conclude, by (6), that γ_1 is not a 4-D geodesic. Then consider the curve c_1, defined on $[\![0,q_1/q]\!]$ as $c_1(s)=\gamma_1(q/q_1s)$. Clearly c_1 connects p_0 and p_1, is timelike, future-pointing and solves Eq. (2).

Now assume that $q<0$. Arguing as above, we find a 5-D future-pointing timelike geodesic $\boldsymbol{\gamma_2}$ connecting (p_0,ε) and $(p_1,\upsilon_2+\varepsilon/2)$, where now

$$\upsilon_2 = \inf_{z \in \mathcal{T}_{p_0,p_1}} \left(- \int_0^1 \omega(z)[\dot{z}]ds \right).$$

Now it results that $q_2 = \dot{y}_2 + \omega(\gamma_2)[\dot{\gamma}_2] \leqslant -\varepsilon/2 < 0$. So $c_2 = \gamma_2((q/q_2)s)$ is the desired solution. □

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Covariants, joint invariants and the problem of equivalence in the invariant theory of Killing tensors defined in pseudo-Riemannian spaces of constant curvature

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The invariant theory of Killing tensors (ITKT) is extended by introducing the new concepts of covariants and joint invariants of (product) vector spaces of Killing tensors defined in pseudo-Riemannian spaces of constant curvature. The covariants are employed to solve the problem of classification of the orthogonal coordinate webs generated by nontrivial Killing tensors of valence two defined in the Euclidean and Minkowski planes. Illustrative examples are provided. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1805728]

I. INTRODUCTION

The second half of the 19th century saw the development of the post-"Theorema Egregium of Gauss" differential geometry going in two major directions. Thus, Riemann[1] generalized Gauss's geometry of surfaces in the Euclidean space by introducing the concept of a differentiable manifold of arbitrary dimension and defining the inner product in terms of the metric tensor on the spaces of tangent vectors. This remarkable work has evolved in time into what is known today as (Riemannian) differential geometry. The other direction originated in the celebrated "Erlangen Program" of Klein.[2,3] According to his manifesto any branch of geometry can be interpreted as an invariant theory with respect to a specific transformation group. Moreover, the main goal of any geometry is the determination of those properties of geometrical figures that remain unchanged under the action of a transformation group. One of the main contributions of Cartan to differential geometry, in particular with his moving frames method,[4] is the blending of these two directions into a single theory. An excellent exposition of this fact can be found in Sharpe[5] (see also, for example, Arvanitoyeorgos[6]). The following diagram presented in Ref. 5 elucidates the relationship among the different approaches to geometry described above:

$$\begin{array}{ccc} \text{Euclidean Geometry} & \overset{\text{generalization}}{\longrightarrow} & \text{Klein Geometries} \\ \downarrow\text{generalization} & & \text{generalization}\downarrow \\ \text{Riemannian Geometry} & \overset{\text{generalization}}{\longrightarrow} & \text{Cartan Geometries} \end{array} \tag{1}$$

Being a result of the natural fusion of classical invariant theory (CIT) and the (geometric) study of Killing tensors defined in pseudo-Riemannian manifolds of constant curvature, the invariant theory of Killing tensors (ITKT) formed recently a new direction of research,[7–16] which, in view of the above, can be rightfully placed into the theory initiated by Cartan. This is especially

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evident in the study of vector spaces of Killing tensors of valence two. Indeed, by now a number of vector spaces of Killing tensors have been investigated from this viewpoint by means of determining the corresponding sets of fundamental *invariants* and, much like in CIT, using them to solve the problem of equivalence in each case. These results have been employed in applications arising in the *theory of orthogonal coordinate webs*,[17–25,16,12,7] where Killing tensors of valence two play a pivotal role (see Ref. 22 for a complete list of references). Admittedly, an orthogonal coordinate web is an integral part of the geometry of the underlying pseudo-Riemmanian manifold. Therefore the problem of group invariant classification of orthogonal coordinate webs in a specific pseudo-Riemannian space of constant curvature is a problem of Klein's approach to geometry, as well as that of Riemann, both leading to the theory due to Cartan [see the diagram (1)].

The main goal of this paper is to further the development of the invariant theory of Killing tensors by introducing the concepts of a *covariant* and a *joint invariant*. In this setting they can be introduced by establishing a natural extension of the main ideas of CIT to the geometric study of Killing tensors in pseudo-Riemannian geometry. Furthermore, we employ the latest generalization of Cartan's method of moving frames due to Fels and Olver[26,27] (see also Refs. 4 and 28–32 for more details and references) to determine complete systems of fundamental covariants for the vector spaces of Killing tensors of valence two defined in the Euclidean and Minkowski planes. The covariants are employed to classify in both cases orthogonal coordinate webs generated by Killing tensors. We also compare the results with the classifications of the orthogonal webs defined in the Minkowski plane obtained in McLenaghan *et al.*[12,15] by means of invariants only.

II. INVARIANT THEORY OF KILLING TENSORS (ITKT)

In this section we establish the requisite language and recall the basic notions of the invariant theory of Killing tensors (ITKT) defined in pseudo-Riemannian spaces of constant curvature. More specifically, we review what is known about isometry group invariants and extend the theory by introducing the concepts of *covariants* and *joint invariants* of product vector spaces of Killing tensors in ITKT. Let $(M,\mathbf{g})$ be a pseudo-Riemannian manifold, dim $M=n$.

Definition 2.1: A Killing tensor $\mathbf{K}$ of valence p defined in $(M,\mathbf{g})$ *is a symmetric* $(p,0)$ *tensor satisfying the Killing tensor equation,*

$$[\mathbf{K},\mathbf{g}]=0, \tag{2}$$

where $[,]$ *denotes the Schouten bracket.*[33] *When* $p=1$, $\mathbf{K}$ *is said to be a* Killing vector (infinitesimal isometry) *and the equation (2) reads*

$$\mathcal{L}_{\mathbf{K}}\mathbf{g}=0,$$

where $\mathcal{L}$ *denotes the Lie derivative operator.*

Remark 2.1: Throughout this paper, unless otherwise specified, $[,]$ denotes the Schouten bracket, which is a generalization of the usual Lie bracket of vector fields.

Killing tensors appear naturally in many problems of classical mechanics, general relativity, field theory, and other areas. To demonstrate this fact, let us consider the following example.

Example 2.1: Let $(\mathbf{X}_H,\mathbf{P}_0,H)$ be a Hamiltonian system defined on $(M,\mathbf{g})$ by a natural Hamiltonian H of the form

$$H(\mathbf{q},\mathbf{p})=\tfrac{1}{2}g^{ij}p_ip_j+V(\mathbf{q}),\quad i,j=1,\ldots,n, \tag{3}$$

where g^{ij} are the contravariant components of the corresponding metric tensor $\mathbf{g}$, $(\mathbf{q},\mathbf{p})\in T^*M$ are the canonical position-momenta coordinates and the Hamiltonian vector field $\mathbf{X}_H$ is given by

$$\mathbf{X}_H = [\mathbf{P}_0, H] \tag{4}$$

with respect to the canonical Poisson bi-vector $\mathbf{P}_0 = \Sigma_{i=1}^{n} \partial/\partial q^i \wedge \partial/\partial p_i$. Assume also that the Hamiltonian system defined by (3) admits a first integral of motion F which is a polynomial function of degree m in the momenta:

$$F(\mathbf{q},\mathbf{p}) = K^{i_1 i_2 \cdots i_m}(\mathbf{q}) p_{i_1} p_{i_2} \cdots p_{i_m} + U(\mathbf{q}), \tag{5}$$

where $1 \leqslant i_1, \ldots, i_m \leqslant n$. Since the functions H and F are in involution, the vanishing of the Poisson bracket defined by $\mathbf{P}_0$:

$$\{H,F\}_0 = \mathbf{P}_0 \,\mathrm{d}\, H \,\mathrm{d}\, F = [[\mathbf{P}_0, H], F] = 0 \tag{6}$$

yields

$$[\mathbf{K}, \mathbf{g}] = 0 \quad \text{(Killing tensor equation)} \tag{7}$$

and

$$K^{i_1 i_2 \cdots i_m} \frac{\partial V}{\partial q^{i_1}} p_{i_2} \cdots p_{i_m} = g^{ij} \frac{\partial U}{\partial q^i} p_j \quad \text{(compatibility condition)}, \tag{8}$$

where the symmetric $(m,0)$-tensor $\mathbf{K}$ has the components $K^{i_1 i_2 \cdots i_m}$ and $1 \leqslant i, j, i_1, \ldots, i_m \leqslant n$. Clearly, in view of Definition 2.1 the equation (7) confirms that $\mathbf{K}$ is a Killing tensor. Furthermore, in the case $m=2$ (see Benenti[22]) the compatibility condition (8) reduces to $\mathbf{K} \,\mathrm{d}\, V = \mathbf{g} \,\mathrm{d}\, U$ or $\mathrm{d}(\hat{\mathbf{K}} \,\mathrm{d}\, V) = 0$, where the (1,1)-tensor $\hat{\mathbf{K}}$ is given by $\hat{\mathbf{K}} = \mathbf{K}\mathbf{g}^{-1}$. We also note that the vanishing of the Poisson bracket (6) and the assumed form of the first integral F (5) imply the following additional conditions:

$$\partial_i U = 0, \quad K^{i_1 i_2 \cdots i_m} \partial_{i_1} V = 0.$$

Indeed, the right-hand side (RHS) of (5) does not have the terms which are polynomials of $\mathbf{p}$ of degrees less than m.

In view of linear properties of the Schouten bracket the sets of Killing tensors of the same valence form vector spaces in $(M,\mathbf{g})$. Let $\mathcal{K}^p(M)$ denote the vector space of Killing tensors of valence $p \geqslant 1$ defined in $(M,\mathbf{g})$. Assume also $\dim M = n$. Then if $(M,\mathbf{g})$ is a pseudo-Riemannian space of constant curvature, the dimension d of the corresponding vector space $\mathcal{K}^p(M)$ for a given $p \geqslant 1$ is determined by the *Delong–Takeuchi–Thompson (DTT) formula*,[34–36]

$$d = \dim \mathcal{K}^p(M) = \frac{1}{n}\binom{n+p}{p+1}\binom{n+p-1}{p}, \quad p \geqslant 1. \tag{9}$$

That being the case, a Killing tensor of valence $p \geqslant 1$ defined in a pseudo-Riemannian space $(M,\mathbf{g})$ of constant curvature can be viewed as an algebraic object, or, an element of $\mathcal{K}^p(M)$. Note the vector space $\mathcal{K}^p(M)$ for a fixed $p \geqslant 1$ is determined by d arbitrary parameters $(\alpha_1, \ldots, \alpha_d)$, where $d = \dim \mathcal{K}^p(M)$ is given by (9). This approach to the study of Killing tensors introduced in Ref. 15 differs significantly from the more conventional approach based on the property that Killing tensors defined in pseudo-Riemannian spaces of constant curvature are sums of symmetrized tensor products of Killing vectors (see, for example, Ref. 36). Moreover, the idea leads to a natural link between the study of vector spaces of Killing tensors and the classical theory of invariants of vector spaces of homogeneous polynomials, which has become in the last decade a growth industry once again (see Olver[39] and the references therein). Thus, it has been shown in a series of recent papers[11,16,10,12–15] that one can utilize the basic ideas of classical invariant theory in the study of Killing tensors defined in pseudo-Riemannian spaces of constant curvature. The concept of an *invariant* of $\mathcal{K}^p(M)$ was introduced in Ref. 16 in the study of nontrivial Killing tensors of the vector space $\mathcal{K}^2(\mathbb{R}^2)$ generating orthogonal coordinate webs in the Euclidean plane.

A. Invariants

It has been shown that one can determine the action of the isometry group $I(M)$ in the d-dimensional space $\Sigma \simeq \mathbb{R}^d$ defined by the parameters $\alpha_1, \ldots, \alpha_d$. In this view, the action is induced by the corresponding action of $I(M)$ in $\mathcal{K}^p(M)$, which, in turn, is induced by the action of $I(M)$ in M. More specifically, it induces the corresponding transformation laws for the parameters $(\alpha_1, \ldots, \alpha_d)$ given by

$$\begin{aligned} \tilde{\alpha}_1 &= \tilde{\alpha}_1(\alpha_1, \ldots, \alpha_d, g_1, \ldots, g_r), \\ \tilde{\alpha}_2 &= \tilde{\alpha}_2(\alpha_1, \ldots, \alpha_d, g_1, \ldots, g_r), \\ &\vdots \\ \tilde{\alpha}_d &= \tilde{\alpha}_d(\alpha_1, \ldots, \alpha_d, g_1, \ldots, g_r), \end{aligned} \tag{10}$$

where $g_1, \ldots, g_r$ are local coordinates on $I(M)$ that parametrize the group and $r = \dim I(M) = \frac{1}{2}n(n+1)$. The formulas (10) can be obtained in each case by making use of the standard transformation rules for tensor components. We note that the action of $I(M)$ can be considered in the spaces M and Σ concurrently, provided there is an isomorphism between the corresponding group actions (see below).

Definition 2.2: Let $(M, \mathbf{g})$ *be a pseudo-Riemannian manifold of constant curvature. For a fixed* $p \geqslant 1$ *consider the corresponding space* $\mathcal{K}^p(M)$ *of Killing tensors of valence p defined in* $(M, \mathbf{g})$. *A smooth function* $\mathcal{I}: \Sigma \to \mathbb{R}$ *defined in the space of functions on the parameter space* Σ *is said to be an* $I(M)$ invariant of the vector space $\mathcal{K}^p(M)$ *iff it satisfies the condition*

$$\mathcal{I} = F(\alpha_1, \ldots, \alpha_d) = F(\tilde{\alpha}_1, \ldots, \tilde{\alpha}_d) \tag{11}$$

under the transformation laws (10) induced by the isometry group $I(M)$.

The main problem of invariant theory is to describe the whole space of invariants (covariants, joint invariants) for a given vector space under the action of a group. To solve this problem one has to find a set of *fundamental invariants (covariants, joint invariants)* with the property that any other invariant (covariant, joint invariant) is a (analytic) function of the fundamental invariants (covariants, joint invariants). The fundamental theorem on invariants of a regular Lie group action[39] determines the number of fundamental invariants required to define the whole of the space of $I(M)$ invariants.

Theorem 2.1: *Let G be a Lie group acting regularly on an m-dimensional manifold X with s-dimensional orbits. Then, in a neighborhood N of each point* $x_0 \in X$, *there exist* $m-s$ *functionally independent G invariants* $\Delta_1, \ldots, \Delta_{m-s}$. *Any other G-invariant* $\mathcal{I}$ *defined near* x_0 *can be locally uniquely expressed as an analytic function of the fundamental invariants through* $\mathcal{I} = F(\Delta_1, \ldots, \Delta_{m-s})$.

Hence, if we assume that the group $I(M), \dim I(M) = r = \frac{1}{2}n(n+1)$ acts in a subspace Σ_r of the parameter space Σ defined by the corresponding $\mathcal{K}^p(M)$, $p \geqslant 1$ regularly with r-dimensional orbits, then, according to Theorem 2.1, the number of fundamental invariants required to describe the whole space of $I(M)$ invariants of $\mathcal{K}^p(M)$ is $d-r$, where d is given by (9) (note $d \geqslant r$). This has been shown to be the case for the vector spaces $\mathcal{K}^2(\mathbb{R}^2)$,[16] $\mathcal{K}^2(\mathbb{R}^2_1)$,[12] $\mathcal{K}^3(\mathbb{R}^2)$,[10] and $\mathcal{K}^2(\mathbb{R}^3)$,[7] where $\mathbb{R}^2, \mathbb{R}^2_1$, and $\mathbb{R}^3$ denote the Euclidean, Minkowski planes and the Euclidean space, respectively. The dimension of the orbits of the isometry group $I(M)$ acting in Σ is not always the same as the dimension of the group. For example, this is the case for the vector space $\mathcal{K}^1(\mathbb{R}^3)$.[11] To determine the dimension of the orbits one can use the infinitesimal generators of the group $I(M)$ in Σ.

In what follows we use the approach introduced in Ref. 15. Let $\mathbf{X}_1, \ldots, \mathbf{X}_r \in \mathcal{X}(M)$ be the infinitesimal generators (Killing vector fields) of the Lie group $I(M)$ acting on M. Note $\mathrm{Span}\{\mathbf{X}_1, \ldots, \mathbf{X}_r\} = \mathcal{K}^1(M) = i(M)$, where $i(M)$ is the Lie algebra of the Lie group $I(M)$. For a fixed $p \geqslant 1$, consider the corresponding vector space $\mathcal{K}^p(M)$. To determine the action of $I(M)$ in the

space Σ, we find first the infinitesimal generators of $I(M)$ in Σ. Consider Diff Σ, it defines the corresponding space Diff $\mathcal{K}^p(M)$, whose elements are determined by the elements of Diff Σ in an obvious way. Let $\mathbf{K}^0 \in \text{Diff}\,\mathcal{K}^p(M)$. Note $\mathbf{K}^0$ is determined by d parameters $\alpha_i^0(\alpha_1,\ldots,\alpha_d)$, $i=1,\ldots,d$, which are functions of $\alpha_1,\ldots,\alpha_d$—the parameters of Σ. Define now a map $\pi:\text{Diff}\,\mathcal{K}^p(M)\to\mathcal{X}(\Sigma)$, given by

$$\mathbf{K}^0 \to \sum_{i=1}^{d} \alpha_i^0(\alpha_1,\ldots,\alpha_d)\frac{\partial}{\partial\,\alpha_i}. \tag{12}$$

To specify the action of $I(M)$ in Σ, we must find the counterparts of the generators $\mathbf{X}_1,\ldots,\mathbf{X}_r$ in $\mathcal{X}(\Sigma)$. Consider the composition $\pi\circ\mathcal{L}$, where π is defined by (12) and $\mathcal{L}$ is the Lie derivative operator. Let $\mathbf{K}$ be the general Killing tensor of $\mathcal{K}^p(M)$, in other words $\mathbf{K}$ is the general solution to the Killing tensor equation (2). Note, for $p=2$ we have $\mathbf{K}=\text{Span}\{\mathbf{g},\mathbf{K}_1,\ldots,\mathbf{K}_{d-1}\}$, where $\{\mathbf{g},\mathbf{K}_1,\ldots,\mathbf{K}_{d-1}\}$ is a basis of the vector space $\mathcal{K}^2(M)$ and $\mathbf{g}$ is the metric of $(M,\mathbf{g})$. Next, define

$$\mathbf{V}_i = \pi\mathcal{L}_{\mathbf{X}_i}\mathbf{K}, \quad i=1,\ldots,r. \tag{13}$$

The composition map $\pi\circ\mathcal{L}:i(M)\to\mathcal{X}(\Sigma)$ maps the generators $\mathbf{X}_1,\ldots,\mathbf{X}_r$ to $\mathcal{X}(\Sigma)$.

Conjecture 2.1 (Ref. 10): Suppose the generators $\mathbf{X}_1,\ldots,\mathbf{X}_r$ of $i(M)$ satisfy the following commutator relations:

$$[\mathbf{X}_i,\mathbf{X}_j] = c_{ij}^k\mathbf{X}_k, \quad i,j,k=1,\ldots,r, \tag{14}$$

where c_{ij}^k, $i,j,k=1,\ldots,r$ are the structural constants. Then the corresponding vector fields $\mathbf{V}_i \in \mathcal{X}(\Sigma)$, defined by (13) satisfy the same commutator relations,

$$[\mathbf{V}_i,\mathbf{V}_j] = c_{ij}^k\mathbf{V}_k, \quad i,j,k=1,\ldots,r. \tag{15}$$

Therefore the map $F_* := \pi\circ\mathcal{L}:i(M)\to i_\Sigma(M)$ is a Lie algebra isomorphism, where $i_\Sigma(M)$ is the Lie algebra generated by $\mathbf{V}_1,\ldots,\mathbf{V}_r$.

We emphasize that the technique of the Lie derivative deformations used here is a very powerful tool. It was used before, for example, in Ref. 37 to generate compatible Poisson bivectors in the theory of bi-Hamiltonian systems. The idea introduced in Ref. 37 was utilized in Ref. 38 and applied to a different class of integrable systems. The validity of the formula (15) can be confirmed directly on a case by case basis, provided that the general form of a Killing tensor $\mathbf{K}^p \in \mathcal{K}^p(M)$ is available. The proof of the general statement of Conjecture 2.1 will be published elsewhere.[8]

Remark 2.2: Alternatively, the generators (13) can be obtained from the formulas for the action of the group (10) in the usual way taking into account that a Lie algebra is the tangent space at the unity of the corresponding Lie group. We note, however, that in this way the formulas (10) are not easy to derive in general.

In view of the isomorphism exhibited in the conjecture and the fact that invariance of a function under an entire Lie group is equivalent to the infinitesimal invariance under the infinitesimal generators of the corresponding Lie algebra one can determine a set of fundamental invariants by solving the system of PDEs

$$\mathbf{V}_i(F) = 0, \quad i=1,\ldots,r \tag{16}$$

for an analytic function $F:\Sigma\to\mathbb{R}$, where the vector fields $\mathbf{V}_i$, $i=1,\ldots,r$ are the generators defined by (13). As is specified by Theorem 2.1, the general solution to the system (16) is an analytic function F of the fundamental invariants. The number of fundamental invariants is $d-s$, where d is specified by the DTT formula (9) and s is the dimension of the orbits of $I(M)$ acting regularly in the parameter space Σ. To determine s and the subspaces of Σ where the isometry group acts with orbits of the same dimension, one employs the result of the following proposition.[39]

Proposition 2.1: *Let a Lie group G act on X, $\mathfrak{g}$ is the corresponding Lie algebra and let $x \in X$. The vector space $S|_x = \mathrm{Span}\{\mathbf{V}_i(x) \,|\, \mathbf{V_i} \in \mathfrak{g}\}$ spanned by all vector fields determined by the infinitesimal generators at x coincides with the tangent space to the orbit $\mathcal{O}_x$ of G that passes through x, so $S|_x = T\mathcal{O}_x|_x$. In particular, the dimension of $\mathcal{O}_x$ equals the dimension of $S|_x$. Moreover, the isotropy subgroup $G_x \subset G$ has dimension* $\dim G - \dim \mathcal{O}_x = r - s$.

Example 2.2: Consider the action of the isometry group $I(\mathbb{R}^2_1)$ on the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$. More information about the geometry of Minkowski plane $\mathbb{R}^2_1$ can be found in the monograph by Thompson.[40] The general form of the elements of $\mathcal{K}^2(\mathbb{R}^2_1)$ in terms of the standard pseudo-Cartesian coordinates (t,x) is given by

$$\mathbf{K} = (\alpha_1 + 2\alpha_4 x + \alpha_6 x^2)\frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + (\alpha_3 + \alpha_4 t + \alpha_5 x + \alpha_6 t x)\frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + (\alpha_2 + 2\alpha_5 t + \alpha_6 t^2)\frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}. \tag{17}$$

The isometry group $I(\mathbb{R}^2_1)$ acts in the Minkowski plane $\mathbb{R}^2_1$ parametrized by (t,x) as follows:

$$\begin{pmatrix} \tilde{t} \\ \tilde{x} \end{pmatrix} = \begin{pmatrix} \cosh\phi & \sinh\phi \\ \sinh\phi & \cosh\phi \end{pmatrix}\begin{pmatrix} t \\ x \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix}, \tag{18}$$

where $\phi, a, b \in \mathbb{R}$ are local coordinates that parametrize the group $I(\mathbb{R}^2_1)$. The generators of the Lie algebra $i(\mathbb{R}^2_1)$ of the isometry group with respect to the coordinates (t,x) take the following form:

$$\mathbf{T} = \frac{\partial}{\partial t}, \quad \mathbf{X} = \frac{\partial}{\partial x}, \quad \mathbf{H} = x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x} \tag{19}$$

corresponding to t and x translations and (hyperbolic) rotation, given with respect to the standard pseudo-Cartesian coordinates (t,x). Note the generators (19) of the Lie algebra $i(\mathbb{R}^2_1)$ enjoy the following commutator relations:

$$[\mathbf{T},\mathbf{X}] = 0, \quad [\mathbf{T},\mathbf{H}] = \mathbf{X}, \quad [\mathbf{X},\mathbf{H}] = \mathbf{T}. \tag{20}$$

We use the formula (18) and the transformation laws for the components of (2, 0) tensors

$$\tilde{K}^{ij}(\tilde{y}^1,\tilde{y}^2,\tilde{\alpha}_1,\ldots,\tilde{\alpha}_6) = K^{k\ell}(y^1,y^2,\alpha_1,\ldots,\alpha_6)\frac{\partial \tilde{y}^i}{\partial y^k}\frac{\partial \tilde{y}^j}{\partial y^\ell}, \quad i,j,k,\ell = 1,2, \tag{21}$$

where the tensor components K^{ij} are given by (17), $y^1 = t, y^2 = x$. In view of (17), (18), and (21) the transformation laws (10) for the parameters α_i, $i = 1,\ldots,6$ take in this case the following form (see also Refs. 23 and 12),

$$\begin{aligned}
\tilde{\alpha}_1 &= \alpha_1 \cosh^2\phi + 2\alpha_3 \cosh\phi \sinh\phi + \alpha_2 \sinh^2\phi + \alpha_6 b^2 - 2(\alpha_4 \cosh\phi + \alpha_5 \sinh\phi)b, \\
\tilde{\alpha}_2 &= \alpha_1 \sinh^2\phi + 2\alpha_3 \cosh\phi \sinh\phi + \alpha_2 \cosh^2\phi + \alpha_6 a^2 - 2(\alpha_5 \cosh\phi + \alpha_4 \sinh\phi)a, \\
\tilde{\alpha}_3 &= \alpha_3(\cosh^2\phi + \sinh^2\phi) + (\alpha_1 + \alpha_2)\cosh\phi \sinh\phi - (a\alpha_4 + b\alpha_5)\cosh\phi \\
&\quad - (a\alpha_5 + b\alpha_4)\sinh\phi + \alpha_6 ab, \\
\tilde{\alpha}_4 &= \alpha_4 \cosh\phi + \alpha_5 \sinh\phi - \alpha_6 b, \\
\tilde{\alpha}_5 &= \alpha_4 \sinh\phi + \alpha_5 \cosh\phi - \alpha_6 a, \\
\tilde{\alpha}_6 &= \alpha_6.
\end{aligned} \tag{22}$$

We note that the corresponding transformation formulas for the parameters obtained in Ref. 12

were derived for *covariant* Killing tensors. Accordingly, they differ somewhat from (22) presented above [compare with (7.6) in Ref. 12]. According to Proposition 2.1, in order to determine the subspaces of Σ where the orbits have the same dimensions, one must check the subspaces of Σ where the system (16) retains its rank. In many cases the system of PDEs (16) can be solved by the method of characteristics. The determination of fundamental invariants by solving (16) is the key idea used in Ref. 15 to adapt the *method of infinitesimal generators* to the problem of finding fundamental invariants of Killing tensors under the action of the isometry group. When the method of characteristic fails, one can employ the *method of undetermined coefficients* to find a set of fundamental invariants.[11,7] Alternatively, a set of fundamental invariants can be determined by using the *method of moving frames* (see Sec. III for more details). To determine the space of $I(\mathbb{R}^2_1)$ invariants, we employ the procedure described above and derive the corresponding infinitesimal generators $\mathbf{V}_i$, $i=1, 2, 3$ by the formula (13),

$$\mathbf{V}_1 = \alpha_4\frac{\partial}{\partial\,\alpha_3} + 2\alpha_5\frac{\partial}{\partial\,\alpha_2} + \alpha_6\frac{\partial}{\partial\,\alpha_5},$$

$$\mathbf{V}_2 = \alpha_5\frac{\partial}{\partial\,\alpha_3} + 2\alpha_4\frac{\partial}{\partial\,\alpha_1} + \alpha_6\frac{\partial}{\partial\,\alpha_4}, \tag{23}$$

$$\mathbf{V}_3 = -2\alpha_3\frac{\partial}{\partial\,\alpha_1} - \alpha_5\frac{\partial}{\partial\,\alpha_4} - (\alpha_1+\alpha_2)\frac{\partial}{\partial\,\alpha_3} - 2\alpha_3\frac{\partial}{\partial\,\alpha_2} - \alpha_4\frac{\partial}{\partial\,\alpha_5},$$

and then solve by the method of characteristic the corresponding system of PDEs (16) with respect to (23). Note the vector fields $-\mathbf{V}_i$, $i=1, 2, 3$ satisfy the same commutator relations as (19) [see (20)], which confirms Conjecture 2.1. Ultimately, this leads to the following theorem.

Theorem 2.2: *Any algebraic $I(\mathbb{R}^2_1)$-invariant I of the subspace of the parameter space Σ of $\mathcal{K}^2(\mathbb{R}^2_1)$ defined by the condition that the vector fields (23) are linearly independent can be (locally) uniquely expressed as an analytic function,*

$$I = F(\mathcal{I}_1,\mathcal{I}_2,\mathcal{I}_3),$$

where the fundamental invariants $\mathcal{I}_i$, $i=1, 2, 3$ are given by

$$\mathcal{I}_1 = (\alpha_4^2+\alpha_5^2-\alpha_6(\alpha_1+\alpha_2))^2 - 4(\alpha_3\alpha_6-\alpha_4\alpha_5)^2,$$

$$\mathcal{I}_2 = \alpha_6(\alpha_1-\alpha_2) - \alpha_4^2 + \alpha_5^2, \tag{24}$$

$$\mathcal{I}_3 = \alpha_6.$$

The fact that $\mathcal{I}_3=\alpha_6$ is a fundamental $I(\mathbb{R}^2_1)$ invariant of the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$ trivially follows from the transformation formulas (22). The fundamental $I(\mathbb{R}^2_1)$-invariant $\mathcal{I}_1$ was derived in Refs. 12 and 15 in the study of the five-dimensional subspace of nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}^2_1)$. As expected, in this case by Theorem 2.1, we have obtained 6 (dimension of the space) -3 (dimension of the orbits) $=3$ fundamental $I(\mathbb{R}^2_1)$ invariants of the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$.

B. Covariants

Consider now the action of the isometry group $I(M)$ on the product space $\mathcal{K}^p(M)\times M$, $p\geqslant 1$. As above it induces the transformation laws on the *extended parameter space* $\Sigma\times M$, where Σ is the parameter space of the vector space $\mathcal{K}^p(M)$,

$$\begin{gathered}\tilde{\alpha}_1 = \tilde{\alpha}_1(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r),\\ \tilde{\alpha}_2 = \tilde{\alpha}_2(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r), \quad \ldots,\\ \tilde{\alpha}_d = \tilde{\alpha}_d(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r),\\ \tilde{x}_1 = \tilde{x}_1(x_1,\ldots,x_n,g_1,\ldots,g_r),\\ \tilde{x}_2 = \tilde{x}_2(x_1,\ldots,x_n,g_1,\ldots,g_r), \quad \ldots,\\ \tilde{x}_n = \tilde{x}_n(x_1,\ldots,x_n,g_1,\ldots,g_r),\end{gathered} \tag{25}$$

where as before $\alpha_1,\ldots,\alpha_d$ are the parameters of $\mathcal{K}^p(M)$ that define $\Sigma, g_1,\ldots,g_r$, $r=\frac{1}{2}n(n+1)$ are local parameters parametrizing the group $I(M)$ and $x_1,\ldots,x_n$ are local coordinates on the manifold M.

Definition 2.3: An $I(M)$ covariant of the vector space $\mathcal{K}^p(M)$ $p\geqslant 1$ is a function $C:\Sigma\times M\rightarrow\mathbb{R}$ satisfying the condition

$$C = F(\alpha_1,\ldots,\alpha_d,x_1,\ldots,x_n) = F(\tilde{\alpha}_1,\ldots,\tilde{\alpha}_d,\tilde{x}_1\ldots,\tilde{x}_n) \tag{26}$$

under the transformation laws (25) induced by the isometry group $I(M)$, where Σ is the parameter space of $\mathcal{K}^p(M)$.

Conjecture 2.1 entails the following corollary.

Corollary 2.1: Consider the product vector space $\mathcal{K}^p(M)\times M$, $p\geqslant 1$. Define the vector fields

$$\mathbf{V}_i' := \mathbf{V}_i + \mathbf{X}_i, \quad i=1,\ldots,r, \tag{27}$$

where $\mathbf{V}_i, i=1,\ldots,r$ are the infinitesimal generators of the Lie algebra $i(M)$ in the parameter space Σ of the vector space $\mathcal{K}^p(M)$ obtained via (13) and $\mathbf{X}_i, i=1,\ldots,r$ are the generators of $i(M)$. Then the vector fields $\mathbf{V}_1',\ldots,\mathbf{V}_r'$ enjoy the same commutator relations as the generators $\mathbf{X}_1,\ldots,\mathbf{X}_r$ of $i(M)$ in $\mathcal{X}(M)$:

$$[\mathbf{V}_i',\mathbf{V}_j'] = c_{ij}^k\mathbf{V}_k', \quad i,j,k=1,\ldots,r, \tag{28}$$

where the structural constants c_{ij}^k are as in (14).

Proof: Straightforward. □

Therefore, in view of the above, $I(M)$ covariants of a vector space $\mathcal{K}^p(M)$ can be obtained by solving the corresponding system of PDEs generated by the vector fields (27):

$$\mathbf{V}_i'(F) = 0, \quad i=1,\ldots,r. \tag{29}$$

Alternatively, one can employ the method of moving frames. To demonstrate how it works in the framework of ITKT we shall employ the method in Sec. III to compute the covariants of the vector spaces $\mathcal{K}^2(\mathbb{R}^2)$ and $\mathcal{K}^2(\mathbb{R}_1^2)$.

C. Joint invariants

Consider now the action of the isometry group $I(M)$ on the product space $\mathcal{K}^\ell(M)\times\mathcal{K}^m(M)\times\cdots\times\mathcal{K}^q(M)$, $\ell,m,\ldots,q\geqslant 1$. Let $\alpha_1,\ldots,\alpha_d,\beta_1,\ldots,\beta_e,\ldots,\gamma_1,\ldots,\gamma_f$ be the parameters of the vector spaces $\mathcal{K}^\ell(M),\mathcal{K}^m(M),\ldots,\mathcal{K}^q(M)$, respectively, where $d,e,\ldots,f$ are the corresponding dimensions determined by (9). Then the action of the isometry group $I(M)$ induces the corresponding transformation laws for the parameters $\alpha_1,\ldots,\alpha_d,\beta_1,\ldots,\beta_e,\ldots,\gamma_1,\ldots,\gamma_f$:

$$\tilde{\alpha}_1 = \tilde{\alpha}_1(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r),$$

$$\tilde{\alpha}_2 = \tilde{\alpha}_2(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r), \quad \ldots,$$

$$\tilde{\alpha}_d = \tilde{\alpha}_d(\alpha_1,\ldots,\alpha_d,g_1,\ldots,g_r), \quad \ldots,$$

$$\tilde{\beta}_1 = \tilde{\beta}_1(\beta_1,\ldots,\beta_e,g_1,\ldots,g_r), \quad \ldots,$$

$$\tilde{\beta}_2 = \tilde{\beta}_2(\beta_1,\ldots,\beta_e,g_1,\ldots,g_r), \quad \ldots, \tag{30}$$

$$\tilde{\beta}_e = \tilde{\beta}_e(\beta_1,\ldots,\beta_e,g_1,\ldots,g_r), \quad \ldots,$$

$$\tilde{\gamma}_1 = \tilde{\gamma}_1(\gamma_1,\ldots,\gamma_f,g_1,\ldots,g_r),$$

$$\tilde{\gamma}_2 = \tilde{\gamma}_2(\gamma_1,\ldots,\gamma_f,g_1,\ldots,g_r), \quad \ldots,$$

$$\tilde{\gamma}_f = \tilde{\gamma}_f(\gamma_1,\ldots,\gamma_f,g_1,\ldots,g_r),$$

where as before $g_1,\ldots,g_r$ are local coordinates on $I(M)$ that parametrize the group and $r = \dim I(M) = \frac{1}{2}n(n+1)$. This observation leads us to introduce the concept of a *joint $I(M)$-invariant*.

Definition 2.4: *A* joint $I(M)$ invariant *of the product space $\mathcal{K}^\ell(M)\times\mathcal{K}^m(M)\times\cdots\times\mathcal{K}^q(M)$, is a function $J:\Sigma^\ell\times\Sigma^m\times\cdots\times\Sigma^q\to\mathbb{R}$ satisfying the condition*

$$J = F(\alpha_1,\ldots,\alpha_d,\beta_1\ldots,\beta_e,\ldots,\gamma_1\ldots,\gamma_f)$$

$$= F(\tilde{\alpha}_1,\ldots,\tilde{\alpha}_d,\tilde{\beta}_1\ldots,\tilde{\beta}_e,\ldots,\tilde{\gamma}_1\ldots,\tilde{\gamma}_f) \tag{31}$$

under the transformation laws (30) induced by the isometry group $I(M)$.

In this case again Conjecture 2.1 entails the following corollary.

Corollary 2.2: Consider the product vector space,

$$\mathcal{K} = \mathcal{K}^\ell(M)\times\mathcal{K}^m(M)\times\cdots\times\mathcal{K}^q(M), \tag{32}$$

where $\ell,m,\ldots,q\geqslant 1$. Define the vector fields

$$\tilde{\mathbf{V}}_i := \mathbf{V}_i^\ell + \mathbf{V}_i^m + \cdots + \mathbf{V}_i^q, \quad i=1,\ldots,r, \tag{33}$$

where $\{\mathbf{V}_i^\ell\},\{\mathbf{V}_i^m\},\ldots,\{\mathbf{V}_i^q\}$, $i=1,\ldots,r$ are the sets of infinitesimal generators of the Lie algebra $i(M)$ in the parameter spaces $\Sigma^\ell,\Sigma^m,\ldots,\Sigma^q$ of the vector spaces $\mathcal{K}^\ell(M),\mathcal{K}^q(M),\ldots,\mathcal{K}^n(M)$, respectively, obtained via (13). Then the vector fields $\tilde{\mathbf{V}}_1,\ldots,\tilde{\mathbf{V}}_r$ enjoy the same commutator relations as the generators $\mathbf{X}_1\ldots,\mathbf{X}_r$ of $i(M)$ in $\mathcal{X}(M)$:

$$[\tilde{\mathbf{V}}_i,\tilde{\mathbf{V}}_j] = c_{ij}^k\tilde{\mathbf{V}}_k, \quad i,j,k=1,\ldots,r, \tag{34}$$

where the structural constants c_{ij}^k are as in (14).

Proof: Straightforward. □

Example 2.3: Consider the product vector space $\mathcal{K}^1(\mathbb{R}^2)\times\mathcal{K}^2(\mathbb{R}^2)$. The general form of the elements of $\mathcal{K}^1(\mathbb{R}^2)$ (Killing vectors) with respect to the Cartesian coordinates is given by

$$\mathbf{K}^1 = (\alpha_1 + \alpha_3 y)\frac{\partial}{\partial x} + (\alpha_2 - \alpha_3 x)\frac{\partial}{\partial y}, \tag{35}$$

while the (contravariant) elements of $\mathcal{K}^2(\mathbb{R}^2)$ assume the following general form with respect to the same coordinate system:

$$\mathbf{K}^2 = (\beta_1 + 2\beta_4 y + \beta_6 y^2)\frac{\partial}{\partial x} \odot \frac{\partial}{\partial x} + (\beta_3 - \beta_4 x - \beta_5 y - \beta_6 xy)\frac{\partial}{\partial x} \odot \frac{\partial}{\partial y}$$
$$+ (\beta_2 + 2\beta_5 x + \beta_6 x^2)\frac{\partial}{\partial y} \odot \frac{\partial}{\partial y}, \tag{36}$$

where $\odot$ denotes the symmetric tensor product. The formulas (35) and (36) put in evidence that the corresponding parameter spaces Σ^1 and Σ^2 are determined by the three parameters $\alpha_i, i=1,\ldots,3$ and the six parameters $\beta_i, i=1,\ldots,6$, respectively. Let $I(\mathbb{R}^2)$ be the proper Euclidean group that consists of the orientation-preserving isometries of $\mathbb{R}^2$ (rigid motions). Its action in $\mathbb{R}^2$ can be described as the semidirect product of rotations and translations. In view of its standard parametrization, we have the transformation of the Cartesian coordinates $\mathbf{x}=(x,y)$,

$$\tilde{\mathbf{x}} = R_\theta \mathbf{x} + \mathbf{a}, \quad R_\theta = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \in \mathrm{SO}(2), \quad \mathbf{a} = (a,b) \in \mathbb{R}^2. \tag{37}$$

Note, the generators of $i(\mathbb{R}^2)=\mathcal{K}^1(\mathbb{R}^2)$, which is the Lie algebra of the Lie group $I(\mathbb{R}^2)$, are given with respect to the Cartesian coordinates by

$$\mathbf{X} = \frac{\partial}{\partial x}, \quad \mathbf{Y} = \frac{\partial}{\partial y}, \quad \mathbf{R} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}, \tag{38}$$

whose flows are translations and a rotation, respectively. Employing the construction (13), we derive two triples of the vector fields representing the generators (38) in $\mathcal{X}(\Sigma^1)$

$$\mathbf{V}_1^1 = -\alpha_3\frac{\partial}{\partial \alpha_2},$$

$$\mathbf{V}_2^1 = \alpha_3\frac{\partial}{\partial \alpha_1}, \tag{39}$$

$$\mathbf{V}_3^1 = \alpha_1\frac{\partial}{\partial \alpha_2} - \alpha_2\frac{\partial}{\partial \alpha_1},$$

and $\mathcal{X}(\Sigma^2)$,

$$\mathbf{V}_1^2 = -2\beta_5\frac{\partial}{\partial \beta_2} - \beta_4\frac{\partial}{\partial \beta_3} + \beta_6\frac{\partial}{\partial \beta_5},$$

$$\mathbf{V}_2^2 = 2\beta_4\frac{\partial}{\partial \beta_1} - \beta_5\frac{\partial}{\partial \beta_3} + \beta_6\frac{\partial}{\partial \beta_6}, \tag{40}$$

$$\mathbf{V}_3^2 = -2\beta_3\left(\frac{\partial}{\partial \beta_1} - \frac{\partial}{\partial \beta_2}\right) + (\beta_1 - \beta_2)\frac{\partial}{\partial \beta_3} + \beta_5\frac{\partial}{\partial \beta_4} - \beta_4\frac{\partial}{\partial \beta_5},$$

respectively. We note that in view of Conjecture 2.1 both the vector fields (39) and the vector fields (40) satisfy the same commutator relations as the generators of $i(\mathbb{R}^2)$ (38). By Corollary 2.2

this fact entails immediately that the vector fields $\{\tilde{\mathbf{V}}_i\}$, $i=1, 2, 3$ defined by

$$\tilde{\mathbf{V}}_i := \mathbf{V}_i^1 + \mathbf{V}_i^2, \quad i = 1,2,3 \tag{41}$$

also enjoy the same commutator relations. This property can be also verified directly. Therefore we have determined the action of $I(\mathbb{R}^2)$ in the product space $\Sigma^1 \times \Sigma^2$. To determine the dimension of the orbits of the group we use the result of Propositon 2.1. Thus, the orbits of the isometry group $I(\mathbb{R}^2)$ acting in $\Sigma^1 \times \Sigma^2$ are three dimensional in the subspace $\mathcal{S}_3 \subset \Sigma^1 \times \Sigma^2$, where the generators (41) are linearly independent. According to Theorem 2.1, the number of fundamental invariants in $\mathcal{S}_3$ is 9 (dimension of $\Sigma^1 \times \Sigma^2$) -3 (dimension of the orbits in $\mathcal{S}_3$) $=6$. Some of these fundamental invariants may be the fundamental invariants of the group action in the vector spaces $\mathcal{K}^1(\mathbb{R}^2)$ and $\mathcal{K}^2(\mathbb{R}^2)$. Indeed, it is instructive at this point to review the transformations imposed on the nine parameters $(\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6)$ of the product space $\Sigma^1 \times \Sigma^2$ by the group action:

$$\tilde{\alpha}_1 = \alpha_1 \cos\theta - \alpha_2 \sin\theta - b\alpha_3,$$

$$\tilde{\alpha}_2 = \alpha_1 \sin\theta + \alpha_2 \cos\theta + a\alpha_3,$$

$$\tilde{\alpha}_3 = \alpha_3,$$

$$\tilde{\beta}_1 = \beta_1 \cos^2\theta - 2\beta_3 \cos\theta \sin\theta + \beta_2 \sin^2\theta - 2b\beta_4 \cos\theta - 2b\beta_5 \sin\theta + \beta_6 b^2,$$

$$\tilde{\beta}_2 = \beta_1 \sin^2\theta - 2\beta_3 \cos\theta \sin\theta + \beta_2 \cos^2\theta - 2a\beta_5 \cos\theta + 2a\beta_4 \sin\theta + \beta_6 a^2, \tag{42}$$

$$\tilde{\beta}_3 = (\beta_1 - \beta_2)\sin\theta \cos\theta + \beta_3(\cos^2\theta - \sin^2\theta) + (a\beta_4 + b\beta_5)\cos\theta + (a\beta_5 - b\beta_4)\sin\theta - \beta_6 ab,$$

$$\tilde{\beta}_4 = \beta_4 \cos\theta + \beta_5 \sin\theta - \beta_6 b,$$

$$\tilde{\beta}_5 = \beta_5 \cos\theta - \beta_4 \sin\theta - \beta_6 a,$$

$$\tilde{\beta}_6 = \beta_6,$$

where (θ, a, b) given by (37) parametrize the isometry group $I(\mathbb{R}^2)$. Hence, the dimension of the orbits in this subspace coincides with the dimension of the group. We also observe that α_3 and β_6 are fundamental $I(\mathbb{R}^2)$ invariants of the group action in $\Sigma^1 \times \Sigma^2$.

To determine the remaining four fundamental invariants we use the method of characteristics to solve the system of linear PDEs,

$$\tilde{\mathbf{V}}_i(F) = 0, \quad i = 1,2,3, \tag{43}$$

where $F: \Sigma^1 \times \Sigma^2 \to \mathbb{R}$ and the vector fields $\tilde{\mathbf{V}}_i$, $i=1, 2, 3$ are given by (41). Having solved the system of PDEs (43), we have therefore proven the following result.

Theorem 2.3: *Any algebraic joint $I(\mathbb{R}^2)$-invariant I defined over the subspace of $\Sigma^1 \times \Sigma^2$ where the vector fields (41) are linearly independent can be locally uniquely expressed as an analytic function,*

$$I = F(\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3, \mathcal{I}_4, \mathcal{J}_1, \mathcal{J}_2),$$

where the fundamental joint $I(\mathbb{R}^2)$-invariants $\mathcal{I}_i, \mathcal{J}_j$, $i=1,\ldots, 4$, $j=1, 2$ are given by

$$\mathcal{I}_1 = [\beta_6(\beta_1 - \beta_2) + \beta_5^2 - \beta_4^2]^2 + 4(\beta_3\beta_6 + \beta_4\beta_5)^2,$$

$$\mathcal{I}_2 = \beta_6(\beta_1 + \beta_2) - \beta_4^2 - \beta_5^2,$$

$$\mathcal{I}_3 = \beta_6, \qquad \mathcal{I}_4 = \alpha_3, \tag{44}$$

$$\mathcal{J}_1 = (\beta_6\alpha_2 + \beta_5\alpha_3)^2 + (\beta_6\alpha_1 - \beta_4\alpha_3)^2,$$

$$\mathcal{J}_2 = (\beta_6\alpha_2 + \alpha_3\alpha_5)(\beta_6\beta_2 - \beta_5^2) + 2(\beta_3\beta_6 + \beta_4\beta_5)(\beta_6\alpha_1 - \beta_4\alpha_3).$$

The fundamental joint $I(\mathbb{R}^2)$ invariants $\mathcal{I}_i$, $i=1, 2, 3$ are the fundamental $I(\mathbb{R}^2)$ invariants of the vector space $\mathcal{K}^2(\mathbb{R}^2)$ ($\mathcal{I}_1$ was derived in Ref. 15), while $\mathcal{I}_4$ is the fundamental $I(\mathbb{R}^2)$ invariant of the vector space $\mathcal{K}^1(\mathbb{R}^2)$. Note the fundamental $I(\mathbb{R}^2)$ invariants $\mathcal{J}_1$ and $\mathcal{J}_2$ are "truly" joint $I(\mathbb{R}^2)$ invariants of the vector spaces $\mathcal{K}^1(\mathbb{R}^2)$ and $\mathcal{K}^2(\mathbb{R}^2)$. Therefore we have introduced an analogue of the concept of a joint invariant in the classical invariant theory of homogeneous polynomials (refer to Ref. 41 for more details). The problem of the determination of fundamental invariants, solved in this section for a particular (product) vector space of Killing tensors (Theorem 2.3) by the *method of infinitesimal generators*, can also be solved by the purely algebraic *method of moving frames*. This is the subject of the considerations that follow.

III. THE METHOD OF MOVING FRAMES

The method of moving frames, introduced originally by Cartan,[4] is a powerful technique that can be employed to solve a wide range of equivalence-type problems. In its original interpretation it is based on an equivariant map from the space of submanifolds to a bundle of frames. The simplest example of a moving frame is the Frenet frame $\{\mathbf{t}, \mathbf{n}\}$ of a regular curve $\gamma \in \mathbb{R}^2$ parametrized by its arc length. In this case the equivariant map assigns to each point on the curve $\gamma(s)$ the corresponding frame $\{\mathbf{t}(s), \mathbf{n}(s)\}$. Clearly, the moving frame along γ can be obtained from a fixed frame via a combination of rotations and/or translations. This puts in evidence that there is a natural isomorphism between the moving frame and the orientation-preserving isometry group (Euclidean group) $I(\mathbb{R}^2)$. This is the essence of the later generalizations of the moving frame method,[28–30] where the moving frame was viewed as an equivariant map from the space of submanifolds to the group itself. In recent works by Fels and Olver[26,27] the classical moving frame method was further generalized to completely general transformation groups, including infinite-dimensional Lie pseudogroups (see also Kogan[32]). Ultimately, the authors have succeeded in bringing the theory up to the level where the bundle of frames is no longer needed. We very briefly review the basic definitions and results of the moving frames theory in its modern formulation (for a complete review, see Ref. 39).

Definition 3.1: A moving frame *is a smooth, G-equivariant map $\rho: M \to G$, where G is an r-dimensional group acting smoothly on an n-dimensional underlying manifold M.*

Theorem 3.1: *A moving frame exists in a neighborhood of a point $\mathbf{x} \in M$ iff G acts freely and regularly near* $\mathbf{x}$.

To construct a moving frame, one employs Cartan's *normalization method*.[4]

Theorem 3.2: *Let G act freely and regularly on M and let $K \subset M$ be a (local) cross section to the group orbits. Given $\mathbf{x} \in M$, let $\mathbf{g} = \rho(\mathbf{x})$ be the unique group element that maps $\mathbf{x}$ to the cross section: $\mathbf{g} \cdot \mathbf{x} = \rho(\mathbf{x}) \cdot \mathbf{x} \in K$. Then $\rho: M \to G$ is a right moving frame.*

More specifically, let $\mathbf{x} = (x_1, \ldots, x_n) \in M$ be local coordinates. Consider the explicit formulas

for the coordinate transformations induced by the action of $G:\omega(\mathbf{g},\mathbf{x})=\mathbf{g}\cdot\mathbf{x}$. The right moving frame $\mathbf{g}=\rho(\mathbf{x})$ can be constructed by making use of a *coordinate cross section*,

$$K=\{x_1=c_1,x_2=c_2,\ldots,x_r=c_r\},$$

where c_i, $i=1,\ldots,r$ are some constants and solving the corresponding *normalization equations*

$$\omega_1(\mathbf{g},\mathbf{x})=c_1,\quad \omega_2(\mathbf{g},\mathbf{x})=c_2,\quad \ldots,\quad \omega_r(\mathbf{g},\mathbf{x})=c_r, \tag{45}$$

for the group G locally parametrized by $\mathbf{g}=(g_1,\ldots,g_r)$ in terms of the local coordinates $(x_1,\ldots,x_n)$. Substituting the resulting expressions for $g_1,\ldots,g_r$ in terms of the local coordinates $(x_1,\ldots x_n)$ into the remaining $n-r$ formulas for the transformation rules $\omega(\mathbf{g},\mathbf{x})=\mathbf{g}\cdot\mathbf{x}$ yields a complete set of fundamental invariants for the action of G on M.

Theorem 3.3: *If* $\mathbf{g}=\rho(\mathbf{x})$ *is the moving frame solution to the normalization equations (45), then the functions*

$$\mathcal{I}_1(\mathbf{x})=\omega_{r+1}(\rho(\mathbf{x}),\mathbf{x}),\ldots,\mathcal{I}_{n-r}(\mathbf{x})=\omega_n(\rho(\mathbf{x}),\mathbf{x}) \tag{46}$$

form a complete system of functionally independent fundamental G invariants.

Let us now illustrate the procedure and demonstrate how the method of moving frames can be effectively applied to the problem of the determination of the fundamental invariants of the isometry group in the invariant theory of Killing tensors.

Example 3.1: Consider the extended vector space $\mathcal{K}^2(\mathbb{R}^2)\times\mathbb{R}^2$. The corresponding extended parameter space $\Sigma\times\mathbb{R}^2$ is determined by the parameters $\beta_1,\ldots,\beta_6,x,y$, where β_i, $i=1,\ldots,6$ are as in (36) and x,y are the standard Cartesian coordinates. The isometry group $I(\mathbb{R}^2)$ acting on $\mathcal{K}^2(\mathbb{R}^2)\times\mathbb{R}^2$ induces the corresponding transformations on the extended parameter space $\Sigma\times\mathbb{R}^2$ (25), which in this case take the following form:

$$\tilde{\beta}_1=\beta_1\cos^2\theta-2\beta_3\cos\theta\sin\theta+\beta_2\sin^2\theta-2b\beta_4\cos\theta-2b\beta_5\sin\theta+\beta_6b^2,$$

$$\tilde{\beta}_2=\beta_1\sin^2\theta-2\beta_3\cos\theta\sin\theta+\beta_2\cos^2\theta-2a\beta_5\cos\theta+2a\beta_4\sin\theta+\beta_6a^2,$$

$$\tilde{\beta}_3=(\beta_1-\beta_2)\sin\theta\cos\theta+\beta_3(\cos^2\theta-\sin^2\theta)+(a\beta_4+b\beta_5)\cos\theta+(a\beta_5-b\beta_4)\sin\theta-\beta_6ab,$$

$$\begin{aligned}\tilde{\beta}_4&=\beta_4\cos\theta+\beta_5\sin\theta-\beta_6b,\\ \tilde{\beta}_5&=\beta_5\cos\theta-\beta_4\sin\theta-\beta_6a,\end{aligned} \tag{47}$$

$$\tilde{\beta}_6=\beta_6,$$

$$\tilde{x}=x\cos\theta-y\cos\theta+a,$$

$$\tilde{y}=x\sin\theta+y\cos\theta+b.$$

Next, we construct a moving frame by using the cross section (for example),

$$K=\{\beta_3=\beta_4=\beta_5=0\}, \tag{48}$$

which yields the corresponding normalization equations,

$$0 = (\beta_1 - \beta_2)\sin\theta\cos\theta + \beta_3(\cos^2\theta - \sin^2\theta) + (a\beta_4 + b\beta_5)\cos\theta + (a\beta_5 - b\beta_4)\sin\theta - \beta_6 ab,$$

$$0 = \beta_4\cos\theta + \beta_5\sin\theta - \beta_6 b, \tag{49}$$

$$0 = \beta_5\cos\theta - \beta_4\sin\theta - \beta_6 a.$$

Solving (49) for the parameters $a, b,$ and θ, we obtain the moving frame map $\rho: \Sigma \times \mathbb{R}^2 \to I(\mathbb{R}^2)$ determined by the following formulas:

$$a = \frac{\beta_5\cos\theta - \beta_4\sin\theta}{\beta_6},$$

$$b = \frac{\beta_4\cos\theta + \beta_5\sin\theta}{\beta_6}, \tag{50}$$

$$\theta = \frac{1}{2}\arctan\frac{2(\beta_3\beta_6 + \beta_4\beta_5)}{\beta_6(\beta_1 - \beta_2) - \beta_4^2 + \beta_5^2}.$$

It was observed in Ref. 11 that the method of moving frames could be used to solve the problem of the determination of fundamental invariants of vector spaces of Killing tensors under the action of the isometry group. Indeed, having derived the moving frame map (50) and the transformation laws (47), we can now make use of the result of Theorem 3.3 and determine a set of fundamental $I(\mathbb{R}^2)$ covariants of $\mathcal{K}^2(\mathbb{R}^2)$. Substituting (50) into (47), by Theorem 3.3, we arrive at the following result.

Theorem 3.4: *Consider the vector space $\mathcal{K}^2(\mathbb{R}^2)$. Any algebraic $I(\mathbb{R}^2)$-covariant C defined over the subspace of $\Sigma \times \mathbb{R}^2$ where the isometry group $I(\mathbb{R}^2)$ acts freely and regularly with three-dimensional orbits can be locally uniquely expressed as an analytic function,*

$$C = F(\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3, \mathcal{C}_1, \mathcal{C}_2),$$

where the fundamental $I(\mathbb{R}^2)$-covariants $\mathcal{I}_i, \mathcal{C}_j$, $i = 1, 2, 3$, $j = 1, 2$ are given by

$$\mathcal{I}_1 = [\beta_6(\beta_1 - \beta_2) + \beta_5^2 - \beta_4^2]^2 + 4(\beta_3\beta_6 + \beta_4\beta_5)^2,$$

$$\mathcal{I}_2 = \beta_6(\beta_1 + \beta_2) - \beta_4^2 - \beta_5^2,$$

$$\mathcal{I}_3 = \beta_6, \tag{51}$$

$$\mathcal{C}_1 = (\beta_6 x + \beta_5)^2 + (\beta_6 y + \beta_4)^2,$$

$$\mathcal{C}_2 = [(\beta_6 x + \beta_5)^2 - (\beta_6 y + \beta_4)^2](\beta_5^2 - \beta_4^2 + \beta_6(\beta_1 - \beta_2)) + 4(\beta_6 x + \beta_5)(\beta_6 y + \beta_4)(\beta_6\beta_3 + \beta_4\beta_5),$$

where Σ is the parameter space of $\mathcal{K}^2(\mathbb{R}^2)$.

We immediately observe that the functions $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$ constitute in fact a set of fundamental $I(\mathbb{R}^2)$ invariants of the vector space $\mathcal{K}^2(\mathbb{R}^2)$, while the functions $\mathcal{C}_1$ and $\mathcal{C}_2$ are "truly" fundamental $I(\mathbb{R}^2)$ covariants of the vector space $\mathcal{K}^2(\mathbb{R}^2)$. We also observe that the fundamental covariant $\mathcal{C}_1$ can be expressed as

$$\mathcal{C}_1 = \mathcal{I}_3 \operatorname{tr} \hat{\mathbf{K}} - \mathcal{I}_2,$$

where the (1, 1)-tensor $\hat{\mathbf{K}}$ is given by $\hat{\mathbf{K}} = \mathbf{K}\mathbf{g}^{-1}$. This observation immediately suggests that $\operatorname{tr} \hat{\mathbf{K}}$ is a fundamental $I(\mathbb{R}^2)$ covariant of $\mathcal{K}^2(\mathbb{R}^2)$. We note, however, that the function $\det \hat{\mathbf{K}}$ is not a fundamental $I(\mathbb{R}^2)$ covariant of $\mathcal{K}^2(\mathbb{R}^2)$.

Consider a similar example.

Example 3.2: Let $\mathcal{K}^2(\mathbb{R}^2_1) \times \mathbb{R}^2_1$ be the extended vector space of $\mathcal{K}^2(\mathbb{R}^2_1)$. The action of the isometry group $I(\mathbb{R}^2_1)$ in the Minkowski plane $\mathbb{R}^2_1$ is given by (18), while the corresponding action in the parameter space Σ of $\mathcal{K}^2(\mathbb{R}^2_1)$ is given by (22). The transformation laws (22) combined with the transformations (18) yield an analogue of (47). Next, we proceed as in Example 3.1. The resulting moving frame map $\rho: \Sigma \times \mathbb{R}^2_1 \to I(\mathbb{R}^2_1)$ is given by

$$a = \frac{\alpha_4 \sinh \phi + \alpha_5 \cosh \phi}{\alpha_6},$$

$$b = \frac{\alpha_4 \cosh \phi + \alpha_5 \sinh \phi}{a_6}, \tag{52}$$

$$\phi = \frac{1}{2} \operatorname{arctanh} \frac{2(\alpha_3\alpha_6 - \alpha_4\alpha_5)}{\alpha_4^2 + \alpha_5^2 - \alpha_6(\alpha_1 + \alpha_2)}.$$

Now we can continue as in the previous example to determine a set of fundamental $I(\mathbb{R}^2_1)$ covariants of the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$.

Theorem 3.5: *Consider the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$. Any algebraic $I(\mathbb{R}^2_1)$ covariant C defined over the subspace of $\Sigma \times \mathbb{R}^2_1$ where the isometry group $I(\mathbb{R}^2_1)$ acts freely and regularly with three-dimensional orbits can be locally uniquely expressed as an analytic function*

$$C = F(\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3, \mathcal{C}_1, \mathcal{C}_2),$$

where the fundamental $I(\mathbb{R}^2_1)$ covariants $\mathcal{I}_i, \mathcal{C}_j$, $i = 1, 2, 3$, $j = 1, 2$ are given by

$$\mathcal{I}_1 = [\alpha_4^2 + \alpha_5^2 - \alpha_6(\alpha_1 + \alpha_2)]^2 - 4(\alpha_3\alpha_6 - \alpha_4\alpha_5)^2,$$

$$\mathcal{I}_2 = (\alpha_1 - \alpha_2)\alpha_6 - \alpha_4^2 + \alpha_5^2,$$

$$\mathcal{I}_3 = \alpha_6, \tag{53}$$

$$\mathcal{C}_1 = (\alpha_6 t + \alpha_5)^2 - (\alpha_6 x + \alpha_4)^2,$$

$$\mathcal{C}_2 = [(\alpha_6 t + \alpha_5)^2 + (\alpha_6 x + \alpha_4)^2](\alpha_4^2 + \alpha_5^2 - \alpha_6(\alpha_1 + \alpha_2)) + 4(\alpha_6 t + \alpha_5)(\alpha_6 x + \alpha_4)(\alpha_3\alpha_6 - \alpha_4\alpha_5),$$

where Σ is the parameter space of $\mathcal{K}^2(\mathbb{R}^2_1)$.

The conclusion is similar to that following Theorem 3.4. Thus, we observe again that the functions $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$ constitute in fact a set of fundamental $I(\mathbb{R}^2_1)$ invariants of the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$, while the functions $\mathcal{C}_1$ and $\mathcal{C}_2$ are "truly" fundamental $I(\mathbb{R}^2_1)$ covariants of the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$.

IV. EQUIVALENCE CLASSES OF VECTOR SPACES $\mathcal{K}^2(\mathbb{R}^2)$ AND $\mathcal{K}^2(\mathbb{R}^2_1)$

In this section we use the results obtained in the preceding section to solve the problems of equivalence for the vector subspaces of *nontrivial* Killing tensors of $\mathcal{K}^2(\mathbb{R}^2)$ and $\mathcal{K}^2(\mathbb{R}^2_1)$. As is well-known[22] the elements of these subspaces generate *orthogonal coordinate webs* in $\mathbb{R}^2$ and $\mathbb{R}^2_1$,

TABLE I. Invariant classification of the orthogonal coordinate webs in $\mathbb{R}^2$ by means of $I(\mathbb{R}^2)$ invariants.

Equivalence class	$\mathcal{I}_1$	$\mathcal{I}_3$	Orthogonal web
EC1	0	0	Cartesian
EC2	0	$\neq 0$	Polar
EC3	$\neq 0$	0	Parabolic
EC4	$\neq 0$	$\neq 0$	Elliptic–hyperbolic

respectively, provided the Killing tensors in question have distinct (and real) eigenvalues. The problem of equivalence in this case is the problem of classification of orthogonal coordinate webs. On the other hand, from the invariant theory point of view the problem of equivalence and the related canonical form problem are intimately related to the problem of the determination of fundamental invariants (covariants, joint invariants).

A. The vector space $\mathcal{K}^2(\mathbb{R}^2)$

Let $\mathcal{K}^2_{nt}(\mathbb{R}^2) \subset \mathcal{K}^2(\mathbb{R}^2)$ be the vector subspace of nontrivial Killing two tensors defined in the Euclidean plane $\mathbb{R}^2$. "Nontrivial" in this context means that none of the elements of $\mathcal{K}^2_{nt}(\mathbb{R}^2)$ is a multiple of the metric of $\mathbb{R}^2$. Clearly $\dim \mathcal{K}^2_{nt}(\mathbb{R}^2) = 5$. It has been established in Refs. 13,14,16 that the functions $\mathcal{I}_1$ and $\mathcal{I}_3$ given by (51) are the fundamental $I(\mathbb{R}^2)$ invariants of $\mathcal{K}^2_{nt}(\mathbb{R}^2)$. Moreover, they can be used to solve the problem of classification of orthogonal coordinate webs in the Euclidean plane. The fundamental $I(\mathbb{R}^2)$ invariants divide the vector subspace $\mathcal{K}^2_{nt}(\mathbb{R}^2)$ into four equivalence classes. The elements within each equivalence class generate a particular orthogonal web (see Ref. 13 for more details). These results are summarized in Table I. Clearly, any (analytic) $I(\mathbb{R}^2)$ covariant of the vector subspace $\mathcal{K}^2_{nt}(\mathbb{R}^2)$ takes the following general form:

$$C = F(\mathcal{I}_1, \mathcal{I}_3, \mathcal{C}_1, \mathcal{C}_2),$$

where the functions $\mathcal{I}_1, \mathcal{I}_3, \mathcal{C}_1$, and $\mathcal{C}_2$ are given by (51).

The same classification can be done by means of the fundamental $I(\mathbb{R}^2)$ covariants $\mathcal{C}_1$ and $\mathcal{C}_2$ given by (51). The results are summarized in Table II.

Recall that in most of the problems studied so far within ITKT the associated *canonical form problem* has been solved for vector spaces of Killing tensors of valence two via transforming the corresponding Killing tensors in orthogonal coordinates back to the original (pseudo-)Cartesian coordinates by using the standard transformations from the orthogonal coordinates to (pseudo-) Cartesian coordinates (see, for example, Refs. 7,12,13,16). In the problems involving Killing tensors of valence two (with distinct eigenvalues and integrable eigenvectors) the equivalence classes (ECs) of the corresponding vector spaces are associated with the corresponding orthogonal coordinate webs and so such an approach seems to be natural.

However, one may wish to solve the canonical form problem for vector spaces of Killing tensors of valences higher than two, in which case a connection with the theory of orthogonal

TABLE II. Invariant classification of the orthogonal coordinate webs in $\mathbb{R}^2$ by means of $I(\mathbb{R}^2)$ covariants.

Equivalence class	$\mathcal{C}_1$	$\mathcal{C}_2$	Orthogonal web
EC1	0	0	Cartesian
EC2	Positive–definite	0	Polar
EC3	1	1	Parabolic
EC4	Positive–definite	Indefinite	Elliptic–hyperbolic

coordinate webs is not evident. In such a case, another, more general approach can be adapted from CIT[39] to the study of Killing tensors. Indeed, recall first the following definitions and results.[39]

Definition 4.1: Two submanifolds $N,P\subset X$ are said to intersect transversally *at a common point $x_0\in N\cap P$ if they have no nonzero tangent vectors in common: $TN|_{x_0}\cap TP|_{x_0}=\{0\}$.*

Definition 4.2: Let G be a Lie transformation group that acts regularly on an m-dimensional manifold X with s-dimensional orbits. A (local) cross section *is an $(m-s)$-dimensional submanifold $K\subset X$ such that K intersects each orbit transversally and at most once.*

Proposition 4.1: If a Lie group G acts regularly on a manifold X, then one can construct a local cross section K passing through any point $x\in X$.

One can define a *coordinate cross section K*, in which case the first *s* coordinates themselves define a coordinate cross section[39]

$$K=\{x_1=c_1,\ldots,x_s=c_s\} \tag{54}$$

iff

$$\frac{\partial(\Delta_1,\ldots,\Delta_{m-s})}{\partial(x_{s+1},\ldots,x_m)}\neq 0, \tag{55}$$

where $\Delta_1,\ldots,\Delta_{m-s}$ are the fundamental invariants of the group action. Then, in view of the above, we can obtain canonical forms of the equivalence classes set by the fundamental invariants as intersections of the coordinate cross sections and the level sets (invariant submanifolds) defined by the fundamental group invariants. To illustrate this simple procedure consider the following example.

Example 4.1: Consider $\mathcal{K}^2_{nt}(\mathbb{R}^2)\subset\mathcal{K}^2(\mathbb{R}^2)$. Without loss of generality we can assume that the elements of the vector subspace $\mathcal{K}^2_{nt}(\mathbb{R}^2)$ enjoy the following general form:

$$\mathbf{K}^2_{nt}=(\beta_1'+2\beta_4y+\beta_6y^2)\frac{\partial}{\partial x}\odot\frac{\partial}{\partial x}+(\beta_3-\beta_4x-\beta_5y-\beta_6xy)\frac{\partial}{\partial x}\odot\frac{\partial}{\partial y}+(2\beta_5x+\beta_6x^2)\frac{\partial}{\partial y}\odot\frac{\partial}{\partial y}, \tag{56}$$

where $\beta_1'=\beta_1-\beta_2$ and the parameters β_i, $i=1,\ldots,6$ are as in (36). The four equivalence classes EC1–4 of $\mathcal{K}^2_{nt}(\mathbb{R}^2)$ have been classified in Table I and Table II. The Killing tensors within each equivalence class share the same geometrical properties, that is they define the same orthogonal coordinate webs equivalent up to the action of the isometry group $I(\mathbb{R}^2)$. This fact can be used to select appropriate canonical forms for each of the four equivalence classes. Thus, one can consider the Killing tensors in terms of the orthogonal coordinates (u,v) (see Ref. 16) and then use the standard coordinate transformations from the orthogonal (u,v) coordinates to the Cartesian coordinates (x,y) in order to determine the corresponding canonical forms for EC1–4. Alternatively, one can proceed by using the coordinate cross sections. The procedure is outlined below.

EC1: In this case the parameter space Σ' defined by the five parameters of (56) can be intersected by the coordinate cross section,

$$K_1=\{\beta_3=\beta_4=\beta_5=0\}. \tag{57}$$

Taking into account (56) and the corresponding formulas for $\mathcal{I}_1$ and $\mathcal{I}_3$ given by (51), we conclude that all but one (β_1') parameters vanish in this case. The parameter β_1' is arbitrary, without loss of generality we can set $\beta_1'=1$, which leads to the canonical form

$$\mathbf{K}_{\mathrm{I}}=\frac{\partial}{\partial x}\odot\frac{\partial}{\partial x}. \tag{58}$$

Alternatively, we could have used the coordinate cross section,

$$K_2 = \{\beta_1' = \beta_4 = \beta_5 = 0\}, \tag{59}$$

which would have led to the canonical form

$$\mathbf{K}_{\mathrm{I}}' = \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y}. \tag{60}$$

Note the canonical forms (58) and (60) are equivalent up to a rotation.

EC2: Reason as in EC1 above. Either of the coordinate cross sections (57) or (59) leads to the canonical form

$$\mathbf{K}_{\mathrm{II}} = y^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x} - xy \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y} + x^2 \frac{\partial}{\partial y} \odot \frac{\partial}{\partial y}. \tag{61}$$

EC3: First, note that the condition $\mathcal{I}_1 \neq 0, \mathcal{I}_3 = 0$ (see Table I) prompts $\beta_4^2 + \beta_5^2 \neq 0$. Therefore the coordinate cross sections that can be used in this case are

$$K_3 = \{\beta_1' = \beta_3 = \beta_4 = 0\} \tag{62}$$

and

$$K_4 = \{\beta_1' = \beta_3 = \beta_5 = 0\}, \tag{63}$$

which lead to the canonical forms

$$\mathbf{K}_{\mathrm{III}} = -y \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y} + 2x \frac{\partial}{\partial y} \odot \frac{\partial}{\partial y} \tag{64}$$

and

$$\mathbf{K}_{\mathrm{III}}' = 2y \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x} - x \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y}, \tag{65}$$

respectively. Note the canonical forms (64) and (65) are equivalent up to a rotation.

EC4: In this case we can use either of the coordinate cross sections (57) or (59). Intersecting the common level set defined by $\mathcal{I}_1 \neq 0, \mathcal{I}_3 \neq 0$ (see Table I) with (57) yields the canonical form

$$\mathbf{K}_{\mathrm{IV}} = (\beta_1' + y^2) \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x} - xy \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y} + x^2 \frac{\partial}{\partial y} \odot \frac{\partial}{\partial y}, \tag{66}$$

while with (59)—the canonical form

$$\mathbf{K}_{\mathrm{IV}}' = y^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x} + (\beta_3 - xy) \frac{\partial}{\partial x} \odot \frac{\partial}{\partial y} + x^2 \frac{\partial}{\partial y} \odot \frac{\partial}{\partial y}. \tag{67}$$

Note the canonical forms (66) and (67) are equivalent up to a rotation and rescaling.

B. The vector space $\mathcal{K}^2(\mathbb{R}_1^2)$

The problem of classification of the 10 orthogonal coordinate webs defined in the Minkowski plane $\mathbb{R}_1^2$ was initially solved by Kalnins[23] in 1975. The approach used in Ref. 23 is based on the property that the Killing tensors defined in pseudo-Riemannian spaces of constant curvature are the sums of symmetrized tensor products of Killing vectors. In Ref. 23 different combinations (as symmetric tensor products) of the basic Killing vectors (19) were analyzed modulo the action of the eight-dimensional discrete group $\mathcal{R}$ of permutations of coordinates and reflections of the signature of the Minkowski metric $\mathbf{g} = \mathrm{diag}(1, -1)$ given in terms of the pseudo-Cartesian coordinates (t, x) (see below). A different approach was used in Rastelli,[42] where the 10 orthogonal webs were classified based on the algebraic properties of the nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}_1^2)$. More

specifically, the author made use of the points where the eigenvalues of such Killing tensors coincide (singular points). Finally, McLenaghan *et al.*[12,15] employed a set of the fundamental $I(\mathbb{R}_1^2)$ invariants of the vector subspace of nontrivial Killing tensors of $\mathcal{K}^2(\mathbb{R}_1^2)$ to classify the 10 orthogonal webs defined in $\mathbb{R}_1^2$. The problem appeared to be incommensurably more challenging than the problem of classification of the orthogonal coordinate webs in $\mathbb{R}^2$.[13,16] The reason is simple: In both cases one has two fundamental invariants at one's disposal, while the number of orthogonal coordinate webs is four (Euclidean plane) and 10 (Minkowski plane). In the latter case the problem was solved[12,15] by introducing the concept of a *conformal* $I(\mathbb{R}_1^2)$ *invariant*, which was used to generate additional *discrete* $I(\mathbb{R}_1^2)$ invariants. To solve the problem, the authors had to investigate the effect of the eight-dimensional discrete group $\mathcal{R}$ on the discrete $I(\mathbb{R}_1^2)$ invariants. Unordered pairs (as the objects preserved by the discrete group) of discrete invariants along with one of the fundamental invariants were used to solve the problem. In what follows, we propose a simpler solution based on the fundamental $I(\mathbb{R}_1^2)$ covariants obtained in the preceding section.

Let $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)\subset\mathcal{K}^2(\mathbb{R}_1^2)$ be the vector subspace of nontrivial Killing two tensors defined in the Minkowski plane $\mathbb{R}_1^2$. Here "nontrivial" has the same meaning as above. Again $\dim\mathcal{K}_{nt}^2(\mathbb{R}_1^2)=5$. Without loss of generality we can assume that in terms of the pseudo-Cartesian coordinates (t,x) the general form of the elements of $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)$ is given by

$$\mathbf{K}=(\alpha_1'+2\alpha_4x+\alpha_6x^2)\frac{\partial}{\partial t}\odot\frac{\partial}{\partial t}+(\alpha_3+\alpha_4t+\alpha_5x+\alpha_6tx)\frac{\partial}{\partial t}\odot\frac{\partial}{\partial x}+(2\alpha_5t+\alpha_6t^2)\frac{\partial}{\partial x}\odot\frac{\partial}{\partial x},\tag{68}$$

where $\alpha_1'=\alpha_1+\alpha_2$ and the parameters α_i, $i=1,\ldots,6$ are as in (17). Note that in this case the parameter space Σ' is determined by the five parameters $\alpha_1',\alpha_3,\alpha_4,\alpha_5$, and α_6. Our next observation is that by Theorem 3.5 any $I(\mathbb{R}_1^2)$ covariant of $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)$ enjoys the form

$$C=F(\mathcal{I}_1,\mathcal{I}_3,\mathcal{C}_1,\mathcal{C}_2),$$

where the functions $\mathcal{I}_1,\mathcal{I}_3,\mathcal{C}_1$, and $\mathcal{C}_2$ are given by (53). As in the case of $\mathcal{K}_{nt}^2(\mathbb{R}^2)$ we can use $\mathcal{I}_1,\mathcal{I}_3,\mathcal{C}_1$, and $\mathcal{C}_2$ to classify the 10 orthogonal webs. However, in view of the number of cases we must use these functions concurrently. Before doing so, we check the effect of $\mathcal{R}$ on $\mathcal{I}_1,\mathcal{I}_3,\mathcal{C}_1$, and $\mathcal{C}_2$. Recall[23,12] that the group (under composition) $\mathcal{R}=\langle R_1,R_2\rangle$ consists of eight discrete transformations generated by

$$R_1:\quad \tilde{t}=t,\quad \tilde{x}=-x\quad\text{(spatial reflections)},$$

$$R_2:\quad \tilde{t}=x,\quad \tilde{x}=t\quad\text{(permutation)}.\tag{69}$$

Note the group $\mathcal{R}$ [along with the isometry group $I(\mathbb{R}_1^2)$] preserves the geometry of the 10 orthogonal webs defined in the Minkowski plane. Recall next[12] that R_1 and R_2 induce the following transformations on the parameters α_i, $i=1,\ldots,6$ of $\mathcal{K}^2(\mathbb{R}_1^2)$ [see (36)]:

$$R_1:\quad \tilde{\alpha}_1=\alpha_1,\quad \tilde{\alpha}_2=\alpha_2,\quad \tilde{\alpha}_3=-\alpha_3,\quad \tilde{\alpha}_4=-\alpha_4,\quad \tilde{\alpha}_5=\alpha_5,\quad \tilde{\alpha}_6=\alpha_6,$$

$$R_2:\quad \tilde{\alpha}_1=\alpha_2,\quad \tilde{\alpha}_2=\alpha_1,\quad \tilde{\alpha}_3=\alpha_3,\quad \tilde{\alpha}_4=\alpha_5,\quad \tilde{\alpha}_5=\alpha_4,\quad \tilde{\alpha}_6=\alpha_6.\tag{70}$$

It follows immediately that the fundamental $I(\mathbb{R}_1^2)$ covariants $\mathcal{I}_1,\mathcal{I}_3,\mathcal{C}_1$, and $\mathcal{C}_2$ remain unchanged under the transformations (70) induced by the group $\mathcal{R}$. We conclude therefore that we can use them in the classification of the 10 orthogonal webs. Recall that the vector subspace $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)$ can be divided into 10 equivalence classes EC1–10 within each of which the corresponding elements generate the *same orthogonal coordinate web* (for more details see Refs. 23 and 12). We consider next the 10 *canonical elements* determined in Ref. 12 representing each class EC1–10 by transforming them to contravariant form and making them compatible with the general form (68) by adding multiples of the metric when necessary. The latter operation does not affect the geometry

of the coordinate webs generated by the canonical elements. We arrive at the following list:

$$\text{EC1} \quad \mathbf{K}_1 = \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t}, \tag{71}$$

$$\text{EC2} \quad \mathbf{K}_2 = x^2 \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + tx \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{72}$$

$$\text{EC3} \quad \mathbf{K}_3 = \left(\frac{1}{2} - x\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \left(\frac{1}{4} - \frac{1}{2}t + \frac{1}{2}x\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + t \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{73}$$

$$\text{EC4} \quad \mathbf{K}_4 = x \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + 2t \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{74}$$

$$\text{EC5} \quad \mathbf{K}_5 = \left(2k^2 - \frac{1}{4}x^2\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} - \frac{1}{4}tx \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} - \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{75}$$

$$\text{EC6} \quad \mathbf{K}_6 = \left(\frac{1}{4} + \frac{1}{4}x^2\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \left(\frac{1}{4} + \frac{1}{4}tx\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{76}$$

$$\text{EC7} \quad \mathbf{K}_7 = \left(-\frac{1}{2} + \frac{1}{4}x^2\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \left(-\frac{1}{4} + \frac{1}{4}tx\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{77}$$

$$\text{EC8} \quad \mathbf{K}_8 = \frac{1}{4}x^2 \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \left(-k^2 + \frac{1}{4}tx\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{78}$$

$$\text{EC9} \quad \mathbf{K}_9 = \left(2k^2 + \frac{1}{4}x^2\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \frac{1}{4}tx \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{79}$$

$$\text{EC10} \quad \mathbf{K}_{10} = \left(-2k^2 + \frac{1}{4}x^2\right) \frac{\partial}{\partial t} \odot \frac{\partial}{\partial t} + \frac{1}{4}tx \frac{\partial}{\partial t} \odot \frac{\partial}{\partial x} + \frac{1}{4}t^2 \frac{\partial}{\partial x} \odot \frac{\partial}{\partial x}, \tag{80}$$

where the parameter k is a $I(\mathbb{R}_1^2)$ invariant of $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)$. In view of Theorem 2.2 (see also Theorem 3.5), it can be represented via the fundamental $I(\mathbb{R}_1^2)$ invariants. Indeed, the corresponding formulas were found in Ref. 12,

$$\text{EC5, EC9, EC10:} \quad k^2 = \frac{\sqrt{\mathcal{I}_1}}{\mathcal{I}_3} \quad (\mathcal{I}_1 > 0),$$

$$\text{EC8:} \quad k^2 = \frac{\sqrt{-\mathcal{I}_1}}{\mathcal{I}_3} \quad (\mathcal{I}_1 < 0). \tag{81}$$

Note the canonical forms (71)–(80) are compatible with the general form given by (68). Following the procedure devised in Ref. 12, we use the canonical forms (71)–(80) to evaluate the corresponding values of the fundamental $I(\mathbb{R}_1^2)$ covariants $\mathcal{I}_1, \mathcal{I}_3, \mathcal{C}_1, \mathcal{C}_2$ and employ the results to distinguish the elements belonging to different equivalence classes EC1–10. The elements of $\mathcal{K}_{nt}^2(\mathbb{R}_1^2)$ must have the same values of $\mathcal{I}_1, \mathcal{I}_3, \mathcal{C}_1$, and $\mathcal{C}_2$. We note however that these functions do not distinguish EC1 from EC3 and EC6 from EC8. Therefore we have to derive some auxiliary $I(\mathbb{R}_1^2)$

invariants to complete the classification scheme. Indeed, consider the vector space $\mathcal{K}^2(\mathbb{R}^2_1)$ under the action of the isometry group $I(\mathbb{R}^2_1)$. Since $\mathcal{I}_3$ is a fundamental $I(\mathbb{R}^2_1)$ invariant, we can consider the level set

$$\mathcal{S}_{\mathcal{I}_3} = \{(\alpha_1, \ldots, \alpha_5) \in \Sigma | \quad \mathcal{I}_3 = 0\}. \tag{82}$$

Note $\mathcal{S}_{\mathcal{I}_3}$ is an $I(\mathbb{R}^2_1)$-invariant submanifold in Σ defined by the parameters α_i, $i=1,\ldots,5$. Next we prove the following result by using the techniques exhibited in Sec. II.

Lemma 4.1: Any algebraic $I(\mathbb{R}^2_1)$ invariant I of the $I(\mathbb{R}^2_1)$-invariant submanifold $\mathcal{S}_{\mathcal{I}_3}$ defined by (82) can be (locally) uniquely expressed as an analytic function

$$I = F(\mathcal{I}'_1, \mathcal{I}'_2),$$

where the fundamental invariants $\mathcal{I}'_i$, $i=1, 2$ are given by

$$\mathcal{I}'_1 = \alpha_4^2 - \alpha_5^2,$$

$$\mathcal{I}'_2 = 2\alpha_3\alpha_4\alpha_5 - \alpha_2\alpha_4^2 - \alpha_1\alpha_5^2, \tag{83}$$

provided the group acts in $\mathcal{S}_{\mathcal{I}_3}$ with three-dimensional orbits.

We note that the fundamental $I(\mathbb{R}^2_1)$ invariants $\mathcal{I}'_1$ and $\mathcal{I}'_2$ still cannot be used in the problem of classification of the elements of $\mathcal{K}^2_{nt}(\mathbb{R}^2_1)$. In particular, $\mathcal{I}'_2$ appears to be a function of $\alpha_1, \alpha_2, \alpha_3, \alpha_4$, and α_5 (not $\alpha'_1, \alpha_3, \alpha_4, \alpha_5$). However, under the additional *invariant* condition

$$\mathcal{I}'_1 = \alpha_4^2 - \alpha_5^2 = 0 \tag{84}$$

it assumes the following form:

$$\mathcal{I}'_2 = 2\alpha_3\alpha_4\alpha_5 - \alpha'_1\alpha_4^2, \tag{85}$$

where $\alpha'_1 = \alpha_1 + \alpha_2$. We immediately recognize the $I(\mathbb{R}^2_1)$-invariant (85) to be an $I(\mathbb{R}^2_1)$ invariant of the submanifold in $\mathcal{S}_{\mathcal{I}_3}$ determined by the condition (84). Hence, $\mathcal{I}'_2$ given by (85) can be used to distinguish between EC1 and EC3.

Next, in order to distinguish between the elements of EC6 and EC8, introduce the following auxiliary $I(\mathbb{R}^2_1)$ invariant:

$$\mathcal{I}^* := k^4\mathcal{I}_3 + \mathcal{I}_1, \tag{86}$$

where k is given by (81) (the formula for EC8). We note that $\mathcal{I}^*$ given by (86) is an $I(\mathbb{R}^2_1)$ invariant. The values of $\mathcal{I}_1$ and $\mathcal{I}_3$ evaluated with respect to the parameters of the canonical form EC8 given by (78) are

$$\mathcal{I}_1 = -\frac{k^4}{4}, \quad \mathcal{I}_3 = \frac{1}{4}.$$

Therefore the $I(\mathbb{R}^2_1)$ invariant $\mathcal{I}^* = 0$, whenever the Killing tensor in question belongs to EC8. The classification scheme is now complete. We summarize the results in Table III.

Using the results obtained we can devise a general algorithm of classification for the elements of the vector spaces $\mathcal{K}^2(\mathbb{R}^2)$ and $\mathcal{K}^2(\mathbb{R}^2_1)$. It consists of the following two steps. Let $\mathbf{K} \in \mathcal{K}^2(\mathbb{R}^2) \times (\mathcal{K}^2(\mathbb{R}^2_1))$.

(i) If $\mathbf{K}$ has arbitrary constants, decompose $\mathbf{K}$ as follows:

TABLE III. Invariant classification of the orthogonal coordinate webs in $\mathbb{R}_1^2$ by means of $I(\mathbb{R}_1^2)$ invariants and covariants.

Equivalence class	$\mathcal{I}_1$	$\mathcal{I}_3$	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{I}_1'$	$\mathcal{I}_2'$	$\mathcal{I}^*$
EC1	0	0	0	0	0	0	
EC2	0	$\neq 0$	Indefinite	0			
EC3	0	0	0	0	0	$\neq 0$	
EC4	$\neq 0$	0	1	1			
EC5	$\neq 0$	$\neq 0$	Indefinite	Positive–definite			
EC6	$\neq 0$	$\neq 0$	Indefinite	Indefinite			$\neq 0$
EC7	0	$\neq 0$	Indefinite	Positive–definite			
EC8	$\neq 0$	$\neq 0$	Indefinite	Indefinite			0
EC9	$\neq 0$	$\neq 0$	Indefinite	Negative–definite			
EC10	$\neq 0$	$\neq 0$	Indefinite	Positive–definite			

$$\mathbf{K} = \ell_0 \mathbf{g} + \sum_{i=1}^{5} \ell_i \mathbf{K}_i, \tag{87}$$

where ℓ_i, $i=1,\ldots,5$ are the arbitrary constants. Note $\Sigma_{i=1}^5 \ell_i \mathbf{K}_i \in \mathcal{K}_{nt}^2(\mathbb{R}^2)(\mathcal{K}_{nt}^2(\mathbb{R}_1^2))$. Clearly, $\mathbf{K} \in \mathcal{K}_{nt}^2(\mathbb{R}^2)(\mathcal{K}_{nt}^2(\mathbb{R}_1^2))$ iff $\ell_0 = 0$.

(ii) Each Killing tensor in the representation (87) represents one of the equivalence classes (and thus, an orthogonal coordinate web), provided it has real eigenvalues in the case of the vector space being $\mathcal{K}^2(\mathbb{R}_1^2)$. We can determine which one by evaluating the corresponding $I(\mathbb{R}^2)$ and $I(\mathbb{R}_1^2)$ invariants and covariants and then using the information provided in Table I or Table II for the Killing tensors defined in the Euclidean plane and Table III defined in the Minkowski plane.

The problem of classification is therefore solved.

Remark 4.1: We note that EC5 and EC10 are characterized by the same values of the fundamental $I(\mathbb{R}_1^2)$ convariants. It agrees with the geometry of the corresponding orthogonal webs, namely they determine two distinct coordinate systems that cover two disjoint areas of the same space (see Miller[25] for more details).

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On perturbations of Dirac operators with variable magnetic field of constant direction

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We carry out the spectral analysis of matrix valued perturbations of three-dimensional Dirac operators with variable magnetic field of constant direction. Under suitable assumptions on the magnetic field and on the pertubations, we obtain a limiting absorption principle, we prove the absence of singular continuous spectrum in certain intervals and state properties of the point spectrum. Various situations, for example, when the magnetic field is constant, periodic or diverging at infinity, are covered. The importance of an internal-type operator (a two-dimensional Dirac operator) is also revealed in our study. The proofs rely on commutator methods. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND MAIN RESULTS

We consider a relativistic spin-$\frac{1}{2}$ particle evolving in $\mathbb{R}^3$ in presence of a variable magnetic field of constant direction. By virtue of the Maxwell equations, we may assume with no loss of generality that the magnetic field has the form $\vec{B}(x_1,x_2,x_3)=(0,0,B(x_1,x_2))$. So the unperturbed system is described, in the Hilbert space $\mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$, by the Dirac operator

$$H_0 := \alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3 P_3 + \beta m,$$

where $\beta\equiv\alpha_0,\alpha_1,\alpha_2,\alpha_3$ are the usual Dirac–Pauli matrices, m is the strictly positive mass of the particle and $\Pi_j := -i\partial_j - a_j$ are the generators of the magnetic translations with a vector potential $\vec{a}(x_1,x_2,x_3)=(a_1(x_1,x_2),a_2(x_1,x_2),0)$ that satisfies $B=\partial_1 a_2-\partial_2 a_1$. Since $a_3=0$, we have written $P_3 := -i\partial_3$ instead of Π_3.

In this paper we study the stability of certain parts of the spectrum of H_0 under matrix valued perturbations V. More precisely, if V satisfies some natural hypotheses, we shall prove the absence of singular continuous spectrum and the finiteness of the point spectrum of $H := H_0+V$ in intervals of $\mathbb{R}$ corresponding to gaps in the symmetrized spectrum of the operator $H^0 := \sigma_1\Pi_1+\sigma_2\Pi_2+\sigma_3 m$ in $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2)$. The matrices σ_j are the Pauli matrices and the symmetrized spectrum σ^0_{sym} of H^0 is the union of the spectra of H^0 and $-H^0$. We stress that our analysis does not require any restriction on the behavior of the magnetic field at infinity. Nevertheless, the pertinence of our work depends on a certain property of the internal-type operator H^0; namely, the size and the number of gaps in σ^0_{sym}. We refer to Refs. 2, 7, 10, 12, and 16 for various results on the spectrum of H^0, especially in the situations of physical interest, for example, when B is constant, periodic or diverges at infinity.

Technically, this work relies on commutator methods initiated by Mourre[14] and extensively developed in Ref. 1. For brevity we shall constantly refer to the latter reference for notations and definitions. Our choice of a conjugate operator enables us to treat Dirac operators with general

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magnetic fields provided they point in a constant direction. On the other hand, as already put into evidence in Ref. 9, the use of a conjugate operator with a matrix structure has a few "rather awkward consequences" for long-range perturbations. We finally mention that this study is the counterpart for Dirac operators of Ref. 13, where only Schrödinger operators are considered. Unfortunately, the intrinsic structure of the Dirac equation prevents us from using the possible magnetic anisotropy to control the perturbations (see Remark 3.2 for details).

We give now a more precise description of our results. For simplicity we impose the continuity of the magnetic field and avoid perturbations with local singularities. Hence we assume that B is a $C(\mathbb{R}^2;\mathbb{R})$-function and choose any vector potential $\vec{a}=(a_1,a_2,0)\in C(\mathbb{R}^2;\mathbb{R}^3)$, e.g. the one obtained by means of the transversal gauge.[16] The definitions below concern the admissible perturbations. In the long-range case, we restrict them to the scalar type in order not to impose unsatisfactory constraints. In the sequel, $\mathcal{B}_{\mathrm{h}}(\mathbb{C}^4)$ stands for the set of 4×4 Hermitian matrices, and $\|\cdot\|$ denotes the norm of the Hilbert space $\mathcal{H}:=\mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$ as well as the norm of $\mathcal{B}(\mathcal{H})$, the set of bounded linear operators on $\mathcal{H}$. $\mathbb{N}:=\{0,1,2,\ldots\}$ is the set of natural numbers. ϑ is an arbitrary $C^\infty([0,\infty))$-function such that $\vartheta=0$ near 0 and $\vartheta=1$ near infinity. Q_j is the multiplication operator by the coordinate x_j in $\mathcal{H}$, and the expression $\langle\cdot\rangle$ corresponds to $\sqrt{1+(\cdot)^2}$.

Definition 1.1: Let V be a multiplication operator associated with an element of $\mathsf{L}^\infty(\mathbb{R}^3;\mathcal{B}_{\mathrm{h}}(\mathbb{C}^4))$.

(a) *V is small at infinity if* $\lim_{r\to\infty}\|\vartheta(\langle Q\rangle/r)V\|=0$,
(b) *V is short-range if* $\int_1^\infty\|\vartheta(\langle Q_3\rangle/r)V\|\mathrm{d}r<\infty$,
(c) *Let V_L be in $C^1(\mathbb{R}^3;\mathbb{R})$ with $x\mapsto\langle x_3\rangle(\partial_j V_{\mathrm{L}})(x)$ in $\mathsf{L}^\infty(\mathbb{R}^3;\mathbb{R})$ for $j=1,2,3$, then $V:=V_{\mathsf{L}}$ is* long-range if

$$\int_1^\infty\left\|\vartheta\left(\frac{\langle Q_3\rangle}{r}\right)\langle Q_3\rangle(\partial_j V)\right\|\frac{\mathrm{d}r}{r}<\infty \text{ for } j=1,2,3.$$

Note that Definitions 1.1.(b) and 1.1.(c) differ from the standard ones: The decay rate is imposed only in the x_3 direction.

We are in a position to state our results. Let $\mathcal{D}(\langle Q_3\rangle)$ denote the domain of $\langle Q_3\rangle$ in $\mathcal{H}$, then the limiting absorption principle for H is expressed in terms of the Banach space $\mathcal{G}:=(\mathcal{D}(\langle Q_3\rangle),\mathcal{H})_{1/2,1}$ defined by real interpolation.[1] For convenience, we recall that $\mathcal{D}(\langle Q_3\rangle^s)$ is contained in $\mathcal{G}$ for each $s>1/2$.

Theorem 1.2: *Assume that B belongs to $C(\mathbb{R}^2;\mathbb{R})$, and that V belongs to $\mathsf{L}^\infty(\mathbb{R}^3;\mathcal{B}_{\mathrm{h}}(\mathbb{C}^4))$, is small at infinity and can be written as the sum of a short-range and a long-range matrix valued function. Then*

(a) *The point spectrum of the operator H in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ is composed of eigenvalues of finite multiplicity and with no accumulation point in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$.*
(b) *The operator H has no singular continuous spectrum in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$.*
(c) *The limits $\lim_{\varepsilon\to+0}\langle\psi,(H-\lambda\mp i\varepsilon)^{-1}\psi\rangle$ exist for each $\psi\in\mathcal{G}$, uniformly in λ on each compact subset of $\mathbb{R}\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(H)\}$.*

The limiting absorption principle (c), together with the inclusions mentioned before the theorem, lead to locally H-smooth operators. They imply the existence of local wave operators.

Corollary 1.3: Let V belong to $\mathsf{L}^\infty(\mathbb{R}^3;\mathcal{B}_{\mathrm{h}}(\mathbb{C}^4))$ and be small at infinity. Assume there exists some $s>1$ such that $\langle Q_3\rangle^s V\in\mathcal{B}(\mathcal{H})$. Then for each open set $J\subset\mathbb{R}\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(H)\}$, the local wave operators $\text{s-}\lim_{t\to\pm\infty}e^{itH_0}e^{-itH}E^H(J)$ *exist and their ranges are equal to $E^{H_0}(J)$, where E^H and E^{H_0} are the spectral measures of H and H_0, respectively.*

Remark 1.4: H_0-bounded perturbations (with relative bound less than one) may also be treated with some slight adaptations of Definition 1.1. In particular Coulomb-type potentials and Zeeman effect [11] could be considered for certain magnetic fields and vector potentials. However, to our knowledge, there is not any explicit class of H_0-bounded perturbations for arbitrary continuous magnetic fields. For this reason, we concentrate on bounded potentials V only, and thus

present a simplified version of a more general, and more complicated, perturbation theory.

The above statements seem to be new for such a general magnetic field. In the special but important case of a nonzero constant magnetic field B_0, the admissible perturbations introduced in Definition 1.1 are more general than those allowed in Ref. 17. We stress that in this situation σ^0_{sym} is equal to $\{\pm\sqrt{2nB_0+m^2}: n\in\mathbb{N}\}$, which implies that there are plenty of gaps where our analysis gives results. On the other hand, if $B(x_1,x_2)\to 0$ as $|(x_1,x_2)|\to\infty$, our treatment gives no information since both $(-\infty,-m]$ and $[m,\infty)$ belong to σ^0_{sym}. We finally mention Ref. 3 for related work on perturbations of magnetic Dirac operators.

II. MOURRE ESTIMATE FOR THE OPERATOR H_0

A. Preliminaries

Let us start by recalling some known results. The operator H_0 is essentially self-adjoint on $\mathcal{D}:=C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ [Ref. 5, Thm. 2.1]. Its spectrum is symmetric with respect to 0 and does not contain the interval $(-m,m)$ [Ref. 16, Cor. 5.14]. Thus the subset $H_0\mathcal{D}$ is dense in $\mathcal{H}$ since $\mathcal{D}$ is dense in $\mathcal{D}(H_0)$ (endowed with the graph topology) and H_0 is a homeomorphism from $\mathcal{D}(H_0)$ onto $\mathcal{H}$.

We now introduce a suitable representation of the Hilbert space $\mathcal{H}$. We consider the partial Fourier transformation

$$\mathcal{F}:\mathcal{D}\to\int_{\mathbb{R}}^{\oplus}\mathcal{H}_{12}\mathrm{d}\xi,\quad (\mathcal{F}\psi)(\xi):=\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}e^{-i\xi x_3}\psi(\cdot,x_3)\mathrm{d}x_3, \tag{2.1}$$

where $\mathcal{H}_{12}:=\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^4)$. This map extends uniquely to a unitary operator from $\mathcal{H}$ onto $\int_{\mathbb{R}}^{\oplus}\mathcal{H}_{12}\mathrm{d}\xi$, which we denote by the same symbol $\mathcal{F}$. As a first application, one obtains the following direct integral decomposition of H_0:

$$\mathcal{F}H_0\mathcal{F}^{-1}=\int_{\mathbb{R}}^{\oplus}H_0(\xi)\mathrm{d}\xi,$$

where $H_0(\xi)$ is a self-adjoint operator in $\mathcal{H}_{12}$ acting as $\alpha_1\Pi_1+\alpha_2\Pi_2+\alpha_3\xi+\beta m$ on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$. In the following remark we draw the connection between the operator $H_0(\xi)$ and the operator H^0 introduced in Sec. I. It reveals the importance of the internal-type operator H^0 and shows why its negative $-H_0$ also has to be taken into account.

Remark 2.1: The operator $H_0(0)$ acting on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$ is unitarily equivalent to the direct sum operator $\left(\begin{smallmatrix} m & \Pi_- \\ \Pi_+ & -m\end{smallmatrix}\right)\oplus\left(\begin{smallmatrix} m & \Pi_+ \\ \Pi_- & -m\end{smallmatrix}\right)$ acting on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^2)\oplus C_0^\infty(\mathbb{R}^2;\mathbb{C}^2)$, where $\Pi_\pm:=\Pi_1\pm i\Pi_2$. Now, these two matrix operators act in $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2)$ and are essentially self-adjoint on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^2)$ [Ref. 5, Thm. 2.1]. However, the first one is nothing but H^0, while the second one is unitarily equivalent to $-H^0$ (this can be obtained by means of the abstract Foldy–Wouthuysen transformation [Ref. 16, Thm. 5.13]). Therefore, $H_0(0)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$ and

$$\sigma[H_0(0)]=\sigma(H^0)\cup\sigma(-H^0)\equiv\sigma^0_{\mathrm{sym}}.$$

Moreover, there exists a relation between $\sigma[H_0(\xi)]$ and σ^0_{sym}. Indeed, for $\xi\in\mathbb{R}$ *fixed, one can show that $H_0(\xi)^2=H_0(0)^2+\xi^2$ on $\mathcal{D}(H_0(\xi)^2)=\mathcal{D}(H_0(0)^2)$, so that*

$$\sigma[H_0(\xi)^2]=\sigma[H_0(0)^2+\xi^2]=(\sigma[H_0(0)])^2+\xi^2=(\sigma^0_{\mathrm{sym}})^2+\xi^2, \tag{2.2}$$

where the spectral theorem has been used for the second equality. Since the spectrum of $H_0(\xi)$ is symmetric with respect to 0 [Ref. 16, Cor. 5.14], it follows that

$$\sigma[H_0(\xi)]=-\sqrt{(\sigma^0_{\mathrm{sym}})^2+\xi^2}\cup\sqrt{(\sigma^0_{\mathrm{sym}})^2+\xi^2}.$$

Define $\mu_0:=\inf|\sigma^0_{\mathrm{sym}}|$ (which is bigger or equal to m because H^0 has no spectrum in $(-m,m)$ [Ref. 16, Cor. 5.14]). Then from the direct integral decomposition of H_0, one readily gets

$$\sigma(H_0) = (-\infty, -\mu_0] \cup [\mu_0, +\infty). \tag{2.3}$$

We conclude the section by giving two technical lemmas in relation with the operator H_0^{-1}. Proofs can be found in an Appendix.

Lemma 2.2:

(a) *For each* $n \in \mathbb{N}$, $H_0^{-n}\mathcal{D}$ *belongs to* $\mathcal{D}(Q_3)$,
(b) $P_3 H_0^{-1}$ *is a bounded self-adjoint operator equal to* $H_0^{-1}P_3$ *on* $\mathcal{D}(P_3)$. *In particular,* $H_0^{-1}\mathcal{H}$ *belongs to* $\mathcal{D}(P_3)$.

One may observe that, given a $C^1(\mathbb{R};\mathbb{C})$-function f with f' bounded, the operator $f(Q_3)$ is well-defined on $\mathcal{D}(Q_3)$. Thus $f(Q_3)H_0^{-n}\mathcal{D}$ is a subset of $\mathcal{H}$ for each $n \in \mathbb{N}$. The preceding lemma and the following simple statement are constantly used in the sequel.

Lemma 2.3: Let f *be in* $C^1(\mathbb{R};\mathbb{C})$ *with* f' *bounded, and* $n \in \mathbb{N}$. *Then*

(a) $iH_0^{-1}f(Q_3) - if\,(Q_3)H_0^{-1}$ *is equal to* $-H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}$ *on* $H_0^{-n}\mathcal{D}$,
(b) $P_3H_0^{-1}f(Q_3) - f(Q_3)P_3H_0^{-1}$ *is equal to* $i(P_3H_0^{-1}\alpha_3 - 1)f'(Q_3)H_0^{-1}$ *on* $\mathcal{D}$.

Both right terms belong to $\mathcal{B}(\mathcal{H})$. For shortness we shall denote them by $[iH_0^{-1}, f(Q_3)]$ and $[P_3H_0^{-1}, f(Q_3)]$, respectively.

B. The conjugate operator

The aim of the present section is to define an appropriate operator conjugate to H_0. To begin with, one observes that $Q_3P_3H_0^{-1}\mathcal{D} \subset \mathcal{H}$ as a consequence of Lemma 2.2. In particular, the formal expression

$$A := \frac{1}{2}(H_0^{-1}P_3Q_3 + Q_3P_3H_0^{-1}) \tag{2.4}$$

leads to a well-defined symmetric operator on $\mathcal{D}$.

Proposition 2.4: The operator A is essentially self-adjoint on $\mathcal{D}$ *and its closure is essentially self-adjoint on any core for* $\langle Q_3\rangle$.

Proof: The claim is a consequence of Nelson's criterion of essential self-adjointness [Ref. 15 Thm. X.37] applied to the triple $\{\langle Q_3\rangle, A, \mathcal{D}\}$. Let us simply verify the two hypotheses of that theorem. By using Lemmas 2.2 and 2.3, one first obtains that for all $\psi \in \mathcal{D}$:

$$\|A\psi\| = \left\| \left(P_3H_0^{-1}Q_3 - \frac{1}{2}[P_3H_0^{-1}, Q_3] \right)\psi \right\| \leqslant c\|\langle Q_3\rangle\psi\|,$$

for some constant $c > 0$ independent of ψ. Then, for all $\psi \in \mathcal{D}$ one has

$$\langle A\psi, \langle Q_3\rangle\psi\rangle - \langle \langle Q_3\rangle\psi, A\psi\rangle = i\,\mathrm{Im}\langle Q_3\psi, [P_3H_0^{-1}, \langle Q_3\rangle]\psi\rangle = i\,\mathrm{Re}\langle(\alpha_3P_3H_0^{-1} - 1)Q_3\psi, Q_3\langle Q_3\rangle^{-1}H_0^{-1}\psi\rangle.$$

A few more commutator calculations, using again Lemma 2.3 with $f(Q_3) = \langle Q_3\rangle^{1/2}$, lead to the following result: For all $\psi \in \mathcal{D}$, there exists a constant $d > 0$ independent of ψ such that

$$|\langle A\psi, \langle Q_3\rangle\psi\rangle - \langle \langle Q_3\rangle\psi, A\psi\rangle| \leqslant d\|\langle Q_3\rangle^{1/2}\psi\|^2.$$

□

As far as we know, the operator (2.4) has never been employed before for the study of magnetic Dirac operators. In Ref. 17, a slightly different conjugate operator has been introduced for Dirac operators with constant magnetic field, namely

$$A = \frac{1}{2} U_{\mathrm{FW}}^{-1} (\langle P_3 \rangle^{-1} P_3 Q_3 + Q_3 P_3 \langle P_3 \rangle^{-1}) \beta U_{\mathrm{FW}},$$

where U_{FW} is the Foldy–Wouthuysen transformation that diagonalizes H_0. Though this operator could also be used in our more general context, it presents the major drawback of making the perturbation theory somewhat more complicated.

C. Strict Mourre estimate for H_0

We now gather some results on the regularity of H_0 with respect to A. We recall that $\mathcal{D}(H_0)^*$ is the adjoint space of $\mathcal{D}(H_0)$ and that one has the continuous dense embeddings $\mathcal{D}(H_0) \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{D}(H_0)^*$, where $\mathcal{H}$ is identified with its adjoint through the Riesz isomorphism.

Proposition 2.5:

(a) *The quadratic form* $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$ *extends uniquely to the bounded form defined by the operator* $-H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1} \in \mathcal{B}(\mathcal{H})$.

(b) *The group* $\{e^{itA}\}_{t\in\mathbb{R}}$ *leaves* $\mathcal{D}(H_0)$ *invariant.*

(c) *The quadratic form*

$$\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1}\psi\rangle, \tag{2.5}$$

extends uniquely to a bounded form on $\mathcal{H}$.

In the framework of Ref. 1, the statements of (a) and (c) mean that H_0 is of class $C^1(A)$ and $C^2(A)$, respectively.

Proof:

(a) For any $\psi \in \mathcal{D}$, one gets

$$\begin{aligned} 2(\langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle) &= \langle [iH_0^{-1}, Q_3]\psi, P_3 H_0^{-1}\psi\rangle + \langle P_3 H_0^{-1}\psi, [iH_0^{-1}, Q_3]\psi\rangle \\ &= -\langle H_0^{-1}\psi, (\alpha_3 P_3 H_0^{-1} + H_0^{-1}\alpha_3 P_3) H_0^{-1}\psi\rangle, \end{aligned} \tag{2.6}$$

where we have used Lemmas 2.2 and 2.3. Furthermore, one has

$$H_0^{-1}\alpha_3 = -\alpha_3 H_0^{-1} + 2H_0^{-1} P_3 H_0^{-1}, \tag{2.7}$$

as an operator identity in $\mathcal{B}(\mathcal{H})$. When inserting (2.7) into (2.6), one obtains the equality

$$\langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle = -\langle \psi, H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1}\psi\rangle. \tag{2.8}$$

Since $\mathcal{D}$ is a core for A, the statement is obtained by density. We shall write $[iH_0^{-1}, A]$ for the bounded extension of the quadratic form $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$.

(b) Since $\mathcal{D}(H_0)$ is not explicitly known, one has to invoke an abstract result in order to show the invariance. Let $[iH_0, A]$ be the operator in $\mathcal{B}(\mathcal{D}(H_0), \mathcal{D}(H_0)^*)$ associated with the unique extension to $\mathcal{D}(H_0)$ of the quadratic form $\psi \mapsto \langle H_0\psi, iA\psi\rangle - \langle A\psi, iH_0\psi\rangle$ defined for all $\psi \in \mathcal{D}(H_0) \cap \mathcal{D}(A)$. Then $\mathcal{D}(H_0)$ is invariant under $\{e^{itA}\}_{t\in\mathbb{R}}$ if H_0 is of class $C^1(A)$ and if $[iH_0, A]\mathcal{D}(H_0) \subset \mathcal{H}$ [Ref. 8, Lemma 2]. From Eq. (2.8) and [Ref. 1, Eq. (6.2.24)], one obtains the following equalities valid in form sense on $\mathcal{H}$:

$$-H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1} = [iH_0^{-1}, A] = -H_0^{-1}[iH_0, A]H_0^{-1}.$$

Thus $[iH_0, A]$ and $(P_3 H_0^{-1})^2$ are equal as operators in $\mathcal{B}(\mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. But since the latter belongs to $\mathcal{B}(\mathcal{H})$, $[iH, A]\mathcal{D}(H_0)$ is included in $\mathcal{H}$.

(c) The boundedness on $\mathcal{D}$ of the quadratic form (2.5) follows by inserting (2.4) into the r.h.s. term of (2.5) and by applying repeatedly Lemma 2.3 with $f(Q_3) = Q_3$. Then one concludes by using the density of $\mathcal{D}$ in $\mathcal{D}(A)$. □

From now on we shall simply denote the closure in $\mathcal{H}$ of $[iH_0,A]$ by $T=(P_3H_0^{-1})^2\in\mathcal{B}(\mathcal{H})$. One interest of this operator is that $\mathcal{F}T\mathcal{F}^{-1}$ is boundedly decomposable [Ref. 6, Prop. 3.6], more precisely:

$$\mathcal{F}T\mathcal{F}^{-1}=\int_{\mathbb{R}}^{\oplus}T(\xi)\mathrm{d}\xi \text{ with } T(\xi)=\xi^2H_0(\xi)^{-2}\in\mathcal{B}(\mathcal{H}_{12}).$$

In the following definition, we introduce two functions giving the optimal value to a Mourre-type inequality. Remark that slight modifications have been done with regard to the usual definition [Ref. 1, Sec. 7.2.1].

Definition 6: Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and assume that S is a symmetric operator in $\mathcal{B}(\mathcal{D}(H),\mathcal{D}(H)^*)$. Let $E^H(\lambda;\varepsilon):=E^H((\lambda-\varepsilon,\lambda+\varepsilon))$ be the spectral projection of H for the interval $(\lambda-\varepsilon,\lambda+\varepsilon)$. Then, for all $\lambda\in\mathbb{R}$ and $\varepsilon>0$, we set

$$\varrho_H^S(\lambda;\varepsilon):=\sup\{a\in\mathbb{R}:E^H(\lambda;\varepsilon)SE^H(\lambda;\varepsilon)\geqslant aE^H(\lambda;\varepsilon)\},$$

$$\varrho_H^S(\lambda):=\sup_{\varepsilon>0}\varrho_H^S(\lambda;\varepsilon).$$

Let us make three observations: The inequality $\varrho_H^S(\lambda;\varepsilon')\leqslant\varrho_H^S(\lambda;\varepsilon)$ holds whenever $\varepsilon'\geqslant\varepsilon$, $\varrho_H^S(\lambda)=+\infty$ if λ does not belong to the spectrum of H, and $\varrho_H^S(\lambda)\geqslant 0$ for all $\lambda\in\mathbb{R}$ if $S\geqslant 0$. We also mention that in the case of two self-adjoint operators H and A in $\mathcal{H}$, with H of class $C^1(A)$ and $S:=[iH,A]$, the function $\varrho_H^S(\cdot)$ is equal to the function $\varrho_H^A(\cdot)$ defined in [Ref. 1, Eq. 7.2.4]. Taking advantage of the direct integral decomposition of H_0 and T, one obtains for all $\lambda\in\mathbb{R}$ and $\varepsilon>0$:

$$\varrho_{H_0}^T(\lambda;\varepsilon)=\operatorname*{ess\,inf}_{\xi\in\mathbb{R}}\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon). \tag{2.9}$$

Now we can deduce a lower bound for $\varrho_{H_0}^T(\cdot)$.

Proposition 2.7: One has

$$\varrho_{H_0}^T(\lambda)\geqslant\inf\left\{\frac{\lambda^2-\mu^2}{\lambda^2}:\mu\in\sigma_{\mathrm{sym}}^0\cap[0,|\lambda|]\right\}, \tag{2.10}$$

with the convention that the infimum over an empty set is $+\infty$.

Proof: We first consider the case $\lambda\geqslant 0$.

(i) Recall from (2.3) that $\mu_0\equiv\inf|\sigma_{\mathrm{sym}}^0|=\inf\{\sigma(H_0)\cap[0,+\infty)\}$. Thus, for $\lambda\in[0,\mu_0)$ the l.h.s. term of (2.10) is equal to $+\infty$, since λ does not belong to the spectrum of H_0. Hence (2.10) is satisfied on $[0,\mu_0)$.

(ii) If $\lambda\in\sigma_{\mathrm{sym}}^0$, then the r.h.s. term of (2.10) is equal to 0. However, since T is positive, $\varrho_{H_0}^T(\lambda)\geqslant 0$. Hence the relation (2.10) is again satisfied.

(iii) Let $0<\varepsilon<\mu_0<\lambda$. Direct computations using the explicit form of $T(\xi)$ and the spectral theorem for the operator $H_0(\xi)$ show that for ξ fixed, one has

$$\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon)=\inf\left\{\frac{\xi^2}{\rho^2}:\rho\in(\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma[H_0(\xi)]\right\}\geqslant\frac{\xi^2}{(\lambda+\varepsilon)^2}. \tag{2.11}$$

On the other hand, one has $\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon)=+\infty$ if $(\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma[H_0(\xi)]=\emptyset$, and *a fortiori*

$$\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon)=+\infty \text{ if } ((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2)\cap\sigma[H_0(\xi)^2]=\emptyset.$$

Thus, by taking into account Eqs. (2.9) and (2.11), the previous observation and relation (2.2), one obtains that

$$\varrho^T_{H_0}(\lambda;\varepsilon) \geqslant \operatorname{ess\,inf}\left\{ \frac{\xi^2}{(\lambda+\varepsilon)^2} : \xi^2 \in ((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2) - (\sigma^0_{\rm sym})^2 \right\}. \tag{2.12}$$

Suppose now that $\lambda \notin \sigma^0_{\rm sym}$, define $\mu := \sup\{\sigma^0_{\rm sym} \cap [0,\lambda]\}$ and choose $\varepsilon > 0$ such that $\mu < \lambda - \varepsilon$. Then the inequality (2.12) implies that

$$\varrho^T_{H_0}(\lambda;\varepsilon) \geqslant \frac{(\lambda-\varepsilon)^2 - \mu^2}{(\lambda+\varepsilon)^2}.$$

Hence the relation (2.10) follows from the above formula when $\varepsilon \to 0$.

For $\lambda < 0$, similar arguments lead to the inequality

$$\varrho^T_{H_0}(\lambda) \geqslant \inf\left\{ \frac{\lambda^2 - \mu^2}{\lambda^2} : \mu \in \sigma^0_{\rm sym} \cap [\lambda,0] \right\}.$$

The claim is then a direct consequence of the symmetry of $\sigma^0_{\rm sym}$ with respect to 0. □

The above proposition implies that we have a strict Mourre estimate, i.e., $\varrho^T_{H_0}(\cdot) > 0$, on $\mathbb{R} \setminus \sigma^0_{\rm sym}$. Moreover it is not difficult to prove that $\varrho^T_{H_0}(\lambda) = 0$ whenever $\lambda \in \sigma^0_{\rm sym}$. It follows that the conjugate operator A does not allow to get spectral informations on H_0 in the subset $\sigma^0_{\rm sym}$.

III. MOURRE ESTIMATE FOR THE PERTURBED HAMILTONIAN

In the sequel, we consider the self-adjoint operator $H := H_0 + V$ with a potential V that belongs to $\mathsf{L}^\infty(\mathbb{R}^3;\mathcal{B}_{\rm h}(\mathbb{C}^4))$. The domain of H is equal to the domain $\mathcal{D}(H_0)$ of H_0. We first give a result on the difference of the resolvents $(H-z)^{-1} - (H_0-z)^{-1}$ and, as a corollary, we obtain the localization of the essential spectrum of H.

Proposition 3.1: Assume that V is small at infinity. Then for all $z \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H_0))$ the difference $(H-z)^{-1} - (H_0-z)^{-1}$ is a compact operator. It follows in particular that $\sigma_{\rm ess}(H) = \sigma_{\rm ess}(H_0)$.

Proof: Since V is bounded and small at infinity, it is enough to check that H_0 is locally compact [Ref. 16, Sec. 4.3.4]. However, the continuity of $\vec{a}$ implies that $\mathcal{D}(H_0) \subset \mathcal{H}^{1/2}_{\rm loc}$ [Ref. 4, Thm. 1.3]. Hence the statement follows by usual arguments. □

Remark 3.2: In the study of an analogous problem for Schrödinger operators,[13] the authors prove a result similar to Proposition 3.1 without assuming that the perturbation is small at infinity (it only has to be small with respect to B in a suitable sense). Their proof mainly relies on the structural inequalities $H_{\rm Sch} := \Pi_1^2 + \Pi_2^2 + P_3^2 \geqslant \pm B$. In the Dirac case, the counterpart of these turn out to be

$$H_0^2 \geqslant 2B \cdot \operatorname{diag}(0,1,0,1) \text{ and } H_0^2 \geqslant -2B \cdot \operatorname{diag}(1,0,1,0),$$

where diag(…) *stands for a diagonal matrix. If we assume that the magnetic field is bounded from below, the first inequality enables us to treat pertubations of the type* $\operatorname{diag}(V_1,V_2,V_3,V_4)$ *with V_2, V_4 small with respect to the magnetic field and V_1, V_3 small at infinity in the original sense. If the magnetic field is bounded from above, the second inequality has to be used and the role of V_2, V_4 and V_1, V_3 are interchanged. However, the unnatural character of these perturbations motivated us not to include their treatment in this paper.*

In order to obtain a limiting absorption principle for H, one has to invoke some abstract results. An optimal regularity condition of H with respect to A has to be satisfied. We refer to Ref. 1, Chap. 5 for the definitions of $\mathcal{C}^{1,1}(A)$ and $\mathcal{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$, and for more explanations on regularity conditions.

Proposition 3.3: Let V be a short-range or a long-range potential. Then H is of class $\mathcal{C}^{1,1}(A)$.

Proof: Since $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H) = \mathcal{D}(H_0)$ invariant, it is equivalent to prove that H belongs to $\mathcal{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$ [Ref. 1, Thm. 6.3.4.(b)]. But in Proposition 2.5.(c), it has already been shown that H_0 is of class $C^2(A)$, so that H_0 is of class $\mathcal{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$. Thus it is enough to

prove that V belongs to $\mathcal{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$. In the short-range case, we shall use Ref. 1, Thm. 7.5.8, which implies that V belongs to $\mathcal{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$. The conditions needed for that theorem are obtained in points (i) and (ii) below. In the long-range case, the claim follows by Ref. 1, Thm. 7.5.7, which can be applied because of points (i), (iii), (iv), and (v) below.

(i) We first check that $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ is a polynomially bounded C_0-group in $\mathcal{D}(H_0)$ and in $\mathcal{D}(H_0)^*$. Lemma 2.3.(a) (with $n=0$ and $f(Q_3)=\langle Q_3\rangle$) implies that H_0 is of class $C^1(\langle Q_3\rangle)$. Furthermore, by an argument similar to that given in part (b) of the proof of Proposition 2.5, one shows that $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H_0)$ invariant. Since $H_0e^{it\langle Q_3\rangle}-e^{it\langle Q_3\rangle}H_0$, defined on $\mathcal{D}$, extends continuously to the operator $t\alpha_3Q_3\langle Q_3\rangle^{-1}e^{it\langle Q_3\rangle}\in\mathcal{B}(\mathcal{H})$, one gets that $\|e^{it\langle Q_3\rangle}\|_{\mathcal{B}(\mathcal{D}(H_0))}\leqslant \mathrm{Const.}\langle t\rangle$ for all $t\in\mathbb{R}$, i.e., the polynomial bound of the C_0-group in $\mathcal{D}(H_0)$. By duality, $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ extends to a polynomially bounded C_0-group in $\mathcal{D}(H_0)^*$ [Ref. 1, Prop. 6.3.1]. The generators of these C_0-groups are densely defined and closed in $\mathcal{D}(H_0)$ and in $\mathcal{D}(H_0)^*$, respectively; both are simply denoted by $\langle Q_3\rangle$.

(ii) Since $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H_0)$ invariant, one may also consider the C_0-group in $\mathcal{D}(H_0)$ obtained by restriction and the C_0-group in $\mathcal{D}(H_0)^*$ obtained by extension. The generator of each of these C_0-groups will be denoted by A. Let $\mathcal{D}(A;\mathcal{D}(H_0)):=\{\varphi\in\mathcal{D}(H_0)\cap\mathcal{D}(A):A\varphi\in\mathcal{D}(H_0)\}$ be the domain of A in $\mathcal{D}(H_0)$, and let $\mathcal{D}(A^2;\mathcal{D}(H_0)):=\{\varphi\in\mathcal{D}(H_0)\cap\mathcal{D}(A^2):A\varphi,A^2\varphi\in\mathcal{D}(H_0)\}$ be the domain of A^2 in $\mathcal{D}(H_0)$. We now check that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$, defined on $\mathcal{D}(A;\mathcal{D}(H_0))$ and on $\mathcal{D}(A^2;\mathcal{D}(H_0))$, respectively, extend to operators in $\mathcal{B}(\mathcal{D}(H_0))$. After some commutator calculations performed on $\mathcal{D}$ and involving Lemma 2.3, one first obtains that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A$ are, respectively, equal on $\mathcal{D}$ to some operators S_1 and $S_2\langle Q_3\rangle^{-1}$ in $\mathcal{B}(\mathcal{H})$, where S_1 and S_2 are polynomials in H_0^{-1}, $P_3H_0^{-1}$, α_3 and $f(Q_3)$ for bounded functions f with bounded derivatives. Since $\mathcal{D}$ is a core for A, these equalities even hold on $\mathcal{D}(A)$. Hence one has on $\mathcal{D}(A^2)$:

$$\langle Q_3\rangle^{-2}A^2=(\langle Q_3\rangle^{-2}A)A=S_2\langle Q_3\rangle^{-1}A=S_2S_1.$$

In consequence, $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$ are equal on $\mathcal{D}(A)$ and on $\mathcal{D}(A^2)$, respectively, to operators expressed only in terms of H_0^{-1}, $P_3H_0^{-1}$, α_3, and $f(Q_3)$ for bounded functions f with bounded derivatives. Moreover, one easily observes that these operators and their products belong to $\mathcal{B}(\mathcal{D}(H_0))$. Thus, it follows that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$ are equal on $\mathcal{D}(A;\mathcal{D}(H_0))$ and on $\mathcal{D}(A^2;\mathcal{D}(H_0))$, respectively, to some operators belonging to $\mathcal{B}(\mathcal{D}(H_0))$.

(iii) By duality, the operator $(\langle Q_3\rangle^{-1}A)^*$ belongs to $\mathcal{B}(\mathcal{D}(H_0)^*)$. Now, for $\psi\in\mathcal{D}(H_0)^*$ and $\varphi\in\mathcal{D}(A;\mathcal{D}(H_0))$, one has

$$\langle(\langle Q_3\rangle^{-1}A)^*\psi,\varphi\rangle=\langle\psi,\langle Q_3\rangle^{-1}A\varphi\rangle=\langle\langle Q_3\rangle^{-1}\psi,A\varphi\rangle, \tag{3.13}$$

where $\langle\cdot,\cdot\rangle$ denotes the duality between $\mathcal{D}(H_0)$ and $\mathcal{D}(H_0)^*$. Since $\langle Q_3\rangle^{-1}$ is a homeomorphism from $\mathcal{D}(H_0)^*$ to the domain of $\langle Q_3\rangle$ in $\mathcal{D}(\mathcal{H}_0)^*$, it follows from (3.13) that the domain of $\langle Q_3\rangle$ in $\mathcal{D}(H_0)^*$ is included in the domain of A in $\mathcal{D}(H_0)^*$ (the adjoint of the operator A in $\mathcal{D}(H_0)$ is equal to the operator $-A$ in $\mathcal{D}(H_0)^*$).

(iv) The inequality $r\|(\langle Q_3\rangle+ir)^{-1}\|_{\mathcal{B}(\mathcal{D}(H_0)^*)}\leqslant\mathrm{Const.}$ for all $r>0$ is obtained from relation (A1), given in the proof of Lemma 2.3, with $f(Q_3)=(\langle Q_3\rangle+ir)^{-1}$.

(v) Assume that V is a long-range (scalar) potential. Then the following equality holds in form sense on $\mathcal{D}$:

$$2[iV,A]=-Q_3(\partial_3V)H_0^{-1}-H_0^{-1}Q_3(\partial_3V)+[iV,H_0^{-1}]Q_3P_3+P_3Q_3[iV,H_0^{-1}], \tag{3.14}$$

with $[iV,H_0^{-1}]=\Sigma_{j=1}^3H_0^{-1}\alpha_j(\partial_jV)H_0^{-1}$. Using Lemma 2.3a, one gets that the last two terms in (3.14) are equal in form sense on $\mathcal{D}$ to

$$2\ \mathrm{Re}\sum_{j=1}^{3} H_0^{-1}\alpha_j Q_3(\partial_j V)P_3 H_0^{-1} - 2\ \mathrm{Im}\sum_{j=1}^{3} H_0^{-1}\alpha_j(\partial_j V)H_0^{-1}\alpha_3 P_3 H_0^{-1}.$$

It follows that $[iV,A]$, defined in form sense on $\mathcal{D}$, extends continuously to an operator in $\mathcal{B}(\mathcal{H})$. Now let ϑ be as in Definition 1.1. Then a direct calculation using the explicit form of $[iV,A]$ obtained above implies that

$$\left\| \vartheta\left(\frac{\langle Q_3\rangle}{r}\right)[iV,A] \right\| \leqslant \mathrm{C}\sum_{j=1}^{3} \left\| \vartheta\left(\frac{\langle Q_3\rangle}{r}\right)\langle Q_3\rangle(\partial_j V) \right\| + \frac{\mathrm{D}}{r},$$

for all $r>0$ and some positive constants C and D. □

As a direct consequence, one obtains that

Lemma 3.4: If V satisfies the hypotheses of Theorem 1.2, then A is conjugate to H on $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$.

Proof: Proposition 3.3 implies that both H_0 and H are of class $\mathcal{C}^{1,1}(A)$. Furthermore, the difference $(H+i)^{-1}-(H_0+i)^{-1}$ is compact by Proposition 3.1, and $\varrho^T_{H_0}>0$ on $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ due to Proposition 2.7. Hence the claim follows by [Ref. 1, Thm. 7.2.9 & Prop. 7.2.6]. □

We can finally give the proof of Theorem 1.2.

Proof of Theorem 1.2: Since A is conjugate to H on $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ by Lemma 3.4, the assertions (a) and (b) follow by the abstract conjugate operator method [Ref. 1, Cor. 7.2.11 & Thm. 7.4.2].

The limiting absorption principle directly obtained via Ref. 1, Thm. 7.4.1 is expressed in terms of some interpolation space, associated with $\mathcal{D}(A)$, and of its adjoint. Since both are not standard spaces, one may use Ref. 1, prop. 7.4.4 for the Friedrichs couple $(\mathcal{D}(\langle Q_3\rangle),\mathcal{H})$ to get the statement (c). In order to verify the hypotheses of that proposition, one has to check that for each $z\in\mathbb{C}\setminus\sigma(H)$ the inclusion $(H-z)^{-1}\mathcal{D}(\langle Q_3\rangle)\subset\mathcal{D}(A)$ holds. However, since $\mathcal{D}(\langle Q_3\rangle)$ is included in $\mathcal{D}(A)$ by Proposition 2.4, it is sufficient to prove that for each $z\in\mathbb{C}\setminus\sigma(H)$ the operator $(H-z)^{-1}$ leaves $\mathcal{D}(\langle Q_3\rangle)$ invariant. Since $\mathcal{D}(H)=\mathcal{D}(H_0)$ is left invariant by the group $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ (see Proposition 3.3 (i)) one easily gets from Ref. 1, Thm. 6.3.4.(a) that H is of class $C^1(\langle Q_3\rangle)$, which implies the required invariance of $\mathcal{D}(\langle Q_3\rangle)$ [Ref. 1, Thm. 6.2.10.(b)]. □

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APPENDIX

Proof of Lemma 2.2: (a) Let φ, ψ be in $\mathcal{D}$. Using the transformation (2.1), one gets

$$\langle H_0^{-n}\varphi, Q_3\psi\rangle = \int_{\mathbb{R}} \langle H_0(\xi)^{-n}(\mathcal{F}\varphi)(\xi), (i\partial_\xi\mathcal{F}\psi)(\xi)\rangle_{\mathcal{H}_{12}}\mathrm{d}\xi.$$

Now the map $\mathbb{R}\ni\xi\mapsto H_0(\xi)^{-n}\in\mathcal{B}(\mathcal{H}_{12})$ is norm differentiable with its derivative equal to $-\Sigma_{j=1}^{n}H_0(\xi)^{-j}\alpha_3 H_0(\xi)^{j-n-1}$. Hence $\{\partial_\xi[H_0(\xi)^{-n}(\mathcal{F}\varphi)(\xi)]\}_{\xi\in\mathbb{R}}$ belongs to $\int_{\mathbb{R}}^{\oplus}\mathcal{H}_{12}\mathrm{d}\xi$. Thus one can perform an integration by parts (with vanishing boundary contributions) and obtain

$$\langle H_0^{-n}\varphi, Q_3\psi\rangle = \int_{\mathbb{R}} \langle i\partial_\xi[H_0(\xi)^{-n}(\mathcal{F}\varphi)(\xi)], (\mathcal{F}\psi)(\xi)\rangle_{H_{12}}\mathrm{d}\xi.$$

It follows that $|\langle H_0^{-n}\varphi, Q_3\psi\rangle|\leqslant \mathrm{const.}\|\psi\|$ for all $\psi\in\mathcal{D}$. Since Q_3 is essentially self-adjoint on $\mathcal{D}$, this implies that $H_0^{-n}\varphi$ belongs to $\mathcal{D}(Q_3)$.

(b) The boundedness of $P_3H_0^{-1}$ is a consequence of the estimate

$$\operatorname*{ess\,sup}_{\xi\in\mathbb{R}}\|\xi H_0(\xi)^{-1}\|_{\mathcal{B}(\mathcal{H}_{12})}=\operatorname*{ess\,sup}_{\xi\in\mathbb{R}}\left\|\frac{|\xi|}{[H_0(0)^2+\xi^2]^{1/2}}\right\|_{\mathcal{B}(\mathcal{H}_{12})}<\infty$$

and of the direct integral formalism [Ref. 6, Prop. 3.6 & 3.7]. The remaining assertions follow by standard arguments. □

Proof of Lemma 2.3: (a) One first observes that the following equality holds on $\mathcal{D}$:

$$iH_0^{-1}f(Q_3)H_0=-H_0^{-1}\alpha_3 f'(Q_3)+if(Q_3). \tag{A1}$$

Now, for $\varphi,\psi\in\mathcal{D}$ and $\eta\in H_0^n\mathcal{D}$, one has

$$\begin{aligned}
&\langle\varphi,iH_0^{-1}f(Q_3)\,\eta\rangle-\langle\varphi,if(Q_3)H_0^{-1}\eta\rangle\\
&\quad=\langle\varphi,iH_0^{-1}f(Q_3)H_0\psi\rangle+\langle\varphi,iH_0^{-1}f(Q_3)(\eta-H_0\psi)\rangle-\langle\overline{f}(Q_3)\varphi,iH_0^{-1}\eta\rangle\\
&\quad=-\langle\varphi,H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}\eta\rangle-\langle\varphi,H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}(H_0\psi-\eta)\rangle\\
&\qquad+\langle\overline{f}(Q_3)\varphi,iH_0^{-1}(H_0\psi-\eta)\rangle+\langle\overline{f}(Q_3)H_0^{-1}\varphi,i(\eta-H_0\psi)\rangle,
\end{aligned}$$

where we have used (A1) in the last equality for the term $\langle\varphi,iH_0^{-1}f(Q_3)H_0\psi\rangle$. Hence there exists a constant c (depending on φ) such that

$$\left|\langle\varphi,iH_0^{-1}f(Q_3)\,\eta\rangle-\langle\varphi,if(Q_3)H_0^{-1}\eta\rangle+\langle\varphi,H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}\eta\rangle\right|\leqslant c\|\eta-H_0\psi\|.$$

Then the statement is a direct consequence of the density of $H_0\mathcal{D}$ and $\mathcal{D}$ in $\mathcal{H}$.

(b) This is a simple corollary of the point (a). □

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Enhanced binding revisited for a spinless particle in nonrelativistic QED

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We consider a spinless particle coupled to a quantized Bose field and show that such a system has a ground state for two classes of short-range potentials which are alone too weak to have a zero-energy resonance. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1793329]

I. INTRODUCTION AND MAIN RESULTS

Our aim in this paper is to prove the existence of the ground state for a spinless nonrelativistic particle interacting with a short-range potential and coupled to a quantized radiation field. We want to show that this can be achieved using the threshold-coupling behavior of the corresponding Schrödinger operator, without using explicitly the zero-energy resonance property.

Let us begin by specifying the classes of potentials to be considered. Throughout the paper we suppose that (i) $V \in L^\infty$ is nonzero and attractive, $V \leqslant 0$, and (ii) V belongs to $L^{3/2}(\mathbb{R}^3)$, which is well known to ensure, in particular, that V lies in the Rollnik class, i.e.,

$$\|V\|_R^2 := \iint_{\mathbb{R}^6} \frac{|V(x)||V(y)|}{|x-y|^2} dx\, dy < +\infty.$$

Finally, we adopt one of the following assumptions: (iii) V is *strictly* attractive, $V < 0$, and satisfies the inequality

$$|\Delta V| \leqslant C|V|, \tag{1.1}$$

with a positive constant C, or alternatively (iii′) V is compactly supported with ΔV integrable. We will say more on the meaning of these assumptions in the remarks following Theorem 1 below. Here we just comment that our goal is to explain the above indicated idea, rather than to push for an optimal result, and therefore the stated assumptions leave ample room for improvements.

We denote by H_λ the family of Schrödinger operators $H_\lambda := p^2 + \lambda V$ on $L^2(\mathbb{R}^3)$ for positive parameters λ. Its eigenvalues are monotonically decreasing functions of λ in $[0, +\infty)$, and it is

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well known that at some positive critical value λ_0, which is called the "coupling-constant threshold" an eigenvalue emerges from the continuum. More precisely, if $\lambda \leqslant \lambda_0$, H_λ has no negative eigenvalues, whereas when $\lambda > \lambda_0$ it has at least one bound state.

We now couple this Schrödinger operator to the radiation field and consider the so-called *Pauli–Fierz operator,*

$$H_\alpha^V = (p + \sqrt{\alpha}\, A(x))^2 + H_f + \lambda V, \tag{1.2}$$

acting on the Hilbert space,

$$\mathcal{H} = L^2(\mathbb{R}^3;\mathbb{C}) \otimes \mathcal{F},$$

where $\mathcal{F} = \oplus_{n=0}^{+\infty} L_b^2(\mathbb{R}^{3n};\mathbb{C})$ is the Fock space for the photon field and $L_b^2(\mathbb{R}^{3n})$ is the space of symmetric functions in $L^2(\mathbb{R}^{3n})$ representing n-photon states, with $n=0$ corresponding to the one-dimensional vacuum sector. Following the usual convention we abuse notation and use the same symbol for H_f and $I \otimes H_f$, etc. The operator H_α^V is essentially self-adjoint on $\mathcal{D}(\Delta) \cap \mathcal{D}(H_f)$, where the symbol $\mathcal{D}$ denotes the operator domain—see Bach, Fröhlich, and Sigal (1999) and Hiroshima (2002).

We denote the ground state energy as

$$E(\alpha, \lambda V) := \inf \text{ spec } H_\alpha^V, \tag{1.3}$$

and the spectrum is then the half-line $[E(\alpha, \lambda V), +\infty)$. In Griesemer, Lieb, and Loss (2001), Theorem 3.1, the authors show under rather weak assumptions about the potential V that, in the case when $\lambda > \lambda_0$, i.e. when the Schrödinger operator $-\Delta + \lambda V$ has a ground state, it persists after coupling to the radiation field. Moreover, in Hainzl, Vougalter, and Vugalter (2003), the authors prove for a particular class of potentials that in the case when $\lambda = \lambda_0$, the coupling to the field can create a ground state for small coupling constant α, despite the fact that the underlying Schrödinger operator $-\Delta + \lambda_0 V$ has no ground state. Recall also that in the case of a particle with spin the same result was proved by two of the present authors in Catto and Hainzl (2004); a different proof is given in Chen, Vougalter, and Vugalter (2003).

Our goal here is to show that $E(\alpha, \lambda V)$ is an eigenvalue of H_α^V for coupling in some interval $(\gamma, \lambda_0]$, with $\lambda_0 - \gamma = \mathcal{O}(\alpha)$ for α small. It means that we do not require the existence of a zero-energy resonance in the absence of the field. This is due to the fact that, in contrast to the other existing work quoted above, we employ a tool adopted from Klaus and Simon (1980) which makes it possible to estimate "how much" the binding is enhanced.

The strategy of proof will be based on the expansion of the self-energy in powers of α, as provided in Hainzl (2003), Hainzl (2002), Hainzl, Vougalter, and Vugalter (2003), and Catto and Hainzl (2004), and by checking that the Griesemer–Lieb–Loss criterium [i.e., inequality (2.1) below] is satisfied for α small enough. To this aim we use the coupling constant threshold expansion of Klaus and Simon (1980), which will allow us to demonstrate the enhanced binding for the class of potentials indicated above. For any ultraviolet cutoff Λ our result holds true for α sufficiently small. In fact for a large class of potentials (see Remark 3) the physical value of α is in the range of validity, since we will fix the photon energy cutoff to be mc^2. This is physically reasonable, since for larger values nonrelativistic QED might no longer be applicable due to the fact that pair-production can take place.

Recall that in the dipole approximation, in the case of a large coupling α the enhanced binding was shown earlier by Hiroshima and Spohn (2001); see also Arai and Kawano (2003) in the context of linear coupling.

We fix units in such a way that the Planck constant $\hbar = 1$, the speed of light $c = 1$, and the electron mass $m = \frac{1}{2}$. The electron charge is then given by $e = \sqrt{\alpha}$, with $\alpha \approx 1/137$ being the fine structure constant. In the present paper α plays the role of a small, dimensionless number which measures the coupling to the radiation field. Our results hold for *sufficiently small values* of α. The operator $p = -i\nabla$ is the electron momentum while A is the quantized magnetic vector potential, which is given by

$$A(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\chi(|k|)}{2\pi|k|^{1/2}} \varepsilon^\lambda(k)[a_\lambda(k)e^{ik\cdot x} + a_\lambda^*(k)e^{-ik\cdot x}]\mathrm{d}k,$$

where the annihilation and creation operators a_λ and a_λ^*, respectively, satisfy the usual commutation relations,

$$[a_\nu(k), a_\lambda^*(q)] = \delta(k-q)\,\delta_{\lambda,\nu},$$

and

$$[a_\lambda(k), a_\nu(q)] = 0, \quad [a_\lambda^*(k), a_\nu^*(q)] = 0.$$

In the following we use the notation

$$A(x) = D(x) + D^*(x). \tag{1.4}$$

The vectors $\varepsilon^\lambda(k) \in \mathbb{R}^3$ in $A(x)$ are orthonormal polarization vectors perpendicular to k which are chosen in a such a way that

$$\varepsilon^2(k) = \frac{k}{|k|} \wedge \varepsilon^1(k). \tag{1.5}$$

The function $\chi(|k|)$ describes the ultraviolet cutoff for the interaction at large wave-numbers k. For the sake of simplicity we choose for χ the Heaviside function $\Theta(\Lambda - |k|)$; more general cutoff functions would work, however, let us emphasize the fact that we shall sometimes use the radial symmetry of χ in the proofs. Throughout the paper we assume $\Lambda = 1$. This corresponds to the energy mc^2 in our system of units and represents a natural upper bound to which the validity of the nonrelativistic QED can be extended.

The photon field energy H_f is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a_\lambda^*(k) a_\lambda(k)\mathrm{d}k, \tag{1.6}$$

and the field momentum reads

$$P_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} k a_\lambda^*(k) a_\lambda(k)\mathrm{d}k. \tag{1.7}$$

Since $\mathcal{H}$ can be also written as $\oplus_{n=0}^{+\infty} L^2(\mathbb{R}^3;\mathbb{C}) \otimes L_b^2(\mathbb{R}^{3n};\mathbb{C}^{2n})$ we can express a general vector $\Psi \in \mathcal{H}$ as a direct sum,

$$\Psi = \bigoplus_{n=0}^{\infty} \psi_n, \tag{1.8}$$

where $\psi_n = \psi_n(x, k_1, \ldots, k_n)$ is an n-photon state. For simplicity, we do not include the variables corresponding to the polarization of the photons.

To simplify further the notation, we introduce the unitary transformation

$$U = \mathrm{e}^{\mathrm{i}P_f \cdot x} \tag{1.9}$$

acting on $\mathcal{H}$. Since

$$UA(x)U^* = A(0)$$

and

$$UpU^* = p - P_f, \tag{1.10}$$

we obtain

$$UH_\alpha^V U^* = (p - P_f + \sqrt{\alpha}A)^2 + H_f + \lambda V, \tag{1.11}$$

where $A=A(0)$. The operator U preserves spectral properties, in particular,

$$\inf \operatorname{spec}[UH_\alpha^V U^*] = \inf \operatorname{spec} H_\alpha^V. \tag{1.12}$$

Thus we shall rather work with $UH_\alpha^V U^*$ in the following; abusing the notation we will use again the symbol H_α^V for it.

Our main result is the following.

Theorem 1: *Adopt the assumptions (i), (ii), and either (iii) or (iii′). Then there exists a function* $g:\mathbb{R}^+ \to (0,1)$ *such that for any small enough* α *and all* $\lambda \in (\lambda_0(1-g(\alpha)), \lambda_0]$, *the spectral threshold* $E(\alpha, \lambda V)$ *is an eigenvalue of* H_α^V.

Remark 1: The assumptions about the potential combine different types of requirements. For instance, hypotheses involving the Laplacian, i.e., (1.1) or $\Delta V \in L^1$ impose restrictions mainly on local regularity of the potential. On the other hand, the integrability condition (ii) which guarantees the Rollnik property regulates the potential decay; on a heuristic level one may say that it should behave as $|x|^{-2-\epsilon}$ at infinity.

Remark 2: It comes out of the proof that $g(\alpha)$ is of order of α, more specifically, the relation (2.37) shows that $g(\alpha)=c\alpha+\mathcal{O}(\alpha^2 \ln \alpha)$ with $c>0$ holds as $\alpha \to 0$. It is important that we get in this way an asymptotical *lower* bound to $g(\alpha)$ which allows us to assess how much the binding is enhanced.

Remark 3: In connection with the previous remark we want to emphasize that all the constants appearing in the proof can be evaluated explicitly. Assuming that we choose a potential V such that the constants $C, b(V)$ in (1.1) and (2.39), respectively, are of the order of one, it turns out that Theorem 1 holds for $\alpha \lesssim 10^{-2}$ which covers the physically important case.

Remark 4: We have recalled above the results of Griesemer, Lieb, and Loss (2001) and Hainzl, Vougalter, and Vugalter (2003), the latter using the existence of a zero-energy resonance state together with a continuity argument which shows that H_α^V has a bound state for values of λ slightly below λ_0. As we have said our strategy is similar but the proof is more constructive, in particular, it provides a rough estimate on how far below λ_0 one can descend to still ensure the existence of a ground state. In addition our method covers a different and in several respects a wider class of potentials V, in particular, we require neither a compact support nor the radial symmetry of the potential.

Remark 5: Using the methods of Catto and Hainzl (2004), Theorem 1 can also be proven for the case of particles with spin. Unfortunately the numbers of inequalities needed increase dramatically. For that reason we restricted our attention to the more convenient case of bosons.

II. PROOF OF THEOREM I

Let $0<\lambda \leq \lambda_0$. According to Griesemer, Lieb, and Loss (2001), the ground state exists provided

$$E(\alpha, \lambda V) < E(\alpha, 0), \tag{2.1}$$

where $E(\alpha,0)$ is the electron self-energy. Thus we are going to construct a trial state $\Psi \in L^2(\mathbb{R}^3) \otimes \mathcal{F}$ which ensures that the last inequality is satisfied,

$$(\Psi; H_\alpha^V \Psi) < E(\alpha,0)\|\Psi\|^2. \tag{2.2}$$

The strategy of proof is as follows: we will compare the respective expansions of $E(\alpha,0)$ and $(\Psi; H_\alpha^V \Psi)$ for the trial state Ψ in terms of the coupling constant α. From Hainzl (2003) and

Hainzl, Vougalter, and Vugalter (2003) we already know the first three terms in the Taylor expansion of the former, namely

$$|E(\alpha,0) - \alpha\pi^{-1} + \alpha^2\langle 0|DD\mathcal{A}_\alpha^{-1}D*D*|0\rangle| \leqslant C_{\mathrm{self}}\alpha^3, \tag{2.3}$$

for some positive constant C_{self}, where $|0\rangle$ is the vacuum vector, $\langle\cdot;\cdot\rangle$ denotes the scalar product in the photon Fock space $\mathcal{F}$, and with

$$\mathcal{A}_\alpha = P_f^2 + H_f + 2\alpha D*D. \tag{2.4}$$

Recall that actually in Hainzl, Vougalter, and Vugalter (2003) the proof is given for $\mathcal{A}_0$ instead of $\mathcal{A}_\alpha$ in the second-order term in (2.3), but the same argument carries through *mutatis mutandis* to the present case.

Consider now a quantity $g(\alpha) \in (0,1)$, to be determined later, and observe that when the coupling parameter λ satisfies

$$(1 - g(\alpha))\lambda_0 < \lambda \leqslant \lambda_0,$$

then the Schrödinger operator,

$$h_\alpha^\lambda := (1 - g(\alpha))p^2 + \lambda V,$$

has a negative eigenvalue $e_\lambda(\alpha) := -|e_\lambda|$ at the bottom of the spectrum. This trivially follows from the inequality $\lambda/[1-g(\alpha)] > \lambda_0$ and our choice of λ_0 to be critical. We denote by ψ_λ a corresponding eigenstate which may be chosen without loss of generality as real-valued and normalized in L^2. Our trial function, to be inserted into (2.2), will involve only two photons being of the form

$$\Psi = \psi_\lambda \oplus \psi_1 \oplus \psi_2 \oplus \cdots, \tag{2.5a}$$

with

$$\psi_1 = -2\sqrt{\alpha}L^{-1}D*p\psi_\lambda \tag{2.5b}$$

and

$$\psi_2 = -\alpha L^{-1}D*D*\psi_\lambda. \tag{2.5c}$$

The operator L on $L^2(\mathbb{R}^3)\otimes\mathcal{F}$ appearing in here is defined by

$$L = (1 - g(\alpha))(p - P_f)^2 + \lambda V + |e_\lambda| + H_f + 2\alpha D*D; \tag{2.6}$$

the definitions (2.5b) and (2.5c) make sense because L is invertible on the orthogonal complement of the vacuum sector $L^2(\mathbb{R}^3)\otimes\mathbb{C}|0\rangle$; this follows from the fact that it is unitarily equivalent to $h_\alpha^\lambda + |e_\lambda| + H_f + 2\alpha D*(x)D(x)$ by means of the operator (1.9). Note that, with the abuse of notation mentioned in the opening, we often use ψ_λ as a shorthand for $\psi_\lambda\otimes|0\rangle$.

The canonical commutation relations yield the identity

$$A^2 = D*D* + DD + 2D*D + \frac{1}{\pi};$$

using it together with commutativity of P_f with D, $D*$, we find that

$$(\Psi;H_\alpha^V\Psi) = g(\alpha)\|P\Psi\|^2 + \left[\frac{\alpha}{\pi} - |e_\lambda|\right]\|\Psi\|^2 + (\Psi;L\Psi) + 2\Re(\Psi;[2\sqrt{\alpha}PD* + \alpha D*D*]\Psi)$$
$$+ (\psi_\lambda;(h_\alpha^\lambda + |e_\lambda|)\psi_\lambda), \tag{2.7}$$

where $P := p - P_f$ denotes the total momentum; the last term on the right-hand side of (2.7) cancels by definition of e_λ, h_α^λ, and ψ_λ.

Let us further remark that it will be convenient in the following to replace the field Hamiltonian H_f by $\widetilde{H}_f := H_f + \alpha^3$ in order to avoid dealing with the logarithmically divergent infrared terms; this trick was already used in Hainzl and Seiringer (2002), Catto and Hainzl (2004), and Hainzl, Hirokawa, and Spohn (2003). It amounts to adding an extra $-\alpha^3\|\Psi\|^2$ term at the right-hand side of (2.7) which does not change, of course, the expansion up to the second order in α. Observe that by our choice of Ψ the identity

$$\begin{aligned}(\Psi; L\Psi) + 2\Re(\Psi; [2\sqrt{\alpha}PD^* + \alpha D^* D^*]\Psi) \\ = (\psi_\lambda; L\psi_\lambda) - 2\Re(\psi_\lambda; -\alpha DDL^{-1}(-2\sqrt{\alpha}PD)^* L^{-1}(-2\sqrt{\alpha}PD)^*\psi_\lambda) \\ - \|L^{-1/2}[2\sqrt{\alpha}PD^* + \alpha D^* D^*]\psi_\lambda\|^2, \end{aligned} \tag{2.8}$$

holds, and the same is true if we replace L in the last relation by $\widetilde{L}$ referring to $\widetilde{H}_f$. Thus we obtain

$$\begin{aligned}(\Psi; \widetilde{H}_\alpha^V \Psi) = g(\alpha)\|P\Psi\|^2 + \left[\frac{\alpha}{\pi} - |e_\lambda| - \alpha^3\right]\|\Psi\|^2 - 4\alpha\|\widetilde{L}^{-1/2}D^* p\psi_\lambda\|^2 - \alpha^2(\psi_\lambda; DD\widetilde{L}^{-1}D^* D^*\psi_\lambda) \\ + 8\alpha^2\Re(\widetilde{L}^{-1}D^* D^*\psi_\lambda; PD^*\widetilde{L}^{-1}D^* p\psi_\lambda), \end{aligned} \tag{2.9}$$

where $\widetilde{H}_\alpha^V$ refers again to $\widetilde{H}_f$. On the other hand, apart from taming the infrared singularity the extra term is irrelevant, as long as we are looking for an effect of an order of α^2. This is why we will abuse notation writing nontilded quantities everywhere except the one place where this Hamiltonian shift indeed matters, that is, in the proof of Lemma 2.4.

To estimate the last term at the right-hand side of (2.9), notice that the Cauchy–Schwarz inequality yields

$$8\alpha^2|(L^{-1}D^* D^*\psi_\lambda; PD^* L^{-1}D^* p\psi_\lambda)| \leqslant \frac{4\alpha^3}{a}\|L^{-1/2}PDL^{-1}D^* D^*\psi_\lambda\|^2 + 4\alpha a\|L^{-1/2}D^* p\psi_\lambda\|^2, \tag{2.10}$$

with a positive constant a to be chosen later. The last term can be combined with the similar term in (2.9) giving

$$\begin{aligned}(\Psi; H_\alpha^V \Psi) \leqslant g(\alpha)\|P\Psi\|^2 - |e_\lambda|\|\Psi\|^2 + \frac{\alpha}{\pi}\|\Psi\|^2 - 4\alpha(1-a)\|L^{-1/2}D^* p\psi_\lambda\|^2 \\ - \alpha^2(\psi_\lambda; DDL^{-1}D^* D^*\psi_\lambda) + \frac{4\alpha^3}{a}\|L^{-1/2}PDL^{-1}D^* D^*\psi_\lambda\|^2. \end{aligned} \tag{2.11}$$

To estimate further the terms appearing in (2.10) we need a series of technical lemmata.

Lemma 2.1: The following inequality holds:

$$(\psi_\lambda; DDL^{-1}D^* D^*\psi_\lambda) \geqslant \langle 0|DD\mathcal{A}_\alpha^{-1}D^* D^*|0\rangle + g(\alpha)C_1, \tag{2.12}$$

where

$$C_1 := \|P_f\mathcal{A}_\alpha^{-1}D^* D^*|0\rangle\|^2.$$

Proof: We denote $L = \mathcal{Q} + b$, with

$$\mathcal{Q} = (1-g(\alpha))(p^2 + P_f^2) + \lambda V + |e_\lambda| + H_f + 2\alpha D^* D,$$

and $b = -2(1-g(\alpha))pP_f$, and we use twice the second resolvent equation,

$$(\mathcal{Q}+b)^{-1}=\mathcal{Q}^{-1}-\mathcal{Q}^{-1}b\mathcal{Q}^{-1}+\mathcal{Q}^{-1}b(\mathcal{Q}+b)^{-1}b\mathcal{Q}^{-1}\geqslant\mathcal{Q}^{-1}-\mathcal{Q}^{-1}b\mathcal{Q}^{-1}, \tag{2.13}$$

where the inverse of $\mathcal{Q}+b$ and the last inequality makes sense in the complement to the vacuum sector where the operator is strictly positive as we have remarked above. Hence we have

$$(\psi_\lambda;DDL^{-1}D*D*\psi_\lambda)\geqslant(\psi_\lambda;DD\mathcal{Q}^{-1}D*D*\psi_\lambda)+2(1-g(\alpha))(\psi_\lambda;DD\mathcal{Q}^{-1}pP_f\mathcal{Q}^{-1}D*D*\psi_\lambda). \tag{2.14}$$

Furthermore, the second term at the right-hand side vanishes. To check this claim, recall that ψ_λ belongs by construction to the null-space of $h_\alpha^\lambda+|e_\lambda|$, and that h_α^λ commutes with the operator

$$\mathcal{K}:=(1-g(\alpha))P_f^2+H_f+2\alpha D*D.$$

It follows easily that

$$\mathcal{Q}^{-1}D*D*\psi_\lambda=\mathcal{K}^{-1}D*D*\psi_\lambda, \tag{2.15}$$

and therefore

$$(\psi_\lambda;DD\mathcal{Q}^{-1}pP_f\mathcal{Q}^{-1}D*D*\psi_\lambda)=(\psi_\lambda;p\psi_\lambda)\langle 0|DD\mathcal{K}^{-1}P_f\mathcal{K}^{-1}D*D*|0\rangle=0,$$

because ψ_λ is real-valued as indicated above making the first factor zero.

Using (2.15) again, we find that the first term reads as

$$\begin{aligned}(\psi_\lambda;DD\mathcal{Q}^{-1}D*D*\psi_\lambda)&=(\psi_\lambda;DD\mathcal{K}^{-1}D*D*\psi_\lambda)\\&=\|\psi_\lambda\|^2\langle 0|DD\mathcal{K}^{-1}D*D*|0\rangle\geqslant\langle 0|DD\mathcal{A}_\alpha^{-1}D*D*|0\rangle+g(\alpha)\\&\quad\times\langle 0|DD\mathcal{A}_\alpha^{-1}P_f^2\mathcal{A}_\alpha^{-1}D*D*|0\rangle,\end{aligned} \tag{2.16}$$

where in the last line we used the fact that ψ_λ is normalized together with the second resolvent equation and positivity of $\mathcal{K}$ in the complement of the vacuum sector. Hence we have the following claim. □

Lemma 2.2: For any positive constant μ we have

$$\|L^{-1/2}D*p\psi_\lambda\|^2\geqslant[C_4(\mu)+\mu C_3(\mu)]\|p\psi_\lambda\|^2-\frac{\lambda}{2}C_3(\mu)(\psi_\lambda;\Delta V\psi_\lambda), \tag{2.17}$$

with

$$C_3(\mu)=\tfrac{2}{3}\langle 0|D(\mathcal{K}+\mu)^{-2}D*|0\rangle \tag{2.18}$$

and

$$C_4(\mu)=\tfrac{2}{3}\langle 0|D(\mathcal{K}+\mu)^{-1}D*|0\rangle. \tag{2.19}$$

Proof: Using the relation analogous to (2.13), we find

$$\begin{aligned}pDL^{-1}D*p\geqslant{}&pD(\mathcal{K}+\mu)^{-1}D*p-pD(\mathcal{K}+\mu)^{-1}[-2pP_f(1-g(\alpha))+h_\alpha^\lambda+|e_\lambda|-\mu]\\&\times(\mathcal{K}+\mu)^{-1}D*p.\end{aligned}$$

Again, since ψ_λ is real valued the term containing pP_f vanishes; notice that the same conclusion can also be made using symmetry of the cutoff function. Since $\mathcal{K}$ acts on photon variables whereas h_α^λ acts on those of the electron, the two operators commute and the second term at the right-hand side of the last estimate can be rewritten as

$$(\psi_\lambda; pD(\mathcal{K}+\mu)^{-1}[-2pP_f(1-g(\alpha))+h_\alpha^\lambda+|e_\lambda|-\mu](\mathcal{K}+\mu)^{-1}D*p\psi_\lambda)$$
$$= C_3(\mu)(p\psi_\lambda; (h_\alpha^\lambda+|e_\lambda|-\mu)p\psi_\lambda), \tag{2.20}$$

with $C_3(\mu)$ given by (2.18). Observing that ψ_λ belongs to the null-space of $h_\alpha^\lambda+|e_\lambda|$ we can further cast a part of the last expression into the form

$$(p\psi_\lambda; (h_\alpha^\lambda+|e_\lambda|)p\psi_\lambda) = -\tfrac{1}{2}(\psi_\lambda; [p,[p,h_\alpha^\lambda+|e_\lambda|]]\psi_\lambda) = \frac{\lambda}{2}(\psi_\lambda; \Delta V\psi_\lambda), \tag{2.21}$$

to obtain

$$(p\psi_\lambda; (h_\alpha^\lambda+|e_\lambda|-\mu)p\psi_\lambda) = -\mu\|p\psi_\lambda\|^2+\frac{\lambda}{2}(\psi_\lambda; \Delta V\psi_\lambda).$$

On the other hand,

$$(\psi_\lambda; pD(\mathcal{K}+\mu)^{-1}D*p\psi_\lambda) = C_4(\mu)\|p\psi_\lambda\|^2,$$

with $C_4(\mu)$ given by (2.19), which concludes the proof. □

Our next auxiliary result is the following.

Lemma 2.3: Let $\alpha>0$ and $0<\lambda\leq\lambda_0$, then for any positive number $g(\alpha)<1-\lambda/\lambda_0$ there are positive constants β and $C(V)$ such that

$$p^2 \leqslant \beta(h_\alpha^\lambda+|e_\lambda|)+C(V). \tag{2.22}$$

Proof: For the inequality (2.22) to hold, the constant β which appears at the right-hand side has obviously to satisfy the inequality $\beta>1/[1-g(\alpha)]$, or equivalently $\beta(1-g(\alpha))-1>0$. We fix an arbitrary β with this property, to be specified later. Next we notice that inequality (2.22) will follow from

$$p^2+\lambda\tilde{V}\geqslant -\tilde{C}(V),$$

with

$$\tilde{V}:=\frac{1}{1-g(\alpha)-\beta^{-1}}V, \quad \tilde{C}(V):=\frac{C(V)}{\beta(1-g(\alpha))-1},$$

because the last inequality is equivalent to (2.22) with the term $|e_\lambda|$ at the right-hand side neglected. In other words, it is sufficient that the Schrödinger operator $p^2+\lambda\tilde{V}$ has no spectrum below $-\tilde{C}(V)$. From the proof of the Birman-Schwinger bound in Reed and Simon (1975), Theorem XIII.10, and the fact that $\tilde{V}$ is nonpositive it follows that this happens if and only if

$$\frac{\lambda^2}{16\pi^2}\iint_{\mathbb{R}^6}\frac{|\tilde{V}(x)||\tilde{V}(y)|}{|x-y|^2}e^{-2\sqrt{\tilde{C}(V)}|x-y|}\,dx\,dy<1. \tag{2.23}$$

Let us denote by $\mathcal{K}_m$ the function $x\mapsto e^{-\sqrt{m}|x|}/4\pi|x|^2$ with a fixed positive m which represents the resolvent kernel in the above expression; it is clear that $\mathcal{K}_m$ belongs to $L^1(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3}\mathcal{K}_m(x)dx=1/\sqrt{m}$. We employ these observations in the following chain of inequalities:

$$\frac{\lambda^2}{16\pi^2}\iint_{\mathbb{R}^6}\frac{|\tilde{V}(x)||\tilde{V}(y)|}{|x-y|^2}e^{-2\sqrt{\tilde{C}(V)}|x-y|}\,dx\,dy=\frac{\lambda^2}{4\pi(1-g(\alpha)-\beta^{-1})^2}\int_{\mathbb{R}^3}(V\star K_{4\tilde{C}(V)})(x)V(x)dx$$
$$\leqslant\frac{\lambda^2}{4\pi(1-g(\alpha)-\beta^{-1})^2}\|V\|_{L^2}^2\|K_{4\tilde{C}(V)}\|_{L^1}$$
$$\leqslant\frac{\lambda^2}{8\pi(1-g(\alpha)-\beta^{-1})^2\sqrt{\tilde{C}(V)}}\|V\|_{L^2}^2,$$

where in the second and third line we used Cauchy–Schwarz and Young inequalities, respectively. Thus the bound (2.23) will be satisfied if the last expression is smaller than one. For a fixed $\beta>2(1-g(\alpha))^{-1}$ we can estimate $(1-g(\alpha)-\beta^{-1})^{-1/2}$ by $\sqrt{\beta}$, and consequently, the inequality (2.22) will hold uniformly in $\lambda\in[0;\lambda_0)$, as long as the positive constant $C(V)$ is chosen large enough to satisfy

$$\frac{\lambda_0^2\sqrt{\beta}\|V\|_{L^2}^2}{8\pi(1-g(\alpha)-\beta^{-1})^{3/2}}<\sqrt{\tilde{C}(V)}, \tag{2.24}$$

which we set out to prove. □

Note that the constants can be chosen explicitly. The left-hand side of (2.24) diverges as $\beta\to\infty$ and in the allowed interval it has a unique minimum at $\beta=4/[1-g(\alpha)]$ where it attains the value $2\lambda_0^2\|V\|_{L^2}^2/3\sqrt{3}\pi(1-g(\alpha))^2$. In other words, the lemma is valid for this β and

$$C(V)=\left(\frac{2\lambda_0^2\|V\|_{L^2}^2}{3\pi(1-g(\alpha))^2}\right)^2.$$

The reader may wonder that we have not used here fully our assumptions about the potential because for a bounded function $V\in L^2$ is a weaker requirement than $V\in L^{3/2}$, however, without the latter our main premise about the existence of the coupling constant threshold may not be valid.

Lemma 2.4 : The following estimates hold:

$$\|PL^{-1}D*D*\psi_\lambda\|^2\leqslant C_5 \tag{2.25}$$

and

$$\|PL^{-1}D*p\psi_\lambda\|^2\leqslant C_6(\alpha)\|p\psi_\lambda\|^2, \tag{2.26}$$

with positive C_5 and $C_6(\alpha)$ given in (2.28) and (2.29) below, depending on β and $C(V)$ of the previous lemma. Using the shifted Hamiltonian $\tilde{H}_f:=H_f+\alpha^3$, we have $C_6(\alpha)\sim\ln(\alpha^{-3})$ as $\alpha\to 0+$.

Proof: By means of (2.22) we get the estimates

$$L^{-1}P^2L^{-1}\leqslant L^{-1}[\beta(h_\alpha^\lambda+|e_\lambda|)+C(V)]L^{-1}\leqslant\frac{\beta}{2}H_f^{-1}+C(V)H_f^{-2}, \tag{2.27}$$

valid in the appropriate part of the state space, namely, when sandwiched between vectors annulated by P_f; in the second inequality we used the fact that for any pair of commuting operators B,C with C strictly positive we have $(B+C)^{-1}B(B+C)^{-1}\leqslant\frac{1}{2}C^{-1}$. In this way we arrive at

$$\|PL^{-1}D*D*\psi_\lambda\|^2\leqslant\left[\frac{\beta}{2}\langle 0|DDH_f^{-1}D*D*|0\rangle+C(V)\langle 0|DDH_f^{-2}D*D*|0\rangle\right]:=C_5 \tag{2.28}$$

and

$$\|PL^{-1}D*p\psi_\lambda\|^2 \leqslant \|p\psi_\lambda\|^2\frac{2}{3}\left[\frac{\beta}{2}\langle 0|DH_f^{-1}D*|0\rangle + C(V)\langle 0|DH_f^{-2}D*|0\rangle\right] := \|p\psi_\lambda\|^2 C_6(\alpha). \tag{2.29}$$

Now we come to the place where the shift matters because without it the right-hand side of (2.29) is infrared divergent. With the replacement $H_f \to H_f + \alpha^3$ we have

$$\langle 0|D[H_f+\alpha^3]^{-2}D*|0\rangle = 8\pi\int_0^1 d|k|\frac{|k|}{[|k|+\alpha^3]^2} = 8\pi(\ln(\alpha^{-3}) + \alpha^3 - 1), \tag{2.30}$$

which concludes the argument. Let us stress that this trick is mainly used for convenience since even without it the term on the left-hand side of (2.29) is finite, which can be seen by repeating the argument in Hainzl and Seiringer (2002), Eq. (4.4). □

Finally we come to our last technical result.

Lemma 2.5: Under the assumption (iii′) there is a positive constant C such that

$$|(\psi_\lambda; \Delta V\psi_\lambda)| \leqslant C(\psi_\lambda; |V|\psi_\lambda). \tag{2.31}$$

Proof: Since $V \in L^\infty$ the ground state is represented on $G := \mathrm{supp}V$ by a positive smooth function. Hence $\rho(\lambda) := \sup_G \psi_\lambda (\inf_G \psi_\lambda)^{-1}$ makes sense and satisfies $1 \leqslant \rho(\lambda) < \infty$; the same is true for $\lambda = (1-g(\alpha))\lambda_0$ corresponding to the zero-energy resonance. Using the standard estimate [Reed and Simon (1975), Thm. IX.28] one can check that $\lambda \mapsto \psi_\lambda$ is continuous in the $\|\cdot\|_\infty$ norm which implies continuity of the function ρ. Consequently, there are positive m and M such that

$$0 < m \leqslant \tilde{\psi}_\lambda(x) \leqslant M < \infty \tag{2.32}$$

holds for all $x \in G$, $\lambda \in]\lambda_0(1-g(\alpha)); \lambda_0]$, and a suitable family of non-normalized solutions (for ψ_λ both the infimum and supremum vanish, of course, as we approach the zero-energy resonance). It follows that

$$(\tilde{\psi}_\lambda; \Delta V\tilde{\psi}_\lambda) \leqslant M^2\|\Delta V\|_{L^1}, \tag{2.33}$$

while $(\tilde{\psi}_\lambda; |V|\tilde{\psi}_\lambda) \geqslant m^2\|V\|_{L^1}$ is positive, so it can majorize (2.33) when multiplied by a sufficiently large C. □

Now we are ready to complete the proof of the theorem. From the definitions of ψ_1 and ψ_2 and with the help of (2.25) and (2.26) we get

$$g(\alpha)\|P\Psi\|^2 \leqslant g(\alpha)(1 + 4\alpha C_6(\alpha))\|p\psi_\lambda\|^2 + \alpha^2 g(\alpha)C_5. \tag{2.34}$$

Using our assumptions about V we can write

$$(\psi_\lambda; |V|\psi_\lambda) = -(\psi_\lambda; V\psi_\lambda) = (1-g(\alpha))\|p\psi_\lambda\|^2 + |e_\lambda|,$$

which yields an estimate to the last term at the right-hand side of (2.17),

$$\|L^{-1/2}D*p\psi_\lambda\|^2 \geqslant \left[C_4(\mu) + \mu C_3(\mu) - \frac{\lambda}{2}C_3(\mu)C(1-g(\alpha))\right]\|p\psi_\lambda\|^2 - \frac{\lambda}{2}C_3(\mu)C|e_\lambda|; \tag{2.35}$$

in case of (iii) this follows from (1.1), whereas for (iii′) we employ Lemma 2.5. Next we insert into (2.11) from (2.34) and (2.35); in combination with Lemma 2.1 we obtain

$$(\Psi;H_\alpha^V\Psi) \leqslant \frac{\alpha}{\pi}\|\Psi\|^2 - \alpha^2\langle 0|DD\mathcal{A}_\alpha^{-1}D*D*|0\rangle \tag{2.36a}$$

$$-|e_\lambda|\|\Psi\|^2 + \alpha|e_\lambda|2\lambda C_3(\mu)C(1-a) \tag{2.36b}$$

$$+\left[g(\alpha)(1+4\alpha C_6(\alpha)-2\alpha(1-a)\lambda C_3(\mu)C)-4\alpha(1-a)\right.$$
$$\left.\times\left[C_4(\mu)+\mu C_3(\mu)-\frac{\lambda}{2}C_3(\mu)C\right]\right]\|p\psi_\lambda\|^2 \tag{2.36c}$$

$$+\alpha^2 g(\alpha)C_5 - \alpha^2 g(\alpha)C_1 + \tag{2.36d}$$

$$+\frac{4\alpha^3}{a}\|L^{-1/2}PDL^{-1}D*D*\psi_\lambda\|^2. \tag{2.36e}$$

Notice first that the term (2.36e) behaves as $\mathcal{O}(\alpha^3)$ for $\alpha\to 0$ which follows, e.g., from Hainzl, Hirokawa, and Spohn (2003), Lemma 15(v); thus it is irrelevant for the argument in the same way as the shift coming from the infrared regularization.

The main idea is now to choose the function $g(\alpha)$ in such a way that it cancels the factor in front of $\|p\psi_\lambda\|^2$ in (2.36c); this yields

$$g(\alpha) = \frac{4\alpha(1-a)\left[C_4(\mu)+\mu C_3(\mu)-\frac{\lambda}{2}C_3(\mu)C\right]}{1+4\alpha C_6(\alpha)-2\alpha(1-a)\lambda C_3(\mu)C}. \tag{2.37}$$

We choose also $\mu=(\lambda/2)C$ and fix the parameter in (2.10) by setting

$$1-a := \min\{(4C_4(\mu))^{-1}, C_6(\alpha)(\mu C_3(\mu))^{-1}, 3/4\};$$

this yields $g(\alpha)\leqslant\alpha$ which means that (2.36d) $=\mathcal{O}(\alpha^3)$.

On the other hand, since

$$\|\Psi\|^2 = 1 + 4\alpha\|L^{-1}D*p\psi_\lambda\|^2 + \alpha^2\|L^{-1}D*D*\psi_\lambda\|^2 = 1+\mathcal{O}(\alpha), \tag{2.38}$$

we deduce from (2.3) that

$$(2.36a) = E(\alpha,0)\|\Psi\|^2 + \mathcal{O}(\alpha^3).$$

We denote by $E(\beta)$ the bottom of the spectrum of $p^2+\beta V$, i.e.,

$$E(\beta) := \inf \operatorname{spec}(p^2+\beta V).$$

We have $E(\lambda_0)=0$ by assumption, and since the ground state represents always case (A) in the terminology of Klaus and Simon (1980); in other words, zero is not an eigenvalue of $p^2+\lambda_0 V$; we know that

$$E(\beta) = -b(V)(\beta-\lambda_0)^2 + \mathcal{O}((\beta-\lambda_0)^3), \tag{2.39}$$

holds for $\beta\geqslant\lambda_0$, close to λ_0, and for some positive constant $b(V)$ depending only on the potential V. Notice that the above asymptotic expansion coming from Klaus and Simon (1980), Theorem 2.3 was derived there for $V\in C_0^\infty(\mathbb{R}^3)$, however, an extension to the Rollnik class is straightforward. Recall now that

$$|e_\lambda| = -(1-g(\alpha))E(\lambda(1-g(\alpha))^{-1}).$$

Since $(1-g(\alpha))\lambda_0 < \lambda \leqslant \lambda_0$ holds by assumption and $g(\alpha)=\mathcal{O}(\alpha)$, we have

$$\lambda(1-g(\alpha))^{-1} - \lambda_0 \leqslant \lambda_0 g(\alpha)(1-g(\alpha))^{-1} = \mathcal{O}(\alpha),$$

and therefore

$$|e_\lambda| = b(V)\left(\frac{\lambda}{1-g(\alpha)} - \lambda_0\right)^2 + \mathcal{O}(\alpha^3),$$

where the first term at the right-hand side is $\mathcal{O}(\alpha^2)$. Returning to (2.36) we conclude from the last claim that the second term in (2.36b) is of order of α^3. This yields for all λ in the considered range and for small α the asymptotic inequality,

$$E(\alpha,\lambda V) \leqslant E(\alpha,0) - |e_\lambda| + \mathcal{O}(\alpha^3).$$

Since $b(V)>0$ the second term at the right-hand side is negative and dominates over the error for α sufficiently small. This demonstrates that the sought inequality (2.1) is valid under the assumptions we have made and thus it proves Theorem 1.

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Two-dimensional Riemannian and Lorentzian geometries from second-order ODE's

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In this paper we give an alternative geometrical derivation of the results recently presented by García-Godínez, Newman, and Silva-Ortigoza on the class of all two-dimensional Riemannian and Lorentzian metrics from second-order ODE's which are in duality with the two-dimensional Hamilton–Jacobi equation. We show that, as it happens in the null surface formulation of general relativity, the Wünschmann-type condition can be obtained as a requirement of a vanishing torsion tensor. Furthermore, from these second-order ODE's we obtain the associated Cartan connections. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In a couple of recent works, García-Godínez, Newman, and Silva-Ortigoza (GNS) presented the (pseudo-)Riemannian geometries which are hidden in a certain class of differential equations (those which satisfy a Wünschmann-type condition, $I_{\mathrm{GNS}}=0$). In the first of these works,[1] they studied how to obtain all two-dimensional Riemannian and Lorentzian metrics from a certain class of second-order ODE's. Furthermore, in Ref. 2, they extended their work and showed how to get all three-dimensional metrics from a certain class of three second-order PDE's and also from a certain class of third-order ODE's. From now on, we will say that these equations are in the GNS class.

The special status of these ODE's and PDE's is that they are in duality with the Hamilton–Jacobi equation. For example, if we have a second-order ODE in the GNS class,

$$u''=\Lambda(u,u',s), \tag{1}$$

and if we know a solution $u=Z(x^a,s)$, with $x^a=(x^1,x^2)$ integration constants, then this solution automatically satisfies the two-dimensional Hamilton–Jacobi equation:

$$g^{ab}\nabla_a Z\nabla_b Z=1, \tag{2}$$

where ∇_a means a differentiation with respect to x^a, and g^{ab}, is a (pseudo-)Riemannian metric constructed from Λ and its derivatives.

All these problems share similar characteristics with the problem of the null surface formulation (NSF) of general relativity in three and four dimensions.[3–6] In NSF, from a certain class of differential equations, known as the Wünschmann class, one can construct all three- and four-dimensional conformal Lorentzian metrics. The three-dimensional conformal metrics are obtained from a class of third-order ODE,

$$u'''=F(u,u',u'',s), \tag{3}$$

with F satisfying the so-called Wünschmann condition $I[F]=0$. Likewise, the four-dimensional metrics are obtained from a pair of second-order PDE's,

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$$u_{ss} = \Lambda(s, s^*, u, u_s, u_{s^*}, u_{ss^*}),$$
$$u_{s^*s^*} = \Lambda^*(s, s^*, u, u_s, u_{s^*}, u_{ss^*}), \tag{4}$$

where s and s^* are complex variables, and Λ and Λ^* satisfy the generalized Wünschmann condition $W[\Lambda, \Lambda^*]=0$ and its complex conjugate. It can be shown that $I[F]$ and $W[\Lambda, \Lambda^*]$ are invariant under contact transformations.[7–9] Again, these equations are in duality with another equation, namely the eikonal equation,

$$g^{ab}\nabla_a Z \nabla_b Z = 0. \tag{5}$$

and the level surfaces of the solution $u=Z(x^a, s)$ to (3), or $u=Z(x^a, s, s^*)$ to (4) are null surfaces of the respective metrics that they generate.

In NSF, the Wünschmann condition can be obtained in several ways.[3,10–12] Two of these were used by GNS to obtain the Wünschmann-type condition for differential equations in duality with the Hamilton–Jacobi equation. There exists a third method which is used in NSF, the torsion-free method, and from which one can obtain not only the Wünschmann class and its respective metrics, but also more geometrical structures associated to the equations, in particular all normal Cartan conformal connections.[13,12] In this paper we show that this method can also be applied to the problem of (pseudo-)Riemannian metrics discussed by GNS. In particular, we show how the torsion-free condition restricts the class of second-order ODE's to those belonging to the GNS class and such that we get all two-dimensional Riemannian and Lorentzian metrics, and respective Cartan connections.

In Sec. II we briefly present the notation and basic concepts about the geometry of second-order ODE's. In Sec. III, we show how to get the GNS class from the torsion-free condition, and construct the associated Cartan connections. Finally, in the conclusions, we discuss the extension of this approach to the problem of the GNS class of third-order ODE's.

II. NOTATION AND BASIC NOTIONS

Let the second-order ODE be

$$u'' = \Lambda(u, u', s), \tag{6}$$

where $s \in \mathbb{R}$ is the independent variable, and the primes denote derivative of the dependent variable u with respect to s.

On the jet-space J^1 with local coordinates (s, u, u') we consider the Pfaffian system $\mathcal{P}$

$$\omega^1 = \mathrm{d}u - u'\,\mathrm{d}s, \tag{7}$$

$$\omega^2 = \mathrm{d}u' - \Lambda\,\mathrm{d}s. \tag{8}$$

Local solutions of (6) are in one-to-one correspondence with integral curves γ: $\mathbb{R} \to J^1$ of $\mathcal{P}$ satisfying $\gamma^*\,\mathrm{d}s \neq 0$. These curves are generated by the vector field on J^1 given by

$$e_s \equiv D = \frac{\partial}{\partial s} + u'\frac{\partial}{\partial u} + \Lambda\frac{\partial}{\partial u'}. \tag{9}$$

We will restrict the domain of Λ to a open neighborhood U of J^1 where Λ is C^∞ and the Cauchy problem is well posed. Then, it follows from Frobenius theorem that the solution space M is a two-dimensional C^∞ manifold, and we will denote a given local coordinates system on it by $x^a = (x^1, x^2)$. It means that we can construct a map Z: $M \times \mathbb{R} \to \mathbb{R}$, $u=Z(x^a, s)$, such that by a given $x_0^a \in M$ the map $u=Z(x_0^a, s)$ is a solution of (6).

Then, if on $M \times \mathbb{R}$ we define a Pfaffian system $\mathcal{S}$ generated by

$$\beta^1 = Z_a \, \mathrm{d}x^a,$$

$$\beta^2 = Z'_a \, \mathrm{d}x^a$$

(where primes mean derivatives on s, and $Z_a = \partial_a Z$), it follows that there exist a diffeomorphism $\zeta\colon J^1 \to M \times \mathbb{R}$ which pulls back the Pfaffian system $\mathcal{S}$ on the system $\mathcal{P}$, i.e.,

$$\zeta^* \mathcal{S} = \mathcal{P}. \tag{10}$$

We will make use of this diffeomorphism later.

III. RIEMANNIAN AND LORENTZIAN GEOMETRIES FROM SECOND-ORDER ODE's

From ω^1, ω^2 which generate the Pfaffian system $\mathcal{P}$, we construct the following one-forms:

$$\theta^1 = \frac{1}{\sqrt{2}}(\omega^1 + a\omega^2), \tag{11}$$

$$\theta^2 = \frac{1}{\sqrt{2}}(\omega^1 - a\omega^2), \tag{12}$$

where $a = a(s, u, u')$ is a nonvanishing function to be determined. Next, we construct a degenerate metric on J^1,

$$h(u, u', s) = 2\theta^{(1} \otimes \theta^{2)} = \eta_{ij} \theta^i \otimes \theta^j, \tag{13}$$

where

$$\eta_{ij} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Note that if $a^2 > 0$, then θ^1 and θ^2 behave as null real vectors, and if $a^2 < 0$, they are complex null vectors.

Let ω^i_j be a connection such that we have the following.

(A) The connection is skew-symmetric,

$$\omega_{ij} = \omega_{[ij]}, \tag{14}$$

where $\omega_{ij} = \eta_{ik}\omega^k{}_j$.

(B) The one-forms θ^1 and θ^2 satisfy the Cartan's torsion-free first structure equations,

$$T^i \equiv \mathrm{d}\theta^i + \omega^k{}_j \wedge \theta^j = 0. \tag{15}$$

Now, we state and prove the following theorem.

Theorem: *The Torsion-free condition on the skew-symmetric connection:*

(1) *uniquely determines the connection, with the only nonvanishing component given by*

$$\omega_{[12]} = -\frac{1}{\sqrt{2}}(\ln a)_u \theta^1 + \frac{1}{\sqrt{2}}(\ln a)_u \theta^2 + \frac{1}{a}\mathrm{d}s, \tag{16}$$

(2) *uniquely determines the function a in terms of* Λ,

$$a^2 = \frac{1}{\Lambda_u}, \tag{17}$$

(3) *impose a Wünschmann-type condition on* Λ,

$$I_{\mathrm{GNS}} = Da + a\Lambda_{u'} = 0. \tag{18}$$

Proof: From (11) and (12) we have

$$\mathrm{d}\theta^1 = -\frac{1}{\sqrt{2}a}a_u\theta^1\wedge\theta^2 - \frac{1}{2a}(1 + Da + a^2\Lambda_u + a\Lambda_{u'})\theta^1\wedge\mathrm{d}s - \frac{1}{2a}(-1 - Da + a^2\Lambda_u - a\Lambda_{u'})\theta^2\wedge\mathrm{d}s, \tag{19}$$

$$\mathrm{d}\theta^2 = \frac{1}{\sqrt{2}a}a_u\theta^1\wedge\theta^2 + \frac{1}{2a}(-1 + Da + a^2\Lambda_u + a\Lambda_{u'})\theta^1\wedge\mathrm{d}s + \frac{1}{2a}(1 - Da + a^2\Lambda_u - a\Lambda_{u'})\theta^2\wedge\mathrm{d}s. \tag{20}$$

The condition of free torsion (15) reads

$$\mathrm{d}\theta^1 - \omega_{[12]}\wedge\theta^1 = 0, \tag{21}$$

$$\mathrm{d}\theta^2 + \omega_{[12]}\wedge\theta^2 = 0, \tag{22}$$

and by solving these equations we get

$$\omega_{[12]} = -\frac{1}{\sqrt{2}}(\ln a)_u\theta^1 + \frac{1}{\sqrt{2}}(\ln a)_u\theta^2 + \frac{1}{2a}(1 + Da + a^2\Lambda_u + a\Lambda_{u'})\mathrm{d}s, \tag{23}$$

together for the three conditions,

$$(-1 - Da + a^2\Lambda_u - a\Lambda_{u'}) = 0, \tag{24}$$

$$(-1 + Da + a^2\Lambda_u + a\Lambda_{u'}) = 0, \tag{25}$$

$$(Da + a\Lambda_{u'}) = 0. \tag{26}$$

Finally, from (23), and the conditions (24), (25), and (26) we get the results stated in the theorem. Q.E.D.

Note now, that with the map ζ: $J^1\to M\times\mathbb{R}$ discussed in Sec. II, we have a one-parameter family of (pseudo-)Riemannian metrics in the solution space M (Riemannian metrics if $\Lambda_u<0$, and Lorentzian metrics if $\Lambda_u>0$), i.e., we have the following family of metrics:

$$g(x^a,s) = (\zeta^{-1})^* h, \tag{27}$$

or written in coordinates,

$$g(x^a,s) = \beta^1\otimes\beta^1 - \frac{1}{\Lambda_u}\beta^2\otimes\beta^2 = \left[Z_aZ_b - \frac{1}{\Lambda_u}Z'_aZ'_b\right]\mathrm{d}x^a\,\mathrm{d}x^b. \tag{28}$$

In fact, they are equivalents, because it is easy to show that h satisfies

$$\mathfrak{L}_{e_s}h = 0. \tag{29}$$

Finally, let us collect the one-forms θ^i and ω^i_j into the matrix-valued one-form

$$\omega_c = \begin{pmatrix} 0 & 0 & 0 \\ \theta^1 & -\omega_{[12]} & 0 \\ \theta^2 & 0 & \omega_{[12]} \end{pmatrix},$$

and let us study two cases.

(a) $\Lambda_u > 0$: In this case we have a Lorentzian metric, and ω_c takes its values in the Lie algebra of $\mathrm{SO}(1,1) \rtimes \mathrm{R}^2$.

This matrix valued one-form can be regarded as a $\mathrm{SO}(1,1) \rtimes \mathrm{R}^2$ Cartan connection[14] on the principal bundle $\mathrm{SO}(1,1) \to \mathrm{P} \to M$ with associated curvature $\Omega_c = \mathrm{d}\omega_c + \omega_c \wedge \omega_c$ given by

$$\Omega_c = \begin{pmatrix} 0 & 0 & 0 \\ T^1 & \Omega_1^1 & \Omega_2^1 \\ T^2 & \Omega_1^2 & \Omega_2^2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -R & 0 \\ 0 & 0 & R \end{pmatrix}, \tag{30}$$

where $\Omega_j^i = \mathrm{d}\omega_j^i + \omega_k^i \wedge \omega_j^k$ is the standard curvature, and

$$R = -\frac{1}{a} a_{uu} \theta^1 \wedge \theta^2. \tag{31}$$

(b) $\Lambda_u < 0$: In this case we have a Riemannian metric, and ω_c takes its values in the Lie algebra of $\mathrm{SO}(2) \rtimes \mathrm{R}^2$.

This construction gives a $\mathrm{SO}(2) \rtimes \mathrm{R}^2$ Cartan connection on the principal bundle $\mathrm{SO}(2) \to \mathrm{P} \to M$ with associated curvature $\Omega_c = \mathrm{d}\omega_c + \omega_c \wedge \omega_c$ given by a similar formula to (30).

IV. CONCLUSIONS

In this paper we show that, as it happens in NSF, all two-dimensional Riemannian and Lorenztian metrics can be obtained from the geometrical condition of a torsion-free connection. Furthermore, we construct all associated Cartan connections to these equations. This approach can be extended to the study of third-order ODE and a pair of second-order PDE's, but the choice of the differential quadratic form h, is not *a priori* so clear. In fact, all these problems should be studied with the Cartan's equivalence method[15] applied to differential equation under a subgroup of contact transformations: the canonical transformations. With this algorithmic method, the group arising from these equations can be naturally obtained as the group of allowed transformations in the study of the equivalence problem. Work in this area has begun.

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Comments on matter collineations of plane symmetric, cylindrically symmetric, and spherically symmetric space–times

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Recently matter collineations (MCs) of plane symmetric static[1] and cylindrically symmetric static space–times[2] have been presented. Earlier, the same author also classified spherically symmetric static space–times according to their MCs.[3] For an energy-momentum tensor $\mathbf{T}$, we call $\boldsymbol{\xi}$ an MC if

$$\pounds_{\boldsymbol{\xi}}\mathbf{T} = 0. \tag{1}$$

In component form, Eq. (1) becomes the MC equation

$$T_{ab,c}\xi^{c} + T_{ac}\xi^{c}{}_{,b} + T_{bc}\xi^{c}{}_{,a} = 0.$$

In these equations, if $\mathbf{T}$ is replaced by the Ricci tensor $\mathbf{R}$ then the vector $\boldsymbol{\xi}$ is called a Ricci collineation (RC). Noting the apparently similar form of the equations and the role of the matter and Ricci tensors in the Einstein field equations (EFEs)

$$R_{ab} - \tfrac{1}{2}Rg_{ab} = \kappa T_{ab}, \tag{2}$$

the author merely replaced the Ricci tensor by the matter tensor in Refs. 4–6 for the classification according to RCs of plane symmetric, cylindrically symmetric, and spherically symmetric static space–times, respectively. All that remains to be done is to check that the RCs satisfy the MC equations. Even if he has done so, errors persist in his papers. For example, because of the error in calculations the Lie algebra for a case, as given in Eq. (B47) of Ref. 4, does not close. This error has been carried over in Eqs. (43) of his paper (Ref. 1). (A typographical error there is carried over as well.) Now, as plane symmetry can locally be considered as a special case of cylindrical symmetry, this particular case appears in Ref. 5 also, where it has been corrected. This correction has been carried over into Eqs. (27) of his paper (Ref. 2) as well, but the author has not cited these papers.

It is worth mentioning a serious misconception in the three subject papers (Refs. 1–3) that was not imported from the Ricci collineation papers. The author says that there are "three, four, five, six, seven, or ten MCs out of which three are isometries and the rest are proper."[1,2] He has assumed that the isometry group is minimal. This is simply incorrect as there are numerous cases of nonminimal isometry groups. It is possible that all the four, five, six, seven, or ten MCs may be isometries and there may be no proper MCs. A similar problem arises for the spherically symmetric case.[3]

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We also mention here that Ref. 7, on the same subject as Ref. 1, does not only classify the plane symmetric space–times (with the correct Lie algebras provided) but it discusses the issue of the relationship between the RCs and MCs and also provides a number of explicit examples for that purpose. We will not go into further detail on this because this is the subject of a separate full-length study[8] in itself.

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Addendum: Symmetries of the energy-momentum tensor

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In recent papers [J. Math. Phys. **44**, 5142 (2003); **45**, 1518 (2003); **45**, 1532 (2004)] we have discussed matter symmetries of nonstatic spherically symmetric space–times, static plane symmetric space–times, and cylindrically symmetric static space–times. These have been classified for both cases when the energy-momentum tensor is nondegenerate and also when it is degenerate. Here we add up some consequences and the missing references about the Ricci tensor. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1777404]

Recently, we have presented a detailed analysis of matter collineations (MCs) for nonstatic spherically symmetric space–times,[1] static plane symmetric space–times,[2] and cylindrically symmetric static space–times.[3] We have discussed in detail the matter symmetries for each of the metrics and have found the corresponding constraint equations. In general, it is not easy to solve these constraint equations, sometimes the solution of the constraint equations may not exist. We have constructed some examples which help us in exploring the difference between RCs and MCs.

It is usually believed that matter and Ricci symmetries are the similar symmetries and one can find MCs directly from the RCs. However, this is not true in general. This has been shown in many papers on this topic.[1–9] In this short communication, we express this difference with examples. Further, we add up some references missing in Refs. 1–3 which should have been inserted there.

Let (M,g) be a space–time manifold with signature $(+,-,-,-)$. It is assumed that the manifold M, and the metric g, are smooth. Einstein's field equations (EFEs), which relate the geometry and matter, are given by

$$R_{ab} - \tfrac{1}{2}Rg_{ab} \equiv G_{ab} = \kappa T_{ab} \quad (a,b = 0,1,2,3), \tag{1}$$

where κ is the gravitational constant, G_{ab} is the Einstein tensor, R_{ab} is the Ricci, and T_{ab} is the matter (energy-momentum) tensor. Also, $R=g^{ab}R_{ab}$ is the Ricci scalar. It is obvious from EFEs that for vacuum space–times, $R_{ab}=T_{ab}$ and consequently, RCs and MCs are similar in this special case.

We define a differentiable vector field ξ on M to be a matter collineation if $\pounds_\xi T_{ab}=0$ which can be written in component form as

$$T_{ab,c}\xi^c + T_{ac}\xi^c_{,b} + T_{cb}\xi^c_{,a} = 0, \tag{2}$$

where $\pounds$ is the Lie derivative operator, ξ^a is the symmetry or collineation vector. Since the Einstein tensor is related to the matter content of the space–time by the EFEs, the investigation of MCs seems to be more relevant from the viewpoint of physics. Here we would not give details of the calculations as the procedure has been explicitly given in the papers.[1–3] Rather we would explore the difference of RCs and MCs for nonstatic spherically symmetric, static plane symmetric, and cylindrically symmetric static space–times with the help of examples.

The most general form of the metric for a spherically symmetric space–time is given by

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$$ds^2 = e^{\nu(t,r)}\,dt^2 - e^{\mu(t,r)}\,dr^2 - e^{\lambda(t,r)}\,d\Omega^2, \tag{3}$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta\, d\phi^2$. The surviving components of the energy-momentum tensor are $T_{00}, T_{01}\ T_{11}, T_{22}, T_{33}$, where $T_{33} = \sin^2\theta T_{22}$. We have found[1] that, for the nondegenerate case, there exist either four, six, seven or ten independent MCs in which four are isometries and the rest are the proper. For the degenerate case, most of the cases give the infinite-dimensional MCs. The worth-noting cases are those where the energy-momentum tensor is degenerate but the group of MCs is finite dimensional, i.e., four or ten. Similar analysis has been given in the paper[10] for the Ricci tensor. It can be seen from the comparison of the two papers[1,10] that MCs and RCs turn out to be the same but the constraint equations are entirely different. For example, in the Einstein/anti-Einstein metric, we obtain seven MCs[5] but RCs are infinite dimensional.

The metric for static plane symmetric space–times is given in the form[11]

$$ds^2 = e^{\nu(x)}\,dt^2 - dx^2 - e^{\mu(x)}(dy^2 + dz^2). \tag{4}$$

The surviving components of the energy-momentum tensor are T_0, T_1, T_2, T_3, where $T_3 = T_2$. When we solve MC equations for the static plane symmetric space–times it turns out[2] that the nondegenerate case yields either four, five, six, seven or ten independent MCs in which four are isometries and the rest are proper. We have also obtained three interesting cases where the energy-momentum tensor is degenerate but the group of MCs is finite dimensional which are either four, six or ten.

Again when we compare the analysis given in the two papers,[2,12] it is concluded that RCs and MCs are similar but with different constraint equations. We can construct some examples by solving these constraint equations which exhibit the difference between RCs and MCs admitted by the space–time. Consider the following plane symmetric static space–time:

$$ds^2 = (ax + b)^2\,dt^2 - dx^2 - (cx + d)^2(dy^2 + dz^2), \tag{5}$$

where $a, b, c, d \in \Re, ac \neq 0 \neq ad - bc$. In this example, we obtain five MCs in which three are the usual isometries and the remaining two are proper MCs but the RCs are infinite dimensional.

The most general form of cylindrically symmetric static space–time is given by

$$ds^2 = e^{\nu(r)}\,dt^2 - dr^2 - e^{\lambda(r)}\,d\theta^2 - e^{\mu(r)}\,dz^2. \tag{6}$$

The only nonzero components of the energy-momentum tensor turn out to be $T_{00}, T_{11}, T_{22}, T_{33}$. We have found[3] that the nondegenerate energy-momentum tensor gives either three, four, five, six, seven or ten independent MCs in which three are isometries and the rest are proper. There are four worth-mentioning cases where we have obtained the group of MCs finite dimensional, even the energy-momentum tensor is degenerate, i.e., either three, four, five or ten. It can be seen from the two papers[3,13] that RCs and MCs become similar but the constraints are different. Here we present examples by solving these constraints which give different space–times for the two collineations.

The following cylindrically symmetric metric,

$$ds^2 = \cosh^2 cr\,dt^2 - dr^2 - (\cosh cr)^{-1}\,d\theta^2 - (\cosh cr)^{-1}\,dz^2, \tag{7}$$

where c is an arbitrary constant, admits four MCs and also four isometries but it has seven RCs. The space–time

$$ds^2 = (r/r_0)^{2a}\,dt^2 - dr^2 - (r/r_0)^{2a}\,d\theta^2 - (r/r_0)^{2a}\,dz^2, \tag{8}$$

where a and r_0 are arbitrary constants such that $a \neq 0, 1$, admits ten MCs with six KVs but seven RCs. Taking $\nu = \lambda = \mu$ in Eq. (6), this metric admits six MCs and also six KVs but seven RCs. The following space–time,

$$ds^2 = (\cosh cr)^{-1}\,dt^2 - dr^2 - \cosh^2 cr\,d\theta^2 - (\cosh cr)^{-1}\,dz^2, \tag{9}$$

has four MCs and also four KVs but seven RCs.

In this addendum, we have provided examples which clearly indicate the difference of the symmetries for the Ricci and matter tensors. Also, we have incorporated the missing references in the previous papers.[1–3] It is mentioned here that RCs and MCs will exactly be similar for those space–times where $R_{ab}=T_{ab}$ or equivalently for vacuum space–times. For example, in the case of Schwarzschild metric, every direction is RC/MC.

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Almost sharp quantum effects

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Quantum effects are represented by operators on a Hilbert space satisfying $0 \leqslant A \leqslant I$, and sharp quantum effects are represented by projection operators. We say that an effect A is almost sharp if $A=PQP$ for projections P and Q. We give simple characterizations of almost sharp effects. We also characterize effects that can be written as longer products of projections. For generality we first work in the formalism of von Neumann algebras. We then specialize to the full operator algebra $B(H)$ and to finite dimensional Hilbert spaces. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1806532]

I. INTRODUCTION

Let H be a complex Hilbert space that represents the state space of a quantum system $\mathcal{S}$. The set of *effects* $\mathcal{E}(H)$ for $\mathcal{S}$ is the set of operators on H satisfying $0 \leqslant A \leqslant I$. Effects represent yes–no measurements that may be unsharp (imprecise, fuzzy). It is interesting that many of the important classes of quantum operators are given by subsets of $\mathcal{E}(H)$. For example, the *sharp* yes–no measurements are represented by the set of projection operators $\mathcal{P}(H) \subset \mathcal{E}(H)$. A *state* for $\mathcal{S}$ is represented by an operator $W \in \mathcal{E}(H)$ satisfying $\mathrm{tr}(W)=1$. We call W a *density operator* and denote the set of density operators by $\mathcal{D}(H)$. The *pure states* for $\mathcal{S}$ are given by $\mathcal{D}(H) \cap \mathcal{P}(H)$.

The probability that $A \in \mathcal{E}(H)$ has values yes (or is true) in the state $W \in \mathcal{D}(H)$ is given by $p_W(A)=\mathrm{tr}(WA)$. If W happens to be a pure state corresponding to the unit vector ψ, then $p_W(A) = \langle A\psi, \psi \rangle$. In particular, sharp effects are called *quantum events* and the probability that event $Q \in \mathcal{P}(H)$ occurs in the state $W \in \mathcal{D}(H)$ is $p_W(Q)=\mathrm{tr}(WQ)$. For $P, Q \in \mathcal{P}(H)$ we define the *conditional probability of Q given P* in the state W by

$$p_W(Q|P) = \frac{\mathrm{tr}(PWPQ)}{\mathrm{tr}(WP)} = \frac{\mathrm{tr}(WPQP)}{\mathrm{tr}(WP)}$$

from which we obtain

$$p_W(PQP) = \mathrm{tr}(WPQP) = p_W(P)p_W(Q|P). \tag{1.1}$$

Now (1.1) is analogous to the traditional probability formula

$$p(A \cap B) = p(A)p(B|A)$$

so in some sense PQP corresponds to an intersection of events. However, in general $p_W(PQP) \neq p_W(QPQ)$ so the order of measurements is relevant. In fact, $P \circ Q = PQP$ corresponds to a sequential measurement in which we measure P first and Q second. We call $P \circ Q$ the *sequential product* of P and Q (see Refs. 2 and 3). More generally, we define the *sequential product* $A \circ B = A^{1/2}BA^{1/2} \in \mathcal{E}(H)$ for any $A, B \in \mathcal{E}(H)$ but our main interest is in sequential products of sharp effects. The form $P \circ Q = PQP$ for projective measurements is well established, but the general form $A \circ B = A^{1/2}BA^{1/2}$ is not unique and depends on the particular measurement technique. In general, we may have a sequential product given by C^*BC where C is any operator satisfying $C^*C=A$. Note however that $C=A^{1/2}$ is the simplest such operator and moreover in this case $C \in \mathcal{E}(H)$. The next result gives some of the important properties of the sequential product.

Theorem 1 (Ref. 3): *Let $A, B \in \mathcal{E}(H)$, $P, Q \in \mathcal{P}(H)$. Then*

(1) $A\circ B=B\circ A$ *if and only if* $AB=BA$.
(2) *If* $A\circ B\in\mathcal{P}(H)$ *then* $AB=BA$.
(3) $P\circ Q\in\mathcal{P}(H)$ *if and only if* $PQ=QP$.

If $AB=BA$ we say that A and B are *compatible*. Physically, compatible effects correspond to effects that are simultaneously measurable. Thus, A and B are simultaneously measurable if and only if their order of measurement is irrelevant. A state $W\in\mathcal{D}(H)$ is *faithful* if $\mathrm{tr}(WA)=0$ for $A\in\mathcal{E}(H)$ implies that $A=0$. The next result gives an interesting probabilistic characterization of compatible sharp effects.

Corollary 2: For $P,Q\in\mathcal{P}(H)$ *and faithful* $W\in\mathcal{D}(H)$, $PQ=QP$ *if and only if* $p_W(Q\circ P)\leqslant p_W(Q\circ(P\circ Q))$.

Proof: Suppose that $p_W(Q\circ P)\leqslant p_W(Q\circ(P\circ Q))$. Then

$$\mathrm{tr}[W(QPQ-QPQPQ)]\leqslant 0.$$

It is easy to check that $PQP\leqslant P$ and it follows that $QPQPQ\leqslant QPQ$. Hence, $QPQ-QPQPQ\in\mathcal{E}(H)$ so that

$$\mathrm{tr}[W(QPQ-QPQPQ)]=0.$$

Since W is faithful, we conclude that

$$QPQ=QPQPQ=(QPQ)^2.$$

Thus, $Q\circ P=QPQ\in\mathcal{P}(H)$ so by part 3 of Theorem 1, $PQ=QP$. The converse is trivial. ■

The next corollary solves Problem 11028 in the American Mathematical Monthly [Vol. 110, p. 636 (2003)].

Corollary 3: Let $\dim(H)=n<\infty$ *and let* $P,Q\in\mathcal{P}(H)$. *Then* $PQ\in\mathcal{P}(H)$ *if and only if* $\mathrm{tr}(PQ)=\mathrm{tr}(PQPQ)$.

Proof: Notice that $W=(1/n)I\in\mathcal{D}(H)$ is faithful and

$$p_W(Q\circ P)=\mathrm{tr}(WQPQ)=\frac{1}{n}\mathrm{tr}(QPQ)=\frac{1}{n}\mathrm{tr}(PQ).$$

Assuming that $\mathrm{tr}(PQ)=\mathrm{tr}(PQPQ)$ we have that

$$p_W(Q\circ P)=\frac{1}{n}\mathrm{tr}(QPQP)=p_W(Q\circ(P\circ Q)).$$

By Corollary 1.2 we have $PQ=QP$ so that $PQ\in\mathcal{P}(H)$. The converse is trivial. ■

One of our main concerns is to characterize effects of the form $A=P\circ Q$ for $P,Q\in\mathcal{P}(H)$. Such effects are called *almost sharp* because they may be obtained by measuring two sharp effects. In a sense, almost sharp effects are "close" to being sharp and we shall present a simple characterization of such effects. Defining the *negation* of $A\in\mathcal{E}(H)$ by $A'=I-A$, we see immediately that $A'\in\mathcal{E}(H)$. We say that A is *nearly sharp* if both A and A' are almost sharp. We shall show that the set of nearly sharp effects has the structure of an orthocomplemented partially ordered set.

Letting $\mathcal{P}_1(H)=\mathcal{P}(H)$ and $\mathcal{P}_2(H)$ be the set of almost sharp elements we see that

$$\mathcal{P}_2(H)=\{A\in\mathcal{E}(H):A=P_1\circ P_2,P_1,P_2\in\mathcal{P}(H)\}$$

and it follows from part 3 of Theorem 1 that $\mathcal{P}_2(H)$ strictly contains $\mathcal{P}_1(H)$. We shall show that

$$\mathcal{P}_3(H)=\{A\in\mathcal{E}(H):A=P_1\circ(P_2\circ P_3),P_1,P_2,P_3\in\mathcal{P}(H)\}$$

strictly contains $\mathcal{P}_2(H)$ if dim (H) is sufficiently large. This suggests the natural problem of when $A\in\mathcal{E}(H)$ has the form

$$A = P_1 \circ (P_2 \circ \cdots \circ (P_{n-1} \circ P_n)). \tag{1.2}$$

Writing (1.2) in terms of operator products gives

$$A = P_1 P_2 \cdots P_{n-1} P_n P_{n-1} \cdots P_2 P_1.$$

We shall also characterize effects that have the form (1.2)

For generality we shall first work in the formalism of a von Neumann algebra. We then consider the full operator algebra $B(H)$ for H separable. Finally, we show that simplifications and further insights can be obtained from considering finite dimensional Hilbert spaces.

II. EFFECTS ON VON NEUMANN ALGEBRAS

Let M be a von Neumann algebra on a Hilbert space H. The set of effects in M is

$$\mathcal{E}(M) = \{A \in M : 0 \leqslant A \leqslant I\}$$

and the set of projections or sharp effects in M is

$$\mathcal{P}(M) = \{P \in M : P = P^* = P^2\} \subset \mathcal{E}(M).$$

For $P, Q \in \mathcal{P}(M)$, according to the usual comparison of projections we define $P \leqslant Q$ if there exists a partial isometry $U \in M$ such that $U^*U = P$ and $UU^* \leqslant Q$. Notice that UU^* is a projection whose range is contained in the range of Q.

For $A \in \mathcal{E}(M)$ we define P_A to be the projection onto the closure of the range of A. It can be shown that

$$P_A = \lim_{n \to \infty} A^{1/n}$$

in the strong operator topology so that $P_A \in M$. Moreover, $P_A A = A P_A = A$. Letting N_A be the projection onto the null space of A we have that

$$N_A = I - P_A = (P_A)'.$$

It is easy to check that P_A is the smallest projection satisfying $A \leqslant P_A$, $N_{A'}$ is the largest projection satisfying $N_{A'} \leqslant A$ and that

$$N_{A'} = \lim_{n \to \infty} A^n.$$

It follows that $N_A = \lim_{n \to \infty} (A')^n$ and hence

$$N_{A'} A = A N_{A'} = N_{A'}.$$

Notice that if $A \in \mathcal{E}(M)$ has the form $A = PQP$ for some $P, Q \in \mathcal{P}(M)$, then we also have that $A = P_A Q P_A$.

Lemma 4: For $A \in \mathcal{E}(M)$ we have that $P_{AA'} = P_A - N_{A'}$.

Proof: It is clear that $AA' \in \mathcal{E}(M)$, $AA' \leqslant A$, and $AA' \leqslant A'$. Hence, $P_{AA'} \leqslant P_A$, $P_{AA'} \leqslant P_{A'}$, and it follows that $N_A \leqslant N_{AA'}$ and $N_{A'} \leqslant N_{AA'}$. Since N_A and $N_{A'}$ are mutually orthogonal we conclude that $N_A + N_{A'} \leqslant N_{AA'}$. To prove the reverse inequality, let $x \neq 0$ satisfying $N_{AA'} x = x$. Write $x = Ax + A'x$ and notice that $A'(Ax) = 0$ and $A(A'x) = 0$. Then $Ax = N_{A'}(Ax)$ and $A'x = N_A(A'x)$. Since $N_{A'} A = N_{A'}$ and $N_A A' = N_A$, we have that $x = N_A x + N_{A'} x$. We conclude that $N_A + N_{A'} = N_{AA'}$. Therefore

$$P_{AA'} = I - N_{AA'} = I - N_A - N_{A'} = P_A - N_{A'}.$$

■

In the process of proving Lemma 4 we also obtained the interesting result $N_A + N_{A'} = N_{AA'}$.

The motivation for the next theorem is the following: If $0 \leqslant A \leqslant I$, then

$$\begin{pmatrix} A & \sqrt{AA'} \\ \sqrt{AA'} & A' \end{pmatrix}$$

is a projection whose compression to the (1,1) component is A.

Theorem 5: *An effect $A\in\mathcal{E}(M)$ is almost sharp if and only if $P_{AA'}\leqslant N_A$.*

Proof: Suppose that $P_{AA'}\leqslant N_A$. Then there exists a partial isometry $U\in M$ such that $U^*U=P_{AA'}$ and $UU^*\leqslant N_A$. Then U maps the range of $P_{AA'}$ into the range of N_A and U^* maps the range of N_A into the range of $P_{AA'}$. Notice that $N_{A'}=P_A-P_{AA'}$, $P_{AA'}$, and N_A are mutually orthogonal projections satisfying

$$N_A+N_{A'}+P_{AA'}=I. \tag{2.1}$$

Define Q_1 by the formula

$$Q_1=P_{AA'}AP_{AA'}+P_{AA'}\sqrt{AA'}U^*N_A+N_AU\sqrt{AA'}P_{AA'}+N_AUA'U^*N_A.$$

It is clear that $Q_1=Q_1^*$ and to show that $Q_1\in\mathcal{P}(M)$ we have

$$\begin{aligned} Q_1^2=&P_{AA'}(A^2+\sqrt{AA'}U^*N_AU\sqrt{AA'})P_{AA'}+P_{AA'}(AP_{AA'}\sqrt{AA'}U^*+\sqrt{AA'}U^*N_AUA'U^*)N_A\\ &+N_A(U\sqrt{AA'}P_{AA'}A+UA'U^*N_AU\sqrt{AA'})P_{AA'}+N_A(U\sqrt{AA'}P_{AA'}\sqrt{AA'}U^*\\ &+UA'U^*N_AUA'U^*)N_A. \end{aligned} \tag{2.2}$$

Notice that

$$U=N_AU=UP_{AA'}=N_AUP_{AA'} \tag{2.3}$$

and hence

$$P_{AA'}=U^*N_AU. \tag{2.4}$$

By (2.4) the first term in (2.2) becomes

$$P_{AA'}(A^2+AA')P_{AA'}=P_{AA'}AP_{AA'}.$$

By (2.4) again, the second term in (2.2) becomes

$$P_{AA'}(A\sqrt{AA'}U^*+A'\sqrt{AA'}U^*)N_A=P_{AA'}\sqrt{AA'}U^*N_A.$$

In a similar way, the third term in (2.2) becomes

$$N_A(UA\sqrt{AA'}+UA'\sqrt{AA'})P_{AA'}=N_AU\sqrt{AA'}P_{AA'}.$$

Finally, by (2.3) and (2.4) the fourth term in (2.2) becomes

$$N_AU(AA'+P_{AA'}A'A')U^*N_A=N_AU(AA'+A'A')U^*N_A=N_AUA'U^*N_A.$$

We conclude that $Q_1\in\mathcal{P}(M)$. To show that $Q_1\leqslant P_{AA'}+N_A$ we have that

$$Q_1(P_{AA'}+N_A)=(P_{AA'}+N_A)Q_1=Q_1.$$

Since $N_{A'}$ is orthogonal to $P_{AA'}$ and N_A we see that

$$Q=N_{A'}+Q_1\in\mathcal{P}(M).$$

Since $N_{A'}\leqslant A\leqslant P_A$, $P_{AA'}\leqslant P_A$, and $P_AN_A=0$ we have by Lemma 4 that

$$P_AQP_A = P_AN_{A'}P_A + P_AQ_1P_A = N_{A'} + P_{AA'}Q_1P_{AA'} = N_{A'} + P_{AA'}AP_{AA'}$$
$$= N_{A'} + (P_A - N_{A'})A(P_A - N_{A'}) = N_{A'} + (P_A - N_{A'})A$$
$$= N_{A'} + P_AA - N_{A'}A = N_{A'} + A - N_{A'} = A.$$

Conversely, suppose that there exists a $Q \in \mathcal{P}(M)$ such that $A = P_AQP_A$. Letting $B = P_AQN_A$ we have that $BB^* \geqslant 0$ and

$$BB^* = P_AQN_AQP_A = P_AQ(I - P_A)QP_A = P_AQP_A - P_AQP_AQP_A = A - A^2 = AA'.$$

Using the polar decomposition of B we find a partial isometry $U \in M$, with initial space P_{B^*}, the range of B^*, and final space P_B, the range of B, such that $B = \sqrt{AA'}U$. Now

$$P_B = P_{BB^*} = P_{AA'}$$

and since $P_{B^*} \leqslant N_A$ we obtain that $UU^* = P_{AA'}$ and $U^*U \leqslant N_A$. Hence, $P_{AA'} \leqslant N_A$. ■

We can gain an intuitive feeling for Theorem 5 as follows. Since $AA' = A - A^2$ we see that A is sharp iff $AA' = 0$ or equivalently $P_{AA'} = 0$. Now Theorem 5 states that A is almost sharp if and only if $P_{AA'}$ is not too big in the sense that $P_{AA'}$ is dominated by N_A. Recall that a *factor* is a von Neumann algebra with trivial center and that in this case all projections are comparable relatively to $\leqslant$. It follows that projections have a well-defined dimension $\dim(P)$ in a factor.

Corollary 6: If M is a factor, then an effect $A \in \mathcal{E}(M)$ is almost sharp if and only if $\dim(P_{AA'}) \leqslant \dim(N_A)$.

Corollary 6 is not true if M is not a factor even when there is a well-defined dimension function. To show this, let M_n be the matrix algebra of $n \times n$ complex matrices and let M be the von Neumann algebra $M = M_n \oplus M_n$. Let $I_n \in M_n$ be the identity matrix and let

$$A = \frac{1}{2}I_n \oplus 0 = \begin{bmatrix} 1/2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1/2 \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{bmatrix} \in M_n \oplus M_n.$$

Then $\dim(P_{AA'}) = \dim(N_A) = n$ but A cannot be written in the form P_AQP_A for some projection Q in $M = M_n \oplus M_n$.

Applying Corollary 6, a moment thought shows that $A \in \mathcal{E}(M)$ is almost sharp if and only if A^n is almost sharp for every positive integer n. This gives the nontrivial result that if $A = P_AQP_A$ for $Q \in \mathcal{P}(M)$, then $A^n = P_AQ_nP_A$ for some $Q_n \in \mathcal{P}(M)$.

In a type III factor, all proper projections are equivalent (have the same dimension). Recall that if A is not invertible, then A is *singular*.

Corollary 7: Let M be a type III factor and let $A \in \mathcal{E}(M)$ with $A \neq I$. Then A is almost sharp if and only if A is singular.

Proof. Suppose A is invertible and $A = P_AQP_A$ for some $Q \in \mathcal{P}(M)$. Since $A \leqslant P_A$, P_A is also invertible which implies that $P_A = I$. Hence, $A = Q$ which implies that $A = I$. Conversely, suppose that $A \neq 0$ and that A is singular. Then $P_{AA'} \neq I$ and $N_A \neq 0$. The result follows from Corollary 6. ■

Recall that an effect $A \in \mathcal{E}(M)$ is *nearly sharp* if A and A' are both almost sharp.

Corollary 8: An effect $A \in \mathcal{E}(M)$ is nearly sharp if and only if $P_{AA'} \leqslant N_A$ and $P_{AA'} \leqslant N_{A'}$. If M is a factor, then $A \in \mathcal{E}(M)$ is nearly sharp if and only if $\dim(P_{AA'}) \leqslant \dim(N_A)$ *and* $\dim(P_{AA'}) \leqslant \dim(N_{A'})$.

An *orthoposet* is a system $(\mathcal{P}, \leqslant, ', 0, 1)$ where $(\mathcal{P}, \leqslant, 0, 1)$ is a bounded poset and $': \mathcal{P} \to \mathcal{P}$ satisfies $a'' = a$, $a \leqslant b$ implies $b' \leqslant a'$ and $a \wedge a' = 0$. An orthoposet $\mathcal{P}$ is *orthomodular* if $a \leqslant b'$ implies $a \vee b$ exists and $a \leqslant b$ implies $b = a \vee (b \wedge a')$. It is well known that $\mathcal{P}(M)$ forms an orthomodular lattice.[1]

Corollary 9: If $\mathcal{E}(M)_{ns}$ is the set of nearly sharp elements in $\mathcal{E}(M)$, then $(\mathcal{E}(M)_{ns}, \leqslant, ', 0, 1)$ is an orthoposet.

Proof: All the properties of an orthoposet are clear except for the condition $A \wedge A' = 0$ for every $A \in \mathcal{E}(M)_{ns}$. To verify this condition suppose that $B \in \mathcal{E}(M)_{ns}$ with $B \leqslant A$ and $B \leqslant A'$. Then $B \leqslant (A + A')/2 = \frac{1}{2}I$. Since $(\frac{1}{2}I)' = \frac{1}{2}I$, it follows that $\frac{1}{2}I \leqslant B'$ so that $N_{B'} = 0$. Since $B \in \mathcal{E}(M)_{ns}$, by Theorem 5, $P_{BB'} \leqslant N_{B'}$ so that $P_{BB'} = 0$. Hence, $BB' = 0$. Since $B' \geqslant \frac{1}{2}I$ we conclude that $B = 0$ and it follows that $A \wedge A' = 0$. ■

III. EFFECTS ON $B(H)$

Let H be a separable Hilbert space and let M be the factor $B(H)$ consisting of all bounded linear operators on H. As in Sec. I, we use the notation $\mathcal{E}(H)$, $\mathcal{P}(H)$ for $\mathcal{E}(M)$, $\mathcal{P}(M)$, respectively. For $P \in \mathcal{P}(H)$ we define

$$[0, P] = \{A \in \mathcal{E}(H) : 0 \leqslant A \leqslant P\}.$$

Theorem 10:

(1) *If $P \in \mathcal{P}(H)$ with $\dim(P') = \infty$, then*

$$[0, P] = \{P_1 Q P_1 : Q, P_1 \in \mathcal{P}(H), P_1 \leqslant P\}.$$

(2) *If $P \in \mathcal{P}(H)$ with $\dim(P) = \dim(P') = \infty$, then $A \in \mathcal{E}(H)$ satisfies $AP = PA$ if and only if $A = P_1 Q P_1 + P_2 R P_2$ with $P_1, P_2, Q, R \in \mathcal{P}(H)$ and $P_1 \leqslant P$, $P_2 \leqslant P'$.*

Proof: (1) If $A = P_1 Q P_1$, then $0 \leqslant A \leqslant P_1 \leqslant P$ so $A \in [0, P]$. Conversely, if $0 \leqslant A \leqslant P$, then $P_A \leqslant P$ and hence $N_A \geqslant P'$. Thus $\dim(N_A) = \infty$ and the result follows from Corollary 6.

(2) If $A = P_1 Q P_1 + P_2 R P_2$ with the given properties, it is clear that $AP = PA$. Conversely, suppose that $AP = PA$. Then we can write $A = PAP + P'AP'$. Since $PAP \in [0, P]$ and $P'AP' \in [0, P']$ the result follows from part (1). ■

A projection P is an example of a simple *superselection rule* and an $A \in \mathcal{E}(H)$ satisfying $AP = PA$ is said to satisfy the superselection rule P. Part (2) of Theorem 10 states that if $\dim(P) = \dim(P') = \infty$, then $A \in \mathcal{E}(H)$ satisfies the superselection rule P if and only if A is the sum of two nearly sharp elements, $A = A_1 + A_2$, where A_1 is contained in the *superselection sector* $[0, P]$ and A_2 is contained in the superselection sector $[0, P']$.

Suppose $P \in \mathcal{P}(H)$ with $\dim(P) = \dim(P') = \infty$. If $A \in [0, P]$ then by Part (1) of Theorem 10, A is almost sharp. If $A, B \in [0, P]$ and $A + B \in \mathcal{E}(H)$, then $A + B \in [0, P]$. It follows that $[0, P]$ is an *effect algebra with unit P* (see Refs. 1 and 2). If $A \in [0, P]$, then $\lambda A \in [0, P]$ for every $\lambda \in [0, 1]$ and it follows that $[0, P]$ is a *convex* effect algebra.[1] Finally, if $A, B \in [0, P]$ then $A \circ B \leqslant A \leqslant P$ where $A \circ B = A^{1/2} B A^{1/2}$. Hence, $A \circ B \in [0, P]$ and we conclude that $[0, P]$ is a *sequential effect algebra*[2] of almost sharp effects. Notice however, that if $A \in [0, P]$ then $A = P_A Q P_A$ where $P_A \in [0, P]$ but $Q \notin [0, P]$ in general.

We now consider the question of when $A \in \mathcal{E}(H)$ has the form

$$A = P_1 P_2 \cdots P_n Q P_n \cdots P_2 P_1 \tag{3.1}$$

for $\mathcal{P}_i, Q \in P(H)$ for $i = 1, \ldots, n$. To answer this question we shall need some preliminary results. If $\dim(N_A) = \infty$, then by Corollary 6, A is almost sharp so that A certainly has the form (3.1). We therefore assume that $\dim(N_A) < \infty$.

Lemma 11:

(1) *Suppose that $A, B \in \mathcal{E}(H)$ satisfy $A = P_A B P_A$, $\dim(N_A) < \infty$, and $\dim(P_{AA'}) = \infty$. Then $\dim(N_B) < \infty$ and $\dim(P_{BB'}) = \infty$.*

(2) *If $A \in \mathcal{E}(H)$ satisfies $\dim(N_A) < \infty$ and $\dim(P_{AA'}) = \infty$, then A does not have the form* (3.1).

Proof: (1) We first show that $\dim(N_B) \leqslant \dim(N_A)$. If this is not true, then there exists a nonzero vector $x \in \ker(B) \ominus \ker(A)$. But then $P_A x = x$ and we have that $Ax = P_A B P_A x = P_A B x = 0$. Hence

$x \in \ker(A)$ which is a contradiction. We now show that $\dim(P_{BB'}) = \infty$. If $\dim(P_{BB'}) < \infty$, then by (2.1) we have that

$$\dim(P_{B'}) = \dim(I - N_{B'}) = \dim(N_B + P_{BB'}) < \infty.$$

Hence, B' is a finite rank operator and it follows that $B = I - B'$ is the identity plus a finite rank map. Since $P_A = I - N_A$ and N_A has finite rank, we conclude that $A = P_A B P_A$ is also the identity plus a finite rank operator. But this contradicts the fact that $\dim(P_{AA'}) = \infty$.

(2) Suppose on the contrary that A has the form (3.1) for some integer n. For each $i = 1, 2, \ldots, n-1$, let

$$B_i = P_{i+1} P_{i+2} \cdots P_n Q P_n \cdots P_{i+2} P_{i+1}.$$

Then $A = P_1 B P_1$, $B_i = P_{i+1} B_{i+1} P_{i+1}$ for $i = 1, \ldots, n-2$, and $B_{n-1} = P_n Q P_n$. By Corollary 6

$$\dim(P_{B_{n-1} B'_{n-1}}) \leqslant \dim(N_{B_{n-1}}).$$

On the other hand, by successive applications of part (1) of this theorem we deduce that $\dim(N_{B_{n-1}}) < \infty$ and $\dim(P_{B_{n-1} B'_{n-1}}) = \infty$. ■

For the remaining case, assume that $\dim(N_A) = k < \infty$ and $\dim(P_{AA'}) = m < \infty$.

Lemma 12: Suppose that $A, B \in \mathcal{E}(H)$, *that* $\dim(N_A) = k < \infty$, $\dim(P_{AA'}) = m > k$ *and* $A = P_A B P_A$. *Then* $\dim(N_B) \leqslant k$ *and* $\dim(P_{BB'}) \geqslant m - k$. *Moreover, there exists a* $B \in \mathcal{E}(H)$ *such that* $A = P_A B P_A$, $\dim(N_B) = k$, *and* $\dim(P_{BB'}) = m - k$.

Proof: That $\dim(N_B) \leqslant k$ follows from part (1) of Lemma 11. To show that $\dim(P_{BB'}) \geqslant m - k$, define

$$\widetilde{A} = (N_A + P_{AA'}) A (N_A + P_{AA'}) = P_{AA'} A P_{AA'},$$

$$\widetilde{B} = (N_A + P_{AA'}) B (N_A + P_{AA'}),$$

and think of them as being defined in the range of $N_A + P_{AA'}$ which is a $k+m$ dimensional Hilbert space. It is easy to check that $P_{\widetilde{A}} = P_{AA'}$ and that $P_{\widetilde{A}} \widetilde{B} P_{\widetilde{A}} = P_{AA'} B P_{AA'} = P_{AA'} A P_{AA'} = \widetilde{A}$. The eigenvalues of $\widetilde{A}$ are

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_m > 0,$$

where 0 has multiplicity k and $1 > \lambda_1$. The eigenvalues of $\widetilde{B}$ are

$$s_1 \geqslant \cdots \geqslant s_k \geqslant s_{k+1} \geqslant \cdots \geqslant s_m \geqslant s_{m+1} \geqslant \cdots \geqslant s_{m+k},$$

where $1 \geqslant s_1$ and $s_{m+k} \geqslant 0$. Since $\widetilde{A}$ is the compression of $\widetilde{B}$ to a k-codimensional space, it follows from Cauchy's interlacing theorem[4] that

$$s_j \geqslant \lambda_j \geqslant s_{j+k} \qquad \text{for } j = 1, \ldots, m.$$

We then obtain that $0 < \lambda_m \leqslant s_m$ and $s_{k+1} \leqslant \lambda_1 < 1$. This implies that $1 > s_{k+1} \geqslant \cdots \geqslant s_m > 0$ and it follows that $\dim(P_{\widetilde{B}\widetilde{B}'}) \geqslant m - k$. To see that $\dim(P_{BB'}) = \dim(P_{\widetilde{B}\widetilde{B}'})$, consider $\widetilde{A}$ and $\widetilde{B}$ as operators on $N_A + P_{AA'}$ and represent A and B by the block matrices

$$A = \begin{pmatrix} I_{N_{A'}} & 0 \\ 0 & \widetilde{A} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} I_{N_{A'}} & 0 \\ 0 & \widetilde{B} \end{pmatrix}.$$

Then notice that

$$BB' = \begin{pmatrix} I_{N_{A'}} & 0 \\ 0 & \widetilde{B} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \widetilde{B}' \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \widetilde{B}\widetilde{B}' \end{pmatrix}.$$

To check the second assertion, consider the effect defined on $P_{AA'}+N_A$,

$$\widetilde{B} = \begin{pmatrix} \lambda_1 & \cdots & 0 & \cdots & 0 & \sqrt{\lambda_1(1-\lambda_1)} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k & \cdots & 0 & 0 & \cdots & \sqrt{\lambda_k(1-\lambda_k)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & \cdots & \lambda_m & 0 & \cdots & 0 \\ \sqrt{\lambda_1(1-\lambda_1)} & \cdots & 0 & \cdots & 0 & 1-\lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\lambda_k(1-\lambda_k)} & \cdots & 0 & 0 & \cdots & 1-\lambda_k \end{pmatrix}.$$

It is easy to check that $\widetilde{A}=P_{\widetilde{A}}\widetilde{B}P_{\widetilde{A}}$. Since

$$\begin{pmatrix} \lambda_i & \sqrt{\lambda_i(1-\lambda_i)} \\ \sqrt{\lambda_i(1-\lambda_i)} & I-\lambda_i \end{pmatrix}$$

is unitarily equivalent to $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ for every $i\leqslant k$, it follows that $\widetilde{B}$ has eigenvalues

$$0,\ldots,0,\lambda_{k+1},\lambda_{k+2},\ldots,\lambda_m,1,\ldots,1,$$

where the multiplicity of 0 and 1 are each k. Since $A=N_{A'}+\widetilde{A}$ we define $B=N_{A'}+\widetilde{B}$ and we are finished. ■

Lemma 13: Suppose that $\dim(N_A)=k>0$, $\dim(P_{AA'})=m$ *and* A *has the form (3.1). Then* $n\geqslant m/k$.

Proof: The case $n=1$ follows from Corollary 6. Assume that the result is true for $n-1$ and suppose that A has the form (3.1). Then

$$B = P_2\cdots P_nQP_n\cdots P_2$$

satisfies the hypothesis and we conclude that

$$n-1 \geqslant \frac{\dim(P_{BB'})}{\dim(N_B)}.$$

By Lemma 12 we have that $\dim(N_B)\leqslant k$ and $\dim(P_{BB'})\geqslant m-k$. Hence, $n-1\geqslant m-k/k$ so that $n\geqslant m/k$. ■

Lemma 14: Suppose that $A\in\mathcal{E}(H)$ *with* $\dim(N_A)=k>0$ and $\dim(P_{AA'})=m$. *Then for any* $n\geqslant m/k$, A *has a representation of the form* (3.1).

Proof: If $m\leqslant k$, by Corollary 6 we can write $A=PQP$ and we are finished. We now assume that $m>k$. By Lemma 12 we can find $B_1\in\mathcal{E}(H)$ such that $A=P_AB_1P_A$, $\dim(N_{B_1})=k$ and $\dim(P_{B_1B_1'})=m-k$. If $m-k\leqslant k$, by Corollary 6 we can write $B_1=PQP$ which implies that

$$A = P_APQPP_A.$$

In this case $m/k\leqslant 2$ and we again are finished. If on the other hand, $m-k>k$, by Lemma 12 we find $B_2\in\mathcal{E}(H)$ such that $B_1=P_{B_1}B_2P_{B_1}$, $\dim(N_{B_2})=k$ and $\dim(P_{B_2B_2'})=m-2k$. If $m-2k\leqslant k$ we are again finished, otherwise there exists $B_3\in\mathcal{E}(H)$ such that $B_2=P_{B_2}B_3P_{B_2}$, $\dim(N_{B_3})=k$ and $\dim(P_{B_3B_3'})=m-3k$. Proceeding this way, we can find n such that $m-(n-1)k\leqslant k$ and we prove the result. ■

Applying these lemmas, we obtain the following.

Theorem 15: *Let $A\in\mathcal{E}(H)$ with H separable and $A\neq I$. Then A has the form (3.1) if and only if* $\dim(N_A)=\infty$ or $0<\dim(N_A)<\infty$ *and* $\dim(P_{AA'})<\infty$.

For $A\in\mathcal{E}(H)$ we define the *fuzzy index* $f(A)$ to be the smallest integer n so that A has the form (3.1). Then A is sharp if and only if $f(A)=0$ and A is almost sharp if and only if $f(A)$ is 0 or 1. By convention, if no such n exists then $f(A)=\infty$. For m,k positive integers we denote the smallest integer greater than or equal to m/k by $\lceil m/k\rceil$. We extend this definition to include values 0 and ∞ for m and k by defining

$$\left\lceil\frac{m}{k}\right\rceil=\begin{cases}\infty & \text{if} \quad k=0 \text{ and } m\neq 0,\\ 0 & \text{if} \quad m=0,\\ 1 & \text{if} \quad k=\infty \text{ and } m\neq 0,\\ \infty & \text{if} \quad m=\infty \text{ and } k\neq\infty.\end{cases}$$

The next result again follows from the previous lemmas.

Theorem 16: *Let $A\in\mathcal{E}(H)$ with H separable. Then*

$$f(A)=\left\lceil\frac{\dim(P_{AA'})}{\dim(N_A)}\right\rceil.$$

The fuzzy index $f(A)$ designates the fewest number of sharp effects whose sequential product gives $A\in\mathcal{E}(H)$. Since sharp effects are frequently thought of as filters such as polarization filters on an optical bench, $f(A)$ is the fewest number of filters that can be placed in series to give the same effect A. Theorem 15 characterizes when $f(A)$ is finite and Theorem 16 provides the value of $f(A)$ as a simple function of A.

IV. FINITE DIMENSIONAL EFFECTS

We now show that we can obtain further insights and some simpler proofs for the set $\mathcal{E}(H)$ on a finite dimensional Hilbert space. Although finite dimensional Hilbert spaces may seem restrictive for quantum systems, there are important fields such as quantum computation and information theory that are based on such spaces.[5]

Let $A\in\mathcal{E}(H)$ where $\dim(H)<\infty$. We define the following non-negative integers:

$$n_0(A)=\dim(N_A),$$

$$n_1(A)=\dim(N_{A'}),$$

$$n(A)=\dim(H)-n_0(A)-n_1(A).$$

Notice that $n_0(A)$ is the multiplicity of the eigenvalue 0, $n_1(A)$ is the multiplicity of the eigenvalue 1, and $n(A)$ is the number of eigenvalues λ with $0<\lambda<1$ including multiplicity.

Lemma 17: If $A\in\mathcal{E}(H)$ with $\dim(H)<\infty$, *then* $n(A)=\dim(P_{AA'})=rank(P_A-A)$.

Proof: By diagonalizing A we can assume without loss of generality that A has the form

$$A=\operatorname{diag}(\lambda_1,\ldots,\lambda_m,1,\ldots,1,0,\ldots,0), \tag{4.1}$$

where $0<\lambda_i<1$ for $i=1,\ldots,m$. We then have that

$$AA'=\operatorname{diag}(\lambda_1(1-\lambda_1),\ldots,\lambda_m(1-\lambda_m),0,\ldots,0,0,\ldots,0),$$

and

$$P_A-A=\operatorname{diag}(1-\lambda_1,\ldots,1-\lambda_m,0,\ldots,0,0,\ldots,0).$$

It follows that $\dim(P_{AA'})=\operatorname{rank}(P_A-A)=n(A)=m$. ■

The next result follows from Corollary 6 and Lemma 17. However, we give a much shorter proof which relies on the fact that $\dim(H)<\infty$.

Theorem 18: *Let* $A\in\mathcal{E}(H)$ *with* $\dim(H)<\infty$.

(1) *A is almost sharp if and only if* $n(A)\leqslant n_0(A)$.
(2) *A is nearly sharp if and only if* $n(A)\leqslant\min\{n_0(A),n_1(A)\}$.

Proof: (1) Suppose $A=P_AQP_A$ for $Q\in\mathcal{P}(H)$. Then by Lemma 17 we have that

$$\begin{aligned} n(A)&=\operatorname{rank}(P_A-A)=\operatorname{rank}(P_A(I-Q)P_A)\leqslant\operatorname{rank}(I-Q)\\ &=\dim(N_Q)\leqslant\dim(N_{P_AQP_A})=\dim(N_A)=n_0(A). \end{aligned}$$

Conversely, suppose that $m=n(A)\leqslant n_0(A)$. Without loss of generality we can represent A as a diagonal matrix (4.1) Let.

$$\Lambda=\operatorname{diag}(\lambda_1,\ldots,\lambda_m)=\begin{pmatrix}\lambda_1&\cdots&0\\ \vdots&\ddots&\vdots\\ 0&\cdots&\lambda_m\end{pmatrix}\in M_m,$$

and represent A by the block matrix,

$$A=\begin{pmatrix}\Lambda&0&0\\ 0&I_{n_1(A)}&0\\ 0&0&0_{n_0(A)}\end{pmatrix}.$$

Since $m\leqslant n_0(A)$, we can split the last block into a $m\times m$ block and an $l\times l$ block, where $l=n_0(A)-m$. Let Q be the block matrix

$$Q=\begin{pmatrix}\Lambda&0&\sqrt{\Lambda(I_m-\Lambda)}&0\\ 0&I_{n_1(A)}&0&0\\ \sqrt{\Lambda(I_m-\Lambda)}&0&I_m-\Lambda&0\\ 0&0&0&0_l\end{pmatrix}.$$

It is easy to check that $P_AQP_A=A$ and that $Q\in\mathcal{P}(H)$.

The proof of (2) follows directly from (1). ■

We may think of $n(A)$ as the number of fuzzy eigenvalues of A and $n_0(A)+n_1(A)$ as the number of sharp eigenvalues. As one might expect, the almost (or nearly) sharpness of A depends on $n(A)$ compared to $n_0(A)$ and $n_1(A)$ and this is the content of Theorem 18. Moreover, it follows from Theorem 16 and Lemma 17 that if $\dim(H)<\infty$ then

$$f(A)=\left\lceil\frac{n(A)}{n_0(A)}\right\rceil.$$

We now consider some examples in $\mathcal{E}(\mathbb{C}^3)$. Let $0<\lambda_i<1$ for $i=1,2,3$, and consider the following effects:

$$A=\begin{pmatrix}\lambda_1&0&0\\ 0&\lambda_2&0\\ 0&0&\lambda_3\end{pmatrix},\quad B=\begin{pmatrix}\lambda_1&0&0\\ 0&\lambda_2&0\\ 0&0&0\end{pmatrix},$$

$$D=\begin{pmatrix}\lambda_1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \text{and } E=\begin{pmatrix}\lambda_1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

Then A and B are not almost sharp, D is almost sharp but it is not nearly sharp and E is nearly sharp. The fuzzy indexes are $f(A)=\infty$, $f(B)=2$, $f(D)=f(E)=1$. The decomposition $E=P_EQP_E$ has the following form:

$$\begin{pmatrix}\lambda_1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda_1 & 0 & \sqrt{\lambda_1(1-\lambda_1)}\\ 0 & 1 & 0\\ \sqrt{\lambda_1(1-\lambda_1)} & 0 & 1-\lambda_1\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

Although E is almost sharp, λE for $0<\lambda<1$ is not almost sharp. Our last result follows from Theorem 18.

Theorem 19: *Let $A\in\mathcal{E}(H)$, $A\neq I$, with* $\dim(H)<\infty$. *Then A has the form (3.1) if and only if A is singular*.

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Inhomogeneous quantum groups for particle algebras

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We construct the inhomogeneous quantum groups FIO(d) and BISp($2d$) and investigate their Hopf algebra structure. FIO(d) and BISp($2d$) leave the algebra of fermion and boson creation/annihilation operators invariant, respectively. We also present the corresponding R-matrices. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The importance of inhomogeneous groups in physics cannot be overestimated. Well known examples are the Poincaré and Galilean groups. Deformations of inhomogeneous Lie groups lead to inhomogeneous quantum groups. This procedure entails the deformation of the function algebra over the classical group and/or the deformation of the enveloping algebra of the Lie algebra.[1,2]

In the present paper we will construct a different type of inhomogeneous quantum groups by considering their action on the algebra of fermionic and bosonic creation/annihilation operators. The algebra of such operators for particles obeying fermionic and bosonic statistics are defined by

$$[c_i, c_j^*]_\pm = \mathbf{1}\delta_{ij},$$

$$[c_i, c_j]_\pm = 0. \tag{1.1}$$

All known particles in physics are bosons and fermions and thus obey (1.1). In Quantum Field Theory the discrete indices are replaced by continuous momentum indices.

As a motivation for the next section, in which we clothe our calculation with compact and standard notation using the language of Hopf algebra, we investigate the nature of the transformation parameters which mixes up the creation and annihilation operators together with the identity element of the algebra as

$$c_i \mapsto c_i' = \alpha_{ik} \otimes c_k + \beta_{ik} \otimes c_k^* + \gamma_i \otimes \mathbf{1},$$

$$c_i^* \mapsto c_i'^* = \alpha_{ik}^* \otimes c_k^* + \beta_{ik}^* \otimes c_k + \gamma_i^* \otimes \mathbf{1}, \quad i,k = 1,2,\ldots,d. \tag{1.2}$$

Here, the minimal assumption we presume is that the homogeneous parameters $\alpha_{ik}, \alpha_{ik}^*, \beta_{ik}, \beta_{ik}^*$ commute among themselves in accordance with the results found in Ref. 3 for FIO(2). Note that the $*$ structure is of some physical significance and will be discussed in Sec. III. We directly impose the invariance of the above algebras under the above transformation. As they stand, they are defined equally for fermions and bosons. As we will see, this seemingly simple transformation consists of parameters which turn out to belong to a Hopf algebra with respective numerical R-matrices.

Now, using the algebra of the original operators, we calculate the (anti-)commutator of the transformed operators, for example, for the first commutation relation, we have

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$$[c_i', c_j'^*]_\pm = [(\alpha_{ik} \otimes c_k + \beta_{ik} \otimes c_k^* + \gamma_i \otimes \mathbf{1}), (\alpha_{jl}^* \otimes c_l^* + \beta_{jl}^* \otimes c_l + \gamma_j^* \otimes \mathbf{1})]_\pm$$
$$= \{\{\alpha_{ik}\alpha_{jl}^* \pm \beta_{ik}\beta_{jl}^*\}\delta_{kl} + [\gamma_i, \gamma_j^*]_\pm\} \otimes \mathbf{1} + \{[\gamma_i, \beta_{jk}^*]_\pm + [\alpha_{ik}, \gamma_j^*]_\pm\} \otimes c_k + \{[\gamma_i, \alpha_{jk}^*]_\pm$$
$$+ [\beta_{ik}, \gamma_j^*]_\pm\} \otimes c_k^*. \tag{1.3}$$

Exploiting the canonical isomorphism $\mathbb{C} \otimes \mathcal{A} \cong \mathcal{A}$ for the tensor product defined over the field $\mathbb{C}$, for the vector space $\mathcal{A}$, this must be equal to

$$\delta_{ij}\mathbf{1} \cong \delta_{ij} \otimes \mathbf{1} = [c_i', c_j'^*]_\pm \otimes \mathbf{1}. \tag{1.4}$$

Upon requiring the transformations to be an algebra homomorphism, one assumes the relations

$$\alpha_{ik}\alpha_{jk}^* \pm \beta_{ik}\beta_{jk}^* + [\gamma_i, \gamma_j^*]_\pm = \delta_{ij}, \tag{1.5}$$

together with

$$[\gamma_i, \beta_{jk}^*]_\pm = 0, \quad [\alpha_{ik}, \gamma_j^*]_\pm = 0,$$

$$[\gamma_i, \alpha_{jk}^*]_\pm = 0, \quad [\beta_{ik}, \gamma_j^*]_\pm = 0, \tag{1.6}$$

among the elements that parametrize the transformations.

Similarly, for the invariance of the second set of the transformed (anti-) commutators, the straightforward calculation,

$$[c_i', c_j']_\pm = [(\alpha_{ik} \otimes c_k + \beta_{ik} \otimes c_k^* + \gamma_i \otimes \mathbf{1}), (\alpha_{jl} \otimes c_l + \beta_{jl} \otimes c_l^* + \gamma_j \otimes \mathbf{1}\ )]_\pm = \{\alpha_{ik}\beta_{jl} \pm \beta_{ik}\alpha_{jl}\}$$
$$\otimes [c_k, c_l^*]_\pm + [\gamma_i, \gamma_j]_\pm \otimes \mathbf{1} + \{[\beta_{ik}, \gamma_j]_\pm + [\gamma_i, \beta_{jk}]_\pm\} \otimes c_k^* + \{[\alpha_{ik}, \gamma_j]_\pm + [\gamma_i, \alpha_{jk}]_\pm\} \otimes c_k, \tag{1.7}$$

is consistent with the (anti-)commutation relations

$$\alpha_{ik}\beta_{jk} \pm \beta_{ik}\alpha_{jk} + [\gamma_i, \gamma_j]_\pm = 0, \tag{1.8}$$

$$[\beta_{ik}, \gamma_j]_\pm = 0, \quad [\alpha_{ik}, \gamma_j]_\pm = 0. \tag{1.9}$$

These calculations show that it is the inhomogeneous transformation parameters that result in the nontrivial algebraic relations. Collecting all the relations defining the algebra of the transformation parameters we have

$$\alpha_{ik}\beta_{jk} \pm \beta_{ik}\alpha_{jk} + [\gamma_i, \gamma_j]_\pm = 0, \tag{1.10}$$

$$\alpha_{ik}\alpha_{jk}^* \pm \beta_{ik}\beta_{jk}^* + [\gamma_i, \gamma_j^*]_\pm = \delta_{ij}, \tag{1.11}$$

$$[\beta_{ik}, \gamma_j]_\pm = 0, \quad [\alpha_{ik}, \gamma_j]_\pm = 0, \tag{1.12}$$

$$[\beta_{ik}, \gamma_j^*]_\pm = 0, \quad [\alpha_{ik}, \gamma_j^*]_\pm = 0, \tag{1.13}$$

together with the $*$-conjugates of all the relations.

The derivation of the quantum invariance group given above, in fact, mimics the derivation of other matrix quantum groups, such as $GL_q(2)$ or $SL_q(2)$ that leave the underlying quantum plane with coordinates (x,y) and the 1-forms, the differentials of x and y, (ξ, η) having the (anti-)commutations

$$xy = qyx, \quad \xi\eta = -q^{-1}\eta\xi, \quad \xi^2 = 0, \quad \eta^2 = 0, \tag{1.14}$$

invariant. In this way, the study of the automorphisms of noncommutative spaces naturally leads to the notion of the quantum groups.[4] In our case the matrix quantum group acts, exclusively, on the vector space which is either fermionic or bosonic in nature.

Intending to emphasize the action of the transformations on the creation/annihilation operators rather than the algebra of creation/annihilation operators, we write the transformation parameters as a quantum matrix and the elements of the particle algebra as a column vector.

II. QUANTUM GROUPS, FIO($2d$) AND BISp($2d$)

If we are to emphasize that the action of the quantum matrix group on the algebra of creation/annihilation operators, we form $(2d+1)$-dimensional column vectors $\mathbf{C} \equiv [c_i, c_i^*, \mathbf{1}]^t$ on which the action is defined via

$$\mathbf{C}' = \mathbf{M} \dot{\otimes} \mathbf{C}, \tag{2.1}$$

or supplying the indices,

$$\mathbf{C}'^i = M^i_k \otimes \mathbf{C}^k, \tag{2.2}$$

where $\mathbf{C}^k$ is the kth entry of the column vector $\mathbf{C}$ and the quantum matrix $\mathbf{M}$ is given by

$$\mathbf{M} = \left[\begin{array}{cc|c} \alpha_{ij} & \beta_{ij} & \gamma_i \\ \beta^*_{ij} & \alpha^*_{ij} & \gamma^*_i \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{1} \end{array}\right] \equiv \left[\begin{array}{c|c} \mathbf{A} & \Gamma \\ \hline 0 & \mathbf{1} \end{array}\right]. \tag{2.3}$$

If the elements of the matrix $\mathbf{M}$ satisfy the relations (1.10)–(1.13) we will name the corresponding quantum groups as the Fermionic Inhomogeneous Orthogonal Group (FIO) and the Bosonic Inhomogeneous Symplectic Quantum Group (BISp), respectively, for the upper and the lower signs. In this section this definition will be made more rigorous by defining the corresponding R-matrices.

The space of vectors $\mathbf{C}$, built out of the generators of the algebras (1.1), is therefore a left M-comodule for the bialgebra defined by all the relations among the transformation parameters obtained in the first section. In order to be able to make the algebra of the transformation parameters (1.10)–(1.13) into a bialgebra, it is convenient to define the vectors

$$\mathbf{C}_1\mathbf{C}_2 = \begin{bmatrix} c_1\mathbf{C} \\ c_2\mathbf{C} \\ \vdots \\ c_d\mathbf{C} \\ c_1^*\mathbf{C} \\ c_2^*\mathbf{C} \\ \vdots \\ c_d^*\mathbf{C} \\ \mathbf{1}\cdot\mathbf{C} \end{bmatrix}, \quad \mathbf{C}_2\mathbf{C}_1 = \begin{bmatrix} \mathbf{C}c_1 \\ \mathbf{C}c_2 \\ \vdots \\ \mathbf{C}c_d \\ \mathbf{C}c_1^* \\ \mathbf{C}c_2^* \\ \vdots \\ \mathbf{C}c_d^* \\ \mathbf{C}\cdot\mathbf{1} \end{bmatrix}, \tag{2.4}$$

where both $\mathbf{C}_1\mathbf{C}_2$ and $\mathbf{C}_2\mathbf{C}_1$ carry double indices as $(\mathbf{C}_1\mathbf{C}_2)^{ij}$, for example, $(\mathbf{C}_1\mathbf{C}_2)^{(d+1)k} = c_1^* \cdot \mathbf{C}^k$, etc. Since these two indexed column vectors cover all possible "multiplications" in the algebra of creation/annihilation operators, it is possible to write Eqs. (1.1) as a matrix equation in the form

$$R\mathbf{C}_1\mathbf{C}_2 = \mathbf{C}_2\mathbf{C}_1, \tag{2.5}$$

where the entries of the $(2d+1)\times(2d+1)$ matrix R are also labeled by double indices as R^{ik}_{lm}. With all these new conventions, the invariance of the algebras defined by Eqs. (1.1) under the action (2.1) boils down to

$$R^{ij}_{kl}(\mathbf{C}'_1\mathbf{C}'_2)^{kl} = (\mathbf{C}'_2\mathbf{C}'_1)^{ij}. \tag{2.6}$$

Given the relation between $\mathbf{C}$ and $\mathbf{C}'$ as $\mathbf{C}'=\mathbf{M}\dot{\otimes}\mathbf{C}$ and the original algebra (1.10)–(1.13), eventually, Eqs. (2.1) and (2.5) are consistent with

$$RM_1M_2 = M_2M_1R, \tag{2.7}$$

where $M_1=\mathbf{M}\otimes 1$, $M_2=1\otimes\mathbf{M}$, and the numerical matrices $R^{-1},R\in M_{(2d+1)^2}(\mathbb{C})\otimes M_{(2d+1)^2}(\mathbb{C})$. Actually, Eq. (2.7) is a just proper way of writing the algebra defined in Eqs. (1.10)–(1.13). It also reflects the fact that the R matrix is of fundamental importance for quantum groups; in that it expresses how the multiplication $(M_1M_2)^{ij}_{kl}=M^i_kM^j_l$ is related to the opposite multiplication, that is, $(M_2M_1)^{ij}_{kl}=M^j_lM^i_k$. As the consistency conditions for the associativity of the multiplication in the algebra generated by M^i_k, the R matrix satisfies the quantum Yang–Baxter equation,

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}, \tag{2.8}$$

where, $R_{12},R_{13},R_{23}\in(M_{(2d+1)^2})^{\otimes 3}$ and $(R_{12})^{ijk}_{lmn}=R^{ij}_{lm}\delta^k_n$, etc.

A quantum group is a noncommutative and noncocommutative Hopf algebra $\mathbf{H}$ with quasitriangular structure $\mathcal{R}\in\mathbf{H}\otimes\mathbf{H}$ (Drinfel'd).[5] There are different lines of approach to the quantum groups depending on the usage and/or the purpose. For example, the commutative algebra of functions on a group manifold, for which the noncocommutative coproduct defined by pointwise multiplication, carries a natural Hopf algebra setting (together with appropriate antipode and counit).[6,7]

The vector fields on the group manifold are dual to the functions on the manifold, in the sense that they act on the function algebra as derivations. As for the algebra of functions, the universal enveloping algebra, $U(\mathfrak{g})$ can also be equipped with the Hopf algebra setting by defining an appropriate (primitive) bialgebra structure and an antipode. The noncommutative (Lie) product on $U(\mathfrak{g})$, inherited from $\mathfrak{g}$, corresponds to the noncocommutative coproduct on the algebra of functions, whereas the cocommutative product on $U(\mathfrak{g})$ corresponds to the commutative product on the algebra of functions. In the case of complex semisimple Lie algebra $\mathfrak{g}$, there is a standard way of defining the deformed quantum enveloping algebra $U_q(\mathfrak{g})$.[8,9]

The duality of two different approaches, crudely mentioned above, turn out to hold when the respective algebras are deformed. The simplest nontrivial example is that $SL_q(2)$ is dual to $U_q(\mathfrak{sl}_2)$. However, there are examples of quantum groups that do not belong to any of the above two types;[6] the quantum groups presented here can be considered to fit into the former construction. As in the example presented here, both the use and the importance of abstract Hopf algebras (quantum groups) in applications to physics emerges when they act on other structures, carrying concrete physical relevance.[10] If a Hopf algebra has a quasitriangular structure $\mathcal{R}\in\mathbf{H}^{\otimes 2}$, which controls the noncocommutativity of the coproduct, in the dual Hopf algebra (if it can be found) the noncommutativity of the multiplication is controlled by the numerical R matrix. The quasitriangular structure $\mathcal{R}$ is often called the universal R matrix, probably for the reason that it produces the matrix solutions of the quantum Yang–Baxter equation on all of its modules, and while the dual producing solutions of the Yang–Baxter on all of its comodules.[7]

Returning to our presentation, we need to prove that the coassociative coproduct $\Delta:\mathbf{M}\mapsto\mathbf{M}\otimes\mathbf{M}$ defined by

$$\Delta(\mathbf{M}) = \mathbf{M}\dot{\otimes}\mathbf{M}, \tag{2.9}$$

together with the antipode $S:\mathbf{M}\mapsto\mathbf{M}, S(\mathbf{M})=\mathbf{M}^{-1}$ as an anti-algebra map and the counit map $\varepsilon:\mathbf{M}\mapsto\mathbb{C}$ given by $\varepsilon(\mathbf{M})=I_{(2d+1)\times(2d+1)}$, defines the matrix quantum groups which we name as the fermionic orthogonal and the bosonic symplectic inhomogeneous quantum groups without referring to any $*$ structure. We denote these quantum groups as FIO$(2d,\mathbb{C})$, and BISp$(2d,\mathbb{C})$, respectively. The coproduct $\Delta:\mathbf{M}\mapsto\mathbf{M}\otimes\mathbf{M}$ should be an algebra homomorphism, in order to make the algebra (2.7) into a bialgebra: $\Delta(\mathbf{M}\mathbf{M}')=\Delta(\mathbf{M})\Delta(\mathbf{M}')$ for all the elements in the algebra (2.7). We will come back to this point after we present the different $*$-conjugation choices for FIO and BISp in the following section.

III. $*$-STRUCTURE AND REAL FORMS

In this section, we will obtain FIO$(2d,\mathbb{R})$ and BISp$(2d,\mathbb{R})$ by changing the $*$-conjugation relations among the M^i_k, for $d=1$ and generalize what we find to the $(2d+1)$-dimensional case for fermions.

The boson algebra in Eqs. (1.1), unlike the fermion algebra, has a corresponding classical counterpart, the Poisson algebra of functions over the cotangent bundle of the configuration space of the corresponding classical system. The Poisson bracket makes the algebra of functions becomes an ∞-dimensional Lie algebra and the definition of the Poisson bracket requires a nondegenerate, closed 2-form Ω, the symplectic form. In terms of canonical coordinates p^i, q_i, it has constant components $\Omega=\Sigma dp^i\wedge dq_i$ so that $\{p^i,q_j\}=\delta^i_j$. An odd dimensional manifold cannot accommodate a nondegenerate symplectic two form and the quantum counterpart must also be even dimensional.

After this digression, we first take the simplest example FIO$(2,\mathbb{C})$ and its action on the fermion algebra (1.1). It acts on the column vector $\mathbf{C}=[c,c^*,\mathbf{1}]^t$ via (2.1) and the conjugation in the entries of $\mathbf{M}$ is forced by the fermion algebra defined in Eqs. (1.1). Hence, the $*$-conjugation in the Hopf algebra $\mathbf{M}$ directly reflects the choice of the vector $\mathbf{C}$. What if one begins with another choice of the column vector $\mathbf{C}$? If we begin with the column vector $\hat{\mathbf{C}}=[1/\sqrt{2}(c+c^*), i/\sqrt{2}(c-c^*),\mathbf{1}]^t$, accordingly the $*$-conjugation relations among $\{M^i_k\}_{i,k=1,2,3}$ changes. It is easy to see that the vectors $\hat{\mathbf{C}}$ and $\mathbf{C}$ are related by

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{2}}\left[\begin{array}{cc|c} 1 & 1 & 0 \\ i & -i & 0 \\ \hline 0 & 0 & \sqrt{2} \end{array}\right]\mathbf{C} \equiv U\mathbf{C}, \tag{3.1}$$

where $U^\dagger=U^{-1}$. If one relabels the entries of $\hat{\mathbf{C}}$ as

$$a_1 \equiv \frac{1}{\sqrt{2}}(c+c^*),$$

$$a_2 \equiv \frac{i}{\sqrt{2}}(c-c^*), \tag{3.2}$$

the anti-commutation relations for these new operators can be derived from the anti-commutation relations among the original operators c,c^*. This is the same thing as the corresponding quantum matrices $\hat{\mathbf{M}}$ and $\mathbf{M}$ are related by a similarity transformation. Therefore, in turn, it is possible to obtain the algebra of $\{\hat{M}^i_k\}_{i,k=1,2,3}$ from those of $\{M^i_k\}_{i,k=1,2,3}$. If we denote the entries of the new matrix as

$$\hat{\mathbf{M}} \equiv \left[\begin{array}{c|c} \mathbf{A} & \mathbf{\Gamma} \\ \hline 0 & \mathbf{1} \end{array}\right], \quad \mathbf{A} \equiv \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad \mathbf{\Gamma} \equiv \begin{bmatrix} \Gamma_1 \\ \Gamma_2 \end{bmatrix}, \tag{3.3}$$

we have

$$\hat{\mathbf{M}} = \left[\begin{array}{cc|c} A_{11} & A_{12} & \Gamma_1 \\ A_{21} & A_{22} & \Gamma_2 \\ \hline 0 & 0 & 1 \end{array}\right] = \left[\begin{array}{cc|c} \mathrm{Re}(\alpha+\beta) & \mathrm{Im}(\alpha-\beta) & \sqrt{2}\mathrm{Re}\ \gamma \\ -\mathrm{Im}(\alpha+\beta) & \mathrm{Re}(\alpha-\beta) & \sqrt{2}\mathrm{Im}\ \gamma^* \\ \hline 0 & 0 & 1 \end{array}\right]. \tag{3.4}$$

If we invert the above relations we obtain

$$\alpha = 1/2(A_{11} + A_{22}) + i/2(A_{12} - A_{21}),$$

$$\beta = 1/2(A_{11} - A_{22}) - i/2(A_{12} + A_{21}). \tag{3.5}$$

Now calculating the anticommutators $[\Gamma_i, \Gamma_j]_+$, using (3.4) and the algebra of $\alpha, \alpha^*, \beta, \beta^*, \gamma, \gamma^*$, we have

$$[\Gamma_1, \Gamma_2]_+ = \frac{1}{2}(\alpha + \beta^*)(\alpha^* + \beta) - \frac{1}{2}(\alpha - \beta^*)(\alpha^* - \beta),$$

$$2\Gamma_1^2 = 1 - (\alpha + \beta^*)(\alpha^* + \beta),$$

$$2\Gamma_2^2 = 1 - (\alpha - \beta^*)(\alpha^* - \beta). \tag{3.6}$$

Using (3.5), we can convert rhs of the above anticommutators also in terms of the self conjugate variables as

$$[\Gamma_1, \Gamma_2]_+ = -A_{11}A_{21} - A_{12}A_{22},$$

$$2\Gamma_1^2 = 1 - A_{11}^2 - A_{12}^2,$$

$$2\Gamma_2^2 = 1 - A_{22}^2 - A_{21}^2, \tag{3.7}$$

all of which combine into the equation

$$[\Gamma_i, \Gamma_j]_+ = \delta_{ij} - A_{ik}A_{jk}, \quad i,j = 1,2. \tag{3.8}$$

For BISp$(2,\mathbb{R})$, similar linear algebra calculations yields

$$[\Gamma_1, \Gamma_2]_- = i\{1 - A_{11}A_{22} + A_{12}A_{21}\}. \tag{3.9}$$

Moreover, since the transformations by U do not mix the homogeneous parameters with the inhomogeneous ones, the (anti-)commutation relations involving the homogeneous parts remain intact. Eventually, for the BISp(2), by introducing the matrix

$$G^- \equiv \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \tag{3.10}$$

the (anti-)commutation relations with real parameters bosonic transformation parameters can be written as

$$[\Gamma_i,\Gamma_j]_- = (G^- - \mathbf{A}G^-\mathbf{A}^t)_{ij}. \tag{3.11}$$

As mentioned in the digression in the beginning of this section, the matrix G^- is related to the symplectic form Ω and generalizes to even dimensions only.

Our aim is to treat both FIO and BISp on the same footing, thus rewritten as in Eq. (3.11), both real forms FIO$(2d,\mathbb{R})$ and BISp$(2d,\mathbb{R})$ can be fused into a single set of equations by denoting $G^+ \equiv \mathbf{1}_{2\times 2}$ as

$$[\Gamma_i,\Gamma_j]_\pm = G^\pm - \mathbf{A}G^\pm\mathbf{A}^t{}_{ij}. \tag{3.12}$$

By the "real form" we refer to the particular $*$-conjugation relation among the algebra transformation, not to the elements of the corresponding R-matrices. With the additional ingredients $G^\pm$, the coproduct defined as $\Delta(\hat{\mathbf{M}})=\hat{\mathbf{M}}\dot{\otimes}\hat{\mathbf{M}}$ extends as an algebra homomorphism to make the algebras defined in Eqs. (3.12) bialgebras. Explicitly, for the real forms, the coproducts for the elements of the matrix $\hat{\mathbf{M}}$,

$$\Delta(\Gamma_i) = \sum_k A_{ik}\otimes\Gamma_k + \Gamma_i\otimes 1, \quad \Delta(A_{ij}) = \sum_n A_{in}\otimes A_{nj}, \tag{3.13}$$

respect the relations (3.12):

$$\begin{aligned}
\Delta([\Gamma_i,\Gamma_j]_\pm) &= \sum_{k,n} A_{ik}A_{jk}\otimes[\Gamma_i,\Gamma_j]_\pm + [\Gamma_i,\Gamma_j]_\pm \otimes \mathbf{1} \\
&= \sum_{k,n} A_{ik}A_{jn}\otimes\{(G^\pm)_{kn} - A_{kp}A_{nr}(G^\pm)_{pr}\} + \{(G^\pm)_{ij} - A_{ik}A_{jn}(G^\pm)_{kn}\}\otimes\mathbf{1} \\
&= (G^\pm)_{ij}\otimes\mathbf{1} - \sum_{k,n} A_{ik}A_{jn}\otimes(G^\pm)_{pr}A_{kp}A_{nr} \\
&= (G^\pm)_{ij}\Delta(\mathbf{1}) - \sum_{p,r}(G^\pm)_{pr}\Delta(A_{ip})\Delta(A_{jr}) = \Delta((G^\pm - \mathbf{A}G^\pm\mathbf{A}^t)_{ij}),
\end{aligned} \tag{3.14}$$

where we have exploited the coproduct

$$\Delta\left(\sum_k A_{ik}A_{jk}\right) = \sum_k \Delta(A_{ik}A_{jk}) = \sum_k \Delta(A_{ik})\Delta(A_{jk}) = \sum_{k,n,p} A_{in}A_{jp}\otimes A_{nk}A_{pk}, \tag{3.15}$$

reading it from right to left. As a result, both FIO(2) and BISp(2) satisfy the Hopf Algebra axioms independent of the $*$-structure, with the antipode

$$S(\hat{\mathbf{M}}) = \hat{\mathbf{M}}^{-1} \equiv \left[\begin{array}{c|c} \mathbf{A}^{-1} & -\mathbf{A}^{-1}\mathbf{\Gamma} \\ \hline \mathbf{0} & \mathbf{1} \end{array}\right], \tag{3.16}$$

and the counit $\varepsilon(\hat{\mathbf{M}})=I_{4\times 4}$. For the fermions, the arguments of this section concerning the $*$-structures do not touch upon the dimensionality of the vectors $\mathbf{C}$ and can easily be extended to any dimension d that can be either odd or even. But in the case of bosons different $*$-conjugation choices exist in even dimensions only. The next section is devoted to the systematic calculation of their numerical R-matrices.

IV. *R*-MATRICES FOR FIO(*d*), BISp(2*d*)

Because the R-matrices of the quantum groups FIO(d) and BISp$(2d)$ follow a pattern that is easy to figure out for increasing d, we will present only the R-matrices for $d=2$ and for both $*$-choices in the previous section as 9×9 matrices. In light of these, we give the nonzero elements of the R-matrices for $d>2$, which are not easy to display as matrices fitting to the page.

For the convenience of the notation and ease for calculation, we relabel the elements of FIO(2,$\mathbb{C}$) and BISp(2,$\mathbb{C}$) as

$$\mathbf{M} = [M_k^i] = \begin{bmatrix} M_1^1 & M_2^1 & M_3^1 \\ M_1^2 & M_2^2 & M_3^2 \\ M_1^3 & M_2^3 & M_3^3 \end{bmatrix} \equiv \begin{bmatrix} \alpha & \beta & \gamma \\ \beta^* & \alpha^* & \gamma^* \\ 0 & 0 & \mathbf{1} \end{bmatrix}, \tag{4.1}$$

and similarly for the real forms which we denoted by $\hat{\mathbf{M}}$. If we supply the indices to Eq. (2.7), we have

$$R_{kl}^{ij}(M_1)_{cd}^{kl}(M_2)_{ab}^{cd} = (M_2)_{cd}^{ij}(M_1)_{kl}^{cd}R_{ab}^{kl},$$

$$R_{kl}^{ij}M_c^k\delta_d^l\delta_a^cM_b^d = \delta_c^iM_d^jM_k^c\delta_l^dR_{ab}^{kl},$$

$$R_{ab}^{ik}M_j^aM_l^b = M_b^kM_a^iR_{jl}^{ab}, \tag{4.2}$$

where all the indices runs over the same range, $i,j,k,l,a,b=1, 2, 3$. From this matrix equation it is possible to extract the R-matrices using (1.10)–(1.13) as

$$R = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{4.3}$$

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{4.4}$$

for the FIO(2,$\mathbb{C}$) and the BISp(2,$\mathbb{C}$), respectively. Because the real forms are just a particular choice of the $*$-structure, it is possible to guess the numerical R-matrices for the FIO(2,$\mathbb{R}$) and the BISp(2,$\mathbb{R}$) by inspecting those of FIO(2,$\mathbb{C}$) and the BISp(2,$\mathbb{C}$) together with their corresponding algebra (3.12). Besides, since FIO(2) can be extended to FIO(d) for both even and odd d, it is practical to work with its real forms.

The only nontrivial (anti-)commutation relations involve the inhomogeneous parameters, therefore the only difference between the R-matrices of the real forms and those above also involve R_{33}^{ik} components. In fact, the $d=2$ real forms have the R-matrices are

$$R=\begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{4.5}$$

$$R=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{4.6}$$

for the FIO$(2,\mathbb{R})$ and the BISp$(2,\mathbb{R})$, respectively. Note that the R-matrix for FIO(2) is a 9×9 matrix, likewise the R-matrix for FIO(d) is $(d+1)^2\times(d+1)^2$-dimensional, etc. In all the R-matrices given above the places of the nonzero elements of their last columns refer to the (anti-)commutation relations of the pairwise $*$-conjugate elements of the vector **C**. For example, for FIO$(2,\mathbb{C})$, the equations,

$$R^{12}_{ab}M^a_3M^b_3=M^2_bM^1_aR^{ab}_{33}, \tag{4.7}$$

$$R^{21}_{ab}M^a_3M^b_3=M^1_bM^2_aR^{ab}_{33}, \tag{4.8}$$

dictate that the nonzero elements of the last column to be R^{12}_{33}, R^{21}_{33}, and R^{33}_{33}. Similarly for FIO$(2,\mathbb{R})$ it is easy to see that

$$R^{11}_{ab}M^a_3M^b_3=M^1_bM^1_aR^{ab}_{33}, \tag{4.9}$$

$$R^{22}_{ab}M^a_3M^b_3=M^2_bM^2_aR^{ab}_{33}, \tag{4.10}$$

dictate the nonzero elements to be R^{11}_{33}, R^{22}_{33}, and R^{33}_{33}. However, the relative signs of all the nonzero entries can be obtained by inspecting the other components in matrix equations (4.2). One can show that these observations also hold for BISp and for higher dimensions. Keeping these considerations in mind, it can be shown that the nonzero diagonal elements of the $(2d+1)^2\times(2d+1)^2$ R-matrix for FIO$(2d,\mathbb{C})$ are

$$R^{ik}_{ik}=\begin{cases} -1, & \text{if } \forall\, i,k<2d, \\ +1, & \text{if}\begin{cases} i\leqslant(2d+1), & \text{with } k=(2d+1), \\ k\leqslant(2d+1), & \text{with } i=(2d+1), \end{cases} \end{cases} \tag{4.11}$$

whereas the nonzero off-diagonal entries are

$$R^{i}{}_{(2d+1)(2d+1)}^{k}=\begin{cases}+1, & \text{if}\begin{cases} i=k+d, & k<i<d,\\ k=i+d, & i<k<d,\end{cases}\\ 0, & \text{otherwise}.\end{cases} \tag{4.12}$$

Now, for the real forms FIO$(d,\mathbb{R})$, with which we refer to the fact that its elements are equal to their $*$-conjugates, R-matrices can be given in a unified manner in arbitrary dimension d. In accordance with this choice of $*$-conjugation, only the position of the off-diagonal nonzero elements change places. The nonzero elements of the $(d+1)^2\times(d+1)^2$ R-matrices for FIO$(d,\mathbb{R})$ are

$$R_{ik}^{ik}=\begin{cases}-1, & \text{if } \forall\, i,k<(d+1),\\ +1, & \text{if}\begin{cases} i\leqslant(d+1), & \text{with } k=(d+1),\\ k\leqslant(d+1), & \text{with } i=(d+1),\end{cases}\end{cases} \tag{4.13}$$

$$R^{i}{}_{(d+1)(d+1)}^{k}=\begin{cases}+1, & \text{if } i=k,\\ 0, & \text{otherwise}.\end{cases} \tag{4.14}$$

Similarly, the off-diagonal nonzero elements the R-matrices for BISp$(2d,\mathbb{C})$ are

$$R^{i}{}_{(2d)(2d)}^{k}=\begin{cases}+1, & \text{if } i=k+d, \quad k<i<d,\\ -1, & \text{if } k=i+d, \quad i<k<d,\\ 0, & \text{otherwise},\end{cases} \tag{4.15}$$

with all the diagonal entries $R_{ik}^{ik}=1$. Last, for the BISp$(2d,\mathbb{R})$, with the elements having self $*$- conjugation relations, the nonzero off-diagonal elements turn out to be a complex unit number up to sign. The relative sign of these terms are also inherited from the $*$-conjugate pairs of operators. They are given by

$$R^{l}{}_{(2d)(2d)}^{k}=\begin{cases}+i, & \text{if } l=k+d, \quad k<l<d,\\ -i, & \text{if } k=l+d, \quad l<k<d,\\ 0, & \text{otherwise},\end{cases} \tag{4.16}$$

in addition to the elements along the diagonal all of which are equal to 1.

V. CONCLUSION AND FUTURE PERSPECTIVE

The inhomogeneous quantum groups we obtained constructively in a somewhat more generalized form than they appear in Refs. 3 and 11 are richer, in content, than one expects.

Considering the matrix quantum group FIO(2), the homogeneous part of the matrix can be identified with the group $SU(1,1)\simeq Sp(2,\mathbb{R})$ and it is the inhomogeneous parameters that makes the algebra (2.7) noncommutative. The noncommutativity is controlled by the numerical matrix R. Moreover, the partitioning the quantum matrix $\mathbf{M}$ indicated by Eqs. (3.12), makes it possible to define various subgroups of the quantum groups FIO(d) and BISp$(2d)$, yielding as well the different classical groups in appropriate limits.[12] Also, dropping all the homogeneous parameters, the algebra of the remaining inhomogeneous parameters is equivalent to the algebra on which they act (1.1).

To construct a quantum group that act on systems carrying both fermions and bosons at the same framework may be a valuable construction, since interesting and also physically realizable mathematical models involve interaction. In this respect, it may be interesting to look for a scheme which can combine the FIO and BISp, as a supersymmetry theory.

A two-dimensional irreducible representation of the fermion algebra (1.1) is the algebra of the Pauli matrices $\sigma_{\mp}=1/2(\sigma_1\mp i\sigma_2)$. Since the inhomogeneous parameters can be identified with the algebra (1.1) setting the homogeneous parameters zero, if one pursues this correspondence for

arbitrary dimensions, in terms of the Clifford algebra, similar to those given in Ref. 3, this may help to put a differential geometric structure on the quantum groups FIO(d).[13]

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An algorithm for quaternionic linear equations in quaternionic quantum theory

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By means of complex representation and companion vector, in this paper we introduce a definition of rank of a quaternion matrix, study the problems of quaternionic linear equations, and obtain an algorithm for quaternionic linear equations in quaternionic quantum theory. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In the study of theory of quaternionic quantum mechanics and some applied disciplines (Finkelstein *et al.*, 1962; Adler and co-workers, 1985, 1986, 1988, 1995, 1997; Sutcliffe, 2003), one often encounters a problem of solution of quaternionic linear equations. Because of the noncommutation of quaternions, the solution of quaternionic linear equations is more difficult. In order to solve quaternionic linear equations, the author (Adler, 1995) changed the quaternionic linear equations into a two-component complex quaternionic linear equations, and turned the problem of quaternionic linear equations into that of complex linear equations. This paper, by means of complex representation and companion vector, studies the problems of quaternionic linear equations, and gives a technique of computing quaternionic linear equations in quaternionic quantum theory.

Let $\mathbf{R}$ denote the real number field, $\mathbf{C}=\{a+b\sqrt{-1}\,|\,a,b\in\mathbf{R}\}$ the complex number field, $\mathbf{Q}$ the quaternion number field. Let $\mathbf{F}^{m\times n}$ denote the set of $m\times n$ matrices on a field $\mathbf{F}$. For any $A\in\mathbf{C}^{m\times n}$, $\overline{A}$ and A^T denote the conjugate and the transpose of the matrix A, respectively.

For any quaternion $x=x_0+x_1i+x_2j+x_3k=y+zj\in\mathbf{Q}$, in which $x_i\in\mathbf{R}$, and $i^2=j^2=k^2=-1$, $ij=-ji=k$, and quaternion matrix $A\in\mathbf{Q}^{m\times n}$, the complex representation of quaternion x and A are, respectively, defined to be

$$x^f=\begin{pmatrix} x_0+x_1\sqrt{-1} & x_2+x_3\sqrt{-1} \\ -x_2+x_3\sqrt{-1} & x_0-x_1\sqrt{-1}\end{pmatrix}=\begin{pmatrix} y & z \\ -\overline{z} & \overline{y}\end{pmatrix}\in\mathbf{C}^{2\times 2}, \tag{1.1}$$

and

$$A^f=(a_{ij}^f)=\left(\begin{pmatrix} y_{ij} & z_{ij} \\ -\overline{z}_{ij} & \overline{y}_{ij}\end{pmatrix}\right)\in\mathbf{C}^{2m\times 2n}. \tag{1.2}$$

Let $A\in\mathbf{Q}^{m\times n}$, $B\in\mathbf{Q}^{n\times s}$; by the definition of complex representation we easily get the following results:

$$(AB)^f=A^fB^f, \tag{1.3}$$

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$$\overline{A^f} = P_m^T A^f P_n, \tag{1.4}$$

where

$$P_t = \mathrm{diag}(J, J, \ldots, J), \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

and $PP^T = I$.

If $\alpha = (x_1, x_2, \ldots, x_{2n})^T \in \mathbf{C}^{2n\times 1}$, then the companion vector α^c of vector α is defined to be $\alpha^c = (-\overline{x_2}, \overline{x_1}, -\overline{x_4}, \overline{x_3}, \ldots, -\overline{x_{2n}}, \overline{x_{2n-1}})^T \in \mathbf{C}^{2n\times 1}$.

For any quaternion matrix $A \in \mathbf{Q}^{m\times n}$, by the definition of the complex representation of a quaternion matrix there exist complex vectors $\alpha_1, \alpha_2, \ldots, \alpha_n$ such that $A = (\alpha_1, \alpha_1^c, \alpha_2, \alpha_2^c, \ldots, \alpha_n, \alpha_n^c)$.

By the definition of the companion vector we easily prove that if complex vectors $\alpha_1, \alpha_1^c, \alpha_2, \alpha_2^c, \ldots, \alpha_s$ are linearly independent, then complex vectors $\alpha_1, \alpha_1^c, \alpha_2, \alpha_2^c, \ldots, \alpha_s, \alpha_s^c$ are also linearly independent.

From the statement above we get the following result.

Proposition 1.1: Let $A \in \mathbf{Q}^{n\times n}$. Then the rank of complex representation matrix A^f is even.

II. RANK OF QUATERNION MATRICES

In this section, we introduce a definition of rank of quaternion matrices by means of complex representation and a companion vector.

For any quaternion matrix $A \in \mathbf{Q}^{m\times n}$, from Proposition 1.1 we know that the rank of A^f is even, the rank of A is defined to be $\mathrm{rank}(A) = \frac{1}{2}\mathrm{rank}(A^f)$.

By the definition of rank and (1.3) we easily know that almost all the equalities and inequalities of rank to complex matrices hold to quaternion matrices. For instance, if $A \in \mathbf{Q}^{m\times n}$, $B \in \mathbf{Q}^{n\times s}$, then

$$\mathrm{rank}(AB) \leqslant \min\{\mathrm{rank}(A), \mathrm{rank}(B)\}.$$

But $\mathrm{rank}(A)$ and $\mathrm{rank}(A^T)$ are not always the same. For example,

$$A = \begin{pmatrix} 1 & i \\ j & k \end{pmatrix}, \quad \mathrm{rank}(A) \neq \mathrm{rank}(A^T).$$

III. QUATERNIONIC LINEAR EQUATIONS

In this section, we study the solution of quaternionic linear equations $Ax = \beta$ and $AXB = C$, and give a technique of finding a solution of the quaternionic linear equations in quaternionic quantum mechanics and quantum fields.

If $A \in \mathbf{Q}^{m\times n}$, $\beta \in \mathbf{Q}^{m\times 1}$, then by the definition of complex representation and (1.3), $Ax = \beta$ if and only if $A^f x^f = \beta^f$. That is $Ax = \beta$ has a solution x if and only if $A^f Y = \beta^f$ has a solution $Y = x^f$.

If Y is a solution of $A^f Y = \beta^f$, by (1.4),

$$A^f Y = \beta^f \Leftrightarrow \overline{A^f}(P_n^T Y P_1) = \overline{\beta^f} \Leftrightarrow A^f(P_n^T \overline{Y} P_1) = \beta^f, \tag{3.1}$$

i.e., $P_n^T \overline{Y} P_1$ is a solution of $A^f Y = \beta^f$, therefore

$$\hat{Y} = \frac{1}{2}(Y + P_n^T \overline{Y} P_1) \tag{3.2}$$

is also a solution of $A^f Y = \beta^f$. Let

$$Y=(Y_{l1})\in \mathbf{C}^{2n\times 2},\quad Y_{l1}=\begin{pmatrix} z_{l1} & z_{l2}\\ z_{l3} & z_{l4}\end{pmatrix}\in \mathbf{C}^{2\times 2},\quad l=1,2,\ldots,n. \tag{3.3}$$

It is easy to get, by direct calculation,

$$\hat{Y}=(\hat{Y}_{l1})\in \mathbf{C}^{2n\times 2},\quad \hat{Y}_{l1}=\begin{pmatrix} \hat{z}_{l1} & \hat{z}_{l2}\\ -\overline{\hat{z}_{l2}} & \overline{\hat{z}_{l1}}\end{pmatrix}\in \mathbf{C}^{2\times 2},\quad l=1,2,\ldots,n, \tag{3.4}$$

in which

$$\hat{z}_{l1}=\frac{1}{2}(z_{l1}+\overline{z_{l4}}),\quad \hat{z}_{l2}=\frac{1}{2}(z_{l2}-\overline{z_{l3}}). \tag{3.5}$$

From (3.4) we construct a quaternion matrix,

$$x=(x_{l1})\in \mathbf{C}^{n\times 1},\quad x_{l1}=\hat{z}_{l1}+\hat{z}_{l2}j=\frac{1}{2}(1,-j)\hat{Y}_{l1}\begin{pmatrix}1\\ j\end{pmatrix},\quad l=1,2,\ldots,n. \tag{3.6}$$

Therefore we have

$$x=\frac{1}{2}(1,-j,1,-j,\ldots,1,-j)\hat{Y}\begin{pmatrix}1\\ j\end{pmatrix}=\frac{1}{4}(1,-j,1,-j,\ldots,1,-j)(Y+P_n^T\overline{Y}P_1)\begin{pmatrix}1\\ j\end{pmatrix}.$$

Clearly $x_{l1}^f=\hat{Y}_{l1}$, and $x^f=\hat{Y}$. This means that $x^f=\hat{Y}$ is a solution of $A^fY=\beta^f$, so x is a solution of $Ax=\beta$.

From the statement above we get following result.

Theorem 3.1: Let $A\in \mathbf{Q}^{m\times n}$, $\beta\in \mathbf{Q}^{m\times 1}$. Then quaternionic linear equations $Ax=\beta$ have a solution if and only if $\mathrm{rank}(A)=\mathrm{rank}(A,\beta)$, i.e., $Ax=\beta$ has a solution if and only if $A^fY=\beta^f$ has a solution, in which case, if Y is a solution to $A^fY=\beta^f$, then the following quaternion is a solution to $Ax=\beta$:

$$x=\frac{1}{4}(1,-j,1,-j,\ldots,1,-j)(Y+P_n^T\overline{Y}P_1)\begin{pmatrix}1\\ j\end{pmatrix}. \tag{3.7}$$

Moreover, if $\mathrm{rank}(A)=\mathrm{rank}(A,\beta)=n$, then quaternionic linear equations $Ax=\beta$ have a unique solution.

Remark: Theorem 3.1 gives not only sufficient and necessary conditions for quaternionic linear equations $Ax=\beta$ to have a solution, but also a technique of finding a solution to quaternionic linear equations $Ax=\beta$. When the quaternionic linear equations $Ax=\beta$ have a solution, we can find a solution by a solution of complex representation equation $A^fY=\beta^f$ from the formula (3.7). Theorem 3.1 turns the problem of the solution of quaternionic linear equations into that of the solution of complex linear equations by means of complex representations of quaternion matrices.

Similarly we easily get the following result.

Theorem 3.2: Let $A\in \mathbf{Q}^{m\times n}$, $B\in \mathbf{Q}^{p\times q}$, $C\in \mathbf{Q}^{m\times q}$. Then quaternionic matrix equation $AXB=C$ has a solution if and only if $\mathrm{rank}(A)=\mathrm{rank}(A,C)$ and $\mathrm{rank}(B)=\mathrm{rank}\binom{B}{C}$, i.e., quaternionic matrix equation $AXB=C$ has a solution if and only if complex matrix equation $A^fYB^f=C^f$ has a solution, in which case, if Y is a solution to complex matrix equation $A^fYB^f=C^f$, then the following matrix is a solution to $AXB=C$:

$$x=\frac{1}{4}(1,-j,1,-j,\ldots,1,-j)(Y+P_n^T\overline{Y}P_q)(1,j,1,j,\ldots,1,j)^T. \tag{3.8}$$

Moreover, if $\mathrm{rank}(A)=\mathrm{rank}(A,C)=n$ and $\mathrm{rank}(B)=\mathrm{rank}\binom{B}{C}=p$, then quaternionic matrix equation $AXB=C$ has a unique solution.

IV. EXAMPLE

Example: Let

$$A=\begin{pmatrix} i & 1+j \\ -1+j & -k \end{pmatrix}, \quad \beta=\begin{pmatrix} i \\ -1 \end{pmatrix}.$$

Find all solutions of quaternionic linear equations $Ax=\beta$.

It is easy to find the A^f and β^f by the definition of complex representation, and

$$A^f=\begin{pmatrix} i & 0 & 1 & 1 \\ 0 & -i & -1 & 1 \\ -1 & 1 & 0 & -i \\ -1 & -1 & -i & 0 \end{pmatrix}, \quad \beta^f=\begin{pmatrix} i & 0 \\ 0 & -i \\ -1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\mathrm{rank}(A^f)=\mathrm{rank}(A^f,\beta^f)=4$, i.e., $\mathrm{rank}(A)=\mathrm{rank}(A,\beta)=2$, then quaternionic linear equations $Ax=\beta$ have a unique solution.

Since $\mathrm{rank}(A^f)=\mathrm{rank}(A^f,\beta^f)=4$, so $A^fY=\beta^f$ has a unique solution. The unique solution is easily found to be

$$Y=\begin{pmatrix} \frac{2}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} \\ \frac{i}{3} & 0 \\ 0 & -\frac{i}{3} \end{pmatrix}.$$

By (3.7), we easily find the unique solution x of quaternionic linear equations $Ax=\beta$, and

$$x=\frac{1}{4}(1,-j,1,-j)(Y+P_2^T\overline{Y}P_1)\begin{pmatrix} 1 \\ j \end{pmatrix}=\begin{pmatrix} \frac{2}{3}+\frac{1}{3}j \\ \frac{1}{3}i \end{pmatrix}.$$

By means of a complex representation and companion vector, this paper introduces a definition of rank of a quaternion matrix, studies the solutions of quaternionic linear equations, gives sufficient and necessary conditions for the quaternionic linear equations to have a solution, and obtains a technique of finding a solution to quaternionic linear equations. This paper turns the problem of quaternionic linear equations into that of complex linear equations, changes noncommutative quaternion problems to a complex question, and provides a practical algorithm of the solution of quaternionic linear equations in quaternionic quantum theory.

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Intersecting hypersurfaces in dimensionally continued topological density gravitation

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We consider intersecting hypersurfaces in curved spacetime with gravity governed by a class of actions which are topological invariants in lower dimensionality. Along with the Chern–Simons boundary terms there is a sequence of intersection terms that should be added in the action functional for a well defined variational principle. We construct them in the case of Characteristic Classes, obtaining relations which have a general topological meaning. Applying them on a manifold with a discontinuous connection 1-form we obtain the gravity action functional of the system and show that the junction conditions can be found in a simple algebraic way. At the sequence of intersections there are localized independent energy tensors, constrained only by energy conservation. We work out explicitly the simplest nontrivial case. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1794841]

I. INTRODUCTION

General relativity can be generalized to a manifold with a boundary. The inclusion of a certain boundary term (Gibbons–Hawking) makes the action principle well defined on the boundary. Also, singular hypersurfaces of matter[1] can be incorporated into a manifold with piece-wise differentiable metric.[2] We will see that these are part of the general properties of actions built out of dimensionally continued topological invariants. The Einstein–Hilbert action of General Relativity is the dimensionally continued form of the two-dimensional Euler Characteristic. A linear combination of terms which are dimensionally continued Euler densities in arbitrary dimensions is known variously as Lovelock or Lanczos–Lovelock or Gauss–Bonnet gravity. It has been studied extensively[3–6] and the boundary action has been constructed.[7–9]

An interesting problem in gravity is the study of collisions of shells of matter.[10–12] Brane-world models of matter on the intersection of co-dimension 1 branes were studied and it was found that the Gauss–Bonnet term was needed in order to get a tension on the intersection in a natural way.[13] The Gauss–Bonnet term is the dimensionally continued 4-dimensional Euler density. We address this problem of intersections and collisions of co-dimension 1 hypersurfaces in a more generalized way, motivated by the properties of the topological invariants.

A topological invariant "action" contains no local degrees of freedom. The only information it encodes is topological. As such, it is independent of the local form of the metric. We consider actions which are topological in a certain dimensionality and then generalize to higher dimensions. These actions have the property that the independent infinitesimal variation of the action with respect to the connection is a total derivative.

We consider a smooth manifold with embedded arbitrarily intersecting hypersurfaces of singular matter. We can view a hypersurface as the shared boundary of two adjacent regions. The gravity of localized matter can be described by a boundary action. As in Ref. 13, we allow for the possibility of matter being localized on the surfaces of intersection also. The spacetime is divided

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up into polyhedral regions bounded by piece-wise smooth hypersurfaces—like a matrix of cells. We show that this situation is compatible with any theory of gravity based on a dimensionally continued topological invariant.

We exploit the topological nature of the theory to write the action in terms of different connections in different regions. This generates our surface actions remarkably simply. We can derive the Israel junction conditions and the junction conditions for any intersections in a purely algebraic way.

In Sec. II we review basic material on topological densities, introducing Characteristic Classes on a manifold with boundary. In Sec. III A we derive the intersection forms generalizing Chern–Simons forms and in Sec. III B we construct the action functional of gravity in the presence of intersecting hypersurfaces employing the properties of the intersection forms. The topological theory is dealt with in Sec. III B 1 and the dimensionally continued case of interest is dealt with in Sec. III B 2. In Sec. IV we work out a simple example along with the energy exchange relations in that case.

II. TOPOLOGICAL DENSITIES AND GRAVITATION

Let M be a manifold with a Riemannian or Lorentzian metric g and a Levi-Cività connection. Let ω be the connection 1-form and Ω the curvature form. For dim $M=2n$ consider the integral

$$\int_M f(\Omega,\ldots\Omega), \quad f(\Omega,\ldots,\Omega)=\Omega^{a_1a_2}\wedge\cdots\wedge\Omega^{a_{2n-1}a_{2n}}\epsilon_{a_1\cdots a_{2n}}, \tag{1}$$

where $\epsilon_{\ldots}$ is the fully anti-symmetric symbol and $\epsilon_{1\cdots 2n}=+1$ and the integral is assumed to exist. The frame E is ortho-normal in the sense that $g(E^a,E^b)=\delta^{ab}$ in the Riemannian case and $g(E^a,E^b)=\eta^{ab}=\mathrm{diag}(-1,1,\ldots,1)$ in the Lorentzian case.

When g is Riemannian and M is compact and oriented $f(\Omega,\ldots,\Omega)$ represents the Euler class. The integral over M, normalized properly, gives the Euler number of M, according to the renowned Gauss–Bonnet–Chern Theorem.[14] There are more general (and precise) definitions than the one we give here. The details are in the textbooks[15–17] but we only need to point out the similarity and make intelligible borrowing of tools from global differential geometry. $f(\Omega,\ldots,\Omega)$ will be called the Euler density. In general an invariant whose integral over M gives a topological invariant of M will be called topological density.

Let us now repeat the Chern–Weil construction and show that under a continuous change of the connection, $\omega\to\omega'$, $f(\Omega,\ldots,\Omega)$ changes by an exact form. In fact we are only going to need f to be invariant, symmetric and multi-linear. These general properties are provided by the invariant polynomials and lead to the so-called Characteristic Classes, of which the Euler class is an example. The following applies globally on the principal bundle but it is sufficient for our purpose to work on the manifold.

Define

$$\omega_t=t\omega+(1-t)\omega'.$$

Call

$$\theta=\omega-\omega'$$

and note that

$$\theta=\frac{d}{dt}\omega_t,$$

and for the curvature associated with ω_t,

$$\Omega_t = d\omega_t + \omega_t \wedge \omega_t, \tag{2}$$

that

$$\frac{d}{dt}\Omega_t = D_t\theta, \tag{3}$$

where D_t is the covariant derivative associated with ω_t. Then

$$\begin{aligned} f(\Omega, \ldots, \Omega) - f(\Omega', \ldots, \Omega') &= \int_0^1 dt \frac{d}{dt} f(\Omega_t, \ldots, \Omega_t) = n \int_0^1 dt f(d\Omega_t/dt, \Omega_t, \ldots, \Omega_t) \\ &= n \int_0^1 dt f(D_t\theta, \Omega_t, \ldots, \Omega_t) = n \int_0^1 dt df(\theta, \Omega_t, \ldots, \Omega_t), \end{aligned} \tag{4}$$

where symmetry and multi-linearity of f have been used, as well as $D_t\Omega_t = 0$.

If we define

$$\mathcal{L}(\omega) = f(\Omega, \ldots, \Omega) \tag{5}$$

and

$$\mathcal{L}(\omega, \omega') = -n \int_0^1 dt f(\omega - \omega', \Omega_t, \ldots, \Omega_t), \tag{6}$$

we can write

$$\mathcal{L}(\omega) = \mathcal{L}(\omega') - d\mathcal{L}(\omega, \omega'). \tag{7}$$

Now, assume that, for example, M is noncompact and without a boundary. If $\mathcal{L}(\omega, \omega')$ vanishes fast enough asymptotically,

$$\int_M \mathcal{L}(\omega) \tag{8}$$

(assumed to exist) does not depend on ω. It is this property that makes $\mathcal{L}(\omega)$ so useful when, with a little modification, it is used as a Lagrangian for gravity for dim $M > 2n$.

Define the $(d\text{-}r)$-form [which is a natural $(d\text{-}r)$-dimensional volume element]:

$$e_{a_1 a_2 \cdots a_r} = \frac{1}{(d-r)!} \epsilon_{a_1 a_2 \cdots a_d} E^{a_{r+1}} \wedge \cdots \wedge E^{a_d}. \tag{9}$$

The associated dimensionally continued Euler density for $d > 2n$ is

$$\mathcal{L}_g(\omega, e) = f(\Omega, \ldots, \Omega, e) = \Omega^{a_1 b_1} \wedge \Omega^{a_2 b_2} \wedge \cdots \wedge \Omega^{a_n b_n} \wedge e_{a_1 b_1 a_2 b_2 \cdots a_n b_n}, \tag{10}$$

which is also an invariant.

Then, the Euler–Lagrange variation with respect to ω in

$$\int_M \mathcal{L}_g(\omega, e), \tag{11}$$

noting that $\delta\Omega = D(\delta\omega)$, vanishes by the Bianch identity and the assumed zero torsion condition $DE^a = 0$.[18] The equations of motion are obtained simply by the Euler–Lagrange variation of the frame, applying the formula

$$\delta e_{a_1\cdots a_r} = \delta E^{a_{r+1}} \wedge e_{a_1\cdots a_r a_{r+1}}, \tag{12}$$

in a purely algebraic way.

In the next section we find how the action (10) is re-expressed in the presence of hypersurfaces and their intersections, by generalizing (7) appropriately, and show that the equations of motion (junction conditions) are still obtained from the mere variation of the frame.

III. TOPOLOGICAL DENSITIES ON MANIFOLDS CONTAINING INTERSECTING HYPERSURFACES

A hypersurface is understood as a smooth co-dimension 1 subspace of the manifold where the connection form exhibits discontinuity or as a (higher co-dimension) intersection of such discontinuities.

Integrating $\mathcal{L}(\omega)$ over the manifold, when ω is the discontinuous connection form, one has to add a Chern–Simons term integrated over the discontinuity for the final result to have well-defined variations with respect to ω (and to be diffeomorphism invariant). If discontinuities intersect, in all possible ways, one should, in general, add appropriate generalizations of the Chern–Simons forms integrated over the intersections.

A discontinuity can be thought of as the common boundary of two d-dimensional (bulk) regions. The intersection of discontinuities can be thought of as common subspaces of the (not smooth) boundaries of a larger number of bulk regions. It is also helpful to think of them as singular overlaps (at the boundaries) or intersections of two or more bulk regions.

With this in mind, we first find generalizations of the Chern–Simons forms.

A. From boundary to intersection action terms

Given an invariant polynomial, we found in the previous section a relation of the form of (7) by interpolating between the given connection ω and an arbitrary one ω'. We can continue by interpolating between the latter and a new connection. In general, let us define the p-parameter family of connections, interpolating between $p+1$ connections, $\omega^1, \ldots, \omega^{p+1}$,

$$\omega_p = \omega_{t_1\cdots t_p} = \omega^1 - (1-t_1)\theta^1 - \cdots - (1-t_1)\cdots(1-t_p)\theta^p, \tag{13}$$

where

$$\theta^r = \omega^r - \omega^{r+1}, \quad r = 1, \ldots, p. \tag{14}$$

Note: For the purposes of Sec. III A and Eqs. (38)–(44) only, the subscript p refers to a function of $t_1, \ldots, t_p$.

Define

$$\frac{\partial}{\partial t_q}\omega_p = \frac{\partial}{\partial t_q}\omega_{t_1\cdots t_p} = \sum_{r\geqslant q}^{p} (1-t_1)\cdots\widehat{(1-t_q)}\cdots(1-t_r)\theta^r = \theta^q_{t_1\cdots\widehat{t_q}\cdots t_p} = \theta^q_p, \tag{15}$$

where the over caret means that the index is omitted. Note that

$$\omega_{t_1\cdots t_p}\big|_{t_r=0} = \omega_{t_1\cdots t_{r-1}t_{r+1}\cdots t_p}, \tag{16}$$

setting the connection $\omega^r = 0$. This will be useful below. Let Ω_p be the p-parameter curvature 2-form associated with ω_p. Then

$$\frac{\partial}{\partial t_q}\Omega_p = \frac{\partial}{\partial t_q}\Omega_{t_1\cdots t_p} = D_{t_1\cdots t_p}\theta^q_{t_1\cdots\widehat{t_q}\cdots t_p} = D_p\theta^q_p. \tag{17}$$

There is also a "Bianchi identity" for Ω_p,

$$D_p\Omega_p = 0; \tag{18}$$

D_p is the covariant derivative associated with ω_p.

Proposition 1: We introduce a $(p+1)$-point term with $p+1$ connection entries. We now show that the $(p+1)$-point generalization of the 2-point Chern–Simons term takes the form

$$\mathcal{L}(\omega^1, \ldots, \omega^{p+1}) = \eta_p \frac{n!}{(n-p)!} \int_0^1 dt_1 \cdots dt_p f(\theta_p^1, \theta_p^2, \ldots, \theta_p^p, \Omega_p, \ldots, \Omega_p), \tag{19}$$

where $\eta_p = (-1)^{p(p+1)/2}$. These terms obey the following rule:

$$\sum_{s=1}^{p+1} (-1)^{s-p-1} \mathcal{L}(\omega^1, \ldots, \widehat{\omega^s}, \ldots, \omega^{p+1}, \omega^{p+2}) = \mathcal{L}(\omega^1, \ldots, \omega^{p+1}) + d\mathcal{L}(\omega^1, \ldots, \omega^{p+1}, \omega^{p+2}). \tag{20}$$

Proof: If we define

$$\omega_{t_{p+1}}^{p+1} = t_{p+1}\omega^{p+1} + (1 - t_{p+1})\omega^{p+2}, \tag{21}$$

then

$$\mathcal{L}(\omega^1, \ldots, \omega_{t_{p+1}}^{p+1}) = \eta_p \frac{n!}{(n-p)!} \int_0^1 dt_1 \cdots dt_p f(\theta_{p+1}^1, \theta_{p+1}^2, \ldots, \theta_{p+1}^p, \Omega_{p+1}, \ldots, \Omega_{p+1}).$$

We have

$$\begin{aligned}\mathcal{L}(\omega^1, \ldots, \omega^p, \omega^{p+1}) - \mathcal{L}(\omega^1, \ldots, \omega^p, \omega^{p+2}) &= \int_0^1 dt_{p+1} \frac{\partial}{\partial t_{p+1}} \mathcal{L}(\omega^1, \ldots, \omega^p, \omega_{t_{p+1}}^{p+1}) \\ &= \eta_p \frac{n!}{(n-p)!} \int_0^1 dt_1 \cdots dt_p dt_{p+1} \frac{\partial}{\partial t_{p+1}} \\ &\quad \times f(\theta_{p+1}^1, \theta_{p+1}^2, \ldots, \theta_{p+1}^p, \Omega_{p+1}, \ldots, \Omega_{p+1}).\end{aligned}$$

From the multi-linearity of the invariant polynomial f we have

$$\begin{aligned}\frac{\partial}{\partial t_{p+1}} f(\theta_{p+1}^1, \theta_{p+1}^2, \ldots, \theta_{p+1}^p, \Omega_{p+1}, \ldots, \Omega_{p+1}) &= \sum_{r=1}^{p} f\left(\theta_{p+1}^1, \ldots, \frac{\partial}{\partial t_{p+1}} \theta_{p+1}^r, \ldots, \theta_{p+1}^p, \Omega_{p+1}, \ldots, \Omega_{p+1}\right) \\ &\quad + (n-p) f\left(\theta_{p+1}^1, \theta_{p+1}^2, \ldots, \theta_{p+1}^p, \frac{\partial}{\partial t_{p+1}} \Omega_{p+1}, \ldots, \Omega_{p+1}\right).\end{aligned}$$

Using (17), we can write the last term as

$$\begin{aligned}&(n-p)(-1)^p df(\theta_{p+1}^1, \theta_{p+1}^2, \ldots, \theta_{p+1}^p, \theta_{p+1}^{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}) \\ &- (n-p) \sum_{s=1}^{p} (-1)^{p+s-1} f(\theta_p^1, \ldots, D_{p+1}\theta_{p+1}^s, \ldots, \theta_{p+1}^{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}),\end{aligned}$$

and using again (17) in the last term we obtain

$$-\sum_{s=1}^{p}(-1)^{p+s-1}\frac{\partial}{\partial t_s}f(\theta^1_{p+1},\ldots,\widehat{\theta^s_{p+1}},\ldots,\theta^{p+1}_{p+1},\Omega_{p+1},\ldots,\Omega_{p+1})$$
$$+\sum_{s=1}^{p}(-1)^{p+s-1}\sum_{r=1,\neq s}^{p+1}f\left(\theta^1_{p+1},\ldots,\frac{\partial}{\partial t_s}\theta^r_{p+1},\ldots,\widehat{\theta^s_{p+1}},\ldots,\theta^p_{p+1},\theta^{p+1}_{p+1},\Omega_{p+1},\ldots,\Omega_{p+1}\right).$$

In all

$$(n-p)(-1)^p df(\theta^1_{p+1},\theta^2_{p+1},\ldots,\theta^p_{p+1},\theta^{p+1}_{p+1},\Omega_{p+1},\ldots,\Omega_{p+1})$$
$$-\sum_{s=1}^{p}(-1)^{p+s-1}\frac{\partial}{\partial t_s}f(\theta^1_{p+1},\ldots,\widehat{\theta^s_{p+1}},\ldots,\theta^{p+1}_{p+1},\Omega_{p+1},\ldots,\Omega_{p+1})$$
$$+\sum_{s=1}^{p+1}(-1)^{p+s-1}\sum_{r=1,\neq s}^{p+1}f\left(\theta^1_{p+1},\ldots,\frac{\partial}{\partial t_s}\theta^r_{p+1},\ldots,\widehat{\theta^s_{p+1}},\ldots,\theta^p_{p+1},\theta^{p+1}_{p+1},\Omega_{p+1},\ldots,\Omega_{p+1}\right).$$

Note now that

$$\frac{\partial}{\partial t_s}\theta^r_{p+1}=\frac{\partial}{\partial t_s}\frac{\partial}{\partial t_r}\omega_{p+1}=\frac{\partial}{\partial t_r}\theta^s_{p+1};\tag{22}$$

then, in the last term, if we split the sum into $r<s$ and $r>s$, changing variables $r\leftrightarrow s$ in the latter and using this identity we see that the term vanishes. We have shown then that $(p+1)$-point $\mathcal{L}_{p+1}$ defined in (19) obeys a rule,

$$\sum_{s=1}^{p+1}(-1)^{s-p-1}\mathcal{L}(\omega^1,\ldots,\widehat{\omega^s},\ldots,\omega^{p+1},\omega^{p+2})=\mathcal{L}(\omega^1,\ldots,\omega^{p+1})+d\mathcal{L}(\omega^1,\ldots,\omega^{p+1},\omega^{p+2}).$$

The relation (16) has been used. □

It is not hard to show that $\mathcal{L}$ is fully anti-symmetric in its entries, so we can write the above in the form

$$\sum_{s=1}^{p+1}\mathcal{L}(\omega^1,\ldots,\omega^{s-1},\omega',\omega^{s+1},\ldots,\omega^{p+1})=\mathcal{L}(\omega^1,\ldots,\omega^{p+1})+d\mathcal{L}(\omega^1,\ldots,\omega^{p+1},\omega'),\tag{23}$$

where ω' is arbitrary.

As θ^r is a 1-form we have $f(\ldots,\theta^r,\ldots,\theta^r,\ldots,\Omega_p,\ldots\Omega_p)=0$ and we can write (19) explicitly in terms of $\theta^r=\omega^r-\omega^{r+1}$, $r=1\ldots p$ in the form

$$\mathcal{L}(\omega^1,\ldots,\omega^{p+1})=\int_0^1 dt_1\cdots dt_p\zeta_p f(\theta^1,\theta^2,\ldots\theta^p,\Omega_p,\ldots,\Omega_p),\tag{24}$$

$$\zeta_p=(-1)^{p(p+1)/2}\frac{n!}{(n-p)!}\prod_{r=1}^{p-1}(1-t_r)^{p-r}.\tag{25}$$

Let us show that $\mathcal{L}_p$'s, constructed from Characteristic Classes, are invariant under local Lorentz transformations. The connections transform as

$$\omega^r_{(g)}=g^{-1}\omega^r g+g^{-1}\,dg,\tag{26}$$

for all $r=1,\ldots,p+1$, where g belongs to the adjoint representation of SO(d-1,1). Then, $\theta^r_{(g)}=g^{-1}\theta^r g$ and $\Omega_{p(g)}=g^{-1}\Omega_p g$, so [20]

$$\mathcal{L}(\omega^1_{(g)}, \ldots, \omega^{p+1}_{(g)}) = \mathcal{L}(\omega^1, \ldots, \omega^{p+1}). \tag{27}$$

In fact, one can derive (23) without reference to the invariant polynomial, by use of the Poincare lemma and the following observation [inspired by the form of (23)]. If $f(x_1, \ldots, x_n)$ is an anti-symmetric function of n variables and

$$Af(x_1, \ldots x_p, x_{p+1}) = f(x_1, \ldots x_p) - \sum_{i=1}^{p} f(x_1, \ldots, x_{i-1}, x_{p+1}, x_{i+1}, \ldots, x_p) \tag{28}$$

(antisymmetrizing over $n+1$ variables) then $AAf(x_1, \ldots, x_{p+2}) = 0$. The proof is trivial.

We can now show (23) by induction, assuming only that $\mathcal{L}(\omega)$ obeys (7). That is, it is true for the $p=0$ case. Assume (23) for $p=k-1$ [let us use the symbol $\mathcal{L}_k(\omega^1 \ldots \omega^k)$ for the intersection forms in this proof],

$$A\mathcal{L}_k(\omega^1 \cdots \omega^{k+1}) = -\, d\mathcal{L}_{k+1}(\omega^1 \cdots \omega^{k+1}). \tag{29}$$

Then $dA\mathcal{L}_{k+1}(\omega^1 \cdots \omega^{k+2}) = 0$. By the Poincare lemma we have that there exists an invariant form, locally, such that

$$A\mathcal{L}_{k+1}(\omega^1 \cdots \omega^{k+2}) = -\, d\mathcal{L}_{k+2}(\omega^1 \cdots \omega^{k+2}), \tag{30}$$

which completes the induction. (19) is *a* solution of the general relation (23).

There is similarity between our composition rule and Stora–Zumino descent equations.[21] The reason is the existence in both cases of a nilpotent operator, A in our case and the fermionic BRST operator there, which commutes and anticommutes, respectively, with the derivative operator d.

B. Manifolds with discontinuous connection 1-form

We now construct the action functional of gravity on a manifold containing intersecting surfaces. It will also enable us to draw conclusions for arbitrary intersections of hypersurfaces for a general dimensionally continued topological density.

1. Topological density

If the functional $\int_M \mathcal{L}$ is independent of the C^0 metric of the manifold M, then it can be evaluated using a continuous connection as well as a connection that is discontinuous at some subspaces (namely there are hypersurfaces involved). That is, the result will be the same. We use this formal equivalence to give a meaning to $\int_M \mathcal{L}(\omega)$ when ω is discontinuous.

Let us start with the case of a topological density $\mathcal{L}(\omega_0)$ of a continuous connection ω_0 integrated over M which contains a single hypersurface. Label 1 and 2 the regions of M separated by the hypersurface. Introduce two connections, ω_1 and ω_2, which are smooth in the regions 1 and 2, respectively. We now write

$$\int_M \mathcal{L}(\omega_0) = \int_1 \mathcal{L}(\omega_1) + d\mathcal{L}(\omega_1, \omega_0) + \int_2 \mathcal{L}(\omega_2) + d\mathcal{L}(\omega_2, \omega_0). \tag{31}$$

Label the surface, oriented with respect to region 1, with 12 (formally $\int_{12} = -\int_{21}$):

$$\begin{aligned}\int_M \mathcal{L}(\omega_0) &= \int_1 \mathcal{L}(\omega_1) + \int_2 \mathcal{L}(\omega_2) + \int_{12} \mathcal{L}(\omega_1, \omega_0) - \mathcal{L}(\omega_2, \omega_0) \\ &= \int_1 \mathcal{L}(\omega_1) + \int_2 \mathcal{L}(\omega_2) + \int_{12} \mathcal{L}(\omega_1, \omega_2) + d\mathcal{L}(\omega_1, \omega_2, \omega_0).\end{aligned} \tag{32}$$

That is, for a smooth surface the rhs is independent of ω_0.

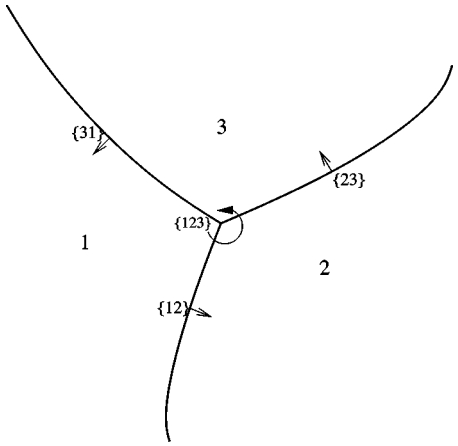

FIG. 1. The simplicial intersection of co-dimension 2 ($h=2$). The totally antisymmetric symbol {123} specifies the intersection including the orientation.

Consider now a sequence of co-dimension $p=1,2,3,\ldots,h$ hyper-surfaces which are intersections of $p+1=2,3,\ldots,h+1$ bulk regions, respectively. We will use the terms intersection and hypersurface alternatively. A co-dimension p hyper-surface is labeled by $i_0\cdots i_p$ where $i_0,\ldots,i_p$ are the labels of the bulk regions which intersect there. We call this configuration a simplicial intersection.

We take the example $h=2$ (Fig. 1), where the intersections are {12}, {13}, {23}, {123}. An exact form integrated over {12} will contribute at {123} the opposite that when integrated over {21}, that is, for the latter integration the intersection can be labeled by $-123=213$, if we assume anti-symmetry of the label. The arrows of positive orientations in Fig. 1 tell us that a fully anti-symmetric symbol {123} will adequately describe the orientations of the intersection 123. This is in contrast to the nonsimplicial intersection (Fig. 2).

Definition 2 (for a simplicial intersection): $\{i_0\cdots i_p\}$ is the set $\overline{i_0}\cap\cdots\cap\overline{i_p}$ where $\overline{i_r}$ is the closure of the open set i_r (a bulk region). $\overline{i_r}$ overlap such that $\partial i_r=\Sigma_{s=0,\neq r}^{h}\,\overline{i_r}\cap\overline{i_s}$ and $i_r\cap i_s=\varnothing$ for all $s\neq r$. This formalises our definitions at the beginning of Sec. II. By $\partial(\overline{A}\cap\overline{B})=(\partial\overline{A}\cap\overline{B})\cup(\overline{A}\cap\partial\overline{B})$, for A, B open sets, we can write

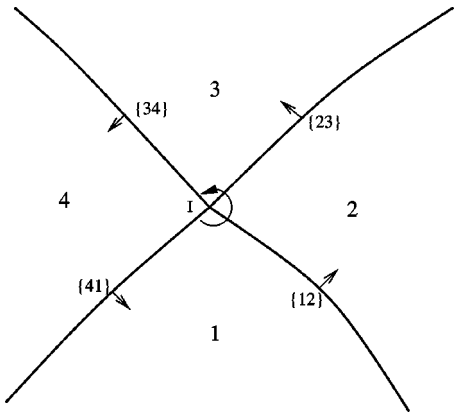

FIG. 2. A nonsimplicial intersection of co-dimension 2 ($h=2$). The intersection, including the orientation, would not be properly represented by the totally anti-symmetric symbol {1234}.

$$\partial\{i_0\cdots i_p\}=\sum_{i_{p+1}}\{i_0\cdots i_{p+1}\}. \tag{33}$$

Full anti-symmetry of the symbol $\{i_0\cdots i_p\}$ keeps track of the orientations properly in (33). As a check,

$$\partial^2\{i_0\cdots i_p\}=\sum_{i_{p+1},i_{p+2}}\{i_0\cdots i_{p+1}i_{p+2}\}=0.$$

Lemma 3: When all intersections are simplicial intersections, with no localized curvature, the contribution from each intersection $\{i_1\cdots i_k\}$ is

$$\int_{\{i_1\cdots i_k\}}\mathcal{L}(\omega_{i_1},\ldots,\omega_{i_k}), \tag{34}$$

up to a boundary term on ∂M.

By "no localized curvature," it is meant that the distributional part of the Riemann curvature tensor must have its support only on co-dimension 1 hypersurfaces and not on lower-dimensional intersections. This is an important condition. We require this in order to have a well-defined ortho-normal frame at the intersections.

Proof: Assume, for $l<h$, we can write

$$\int_M\mathcal{L}(\omega_0)=\sum_{k=1}^{l-1}\frac{1}{k!}\sum_{i_1\cdots i_k}\int_{\{i_1\cdots i_k\}}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_k})+\frac{1}{l!}\sum_{i_1\cdots i_l}\int_{\{i_1\cdots i_l\}}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_l})+d\mathcal{L}(\omega_{i_1}\cdots\omega_{i_l},\omega_0). \tag{35}$$

We have already seen that this is true for $l=1$ and $l=2$. The exact form gives

$$\frac{1}{l!}\sum_{i_1\cdots i_li_{l+1}}\int_{\{i_1\cdots i_li_{l+1}\}}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_l},\omega_0),$$

+ a term on ∂M. From the anti-symmetry of $\{i_1\cdots i_li_{l+1}\}$ and of $\mathcal{L}$ we have

$$\frac{1}{l!}\sum_{i_1\cdots i_{l+1}}\int_{\{i_1\cdots i_li_{l+1}\}}\frac{1}{l+1}\sum_{r=1}^{l+1}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_{r-1}},\omega_0,\omega_{i_{r+1}}\cdots\omega_{i_{l+1}}).$$

Applying the composition rule we get

$$\int_M\mathcal{L}(\omega_0)=\sum_{k=1}^{l}\frac{1}{k!}\sum_{i_1\cdots i_k}\int_{\{i_1\cdots i_k\}}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_k})+\frac{1}{(l+1)!}\sum_{i_1\cdots i_{l+1}}\int_{\{i_1\cdots i_{l+1}\}}\mathcal{L}(\omega_{i_1}\cdots\omega_{i_{l+1}})+d\mathcal{L}(\omega_{i_1}\cdots\omega_{i_{l+1}},\omega_0). \tag{36}$$

Finally we note that the total derivative term on the highest co-dimension intersections (order h), can only contribute to ∂M. So by induction we have proved the Lemma.

Note that apart from our composition formula we have used only Stokes's theorem, which is valid on a topologically nontrivial manifold M assuming a partition of unity f_i subordinated to a chosen covering. By (27) each of the terms appearing will be invariant w.r.t. the structure group. So the last formula is valid over M understanding each $\mathcal{L}$ as $\Sigma_i\, f_i\mathcal{L}$. □

We began with a smooth manifold with an Euler Density action which is completely independent of the choice of ω_0. This gives only a topological invariant of the manifold and is entirely independent of any embedded hypersurfaces. The ω_i's, as well as their number, are arbitrary also. So we see that we have constructed a "theory of gravity," in the presence of arbitrarily intersecting hypersurfaces of discontinuity in the connection, which is a topological invariant. It is a trivial

theory in that the action is completely insensitive to these hypersurfaces. The "gravitational" equations of motion vanish identically, regardless of the geometry, providing no way to relate geometry to energy–momentum.

2. Dimensionally continued Euler densities

Now we consider the dimensionally continued Euler density for arbitrarily intersecting hypersurfaces separating bulk regions counted by i. We postulate the action

$$S_g = \sum_i \int_i \mathcal{L}_g(\omega_i, e) + \sum_{k=2}^{h} \frac{1}{k!} \sum_{i_1 \cdots i_k} \int_{\{i_1 \cdots i_k\}} \mathcal{L}_g(\omega_{i_1}, \ldots, \omega_{i_k}, e). \tag{37}$$

We will show that this action is "one and a half order" in the connection. We will need to revisit our derivation of the composition rule in Sec. III A, this time interpolating between the different metric functions $E^i(x)$, where the index represents the region (the local Lorentz index being suppressed). Physically, we require the metric being continuous at a surface $\Sigma_{1\cdots p+1}$: $i^* E^i = E$ which implies $i^*(e^i) = e$. Here i^* is the pullback of the embedding of $\Sigma_{1\cdots p+1}$ into M. We will see that this continuity condition arises naturally from the action principle. Define the Lagrangian on the surface $\Sigma_{1\cdots p+1}$ to be

$$\mathcal{L}(\omega^1, \ldots, \omega^{p+1}, e) = \int_0^1 dt_1 \cdots dt_p \zeta_p f(\theta^1, \theta^2, \ldots, \theta^p, \Omega_p, \ldots, \Omega_p, e_p),$$

$$(e_p)_{a_1 \cdots a_{2n}} = \frac{1}{(d-2n)!} (E_p)^{a_{2n+1}} \wedge \cdots \wedge (E_p)^{a_d} \epsilon_{a_1 \cdots a_d}, \tag{38}$$

where $E_p = E^1 - (1-t_1)(E^1 - E^2) - \cdots - (1-t_1)\cdots(1-t_p)(E^p - E^{p+1})$ and ζ_p is given by (25).

Following through the calculation of Sec. III A, we pick up extra terms, involving derivatives of E_{p-1}, from using the Leibnitz Rule on f:

$$\begin{aligned} &\frac{\partial}{\partial t_{p+1}} f(\theta^1_{p+1}, \theta^2_{p+1}, \ldots, \theta^p_{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, e_{p+1}) \\ &\quad = \sum_{s=1}^{p+1} f\left(\theta^1_{p+1}, \ldots, \widehat{\theta^s_{p+1}}, \ldots, \theta^{p+1}_{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, \frac{\partial e_{p+1}}{\partial t_s}\right) \\ &\qquad + (n-p) f(\theta^1_{p+1}, \theta^2_{p+1}, \cdot\, \theta^{p+1}_{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, D_{p+1} e_{p+1}) + (\cdots). \end{aligned}$$

The $(\cdots)$ are terms which appear just as in Sec. III A.

We will verify our assertion that the action is one-and-a-half order by infinitesimally varying the metric and connection in one region. We vary them as independent fields. Using t_{p+1} to interpolate between E^{p+1} and $E^{p+1} + \delta E^{p+1}$ and the corresponding variation of ω^{p+1}:

$$\delta\mathcal{L}(\omega^1, \ldots, \omega^{p+1}, e) = \int_0^1 dt_1 \cdots dt_{p+1} \zeta_p \Xi + (\cdots), \tag{39}$$

$$\begin{aligned} \Xi = &\prod_{i=1}^{p} (1-t_i) \sum_{s=1}^{p} f\left(\theta^1_{p+1}, \ldots, \widehat{\theta^s_{p+1}}, \ldots, \delta\omega^{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, \frac{\partial e_{p+1}}{\partial t_s}\right) \\ &- f\left(\theta^1_{p+1}, \ldots, \theta^p_{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, \frac{\partial e_{p+1}}{\partial t_{p+1}}\right) + \prod_{i=1}^{p} (1-t_i)(n-p+1) \\ &\times f(\theta^1_{p+1}, \ldots, \theta^p_{p+1}, \delta\omega^{p+1}, \Omega_{p+1}, \ldots, \Omega_{p+1}, D_{p+1} e_{p+1}). \end{aligned} \tag{40}$$

The $(\cdots)$ are terms which will cancel when intersections are taken into account, just as in the topological theory (provided that the metric is continuous). Above, we have made use of $\theta^{p+1}_{p+1} = -(1-t_1)\cdots(1-t_p)\,\delta\omega^{p+1}$.

We require the vanishing of the terms in (40) involving $\delta\omega^{p+1}$. Now $E_{p+1} = E^1 - (1-t_1)(E^1 - E^2) - \cdots + (1-t_1)\cdots(1-t_{p+1})\,\delta E^{p+1}$. Making use of formula (12),

$$\frac{\partial}{\partial t_s}(e_{p+1})_{a_1\cdots a_{2n}} = \frac{\partial}{\partial t_s}(E_{p+1})^b \wedge (e_{p+1})_{a_1\cdots a_{2n}b}$$
$$= \sum_{i=1}^{p} (1-t_1)\cdots\widehat{(1-t_s)}\cdots(1-t_i)(E^i - E^{i+1})^b \wedge (e_p)_{a_1\cdots a_{2n}b} + \mathcal{O}(\delta E^{p+1}). \quad (41)$$

So we see the first term in (40) vanishes if $i^*(E^{i+1}) = i^*(E^i)$ for all $i = 1\cdots p+1$, i.e., the metric is continuous. Given this, we see that

$$\begin{aligned} i^*(D_{p+1}E_{p+1}) = i^*(dE_{p+1} + \omega_{p+1}\wedge E_{p+1}) &= i^*\big(d\{E^1 + t_1(E^2 - E^1) + \cdots t_1\cdots t_{p+1}\delta E^{p+1}\} \\ &\quad + \{\omega_1 + t_1\theta^1 + \cdots + t_1\cdots t_p\delta\omega_{p+1}\}\wedge(E \\ &\quad + t_1\cdots t_{p+1}\delta E^{p+1})\big) \\ &= i^*\Bigg(D(\omega^1)E^1 + \sum_{i=1}^{p} t_1\cdots t_i(D(\omega^{i+1})E^{i+1} - D(\omega^i)E^i) \\ &\quad + \mathcal{O}(\delta\omega^{p+1}) + \mathcal{O}(\delta E^{p+1})\Bigg). \end{aligned} \quad (42)$$

The third term in (40) already contains a $\delta\omega^{p+1}$ apart from the $D_{p+1}e_{p+1}$. $D_{p+1}e_{p+1}$ is proportional to $D_{p+1}E_{p+1}$ so to first order in δE^p, this term vanishes if $D(\omega^i)E^i = 0$ for all $i = 1\ldots p$.[23]

The only nonvanishing term in (40) is the second which involves

$$\frac{\partial}{\partial t_{p+1}}(e_{p+1})_{a_1\cdots a_{2n}} = -(1-t_1)\cdots(1-t_p)(\delta E^{p+1})^b \wedge (e_{p+1})_{a_1\cdots a_{2n}b} = -(\delta e_p)_{a_1\cdots a_{2n}}.$$

So we arrive at a simple expression for the variation of the action, once the equation of motion for the connection and continuity of the metric have been substituted:

$$\delta\mathcal{L}(\omega^1, \ldots, \omega^{p+1}, e) = \int_0^1 dt_1\cdots dt_p\zeta_p f(\theta^1, \ldots, \theta^p, \Omega_p, \ldots, \Omega_p, \delta e) + (\cdots).$$

Then, variation of an ω_i will vanish automatically upon imposing the zero torsion condition and the continuity of the metric at the intersections.[24] Second, from the variation of the frame E^a we obtain a field equation for gravitation and its relation to the matter present, by

$$\delta_E S_g + \delta_E S_{\text{matter}} = 0. \quad (43)$$

The field equations are actually algebraically obtained, on the gravity side, using (12). Note that although intersections describe physically a situation such as collisions, there is a nonzero energy momentum tensor at the intersection when the theory is not linear in the curvature 2-form. The dimensionally continued nth Euler density produces a nonzero energy tensor down to d-n dimensional intersections. Explicitly, the gravitational equation of motion for a fundamental intersection $\Sigma_{1\cdots p+1}$, carrying localized matter $\mathcal{L}_{m(1\cdots p+1)}$ is

$$\int_0^1 dt_1\cdots dt_p\zeta_p\theta^1\wedge\cdots\wedge\theta^p\wedge(\Omega_p)^{n-p}\wedge\delta E\wedge e = \delta_E\mathcal{L}_{m(1\cdots p+1)}. \quad (44)$$

We have dropped the local frame index and $(\Omega_p)^{n-p} = \Omega_p\wedge\cdots\wedge\Omega_p$.

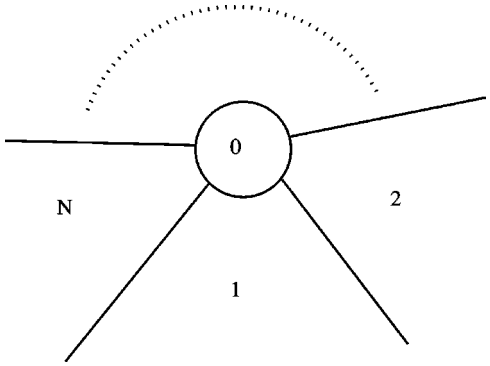

FIG. 3. The nonfundamental intersection viewed as the limit $\{0\}\to I$, where I is a co-dimension 2 surface.

IV. AN EXPLICIT EXAMPLE

We calculate the Lagrangian of the simplest intersection, that of N d-1-dimensional (non-null) surfaces intersecting at the same d-2-dimensional (non-null) surface. We then find explicitly the equations of motion for the intersection in the simplest topological density such that equations of motion are nontrivial, the $n=2$ Euler density (Gauss–Bonnet term). We also express the energy conservation in the form of relations among the energy tensors involved in this case.

A. Equation of motion

We can treat the nonsimplicial intersection with a 2-dimensional normal space as follows. We divide the space–time into $N+1$ regions formed by N surfaces intersecting a cylinder in the middle. Taking the cross section of the system, we see a circle with N outgoing lines, without further intersections (Fig. 3). We call ω the connection inside the circle and ω_i the connections of the N regions formed outside between the lines. We are going to take the limit of the circle to zero size. The intersections are N lowest-dimensional simplicial intersections. We calculate the contributions at the intersections implying that they are integrated over the same surface.

The action functional of the hypersurfaces is

$$\int_{12}\mathcal{L}(\omega_1\omega_2)+\int_{23}\mathcal{L}(\omega_2\omega_3)+\cdots+\int_{N1}\mathcal{L}(\omega_N\omega_1). \tag{45}$$

In order to calculate the equation of motion explicitly in terms of intrinsic and extrinsic curvature tensors we should introduce the connection ω_{ij} associated with the induced metric at the common boundaries. Using the composition rule

$$\mathcal{L}(\omega_i\omega_j)=\mathcal{L}(\omega_i\omega_{ij})+\mathcal{L}(\omega_{ij}\omega_j)-d\mathcal{L}(\omega_i\omega_j\omega_{ij}), \tag{46}$$

we obtain one set of contributions at the intersection, when the common boundary connections are involved.

From the N fundamental intersection, $k=3$ terms in (37), we have

$$\mathcal{L}(\omega_1\omega_2\omega)+\mathcal{L}(\omega_2\omega_3\omega)+\cdots+\mathcal{L}(\omega_N\omega_1\omega). \tag{47}$$

Up to total derivatives, the expression is independent of the connection ω, but depends only on the bulk region connections ω_i. Adding trivially a set of terms $\mathcal{L}(\omega_i\omega_1\omega)+\mathcal{L}(\omega_1\omega_i\omega)=0$, $i=3\ldots N$, and using the composition rule we have

$$\mathcal{L}(\omega_1\omega_2\omega_3)+\mathcal{L}(\omega_1\omega_3\omega_4)+\cdots+\mathcal{L}(\omega_1\omega_{N-1}\omega_N), \tag{48}$$

plus an exact form containing ω. The variation of (47) with respect to the frame gives us the equation of motion.

If we want to express things in terms of extrinsic curvatures, we can use

$$\mathcal{L}(\omega_i\omega_j\omega) + \mathcal{L}(\omega_i\omega\omega_{ij}) + \mathcal{L}(\omega\omega_j\omega_{ij}) = \mathcal{L}(\omega_i\omega_j\omega_{ij}) \tag{49}$$

(dropping the exact forms integrated on the smooth infinite intersection) and (46) and (47) to obtain finally

$$\mathcal{L}_{d-2} = (12) + (23) + \cdots + (N1); \quad (ij) = \mathcal{L}(\omega_i\omega_{ij}\omega) - \mathcal{L}(\omega_j\omega_{ij}\omega). \tag{50}$$

Clearly ω can be taken as the connection associated with the induced metric of the intersection. Now we can express everything in terms of the bulk region connections, the second fundamental forms $\theta_{i|ij}$ of the surface $\{ij\}$ induced by the region i and the χ_{ij}, the second fundamental form of the intersection regarded as the boundary of $\{ij\}$:

$$\theta_{iij} = \omega_i - \omega_{ij}, \quad \chi_{ij} = \omega_{ij} - \omega. \tag{51}$$

Note that, as the form of the Lagrangian suggests, we could directly try to build the Lagrangian by applying the method Sec. II directly without the use of a simplicial intersection and limiting cases. That is, there is nothing singular in the limit taken.

In order to write the simplest nontrivial equation of motion for the common intersection of N d-1-dimensional surfaces, we consider the $n=2$ dimensionally continued Euler density. Applying (19) or (24) we find easily

$$\mathcal{L}(\omega_i\omega_{ij}\omega) = f(\theta_{i\,ij}, \chi_{ij}). \tag{52}$$

As noted above, formula (48), the equation of motion for $\mathcal{L}_{d-2}$ w.r.t. the connection which remains vanished via the assumed zero torsion condition in the dimensionally continued theory. Varying the frame E^a we obtain the equations of motion. We define the gravity Lagrangian as $\mathcal{L}_g = \mathcal{L}^{(1)} + \alpha_1 \mathcal{L}^{(2)}$, where $\mathcal{L}^{(n)}$ is the n-th Euler Density and α_1 is the constant of dimension (length)^2, the coupling of the Gauss–Bonnet term. We express the second fundamental form θ^{ab} in terms of the extrinsic curvature K_{ab} by

$$\theta^{ab} = \theta^{cab} E_c, \quad \text{where} \quad \theta^{cab} = -\epsilon(n) 2 n^{[a} \boldsymbol{\nabla}^{\,b]} n^c = -\epsilon(n) 2 n^{[a} K^{\,b]c}, \tag{53}$$

where n^μ is the normal vector of a $(d$-1)-dimensional surface embedded in a given bulk and it carries the same indices as the θ^{ab} [see (51)] and $K_{\mu\nu} = h^\rho_\mu \boldsymbol{\nabla}_\rho n_\nu$ with $h_{\mu\nu} = g_{\mu\nu} - \epsilon(n) n_\mu n_\nu$, $\epsilon(n) = n_\mu n^\mu = \pm 1$. The vielbein e^μ_a and its inverse e^a_μ is used to change from spacetime to local frame indices. χ^{ab} is defined similarly for v^μ, the normal vector of the intersection embedded in a given $(d$-1)-dimensional hypersurface and it carries the same indices as χ^{ab}, and the extrinsic curvature $C_{\mu\nu} = \gamma^\rho_\mu h^\sigma_\nu \boldsymbol{\nabla}_\rho v_\sigma$ with $\gamma_{\mu\nu} = h_{\mu\nu} - \epsilon(v) v_\mu v_\nu$. We have

$$2\alpha_1 \sum \epsilon(n)\epsilon(v) \left\{ (\mathcal{K}\overline{C})^{ab} + (\overline{\mathcal{K}}C)^{ab} - \frac{1}{2}\gamma^{ab} \mathrm{Tr}(\mathcal{K}\overline{C} + \overline{\mathcal{K}}C) \right\} = -T^{ab}_{d-2}, \tag{54}$$

where $\mathcal{K}_{ab}$ is the projection of K_{ab} on the intersection. Clearly the sum in (54) is over all terms in (50), one for each embedding of each $(d$-1)-surface in the adjacent bulk region. We use the notation $\overline{\mathcal{K}}_{ab} = \mathcal{K}_{ab} - \gamma_{ab}\mathcal{K}$, where $\mathcal{K} = \gamma^{ab}\mathcal{K}_{ab}$, and compact matrix multiplication, for example $(\mathcal{K}\overline{C})^{ab} = \mathcal{K}^c_a \overline{C}^{cb}$. T^{ab}_{d-2} is the energy momentum tensor which in general should be localized at the intersection.

B. Energy conservation at the intersection

Let us see the implications of these results for the question of energy conservation. We recall that the local expression of the energy-momentum tensor conservation is related to the diffeomorphism invariance of the action, under which the metric tensor changes as $\delta g_{ab} = 2\boldsymbol{\nabla}_{(a}\,\xi_{\,b)}$ where $\xi^a = \delta x^a(x)$ are infinitesimal coordinate transformations. Note that $2\boldsymbol{\nabla}_{(a}\xi_{b)} = \delta g_{ab}$ has to be continuous.

Let us first consider the case of an intersection whose action term is zero. Let N regions intersect, labeled by i, at a common intersection I. We write the energy exchange relations in the system as

$$\delta_\xi S_{\text{matter}} = \sum_i \int_i T_d^{ab} \boldsymbol{\nabla}_a \xi_b + \frac{1}{2} \sum_{i,j=i\pm1} \int_{ij} T_{d-1}^{ab} \boldsymbol{\nabla}_a \xi_b = 0, \tag{55}$$

where the normal vectors obey $n_{ij} = -n_{ji}$, $j = i \pm 1$. Then by $\xi_b = \xi_{\|b} + \epsilon(n) n_b n^c \xi_c$ with $\xi_{\|b} = h_b^c \xi_c$ we obtain

$$\begin{aligned} &- \sum_i \int_i \boldsymbol{\nabla}_a T_d^{ab} \xi_b + \sum_{ij} \int_{ij} \epsilon(n) n_a T_d^{ab} h_b^c \xi_c - \frac{1}{2} D_a T_{d-1}^{ab} \xi_b + \sum_{ij} \int_{ij} n_a T_d^{ab} n_b n^c \xi_c \\ &\quad + \frac{1}{2} T_{d-1}^{ab} K(n)_{ab} \epsilon(n) n^c \xi_c + \int_I \sum_{ij} \frac{1}{2} \epsilon(v) v_a T_{d-1}^{ab} \xi_b = 0, \end{aligned} \tag{56}$$

where $K(n)_{ab} = h_a^c \boldsymbol{\nabla}_c n_b$ and $n^a; K_{ab}$ carries an index ij. Also $j = i \pm 1$; the same for v^a which is the normal on I induced by ij pointing outwards. Recall that integrals are taken over the interiors of the sets. Along with the known relations we then obtain the ones related with the intersection

$$\sum \epsilon(v) v_a T_{d-1}^{ab} \gamma_b^c = 0, \quad \sum v_a T_{d-1}^{ab} v_b v^c = 0, \tag{57}$$

where the sum is over all shared boundaries. γ_{ab} is the induced metric at I.

Equation (57) implies that the total energy current density at the intersection or collision is zero. This is valid though when the energy tensor at the intersection vanishes identically. On the other hand, as we have learned, the energy tensor is not zero in general and the energy conservation has to take into account this lower-dimensional energy tensor existing at the intersection hypersurface. In such a case there is an additional term in (55) that can be written as

$$\frac{1}{2N} \int_I \sum_{ij} T_{d-2}^{ab} \boldsymbol{\nabla}_a \xi_b, \tag{58}$$

where we sum over the contribution from each side of every shared boundary for N regions. T_{d-2}^{ab} is the total energy momentum tensor on I. We decompose $\xi_b = \xi_{\|b} + \epsilon(n) n_b n^c \xi_c + \epsilon(v) v_b v^c \xi_c$ where $\xi_{\|b} = \gamma_b^c \xi_c$. We then have

$$- \int_I \mathcal{D}_a T_{d-2}^{ab} \xi_{\|b} + \int_I \mathcal{D}_a (T_{d-2}^{ab} \xi_{\|b}) + \int_I T_{d-2}^{ab} \frac{1}{N} \sum_{ij} (\epsilon(n) \mathcal{K}_{ab} n^c + \epsilon(v) C_{ab} v^c) \xi_c; \tag{59}$$

$\mathcal{D}$ is the covariant derivative associated with γ. The second term is useful when the intersection is not smooth itself. The energy exchange relation are then

$$\sum \epsilon(v) v_a T_{d-1}^{ab} \gamma_b^c = \mathcal{D}_a T_{d-2}^{ac} \sum v_a T_{d-1}^{ab} v_b v^c + T_{d-2}^{ab} \frac{1}{N} \sum_{ij} (\epsilon(n) \mathcal{K}_{ab} n^c + \epsilon(v) C_{ab} v^c) = 0, \tag{60}$$

where the first sums are over all shared boundaries.

For a collision of hypersurfaces, the intersection surface will be space-like. The v vectors are time-like (velocity) vectors. We assume the hypersurface matter of the form

$$v^a v^b T_{ab} = \rho, \quad \gamma_c^a T_{ab} v^b = 0. \tag{61}$$

The first of (57) is satisfied automatically while the second becomes

$$\sum_{\Lambda} \rho_{\Lambda} v_{\Lambda}^{a} = 0, \tag{62}$$

where the upper case greek index counts the hypersurfaces. We can recover the results of Langlois, Maeda, and Wands[11] by first introducing the ortho-normal basis at the intersection. The basis is taken to line up with the two vectors v_{Λ} and n_{Λ} of one of the hypersurfaces:

$$E_{(0)} = v_{\Lambda}, \quad E_{(1)} = n_{\Lambda}. \tag{63}$$

We can write the other v vectors in the following way, motivated by special relativity,

$$v_{\Xi} = \gamma_{\Xi|\Lambda} E_{(0)} + \gamma_{\Xi|\Lambda} \beta_{\Xi|\Lambda} E_{(1)}, \tag{64}$$

where the β and γ have the usual interpretation from S.R. Hence, the two components of Eq. (62) are

$$\sum_{\Xi} \rho_{\Xi} \gamma_{\Xi|\Lambda} = 0, \tag{65}$$

$$\sum_{\Xi} \rho_{\Xi} \gamma_{\Xi|\Lambda} \beta_{\Xi|\Lambda} = 0. \tag{66}$$

These are the results found in Ref. 11; they are conservation of energy and momentum, respectively.

The hypersurfaces obey the same rules in terms of the local inertial frame as do point particle collisions in two dimensions. This is true for quite general bulk backgrounds. The only essential feature is the absence of a deficit angle at the collision. This means that there is a well-defined local inertial frame at the collision and the S.R. addition of velocities applies.

We have calculated the contribution to the energy–momentum tensor at the collision due to the junction conditions. Our calculation implicitly assumed that there was no conical singularity (see the footnote to Lemma 3). There may be some correction to this from a conical singularity. If we impose some reasonable energy condition such as the dominant energy condition, this space-like matter should vanish—the two contributions should cancel. The assumption of no conical deficit is then justified for the *Einstein* theory, because we have seen that there is no contribution due to the junction conditions. But this would not be so for the Gauss–Bonnet theory. In that case, the cancellation would demand that there be a conical singularity at the collision. Conversely, if we impose that there be no such singularity, we must have space-like matter localized at the collision.

Since completion of this work, intersecting branes in Lovelock gravity have been studied by Lee and Tasinato[25] and by Navarro and Santiago.[26] A further analysis of the geometry of intersections has been done by us in Ref. 27.

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Asymptotic upper bounds for the entropy of orthogonal polynomials in the Szegő class

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We give an asymptotic upper bound as $n\to\infty$ for the entropy integral, $E_n(w) = -\int p_n^2(x)\log(p_n^2(x))w(x)dx$, where p_n is the nth degree orthonormal polynomial with respect to a weight $w(x)$ on $[-1,1]$ which belongs to the Szegő class. We also study two functionals closely related to the entropy integral. First, their asymptotic behavior is completely described for weights w in the Bernstein class. Then, as for the entropy, we obtain asymptotic upper bounds for these two functionals when $w(x)$ belongs to the Szegő class. In each case, we give conditions for these upper bounds to be attained. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In the framework of the density functional theory (see, e.g., Refs. 6 and 11), the physical and chemical properties of fermionic systems are described by means of the single-particle probability densities. If $\Psi(\vec{r})$ is the wave function of a single-particle system in a (D-dimensional) position space, and $\hat{\Psi}(\vec{p})$ is the corresponding wave function in momentum space [that is, the Fourier transform of $\Psi(\vec{r})$], then the position and momentum densities of the system are given by

$$\rho(\vec{r}) = |\Psi(\vec{r})|^2, \quad \gamma(\vec{p}) = |\hat{\Psi}(\vec{p})|^2,$$

respectively. It is known that the Boltzmann–Gibbs–Shannon position–space entropy,

$$S(\rho) = -\int \rho(\vec{r})\log\,\rho(\vec{r})d\vec{r},$$

measures the uncertainty in the localization of the particle in space (lower entropy indicates a more concentrated wave function, with the associated higher accuracy in predicting the localization of the particle). The similar is true for the momentum–space entropy,

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$$S(\gamma) = -\int \gamma(\vec{p})\log\ \gamma(\vec{p})d\vec{p}.$$

These quantities have importance in the study of the structure and dynamics of atomic and molecular systems; we refer the reader to the survey[5] and to references therein. Both $S(\rho)$ and $S(\gamma)$ also play a role in a generalization of the Heisenberg uncertainty relation: it has been established[3] that for any pair of densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ in D-dimensional space, we have the sharp inequality

$$S(\rho) + S(\gamma) \geqslant D(1 + \log\ \pi), \tag{1}$$

which expresses quantitatively the impossibility of the simultaneous localization of a pair of observables with no common eigenstates.

It is well known that the wave function of many important systems, such as D-dimensional harmonic oscillator and hydrogen atom, are expressible in terms of families of orthogonal polynomials. It is not surprising that, as it has been shown in Refs. 4 and 13, the computation of the entropies $S(\rho)$ and $S(\gamma)$ usually can be reduced to integrals involving these polynomials.

Let ν be a positive unit Borel measure on $\Delta := [-1,1]$ and let

$$p_n(x) = \gamma_n \prod_{j=1}^{n} (x - \zeta_j^{(n)}), \quad \gamma_n > 0, \quad n \in \mathbb{N},$$

denote the corresponding sequence of *orthonormal* polynomials such that

$$\int p_n(x)p_m(x)d\nu(x) = \delta_{mn}, \quad m,n \in \mathbb{N}.$$

We define the *information entropy* of the polynomials $p_n(x)$ as

$$E_n = E_n(\nu) = -\int p_n^2(x)\log(p_n^2(x))d\nu(x). \tag{2}$$

Throughout the paper, we will assume that the orthogonality measure ν is absolutely continuous with respect to the Lebesgue measure λ on Δ with the Radon–Nikodym derivative

$$d\nu/d\lambda = \nu'(x) = w(x), \quad w \in L^1(\Delta).$$

For normalization purposes, we will always assume that the weight w is unitary, i.e.,

$$\int_{\Delta} w(x)dx = 1. \tag{3}$$

The information entropy will be indistinctly denoted by $E_n(\nu)$ and $E_n(w)$. We follow this convention below for other notations.

The asymptotic behavior of E_n as $n \to \infty$ has a special interest in the study of the so-called Rydberg states of quantum-mechanical systems. Besides physical motivations, there are some fascinating aspects of this problem because of a certain universal behavior of related integrals, and because of a close connection of the entropy E_n with important functionals of the normalized zero counting measures of the polynomials p_n,

$$\mu_n = \frac{1}{n}\sum_{j=1}^{n} \delta_{\zeta_j^{(n)}}, \quad n > 0,$$

and of the following probability measures ν_n:

$$d\nu_n(x) = p_n^2(x)d\nu(x), \quad n \geqslant 0$$

(note that $\nu_0 = \nu$). Both measures are standard objects of study in the analytic theory of orthogonal polynomials. For instance, the normalized zero counting measure μ_n is closely connected with the nth root asymptotics of p_n, and as was shown in Ref. 12, ν_n is associated with the behavior of the ratio p_{n+1}/p_n as $n \to \infty$.

If μ and ν are positive Borel measures on $\mathbb{C}$, then their *mutual entropy* is defined as

$$S(u,v) = \begin{cases} -\infty & \text{if } \mu \text{ is not } \nu\text{-absolutely continuous,} \\ -\int \log\left(\dfrac{d\mu}{d\nu}\right)d\mu & \text{if } \mu \text{ is } \nu\text{-absolutely continuous,} \end{cases}$$

and their *mutual logarithmic energy* as

$$I(\nu,\mu) = -\int\int \log|z-t|d\nu(t)d\mu(z).$$

With these notations the entropy (2) is equivalently rewritten as

$$E_n(\nu) = S(\nu_n,\nu) = -2\log\gamma_n + 2n\, I(\mu_n,\nu_n). \tag{4}$$

In particular, from a classical Jensen's inequality for integrals, it follows immediately that if both μ and ν are unit measures on Δ, then $S(\mu,\nu) \leqslant 0$, with equality if and only if $\mu = \nu$. Hence,

$$E_n(\nu) \leqslant 0,$$

with equality if and only if $n = 0$.

Aptekarev *et al.*[1] considered two subfamilies of the usual Szegő class of weights on Δ, namely the Jacobi weights and the Bernstein-Szegő class (weights being bounded above, bounded away from zero, and satisfying a Dini–Lipschitz condition). In this last case it is known that the asymptotic formula for the orthogonal polynomials p_n holds uniformly in Δ, as n tends to infinity. With these assumptions it has been proved in Ref. 1 that

$$\lim_{n\to\infty} E_n(w) = S(\rho,w) + \log(2) - 1, \tag{5}$$

where

$$\rho(x) = 1/(\pi\sqrt{1-x^2})$$

denotes the Chebyshev unit weight on Δ. We are concerned here with the problem of whether a weaker form of this equality holds in the Szegő class of weights. We will show that the right-hand side of (5) is actually an asymptotic upper bound for the entropy $E_n(w)$ when the weight w satisfies the Szegő condition [see assumption (6) below]. Furthermore, the expression (2) for the entropy can be naturally split into two functionals, which have simple asymptotic behaviors when w belongs to the Bernstein class (see Proposition 1). The situation with the Bernstein class is in a sense optimal: the corresponding limits provide asymptotic upper bounds for w in the whole Szegő class. We also give conditions for the entropy and the two functionals to tend to their upper bounds as the degree n becomes large.

Finally, we must mention that in the case of an unbounded support of the weight of orthogonality interesting results concerning the asymptotics of the E_n and related functionals have been obtained recently in Ref. 9.

II. STATEMENTS OF RESULTS

The weighted L^p norm of a function f with respect to a weight k on Δ will be denoted by

$$\|f\|_{L^p(k)} = \left(\int_\Delta |f(x)|^p k(x) dx \right)^{1/p}, \quad 1 \leqslant p \leqslant \infty.$$

We will simply write L^p when $k \equiv 1$ on Δ.

Though our main interest in this paper lies in the Szegő class of weights, some other classes appear at different places. We recall the definitions of these classes now.

The *Erdős–Turan class* $\mathcal{ET}$ consists of weights $w \in L^1$ such that $w > 0$ almost everywhere on Δ.

The *Szegő class* $\mathcal{S}$ consists of weights $w \in L^1$ such that

$$\log(w_0) \in L^1(\rho), \tag{6}$$

where

$$w_0(x) := w(x)/\rho(x) = \pi\sqrt{1-x^2}w(x)$$

denotes the trigonometric weight corresponding to w. The fact that $w_0 \in L^1(\rho)$ implies $\log^+(w_0) \in L^1(\rho)$, where, as usual, we denote

$$\log^+(x) = \max\{\log(x), 0\}, \quad x > 0.$$

Hence, condition (6) is actually equivalent to

$$S(\rho, w) = \int_\Delta \log(w_0(x))\rho(x)dx > -\infty. \tag{7}$$

Note that (6) and (7) can equivalently be rewritten as $\log(w) \in L^1(\rho)$ and

$$\int_\Delta \log(w(x))\rho(x)dx > -\infty,$$

respectively.

Finally, the *Bernstein class* $\mathcal{B}$ consists of weights w such that w_0 is given by the reciprocal of a positive polynomial on Δ. As it is well-known, the class $\mathcal{B}$ is an important class useful for establishing asymptotic properties in the Szegő theory of orthogonal polynomials. Obviously, one has the following inclusions $\mathcal{B} \subset \mathcal{S} \subset \mathcal{ET}$.

We will also use the notations

$$f_n(x) := p_n(x)\sqrt{w_0(x)}, \tag{8}$$

and for $M > 0$,

$$\Delta_n(M) := \{x \in \Delta : |f_n(x)| \geqslant M\}. \tag{9}$$

One of the main results of the paper is the following theorem.

Theorem 1: *Assume that the weight w belongs to the Szegő class* $\mathcal{S}$*. Then, for all* $M > \sqrt{2}$,

$$E_n(w) = S(\rho, w) + \log(2) - 1 - \int_{\Delta_n(M)} p_n^2(x)\log^+(p_n^2(x))w(x)dx + o(1), \quad n \to \infty. \tag{10}$$

As a simple consequence of the above formula, we obtain the following asymptotic upper bound together with necessary and sufficient conditions for equality.

Corollary 1: Assume that the weight w belongs to the Szegő class $\mathcal{S}$*. Then the following asymptotic upper bound for the entropy holds:*

$$\limsup_{n\to\infty} E_n(w) \leqslant S(\rho, w) + \log(2) - 1. \tag{11}$$

Moreover, for a subsequence $n \in \Lambda \subset \mathbb{N}$,

$$\lim_{n\in\Lambda} E_n(w) = S(\rho,w) + \log(2) - 1, \tag{12}$$

if and only if there exists a constant $M > \sqrt{2}$, *such that*

$$\lim_{n\in\Lambda} \int_{\Delta_n(M)} p_n^2(x)\log^+(p_n^2(x))w(x)dx = 0. \tag{13}$$

In this case (13) is valid for all $M > \sqrt{2}$.

Furthermore, (13) holds if there exists $\varepsilon > 0$ *such that either*

$$\sup_{n\in\Lambda} \int_\Delta (\log^+(p_n^2(x)))^{1+\varepsilon} p_n^2(x)w(x)dx < \infty \quad or \quad \sup_{n\in\Lambda} \int_\Delta (p_n^2(x))^{1+\varepsilon} w(x)dx < \infty. \tag{14}$$

Remark 1: Notice that the findings of Ref. 1 on Bernstein–Szegő polynomials are included in Corollary 1 since for $w \in \mathcal{B}$, $\log(w_0)$ is bounded and the f_n are uniformly bounded in $[-1,1]$. In contrast, the case of Jacobi polynomials requires some extra considerations. One knows that for the orthonormal Jacobi polynomials there exists a constant c such that for $n \geqslant 0$ and $x \in [-1,1]$,

$$|P_n^{(\alpha,\beta)}(x)| \cdot \left(\sqrt{1-x} + \frac{1}{n}\right)^{\alpha+1/2} \left(\sqrt{1+x} + \frac{1}{n}\right)^{\beta+1/2} \leqslant c/\sqrt{\pi}.$$

Taking into account that here $w_0(x) = \pi(1-x)^{\alpha+1/2}(1+x)^{\beta+1/2}$, we find that for $p_n = P_n^{(\alpha,\beta)}$,

$$(p_n(x))^{2+\varepsilon} w_0(x) \leqslant c\sqrt{\pi} \left(\frac{1-x}{(\sqrt{1-x}+1/n)^{2+\varepsilon}}\right)^{\alpha+1/2} \left(\frac{1+x}{(\sqrt{1+x}+1/n)^{2+\varepsilon}}\right)^{\beta+1/2},$$

and the second condition in (14) is satisfied.

Remark 2: An inequality weaker than (11) is a straightforward consequence of the asymptotic behavior of the measures ν_n. Indeed, if $w \in \mathcal{ET}$, we know from Rakhmanov's Theorem[12] that $d\nu_n(x) \to \rho(x)dx$ as $n \to \infty$ in the weak-* topology. It follows from the weak upper semicontinuity of the mutual entropy (Ref. 7, Corollary 5.3) that lim sup $E_n(w) =$ lim sup $S(\nu_n, w) \leqslant S(\rho, w)$. In particular, it shows that if the weight w is in $\mathcal{ET}\backslash\mathcal{S}$,

$$\lim_{n\to\infty} E_n(w) = -\infty.$$

Nevertheless, it seems that a semicontinuity argument for the entropy does not allow us to explain the additional term $\log(2)-1$ occurring on the right-hand side of (12).

The information entropy for Chebyshev polynomials orthonormal with respect to ρ has been computed in Refs. 4,14:

$$E_n(\rho) = \log(2) - 1, \quad \text{for} \quad n \geqslant 1. \tag{15}$$

Intuitively, Chebyshev polynomials are the most "uniformly" distributed polynomials, both for each n and asymptotically as $n \to \infty$. This fact is formally set in the next corollary.

Corollary 2: If

$$\limsup_{n\to\infty} E_n(w) \geqslant \log(2) - 1, \tag{16}$$

then $w = \rho$ *and* $E_n(w) = \log(2) - 1$, $n \geqslant 1$.

The proof is a simple consequence of inequality (11). Indeed, from this inequality, we see that (16) can only happen if $S(\rho,w) = 0$ that is $\rho = w$.

Now we exploit the connection between the entropy $E_n(w)$ and the mutual energy $I(\mu_n, \nu_n)$ given in (4). It is well known that in the class $\mathcal{ET}$ both μ_n and ν_n tend (as $n \to \infty$) to the Chebyshev (equilibrium) distribution given by the weight ρ on Δ. In particular, from the convexity properties of the mutual energy it follows that

$$\lim_{n\to\infty} I(\mu_n, \nu_n) = I(\rho, \rho) = \log(2).$$

What is more surprising is that the next term of the asymptotic expansion of $I(\mu_n, \nu_n)$ also exhibits a "universal" behavior, in the sense that it does not depend on the choice of the weight w. Namely, if the entropy $E_n(w)$ satisfies (12), then the following result is a direct consequence of (4) and the well known asymptotic behavior of the leading coefficient of p_n [see (29)].

Corollary 3: Assume w is a weight in the Szegő class $\mathcal{S}$ and condition (13) is satisfied. Then the mutual energy $I(\mu_n, \nu_n)$ has the following asymptotic expansion:

$$I(\mu_n, \nu_n) = \log(2) - \frac{1}{2n} + o\left(\frac{1}{n}\right), \quad n \in \Lambda, \quad n \to \infty.$$

This remarkable fact certainly deserves further study.

Another aim of the paper is to study two related functionals F_n and G_n, whose sum equals the entropy,

$$E_n(w) = F_n(w) + G_n(w),$$

and which are defined by

$$F_n(w) = -\int_\Delta \log(p_n^2(x) w_0(x)) p_n^2(x) w(x) dx = S(f_n^2 \rho, \rho), \tag{17}$$

and

$$G_n(w) = \int_\Delta \log(w_0(x)) p_n^2(x) w(x) dx = -S(p_n^2 w, p_n^2 \rho). \tag{18}$$

We will see that the functional F_n also exhibits a "universal" behavior, while G_n is sensitive to a particular choice of the weight w, and is related naturally with the mutual entropy $S(\rho, w)$. Functionals F_n and G_n have a particularly nice behavior for w in the Bernstein class $\mathcal{B}$:

Proposition 1: Let S be a polynomial of degree $2N$ $(N \geqslant 0)$ such that $S(x) > 0$ for $x \in \Delta$, and assume that the orthogonality weight satisfies

$$w_0(x) = \frac{1}{S(x)}, \quad x \in \Delta.$$

Then

$$F_n(w) = \log(2) - 1, \quad \textit{for} \quad n > N. \tag{19}$$

Moreover,

$$\lim_{n\to\infty} G_n(w) = S(\rho, w), \tag{20}$$

and this limit takes place with a geometric rate. Consequently, the same holds true for the limit in (5).

The conjecture that constant entropy $E_n(w)$ is a (yet another) characterization of Chebyshev polynomials [cf. (15)] belongs to Golinsky. We were able to prove it in the Bernstein class $\mathcal{B}$.

Proposition 2: Let $w \in \mathcal{B}$ such that $E_n(w)$ is constant for all sufficiently large n. Then $w = \rho$.

Since Bernstein weights are suitable as approximation tool for the whole Szegő class, we could expect the asymptotic behavior from Proposition 1 to hold in a more general setting. Nevertheless, the behavior of the entropy, as well as the behavior of the two functionals F_n and G_n is extremely sensitive to the growth of $p_n^2 w$, which may affect convergence. In general, the following expression for the first functional F_n holds true:

Theorem 2: *Assume the weight w belongs to the Szegő class $\mathcal{S}$. Then, for all $M>\sqrt{2}$,*

$$F_n(w) = \log(2) - 1 - \int_{\Delta_n(M)} \log(f_n^2(x)) f_n^2(x)\rho(x)dx + o(1), \quad n \to \infty. \tag{21}$$

Again, as a simple consequence of the above formula, we get the following corollary.

Corollary 4: Assume the weight w belongs to the Szegő class $\mathcal{S}$. Then, the following asymptotic upper bound for F_n holds:

$$\limsup_{n\to\infty} F_n(w) \leqslant \log(2) - 1. \tag{22}$$

Moreover, for a subsequence $n \in \Lambda \subset \mathbb{N}$,

$$\lim_{n\in\Lambda} F_n(w) = \log(2) - 1, \tag{23}$$

if and only if there exists a constant $M>\sqrt{2}$, such that

$$\lim_{n\in\Lambda} \int_{\Delta_n(M)} f_n^2(x)\log(f_n^2(x))\rho(x)dx = 0, \tag{24}$$

for f_n and $\Delta_n(M)$ defined in (8) and (9), respectively. In this case, (24) is valid for every $M>\sqrt{2}$.

Furthermore, (24) holds if there exists an $\varepsilon>0$ such that either

$$\sup_{n\in\Lambda} \int_{\Delta} (\log^+(f_n^2(x)))^{1+\varepsilon} f_n^2(x)\rho(x)dx < \infty \quad \text{or} \quad \sup_{n\in\Lambda} \int_{\Delta} (f_n^2(x))^{1+\varepsilon}\rho(x)dx < \infty. \tag{25}$$

Remark 3: The method of proof of Theorem 2 can be applied to larger classes of weights. In fact, we only need an L^2 asymptotics of the polynomials p_n on the support Δ of the measure ν, and that has been extended beyond the Szegő class. For instance, using our technique we can prove that (11) is valid for weights $w \in \mathcal{F}(dini)$, introduced in Ref. 8.

Remark 4: Apparently, a necessary condition for (25) is that $w_0 \log(w_0) \in L^1(\rho)$ [cf. with (6)]. If $\log(w_0) \in L^\infty$ then there is equivalence between conditions (13) and (24), and between (14) and (25), respectively.

Concerning the second functional G_n, we use a result from Ref. 10 to deduce the following proposition.

Proposition 3: Assume the weight w belongs to the Szegő class $\mathcal{S}$ and $\log^+(w_0) \in L^\infty$; *then*

$$\limsup_{n\to\infty} G_n(w) \leqslant S(\rho,w) = \int_{\Delta} \log(w_0(x))\rho(x)dx. \tag{26}$$

Similarly, assume that $\log^-(w_0) \in L^\infty$; then

$$\liminf_{n\to\infty} G_n(w) \geqslant S(\rho,w) = \int_{\Delta} \log(w_0(x))\rho(x)dx. \tag{27}$$

Hence, if $\log(w_0) \in L^\infty$, *then*

$$\lim_{n\to\infty} G_n(w) = S(\rho,w).$$

Furthermore, if the weight w belongs to the set $\mathcal{ET}\backslash\mathcal{S}$, *the assumption* $\log^+(w_0)\in L^\infty$ *still implies inequality (26). In this case, (26) simplifies to* $\lim_{n\to\infty}G_n(w)=-\infty$.

III. PROOFS OF THEOREMS 1 AND 2, COROLLARIES 1 AND 4

Before entering the proofs of our results, let us state two preliminary lemmas. The first one is borrowed from Ref. 1.

Lemma 1 (Ref. 1, Lemma 2.1): Let g be a continuous function on $\mathbb{R}$, $g(\theta+\pi)=g(\theta)$, $f\in L^1([0,\pi])$, *and let* $\gamma(\theta)$ *be a function that is measurable and almost everywhere finite on* $[0,\pi]$. *Then, as* $n\to\infty$,

$$\int_0^\pi g(n\theta+\gamma(\theta))f(\theta)d\theta\to\frac{1}{\pi}\int_0^\pi g(\theta)d\theta\int_0^\pi f(\theta)d\theta.$$

As remarked in Ref. 1, when $\gamma(\theta)=0$ and $g\in L^\infty[0,\pi]$, the statement of the lemma becomes a well-known result of Fejer; cf. Ref. 2, Chap. I, Sec. 20.

As the second main ingredient in our proofs let us recall the Szegő asymptotics for $f_n(x)=\sqrt{w_0(x)}p_n(x)$: if

$$g_n(x)=\sqrt{2}\cos(n\arccos x+\gamma(x)),$$

where

$$\gamma(x)=\frac{1}{2\pi}\int_\Delta\frac{\log w_0(x)-\log w_0(t)}{x-t}\sqrt{\frac{1-x^2}{1-t^2}}dt$$

is the harmonic conjugate function to $\log w_0$; then in the Szegő class $\mathcal{S}$, one has

$$\lim_{n\to\infty}\|f_n-g_n\|_{L^2(\rho)}=0, \tag{28}$$

and

$$\lim_{n\to\infty}\log\left(\frac{\gamma_n}{2^n}\right)=-\frac{1}{2}(\log(2)+S(\rho,w)). \tag{29}$$

The mutual entropy on the right-hand side of (29) is known as the Szegő constant for the weight w. Since the entropy integral is very sensitive to the growth of $f_n^2=p_n^2w_0$, the following lemma will be useful; roughly speaking, it shows that the subsets $\Delta_n(M)$, defined in (9), have no influence on the L^2 asymptotics (28):

Lemma 2: For $w\in\mathcal{S}$,

$$\lim_{n\to\infty}\int_{\Delta_n(M)}\rho(x)dx=0, \tag{30}$$

for every $M>\sqrt{2}$. *Furthermore, let* $\widetilde{f}_n$, $n\geqslant 0$, *be the sequence of truncated functions,*

$$\widetilde{f}_n(x):=\begin{cases}f_n(x), & \text{for } x\in\Delta\setminus\Delta_n(M),\\ 1, & \text{for } x\in\Delta_n(M).\end{cases} \tag{31}$$

Then

$$\lim_{n\to\infty}\|\widetilde{f}_n-g_n\|_{L^2(\rho)}=0. \tag{32}$$

Proof: Observe first that by the Cauchy–Schwarz inequality,

$$\int_\Delta |f_n^2(x) - g_n^2(x)|\rho(x)dx \leqslant \|f_n + g_n\|_{L^2(\rho)} \cdot \|f_n - g_n\|_{L^2(\rho)} \leqslant (\|f_n\|_{L^2(\rho)} + \|g_n\|_{L^2(\rho)}) \cdot \|f_n - g_n\|_{L^2(\rho)},$$

so that

$$\int_\Delta |f_n^2(x) - g_n^2(x)|\rho(x)dx \leqslant (1 + \sqrt{2})\|f_n - g_n\|_{L^2(\rho)}. \tag{33}$$

Now we can show that the Chebyshev (and hence, Lebesgue) measure of $\Delta_n(M)$ is asymptotically vanishing: by (33),

$$\begin{aligned}(M^2 - 2)\int_{\Delta_n(M)} \rho(x)dx &\leqslant \int_{\Delta_n(M)} (f_n^2(x) - 2)\rho(x)dx \\ &\leqslant \int_{\Delta_n(M)} |f_n^2(x) - g_n^2(x)|\rho(x)dx \leqslant (1 + \sqrt{2})\|f_n - g_n\|_{L^2(\rho)},\end{aligned}$$

the right-hand side tending to zero as $n \to \infty$ by (28); this proves (30). Moreover, since $|\tilde{f}_n(x)| = 1$ and $|g_n(x)| \leqslant \sqrt{2}$ for $x \in \Delta_n(M)$, we have by (33),

$$\begin{aligned}\|\tilde{f}_n - g_n\|_{L^2(\rho)}^2 &= \int_{\Delta \setminus \Delta_n(M)} |f_n(x) - g_n(x)|^2\rho(x)dx + \int_{\Delta_n(M)} |\tilde{f}_n(x) - g_n(x)|^2\rho(x)dx \\ &\leqslant (1 + \sqrt{2})\|f_n - g_n\|_{L^2(\rho)} + 3\int_{\Delta_n(M)} \rho(x)dx.\end{aligned}$$

It remains to use (28) and (30) to see that (32) is satisfied. □

A. Proof of Theorem 1

Fix arbitrary $M > \sqrt{2}$ and let $\Delta_n(M)$ and $\tilde{f}$ be as defined in (9) and (31), respectively. We write the entropy as

$$E_n(w) = S(f_n^2\rho, w) = S(g_n^2\rho, w) + [S(\tilde{f}_n^2\rho, w) - S(g_n^2\rho, w)] + [S(f_n^2\rho, w) - S(\tilde{f}_n^2\rho, w)]. \tag{34}$$

In three steps let us prove that the first term on the right has as a limit the first three terms on the right-hand side of (1), the second term tends to 0, and the third term is asymptotically negative and related to the integral in (1).

Let

$$\mathcal{R}(y) = y^2 \log(y^2), \quad y \in \mathbb{R}.$$

From Lemma 1 we get

$$\begin{aligned}\lim_{n\to\infty} S(g_n^2\rho, w) &= -\lim_{n\to\infty}\int_0^\pi \mathcal{R}(g_n(\cos(\theta)))\frac{d\theta}{\pi} + \lim_{n\to\infty}\int_0^\pi \log(w_0(\cos(\theta)))g_n^2(\cos(\theta))\frac{d\theta}{\pi} \\ &= -\int_0^\pi \mathcal{R}(\sqrt{2}\cos(\theta))\frac{d\theta}{\pi} + \int_0^\pi 2\cos^2(\theta)\frac{d\theta}{\pi}\int_0^\pi \log(w_0(\cos(\theta)))\frac{d\theta}{\pi} \\ &= E_1(\rho) + S(\rho, w) = \log(2) - 1 + S(\rho, w).\end{aligned} \tag{35}$$

Hence the first term on the right-hand side of (34) has the required limit. The second term in (34) can be written as

$$S(\widetilde{f}_n^2\rho,w)-S(g_n^2\rho,w)=\int_\Delta\left[\mathcal{R}\left(\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right)-\mathcal{R}\left(\frac{g_n(x)}{\sqrt{w_0(x)}}\right)\right]w(x)dx. \tag{36}$$

Recall that both $\widetilde{f}_n$ and g_n are uniformly bounded on Δ by M, and hence for $x\in\Delta$,

$$\left|\mathcal{R}\left(\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right)\right|w_0(x)\leqslant|\mathcal{R}(\widetilde{f}_n(x))|+|\log(w_0(x))|\widetilde{f}_n^2(x)\leqslant M^2\log M^2+M^2|\log(w_0(x))|=:h(x),$$

where $h\in L^1(\rho)$ by assumption (6). Similarly,

$$\left|\mathcal{R}\left(\frac{g_n(x)}{\sqrt{w_0(x)}}\right)\right|w_0(x)\leqslant h(x),\quad x\in\Delta.$$

The integral in (36) will be split into two parts depending on whether w_0 is small or large. Fix an arbitrary $0<\varepsilon<1$; by the monotone convergence theorem there exists a constant $C=C(\varepsilon)$ such that

$$0\leqslant\int_{h(x)>C}h(x)\rho(x)dx=\int_\Delta h(x)\rho(x)dx-\int_{h(x)\leqslant C}h(x)\rho(x)dx<\varepsilon.$$

Defining $\tau:=M^2\exp(-C/M^2)$ we see that $w_0(x)<\tau$ implies that $h(x)>C$, and hence

$$\left|\int_{w_0(x)<\tau}\left[\mathcal{R}\left(\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right)-\mathcal{R}\left(\frac{g_n(x)}{\sqrt{w_0(x)}}\right)\right]w(x)dx\right|\leqslant 2\int_{w_0(x)<\tau}h(x)\rho(x)dx\leqslant 2\varepsilon.$$

On the other hand, if $w_0(x)\geqslant\tau$, then

$$\left|\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right|\leqslant\frac{M}{\sqrt{w_0(x)}}\leqslant\frac{M}{\sqrt{\tau}}=e^{C/(2M^2)}=:C_1,$$

and the same inequality is valid for $g_n/\sqrt{w_0}$. Taking into account that $\mathcal{R}$ is smooth,

$$\begin{aligned}\left|\mathcal{R}\left(\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right)-\mathcal{R}\left(\frac{g_n(x)}{\sqrt{w_0(x)}}\right)\right|&\leqslant\max_{|y|\leqslant C_1}|\mathcal{R}'(y)|\left|\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}-\frac{g_n(x)}{\sqrt{w_0(x)}}\right|\\&\leqslant\max_{|y|\leqslant C_1}|2y(1+\log(y^2))|\left|\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}-\frac{g_n(x)}{\sqrt{w_0(x)}}\right|\\&\leqslant C_2\left|\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}-\frac{g_n(x)}{\sqrt{w_0(x)}}\right|,\end{aligned}$$

with $C_2:=\max\{4e^{-3/2},2C_1(1+\log(C_1^2))\}$. Hence, using the Cauchy–Schwarz inequality,

$$\left|\int_{w_0(x)\geqslant\tau}\left[\mathcal{R}\left(\frac{\widetilde{f}_n(x)}{\sqrt{w_0(x)}}\right)-\mathcal{R}\left(\frac{g_n(x)}{\sqrt{w_0(x)}}\right)\right]w(x)dx\right|\leqslant C_2\|(\widetilde{f}_n-g_n)\sqrt{w_0(x)}\|_{L^1(\rho)}\leqslant C_2\|\widetilde{f}_n-g_n\|_{L^2(\rho)},$$

which by (32) tends to 0 as $n\to\infty$. Taking into account that $\varepsilon\in(0,1)$ was chosen arbitrarily, we conclude that

$$S(\widetilde{f}_n^2\rho,w)-S(g_n^2\rho,w)\to 0,\quad n\to\infty. \tag{37}$$

Thus, for establishing the expression for the entropy in Theorem 1, it only remains to examine the last bracket on the right-hand side of (34). Notice that since $\widetilde{f}_n=f_n$ on $\Delta\setminus\Delta_n(M)$,

$$S(f_n^2\rho,w)-S(\tilde{f}_n^2\rho,w)=-\int_{\Delta_n(M)}p_n^2(x)\log(p_n^2(x))w(x)dx+\int_{\Delta_n(M)}\log\left(\frac{1}{w_0(x)}\right)\rho(x)dx$$
$$=-\int_{\Delta_n(M)}p_n^2(x)\log^+(p_n^2(x))w(x)dx+\int_{\tilde{\Delta}_n(M)}p_n^2(x)|\log(p_n^2(x))|w(x)dx$$
$$-\int_{\Delta_n(M)}\log(w_0(x))\rho(x)dx,$$

where

$$\tilde{\Delta}_n(M)=\{x\in\Delta_n(M):p_n^2(x)<1\}\subset\Delta_n(M).$$

Observing that, for $p_n^2(x)\leqslant 1$, we have $0\leqslant p_n^2(x)\,|\log(p_n^2(x))|\leqslant 1$, we obtain

$$0\leqslant\int_{\tilde{\Delta}_n(M)}p_n^2(x)|\log(p_n^2(x))|w(x)dx\leqslant\int_{\Delta_n(M)}w(x)dx=\int_{\Delta_n(M)}w_0(x)\rho(x)dx.$$

Since $w_0\in L^1(\rho)$, $\log(w_0)\in L^1(\rho)$, by the absolute continuity of the Lebesgue integral, relation (30) implies that

$$\lim_{n\to\infty}\int_{\Delta_n(M)}w_0(x)\rho(x)dx=0,\quad\text{and}\quad\lim_{n\to\infty}\int_{\Delta_n(M)}\log(w_0(x))\rho(x)dx=0,\tag{38}$$

showing that

$$S(f_n^2\rho,w)-S(\tilde{f}_n^2\rho,w)=-\int_{\Delta_n(M)}p_n^2(x)\log^+(p_n^2(x))w(x)dx+o(1),\quad n\to\infty.\tag{39}$$

Hence, gathering (35), (37), and (39) in (34), we get (10). □

B. Proof of Corollary 1

Since

$$\int_{\Delta_n(M)}p_n^2(x)\log^+(p_n^2(x))w(x)dx\geqslant 0,$$

relation (11) is a trivial consequence of Theorem 1. Suppose now that (13) holds for some $M>\sqrt{2}$, then (12) follows immediately from (10). Conversely, if (12) is true then it follows from Theorem 1 that (13) holds for all $M>\sqrt{2}$.

In order to prove that (14) is sufficient for (13), notice that, by Hölder's inequality,

$$\int_{\Delta_n(M)}p_n^2(x)\log^+(p_n^2(x))w(x)dx\leqslant\left(\int_{\Delta_n(M)}p_n^2(x)(\log^+(p_n^2(x)))^{1+\varepsilon}w(x)dx\right)^{1/(1+\varepsilon)}$$
$$\times\left(\int_{\Delta_n(M)}p_n^2(x)w(x)dx\right)^{1-1/(1+\varepsilon)}.\tag{40}$$

Furthermore,

$$\int_{\Delta_n(M)} p_n^2(x)w(x)dx \leqslant \int_{\Delta_n(M)} [f_n^2(x) - g_n^2(x)]\rho(x)dx + \int_{\Delta_n(M)} g_n^2(x)\rho(x)dx$$
$$\leqslant \int_{\Delta_n(M)} [f_n^2(x) - g_n^2(x)]\rho(x)dx + 2\int_{\Delta_n(M)} \rho(x)dx$$
$$\leqslant (1+\sqrt{2})\|f_n - g_n\|_{L^2(\rho)} + 2\int_{\Delta_n} \rho(x)dx = o(1), \quad n \to \infty,$$

where we have used (28), (30), and (33).

If we assume that the first condition in (14) holds, then the first factor on the right-hand side of (40) is uniformly bounded in n, and (13) follows.

Finally, notice that the second condition in (14) implies the first one since $\log^+(z) \leqslant z$ for $z \geqslant 0$, and hence

$$(\log^+(y))^{1+\varepsilon} = \left(\frac{1+\varepsilon}{\varepsilon}\right)^{1+\varepsilon} (\log^+(y^{\varepsilon/(1+\varepsilon)}))^{1+\varepsilon} \leqslant \left(\frac{1+\varepsilon}{\varepsilon}\right)^{1+\varepsilon} y^{\varepsilon}, \quad y \geqslant 0.$$

□

C. Proof of Theorem 2

Our proof for Theorem 2 follows closely the arguments of the proof of Theorem 1, but some parts simplify. As before let $\mathcal{R}(y) = y^2 \log(y^2)$, $y \in \mathbb{R}$, and fix $M > \sqrt{2}$. We write the functional as follows:

$$F_n(w) = \int_\Delta [-\mathcal{R}(g_n(x))]\rho(x)dx + \int_\Delta [\mathcal{R}(g_n(x)) - \mathcal{R}(\tilde{f}_n(x))]\rho(x)dx + \int_\Delta [\mathcal{R}(\tilde{f}_n(x))$$
$$- \mathcal{R}(f_n(x))]\rho(x)dx. \tag{41}$$

Here the first integral on the right-hand side of (41) has the limit $E_1(\rho) = \log(2) - 1$ by Lemma 1. The last one can be written as

$$\int_\Delta [\mathcal{R}(\tilde{f}_n(x)) - \mathcal{R}(f_n(x))]\rho(x)dx = -\int_{\Delta_n(M)} \log(f_n^2(x)) f_n^2(x)\rho(x)dx \leqslant 0,$$

the right-hand side coinciding with the integral in (21). Thus Theorem 2 follows by showing that the second integral on the right-hand side of (41) is asymptotically vanishing. Recalling that $|\tilde{f}_n(x)|$ and $|g_n(x)|$ are uniformly bounded by M for all $n \geqslant 0$ and $x \in \Delta$, we obtain

$$\left| \int_\Delta [\mathcal{R}(g_n(x)) - \mathcal{R}(\tilde{f}_n(x))]\rho(x)dx \right|$$
$$\leqslant \max_{y \in [-M,M]} |\mathcal{R}'(y)| \int_\Delta |g_n(x) - \tilde{f}_n(x)|\rho(x)dx$$
$$\leqslant M^2(1 + \log M^2)\|g_n - \tilde{f}_n\|_{L^1(\rho)} \leqslant M^2(1 + \log M^2)\|g_n - \tilde{f}_n\|_{L^2(\rho)},$$

the term on the right tending to zero as $n \to \infty$ by (32). □

D. Proof of Corollary 4

Since

$$\int_{\Delta_n(M)} f_n^2(x)\log(f_n^2(x))\rho(x)dx \geqslant 0,$$

relation (22) is a trivial consequence of Theorem 2. Suppose now that (24) holds for some $M>\sqrt{2}$; then (23) follows immediately from (21). Conversely, if (23) is true then it follows from Theorem 2 that (24) holds for all $M>\sqrt{2}$.

In order to prove that the first condition in (25) (which clearly is weaker than the second one) is sufficient for (24), notice that, by Hölder's inequality,

$$\int_{\Delta_n} f_n^2(x)\log^+(f_n^2(x))\rho(x)dx \leqslant \left(\int_{\Delta_n} f_n^2(x)(\log^+(f_n^2(x)))^{1+\varepsilon}\rho(x)dx\right)^{1/(1+\varepsilon)}\left(\int_{\Delta_n} f_n^2(x)\rho(x)dx\right)^{1-1/(1+\varepsilon)},$$

and we may conclude as in the proof of Corollary 1 that the second factor on the right-hand side tends to zero. □

IV. PROOFS OF PROPOSITIONS 1, 2, AND 3

A. Proof of Proposition 1

Let us make the change of variables $x=(z+1/z)/2$. It is well known that since $S(x)>0$ on Δ we may write S as

$$S(x) = |q(z)|^2 = q(z)q(1/z), \tag{42}$$

with q a polynomial of degree $2N$ with real coefficients having all its zeros outside the disk and $q(0)>0$. Moreover,

$$p_n(x) = \frac{1}{\sqrt{2}}(z^n q(z^{-1}) + z^{-n}q(z)) \tag{43}$$

is the orthonormal polynomial of degree $n>N$ with respect to the Bernstein weight ρ/S. Introducing the Blaschke product,

$$B_n(z) = z^{2n}q(1/z)/q(z), \quad n \geqslant N, \tag{44}$$

we find that

$$p_n^2(x)w_0(x) = \tfrac{1}{2}|1+B_n(z)|^2 = 1 + \tfrac{1}{2}(B_n(z)+B_n(1/z)), \quad |z|=1.$$

Since, for $n>N$, $B_n(0)=0$, and B_n is analytic in the disk, we have

$$\begin{aligned}\log(2) - F_n(w) &= \log(2) + \int \log(p_n^2(x)w_0(x))p_n^2(x)w_0(x)\rho(x)dx \\ &= \frac{1}{2\pi}\int_{|z|=1}\log(|1+B_n(z)|^2)\left[1+\frac{1}{2}(B_n(z)+B_n(1/z))\right]|dz| \\ &= \mathrm{Re}\left(\frac{1}{2\pi i}\int_{|z|=1}\log(1+B_n(z))[2+B_n(z)+B_n(1/z)]\frac{dz}{z}\right).\end{aligned}$$

Since $|B_n(z)|<1$ for $|z|<1$, the function $\log(1+B_n)[2+B_n]$ is holomorphic inside the disk and vanishes at the origin. Thus,

$$\log(2) - F_n(w) = \mathrm{Re}\left(\frac{1}{2\pi i}\int_{|z|=1}\log(1+B_n(z))B_n(1/z)\frac{dz}{z}\right) \tag{45}$$

$$= \mathrm{Re}\left(\frac{1}{2\pi i} \int_{|z|=1} \frac{\log(1+B_n(z))}{B_n(z)} \frac{dz}{z} \right), \tag{46}$$

where we have used that $B_n(1/z) = 1/B_n(z)$. Observe that the last integrand is analytic in a neighborhood of the unit circle, and we can integrate along a smaller circle $|z| = r < 1$, where $|B_n(z)| < 1$. Replacing the log by its uniformly convergent Taylor expansion we get finally that this integral equals 1, which proves (19).

On the other hand, by a similar reasoning we have

$$\begin{aligned} G_n(w) &= \int_{-1}^{1} \log(w_0(x)) p_n(x)^2 w(x) dx \\ &= -2\mathrm{Re}\left(\frac{1}{2\pi i} \int_{|z|=1} \log(q(z)) \left[1 + \frac{1}{2}(B_n(z) + B_n(1/z)) \right] |dz| \right) \\ &= -2 \log(q(0)) - \frac{1}{2\pi i} \int_{|z|=1} \log(q(z)) B_n(1/z) \frac{dz}{z}. \end{aligned} \tag{47}$$

Note that in the last expression of (47), taking the real part is not necessary since q and B_n are real functions. Integrating now along $|z| = R > 1$, we observe that $|B_n(1/z)|$ becomes geometrically small, there which yields a geometric rate of convergence for

$$\lim_{n\to\infty} G_n(w) = -2 \log(q(0)) = -\mathrm{Re} \frac{1}{\pi} \int_{|z|=1} \log(q(z)) \frac{dz}{z} = S(\rho, w),$$

which proves (20). □

B. Proof of Proposition 2

From the computations of $F_n(w)$ and $G_n(w)$ in the proof of Proposition 1, see (45) and (47), we know that $E_n(w)$ is constant for n large, say $n > N_0 > N$, if and only if

$$\frac{1}{2\pi i} \int_{|z|=1} \frac{B_N(1/z) \log(q(z))}{z^{2n-2N}} \frac{dz}{z} = 0, \quad n > N_0, \tag{48}$$

where the polynomial q and the Blaschke product B_N are defined by (42) and (44), respectively. Since $\log(q(z))$ is analytic in some neighborhood $\mathcal{U}$ of the unit disk, we may conclude that $\log(q(z)) B_N(1/z)$ is meromorphic in $\mathcal{U}$, and thus can be written as

$$B_N(1/z) \log(q(z)) = r(z) + f(z), \quad z \in \mathcal{U}, \tag{49}$$

where r is a rational function such that $z^{2N} q(1/z) r(z)$ is a polynomial of degree at most $2N-1$, and f is analytic in $\mathcal{U}$. Since r is analytic outside the unit disk and grows like at most $1/z$ at infinity, we deduce

$$\frac{1}{2\pi i} \int_{|z|=1} \frac{r(z)}{z^{2n-2N}} \frac{dz}{z} = 0, \quad n > N_0,$$

which implies, together with (48) and (49), that

$$\frac{1}{2\pi i} \int_{|z|=1} \frac{f(z)}{z^{2n-2N}} \frac{dz}{z} = 0, \quad n > N_0.$$

Hence, all sufficiently high even Taylor coefficients of f vanish. As a consequence, $f(z) + f(-z) = P(z)$ is a polynomial, and

$$B_N(1/z)\log(q(z)) + B_N(-1/z)\log(q(-z)) = r(z) + r(-z) + P(z), \quad |z| \leqslant 1. \tag{50}$$

Since the right-hand side of (50) is a rational function, the principle of analytic continuation applies, showing that (50) actually holds everywhere in $\mathbb{C}$. First, assume that the polynomial q is even, that is $q(z)=q(-z)$, $z \in \mathbb{C}$. Then, it follows from (50) that $\log(q(z))$ is a rational function so that q can only be a constant, namely 1 by the normalization (3) of the weight w. Second, assume that the polynomial q is not even (hence different from a constant). It implies the existence of some root $\alpha \in \mathbb{C}$ of q such that either $q(-\alpha) \neq 0$ or $-\alpha$ is a root of q of different multiplicity than that of α. Note that $\alpha \neq 0$ since, by assumption, $q(0) > 0$. Then we get a contradiction. Indeed, in view of the definition (44) of B_N, we readily observe that the left-hand side of (50) has a branch point at α while the right-hand side has not. Hence, $q(z)$ is constant, equal to 1, and the proof of Proposition 2 is finished. □

C. Proof of Proposition 3

Choosing $p=2$ and $g=|\log(w_0)w|^{1/2} \in L^1$ in Theorem 2 of Ref. 10 shows that

$$\liminf_{n\to\infty} \int_\Delta |\log(w_0(x))| p_n^2(x) w(x) dx \geqslant \int_\Delta |\log(w_0(x))| \rho(x) dx, \tag{51}$$

for any weight w in the Erdős–Turan class $\mathcal{ET}$. If $\log^+(w_0) \in L^\infty$, there exists a constant $C>1$ such that $w_0(x) \leqslant C$, $x \in \Delta$. Hence $|\log(w_0/C)| = -\log(w_0/C)$ and substracting $\log(C)$ to both sides of (51), we get (26) since

$$\int_\Delta \rho(x) dx = \int_\Delta p_n^2(x) w(x) dx = 1.$$

A similar reasoning shows (27) when $\log^-(w_0) \in L^\infty$. Since this argument applies for any weight in the Erdős–Turan class, the last assertion in the proposition also follows. □

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Recovering the M-channel Sturm-Liouville operator from M+1 spectra

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For a system of M coupled Schrödinger equations, the relationship is found between the vector-valued norming constants and $M+1$ spectra corresponding to the same potential matrix but different boundary conditions. Under a special choice of particular boundary conditions, this equation for norming vectors has a unique solution. The double set of norming vectors and associated spectrum of one of the $M+1$ boundary value problems uniquely specifies the matrix of potentials in the multichannel Schrödinger equation. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1794844]

I. INTRODUCTION

Consider the system of coupled one-dimensional Schrödinger equations

$$-\frac{d^2}{dx^2}\Psi_\alpha(x)+\sum_\beta V_{\alpha\beta}(x)\Psi_\beta(x)=(E-\varepsilon_\alpha)\Psi_\alpha(x),\quad \alpha=1,\ldots,M. \tag{1}$$

In this system, each equation is referred to as a "channel" and ε_α's are the energies of channel "thresholds." Once $E\geqslant\varepsilon_\alpha$, it is said that α's threshold becomes open. The system (1) is a matrix generalization of the ordinary one-dimensional Schrödinger equation. The coupled Schrödinger equations originate in the Feshbach's unified theory, see Ref. 1, of nuclear reactions and correspond to so-called approximation of the strong coupling [when a finite number of equations in (1) is left]. Now, that method, renewed and generalized (see, e.g., Ref. 2), finds a lot of applications and, rightfully, is one of the most universal tools for microscopic description of systems with many degrees of freedom (nuclear structure, reactions, molecules, etc).

The inverse problem for multichannel Schrödinger Eq. (1) has also been developed.[3–5] As in one-channel case, one can uniquely restore the potential matrix $V_{\alpha\beta}(x)$ from the spectral measure that, e.g., for the case of bounded interval, is specified by the complete set of eigenvalues E_n and so-called norming vectors (spectral weight vectors) $\gamma_\alpha(E_n)$. These vectors characterize the behavior of the normalized wave functions $\Psi_\alpha(x,E_n)$ at one of the boundaries of interval (or at the origin for a half-axis problem, etc.), see also below.

At the same time, in the one-channel case we have more variants of the inverse problem. Among them, there is a statement of an inverse eigenvalue problem on a bounded interval where no norming constants occur. Namely, the potential is uniquely recovered from a knowledge of only two different spectra, each for a distinct pair of homogeneous boundary conditions (with the same potential).[6] There were established necessary and sufficient conditions of the solvability of the inverse Sturm–Liouville problem from two-spectra, see, e.g., Ref. 7.

Until now, one attempt to generalize this theorem to the multichannel Sturm–Liouville operator has been known to the author—see Ref. 8 (the case of a finite-difference operator). Though not complete, this work gave an idea of the existence of such a generalization in principle. No doubt, the possibility of deriving potential matrix from a certain set of spectra would contribute to the

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multichannel inverse problem theory. In the present article, results concerning that problem are obtained. It is found that $M+1$ spectra determine the $V_{\alpha\beta}(x)$ and, under special conditions, it is possible to uniquely restore multichannel Sturm–Liouville operator.

The central idea of this article is to derive the relationship between $M+1$ spectra and M-component norming vector $\gamma_\alpha(E_n)$ associated with one of the $M+1$ boundary value problems on a finite interval (which may be a good model for a description of the compacted system with bound states). Then, having the double set of eigenvalues and norming vectors, one can uniquely restore an interaction matrix by the Gel'fand–Levitan inversion procedure on finite interval. The reader can get acquainted with a multichannel extension of the inverse problem in, e.g., Ref. 5, p. 135 (Sec. IX.4 "Coupled Channels").

The next section is devoted to setting forth these results. We shall find the sought expression which, however, does not guarantee the uniqueness in itself. Only under a special choice of boundary conditions can it be represented in a form of system of linear algebraic equations which give a simple criterion of the uniqueness and solvability. For the sake of the reader's convenience, the narrative is organized so that it goes partially in parallel with standard derivation of two spectra formulas given in Ref. 7, Chap. 3.

II. DERIVATION OF THE FORMULA FOR NORMING VECTOR

We are beginning this section with preliminary notations. Let us rewrite the system (1) in a more symbolic form as follows:

$$-\frac{d^2}{dx^2}y(x)+\hat{V}(x)y(x)=\lambda y(x), \quad x\in[0,a], \tag{2}$$

where y stands for the whole vector-column solution

$$y(x)\equiv\begin{pmatrix}\Psi_1(x)\\ \vdots\\ \Psi_M(x)\end{pmatrix},$$

and

$$\hat{V}\equiv V_{\alpha\beta}+\varepsilon_\alpha\delta_{\alpha\beta}, \quad \lambda\equiv E.$$

The potential matrix is the real symmetric matrix of continuous functions, $x\in[0,a]$. In this article, the hat will always stand for the matrix. Next, we add to Eq. (2) the following boundary conditions:

$$\begin{cases} y'(0)-\hat{h}y(0)=0, & y'(a)+\hat{H}y(a)=0,\\ y_i'(0)-\hat{h}_i y_i(0)=0, & y_i'(a)+\hat{H}y_i(a)=0, \quad i=1,\ldots,M, \end{cases} \tag{3}$$

where we take $\hat{h}$, $\hat{h}_i$, and $\hat{H}$ to all be the real symmetric matrices. We denote the spectra of the M+1 problems (2) and (3) by $\{\lambda_n\}_{n=1}^{\infty}$ and $\{\lambda_n^i\}_{n=1}^{\infty}$, respectively. There is no theorem of interlacing of the spectra in the M-channel case, $M>1$. So, we additionally require that no spectrum degeneracy should occur.

Let us denote by $\hat{\phi}(x,\lambda)$ and $\hat{\chi}_i(x,\lambda)$ the matrix solutions of Eq. (2) satisfying the initial conditions

$$\hat{\phi}(0,\lambda)=\hat{1}, \quad \hat{\phi}'(x,\lambda)|_{x=0}=\hat{h}, \quad \hat{\chi}_i(0,\lambda)=\hat{1}, \quad \hat{\chi}_i'(x,\lambda)|_{x=0}=\hat{h}_i, \tag{4}$$

where the prime stands for the derivative with respect to x. In what follows we shall use the prime to denote this derivative. A matrix solution of (2) means that each column of the matrix is a vector-solution, only satisfying a specific initial (boundary) condition. Eigenvalues of the boundary value problems (2) and (3) coincide with zeros of determinants of the matrices

$$\begin{cases} \hat{\Phi}(\lambda) = \overline{\hat{\phi}}'(x,\lambda)|_{x=a} + \overline{\hat{\phi}}(a,\lambda)\hat{H}, \\ \hat{\Phi}_i(\lambda) = \overline{\hat{\chi}}_i'(x,\lambda)|_{x=a} + \overline{\hat{\chi}}_i(a,\lambda)\hat{H}, \end{cases} \tag{5}$$

where the bar sign denotes transpose.

Now we introduce the norming vectors associated with the spectrum $\{\lambda_n\}_{n=1}^{\infty}$

$$\gamma_{\lambda_n} \equiv \begin{pmatrix} \gamma_1(\lambda_n) \\ \vdots \\ \gamma_M(\lambda_n) \end{pmatrix},$$

such that

$$\hat{\phi}(x,\lambda_n)\gamma_{\lambda_n} = y(x,\lambda_n) \tag{6}$$

with $y'(x,\lambda_n)|_{x=a} + \hat{H}y(a,\lambda_n) = 0$ and $\int_0^a \Sigma_{\alpha=1}^M [\Psi_\alpha(x,\lambda_n)]^2 dx = 1$. Likewise, for the spectra $\{\lambda_n^i\}_{n=1}^{\infty}$

$$\gamma_{\lambda_n^i} \equiv \begin{pmatrix} \gamma_1(\lambda_n^i) \\ \vdots \\ \gamma_M(\lambda_n^i) \end{pmatrix},$$

such that

$$\hat{\chi}_i(x,\lambda_n^i)\gamma_{\lambda_n^i} = y_i(x,\lambda_n^i) \tag{7}$$

with $y_i'(x,\lambda_n^i)|_{x=a} + \hat{H}y_i(a,\lambda_n^i) = 0$ and $\int_0^a \Sigma_{\alpha=1}^M [\Psi_\alpha(x,\lambda_n^i)]^2 dx = 1$. Let us also introduce the function γ_λ (versus λ) such that $\gamma_\lambda = \gamma_{\lambda_n}$ when $\lambda = \lambda_n$ and $\gamma_\lambda = \gamma_{\lambda_n^i}$ when $\lambda = \lambda_n^i$. That function makes sense at the points λ_n and λ_n^i only. In between, we have the freedom to specify it arbitrarily. We can only require this function to be continuously differentiable and have no singularities, $\gamma_\lambda \neq 0$.

We take

$$f_i(x,\lambda) \equiv \overline{\gamma_\lambda}\overline{\hat{\chi}}_i(x,\lambda) + m_i(\lambda)\overline{\gamma_\lambda}\overline{\hat{\phi}}(x,\lambda), \tag{8}$$

where $m_i(\lambda)$ is scalar and we require that

$$f_i'(x,\lambda)_{x=a} + f_i(a,\lambda)\hat{H} = 0 \Rightarrow \tag{9}$$

$$m_i(\lambda)[\overline{\gamma_\lambda}\overline{\hat{\phi}}'(x,\lambda)|_{x=a} + \overline{\gamma_\lambda}\overline{\hat{\phi}}(a,\lambda)\hat{H} = -[\overline{\gamma_\lambda}\overline{\hat{\chi}}_i'(x,\lambda)|_{x=a} + \overline{\gamma_\lambda}\overline{\hat{\chi}}_i(a,\lambda)\hat{H}. \tag{10}$$

Comparing with (5) we have

$$m_i(\lambda) = -\frac{\overline{\Phi}_i(\lambda)\Phi(\lambda)}{\overline{\Phi}(\lambda)\Phi(\lambda)}, \tag{11}$$

where we denote $\Phi(\lambda) \equiv \overline{\hat{\Phi}}(\lambda)\gamma_\lambda$ and $\Phi_i(\lambda) \equiv \overline{\hat{\Phi}}_i(\lambda)\gamma_\lambda$.

Next, employing the well known Green formula we have

$$(\lambda - \lambda_n)\int_0^a f_i(x,\lambda)\hat{\phi}(x,\lambda_n)\gamma_{\lambda_n}dx = f_i'(x,\lambda)|_{x=0}\hat{\phi}(0,\lambda_n)\gamma_{\lambda_n} - f_i(0,\lambda)\hat{\phi}'(x,\lambda)|_{x=0}\gamma_{\lambda_n} = \overline{\gamma_\lambda}(\hat{h}_i - \hat{h})\gamma_{\lambda_n}.$$

From the other hand,

$$(\lambda-\lambda_n)\int_0^a f_i(x,\lambda)\hat{\phi}(x,\lambda_n)\gamma_{\lambda_n}dx=(\lambda-\lambda_n)\int_0^a \overline{\gamma_\lambda}\overline{\hat{\chi}}_i(x,\lambda)\hat{\phi}(x,\lambda_n)\gamma_{\lambda_n}dx-(\lambda-\lambda_n)$$
$$\times\int_0^a \frac{\overline{\Phi}_i(\lambda)\Phi(\lambda)}{\overline{\Phi}(\lambda)\Phi(\lambda)}\overline{\gamma_\lambda}\overline{\hat{\phi}}(x,\lambda)\hat{\phi}(x,\lambda_n)\gamma_{\lambda_n}dx=\overline{\gamma_\lambda}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}, \tag{12}$$

where we used, in the two last formulas, the definitions (4), (8), and (11). The last equality follows from the fact that the matrices in (3) are symmetric.

Let us pass to the limit $\lambda\to\lambda_n$. Then the Eq. (12) goes over into

$$-\frac{\frac{d}{d\lambda}[\overline{\Phi}(\lambda)\Phi(\lambda)]|_{\lambda=\lambda_n}}{\overline{\Phi}_i(\lambda_n)\Phi(\lambda_n)}\overline{\gamma_{\lambda_n}}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}=1, \tag{13}$$

where we used the L' Hospital rule and definition (6).

We shall prove that this formula can be represented as

$$(\lambda_n^i-\lambda_n)^{-1}\prod_{\substack{\mu=1\\ \mu\neq n}}^{\infty}\frac{\lambda_\mu-\lambda_n}{\lambda_\mu^i-\lambda_n}\overline{\gamma_{\lambda_n}}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}=1. \tag{14}$$

Since $\Phi(\lambda)$ and $\Phi_i(\lambda)$ are the entire holomorphic functions they are determined (to within constant multipliers) by their zeros and, hence, can be represented as follows:

$$\Phi(\lambda)=C\prod_{\mu=1}^{\infty}\left(1-\frac{\lambda}{\lambda_\mu}\right);\quad \Phi_i(\lambda)=C_i\prod_{\nu=1}^{\infty}\left(1-\frac{\lambda}{\lambda_\nu^i}\right). \tag{15}$$

Substituting (15) into (13) we have

$$\frac{\frac{1}{\lambda_n}\prod_{\substack{\mu=1\\ \mu\neq n}}^{\infty}\left(1-\frac{\lambda_n}{\lambda_\mu}\right)\overline{C}C}{\prod_{\nu=1}^{\infty}\left(1-\frac{\lambda_n}{\lambda_\nu^i}\right)\overline{C}_iC}\overline{\gamma_{\lambda_n}}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}=1. \tag{16}$$

Now we have to ascertain the expression for the $\overline{C}C/\overline{C}_iC$. We shall need some knowledge about an asymptotic behavior of the solutions of (2). First of all, these equations become uncoupled in the limit $\lambda\to\infty$. So, as in the one-channel case, we have $\lim_{\lambda\to\infty}\hat{\Phi}(\lambda)\{\hat{\Phi}_i(\lambda)\}^{-1}=1$, and the same for the transpose of these matrices. Here the limit is taken for the diverging sequence $\lambda\equiv\lambda(k)=k^{2\pm\varepsilon}+O(1)$ for any $\varepsilon>0$ and k being integer and sufficiently large [we choose such a sequence lest $\lambda(k)$ should coincide with M+1 spectra at even if one point].

Taking this into account we obtain

$$\frac{\overline{C}C}{\overline{C}_iC}\prod_{\mu=1}^{\infty}\frac{\lambda_\mu^i}{\lambda_\mu}\lim_{\lambda\to\infty}\prod_{\mu=1}^{\infty}\frac{\lambda_\mu-\lambda}{\lambda_\mu^i-\lambda}=1. \tag{17}$$

We have the following asymptotic formulas for λ and λ^i: $\lambda_\mu=(\pi/a)^2\mu^2+O(1)$ and the same for λ^i. Then $\lambda_\mu^i-\lambda_\mu=O(1)$ and the series $\Sigma_\mu^\infty|(\lambda_\mu-\lambda_\mu^i)/(\lambda_\mu^i-\lambda)|$ converges uniformly as $\lambda\to\infty$ on the set $\mathbb{R}\setminus(\lambda_\mu\cup\lambda_\mu^i)$. Hence, we can pass to the limit in each term of the infinite product

$$\lim_{\lambda\to\infty}\prod_{\mu=1}^{\infty}\frac{\lambda_\mu-\lambda}{\lambda_\mu^i-\lambda}=\lim_{\lambda\to\infty}\prod_{\mu=1}^{\infty}\left(1+\frac{\lambda_\mu-\lambda_\mu^i}{\lambda_\mu^i-\lambda}\right)=1. \tag{18}$$

We see from (18) and (17) that

$$\frac{\overline{C}C}{\overline{C_i}C}\prod_{\mu=1}^{\infty}\frac{\lambda_\mu^i}{\lambda_\mu}=1. \tag{19}$$

At last, we can obtain the final expression for γ_{λ_n}. Substituting (19) into (16) we have the formula (14)—the system of M equations ($i=1,\dots,M$) for determining M components of γ_{λ_n}.

In the one-channel case the formula (14) goes over into the known expression for two spectra

$$(\lambda_n^2-\lambda_n^1)^{-1}\prod_{\substack{\mu=1\\ \mu\neq n}}^{\infty}\frac{\lambda_\mu^1-\lambda_n^1}{\lambda_\mu^2-\lambda_n^1}(h_2-h_1)\gamma_{\lambda_n}^2=1, \tag{20}$$

where the matrix values become scalars, and we denote, by indices 1 and 2, two spectra determining scalar norming factor γ_{λ_n}.

The system (14) is not linear one: Each row in it contains the quadratic form $\overline{\gamma}_{\lambda_n}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}$. Hence, these equations cannot be solved uniquely in general (including solvability itself). In other words, we have to impose some constraint on choosing the matrices $\hat{h}_i$, i.e., the difference $\hat{h}_i-\hat{h}$. Among other possibilities, we give several realizations which will allow a unique solvability of the system (14).

(i) The symmetric matrix $\hat{h}_i-\hat{h}\equiv\hat{\xi}^{(i)}$ has the form of a Jacobi matrix

$$\hat{\xi}^{(i)}=\begin{pmatrix}\xi_{11}^{(i)} & \xi_{12}^{(i)} & 0 & 0 & . & . & 0\\ \xi_{12}^{(i)} & 0 & \xi_{23}^{(i)} & 0 & . & . & .\\ 0 & \xi_{23}^{(i)} & 0 & \xi_{34}^{(i)} & . & . & .\\ . & . & . & . & . & . & .\\ . & . & . & . & . & . & \xi_{M-1M}^{(i)}\\ 0 & . & . & . & 0 & \xi_{M-1M}^{(i)} & 0\end{pmatrix}, \tag{21}$$

where the main diagonal contains only one nonzero element, $\xi_{11}^{(i)}$. Then

$$\overline{\gamma}_{\lambda_n}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}=\xi_{11}^{(i)}\gamma_1(\lambda_n)^2+2\sum_{k\neq 1}^{M}\xi_{k-1k}^{(i)}\gamma_{k-1}(\lambda_n)\gamma_k(\lambda_n). \tag{22}$$

Introducing the variables $\omega_1\equiv\gamma_1(\lambda_n)^2$ and $\omega_k\equiv\gamma_{k-1}(\lambda_n)\gamma_k(\lambda_n), k=2,\dots,M$ we can rewrite the last expression as follows:

$$\overline{\gamma}_{\lambda_n}(\hat{h}_i-\hat{h})\gamma_{\lambda_n}=\xi_{11}^{(i)}\omega_1+2\sum_{k\neq 1}^{M}\xi_{k-1k}^{(i)}\omega_k. \tag{23}$$

Then (14) becomes the system of linear algebraic equations for the variables ω. If $\omega_1=\gamma_1(\lambda_n)^2>0$, then $\gamma_1(\lambda_n)=\pm\omega_1^{1/2}$, $\gamma_2(\lambda_n)=\mp\omega_2/\omega_1^{1/2}$ and so forth. The sign in front of $\omega_1^{1/2}$ in the expression for $\gamma_1(\lambda_n)$ determines the common sign for γ_{λ_n} and, hence, is inessential: The whole vector-valued wave function is determined to within sign ($\pm$). With the nonzero element $\xi_{ll}^{(i)}\neq 0, l\neq 1$ positioned in arbitrary place of the main diagonal, the scheme is analogous.

(ii) The matrix $\hat{h}_i-\hat{h}\equiv\hat{\zeta}^{(i)}$ is represented as follows:

$$\hat{\zeta}^{(i)} = \begin{pmatrix} 0 & . & 0 & \zeta_{1l}^{(i)} & 0 & . & 0 \\ . & . & . & . & . & . & . \\ . & . & 0 & \zeta_{l-1l}^{(i)} & 0 & . & . \\ \zeta_{l1}^{(i)} & . & \zeta_{ll-1}^{(i)} & \zeta_{ll}^{(i)} & \zeta_{ll+1}^{(i)} & . & \zeta_{lM}^{(i)} \\ . & . & 0 & \zeta_{l+1l}^{(i)} & 0 & . & 0 \\ . & . & . & . & . & . & . \\ 0 & . & 0 & \zeta_{Ml}^{(i)} & 0 & . & 0 \end{pmatrix}, \tag{24}$$

i.e., the matrix contains one nonzero row and one nonzero column which cross each other in a place of the entry $\zeta_{ll}^{(i)}$. For the quadratic form we have (using the symmetry of $\hat{h}_i - \hat{h}$)

$$\overline{\gamma}_{\lambda_n}(\hat{h}_i - \hat{h})\gamma_{\lambda_n} = \zeta_{ll}^{(i)}\gamma_l(\lambda_n)^2 + 2\sum_{k\neq l}^{M} \zeta_{lk}^{(i)}\gamma_l(\lambda_n)\gamma_k(\lambda_n). \tag{25}$$

Introducing new variables $\theta_k \equiv \gamma_l(\lambda_n)\gamma_k(\lambda_n)$, $k \neq l$, and $\theta_l \equiv \gamma_l(\lambda_n)^2$ we can now look upon (14) as a linearized system again

$$(\lambda_n^i - \lambda_n)^{-1}\prod_{\substack{\mu=1 \\ \mu\neq n}}^{\infty} \frac{\lambda_\mu - \lambda_n}{\lambda_\mu^i - \lambda_n}\left\{ \zeta_{ll}^{(i)}\theta_l + 2\sum_{k\neq l}^{M} \zeta_{lk}^{(i)}\theta_k \right\} = 1. \tag{26}$$

After deriving θ_i, one can obtain $\gamma_i(\lambda_n)$ trivially. Of course, the solvability in this case depends on whether the corresponding determinant for the system (26) is nonzero and $\theta_l > 0$.

In all the cases, the knowledge of the complete set $\{\lambda_n, \gamma_{\lambda_n}\}_{n=1}^{\infty}$ allows a unique restoration of the potential matrix by the standard Gel'fand–Levitan theory (its multichannel generalization).

III. CONCLUSIONS

In this article, the relationship is established between components of the norming vector γ_{λ_n} associated with a certain boundary value problem (with the spectrum $\{\lambda_n\}_{n=1}^{\infty}$) and the spectra (including $\{\lambda_n\}_{n=1}^{\infty}$) of $M+1$ multichannel Sturm-Liouville operators with the same potential matrix $V_{\alpha\beta}(x)$ but different boundary conditions. As a matter of fact, the central result is formula (14). Though giving no unique solutions in general, it can get linear if we require the matrices $\hat{h}_i$ to be of special type. Hence, the uniqueness of the multichannel inverse eigenvalue problem from $M+1$ spectra is however possible for a particular class of boundary conditions. The problem of specifying the necessary and sufficient conditions needs a special examination. It is clear that scrutinizing the asymptotic behavior of the spectra with different boundary conditions will be required. It is closely associated with specifying the class of differentiable functions the $V_{\alpha\beta}(x)$ pertain to. So, the results given present only an intermediate stage in investigations on the subject.

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Semiclassical wave-packet scattering in one and two dimensions

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We prove that under short range potentials a semiclassical wave packet's propagation is accurate for infinite times in the $\hbar \to 0$ limit. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1780613]

I. INTRODUCTION

Semiclassical analysis is the study of the connections between the quantum dynamics and the corresponding classical dynamics in the $\hbar \to 0$ limit. Consider the quantum dynamics determined by the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left\{ -\frac{\hbar^2}{2}\Delta_x + V(x) \right\} \psi(x,t). \tag{1}$$

Following the prescription defined in Refs. 1–5 one can construct approximate solutions to this equation whose time propagation is determined by the corresponding classical mechanics. These wave packets depend explicitly on the corresponding classical dynamics of the system, $\hbar$, and position. These semiclassical wave packets can be used to approximate the quantum dynamics.[1–5] Here we present a result for the semiclassical wave packets that is uniform in time. This result is an extension of a known result[1] to one and two space dimensions.

The organization of the paper is as follows: In Sec. II we present the construction of the semiclassical wave packets. In Sec. III we introduce the needed results from classical scattering theory. In Sec. IV we state and prove Theorem 1, the main result of the paper for $n=1$, referring the reader to some technical lemmas from Sec. V. In Sec. VI we provide the necessary tools needed to extend the proof to two dimensions.

Throughout we adopt standard multi-index notation.[7] The inner products are linear in the second term, conjugate linear in the first. Furthermore, we assume that our potential is "short range," i.e., $V(x)$ satisfies the short-range assumption (D) if for any multi-index α such that $|\alpha| = 0,1,2,3$, there exists $C_{|\alpha|} > 0$, $0 < \nu < 1$, such that

$$|(D^\alpha V)(x)| \leqslant C_{|\alpha|}(1+|x|)^{-1-|\alpha|-\nu}.$$

Notice that if a potential is short range then

$$V(x) \in L^p(\mathbb{R}^n) \text{ for } p > \max\left\{ \frac{n}{1+\nu}, 1 \right\}$$

and

$$V(x)(1+x)^{-[(n/2)-1]+(\nu/2)} \in L^2(\mathbb{R}^n).$$

So, for $n=1,2$ our potentials are in $L^2(\mathbb{R}^n)$.

II. SEMICLASSICAL WAVE PACKETS

Here we present a definition of the semiclassical wave packets. Our construction is analogous to the standard construction of the harmonic oscillator eigenstates using raising and lowering operators. Greater detail on the construction presented here can be found in Ref. 4. Let $a,\ \eta \in \mathbb{R}^n$, and $\hbar > 0$. Furthermore assume that A and B are complex $n \times n$ matrices satisfying

$$A^t B - B^t A = 0, \tag{2}$$

$$A^* B + B^* A = 2I. \tag{3}$$

Conditions (2) and (3) are known to be equivalent to the following four conditions assumed in Ref. 1:

(i) A and B are invertible;
(ii) the real and imaginary parts of BA^{-1} are both real symmetric;
(iii) $\mathrm{Re}\, BA^{-1}$ is strictly positive definite;
(iv) $(\mathrm{Re}\, BA^{-1})^{-1} = AA^*$.

Let $p = -i\hbar\nabla_x$ be the momentum operator. For any $v \in \mathbb{C}^n$ we define associated raising and lowering operators by

$$\mathcal{A}(A,B,\hbar,a,\eta,v)^* = \frac{1}{\sqrt{2\hbar}}[\langle B\overline{v},(x-a)\rangle - i\langle A\overline{v},(p-\eta)\rangle]$$

and

$$\mathcal{A}(A,B,\hbar,a,\eta,v) = \frac{1}{\sqrt{2\hbar}}[\langle \overline{B}v,(x-a)\rangle + i\langle \overline{A}v,(p-\eta)\rangle].$$

Let $\{e_j\}$ be any orthonormal basis for $\mathbb{R}^n$, and define

$$\mathcal{A}_j(A,B,\hbar,a,\eta)^* = \mathcal{A}(A,B,\hbar,a,\eta,e_j)^*,$$

$$\mathcal{A}_j(A,B,\hbar,a,\eta) = \mathcal{A}(A,B,\hbar,a,\eta,e_j).$$

Then we can define

$$\mathcal{A}(A,B,\hbar,a,\eta)^* = \frac{1}{\sqrt{2\hbar}}[B^*(x-a) - iA^*(p-\eta)],$$

$$\mathcal{A}(A,B,\hbar,a,\eta) = \frac{1}{\sqrt{2\hbar}}[B^t(x-a) + iA^t(p-\eta)],$$

where the representation is in terms of the above basis. Define $\phi_0(A,B,\hbar,a,\eta,\cdot)$ to be a normalized vector with respect to $L^2(\mathbb{R}^n)$ such that

$$\mathcal{A}(A,B,\hbar,a,\eta)\phi_0(A,B,\hbar,a,\eta,\cdot) = 0.$$

It is seen that

$$\phi_0(A,B,\hbar,a,\eta,x) = (\pi\hbar)^{-n/4}(\det(A))^{-1/2}\exp\{-\langle (x-a),BA^{-1}(x-a)\rangle/(2\hbar) + i\langle \eta,(x-a)\rangle/\hbar\}.$$

Here a particular choice of phase is being made. For any multi-index k, we define

$$\phi_k(A,B,\hbar,a,\eta,x) = \frac{1}{\sqrt{k!}}(\mathcal{A}_1(A,B,\hbar,a,\eta)^*)^{k_1} \times \cdots \times (\mathcal{A}_n(A,B,\hbar,a,\eta)^*)^{k_n}\phi_0(A,B,\hbar,a,\eta,x).$$

Remark: The only ambiguity here is in the choice of sign on $(\det(A))^{-1/2}$, it is chosen depending on the initial conditions and continuity.

Remark: The functions $\phi_k(A,B,\hbar,a,\eta,\cdot)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$.[4]

Let $S(t)$ be in $\mathbb{R}$, $a(t)$, $\eta(t)$ be vectors in $\mathbb{R}^n$, $A(t)$, $B(t)$ be complex $n\times n$ matrices all governed by the following system of ordinary differential equations:

$$\dot{a}(t) = \eta(t),$$

$$\dot{\eta}(t) = -\vec{\nabla} V(a(t)),$$

$$\dot{A}(t) = iB(t), \tag{4}$$

$$\dot{B}(t) = iV^{(2)}(a(t))A(t),$$

$$\dot{S}(t) = \frac{(\eta(t))^2}{2} - V(a(t)),$$

suppose the initial conditions given such that $A(0)$, $B(0)$ together satisfy (2) and (3) and $S(0)=0$. It is known that $A(t)$, $B(t)$ together still satisfy (2) and (3).[4]

Remark: Let

$$W_{a(t)}(x) = V(a(t)) + \langle V^{(1)}(a(t)),(x-a(t))\rangle + \tfrac{1}{2}\langle (x-a(t)),V^{(2)}(a(t))(x-a(t))\rangle,$$

the functions $\psi(x,t)=e^{iS(t)/\hbar}\phi_k(A(t),B(t),\hbar,a(t),\eta(t),x)$ provide exact solutions to the time dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2}\Delta_x\psi(x,t) + W_{a(t)}(x)\psi(x,t).$$

We state a result about the wave packets that will be used later. The reference is Ref. 4.

Lemma 1: Suppose $V\in C^3(\mathbb{R}^n)$ *satisfies* $-C_1\leqslant V(x)\leqslant C_2e^{Mx^2}$ *for some* C_1, C_2 *and* M. *Let* $(A(t),B(t),a(t),\eta(t),S(t))$ *be a solution to the system (4) with appropriate initial conditions. Let* $H(\hbar)=-(\hbar^2/2)\Delta+V(x)$. *Then there exists some* $C(k,t)$ *such that*

$$\|e^{-itH(\hbar)/\hbar}\phi_k(A(0),B(0),\hbar,a(0),\eta(0),x) - e^{-iS(t)/\hbar}\phi_k(A(t),B(t),\hbar,a(t),\eta(t),x)\| \leqslant C(k,t)\hbar^{1/2}. \tag{5}$$

Using these semiclassical wave packets one can now attempt to provide a construction for approximate solutions to the Schrödinger equation and prove accuracy estimates. For details on this see Refs. 1–5.

III. CLASSICAL SCATTERING

Existence of scattering states in classical mechanics is crucial to our study.

Lemma 2: Let $V(x)$ *satisfy the short-range assumption* (D). *Given any* $(a_-,\eta_-)\in\mathbb{R}^{2n}$ *such that* $\eta_-\neq 0$. *Let* A_-, *and* B_- *be complex* $n\times n$ *matrices satisfying conditions (2) and (3) then there exist a unique solution* $[a(t),\eta(t),A(t),B(t),S(t)]$ *to the system (4) such that*

$$\lim_{t\to-\infty}|a(t) - a_- - \eta_- t| = 0,$$

$$\lim_{t\to-\infty}|\eta(t) - \eta_-| = 0,$$

$$\lim_{t\to-\infty}|S(t)-t\eta_-^2/2|=0, \tag{6}$$

$$\lim_{t\to-\infty}\|A(t)-A_--iB_-t\|=0,$$

$$\lim_{t\to-\infty}\|B(t)-B_-\|=0.$$

Moreover, there exists $n\times n$ *complex matrices* A_+, B_+ *satisfying (2) and (3) and a closed set* E *of measure zero contained in* $\mathbb{R}^{2n}$ *such that* $(a_-,\eta_-)\in\mathbb{R}^{2n}\backslash E$ *implies the existence of* $(a_+,\eta_+)\in\mathbb{R}^{2n}$ *with* $\eta_+\neq 0$, $S_+\in R$ *such that*

$$\lim_{t\to\infty}|a(t)-a_+-\eta_+t|=0,$$

$$\lim_{t\to\infty}|\eta(t)-\eta_+|=0,$$

$$\lim_{t\to\infty}\|A(t)-A_+-iB_+t\|=0, \tag{7}$$

$$\lim_{t\to\infty}\|B(t)-B_+\|=0,$$

$$\lim_{t\to\infty}|S(t)-S_+-t\eta_+^2/2|=0.$$

This result basically says that given an incoming free state we can find an interacting state that approaches it at infinite negative time. Then for almost any free incoming state there exists a free outgoing state that approximates the interaction state at infinite time. In the language of scattering, the above theorem is existence, uniqueness of scattering operators coupled with asymptotic completeness. The proof of this for the position and momentum variables $a(t)$, $\eta(t)$, is given in Ref. 8, the proof for the spreading variables $A(t)$, $B(t)$ and the action variable $S(t)$, is given in Ref. 1.

IV. STATEMENT AND PROOF OF THE MAIN RESULT FOR $N=1$

Let

$$H(\hbar)=-\frac{\hbar^2}{2}\Delta_x+V(x)$$

and

$$H_1(t,\hbar)=-\frac{\hbar^2}{2}\Delta_x+W_{a(t)}(x),$$

with corresponding unitary propagators $U(t)$ and $U_1(t,0)$, respectively. Recall

$$U_1(t,0)\phi_0(A(0),B(0),\hbar,a(0),\eta(0),x)=e^{iS(t)/\hbar}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x).$$

Theorem 1: *If* $V(x)$ *satisfies the short-range assumption* (D), *then there exists* C, $\lambda>0$, *both independent of* t *and* $\hbar$ *such that*

$$\|U(t)\phi_0(A(0),B(0),\hbar,a(0),\eta(0),\cdot)-e^{iS(t)/\hbar}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\|_2\leqslant C\hbar^{\lambda}$$

for all $t\in(-\infty,\infty)$, $\hbar\in(0,1)$, *any* $A(0)$, $B(0)$ *satisfying Eqs. (2) and (3) and almost all* $a(0)$, $\eta(0)$.

Remark: The theorem is an analogous statement to that of lemma 2 for the semiclassical wave packets.

The proof given in Ref. 1 that is restricted to $n \geqslant 3$ uses the fact that the wave packet decays as $t^{-n/2}$, and thus the wave packet is itself in L^1 when $n \geqslant 3$. For $n=1$ and $n=2$ we remove the portion of the state that has small asymptotic momentum. This portion of the wave packet is $O(\hbar^{1/2})$. The remaining portion of the wave packet decays fast enough in t to prove the estimates we need. Our idea is to write the wave packet as

$$\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x) = \frac{p}{\eta}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x) + \frac{\eta - p}{\eta}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)$$

and then drop the second term at time 0 in order to get the asymptotics to cancel out correctly. The intuition is that the second term above is on the order of $\sqrt{\hbar}$ at time zero and can be disregarded in the semiclassical limit. The idea to write the wave packet in this way was inspired by Ref. 6 and many ideas from this paper can be seen in the proof. We need the portion of the wave packet that is not disregarded to be propogated exactly by the semiclassics given in Sec. II, therefore we write the wave packet as

$$\begin{aligned}
\phi_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) &= \left\{1 + \frac{(x-a(\tau))iB_+}{A(\tau)\eta_+}\right\}\phi_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) \\
&\quad - \frac{(x-a(\tau))iB_+}{A(\tau)\eta_+}\phi_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) \\
&= \left\{1 + \frac{(x-a(\tau))iB_+}{A(\tau)\eta_+}\right\}\phi_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) \\
&\quad - \sqrt{\frac{\hbar}{2}}\frac{iB_+}{\eta_+}\phi_1(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) \\
&= \tilde{\phi}_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x) \\
&\quad - \sqrt{\frac{\hbar}{2}}\frac{iB_+}{\eta_+}\phi_1(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x). \qquad (8)
\end{aligned}$$

We have used the fact that in one dimension

$$\phi_1(A(t),B(t),\hbar,a(t),\eta(t),x) = \sqrt{\frac{2}{\hbar}}\frac{(x-a(t))}{A(t)}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x). \qquad (9)$$

The argument of the theorem almost exactly follows the argument in Ref. 1. Besides the introduction of the modified wave packet the changes that we have made are imbedded in technical lemmas 3 and 4.

Proof of Theorem 1 for $n=1$: Let $\mu < 1$, $\epsilon \in (0, \frac{1}{6})$, and define

$$\chi_1(\hbar,a(t),x) = \begin{cases} 1 & \text{if } |x-a(t)| \leqslant (1+|a(t)|)\mu\hbar^{1/2-\epsilon}, \\ 0 & \text{otherwise.} \end{cases}$$

Define $\chi_2(\hbar,a(t),x) = 1 - \chi_1(\hbar,a(t),x)$. Now define $\tilde{\phi}_0(A(\tau),B(\tau),\hbar,a(\tau),\eta(\tau),x)$ as above and proceed to calculate. By (8) and since $\{U(t) - U_1(t,0)\}$ is bounded by lemma 2 it is clear that

$$\begin{aligned}
&\|\{U(t) - U_1(t,0)\}\phi_0(A(0),B(0),\hbar,a(0),\eta(0),\cdot)\|_2 \\
&\quad \leqslant \|\{U(t) - U_1(t,0)\}\tilde{\phi}_0(A(0),B(0),\hbar,a(0),\eta(0),\cdot)\|_2 + k\sqrt{\hbar}, \qquad (10)
\end{aligned}$$

where

$$k = \frac{|B_+|}{\sqrt{2}|\eta_+|}.$$

By the fundamental theorem of calculus,

$$\begin{aligned}
&\|\{U(t) - U_1(t,0)\}\tilde{\phi}_0(A(0),B(0),\hbar,a(0),\eta(0),\cdot)\|_2 \\
&\quad = \left\| \int_0^t \frac{d}{ds}\{U(s) - U_1(s,0)\}\tilde{\phi}_0(A(0),B(0),\hbar,a(0),\eta(0),\cdot)ds \right\|_2 \\
&\quad \leqslant \hbar^{-1}\int_0^t \|\{V(\cdot) - W_{a(s)}(\cdot)\}\tilde{\phi}_0(A(s),B(s),\hbar,a(s),\eta(s),\cdot)\|_2\, ds. \qquad (11)
\end{aligned}$$

Analyzing the integrand in the last expression,

$$\begin{aligned}
&\|\{V(x) - W_{a(s)}(x)\}\tilde{\phi}_0(A(s),B(s),\hbar,a(s),\eta(s),x)\|_2 \\
&\quad \leqslant \|\{V(x) - W_{a(s)}(x)\}\chi_1(\hbar,a(s),x)\tilde{\phi}_0(A(s),B(s),\hbar,a(s),\eta(s),x)\|_2 \\
&\qquad + \|V(x)\chi_2(\hbar,a(s),x)\tilde{\phi}_0(A(s),B(s),\hbar,a(s),\eta(s),x)\|_2 \\
&\qquad + \|W_{a(s)}(x)\chi_2(\hbar,a(s),x)\tilde{\phi}_0(A(s),B(s),\hbar,a(s),\eta(s),x)\|_2 = \mathrm{I}(s) + \mathrm{II}(s) + \mathrm{III}(s). \qquad (12)
\end{aligned}$$

If $|x-a(s)| \leqslant (1+|a(s)|)\mu\hbar^{1/2-\epsilon}$ then following the analysis from Ref. 1 we let $z_* \in \mathcal{Z} = \{z = rx + (1-r)y\}$ such that $|z_*| \leqslant |z|$ for all $z \in \mathcal{Z}$. By the fundamental theorem of calculus and the triangle inequality it can be seen that

$$|V_2(x) - V_2(y)| \leqslant C_3(1+|z|)^{-4-\nu}|x-y| \leqslant C_3(1+|y|-|y-z|)^{-4-\nu} \leqslant C_3[(1-\mu)(1+|y|)^{-4-\nu}|x-y| \ , \qquad (13)$$

where C_3 is taken from the short-range assumption. From here it follows that

$$\|\chi_1(\hbar,a(s),x)(V(x) - W_{a(s)}(x))\|_\infty \leqslant C_3(1+|a(s)|)^{-1-\nu}\hbar^{3/2-3\epsilon}. \qquad (14)$$

Hence

$$\mathrm{I}(s) \leqslant C_3(1+|a(s)|)^{-1-\nu}\hbar^{3/2-3\epsilon}\left(1 + k\sqrt{\frac{\hbar}{2}}\right).$$

Again we follow the argument in Ref. 1. Due to continuity and asymptotics of the classical quantities $a(s)$, $A(s)$ that

$$\begin{aligned}
\mathrm{II}(s) &\leqslant \left\| \chi_2(\hbar,a(s),x)\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_\infty \left\| \chi_2(\hbar,a(s),x)V(x)\left(1 + \frac{(x-a(s))iB_+}{A(s)\eta_+}\right)\right. \\
&\quad \left. \times(\pi\hbar)^{-1/4}(A(s))^{-1/2}\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_2 \\
&\leqslant \exp\{-C'\hbar^{-2\epsilon}\}\left\| \chi_2(\hbar,a(s),x)V(x)\left(1 + \frac{(x-a(s))iB_+}{A(s)\eta_+}\right)\right. \\
&\quad \left. \times(\pi\hbar)^{-1/4}(A(s))^{-1/2}\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_2, \qquad (15)
\end{aligned}$$

where C' is some constant independent of s and $\hbar$. By lemma 5.1 and dividing by $A(s)\eta_+$ there exists C_V, T_1 such that for $s > T_1$,

$$\mathrm{II}(s) \leqslant C_V \hbar^{-1/2-\nu/2} \exp\{-C'\hbar^{-2\epsilon}\}|s|^{-1-\nu/2}.$$

We can do the same thing with $\mathrm{III}(s)$ as well. By lemma 5.2 there exists T_2, C_W such that for $s > T_2$,

$$\mathrm{III}(s) \leqslant C_W \hbar^{-1} \exp\{-C'\hbar^{-2\epsilon}\}|s|^{-1-\nu}.$$

The theorem is now proven by taking $T = \max\{T_1, T_2\}$ and writing for $t > T$,

$$\hbar^{-1}\int_0^t (\mathrm{I}(s) + \mathrm{II}(s) + \mathrm{III}(s))\mathrm{d}s = \hbar^{-1}\left\{\int_0^T (\mathrm{I}(s) + \mathrm{II}(s) + \mathrm{III}(s))\mathrm{d}s + \int_0^t (\mathrm{I}(s) + \mathrm{II}(s) + \mathrm{III}(s))\mathrm{d}s\right\}.$$

The first term is bounded by some $C_T\hbar^{1/2}$ by lemma 1. The second term is bounded by some $C\hbar^{-2}\exp\{-C'\hbar^{-2\epsilon}\} + C_3\hbar^{1/2-3\epsilon}$ by the work shown here. In order to propagate to large negative times we write the modified wave packet with η_-, B_- in place of η_+, B_+ and the details are the same. □

V. TECHNICAL LEMMAS

Lemma 3: In space dimension one if $V(x)$ satisfies the short-range assumption (D), then there exists some constant C such that for t sufficiently large, $\hbar \in (0,1)$,

$$\left\| \chi_2(\hbar, a(t), x) V(x)\{\eta_+ A(t) + (x - a(t))iB_+\}(\pi\hbar)^{-1/4}(A(t))^{-1/2} \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \leqslant C\hbar^{-1/2-\nu/2}t^{-\nu/2},$$

where $\chi_2(\hbar, a(t), x)$ is as defined in the proof of Theorem 1.

Proof: Let $k_1 > 0$. By lemma 2 there exists T such that $t > T$ implies that

$$\begin{aligned}&\left\| \chi_2(\hbar, a(t), x) V(x)\{\eta_+ A(t) + (x - a(t))iB_+\}(\pi\hbar)^{-1/4}(A(t))^{-1/2} \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \\ &\quad \leqslant \left\| \chi_2(\hbar, a(t), x) V(x) \cdot \{\eta_+(A_+ + iB_+t) + (x - a_+ - \eta_+ t)iB_+\} \right. \\ &\qquad \left. \times (\pi\hbar)^{-1/4}(A(t))^{-1/2} \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 + k_1\hbar^{-1/4}|A(t)|^{-1/2}. \end{aligned} \tag{16}$$

Using the triangle inequality we find that

$$\begin{aligned}&\left\| \chi_2(\hbar, a(t), x) V(x) \cdot \{\eta_+(A_+ + iB_+t) + (x - a_+ - \eta_+ t)iB_+\}(\pi\hbar)^{-1/4}(A(t))^{-1/2} \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \\ &\quad \leqslant \left\| V(x)[\eta_+ A_+](\pi\hbar)^{-1/4}(A^{-1/2}(t)) \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 + \left\| \chi_2(\hbar, a(t), x) V(x)[iB_+(x - a_+)] \right. \\ &\qquad \left. \times (\pi\hbar)^{-1/4}(A^{-1/2}(t)) \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2. \end{aligned} \tag{17}$$

Since $V(x) \in L^2(\mathbb{R})$ we have some constant k_2 such that for large enough t,

$$\left\| V(x)[\eta_+ A_+](\pi\hbar)^{-1/4}(A^{-1/2}(t)) \exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \leqslant k_2\hbar^{-1/4}t^{-1/2}. \tag{18}$$

Similarly,

$$\left\| \chi_2(\hbar,a(t),x)V(x)[iB_+(x-a_+)](\pi\hbar)^{-1/4}(A^{-1/2}(t))\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2$$
$$\leqslant \|iB_+V(x)(x-a_+)^{1/2+\nu/2}\|_2 \left\| \chi_2(\hbar,a(t),x)(\pi\hbar)^{-1/4}(A(t))^{-1/2}(x-a_+)^{1/2-\nu/2} \times\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_\infty. \tag{19}$$

The first factor is a constant independent of t and $\hbar$. Evaluating the second term further we see that

$$\left\| \chi_2(\hbar,a(t),x)(\pi\hbar)^{-1/4}(A(t))^{-1/2}(x-a_+)^{1/2-\nu/2}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_\infty$$
$$= \left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}}\frac{(x-a(t))^{1/2-\nu/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_\infty$$
$$\leqslant \left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}}\right\|_\infty \left\| \chi_2(\hbar,a(t),x)\frac{(x-a(t))^{1/2-\nu/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_\infty$$
$$\leqslant \left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}}\right\|_\infty \frac{\hbar^{-\nu/4+\epsilon\nu/2}}{(\mu(1+|a(t)|))^{\nu/2}}\left\| \frac{(x-a(t))^{1/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_\infty. \tag{20}$$

The second norm in the last expression is bounded by a constant. For the first norm we see that

$$\left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}}\right\|_\infty \leqslant \max\left\{1,\left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)}{(x-a(t))}\right\|_\infty\right\}. \tag{21}$$

Now we see that

$$\left\| \chi_2(\hbar,a(t),x)\frac{(x-a_+)}{(x-a(t))}\right\|_\infty \leqslant \left\| \chi_2(\hbar,a(t),x)\frac{(x-a(t)+a(t)-a_+)}{(x-a(t))}\right\|_\infty 1+\left\| \chi_2(\hbar,a(t),x)\frac{(a(t)-a_+)}{(x-a(t))}\right\|_\infty$$
$$\leqslant 1+\left\| \chi_2(,a(t),x)\frac{(a(t)-a_+)}{(1+a(t))\mu\hbar^{1/2-\nu/2}}\right\|_\infty \leqslant 1+k_3\hbar^{-1/2+\nu/2}, \tag{22}$$

where k_3 is a constant independent of t and $\hbar$. The lemma now follows. □

Lemma 4: If $V(x)$ satisfies the short-range assumption (D), then there exists some constant C such that for large enough t, and $\hbar\in(0,1)$,

$$\left\| W_{a(t)}(x)\left[1+\sqrt{\frac{\overline{A}(t)}{A(t)}}\frac{(x-a(t))iB_+}{|A(t)|\eta_+}\right](\pi\hbar)^{-1/4}(A^{-1/2}(t))\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \leqslant C\hbar^{-1}t^{-1-\nu}.$$

Proof: Since $V(x)$ satisfies the short-range condition there exists C_j, $j=0,1,2$ such that

$$\left\| W_{a(t)}(x)\left[1+\sqrt{\frac{\overline{A(t)}}{A(t)}}\frac{(x-a(t))iB_+}{|A(t)|\eta_+}\right](\pi\hbar)^{-1/4}(A^{-1/2}(t))\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2$$
$$\leqslant \sum_{j=0}^{2} C_j(1+|a(t)|)^{-1-j-\nu}\cdot|A(t)|^j\cdot 2^j\cdot\hbar^{j/2}\left\|\left(\frac{(x-a(t))}{2|A(t)|\hbar^{1/2}}\right)^j\cdot\left\{1+\sqrt{\frac{\overline{A(t)}}{A(t)}}\frac{(x-a(t))iB_+}{|A(t)|\eta_+}\right\}\right.$$
$$\left.\times(\pi\hbar)^{-1/4}(A(t))^{-1/2}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2. \tag{23}$$

By explicit evaluation, we see that the norms in the last expression are bounded by constants independent of t and $\hbar$. □

VI. EXTENSION TO TWO DIMENSIONS

The extension of this result to two dimensions has a few complications due to the structure of higher order states in more than one dimension. Here we point out the changes that need to be made in the proof of Theorem 1 in order to extend it to $n=2$. The techniques follow the construction given in Ref. 3. We present this in a less general manner for the sake of clarity. Let $\{e_1,e_2\}$ be the standard basis for $\mathbb{R}^2$. By the polar decomposition theorem for all t there exists a unique unitary matrix $U_A(t)$ such that $A(t)=|A(t)|U_A(t)$. We then define

$$\tilde{H}_1(v,x)=2\langle v,x\rangle$$

and

$$H_{e_j}(A(t);x)=\tilde{H}_1(U_A(t)e_j,x).$$

Now we proceed to define the higher order wave packet,

$$\phi_{e_j}(A(t),B(t),\hbar,a(t),\eta(t),x)=2^{-1/2}H_{e_j}(A(t);\hbar^{-1/2}|A(t)|^{-1}(x-a(t)))\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x) \tag{24}$$

$$=2^{1/2}\langle U_A(t)e_j,\hbar^{-1/2}|A(t)|^{-1}(x-a(t))\rangle\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x). \tag{25}$$

Now define

$$\tilde{\phi}_0(A(t),B(t),\hbar,a(t),\eta(t),x)=\left\{1+\left\langle U_A(t)e_1,\frac{i|A(t)|^{-1}B_+(x-a(t))}{\langle e_1,\eta_+\rangle}\right\rangle\right\}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x) \tag{26}$$

and the modified wave packet is again propagated as in Theorem 1. Since we have assumed that $\eta_+\neq 0$ we can use e_2 instead of e_1 if $\langle e_1,\eta_+\rangle=0$. Recall

$$U_A(t)=|A(t)|^{-1}A(t),$$

implying

$$U_A^*(t)=A^{-1}(t)|A(t)|,$$

and so similar to the analysis in one dimension we have

$$\tilde{\phi}_0(A(t),B(t),\hbar,a(t),\eta(t),x) = \left\{ \frac{\langle e_1,\eta_+\rangle}{\langle e_1,\eta_+\rangle} + \left\langle e_1, \frac{iA^{-1}(t)B_+(x-a(t))}{\langle e_1,\eta_+\rangle} \right\rangle \right\} \phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)$$

$$= \frac{1}{\langle e_1,\eta_+\rangle} \langle e_1, \eta_+ + A^{-1}(t)(x-a(t))iB_+\rangle \phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)$$

$$= \frac{1}{\langle e_1,\eta_+\rangle} \langle e_1, A^{-1}(t)\{A(t)\eta_+ + (x-a(t))iB_+\}\rangle \phi_0(A(t),B(t),\hbar,a(t),\eta(t),x). \tag{27}$$

Noting that

$$V(x)(1+x)^{\nu/2} \in L^2(\mathbb{R}^2)$$

and thus

$$\|iB_+V(x)(x-a_+)^{\nu/2}\|_2$$

is constant in place of

$$\|iB_+V(x)(x-a_+)^{1/2+\nu/2}\|_2$$

in the one dimensional case, the proof is now analogous to the proof for $n=1$.

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Analytic solution for entangled two-qubit in a cavity field

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An exact solution of the time-dependent master equation that describes the evolution of two two-level qubits (ions or atoms) within a perfect cavity for the case of multiphoton transition and in the presence of both the Stark shift and phase shift is obtained. Employing this solution, the significant features of the entanglement when a second qubit is allowed to interact with cavity mode and becomes entangled with the first qubit are investigated in the context of the measure defined by negative eigenvalues for the partial transposition of the density operator. The effects of Stark shift, distance between the two qubits, and an instantaneous phase shift experienced by the second qubit on the entanglement and probability amplitudes are indicated. It has been shown that the entanglement as well as the intensity are markedly affected by different parameters when the nonlinear two-photon process is involved. Moreover, the quasiprobability distribution function is investigated before and after the sudden phase shift experienced by the second qubit. We believe that this may throw some light on the question of the entanglement of multi-qubit systems. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1795986]

I. OVERVIEW

Investigations into the emerging science of quantum information has led to the widespread belief that entanglement in states shared between two systems can be used as a resource in nonclassical applications.[1–3] The theory of quantum entanglement has occupied a central place in modern research because of its promise of enormous utility in quantum computing, cryptography, etc.[4–8] A major thrust of current research is to find a quantitative measure of entanglement for general states. One of the most intriguing problems of quantum mechanics is the interpretation of the measurement process (for an overview of fundamental problems in quantum measurement, see, for example, Refs. 9–11). The reason for this central role of the measurement process is the absence of fundamental, elements of reality, that would simultaneously characterize both the dynamics and the measurement results. At this end, in quantum information, the maximally entangled states have a special significance.

For the experiments in the newest fields of physics, quantum computing, quantum communication, and quantum cryptography[4–8] the quantitative analysis of the multiqubit or ion is of substantial interest.[12] The dipole-dipole interaction between two atoms can be understood through the exchange of virtual photons and depends on the transition dipole moment of the levels involved. It can be characterized by complex coupling constants, or by their real and imaginary parts, where the former affect decay constants and the latter lead to level shifts.[13] There is an inherent interest in analytical and nonperturbative solutions of multiatom interacting with the cavity field problems, all the more considering quantum systems with more than one particle. One example of such a

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kind is the system of two two-level qubits in an electromagnetic field.[14–20] Entanglement of identical particles is a property dependent on which single-particle basis is chosen, as any operation should act on each identical particle in the same way. Indeed, individual particles are excitations of a quantum field, and the single-particle basis defines which set of particles are used in representing the many-particle state.[21]

One aim of the present article is to extend the previous models to a much more general model. To be more precise, we assume that two two-level atoms (two qubits) share a bipartite system, taking into account the multiphoton transition and the presence of Stark shift with the second qubit undergoing phase shift. Another principal aim is to elucidate the extent to which mixed entangled states can affect the entanglement. The emphasis being put on the investigation of the entanglement in a more general situation in which the two atoms (qubits) share a mixed state, rather than a pure state. The issue of attributing objective properties to the constituents of a quantum system composed of identical atoms, does not turn out to be a straightforward generalization of just the analyzed case involving distinguishable atoms, and the problem of entanglement has to be reconsidered. If a system interacts unitarily with an imperfectly known environment, the subdynamics of the system, averaged over the unknown states of the environment is nonunitary, and can take a pure state to a mixed state. In general it is known that there are also cases when entangled states are mixed with other entangled states and where the sum is separable.

The outline of this article is arranged as follows: In Sec. II, we give notation and definitions of the model and its analytical solution to be used in the rest of the article. The entanglement measure calculation is presented in Sec. III. By a numerical computation, we examine the influence of distance between the qubits, Stark shift, and phase shift on the evolution of the measure of entanglement which will be defined in terms of the negative eigenvalues of the partial transposition. Finally, Sec. IV has few concluding remarks, and few avenues for further investigations are indicated.

II. TWO QUBITS MODEL

To set the stage, we first begin with a discussion of where the two-qubit model comes from. Therefore, the physical system on which we focus is a two three-level harmonically trapped ions with its center-of-mass motion quantized. The ions are subjected to a laser field. This model differs from the standard micromaser setup in that instead of a single qubit we have assumed a pair of qubits interacting with a single mode of the cavity field. The position of the first qubit in the cavity is fixed and the second qubit is at some distance L from it. This distance will be a variable parameter of the problem.[9–11] Our interest lies in the case where the Stark shift and phase shift are included. The electronic levels $|a\rangle$ and $|b\rangle$ are assumed to be metastable and coupled via a laser field of the form

$$E(\hat{x},t) = E_0 \exp[i(\hat{k}\,.\,\hat{x} - \omega t + \phi(t))], \tag{1}$$

where E_0 is the strength of the electric field, $\hat{k}$ is the wave vector of the driving laser field, $\hat{x}$ is the position operator associated with the center-of-mass motion, and ω is the laser frequency. We denote by $\phi(t)$ the fluctuations in the laser phase. Therefore, we can express the center-of-mass position in terms of the creation and annihilation operators of the one-dimensional trap, namely,

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega_s}}(\hat{a}^\dagger + \hat{a}) = \Delta x(\hat{a}^\dagger + \hat{a}). \tag{2}$$

We denote by $\hat{a}$ and $\hat{a}^\dagger$ the annihilation and creation operators and ω_s is the vibrational frequency related to the center-of-mass harmonic motion along the direction $\hat{x}$. In the absence of the rotating wave approximation, the trapped ions Hamiltonian that describes the system between detections may be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{3}$$

where

$$\hat{H}_0 = \hbar\omega_s \hat{a}^\dagger \hat{a} + \sum_{i=a,b,c} \hbar\omega_i |i\rangle\langle i|,$$

$$\hat{H}_1 = \hbar \sum_{i=1}^{2} \{(\lambda_1^{(i)} e^{-i(k_i.\hat{x}-\omega t+\phi_i)} S_{bc}^{(i)} + \text{H.c.}) + (\lambda_2^{(i)} e^{-i(k_i.\hat{x}-\omega t+\phi_i)} S_{ac}^{(i)} + \text{H.c.})\}. \tag{4}$$

The transition in the three-level ions is characterized by the dipole matrix element $\lambda_j^{(i)}$ where $S_{lm}^{(i)} = |l^{(i)}\rangle\langle m^{(i)}|$ $(l,m=a,b,c)$ being the considered three atomic levels. For the sake of simplicity (but without loss of generality), we have assumed to deal with the case in which $\phi_1 = 0$, $\phi_2 = \phi$ and the level $|c\rangle$ is assumed to be dipole-coupled to both the levels $|a\rangle$ and $|b\rangle$ via a far detuned laser field. While this is straightforward, it is often the case that it is simpler to work in the interaction picture in which the Hamiltonian (4) evolves in time according to the interaction with the vacuum field. If we express the center-of-mass position in terms of the creation and annihilation operators, the interaction part of Eq. (4) becomes

$$\begin{aligned}\hat{H}_{\text{int}} = &-\hbar\Delta \sum_{i=1}^{2} (S_{bb}^{(i)} + S_{aa}^{(i)}) + \hbar(\lambda_1^{(1)} e^{-i\eta(\hat{a}^\dagger+\hat{a})} S_{bc}^{(1)} + \text{H.c.}) + \hbar(\lambda_2^{(1)} e^{-i\eta(\hat{a}^\dagger+\hat{a})} S_{ac}^{(1)} + \text{H.c.}) \\ &+ \hbar(\lambda_1^{(2)} e^{-i\eta(\hat{a}^\dagger+\hat{a})} S_{bc}^{(2)} e^{-i\phi} + \text{H.c.}) + \hbar(\lambda_2^{(2)} e^{-i\eta(\hat{a}^\dagger+\hat{a})} S_{ac}^{(2)} e^{-i\phi} + \text{H.c.}),\end{aligned} \tag{5}$$

where $\eta = k\sqrt{\hbar/2M\omega_s}$, is the Lamb–Dicke parameter. In Eq. (5) the time-dependent factor is eliminated in the interaction picture, since $\omega_c - (\omega_b + \Delta) = m\omega_s$ and $\omega_c - (\omega_a + \Delta) = m\omega_s$. We assume the Lamb–Dicke regime with small η. In order to obtain this we detune the laser frequency ω to the mth vibrational red sideband. Also, we apply the rotating wave approximation discarding the rapidly oscillating terms and selecting the terms that oscillate with minimum frequency.[22] In these limits we can expand the interaction Hamiltonian to lowest order in η. The resulting effective Hamiltonian may be written as

$$\begin{aligned}\hat{H}_{\text{int}} = &-\hbar\Delta \sum_{i=1}^{2} (S_{bb}^{(i)} + S_{aa}^{(i)}) + \hbar\gamma_1^{(1)}(\hat{a}^{\dagger m} S_{bc}^{(1)} + \text{H.c.}) + \hbar\gamma_2^{(1)}(\hat{a}^{\dagger m} S_{ac}^{(1)} + \text{H.c.}) + \hbar\gamma_1^{(2)}(\hat{a}^{\dagger m} S_{bc}^{(2)} e^{-i\phi} + \text{H.c.}) \\ &+ \hbar\gamma_2^{(2)}(\hat{a}^{\dagger m} S_{ac}^{(2)} e^{-i\phi} + \text{H.c.}),\end{aligned} \tag{6}$$

with new coupling parameter $\gamma_i^{(j)}$ including the Dicke parameter in its definition. The analysis of such a Hamiltonian model can be carried out, providing eliminating of the nonresonantly coupled atomic level $|c\rangle$ adiabatically in the same manner as the standard JCM. Indeed, due to the large detuning, the transitions for instance from the level $|a\rangle$ to the level $|c\rangle$ are very fast and immediately followed by decays on the atomic level $|b\rangle$. Therefore, considering only coarse grained observables, meaning that the system is observed at a rough enough time scale, effectively eliminates the far detuned level, namely, at such a time scale, the only observables and hence meaningful dynamical behaviors, involve levels $|a\rangle$ and $|b\rangle$ as a result of time averaging second-order processes having $|c\rangle$ as an intermediate virtual level. This procedure hence suppresses the fine dynamics, that is it sacrifices any information concerning the fast dynamics the third level is involved in. So that the effective Hamiltonian of the system for $m=1$ in Eq. (6), including the ac-Stark shift, in the dipole and rotating wave approximation, can be written as[14–20] $(\hbar = 1)$

$$\hat{H} = \hat{a}^{\dagger}\hat{a}(\beta_1 S_{ba}^{(1)} S_{ab}^{(1)} + \beta_2 S_{ab}^{(1)} S_{ba}^{(1)}) + \hat{a}^{\dagger}\hat{a}(\beta_1 S_{ba}^{(2)} S_{ab}^{(2)} + \beta_2 S_{ab}^{(2)} S_{ba}^{(2)}) + \omega\hat{a}^{\dagger}\hat{a} + \omega(S_{aa}^{(1)} - S_{bb}^{(1)}) + \omega(S_{aa}^{(2)} - S_{bb}^{(2)}) + \gamma_1(S_{ab}^{(1)}\hat{a}^2 + \text{H.c.}) + \gamma_2(e^{i\phi} S_{ab}^{(2)}\hat{a}^2 + \text{H.c.}). \tag{7}$$

We denote by β_1 and β_2 the intensity-dependent Stark shifts, that are due to the virtual transitions to the intermediate relay level and $\gamma_i = \eta^2 \gamma_1^{(i)} \gamma_2^{(i)} / \Delta$.

It has been shown that entangled states in a two-atom system can be created by a continuous driving of the atoms with a coherent or chaotic thermal field, or by a pulse excitation followed by a continuous observation of radiative decay.[23] To begin with, we shall choose the following mixed state:

$$\rho = r|e_1, g_2\rangle\langle e_1, g_2| + (1-r)|g_1, e_2\rangle\langle g_1, e_2| \in \mathfrak{S}_A. \tag{8}$$

We may write the initial state of the field in vacuum state as

$$\varpi = |0\rangle\langle 0| \in \mathfrak{S}_F. \tag{9}$$

The continuous map $\mathcal{E}_t^*$ describing the time evolution between the qubits and the field is defined by the unitary evolution operator generated by $\hat{H}$ such that

$$\mathcal{E}_t^* : \mathfrak{S}_A \rightarrow \mathfrak{S}_A \otimes \mathfrak{S}_F,$$

$$\mathcal{E}_t^* \rho = \hat{U}_t(\rho \otimes \varpi)\hat{U}_t^*. \tag{10}$$

The interaction Hamiltonian, in this case, leads to an exactly solvable time evolution operator. Resuming our analysis, the time evolution operator can be written as

$$\hat{U}_t \equiv \exp\left(-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'\right), \tag{11}$$

i.e., $\hat{U}_t$ satisfies the interaction picture Schrödinger equation. Most of the authors who have treated multiqubits systems interacting with cavity fields have dealt with the case in which the Stark shift has been ignored.[9–11] However, in reality it cannot be ignored. Our interest in the current article lies in looking for a time dependent analytical solution even when the Stark shift and phase shift are nonzero. Using the above equations, in the interaction picture and after some algebraic manipulations we find that the final state $\mathcal{E}_t^*\rho$ at any time $t > 0$ is given by

$$\mathcal{E}_t^* \rho = \sum_{i=1}^{3}\sum_{j=1}^{3} U_{ij}(t)|\psi_i\rangle\langle\psi_j|, \tag{12}$$

where

$$U_{11}(t) = rA_tA_t^* + (1-r)B_tB_t^*, \quad U_{12}(t) = rA_tC_t^* + (1-r)B_tC_t^*,$$

$$U_{13}(t) = rA_tB_t^* + (1-r)B_tA_t^*, \quad U_{22}(t) = C_tC_t^*,$$

$$U_{23}(t) = rC_tB_t^* + (1-r)C_tA_t^*, \quad U_{33}(t) = rB_tB_t^* + (1-r)A_tA_t^*, \tag{13}$$

$\rho_{ij}(t) = \rho_{ji}^*(t)$, and

$$A_t = -\frac{\gamma_2^2}{\mu_1} - \frac{\gamma_1^2 \exp(-i2\beta_1 t)}{\mu_1}\left(\cos \mu t + i2\beta_1 \frac{\sin \mu t}{\mu}\right),$$

$$B_t = -\frac{\gamma_1^* \gamma_2 \exp(i\phi)\exp(-i2\beta_1 t)}{\mu_1}\left(\cos \mu t + 2\beta_1 \frac{\sin \mu t}{\mu}\right) + \frac{\gamma_1^* \gamma_2 \exp(i\phi)}{\mu_1},$$

$$C_t = -i2\gamma_1^* \exp(-i2\beta_1 t)\frac{\sin \mu t}{\mu}, \tag{14}$$

and

$$\mu = \sqrt{4\beta_1^2 + 2(\gamma_1^2 + \gamma_2^2)}, \quad \mu_1 = (\gamma_1^2 + \gamma_2^2),$$

$$\psi_1 = |e_1, g_2, 0\rangle, \quad \psi_2 = |g_1, e_2, 0\rangle, \quad \psi_3 = |g_1, g_2, 2\rangle. \tag{15}$$

We have therefore obtained an analytical solution of the final state of the system for this general model. Having obtained the explicit form of the final state of the system under consideration, we are therefore in a position to discuss the statistical properties of the system.

III. ENTANGLEMENT

The characterization and classification of entanglement in quantum mechanics is one of the cornerstones of the emerging field of quantum information theory. Although an entangled two-qubit state $\mathcal{E}_t^* \rho$ is not equal to the product $\mathcal{E}_t^* \rho_1$ and $\mathcal{E}_t^* \rho_2$ of the two single-qubit states contained in it, it may very well be a convex sum of such products. In general it is known that microscopic entangled states are found that to be very stable, for example electron-sharing in atomic bonding and two-qubit entangled photon states generated by parametric down conversion. Entanglement as one of the most nonclassical features of quantum mechanics is usually arisen from quantum correlations between separated subsystems which cannot be created by local actions on each subsystem. By definition, a mixed state of a bipartite system is said to be nonentangled if it can be written as a convex combination of pure product states. Although, in the case of pure states of bipartite systems it is easy to check whether a given state is entangled or not, the question is yet an open problem in the case of mixed states. There is also an increasing attention in quantifying entanglement, particularly for mixed states of a bipartite system.[24–38]

In this article, we take the measure of negative eigenvalues for the partial transposition of the density operator. It was proved that the negativity is an entanglement monotone,[38] hence, the negativity is a good entanglement measure. According to the Peres[39] and Horodecki *et al.*[40] condition for separability,[39,40] a two-qubit state for the given set of parameter values is entangled if and only if its partial transpose is negative. The measure of entanglement can be defined in terms of the negative eigenvalues of the partial transposition in the following form[36,37]

$$I_{\mathcal{E}_t^* \rho}(t) = 2 \max(0, -\lambda_{\text{neg}}), \tag{16}$$

where λ_{neg} is the sum of the negative eigenvalues of the partial transposition of the time-dependent reduced atomic density matrix ρ^a, which can be obtained by tracing out the field variables

$$\rho^a = \text{Tr}_f(\mathcal{E}_t^* \rho). \tag{17}$$

In the two qubit system $(C^2 \otimes C^2)$ it can be shown that the partial transpose of the density matrix can have at most one negative eigenvalue.[40] The partial transposition of ρ^{aT} has four eigenvalues one of which is negative, then the entanglement is given by

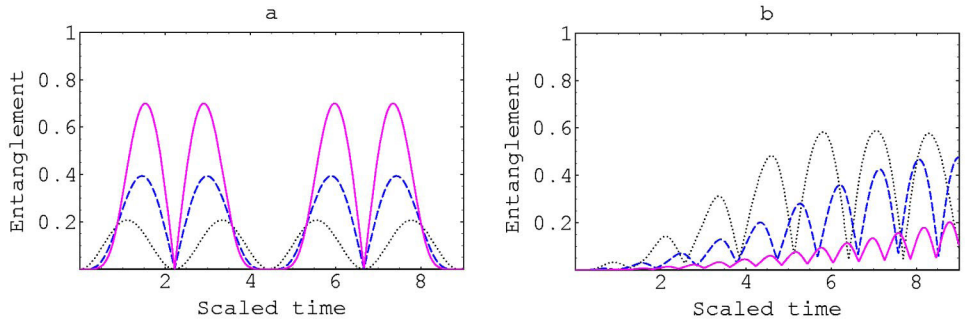

FIG. 1. This figure presents the results of a numerical calculation of the time evolution of the negativity as a measure of entanglement. The parameters $\phi=0$, and $L=0$, where (a) $r=0.2$ (solid curve), $r=0.6$ (dashed curve), and $r=1$ (dotted curve) and (b) $r=0.2$, $\beta_1=5\gamma$ (solid curve), $\beta=3\gamma$ (dashed curve), and $\beta_1=2\gamma$ (dotted curve).

$$I_{\varepsilon_t^*\rho}(t)=\sqrt{U_{33}^2(t)+4U_{21}(t)U_{12}(t)}-U_{33}(t).$$

The entanglement measure then ensures the scale between 0 and 1 and monotonously increases as entanglement grows. An important situation is that, when $I_{\varepsilon_t^*\rho}(t)=0$ the two qubits are separable and $I_{\varepsilon_t^*\rho}(t)=1$ indicates maximum entanglement between the two qubits. It was proved[38] that the negativity is an entanglement monotone, and hence is a good entanglement measure.

An interesting question is whether or not the entanglement is affected by the different parameters of the present system with the initial state in which one of the qubits is prepared in its excited state and the other in the ground state. In particular, the mixed state parameter r, the Stark shift parameter β_1, the distance between the qubits L, and the phase shift ϕ. A numeric evaluation of the entanglement measure leads to the plot in Fig. 1(a). We consider the coupling of the first qubit is taken to be constant $\gamma_1=\gamma$. Although we allow the second qubit to be at a distance L away and experience a variable qubit field coupling $\gamma_2=\gamma\cos kL$ (where we set $\beta_1=0$, $L=0$, $\phi=0$, and $r=1$). It is shown that the two qubits are entangled in this case, with the maximum value $I_{\varepsilon_t^*\rho}(t)\approx 0.2$ for $r=1$, $I_{\varepsilon_t^*\rho}(t)\approx 0.4$ for $r=0.6$ and $I_{\varepsilon_t^*\rho}(t)\approx 0.7$ for $r=0.2$. In all these cases we see that for some interaction times the entanglement is equal to zero, this period is increased with decreasing the parameter r. We now consider the two qubits interacting with the cavity field in the presence of Stark shift parameter β_1, where we set three different values of β_1 for the sake of comparison [see Fig. 1(b)]. It is remarkable to see that with the value of the Stark shift parameter, $\beta_1=2\gamma$ the entanglement is nearly zero for the initial period of the interaction time. This period increases with increasing the Stark shift. Also, the maximum value of the entanglement is decreased with increasing β_1. In this case we can say that, when the system is allowed to evolve without applying a phase shift, the entanglement degree is a periodic function of time. This is particularly because of the nonlinear nature of the coupling in this case (two-photon process).

We now pause to touch on certain entanglement features when a phase shift is applied to the second qubit at the time τ. To this end we consider the same values of the other parameters similar to Fig. 1(a). Three important values for the timing of the phase shift, namely, $\tau=\pi(J\pm 0.25)$, 3π, and $J\pi$ (here $J=3$) corresponding to the maximum and minimum values of the probability of emission of photon pair. This is illustrated in Fig. 2, where we have shown the time evolution of the entanglement for different values of the timing of the phase shift and $\phi=\pi/2$. First of all, we note that the regular behavior has been seen only for the case when $\tau=3\pi$. While for the other two values, i.e., for $\tau=\pi(J\pm 0.25)$, we see that there are two maximum values of the entanglement $I_{\varepsilon_t^*\rho}(t)\approx 0.5$ and 0.97. This situation is quite different from the maximum values of the entanglement at $\tau=3\pi$, where the two peaks have the same maximum value at $I_{\varepsilon_t^*\rho}(t)\approx 0.85$. It should be noted that the entanglement vanish for some period of the interaction time only when $\tau=3\pi$. These properties show that the role played by the timing of the phase shift on the entanglement is essential. Interestingly, when r is taken to be nonzero $(r=0.2)$, the values of the maximum en-

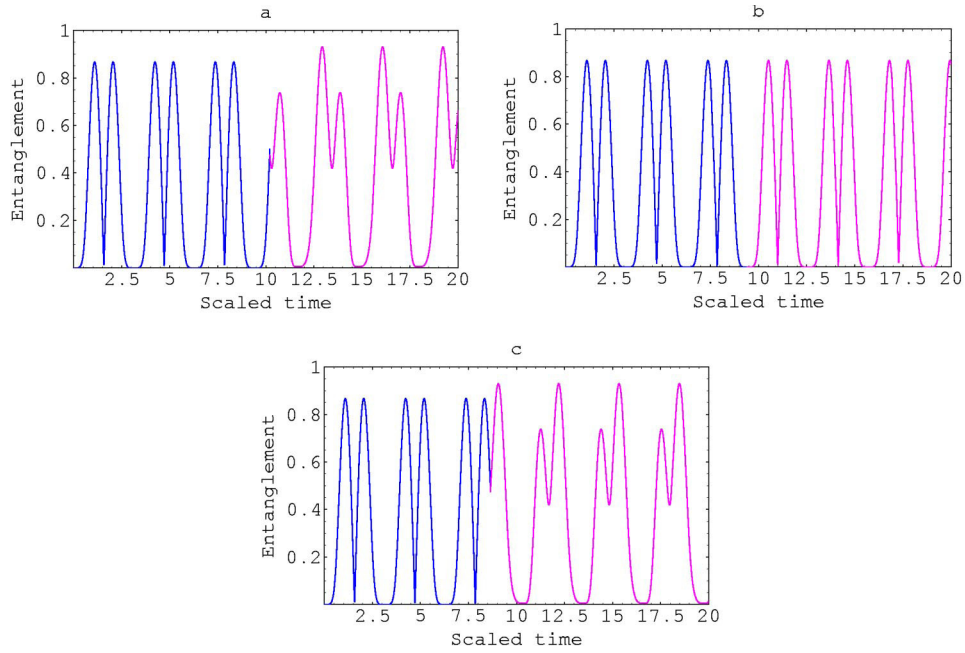

FIG. 2. This figure presents the results of a numerical calculation of the time evolution of the negativity as a measure of entanglement. $\phi=\pi/4$, $\beta_1=0$, $L=0$ and for different values of the timing of an applied phase step τ, where (a) $\tau=13\pi/4$, (b) $\tau=4\pi$, and (c) $\tau=11\pi/4$.

tanglement are decreased, indicating that the mixed state setting leads to a decreasing of the qubit-qubit entanglement. While the qubit-qubit entanglement has the same feature for different values of the mixed state parameter r, the change only occurs on the amplitude of the oscillations (see Fig. 2).

In the previous discussion, we have discussed different excitation processes which can prepare two qubits in the asymmetric state and we have assumed that both the qubits in the same position, i.e., $L=0$. This assumption is only valid if the coupling parameters $\gamma_1=\gamma_2$. The analysis involved single mode cavities, but ignored spontaneous emission from the qubits and the cavity damping. Here, we will extend this analysis to consider that two qubits separated by an arbitrary distance L, and we would like to highlight briefly why the qubit-qubit entanglement measure might have different features in the presence of the distance between the qubits. Figure 3(a) shows the basic features of the behavior of the qubit-qubit entanglement with different values of the distance between the qubits L. We remark that the entanglement has some kind of periodicity [see Fig. 3(a)] when $L=\pi/2k$. It is important to note here that, the minimum value of the entanglement is

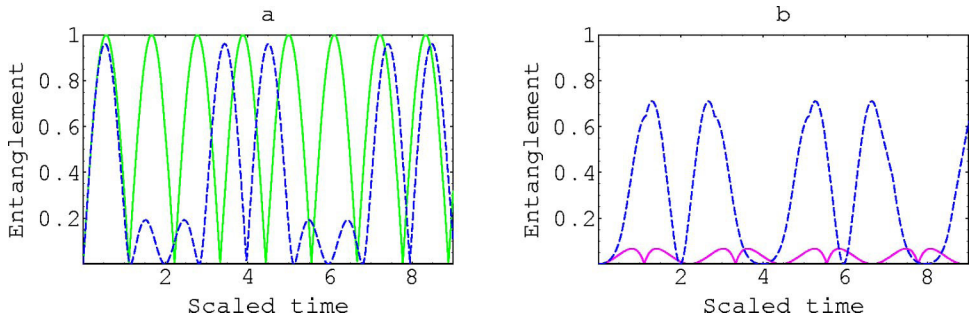

FIG. 3. Plot of the negativity as a measure of entanglement against the scaled time γt, the parameters $\beta_1=0$, $\phi=0$, and $r=1$, where (a) $kL=\pi/2$ (solid curve), and $kL=\pi/3$ (dotted curve). (b) The same as (a) but $r=0.2$.

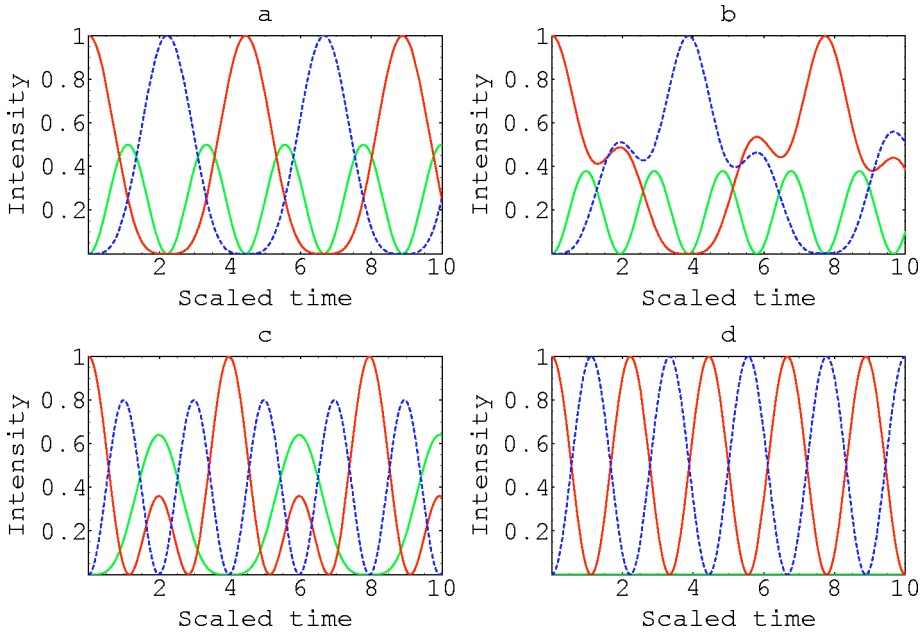

FIG. 4. This figure presents the results of the numerical calculations of the time evolution of the probability of the first qubit in excited state (solid line), probability of the second qubit in excited state (dotted line), and probability of emission of photon pair (dashed line), where (a) $\phi=0$, $\beta_1=0$, $kL=0$, $r=1$, (b) $\beta_1=0.8\gamma$, (c) $\phi=0$, $\beta_1=0$, $kL=\pi/3$, $r=1$, and (d) $\phi=0$, $\beta_1=0$, $kL=\pi/2$, $r=1$.

achieved, i.e., $I_{\mathcal{E}_t^*\rho}(t)\approx 0$ which means that the two qubits are separable and also the maximum values $I_{\mathcal{E}_t^*\rho}(t)=1$ is reached which indicates maximum entanglement between the two qubits. Therefore, one can say that an appropriate choice of distance between the two qubits leads to, on one hand, a complete separability between the qubits at other values of the interaction time and on the other hand maximum entanglement in other intervals of the interaction time. Meanwhile, the general feature of the entanglement in the case $L=\pi/3k$ is dramatically changed [see Fig. 3(a)]. This behavior is affected once the mixed state parameter r is decreased [see Fig. 3(b)]. It is noticed that the amount of entanglement is strongly decreased due to setting $L=\pi/2k$ and $r=0.2$, while it increased again when $L=\pi/3k$. Generally speaking, because of the influence of a mixed state parameter on entanglement, the amplitude of local maxima and minima decrease with increasing the deviation of r from the unity. However, as r takes values close to the unity we return to the same behavior in the initial pure state setting, i.e., $\rho=|e_1,g_2\rangle\otimes\langle e_1,g_2|$. However a slight change in r therefore, dramatically alters the entanglement. This is remarkable as the entanglement is strongly dependent on the initial state, which can be entangled or unentangled. Here, we clarify that it can be done by using a different initial state, which is strongly affected by the qubit number representation. This naturally leads to the use of occupation numbers of different single-qubit basis states in quantifying identical-qubits entanglement even when the number of qubits is conserved. The occupation-numbers of different modes have already been used in quantum computing.[41]

To this end, we devote the discussion in Fig. 4 to consider the effect of these different parameters on the probability of the first qubit (or atom) in excited state, the probability of the second qubit in excited state and probability of emission of photon pair. We would like to remark that when qubit 2 is initially prepared in either $|g_2\rangle$ $(r=1)$ or $|e_2\rangle$ $(r=0)$, which are stationary states for qubit 2, there will be substantial changes to the evolution of qubit 1 due to phase shifts introduced in the field through the dispersive interaction. The subsystem qubit 2 plays the role of a single qubit reservoir,[42] in the sense that it will induce modifications in the subsystem qubit 1 without having its state changed. If we increase the value of Stark shift parameter $\beta_1=0.8\gamma$, we have the situation shown in Fig. 4(b). We note a stronger modulation in the oscillations and a clear departure from ordinary Rabi oscillations is verified (see Fig. 4). The populations clearly exhibit

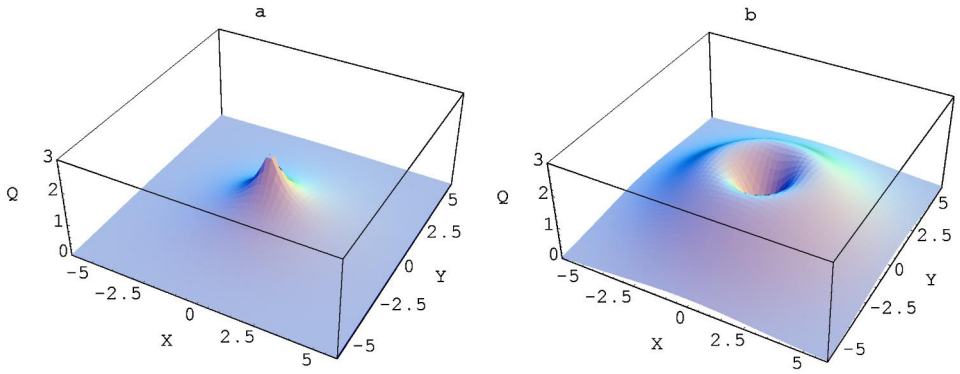

FIG. 5. Plot of quasiprobability function (Q-function) as a function of $X=\mathrm{Re}(\alpha)$ and $Y=\mathrm{Im}(\alpha)$, where the coherent state here is given by $|\alpha\rangle=\exp[-|\alpha|^2/2]\alpha^n/\sqrt{n!}|n\rangle$, $\alpha=X+iY$. The scaled time $\gamma t=\pi/2$, $L=0$, $\beta_1=0$, $r=1$. (a) corresponds to the case where the phase shift $\phi=\pi/2$, the timing of phase shift $\tau=13\pi/4$ and (b) the same as in (a) but $\tau=3\pi$.

the characteristic features observed in the entanglement behavior and provide us with information about the discrete nature of the quantized atom-field interaction. The remaining task is to identify and compare the results presented above for the entanglement degree with another accepted entanglement measure such as the concurrence.[43] One, possibly not very surprising, principal observation is that the numerical calculations corresponding to the same parameters, which have been considered above, give nearly the same behavior. This means that both the entanglement due to the negativity and concurrence measures are qualitatively the same.

There exists a neat explanation from the phase space point of view. Next, we will compute the relevant field quasiprobability in phase space. The Q-function computed for the field reduced density matrix $\rho^f(t)$ in the following form:

$$Q(\alpha)=\frac{1}{\pi}\langle\alpha|\rho^f(t)|\alpha\rangle,$$

where $|\alpha\rangle$ is a coherent state. The quasiprobability will be obtained in terms of probability amplitudes and photon occupation amplitudes. We now attempt to identify regions in the three-dimensional space spanned by the quasiprobability function that is inhabited by physical states, i.e., characterized by legitimate density matrices. Since the timing of an applied phase step has a large influence on the result, therefore to complete our work we shall consider in this discussion the quasiprobability function and how it is affected by the phase step in two different cases. For this purpose we have plotted Figs. 5 taking into consideration the same values of all parameters as in the above figures. For instance we have depicted the Q-function in Fig. 5(a) for $\beta_1=0$, $L=0$, $r=1$, and $\gamma t=\pi/2$, when the timing of an applied phase step $\tau=11\pi/4$ and $\phi=\pi/2$. We observe in general there is no change in the figure shape, i.e., there is no influence on the Q-function. The Q-function feature is exactly similar to that observed in the absence of the phase shift. As soon as we increase the values of τ such that $\tau=3\pi$, which means that the phase step is applied at the moment of maximum probability of pair photon emission, then we can observe a drastic change occurring in the function behavior. Therefore the shape of the quasiprobability is very sensitive to the choice of the application time of the phase step. Meanwhile, the general feature of the quasiprobability distribution function in the case $\tau=13\pi/4$, is almost identical to that in the previous case in which the timing of an applied phase step $\tau=11\pi/4$.

IV. CONCLUSION

We have investigated the entanglement in the context of an ensemble of two identical qubits (or atoms) coupled to a cavity field which can become entangled with one another, even when they do not interact directly with each other. We have treated the more general case where initial states

of the two qubits can be mixed with any state of the field. We have obtained an exact solution of the density operator taking into account the presence of Stark shift and an instantaneous phase shift experienced by one of the atoms that can be easily interpreted physically, and thus provides insight into the behavior of more complicated multiqubit systems. It is found that entangled pure states for this generalized case did not have the same entanglement as the mixed state case. Entanglement is measured via the negativity, currently defined only for an arbitrary system of two qubits, but similar analysis can in principle be applied to other systems such as a bipartite system with arbitrary dimensions. The influences of the Stark shift and the distance between the two-qubits have been presented. We have elucidated our studies by giving a detailed analysis and explanation of the predicted entanglement, intensity, and quasiprobability phenomena with nonzero values of the phase shift. The effect of phase shift is discussed when we apply a phase step at the moment of the maximum or minimum probability of photon pair emission. Finally, we have noted that the inclusion of the Stark shift in the present model, under suitable conditions, could lead to zero values of the entanglement, an effect that may have important consequences in other nonlinear processes. Finally, in addition to quantum computing implementations involving identical particles, the result here is also useful for many-body physics.

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A Wronskian of Jost solutions

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Based on the standard fact that any matrix potential $u=u(x)$ determines a family of Jost solutions whose parameter runs analytically (continuously) on the (closed) half planes, respectively, the zeros of a suitable matrix valued Wronskian of a Jost solution pair are explored. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Jost and Faddeev and their Wronskians play a crucial role in the direct and inverse scattering theory of the usual Schrödinger equation on the line (see, e.g., Deif and Trubowitz in Ref. 1). The fact that the Jost solutions are scalar functions allows one to prove that their Wronskians depend only of the spectral variable, to relate it to the entries of the scattering matrix and to the bound states as well as to use it as a tool for studying asymptotic properties for small values of the spectral variable.

All of this changes when studying the matrix equation of Schrödinger-type where the Jost solutions generalize and become matrix functions. One can define the Wronskian following Wadati and Kamijo in Ref. 2, Martínez Alonso and Olmedilla in Ref. 3, and Aktosun, Klaus and Van der Mee in Ref. 4. The basic facts such as dependence upon the spectral variable, relationship to scattering matrix coefficients and bound states and facilitation of the study of asymptotic behavior as the spectral variable tends to zero, still go through. The major inconvenience is the need to study the direct and inverse theory for the matrix equation of Schrödinger-type on the line for matrix potentials together with its adjoint at the same time, or to restrict oneself to self-adjoint potentials.

Here we shall consider a different way to define a Wronskian that only involves data pertaining to the matrix potential but not to its adjoint. It has the disadvantage that depends not only on the spectral variable and does not satisfy an antisymmetry relation but allows one to relate its zeros to the bound states. The goal of this work is to show that, under suitable conditions, the number of zeros is finite.

There will be four additional sections. Section II will be dedicated to quoting issues about the existence and asymptotic behavior for large values of both spatial and spectral variables of the Jost and Faddeev matrix solutions of Schrödinger-type for any matrix potential. Section III will deal with the analyticity and continuity on the half planes and the closed half planes, respectively, of the Faddeev and Jost matrix solutions and their derivatives with respect to the spectral variable including the asymptotic behavior for small values. All of this material in these sections is standard. Its formulation and proofs are as those for the usual Faddeev and Jost solutions (see Ref. 4). In Sec. IV we shall define a Wronskian for the Jost matrix solutions, state and prove its properties that imply that, under certain conditions its zeros form a discrete set in the upper half plane. In the last section (Sec. V), we shall give some comments and conclude from the results of Sec. IV that the number of bound state wave numbers is finite for suitable non-self-adjoint matrix potential.

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II. JOST AND FADDEEV SOLUTIONS

By a matrix potential u of Faddeev type we shall mean a square-matrix-valued function $u=(u_{ij})_{1\leqslant i,j\leqslant n}$, where n is a positive integer fixed, defined on the real line whose entry functions u_{ij} are complex valued integrable functions satisfying the Faddeev condition (see Ref. 5): $\int_{-\infty}^{\infty}(1+|x|)|u_{ij}|<\infty, 1\leqslant i,j\leqslant n$

For these (nonself-adjoint) matrix potentials of Faddeev-type there exists a one-parametric family of solutions for the spectral problem for the matrix equation of Schrödinger-type.

Proposition 2.1: *Let u be a matrix potential of Faddeev-type. Then the spectral problem*

$$\varphi_{xx}+k^2\varphi=u\varphi, \tag{2.1}$$

has a solution for each complex number k, i.e., a C^1-square matrix valued function $x\mapsto\phi(x,k)$ with second derivative defined on the real line satisfying the differential matrix equation in (2.1).

The second order linear differential matrix equation (2.1) may be converted into an integral matrix equation of Volterra-type for which we need a classification of solutions according to their asymptotic behavior. For instance,

$$e^{-kix}\psi_+(x,k)=\int_x^{\infty}\frac{1-e^{2ik(y-x)}}{2ik}e^{-kiy}u(y)\psi_+(y,k)dy.$$

For all real k the iterates are dominated in the spectral norm by the corresponding iterate of the scalar equation $s(x,\kappa)=1+\int_x^{\infty}(y-x)\|u(y)\|s(y,\kappa)dy$, implying (see Ref. 1)

$$\begin{aligned}\left\|e^{-i\kappa x}\psi_+(x,k)-I_{n\times n}\right\|<s(x,k)-1&=\sum_{\ell=1}^{\infty}\frac{1}{\ell}\left[(1+\max(0,-x))\int_x^{\infty}(1+|y|)\|u(y)\|dy\right]^{\ell}\\&=\exp([1+\max(0,-x)]\int_x^{\infty}(1+|y|)\|u(y)\|dy)-1\\&\leqslant\exp\left(\int_x^{\infty}(1+|y|)\|u(y)\|dy\right)-1, x\geqslant 0,\end{aligned} \tag{2.2}$$

where we used that $\max(0,-x)=0$ for $x\geqslant 0$ and $\|\cdot\|$ is any norm over the complex $n\times n$ matrices. Since u is a matrix potential of Faddeev-type, we have $\int_x^{\infty}(1+|y|)\|u(y)\|dy\to 0$ as $x\to+\infty$. Hence given a positive number $\epsilon>0$, there exists a positive number N such that $\|e^{-i\kappa x}\psi_+(x,k)-\mathrm{I}_{n\times n}\|<\epsilon$, for all k, Im $k\geqslant 0$ and $x>N$. All of this is summarized as follows.

Proposition 2.2: *Let u be a matrix potential of Faddeev-type. Then there exist unique C^1 matrix solutions with second derivative, $x\mapsto\phi_{\pm}(x,k)$, $x\mapsto\psi_{\pm}(x,k)$ for the spectral (2.1) problem with the following asymptotic behavior.*

On the closed upper half k plane,

$\phi_+(x,k)\sim e^{-ixkI_{n\times n}}$ *as* $x\to-\infty$, $\psi_+(x,k)\sim e^{ixkII_{n\times n}}$ *as* $x\to\infty$.

On the closed lower half k plane,

$\phi_-(x,k)\sim e^{ixkI_{n\times n}}$ *as* $x\to-\infty$, $\psi_-(x,k)\sim e^{-ixkI_{n\times n}}$ *as* $x\to\infty$, *and are called the Jost solutions.*

The Jost solutions $\psi_{\pm}$, $\phi_{\pm}$ without the factors $e^{\pm ixk}$, for example $m_+(x,k)=e^{-2kix}\psi_+(x,k)$, are here denoted by $m_{\pm}$, $\hat{m}_{\pm}$ and called the Faddeev solutions (see Ref. 4), respectively.

In the sequel, the statements will be formulated in terms of the Jost and Faddeev solutions pertaining to the matrix potential u of Faddeev-type.

Corollary 2.3: *There exist a number $\mathcal{N}$ and a neighborhood $V(x_0)$ for each real number x_0 in the interval $(\mathcal{N},+\infty)$ such that the function $k\mapsto[\psi_+(x,k)]^{-1}$ is well-defined on the whole closed upper half plane for all $x\in V(x_0)$, or equivalently, the function $x\mapsto[\psi_+(x,k)]^{-1}$ is well defined on $V(x_0)$ for all k, Im $k\geqslant 0$.*

Proof: It is enough to prove that there exist a number $\mathcal{N}$ and a neighborhood $V(x_0)$ for each real number x_0 in the interval $(\mathcal{N},+\infty)$ such that the $n\times n$ matrix $\psi_+(x,\kappa)$ is invertible for all k, Im $k\geqslant 0$ and for all $x\in V(x_0)$. First of all define $G(x)=(1+\max(0,-x))\int_x^{\infty}(1+|y|)\|u(y)\|dy$. We

have just seen that for $k, \operatorname{Im} k \geqslant 0$ $\|e^{-i\kappa x}\psi_+(x,k) - \mathrm{I}_{n\times n}\| < \exp[G(x)] - 1$ [see inequality in (2.2)]. Thus $\psi_+(x,k)$ is a nonsingular $n\times n$ matrix for every $k, \operatorname{Im} k \geqslant 0$ if the last member of this estimate is strictly less than 1. The latter is equivalent to requiring that the expression $G(x) < \ln(2)$. However, $G(x)$ is monotonically nonincreasing in x, tends to $+\infty$ as $x \to -\infty$ (unless $u(x) = 0$ almost everywhere) and vanishes as $x \to \infty$. Letting $\mathcal{N}$ stand for the supremum of all real x for which $G(x) = \ln(2)$, we see that $[\psi_+(x,k)]^{-1}$ is well-defined for all $x > \mathcal{N}$, irrespective of the choice of $k, \operatorname{Im} k \geqslant 0$. Thus for any real fixed $x_0 \in (\mathcal{N}, \infty)$, by choosing as $V(x_0)$, the entire interval itself $(\mathcal{N}, \infty)$ or any open subset of it containing x_0, we get the claim. □

The Jost solutions have the following asymptotic behavior of the spectral variable and asymptotic relations.

Proposition 2.4: *For x on the real line,*

$\phi_+(x,k) \sim e^{-ix\mathrm{k}\mathrm{I}_{n\times n}}$, $\psi_+(x,k) \sim e^{ix\mathrm{k}\mathrm{I}_{n\times n}}$ *as* $k \to \infty$, $\operatorname{Im} k \geqslant 0$

$\phi_-(x,k) \sim e^{ix\mathrm{k}\mathrm{I}_{n\times n}}$, $\psi_-(x,k) \sim e^{-ix\mathrm{k}\mathrm{I}_{n\times n}}$ *as* $k \to \infty$, $\operatorname{Im} k \leqslant 0$.

Proposition 2.5: *There exist unique matrix functions* a_ℓ, a_r, $b_\ell b_r$ *such that we have the asymptotic relations* $\psi_+(x,\kappa) \sim (e^{i\kappa x}a_\ell(k) + e^{-i\kappa x}b_\ell(\kappa))$ *as* $x \to -\infty$ *and* $\phi_+(x,\kappa) \sim e^{-i\kappa x}a_r(\kappa) + e^{i\kappa x}b_r(\kappa)$ *as* $x \to +\infty$ *for* $\kappa \neq 0$ *on the real line.*

III. ANALYTICITY AND CONTINUITY OF THE JOST AND FADDEEV SOLUTIONS

Theorem 3.1: *Let u a matrix potential of Faddeev type. Then*

(1) *The functions* $k \mapsto (d^\ell m_+/dx^\ell)(x,k)$, $k \mapsto (d^\ell \hat{m}_+/dx^\ell)(x,k)$ *are analytic on the open upper half plane. Fix a complex number* k_0 $\operatorname{Im} k_0 \geqslant 0$.

(2) *On* $[\alpha, +\infty)$, $(d^\ell m_+/dx^\ell)(x,k) \sim (d^\ell m_+/dx^\ell)(x,k_0)$ *as* $k \to k_0, \operatorname{Im} k \geqslant 0$, *and on* $(-\infty, \beta]$, $(d^\ell \hat{m}_+/dx^\ell)(x,k) \sim (d^\ell \hat{m}_+/dx^\ell)(x,k_0)$ *as* $k \to k_0, \operatorname{Im} k \geqslant 0$, *where* α, β *are any real numbers fixed and* $\ell = 0, 1$.

(3) *Similar results hold for the maps* $k \mapsto (d^\ell m_-/dx^\ell)(x,k)$, $k \mapsto (d^\ell \hat{m}_-/dx^\ell)(x,k)$, $\ell = 0, 1$.

Remark: The proof for $\ell = 1$ follows at once from establishing the result for $\ell = 0$. For the Jost solutions, the conclusion of Theorem 3.1 can only be true on the close half planes uniformly for x in any finite interval of the real line, respectively. Note $\lim_{x\to\infty}\psi_+(x,\kappa) = \lim_{x\to\infty}\lim_{\substack{k\to\kappa \\ \operatorname{Im} k>0}} \psi_+(x,k)$ does not exist for real $\kappa \neq 0$ and for $\kappa = 0$ such limit is equal to $\mathrm{I}_{n\times n}$ because $\psi_+(x,\kappa) \sim e^{x\kappa\mathrm{I}_{n\times n}}$ as x goes to ∞, but $\lim_{\substack{k\to\kappa \\ \operatorname{Im} k>0}} \lim_{x\to\infty}\psi_+(x,k) = 0_{n\times n}$. Hence for Jost solutions the uniform convergence as in Theorem 3.1 is only true for any real κ and x in a finite interval.

Theorem 3.1 has a straightforward consequence for the Faddeev and Jost solutions.

Corollary 3.2: *The Faddeev and Jost solutions together with their derivatives respect to the spatial variable x are analytic on the open half planes and continuous on the closed upper half planes, respectively.*

IV. A WRONSKIAN OF THE JOST SOLUTIONS

Let us consider the Wronskian (see Ref. 6)

$$W(\psi,\varphi) = \psi\psi'\psi^{-1}\varphi - \psi\varphi' = -\psi^2\frac{d}{dx}(\psi^{-1}\varphi), \tag{4.1}$$

where a prime indicates derivative respect the variable x.

In contrast to the Wronskian 2-4, $W(\psi,\varphi) = [\psi']^\dagger\varphi - [\psi]^\dagger\varphi'$, ours depends on where ψ^{-1} is defined and on the variable x, and does not satisfy the usual antisymmetry relation $W(\psi,\phi) = -W(\phi,\psi)^\dagger$ but allows one to relate it to the bound states for sufficiently large real numbers x_0 which is sufficient for the purposes of this work.

By virtue Corollary 2.3, the Wronskian is defined on the closed upper half plane for any real number fixed x_0 large enough and Corollary 3.2 implies its analyticity and continuity.

Proposition 4.1: Let x_0 *be a fixed real number large enough according to the Corollary 2.3.*

Then the Wronskian $k\mapsto W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)$ *is defined on the closed upper half plane, analytic on the open upper half plane and continuous on the closed upper half plane.*

Similar results for the matrix Wronskian $W(\psi_-,\phi_-)$ can be obtained in the same way. In the sequel, we generate results only for the matrix Wronskian in (4.1) for the Jost solution ψ_+, ϕ_+.

Proposition 4.2: The set $\mathcal{W}_{x_0}=\{k,\operatorname{Im}k\geqslant 0: W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)=0\}$ *is bounded for any fixed real number* x_0 *large enough as in the previous proposition.*

Proof: By Proposition 2.3, $W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)\sim(-2ik)\mathrm{I}_{n\times n}$ as $k\to\infty$, $\operatorname{Im}k\geqslant 0$. Therefore, the set $\mathcal{W}_{x_0}$ is bounded as a set of the closed upper half plane for any real number x_0 large enough.

From now on x_0 will be a fixed real number large enough which means a real number chosen according to Corollary 2.3.

Proposition 4.3: The set $\mathcal{W}_{x_0}$ *satisfies that*

$$\mathcal{W}_{x_0}=\{k,\operatorname{Im}k\geqslant 0:\exists\ \text{a matrix } c=c(k)\ \text{such that}\ \phi_+(\cdot,k)\equiv\psi_+(\cdot,k)c\}.$$

Proof: Fix x_0 a real number as the statement, i.e., as in Corollary 2.3.

Let k_0 a complex number in the closed upper half plane ($\operatorname{Im}k_0\geqslant 0$) where $\phi_+(\cdot,k_0)\equiv\psi_+(\cdot,k_0)c$ being $c=c(k_0)$ a constant matrix. It is straightforward to see that by replacing this identity in the expression of the Wronskian given in (5.1) $W(\psi_+(\cdot,k_0),\phi_+(\cdot,k_0))(x)=0_{n\times n}$ for any x on the real line, where $\psi_+(x,k_0)$ is defined (Corollary 2.3) in particular for $x=x_0$. Thus $\mathcal{W}_{x_0}$ contains the set.

Take $k_0\in\mathcal{W}_{x_0}$. By Corollary 2.3, $x\mapsto[\psi_+(x,k_0)]^{-1}$ is well-defined on a neighborhood $V(x_0)$ $(k_0,\operatorname{Im}k_0\geqslant 0)$. Thus write $\phi_+(x,k_0)=\psi_+(x,k)c(x,k_0)$ for $x\in V(x_0)$, where $x\mapsto c(x,k_0)$ is differentiable at $x=x_0$ and the Wronskian $x\mapsto W(\psi(\cdot,k_0),\phi(\cdot,k_0))(x)$ is well-defined on $V(x_0)$. Since $W(\psi_+(\cdot,k_0),\phi_+(\cdot,k_0))(x_0)$ vanishes, then in view of (4.1), $W(\psi_+(\cdot,k_0),\phi_+(\cdot,k_0))(x_0)=\psi_+(x_0,k_0)c'(x_0,k_0)=0_{n\times n}$. From this and the choice of $x\mapsto c(x,k_0)$,

$$\phi_+(x_0,k_0)=\psi_+(x_0,k_0)c$$

$$\phi'_+(x_0,k_0)=\psi'_+(x_0,k_0)c,$$

being $c=c(x_0,k_0)$. Thus ϕ_+, ψ_+c are two solutions of the second order linear diferential equation (2.1) that agree at x_0 as well as their derivatives. By uniqueness, we have that $\phi_+(\cdot,k_0)\equiv\psi_+(\cdot,k_0)c$. Hence $\mathcal{W}_{x_0}$ is contained in the set, which finally proves the claim. □

Proposition 4.4: $\mathcal{W}_{x_0}$ *is a discrete set of the open upper half plane.*

Proof: This follows at once because the Wronskian $k\mapsto W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)$ is analytic on the open upper half plane (Proposition 4.1), therefore, its zeros are isolated in the upper half plane showing the claim. □

Proposition 4.5: Let $\kappa_0\neq 0$ *be a real number where the zeros in the open upper half plane of the Wronskian* $k\mapsto W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)$ *accumulate. Then* $a_r(\kappa_0)=0$.

Proof: Let κ_0 be as in the statement. By Proposition 4.5 the Wronskian is continuous on the closed upper half plane which shows that $W(\psi_+(\cdot,\kappa_0),\phi_+(\cdot,\kappa_0))(x_0)=0$. By virtue of Proposition there exists a constant $c=c(\kappa_0)$ such that $\phi_+(x_0,\kappa_0)=\psi_+(x_0,\kappa_0)c$. This together with Proposition 2.5 imply $\phi_+(x,\kappa_0)\sim e^{ix\kappa_0}c$ and $\phi_+(x_0,\kappa_0)\sim(e^{-ix\kappa}a_r(\kappa_0)+e^{ix\kappa_0}b_r(\kappa_0))$ as $x\to+\infty$. Thus $a_r(\kappa_0)=0$. □

Proposition 4.6: Assume the existence of $\lim_{k\to 0} W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)/k$ *and the accumulation of zeros of the Wronskian* $k\overset{\operatorname{Im}k\geqslant 0}{\mapsto}W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)$ *to* $k_0=0$. *Then* $(d/d\kappa)W(\psi_+(\cdot,\kappa),\phi_+(\cdot,\kappa))(x_0)\big|_{\kappa_0=0}=0$.

Proof: Let $\{k_n\}_n$ be a sequence of complex numbers in the upper half plane ($\operatorname{Im}k_n>0$) which accumulates to 0 and where $k\mapsto W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)$ vanishes. Then $W(\psi_+(\cdot,k_n),\phi_+(\cdot,k_n))\times(x_0)/k_n=0$ for all n. Hence by the first part of the hypothesis $(d/d\kappa)W(\psi_+(\cdot,\kappa),\phi_+(\cdot,\kappa))\times(x_0)\big|_{\kappa_0=0}=\lim_{k\to 0} W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)/k=0_{n\times n}$ where we use the fact that $W(\psi_+(\cdot,0),\phi_+(\cdot,0))(x_0)=0$. □

V. CONCLUSIONS

The usual Schrödinger equation has scalar Jost solutions $\psi_+(x,k)\sim e^{ikx}$ as $x\to+\infty$, $\phi_+(x,k)\sim e^{-ikx}$ as $x\to-\infty$. This fact allows to prove that their Wronskian $W(\psi_+,\phi_+)=\psi_+'\phi_+-\psi_+\phi_+'$ is independent of the real variable x and to relate it to the scattering coefficients by using the asymptotic relations for κ in the real line $\psi_+(x,\kappa)\sim a_\ell(k)e^{i\kappa x}+b_\ell(\kappa)e^{-i\kappa x}$ as $x\to-\infty$ and $\phi_+(x,\kappa)\sim a_r(\kappa)e^{-i\kappa x}+b_r(\kappa)e^{i\kappa x}$ as $x\to-\infty$, $\kappa\neq0$. It also allows one to relate bound state wave-numbers to the Wronskian which arise as zeros of $a_\ell(k)=a_r(k)$ on the positive imaginary axis and to use it as a tool for studying asymptotic properties as $k\to0$, $\mathrm{Im}\,k\geqslant0$. Since, in addition, $|a_\ell(\kappa)|^2-|b_\ell(\kappa)|^2=1$ for real $\kappa\neq0$, the continuity of $k\mapsto a_\ell(k)$ in the closed upper half plane implies the finiteness of the number of bound state wave numbers (it also implies that they cannot accumulate to any real number $\kappa\neq0$).

As we have seen this changes when studying the $n\times n$ matrix equation of Schrödinger type where the Jost solutions generalize and become $n\times n$ matrix functions. One may consider the Wronskian $W(\psi_+,\phi_+)=[\psi_+']^\dagger\phi_+-[\psi_+]^\dagger\phi_+'$, where † denotes the conjugate transpose, ϕ_+ is a Jost solution pertaining to the $n\times n$ matrix potential $u(x)$, and ψ_+ is a Jost solution pertaining to the matrix potential $u(x)^\dagger$. The basic stuff such as x-independence, relationships to scattering coefficients and bound states and facilitation of the study of small k asymptotic, still go through (see Ref. 4). The major drawback is the need to study the direct and inverse scattering theory for the matrix Schrödinger equations on the line for the potentials u and $u^\dagger$ at the same time, or to restrict oneself to self-adjoint potentials. On the other hand, one may consider the Wronskian $W(\psi,\varphi)=-\psi^2(d/dx)(\psi^{-1}\varphi)$ to obtain a Wronskian which is not well-defined for all ψ, not independent of the spatial variable x and does not satisfy an usual antisymmetry relation $W(\psi,\phi)=-W(\phi,\psi)^\dagger$ but only involves data pertaining to u (and not data pertaining to $u^\dagger$) and allows to relate it to the bound states (also to the scattering matrix coefficients).

It is indicated by Boris Pavlov (see Refs. 7 and 8) that the (scalar) Schrödinger equation on the half-line with complex potential has finitely many discrete eigenvalues if the potential decays exponentially, but often infinitely many discrete eigenvalues if the potential decays algebraically. It is a standard argument, involving the observation that the resolvent of the full-line Schrödinger equation is a rank one perturbation of the direct sum of the resolvents of the Schrödinger equations on the positive and negative half-lines, to see that this result goes through for the Schrödinger equation with complex potential on the full line. The standard result that Schrödinger equations with a Faddeev class potential [i.e., one where $(1+|x|)q(x)$ belongs to L^1] has only finitely many discrete eigenvalues, is only true for real potentials. Here it has been studied a generalization of the class of Schrödinger equations considered by Boris Pavlov, but has assumed a Faddeev-type of condition on the matrix potential. Unfortunately, the standard argument of excluding accumulation of discrete eigenvalues on the real line requires that $\|a_l(k)\|\geqslant1$. However, the identity $a_l(k)^\dagger a_l(k)-b_l(k)^\dagger b_l(k)=I_{n\times n}$ on which this can be based, has only been proved for selfadjoint matrix potentials (see Ref. 4). For complex potentials ($n=2$) this identity would imply that $a_l(k_0)=0$ and $b_l(k_0)=\pm i$ at a real numbers k_0 where the discrete eigenvalues accumulate (here it is used that $k\mapsto a_l(k)$ is continuous in the closed upper half plane). Thus even in the case that this identity will hold, we cannot conclude that the number of discrete eigenvalues is finite for a matrix potential which is not self-adjoint.

It is well-known that the norm of Jost solution $\phi_+(\cdot,k_0)$ which is a bound state is a square integrable function, therefore, the complex number k_0 belongs to the open upper half plane, i.e., $\mathrm{Im}\,k_0>0$ and there exists a constant matrix $c=c(k_0)$ such that $\phi_+(\cdot,k_0)\equiv\psi_+(\cdot,k_0)c$. This fact together with the discussion in the previous section yield to the following conclusion.

Theorem 5.1: Assume the existence of $\lim_{\substack{k\to0\\ \mathrm{Im}\,k\geqslant0}} W(\psi_+(\cdot,k),\phi_+(\cdot,k))(x_0)/k\neq0$ *and* $a_r(\kappa)\neq0$ *for real* $\kappa\neq0$. *Then the number of bound state wave numbers is finite.*

Proof: Let x_0 be a number large enough as indicated in the Corollary 2.3. In view of Proposition 4.3, we only need to consider the cardinality of $\mathcal{W}_{x_0}$. Given a complex number $k_0\in\mathcal{W}_{x_0}$, $\mathrm{Im}\,k_0>0$, the discreteness of $\mathcal{W}_{x_0}$ (Proposition 4.4) shows that there exist a neighborhood $V(k_0)$,

such that $\mathcal{W}_{x_0} \cap V(k_0) = \{k_0\}$ (the zeros of the Wronskian cannot accumulate to complex numbers in the upper half plane).

Consider a real number $\kappa_0 \neq 0$. In view of Proposition 4.5 and $a(\kappa_0) \neq 0$ by hypothesis, the zeros of the Wronskian cannot accumulate to κ_0. In addition, by virtue of Proposition 4.6 and $\lim_{\substack{k\to 0 \\ \text{Im } k\geqslant 0}} W(\psi_+(\cdot,k), \phi_+(\cdot,k))(x_0)/k \neq 0$ by hypothesis, the zeros of the Wronskian cannot accumulate to 0. Thus the zeros of the Wronskian in the upper half plane cannot accumulate to a real numbers. In consequence, for each real number k_0, we can find a neighborhood $V(k_0)$ such that $\mathcal{W}_{x_0} \cap V(k_0) = \emptyset$, $k_0 \neq 0$ and $\mathcal{W}_{x_0} \cap V(0) = \{0\}$. Note that $\cup_{k,\text{Im } k>0} V(k) \cup \cup_{k,\text{Im } k=0} V(k)$ is an open covering for $\overline{\mathcal{W}_{x_0}}$ which is a compact set of the closed upper half plane (Proposition 4.2). Hence there exist a finite collection of complex numbers $k_i, \text{Im } k_i > 0, i = 1, \ldots, \ell_1$, and real numbers $\kappa_j, j = 1, \ldots, \ell_2$, such that $\cup_{i=1}^{\ell_1} V(k_i) \cup \cup_{j=1}^{\ell_2} V(\kappa_j) \supseteqq \overline{\mathcal{W}_{x_0}}$. By the choice of the covering, we must have $\{k_1, \ldots, k_{\ell_1}\} \cup \{\kappa_1, \ldots, \kappa_{\ell_2}\} \supseteqq \mathcal{W}_{x_0}$. Since the set of the bound state wave numbers is a subset of both the open upper half plane and $\mathcal{W}_{x_0}$ sets, it is totally contained in $\{k_1, \ldots, k_{\ell_1}\}$, which shows the claim. □

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On the Bose condensation in some model of a nonideal Bose gas

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A model of a nonideal Bose gas with a repulsive interaction is considered. It is proved that there is not macroscopic occupation of the ground state in the thermodynamic limit in this model, but nevertheless the generalized condensation occurs. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1795971]

I. INTRODUCTION

The experimental creation of Bose condensates (for a review of the theory of trapped Bose-condensed gases with extensive references in the literature see Ref. 1) has sparked interest in their properties. One of the most important and knotty problems is connected with the rigorous proof of the existence (or absence) of Bose condensation for nonideal (imperfect) Bose systems. Another aspect which in particular has received much attention is the relation between nature of interparticle interaction and Bose condensation.

Schröder[2] considered a model of a nonideal Bose gas contained in a d-dimensional ($d \geqslant 3$) cubical box with Dirichlet boundary conditions on two opposite faces and periodic boundary conditions on the remaining surface. From the results of this work the absence of macroscopic occupation of the zero momentum one particle state was ensued. In Ref. 3 the model formally looking like Schröder's model has been studied. The Hamiltonian of Michoel and Verbeure[3] differs from the Huang–Yang–Luttinger Hamiltonian[4] by the plus sign in the additional term, which is purely quantum mechanical contribution to the mean-field interaction energy. Michoel and Verbeure, referring to the approximation theorem proved in Ref. 5 showed that their model has so-called nonextensive Bose condensation, i.e., there is generalized condensation[6,7] without macroscopic occupation of the ground state level.

In the following a model of a nonideal Bose gas, which is some minimal generalization of the Michoel–Verbeure model, is considered. By the Bogoliubov method[8–10] we prove that there is no Bose condensation,[11] in which the total condensate is in the ground state so that the ground state is macroscopically occupied. The aim of this article is to analyze the simple diagonal model within the framework of the general ideas and methods, which are referred to as the Bogoliubov theory of superfluidity. They were introduced in Refs. 8 and 9 and later further extended by Ginibre.[10]

In Sec. II we give a definition of the model and present the main result. In Sec. III we prove the main theorem. Section IV contains a few concluding remarks. In particular, using the method of Ref. 3 we prove that the model has the generalized condensation.

II. MODEL AND MAIN RESULT

We consider a system of spinless identical nonrelativistic bosons of mass m enclosed in a centered hypercubic box $\Lambda \subset \mathbb{R}^d$, $d \geqslant 3$, of volume $V=|\Lambda|=L^d$ with periodic boundary conditions for the wave functions. The Hamiltonian of the model is given by

$$\hat{H}_\Lambda = \sum_{p \in \Lambda^*} \epsilon_p \hat{n}_p + \frac{\lambda}{V} \hat{N}_\Lambda^2 + \frac{g}{2V} \sum_{p \in \Lambda^*} \hat{n}_p^2, \tag{1}$$

where $\epsilon_p = p^2/(2m)$, positive constants λ and g do not depend on V,

$$\hat{N}_\Lambda = \sum_{p \in \Lambda^*} \hat{n}_p, \hat{n}_p = \hat{a}_p^\dagger \hat{a}_p.$$

Here $\hat{a}_p^\# = \{\hat{a}_p^\dagger \text{ or } \hat{a}_p\}$ are the usual boson creation (annihilation) operators for the one-particle state $\psi_p(x) = V^{-1/2} \exp(ipx)$, $p \in \Lambda^*$, $x \in \Lambda$, acting on the Fock space $F_\Lambda = \oplus_{n=0}^\infty \mathcal{H}_{\mathrm{B}}^{(n)}$, where $\mathcal{H}_{\mathrm{B}}^{(n)} \equiv [L^2(\Lambda^n)]_{\mathrm{symm}}$ is the symmetrized n-particle Hilbert space appropriate for bosons, and $\mathcal{H}_{\mathrm{B}}^{(0)} \equiv \mathbb{C}$. The sums in (1) run over the dual set

$$\Lambda^* = \left\{ p \in \mathbb{R}^d : p_j = \frac{2\pi}{L} n_j, n_j = 0, \pm 1, \pm 2, \ldots, j = 1, 2, \ldots, d \right\}.$$

The Michoel-Verbeure model is a special case of (1) where $g = \lambda$. Obviously, the Hamiltonian (1) is superstable.[12]

Let us prove, that in the case of model (1) for every $p \in \Lambda^* \setminus \{0\}$

$$\lim_{V \to \infty} \frac{\langle \hat{n}_p \rangle_{\hat{H}_\Lambda(\mu)}}{V} = 0, \tag{2}$$

where $\langle \cdots \rangle_{\hat{H}_\Lambda(\mu)}$ denotes the finite-volume grand-canonical Gibbs state for the Hamiltonian $\hat{H}_\Lambda(\mu) \equiv \hat{H}_\Lambda - \mu \hat{N}_\Lambda$ and μ is the chemical potential.

First, we define the Bogoliubov inner product[13–15] (or the Duhamel two-point function) for the Hamiltonian $\hat{\Gamma}$ and for any two operators $\hat{A}$, $\hat{B}$ by

$$(\hat{A}, \hat{B})_{\hat{\Gamma}} = \int_0^1 dx \langle e^{x\beta\Gamma} \hat{A} e^{-x\beta\Gamma} \hat{B} \rangle_{\hat{\Gamma}}. \tag{3}$$

Here $\langle \cdots \rangle_{\hat{\Gamma}}$ denotes the appropriate thermal average with respect to the Hamiltonian $\hat{\Gamma}$ and the inverse temperature β. The Bogoliubov inner product is positive semidefinite. It also satisfies the symmetry property, so

$$(\hat{A}, \hat{B})_{\hat{\Gamma}} = (\hat{B}, \hat{A})_{\hat{\Gamma}}, (\hat{A}^\dagger, \hat{A})_{\hat{\Gamma}} \geqslant 0. \tag{4}$$

The properties (4) follow from the definition (3). Noting that

$$\mathrm{tr}(e^{-x\beta\Gamma}[\hat{A}, \beta\hat{\Gamma}] e^{-(1-x)\beta\hat{\Gamma}} \hat{B}) = \frac{d}{dx} \mathrm{tr}(e^{-x\beta\Gamma} \hat{A} e^{-(1-x)\beta\hat{\Gamma}} \hat{B})$$

we have the relation

$$\langle [\hat{A}, \hat{B}] \rangle_{\hat{\Gamma}} = ([\hat{A}, \beta\hat{\Gamma}], \hat{B})_{\hat{\Gamma}}. \tag{5}$$

We then prove the following result.

Lemma 1: In the case of model (1) for every $p \in \Lambda^* \setminus \{0\}$ one has

$$(\hat{a}_p^\dagger, \hat{a}_p)_{\hat{H}_\Lambda} \leqslant (\beta\epsilon_p)^{-1}, \tag{6}$$

with the Bogoliubov inner product defined in the canonical ensemble.

Proof: Take $\hat{A} = \hat{a}_p$, $\hat{B} = \hat{a}_p^\dagger$, $\hat{\Gamma} = \hat{H}_\Lambda$ in the equality (5). Then it becomes

$$1 = \beta\epsilon_p (\hat{a}_p^\dagger, \hat{a}_p)_{\hat{H}_\Lambda} + \beta (\hat{a}_p^\dagger, \hat{C}_p \hat{a}_p)_{\hat{H}_\Lambda}, \tag{7}$$

where

$$\hat{C}_p \equiv \frac{2}{V}\left(\frac{g}{2}\hat{n}_p + \lambda\hat{N}\right) + \frac{1}{V}\left(\lambda + \frac{g}{2}\right). \tag{8}$$

Note that $\hat{C}_p$ is a positive Hermitian operator and it commutes with $\hat{H}_\Lambda$. Then, because of (4), the second term in the right-hand side of (7) is non-negative. This completes the proof of Lemma 1.

Note that the inequality (6) has a highly general nature, expressing a so-called local Gaussian domination property.[16]

Lemma 2: In the case of model (1) the condition

$$\lim_{V\to\infty}\frac{1}{V}\langle\hat{n}_p\rangle_{\hat{H}_\Lambda} = 0 \tag{9}$$

is satisfied for every $p \in \Lambda^* \setminus \{0\}$, *where* $\langle\cdots\rangle_{\hat{H}_\Lambda}$ *denotes the finite-volume canonical Gibbs state for the Hamiltonian* $\hat{H}_\Lambda$.

Proof: Use the Falk-Bruch inequality.[14,17] Then

$$\langle\hat{n}_p\rangle_{\hat{H}_\Lambda} \leqslant \frac{1}{2}\left[\sqrt{c_p^{(0)}b_p^{(0)}}\coth\sqrt{\frac{c_p^{(0)}}{4b_p^{(0)}}} - 1\right], \tag{10}$$

where

$$b_p \equiv (\hat{a}_p^\dagger, \hat{a}_p)_{\hat{H}_\Lambda} \leqslant b_p^{(0)} = (\beta\epsilon_p)^{-1},$$

$$c_p \equiv \langle[\hat{a}_p^\dagger, [\beta\hat{H}_\Lambda, \hat{a}_p]]\rangle_{\hat{H}_\Lambda} \leqslant c_p^{(0)} = \beta\left(\epsilon_p + 2\lambda\rho + \frac{2}{V}(\lambda+g)\langle\hat{n}_p\rangle_{\hat{H}_\Lambda} + \frac{1}{V}\left(\lambda + \frac{g}{2}\right)\right),\ c_p^{(0)} \geqslant 0$$

and ρ is the mean number of particles per unit volume for model (1). From $\coth x < 1 + 1/x$, $x > 0$, one deduces

$$\frac{1}{V}\langle\hat{n}_p\rangle_{\hat{H}_\Lambda} \leqslant \frac{1}{2V}\left[\sqrt{\frac{\epsilon_p + 2\lambda\rho + (\lambda+g)\langle\hat{n}_p\rangle_{\hat{H}_\Lambda}/V + (\lambda+g/2)/V}{\epsilon_p}} + \frac{2}{\beta\epsilon_p} - 1\right].$$

Since

$$\inf_{p\in\Lambda^*\setminus\{0\}}\epsilon_p = \frac{2\pi^2}{m}V^{-2/3},$$

we obtain $\langle\hat{n}_p\rangle_{\hat{H}_\Lambda}/V \sim V^{-1/3}$. The Lemma 2 is proved.

Condition (2) is a consequence of condition (9). It follows from the formula

$$\langle\hat{n}_p\rangle_{\hat{H}_\Lambda(\mu)} = \Xi_\Lambda^{-1}\sum_{N=0}^{\infty}\exp\left[-\beta V\left(f_N - \mu\frac{N}{V}\right)\right]\langle\hat{n}_p\rangle_{\hat{H}_\Lambda}, \tag{11}$$

where the grand canonical partition function is given by

$$\Xi_\Lambda = \sum_{N=0}^{\infty}\exp\left[-\beta V\left(f_N - \mu\frac{N}{V}\right)\right]$$

and N-particle free energy is

$$f_N = -\frac{1}{\beta V}\ln\mathrm{tr}_{\mathcal{H}_{\mathrm{B}}^{(N)}}e^{-\beta\hat{H}_\Lambda}.$$

Namely, let us define $\overline{\rho}$ by the condition

$$\inf_{N/V} F_N\left(\frac{N}{V}\right) = F_N(\overline{\rho}) \equiv \overline{F}_N.$$

In virtue of convexity of the free energy as a function of ρ[12] for $N/V - \overline{\rho} > \xi > 0$ one gets

$$F_N\left(\frac{N}{V}\right) \geqslant a_1 + a_2\left(\frac{N}{V} - \overline{\rho} - \xi\right),$$

where $a_1 = F_N(\overline{\rho}+\xi) \geqslant \overline{F}_N + \sigma$, $\sigma > 0$, $a_2 = F_N'(\overline{\rho}+\xi) > 0$. Furthermore, for $|N/V - \overline{\rho}| < \xi' < \xi$ we have $F_N \leqslant \overline{F}_N + \sigma/2$. Then we can write the following lower bound:

$$\Xi_\Lambda \geqslant \sum_{|N/V-\overline{\rho}|<\xi'} \exp(-\beta V F_N) \geqslant 2\xi' V \exp\left[-\beta V\left(\overline{F}_N + \frac{\sigma}{2}\right)\right].$$

From Lemma 2 and (11) we get, for every $p \in \Lambda^* \setminus \{0\}$ and V large enough,

$$\begin{aligned}
\langle \hat{n}_p \rangle_{\hat{H}_\Lambda(\mu)} &\leqslant c_1 \Xi_\Lambda^{-1} \sum_{N=0}^{\infty} N^{2/3} \exp(-\beta V F_N) \\
&= c_1 \Xi_\Lambda^{-1} \sum_{0 \leqslant N \leqslant V(\overline{\rho}+\xi)} N^{2/3} \exp(-\beta V F_N) + c_1 \Xi_\Lambda^{-1} \sum_{N \geqslant V(\overline{\rho}+\xi)} N^{2/3} \exp(-\beta V F_N) \\
&\leqslant c_1 (\overline{\rho}+\xi)^{2/3} V^{2/3} + c_1 \Xi_\Lambda^{-1} \sum_{N \geqslant V(\overline{\rho}+\xi)} N^{2/3} \exp\left\{-\beta V\left[a_1 + a_2\left(\frac{N}{V} - \overline{\rho} - \xi\right)\right]\right\} \\
&\leqslant c_1 (\overline{\rho}+\xi)^{2/3} V^{2/3} + c_2 \exp\left(-\frac{\sigma V}{2}\right),
\end{aligned}$$

where c_1 and c_2 are some positive constants. (2) follows from the last relation.

To study the behavior of $\langle \hat{n}_0 \rangle_{\hat{H}_\Lambda(\mu)}/V$ we are concerned with the Bogoliubov–Ginibre approach. Let us first rewrite the Hamiltonian $\hat{H}_\Lambda(\mu)$ in the form

$$\begin{aligned}
\hat{H}_\Lambda(\mu) = &-\mu \hat{a}_0^\dagger \hat{a}_0 + \sum_{p \in \Lambda^*, p \neq 0} (\epsilon_p - \mu) \hat{n}_p + \frac{\lambda}{V}\left[\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_0 + 2\hat{a}_0^\dagger \hat{a}_0 \sum_{p \in \Lambda^*, p \neq 0} \hat{n}_p + \left(\sum_{p \in \Lambda^*, p \neq 0} \hat{n}_p\right)^2\right] \\
&+ \frac{a}{2V}\left(\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_0 + \sum_{p \in \Lambda^*, p \neq 0} \hat{n}_p^2\right). \qquad (12)
\end{aligned}$$

According to the Bogoliubov method,[18] we now replace

$$\hat{a}_0 \to c V^{1/2}, \quad \hat{a}_0^\dagger \to \overline{c} V^{1/2}, \qquad (13)$$

where $c \in \mathbb{C}$ and the bar means complex conjugation. So we have the approximating Hamiltonian

$$\hat{H}_\Lambda(\mu, c) = \hat{H}_\Lambda^{(0)}(\mu, c) + \hat{H}_\Lambda'(\mu), \qquad (14)$$

where

$$\hat{H}_\Lambda^{(0)}(\mu, c) = V\left(\lambda |c|^2 - \mu + \frac{g}{2}|c|^2\right)|c|^2 + \left(\lambda + \frac{g}{2}\right)|c|^2 + 2\lambda |c|^2 \hat{N}_\Lambda',$$

$$\hat{H}'_\Lambda(\mu) = \sum_{p\in\Lambda^*,p\neq 0} (\epsilon_p - \mu)\hat{n}_p + \frac{\lambda}{V}\hat{N}'^2_\Lambda + \frac{g}{2V}\sum_{p\in\Lambda^*,p\neq 0}\hat{n}^2_p, N'_\Lambda \equiv \sum_{p\in\Lambda^*,p\neq 0}\hat{n}_p.$$

After the canonical gauge transformation to boson operators $\hat{a}^{\#}_p \to \exp(\pm i \arg c)\hat{a}^{\#}_p$ note that Hamiltonian (14) depends only on $c=|c|\equiv\sqrt{\rho_0}$, $\rho_0 \geqslant 0$.

Define the grand-canonical pressures

$$p_\Lambda = (\beta V)^{-1} \ln \mathrm{tr}_{F_\Lambda} \exp[-\beta\hat{H}_\Lambda(\mu)]$$

and

$$p_\Lambda(c) = (\beta V)^{-1} \ln \mathrm{tr}_{F_\Lambda} \exp[-\beta\hat{H}_\Lambda(\mu,c)]$$

associated with Hamiltonians $\hat{H}_\Lambda(\mu)$ and $\hat{H}_\Lambda(\mu,c)$, respectively.

Theorem: *The model Hamiltonian (1) and the approximating Hamiltonian (14) are thermodynamically equivalent in accordance to Wentzel,*[19] *i.e.,*

$$\lim_{V\to\infty}\sup_c p_\Lambda(c) = \lim_{V\to\infty} p_\Lambda \equiv p.$$

The proof of this theorem is given in Sec. III.

Theorem states that the self-consistency parameter c in the Bogoliubov-Ginibre method is determined by the condition that the approximate pressure $p_\Lambda(c)$ be maximal. If an appropriate equation (self-consistency equation) has the nontrivial solution (this equation always has the trivial solution $c=0$ for gauge invariant Hamiltonians), then we prove that Bose condensation actually occurs in the system under consideration[20]

$$\rho_0 = \lim_{V\to\infty} \frac{\langle \hat{a}^\dagger_0 \hat{a}_0\rangle_{\hat{H}_\Lambda(\mu)}}{V} > 0. \tag{15}$$

An absence of the nontrivial solution implies an absence of the Bose condensate. Let us prove, that the last just and is realized in a considered case.

A necessary condition for $p_\Lambda(c)$ to be maximum is

$$\left\langle \frac{\partial \hat{H}^{(0)}_\Lambda(\mu,c)}{\partial c} \right\rangle_{\hat{H}_\Lambda(\mu,c)} = 0.$$

By explicit calculations we get the following equation to obtain a nontrivial solution

$$g\rho_0 = \mu - 2\lambda\rho_0 - \frac{2\lambda}{V}\sum_{p\in\Lambda^*,p\neq 0}\langle\hat{n}_p\rangle_{\hat{H}_\Lambda(\mu,c)} - \frac{1}{V}\left(\lambda + \frac{g}{2}\right). \tag{16}$$

Prove that for V sufficiently large (16) does not have a positive solution $\rho_0 > 0$. Use the inequality[13,21]

$$\langle[\hat{A},[\hat{H},\hat{A}^\dagger]]\rangle_{\hat{H}} \geqslant 0, \tag{17}$$

which is valid for any operator $\hat{A}$ and for any self-conjugate superstable Hamiltonian $\hat{H}$. Take $\hat{A} = \hat{a}^\dagger_p (p\neq 0)$, $\hat{H}=\hat{H}_\Lambda(\mu,c)$. One gets

$$\mu - 2\lambda\rho_0 - \frac{2\lambda}{V}\sum_{p\in\Lambda^*,p\neq 0}\langle\hat{n}_p\rangle_{\hat{H}_\Lambda(\mu,c)} - \frac{1}{V}\left(\lambda + \frac{g}{2}\right) \leqslant \epsilon_p + \frac{2}{V}(\lambda+g)\langle\hat{n}_p\rangle_{\hat{H}_\Lambda(\mu,c)} \tag{18}$$

for all $p\in\Lambda^*\setminus\{0\}$. As in the case of Hamiltonian (1) (see Lemma 2) we get

$$\lim_{V\to\infty} \frac{1}{V}\langle \hat{n}_p\rangle_{\hat{H}_\Lambda(\mu,c)} = 0$$

for all $p \in \Lambda^* \setminus \{0\}$. Hence the right-hand side of (18) can be made arbitrarily small for V sufficiently large. Thus we conclude that for $V\to\infty$ and for any $g>0$ Eq. (16) does not have a positive solution $\rho_0 > 0$.

III. PROOF OF THEOREM

The following fact[10] will be needed below.

Lemma 3: $p_\Lambda \geqslant p_\Lambda(c)$ *for all* $c \in \mathbb{C}$.

For later purpose, we remind a convenient definition of the Bogoliubov approximation, which was proposed by Ginibre. The boson Fock space F_Λ is isomorphic to the tensor product $F_{0\Lambda} \otimes F'_\Lambda$, where $F_{0\Lambda}$ and F'_Λ are the symmetric tensor algebras constructed on the one-dimensional subspace of the constant functions $\psi_0 = V^{-1/2}$, and on its orthogonal complement, respectively. For any complex $c \in \mathbb{C}$, we consider in $F_{0\Lambda}$ the coherent vector

$$|c\rangle = \exp\left(-V\frac{|c|^2}{2}\right)\sum_{n=0}^{\infty}\frac{1}{n!}(V^{1/2}c)^n(\hat{a}_0^\dagger)^n|0\rangle,$$

where $|0\rangle$ is the vacuum vector of F_Λ. Then $\hat{a}_0|c\rangle = c|c\rangle$. To every operator $\hat{A}$ on F_Λ and any complex number c, we can associate the operator $\hat{A}(c)$ on F'_Λ defined by its quadratic form

$$\langle \varphi'_1|\hat{A}(c)|\varphi'_2\rangle = \langle \varphi'_1 \otimes c|\hat{A}|\varphi'_2 \otimes c\rangle,$$

where the vectors $|\varphi'_1\rangle$, $|\varphi'_2\rangle$ lie in F'_Λ. The transformation from the operator $\hat{A}$ to operator $\hat{A}(c)$ is called by Bogoliubov approximation of $\hat{A}$. This transformation consists in replacing $\hat{a}_0$ and $\hat{a}_0^\dagger$ by $c\sqrt{V}$ and $\bar{c}\sqrt{V}$ in $\hat{A}$, after $\hat{A}$ has been expanded as a normal Vick form. Taking into account these definitions, we have

$$\begin{aligned}
\mathrm{tr}_{F'_\Lambda} \exp[-\beta\hat{H}_\Lambda(\mu,c)] &= \sup_{\{|\varphi'_n\rangle\}} \sum_n \exp[-\beta\langle \varphi'_n|\hat{H}_\Lambda(\mu,c)|\varphi'_n\rangle] \\
&= \sup_{\{|\varphi'_n\rangle\}} \sum_n \exp[-\beta\langle \varphi'_n \otimes c|\hat{H}_\Lambda(\mu)|\varphi'_n \otimes c\rangle] \\
&\leqslant \sup_{\{|\varphi'_n\rangle\}} \sum_n \langle \varphi'_n \otimes c|\exp[-\beta\hat{H}_\Lambda(\mu)]|\varphi'_n \otimes c\rangle \leqslant \mathrm{tr}_{F_\Lambda} \exp[-\beta\hat{H}_\Lambda(\mu)].
\end{aligned}$$

The sup in these relations is taken over all possible orthonormal bases of F'_Λ contained in the form domain of $\hat{H}_\Lambda(\mu,c)$. The former inequality is the Peierls's inequality. The latter is the immediate consequence of the definition of Bogoliubov's approximation, since, as the coherent vector $|c\rangle$ can be taken as the first vector of an orthonormal basis in $F_{0\Lambda}$. This ends the proof of Lemma 3.

We prove the Theorem.

(1) By the Bogoliubov inequality[13] and Lemma 3 one gets

$$0 \leqslant p_\Lambda - p_\Lambda(c) \leqslant \frac{1}{V}\langle \hat{H}_\Lambda(\mu,c) - \hat{H}_\Lambda(\mu)\rangle_{\hat{H}_\Lambda(\mu)}. \tag{19}$$

In order to write the average in the right-hand side of (19), it will be helpful to express the Hamiltonian $\hat{H}_\Lambda(\mu,c)$ by a Taylor expansion around $\hat{a}_0^\#$. Then

$$\hat{H}_\Lambda(\mu,c)-\hat{H}_\Lambda(\mu)=-\hat{A}^\dagger[\hat{a}_0,\hat{H}_\Lambda(\mu)]+\text{H.c.}+\frac{1}{2}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,\hat{H}_\Lambda(\mu)]]+\text{H.c.}+\hat{A}^\dagger[\hat{a}_0,[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger]]\hat{A}$$
$$-\frac{1}{2}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger]]]\hat{A}+\text{H.c.}+\frac{1}{4}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,[[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger],\hat{a}_0^\dagger]]]\hat{A}\hat{A}, \tag{20}$$

where $\hat{A}\equiv\hat{a}_0-c\sqrt{V}$, $\hat{A}^\dagger\equiv\hat{a}^\dagger-\bar{c}\sqrt{V}$. The third- and fourth-order terms in (20) are bounded by

$$-\frac{1}{2}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger]]]\hat{A}+\text{H.c.}+\frac{1}{4}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,[[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger],\hat{a}_0^\dagger]]]\hat{A}\hat{A}$$
$$=-\frac{3}{2V}(2\lambda+g)\left(\hat{A}^2+\frac{2}{3}c\sqrt{V}\hat{A}\right)^\dagger\left(\hat{A}^2+\frac{2}{3}c\sqrt{V}\hat{A}\right)+\frac{2}{3}(2\lambda+g)|c|^2\hat{A}^\dagger\hat{A}\leqslant\frac{2}{3}(2\lambda+g)|c|^2\hat{A}^\dagger\hat{A}. \tag{21}$$

The terms of first and second order can be combined to give

$$-\hat{A}^\dagger[\hat{a}_0,\hat{H}_\Lambda(\mu)]+\text{H.c.}+\frac{1}{2}\hat{A}^\dagger\hat{A}^\dagger[\hat{a}_0,[\hat{a}_0,\hat{H}_\Lambda(\mu)]]+\text{H.c.}+\hat{A}^\dagger[\hat{a}_0,[\hat{H}_\Lambda(\mu),\hat{a}_0^\dagger]]\hat{A}$$
$$=-\frac{1}{2}[\hat{A}^\dagger\hat{A},[\hat{H}_\Lambda(\mu),\hat{A}^\dagger\hat{A}]]+2\hat{A}^\dagger[\hat{A},[\hat{H}_\Lambda(\mu),\hat{A}^\dagger]]\hat{A}-\frac{3}{2}\hat{A}^\dagger[\hat{A},\hat{H}_\Lambda(\mu)]-\frac{3}{2}[\hat{H}_\Lambda(\mu),\hat{A}^\dagger]\hat{A}. \tag{22}$$

Because of (17), the Gibbs average of the first term in the right-hand side of (22) is negative and can be dropped, since we are looking for an upper bound in (19). Since

$$[\hat{A},[\hat{H}_\Lambda(\mu),\hat{H}^\dagger]]=-\mu+\frac{1}{V}(2\lambda+g)+\frac{1}{V}(2\lambda+g)2\hat{a}_0^\dagger\hat{a}_0+\frac{2\lambda}{V}\hat{N}'_\Lambda\leqslant-\mu+\frac{1}{V}(2\lambda+g)+\frac{2}{V}(2\lambda+g)\hat{N}_\Lambda,$$

we have

$$2\hat{A}^\dagger[\hat{A},[\hat{H}_\Lambda(\mu),\hat{A}^\dagger]]\hat{A}\leqslant2\left(\frac{2\lambda+g}{V}-\mu\right)\hat{A}^\dagger\hat{A}+4\frac{2\lambda+g}{V}\hat{A}\hat{N}_\Lambda\hat{A}. \tag{23}$$

We consider the last two terms in the right-hand side of (22). Their averages with respect to $\hat{H}_\Lambda(\mu)$ do not depend on c, and are real and equal. Furthermore,

$$-2\langle\hat{A}^\dagger[\hat{A},\hat{H}_\Lambda(\mu)]\rangle_{\hat{H}_\Lambda(\mu)}=\langle[\hat{A}^\dagger,[\hat{H}_\Lambda(\mu),\hat{A}]]\rangle_{\hat{H}_\Lambda(\mu)}+\langle[\hat{A}^\dagger,[\hat{H}_\Lambda(\mu),\hat{A}]]_+\rangle_{\hat{H}_\Lambda(\mu)}, \tag{24}$$

where $[\ldots,\ldots]_+$ is the anticommutator. The first term in (24) is bounded by

$$\langle[\hat{A}^\dagger,[\hat{H}_\Lambda(\mu),\hat{A}]]\rangle_{\hat{H}_\Lambda(\mu)}\leqslant-\mu+\frac{1}{V}(2\lambda+g)+2\frac{2\lambda+g}{V}\rho, \tag{25}$$

where $\rho\equiv\langle\hat{N}_\Lambda\rangle_{\hat{H}_\Lambda(\mu)}$. Using a spectral decomposition of $\hat{H}_\Lambda(\mu)$ one can estimate the second term in (24) as[10]

$$\langle[\hat{A}^\dagger,[\hat{H}_\Lambda(\mu),\hat{A}]]_+\rangle_{\hat{H}_\Lambda(\mu)}\leqslant\langle[\hat{A},[\hat{H}_\Lambda(\mu),\hat{A}^\dagger]]\rangle_{\hat{H}_\Lambda(\mu)}+2\beta^{-1}\langle[\hat{A},\hat{A}^\dagger]_+\rangle_{\hat{H}_\Lambda(\mu)}. \tag{26}$$

Therefore, it follows from (24)–(26) that

$$-\frac{3}{2}\langle\hat{A}^\dagger[\hat{A},\hat{H}_\Lambda(\mu)]\rangle_{\hat{H}_\Lambda(\mu)}-\frac{3}{2}\langle[\hat{H}_\Lambda(\mu),\hat{A}^\dagger]\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}\leqslant-3\mu+\frac{3}{V}(2\lambda+g)+\frac{6}{V}(2\lambda+g)\rho$$
$$+3\beta^{-1}\langle[\hat{A},\hat{A}^\dagger]_+\rangle_{\hat{H}_\Lambda(\mu)}. \tag{27}$$

Collecting (21), (23), and (27) we obtain finally the following upper bound for the average in the right-hand side of the Bogoliubov inequality (19):

$$\langle\hat{H}_\Lambda(\mu,c)-\hat{H}_\Lambda(\mu)\rangle_{\hat{H}_\Lambda(\mu)}\leqslant\frac{2}{3}(2\lambda+g)|c|^2\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}+2\left(-\mu+\frac{1}{V}(2\lambda+g)\right)\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}+\frac{4}{V}(2\lambda+g)$$
$$\times\langle\hat{A}^\dagger\hat{N}_\Lambda\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}+3\beta^{-1}\langle[\hat{A},\hat{A}^\dagger]_+\rangle_{\hat{H}_\Lambda(\mu)}-3\mu+\frac{3}{V}(2\lambda+g)+\frac{6}{V}(2\lambda+g)\rho. \tag{28}$$

(2) The next step in the proof of Theorem is to obtain an upper bound for $\langle\hat{N}_\Lambda\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}$. We write this average as

$$\langle\hat{N}_\Lambda\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}=Q_\Lambda+\overline{\rho}\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)},$$

where

$$Q_\Lambda\equiv\left\langle\left(\frac{\hat{N}_\Lambda}{V}-\overline{\rho}\right)\hat{A}^\dagger\hat{A}\right\rangle_{\hat{H}_\Lambda(\mu)}$$

denotes the grand-canonical average and the positive number $\overline{\rho}$ will be defined below. The average Q_Λ can be written as

$$Q_\Lambda=\Xi_\Lambda^{-1}\sum_{N=0}^{\infty}\left(\frac{N}{V}-\overline{\rho}\right)\exp(-\beta VF_N)\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda}, \tag{29}$$

where $F_N\equiv f_N-\mu N/V$, f_N represents the free-energy density and Ξ_Λ is the grand-canonical partition function associated with the Hamiltonian $\hat{H}_\Lambda$.

Let us partition the set $\{N\}$ and write the average (29) as

$$Q_\Lambda\equiv Q_\Lambda^{(1)}+Q_\Lambda^{(2)}+Q_\Lambda^{(3)}.$$

Now, we have to estimate from above the every term in this decomposition.

$$Q_\Lambda^{(1)}\equiv\Xi_\Lambda^{-1}\sum_{0\leqslant N<V\overline{\rho}}\left(\frac{N}{V}-\overline{\rho}\right)\exp(-\beta VF_N)\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda}\leqslant 0,$$

$$Q_\Lambda^{(2)}\equiv\Xi_\Lambda^{-1}\sum_{V\overline{\rho}\leqslant N\leqslant V(\overline{\rho}+\xi)}\left(\frac{N}{V}-\overline{\rho}\right)\exp(-\beta VF_N)\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda}\leqslant\xi\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}_\Lambda(\mu)}.$$

Here $\xi>0$. Finally, we estimate the last term $Q_\Lambda^{(3)}$. The free energy is the convex function of ρ, so we have

$$F_N\left(\frac{N}{V}\right)\geqslant a_1+a_2\left(\frac{N}{V}-\overline{\rho}-\xi\right), \tag{30}$$

where $a_1=F_N(\overline{\rho}+\xi)$, $a_2=F_N'(\overline{\rho}+\xi)>0$ and $\overline{\rho}$ is defined by the condition

$$\inf_{N/V} F_N\left(\frac{N}{V}\right) = F_N(\overline{\rho}) \equiv \overline{F}_N.$$

Using (30), we obtain

$$\begin{aligned}
Q_\Lambda^{(3)} &\equiv \Xi_\Lambda^{-1} \sum_{N>V(\overline{\rho}+\xi)} \left(\frac{N}{V}-\overline{\rho}\right)\exp(-\beta V F_N)\langle \hat{A}^\dagger \hat{A}\rangle_{\hat{H}_\Lambda} \\
&\leqslant \Xi_\Lambda^{-1} \sum_{N>V(\overline{\rho}+\xi)} \left(\frac{N}{V}-\overline{\rho}\right)\exp\left\{-\beta V\left[a_1 + a_2\left(\frac{N}{V}-\overline{\rho}-\xi\right)\right]\right\}\langle \hat{A}^\dagger \hat{A}\rangle_{\hat{H}_\Lambda} \\
&\leqslant \Xi_\Lambda^{-1} \sum_{N>V(\overline{\rho}+\xi)} \left(\frac{N}{V}-\overline{\rho}\right)\exp\left\{-\beta V\left[a_1 + a_2\left(\frac{N}{V}-\overline{\rho}-\xi\right)\right]\right\}(N+|c|^2 V) \\
&= \Xi_\Lambda^{-1}\frac{1}{V}\exp(-\beta V a_1) \sum_{N>V(\overline{\rho}+\xi)} (N-V\overline{\rho})^2 \exp\{-\beta a_2[N-V(\overline{\rho}+\xi)]\} + \Xi_\Lambda^{-1}(\overline{\rho}+|c|^2) \\
&\quad \times \exp(-\beta V a_1) \sum_{N>V(\overline{\rho}+\xi)} (N-V\overline{\rho})^2 \exp\{-\beta a_2[N-V(\overline{\rho}+\xi)]\} \\
&= \Xi_\Lambda^{-1}\exp(-\beta V a_1)\left[\frac{1}{V}\frac{e^{-\beta a_2}(1+e^{-\beta a_2})}{(1-e^{-\beta a_2})^2} + 2\xi\frac{e^{-\beta a_2}}{(1-e^{-\beta a_2})^2} + \xi^2 V\frac{1}{1-e^{-\beta a_2}}\right. \\
&\quad \left. + (\overline{\rho}+|c|^2)\left(\frac{e^{-\beta a_2}}{(1-e^{-\beta a_2})^2} + \ + \xi V\frac{1}{1-e^{-\beta a_2}}\right)\right].
\end{aligned} \tag{31}$$

Let us find the lower bound for Ξ_Λ. The convexity implies that for any $\sigma>0$ and any sufficiently small ξ', $|N/V-\overline{\rho}|<\xi'<\xi$, one has $\overline{F}_N \leqslant F_N \leqslant \overline{F}_N + \sigma/2$. Then

$$\Xi_\Lambda \geqslant \sum_{|N/V-\overline{\rho}|<\xi'} \exp(-\beta V F_N) \geqslant 2\xi' V \exp\left[-\beta V\left(\overline{F}_N + \frac{\sigma}{2}\right)\right]. \tag{32}$$

Putting together the bounds (31) and (32), we obtain

$$Q_\Lambda^{(3)} \leqslant a_3 \exp\left[-\beta V\left(a_1 - \overline{F}_N - \frac{\sigma}{2}\right)\right] \leqslant a_3 \exp\left(-\beta V\frac{\sigma}{2}\right),$$

with some positive constant a_3.

Collecting the estimates above, we obtain that there exist some positive constants u and v, independent on V, such that

$$\frac{1}{V}\langle \hat{A}^\dagger \hat{N}_\Lambda \hat{A}\rangle_{\hat{H}_\Lambda(\mu)} \leqslant u + v\langle \hat{A}^\dagger \hat{A}\rangle_{\hat{H}_\Lambda(\mu)}. \tag{33}$$

Therefore, it follows from (33) that there exist two positive constants σ_1 and σ_2, independent on V, such that

$$\langle \hat{H}_\Lambda(\mu,c) - \hat{H}_\Lambda(\mu)\rangle_{\hat{H}_\Lambda(\mu)} \leqslant \sigma_1 + \frac{\sigma_2}{2}\langle \hat{A}^\dagger \hat{A}\rangle_{\hat{H}_\Lambda(\mu)}. \tag{34}$$

(3) It remains to prove that

$$\lim_{V\to\infty} \inf_c \left[\frac{1}{V}\langle \hat{H}_\Lambda(\mu,c) - \hat{H}_\Lambda(\mu)\rangle_{\hat{H}_\Lambda(\mu)}\right] = 0. \tag{35}$$

The proof is a standard application of the Bogoliubov method.[21] Since in the approximating Hamiltonian the gauge symmetry is broken, we introduce

$$\hat{H}_\Lambda^{(\nu)}(\mu) \equiv \hat{H}_\Lambda(\mu) - \sqrt{V}(\overline{\nu}\hat{a}_0 + \nu\hat{a}_0^\dagger),$$

$$\hat{H}_\Lambda^{(\nu)}(\mu, c) \equiv \hat{H}_\Lambda(\mu, c) - V(\overline{\nu c} + \nu\overline{c})$$

with sources $\nu \in \mathbb{C}$ breaking the symmetry of $\hat{H}_\Lambda(\mu)$. The best bound in (34) is obtained for $c^* = \langle \hat{a}_0/\sqrt{V}\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)}$, $|c^*| \leqslant M < \infty$. By the Harris inequality[22] one gets

$$\frac{1}{2}\langle [\delta\hat{a}_0^\dagger, \delta\hat{a}_0]_+\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)} \leqslant (\delta\hat{a}_0^\dagger, \delta\hat{a}_0)_{\hat{H}_\Lambda^{(\nu)}(\mu)} + \frac{\beta}{12}\langle [\delta\hat{a}_0, [\hat{H}_\Lambda^{(\nu)}(\mu), \delta\hat{a}_0^\dagger]]\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)}, \tag{36}$$

where $\delta\hat{a}_0^\# = \hat{a}_0^\# - \langle \hat{a}_0^\#\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)}$. The second term in the right-hand side of (36) is bounded by

$$\langle [\delta\hat{a}_0, [\hat{H}_\Lambda^{(\nu)}(\mu), \delta\hat{a}_0^\dagger]]\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)} \leqslant -\mu + 4\left(\lambda + \frac{g}{2}\right)\rho_\Lambda^{(\nu)}, \tag{37}$$

where $\rho_\Lambda^{(\nu)} \equiv \langle \hat{N}_\Lambda\rangle_{\hat{H}_\Lambda^{(\nu)}}/V < \infty$. To get an upper estimate for the first term in the right-hand side of (36), use the formula

$$(\delta\hat{a}_0^\dagger, \delta\hat{a}_0)_{\hat{H}_\Lambda^{(\nu)}(\mu)} = \beta^{-1}\frac{\partial^2 p_\Lambda^{(\nu)}}{\partial\overline{\nu}\partial\nu},$$

with $p_\Lambda^{(\nu)} \equiv (\beta V)^{-1}\ln \mathrm{tr}_{F_\Lambda} \exp[-\beta\hat{H}_\Lambda^{(\nu)}(\mu)]$. Without restriction we may assume that $\overline{\nu} = \nu = r \geqslant 0$. Then

$$(\delta\hat{a}_0^\dagger, \delta\hat{a}_0)_{\hat{H}_\Lambda^{(\nu)}(\mu)} = \frac{1}{4\beta r}\frac{d}{dr}\left(r\frac{dp_\Lambda^{(\nu)}}{dr}\right). \tag{38}$$

Denoting

$$\Delta(r) \equiv p_\Lambda^{(\nu)} - \sup_c p_\Lambda^{(\nu)}(c),$$

and using relations (19), (34), (36), and (37), we get

$$\Delta(r) \leqslant V^{-1}[\sigma_3 + \sigma_2(\delta\hat{a}_0^\dagger, \delta\hat{a}_0)_{\hat{H}_\Lambda^{(\nu)}(\mu)}], \tag{39}$$

where $\sigma_3 = \sigma_1 + \sigma_2\beta[4(\lambda + g/2)\rho_\Lambda^{(\nu)} - \mu]/12$. Multiply both sides of (39) by r, integrate over r from R to $R+\varepsilon$, and use the formula (38). Then

$$\int_R^{R+\varepsilon} r\Delta(r)dr \leqslant V^{-1}\left[\sigma_3\frac{(R+\varepsilon)^2 - R^2}{2} + \frac{\sigma_2}{4\beta}\left(r\frac{dp_\Lambda^{(\nu)}}{dr}\right)\Bigg|_R^{R+\varepsilon}\right].$$

Note now, that

$$\frac{dp_\Lambda^{(\nu)}}{dr} = \frac{2}{V}\langle \hat{a}_0\rangle_{\hat{H}_\Lambda^{(\nu)}(\mu)} \leqslant 2\sqrt{\rho_\Lambda^{(\nu)}}. \tag{40}$$

Therefore,

$$\int_R^{R+\varepsilon} r\Delta(r)dr \leqslant V^{-1}\left[\sigma_3\frac{(R+\varepsilon)^2 - R^2}{2} + \frac{\sigma_2}{2\beta}\sqrt{\rho_\Lambda^{(\nu)}}(2R+\varepsilon)\right]. \tag{41}$$

Take into account, that

$$\left|\frac{d\Delta(r)}{dr}\right| \leqslant 2(\sqrt{\rho_\Lambda^{(\nu)}}+M). \tag{42}$$

This estimate follows from the definition of $\Delta(r)$ and (40). The last inequality gives

$$\Delta(R) \leqslant \Delta(r) + 2(r-R)(\sqrt{\rho_\Lambda^{(\nu)}}+M), \tag{43}$$

where $r \in [R, R+\varepsilon]$. Multiplying (38) by r and integrating, we have

$$\Delta(R)\frac{(R+\varepsilon)^2-R^2}{2} \leqslant \int_R^{R+\varepsilon} r\Delta(r)dr + 2(\sqrt{\rho_\Lambda^{(\nu)}}+M)\left(\frac{r^3}{3}-R\frac{r^2}{2}\right)\Bigg|_R^{R+\varepsilon}.$$

Using (41), we get

$$\Delta(R) \leqslant \frac{1}{V}\left[\sigma_3 + \frac{\sigma_2}{\beta\varepsilon}\sqrt{\rho_\Lambda^{(\nu)}} + (\sqrt{\rho_\Lambda^{(\nu)}}+M)\varepsilon\frac{R+\frac{2\varepsilon}{3}}{R+\frac{\varepsilon}{2}}\right]. \tag{44}$$

Minimizing the right-hand side of (44) one obtains that for $V\to\infty$ the best choice of ε is $\varepsilon \sim 1/\sqrt{V}$, which gives $\Delta(R) \leqslant \eta V^{-1/2}$, where η is independent of V and can be taken independent of R in any bounded interval. For $\nu=0$ this implies (35). This finishes the proof of the Theorem.

IV. CONCLUSION

For $\lambda=0$ the Bogoliubov method implies the absence of Bose condensation also. In this case an appropriate self-consistency equation has the trivial solution only. On the other hand, for $g=0$ and $\lambda>0$ (mean field model) a self-consistency equation in the thermodynamic limit takes the degenerate form $(\mu-2\lambda\rho)c=0$ as for free bosons. Condensation can occur only at $\mu=2\lambda\rho$, and the density ρ_0 of the condensate is not determined by the equation.

The results of Michoel and Verbeure[3] on the nonextensive Bose condensation can be extended to our case. Let us take into account the correlation inequality[23,24]

$$\beta\langle\hat{A}[\hat{H},\hat{A}]\rangle_{\hat{H}} \geqslant \langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}} \ln\frac{\langle\hat{A}^\dagger\hat{A}\rangle_{\hat{H}}}{\langle\hat{A}\hat{A}^\dagger\rangle_{\hat{H}}} \tag{45}$$

for all local observables $\hat{A}$ belonging to the domain of $[\hat{H},\ldots]$. Taking $\hat{A}=\hat{a}_k$, $\hat{H}=\hat{H}_\Lambda(\mu)$ in (45), one gets

$$\langle\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)} \ln(1+\langle\hat{n}_k\rangle^{-1}_{\hat{H}_\Lambda(\mu)}) \geqslant \beta\Bigg[(\varepsilon_k-\mu)\langle\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)} + \frac{g}{V}\langle\hat{n}_k^2\rangle_{\hat{H}_\Lambda(\mu)} + \frac{2\lambda}{V}\langle\hat{n}_k\hat{N}_\Lambda\rangle_{\hat{H}_\Lambda(\mu)} - \frac{1}{V}\left(\lambda+\frac{g}{2}\right) \times\langle\hat{n}_k\hat{N}_\Lambda\rangle_{\hat{H}_\Lambda(\mu)}\Bigg]. \tag{46}$$

Referring to (17) with $\hat{H}=\hat{H}_\Lambda(\mu)$, $\hat{A}=\hat{n}_k^{1/2}\hat{a}_p$, $p\neq k$, we have

$$\left\langle\left(\mu-\frac{2\lambda}{V}\hat{N}_\Lambda\right)\hat{n}_k\right\rangle_{\hat{H}_\Lambda(\mu)} \leqslant \epsilon_p\langle\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)} + \frac{1}{V}\left(\lambda+\frac{g}{2}\right)\langle\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)} + \frac{2}{V}(\lambda+g)\langle\hat{n}_p\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)}, \quad p\neq k. \tag{47}$$

Inserting (47) into (46) and using the bound $\langle\hat{n}_k^2\rangle_{\hat{H}_\Lambda(\mu)} \geqslant 0$, we get for $p\neq k$

$$\langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \ln(1 + \langle \hat{n}_k \rangle^{-1}_{\hat{H}_\Lambda(\mu)}) \geqslant \beta \left[\left(\epsilon_k - \epsilon_p - \frac{2\lambda + g}{V} \right) \langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} - \frac{2(\lambda + g)}{V} \langle \hat{n}_p \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \right].$$

Take $\delta > 0$ arbitrary, $|k| \geqslant \delta$ and $|p| \leqslant \delta/2$. Then for every V,

$$\langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \ln(1 + \langle \hat{n}_k \rangle^{-1}_{\hat{H}_\Lambda(\mu)}) \geqslant c_k \langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} - \frac{2\beta}{V}(\lambda + g) \langle \hat{n}_p \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)},$$

where

$$c_k \equiv \beta \left(\epsilon_k - \frac{\delta^2}{8m} - \frac{2\lambda + g}{V} \right).$$

Solving the last inequality with respect to $\langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)}$, one has

$$\langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \leqslant (e^{c_k} - 1)^{-1} + \frac{2\beta}{V}(\lambda + g) \langle \hat{n}_p \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} (1 - e^{-c_\delta})^{-1}, \tag{48}$$

where $c_\delta \equiv c_k|_{|k|=\delta}$. (46) gives

$$\beta \left[\left(-\epsilon_p + \mu + \frac{1}{V} \left(\lambda + \frac{g}{2} \right) \right) \langle \hat{n}_p \rangle_{\hat{H}_\Lambda(\mu)} - \frac{2\lambda}{V} \langle \hat{n}_p \hat{N}_\Lambda \rangle_{\hat{H}_\Lambda(\mu)} \right] \geqslant -1. \tag{49}$$

Taking $\hat{H} = \hat{H}_\Lambda(\mu)$, $\hat{A} = \hat{a}^\dagger_p$ in the inequality (17), we have

$$\mu \leqslant \epsilon_p + 2\lambda\rho + \frac{2}{V}(\lambda + g) \langle \hat{n}_p \rangle_{\hat{H}_\Lambda(\mu)} + \frac{1}{V} \left(\lambda + \frac{g}{2} \right).$$

Putting this into (49) gives

$$\frac{2\lambda}{V^2} \langle \hat{n}_p \hat{N}_\Lambda \rangle_{\hat{H}_\Lambda(\mu)} \leqslant \frac{1}{\beta V} + \left[2\lambda\rho + \frac{1}{V}(2\lambda + g) \right] \frac{\langle \hat{n}_p \rangle_{\hat{H}_\Lambda(\mu)}}{V} + \frac{2(\lambda + g)}{V^2} \langle \hat{n}_p \rangle^2_{\hat{H}_\Lambda(\mu)}.$$

Using Theorem and formula (2), we get

$$\frac{1}{V^2} \langle \hat{n}_p \hat{N}_\Lambda \rangle_{\hat{H}_\Lambda(\mu)} < \varepsilon \tag{50}$$

for every $\varepsilon > 0$, V large enough and $p \in \Lambda^*$. Since

$$\frac{1}{V} \sum_{k \in \Lambda^*, |k| < \delta} \langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} = \rho - \frac{1}{V} \sum_{k \in \Lambda^*, |k| \geqslant \delta} \langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)},$$

the inequality (48) implies that for $|p| \leqslant \delta/2$

$$\frac{1}{V} \sum_{k \in \Lambda^*, |k| < \delta} \langle \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \geqslant \rho - \frac{1}{V} \sum_{k \in \Lambda^*, |k| \geqslant \delta} (e^{c_k} - 1)^{-1} - \frac{2\beta(\lambda + g)}{V} \sum_{k \in \Lambda^*, |k| \geqslant \delta} \langle \hat{n}_p \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} (1 - e^{-c_\delta})^{-1}. \tag{51}$$

Take $\varepsilon > 0$ arbitrary and V large enough such that (50) is satisfied. Then

$$\frac{1}{V^2} \sum_{k \in \Lambda^*, |k| \geqslant \delta} \langle \hat{n}_p \hat{n}_k \rangle_{\hat{H}_\Lambda(\mu)} \leqslant \frac{1}{V^2} \langle \hat{n}_p \hat{N}_\Lambda \rangle_{\hat{H}_\Lambda(\mu)} < \varepsilon.$$

Finally, we have from (51) that

$$\lim_{\delta\to 0}\lim_{V\to\infty}\frac{1}{V}\sum_{k\in\Lambda^*,|k|<\delta}\langle\hat{n}_k\rangle_{\hat{H}_\Lambda(\mu)}\geqslant\rho-\int_{\mathbb{R}^d}\frac{dk}{(2\pi)^d}\frac{1}{e^{\beta\epsilon_k}-1}.$$

Hence for every $\rho>0$ there exists $\beta_c>0$, defined by

$$\rho=\int_{\mathbb{R}^d}\frac{dk}{(2\pi)^d}\frac{1}{e^{\beta_c\epsilon_k}-1},$$

such that for all $\beta>\beta_c$ the generalized condensation, also called frgmentation, takes place.

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Solution of the dual reflection equation for $A_{n-1}^{(1)}$ solid-on-solid model

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We obtain a diagonal solution of the *dual reflection* equation for the elliptic $A_{n-1}^{(1)}$ solid-on-solid model. The isomorphism between the solutions of the reflection equation and its dual is studied. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Two-dimensional lattice spin models in statistical mechanics have traditionally been solved by imposing periodic boundary condition. The Yang–Baxter equation[1,2]

$$R_{12}(u_1-u_2)R_{13}(u_1-u_3)R_{23}(u_2-u_3)=R_{23}(u_2-u_3)R_{13}(u_1-u_3)R_{12}(u_1-u_2), \tag{1.1}$$

together with such boundary condition then leads to families of commuting row *transfer matrices* and hence solvability.[2] The work of Sklyanin[3] shows that, by using the reflection equation (RE) introduced by Cherednik[4]

$$R_{12}(u_1-u_2)K_1(u_1)R_{21}(u_1+u_2)K_2(u_2)=K_2(u_2)R_{12}(u_1+u_2)K_1(u_1)R_{21}(u_1-u_2), \tag{1.2}$$

it is also possible to construct families of commuting *double-row transfer matrices* for vertex models with open boundary conditions. Then such a scheme has been generalized to *face-type* solid-on-solid (SOS) models.[5,6]

In order to construct the *double-row transfer matrices*, besides the RE, one needs the dual reflection equation whose explicit form is related with the crossing-unitarity relation of the R-matrix.[3,7,5,6] For the $\mathbb{Z}_n$ Belavin model,[8] the dual RE reads[6]

$$R_{12}(u_2-u_1)\tilde{K}_1(u_1)R_{21}(-u_1-u_2-nw)\tilde{K}_2(u_2)=\tilde{K}_2(u_2)R_{12}(-u_1-u_2-nw)\tilde{K}_1(u_1)R_{21}(u_2-u_1), \tag{1.3}$$

where w is the crossing parameter of the R-matrix. Moreover, there exists a *simple-form* isomorphism between the solution of the RE (1.2) and that of its dual (1.3)

$$\tilde{K}(u)=K\left(-u-\frac{nw}{2}\right). \tag{1.4}$$

However, for integrable SOS models, due to the complicated crossing-unitarity relation of R-matrix (Boltzmann weight) (2.18),[9,10] the dual RE (3.2) contains the face-type parameters $\{\lambda_j\}$ in addition to the spectral parameter. A generalized isomorphism between the solutions to the RE and its dual for SOS models, if exists, is yet to be found. In this sense, the dual RE for the

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face-type models has got its own *independent* role in contrast with the vertex model.

The RE of SOS models has been solved to give the diagonal K-matrices for the $A_n^{(1)}$, $B_n^{(1)}$, $C_n^{(1)}$, $D_n^{(1)}$, $A_{2n}^{(2)}$, and $A_{2n+1}^{(2)}$ SOS models.[11] But the generic (nondiagonal) K-matrix is known only for the $A_1^{(1)}$ SOS model.[12,5] However, the dual RE of the face type was solved only for the $A_1^{(1)}$ SOS model.[5] In this article, we consider the dual RE for the $A_{n-1}^{(1)}$ SOS model. After briefly reviewing the face-vertex correspondence between the $\mathbb{Z}_n$ Belavin model and the $A_{n-1}^{(1)}$ SOS model,[14] we construct the isomorphism between the solution of the RE and its dual for the $A_{n-1}^{(1)}$ SOS model in Sec. III. In Sec. IV, we derive a diagonal solution to the dual RE by solving directly. Then we prove that our diagonal solution to the dual RE can be obtained through the isomorphism transformation (3.16) from the diagonal solution[11] of RE by a special choice of the free parameter λ'. The final section is for conclusions.

II. REFLECTION EQUATION AND ITS DUAL FOR $A_{n-1}^{(1)}$ SOS MODEL

A. $\mathbb{Z}_n$ Belavin R-matrix

Let us fix τ such that $\mathrm{Im}(\tau)>0$ and a generic complex number w. Introduce the following elliptic functions:

$$\theta\begin{bmatrix} a \\ b \end{bmatrix}(u,\tau) = \sum_{m=-\infty}^{\infty} \exp\{\sqrt{-1}\pi[(m+a)^2\tau + 2(m+a)(u+b)]\}, \tag{2.1}$$

$$\theta^{(j)}(u) = \theta\begin{bmatrix} \frac{1}{2} - \frac{j}{n} \\ \frac{1}{2} \end{bmatrix}(u, n\tau), \quad \sigma(u) = \theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u,\tau). \tag{2.2}$$

Among them the σ-function satisfies the following identity:

$$\begin{aligned} &\sigma(u+x)\sigma(u-x)\sigma(v+y)\sigma(v-y) - \sigma(u+y)\sigma(u-y)\sigma(v+x)\sigma(v-x) \\ &\quad = \sigma(u+v)\sigma(u-v)\sigma(x+y)\sigma(x-y), \end{aligned} \tag{2.3}$$

which will be useful in the following. [Our σ-function is the ϑ-function $\vartheta_1(u)$.[13] It has the following relation with the *Weierstrassian* σ-function if denoted by $\sigma_w(u)$: $\sigma_w(u) \propto e^{\eta_1 u^2}\sigma(u)$, $\eta_1 = \pi^2\left(\frac{1}{6} - 4\Sigma_{n=1}^{\infty} nq^{2n}/(1-q^{2n})\right)$ and $q = e^{\sqrt{-1}\tau}$.]

Let $R^B(u) \in \mathrm{End}(\mathbb{C}^n \otimes \mathbb{C}^n)$ be the $\mathbb{Z}_n$ Belavin R-matrix[8] given by

$$R^B(u) = \sum_{i,j,k,l} R_{ij}^{kl}(u) E_{ik} \otimes E_{lj}, \tag{2.4}$$

in which E_{ij} is the matrix with elements $(E_{ij})_k^l = \delta_{jk}\delta_{il}$. The coefficient functions are[9]

$$R_{ij}^{kl}(u) = \begin{cases} \dfrac{h(u)\sigma(w)\theta^{(i-j)}(u+w)}{\sigma(u+w)\theta^{(i-k)}(w)\theta^{(k-j)}(u)} & \text{if } i+j = k+l \bmod n, \\ 0 & \text{otherwise.} \end{cases} \tag{2.5}$$

Here we have set

$$h(u)=\frac{\prod_{j=0}^{n-1}\theta^{(j)}(u)}{\prod_{j=1}^{n-1}\theta^{(j)}(0)}. \tag{2.6}$$

The R-matrix satisfies the quantum Yang–Baxter Eq. (1.1) and the following unitarity and crossing-unitarity relations:[15]

$$\text{Unitarity: } R^B{}_{12}(u)R^B_{21}(-u)=id, \tag{2.7}$$

$$\text{Crossing-unitarity: } (R^B)^{t_2}_{21}(-u-nw)(R^B)^{t_2}_{12}(u)=\frac{e^{\sqrt{-1}nw}\sigma(u)\sigma(u+nw)}{\sigma(u+w)\sigma(u+nw-w)}id, \tag{2.8}$$

where t_i denotes the transposition in the ith space.

B. $A^{(1)}_{n-1}$ SOS R-matrix and face-vertex correspondence

Let $\{\epsilon_i|i=1,2,\ldots,n\}$ be the orthonormal basis of the vector space $\mathbb{C}^n$ such that $\langle\epsilon_i,\epsilon_j\rangle=\delta_{ij}$. The A_{n-1} simple roots are $\{\alpha_i=\epsilon_i-\epsilon_{i+1}|i=1,\ldots,n-1\}$ and the fundamental weights $\{\Lambda_i|i=1,\ldots,n-1\}$ satisfying $\langle\Lambda_i,\alpha_j\rangle=\delta_{ij}$ are given by

$$\Lambda_i=\sum_{k=1}^{i}\epsilon_k-\frac{i}{n}\sum_{k=1}^{n}\epsilon_k.$$

Set

$$\hat{i}=\epsilon_i-\overline{\epsilon},\ \overline{\epsilon}=\frac{1}{n}\sum_{k=1}^{n}\epsilon_k,\ i=1,\ldots,n,\ \text{then}\ \sum_{i=1}^{n}\hat{i}=0. \tag{2.9}$$

For each dominant weight $\Lambda=\Sigma_{i=1}^{n-1}a_i\Lambda_i$, $a_i\in\mathbb{Z}^+$, there exists an irreducible highest weight finite-dimensional representation V_Λ of A_{n-1} with the highest vector $|\Lambda\rangle$. For example the fundamental vector representation is V_{Λ_1}.

Let $\mathfrak{h}$ be the Cartan subalgebra of A_{n-1} and $\mathfrak{h}^*$ be its dual. A finite-dimensional diagonalizable $\mathfrak{h}$-module is a complex finite-dimensional vector space W with a weight decomposition $W=\oplus_{\mu\in\mathfrak{h}^*}W[\mu]$, so that $\mathfrak{h}$ acts on $W[\mu]$ by $xv=\mu(x)v$, $(x\in\mathfrak{h},v\in W[\mu])$. For example, the fundamental vector representation $V_{\Lambda_1}=\mathbb{C}^n$, the nonzero weight spaces $W[\hat{i}]=\mathbb{C}\epsilon_i$, $i=1,\ldots,n$.

For a generic $\lambda\in\mathbb{C}^n$, define

$$\lambda_i=\langle\lambda,\epsilon_i\rangle,\ \lambda_{ij}=\lambda_i-\lambda_j,\ |\lambda|=\sum_{l=1}^{n}\lambda_l,\ i,j=1,\ldots,n. \tag{2.10}$$

Let $R(z,\lambda)\in\mathrm{End}(\mathbb{C}^n\otimes\mathbb{C}^n)$ be the R-matrix of the $A^{(1)}_{n-1}$ SOS model given by

$$R(z,\lambda)=\sum_{i=1}^{n}R^{ii}_{ii}(z,\lambda)E_{ii}\otimes E_{ii}+\sum_{i\neq j}\{R^{ij}_{ij}(z,\lambda)E_{ii}\otimes E_{jj}+R^{ji}_{ij}(z,\lambda)E_{ji}\otimes E_{ij}\}. \tag{2.11}$$

The coefficient functions are

$$R^{ii}_{ii}(z,\lambda)=1,\ R^{ij}_{ij}(z,\lambda)=\frac{\sigma(z)\sigma(\lambda_{ij}w-w)}{\sigma(z+w)\sigma(\lambda_{ij}w)}, \tag{2.12}$$

$$R_{ij}^{ji}(z,\lambda)=\frac{\sigma(w)\sigma(z+\lambda_{ij}w)}{\sigma(z+w)\sigma(\lambda_{ij}w)}, \tag{2.13}$$

and λ_{ij} is defined in (2.10). The R-matrix satisfies the dynamical (modified) quantum Yang–Baxter equation

$$\begin{aligned}&R_{12}(z_1-z_2,\lambda-h^{(3)})R_{13}(z_1-z_3,\lambda)R_{23}(z_2-z_3,\lambda-h^{(1)})\\&\quad=R_{23}(z_2-z_3,\lambda)R_{13}(z_1-z_3,\lambda-h^{(2)})R_{12}(z_1-z_2,\lambda),\end{aligned} \tag{2.14}$$

with unitarity relation

$$R_{12}(u,\lambda)R_{21}(-u,\lambda)=id. \tag{2.15}$$

We adopt the notation: $R_{12}(z,\lambda-h^{(3)})$ acts on a tensor $v_1\otimes v_2\otimes v_3$ as $R(z,\lambda-\mu)\otimes id$ if $v_3\in W[\mu]$. Let us introduce

$$\tilde{R}(u,\lambda)_{ij}^{kl}=R(u,\lambda)_{ij}^{kl}\left\{\frac{f_2(\lambda;k)}{f_2(\lambda+\hat{k};k)}\frac{f_2(\lambda+\hat{i}+\hat{j};i)}{f_2(\lambda+\hat{j};i)}\right\}, \tag{2.16}$$

$$f_2(\lambda;j)=\prod_{k\neq j}\frac{\sigma(\lambda_{jk}w)}{\sigma(w)}. \tag{2.17}$$

The R-matrix satisfies the following crossing-unitarity relation[6]

$$\sum_{i_2,j_2=1}^{n}\tilde{R}(-u-nw,\lambda-\hat{j}_2)_{j_1\ j_2}^{i_1\ i_2}R(u,\lambda-\hat{j}_2)_{i_3\ j_2}^{i_2\ j_3}=\frac{e^{\sqrt{-1}nw}\sigma(u)\sigma(u+nw)}{\sigma(u+w)\sigma(u+nw-w)}\delta_{i_3}^{i_1}\delta_{j_3}^{j_1}. \tag{2.18}$$

Let us introduce an intertwiner—a n-component column vector $\phi_{\lambda,\lambda-\hat{j}}(u)$ whose kth element is

$$\phi_{\lambda,\lambda-\hat{j}}^{(k)}(u)=\theta^{(k)}(u+nw\lambda_j). \tag{2.19}$$

Using the intertwiner, the face-vertex correspondence can be written as[14]

$$R_{12}^{B}(u_1-u_2)\phi_{\lambda,\lambda-\hat{i}}(u_1)\otimes\phi_{\lambda-\hat{i},\lambda-\hat{i}-\hat{j}}(u_2)=\sum_{kl}R(u_1-u_2,\lambda)_{ij}^{kl}\phi_{\lambda-\hat{l},\lambda-\hat{l}-\hat{k}}(u_1)\otimes\phi_{\lambda,\lambda-\hat{l}}(u_2). \tag{2.20}$$

Then the Yang–Baxter equation of the $\mathbb{Z}_n$ Belavin R-matrix $R^B(u)$ (1.1) is equivalent to the dynamical Yang–Baxter equation of the $A_{n-1}^{(1)}$ SOS R-matrix $R(u,\lambda)$ (2.14).

III. RE AND DUAL RE FOR $A_{n-1}^{(1)}$ SOS MODEL

In this section, using the intertwiner between the $\mathbb{Z}_n$ Belavin R-matrix and that of the $A_{n-1}^{(1)}$ SOS model, we construct the isomorphism between the solution of the RE for the $A_{n-1}^{(1)}$ SOS model and that of its dual from the isomorphism (1.4).

A. RE and its dual for SOS model

The RE of the K-matrix $\mathcal{K}(\lambda|u)$ for the face-type SOS model was given as follows:[5,12,16,17]

$$\sum_{i_1,i_2}\sum_{j_1,j_2} R(u_1-u_2,\lambda)_{i_1}^{i_0}{}_{j_1}^{j_0}\mathcal{K}(\lambda+\hat{j}_1+\hat{i}_2|u_1)_{i_2}^{i_1}R(u_1+u_2,\lambda)_{j_2}^{j_1}{}_{i_3}^{i_2}\mathcal{K}(\lambda+\hat{j}_3+\hat{i}_3|u_2)_{j_3}^{j_2}$$
$$=\sum_{i_1,i_2}\sum_{j_1,j_2}\mathcal{K}(\lambda+\hat{j}_1+\hat{i}_0|u_2)_{j_1}^{j_0}R(u_1+u_2,\lambda)_{i_1}^{i_0}{}_{j_2}^{j_1}\mathcal{K}(\lambda+\hat{j}_2+\hat{i}_2|u_1)_{i_2}^{i_1}R(u_1-u_2,\lambda)_{j_3}^{j_2}{}_{i_3}^{i_2}. \quad (3.1)$$

The dual RE of the K-matrix $\tilde{\mathcal{K}}(\lambda|u)$ was written down by[5,6]

$$\sum_{i_1,i_2}\sum_{j_1,j_2} R(u_2-u_1,\lambda)_{i_1}^{i_0}{}_{j_1}^{j_0}\tilde{\mathcal{K}}(\lambda+\hat{j}_1+\hat{i}_1|u_1)_{i_2}^{i_1}\tilde{R}(-u_1-u_2-nw,\lambda)_{j_2}^{j_1}{}_{i_3}^{i_2}\tilde{\mathcal{K}}(\lambda+\hat{j}_2+\hat{i}_3|u_2)_{j_3}^{j_2}$$
$$=\sum_{i_1,i_2}\sum_{j_1,j_2}\tilde{\mathcal{K}}(\lambda+\hat{j}_0+\hat{i}_0|u_2)_{j_1}^{j_0}\tilde{R}(-u_1-u_2-nw,\lambda)_{i_1}^{i_0}{}_{j_2}^{j_1}\tilde{\mathcal{K}}(\lambda+\hat{j}_2+\hat{i}_1|u_1)_{i_2}^{i_1}R(u_2-u_1,\lambda)_{j_3}^{j_2}{}_{i_3}^{i_2}, \quad (3.2)$$

where $\tilde{R}(u,\lambda)$ is defined in (2.16) for the $A_{n-1}^{(1)}$ SOS model. The explicit expressions of $\tilde{R}(u,\lambda)$ for other types of SOS models were given in Ref. 6. Because of the *nontrivial* dependence on the face-type parameters $\{\lambda_j\}$, the dual RE of SOS models should be treated separately in contrast with those of the vertex models.

As in the Sklyanin scheme for the vertex models, one can construct families of commuting *double-row transfer matrices* for the SOS model with open boundary condition in terms of the K-matrices $\mathcal{K}(\lambda|u)$ and $\tilde{\mathcal{K}}(\lambda|u)$.[5,6]

B. Isomorphism between the solutions of the RE and its dual for $A_{n-1}^{(1)}$ SOS model

Thanks to the face-vertex correspondence between the $\mathbb{Z}_n$ Belavin vertex model and the $A_{n-1}^{(1)}$ SOS model (2.20), we can construct the isomorphism between the solutions of the RE and its dual for the $A_{n-1}^{(1)}$ SOS model from the isomorphism (1.4) of the $\mathbb{Z}_n$ Belavin vertex model.

Let us introduce other types of intertwiners $\overline{\phi}$ and $\tilde{\phi}$ satisfying the following orthogonality conditions:

$$\sum_k \overline{\phi}^{(k)}_{\lambda,\lambda-\hat{i}}(u)\phi^{(k)}_{\lambda,\lambda-\hat{j}}(u)=\delta_{ij}, \quad (3.3)$$

$$\sum_k \tilde{\phi}^{(k)}_{\lambda+\hat{i},\lambda}(u)\phi^{(k)}_{\lambda+\hat{j},\lambda}(u)=\delta_{ij}. \quad (3.4)$$

One can derive the "completeness" relations from the above conditions

$$\sum_k \overline{\phi}^{(i)}_{\lambda,\lambda-\hat{k}}(u)\phi^{(j)}_{\lambda,\lambda-\hat{k}}(u)=\delta_{ij}, \quad (3.5)$$

$$\sum_k \tilde{\phi}^{(i)}_{\lambda+\hat{k},\lambda}(u)\phi^{(j)}_{\lambda+\hat{k},\lambda}(u)=\delta_{ij}, \quad (3.6)$$

and the following relation between the intertwiners $\overline{\phi}$ and $\tilde{\phi}$ from their definitions (3.3) and (3.4):[6]

$$\overline{\phi}_{\lambda+\hat{j},\lambda}(u)=\frac{\sigma\left(u+w|\lambda|-\frac{n-1}{2}-w\right)}{\sigma\left(u+w|\lambda|-\frac{n-1}{2}\right)}\left\{\prod_{k\neq j}\frac{\sigma(\lambda_{jk}w)}{\sigma(\lambda_{jk}w+w)}\right\}\tilde{\phi}_{\lambda+\hat{j},\lambda}(u-nw). \quad (3.7)$$

Noting the fact $\langle\overline{\epsilon},\epsilon_j\rangle=1/n$ and the definition of the intertwiner (2.19), one can derive the following relations: for $\forall\alpha\in\mathbb{C}$

$$\phi_{\lambda+\alpha\bar{\epsilon}_{\hat{i}},\lambda+\alpha\bar{\epsilon}_{\hat{j}}}(u)=\phi_{\lambda,\lambda-\hat{j}}(u+\alpha w), \tag{3.8}$$

$$\overline{\phi}_{\lambda+\alpha\bar{\epsilon}_{\hat{i}},\lambda+\alpha\bar{\epsilon}_{\hat{j}}}(u)=\overline{\phi}_{\lambda,\lambda-\hat{j}}(u+\alpha w), \tag{3.9}$$

$$\tilde{\phi}_{\lambda+\alpha\bar{\epsilon}_{\hat{i}},\lambda+\alpha\bar{\epsilon}_{\hat{j}}}(u)=\tilde{\phi}_{\lambda,\lambda-\hat{j}}(u+\alpha w). \tag{3.10}$$

Define

$$\mathcal{K}(\lambda|u)_i^j=\sum_{s,t}\tilde{\phi}^{(s)}_{\lambda-\hat{i}+\hat{j},\lambda-\hat{i}}(u)K(u)_t^s\phi^{(t)}_{\lambda,\lambda-\hat{i}}(-u), \tag{3.11}$$

$$\tilde{\mathcal{K}}(\lambda|u)_i^j=\sum_{s,t}\overline{\phi}^{(s)}_{\lambda,\lambda-\hat{j}}(-u)\tilde{K}(u)_t^s\phi^{(t)}_{\lambda-\hat{j}+\hat{i},\lambda-\hat{j}}(u). \tag{3.12}$$

Then we have

Theorem 1 (Ref. 6): *The above relations (3.11) and (3.12) map the solutions $K(u)$ and $\tilde{K}(u)$ to the RE (1.2) and the dual (1.3) for the $\mathbb{Z}_n$ Belavin R-matrix to the solutions $\mathcal{K}(\lambda|u)$ and $\tilde{\mathcal{K}}(\lambda|u)$ to the RE (3.1) and the dual (3.2) for the $A^{(1)}_{n-1}$ SOS R-matrix, and vice versa.*

Using the relations (3.5) and (3.6), one can invert (3.11)

$$K(u)_t^s=\sum_{i,j}\phi^{(s)}_{\lambda-\hat{i}+\hat{j},\ \lambda-\hat{i}}(u)\mathcal{K}(\lambda|u)_i^j\overline{\phi}^{(t)}_{\lambda,\lambda-\hat{i}}(-u). \tag{3.13}$$

Using the isomorphism (1.4) between the solutions of the RE and the dual RE for the $\mathbb{Z}_n$ Belavin R-matrix, the relations (3.5), (3.6), and (3.12), we have

$$\begin{aligned}\tilde{\mathcal{K}}(\lambda|u)_\mu^\nu&=\sum_{s,t}\overline{\phi}^{(s)}_{\lambda,\lambda-\hat{\nu}}(-u)\tilde{K}(u)_t^s\phi^{(t)}_{\lambda-\hat{\nu}+\hat{\mu},\lambda-\hat{\nu}}(u)\\&=\sum_{s,t}\overline{\phi}^{(s)}_{\lambda,\ \lambda-\hat{\nu}}(-u)K\left(-u-\frac{nw}{2}\right)_t^s\phi^{(t)}_{\lambda-\hat{\nu}+\hat{\mu},\ \lambda-\hat{\nu}}(u)\\&=\sum_{i,j}\sum_{s,t}\overline{\phi}^{(s)}_{\lambda,\ \lambda-\hat{\nu}}(-u)\phi^{(s)}_{\lambda'-\hat{i}+\hat{j},\ \lambda'-\hat{i}}\left(-u-\frac{nw}{2}\right)\mathcal{K}\left(\lambda'|-u-\frac{nw}{2}\right)_i^j\\&\quad\times\overline{\phi}^{(t)}_{\lambda',\ \lambda'-\hat{i}}\left(u+\frac{nw}{2}\right)\phi^{(t)}_{\lambda-\hat{\nu}+\hat{\mu},\ \lambda-\hat{\nu}}(u)\\&=\sum_{i,j}M(\lambda,\lambda'-\hat{i}|-u)_j^\nu\mathcal{K}\left(\lambda'|-u-\frac{nw}{2}\right)_i^jM\left(\lambda',\lambda-\hat{\nu}|u+\frac{nw}{2}\right)_\mu^i,\end{aligned} \tag{3.14}$$

where $\lambda'\in\mathbb{C}^n$ is arbitrary and a *crossing matrix* $M(\lambda,\lambda'|u)_j^\nu$ is defined by

$$M(\lambda,\lambda'|u)_j^\nu=\sum_t\overline{\phi}^{(t)}_{\lambda,\ \lambda-\hat{\nu}}(u)\phi^{(t)}_{\lambda'+\hat{j},\lambda'}\left(u-\frac{nw}{2}\right). \tag{3.15}$$

Finally, we obtain

Theorem 2: *The solutions to the RE (3.1) and the dual (3.2) for the $A^{(1)}_{n-1}$ SOS R-matrix have the following isomorphism:*

$$\tilde{\mathcal{K}}(\lambda|u)_\mu^\nu=\sum_{i,j}M(\lambda,\lambda'-\hat{i}|-u)_j^\nu\mathcal{K}\left(\lambda'|-u-\frac{nw}{2}\right)_i^jM\left(\lambda',\lambda-\hat{\nu}|u+\frac{nw}{2}\right)_\mu^i, \tag{3.16}$$

where $\lambda'\in\mathbb{C}^n$ is arbitrary.

We remark that the crossing matrix (3.15) is generally *nondiagonal*. Hence, the corresponding

$\tilde{\mathcal{K}}(\lambda|u)$ of the solution to the dual RE (3.2) obtained by the isomorphism (3.16) from the diagonal solution[11] to RE is generally nondiagonal, too, except for the case that a special choice of "*moduli*" parameter λ' is chosen as (4.5) (this special case will be clarified later in the next section). However, in order to diagonalize the corresponding *double-row transfer matrices* for the $A_{n-1}^{(1)}$ SOS model by the algebraic Bethe ansatz method, one needs $\mathcal{K}(\lambda|u)$ and $\tilde{\mathcal{K}}(\lambda|u)$ both diagonal.[18,19] In the next section, we shall search for a diagonal $\tilde{\mathcal{K}}(\lambda|u)$.

IV. DIAGONAL SOLUTION OF THE DUAL RE FOR $A_{n-1}^{(1)}$ SOS MODEL

In this section we look for the diagonal solution to the dual RE (3.2) for the $A_{n-1}^{(1)}$ SOS model, namely, the *K*-matrix $\tilde{\mathcal{K}}(\lambda|u)$ of following form:

$$\tilde{\mathcal{K}}(\lambda|u)_i^j = \tilde{k}(\lambda|u)_i \delta_i^j, \tag{4.1}$$

where $\{\tilde{k}(\lambda|u)_i\}$ are the functions of the face parameters $\{\lambda_j\}$ and the spectral parameter u. From directly solving the Eq. (3.2), we have

Theorem 3: For

$$\tilde{k}(\lambda|u)_i = \left\{ \prod_{k\neq i} \frac{\sigma(\lambda_{ik}w - w)}{\sigma(\lambda_{ik}w)} \right\} \frac{\sigma\left(\lambda_i w + \overline{\xi} + u + \frac{nw}{2}\right)}{\sigma\left(\lambda_i w + \overline{\xi} - u - \frac{nw}{2}\right)} f(u,\lambda), \tag{4.2}$$

in which $\overline{\xi}$ is a free parameter and $f(u,\lambda)$ is any nonvanishing function of λ and u, the diagonal K-matrix $\tilde{\mathcal{K}}(\lambda|u)$ with entries (4.1) and (4.2) is a solution to the dual RE (3.2) for the $A_{n-1}^{(1)}$ SOS model.

Proof: Substituting $\tilde{\mathcal{K}}(\lambda|u)$ of form (4.1) into the dual RE (3.2) for the $A_{n-1}^{(1)}$ SOS model, one finds the only nontrivial conditions of $\tilde{k}(\lambda|u)_i$ are

$$\begin{aligned}
&R(u_2-u_1,\lambda)_{ji}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_1)_j\tilde{R}(-u_1-u_2-nw,\lambda)_{ji}^{ij}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_2)_j \\
&\quad + R(u_2-u_1,\lambda)_{ij}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_1)_i\tilde{R}(-u_1-u_2-nw,\lambda)_{ji}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_2)_j \\
&= R(u_2-u_1,\lambda)_{ji}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_1)_i\tilde{R}(-u_1-u_2-nw,\lambda)_{ij}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_2)_i \\
&\quad + R(u_2-u_1,\lambda)_{ji}^{ij}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_1)_j\tilde{R}(-u_1-u_2-nw,\lambda)_{ji}^{ji}\tilde{k}(\lambda+\hat{i}+\hat{j}|u_2)_i,\ i\neq j.
\end{aligned}$$

Substituting (2.16) and (4.2) into the above equation, the dual RE (3.2) is equivalent to the following equation:

$$\begin{aligned}
&\left\{ \sigma(u_- + \lambda_{ij}w)\sigma(u_+) - \sigma(u_-)\sigma(u_+ - \lambda_{ij}w)\frac{\sigma(\lambda_j w + \overline{\xi'} - u_1')\sigma(\lambda_i w + \overline{\xi'} + u_1')}{\sigma(\lambda_j w + \overline{\xi'} + u_1')\sigma(\lambda_i w + \overline{\xi'} - u_1')} \right\} \\
&\quad \times \frac{\sigma(\lambda_j w + \overline{\xi'} - u_2')\sigma(\lambda_i w + \overline{\xi'} + u_2')}{\sigma(\lambda_j w + \overline{\xi'} + u_2')\sigma(\lambda_i w + \overline{\xi'} - u_2')} \\
&= \sigma(u_+ + \lambda_{ij}w)\sigma(u_-) - \sigma(u_+)\sigma(u_- - \lambda_{ij}w)\frac{\sigma(\lambda_j w + \overline{\xi'} - u_1')\sigma(\lambda_i w + \overline{\xi'} + u_1')}{\sigma(\lambda_j w + \overline{\xi'} + u_1')\sigma(\lambda_i w + \overline{\xi'} - u_1')},
\end{aligned} \tag{4.3}$$

where $u_- = u_1' - u_2'$, $u_+ = u_1' + u_2'$, $u_i' = -u_i - nw/2$, $\overline{\xi'} = \overline{\xi} + (n-2)/nw$. Equation (4.3) is a consequence of the identity (2.3). Then we complete our proof.

Now we shall study the relation between our solution of the dual RE and the diagonal solution of RE which was given as follows:[11]

$$\mathcal{K}(\lambda|u)_i^j = k(\lambda|u)_i \delta_i^j = g(u,\lambda)\frac{\sigma(\lambda_i w+\xi-u)}{\sigma(\lambda_i w+\xi+u)}\delta_i^j. \tag{4.4}$$

Here, $g(\lambda|u)$ is any nonvanishing function of λ and u, and ξ is a free parameter. Let us choose

$$\lambda' = \lambda + \frac{n}{2}\overline{\epsilon} \Rightarrow \lambda_i' = \lambda_i + \tfrac{1}{2}, \tag{4.5}$$

the vector $\overline{\epsilon}$ is defined in (2.9). Using the relation (3.8), the crossing matrix $M(\lambda,\lambda+(n/2)\overline{\epsilon}-\hat{i}|u)_i^\nu$ defined in (3.15) becomes simple

$$M\left(\lambda,\lambda+\frac{n}{2}\overline{\epsilon}-\hat{i}|u\right)_i^\nu = \sum_t \overline{\phi}^{(t)}_{\lambda,\lambda-\hat{\nu}}(u)\phi^{(t)}_{\lambda+(n/2)\overline{\epsilon},\lambda+(n/2)\overline{\epsilon}-\hat{\nu}}\left(u-\frac{nw}{2}\right) = \sum_t \overline{\phi}^{(t)}_{\lambda,\lambda-\hat{i}}(u)\phi^{(t)}_{\lambda,\lambda-\hat{i}}(u) = \delta_i^\nu. \tag{4.6}$$

The resulting solution to the dual RE by the isomorphism transformation (3.16) from the diagonal solution to RE is

$$\widetilde{\mathcal{K}}(\lambda|u)_\mu^\nu = k\left(\lambda+\frac{n}{2}\overline{\epsilon}|-u-\frac{nw}{2}\right)_\nu M\left(\lambda+\frac{n}{2}\overline{\epsilon},\lambda-\hat{\nu}|u+\frac{nw}{2}\right)_\mu^\nu. \tag{4.7}$$

The relations (3.7) and (4.5) enable us to further simplify the expression of the crossing matrix $M(\lambda+(n/2)\overline{\epsilon},\lambda-\hat{\nu}|u+nw/2)_\mu^\nu$:

$$\begin{aligned}
M\left(\lambda+\frac{n}{2}\overline{\epsilon},\lambda-\hat{\nu}|u+\frac{nw}{2}\right)_\mu^\nu &= \frac{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n-2}{2}w-\frac{n-1}{2}\right)}{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n}{2}w-\frac{n-1}{2}\right)}\left\{\prod_{k\neq\nu}\frac{\sigma(\lambda_{\nu k}w-w)}{\sigma(\lambda_{\nu k}w)}\right\}\\
&\quad\times\sum_t \widetilde{\phi}^{(t)}_{\lambda+(n/2)\overline{\epsilon},\lambda+(n/2)\overline{\epsilon}-\hat{\nu}}\left(u-\frac{nw}{2}\right)\phi^{(t)}_{\lambda-\hat{\nu}+\hat{\mu},\lambda-\hat{\nu}}(u)\\
&= \frac{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n-2}{2}w-\frac{n-1}{2}\right)}{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n}{2}w-\frac{n-1}{2}\right)}\left\{\prod_{k\neq\nu}\frac{\sigma(\lambda_{\nu k}w-w)}{\sigma(\lambda_{\nu k}w)}\right\}\\
&\quad\times\sum_t \widetilde{\phi}^{(t)}_{\lambda,\lambda-\hat{\nu}}(u)\phi^{(t)}_{\lambda-\hat{\nu}+\hat{\mu},\lambda-\hat{\nu}}(u)\\
&= \frac{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n-2}{2}w-\frac{n-1}{2}\right)}{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n}{2}w-\frac{n-1}{2}\right)}\left\{\prod_{k\neq\nu}\frac{\sigma(\lambda_{\nu k}w-w)}{\sigma(\lambda_{\nu k}w)}\right\}\delta_\mu^\nu.
\end{aligned}$$

Finally, the resulting solution to the dual RE by the isomorphism transformation (3.16) from the diagonal solution to RE is given by

$$\widetilde{\mathcal{K}}(\lambda|u)_{\mu}^{\nu}=\frac{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n-2}{2}w-\frac{n-1}{2}\right)}{\sigma\left(u+|\lambda-\hat{\nu}|w+\frac{n}{2}w-\frac{n-1}{2}\right)}\left\{\prod_{k\neq\nu}\frac{\sigma(\lambda_{\nu k}w-w)}{\sigma(\lambda_{\nu k}w)}\right\}k\left(\lambda+\frac{n}{2}\overline{|\varepsilon|}-u-\frac{nw}{2}\right)_{\nu}\delta_{\mu}^{\nu}. \tag{4.8}$$

Substituting the diagonal solution of RE (4.4) into the above equation and after redefining the boundary parameter $\overline{\xi}$ and the free nonvanishing function $f(u,\lambda)$, one finds that the resulting diagonal solution (4.8) to the dual RE is exactly the same as (4.2).

V. CONCLUSION AND COMMENTS

By using the face-vertex correspondence (2.20) and the isomorphism (1.4) between the solutions to the RE and its dual for the $\mathbb{Z}_n$ Belavin *R*-matrix, we construct the isomorphism between the solutions to the RE and its dual for the $A_{n-1}^{(1)}$ SOS *R*-matrix. By directly solving the equation, we obtain a diagonal solution to the dual RE. Our solution to the dual RE can also be obtained through the isomorphism transformation (3.16) from the diagonal solution to RE obtained in Ref. 11 by a special choice of the free parameter λ' (4.5). Furthermore, the diagonal $\widetilde{\mathcal{K}}(\lambda|u)$ obtained in this article enables us to diagonalize the *double-row transfer matrices* of the $\mathbb{Z}_n$ Belavin model with open boundary condition described by the diagonal $\mathcal{K}(\lambda|u)$ and the diagonal $\widetilde{\mathcal{K}}(\lambda|u)$.[19]

Alternatively in Ref. 20, the very isomorphism with the special choice of the free parameter λ' (4.5) from the diagonal solution of RE to the diagonal solution of the dual RE was constructed by fusion procedure. However, our *generic* isomorphism transformation (3.16) gives a way to construct a *nondiagonal* solution of the dual RE with additional free parameters $\{\lambda_i'\}$.

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Approximation of sums of oscillating summands in certain physical problems

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The motion of a one-dimensional harmonic oscillator caused by recurring pushes in the absence of friction is considered. In particular, two cases are studied: the case when the pushes become more frequent and the other one when the pushes become less frequent. By means of an application of the Hardy–Littlewood–Vinogradov–Van der Corput theorem on the approximation of exponential sums by shorter ones, new asymptotic formulas for the solution of the problem are obtained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1797552]

I. INTRODUCTION

In some fields of mathematics and mathematical physics the sums of the form

$$S=\sum_{a<k\leqslant b}\varphi(k)e^{2\pi i f(k)} \tag{1}$$

are studied. Here $\varphi(x)$ and $f(x)$ are real functions of real argument, $i^2=-1$. Such sums appear, for example, in number theory in the analysis of the Riemann zeta function, in the solution of the problems, connected with integer points in the domains on plane and in space, in the study of the Fourier series, in the solution of such differential equations as the wave equation, the potential equation, the heat conductivity equation and so on.

We call the number $b-a$ *the length of the sum* S (for the integers a and b, this is the number of the summands in S).

When $\varphi(x)$ and $f(x)$ satisfy certain conditions, the sum S can be replaced with good accuracy by another sum S_1,

$$S_1=\sum_{\alpha<k\leqslant\beta}\Phi(k)e^{2\pi i F(k)}, \tag{2}$$

with the length $\beta-\alpha$, which is much smaller then $b-a$. First relations of the form

$$S=S_1+R, \tag{3}$$

where S, S_1 are the sums (1) and (2), respectively, R is a remainder term, with concrete functions $\varphi(x)$ and $f(x)$, were obtained by Hardy and Littlewood,[1] when they deduced approximate functional equation for the Riemann zeta function $\zeta(s)$ and by Vinogradov,[2] in the study of total numbers of integer points in the domains on plane. In the general form the theorem was proved by Van der Corput[3] (for the recent results connected with the Van der Corput theorem, see Ref. 4).

In each of the above-mentioned papers, some restrictions on the functions $\varphi(x)$ and $f(x)$ were imposed. With certain restrictions on $\varphi(x)$ and $f(x)$ which are convenient for applications, the theorem was proved by Karatsuba in Ref. 5 (see also Ref. 6).

We shall use the following notations:

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(1) *For* $B>0$, $B\to+\infty$, *or* $B\to 0$, *we write*

$$1 \ll \frac{A}{B} \ll 1,$$

if there are constants $C_1>0$ *and* $C_2>0$, *such that*

$$C_1 \leqslant \frac{|A|}{B} \leqslant C_2.$$

(2) *For a real number* α, *the notation* $\|\alpha\|$, *is understood in the following sense:*

$$\|\alpha\| = \min(\{\alpha\}, 1-\{\alpha\}),$$

where $\{\alpha\}$ *is the fractional part of* α.

We formulate the main theorem about replacing of an exponential sum by shorter one in accordance with the equality (3).

Theorem: *Assume that the real functions* $f(x)$ *and* $\varphi(x)$ *satisfy the following conditions on the segment* $[a,b]$ *:*

(1) $f''''(x)$ *and* $\varphi''(x)$ *are continuous;*
(2) *there exist numbers* H, U *and* V *such that* $H>0$, $1\ll U\ll V$, $0<b-a\leqslant V$ *and*

$$\frac{1}{U} \ll f''(x) \ll \frac{1}{U}, \quad \varphi(x) \ll H,$$

$$f'''(x) \ll \frac{1}{UV}, \quad \varphi'(x) \ll \frac{H}{V},$$

$$f''''(x) \ll \frac{1}{UV^2}, \quad \varphi''(x) \ll \frac{H}{V^2}.$$

Then, if we define the numbers x_μ *by the equation*

$$f'(x_\mu) = \mu,$$

we obtain

$$\sum_{a<\mu\leqslant b} \varphi(\mu) e^{2\pi i f(\mu)} = \sum_{f'(a)\leqslant\mu\leqslant f'(b)} C(\mu) Z(\mu) + R, \tag{4}$$

where

$$R = O\left(\frac{HU}{b-a} + HT_a + HT_b + H\log(f'(b) - f'(a) + 2)\right);$$

$$T_j = \begin{cases} 0, & \text{if } f'(j) \text{ is an integer;} \\ \min\left(\dfrac{1}{\|f'(j)\|}, \sqrt{U}\right), & \text{if } \|f'(j)\| \neq 0; \end{cases}$$

$j=a,b$;

$$C(\mu) = \begin{cases} 1, & \text{if } f'(a) < \mu < f'(b); \\ \dfrac{1}{2}, & \text{if } \mu = f'(a) \text{ or } \mu = f'(b); \end{cases}$$

$$Z(\mu)=\frac{1+i}{\sqrt{2}}\frac{\varphi(x_\mu)}{\sqrt{f''(x_\mu)}}e^{2\pi i(f(x_\mu)-\mu x_\mu)}.$$

It is possible to prove this theorem with slightly weaker restrictions on $f(x)$ and $\varphi(x)$, replacing the condition (1) by the following condition

(1^*) *The finite derivatives* $f''''(x)$ *and* $\varphi''(x)$ *exist at every point of the segment* $[a,b]$.

The simplest version of the formulated theorem is the statement, which is called *the Van der Corput lemma* (see Ref. 7, for example).

Lemma (Van der Corput): Let $f(x)$ *be a real differentiable function on the interval* $a<x\leqslant b$. *Moreover, assume that inside this interval it's derivative* $f'(x)$ *is a monotonic and of a constant sign function, and for a constant* δ *such that* $0<\delta<1$ *the function* $f'(x)$ *satisfies the inequality* $|f'(x)|\leqslant\delta$.

Then

$$\sum_{a<k\leqslant b}e^{2\pi if(k)}=\int_a^b e^{2\pi if(x)}dx+\theta\left(3+\frac{2\delta}{1-\delta}\right), \tag{5}$$

where $|\theta|\leqslant 1$.

Remark: If the parameters a and b are integers, then it is possible to replace the relation (5) by the following one:

$$\sum_{a<k\leqslant b}e^{2\pi if(k)}=\int_a^b e^{2\pi if(x)}\,dx+\frac{1}{2}e^{2\pi if(b)}-\frac{1}{2}e^{2\pi if(a)}+\theta\frac{2\delta}{1-\delta}, \tag{6}$$

where $|\theta|\leqslant 1$.

II. STATEMENT OF THE PROBLEM

Our aim in the present paper is to apply the theorem (the lemma) to the solution of the problem of description of dynamics of the harmonic oscillator under the action of recurring pushes. Such an oscillator is an exact or approximate model in many problems of classical and quantum physics.

We consider the simplest example of vibrations of the one-dimensional harmonic oscillator in the absence of friction. The equation of the motion of such an oscillator is (see Ref. 8, for example)

$$\ddot{x}+\omega_0^2x=0, \tag{7}$$

where $\omega_0>0$ is a constant which is called the fundamental frequency of the oscillator vibrations; (7) describes the free oscillations of the harmonic oscillator without the friction:

$$x_0(t)=x_0\,\sin(\omega_0t-\varphi_0), \tag{8}$$

where $x_0=$const and $\varphi_0=$const are the given initial amplitude and phase.

Assume that the pushes act on the oscillator in the successive time moments $0<t_0<t_1<t_2<\cdots<t_n<\cdots$, $t_n\to+\infty$. These pushes give the positive increments the velocity of the oscillator motion: $V_0,V_1,\ldots,V_n,\ldots$. The mathematical description of such a problem presents the Cauchy problem with initial conditions

$$x(0)=X_0;\quad \dot{x}(0)=X_1. \tag{9}$$

For $t>0$, $x(t)$ satisfies the equation (see Ref. 9)

$$\ddot{x} + \omega_0^2 x = \sum_{k=0}^{\infty} V_k \delta(t - t_k), \tag{10}$$

where $\delta(t)$ is the Dirac delta-function:

$$\delta(x) = 0, \quad x \neq 0, \quad \int_{-\infty}^{+\infty} \delta(x)dx = 1.$$

The solution of this problem for $t_{n-1} < t < t_n$ has the following form:

$$x(t) = x_0(t) + S(t) = x_0(t) + \sum_{k=0}^{n-1} V_k \frac{\sin\ \omega_0(t - t_k)}{\omega_0}. \tag{11}$$

Here and below, $x_0(t)$ is the free harmonic vibrations of the oscillator (8).

III. PERIODIC PUSHES OF EQUAL VALUE ACT ON THE OSCILLATOR

The case when the pushes of the form

$$V_k = V,\ t_k = k\tau; \quad \tau = \text{const} > 0; \quad k = 0,1,2, \ldots, n; \quad n \to +\infty; \tag{12}$$

act on the one-dimensional harmonic oscillator is explicitly investigated in Ref. 9. There the solution of the problem (9), (10), (12) in the form

$$x(t) = x_0(t) + \frac{V}{\omega_0} \frac{\sin \dfrac{n\omega_0\tau}{2}}{\sin \dfrac{\omega_0\tau}{2}} \sin\ \omega_0 \left(t - \frac{n-1}{2}\tau \right)$$

is obtained for $t_{n-1} < t < t_n$. It is noted in Ref. 9 that "it is impossible to simplify the sum (11) for arbitrary t_k, V_k." We demonstrate below how applying the theorem (lemma) it is possible to obtain new asymptotic formulas for the solution of the problem (9), (10) also in the case of more complicated, nonperiodic pushes.

IV. THE PUSHES ACTING ON THE OSCILLATOR BECOME MORE FREQUENT

Consider the following example: in the absence of friction the pushes of the form

$$V_k = V,\ t_k = \tau(k + D)^{\beta}; \quad k = 0,1,2, \ldots, n; \quad n \to +\infty; \tag{13}$$

act on the harmonic oscillator, where $V; \tau; \beta; D$ are positive constants, with $D \geqslant 1$, and

$$0 < \beta < 1. \tag{14}$$

Note that the condition (14) means that the pushes become more frequent. For the pushes (13), (14) the sum $S = S(t)$ in (11) takes the form

$$S = \frac{V}{\omega_0} \mathrm{Im} \sum_{k=0}^{n-1} e^{i\omega_0(t - t_k)} = \frac{V}{\omega_0} \mathrm{Im}(e^{i\omega_0 t} S_0), \tag{15}$$

where

$$S_0 = \sum_{k=0}^{n-1} e^{-2\pi i(\omega_0/(2\pi))t_k}.$$

Set

$$f(x) = \frac{\omega_0}{2\pi} t_x = \frac{\omega_0}{2\pi} \tau (x + D)^{\beta}.$$

We note that

$$0 < f'(x) = \frac{\omega_0}{2\pi} \beta \tau (x + D)^{-1+\beta},$$

and for $x \to +\infty, f'(x) \to 0$ monotonically. That is why, defining the number x_1 by the equality

$$\frac{\omega_0}{2\pi} \beta \tau (x_1 + D)^{-1+\beta} = \frac{1}{2},$$

that is

$$x_1 = \left(\frac{\omega_0 \beta \tau}{\pi} \right)^{(1/(1-\beta))} - D,$$

we find that for $x \geqslant x_1$ the derivative $f'(x)$ satisfies the relation

$$0 < f'(x) \leqslant \frac{1}{2}.$$

Let $n_1 = [\max(0, x_1)] + 1, n > n_1$ (here and below $[X]$ means the integer part of the number X). We represent $S_0(t)$ in the form of the sum of two summands

$$S_0(t) = S_1(t) + S_2(t), \tag{16}$$

where

$$S_1(t) = \sum_{0 \leqslant k \leqslant n_1} e^{-2\pi i f(k)}, \tag{17}$$

$$S_2(t) = \sum_{n_1 < k \leqslant n-1} e^{-2\pi i f(k)}. \tag{18}$$

To estimate the sum $S_2(t)$ we apply the Van der Corput lemma; from (6) we obtain

$$S_2(t) = \int_{n_1}^{n-1} e^{-2\pi i f(x)}\, dx + \frac{1}{2} e^{-2\pi i f(n-1)} - \frac{1}{2} e^{-2\pi i f(n_1)} + \theta \frac{2\delta}{1-\delta}, \quad |\theta| \leqslant 1, \tag{19}$$

where

$$0 < \delta = \frac{\omega_0}{2\pi} \beta \tau (n_1 + D)^{-1+\beta} \leqslant \frac{1}{2}.$$

Consider the integral from (19):

$$J = J(n-1) = \int_{n_1}^{n-1} e^{-2\pi i f(x)}\, dx = \int_{n_1}^{n-1} e^{-i\omega_0 \tau (x+D)^{\beta}}\, dx. \tag{20}$$

Making the following change of variables of integration:

$$y = \omega_0 \tau (x + D)^{\beta},$$

we find from (20),

$$J = \beta^{-1}(\omega_0\tau)^{-1/\beta}\int_{\omega_0\tau(n_1+D)^\beta}^{\omega_0\tau(n+D-1)^\beta} y^{1/\beta-1}e^{-iy}\,dy = \beta^{-1}(\omega_0\tau)^{-1/\beta}J_1, \tag{21}$$

where

$$J_1 = \int_A^B y^{1/\beta-1}e^{-iy}\,dy,$$

$$A = \omega_0\tau(n_1+D)^\beta, \quad B = \omega_0\tau(n-1+D)^\beta. \tag{22}$$

Integrating J_1 by parts one time, we obtain

$$J_1 = iB^{1/\beta-1}e^{-iB} - iA^{1/\beta-1}e^{-iA} - i(\beta^{-1}-1)J_2, \tag{23}$$

where

$$J_2 = \int_A^B y^{1/\beta-2}e^{-iy}\,dy. \tag{24}$$

Since from (14) $1/\beta - 1 > 0$, in (23) we get $B^{1/\beta-1} > A^{1/\beta-1}$.

Let us get an upper bound for the integral J_2. Assume at first that $\beta \neq \frac{1}{2}$. From (24) we have

$$J_2 = \; i\int_A^B y^{1/\beta-2}\,de^{-iy} = iy^{1/\beta-2}e^{-iy}\Big|_A^B - i\left(\frac{1}{\beta}-2\right)\int_A^B y^{1/\beta-3}e^{-iy}\,dy.$$

From here,

$$|J_2| \leqslant B^{1/\beta-2} + A^{1/\beta-2} + \left|\frac{1}{\beta}-2\right|\int_A^B y^{1/\beta-3}\,dy \leqslant 2B^{1/\beta-2} + 2A^{1/\beta-2}, \quad \beta \neq \frac{1}{2}.$$

If $\beta = \frac{1}{2}$, then $J_2 = \int_A^B e^{-iy}\,dy$, and $|J_2| \leqslant 2$. Hence, for any $\beta, 0 < \beta < 1$, the inequality

$$|J_2| \leqslant 2B^{1/\beta-2} + 2A^{1/\beta-2} + 2 \tag{25}$$

is valid. From (23)–(25) we obtain

$$J_1 = iB^{1/\beta-1}e^{-iB} - iA^{1/\beta-1}e^{-iA} + \theta_1\frac{2(1-\beta)}{\beta}(B^{1/\beta-2} + A^{1/\beta-2} + 1), \tag{26}$$

$|\theta_1| \leqslant 1$.

From (18)–(22) and (26) we find the following approximation of the sum $S_2(t)$:

$$\begin{aligned} S_2(t) = {} & i(\omega_0\tau\beta)^{-1}(n-1+D)^{1-\beta}e^{-i\omega_0 t_{n-1}} + \theta_1 2(1-\beta)(\omega_0\tau\beta)^{-2}(n-1+D)^{1-2\beta} - i(\omega_0\tau\beta)^{-1}(n_1 \\ & + D)^{1-\beta}e^{-i\omega_0 t_{n_1}} + \theta_1 2(1-\beta)(\omega_0\tau\beta)^{-2}(n_1+D)^{1-2\beta} + \frac{1}{2}e^{-i\omega_0 t_{n-1}} - \frac{1}{2}e^{-i\omega_0 t_{n_1}} \\ & + \theta_1 2(1-\beta)(\omega_0\tau)^{-1/\beta}\beta^{-2} + \theta\frac{2\delta}{1-\delta}, \end{aligned} \tag{27}$$

where $|\theta| \leqslant 1$, $|\theta_1| \leqslant 1$, $0 < \delta \leqslant \frac{1}{2}$, $t_{n_1} = \tau(n_1+D)^\beta$, $t_{n-1} = \tau(n-1+D)^\beta$.

The sum $S_1(t)$ from (17) is estimated in the trivial way by the amount of its summands, that is,

$$S_1(t) = \theta_2(n_1+1), \quad |\theta_2| \leqslant 1. \tag{28}$$

From (16), (27), and (28) we have

$$e^{i\omega_0 t}S_0(t) = i(\omega_0\tau\beta)^{-1}(n-1+D)^{1-\beta}e^{i\omega_0(t-t_{n-1})} + \theta_3 R, \tag{29}$$

where $|\theta_3| \leqslant 1$,

$$R = 2(1-\beta)(\omega_0\tau\beta)^{-2}(n-1+D)^{1-2\beta} + (\omega_0\tau\beta)^{-1}(n_1+D)^{1-\beta} + 2(1-\beta)(\omega_0\tau\beta)^{-2}(n_1+D)^{1-2\beta}$$
$$+ n_1 + 2 + \theta_1 2(1-\beta)\beta^{-2}(\omega_0\tau)^{-1/\beta} + \frac{2\delta}{1-\delta}, \tag{30}$$

$0 < \delta \leqslant \frac{1}{2}$.

The imaginary part of the expression (29) is

$$\mathrm{Im}(e^{i\omega_0 t}S_0(t)) = (\omega_0\tau\beta)^{-1}(n-1+D)^{1-\beta}\cos\,\omega_0(t-t_{n-1}) + \theta_3 R,$$

$|\theta_3| \leqslant 1$.

From here and from (11) and (15) we find the general solution of the problem (9), (10), (13), (14): for $t_{n-1} < t < t_n$,

$$x(t) = x_0(t) + \frac{V}{\omega_0^2\tau\beta}(n-1+D)^{1-\beta}\sin\left(\omega_0 t + \frac{\pi}{2} - \omega_0\tau(n-1+D)^{\beta}\right) + \theta_4 R_0, \tag{31}$$

where $|\theta_4| \leqslant 1, R_0 = (V/\omega_0)R$.

Remark: It is possible to make (27), and therefore the solution of the problem (31), more precise, integrating by parts (22) not once, as it was done above, but several times (see the next paragraph).

V. A SPECIAL CASE OF THE PROBLEM IN WHICH THE PUSHES ACTING ON THE OSCILLATOR BECOME MORE FREQUENT

We consider again the problem (9), (10), (13), (14), but now with such values of the parameters β, τ, D, ω_0, that for the function

$$f'(x) = \frac{\omega_0}{2\pi}\beta\tau(x+D)^{-1+\beta}$$

the relation

$$f'(x)|_{x=0} = \frac{\omega_0}{2\pi}\beta\tau D^{-1+\beta} = \delta < 1 \tag{32}$$

holds. In this case we can apply the Van der Corput lemma to the asymptotic evaluation of the sum S_0 in (15). According to (6) we have

$$S_0 = e^{-i\omega_0 t_0} + \sum_{0<k\leqslant n-1} e^{-i\omega_0 t_k} = J + \theta\left(1 + \frac{2\delta}{1-\delta}\right),$$

where $|\theta| \leqslant 1$,

$$J = J(n-1) = \int_0^{n-1} e^{-i\omega_0 t_x}\,dx = \beta^{-1}(\omega_0\tau)^{-1/\beta}\int_{\omega_0 t_0}^{\omega_0 t_{n-1}} y^{1/\beta\,-1}e^{-iy}\,dy. \tag{33}$$

As before, here $y = \omega_0\tau(x+D)^{\beta}$, $t_0 = \tau D^{\beta}$, $t_{n-1} = \tau(n-1+D)^{\beta}$.

We assume at first that $1/\beta = m \geqslant 2, m$ is an integer. Then from (33) we find

$$\int_{\omega_0 t_0}^{\omega_0 t_{n-1}} y^{m-1}e^{-iy}\,dy = e^{-iy}(iy^{m-1} - i^2(m-1)y^{m-2} + \cdots + i^{3m-2}(m-1)!)\Big|_{\omega_0 t_0}^{\omega_0 t_{n-1}}.$$

From here we obtain

$$\begin{aligned}\mathrm{Im}(e^{i\omega_0 t}S_0) = \beta^{-1}(\omega_0\tau)^{-1/\beta}((\omega_0 t_{n-1})^{m-1}\cos\,\omega_0(t-t_{n-1}) + (\omega_0 t_{n-1})^{m-2}(m-1)\sin\,\omega_0(t-t_{n-1})\\ -(\omega_0 t_{n-1})^{m-3}(m-1)(m-2)\cos\,\omega_0(t-t_{n-1}) - (\omega_0 t_{n-1})^{m-4}(m-1)(m-2)\\ \times(m-3)\sin\,\omega_0(t-t_{n-1}) + \cdots + (m-1)\,!\,\mathrm{Im}(i^{3m-2}e^{i\omega_0(t-t_{n-1})})) + \theta_1 m((\omega_0 t_0)^{m-1}\\ +(m-1)^{m-1}) + \theta\left(1+\frac{2\delta}{1-\delta}\right),\end{aligned}$$

where $|\theta|\leqslant 1$, $|\theta_1|\leqslant 1$. It is possible to rewrite the last expression in the form

$$\mathrm{Im}(e^{i\omega_0 t}S_0) = m(\omega_0\tau)^{-m}A\,\sin(\omega_0(t-t_{n-1})+\varphi) + \theta_2 R, \tag{34}$$

where $|\theta_2|\leqslant 1$,

$$R = m((\omega_0 t_0)^{m-1} + (m-1)^{m-1}) + 1 + \frac{2\delta}{1-\delta}, \tag{35}$$

$$A = \sqrt{A_1^2 + A_2^2}, \tag{36}$$

$$A_1 = (\omega_0 t_{n-1})^{m-1} - (\omega_0 t_{n-1})^{m-3}(m-1)(m-2) + \cdots \sim (\omega_0 t_{n-1})^{m-1}, \tag{37}$$

$$A_2 = (\omega_0 t_{n-1})^{m-2}(m-1) - (\omega_0 t_{n-1})^{m-4}(m-1)(m-2)(m-3) + \cdots \sim (m-1)(\omega_0 t_{n-1})^{m-2}, \tag{38}$$

$$\varphi = \arctan\frac{A_1}{A_2} = \frac{\pi}{2} - \arctan\frac{A_2}{A_1} \sim \frac{\pi}{2}, \tag{39}$$

$m=1/\beta$, $t_0=\tau D^\beta$, $t_{n-1}=\tau(n-1+D)^\beta$, $n\to+\infty$.

From (11), (15), (34) we find the solution of the problem (9), (10), (13), (14), (32): for $t_{n-1}<t<t_n$,

$$x(t) = x_0(t) + \frac{V}{\omega_0\beta}(\omega_0\tau)^{-1/\beta}A\,\sin(\omega_0 t - \omega_0\tau(n-1+D)^\beta + \varphi) + \theta_0 R_0, \tag{40}$$

where $|\theta_0|\leqslant 1$, $R_0=(V/\omega_0)R$, and the values A and φ are defined by (36)–(39).

Remark: We obtained the solution of the problem of the form (40) in the assumption that $1/\beta=m$ is an integer. If $1/\beta$ is not an integer, then defining m by the equality $[1/\beta]=m$, we integrate (33) by parts $m+1$ times, and then we estimate from above by the absolute value of the last "remainder" integral. After that the solution is obtained in the same way as in the case when $1/\beta$ is an integer. The remainder (35) also includes the estimate of the "remainder" integral.

Remark: In the solution (40) the remainder expressed via (35) does not depend on n [compare with the remainder (30) obtained in the previous paragraph].

Remark: Substituting in (40) not the exact values of A and φ, but using the equivalences (37) and (39), we obtain, instead of the forced oscillations (40):

$$\frac{V}{\omega_0\beta}(\omega_0\tau)^{-1/\beta}A\,\sin(\omega_0 t - \omega_0\tau(n-1+D)^\beta + \varphi),$$

the forced oscillations of the problem considered before:

$$\frac{V}{\omega_0^2\tau\beta}(n-1+D)^{1-\beta}\,\sin\left(\omega_0 t + \frac{\pi}{2} - \omega_0\tau(n-1+D)^\beta\right),$$

see (31).

VI. THE PUSHES ACTING ON THE OSCILLATOR BECOME LESS FREQUENT

Consider the following example: the pushes of the form

$$V_k = V, \quad t_k = \tau(k+D)^{\beta}; \quad k = 0,1,2,\dots,n; \quad n \to +\infty; \tag{41}$$

act on the harmonic oscillator in the absence of friction, where V, τ, β, D are positive constants, and also $D \geqslant 1$,

$$1 < \beta < 2. \tag{42}$$

It is easy to see that under the condition (42) the pushes become less frequent. To obtain the solution of the problem (9), (10), (41), (42), we transform the sum S_0 from (15) in the following way. We divide the interval of summation in k into $m+1$ intervals of the form

$$\frac{n-1}{2} < k \leqslant n-1; \quad \frac{n-1}{4} < k \leqslant \frac{n-1}{2}; \dots; \quad 0 \leqslant k \leqslant \frac{n-1}{2^m},$$

where m is a natural number such that

$$2^m \leqslant n-1 < 2^{m+1}.$$

We represent S_0 in the form

$$S_0 = \sum_{0 \leqslant k \leqslant (n-1)2^{-m}} e^{-i\omega_0 t_k} + \sum_{\nu=0}^{m-1} \sum_{(n-1)2^{-\nu-1} < k \leqslant (n-1)2^{-\nu}} e^{-i\omega_0 t_k} = S_1 + S_2, \tag{43}$$

where

$$S_1 = \sum_{0 \leqslant k \leqslant (n-1)2^{-m}} e^{-i\omega_0 t_k} = e^{-i\omega_0 t_0} + e^{-i\omega_0 t_1}, \tag{44}$$

$$S_2 = \sum_{\nu=0}^{m-1} S(\nu), \quad S(\nu) = \sum_{(n-1)2^{-\nu-1} < k \leqslant (n-1)2^{-\nu}} e^{-i\omega_0 t_k}. \tag{45}$$

We transform the sum $S(\nu)$ using a simple variant of the main theorem. We set $\varphi(x)=1$, $H=1$, $T_a = T_b = \sqrt{U}$. Since in the theorem the estimate

$$|Z(\mu)| \leqslant H\sqrt{U} = \sqrt{U},$$

holds, then it is possible to suppose that in the relation (4) each factor $C(\mu)$ is equal to 1. We have

$$S(\nu) = \sum_{A < x \leqslant 2A} e^{-2\pi i f(x)}, \quad \overline{S}(\nu) = \sum_{A < x \leqslant 2A} e^{2\pi i f(x)},$$

where

$$f(x) = \frac{\omega_0 \tau}{2\pi}(x+D)^{\beta}, \tag{46}$$

$A = (n-1)2^{-\nu-1}, 0 \leqslant \nu \leqslant m-1$.

From (46) it follows that

$$f'(x) = \frac{\omega_0 \tau \beta}{2\pi}(x+D)^{\beta-1}, \quad f''(x) = \frac{\omega_0 \tau \beta(\beta-1)}{2\pi}(x+D)^{\beta-2}.$$

If we set $U = d^{-1}(A+D)^{2-\beta}$, where $d = \omega_0 \tau \beta(\beta-1)/(2\pi)$, then for $A \leqslant x \leqslant 2A$ the inequalities $1/(2U) \leqslant f''(x) \leqslant 1/U$ are satisfied.

We define the numbers x_μ by the equality

$$f'(x_\mu) = \frac{\omega_0 \tau \beta}{2\pi}(x_\mu + D)^{\beta-1} = \mu,$$

that is

$$x_\mu = \left(\frac{2\pi}{\omega_0 \tau \beta}\right)^{1/(\beta-1)} \mu^{1/(\beta-1)} - D.$$

Then

$$f(x_\mu) - \mu x_\mu = \frac{\omega_0 \tau}{2\pi}\left(\frac{2\pi}{\omega_0 \tau \beta}\right)^{\beta/(\beta-1)} \mu^{\beta/(\beta-1)} - \left(\frac{2\pi}{\omega_0 \tau \beta}\right)^{1/(\beta-1)} \mu^{1+1/(\beta-1)} + D\mu = -D_1 \mu^{1+1/(\beta-1)} + D\mu,$$

where

$$D_1 = \left(1 - \frac{1}{\beta}\right)\left(\frac{2\pi}{\omega_0 \tau \beta}\right)^{1/(\beta-1)}.$$

Besides,

$$f''(x_\mu) = \frac{\omega_0 \tau \beta(\beta-1)}{2\pi}\left(\frac{2\pi}{\omega_0 \tau \beta}\right)^{(\beta-2)/(\beta-1)} \mu^{(\beta-2)/(\beta-1)} = (\beta-1)\left(\frac{\omega_0 \tau \beta}{2\pi}\right)^{1/(\beta-1)} \mu^{1-1/(\beta-1)}.$$

Since in our example $b=2A$, $a=A$, $U=d^{-1}(A+D)^{2-\beta}$, we get

$$f'(b) - f'(a) = (b-a)f''(\xi) \leqslant \frac{A}{U} = \frac{Ad}{(A+D)^{2-\beta}} \leqslant d(A+D)^{\beta-1}.$$

This implies that the remainder term from (4) takes the form

$$R_\nu = O(UA^{-1} + \sqrt{U} + \log(2 + d(A+D)^{\beta-1})) = O(d^{-1}A^{-1}(A+D)^{2-\beta} + d^{-1/2}(A+D)^{1-\beta/2} + \log(2 + d(A+D)^{\beta-1})) = O(d^{-1/2}(A+D)^{1-\beta/2}) = O(d^{-1/2}A^{1-\beta/2}) = O(d^{-1/2}2^{-\nu(1-\beta/2)}n^{1-\beta/2}).$$

We apply the theorem to the asymptotic evaluation of the sum $\overline{S(\nu)}$. We find

$$\overline{S(\nu)} = \sum_{A<x\leqslant 2A} e^{2\pi i(\omega_0 \tau/(2\pi))(x+D)^\beta} = e^{i(\pi/4)} \sum_{\mu_1<\mu\leqslant\mu_2} (\beta-1)^{-1/2}\left(\frac{\omega_0 \tau \beta}{2\pi}\right)^{-1/(2(\beta-1))} \mu^{-1/2+1/(2(\beta-1))} e^{-2\pi i(D_1\mu^{1+1/(\beta-1)} - D\mu)} + O(R_\nu),$$

or using the complex conjugated sum we get

$$S(\nu) = e^{-i(\pi/4)}(\beta-1)^{-1/2}\left(\frac{\omega_0 \tau \beta}{2\pi}\right)^{-1/(2(\beta-1))} \sum_{\mu_1<\mu\leqslant\mu_2} \mu^{-1/2+1/(2(\beta-1))} e^{2\pi i(D_1\mu^{1+1/(\beta-1)} - D\mu)} + O(R_\nu), \tag{47}$$

where μ are the integers, and also

$$\mu_1 = f'(A) = \frac{\omega_0 \tau \beta}{2\pi}(A+D)^{\beta-1},$$

$$\mu_2 = f'(2A) = \frac{\omega_0 \tau \beta}{2\pi}(2A + D)^{\beta-1}.$$

Substituting (47) into (45) and summing over all ν, or what is the same, over all μ,

$$1 \leqslant \mu \leqslant \frac{\omega_0 \tau \beta}{2\pi}(n - 1 + D)^{\beta-1},$$

we obtain

$$S_2 = e^{-i(\pi/4)}(\beta-1)^{-1/2}\left(\frac{\omega_0\tau\beta}{2\pi}\right)^{-1/(2(\beta-1))} \sum_{1\leqslant\mu\leqslant\omega_0\tau\beta/(2\pi)(n\,-\,1\,+\,D)^{\beta-1}} \mu^{-1/2+1/(2(\beta-1))} e^{2\pi i(D_1\mu^{1+1/(\beta-1)}-D\mu)} + O\left(\sum_{\nu=0}^{m-1} R_\nu\right). \tag{48}$$

From (48) and (43)–(45) we obtain for the sum S_0 the following asymptotic expression:

$$S_0 = e^{-i(\pi/4)}(\beta-1)^{-1/2}\left(\frac{\omega_0\tau\beta}{2\pi}\right)^{-1/(2(\beta-1))} \sum_{1\leqslant\mu\leqslant\omega_0\tau\beta/(2\pi)(n\,-\,1\,+\,D)^{\beta-1}} \mu^{-1/2+1/(2(\beta-1))} \times e^{2\pi i((\beta-1)/\beta(2\pi/(\omega_0\tau\beta))^{1/(\beta-1)}\mu^{1+1/(\beta-1)}-D\mu)} + O(d^{-1/2}n^{1-\beta/2}). \tag{49}$$

Comparing (43) and (49) we see that applying the theorem we approximate the initial sum of n summands by the sum of $n^{\beta-1}, 1<\beta<2$, summands $n\to+\infty$ From (11), (16), and (49) we find the general solution of the problem (9), (10), (41), and (42) in the following form: for $t_{n-1}<t<t_n$,

$$x(t) = x_0(t) + \frac{V}{\omega_0}(\beta-1)^{-1/2}\left(\frac{\omega_0\tau\beta}{2\pi}\right)^{-1/(2(\beta-1))} \mathrm{Im}\left(e^{i(\omega_0 t-\pi/4)} \sum_{1\leqslant\mu\leqslant\omega_0\tau\beta/(2\pi)(n\,-\,1\,+\,D)^{\beta-1}} \mu^{-1/2+1/(2(\beta-1))} \times e^{2\pi i((\beta-1)/\beta(2\pi/(\omega_0\tau\beta))^{1/(\beta-1)}\mu^{1+1/(\beta-1)}-D\mu)}\right) + O(n^{1-\beta/2}). \tag{50}$$

Replacing in (50) the variable of summation μ by k and introducing new parameters,

$$N = \left[\frac{\omega_0\tau\beta}{2\pi}(n - 1 + D)^{\beta-1}\right] + 1;$$

$$A_k = (k+1)^{-1/2+1/(2(\beta-1))};$$

$$T_k = 2\pi\frac{\beta-1}{\beta}\left(\frac{2\pi}{\omega_0\tau\beta}\right)^{1/(\beta-1)}(k+1)^{1+1/(\beta-1)} - 2\pi(k+1)D;$$

$$W = V(\beta-1)^{-1/2}\left(\frac{\omega_0\tau\beta}{2\pi}\right)^{-1/(2(\beta-1))},$$

we obtain the solution of the problem in the following more compact form: for $t_{n-1}<t<t_n$,

$$x(t) = x_0(t) + \frac{W}{\omega_0}\sum_{k=0}^{N-1} A_k \sin\left(\omega_0 t - \frac{\pi}{4} + T_k\right) + O(N^{-1/2+1/(2(\beta-1))}).$$

Remark: In the results obtained above, it is assumed that τ, ω_0, β, and D are constants, and the constants in the remainders of the approximate solutions depend on the parameters τ, ω_0, β and D. In the examples considered above, it is assumed also that the total number of pushes n

must be great enough, that is $n \geqslant n_1(\tau, \omega_0, \beta, D)$.

Remark: It is possible to obtain the asymptotic approximation of the solution $x(t)$*, which is uniform not only in* n*,* $n \to +\infty$ *, but also in the parameters* τ, ω_0, β, D*. However, to obtain such formulas one needs very cumbersome calculations.*

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Error syndrome calculation for graph codes on a one-way quantum computer: Towards a quantum memory

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For realizing a quantum memory the encoded quantum information can be protected against decoherence via repeated decoding and re-encoding operations. This requires us to perform fast encoding and decoding operations. The computational model underlying the one-way quantum computer provides a suitable concept for a fast implementation, which has been solved in a previous article for the encoding operation. In the present paper we show that the missing part, the decoding operation, can also be realized on a one-way quantum computer. This is based on the graph code representation for stabilizer codes, on the one hand, and the relation between cluster states and graph codes, on the other hand. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1797533]

I. INTRODUCTION

The concept of quantum error correcting codes plays a central role for the realization of quantum computational processes. In particular, quantum information, that is stored in a quantum system, has to be protected against decoherence. The states of the "input system" describe the quantum information we wish to store. These input states are given by density operators $\rho \in \mathcal{L}_1(\mathcal{K})$ acting on an "input Hilbert space" $\mathcal{K}$. The second system under consideration is the "output system" whose states are the density operators on an "output Hilbert space" $\mathcal{H}$.

The output system is the one which is present in nature, and in which we wish to encode quantum information. All relevant decoherence processes operating on the output system due to the coupling with the environment. A possible description of decoherence is the following: Consider a one parameter semi-group $t \mapsto T_t, T_t \circ T_s = T_{t+s}$, of channels acting on the observable algebra of all linear operators on $\mathcal{H}$. (In the Heisenberg picture, a channel T is a completely positive map that preserves unit operator.) The channel T_t is interpreted as the process of decoherence (error) that is present at the "time" t. A quantum computational process is only sufficiently reliable if the effect of errors is below a threshold ϵ. We define the "decoherence time" of the system to be the largest time s for which the cb-norm $\|T_s - \mathrm{id}\| \leq \epsilon$ is below the tolerable threshold. For most of the systems, which can be realized in experiments, the decoherence time s is too small for a sensible quantum memory.

In order to protect quantum information, we encode quantum states of the input system into quantum states of the output system. In the Heisenberg picture, which is preferably used here, an encoding operation is described by a channel E that maps the observable algebra $\mathcal{B}(\mathcal{H})$ of the output system into the observable algebra $\mathcal{B}(\mathcal{K})$ of the input system. For receiving the encoded quantum information back, we also need a decoding operation which is a channel D that maps the input observable algebra into the output observable algebra.

We encode states of the input system via a channel E to realize a quantum memory. After a certain time t, the encoded quantum information is corrupted due to the decoherence process T_t. The stored information is recovered by an application of an appropriate decoding operation D. The

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total channel that has been performed operates on the input system and it is given by the composition $E \circ T_t \circ D$. If this channel is close to the identity $\|E \circ T_t \circ D - \mathrm{id}\| \leq \epsilon$, we would have stored our quantum information successfully during the time t. For a reasonable coding scheme, the storing time t is much larger than the decoherence time s of the output system. The ratio t/s can be increased by increasing the ratio $\dim(\mathcal{H})/\dim(\mathcal{K})$ of the dimension of the output system and the dimension of the input system. Thus, increasing the storing time requires a larger amount of resources.

An alternative idea for obtaining large storing times is to concatenate decoding and re-encoding operations. Suppose we are able to store quantum information successfully for a time t. Then we just re-encode the corrected quantum information again, which corresponds to the operation $E \circ T_t \circ D \circ E$. Again the system undergoes decoherence for a further time t. Then the decoding operation is applied once more. The channel $E \circ T_t \circ D \circ E \circ T_t \circ D$ is close to the identity and we have stored our quantum information successfully for a time period $2t$. This heuristic picture is only realistic, if we assume that the decoding re-encoding operation $D \circ E$ can be performed much faster than the typical decoherence time s of the output system.

For realizing a quantum memory, we are therefore interested in "fast implementations" for encoding and decoding operations. The model of one-way quantum computing, introduced by Raussendorf and Briegel,[1–8] suggest being an appropriate base for realizing fast operations due to the intrinsic parallelism of this model. A one-way quantum computer operates on a system of qudits (quantum digits). Elementary operations within this scheme are (a) *local preparation procedures* which address every qudit individually, (b) one *elementary step of a dynamics* that corresponds to two-qudit next-neighbor interactions, (c) *local measurement operations* which operate independent on each qudit, and (d) *conditional local unitary operations*, depending on the measurement outcomes. The parallelism of a one-way quantum computer is based on the dynamics which is a global operation that addresses all qudits at the same time.

The pattern of two-qudit interactions defines a "weighted graph" on the set of qudit positions. Namely, two positions are connected by an edge, if the corresponding qudits interact with each other. The "weight," attached to an edge, is the "strength" of the qudit coupling (which is an integral number for suitable interactions).

As we have discussed in previous articles,[9,10] quantum error correcting codes associated with "graphs" are closely related to one-way quantum computing. The qudits under consideration are grouped into "input" qudits and "output qudits." In Ref. 11 we have shown that every encoding procedure for a graph code can be implemented on a one-way quantum computer by four elementary operations: (1) First one applies an appropriate local preparation procedure: Every output qudit is prepared in the "standard state" $(1/\sqrt{d})(\Sigma_{q \in \mathbb{F}_d}|q\rangle$, where $|q\rangle, q \in \mathbb{F}_d$ is an orthonormal basis labeled by the elements of a finite field $\mathbb{F}$ of order d, that is, d is a power of a prime. (2) One elementary step of a discrete dynamics is performed. This dynamics corresponds to the interaction pattern which is given by the underlying graph. (3) The input qudits are measured independently in the "x-basis," the nonbinary generalization of the σ_x-eigenbasis. (4) Depending on the measurement outcome, a suitable local unitary operation is performed. This scheme can be applied to all stabilizer codes over finite fields,[12] since any such code is equivalent to a graph code.[10,13]

The main result of the present paper is concerned with an implementation of the "decoding operation" of a graph code. It is based on a suitable extension of the coding graph by adding "syndrome vertices" and edges that connect the syndrome vertices with the output vertices in an appropriate manner. The syndrome vertices are the positions of the syndrome qudits which are used to measure the "error syndrome."

Theorem: *For every graph code over a finite field, the syndrome calculation can be implemented one a one-way quantum computer by a sequence of three elementary operations: (1) The input qudits as well as the syndrome qudits are individually prepared in the "standard state." (2) One inverse elementary step of the discrete dynamics, which corresponds to the extended coding graph, is performed. (3) The output qudits are measured independently in the x-basis and the syndrome qudits are measured independently in the z-basis which generalizes the σ_z-eigenbasis to the nonbinary case.*

Remark: The decoding operation can be completed by a conditional local unitary operation: (4) Depending on the measurement outcome of the output and syndrome qudits, a suitable local unitary operation is performed. This correction operation depends on the calculated syndromes and therefore on the class of errors that yield the same syndrome. Recall that the error syndrome is only uniquely determined by the error if the code is nondegenerate. We prove here that for any calculated error syndrome an appropriate local correction operation exists. However, to calculate it explicitly may be an NP hard problem concerning the length of the code.

We mention at this point that both operations, the encoding and the decoding, are based on the same dynamics. This is of course what one expects as far as the implementation of stabilizer codes by quantum circuits (consisting of one- and two-qudit elementary gates) is concerned:[14] The decoding one just uses the reversed circuit.

The paper is organized as follows: In Sec. II, we give some mathematical preliminaries as well as notations and conventions which are used in the subsequent sections. A precise description of the elementary operations that can be performed on a one-way quantum computer is given in Sec. III. The realization of a decoding operation on a one-way quantum computer is presented in Sec. IV. Some technical proofs are given in the Appendix and Sec. IV C in order to keep the article more comprehensive.

II. MATHEMATICAL PRELIMINARIES

The classical configuration space of a "digit" is given by a finite "alphabet" which is a finite field $\mathbb{F}$ of order d. For binary systems we are concerned with the field of two elements $\mathbb{F}_2=\{0,1\}$. A classical register is described by its configurations which are given by tuples $q^I=(q^i)_{i\in I}$ in the vector space $\mathbb{F}^I$. Each position $i\in I$ of the register is given by a "letter q^i" from the alphabet $\mathbb{F}$. It is convenient to identify a vector $a^K=(a^k)_{k\in K}\in\mathbb{F}^K$ with the vector in $\mathbb{F}^I$ that has only nonvanishing components in the subset $K\subset I$. The *phase space* of a register I is modeled by the vector space $\Xi^I=\mathbb{F}^I\oplus\mathbb{F}^I$.

The Hilbert space, describing a quantum register of qudits, is the space $\mathcal{L}_2(\mathbb{F}^I)$ of complex valued functions on $\mathbb{F}^I$ and its complex dimension is $d^{|I|}$ where $|I|$ is the number of elements in I. The scalar product of two functions ψ_1,ψ_2 is given by $\langle\psi_1,\psi_2\rangle=d^{-|I|}\Sigma_{q^I}\overline{\psi_1}(q^I)\psi_2(q^I)$. The algebra $\mathfrak{A}(I)$ of all linear operators on $\mathcal{L}_2(\mathbb{F}^I)$ is the "observable algebra" of the quantum register.

A useful basis of unitary operators in $\mathfrak{A}(I)$ is given by the unitary "Weyl" operators $\mathbf{w}(\xi^I),\xi^I\in\Xi^I$. For a given vector $\xi^I=(p^I,q^I)\in\Xi^I$ in phase space the corresponding Weyl operator is defined by

$$(\mathbf{w}(\xi^I)\psi)(q_1^I)=\chi(p^I,q_1^I)\psi(q_1^I-q^I), \tag{1}$$

with $\psi\in\mathcal{L}_2(\mathbb{F}^I)$. The phases $\chi(p^I,q^I)$ form a symmetric bicharacter of the additive group $\mathbb{F}^I$.[9] If the field $\mathbb{F}$ has characteristic d, then the bicharacter is given by $\chi(p^I,q^I)=\exp(2\pi i d^{-1}\Sigma_{i\in I}p^iq^i)$. By construction, the Weyl operators satisfy a discrete version of the canonical commutation relations,

$$\mathbf{w}(\xi_1^I)\mathbf{w}(\xi_2^I)=\chi(p_2^I,q_1^I)\mathbf{w}(\xi_1^I+\xi_2^I). \tag{2}$$

For a phase space vector $\xi^I=(0^I,q^I)$, the Weyl operator $\mathbf{x}(q^I):=\mathbf{w}(0^I,q^I)$ is a pure *shift* by q^I. On the other hand, the phase space vector $\xi^I=(p^I,0^I)$ corresponds to a *multiplier operator* $\mathbf{z}(p^I):=\mathbf{w}(p^I,0^I)$.

III. ONE-WAY QUANTUM COMPUTING

After a brief introduction into the basic elementary operations of one-way quantum computing, we apply the results of Ref. 11 to derive an implementation of both the encoding and decoding operation, on a one-way quantum computer.

It is convenient to fix one normalized "standard vector" $\Omega_K\in\mathcal{L}_2(\mathbb{F}^K)$ which we choose to be the constant function on $\mathbb{F}^K$. The application of multiplier operators yields an orthonormal basis $(\mathbf{z}(p^K)\Omega_K)_{p^K\in\mathbf{F}^K}$. This basis is called the "x-basis," which is the joint eigenbasis of the shift

operators. Any other product basis can be obtained by applying a local unitary operator $U_K = \otimes_k U_k$ to the x-basis. In particular, the local Fourier transform F_K, which is given by

$$(F_K\psi)(p^K) = \frac{1}{\sqrt{d}^{|K|}} \sum_{q^K} \chi(p^K, q^K)\psi(q^K), \tag{3}$$

transforms the x-basis to the so called z-basis which is nothing else but the joint eigenbasis of the multiplier operators.

The elementary operations are successively applied to a system of multiple qudits, which are grouped into three different types, according to their role. The "input qudits," "output qudits," as well as the "measuring qudits." They are labeled by the sets of vertices I, J, and K, respectively. The corresponding observable algebra (of the full quantum system) is given by $\mathfrak{A}(IJK) = \mathfrak{A}(I) \otimes \mathfrak{A}(J) \otimes \mathfrak{A}(K)$. In order to arrange formulas more clearly, we write $IJKL\cdots$ for the disjoint union $I \cup J \cup K \cup L \cup \cdots$ of sets of qudit positions (vertices).

A. Local preparation

Mathematical description: To each local unitary operator $U_{JK} = \otimes_{j \in JK} U_j$ in $\mathfrak{A}(JK)$ we associate the channel $\mathbf{E}_{U_{JK}}$ which maps an operator $A \in \mathfrak{A}(IJK)$ to

$$\mathbf{E}_{U_{JK}}(A) = \Phi_{JK}^* U_{JK}^* A\, U_{JK} \Phi_{JK} \in \mathfrak{A}(I). \tag{4}$$

Here Φ_{JK} is the isometry which assigns to a vector ψ the tensor product $\Phi_{JK}\psi = \psi \otimes \Omega_{JK}$.

Interpretation: The channel $\mathbf{E}_{U_{JK}}$ describes the *local preparation* which prepares each qudit at position $j \in J$ individually in the state which corresponds to the unit-vector $U_j\Omega_j$.

B. Elementary step of a discrete dynamics

Mathematical description: Let $\Lambda = (\Lambda_j^i)_{i,j \in IJK}$ be the adjacency matrix of a weighted graph with vertices IJK. We define the unitary multiplication operator $u(\Lambda)$ according to

$$(u(\Lambda)\psi)(q^{IJK}) := \tau(q^{IJK})\psi(q^{IJK}), \tag{5}$$

which implements an automorphism α_Λ of $\mathfrak{A}(IJK)$. An operator A is mapped to

$$\boldsymbol{\alpha}_\Lambda(A) = u(\Lambda)^* A u(\Lambda). \tag{6}$$

The phase-valued function $q^{IJK} \to \tau(q^{IJK})$ is chosen in such a way that

$$\tau(q^{IJK} + q_1^{IJK}) = \tau(q^{IJK})\tau(q_1^{IJK})\chi(q_1^{IJK}, \Lambda q^{IJK}) \tag{7}$$

holds for $q^{IJK} + q_1^{IJK} \in \mathbb{F}^{IJK}$.

Remark: For all graphs Λ a phase valued function τ that fulfills (7) exists. To see this, we build the finite-dimensional Abelian C*-algbra which is generated by unitary operators $\mathbf{u}(q^{IJK})$ that fulfill the relations

$$\mathbf{u}(q^{IJK} + q_1^{IJK}) = \mathbf{u}(q^{IJK})\mathbf{u}(q_1^{IJK})\chi(q_1^{IJK}, \Lambda q^{IJK}). \tag{8}$$

Each pure state (character) of this C*-algebra ζ induces a function τ that fullfills (7) by putting $\tau(q^{IJK}) := \zeta(\mathbf{u}(q^{IJK}))$.

To be more concrete, we can give an explicite formula for an appropriate function τ provided the graph Λ has no self-links. In this case, a solution for (7) is given by

$$\tau(q^{IJK}) := \exp\left(\frac{i\pi}{d} \sum_{i,j \in IJK} \Lambda_j^i q^i q^j\right). \tag{9}$$

Interpretation: The weighted graph Λ describes a next-neighbor interaction pattern subject to the dynamics $\boldsymbol{\alpha}_\Lambda$. Two positions i, j are neighbored if the corresponding matrix element of the

adjacency matrix does not vanish $\Lambda^i_j \neq 0$. The value of Λ^i_j corresponds to the strength of the coupling between qudit i and j.

C. Local measurements

Mathematical description: A local measurement operation is determined by a local unitary operator $U_{IK}=U_I\otimes U_K$. The corresponding operation is the channel $\mathbf{M}_{U_{IK}}$ which maps the C*-algebra $\mathcal{C}(\mathbb{F}^{IK},\mathfrak{A}(J))$ of operator valued functions $A:\mathbb{F}^{IK}\to\mathfrak{A}(J)$ to the operator

$$\mathbf{M}_{U_{IK}}(A)=\sum_{p^{IK}} U_{IK}\mathbf{z}(p^{IK})\Phi_{IK}A(p^{IK})\Phi^*_{IK}\mathbf{z}(p^{IK})^*U^*_{IK}, \tag{10}$$

in $\mathfrak{A}(IJK)$. The operators $U_{IK}\mathbf{z}(p^{IK})\Phi_{IK}, p^{IK}\in\mathbb{F}^{IK}$, are a complete family of mutually orthogonal isometries. This implies, in particular, that $\mathbf{M}_{U_{IK}}$ is an algebra homomorphism. Concerning the Heisenberg picture, this is the characteristic property of a projection valued measure. For our purposes, there are two interesting measurement bases: The x-basis corresponding to $U_{IK}=\mathbf{1}_{IK}$ and the z-basis corresponding to $U_{IK}=F_{IK}$.

Interpretation: Local measurements are dual to the local preparation schemes. They describe the individual measurement of a certain subset of qudits which consists here of input and measuring qudits IK. After the measurement operation has been performed, the remaining output qudits at positions J are in a quantum state that depends on the measurement outcome.

D. Conditional phase space translations

Mathematical description: Let f^J_{IK} be a function that maps a configuration $q^{IK}\in\mathbb{F}^{IK}$ to a phase space vector $f^J_{IK}q^{IK}\in\Xi^{IK}$. We associate to f^J_{IK} the *conditional phase space translation* $\mathbf{C}_{f^J_{IK}}$. It is the channel that assigns to an observable $A\in\mathfrak{A}(J)$ the operator valued function $\mathbf{C}_{f^J_{IK}}(A)\in\mathcal{C}(\mathbb{F}^{IK},\mathfrak{A}(J))$ by

$$q^{IK}\mapsto \mathbf{C}_{f^J_{IK}}(A)(q^{IK})=\mathbf{w}(f^J_{IK}q^{IK})A\mathbf{w}(f^J_{IK}q^{IK})^*. \tag{11}$$

Interpretation: After the qudits at the positions IK are measured, a measurement result $q^{IK}\in\mathbb{F}^{IK}$ is received. Depending on this outcome, a phase space translation is performed. The function f^J_{IK} describes a role which the phase space translation $f^J_{IK}q^{IK}$ one has to perform in case a randomly produced measurement result q^{IK} is received.

IV. IMPLEMENTING THE DECODING OPERATION BY A ONE-WAY QUANTUM COMPUTER

The encoding and decoding operation of a quantum error correcting code can be implemented as "quasi-free operations." Concerning the Heisenberg picture, quasi-free operations are channels T from the output algebra $\mathfrak{A}(J)$ into the input algebra $\mathfrak{A}(I)$ that map Weyl operators $\mathbf{w}(\xi^J)$ to a multiples of Weyl operators $T(\mathbf{w}(\xi^J))=\zeta(\xi^J)\mathbf{w}(\xi^I)$. As we have shown in Ref. 11, each quasi-free operation can be implemented on a one-way quatum computer by local preparation, one elementary step of a discrete dynamics (acting globally), a local measurement, and finally a phase space translation conditioned by the measurement outcome. The following definition expresses this in precise mathematical terms.

Definition IV.1: Let Λ be the adjacency matrix of a graph on the union of input vertices I, output vertices J, and syndrome vertices K, let $U_{IK}=\otimes_{i\in IK}U_i\in\mathfrak{A}(IK)$ be a local unitary operator, and let $f^J_{IK}:\mathbb{F}^{IK}\to\Xi^J$ be a function. We associate to the triple $(\Lambda,U_{IK},f^J_{IK})$ the channel $\mathbf{T}_{[\Lambda,U_{IK},f^J_{IK}]}:\mathfrak{A}(J)\to\mathfrak{A}(I)$, which is defined by

$$\mathbf{T}_{[\Lambda,U_{IK},f^J_{IK}]}:=\mathbf{E}_{1_{JK}}\circ\boldsymbol{\alpha}_\Lambda\circ\mathbf{M}_{U_{IK}}\circ\mathbf{C}_{f^J_{IK}}. \tag{12}$$

Interpretation: (1) The channel $\mathbf{E}_{1_{JK}}$ describes the preparation of the output and measuring qudits in the shift invariant standard state. (2) The next-neighbor interaction, which is described by

the graph Λ, is switched on for a definite period of time. This corresponds to the application of one elementary step of the discrete dynamics $\boldsymbol{\alpha}_\Lambda$ which acts globally on "all" qudits IJK. (3) The input and measuring qudits IK are measured in the product basis $(U_{IK}\mathbf{z}(p^{IK})\Omega_{IK})_{p^{IK}\in\mathbb{F}^{IK}}$. For quasi-free operations, the measurement of the input qudits is performed in the x-basis whereas the measurement qudits are either measured in a z- or an x-basis. This corresponds to the choice $U_i=\mathbf{1}_i$ for $i\in I$ and $U_k\in\{\mathbf{1}_k,F_k\}$ for $k\in K$. (4) After the measurement has been performed, one has produced a quantum state of the output qudits J which depends on the measurement outcome $p^{IK}\in\mathbb{F}^{IK}$. In order to realize a pure quantum operation, one has to perform, on the output qudits J, a phase space translation by the vector $f^J_{IK}p^{IK}$ which depends on the measurement outcome p^{IK}.

Note that in general the channels, given by Definition IV.1, are not pure. This requires additional conditions on the graph, on one hand, and on the conditional phase space translation, on the other hand.

A. Quantum error correction

We briefly recall here the concept of a quantum error correcting code that is able to correct errors that occur at a particular number e of qudits. A channel $T:\mathfrak{A}(J)\to\mathfrak{A}(J)$ is localized at a subset $E\subset J$ of qudit positions, if $T(A)=A$ holds for all operators $A\in\mathfrak{A}(J\backslash E)$ that are localized in the complement of E. This means that only the qubits at the positions E are affected by errors. A quantum error correcting code, that is able to correct e errors, is a pair (E,D) that consists of an encoding operation $E:\mathfrak{A}(J)\to\mathfrak{A}(I)$ and a decoding operation $D:\mathfrak{A}(I)\to\mathfrak{A}(J)$ such that the composition $E\circ T\circ D=\mathrm{id}$ is the ideal channel for all T that are localized at any subset E that contains e elements.

B. How to realize the decoder

The encoder and decoder can be related to the same adjacency matrix Λ of a graph on the union of input vertices I, output vertices J, and syndrome vertices L. For the implementation of a reasonable quantum error correcting code, which is able to correct e-errors, the matrix Λ has to fulfill the subsequent three conditions. [The following notation is used: For a matrix Θ^N_M and for two subsets $K\subset M,L\subset N$, we write $\Theta^L_K=(\Theta^l_k)_{l\in L,k\in K}$ for the corresponding sub-block. For a vector a^K we define $\Theta^L_K a^K=(\Sigma_k\Theta^l_k a^k)_{l\in L}$.]

Definition IV.2: The set of e-error correcting graphs $\mathcal{G}_e(I,J,L)$ is defined to consist of all graphs on the union of input vertices I, output vertices J, and syndrome vertices L whose adjacency matrix $\Lambda=(\Lambda^i_j)_{i,j\in IJL}$ fulfills the following conditions.

G-1: The block matrix Λ^J_{IL} is invertible with an inverse $\overline{\Lambda}^{IL}_J$.
G-2: There are no edges that connect input and syndrome vertices, i.e., the block matrix $\Lambda^{IL}_{IL}=0$ vanishes.
G-3: For all sets $E\subset J$ that contain at most $2e$ elements the condition

$$\Lambda^{J\backslash E}_{IE}q^{IE}=0 \text{ implies } q^I=0 \text{ and } \Lambda^I_E q^E=0 \tag{13}$$

is fulfilled.

Description of the encoding operation: As we have shown in Ref. 11, to an e-error correcting graph $\Lambda\in\mathcal{G}_e(I,J,L)$ corresponds the encoding channel $E_\Lambda=\mathbf{T}_{[\Lambda^{IJ}_{IJ},1_I,e^J_I]}$ of an e-error correcting code. Here e^J_I is the function from $\mathbb{F}^I$ to Ξ^J which is defined by

$$e^J_I p^I=(\Lambda^J_J\overline{\Lambda}^J_I p^I,-\overline{\Lambda}^J_I p^I). \tag{14}$$

The encoding scheme only operates on the input and output qudits and depends just on the subgraph Λ^{IJ}_{IJ} where the syndrome vertices are removed.

Interpretation: (1) The output qudits are prepared in the shift invariant state. (2) One step of the discrete dynamics, associated with the subgraph Λ^{IJ}_{IJ} is applied. (3) The input qudits are measured in x-basis. (4) Depending on the measurement outcome, a phase space translation is

done. The relation between the measurement outcome and the phase space translation is described by the "classical device" e_I^J.

Description of the decoding operation: The decoding operation makes use of the same graph $\Lambda \in \mathcal{G}_e(I,J,L)$ as the encoding operation but the vertices are interpreted differently. The output vertices J are now interpreted as inputs and, *vice versa*, the input vertices I as outputs. The syndrome vertices L are measuring vertices, to fix the error syndrome. However, the conditional phase space translation, which is performed after the measurement procedure, is more subtle as for the encoding case and relies on the following theorem:

Theorem IV.1: *Let $\Lambda \in \mathcal{G}_e(I,J,L)$ be an e-error correcting graph (see Definition IV.2). For each $q^L \in \mathbb{F}^L$ there is at most one solution $f_L^I q^L = (p^I, q^I) \in \Xi^I$ of the system of equations,*

$$p^E - \Lambda_{IEL}^J q^{IEL} = 0^J,$$

$$p^I - \Lambda_E^I q^E = 0^I, \tag{15}$$

for some $(p^E, q^E) \in \Xi^J$, provided E contains at most e elements.

Proof: Let us assume that for the two vectors $b^L, q^L \in \mathbb{F}^L$ there are solutions (a^I, b^I) and (p^I, q^I) of the system of equations,

$$a^E = \Lambda_{IEL}^J b^{IEL} \text{ and } a^I = \Lambda_E^I b^E,$$

$$p^E = \Lambda_{IEL}^J q^{IEL} \text{ and } p^I = \Lambda_E^I q^E, \tag{16}$$

respectively. The vectors (a^E, b^E) and (p^E, q^E) have components in a common set $E \subset J$ that contains at most $2e$ elements. This is true if $(a^E, b^E) = (a^K, b^K)$ and $(p^E, q^E) = (p^F, q^F)$ are independently supported in sets K and F that contain at most e elements. The set E is then their union $E = KF$. If $b^L = q^L$ holds, then the identity,

$$a^E - p^E = \Lambda_{IE}^J (b^{IE} - q^{IE}), \tag{17}$$

follows. We split the system of equations (17) into the components, belonging to the subset $E \subset J$ and its complement $J \setminus E$. This yields the identity

$$\Lambda_{IE}^{J \setminus E} (b^{IE} - q^{IE}) = 0^{J \setminus E}, \tag{18}$$

for the components in the complement $J \setminus E$. We conclude, by making use of the condition **G-3** in Definition IV.2, that $b^I = q^I$ holds as well as $\Lambda_E^I b^E = \Lambda_E^I q^E = a^I = p^I$. This implies that for a given vector $q^L = b^L$ there is indeed at most one solution $f_L^I q^L = (p^I, q^I) \in \Xi^I$ of (15). □

With the help of Theorem IV.1, we are able to define the function $d_{JL}^I : \mathbb{F}^{JL} \to \Xi^I$, which determines which conditional phase space translation $d_{JL}^I m^{JL}$ one has to perform if the measurement outcome m^{JL} has been received.

Definition IV.3: The function $d_{JL}^I : \mathbb{F}^{JL} \to \Xi^I$ assigns to each measurement outcome $m^{JL} \in \mathbb{F}^{JL}$ the phase space vector

$$d_{JL}^I m^{JL} := (p^I, q^I - \overline{\Lambda_J^I} m^J), \tag{19}$$

if (p^I, q^I) is the unique solution of (15) for $q^L = m^L + \overline{\Lambda_J^L} m^J$ and

$$d_{JL}^I m^{JL} := 0^I \tag{20}$$

if (15) has no solution for $q^L = m^L + \overline{\Lambda_J^L} m^J$.

The subsequent theorem gives a description of the decoder in terms of elementary operations on a one-way quantum computer.

Theorem IV.2: *Let $\Lambda \in \mathcal{G}_e(I,J,L)$ be an e-error correcting graph and let $D_\Lambda : \mathfrak{A}(I) \to \mathfrak{A}(J)$ be the channel,*

$$D_\Lambda := \mathbf{T}_{[-\Lambda,1_J\otimes F_L,d^I_{JL}]}, \tag{21}$$

where the function d^I_{JL} is given by Definition IV.3. Then the pair (E_Λ, D_Λ) is an e-error correcting code.

Before going into the details of the proof, we comment here how to interprete the operation D_Λ concerning one-way quantum computing. The proof of Theorem IV.2 is postponed to the next subsection "Verifying the correction property" since it requires some technical tools which are provided therein.

Interpretation: We describe now the implementation of the decoder as a four-step procedure of elementary operations on a one-way quantum computer.

Step 1: The input qudits I and the syndrome qudits L are individually prepared in the shift invariant state.
Step 2: One elementary step of the dynamics with respect to the graph $-\Lambda$ is performed.
Step 3: The syndrome qudits L are measured in z-basis and the output qudits J are measured in x-basis which produces a measurement result m^{JL} the "error syndrome."
Step 4: Depending on the "error syndrome" m^{JL} the phase space translation with respect to the vector $d^I_{JL}m^{JL}$ is performed which is the final "correction operation."

C. Verifying the correction property

We can verify that the pair (E_Λ, D_Λ) is an e-error correcting code by making use of the following useful lemmas, where we choose, for the subsequent, a fixed e-error correcting graph $\Lambda \in \mathcal{G}_e(I,J,L)$ with inputs I, outputs J, and syndrome vertices L.

Lemma IV.1: For each $(p^I,q^I) \in \Xi^I$, for each $(p^J,q^J) \in \Xi^J$, and for each $q^L \in \mathbb{F}^L$ the following identities hold:

$$\mathbf{v}_{[\Lambda,q^L]}\mathbf{x}(q^I) = \mathbf{z}(\Lambda^J_I q^I)\mathbf{v}_{[\Lambda,q^L]}, \tag{22}$$

$$\mathbf{w}(p^J,q^J)\mathbf{v}_{[\Lambda,0^L]} = \tau(q^J)\mathbf{z}(p^J - \Lambda^J_J q^J)\mathbf{v}_{[\Lambda,0^L]}\mathbf{z}(-\Lambda^I_J q^J), \tag{23}$$

$$\mathbf{v}_{[\Lambda,q^L]} = \mathbf{z}(\Lambda^J_L q^L)\mathbf{v}_{[\Lambda,0^L]}. \tag{24}$$

Proof of (22): We observe for a vector $\psi \in \mathcal{L}_2(\mathbb{F}^I), (p^I,q^I)$ and q^L that the identity,

$$[\mathbf{v}_{[\Lambda,q^L]}\mathbf{x}(q^I)\psi](b^J) = \sqrt{d}^{|I|-|J|}\sum_{b^I}\tau(b^{IJ}+q^{IL})\psi(b^I), \tag{25}$$

is valid for all b^J. Now, we make use of the fact that the relation $\tau(b^{IJ}+q^{IJ}) = \tau(b^{IJ}+q^L)\chi(\Lambda^J_I q^I, b^J)$ holds where we have used the assumption that $\Lambda^{IL}_{IL}=0$. This implies that the identity (22) is true.

Proof of (23): For a vector $\psi \in \mathcal{L}_2(\mathbb{F}^I)$ and for each p^J,q^J we apply the operator $\mathbf{w}(p^J,q^J)\mathbf{v}_{[\Lambda,0^L]}$ to $\psi \in \mathcal{L}_2(\mathbb{F}^I)$. We find for all $b^J \in \mathbb{F}^J$:

$$[\mathbf{w}(p^J,q^J)\mathbf{v}_{[\Lambda,0^L]}\psi](b^J) = \sqrt{d}^{|I|-|J|}\chi(p^J,b^J)\sum_{b^I}\tau(b^{IJ}-q^J)\psi(b^I). \tag{26}$$

We compute the term $\chi(p^J,b^J)\tau(b^{IJ}-q^J)$ as a product of four phases:

$$\chi(p^J,b^J)\tau(b^{IJ}-q^J) = \tau(q^J)\tau(b^{IJ})\chi(p^J-\Lambda^J_J q^J,b^J)\chi(-\Lambda^I_J q^J,b^I). \tag{27}$$

By means of this decomposition, the vector $\mathbf{w}(p^J,q^J)\mathbf{v}_{[\Lambda,0^L]}\psi$ can be obtained by the following sequence of operations: First we apply the multiplier operator $\psi \mapsto \psi_1 := \mathbf{z}(-\Lambda^I_J q^J)\psi$ which corresponds to multiplying the phases $\chi(-\Lambda^I_J q^J, b^I)$ for all b^I. Then we apply the isometry $\psi_1 \mapsto \psi_2 := \mathbf{v}_{[\Lambda,0^L]}\psi_1$ which corresponds to multiplying the phases $\tau(b^{IJ})$ and summation over the

b^I-variables. In the next step, the multiplier $\psi_2 \mapsto \psi_3 := \mathbf{z}(p^J - \Lambda_J^J q^J)\psi_2$ is performed due to multiplication by the phases $\chi(b^J, p^J - \Lambda_J^J q^J)$. Finally, the constant phase $\tau(q^J)$ remains and we obtain the relation $\mathbf{w}(p^J, q^J)\mathbf{v}_{[\Lambda,0^L]}\psi = \tau(q^J)\psi_3$. More explicitly, the identity

$$\mathbf{w}(p^J, q^J)\mathbf{v}_{[\Lambda,0^L]}\psi = \tau(q^J)\mathbf{z}(p^J - \Lambda_J^J q^J)\mathbf{v}_{[\Lambda,0^L]}\mathbf{z}(-\Lambda_J^I q^J)\psi, \tag{28}$$

is true which proves (23).

Proof of (24): The third identity just follows directly from the definition of the isometries $\mathbf{v}_{[\Lambda,q^L]}$. □

We prove in the Appendix that the channel D_Λ has a representation by Kraus operators $S_{q^L}, q^L \in \mathbb{F}^L$, which are labeled by syndrome configurations. By making use of Lemma A.3, we can formulate the following statement.

Lemma IV.2: If $E \subset J$ is a set that contains at most e elements. For each (p^E, q^E) there exists a $q^L \in \mathbb{F}^L$ such that the identity

$$\tau(q^E)^{-1}\mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]} = \mathbf{v}_{[\Lambda,q^L]}\mathbf{w}(-f_L^I q^L)^* = S_{q^L}, \tag{29}$$

holds where $f_L^I q^L = (p^I, q^I)$ is the unique solution of the system of equations $p^I = \Lambda_E^I q^E$ and $p^E = \Lambda_{IEL}^J q^{IEL}$.

Proof: We make use of Lemma IV.1 in order to prove (29). Combining the identities (22)–(24) we conclude that

$$\tau(q^E)^{-1}\mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]} = \mathbf{z}(p^E - \Lambda_{EIL}^J q^{IEL})\mathbf{v}_{[\Lambda,q^L]}\mathbf{w}(\Lambda_E^I q^E, -q^I)^*, \tag{30}$$

is valid for each $(p^E, q^E) \in \Xi^J$, for each $q^I \in \mathbb{F}^I$, and for each $q^L \in \mathbb{F}^L$. This can be verified as follows: First we conclude from (23) that the left hand side of (29) is equal to $\mathbf{z}(p^E - \Lambda_E^J q^E)\mathbf{v}_{[\Lambda,0^L]}\mathbf{z}(-\Lambda_E^I q^E)$. Then we apply (22) for some $q^I \in \mathbb{F}^I$ which implies that the left hand side of (29) coincides with $\mathbf{z}(p^E - \Lambda_{EI}^J q^{IE})\mathbf{v}_{[\Lambda,0^L]}\mathbf{x}(q^I)\mathbf{z}(-\Lambda_E^I q^E)$. According to (24), we derive for $q^L \in \mathbb{F}^L$ that (30) is indeed true.

We observe that for each (p^E, q^E) there exist a q^L such that that the range of $\mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]}$ coincides with the range of $\mathbf{v}_{[\Lambda,q^L]}$. In fact, we have shown in Ref. 11 that the ranges of isometries $(\mathbf{v}_{[\Lambda,q^L]})_{q^L \in \mathbb{F}^L}$ are the multiplicity spaces of characters of the Abelian algebra, the *stabilizer algebra*, that is generated by the Weyl operators $\mathbf{w}(\Lambda_J^J b^J, b^J)$ with $\Lambda_J^I b^J = 0^I$. This corresponds to the eigenvalue equation $\mathbf{w}(\Lambda_J^J b^J, b^J)\mathbf{v}_{[\Lambda,q^L]} = \tau(b^J - q^L)\mathbf{v}_{[\Lambda,q^L]}$ which can also be verfied by combining (23) and (24) in a suitable way. Since the Weyl operators $\mathbf{w}(p^E, q^E)$ and $\mathbf{w}(\Lambda_J^J b^J, b^J)$ commute up to a phase, the range of the operator $\mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]}$ is a multiplicity space of some character and therefore coincides with the range of $\mathbf{v}_{[\Lambda,q^L]}$ for some q^L, which can be computed in terms of (p^E, q^E) form (23) and (24) and the assumption **G-1** that Λ_{IL}^J is invertible with an inverse $\overline{\Lambda_J^{IL}}$. Namely q^L fulfills the identity $q^L = \overline{\Lambda_J^L}(p^E - \Lambda_E^J q^E)$. We choose $p^I := \Lambda_E^I q^E$ and $q^I := \overline{\Lambda_J^I}(p^E - \Lambda_E^J q^E)$ which implies that the system of equations $p^I = \Lambda_E^I q^E$ and $p^E = \Lambda_{IEL}^J q^{IEL}$ has a solution (p^I, q^I).

We have assumed that the set E contains at most e elements which implies, by Theorem IV.1, that $f_L^I q^L = (p^I, q^I)$ is the *unique* solution of the system of equations, which is completely determined by q^L. Thus the identity (30) becomes

$$\tau(q^E)^{-1}\mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]} = \mathbf{v}_{[\Lambda,q^L]}\mathbf{w}(-f_L^I q^L)^* = S_{q^L}, \tag{31}$$

which concludes the proof. □

Proof of Theorem IV.2: With help of Lemma IV.2 we can prove that the encoder E_Λ and the decoder D_Λ are indeed an e-error correcting code. The Kraus operators of a channel $T: \mathfrak{A}(J) \to \mathfrak{A}(J)$ that are localized in a set $E \subset J$ with at most e elements are spanned by Weyl operators $\mathbf{w}(p^E, q^E)$. In order to verify the identity $E_\Lambda \circ T \circ D_\Lambda = \mathrm{id}$ it is sufficient to show that the operators $S_{q^L}^* \mathbf{w}(p^E, q^E)\mathbf{v}_{[\Lambda,0^L]}, (p^E, q^E) \in \Xi^E, q^L \in \mathbb{F}^L$, are multiples of the identiy. By Lemma IV.2 for each (p^E, q^E) there exists a $b^L \in \mathbb{F}^L$ such that

$$S^*_{q^L}\mathbf{w}(p^E,q^E)\mathbf{v}_{[\Lambda,0^L]} \cong S^*_{q^L}S_{b^L} = \delta(q^L - b^L)\mathbf{1}, \tag{32}$$

where we have used the fact that $(S_{q^L})_{q^L\in\mathbb{F}^L}$ is a complete family of mutually orthogonal isometries. □

Interpretation of the correction procedure: We conclude by making a few remarks on the decoding procedure. The system of equation $p^I = \Lambda^I_E q^E$ and $p^E = \Lambda^J_{IEL} q^{IEL}$ has a unique solution (p^I, q^I), provided the components of the vector (p^E, q^E) has nonvanishing components for a subset E with at most e elements. This fact (Theorem IV.1) is essential for a successful decoding procedure since it identifies the effect of an error operator $\mathbf{w}(p^E, q^E)$ uniquely with an error syndrome q^L. The phase space translation by $f^I_L q^L$ is then the corresponding correction operation which eliminates the effect of the error.

However, if we relax the condition that the error occurs at a set E of at most e qudits, then the decoding operation can fail. For a general error operator $\mathbf{w}(a^J, b^J)$ the identity

$$\tau(b^J)^{-1}\mathbf{w}(a^J,b^J)\mathbf{v}_{[\Lambda,0^L]} = \mathbf{v}_{[\Lambda,q^L]}\mathbf{w}(-a^I,-b^I)^* \tag{33}$$

holds where the error syndrome is related to the error by $q^L = \overline{\Lambda^L_J}(a^J - \Lambda^J_J b^J)$. The protected subspace is affected by the effective error (a^I, b^I) which is given by $a^I := \Lambda^I_E q^E$ and $b^I := \overline{\Lambda^I_J}(a^J - \Lambda^J_J b^J)$. The solution $f^I_L q^L$, which corresponds to some other error (p^E, q^E) on $e = |E|$ qudits, may be different from $(a^I, b^I) \neq f^I_L q^L$. Thus the error (a^J, b^J) causes a nontrivial effective error $\mathbf{w}(-f^I_L q^L)\mathbf{w}(-a^I, -b^I)^*$ on the protected subspace which cannot be corrected by the decoding operation. Namely we have

$$S^*_{q^L}\mathbf{w}(a^J,b^J)\mathbf{v}_{[\Lambda,0^L]} = \tau(b^J)\mathbf{w}(-f^I_L q^L)\mathbf{w}(-a^I,-b^I)^* \neq \mathbf{1}, \tag{34}$$

and the correction procedure fails.

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APPENDIX: KRAUS REPRESENTATIONS FOR THE ENCODER AND THE DECODER

The encoding and decoding operations are channels of the type given by Definition IV.1. We give here a Kraus representation for a general channel of this kind.[15]

Lemma A.1: Let Λ be the adjacency matrix of a graph with input vertices I, output vertices J, and measuring vertices K. Let $U_{IK} \in \mathfrak{A}(IK)$ be a local unitary opertor and let f^I_{KL} be a function form $\mathbb{F}^{IK}$ to Ξ^J. The channel $\mathbf{T}_{[\Lambda,U_{IK},f^J_{IK}]}$ can be represented by d^{IK} Kraus operators,

$$\mathbf{T}_{[\Lambda,U_{IK},f^J_{IK}]}(A) = \sum_{p^{IK}} T^*_{p^{IK}} A T_{p^{IK}}, \tag{A1}$$

where for each $p^{IK} \in \mathbb{F}^{IK}$ the corresponding Kraus operator is given by

$$T_{p^{IK}} = \mathbf{w}(f^J_{IK}p^{IK})\Phi^*_{IK}\mathbf{z}(-p^{IK})U^*_{IK}u(\Lambda)\Phi_{JK}. \tag{A2}$$

Proof: The preparation channel $\mathbf{E}_{1_{JK}}$ is pure and implemented by the isometry Φ_{JK}. The dynamics $\boldsymbol{\alpha}_\Lambda$ is implemented by the unitary operator $u(\Lambda)$. The Kraus operators for the local measurement operation $\mathbf{M}_{U_{IK}}$ are given by the co-isometries $\Phi^*_{IK}\mathbf{z}(-p^{IK})U^*_{IK}$; each of them corresponds to the measurement outcome $p^{IK} \in \mathbb{F}^{IK}$. Finally, the Kraus operators for the conditional phase space translation are the Weyl operators $\mathbf{w}(f^J_{IK}p^{IK}), p^{IK} \in \mathbb{F}^{IK}$. Thus a Kraus representation for the channel $\mathbf{T}_{[\Lambda,U_{IK},f^J_{IK}]}$ is indeed given by the operators

$$T_{p^{IK}} = \mathbf{w}(f^J_{IK} p^{IK})^* \Phi^*_{IK} \mathbf{z}(-p^{IK}) U^*_{IK} u(\Lambda) \Phi_{JK}, \tag{A3}$$

with $p^{IK} \in \mathbb{F}^{IK}$. □

In Ref. 11 it is shown how to associate to an e-error correcting graph $\Lambda \in \mathcal{G}_e(I,J,L)$ (Definition IV.2) a complete family of mutually orthogonal isometries $(\mathbf{v}_{[\Lambda,q^L]})_{q^L \in \mathbb{F}^L}$. Each of the isometries map the input Hilbert space $\mathcal{L}_2(\mathbb{F}^I)$ into the output Hilbert space $\mathcal{L}_2(\mathbb{F}^J)$. For $q^L \in \mathbb{F}^L$, the corresponding isometry is given by

$$(\mathbf{v}_{[\Lambda,q^L]}\psi)(q^J) = \frac{1}{\sqrt{d}^{|J|}} \sum_{q^I} \tau(q^{IJL}) \psi(q^I), \tag{A4}$$

with $\psi \in \mathcal{L}_2(\mathbb{F}^I)$ and $q^J \in \mathbb{F}^J$. The range of $\mathbf{v}_{[\Lambda,q^L]}$ is the protected subspace of a graph code.[9] To point out the relation to the Kraus representation of Lemma A.1 we claim that the the isometry $\mathbf{v}_{[\Lambda,q^L]}$ can also be represented by

$$\mathbf{v}_{[\Lambda,q^L]} = \sqrt{d}^{|I|} \Phi^*_{IL} u(\Lambda) \mathbf{x}(q^L) F_L \Phi_{JL}. \tag{A5}$$

In Ref. 11 we have shown that the following is true.

Lemma A.2: The encoding operation $E_\Lambda = \mathbf{T}_{[\Lambda^{IJ}_{IJ}, 1_I, e^J_I]} : \mathfrak{A}(J) \to \mathfrak{A}(I)$ *is pure and for all* $A \in \mathfrak{A}(J)$ *the identity,*

$$E_\Lambda(A) = \mathbf{v}^*_{[\Lambda,0^L]} A \mathbf{v}_{[\Lambda,0^L]}, \tag{A6}$$

is valid.

By making use of Lemma A.1, we also obtain a useful Kraus representation for the decoding channel in terms of the isometries $\mathbf{v}_{[\Lambda,q^L]}, q^L \in \mathbb{F}^L$. For this purpose, we introduce the function function $f^I_L : \mathbb{F}^L \to \Xi^I$ by $f^I_L q^L = 0^I$ if the equation (15) has no solution for q^L. Otherwise, we put

$$f^I_L q^L = (p^I, q^I), \tag{A7}$$

where the phase space vector (p^I, q^I) is the *unique* solution (Theorem IV.1) of the equation (15), that is, $p^I = \Lambda^I_E q^E$ and $p^E = \Lambda^J_{IEL} q^{IEL}$ holds for some vector (p^E, q^E) which has nonvanishing components in for a set $E \subset J$ which contains at most e elements.

Lemma A.3: The decoding channel $D_\Lambda : \mathfrak{A}(I) \to \mathfrak{A}(J)$ *has a Kraus representation,*

$$D_\Lambda(B) = \sum_{q^L} S_{q^L} B S^*_{q^L}, \tag{A8}$$

where for $q^L \in \mathbb{F}^L$ *the Kraus operator* S_{q^L} *is given by*

$$S_{q^L} = \mathbf{v}_{[\Lambda,q^L]} \mathbf{w}(-f^I_L q^L)^*. \tag{A9}$$

In particular, the operators $(S_{q^L})_{q^L \in \mathbb{F}^L}$ *form a complete family of mutually orthogonal isometries and* D_Λ *is* an **-algebra homomorphism.*

Proof: By Lemma A.1 we conclude that D_Λ has a representation by the Kraus operators,

$$\widetilde{S}_{m^{JL}} := \Phi^*_{IL} u(\Lambda) F_L \mathbf{z}(m^{JL}) \Phi_{JL} \mathbf{w}(d^I_{JL} m^{JL}), \tag{A10}$$

with $m^{JL} \in \mathbb{F}^{JL}$. By the definition of the function d^I_{JL}, the identity $d^I_{JL} m^{JL} = (p^I, q^I - \overline{\Lambda^I_J} m^J)$ holds for $(p^I, q^I) = f^I_L q^L$ and for $m^L = q^L - \overline{\Lambda^L_J} m^J$. Inserting this into (A10) yields

$$\widetilde{S}_{m^{JL}} = \Phi^*_{IL} u(\Lambda) \mathbf{z}(m^J) \mathbf{x}(-q^L + \overline{\Lambda^L_J} m^J) F_L \Phi_{JL} \mathbf{w}(p^I, q^I - \overline{\Lambda^I_J} m^J), \tag{A11}$$

where we have used the relation $F_L \mathbf{z}(q^L) = \mathbf{x}(q_L) F_L$. Since $\mathbf{x}(\overline{\Lambda^I_J} m^J)$ is localized in I and commutes with $F_L \Phi_{JL}$. This yields

$$\tilde{S}_{m^{JL}} \cong \Phi^*_{IL}\mathbf{z}(m^J)u(\Lambda)\mathbf{x}(q^L - \overline{\Lambda}^{IL}_J m^J)F_L\Phi_{JL}\mathbf{w}(p^I,q^I)^*, \tag{A12}$$

where we write $S \cong S'$ if $S = e^{i\theta}S'$ holds for some phase $e^{i\theta}$. In the next step we use the commutation relation $u(\Lambda)\mathbf{x}(a^{IL}) = \mathbf{w}(\Lambda^J_{IL}a^{IL}, a^{IL})u(\Lambda)$ and the fact that Φ^*_{IL} has the invariance property $\Phi^*_{IL}\mathbf{x}(a^{IL}) = \Phi^*_{IL}$. This implies

$$\tilde{S}_{m^{JL}} \cong \Phi^*_{IL}u(\Lambda)F_L\mathbf{z}(q^L)\Phi_{JL}\mathbf{w}(-p^I,-q^I)^* = \frac{1}{\sqrt{d}^{|J|}}S_{q^L}, \tag{A13}$$

where we have used the identity (A5) for the isometry $\mathbf{v}_{[\Lambda,q^L]}$. Thus D_Λ has a representation by the Kraus operators $(S_{q^L})_{q^L\in\mathbb{F}^L}$. We have shown in Ref. 11 that $(\mathbf{v}_{[\Lambda,q^L]})_{q^L\in\mathbb{F}^L}$ is a family of mutually orthogonal isometries and thus the same holds for Kraus operators $(S_{q^L})_{q^L\in\mathbb{F}^L}$ too. That is, $S^*_{q^L}S_{a^L} = \delta(q^L - a^L)\mathbf{1}$ and $\Sigma_{q^L}S_{q^L}S^*_{q^L} = \mathbf{1}$ holds and D_Λ is a homomorphism. □

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Non-null Lie quadratics in E^3

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Interpolation problems in the space SO(3) of rotations of Euclidean 3-space E^3 are reviewed in Secs. I and II as background and motivation to a study of curves in E^3 called Lie quadratics. Except for a special class called null, Lie quadratics have resisted analysis until now. The rest of the present paper is devoted to new results showing non-null Lie quadratics have rich analytical, geometrical, and asymptotic structures: rates of growth are studied using differential equations and inequalities, Lie quadratics are proved to be extendible over the whole of $\mathbb{R}$, and existence of axes is proved under fairly general conditions. Examples show sharpness of many results. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1803609]

I. INTRODUCTION

Interpolating in the group SO(3) of rotations of Euclidean 3-space E^3, and in Riemannian manifolds generally, is a more significant task, in terms of applications and mathematics, than might at first be suspected. To place the new mathematical results of the present paper in context, we first say something about applications and previous mathematical work. Interpolation in SO(3) is very different to the standard problem of interpolation in E^3.

Example 1: *A rigid body K, perhaps a camera, is free to rotate about the origin* **0** *in Euclidean 3-space* E^3. *Configurations* x_i, *and possibly angular velocities* v_i, *are specified at times* $i=0, T$. *The problem is to move K accordingly. At time t the configuration* $x(t)$ *is given by a positively oriented orthonormal frame* $(x_1(t), x_2(t), x_3(t))$ *fixed relative to K. Equivalently,* $x(t)$ *is the rotation matrix*

$$\begin{bmatrix} x_1(t) & x_2(t) & x_3(t) \end{bmatrix} \in \mathrm{SO}(3),$$

and so we have an interpolation problem for a curve $x:[0,T]\to \mathrm{SO}(3)$. *In the simplest case, where angular velocities are not specified at endpoints, the interpolation conditions are*

$$x(0)=x_0, \quad x(T)=x_T. \tag{1}$$

If our elementary problem was posed in E^3, *instead of SO(3), the affine line segment from* x_0 *to* x_T *would probably be chosen as interpolant. However, although SO(3) is contained in the Euclidean space* $M_{3\times 3}\cong E^9$ *of real* 3×3 *matrices, an affine line in* E^9 *intersects SO(3) in at most two points. So line segments are not available for interpolation in SO(3). However SO(3) is covered by open subsets U diffeomorphic to open subsets of* E^3. *Such covers must contain several open sets, because U cannot be the whole of SO*(3). *For instance, rotations may be mapped to Euler angles* $(\psi,\theta,\phi)\in[0,2\pi)\times[0,\pi)\times[0,2\pi)\subset E^3$. *Chart-based interpolation proceeds by mapping* x_0, x_T *to points in* E^3, *interpolating in* E^3 *then mapping the interpolant back into SO(3). This prescription is less straightforward than it sounds. For instance, if the Euler angle of* x_i *are* $(\psi_i,\theta_i,\phi_i)=\Phi(x_i)$ *for* $i=0, T$, *small perturbations in* x_i *can give large changes in* ψ_i, ϕ_i *when* $\theta_i\approx 0$. *Also, whether the* θ_i *are small or not, the chart-based interpolant x may be a very unnatural choice. For example, taking*

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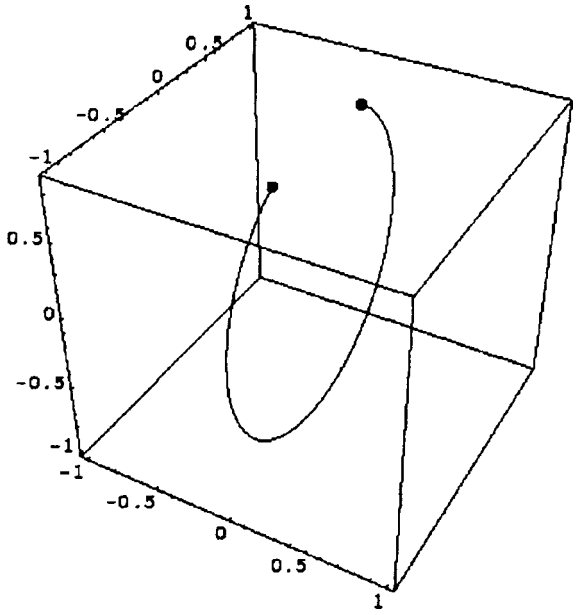

FIG. 1. Lens directions with chart-based linear interpolation.

$$x_{jT} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt{3}/2 & (-1)^j/2 \\ 0 & (-1)^{j+1}/2 & \sqrt{3}/2 \end{bmatrix},$$

where $j=0, 1$, *the curve of directions of the camera lens takes the long way around (Fig. 1).*

Although these difficulties can be ameliorated by switching between charts, this complicates implementation and has unwelcome side effects: the interpolant from x_T *to* x_0 *may be different to that from* x_0 *to* x_T. □

The geometrical difficulties in Example 1 suggest using a more geometrical interpolation scheme, like the following simple method from Riemannian geometry. A *Riemannian metric* on a C^∞ manifold M such as SO(3) is a smooth assignment of inner products to the tangent spaces at each point in M. The *length* $L(x)$ and *energy* $J_1(x)$ *of a smooth curve* $x:[0,T]\to \mathrm{SO}(3)$ are then defined as

$$L(x) = \int_0^T \|x^{(1)}(t)\| \mathrm{d}t \quad \text{and } J_1(x) = \int_0^T \|x^{(1)}(t)\|^2 \, \mathrm{d}t,$$

where the norm $\|\,\|$ is calculated using the Riemannian metric, and superscript (n) means n-fold derivative. Curves satisfying (1) of minimum length and uniform speed are called *minimal geodesics*. They also minimize energy. Geodesics on SO(3) can sometimes be written down in closed form, notably when the metric is *bi-invariant*. In this case rotations are represented by unit quaternions, namely points in the three-dimensional unit sphere $S^3 \subset E^4$, with geodesics represented by arcs of great circles. Interpolation by geodesics effectively deals with the problems raised in Example 1, but is inadequate for most applications.

In Example 1 only two camera configurations x_0, $x_T \in \mathrm{SO}(3)$ are prescribed, whereas in practice x may need to satisfy many such constraints. Piecewise geodesics are inappropriate because, like piecewise-linear curves in E^3, they are usually nondifferentiable at junctions. A simple way to ensure this does not occur is to prescribe derivatives of x at junctions, replacing (1) by

$$x(0)=x_0,\ \ x^{(1)}(0)=v_0,\ \ x(T)=x_T,\ \ x^{(1)}(T)=v_T. \tag{2}$$

If the problem was posed in E^3 a cubic polynomial could satisfy (2), but SO(3) has no nonconstant polynomial curves, and chart-based cubic polynomials are problematic in the same ways as chart-based line segments. On the other hand, geodesics in SO(3) are readily calculable, at least for a bi-invariant metric, and correspond to lines in E^3. This reminds us of the classical *deCastlejau algorithm* for generating polynomial curves in E^3 from line segments.

Replacing line segments by geodesic arcs in the cubic deCastlejau algorithm gives curves in SO(3) capable of satisfying (2), as in Refs. 29 and 12. This elegant and effective method is frequently applied, and has been investigated further in Ref. 11. A recursive form of the deCastlejau algorithm also adapts to Hermite interpolation in SO(3).[19–23] Unlike the Euclidean versions, the adapted nonrecursive and recursive deCastlejau schemes generate different curves in SO(3). Yet another kind of curve results when we insist on an analogue of the important *variation diminishing property*, that cubics in E^3 minimize

$$\int_0^T \|x^{(2)}(t)\|^2\,\mathrm{d}t$$

among curves $x:[0,T]\to E^3$ satisfying (2).

II. RIEMANNIAN CUBICS AND LIE QUADRATICS

A Riemannian manifold comes equipped with a *Levi–Cività covariant derivative* ∇, which is a procedure for differentiating vector fields, whose associated *parallel translation* respects the Riemannian metric. *Riemannian cubics* are critical points of the functional J_2 given by

$$J_2(x)=\int_0^T \|\nabla_{d/\mathrm{d}t}\,x^{(1)}\|^2\,\mathrm{d}t, \tag{3}$$

where $x:[0,T]\to M$ satisfies (2). As shown in Refs. 13 and 26, the Euler–Lagrange equation of J_2 is

$$\nabla^3_{d/\mathrm{d}t}\,x^{(1)}+R(\nabla_{d/\mathrm{d}t}\,x^{(1)},x^{(1)})x^{(1)}=\mathbf{0}, \tag{4}$$

where R is the *Riemannian curvature* of ∇. Let M be SO(3) with a bi-invariant Riemannian metric. Then, as it stands, (4) amounts to 36 nonlinear first order ODEs for 36 scalar functions, with 24 equality constraints, and 36 scalar boundary conditions. The first step in solving this system is the reduction in Ref. 26 of (4) to a second order system of ODEs for $V:[0,T]\to E^3$,

$$V^{(2)}(t)=V^{(1)}(t)\times V(t)+C\ \text{ where } C\in E^3, \tag{5}$$

together with the first order equation

$$x^{(1)}(t)=x(t)B(V(t)), \tag{6}$$

where $B:E^3\to so(3)$ is the linear isomorphism from E^3 onto the space of skew-symmetric 3×3 real matrices given by $B(v)(w)=v\times w$, and $\times$ denotes the vector product in E^3. In Sec. IV of the present paper Eqs. (5) and (6) are shown to be solvable over the whole real line. In Ref. 25, Eq. (6) is solved using at most one quadrature. For any interval $S\subseteq\mathbb{R}$, a curve $V:S\to E^3$ satisfying (5) is called a *Lie quadratic* in E^3. Defining $F:S\to[0,\infty)$ by $F(t)=\|V(t)\|^2$, it follows easily from (5) that

$$F^{(2)}(t)=6\langle C,V(t)\rangle+2b, \tag{7}$$

$$\|V^{(1)}(t)\|^2=2\langle C,V(t)\rangle+b, \tag{8}$$

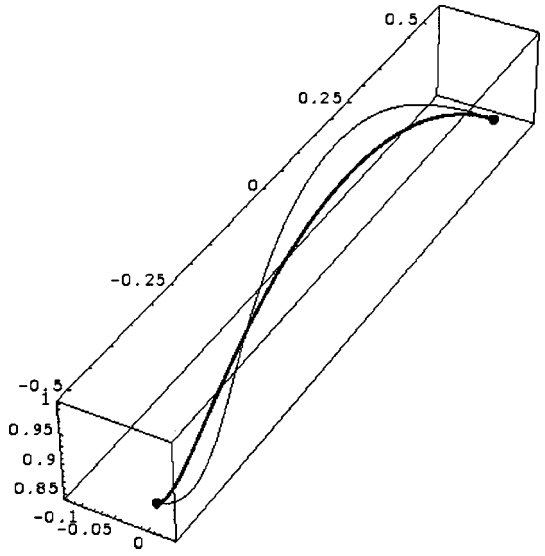

FIG. 2. Lens directions for the Riemannian cubic.

$$\|V^{(2)}(t)\|^2 = c, \tag{9}$$

where b, $c \in \mathbb{R}$ are constant. Set $d = 3(\|C\|^2 + c)$ and $\delta_\pm = 3(\|C\| \pm \sqrt{c})^2$.

Example 2: *Taking* v_0, v_T *as*

$$\begin{bmatrix} 0.0000 & 0.9280 & -0.3725 \\ -0.6175 & -0.1225 & 0.2121 \\ 0.7866 & -0.2121 & -0.1225 \end{bmatrix}, \begin{bmatrix} 0.0000 & -0.2708 & -0.2380 \\ 0.1155 & -0.0224 & -0.0388 \\ 0.3415 & 0.0388 & -0.0224 \end{bmatrix},$$

the curve of lens directions for the Riemannian cubic shown (thick) in Fig. 2 is less wavy in appearance than the curve for the adapted nonrecursive deCastlejau algorithm of Sec. I. These curves were generated in about 7 seconds on a 2 GHz PC running Mathematica. □

There is a special class of Lie quadratics for which quite a lot is known: the Lie quadratic $V: S \to E^3$ is called *null* when its constant C is $\mathbf{0}$. In Ref. 24 null Lie quadratics in E^3 are shown to have constant (usually nonzero) curvature, linearly varying torsion, and two *axes*. The axes are rays through $\mathbf{0}$, to which V becomes C^0 close as $t \to \pm\infty$. The space of null Lie quadratics has rotational symmetry, and individual null quadratics have *internal symmetry*. A Riemannian cubic in SO(3) associated with a null Lie quadratic also has internal symmetries and is asymptotic to a pair of geodesics.

Example 3: Figure 3 shows the null Lie quadratic $V: [0, 26] \to E^3$ *with* $V(0)$, $V^{(1)}(0)$ *taken as*

$$\begin{bmatrix} 3.2734 & 0.6697 & -5.1300 \end{bmatrix}^{\mathbf{T}}, \begin{bmatrix} -0.2320 & -0.0935 & 0.3427 \end{bmatrix}^{\mathbf{T}},$$

where $\mathbf{T}$ *means transpose. The Lie quadratic starts in the lower right, spiralling outwards along an axis pointing upwards and to the left. Around* $V(14)$ *the curve spirals inwards along the other axis, which points to the left and slightly downwards.*

Figure 4 shows the curve x_1 *in* S^2 *of first columns of* $x: [0, 26] \to SO(3)$ *associated with the null Lie quadratic V.*

x_1 *spirals downwards from a closed curve in the upper left, switches, then spirals upwards towards a closed curve in the lower right (note the change in sense of spiralling). The limiting*

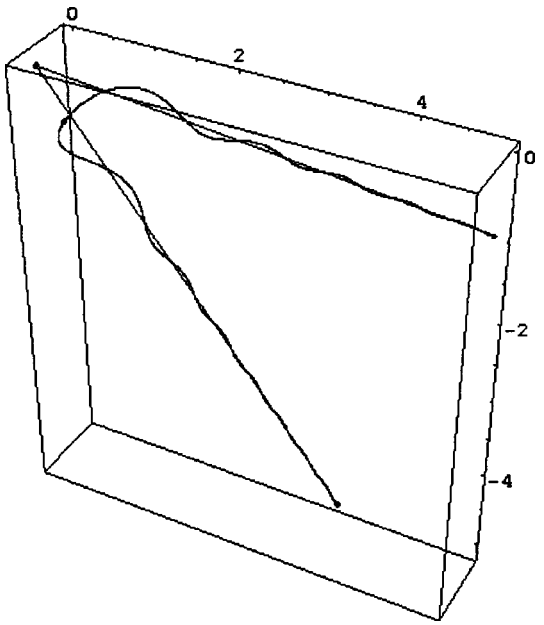

FIG. 3. Null Lie quadratic V in E^3, showing $V(0)$, $V(14.3)$, $V(26)$, and axes.

curves are projections of geodesics in SO(3), namely circles in S^2. Self-symmetry of x is not evident on casual inspection. □

In addition to references already cited, for further background on null Lie quadratics, Riemannian cubics, variational problems, reduction to Lie quadratics, generalizations, and alternatives see Refs. 6, 16, 28, 14, 15, 33–35, 10, 18, 8, 9, 30, and 2. For engineering applications see Refs. 17, 4, 27, 5, 3, 31, and 32.

For the larger class of non-null Lie quadratics V we note that if $A \in \mathrm{SO}(3)$ then $t \mapsto AV(t)$ is a non-null Lie quadratic with constant AC, if $t_0 \in \mathbb{R}$ then $t \mapsto V(t-t_0)$ is a non-null Lie quadratic with

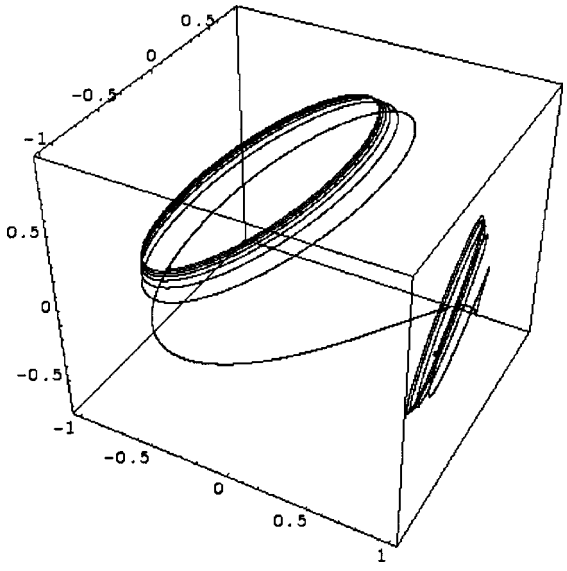

FIG. 4. $x_1:[0,26] \to S^2$, $x_1(0)$, $x_1(14.3)$, $x_1(26)$.

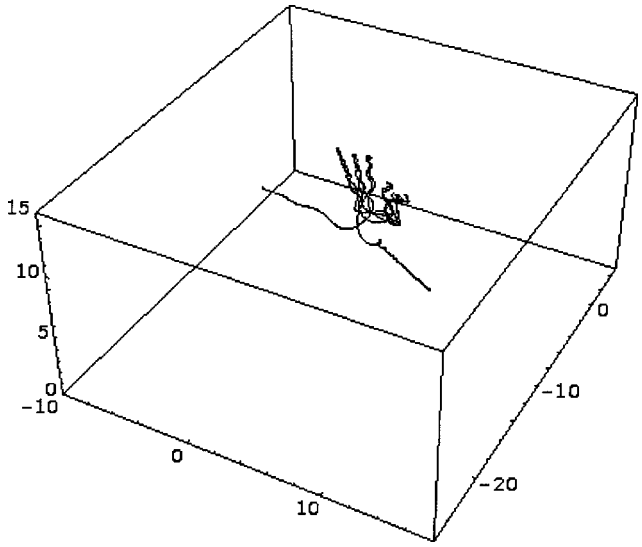

FIG. 5. $V:[-45,30]\to E^3$ computed with 16 significant figures in Example 4.

constant C, and if $0\neq a_1\in\mathbb{R}$ then $t\mapsto a_1V(a_1t)$ is a non-null Lie quadratic with constant a_1^3C. So after a rotation, change of origin, and change of scale a non-null Lie quadratic $V:\mathbb{R}\to E^3$ can be made to satisfy

$$C=\begin{bmatrix}1 & 0 & 0\end{bmatrix}^{\mathbf{T}},\quad V_1(0)=0,\quad \langle V(0),V^{(1)}(0)\rangle=0.$$

The geometry of Lie quadratics is much more complicated in the non-null case.

Example 4: Taking $V(0)=[1.0\ 2.0\ 2.0]^{\mathbf{T}}$, $V^{(1)}(0)=[-1.0\ 1.0\ 1.0]^{\mathbf{T}}$, *and* $C=-[0.4\ 0.5\ 0.75]^{\mathbf{T}}$, *we find*

$$b=8.800\,00,\quad c=20.4742,\quad d=64.34,\quad \delta_-=37.5669,\quad \delta_+=91.1131.$$

Numerical simulation with Mathematica's default 16 *significant figures working precision gives Fig. 5 for* $V:[-45,30]\to E^3$. *The curve appears to spiral backwards and forwards along rays through the origin.* □

From this point onwards the results are new, emphasizing the squared-norm function F of a Lie quadratic V. There are seven theorems, all central to the paper. These emphasize asymptotic properties of V, through a detailed analysis of F and its relationship to the constants $b,c,d,\delta_\pm$.

(i) Lie quadratics in E^3 (whether null or not) extend to Lie quadratics defined on the whole of $\mathbb{R}$ (Corollary 5), as do Riemannian cubics (Theorem 2), and can be sensitive to initial data (Example 5).
(ii) F satisfies various differential inequalities and differential equations (Theorem 1).
(iii) F satisfies a nonlinear third-order differential equation (11) from which follow further inequalities (Corollaries 1 and 2), and a second order equation (14) for $G\equiv(F^{(1)})^2$.
(iv) When $b<0$ F is strictly convex, with $F(t)$ increasing as t^4 for $t\to\pm\infty$ (Theorem 3).
(v) For $b>0$ V can be periodic (Example 6) and sometimes F is multimodal (Example 5).
(vi) For $b\geqslant 0$ V is often unbounded (Theorem 5) and then $F(t)$ increases as t^2 or t^4.
(vii) For $b\geqslant 0$ there are relationships between critical values of F (Theorem 5, Example 9).
(viii) When V is unbounded the angular part $U(t)$ of $V(t)$ converges to a limit $\alpha_\pm(V)$ as $t\to\pm\infty$ (Theorem 6) with $a_\pm\equiv\langle C,\alpha_\pm(V)\rangle\geqslant 0$ (Corollary 9).
(ix) When V is unbounded $F(t)=O(t^2)$ as $t\to\pm\infty$ if and only if $a_\pm=0$ (Theorem 7).
(x) The asymptotic directions $\alpha_\pm(V)$ may be difficult to determine (Example 11).

Properties of F, as well as being of interest in their own right, are the key to the rest of our analysis. Whereas in the null case F is a quadratic polynomial, the possibilities when V is non-null are more various and take a little longer to unfold, starting with some differential equations and inequalities.

III. DIFFERENTIAL EQUATIONS AND INEQUALITIES

Let $V:S\to E^3$ be a Lie quadratic defined on an open interval S, with constant vector C, $F:S\to[0,\infty)$, and associated constants $b,c,d,\delta_\pm$ as defined in Sec. II. A result similar to the following theorem appeared independently in Ref. 1.

Theorem 1: $F\geqslant 0$, $F^{(2)}+b=3\|V^{(1)}\|^2\geqslant 0$,

$$\delta_-\leqslant (F^{(2)}+b)F-\tfrac{3}{4}(F^{(1)})^2=d-F^{(4)}\leqslant\delta_+, \tag{10}$$

and

$$\begin{aligned}48F(F^{(3)})^2-48F^{(1)}(F^{(2)}-2b)F^{(3)}+64b^3+48d^2-96bdF+48b^2F^2+72d(F^{(1)})^2-72bF(F^{(1)})^2\\ +27(F^{(1)})^4-96dFF^{(2)}+96bF^2F^{(2)}-72F(F^{(1)})^2F^{(2)}-48b(F^{(2)})^2+48F^2(F^{(2)})^2+16(F^{(2)})^3\\ -576d\|C\|^2+1728\|C\|^4=0.\end{aligned} \tag{11}$$

Proof: Eliminating $\langle C,V\rangle$ between (7) and (8), $\|V^{(1)}\|^2=\frac{1}{3}(F^{(2)}+b)$. By (9) and (5), $\|V^{(1)}\|^2F-\langle V^{(1)},V\rangle^2+2\langle C,V^{(1)}\times V\rangle+\|C\|^2=c$. Then

$$\tfrac{1}{3}(F^{(2)}+b)F-\tfrac{1}{4}(F^{(1)})^2+2\langle C,V^{(1)}\times V\rangle+\|C\|^2=c.$$

Differentiating (7) twice, and by (5), $F^{(4)}=6\langle C,V^{(1)}\times V+C\rangle$ and consequently

$$\langle C,V^{(1)}\times V\rangle=\tfrac{1}{6}F^{(4)}-\|C\|^2. \tag{12}$$

For (10), it remains to prove $\delta_-\leqslant d-F^{(4)}\leqslant\delta_+$: by (7), $|F^{(4)}|=6|\langle C,V^{(2)}\rangle|\leqslant 6\|C\|\sqrt{c}$. So

$$\delta_-=3(\|C\|-\sqrt{c})^2\leqslant d-F^{(4)}\leqslant 3(\|C\|+\sqrt{c})^2=\delta_+,$$

and this proves (10). Now $F^{(4)}=6\langle C,C\rangle+6\langle C,V^{(1)}\times V\rangle$ by (5), and then

$$\begin{aligned}\left(\frac{F^{(4)}}{6}-\|C\|^2\right)^2&=\|C\|^2(\|V^{(1)}\|^2\|V\|^2-\langle V^{(1)},V\rangle^2)-\|\langle C,V\rangle V^{(1)}-\langle C,V^{(1)}\rangle V\|^2\\ &=\|C\|^2\left(\left(\frac{F^{(2)}+b}{3}\right)F-\frac{(F^{(1)})^2}{4}\right)-\left(\frac{F^{(2)}-2b}{6}\right)^2\left(\frac{F^{(2)}+b}{3}\right)\\ &\quad-\left(\frac{F^{(3)}}{6}\right)^2F+\left(\frac{F^{(2)}-2b}{6}\right)\frac{F^{(3)}}{6}F^{(1)}.\end{aligned}$$

Eliminating $F^{(4)}$ with (10) gives (11). □

Corollary 1: $64b^3F+48d^2F-96bdF^2+48b^2F^3-48b^2(F^{(1)})^2+72dF(F^{(1)})^2-72bF^2(F^{(1)})^2+27F(F^{(1)})^4-96dF^2F^{(2)}+96bF^3F^{(2)}+48b(F^{(1)})^2F^{(2)}-72F^2(F^{(1)})^2F^{(2)}-48bF(F^{(2)})^2+48F^3(F^{(2)})^2-12(F^{(1)})^2(F^{(2)})^2+16F(F^{(2)})^3-576d\|C\|^2F+1728\|C\|^4F\leqslant 0$.

Proof: Equation (11) is quadratic in $F^{(3)}$, with discriminant -192 times the left-hand side. □

Corollary 2: At a critical point t_0 of F where $F(t_0)>0$,

$$(F^{(2)})^3-3b(F^{(2)})^2+3(d-bF-FF^{(2)})^2-108\|C\|^2c+4b^3\leqslant 0.$$

Proof: Set $F^{(1)}=0$ in Corollary 1 and divide both sides by $16F$. □

Writing $G=(F^{(1)})^2$ for $F^{(1)}\neq 0$,

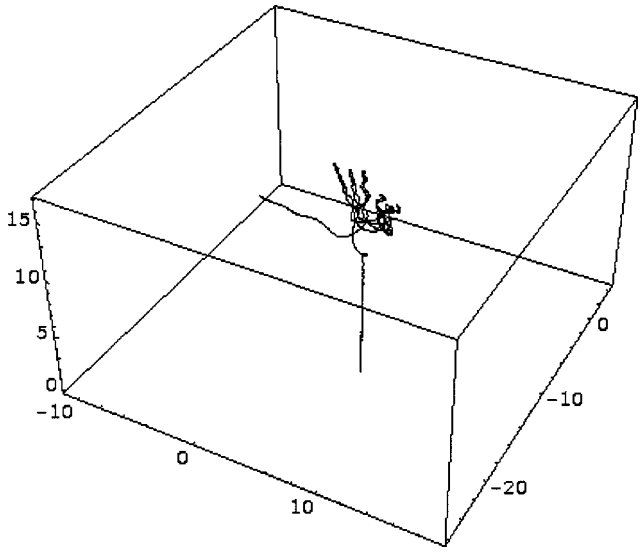

FIG. 6. $V:[-45,30]\to E^3$ computed with 25 significant figures in Example 5.

$$F^{(2)}=\frac{1}{2}\frac{\mathrm{d}G}{\mathrm{d}F},\quad F^{(3)}=\frac{\epsilon}{2}G^{1/2}\frac{\mathrm{d}^2G}{\mathrm{d}F^2},\quad F^{(4)}=\frac{1}{2}G\frac{\mathrm{d}^3G}{\mathrm{d}F^3}+\frac{1}{4}\frac{\mathrm{d}G}{\mathrm{d}F}\frac{\mathrm{d}^2G}{\mathrm{d}F^2},$$

where ϵ is the sign of $F^{(1)}$. Then, from (10) and (11), we have the following.

Corollary 3: In any open interval where $F^{(1)}\neq 0$,

$$2G^2\frac{\mathrm{d}^3G}{\mathrm{d}F^3}+\frac{\mathrm{d}G}{\mathrm{d}F}\frac{\mathrm{d}^2G}{\mathrm{d}F^2}+2F\frac{\mathrm{d}G}{\mathrm{d}F}-3G+4bF-4d=0, \tag{13}$$

and

$$12\frac{\mathrm{d}^2G}{\mathrm{d}F^2}\left(4bG-G\frac{\mathrm{d}G}{\mathrm{d}F}+FG\frac{\mathrm{d}^2G}{\mathrm{d}F^2}\right)+2\left(\frac{\mathrm{d}G}{\mathrm{d}F}\right)^3-12\frac{\mathrm{d}G}{\mathrm{d}F}\left(4F-4bF^2+b\frac{\mathrm{d}G}{\mathrm{d}F}+3FG-F^2\frac{\mathrm{d}G}{\mathrm{d}F}\right)$$
$$+9G(8d-8bF+3G)+48bF(bF-2d)+16(4b^3+3d^2-36d\|C\|^2+108\|C\|^4)=0. \tag{14}$$

□

Despite extreme sensitivity of solutions of (5) to numerical measurements, the evidence suggests these inequalities are sharp.

Example 5: In Example 4, numerical simulation with 16 significant figures working precision gives Fig. 5 for $V:[-45,30]\to E^3$. *Figure 6, using 25 significant figures (our default from now on), is noticeably different, although the two figures share some similarities in general appearance.*

In particular, both Figs. 5 and 6 suggest F is multimodal. The graph of $F|[-45,30]$ *in Fig. 7 shows more detail: eight points of local minimum and seven of local maximum. In Fig. 6, the curve starts from around the right of the front panel, spirals outwards then, after sporadic spiralling in the middle range, spirals outwards to the panel on the left.*

In Fig. 8 $d-F^{(4)}$ *is plotted together with the horizontal lines through* $\delta_\pm$. $F^{(4)}$ *appears is highly oscillatory, and the inequalities in (10) seem sharp.*

Corollary 1 is also sharp, as illustrated by the plot in Fig. 9 of the left-hand side of the inequality.

However, for a null Lie quadratic F is a quadratic polynomial.[24] □

Another basic fact is the extendibility of Riemannian cubics and Lie quadratics from intervals S to the whole of $\mathbb{R}$. The following inequality is needed for the proof in Sec. IV.

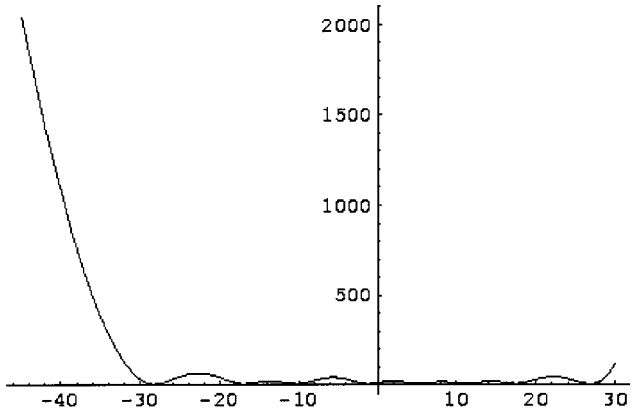

FIG. 7. F in Example 5.

Corollary 4: Given $t_0 \in S$, there are constants $\kappa_0, \kappa_2 > 0$ depending only on $V(t_0)$, $V^{(1)}(t_0)$, $V^{(2)}(t_0)$ such that, for all $t \in S$,

$$\|V(t)\|, \|V^{(1)}(t)\|^2 \leqslant \kappa_2^2 t^2 + \kappa_0^2.$$

Proof: For $t \in S$, $|F^{(4)}(t)| \leqslant 6\|C\|\sqrt{c}$. So when $t \geqslant t_0$, $|F^{(3)}(t)| \leqslant |F^{(3)}(t_0)| + 6\|C\|\sqrt{c}(t-t_0)$. Then $|F^{(2)}(t)| \leqslant k_0 + k_1(t-t_0) + k_2(t-t_0)^2$ where k_0, k_1, k_2 depend only on $V(t_0)$, $V^{(1)}(t_0)$, $V^{(2)}(t_0)$, and so on: $F(t)$ is bounded by a quartic in t, at least for $t \geqslant t_0$, and a similar argument applies for $t < t_0$. So $\|V\|$ is bounded by a quadratic. Because $F^{(2)}$ is bounded by a quadratic so is $\|V^{(1)}\|^2$. □

IV. EXTENDING RIEMANNIAN CUBICS AND LIE QUADRATICS

We prove an extendibility result for Riemannian cubics in SO(3), then use it to prove extendibility for Lie quadratics in E^3. Reference 7 also contains results on extendibility of cubics.

Lemma 1: For some $\delta > 0$, given $t_0 \in \mathbb{R}$, $x_0 \in SO(3)$, and $v_i \in TSO(3)_{x_0}$ with $\|B^{-1}(x_0^{-1}v_i)\| \leqslant 1$ for $0 \leqslant i \leqslant 2$, there is a unique Riemannian cubic $x: (t_0 - \delta, t_0 + \delta) \to SO(3)$ satisfying

$$x(t_0) = x_0, \quad x^{(1)}(t_0) = v_0, \quad \nabla_{d/dt} x^{(1)}\big|_{t_0} = v_1, \quad \text{and} \quad \nabla^2_{d/dt} x^{(1)}\big|_{t_0} = v_2. \tag{15}$$

Proof: Picard's theorem on local unique solvability of ordinary differential equations almost asserts this, but with δ depending on x_0, v_0, v_1, v_2. However SO(3) is compact. Restricting v_0, v_1, v_2 also to lie in a compact set permits a uniform choice of δ. □

Lemma 2: For δ as in Lemma 1, given $t_0 \in \mathbb{R}$, $x_0 \in SO(3)$, and $v_i \in TSO(3)_{x_0}$ for $0 \leqslant i \leqslant 2$, if

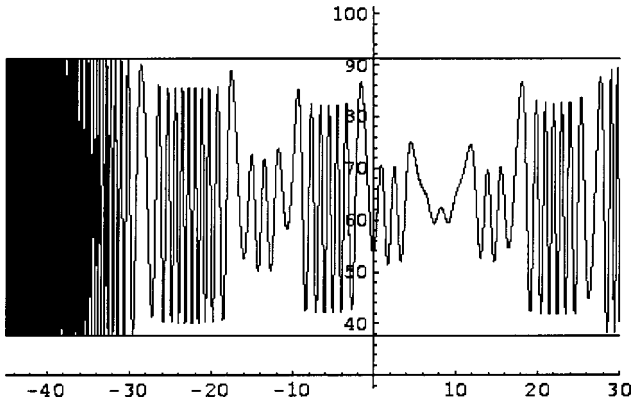

FIG. 8. $d - F^{(4)}$ and $\delta_\pm$ in Example 5.

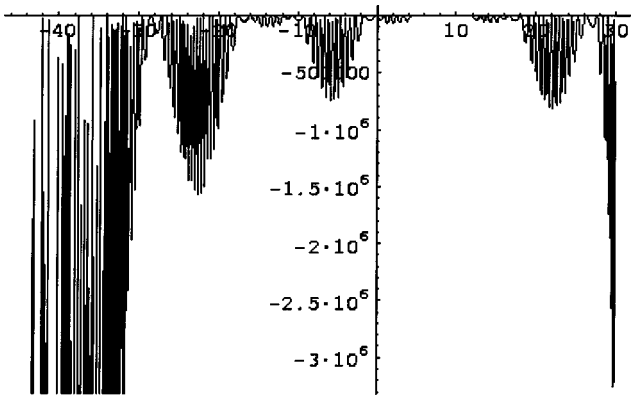

FIG. 9. Corollary 1 in Example 5.

$\lambda \geqslant 1+\max_i \|v_i\|$ *then there is a unique Riemannian cubic* $x:(t_0-\delta/\lambda, t_0+\delta/\lambda)\to SO(3)$ *satisfying (15).*

Proof: Using Lemma 1, let $\hat{x}:(t_0-\delta, t_0+\delta)\to \mathrm{SO}(3)$ be the Riemannian cubic satisfying

$$\hat{x}(t_0)=x_0,\ \ \hat{x}^{(1)}(t_0)=v_0/\lambda,\ \ \ \nabla_{d/dt}\,\hat{x}^{(1)}\big|_{t_0}=v_1/\lambda^2,\ \text{ and }\ \nabla^2_{d/dt}\,\hat{x}^{(1)}\big|_{t_0}=v_2/\lambda^3.$$

Then set $x(t)=\hat{x}(t_0+\lambda(t-t_0))$. □

Theorem 2: *Given* $t_0\in\mathbb{R}$, $x_0\in SO(3)$, *and* v_0, v_1, $v_2\in TSO(3)_{x_0}$, *there is a unique Riemannian cubic* $x:\mathbb{R}\to SO(3)$ *satisfying (15).*

Proof: By Lemma 1, for some $\tilde{\delta}>0$ there is a (Riemannian) cubic $\tilde{x}:(t_0-\tilde{\delta}, t_0+\tilde{\delta})\to \mathrm{SO}(3)$ satisfying (15). If $\tilde{x}$ is not extendible to a cubic on $(t_0-\tilde{\delta},\infty)$, let $\mathcal{T}$ be the set of real numbers T for which $\tilde{x}$ extends to a cubic on $(t_0-\tilde{\delta}, T]$. Set $\overline{T}=\sup\mathcal{T}$ and

$$\lambda=(\kappa_2^2\overline{T^2}+\kappa_0^2+1)^2+\|V^{(2)}(t_0)\|+1.$$

Choose $T\in\mathcal{T}$ with $T>\overline{T}-(\delta/2\lambda)$ and δ as in Lemma 1. By (9) and Corollary 4, the Lie quadratic V associated with a cubic extension $x:(t_0-\delta_0, T]\to \mathrm{SO}(3)$ of $\tilde{x}$ satisfies

$$\|V(t)\|\leqslant \kappa_2^2t^2+\kappa_0^2,\ \ \|V^{(1)}(t)\|\leqslant\sqrt{\kappa_2^2t^2+\kappa_0^2},\ \ \|V^{(2)}(t)\|=\|V^{(2)}(t_0)\|,\ \text{ for } t\in(t_0-\delta_0, T),$$

where κ_0, κ_2 depend only on $\tilde{x}$. By Ref. 26 Lemma 2,

$$\|B^{-1}(x(t)^{-1}x^{(1)}(t))\|=\|V(t)\|\leqslant\lambda-1,$$

$$\|B^{-1}(x(t)^{-1}\nabla_{d/dt}\,x^{(1)})\|=\|V^{(1)}(t)\|\leqslant\lambda-1,$$

$$\|B^{-1}(x(t)^{-1}\nabla^2_{d/dt}\,x^{(1)})\|=\left\|V^{(2)}(t)+\tfrac{1}{2}V(t)\times V^{(1)}(t)\right\|\leqslant\|V^{(2)}(t_0)\|+\tfrac{1}{2}(\kappa_2^2t^2+\kappa_0^2)^{3/2}\leqslant\lambda-1.$$

Applying Lemma 2, with $\hat{T}\equiv T-(\delta/4\lambda)$ in place of t_0, $x\big|[\hat{T}-(\delta/4\lambda), T]$ extends to a cubic defined on $[\hat{T}-(\delta/\lambda), \hat{T}+(3\delta/4\lambda)]$. So x, and therefore $\tilde{x}$, extends to a Riemannian cubic on $[t_0-\tilde{\delta}, \overline{T}+(\delta/4\lambda)]$, namely $\overline{T}+(\delta/4\lambda)\in\mathcal{T}$, contradicting $\overline{T}=\sup\mathcal{T}$. So $\tilde{x}$ is right extendible after all. Left extendibility is proved similarly. Uniqueness follows from Picard's local uniqueness. □

Corollary 5: Given $C\in E^3$, $t_0\in\mathbb{R}$ *and* w_0, $w_1\in E^3$, *there is a unique Lie quadratic* $V:\mathbb{R}\to E^3$ *with constant* C, *satisfying*

$$V(t_0)=w_0\ \text{ and }\ V^{(1)}(t_0)=w_1.$$

Proof: Set $w_2 = w_1 \times w_0 + C$, $x_0 = \mathbf{1}$, $v_0 = B^{-1}w_0$, $v_1 = B^{-1}w_1$, $v_2 = B^{-1}w_2$, apply Theorem 2, and let V be the Lie quadratic associated with the Riemannian cubic $x: \mathbb{R} \to \mathrm{SO}(3)$. □

So there is no loss in restricting attention to Lie quadratics in E^3 defined on the whole of $\mathbb{R}$. We may then ask about rates of growth of $V(t)$, or equivalently of $F(t)$, as $t \to \pm\infty$.

V. RATES OF GROWTH I

By Theorem 1, for a Lie quadratic, $V: \mathbb{R} \to E^3$,

$$F^{(4)} + (F^{(2)} + b)F = \tfrac{3}{4}(F^{(1)})^2 + d, \text{ where } d \geqslant 0. \tag{16}$$

When $d=0$ V is null of the form $V(t) = (t - t_0)\beta$, where $t_0 \in \mathbb{R}$ and $\beta \in E^3$. For $d > 0$, $\tilde{F}$ given by $F(t) = d^{1/3}\tilde{F}(d^{1/6}t)$ satisfies (16) with b replaced by $d^{-2/3}b$ and d by 1. So there would be no real loss of generality in taking $d=1$, but we continue with only the assumption $d > 0$. By Corollary 4, $\limsup_{t\to\pm\infty}[F(t)/t^4] < \infty$ and $\limsup_{t\to\pm\infty}[\|V^{(1)}(t)\|^2/t^2] < \infty$. Sharper results follow from Theorem 1.

Corollary 6: We have $\max\{0, -b/2\} \leqslant \liminf_{t\to\pm\infty}[F(t)/t^2]$ *and* $\limsup_{t\to\pm\infty}[F(t)/t^4] \leqslant \|C\|\sqrt{c}/4$.

Proof: Because $F^{(2)}(t) \geqslant -b$, $F^{(1)}(t) - F^{(1)}(t_0) \geqslant -b(t - t_0)$ for any $t \geqslant t_0 \in \mathbb{R}$. Integrating again,

$$F(t) \geqslant F(t_0) + (t - t_0)F^{(1)}(t_0) - \frac{b}{2}(t - t_0)^2. \tag{17}$$

For $t < t_0$, $F^{(1)}(t) - F^{(1)}(t_0) \leqslant -b(t - t_0)$, and again (17) holds on second integration. Similarly, because

$$F^{(4)}(t) \leqslant d - \delta_- = 6\|C\|\sqrt{c}, \text{ we have } \limsup_{t\to\pm\infty}\frac{F(t)}{t^4} \leqslant \frac{\|C\|\sqrt{c}}{4}.$$

□

Corollary 7: Let t_0 be a point of local minimum of F. Then $bF(t_0) \leqslant \delta_+$.

(1) If $F(t_0) = 0$ then $\delta_- = 0$.
(2) If t_0 is a degenerate critical point then $bF(t_0) \geqslant \delta_-$.

Proof: By (10), $\delta_- \leqslant (F^{(2)}(t_0) + b)F(t_0) \leqslant \delta_+$, where $F^{(2)}(t_0) \geqslant 0$. □

By Theorem 1, for $F^{(1)}F \neq 0$, we have $2\delta_- F^{-5/2} \leqslant 2bF^{-3/2} + (d/dF)(F^{-3/2}G) \leqslant 2\delta_+ F^{-5/2}$ and, integrating over $[F(t_1), F(t_2)]$ where $F^{(1)} > 0$ on $[t_1, t_2]$,

$$\frac{4\delta_-}{3}(\rho^{3/2} - 1) \leqslant 4bF(t_1)\rho(\rho^{1/2} - 1) + G(t_2) - \rho^{3/2}G(t_1) \leqslant \frac{4\delta_+}{3}(\rho^{3/2} - 1), \tag{18}$$

where $\rho \equiv F(t_2)/F(t_1) > 1$.

Theorem 3: *Suppose $b \leqslant 0$. Then F is convex. If $b < 0$ or $\delta_- > 0$ then F is strictly convex and* $\liminf_{t\to\pm\infty}[F(t)/t^4] > 0$.

Proof: By Theorem 1, $F^{(2)} + b \geqslant 0$, and F is convex because $b \leqslant 0$. Similarly, if $b < 0$ then F is strictly convex. For $b \leqslant 0$ and $\delta_- > 0$, $(F^{(2)} + b)F \geqslant \delta_- + \frac{3}{4}(F^{(1)})^2 > 0$ by (10), and again F is strictly convex.

Because F is strictly convex, it is unbounded, has a point t_0 of global minimum, and t_0 is the only critical point. Take $[t_1, t_2] \subset (t_0, \infty)$ in (18), let $t_1 \to t_0^+$, and write $t_2 = t$,

$$G(t) \geqslant 4(\rho^{1/2} - 1)\left(\left(\frac{\delta_-}{3} - bF(t_0)\right)\rho + \frac{\delta_-}{3}\rho^{1/2} + \frac{\delta_-}{3}\right).$$

Given $0 < \epsilon < 1$, choose $t_3 > t_0$ so large that $\rho > \epsilon^2$ for all $t \geqslant t_3$. Then $\rho^{1/2} - 1 \geqslant (1 - \epsilon)\rho^{1/2}$, and

$$F^{(1)}(t) = \sqrt{G(t)} \geqslant \gamma\rho^{3/4}, \text{ where } \gamma \equiv 2\sqrt{(1-\epsilon)\left(\frac{\delta_-}{3} - bF(t_0)\right)}.$$

So $F(t)^{-3/4}(dF/dt) \geqslant \gamma F(t_0)^{-3/4}$ and, integrating again, $F(t)^{1/4} - F(t_3)^{1/4} \geqslant 4\gamma F(t_0)(t-t_0)$, so that $\liminf_{t\to\infty}[F(t)/t^4] \geqslant \gamma$. Now if $F(t_0)=0$ we have $V(t_0)=V^{(1)}(t_0)=\mathbf{0}$, and the unique solution of (5) satisfying these conditions is $V(t)=\frac{1}{2}(t-t_0)^2C$, for which $b=0$. So either $F(t_0)>0$ or $b=0$, and either $b>0$ or $\delta_->0$ by hypothesis. So in any case we have $\gamma>0$, completing the proof for $t \to \infty$. For $t\to-\infty$ consider the Lie quadratic $s\mapsto -V(-s)$. □

VI. POLYNOMIAL SOLUTIONS FOR *F*

Comparing Corollary 6 and Theorem 3, if $b\delta_-<0$ then $F(t)=O(t^4)$ but $F(t)\neq O(t^3)$. On the other hand, F is sometimes bounded when $b>0$.

Example 6: Given a_0, c_0, $t_0 \in \mathbb{R}$, $A \in SO(3)$, define a Lie quadratic,

$$V(t) = a_0 A(-c_0, \cos a_0c_0(t-t_0), \sin a_0c_0(t-t_0)). \tag{19}$$

Then $C=a_0^3c_0A(1,0,0)$, F is constant with value $a_0^2(1+c_0^2)$,

$$b = 3a_0^4c_0^2, \ c = a_0^6c_0^4, \ d = 3a_0^6c_0^2(1+c_0^2) \text{ and } \delta_\pm = 3a_0^6c_0^2(1\pm c_0)^2.$$

If $a_0c_0=0$ then V is constant. Otherwise V is periodic and non-null (the only bounded null Lie quadratics in E^3 are constants).

Conversely, let V be any Lie quadratic in E^3 with F constant. If $C=\mathbf{0}$ then $b=0$ by (7) and then $\|V^{(1)}\|=0$ by (8), namely V is constant. If $C\neq\mathbf{0}$ then, after rotation in E^3 and time dilation, we can suppose $C=(1,0,0)$, so that the first component V_1 of V is $-c_0$. By (5), the other components satisfy

$$V_2^{(2)} = -c_0V_3^{(1)}, \ V_3^{(2)} = c_0V_2^{(1)},$$

giving $V_2=\cos c_0(t-t_0)$, $V_3=\sin c_0(t-t_0)$ for some $t_0\in\mathbb{R}$. So, in any case where F is constant, V has the form (19) after rotation and dilation. □

Example 7: For $b>0$, $c\geqslant 0$, $A\in SO(3)$ and $t_0\in\mathbb{R}$, let V be the null quadratic for which

$$V(t_0) = A(\sqrt{c},0,0), \ V^{(1)}(t_0) = A(0,\sqrt{b},0).$$

Then $F(t)=b(t-t_0)^2+c$, and $d=\delta_+=\delta_-=3c$. Alternatively, F is also realized by the affine Lie quadratic

$$t \mapsto -A(\sqrt{b}(t-t_0), \sqrt{c}, 0),$$

which is non-null for $c>0$. □

Example 8: For $a_0>0$, $c_0\in\mathbb{R}$, $A\in SO(3)$ and $t_0\in\mathbb{R}$, set

$$V(t) = (a_0(t-t_0)^2 + c_0)A(1,0,0).$$

Then V is a Lie quadratic in E^3 with $C=2a_0A(1,0,0)$, $F(t)=(a_0(t-t_0)^2+c_0)^2$,

$$b = -4a_0c_0, \ c = 4a_0^2, \ d = 24a_0^2, \ \delta_+ = 48a_0^2, \text{ and } \delta_- = 0.$$

□

In particular, Examples 6, 7, and 8 give constant, quadratic and quartic solutions of (16) with $F\geqslant 0$, $F^{(2)}+b\geqslant 0$, and $d\geqslant 0$. There are no other examples: all polynomial solutions of (16) have the form

$$a_0(t-t_0)^2 + c_0 \text{ or } (b_0(t-t_0)^2 + d_0)^2, \tag{20}$$

where

(i) $a_0=b$ and $3bc_0=d$, or $a_0=0$ and $bc_0=-d$,
(ii) $24b_0^2=d$ and $4b_0d_0=-b$, or $b_0=0$ and $bd_0^2=d$.

When $b<0$ the solution $F(t)=b(t-t_0)^2+d/(3b)$ of (16) satisfies neither $F\geqslant 0$ nor $F^{(2)}+b\geqslant 0$. In Examples 6, 7, and 8, t_0 is a point of global minimum of F. In Example 6, and in Example 8 when $c_0=0$, t_0 is degenerate.

Theorem 4: *Unless V is one of the periodic Lie quadratics in Example 6,*

(1) the critical points of F are isolated, and
(2) if $F(t_0)>0$ and $F^{(1)}(t_0)=F^{(3)}(t_0)=0$ then $F(t)=(a_0(t-t_0)^2+c_0)^2$ where a_0, $c_0\in\mathbb{R}$,
(3) if t_0 is a degenerate critical point of F either $F^{(3)}(t_0)\neq 0$ or $F(t)=(d/24)(t-t_0)^4$.

Proof: For (2), $F(t_0)$, $F^{(2)}(t_0)$ determine F uniquely as a solution of (16), and all $(F(t_0),F^{(2)}\times(t_0))\in(0,\infty)\times\mathbb{R}$ are realized in Example 8. For (3), F is determined by $F(t_0)\geqslant 0$. Positive values are realized by taking F constant, and 0 is achieved in Example 8 by setting $c_0=0$. If F is constant V appears in Example 6. For (1), if F is nonconstant a critical point then, by (3), t_0 satisfies $F^{(i)}(t_0)\neq 0$ for some $i=2$, 3, 4. So t_0 is isolated. □

Corollary 8: If F is nonconstant its points of local maximum are nondegenerate. □

VII. RATES OF GROWTH II: $b\geqslant 0$

Theorem 5: *Suppose $b\geqslant 0$. If t_0 is a point of local maximum of F, then $\delta_-\leqslant bF(t_0)$. If t_0 is a point of local minimum of F then $bF(t_0)\leqslant\delta_+$, and*

(1) if $F|(t_0,\infty)$ has no critical points and is unbounded, then $3bF(t_0)\leqslant\delta_+$, and either

$$\lim_{t\to\infty}\frac{F(t)}{t^2}=b \text{ or } \liminf_{t\to\infty}\frac{F(t)}{t^4}>0;$$

(2) if $F|(-\infty,t_0)$ has no critical points and is unbounded, then $3bF(t_0)\leqslant\delta_+$, and either

$$\lim_{t\to-\infty}\frac{F(t)}{t^2}=b \text{ or } \liminf_{t\to-\infty}\frac{F(t)}{t^4}>0;$$

(3) if $3bF(t_0)\leqslant\delta_-$ and $\delta_->0$, then t_0 is the only critical point of F, is nondegenerate, and F is unbounded on $[0,\infty)$ and on $(-\infty,0]$;
(4) if $3bF(t_0)<\delta_-$ then

$$\liminf_{t\to\pm\infty}\frac{F(t)}{t^4}>0;$$

(5) for $\delta_->0$, let t_1 be another critical point of F, where F has no critical points between t_0,t_1. Then $3bF(t_0)>\delta_-$ and

$$F(t_1)\geqslant\left(\frac{\mu F(t_0)^{1/2}+\sqrt{4\mu F(t_0)^2-3\mu^2F(t_0)}}{2(F(t_0)-\mu)}\right)^2,\quad \text{where } \mu=\frac{\delta_-}{3b}. \tag{21}$$

If also $3bF(t_0)>\delta_+$ then

$$F(t_1)\leqslant\left(\frac{\mu F(t_0)^{1/2}+\sqrt{4\mu F(t_0)^2-3\mu^2F(t_0)}}{2(F(t_0)-\mu)}\right)^2,\quad \text{where } \mu=\frac{\delta_+}{3b}. \tag{22}$$

Proof: For t_0 a critical point of F, $\delta_-\leqslant(F^{(2)}(t_0)+b)F(t_0)\leqslant\delta_+$, by (10). If t_0 is a point of local maximum then $F^{(2)}(t_0)\leqslant 0$ and therefore $\delta_-\leqslant(F^{(2)}(t_0)+b)F(t_0)\leqslant bF(t_0)$. Similarly, if t_0 is a point of local minimum $F^{(2)}(t_0)\geqslant 0$ and $bF(t_0)\leqslant\delta_+$. For *(1)*, by (18), with $[t_1,t_2]\subset(t_0,\infty)$,

$$\rho^{3/2}\left(4bF(t_1) - G(t_1) - \frac{4\delta_+}{3}\right) - 4bF(t_1)\rho \leqslant -\left(G(t_2) + \frac{4\delta_+}{3}\right), \tag{23}$$

$$\rho^{3/2}\left(4bF(t_1) - G(t_1) - \frac{4\delta_-}{3}\right) - 4bF(t_1)\rho \geqslant -\left(G(t_2) + \frac{4\delta_-}{3}\right). \tag{24}$$

By hypothesis, $\limsup_{t_2\to\infty}\rho=\infty$. By (23), and because $G(t_2)+(4\delta_+/3)\geqslant 0$,

$$4bF(t) - G(t) \leqslant \frac{4\delta_+}{3} \text{ for all } t > t_0.$$

So $3bF(t_0)\leqslant\delta_+$. By (24) if, for any $t_1\geqslant t_0$, $k(t_1)\equiv 4bF(t_1)-G(t_1)-(4\delta_-/3)<0$, then for all $t\geqslant t_1$,

$$G(t) \geqslant -k(t_1)\rho^{3/2} + 4bF(t_1)\rho - \frac{4\delta_-}{3}, \text{ where } \rho = F(t)/F(t_1).$$

Then, as in the proof of Theorem 3, $\liminf_{t\to\infty}[F(t)/t^4]>0$. Alternatively if $k(t)\geqslant 0$ for all $t\geqslant t_0$, then $G(t)<4bF(t)$ and $0\leqslant F^{(1)}(t)<2\sqrt{b}F(t)^{1/2}$. So

$$0 \leqslant F(t) < (F(t_0)^{1/2} + \sqrt{b}(t-t_0))^2,$$

and $\limsup_{t\to\infty}[F(t)/t^2]\leqslant b$. When $b=0$ this proves (*1*), and when $b>0$ we argue as follows. By (23), since ρ is unbounded, $G(t)\geqslant 4bF(t)-(4\delta_+/3)$, for all $t\geqslant t_0$. Eventually the right-hand side is positive, when $t=t_1$ say, and

$$F^{(1)}(t) \geqslant 2(bF - \delta_+)^{1/2},$$

for all $t\geqslant t_1$. Integrating $(bF(t)-\delta_+)^{1/2}\geqslant b(t-t_1)+(bF(t_1)-\delta_+)^{1/2}$, which completes the proof of (*1*).

Now (*2*) follows by applying (*1*) to the Lie quadratic W where $W(s)=-V(2t_0-s)$. The parameters $b,c,d,\delta_\pm$ are the same for W, and C is replaced by $-C$.

For (*3*) $F(t_0)\neq 0$ and t_0 is nondegenerate, by Corollary 7. Taking $t_1\to t_0^+$ in (24),

$$G(t) \geqslant \tfrac{4}{3}(\rho^{1/2}-1)((\delta_- - 3bF(t_0))\rho + \delta_-\rho^{1/2} + \delta_-) \geqslant \tfrac{4}{3}(\rho-1)\delta_-, \tag{25}$$

where $\rho(t)=F(t)/F(t_0)$. In particular $F^{(1)}(t)\neq 0$ for $t\in(t_0,t_1]$ and, since t_0 is a point of local minimum of F, $F^{(1)}$ is positive on $(t_0,t_1]$. So $F|(t_0,t_1]$ is increasing, and $F(t_1)F^{(1)}(t_1)>0$. So $F(t)F^{(1)}(t)>0$ for all $t>t_0$, and (25) still holds. Since F is strictly increasing on (t_0,∞), so is ρ. Also

$$F^{(1)}(t) \geqslant 2\sqrt{\frac{\delta_-}{3}}(\rho-1)^{1/2} = 2\sqrt{\frac{\delta_-}{3}}(F(t)/F(t_0)-1)^{1/2}.$$

Then integration gives $\liminf_{t\to\infty}[F(t)/t^2]>0$, and (*3*) follows by applying this to W in place of V.

For (*4*), given $\lambda\in(0,1)$, choose ρ so large (and t accordingly) so that (25) gives

$$\rho(t)^{-3/4}F^{(1)}(t) \geqslant \lambda\sqrt{\frac{4(\delta_- - 3bF(t_0))}{3}}, \text{ namely } F(t)^{-3/4}F^{(1)}(t) \geqslant \lambda\sqrt{\frac{4(\delta_- - 3bF(t_0))}{3}}F(t_0)^{-3/4}.$$

Integration then proves (*4*) for $t\to\infty$, and applying this to W proves the rest of (*4*).

For (*5*), $bF(t_0)>0$ by (*3*). Also (18) gives $\delta_-(\rho+\rho^{1/2}+1)\leqslant 3bF(t_1)\leqslant\delta_+(\rho+\rho^{1/2}+1)$, where $\rho=F(t_1)/F(t_0)$. Writing $f_i=F(t_i)^{1/2}$,

$$f_1^2(\mu - f_0^2) + f_1(\mu f_0) + \mu f_0^2 \leqslant 0, \tag{26}$$

where $\mu=\delta_-/3b$ and $\mu-f_0^2<0$ by (*3*). So either

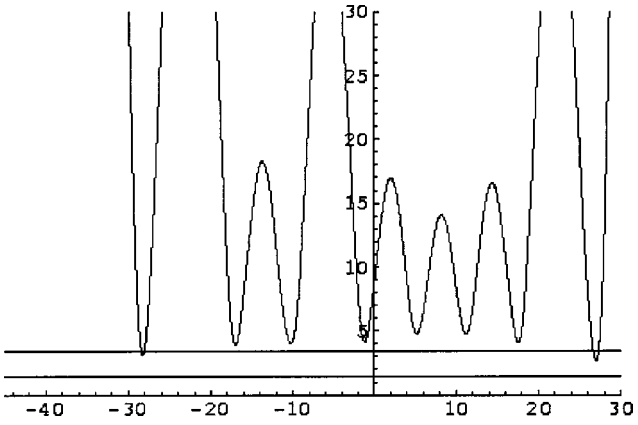

FIG. 10. F in Examples 5 and 9.

$$f_1 \leqslant \frac{\mu f_0 - \sqrt{4\mu f_0^4 - 3\mu^2 f_0^2}}{2(f_0^2 - \mu)} \quad \text{or } f_1 \geqslant \frac{\mu f_0 + \sqrt{4\mu f_0^4 - 3\mu^2 f_0^2}}{2(f_0^2 - \mu)}.$$

Now $(\mu f_0)^2 - (4\mu f_0^4 - 3\mu^2 f_0^2) = 4\mu f_0^2(\mu - f_0^2) < 0$ and, since $f_1 \geqslant 0$, this proves (21). Taking $\mu = \delta_+/3b$, the direction of the inequality in (26) reverses. When also $3bF(t_0) > \delta_+$, namely $\mu - f_0^2 < 0$, (22) follows in similar fashion to (21). □

Notice that when $3bF(t_0) < 2\delta_-$, (21) in (5) of Theorem 5 is stronger than $F(t_0) < F(t_1)$.

Example 9: *Figure 10 plots F in Example 5, with horizontal lines of heights* $\delta_\pm/3b$. *As in, Theorem 5,* $F(t_0) \leqslant \delta_+/3b$ *for every point* t_0 *of local minimum of F. Also notice that* $F(t_0) \leqslant \delta_+/3b$ *only for the first and last observed points* t_0 *of local minimum. Even if we only know* $F|[-20,20]$, *it follows from Part 1 of Theorem 5 that the restriction of F to each of* $(-\infty,-20)$ *and* $(20,\infty)$ *is either bounded or has a point of local minimum.* □

Under fairly general conditions $F(t)$ grows faster than linearly and V can be shown to possess *axes*, generalizing a result for null Lie quadratics. The axes of a non-null Lie quadratic V have non-negative components in the direction of the constant vector C.

VIII. SUPERLINEARITY

Whether $b > 0$ or not, for $V(t) \neq \mathbf{0}$ write $U(t) = V(t)/\|V(t)\|$. Then $U^{(1)} = (V^{(1)}/F^{1/2}) - (F^{(1)}U/2F)$.

Lemma 3: $\|U^{(1)}\| = \sqrt{(d - F^{(4)})/3}/F \leqslant (\|C\| + \sqrt{c})/F$.

Proof: $\|U^{(1)}\|^2 = [4F\|V^{(1)}\|^2 - (F^{(1)})^2]/4F^2 = \left[F(F^{(2)} + b) - \frac{3}{4}(F^{(1)})^2\right]/3F^2 = (d - F^{(4)})/3F^2 \leqslant \delta_+/3F^2$, by Theorem 1. □

Definition 1: *For* $\sigma = \pm$, F *is said to be* σ-superlinear *when, for some* $\epsilon > 0$, *we have* $0 < \liminf_{t \to \sigma\infty}[F(t)/|t|^{1+\epsilon}] < \infty$. □

In Example 6, V is not superlinear. In general,

(i) if F is superlinear then $\epsilon \leqslant 3$, by Corollary 6,
(ii) if $b < 0$ then F is $\pm$ superlinear with $\epsilon = 3$, by Theorem 3,
(iii) for $b \geqslant 0$, if $F(t)$ is unbounded for $\sigma t > 0$, with finitely many critical points t_i satisfying $\sigma t_i > 0$, then F is σ superlinear with ϵ either 1 or 3, by Theorem 5,
(iv) if V is null and nonconstant then F is $\pm$ superlinear with $\epsilon = 1$.

Definition 2: *Let* $\sigma = \pm$, $p \in \mathbb{R}$ *and* $h: \mathbb{R} \to \mathbb{R}$ *be given. A function* $g: \mathbb{R} \to \mathbb{R}$ *is said to be* $O_\sigma(h)$ *when* $\limsup_{t \to \sigma\infty}[g(t)/h(t)] < \infty$. □

Theorem 6: *If F is* σ*-superlinear then* $\alpha_\sigma(V) \equiv \lim_{t \to \sigma\infty} U(t)$ *exists, and*

$$U(t) = \alpha_\sigma(V) + O_\sigma(|t|^{-\epsilon}).$$

Proof: For $r<s$,

$$\|U(s)-U(r)\| \leqslant \int_r^s \|U^{(1)}(t)\|\mathrm{d}t \leqslant \int_r^s \frac{\|C\|+\sqrt{c}}{F(t)}\mathrm{d}t.$$

For $\sigma=+$, the right-hand side is bounded above by $k(r^{-\epsilon}-s^{-\epsilon})$ for some constant $k>0$, at least for r sufficiently large. So $\{U(j): j\geqslant 1\}\subset S^2$ is Cauchy, therefore convergent, then $\lim_{s\to\infty} U(s)$ exists, in the limit as $s\to\infty$ $\|\alpha_+(V)-U(r)\|\leqslant kr^{-\epsilon}$, and similarly for $\sigma=-$. □

Example 10: *Let V be a null Lie quadratic V with $b=1$, $c>0$, and $F(t)=c+t^2$. Set $\tau(t)=\int_0^t[\sqrt{c}/F(t)]\mathrm{d}t=(1/\sqrt{c})\arctan(t/c)$ and $W_2(\tau)\equiv U(t)=(c+t^2)^{-1/2}V(t)$. Differentiating with respect to τ, set $W_1(\tau)\equiv W_2'(\tau)=c^{-1/2}((c+t^2)^{1/2}V^{(1)}-t(c+t^2)^{-1/2}V)$, and $W_3(\tau)\equiv W_1(\tau)\times W_2(\tau)$. Then $W\equiv[W_1\ W_2\ W_3]\in SO(3)$, and*

$$W'(\tau)=\begin{bmatrix} 0 & -1 & c\sec^3(\sqrt{c}\tau) \\ 1 & 0 & 0 \\ -c\sec^3(\sqrt{c}\tau) & 0 & 0 \end{bmatrix} W(\tau),$$

where $\tau\in(-\pi/(2\sqrt{c}),\pi/(2\sqrt{c}))$. So U and therefore V can be found by solving the third-order homogeneous linear differential equation with variable coefficients

$$\cos^3(\sqrt{c}\tau)\frac{d}{d\tau}((y''(\tau)+y(\tau))\cos^3(\sqrt{c}\tau))+c^2y'(\tau)=0,$$

for $y:(-\pi/(2\sqrt{c}),\pi/(2\sqrt{c}))\to\mathbb{R}$. □

Theorem 7: *Let F be σ superlinear. Then*

$$\frac{f(t)}{t^2}=\frac{a_\sigma}{2}+O_\sigma(|t|^{-1}),$$

where $f\equiv F^{1/2}$ and $a_\sigma\equiv\langle C,\alpha_\sigma(V)\rangle$.

Proof: Suppose $\sigma=+$. By (5), $fU^{(2)}+2f^{(1)}U^{(1)}+f^{(2)}U=f^2U^{(1)}\times U+C$, and, since $\|U\|\equiv 1$, taking inner products of both sides with U gives

$$0\leqslant f^{(2)}-\langle C,U\rangle=f\langle U^{(1)},U^{(1)}\rangle\leqslant\frac{\delta_+}{3f^3}=O_+(t^{-3(1+\epsilon)/2}),$$

by Lemma 3 and because F is $+$ superlinear. Then $f^{(2)}(t)=a_++O_+(t^{-\epsilon})$, by Theorem 6. Integrating, for large $t_0<t$,

$$f^{(1)}(t)=a_+(t-t_0)+f^{(1)}(t_0)+O_+(K_1(t)-K_1(t_0)),$$

where $K_1(t)$ is $\ln t$ or $t^{1-\epsilon}/(1-\epsilon)$, according to $\epsilon=1$ or not. Integrating again,

$$f(t)=\frac{a_+(t-t_0)^2}{2}+(t-t_0)f^{(1)}(t_0)+f(t_0)+O_+(K_2(t)-(t-t_0)K_1(t_0)),$$

where $K_2(t)=t\ln t-t_0\ln t_0-t+t_0$, $t_0^{-1}-t^{-1}$, or $(t^{2-\epsilon}-t_0^{2-\epsilon})/((1-\epsilon)(2-\epsilon))$, according to ϵ is 1, 2 or neither. In any case, $f(t)/t^2=(a_+/2)+O_+(t^{-1})$. For $\sigma=-$ apply what has already been proved to the Lie quadratic W given by $W(s)=-V(-s)$, noting that W has constant $-C$ and $\alpha_+(W)=-\alpha_-(V)$. □

Corollary 9: Let F be σ superlinear. Then $\langle C,\alpha_\sigma\rangle\geqslant 0$, and either

(i) $\epsilon=1$, $\langle C,\alpha_\sigma\rangle=0$, *and* $b\geqslant 0$, *or*
(ii) $\epsilon=3$, *or*
(iii) $\langle C,\alpha_\sigma\rangle=0$, $b\geqslant 0$, *and F has critical points t_0 with σt_0 arbitrarily large.*

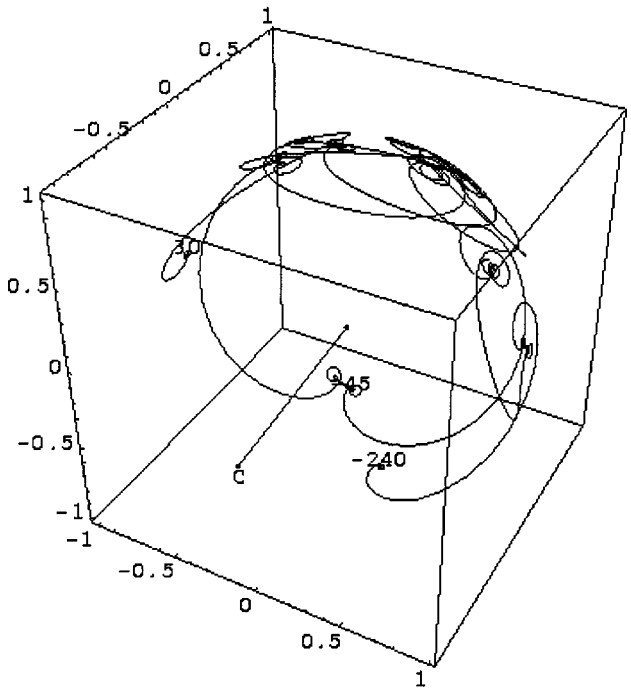

FIG. 11. U in Examples 5, 11.

Proof: If $a_+>0$ then $\epsilon=3$, by Theorem 7. Alternatively, if $a_\sigma=0$ then $b\geqslant 0$ by Theorem 3. Then, by Theorem 5, either $\epsilon=1$ or F has critical points t_0 with σt_0 arbitrarily large. □

Unlike the null case, where convergence to axes is more or less steady, unbounded non-null Lie quadratics in E^3 may explore numerous possibilities before settling on an asymptotic direction, at least when $b>0$.

Example 11: In Example 5, $\langle C,U(-45)\rangle=-0.032\,55$ *and* $\langle C,U(30)\rangle=0.2915$. *So, by Corollary 9,* $U(-45)$ *is far from* $\alpha_-(V)$, *which is not apparent from Figs. 6 and 7. Solving (5) numerically for V over the larger domain* $[-240,30]$, $U:[-240,30]\to S^2$ *is shown in Fig. 11, together with the line segment from* (0,0,0) *to C and labels when* $t=-240,-45,30$. *We find* $\langle C,U(-240)\rangle=0.62375$, *and Corollary 9 permits* $\alpha_-(V)\approx U(-240)$, $\alpha_+(V)\approx U(30)$. □

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q-deformation of $z \to (\alpha z+\beta)/(\gamma z+\delta)$

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We construct the action of the quantum double of $U_q(su(2))$ on the standard Podleś sphere and interpret it as the quantum projective formula generalizing to the q-deformed setting the action of the Lorentz group of global conformal transformations on the ordinary Riemann sphere. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1803610]

I. INTRODUCTION

As it is well known, the Lorentz group $SL(2,\mathbf{C})$ naturally acts on the Riemann sphere S^2 by the conformal transformations

$$z \to \frac{\alpha z+\beta}{\gamma z+\delta}, \quad \alpha,\beta,\gamma,\delta \in \mathbf{C}, \quad \alpha\delta-\beta\gamma=1. \tag{1}$$

The q-deformation of S^2 is referred to as the Podleś sphere (Podleś, 1987). One of the goals of this paper is to find the corresponding q-deformation of the conformal transformations (1). We note that the restriction $\overline{\alpha}=\delta$, $\overline{\gamma}=-\beta$ gives the action of the group SU(2) on S^2 which just corresponds to the standard geometrical rotations of the two-sphere embedded into three-dimensional Euclidean space. The q-deformed version of this SU(2) action was studied in detail by Podleś (1987). However, to our best knowledge, the q-conformal action of the full q-Lorentz group on the Podleś sphere has not yet been reported.

Recall, that the algebra of functions $\mathrm{Fun}(S^2)$ on ordinary two sphere can be viewed as the algebra of those functions on the group SU(2) which are invariant with respect to the right action of the maximal torus U(1) on SU(2). This gives the dual description of the coset $SU(2)/U(1) \equiv S^2$. The group SU(2) acts naturally from the left on this coset and this action can be extended to the action (1) of the Lorentz group $SL(2,\mathbf{C})$ on S^2 since we have a well-known identification $SU(2)/U(1) \equiv SL(2,\mathbf{C})/B$ with B being the Borel subgroup (consisting of upper triangular matrices) of $SL(2,\mathbf{C})$.

In order to construct the q-deformation of the picture just described, we take some inspiration from the theory of Poisson–Lie groups (see Semenov-Tian-Shansky, 1985, and Klimčík, 2004 for the elements). There is the Iwasawa decomposition $SL(2,\mathbf{C})=SU(2)AN$ of the Lorentz group where AN is the subgroup of upper triangular complex 2×2 matrices with real positive numbers on diagonal and unit determinant. AN turns out to be the dual Poisson–Lie group of SU(2) and $SL(2,\mathbf{C})$ is the Drinfeld double of SU(2) in the Poisson–Lie sense of this word. Now the Drinfeld double $SL(2,\mathbf{C})$ acts on Fun(SU(2)): the action of its subgroup SU(2) is induced just by the left multiplication of SU(2) on itself and the subgroup AN acts by the so-called dressing tranformations. This action of the $SL(2,\mathbf{C})$ on Fun(SU(2)) descends to $\mathrm{Fun}(SU(2)/U(1)(\equiv S^2))$ and it turns out to be given by the projective action (1), where z is the standard complex coordinate on the Riemann sphere.

The theory of Poisson–Lie groups is a sort of the semiclassical limit of the theory of q-deformed Hopf algebras for the deformation parameter q approaching 1. Many Poisson–Lie concepts can be directly generalized to the Hopf algebra setting like, e.g., the Drinfeld double or the dressing transformations. In particular, the Poisson–Lie concept of the duality translates into

the famous (Drinfeld, 1986) duality in the world of Hopf algebras. Having in mind the parallels between the Poisson–Lie and the Hopf worlds, it is not difficult to find the q-deformation of the projective formula. We proceed as follows.

The Podleś sphere $\mathrm{Fun}_q(S^2)$ is a one-parameter deformation of the algebra $\mathrm{Fun}(S^2)$. It is generated by the U(1) right-invariant elements of the quantum group $\mathrm{Fun}_q(\mathrm{SU}(2))$. The deformed enveloping algebra $\mathrm{U}_q(\mathrm{su}(2))$ naturally acts on the deformed $\mathrm{Fun}_q(\mathrm{SU}(2))$. [This corresponds to the left action of SU(2) on Fun(SU(2)) just described above.] The Hopf dual $\mathrm{U}_q(an)$ of $\mathrm{U}_q(\mathrm{su}(2))$ acts on $\mathrm{Fun}_q(\mathrm{SU}(2))$ in the Hopf-dressing way. This corresponds to the dressing action of AN on Fun(SU(2)). As noted by Korogodsky (unpublished), the Hopf analogue of the dressing action of $\mathrm{U}_q(an)$ on $\mathrm{Fun}_q(\mathrm{SU}(2))$ is the adjoint action of the Hopf algebra $\mathrm{Fun}_q(\mathrm{SU}(2))$ on itself. This statement is consistent due to the Drinfeld duality isomorphism between $\mathrm{U}_q(an)$ and $\mathrm{Fun}_q(\mathrm{SU}(2))$. The respective actions of $\mathrm{U}_q(an)$ and $\mathrm{U}_q(\mathrm{su}(2))$ on $\mathrm{Fun}_q(\mathrm{SU}(2))$ combine to the action of the Drinfeld double $D(\mathrm{U}_q(\mathrm{su}(2)))$ on $\mathrm{Fun}_q(\mathrm{SU}(2))$. This Drinfeld double is nothing but the q-Lorentz group (see Podleś and Woronowicz, 1990) and the only consistency check of the construction consists in verifying that the action of the q-Lorentz group descends from $\mathrm{Fun}_q(\mathrm{SU}(2))$ on $\mathrm{Fun}_q(S^2)$. It turns out to be the case and thus we obtain the q-deformation of the projective formula (1).

In Sec. II, we describe the action of the quantum double $D(\mathrm{U}_q(\mathrm{su}(2)))$ on the Podleś sphere and in Sec. III we show that it leads to the projective formula (1) in the limit $q\to 1$. We finish with a short outlook.

II. ACTION OF THE DRINFELD DOUBLE $D(\mathrm{U}_q(\mathrm{su}(2)))$ ON THE PODLEŚ SPHERE

First we recall some relevant facts concerning (the $*$-actions of) the Drinfeld double. The reader can mostly find them also in Majid (1995), however, our exposition between Eqs. (9) and (11) is original.

Thus let H be a Hopf algebra, $\tilde{H}$ its dual and H^{cop} the co-opposite Hopf algebra of H. The Drinfeld double $D(H)$ is another Hopf algebra which is generated by its two sub-Hopf algebras H^{cop} and $\tilde{H}$. The coalgebra structure of $D(H)$ is just that of $H^{\mathrm{cop}}\otimes\tilde{H}$, the antipode S_D is given by

$$S_D(U\otimes f)\equiv(1\otimes Sf)(S^{\mathrm{cop}}U\otimes 1)=(S^{\mathrm{cop}}U)''\otimes(Sf)''\langle(S^{\mathrm{cop}}U)',(Sf)'\rangle\langle S^{\mathrm{cop}}(S^{\mathrm{cop}}U)''',(Sf)'''\rangle, \quad (2)$$

and the product is defined by the following cross relations (Majid, 1995):

$$\langle U',f'\rangle(U''\otimes 1)(1\otimes f'')=\langle U'',f''\rangle(1\otimes f')(U'\otimes 1). \quad (3)$$

Here $U\in H^{\mathrm{cop}}$, $f\in\tilde{H}$, $\langle .,.\rangle$ is the duality pairing between H and $\tilde{H}$ and we use the Sweedler notation for the coproduct

$$\Delta^{\mathrm{cop}}(U)=\sum_p U'_p\otimes U''_p\equiv U'\otimes U'', \quad \Delta(f)=f'\otimes f''. \quad (4)$$

The formula (3) is particularly useful if we know the generators and their relations for both algebras H^{cop} and $\tilde{H}$ separately. The set of relations for the algebra structure of $D(H)$ can be then directly obtained from (3) and (4).

If, moreover, H and $\tilde{H}$ are equipped with compatible star structures, then the quantum double $D(H)$ can be also naturally made a $*$-Hopf algebra. Recall that a star $*$ on H is an antilinear antihomorphism of H satisfying $S*S*=Id$, $*^2=Id$, $(*\otimes *)\Delta=\Delta*$, and $*\varepsilon=\varepsilon*$. The standard compatibility relation (cf. Majid, 1995) between the stars on H and $\tilde{H}$ reads

$$\langle U*,f\rangle=\overline{\langle U,(Sf)*\rangle}, \quad U\in H, \quad f\in\tilde{H}. \quad (5)$$

The explicit formula for the star $*$ on $D(H)$ is then uniquely determined as follows:

$$(U \otimes f)^* \equiv (1 \otimes f^*)(U^* \otimes 1) = U^{*\prime\prime} \otimes f^{*\prime\prime}\langle U^{*\prime}, f^{*\prime}\rangle\langle S^{\mathrm{cop}}U^{*\prime\prime\prime}, f^{*\prime\prime\prime}\rangle, \quad U \in H^{\mathrm{cop}}, \quad f \in \tilde{H}, \tag{6}$$

where the star on H^{cop} is the same as that on H.

The algebras H^{cop} and $\tilde{H}$ act (from the left) on $\tilde{H}$, respectively, as

$$U \triangleright h = \langle S^{\mathrm{cop}}(U), h^{\prime}\rangle h^{\prime\prime}, \quad U \in H^{\mathrm{cop}}, \quad h \in \tilde{H}, \tag{7a}$$

$$f \triangleright h = f^{\prime} h S(f^{\prime\prime}), \quad f, h \in \tilde{H}. \tag{7b}$$

We note that $S^{\mathrm{cop}} = S^{-1}$, where S is the antipode of H. Using the basic axioms of Hopf algebras, it is easy to check that the definitions (7a) and (7b) imply

$$\langle U^{\prime}, f^{\prime}\rangle U^{\prime\prime} \triangleright (f^{\prime\prime} \triangleright h) = \langle U^{\prime\prime}, f^{\prime\prime}\rangle f^{\prime} \triangleright (U^{\prime} \triangleright h), \quad U \in H^{\mathrm{cop}}, \quad f, h \in \tilde{H}.$$

By comparing with the defining relation (3), this means that (7a) and (7b) describe in fact the left action of the quantum double $D(H)$ on $\tilde{H}$. Explicitly,

$$(U \otimes f) \triangleright h \equiv U \triangleright (f \triangleright h), \quad U \in H^{\mathrm{cop}}, \quad f, h \in \tilde{H}. \tag{8}$$

It can be also directly checked [with the help of the condition (5)], that this action is compatible with the algebra structure of $\tilde{H}$ and with the $*$-structure on $\tilde{H}$. Explicitly,

$$x \triangleright (fh) = (x^{\prime} \triangleright f)(x^{\prime\prime} \triangleright h), \quad x \in D(H), \; f, h \in \tilde{H}, \tag{9a}$$

$$(x \triangleright f)^* = (S_D(x))^* \triangleright f^*, \quad x \in D(H), \; f \in \tilde{H}. \tag{9b}$$

Now let $k \in H^{\mathrm{cop}}$ be a grouplike self-adjoint element, i.e., $k^* = k$, $\Delta^{\mathrm{cop}}k = k \otimes k$, $\varepsilon(k) = 1$. We can then define a linear space A consisting of invariant elements of $\tilde{H}$ with respect to the right action of k and $S(k)$ on $\tilde{H}$,

$$A = \{f \in \tilde{H}, \; \langle f^{\prime\prime}, k\rangle f^{\prime} \equiv f \triangleleft k = f, \; f \triangleleft S(k) = f\}. \tag{10}$$

We have for $f, g \in A$

$$(fg) \triangleleft k = \langle f^{\prime\prime}g^{\prime\prime}, k\rangle f^{\prime}g^{\prime} = \langle f^{\prime\prime}, k\rangle\langle g^{\prime\prime}, k\rangle f^{\prime}g^{\prime} = fg$$

and, in the same way, $(fg) \triangleleft S(k) = 1$ which means that A is the subalgebra of $\tilde{H}$. We obtain easily also the $*$-stability of A, since for $f \in A$ we have

$$f^* \triangleleft k = \langle f^{*\prime\prime}, k\rangle f^{*\prime} = (\langle f^{\prime\prime}, (S(k))^*\rangle f^{\prime})^* = (f \triangleleft S(k))^* = f^*$$

and, in the same way, $f^* \triangleleft S(k) = (f \triangleleft k)^* = f^*$.

It is not difficult to prove that A is also stable with respect to the action (7a) and (7b) of the quantum double $D(H)$ on $\tilde{H}$. Indeed, we have for the H^{cop} action (7a),

$$U \triangleright (f \triangleleft k) = \langle S^{\mathrm{cop}}(U), f^{\prime}\rangle f^{\prime\prime}\langle f^{\prime\prime\prime}, k\rangle = (U \triangleright f) \triangleleft k, \quad U \in H^{\mathrm{cop}}, \quad f \in \tilde{H}.$$

The proof of stability for $\tilde{H}$ action (7b) is slightly more involved,

$$(h \triangleright f) \triangleleft k = \langle (h^{\prime} f S(h^{\prime\prime}))^{\prime\prime}, k\rangle ((h^{\prime} f S(h^{\prime\prime}))^{\prime} = \langle h^{\prime\prime} f^{\prime\prime} S h^{\prime\prime\prime}, k\rangle h^{\prime} f^{\prime} S h^{\prime\prime\prime\prime} = \langle h^{\prime\prime}, k\rangle\langle f^{\prime\prime}, k\rangle\langle S h^{\prime\prime\prime}, k\rangle h^{\prime} f^{\prime} S h^{\prime\prime\prime\prime}$$

$$= \langle h^{\prime\prime}, kS(k)\rangle\langle f^{\prime\prime}, k\rangle h^{\prime} f^{\prime} S h^{\prime\prime\prime} = \langle f^{\prime\prime}, k\rangle h^{\prime} f^{\prime} S h^{\prime\prime} = h \triangleright (f \triangleleft k), \quad h, f \in \tilde{H}.$$

The same formulas hold true upon replacing $k \to S(k)$.

In the context of our paper, the *-Hopf algebra H will be the standard deformation $U_q(su(2))$ of $U(su(2))$, $\tilde{H}$ will be the corresponding dual deformation $Fun_q(SU(2))$ of $Fun(SU(2))$ and A will be the Podleś sphere $Fun_q(S^2)$. For the sake of mathematical rigor, we should pay attention to the fact that the notion of the dual Hopf algebra needs some clarification in the infinite-dimensional case. Actually, $U_q(su(2))$ and $Fun_q(SU(2))$ are in duality in the sense of Chaps. V.7 and VII.4 of the book by Kassel (1995). The general Drinfeld double formulas (2)–(10) then work with this notion of duality with the bilinear pairing given by Eq. (12d).

For the description of the Hopf algebras $Fun_q(SU(2))$ and $U_q(su(2))$, we use the conventions of Dąbrowski and Sitarz (2003) and Dąbrowski *et al.* (unpublished). Thus let $q\neq 1$ be a real positive number and denote $Fun_q(SU(2))$ a *-Hopf algebra generated by a and b, subject to relations

$$ba=qab,\quad b^*a=qab^*,\ bb^*=b^*b,\quad a^*a+q^2b^*b=1,\quad aa^*+bb^*=1, \tag{11a}$$

equipped with a coproduct

$$\Delta a=a\otimes a-qb\otimes b^*,\quad \Delta b=b\otimes a^*+a\otimes b, \tag{11b}$$

a counit $\varepsilon(a)=1$, $\varepsilon(b)=0$ and an antipode

$$Sa=a^*,\quad Sa^*=a,\quad Sb=-qb,\quad Sb^*=-q^{-1}b^*. \tag{11c}$$

The algebra $Fun_q(SU(2))$ is thus well defined but it is perhaps useful to comment its name. As everywhere in this paper, the symbol $Fun_q(M)$ indicates the deformation of the algebra of a certain class of functions on the ordinary manifold M. If the manifold M is the Lie group then the typical functions in this class are the matrix elements of the finite-dimensional representations of this group (cf. Levendorskii and Soibelman, 2001).

The *-Hopf algebra $U_q(su(2))$ is generated by elements e and (invertible self-adjoint) k, subject to relations

$$ek=qke,\quad k^2-k^{-2}=(q-q^{-1})(e^*e-ee^*), \tag{12a}$$

equipped with a coproduct

$$\Delta k=k\otimes k,\quad \Delta e=e\otimes k+k^{-1}\otimes e, \tag{12b}$$

a counit $\varepsilon(k)=1$, $\varepsilon(e)=0$ and an antipode

$$Se=-q^{-1}e,\quad Se^*=-qe^*,\quad Sk=k^{-1}. \tag{12c}$$

The (nondegenerate) duality pairing between $U_q(su(2))$ and $Fun_q(SU(2))$ is given by the two-dimensional representation of $U_q(su(2))$, i.e.,

$$\langle k,a\rangle=q^{1/2},\quad \langle k,a^*\rangle=q^{-1/2},\quad \langle e,-qb^*\rangle=\langle e^*,b\rangle=1 \tag{12d}$$

with all other couples of generators pairing to 0. It is easy to verify that the star structures on $Fun_q(SU(2))$ and $U_q(su(2))$ are compatible in the sense of Eq. (5).

The Podleś sphere is the algebra $Fun_q(S^2)$ viewed as the subalgebra of $Fun_q(SU(2))$ of right invariant elements with respect to the action of the self-adjoint grouplike elements k and k^{-1} [cf. (10)]. It is generated by

$$B=ab,\quad B^*=b^*a^*,\quad A=bb^*,$$

obeying the following relations:

$$AB=q^2BA,\quad AB^*=q^{-2}B^*A,\quad BB^*=q^{-2}A(1-A),\quad B^*B=A(1-q^2A).$$

The action of the q-Lorentz group $D(U_q(su(2)))$ on $Fun_q(S^2)\subset Fun_q(SU(2))$ is described by the formulas (7a) and (7b). We obtain explicitly

$$k\triangleright B = q^{-1}B, \quad k\triangleright B^* = qB^*, \quad k\triangleright A = A,$$

$$k^{-1}\triangleright B = qB, \quad k^{-1}\triangleright B^* = q^{-1}B^*, \quad k^{-1}\triangleright A = A,$$

$$e\triangleright B = 0, \quad e\triangleright B^* = q^{-1/2} - (q^{3/2} + q^{-1/2})A, \quad e\triangleright A = q^{1/2}B,$$

$$e^*\triangleright B = -q^{-3/2} + (q^{1/2} + q^{-3/2})A, \quad e^*\triangleright B^* = 0, \quad e^*\triangleright A = -q^{-1/2}B^*, \tag{13a}$$

$$a\triangleright B = q^{-1}B + (q - q^{-1})BA, \quad a\triangleright B^* = q^{-1}B^* + (q - q^{-1})AB^*,$$

$$a\triangleright A = q^{-2}A + (1 - q^{-2})A^2,$$

$$a^*\triangleright B = qB + (q - q^3)AB, \quad a^*\triangleright B^* = qB^* + (q - q^3)B^*A,$$

$$a^*\triangleright A = q^2A + (q^2 - q^4)A^2,$$

$$b\triangleright B = (q^2 - 1)B^2, \quad b\triangleright B^* = (1 - q^2)A^2, \quad b\triangleright A = (q^3 - q)BA,$$

$$b^*\triangleright B = (q - q^{-1})A^2, \quad b^*\triangleright B^* = -(q - q^{-1})B^{*2}, \quad b^*\triangleright A = (1 - q^2)AB^*. \tag{13b}$$

We note, that the notion of *-structure is crucial for our paper because the group $SL(2,\mathbf{C})$ (in the context of the conformal transformations acting on the Riemann sphere) is viewed as the *real* group. It is this fact which is the starting point of our strategy to deform the projective formula (1), since the real group $SL(2,\mathbf{C})$ is the Poisson–Lie Drinfeld double of the group SU(2). The concept of reality in the deformed Hopf picture is encoded in the *-structure. Thus we need a star * on our quantum double $D(U_q(su(2))) = SL_q(2,\mathbf{C})$. It is in fact given by the formula (6) uniquely in terms of the standard stars on $U_q(su(2))$ and $Fun_q(SU(2))$ (see Majid, 1995; Dąbrowski *et al.*, unpublished). The star-compatible action of the *-Hopf algebra $D(U_q(su(2)))$ on the *-algebra $Fun_q(SU(2))$ [and on its subalgebra $Fun_q(S^2)$] is the q-deformed version of the statement that the real group $SL(2,\mathbf{C})$ acts on the real algebra Fun(SU(2)) and on its subalgebra $Fun(S^2)$.

III. THE LIMIT $q\to 1$

In this section, we want to show that the action (7a) and (7b) of the quantum double $D(U_q(su(2)))$ on $Fun_q(S^2)$ described explicitly by the formulas (13a) and (13b) gives in the limit $q\to 1$ the same result as the action of the group $SL(2,\mathbf{C})$ on $Fun(S^2)$ induced by the projective formula (1). First of all, the limit $q\to 1$ of $Fun_q(S^2)$ gives the commutative algebra of complex functions on the sphere S^2, generated by

$$\mathcal{B} = \frac{z}{z\bar{z} + 1}, \quad \mathcal{B}^* = \frac{\bar{z}}{z\bar{z} + 1}, \quad \mathcal{A} = \frac{1}{z\bar{z} + 1},$$

where z is the standard complex coordinate on the Riemann sphere given by the stereographic projection.

The subgroup SU(2) of $SL(2,\mathbf{C})$ acts on S^2 via formula (1),

$$z \to \frac{\alpha z + \beta}{-\bar{\beta}z + \bar{\alpha}}, \quad \bar{z} \to \frac{\bar{\alpha}\bar{z} + \bar{\beta}}{-\beta\bar{z} + \alpha}.$$

Its Lie algebra Lie(SU(2)) therefore acts on $Fun(S^2)$ via three vector fields $\mathcal{R}_j$, $j=1,2,3$,

$$\mathcal{R}_3 = i(z\partial_z - \overline{z}\partial_{\overline{z}}), \quad \mathcal{R}_1 + i\mathcal{R}_2 = i(\partial_z + \overline{z}^2\partial_{\overline{z}}), \quad -\mathcal{R}_1 + i\mathcal{R}_2 = i(z^2\partial_z + \partial_{\overline{z}}).$$

The subgroup AN of $\mathrm{SL}(2,C)$ is formed by complex upper-triangular 2×2 matrices with real positive numbers on the diagonal. Its action on S^2 is obtained from the projective formula (1) for the following choice of parameters: $\gamma=0$, Im $\alpha=0$, Re $\alpha>0$, and β an arbitrary complex number. Thus

$$z \to \alpha(\alpha z + \beta), \quad \overline{z} \to \alpha(\alpha\overline{z} + \overline{\beta}).$$

The Lie algebra Lie(AN) therefore acts on Fun(S^2) via three vector fields $\mathcal{T}_j$, $j=0,1,2$,

$$\mathcal{T}_0 = z\partial_z + \overline{z}\partial_{\overline{z}}, \quad \mathcal{T}_2 + i\mathcal{T}_1 = -2\partial_{\overline{z}}, \quad -\mathcal{T}_2 + i\mathcal{T}_1 = 2\partial_z.$$

It is now straightforward to calculate

$$\mathcal{R}_3\mathcal{B} = i\mathcal{B}, \quad \mathcal{R}_3\mathcal{B}^* = -i\mathcal{B}^*, \quad \mathcal{R}_3\mathcal{A} = 0.$$

$$(\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{B} = i(2\mathcal{A}-1), \quad (\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{B}^* = 0, \quad (\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{A} = -i\mathcal{B}^*, \tag{14a}$$

$$(-\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{B} = 0, \quad (-\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{B}^* = i(2\mathcal{A}-1), \quad (-\mathcal{R}_1 + i\mathcal{R}_2)\mathcal{A} = -i\mathcal{B},$$

$$\mathcal{T}_0\mathcal{B} = \mathcal{B}(2\mathcal{A}-1), \quad \mathcal{T}_0\mathcal{B}^* = \mathcal{B}^*(2\mathcal{A}-1), \quad \mathcal{T}_0\mathcal{A} = 2\mathcal{A}(\mathcal{A}-1),$$

$$(\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{B} = 2\mathcal{B}^2, \quad (\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{B}^* = -2\mathcal{A}^2, \quad (\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{A} = 2\mathcal{A}\mathcal{B}, \tag{14b}$$

$$(-\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{B} = 2\mathcal{A}^2, \quad (-\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{B}^* = -2\mathcal{B}^{*2}, \quad (-\mathcal{T}_2 + i\mathcal{T}_1)\mathcal{A} = -2\mathcal{A}\mathcal{B}^*.$$

We recall, that the formulas (14a) and (14b) describe the infinitesimal projective action (1) of the Lie algebra Lie($\mathrm{SL}(2,\mathbf{C})$) on Fun($S^2$). We wish to show that they can be obtained from the formulas (13a) and (13b) in the limit $q\to 1$.

In the limit $q\to 1$, the Hopf algebra $\mathrm{U}_q(\mathrm{su}(2))$ reduces to the enveloping algebra of Lie(SU(2)). Upon the standard identification

$$-ie = -R_1 + iR_2, \quad ie^* = R_1 + iR_2, \quad k = q^{iR_3}, \quad k^{-1} = q^{-iR_3},$$

we indeed obtain in the limit the standard definition of the U(su(2)) (viewed as the Hopf algebra) from the defining relations (12a)–(12c) of $\mathrm{U}_q(\mathrm{su}(2))$. In particular, the commutations relations (12a) give in the limit $[R_j,R_k]=\epsilon_{jkl}R_l$. (Note that $R_j^*=-R_j$.) In the limit $q\to 1$, the action (13a) of $\mathrm{U}_q(\mathrm{su}(2))$ thus gives

$$(R_3\triangleright B)_{q\to 1} = \lim_{q\to 1}\frac{k-1}{i\ln q}\triangleright B = iB, \quad (R_3\triangleright B^*)_{q\to 1} = -iB^*, \quad (R_3\triangleright A)_{q\to 1} = 0.$$

$$\begin{gathered}((R_1 + iR_2)\triangleright B)_{q\to 1} = \lim_{q\to 1}(ie^*\triangleright B) = i(2A-1), \quad ((R_1 + iR_2)\triangleright B^*)_{q\to 1} = 0,\\ ((-R_1 + iR_2)\triangleright B)_{q\to 1} = 0, \quad ((-R_1 + iR_2)\triangleright B^*)_{q\to 1} = \lim_{q\to 1}(-ie\triangleright B^*) = i(2A-1),\end{gathered} \tag{15a}$$

$$((R_1 + iR_2)\triangleright A)_{q\to 1} = -iB^*, \quad ((-R_1 + iR_2)\triangleright A)_{q\to 1} = -iB.$$

Comparing (15a) with (14a), we immediately observe that the $q\to 1$ limit of the $\mathrm{U}_q(\mathrm{su}(2))$ action on the Podleś sphere indeed coincides with the Lie(SU(2)) action induced by the projective formula.

Now we turn our attention to the q-deformation of the action of Lie(AN). We define the following elements of $\mathrm{Fun}_q(\mathrm{SU}(2))$:

$$ {}^qT_0 = \frac{a - a^*}{2(\ln q)}, \quad i^qT_1 + {}^qT_2 = \frac{b}{(\ln q)}, \quad i^qT_1 - {}^qT_2 = \frac{b^*}{(\ln q)} \tag{16a} $$

and calculate

$$ \lim_{q\to 1}({}^qT_0 \triangleright B) = B(2A-1), \quad \lim_{q\to 1}({}^qT_0 \triangleright B^*) = B^*(2A-1), \quad \lim_{q\to 1}({}^qT_0 \triangleright A) = 2A(A-1), $$

$$ \begin{aligned} &\lim_{q\to 1}(i^qT_1 + {}^qT_2) \triangleright B = 2B^2, \quad \lim_{q\to 1}(i^qT_1 + {}^qT_2) \triangleright B^* = -2A^2, \\ &\lim_{q\to 1}(i^qT_1 - {}^qT_2) \triangleright B = 2A^2, \quad \lim_{q\to 1}(i^qT_1 - {}^qT_2) \triangleright B^* = -2B^{*2}, \\ &\lim_{q\to 1}(i^qT_1 + {}^qT_2) \triangleright A = 2AB, \quad \lim_{q\to 1}(i^qT_1 - {}^qT_2) \triangleright A = -2AB^*. \end{aligned} \tag{15b} $$

Comparing (15b) with (14b), we immediately observe that the $q\to 1$ limit of the $\mathrm{Fun}_q(\mathrm{SU}(2))$ action on the Podleś sphere indeed gives the Lie(AN) action induced by the projective formula (1).

The reader may find somewhat mysterious why the $q\to 1$ limit of $\mathrm{Fun}_q(\mathrm{SU}(2))$ contains Lie(AN) generators. The explanation of this fact resides in the famous Drinfeld duality principle which states that there is a natural identification of Hopf algebras $\mathrm{Fun}_g(G)$ and $\mathrm{U}_q(\mathcal{G}^*)$. Here G is a Poisson–Lie group and $\mathcal{G}^*$ is the Lie algebra of its dual Poisson–Lie group G^*. Let us indicate [a rigorous proof would require to give meaning to nonpolynomial functions appearing in (16b)] why the Drinfeld duality takes place in the case $G=\mathrm{SU}(2)$ and $G^*=AN$. The Lie algebra Lie(AN) is generated by three generators T_j, $j=0,1,2$, $T_j^*=-T_j$ obeying the following commutation relations:

$$ [T_0,T_1] = -T_1, \quad [T_0,T_2] = -T_2, \quad [T_1,T_2] = 0. \tag{17} $$

We set

$$ a = q^{T_0}\sqrt{1+q^2(\ln q)^2(T_1^2+T_2^2)}, \quad a^* = \sqrt{1+q^2(\ln q)^2(T_1^2+T_2^2)}\,q^{-T_0}, $$

$$ b = (\ln q)(iT_1 + T_2), \quad b^* = (\ln q)(iT_1 - T_2). \tag{16b} $$

Then it is not difficult to check two things: (1) the formulas (16b) and (17) imply the defining commutation relations (11a) of the Hopf algebra $\mathrm{Fun}_q(\mathrm{SU}(2))$; (2) it holds $\lim_{q\to 1}({}^qT_j) = T_j$.

Remark 1: Note that this explicit relation (16b) between $\mathrm{U}_q(\mathrm{Lie}(AN))$ and $\mathrm{Fun}_q(\mathrm{SU}(2))$ *degenerates* when $q\to 1$. This fact was important for establishing the limit $q\to 1$ of the Hopf adjoint action of $\mathrm{Fun}_q(\mathrm{SU}(2))$ on $\mathrm{Fun}_q(S^2)\subset\mathrm{Fun}_q(\mathrm{SU}(2))$. Indeed, it appears superficially that in the $q\to 1$ limit, the algebra $\mathrm{Fun}_q(\mathrm{SU}(2))$ becomes commutative and the adjoint action trivial. This observation is too naive, however, and the explanation of the paradox resides in the degeneration of the relation (16b) between the sets of generators T_j and a, a^*, b, b^* in the limit $q\to 1$.

Remark 2: We have established the correct $q\to 1$ limit of the quantum double action (7a) and (7b) by performing the detailed calculations with the generators, relations, etc. However, it is also possible to establish it on the conceptual level. First of all, the experts in Poisson–Lie groups and Hopf algebras know that the $q\to 1$ of the adjoint action (7b) of $\mathrm{U}_q(\mathcal{G}^*)$ on itself is indeed the dressing transformation of the Poisson–Lie group G by its dual Poisson–Lie group G^* [here $G=\mathrm{SU}(2)$ and $G^*=AN$]. The reader can find the detailed proof of this fact in the paper of Korogodsky (unpublished). The conceptual proof of the correct $q\to 1$ limit of the formula (7a) is even simpler. Indeed we have the following.

The standard left action of the enveloping algebra U(su(2)) on Fun(SU(2)) is given by left derivations, i.e., if X is an element of su(2) and $h(g)$ is in Fun(SU(2)) then we have

$$(X\triangleright h)(g)=\left.\frac{d}{dt}h(e^{-tX}g)\right|_{t=0}. \tag{18}$$

Recall the coproduct and the counit of the Hopf algebra structure of the nondeformed Fun(SU(2)),

$$(\Delta h)(g_1,g_2)=h(g_1g_2),\quad \varepsilon(h)=h(e),$$

where e is the group unit. Recall also that $S(X)=-X$ for $X\in\mathrm{su}(2)\subset\mathrm{U}(\mathrm{su}(2))$. Finally note the standard formula for the pairing $\langle .,.\rangle$ between $X\in\mathrm{su}(2)$ and $h\in\mathrm{Fun}(\mathrm{SU}(2))$:

$$-\langle X,h\rangle=\varepsilon(X\triangleright h).$$

Setting all of these pieces of information together, we see that (18) can be written as

$$(X\triangleright h)(g)=\left.\frac{d}{dt}h(e^{-tX}g)\right|_{t=0}=\langle S^{-1}(X),h'\rangle h''(g).$$

This is indeed the formula (7a) for $H=\mathrm{U}(\mathrm{su}(2))$ and $\tilde{H}=\mathrm{Fun}(\mathrm{SU}(2))$. In this way, we have verified that the action (7a) of $\mathrm{U}_q(\mathrm{su}(2))$ on $\mathrm{Fun}_q(\mathrm{SU}(2))$ [and, consequently on $\mathrm{Fun}_q(S^2)\subset\mathrm{Fun}_q(\mathrm{SU}(2))$] has the correct $q\to1$ limit, because it is well known that the left action of SU(2) on $S^2=\mathrm{SU}(2)/\mathrm{U}(1)$ is induced by the projective formula (1) for $\overline{\alpha}=\delta$, $\overline{\gamma}=-\beta$.

IV. CONCLUSIONS AND OUTLOOK

We have constructed the q-Lorentz group extension of the natural action of $\mathrm{U}_q(\mathrm{su}(2))$ on the Podleś sphere and shown that it can be naturally interpreted as the q-deformation of the projective formula $z\to(\alpha z+\beta)/(\gamma z+\delta)$ describing the global conformal transformation of the Riemann sphere. Our results are rather mathematical in nature but we believe that they can be used mainly in mathematical physics, e.g., in further studies of braided field theories (cf. Oeckl, 2001) and also in studies of q-differential operators (cf. the q-Dirac operator by Dąbrowski and Sitarz, 2003) on the Podleś sphere. Indeed, our studies suggest to investigate the symmetry properties of those objects not only from the point of view of the action of the $\mathrm{U}_q(\mathrm{su}(2))$ quantum group but also from the point of view of the action of its quantum double.

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Global classical solution of the Vlasov–Maxwell–Landau system near Maxwellians

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We consider a classical model in the kinetic theory of plasma—the Vlasov–Maxwell–Landau system. Global in time classical solutions near Maxwellians are constructed for hard potential and soft potential, i.e., $\gamma \geqslant -1$. The construction of global solution is based on an energy method. Meanwhile, global classical solutions of the Vlasov–Poisson–Landau system near Maxwellians for $\gamma \geqslant -1$ and the exponential decay of such solutions are obtained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1803611]

I. INTRODUCTION

The dynamics of charged dilute particles in plasma physics can be described by the Vlasov–Maxwell–Landau system (see Refs. 1–3),

$$\partial_t F + v \cdot \nabla_x F + \frac{e}{m}\left\{E + \frac{v}{c} \times B\right\} \cdot \nabla_v F = Q[F,F], \quad F(0,x,v) = F_0(x,v), \tag{1.1}$$

where $F(t,x,v)$ is the spatially periodic distribution function for the particles at time $t \geqslant 0$, with spatial coordinates $x=(x_1,x_2,x_3) \in [-\pi,\pi]^3 = T^3$ and velocity $v=(v_1,v_2,v_3) \in R^3$. And e, m, and c denote the magnitude of their charges and mass, the light speed, respectively. The collision between particles is described by the following Landau operator:

$$\begin{aligned} Q[F,G] &= \nabla_v \cdot \left\{ \int_{R^3} \varphi(v-v_*)[F(v_*)\nabla_v G(v) - G(v)\nabla_v F(v_*)]\mathrm{d}v_* \right\} \\ &= \partial_i \int_{R^3} \varphi^{ij}(v-v_*)[F(v_*)\partial_j G(v) - G(v)\partial_j F(v_*)]\mathrm{d}v_*. \end{aligned}$$

In the case of an interaction force $\mathfrak{R}$ between the particles which depends on the interparticle distance r according to an inverse power law $\mathfrak{R}=r^{-s}$ with $s \geqslant 2$, $\varphi^{ij}(v)=\{\delta_{ij}-v_i v_j/|v|^2\}|v|^{\gamma+2}$ where $\gamma=(s-5)/(s-1)$. This leads to the usual classification in terms of hard potential ($\gamma>0$), Maxwellian molecules ($\gamma=0$) or soft potential ($\gamma<0$) (see Ref. 4). The present study is restricted to the case $\gamma \geqslant -1$.

The self-consistent, spatially periodic electromagnetic field $[E(t,x),B(t,x)]$ in (1.1) is coupled with $F(t,x,v)$ through the Maxwell system,

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$$\partial_t E - c\nabla \times B = -4\pi J = -4\pi \int_{R^3} ev F \, dv, \quad \nabla \cdot B = 0,$$

$$\partial_t B + c\nabla \times E = 0, \quad \nabla \cdot E = \rho = 4\pi \int_{R^3} e\{F - \mu\} dv, \tag{1.2}$$

$$E(0,x) = E_0(x), \quad B(0,x) = B_0(x).$$

The Vlasov–Maxwell–Landau system is a classical model in the kinetic theory of plasma and also arises in several branches of continuum physics. This system provides a statistical description of a plasma, in terms of its density $F(t,x,v)$, when the collisions moving particles are taken into account. There are two reduced descriptions of a high-temperature, low-density plasma. One is obtained by assuming that collisions are so rare that they are neglected. The associated model constitutes the Vlasov–Maxwell system, which is investigated by many authors (see Refs. 1 and 5–7). By neglecting the magnetic field ($B \equiv 0$ and $E = \nabla_x \phi$), one obtains the second reduced system, that is, the Vlasov–Poisson–Landau system,

$$\partial_t F + v \cdot \nabla_x F + \frac{c}{m} \nabla_x \phi \cdot \nabla_v F = Q[F,F],$$

$$\Delta \phi = 4\pi \int_{R^3} e\{F - u\} dv, \quad \int_{T^3} \phi \, dx = 0,$$

$$F(0,x,v) = F_0(x,v).$$

There are some investigations about the Vlasov–Poisson–Landau system (see Refs. 1,2,8,9,3). The purpose of this paper is to construct global classical solutions for (1.1) and (1.2) near a global Maxwellian $\mu = (n_0/e)(m/2\pi k T_0)^{3/2} e^{-m|v|^2/2kT_0}$. For convenience, we normalize all the physical constants involved in (1.1) and (1.2) to be one and let the global Maxwellian be $\mu(v) = e^{-|v|^2}$. We define the standard perturbation $f(t,x,v)$ to μ as $F = \mu + \mu^{1/2} f$. It is well known that $Q[\mu,\mu] = 0$. By expanding $Q[\mu + \mu^{1/2} g_1, \mu + \mu^{1/2} g_2]$, we define

$$Q[\mu + \mu^{1/2} g_1, \mu + \mu^{1/2} g_2] \equiv Q[\mu,\mu] + \mu^{1/2}\{K g_1 + A g_2 + \Gamma[g_1,g_2]\}.$$

The system (1.1) for $f(t,x,v)$ turns into

$$[\partial_t + v \cdot \nabla_x + (E + v \times B) \cdot \nabla_v] f - 2E \cdot v \mu^{1/2} + Lf = E \cdot v f + \Gamma[f,f], \tag{1.3}$$

with $f(0,x,v) = f_0(x,v)$ and $L = -A - K$. Notice that A, K, and Γ are defined in the same way as in Ref. 10, namely, $\sigma^i = \varphi^{ij} * [v_j \mu], \sigma^{ij} = \varphi^{ij} * \mu$,

$$Ag = \mu^{-1/2} \partial_i \{\mu^{1/2} \sigma^{ij} [\partial_j g + v_j g]\}, \quad Kg = -\mu^{1/2} \partial_i \{\mu [\varphi^{ij} * \{\mu^{1/2} [\partial_j g + v_j g]\}]\},$$

$$\begin{aligned} \Gamma[g_1,g_2] = {} & \partial_i [\{\varphi^{ij} * [\mu^{1/2} g_1]\} \partial_j g_2] - \{\varphi^{ij} * [v_i \mu^{1/2} g_1]\} \partial_j g_2 - \partial_i [\{\varphi^{ij} * [\mu^{1/2} \partial_j g_1]\} g_2] \\ & + \{\varphi^{ij} * [v_i \mu^{1/2} \partial_j g_1]\} g_2. \end{aligned}$$

The coupled Maxwell system takes the form

$$\partial_t E - c\nabla \times B = -J = -\int_{R^3} fv\mu^{1/2}\,\mathrm{d}v, \quad \nabla \cdot B = 0,$$

$$\partial_t B + c\nabla \times E = 0, \quad \nabla \cdot E = \rho = \int_{R^3} \mu^{1/2} f\,\mathrm{d}v, \tag{1.4}$$

$$E(0,x) = E_0(x), \quad B(0,x) = B_0(x).$$

Obviously, the conservation laws of mass, momentum, and energy of (1.1) hold

$$\frac{d}{\mathrm{d}t}\int_{R^3\times T^3} F(t) = \frac{d}{\mathrm{d}t}\left[\int_{R^3\times T^3} vF(t) + \int_{T^3} E(t)\times B(t)\right] = 0,$$

$$\frac{d}{\mathrm{d}t}\left[\int_{R^3\times T^3} |v|^2 F(t) + \int_{T^3} |E(t)|^2 + |B(t)|^2\right] = 0.$$

Notice that from the Maxwell system and the periodic boundary condition of $E(t,x), (d/\mathrm{d}t)\int_{T^3} B(t,x)\mathrm{d}x \equiv 0$. Thus we have a constant $\overline{B}$ such that $(1/|T^3|)\int_{T^3} B(t,x)\mathrm{d}x = \overline{B}$. By assuming that initially $[F_0, E_0, B_0]$ has the same mass, total momentum, and total energy as the steady state $[\mu, 0, \overline{B}]$, we can rewrite the conservation laws in the terms of the perturbation $[f, E, B]$ as

$$\int_{R^3\times T^3} f(t)\mu^{1/2} = \int_{R^3\times T^3} vf(t)\mu^{1/2} + \int_{T^3} E(t)\times B(t) = 0, \tag{1.5}$$

$$\int_{R^3\times T^3} |v|^2 f(t)\mu^{1/2} + \int_{T^3} |E(t)|^2 + |B(t) - \overline{B}|^2 = 0. \tag{1.6}$$

We shall use $(\cdot,\cdot)$ to denote either the standard L^2 inner product in T^3 or in $T^3\times R^3$. We shall use $\|\cdot\|$ to denote the corresponding norms. Let the multi-indices α and β be $\alpha = [\alpha_0, \alpha_1, \alpha_2, \alpha_3], \beta = [\beta_1, \beta_2, \beta_3]$ with $|\alpha| = \Sigma_{k=0}^3 \alpha_k$ and $|\beta| = \Sigma_{k=1}^3 \beta_k$. We define $\partial_\beta^\alpha \equiv \partial_t^{\alpha_0}\partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\partial_{x_3}^{\alpha_3}\partial_{v_1}^{\beta_1}\partial_{v_2}^{\beta_2}\partial_{v_3}^{\beta_3}$. If each component of β is not greater than that of $\overline{\beta}$'s, we denote it by $\beta \leqslant \overline{\beta}$. We define $\beta < \overline{\beta}$ if $\beta \leqslant \overline{\beta}$, and $|\beta| < |\overline{\beta}|$. We denote $\binom{\beta}{\overline{\beta}}$ by $C_{\overline{\beta}}^{\beta}$.

We define the weighted norm and the high order energy norm as

$$|g|_\sigma^2 = \int_{R^3} [\sigma^{ij}\partial_i g\partial_j g + \sigma^{ij} v_i v_j g^2]\mathrm{d}v, \quad \|g\|_\sigma^2 = \int_{R^3\times T^3} [\sigma^{ij}\partial_i g\partial_j g + \sigma^{ij} v_i v_j g^2]\mathrm{d}x\,\mathrm{d}v,$$

$$E(f(t,x,v)) \equiv \sum_{|\alpha|+|\beta|\leqslant N}\left[\frac{1}{2}\|\partial_\beta^\alpha f(t)\|^2 + \int_0^t \|\partial_\beta^\alpha f(s)\|_\sigma^2\,\mathrm{d}s\right] + \sum_{|\alpha|\leqslant N}[\|\partial^\alpha E(t)\|^2 + \|\partial^\alpha B(t)\|^2],$$

with the initial energy

$$E(f_0) = E(f(0)) \equiv \sum_{|\alpha|+|\beta|\leqslant N}\frac{1}{2}\|\partial_\beta^\alpha f_0\|^2 + \sum_{|\alpha|\leqslant N}[\|\partial^\alpha E_0\|^2 + \|\partial^\alpha B_0\|^2].$$

Throughout this paper, $N \geqslant 8$. The main result in this paper is as follows.

Theorem 1.1: *Assume that $[f_0, E_0, B_0]$ satisfies the conservation laws (1.5) and (1.6). Let $F_0(x,v) = \mu + \mu^{1/2} f_0 \geqslant 0$. There exist $C_0 > 0$ and $M > 0$ such that if $E(f_0) \leqslant M$, then there exists a unique global solution $f(t,x,v)$ to the system (1.3) and (1.4). Moreover, $F(t,x,v) = \mu$*

$+\mu^{1/2}f(t,x,v)\geqslant 0$ *and* $\sup_{0\leqslant t\leqslant\infty}E(f(t))\leqslant C_0E(f_0)$.

For the simpler Vlasov–Poisson–Landau system from (1.3) and (1.4), we have

$$[\partial_t + v\cdot\nabla_x + \nabla_x\phi\cdot\nabla_v]f - 2\nabla_x\phi\cdot v\mu^{1/2} + Lf = \nabla_x\phi\cdot vf + \Gamma[f,f],$$

$$\Delta\phi = \int_{R^3}\mu^{1/2}f\,dv, \quad \int_{T^3}\phi\,dx = 0, \tag{1.7}$$

$$f(0,x,v) = f_0(x,v).$$

We define the same energy norm as the above with $B\equiv 0$ and $E=\nabla_x\phi$. The conservation laws of mass, momentum, and total energy are

$$\int_{R^3\times T^3} f(t)\mu^{1/2} = \int_{R^3\times T^3} vf(t)\mu^{1/2} = 0, \tag{1.8}$$

$$\int_{R^3\times T^3}|v|^2f(t)\mu^{1/2} + \int_{T^3}|\nabla_x\phi(t)|^2 = 0. \tag{1.9}$$

We have the following result for the decay of such a simpler system.

Theorem 1.2: *Assume that f_0 satisfies (1.8) and (1.9). Let $F_0(x,v)=\mu+\mu^{1/2}f_0\geqslant 0$. There exist $C_0>0$ and $M>0$ such that if $E(f_0)\leqslant M$, then there exists a unique global solution $f(t,x,v)$ to the system (1.7). Moreover, $F(t,x,v)=\mu+\mu^{1/2}f(t,x,v)\geqslant 0$ and $\sup_{0\leqslant t\leqslant\infty}E(f(t))\leqslant C_0E(f_0)$.*

Moreover, there is a $\delta^*>0$ such that

$$\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f(t)\|\leqslant E^{1/2}(f_0)e^{-\delta^* t}.$$

Although there are some research about the dynamical problems of the Landau equation (see Refs. 1,4,2,11,12,10,13,14,8,9,3), but few global classical solutions have been constructed except for Refs. 11,12,10, especially little for soft potential, i.e., $\gamma<0$ as pointed out by Desvillettes and Villani in Refs. 11,12, where they have constructed global classical solutions to the spatially homogeneous Landau equation for hard potential $0<\gamma\leqslant 1$. Guo first obtains the global classical solution of the Vlasov–Poisson–Boltzmann near Maxwellians under the hard sphere condition in the pioneering paper, Ref. 15. And then he also shows in Ref. 16 that under the hard sphere condition, global classical solution of the Vlasov–Maxwell–Boltzmann near Maxwellians can be constructed, which is the first result of global solution in this direction. In Ref. 10, the first global classical solution of the Landau equation with $\gamma\geqslant -3$ near Maxwellians can be obtained by original energy method. Zhan establishes the local existence of weak solution of the system (1.1) and (1.2) with initial data of unrestricted size in Ref. 3.

Motivated by the framework used in Ref. 16, we establish the existence and uniqueness of global in time classical solution of the system (1.1) and (1.2) near Maxwellians for both hard potential and soft potential, i.e., $\gamma\geqslant -1$. Although our construction of global solutions is based on an energy method developed in Refs. 15,16,10, we cannot obtain the crucial positivity of the linearized Landau operator L by using the similar argument developed in Refs. 15,17,10. This is because either $-\int E\times B$ in the momentum conservation in (1.5) or $-\|E(t)\|-\|B(t)-\overline{B}\|$ in the reduced energy conservation (1.6) cannot be controlled by $o(1)\|\partial_\beta^\alpha f(t)\|$, due to the presence of the magnetic field $[E(t,x),B(t,x)]$. Instead, we revised the methods in Ref. 16 to obtain it. Furthermore, we introduce the norm $\|\cdot\|_\sigma$ in the total energy and use the following inequality (1.14) with $\gamma\geqslant -1$ in order to control the product of the term $\partial_\beta[vf]$ and the term $\partial_\beta f$ in the energy estimate. However, we cannot control this product by (1.14) when $\gamma<-1$. As for this problem, we consider it in the future.

In the following we give some lemmas which can be found in Ref. 10.

Lemma 1.3: *Let* $|\beta|>0, |\alpha|+|\beta|\leqslant N$. *Then for small* $\eta>0$, *there exists* $C>0$ *and* $C_\eta>0$ *such that*

$$-(\partial_\beta[Ag],\partial_\beta g)\geqslant \|\partial_\beta g\|_\sigma^2-\eta\sum_{|\beta_1|\leqslant|\beta|}\|\partial_{\beta_1} g\|_\sigma^2-C_\eta\|\mu g\|^2, \tag{1.10}$$

$$|(\partial_\beta[Kg_1],\partial_\beta g_2)|\leqslant\left\{\eta\sum_{|\beta_1|\leqslant|\beta|}\|\partial_{\beta_1} g_1\|_\sigma+C_\eta\|\mu g_1\|\right\}\|\partial_\beta g_2\|_\sigma, \tag{1.11}$$

$$\begin{aligned}(\partial_\beta^\alpha\Gamma[g_1,g_2],\partial_\beta^\alpha g_3)\leqslant C\Bigg[&\left\{\sum_{\alpha_1\leqslant\alpha,\beta_1\leqslant\beta}\|\partial_{\beta_1}^{\alpha_1} g_1\|\right\}\left\{\sum_{\alpha_1\leqslant\alpha,\beta_1\leqslant\beta}\|\partial_{\beta_1}^{\alpha_1} g_2\|_\sigma\right\}+\left\{\sum_{\alpha_1\leqslant\alpha,\beta_1\leqslant\beta}\|\partial_{\beta_1}^{\alpha_1} g_1\|_\sigma\right\}\\&\times\left\{\sum_{\alpha_1\leqslant\alpha,\beta_1\leqslant\beta}\|\partial_{\beta_1}^{\alpha_1} g_2\|\right\}\Bigg]\|\partial_\beta^\alpha g_3\|_\sigma.\end{aligned} \tag{1.12}$$

It is well known that the linearized collision operator L is non-negative. And for fixed (t,x), the null space of L is the five dimensional space of $N=\mathrm{span}\{1,v_i,|v|^2\}\mu^{1/2}$, where $1\leqslant i\leqslant 3$. We denote $\{1,v_i,|v|^2\}\mu^{1/2}$ as $\{e_1,e_2,e_3,e_4,e_5\}$ in Ref. 7. We define a projection P_0 in $L^2(R^3)$ for any fixed x as $P_0g(x,v)=\Sigma(g(x,\cdot),e_j)e_j$ and $P_1=I-P_0$ where I is the identity operator.

Lemma 1.4: For any $m>1$, *there is* $0<C(m)<\infty$, *such that*

$$|(\partial_i\sigma^j g_1,g_2)|+|(Kg_1,g_2)|\leqslant\frac{C}{m}|g_1|_\sigma|g_2|_\sigma+C(m)\left\{\int_{|v|\leqslant C(m)}|g_1|^2\,\mathrm{d}v\right\}^{1/2}\left\{\int_{|v|\leqslant C(m)}|g_2|^2\,\mathrm{d}v\right\}^{1/2}. \tag{1.13}$$

Moreover, we have that there exists $c>0$ *and* $\delta>0$ *such that*

$$\|g\|_\sigma^2\geqslant c\|[1+|v|]^{(\gamma+2)/2}g\|^2, \tag{1.14}$$

$$(Lg,g)\geqslant\delta\|P_1g\|_\sigma^2. \tag{1.15}$$

Lemma 1.5: Let $\chi(v)$ *be a smooth function so that* $\{|\chi|+|\nabla\chi|+|\nabla^2\chi|\leqslant C\mu(v/4)$, *then*

$$\left\|\int\partial^\alpha\Gamma[g_1,g_2]\chi\,\mathrm{d}v\right\|\leqslant C\left\{\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} g_1\|\right\}\left\{\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} g_2\|_\sigma\right\}. \tag{1.16}$$

II. ENERGY ESTIMATES

The goal in this section is to construct local in time solutions to the system (1.3) and (1.4). The construction is based on a uniform energy estimate for the following sequence of iterating approximate solutions:

$$[\partial_t+v\cdot\nabla_x+(E^n+v\times B^n)\cdot\nabla_v]F^{n+1}=Q[F^n,F^{n+1}],$$

$$F^{n+1}(0,x,v)=F_0(x,v),$$

together with the coupled Maxwell system:

$$\partial_t E^n - \nabla \times B^n = -J^n = -\int_{R^3} v F^n \, dv, \quad \nabla \cdot B^n = 0,$$

$$\partial_t B^n + \nabla \times E^n = 0, \quad \nabla \cdot E^n = \rho^n = \int_{R^3} \{F^n - \mu\} dv,$$

$$E^n(0,x) = E_0(x), \quad B^n(0,x) = B_0(x).$$

We start with $F^0(t,x,v) = F_0(x,v)$. And then $[E^0(t,x), B^0(t,x)]$ is solved through the Maxwell system with initial datum $[E_0(x), B_0(x)]$. Since $F^{n+1} = \mu + \mu^{1/2} f^{n+1}$, we need to solve f^{n+1} such that

$$\begin{aligned} &[\partial_t + v \cdot \nabla_x + (E^n + v \times B^n) \cdot \nabla_v - (E^n \cdot v) - A] f^{n+1} - 2E^n \cdot v \mu^{1/2} - K f^n = \Gamma[f^n, f^{n+1}], \\ &\partial_t E^n - \nabla \times B^n = -J^n = -\int_{R^3} v f^n \mu^{1/2} \, dv, \quad \nabla \cdot B^n = 0, \end{aligned} \tag{2.1}$$

$$\begin{aligned} &\partial_t B^n + \nabla \times E^n = 0, \quad \nabla \cdot E^n = \rho^n = \int_{R^3} f^n \mu^{1/2} \, dv, \\ &E^n(0,x) = E_0(x), \quad B^n(0,x) = B_0(x), \quad f^{n+1}(0,x,v) = f_0(x,v), \end{aligned} \tag{2.2}$$

starting with $f^0(t,x,v) = f_0(x,v)$. Our goal is to get a uniformly in n estimate for $E(f^{n+1}(t))$. The crucial energy estimate is as follows:

Lemma 2.1: The sequence $\{F^n\}$ is well defined and non-negative. Moreover, there exist $T^*(E(f_0)) > 0$ and $C > 0$ such that for $0 \leq t \leq T^*$ and $E(f_0)$ sufficiently small, then

$$\sup_k E(f^k(t)) \leq C E(f_0). \tag{2.3}$$

Proof: The proof is based on an induction over k. Clearly (2.3) holds when $k = 0$. Assume (2.3) is valid for $k = n$ so that $F^n \geq 0$. We notice that $Q[F^n, F^{n+1}]$ can be written as the linear form on F^{n+1} (see Ref. 10) and then (2.1) is a linear equation on F^{n+1}. For given $F^n \geq 0$, there exists a solution F^{n+1} to the linear equation (2.1). Moreover, $F^{n+1} \geq 0$ since $F_0(x,v) \geq 0$.

To prove (2.3) for $k = n+1$, the first step is to estimate the ∂_β^α derivatives of f^{n+1}. Taking ∂_β^α $(\beta \neq 0)$ of (2.1), multiplying $\partial_\beta^\alpha f^{n+1}$, and then integrating over $T^3 \times R^3$, we obtain

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} \|\partial_\beta^\alpha f^{n+1}\|^2 - (\partial_\beta A[\partial^\alpha f^{n+1}], \partial_\beta^\alpha f^{n+1}) - (\partial_\beta K[\partial^\alpha f^n], \partial_\beta^\alpha f^{n+1}) \\ &\quad = (\partial_\beta^\alpha \Gamma[f^n, f^{n+1}], \partial_\beta^\alpha f^{n+1}) - \sum_{j, \beta_1 < \beta} (C_\beta^{\beta_1} \partial_{\beta - \beta_1} v_j \partial^j \partial_{\beta_1}^\alpha f^{n+1}, \partial_\beta^\alpha f^{n+1}) + (\partial_\beta^\alpha [E^n \cdot v f^{n+1}], \partial_\beta^\alpha f^{n+1}) \\ &\qquad + 2(\partial^\alpha E^n \cdot \partial_\beta [v \mu^{1/2}], \partial_\beta^\alpha f^{n+1}) - \sum_{0 \neq \alpha_1 \leq \alpha} C_\alpha^{\alpha_1} (\partial^{\alpha_1} E^n \cdot \partial_\beta^{\alpha - \alpha_1} \nabla_v f^{n+1}, \partial_\beta^\alpha f^{n+1}) \\ &\qquad - \sum_{0 \neq \alpha_1 \leq \alpha, 0 \neq \beta_1 \leq \beta} C_\alpha^{\alpha_1} C_\beta^{\beta_1} (\partial_{\beta_1} v \times \partial^{\alpha_1} B^n \cdot \partial_\beta^{\alpha - \alpha_1} \nabla_v f^{n+1}, \partial_\beta^\alpha f^{n+1}). \end{aligned} \tag{2.4}$$

We now estimate (2.4) term by term. For any $\eta > 0$, applying Lemma 1.3 and $\|\mu g\| \leq C \|g\|_\sigma$, we deduce

$$
\begin{aligned}
-(\partial_\beta A[\partial^\alpha f^{n+1}],\partial_\beta^\alpha f^{n+1}) &\geqslant \|\partial_\beta^\alpha f^{n+1}\|_\sigma^2 - \eta \sum_{|\beta_1|\leqslant|\beta|} \|\partial_{\beta_1}^\alpha f^{n+1}\|_\sigma^2 - C_\eta \|\partial^\alpha f^{n+1}\|_\sigma^2,\\
-(\partial_\beta K[\partial^\alpha f^n],\partial_\beta^\alpha f^{n+1}) &\geqslant -\left\{\eta \sum_{|\beta_1|\leqslant|\beta|} \|\partial_{\beta_1}^\alpha f^n\|_\sigma + C_\eta \|\mu\partial^\alpha f^n\|\right\}\|\partial_\beta^\alpha f^{n+1}\|_\sigma\\
&\geqslant -\eta \sum_{|\beta_1|\leqslant|\beta|} \|\partial_{\beta_1}^\alpha f^n\|_\sigma^2 - \eta\|\partial_\beta^\alpha f^{n+1}\|_\sigma^2 - C_\eta\|\mu\partial^\alpha f^n\|^2.
\end{aligned}
\tag{2.5}
$$

We now estimate the second term on the right-hand side of (2.4).

$$
\begin{aligned}
\sum_{j,\beta_1<\beta} (C_\beta^{\beta_1}\partial_{\beta-\beta_1} v_j \partial^j \partial_{\beta_1}^\alpha f^{n+1}, \partial_\beta^\alpha f^{n+1}) &\leqslant C \sum_{j,\beta_1<\beta} \|\partial_\beta^\alpha f^{n+1}\|\,\|\partial^j \partial_{\beta-\beta_1}^\alpha f^{n+1}\|\\
&\leqslant \sum_{j,\beta_1<\beta} [\eta\|\partial_\beta^\alpha f^{n+1}\|^2 + C_\eta\|\partial^j\partial_{\beta-\beta_1}^\alpha f^{n+1}\|^2].
\end{aligned}
\tag{2.6}
$$

The fourth term on the right-hand side of (2.4) is bounded by

$$
2(\partial^\alpha E^n \cdot \partial_\beta[v\mu^{1/2}],\partial_\beta^\alpha f^{n+1}) \leqslant C\|\partial^\alpha E^n\|\,\|\partial_\beta^\alpha f^{n+1}\|. \tag{2.7}
$$

We now estimate the fifth term on the right-hand side of (2.4). Recalling that $W^{4,1}(T^3)\subset L^\infty(T^3)$, we have

$$
\begin{aligned}
\sup_x\left[\int_{R^3} |g(x,u)|^2\,\mathrm{d}u\right] &\leqslant C\sum_{|\ell|\leqslant 4}\int_{T^3}\left|\partial^\ell\int_{R^3} g(x,u)\mathrm{d}u\right|^2\mathrm{d}x\\
&\leqslant C\sum_{|\ell_1|+|\ell_2|\leqslant 4}\int_{T^3\times R^3}|\partial^{\ell_1}g(x,u)\partial^{\ell_2}g(x,u)|\mathrm{d}u\,\mathrm{d}x \leqslant C\sum_{|\ell|\leqslant 4}\|\partial^\ell g(x,u)\|^2.
\end{aligned}
\tag{2.8}
$$

We separate two cases. If $|\alpha_1|\geqslant 5$, then $|\alpha-\alpha_1|+4\leqslant|\alpha|-1$. From (2.8), we have

$$
\begin{aligned}
-\sum_{0\neq\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1},\partial_\beta^\alpha f^{n+1}) &\leqslant C\sum_{0\neq\alpha_1\leqslant\alpha}\int_{T^3}|\partial^{\alpha_1}E^n|\\
&\quad\times\left\{\int|\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1}|^2\,\mathrm{d}v\right\}^{1/2}\left\{\int|\partial_\beta^\alpha f^{n+1}|^2\,\mathrm{d}v\right\}^{1/2}\mathrm{d}x\\
&\leqslant C\sum_{0\neq\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\sup_x\left\{\int|\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1}|^2\,\mathrm{d}v\right\}^{1/2}\|\partial_\beta^\alpha f^{n+1}\|\\
&\leqslant C\left\{\sum_{0\neq\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\right\}\cdot\sum_{|\ell|\leqslant|\alpha-\alpha_1|+4}\|\partial_\beta^\ell\nabla_v f^{n+1}\|\cdot\|\partial_\beta^\alpha f^{n+1}\|\\
&\leqslant C\left\{\sum_{0\neq\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\right\}\cdot\sum_{|\ell|\leqslant|\alpha|-1}\|\partial_\beta^\ell\nabla_v f^{n+1}\|\cdot\|\partial_\beta^\alpha f^{n+1}\|.
\end{aligned}
$$

On the other hand, if $|\alpha_1|\leqslant 4$ and $|\alpha_1|+1\leqslant 5$, we have

$$
\begin{aligned}
-\sum_{0\neq\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1},\partial_\beta^\alpha f^{n+1}) &\leqslant C\sum_{0\neq\alpha_1\leqslant\alpha}\sup_x|\partial^{\alpha_1}E^n|\cdot\|\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1}\|\cdot\|\partial_\beta^\alpha f^{n+1}\|\\
&\leqslant C\sum_{0\neq\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|_{H^2}\|\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1}\|\cdot\|\partial_\beta^\alpha f^{n+1}\|\\
&\leqslant C\Big\{\sum_{|\ell|\leqslant|\alpha_1|+2}\|\partial^\ell E^n\|\Big\}\cdot\sum_{0\neq\alpha_1\leqslant\alpha}\|\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1}\|\cdot\|\partial_\beta^\alpha f^{n+1}\|.
\end{aligned}
$$

We thus have a unified estimate ($N\geqslant 8$) for the fifth term as

$$
-\sum_{0\neq\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}\nabla_v f^{n+1},\partial_\beta^\alpha f^{n+1})\leqslant C\Big\{\sum_{|\ell|\leqslant N}\|\partial^\ell E^n\|\Big\}\cdot\Big\{\sum_{|\ell|+|\lambda|\leqslant N}\|\partial_\lambda^\ell f^{n+1}\|\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|. \tag{2.9}
$$

We now estimate the third term on the right-hand side of (2.4). In the case $|\alpha_1|\geqslant 5, |\alpha-\alpha_1|+4\leqslant|\alpha|-1$. From (1.14) in Lemma 1.4 with $\gamma\geqslant -1$, we have

$$
\begin{aligned}
&\sum_{\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}[vf^{n+1}],\partial_\beta^\alpha f^{n+1})\\
&\quad\leqslant C\sum_{\alpha_1\leqslant\alpha}\int_{T^3}|\partial^{\alpha_1}E^n|\Big\{\sum_{\beta_1\leqslant\beta}\int(1+|v|)|\partial_{\beta_1}^{\alpha-\alpha_1}f^{n+1}|^2\,dv\Big\}^{1/2}\cdot\Big\{\int(1+|v|)|\partial_\beta^\alpha f^{n+1}|^2\,dv\Big\}^{1/2}dx\\
&\quad\leqslant C\Big\{\sum_{\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\Big\}\sup_x\Big\{\sum_{\beta_1\leqslant\beta}\int(1+|v|)|\partial_{\beta_1}^{\alpha-\alpha_1}f^{n+1}|^2\,dv\Big\}^{1/2}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma\\
&\quad\leqslant C\Big\{\sum_{\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\Big\}\cdot\Big\{\sum_{|\ell|\leqslant|\alpha-\alpha_1|+4,\beta_1\leqslant\beta}\|(1+|v|)^{1/2}\partial_{\beta_1}^\ell f^{n+1}\|\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma\\
&\quad\leqslant C\Big\{\sum_{\alpha_1\leqslant\alpha}\|\partial^{\alpha_1}E^n\|\Big\}\cdot\Big\{\sum_{|\ell|\leqslant|\alpha-\alpha_1|+4,\beta_1\leqslant\beta}\|\partial_{\beta_1}^\ell f^{n+1}\|_\sigma\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma.
\end{aligned}
$$

Similarly, for $|\alpha_1|\leqslant 4$,

$$
\begin{aligned}
\sum_{\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}[vf^{n+1}],\partial_\beta^\alpha f^{n+1}) &\leqslant C\sum_{\alpha_1\leqslant\alpha}\sup_x|\partial^{\alpha_1}E^n|\cdot\Big\{\sum_{\beta_1\leqslant\beta}\|(1+|v|)^{1/2}\partial_{\beta_1}^{\alpha-\alpha_1}f^{n+1}\|\Big\}\\
&\quad\times\{\|(1+|v|)^{1/2}\partial_\beta^\alpha f^{n+1}\|\}\\
&\leqslant C\Big\{\sum_{|\ell|\leqslant|\alpha_1|+2}\|\partial^\ell E^n\|\Big\}\cdot\Big\{\sum_{\alpha_1\leqslant\alpha,\beta_1\leqslant\beta}\|\partial_{\beta_1}^{\alpha-\alpha_1}f^{n+1}\|_\sigma\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma.
\end{aligned}
$$

We thus conclude from $N\geqslant 8$ that the third term is bounded by

$$
\sum_{\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}(\partial^{\alpha_1}E^n\cdot\partial_\beta^{\alpha-\alpha_1}[vf^{n+1}],\partial_\beta^\alpha f^{n+1})\leqslant C\Big\{\sum_{|\ell|\leqslant N}\|\partial^\ell E^n\|\Big\}\cdot\Big\{\sum_{|\ell|+|\lambda|\leqslant N}\|\partial_\lambda^\ell f^{n+1}\|_\sigma\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma. \tag{2.10}
$$

By the estimate similar to the above, we have that the sixth term on the right-hand side of (2.4) is bounded by

$$
C\Big\{\sum_{|\ell|\leqslant N}\|\partial^\ell B^n\|\Big\}\cdot\Big\{\sum_{|\ell|+|\lambda|\leqslant N}\|\partial_\lambda^\ell f^{n+1}\|_\sigma\Big\}\cdot\|\partial_\beta^\alpha f^{n+1}\|_\sigma. \tag{2.11}
$$

Finally, we estimate the nonlinear collision terms in (2.4). Applying (1.12) in Lemma 1.3, we have

$$(\partial_\beta^\alpha \Gamma[f^n, f^{n+1}], \partial_\beta^\alpha f^{n+1}) \leqslant C\Big[\Big\{\sum \|\partial_{\beta_1}^{\alpha_1} f^n\|\Big\}\Big\{\sum \|\partial_{\beta_1}^{\alpha_1} f^{n+1}\|_\sigma\Big\} + \Big\{\sum \|\partial_{\beta_1}^{\alpha_1} f^n\|_\sigma\Big\}\Big\{\sum \|\partial_{\beta_1}^{\alpha_1} f^{n+1}\|\Big\}\Big]\|\partial_\beta^\alpha f^{n+1}\|_\sigma. \tag{2.12}$$

Integrating over $[0,t]$ of (2.4), collecting the above estimate, and applying the elementary inequality, we have

$$\begin{aligned}
&\frac{1}{2}\|\partial_\beta^\alpha f^{n+1}(t)\|^2 + [\|\partial^\alpha E^{n+1}(t)\|^2 + \|\partial^\alpha B^{n+1}(t)\|^2] + \int_0^t \|\partial_\beta^\alpha f^{n+1}(s)\|_\sigma^2 ds \\
&\leqslant \frac{1}{2}\|\partial_\beta^\alpha f_0\|^2 + [\|\partial^\alpha E_0\|^2 + \|\partial^\alpha B_0\|^2] + C\int_0^t \Big\{\sum_{|\alpha|\leqslant N} \|\partial^\alpha E\|\Big\} \cdot \Big\{\sum_{|\alpha|+|\lambda|\leqslant N} \|\partial_\lambda^\alpha f^{n+1}(s)\|\Big\} ds \\
&\quad + C\int_0^t \sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^n(s)\|^2\, ds + C_\eta \int_0^t \sum_{|\alpha_1|\leqslant N} \|\mu \partial^{\alpha_1} f^n(s)\|^2\, ds + \int_0^t C\Big\{\sum_{|\ell|\leqslant N} [\|\partial^\ell E^n\| + \|\partial^\ell B^n\|]\Big\} \\
&\quad \times \Big\{\sum_{|\ell|+|\lambda|\leqslant N} \|\partial_\lambda^\ell f^{n+1}\|_\sigma\Big\} \cdot \|\partial_\beta^\alpha f^{n+1}\|_\sigma\, ds + C\eta \int_0^t \sum_{|\alpha_1|+|\beta_1|\leqslant N} \|\partial_\beta^\alpha f^{n+1}(s)\|_\sigma^2\, ds \\
&\quad + C_\eta \int_0^t \sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^{n+1}(s)\|_\sigma^2\, ds + C\int_0^t \Big\{\sum_{|\alpha_1|+|\beta_1|\leqslant N} \|\partial_{\beta_1}^{\alpha_1} f^n(s)\|\Big\}\Big\{\sum_{|\alpha_1|+|\beta_1|\leqslant N} \|\partial_{\beta_1}^{\alpha_1} f^{n+1}(s)\|_\sigma\Big\} \\
&\quad \times \|\partial_\beta^\alpha f^{n+1}(s)\|_\sigma\, ds + C\int_0^t \Big\{\sum_{|\alpha_1|+|\beta_1|\leqslant N} \|\partial_{\beta_1}^{\alpha_1} f^n(s)\|_\sigma\Big\}\Big\{\sum_{|\alpha_1|+|\beta_1|\leqslant N} \|\partial_{\beta_1}^{\alpha_1} f^{n+1}(s)\|\Big\}\|\partial_\beta^\alpha f^{n+1}(s)\|_\sigma\, ds.
\end{aligned} \tag{2.13}$$

In the following we consider ∂^α derivatives. Taking ∂^α of (2.1), we get

$$\begin{aligned}
&[\partial_t + v\cdot\nabla_x + (E^n + v\times B^n)\cdot\nabla_v - A]\partial^\alpha f^{n+1} - K[\partial^\alpha f^n] - 2[\partial^\alpha E^n \cdot v]\mu^{1/2} + \partial^\alpha[E^n \cdot v f^{n+1}] \\
&\quad + \sum_{0\neq\alpha_1\leqslant\alpha} C_\alpha^{\alpha_1}[\partial^{\alpha_1} E^n + v\times\partial^{\alpha_1} B^n]\partial^{\alpha-\alpha_1}\nabla_v f^{n+1} = \partial^\alpha \Gamma[f^n, f^{n+1}],
\end{aligned} \tag{2.14}$$

Applying (1.12) in Lemma 1.3 yields

$$\begin{aligned}
(\partial^\alpha \Gamma[f^n, f^{n+1}], \partial^\alpha f^{n+1}) \leqslant C\Bigg[\sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^{n+1}\|_\sigma\Bigg]\Bigg\{\Bigg[\sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^n\|\Bigg]\Bigg[\sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^{n+1}\|_\sigma\Bigg] \\
+ \Bigg[\sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^n\|_\sigma\Bigg]\Bigg[\sum_{|\alpha_1|\leqslant N} \|\partial^{\alpha_1} f^{n+1}\|\Bigg]\Bigg\}.
\end{aligned} \tag{2.15}$$

We notice, from Lemma 1.3 and (1.13) (see Ref. 10), that for any $\eta > 0$ small,

$$\begin{aligned}
-\int_0^t (A[\partial^\alpha f^{n+1}], \partial^\alpha f^{n+1}) - \int_0^t (K[\partial^\alpha f^n], \partial^\alpha f^{n+1}) \geqslant \frac{3}{4}\int_0^t \|\partial^\alpha f^{n+1}(s)\|_\sigma^2\, ds - C\int_0^t \|\partial^\alpha f^{n+1}(s)\|^2\, ds \\
- \eta\int_0^t \|\partial^\alpha f^n(s)\|_\sigma^2\, ds - C_\eta \int_0^t \|\mu\partial^\alpha f^n(s)\|^2\, ds.
\end{aligned} \tag{2.16}$$

It is easily founded that

$$-2[\partial^\alpha E^n \cdot v]\mu^{1/2} = -2[\partial^\alpha E^{n+1}\cdot v]\mu^{1/2} - 2[\partial^\alpha E^{n+1} - \partial^\alpha E^n]\cdot v\mu^{1/2}.$$

Notice that from Maxwell system, the inner product of the first term on the right-hand side of the above equality with $\partial^\alpha f^{n+1}$ is

$$-\int 2\partial^\alpha E^{n+1}\cdot v\mu^{1/2}\partial^\alpha f^{n+1} = -\int 2\partial^\alpha E^{n+1}\partial^\alpha J^{n+1}\,dx = \frac{d}{dt}[\|\partial^\alpha E^{n+1}(t)\|^2 + \|\partial^\alpha B^{n+1}(t)\|^2]. \tag{2.17}$$

And the inner product of the second term with $\partial^\alpha f^{n+1}$ is bounded by

$$C[\|\partial^\alpha E^n\| + \|\partial^\alpha E^{n+1}\|]\|\partial^\alpha_\beta f^{n+1}\|.$$

Multiplying both sides of (2.14) by $\partial^\alpha f^{n+1}$ and using (2.9), (2.11), and (2.15)–(2.17), then integrating over $T^3\times R^3$, we are able to obtain

$$\begin{aligned}
&\frac{1}{2}\|\partial^\alpha f^{n+1}\|^2 + [\|\partial^\alpha E^{n+1}(t)\|^2 + \|\partial^\alpha B^{n+1}(t)\|^2] + \frac{3}{4}\int_0^t \|\partial^\alpha f^{n+1}(s)\|_\sigma^2\,ds \\
&\leqslant \frac{1}{2}\|\partial^\alpha f_0\|^2 + [\|\partial^\alpha E_0\|^2 + \|\partial^\alpha B_0\|^2] + C\int_0^t \|\partial^\alpha f^{n+1}(s)\|^2\,ds + C\int_0^t [\|\partial^\alpha E^n\| + \|\partial^\alpha E^{n+1}\|]\|\partial^\alpha_\beta f^{n+1}(s)\|ds \\
&\quad + \eta\int_0^t \|\partial^\alpha f^n(s)\|_\sigma^2\,ds + C_\eta\int_0^t \|\mu\partial^\alpha f^n(s)\|^2\,ds + \int_0^t C\Big[\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} f^{n+1}\|_\sigma\Big]\Big\{\Big[\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} f^n\|\Big] \\
&\quad \times\Big[\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} f^{n+1}\|_\sigma\Big] + \Big[\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} f^n\|_\sigma\Big]\Big[\sum_{|\alpha_1|\leqslant N}\|\partial^{\alpha_1} f^{n+1}\|\Big]\Big\}ds.
\end{aligned} \tag{2.18}$$

Combining this with (2.13) implies, for any $\eta>0$ small,

$$\begin{aligned}
E(f^{n+1}(t)) &\leqslant CE(f_0) + Ct\sup_{0\leqslant s\leqslant t}E(f^{n+1}(s)) + Ct\sup_{0\leqslant s\leqslant t}E(f^n(s)) + Ct\sup_{0\leqslant s\leqslant t}E(f^{n+1}(s))\sup_{0\leqslant s\leqslant t}E^{1/2}(f^n(s)) \\
&\quad + Ct\sup_{0\leqslant s\leqslant t}E^{1/2}(f^{n+1}(s))\sup_{0\leqslant s\leqslant t}E(f^n(s)).
\end{aligned}$$

Since $\sup_{0\leqslant s\leqslant t}E(f^n(s))\leqslant CE(f_0)$, we have

$$(1 - CT^*E^{1/2}(f_0) - CT^*E(f_0))\sup_{0\leqslant s\leqslant T^*(M)}E(f^{n+1}(s)) \leqslant CE(f_0) + CT^*E(f_0).$$

Choosing T^* and $E(f_0)$ small enough, we conclude the proof of Lemma 2.1.

Theorem 2.2: *For any sufficiently small $M>0$, there exists $T^*(M)>0$ and $M_1>0$ such that if $E(f_0)\leqslant M_1$, then there is a unique classical solution $f(t,x,v)$ to (1.2) in $[0,T^*(M))\times T^3\times R^3$ such that $\sup_{0\leqslant t\leqslant T^*}E(f(t))\leqslant M$ and $E(f(t))$ is continuous over $[0,T^*(M))$. If $F_0(x,v)=\mu+\mu^{1/2}f_0\geqslant 0$, then $F(t,x,v)=\mu+\mu^{1/2}f(t,x,v)\geqslant 0$. Furthermore, the conservation laws (1.5) and (1.6) hold for all $0<t<T^*$ if they are valid initially at $t=0$.*

Proof: Let $F^0(t,x,v)\equiv F_0(x,v)$. Take $n\to\infty$ in Lemma 2.1 to obtain a classical solution f so that $F(x,t,v)=\mu+\mu^{1/2}f(t,x,v)\geqslant 0$.

In order to prove the uniqueness, we assume that there exists another solution g such that $\sup_{0\leqslant s\leqslant T^*}E(g(s))\leqslant M$. Taking the difference, we have

$$\begin{aligned}
\{\partial_t + v\cdot\nabla_x + (E_f + v\times B_f)\cdot\nabla_v + L\}[f-g] &= -[E_f - E_g + v\times(B_f - B_g)]\nabla_v g \\
&\quad + 2[E_f - E_g]\cdot v\mu^{1/2} + E_f\cdot v[f-g] \\
&\quad + [E_f - E_g]\cdot vg + \Gamma[f-g,g] + \Gamma[g,f-g],
\end{aligned}$$

$$\partial_t(E_f-E_g)-\nabla\times(B_f-B_g)=-\int_{R^3}v\mu^{1/2}(f-g)\mathrm{d}v,\quad \nabla\cdot(E_f-E_g)=\int_{R^3}(f-g)\mu^{1/2}\,\mathrm{d}v,$$
$$\partial_t(B_f-B_g)+\nabla\times(E_f-E_g)=0,\quad \nabla\cdot(B_f-B_g)=0, \tag{2.19}$$

with $f(0,x,v)=g(0,x,v)$, $E_f(0,x)=E_g(0,x)$, and $B_f(0,x)=B_g(0,x)$ as well as $L=-A-K$.

By an argument similar to (2.8), we obtain $\sup_x|g|_\sigma^2\leqslant C\Sigma_{|\alpha|\leqslant 4}\|\partial^\alpha g\|_\sigma^2$ (see Ref. 10). We apply Lemma 1.3 and the above estimate to get

$$|([E_f-E_g+v\times(B_f-B_g)]\nabla_v g,f-g)|\leqslant C\left\{\sum_{|\alpha|\leqslant 4}\|\partial^\alpha g\|_\sigma^2\right\}\{\|E_f-E_g\|^2+\|B_f-B_g\|^2\}+\frac{1}{4}\|f-g\|_\sigma^2,$$

$$\begin{aligned}(\Gamma[f-g,g]+\Gamma[g,f-g],f-g)&\leqslant\sum_{|\alpha|\leqslant 4}[\|\partial^\alpha f\|+\|\partial^\alpha g\|]\|f-g\|_\sigma^2\\&\quad+\sum_{|\alpha|\leqslant 4}[\|\partial^\alpha f\|_\sigma+\|\partial^\alpha g\|_\sigma]\|f-g\|_\sigma\|f-g\|\\&\leqslant CM^{1/2}\|f-g\|_\sigma^2+\frac{1}{8}\|f-g\|_\sigma^2+C\sum_{|\alpha|\leqslant 4}[\|\partial^\alpha f\|_\sigma^2+\|\partial^\alpha g\|_\sigma^2]\|f-g\|^2,\end{aligned}$$

$$|([E_f-E_g]\cdot vg,f-g)|\leqslant\frac{1}{4}\|f-g\|_\sigma^2+C\sum_{|\alpha|\leqslant 4}\|\partial^\alpha g\|_\sigma^2\|E_f-E_g\|^2,$$

$$(|E_f\cdot v(f-g)|,|f-g|)\leqslant CM^{1/2}\|f-g\|_\sigma^2.$$

From the Maxwell system in (2.19), we deduce from (2.17) that

$$2([E_f-E_g]\cdot v\mu^{1/2},f-g)=-\frac{\mathrm{d}}{\mathrm{d}t}[\|E_f-E_g\|^2+\|B_f-B_g\|^2].$$

Moreover, from (2.16), we easily know,

$$(L[f-g],f-g)\geqslant\tfrac{1}{2}\|f-g\|_\sigma^2-C\|f-g\|^2.$$

Multiplying (2.19) by $(f-g)$, and collecting the above estimates, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{2}\|f-g\|^2+\|E_f-E_g\|^2+\|B_f-B_g\|^2\right]+\frac{1}{2}\|f-g\|_\sigma^2&\leqslant C\left\{\sum_{|\alpha|\leqslant 4}[\|\partial^\alpha f\|_\sigma^2+\|\partial^\alpha g\|_\sigma^2+1\}\right.\\&\quad\times[\|f-g\|^2+\|E_f-E_g\|^2+\|B_f-B_g\|^2]\\&\quad+\left[CM^{1/2}+\frac{3}{8}\right]\|f-g\|_\sigma^2.\end{aligned}\tag{2.20}$$

If we choose M small enough, the last term on the right-hand side of (2.20) can be absorbed by $\frac{1}{2}\|f-g\|_\sigma^2$. It is easy to know that $\int_0^t\{\Sigma_{|\alpha|\leqslant 4}[\|\partial^\alpha f\|_\sigma^2+\|\partial^\alpha g\|_\sigma^2]\}\mathrm{d}s\leqslant 2M$. Then, we deduce $f\equiv g$ from the Gronwall inequality.

To show the continuity of $E(f(t))$ with respect to t, we use the summation of (2.13) and (2.18) (with $f^n=f^{n+1}=f$) to get

$$|E(f(t))-E(f(s))| \leqslant C[1+\sup_{s\leqslant y\leqslant t} E^{1/2}(f(y))]\int_s^t \sum [\|\partial_\beta^\alpha f(y)\|_\sigma^2]\mathrm{d}y \to 0$$

as $t\to s$. By $F=\mu+\mu^{1/2}f$, it is straightforward to verify that the mass, total momentum, and total energy conservations hold for such solution constructed.

III. POSITIVITY OF *L*

In this section, we shall establish the positivity of the linear operator L for any small solution $[f(t,x,v),E(t,x),B(t,x)]$ to the system (1.3) and (1.4). Together with the Maxwell system, the conservation laws of mass, momentum, and energy play an important role.

Then for $f(t,x,v)$ and fixed (t,x), we know in the introduction that $P_0f=a(t,x)\mu^{1/2}+b(t,x)\cdot v\mu^{1/2}+c(t,x)|v|^2\mu^{1/2}$ for some $a(t,x),c(t,x)$ and vector function $b(t,x)$. Thus we split f as $f=P_0f+P_1f$ in the system (1.3) and (1.4) and we have

$$[\partial_t+v\cdot\nabla_x]P_0f-2E\cdot v\mu^{1/2}=l(P_1f)+h(f), \tag{3.1}$$

where

$$l(P_1f)\equiv-[\partial_t+v\cdot\nabla_x+L]P_1f, \tag{3.2}$$

$$h(f)\equiv-(E+v\times B)\cdot\nabla_v f+E\cdot vf+\Gamma[f,f]. \tag{3.3}$$

Lemma 3.1: Let $\partial^\alpha=\partial_t^{\alpha_0}\partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\partial_{x_3}^{\alpha_3}$, *then* $\partial^\alpha P_0f=P_0\partial^\alpha f$ *and* $\|\partial^\alpha P_0f\|_\sigma^2+\|\partial^\alpha P_1f\|_\sigma^2\geqslant\|\partial^\alpha f\|_\sigma^2$. *There exists* $C>1$ *such that for any* $f\in C_c^\infty(R\times T^3\times R^3)$

$$\frac{1}{C}\|\partial^\alpha P_0f\|_\sigma^2\leqslant\|\partial^\alpha a\|^2+\|\partial^\alpha b\|^2+\|\partial^\alpha c\|^2\leqslant C\|\partial^\alpha P_0f\|^2. \tag{3.4}$$

Proof: A direct computation implies $\partial^\alpha P_0f=P_0\partial^\alpha f$. It is easy to get the second result from the triangle inequality. We substitute $\|\cdot\|_\sigma$ with $P_0\partial^\alpha f=\partial^\alpha a(t,x)\mu^{1/2}+\partial^\alpha b(t,x)\cdot v\mu^{1/2}+\partial^\alpha c(t,x)|v|^2\mu^{1/2}$. Using $\sigma^{ij}\leqslant C[1+|v|]^{\gamma+2}$ and the exponential decay of e_j, we can obtain the first half of (3.4) by a direct computation. For the second half of (3.4), since a,b, and c are the coefficients of a basis to the finite dimensional space N, $|\partial^\alpha a|^2+|\partial^\alpha b|^2+|\partial^\alpha c|^2$ is bounded by $C\int|\partial^\alpha P_0f|^2\,\mathrm{d}v$ for any (t,x). We then deduce (3.4) by a further integration over x.

Lemma 3.2: Let $[f(t,x,v),E(t,x),B(t,x)]$ *be the solution constructed in Theorem 2.2 to (1.3) and (1.4). Then we have*

$$\rho_2\int_{T^3} b(t,x)=-\int_{T^3} B(t,x)\times E(t,x), \tag{3.5}$$

$$\left|\int_{T^3} a(t,x)\right|+\left|\int_{T^3} c(t,x)\right|\leqslant C[\|E\|^2+\|B-\overline{B}\|^2], \tag{3.6}$$

where $\rho_2=\int|v|^2\mu$.

Proof: Plugging $f=P_0f+P_1f$ into the momentum equation (1.5). For fixed (t,x), notice that $(P_1f,e_j)=0$ and $P_0f=a(t,x)\mu^{1/2}+b(t,x)\cdot v\mu^{1/2}+c(t,x)|v|^2\mu^{1/2}$, we have $\int vf\mu^{1/2}\,\mathrm{d}v=b(t,x)\int|v|^2\mu\,\mathrm{d}v$. Hence (3.5) follows from (1.5). Similarly, we have

$$\int f\mu^{1/2}\,\mathrm{d}v=\rho_0a(t,x)+\rho_2c(t,x)\quad\text{and}\quad\int|v|^2f\mu^{1/2}\,\mathrm{d}v=\rho_2a(t,x)+\rho_4c(t,x),$$

where $\rho_i=\int|v|^i\mu\,\mathrm{d}v$. Further integration over T^3, we have (3.6) from the above equations and the Schwartz inequality.

We plug $P_0 f = a(t,x)\mu^{1/2} + b(t,x)\cdot v\mu^{1/2} + c(t,x)|v|^2\mu^{1/2}$ into the left-hand side of (3.1) and expand it as the products of a polynomial in v and $\mu^{1/2}$,

$$\sum_i \left[v_i \partial^i c|v|^2 + [\partial^0 c + \partial^i b]v_i^2 + \sum_{j>i} [\partial^i b_j + \partial^j b_i]v_i v_j + [\partial^0 b_i + \partial^i a - 2E_i]v_i + \partial^0 a \right]\mu^{1/2},$$

where $\partial^0 = \partial_t, \partial^j = \partial_{x_j}$. For any fixed (t,x), this is an expansion of the left-hand side of (3.1) with respect to the basis of $\mu^{1/2}, v_i\mu^{1/2}, v_i^2\mu^{1/2}, v_i v_j \mu^{1/2}$, and $|v|^2 v_i \mu^{1/2}$ denoted by ϵ_j where $1 \leqslant i \neq j \leqslant 3$. Expand the right-hand side of (3.1) with respect to the same basis, and compare with their coefficients on two sides. Then we have

$$(1)\ \nabla_x c = l_c + h_c, \quad (2)\ \partial^0 c + \partial^i b_i = l_i + h_i, \quad (3)\ \partial^0 a = l_a + h_a,$$

$$(4)\ \partial^i b_j + \partial^j b_i = l_{ij} + h_{ij}, \quad i \neq j, \quad (5)\ \partial^0 b_i + \partial^i a - 2E_i = l_{bi} + h_{bi},$$

where $\partial^0 = \partial_t$ and $\partial^j = \partial_{x_j}$. Here $l_c(t,x), l_i(t,x), l_{ij}(t,x), l_{bi}(t,x)$, and $l_a(t,x)$ are the corresponding coefficients of such an expansion of the linear term $l(P_1 f)$, and $h_c(t,x), h_i(t,x), h_{ij}(t,x), h_{bi}(t,x)$, and $h_a(t,x)$ are the corresponding coefficients of the same expansion of the higher order term $h(f)$.

Let ϵ_j^* be the corresponding orthogonal basis of ϵ_j such that for some constants $\lambda^{ij}, \epsilon_j^* = \sum_{i=1}^{13} \lambda^{ij}\epsilon_j$. Then for any fixed $(t,x), l_c(t,x), l_i(t,x), l_{ij}(t,x), l_{bi}(t,x)$, and $l_a(t,x)$ take the form $\sum_{i,n=1}^{13} \lambda^{ij}\lambda^{in}\int_{R^3} l(P_1 f)\epsilon_n(v)\mathrm{d}v$. The same is true after we take ∂^α. Let $|\alpha| \leqslant N-1$. By (3.2), we have that

$$\left\| \int (-[\partial_t + v\cdot\nabla_x]) P_1 \partial^\alpha f \cdot \epsilon_n(v)\mathrm{d}v \right\|^2 \leqslant \int |\epsilon_n(v)|\mathrm{d}v \int_{R^3\times T^3} |\epsilon_n(v)|(|P_1\partial^0\partial^\alpha f|^2 + |v|^2|P_1\nabla_x\partial^\alpha f|^2)\mathrm{d}x\,\mathrm{d}v \leqslant C[\|P_1\partial^0\partial^\alpha f\| + \|P_1\nabla_x\partial^\alpha f\|]^2, \tag{3.7}$$

$$\int LP_1\partial^\alpha f\epsilon_n(v)\mathrm{d}v = \int (-A-K)P_1\partial^\alpha f\epsilon_n(v)\mathrm{d}v.$$

Recalling the expressions of A, K, and ϵ_n, integration by parts and the Schwartz inequality will result in

$$\left\| \int LP_1\partial^\alpha f\epsilon_n(v)\mathrm{d}v \right\|^2 \leqslant C\|P_1\partial^\alpha f\|^2. \tag{3.8}$$

Combining (3.7) and (3.8), we have

$$\left\| \int \partial^\alpha l(P_1 f)\cdot\epsilon_n(v)\mathrm{d}v \right\|^2 \leqslant C[\|P_1\partial^0\partial^\alpha f\| + \|P_1\nabla_x\partial^\alpha f\| + \|P_1\partial^\alpha f\|]^2.$$

Here $\partial^0 = \partial_t$ and we have used the facts that $\partial^\alpha P_1 f = P_1\partial^\alpha f$ and the exponential decay of $\epsilon_n(v)$. The above proof is summarized in the following lemma.

Lemma 3.3: Let $\alpha = [\alpha_0, \alpha_1, \alpha_1, \alpha_2]$, *then for any* $1 \leqslant i, j \leqslant 3$,

$$\sum_{|\alpha|\leqslant N-1} [\|\partial^\alpha l_c\| + \|\partial^\alpha l_i\| + \|\partial^\alpha l_{ij}\| + \|\partial^\alpha l_{bi}\| + \|\partial^\alpha l_a\|] \leqslant C \sum_{|\alpha|\leqslant N} \|P_1\partial^\alpha f\|.$$

Since $\partial^\alpha J = \int_{R^3}\partial^\alpha f v\mu^{1/2}\,\mathrm{d}v$, we easily know that $\|\partial^\alpha J\| \leqslant C\|\partial^\alpha f\|$. Thus, by (1.16) and (1.14) with $\gamma \geqslant -1$, the arguments similar to Lemma 8 in Ref. 16 will imply that the following two lemmas hold.

Lemma 3.4: Let $[f(t,x,v), E(t,x), B(t,x)]$ *be the solution constructed in Theorem 2.2 to (1.3) and (1.4) such that*

$$\sum_{|\alpha|\leqslant N}\left[\tfrac{1}{2}\|\partial^\alpha f(t)\|^2+\|\partial^\alpha E(t)\|^2+\|\partial^\alpha B(t)\|^2\right]\leqslant M, \tag{3.9}$$

with the constant $M>0$ small enough. Then we have

$$\sum_{|\alpha|\leqslant N-1}\left[\|\partial^\alpha h_c\|+\|\partial^\alpha h_i\|+\|\partial^\alpha h_{ij}\|+\|\partial^\alpha h_{bi}\|+\|\partial^\alpha h_a\|\right]\leqslant CM^{1/2}\sum_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma.$$

Lemma 3.5: Let $[f(t,x,v),E(t,x),B(t,x)]$ be the solution constructed in Theorem 2.2 to (1.3) and (1.4). Let the small assumption (3.9) be valid for some $M\leqslant 1$. Then there is a constant $C>0$ such that

$$\sum_{|\alpha|\leqslant N-1}\left[\|\partial^\alpha E(t)\|+\|\partial^\alpha[B(t)-\bar{B}]\|\right]\leqslant C\sum_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma.$$

Theorem 3.6: *Let $[f(t,x,v),E(t,x),B(t,x)]$ be the solution constructed in Theorem 2.2 to (1.3) and (1.4). If the small amplitude assumption (3.9) holds. Then there exists $\delta_M>0$ such that*

$$\sum_{|\alpha|\leqslant N}(L\partial^\alpha f,\partial^\alpha f)\geqslant\delta_M\sum_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma^2.$$

Using Lemmas 3.1–3.5, (1.15), equations (1.1)–(1.5) and (1.14) with $\gamma\geqslant -1$, the arguments similar to those in the proof of Theorem 3 of Ref. 16, except for several differences, will imply Theorem 3.6.

The first difference is to prove the estimate of the purely spatial derivative of $a(t,x)$. The direct calculation implies $\nabla\cdot\partial^\alpha E=\int\partial^\alpha f\ \mu^{1/2}=\rho_0\partial^\alpha a(t,x)+\rho_2\partial^\alpha c(t,x)$. Since $\partial^\alpha c(t,x)$ is controlled by the argument similar to those in Ref. 16, we thus obtain the estimate of the purely spatial derivative of $a(t,x)$ by the same method as in Ref. 16.

The second difference is to prove the estimate of the higher purely temporal derivative $\partial^\alpha b_j$ with $|\alpha|\geqslant 3$. It is clear that the direct calculation implies $J=\rho_2 b(t,x)$. The Maxwell system leads to

$$\partial^{\alpha-1}E-\nabla\times\partial^{\alpha-2}B=-\partial^{\alpha-2}J,\quad \nabla\times\partial^{\alpha-2}B+\nabla\times[\nabla\times\partial^{\alpha-3}E]=0.$$

It is easy to get

$$\partial^{\alpha-1}E+\nabla\times[\nabla\times\partial^{\alpha-3}E]=-\partial^{\alpha-2}J=-\rho_2\partial^{\alpha-2}b.$$

Together with $\partial^{\alpha-1}$ on Eq. (5), we get

$$\begin{aligned}\|\partial^\alpha b_i\|=\|-\partial^i\partial^{\alpha-1}a+2\partial^{\alpha-1}E_i+\partial^{\alpha-1}[l_{bi}+h_{bi}]\|&\leqslant\|\partial^i\partial^{\alpha-1}a\|+2\rho_2\|\partial^{\alpha-2}b_i\|+2\|\nabla\times[\nabla\times\partial^{\alpha-3}E]\|\\&\quad+\|\partial^{\alpha-1}[l_{bi}+h_{bi}]\|.\end{aligned}$$

Thus we have

$$\|\partial^\alpha b_i\|-2\rho_2\|\partial^{\alpha-2}b_i\|\leqslant\|\partial^i\partial^{\alpha-1}a\|+2\|\nabla\times[\nabla\times\partial^{\alpha-3}E]\|+\|\partial^{\alpha-1}[l_{bi}+h_{bi}]\|.$$

The right-hand side of the above inequality is bounded by $C\Sigma_{|\alpha|\leqslant N}\|P_1\partial^\alpha f\|+CM^{1/2}\Sigma_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma$, which can be proved by the same arguments as in Ref. 16. Then we can obtain the estimate of the higher purely temporal derivative $\partial^\alpha b_j$ by a bootstrap argument.

IV. GLOBAL EXISTENCE

In this section, we will prove the existence of global classical solution to the system (1.3) and (1.4). We first derive a refined energy estimate for (1.3) and (1.4).

Theorem 4.1: *Let $[f(t,x,v),E(t,x),B(t,x)]$ be the solution constructed in Theorem 2.2 to (1.3) and (1.4). Let the small amplitude assumption (3.9) be valid. For any given $0\leqslant m\leqslant N$, $|\beta|\leqslant m$, there are constants $C_{|\beta|}>0, C_m^*>0$ and $\delta_m>0$ such that*

$$\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\left[\frac{\mathrm{d}}{\mathrm{d}t}(C_{|\beta|}\|\partial_\beta^\alpha f\|^2+\|\partial^\alpha E(t)\|^2+\|\partial^\alpha B(t)\|^2)+\delta_m\|\partial_\beta^\alpha f\|_\sigma^2\right]\leqslant C_m^* E^{1/2}(f(t))\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2. \tag{4.1}$$

Proof: We use an induction over m, the order of the v-derivatives. For $m=0$, by taking the pure ∂^α derivatives of (1.3), we obtain

$$\begin{aligned}&[\partial_t+v\cdot\nabla_x+(E+v\times B)\cdot\nabla_v-(E\cdot v)]\partial^\alpha f+L[\partial^\alpha f]-2[\partial^\alpha E\cdot v]\mu^{1/2}\\&\quad=\partial^\alpha\Gamma[f,f]-\sum_{0\neq\alpha_1\leqslant\alpha}C_\alpha^{\alpha_1}[\partial^{\alpha_1}E+v\times\partial^{\alpha_1}B]\partial^{\alpha-\alpha_1}\nabla_v f+\sum_{0\neq\alpha_1\leqslant\alpha}C_\alpha^{\alpha_1}\partial^{\alpha_1}E\cdot v\,\partial^{\alpha-\alpha_1}f.\end{aligned} \tag{4.2}$$

Take the inner product with $\partial^\alpha f$ of Eq. (4.2). Recalling estimates (2.15) and (2.17) in Lemma 2.1 with $f^n=f^{n+1}=f$, applying Theorem 3.6 to $L[\partial^\alpha f]$ and summing over $|\alpha|\leqslant N$, we deduce, for some constant $C>0$, that

$$\sum_{|\alpha|\leqslant N}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\|\partial^\alpha f\|^2+\|\partial^\alpha E(t)\|^2+\|\partial^\alpha B(t)\|^2\right)+\delta_0\sum_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma^2\leqslant CE^{1/2}(f(t))\sum_{|\alpha|\leqslant N}\|\partial^\alpha f\|_\sigma^2.$$

This concludes the case for $m=0$ with $C_0=1/2$ and $C_0^*=C$.

Assume the theorem is valid for m. For $|\beta|=m+1$, taking ∂_β^α of (1.3), we obtain

$$\begin{aligned}&[\partial_t+v\cdot\nabla_x+(E+v\times B)\cdot\nabla_v]\partial_\beta^\alpha f-2\partial^\alpha E\cdot\partial_\beta[v\mu^{1/2}]+\partial_\beta[L\partial^\alpha f]+\sum_{\beta_1\neq 0}C_\beta^{\beta_1}\partial_{\beta_1}v\cdot\nabla_x\partial_{\beta-\beta_1}^\alpha f\\&=\sum C_\alpha^{\alpha_1}C_\beta^{\beta_1}\partial^{\alpha_1}E\cdot\partial_{\beta_1}v\,\partial_{\beta-\beta_1}^{\alpha-\alpha_1}f-\sum_{\alpha_1\neq 0}C_\alpha^{\alpha_1}\partial^{\alpha_1}E\nabla_v\partial_\beta^{\alpha-\alpha_1}f-\sum_{\alpha_1\neq 0,\beta_1\neq 0}C_\alpha^{\alpha_1}C_\beta^{\beta_1}\partial_{\beta_1}v\\&\quad\times\partial^{\alpha_1}B\cdot\nabla_v\partial_{\beta-\beta_1}^{\alpha-\alpha_1}f+\sum C_\alpha^{\alpha_1}\partial_\beta\Gamma[\partial^{\alpha_1}f,\partial^{\alpha-\alpha_1}f].\end{aligned} \tag{4.3}$$

From (2.5) in Lemma 2.1, for any $\eta>0$, there is a constant $C_\eta>0$ such that

$$(\partial_\beta[L\partial^\alpha f],\partial_\beta^\alpha f)\leqslant\|\partial_\beta^\alpha f\|_\sigma^2-\eta\sum_{\beta'\leqslant\beta}\|\partial_{\beta'}^\alpha f\|_\sigma^2-C_\eta\|\partial^\alpha f\|_\sigma^2.$$

We can further choose $C_\eta>0$ such that the inner product of the last term on the left-hand side of (4.3) with $\partial_\beta^\alpha f$ is bounded by

$$\eta\|\partial_\beta^\alpha f\|_\sigma^2+C_\eta\sum_{|\beta_1|=1}\|\nabla_x\partial_{\beta-\beta_1}^\alpha f\|_\sigma^2.$$

Since $|\beta|=m+1,|\alpha|\leqslant N-1$ and by Lemma 3.5 and $\|f\|\leqslant\|f\|_\sigma$, we have

$$(2\partial^\alpha E\cdot\partial_\beta[v\mu^{1/2}],\partial_\beta^\alpha f)=(-1)^{|\beta|}(2\partial^\alpha E\cdot\partial_\beta^2[v\mu^{1/2}],\partial^\alpha f)\leqslant C_\mu\|\partial^\alpha E\|\cdot\|\partial^\alpha f\|\leqslant C_\mu\sum_{|\alpha'|\leqslant N}\|\partial^{\alpha'}f\|_\sigma^2.$$

By the arguments similar to those in Lemma 2.1, the inner product of other terms on the right-hand side of (4.3) with $\partial_\beta^\alpha f$ is bounded by $CE^{1/2}(f(t))\Sigma_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2$. We have, by collecting terms and summing over $|\beta|=m+1$ and $|\alpha|+|\beta|\leqslant N$,

$$\sum_{|\beta|=m+1,|\alpha|+|\beta|\leqslant N}\left[\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\partial_\beta^\alpha f(t)\|^2+\|\partial_\beta^\alpha f(t)\|_\sigma^2\right]$$
$$\leqslant \sum_{|\beta|=m+1,|\alpha|+|\beta|\leqslant N}\left[\sum_{|\beta|=m+1}2\eta\|\partial_\beta^\alpha f(t)\|_\sigma^2+(2\eta+C_\mu+C_\eta)\right.$$
$$\left.\times\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f(t)\|_\sigma^2+CE^{1/2}(f(t))\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2\right]$$
$$\leqslant Z_{m+1}\left[\sum_{|\beta|=m+1}2\eta\|\partial_\beta^\alpha f(t)\|_\sigma^2+(2\eta+C_\mu+C_\eta)\right.$$
$$\left.\times\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f(t)\|_\sigma^2+CE^{1/2}(f(t))\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2\right].$$

Here we have used that $\|\partial_\beta^\alpha f(t)\|\leqslant C\|\partial_\beta^\alpha f(t)\|_\sigma$ and Z_{m+1} denotes the number of all possible (α,β) such that $|\beta|\leqslant m+1, |\alpha|+|\beta|\leqslant N$.

By choosing $\eta=1/4Z_{m+1}$, we have, for some constant $C(Z_{m+1})>0$,

$$\sum_{|\beta|=m+1,|\alpha|+|\beta|\leqslant N}\left[\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\partial_\beta^\alpha f(t)\|^2+\frac{1}{2}\|\partial_\beta^\alpha f(t)\|_\sigma^2\right]\leqslant C(Z_{m+1})\left[\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f(t)\|_\sigma^2\right.$$
$$\left.+CE^{1/2}(f(t))\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2\right]. \tag{4.4}$$

We may assume $C(Z_{m+1})\geqslant 1$. Multiply (4.3) by $\delta_m/2C(Z_{m+1})$ and add it to (4.1) for $|\beta|\leqslant m$ to get

$$\sum_{|\beta|=m+1,|\alpha|+|\beta|\leqslant N}\left[\frac{\delta_m}{4C(Z_{m+1})}\frac{\mathrm{d}}{\mathrm{d}t}\|\partial_\beta^\alpha f(t)\|^2+\frac{\delta_m}{4C(Z_{m+1})}\|\partial_\beta^\alpha f(t)\|_\sigma^2\right]$$
$$+\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\left[\frac{\mathrm{d}}{\mathrm{d}t}(C_{|\beta|}\|\partial_\beta^\alpha f\|^2+\|\partial^\alpha E(t)\|^2+\|\partial^\alpha B(t)\|^2)+\delta_m\|\partial_\beta^\alpha f\|_\sigma^2\right]$$
$$\leqslant\frac{\delta_m}{2}\sum_{|\beta|\leqslant m,|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f(t)\|_\sigma^2+\left(C_m^*+\frac{\delta_m}{2}\right)E^{1/2}(f(t))\sum_{|\alpha|+|\beta|\leqslant N}\|\partial_\beta^\alpha f\|_\sigma^2.$$

Absorb the first term on the right-hand side by the last term on the left-hand side. We thus conclude the lemma by letting

$$C_{m+1}^*=C_m^*+\frac{\delta_m}{2},\quad C_{m+1}=\frac{\delta_m}{4C(Z_{m+1})},\quad \delta_{m+1}=\frac{\delta_m}{4C(Z_{m+1})}\leqslant\frac{\delta_m}{2}.$$

Proof of Theorems 1.1 and 1.2: The proof of Theorems 1.1 and 1.2 can be obtained by Theorem 4.1 and the arguments similar to those in the proof of Theorem 1 and Theorem 2 in Ref. 16.

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Upper quantum Lyapunov exponent and parametric oscillators

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We introduce a definition of upper Lyapunov exponent for quantum systems in the Heisenberg representation, and apply it to parametric quantum oscillators. We provide a simple proof that the upper quantum Lyapunov exponent ranges from zero to a positive value, as the parameters range from the classical system's region of stability to the instability region. It is also proved that in the instability region the parametric quantum oscillator satisfies the discrete quantum Anosov relations defined by Emch, Narnhofer, Sewell, and Thirring. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1803926]

I. INTRODUCTION

Several definitions of quantum Lyapunov exponents have been proposed (see Refs. 1–6 and references therein). Due to the fact that there are few examples on which these definitions can be explicitly tested in detail, their range of applicability is not well established. Emch and co-workers[1,2] formulated a definition of quantum Anosov systems, and the associated quantum Lyapunov exponents. This definition of the Lyapunov exponents is however too rigid, and it is not applicable to systems that do not have a global structure with a constant hyperbolicity property. Majewski and Kuna[5] extracted from Ref. 1 a more general definition, that is still too restrictive, since it assumes the existence of certain limits that one cannot expect to be well defined in general. In a quite different approach, Vilela Mendes[6] introduced a definition of the quantum Lyapunov exponents based on the probability density $\rho(x,t)=|\psi(x,t)|^2$ in the position representation. The limitation of this approach is that it singles out the position representation, and thus it is not easily related to the dependence on initial conditions in phase space (x, and p).

In the present paper we propose a definition of the upper quantum Lyapunov exponent that is close in spirit to the ones of Refs. 1 and 5, but is more general and with a wider range of applicability. It is formulated in terms of the evolution of observables in an algebraic setting, and based by analogy on the classical upper Lyapunov exponent, as defined in the general context of cocycles.[7,8] An essential ingredient is the behavior with respect to changes in the initial conditions. In Refs. 1, 3, and 5 these are taken in a very general framework, by considering the variations generated by all the derivations on the algebra of observables. For our definition we restrict the class of variations of initial conditions to those derivations that correspond to translations in phase space, i.e., in x and in p. We illustrate this definition with the example of a parametric quantum oscillator, which shows the utility of the extension.

II. DEFINITION OF THE UPPER QUANTUM LYAPUNOV EXPONENT

Consider a quantum mechanical particle and let $\hat{x}$ and $\hat{p}$ denote its coordinate and momentum operators, on the Hilbert space $\mathcal{H}=L_2(\mathbb{R},\mathrm{d}x)$, with $[\hat{x},\hat{p}]=i\hbar$. We choose the units such that $\hbar=1$. We define the self-adjoint operator

$$L_{\underline{\alpha}} := \alpha_p \hat{p} + \alpha_x \hat{x}, \quad \text{with } \underline{\alpha} \equiv (\alpha_p, \alpha_x) \in \mathbb{R}^2. \tag{1}$$

It defines a derivation[1] $\delta_{\underline{\alpha}}$, acting on operators $A \in \mathcal{A}$, where $\mathcal{A}$ denotes the algebra of observables, by

$$\delta_{\underline{\alpha}} A = [L_{\underline{\alpha}}, A], \ \forall A \in \mathrm{Dom}(\delta_{\underline{\alpha}}), \tag{2}$$

where

$$\mathrm{Dom}(\delta_{\underline{\alpha}}) \equiv \{A \in \mathcal{A} \text{ such that} [L_{\underline{\alpha}}, A] \in \mathcal{A}\}. \tag{3}$$

This derivation may be interpreted as a derivation in the direction of phase space determined by (α_p, α_x) and is thus naturally suggested by classical mechanics.

Let $U(t, t_0)$ denote the unitary propagator which defines the dynamics, with initial time t_0. In order to proceed we must also specify the algebra of observables. Experience with examples[2] suggests the choice of the Weyl algebra $\mathcal{W}$, which consists of finite linear combinations of the operators

$$W(\beta, \gamma) = \exp[i(\beta \hat{x} + \gamma \hat{p})], \quad (\beta, \gamma) \in \mathbb{R}^2. \tag{4}$$

This is particularly natural because $\mathcal{W} \subset \mathrm{Dom}\ \delta_{\underline{\alpha}}$, since

$$[L_{\underline{\alpha}}, W(\beta, \gamma)] = (\alpha_p \beta - \alpha_x \gamma) W(\beta, \gamma). \tag{5}$$

Equivalently,[2] one can consider polynomials in $W = \exp[i(\beta \hat{x} + \gamma \hat{p})]$ with the multiplication law $W(z)W(z') = \exp(i\sigma(z, z'))W(z+z')$, with $z := (\beta, \gamma)$, $z' := (\beta', \gamma')$, and the symplectic form $\sigma(z, z') = (\beta\gamma' - \beta'\gamma)/2$. Note that once the equations (20) and (21) of Theorem 2 have been established, the C^* character of the algebra is inessential: a $*$-algebra is sufficient (see Ref. 1, Remark 3.7, No. 6).

We also assume that the dynamics defines an automorphism of $\mathcal{W}$,

$$U^\dagger(t, t_0) A U(t, t_0) \in \mathcal{W}, \quad \forall A \in \mathcal{W}, \forall t, t_0 \in \mathbb{R}. \tag{6}$$

Under the above assumptions, we can formulate the following.

Definition: The *upper quantum Lyapunov exponent* is defined as

$$\overline{\lambda} = \sup_{\underline{\alpha} \in \mathbb{R}^2} \overline{\lambda}_{\underline{\alpha}}, \tag{7}$$

where

$$\overline{\lambda}_{\underline{\alpha}}(U, L_{\underline{\alpha}}, A, t_0) := \limsup_{t \to \infty} \frac{1}{t} \ln \| [L_{\underline{\alpha}}, A(t, t_0)] \| \tag{8}$$

and

$$A(t, t_0) := U^\dagger(t, t_0) A U(t, t_0) \tag{9}$$

and $A \in \mathcal{W}$. The norm is chosen as $\|A\| = \sup_{\psi \in \mathcal{H}} \|A\psi\| / \|\psi\|$.

Remarks:

(1) This definition is adapted from the general formulation for cocycles described, e.g., in Ref. 8. $\overline{\lambda}$ is expected to be independent of t_0 and of the choice of the observable A, under suitable conditions, e.g.,

$$[L, A(t, t_0)] \neq 0. \tag{10}$$

(2) If the limit in (8) exists, then it is called the Lyapunov exponent $\lambda_{\underline{\alpha}}(U, L, A, t_0)$.

(3) Because of the unitarity of the time evolution, the exponent $\overline{\lambda}_{\underline{\alpha}}$ can also be expressed as

$$\overline{\lambda}_{\underline{\alpha}}(U,L_{\underline{\alpha}},A,t_0) = \limsup_{t\to\infty}\frac{1}{t}\ln\|[L_{\underline{\alpha}}(t_0,t),A]\| \tag{11}$$

with

$$L_{\underline{\alpha}}(t_0,t) := U^{\dagger}(t_0,t)L_{\underline{\alpha}}U(t_0,t). \tag{12}$$

(4) The main differences with the earlier definitions of Refs. 1, 2, and 5 are the lim sup in Eq. (8) and the restriction to the derivations (1) corresponding to directions in phase space.

III. APPLICATION TO PARAMETRICALLY DRIVEN QUANTUM OSCILLATORS

In order to show the usefulness of the above definition, we consider the parametric quantum oscillator,[9–11] one of the simplest paradigms of the transition from regular to unstable behavior in classical mechanics.[12,13] The Hamiltonian (we take the mass=1) is

$$H(t) = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}f(t)\hat{x}^2, \tag{13}$$

where f is a periodic function of period T,

$$f(t+T) = f(t). \tag{14}$$

It is convenient to decompose f as $f(t)=E+f_{za}$ with $E=(1/T)\int_0^T dt\, f(t)$ [and thus $(1/T)\int_0^T dt\, f_{za}(t)=0$]. We will analyze the one parameter family of systems defined by varying the average $E\in\mathbb{R}$.

The classical equation corresponding to (13) is Hill's equation,[14,15]

$$\ddot{x} + f(t)x = 0, \tag{15}$$

which is well known (Ref. 14, Chap. 4, and Ref. 15) to have bands of stability regions S, and instability regions I ("gaps"), when the parameter E is varied.

For the quantum parametric oscillators we will prove the following results:

Theorem 1: For any observable $A=W(\beta,\gamma)$ of the form (4), in the stability region $E\in S$ one has

$$\overline{\lambda}_{\underline{\alpha}}(U,L_{\underline{\alpha}},A,t_0) = 0,\ \forall\ \underline{\alpha},\quad \forall\ t_0. \tag{16}$$

In the instability region $E\in I$, there is a stable direction $\underline{\alpha}_s$, which depends on t_0, for which

$$\overline{\lambda}_{\underline{\alpha}_s}(U,L_{\underline{\alpha}_s},A,t_0) = -\lambda_r < 0, \tag{17}$$

whereas for all other directions $\underline{\alpha}$,

$$\overline{\lambda}_{\underline{\alpha}}(U,L_{\underline{\alpha}},A,t_0) = \lambda_r > 0, \tag{18}$$

where λ_r is the absolute value of the real part of the Floquet exponent of the corresponding classical oscillator defined below in Eq. (32). Thus the upper Lyapunov exponent is

$$\overline{\lambda} = \sup_{\underline{\alpha}}\overline{\lambda}_{\underline{\alpha}} = \lambda_r > 0. \tag{19}$$

There is thus a transition in the upper quantum Lyapunov exponent $\overline{\lambda}$ as the parameter E ranges from the classical system's region of stability to the instability region.

Theorem 2: If we consider the time evolution in the instability region $E\in I$ at discrete times $t_n=n2T$ given by even integer multiples of the period T, there is an unstable eigendirection $\underline{\alpha}_+ \equiv(\alpha_{p^+},\alpha_{x^+})$ such that the corresponding derivation $L_{\underline{\alpha}_+}$ satisfies for all t_n,

$$e^{iL_{\underline{\alpha}_+}s}\, e^{-\lambda_r t_n} U^\dagger(t_n,0) = U^\dagger(t_n,0) e^{iL_{\underline{\alpha}_+}s}, \tag{20}$$

and a stable eigendirection $\underline{\alpha}_- \equiv (\alpha_{p-}, \alpha_{x-})$ such that

$$e^{iL_{\underline{\alpha}_-}s}\, e^{\lambda_r t_n} U^\dagger(t_n,0) = U^\dagger(t_n,0) e^{iL_{\underline{\alpha}_-}s}, \tag{21}$$

where $\lambda_r > 0$ is the real part of the classical Floquet exponent. Thus the system satisfies the discrete quantum Anosov relations defined by Emch, Narnhofer, Sewell, and Thirring.[1–3]

Remarks: This system satisfies the quantum Anosov relations but it lacks two other properties that enter in the definition of quantum Anosov systems as formulated in Refs. 1–3: There is no state that is invariant with respect to $U(t_n,0)$, nor with respect to $e^{iL_{\underline{\alpha}_\pm}s}$ [$U(t_n,0)$ has no eigenvalues for $E \in I$ and there are no translation invariant states in $\mathcal{H} = L_2(\mathbb{R}, dx)$]. However, as it was remarked in Ref. 1 (Remark 3.7, No. 7) the requirement of the invariant state may be dispensed with, depending on the intended application.

The relations (20) and (21) can be written equivalently, by changing $t_n \to -t_n$ as

$$e^{iL_{\underline{\alpha}_+}s}\, e^{\lambda_r t_n} U(t_n,0) = U(t_n,0) e^{iL_{\underline{\alpha}_+}s}, \tag{22}$$

$$e^{iL_{\underline{\alpha}_-}s}\, e^{-\lambda_r t_n} U(t_n,0) = U(t_n,0) e^{iL_{\underline{\alpha}_-}s}. \tag{23}$$

With this representation (22) one can give an intuitive interpretation for the Lyapunov exponent in the Schrödinger picture: We compare the forward time evolution ($t_{n+1} > t_n$) of two initial states ψ and $\psi + \delta\psi$ that are related to each other by a translation in phase space in direction $\underline{\alpha}_+$ of size s. The time evolution $U(t_n,0)[\psi + \delta\psi]$ to time t_n will yield a state $\phi + \delta\phi$, that can be related to $\phi = U(t_n,0)\psi$ by a translation in phase space in the same direction $\underline{\alpha}_+$ but of a size s' that is exponentially amplified $s' = s\, e^{\lambda_r t_n}$. This can be visualized by the following diagram:

$$\begin{array}{ccc} \psi & \overset{U(t_n,0)}{\longrightarrow} & \phi \\ e^{iL_{\underline{\alpha}_+}s}\downarrow & & \downarrow e^{iL_{\underline{\alpha}_+}s\, e^{\lambda_r t_n}} \\ \psi + \delta\psi & \overset{U(t_n,0)}{\longrightarrow} & \phi + \delta\phi \end{array} \tag{24}$$

For Anosov systems this property is satisfied globally for any size s of the translation. The definition of the Lyapunov exponent (11) can be interpreted on the basis of this picture but taking infinitesimally small translations.

In order to determine the upper quantum Lyapunov exponent according to Eq. (11) we first need to calculate $L_{\underline{\alpha}}(t_0,t)$.

Lemma 1:

$$L_{\underline{\alpha}}(t_1;t_2) = \alpha_p(t_1;t_2)\hat{p} + \alpha_x(t_1;t_2)\hat{x} \tag{25}$$

with

$$\alpha_p(t_1;t_2) = e^{(t_1-t_2)\lambda_+} h_{p+}(t_1;t_2) + e^{(t_1-t_2)\lambda_-} h_{p-}(t_1;t_2), \tag{26}$$

$$\alpha_x(t_1;t_2) = e^{(t_1-t_2)\lambda_+} h_{x+}(t_1;t_2) + e^{(t_1-t_2)\lambda_-} h_{x-}(t_1;t_2), \tag{27}$$

and $h_{p\pm}(t_1;t_2)$, $h_{x\pm}(t_1;t_2)$ are periodic functions of the same period T of the function f, and $\lambda_\pm$ are the Floquet exponents associated to the classical dynamics [defined below in Eq. (32)]. In the stability bands $E \in S$, $\lambda_\pm$ are purely imaginary, whereas in the instability regions $E \in I$, $\lambda_\pm$ has a nonvanishing real part, that we will denote $\pm\lambda_r$.

Proof of Lemma 1: The classical equation (15) may be written

$$\frac{d}{dt}\begin{pmatrix} p \\ x \end{pmatrix} = \begin{pmatrix} 0 & -f(t) \\ 1 & 0 \end{pmatrix}\begin{pmatrix} p \\ x \end{pmatrix}. \tag{28}$$

The propagator $F(t,t_0)$ of the classical equation, defined by

$$\begin{pmatrix} p(t) \\ x(t) \end{pmatrix} = F(t,t_0)\begin{pmatrix} p(t_0) \\ x(t_0) \end{pmatrix}, \quad F(t,t) = 1 \ \forall \ t, \tag{29}$$

may be written, by Floquet's theorem[15] as the following.

Lemma 2:

$$F(t,t_0) = G(t)e^{(t-t_0)B}G^{-1}(t_0), \tag{30}$$

where

$$G(t+T) = G(t) \tag{31}$$

is an invertible differentiable matrix, and B a constant traceless matrix.

Thus B is of one of the following three forms:

(1) B has two complex eigenvalues

$$\lambda_{\pm} = \pm(\lambda_r + i\lambda_i) \neq 0 \tag{32}$$

(we choose the notation such that $\lambda_r \geqslant 0$): Thus B is diagonalizable and there are two cases,

(1a) $\lambda_r = 0$ (stable case, band),
(1b) $\lambda_r \neq 0$ (unstable case, gap).

In these two cases one can write

$$F(t,t_0) = G(t)Se^{(t-t_0)\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}}S^{-1}G^{-1}(t_0), \tag{33}$$

where S is some invertible matrix.

(2) $\lambda_{\pm} = 0$.

In this case B is not diagonalizable, and has Jordan canonical form $\left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$. It corresponds to a band edge, which we shall not discuss further in this paper.

Using the fact that the Heisenberg equations of motion for the operators $\hat{x}(t)$ and $\hat{p}(t)$ have the same form as the classical equations for $p(t)$ and $x(t)$, we can write

$$\begin{pmatrix} U^{\dagger}(t,t_0) & \hat{p} & U(t,t_0) \\ U^{\dagger}(t,t_0) & \hat{x} & U(t,t_0) \end{pmatrix} = F(t,t_0)\begin{pmatrix} \hat{p} \\ \hat{x} \end{pmatrix} = g(t)\begin{pmatrix} e^{(t-t_0)\lambda_+} & 0 \\ 0 & e^{(t-t_0)\lambda_-} \end{pmatrix}g^{-1}(t_0)\begin{pmatrix} \hat{p} \\ \hat{x} \end{pmatrix}, \tag{34}$$

with $g(t) \equiv G(t)S$. Writing explicitly the matrix elements $g(t_1) \equiv (g_{ij}(t_1)), g^{-1}(t_2) \equiv (g_{ij}^{-1}(t_2))$, we find, by (26), (27), and (34) that the functions in Eq. (26) are given by

$$h_{p+}(t_1;t_2) = (\alpha_p g_{11}(t_1) + \alpha_x g_{21}(t_1))g_{11}^{-1}(t_2), \tag{35}$$

$$h_{p-}(t_1;t_2) = (\alpha_p g_{12}(t_1) + \alpha_x g_{22}(t_1))g_{21}^{-1}(t_2), \tag{36}$$

$$h_{x+}(t_1;t_2) = (\alpha_p g_{11}(t_1) + \alpha_x g_{21}(t_1))g_{12}^{-1}(t_2), \tag{37}$$

$$h_{x-}(t_1;t_2) = (\alpha_p g_{12}(t_1) + \alpha_x g_{22}(t_1))g_{22}^{-1}(t_2), \tag{38}$$

which are periodic in t_1 and in t_2 since $g(t)$ is periodic.

Proof of Lemma 2: The time evolution is symplectic, thus the Jacobi matrix $F(t,t_0)$ of the map (21) satisfies[12]

$$FJF^T = J, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{39}$$

and hence $\det F = 1$. Thus we may define $e^{BT} := F(T,0)$, i.e., $B := (1/T)\ln F(T,0)$, and define $G(t) := F(t,0)e^{-Bt}$. Then

$$G(t+T) = F(t+T,0)e^{-B(t+T)} = F(t+T,T)F(T,0)e^{-B(t+T)} = F(t,0)e^{-Bt} = G(t),$$

which is Floquet's theorem.[15]

It follows that

$$F(t,t_0) = F(t,0)F(0,t_0) = F(t,0)F^{-1}(t_0,0) = G(t)e^{B(t-t_0)}G^{-1}(t_0),$$

which is (30).

Now $F(T,0) = G(T)e^{BT}G^{-1}(0)$ and $1 = \det F(T,0) = \det(G(T))\det(e^{BT})(\det G(0))^{-1} = \det e^{BT}$ because $G(T) = G(0)$, hence $\mathrm{Tr}\, B = 0$.

Proof of Theorem 1: The Weyl algebra of observables is in the domain of the family of derivations defined as

$$\tilde{\delta}_{\underline{\alpha}}^{t_0,t} A := [L_{\underline{\alpha}}(t_0,t), A] \tag{40}$$

parametrized by the time variable,

$$\mathcal{W} \subset \mathrm{Dom}(\tilde{\delta}_{\underline{\alpha}}^{t_0,t}), \quad \forall\, t_0, t \in \mathbb{R}.$$

Indeed, by (5) and (25), if $A = e^{i(\beta\hat{x}+\gamma\hat{p})}$ then

$$[L_{\underline{\alpha}}(t_0,t), A] = (\alpha_p(t_0,t)\beta - \alpha_x(t_0,t)\gamma)A \in \mathcal{W}. \tag{41}$$

In order to determine the Lyapunov exponent we calculate

$$\|[L_{\underline{\alpha}}(t_0,t), A]\| = |\alpha_p(t_0,t)\beta - \alpha_x(t_0,t)\gamma|, \tag{42}$$

where we have used $\|A\| = 1$. By (26), (27), and (35)–(38) we may write, for $t, t_0 \in \mathbb{R}_+$,

$$\|[L_{\underline{\alpha}}(t_0,t), A]\| = |e^{(t-t_0)\lambda_+}[\{\alpha_p g_{12}(t_0) + \alpha_x g_{22}(t_0)\}(\beta g_{21}^{-1}(t) - \gamma g_{22}^{-1}(t))] + e^{(t-t_0)\lambda_-}[(\alpha_p g_{11}(t_0) + \alpha_x g_{21}(t_0)) \times (\beta g_{11}^{-1}(t) - \gamma g_{12}^{-1}(t))]|, \tag{43}$$

where we have used $\lambda_- = -\lambda_+$. The stable direction $\underline{\alpha}_s$ is determined by the condition that the curly bracket in the first term vanishes,

$$\{\alpha_p g_{12}(t_0) + \alpha_x g_{22}(t_0)\} = 0, \tag{44}$$

which leads to

$$\underline{\alpha}_s \equiv (\alpha_{ps}, \alpha_{xs}) = \eta_s(-g_{22}(t_0), g_{12}(t_0)), \tag{45}$$

where η_s is an arbitrary constant. We remark that the second term in (43) is not identically zero since

$$\alpha_p g_{11}(t_0) + \alpha_x g_{21}(t_0) = \eta_s(-g_{22}(t_0)g_{11}(t_0) + g_{12}(t_0)g_{21}(t_0)) = -\eta_s \det g \neq 0. \tag{46}$$

In this case we can write

$$\|[L_{\underline{\alpha}_s}(t_0,t), A]\| = e^{-t\lambda_r} S(t), \tag{47}$$

where λ_r is the absolute value of the real part of $\lambda_\pm$, and $S(t)$ is a periodic function of t. There is thus a sequence of times $\{t_k \to \infty\}$, such that $S(t_k) > \delta > 0$, for some constant δ, and therefore

$$\bar{\lambda}_{\underline{\alpha}_s}(U,L_{\underline{\alpha}_s},A,t_0) = -\lambda_r + \limsup_{t\to\infty}\frac{1}{t}\ln S(t) = -\lambda_r. \tag{48}$$

For all other directions $\underline{\alpha}$ we can write

$$\|[L_{\underline{\alpha}}(t_0,t),A]\| = e^{t\lambda_r}R(t), \tag{49}$$

where $R(t)$ is the sum of a periodic function and one that is either exponentially decreasing or identically zero. Thus there is a sequence of times $\{t_k\to\infty\}$, such that $R(t_k)>\delta>0$, for some constant δ, and therefore

$$\bar{\lambda}_{\underline{\alpha}}(U,L_{\underline{\alpha}},A,t_0) = \lambda_r + \limsup_{t\to\infty}\frac{1}{t}\ln R(t) = \lambda_r. \tag{50}$$

In the stability bands $E\in S,\lambda_\pm$ are imaginary, and thus $\bar{\lambda}_{\underline{\alpha}}=0$ for all directions $\underline{\alpha}$.

Remark: A simple extension of this proof shows that Theorem 1 is also true for any observable $A\in\mathcal{W}$ provided that $[L_{\underline{\alpha}},A]\neq 0$.

Proof of Theorem 2: We remark first that (20) and (21) are equivalent, by deriving with respect to s at $s=0$ to

$$U^\dagger(t_n,0)L_{\underline{\alpha}_+}U(t_n,0) = e^{-\lambda_r t_n}L_{\underline{\alpha}_+}, \tag{51}$$

$$U^\dagger(t_n,0)L_{\underline{\alpha}_-}U(t_n,0) = e^{\lambda_r t_n}L_{\underline{\alpha}_-}. \tag{52}$$

The eigendirections are thus determined by the conditions

$$L_{\underline{\alpha}_\pm}(t_n,0) = e^{\mp\lambda_\pm t_n}L_{\underline{\alpha}_\pm}(0,0). \tag{53}$$

According to Eqs. (25)–(27), since $h_{p\pm}(t,0)$ and $h_{x\pm}(t,0)$ are T periodic and since $\lambda_-=-\lambda_+$, these conditions will be satisfied.

For $\underline{\alpha}_+$, if $h_{p+}(t_n,0)=h_{p+}(0,0)=0$ and $h_{x+}(t_n,0)=h_{x+}(0,0)$, i.e., according to (35) and (37), if

$$(\alpha_{p+}g_{11}(0)+\alpha_{x+}g_{21}(0))g_{12}^{-1}(0) = 0, \tag{54}$$

$$(\alpha_{p+}g_{11}(0)+\alpha_{x+}g_{21}(0))g_{22}^{-1}(0) = 0. \tag{55}$$

For $\underline{\alpha}_-$, if $h_{p-}(t_n,0)=h_{p-}(0,0)=0$ and $h_{x-}(t_n,0)=h_{x-}(0,0)$, i.e., according to (36) and (38), if

$$(\alpha_{p-}g_{12}(0)+\alpha_{x-}g_{22}(0))g_{22}^{-1}(0) = 0, \tag{56}$$

$$(\alpha_{p-}g_{12}(0)+\alpha_{x-}g_{22}(0))g_{21}^{-1}(0) = 0. \tag{57}$$

Since g^{-1} is nonsingular, g_{12}^{-1} and g_{22}^{-1} cannot both be zero, and therefore for $\underline{\alpha}_-$ we obtain the condition

$$\alpha_{p-}g_{12}(0)+\alpha_{x-}g_{22}(0) = 0, \tag{58}$$

which has the solution

$$\underline{\alpha}_- \equiv (\alpha_{p-},\alpha_{x-}) = \eta_-(-g_{22}(0),g_{12}(0)), \tag{59}$$

where η_- is an arbitrary constant. Since g is nonsingular, g_{12} and g_{22} cannot both be zero, and thus (59) determines the unique stable eigendirection. It coincides for t_0 with the stable $\underline{\alpha}_s$ of Theorem 1, Eq. (45).

By the same type of argument we obtain the unstable eigendirection as

$$\underline{\alpha}_+ \equiv (\alpha_{p+}, \alpha_{x+}) = \eta_+(-g_{21}(0), g_{11}(0)). \tag{60}$$

We remark that

$$e^{2T\lambda_\pm} = e^{\pm 2T\lambda_r} e^{\pm i2T\lambda_i} = e^{\pm 2T\lambda_r}, \tag{61}$$

since in the gaps $E \in I$ the imaginary part λ_i of the Floquet eigenvalues takes constant values of the form

$$\lambda_i = k\frac{2\pi}{2T}, \quad k \in \mathbb{Z}. \tag{62}$$

This can be shown as follows: $\Lambda_\pm \equiv e^{\lambda_\pm T}$ are the eigenvalues of the propagator matrix $F(T,0)$ defined in Eq. (30). Since it is a real matrix with $\det F(T,0)=1$, its eigenvalues are either real or complex conjugate to each other $\Lambda_- = \Lambda_+^*$, in which case $|\Lambda_\pm| = 1$. Therefore, in the instability region $E \in I$ the eigenvalues $\Lambda_\pm = e^{\pm(\lambda_r + i\lambda_i)}$ are necessarily real, and thus $\lambda_i T = k\pi$, $k \in \mathbb{Z}$.

This completes the proof of the Anosov property (51) and (52).

Remark 1: The factor $1/2$ in Eq. (62) explains the need to take time intervals that are multiples of $2T$ in order to have the Anosov property. For the gaps with even k one has the Anosov property also in the discrete times $t_n' = nT$, $n \in \mathbb{Z}$.

Remark 2: We have set $t_0 = 0$ above, but, although the eigenvalues $\lambda_\pm$ do not vary upon variation of t_0, the eigendirections do. This is the reason why we have an Anosov system in discretized time but not in continuous time.

Remark 3: The above example of a quantum Anosov structure is interesting because it is not global in the space of parameters E, i.e., if $E \in S$ it is not realized. For $E \in S$, the upper quantum Lyapunov exponent equals zero, a case which is included in our definition, but not by Refs. 1–3.

Remark 4: The parametric quantum oscillator (13) is, of course, very special, being quadratic in $\hat{x}$ and $\hat{p}$. We have used the fact that the Heisenberg equations of motion for $\hat{x}, \hat{p}$ have the same form as the classical Hamiltonian equations. The dynamics are, however, rich and nontrivial and not explicitly soluble both classically and quantum mechanically: the complexity manifests itself in the fact that the symmetry group of (13) is SU (1,1) rather than the Heisenberg group.[16] The transition in the theorem has a physical interpretation in a model of quadrupole radio-frequency traps (Paul–Penning traps), see Refs. 9, 10, and 17 and references given there.

Remark 5: The case of a quasiperiodic time dependence has a very interesting structure (Refs. 18 and 19), and our approach is, in principle, applicable to this case.

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Fluctuation statistics in networks: A stochastic path integral approach

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We investigate the statistics of fluctuations in a classical stochastic network of nodes joined by connectors. The nodes carry generalized charge that may be randomly transferred from one node to another. Our goal is to find the time evolution of the probability distribution of charges in the network. The building blocks of our theoretical approach are (1) known probability distributions for the connector currents, (2) physical constraints such as local charge conservation, and (3) a time scale separation between the slow charge dynamics of the nodes and the fast current fluctuations of the connectors. We integrate out fast current fluctuations and derive a stochastic path integral representation of the evolution operator for the slow charges. The statistics of charge fluctuations may be found from the saddle-point approximation of the action. Once the probability distributions on the discrete network have been studied, the continuum limit is taken to obtain a statistical field theory. We find a correspondence between the diffusive field theory and a Langevin equation with Gaussian noise sources, leading nevertheless to nontrivial fluctuation statistics. To complete our theory, we demonstrate that the cascade diagrammatics, recently introduced by Nagaev, naturally follows from the stochastic path integral. By generalizing the principle of minimal correlations, we extend the diagrammatics to calculate current correlation functions for an arbitrary network. One primary application of this formalism is that of full counting statistics (FCS), the motivation for why it was developed in the first place. We stress however, that the formalism is suitable for general classical stochastic problems as an alternative approach to the traditional master equation or Doi–Peliti technique. The formalism is illustrated with several examples: Both instantaneous and time averaged charge fluctuation statistics in a mesoscopic chaotic cavity, as well as the FCS and new results for a generalized diffusive wire. © *2004 American Institute of Physics.*
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I. INTRODUCTION

Consider an exclusive nightclub with a long line at the entrance. A bouncer is at the front of the line to keep out the riffraff. At every time step, a person is accepted inside the club with probability p, or rejected with probability $1-p$. Inside the club, people stay for a while and eventually leave. At every time step, the probability a person leaves is q. We want to answer a question such as "what is the probability that Q people leave the club after t time steps?"

Assuming that p and q remain constant, the situation is simple and we can easily solve the relevant probabilistic problem. However, in realistic situations this rarely happens: The management wants to make money. If the club is almost empty, they instruct the bouncer to be less discriminating, while if the club is almost full, the bouncer is to be more discriminating. Thus, p becomes a function of the number of people in the club. People will be more likely to leave if the club is very crowded, so q is also a function of the number of people inside the club. The problem posed now is much more difficult because of the presence of feedback: The elementary processes change in response to the cumulative effect of what they have accomplished in the past.

This simple example captures all the basic features of the problems we wish to consider. Although the example was given with people, the actors in the probability game may be any quantity such as charge, energy, heat, or particles, which we will refer to simply as generalized charge. Similarly, the nightclub can be a mesoscopic chaotic cavity,[1] a birth-death process,[2] a biological membrane channel,[3] etc.

Historically, general stochastic problems are solved with the master equation. The time rate of change of the probability to be in a particular state is given in terms of transition rates to other states. This approach has had great success and leads naturally to the Fokker–Planck and Langevin equations.[4] However, once the master equation is given, the solution is often quite difficult to obtain.

This paper takes a different approach. Rather than beginning with a master equation describing the probability of all processes happening in a unit of time, we make several assumptions from which we can reformulate the problem. Although these assumptions limit the applicability of the theory, when they apply, the problems are much easier to solve. The assumptions are:

- The system we are interested in is a composite system made out of constituent parts. In the nightclub example, the system is made up of three physical regions: Outside the front door, the interior of the club, and outside the back door. The decomposition of a larger system into smaller interacting parts is only meaningful for us if there is a separation of time scales. This means that the charge inside the constituent parts changes on a slower time scale than the fluctuations at the boundaries. In the nightclub example, this simply means that the average time a person spends in the club will be much longer than the typical time needed to enter the door.
- Taken alone, the parts of the composite system have a finite number of simple properties or parameters. The only property of the nightclub that was relevant for the problem was the total number of people in it at any given time. The important element of the line out in front is that it never runs out. All other details are irrelevant.
- In the limit where all parts of the network are very large (so that the elementary transport processes do not affect themselves in the short run), the transport probability distributions between elements are known. In the nightclub example, the probability of getting Q people through the front door after t time steps (given a constant, large number of people inside) is easy to find, because we have assumed that the elementary probability p does not change from trial to trial. The transport probability distribution is simply the binomial distribution[4] where the probability p is a function of the (approximately unchanging) number of people inside. The back door distribution is obtained in the same way.
- There are conservation laws that govern the probabilistic processes. No matter what probability distributions we have, there are certain rules that must be obeyed. The net number of people that enter, stay, and leave the club must be a constant. This means that the time rate of change of the club's occupancy is given by the people-current in minus the people-current out. The people in the line outside are a special case. There is in principle always a replacement, so moving one person inside the club does not affect the properties of the line.

Now, the strategy is to use this information as the starting point to find transport statistics for the combined interacting system. The main result derived is a path integral expression for the conditional probability (taking conservation laws into account) for starting and ending with a given amount of charge at each location after some time has passed. From this conditional probability, specific quantities such as transport statistics through the system, fluctuation statistics of charge at a particular location and the like may be found.

One primary application of this formalism is that of full counting statistics (FCS),[5,6] the motivation for why it was developed in the first place.[7] FCS describes the fluctuations of currents in electrical conductors. It gives the distribution of the probability that a certain number of electrons pass a conductor in a certain amount of time. Mean current flow and shot noise[1] correspond to the first and second cumulant of this distribution. The full distribution (defined by all cumulants) provides a full characterization of the transport properties of an electrical conductor in the long time limit. In the past, FCS was mainly addressed with quantum mechanical tools such as

the scattering theory[5,6,8,9] of coherent conductors, the circuit theory based on Keldysh Green functions,[10–13] or the nonlinear σ model.[14] However, a number of works realized that for semi-classical systems with a large number of conductance channels, shot noise may be calculated without accounting for the phase coherence of the electron.[15–18] These works treat the basic sources of noise quantum mechanically, but calculate the spread of the noise throughout the conductor classically. For specific conductors like diffusive wires and chaotic cavities, this idea has been extended to the calculation of third and fourth cumulants via the cascade principle[19,20] and to the full generating function of FCS.[7,21–23] In the present work, we consider an abstract model instead of any particular example and develop the mathematical foundations of the proposed semi-classical procedure to obtain FCS. We introduce and investigate networks of elements with known transport statistics and show how the FCS of the entire network can be constructed systematically.

The formalism we present is related to a different approach in nonequilibrium statistical physics called the Doi–Peliti technique.[24] The idea is that once the basic master equation governing the time evolution of probability distributions is given, it may be interpreted as a Schrödinger equation which may be cast into a second-quantized language. This quantum problem is then converted into a quantum mechanical path integral (often obeying bosonic or fermionic statistics) from which one may take the continuum limit and use a field theory renormalization group approach with diagrammatic perturbation expansion.[25] This approach is useful in many situations far from equilibrium and has several parallels to our approach. It has been pointed out that this technique is in some sense the classical limit of the quantum mechanical Keldysh formalism,[26] the same tool used in the past to calculate FCS, so this gives another connection with the subject matter we are concerned with.

There are several advantages of our approach. First, we skip the master equation step. If the probability distributions of the connector fluctuations are given, we may immediately construct network distributions. Second, from a computational view, our formulation of the problem is much simpler than starting from first principles for situations where the ingredients we need are available, and results are much easier to obtain than beginning with the master equation alone. Thirdly, our formulation also applies to situations where temporal transition probabilities may be large. Finally, the formalism's physical origin is clear, so the needed mathematical objects are well motivated.

The rest of the paper is organized as follows. In Sec. II, we introduce and develop the general theory. After reviewing elements of probability theory, we derive the stochastic path integral for a network of nodes as well as explore the relationship to the master equation and Doi–Peliti formalism. In Sec. III, the continuum limit is taken to derive a stochastic field theory and link our formalism with the Langevin equation point of view. In Sec. IV, we develop diagrammatics rules to calculate cumulants of the current distribution as well as current correlation functions for an arbitrary network. Section V gives several applications of the theory to different physical situations. We solve the field theory for the mesoscopic wire and demonstrate universality in multiple dimensions as well as present new results for the conditional occupation function and probability distribution. We also consider the problem of charge fluctuation statistics (both instantaneous and time-averaged) in a mesoscopic chaotic cavity. Section VI contains our conclusions.

II. GENERAL FORMALISM

Once we have the basic elements of our theory (the generalized charges), we must specify some spatial structure that they move around on. As we noted in the introduction, the essential structure needed to state the problem are simply points we refer to as nodes, joined by connectors. This defines a network (see Fig. 1). The state of each node α is described by one (effectively continuous) charge Q_α,[27] and $\mathbf{Q}$ is the charge vector describing the charge state of the network. The node's state may be changed by transport: Flow of charges between nodes takes place via the connectors carrying currents $I_{\alpha\beta}$ from node α to node β. The variation of these charges Q_α is given by

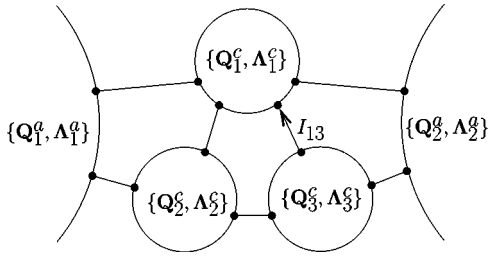

FIG. 1. An arbitrary network. Each node has charge and counting variables $\{\mathbf{Q}_\alpha, \mathbf{\Lambda}_\alpha\}$. The nodes transfer charge via currents $I_{\alpha\beta}$ through the connectors. The absorbed counting fields $(\mathbf{\Lambda}_\alpha^a)$ are constants by definition of the absorbed charges $\mathbf{Q}_\alpha^a$ (see text). Each node may have an arbitrary number of different charge species, $\mathbf{Q}_\alpha = \{Q_\alpha^1, Q_\alpha^2, \ldots, Q_\alpha^j\}$.

$$Q_\alpha(t+\Delta t) - Q_\alpha(t) = \sum_\beta Q_{\alpha\beta}, \tag{1}$$

where the transmitted charges $Q_{\alpha\beta}(t) = \int_0^{\Delta t} dt' I_{\alpha\beta}(t+t')$ are distributed according to $P_{\alpha\beta}(Q_{\alpha\beta}(t))$. The fact that the probabilities $P_{\alpha\beta}(t)$ also depend on the charges $\mathbf{Q}(t)$ is one source of the difficulty of the problem.

Assuming that the probability distributions $P_{\alpha\beta}$ (which depend parametrically on the state of nodes α and β) of the transmitted charges $Q_{\alpha\beta}$ are known, we seek the time evolved probability distribution $\Gamma(\mathbf{Q}, t)$ of the set of charges $\mathbf{Q}$ for a given initial distribution $\Gamma(\mathbf{Q}, 0)$. In other words, one has to find the conditional probability (which we refer to as the evolution operator) $U(\mathbf{Q}, \mathbf{Q}', t)$ such that

$$\Gamma(\mathbf{Q}, t) = \int d\mathbf{Q}' U(\mathbf{Q}, \mathbf{Q}', t) \Gamma(\mathbf{Q}', 0). \tag{2}$$

We assume that there is a separation of time scales, $\tau_0 \ll \tau_C$, between the correlation time of current fluctuations, τ_0, and the slow relaxation time of charges in the nodes, τ_C. As we will show in the next section, this separation of time scales allows us to derive a stochastic path integral representation for the evolution operator,

$$U(\mathbf{Q}_f, \mathbf{Q}_i, t) = \int \mathcal{D}\mathbf{Q}\mathcal{D}\mathbf{\Lambda} \exp\{S(\mathbf{Q}, \mathbf{\Lambda})\}, \tag{3a}$$

$$S(\mathbf{Q}, \mathbf{\Lambda}) = \int_0^t dt' \left[-i\mathbf{\Lambda} \cdot \dot{\mathbf{Q}} + (1/2) \sum_{\alpha\beta} H_{\alpha\beta}(\mathbf{Q}, \lambda_\alpha - \lambda_\beta) \right], \tag{3b}$$

where the vector $\mathbf{\Lambda}$ has components λ_α: Node variables conjugated to the Q_α that impose charge conservation in the network.

In the following, we define the functions $H_{\alpha\beta}$ as the generating functions of the fast currents between nodes α and β. On the time scale $\Delta t \gg \tau_0$, the currents through isolated connectors are Markovian, so that all cumulants (irreducible correlators which are denoted by double angle brackets) of the transmitted charge $\langle\langle (Q_{\alpha\beta})^n \rangle\rangle$ are linear in Δt. Following the standard notation in mesoscopic physics,[28] we define the current cumulants $\langle\langle (\tilde{I}_{\alpha\beta})^n \rangle\rangle$ as the coefficients in

$$\langle\langle (Q_{\alpha\beta})^n \rangle\rangle = \Delta t \langle\langle (\tilde{I}_{\alpha\beta})^n \rangle\rangle, \tag{4}$$

where the tilde symbol has been introduced to distinguish the bare currents of each connector (the sources of noise) from the physical currents $I_{\alpha\beta}$ flowing through that same connector when it is placed into the network. Then the generators $H_{\alpha\beta}$ are defined via the equation

$$\langle\langle(\tilde{I}_{\alpha\beta})^n\rangle\rangle = \left.\frac{\partial^n H_{\alpha\beta}(\mathbf{Q},\lambda_{\alpha\beta})}{(i\,\partial\lambda_{\alpha\beta})^n}\right|_{\lambda_{\alpha\beta}=0}, \tag{5}$$

and thus contain complete information about the statistics of the noise sources. The $\lambda_{\alpha\beta}$ [eventually to be replaced with with $\lambda_\alpha-\lambda_\beta$ in Eq. (3)] is the generating variable for the current $\tilde{I}_{\alpha\beta}$. The notion of current cumulants is useful because they are the time independent objects, and thus have time independent generators, Eq. (5). The generators $H_{\alpha\beta}(\mathbf{Q},\lambda_{\alpha\beta})$ depend in general on the full vector $\mathbf{Q}$ and not just on the generalized charges of the neighboring nodes Q_α and Q_β. This may serve to incorporate long range interactions between distant nodes.

The charge $Q_{\alpha\beta}$ transferred through the connectors [characterized by Eqs. (4) and (5)] may be discrete. However, the charge in the nodes Q_α is treated as an effectively continuous variable in Eqs. (1)–(3). This is justified if many charges in the node participate in transport. Formally, this limit allows a saddle-point evaluation of the propagator (3a).

A. Derivation of the path integral

To derive the path integral Eq. (3), we follow the usual procedure[29] and first discretize time, $t=n\Delta t$ to derive an expression for U that is valid for propagation over one time step Δt. Because of the separation of time scales $\tau_0 \ll \tau_C$, we can consider Δt as an intermediate time scale,

$$\tau_0 \ll \Delta t \ll \tau_C. \tag{6}$$

The left inequality, $\tau_0 \ll \Delta t$, implies that the transmitted charges $Q_{\alpha\beta}$ are Markovian.[4] This means that charges transmitted in separate time intervals are uncorrelated with each other. While it is not necessary to specify the source of the current correlation in the general formulation, it is worth noting two examples. In a mesoscopic point contact, the correlation time τ_0 has the interpretation of the time taken by an electron wavepacket to pass the point contact. In chemical dynamics, it could be the time taken for a long molecule in solution to traverse a filter.

In a time Δt, the probability that charge $Q_{\alpha\beta}$ is transmitted between nodes α and β can be written as the Fourier transform of the exponential of a generating function $S_{\alpha\beta}$:

$$P_{\alpha\beta}(Q_{\alpha\beta},\Delta t) = \int \frac{d\lambda_{\alpha\beta}}{2\pi}\exp\{-i\lambda_{\alpha\beta}Q_{\alpha\beta} + S_{\alpha\beta}(\lambda_{\alpha\beta})\}. \tag{7}$$

The definition of the cumulant of transmitted charge is

$$\langle\langle(Q_{\alpha\beta})^n\rangle\rangle = \left.\frac{\partial^n S_{\alpha\beta}(\lambda_{\alpha\beta})}{(i\,\partial\lambda_{\alpha\beta})^n}\right|_{\lambda_{\alpha\beta}=0}. \tag{8}$$

The Markovian assumption implies that the probability of transmitting charge $Q_{\alpha\beta}$ in time Δt followed by charge $Q'_{\alpha\beta}$ in time $\Delta t'$ through any connector is given by the product of independent probability distributions. This implies that the probability of transmitting charge $Q_{\alpha\beta}$ in time $\Delta t + \Delta t'$ may be calculated by finding all ways of independently transferring charge $Q'_{\alpha\beta}$ in the first step and $Q_{\alpha\beta}-Q'_{\alpha\beta}$ in the second step,

$$P(Q_{\alpha\beta},\Delta t+\Delta t') = \int dQ'_{\alpha\beta}P(Q_{\alpha\beta}-Q'_{\alpha\beta},\Delta t')P(Q'_{\alpha\beta},\Delta t), \tag{9}$$

which takes the form of a convolution of probabilities. Applying a Fourier transform to both sides of Eq. (9) with argument $\lambda_{\alpha\beta}$ decouples the convolution into a product of the two Fourier transformed distributions. Equation (7) implies $S_{\alpha\beta}(\Delta t+\Delta t',\lambda_{\alpha\beta})=S_{\alpha\beta}(\Delta t,\lambda_{\alpha\beta})+S_{\alpha\beta}(\Delta t',\lambda_{\alpha\beta})$. It then immediately follows that the generating function must be linear in time. Therefore, a time independent $H_{\alpha\beta}$ may be introduced: $S_{\alpha\beta}=\Delta t\, H_{\alpha\beta}$. The linear dependence of $S_{\alpha\beta}$ on time implies that all charge cumulants (8) will be proportional to time. Therefore, we define the time independent current cumulants, Eq. (5).

Different connectors are clearly uncorrelated for $\Delta t \ll \tau_C$, which indicates that the total probability distribution of transmitted charges is a product of the independent probabilities in each connector:[30]

$$P[\{Q_{\alpha\beta}\}] = \prod_{\alpha>\beta} P_{\alpha\beta}[Q_{\alpha\beta}, \Delta t]. \tag{10}$$

Thus far, the analysis is only valid for times much smaller than τ_C. For this case, the charges in the nodes will only slightly change. Since we wish to consider longer times, we need to take into account the fact that charge transfer between different nodes will be correlated as charge piles up inside the nodes. This may be accounted for by imposing charge conservation Eq. (1) during the time interval with a delta function,

$$\delta\left(Q_\alpha - Q'_\alpha - \sum_\beta Q_{\alpha\beta}\right) = \int \frac{d\lambda_\alpha}{2\pi} \exp\left\{-i\lambda_\alpha\left[Q_\alpha - Q'_\alpha - \sum_\beta Q_{\alpha\beta}\right]\right\}. \tag{11}$$

Here, Q'_α is the charge in the node before the time interval while Q_α is the charge accumulated in the node after the time interval is over. In Eq. (11), λ_α (referred to as a *counting variable*) plays the role of a Lagrange multiplier. The propagator is obtained by multiplying the constraint (11) and the independent probability distribution (10). Representing the probabilities in their Fourier form (7) then yields

$$\tilde{U}(\mathbf{Q}, \mathbf{Q}', Q_{\alpha\beta}, \Delta t) = \prod_\alpha \int \frac{d\lambda_\alpha}{2\pi} \prod_{\alpha>\beta} \int \frac{d\lambda_{\alpha\beta}}{2\pi} \exp(S),$$

$$S = -i\sum_\alpha \lambda_\alpha \left(Q_\alpha - Q'_\alpha - \sum_\beta Q_{\alpha\beta}\right) + \sum_{\alpha>\beta} [-i\lambda_{\alpha\beta} Q_{\alpha\beta} + \Delta t H_{\alpha\beta}(\mathbf{Q}', \lambda_{\alpha\beta})]. \tag{12}$$

The full propagator $\tilde{U}(\mathbf{Q}, \mathbf{Q}', Q_{\alpha\beta}, \Delta t)$ still keeps track of each individual connector contribution $Q_{\alpha\beta}$. We now integrate out the fast fluctuations to obtain the dynamics of the slow variables. This may be done by using the identity $\Sigma_\alpha \lambda_\alpha \Sigma_\beta Q_{\alpha\beta} = \Sigma_{\alpha>\beta}(\lambda_\alpha Q_{\alpha\beta} + \lambda_\beta Q_{\beta\alpha})$ and $Q_{\alpha\beta} = -Q_{\beta\alpha}$. The integration over $Q_{\alpha\beta}$ gives a delta function of argument $\lambda_{\alpha\beta} - (\lambda_\alpha - \lambda_\beta)$, so that the $\lambda_{\alpha\beta}$ integrals may be trivially done. We obtain

$$U(\mathbf{Q}, \mathbf{Q}', \Delta t) = \prod_\alpha \int \frac{d\lambda_\alpha}{2\pi} \exp\left\{-i\sum_\alpha \lambda_\alpha (Q_\alpha - Q'_\alpha) + \Delta t \sum_{\alpha>\beta} H_{\alpha\beta}(\mathbf{Q}', \lambda_\alpha - \lambda_\beta)\right\}. \tag{13}$$

This is the general result for the one step propagator. If any two nodes are unconnected, $H_{\alpha\beta}$ is zero.

An important comment is in order: Because $H_{\alpha\beta}$ changes slightly over the time period, which in turn affects the probability of transmitting charge through the contacts, it is not clear at what part of the time step $H_{\alpha\beta}$ should be evaluated. This ambiguity exists because our theory is not microscopic. Rather, it takes the microscopic noise generators as an input. This ambiguity gives the freedom of stochastic quantization.[31] The same problem also occurs in quantum mechanical path integrals, and its source there is an ambiguity in operator ordering.[32] As we are interested in the large transporting charge limit, $\gamma \gg 1$, and evaluate the integrals in leading order saddle-point approximation, this ambiguity will not affect the results.[7] For calculations beyond the large transporting charge limit, the canonical variables $\mathbf{Q}$ and $\mathbf{\Lambda}$ need to be properly ordered, which can only be done with a microscopic theory. For example, the master equation discretized in time as discussed in Sec. II D requires the placement of $\mathbf{\Lambda}$ operators in front of $\mathbf{Q}$ operators, since the generating functions $H_{\alpha\beta}$ of the transition probabilities depend on the state of the system at the beginning of the time period.

To extend the propagator (13) to longer times $t = n\Delta t$, we use the composition property of the evolution operator (also known as the Chapman–Kolmogorov equation[4]). This requires separate

$\{Q_\alpha\}$ integrals at each time step, so that for n time steps there will be $n-1$ integrals over $\mathbf{Q}$, while each of the n one-step propagators comes with its own $\mathbf{\Lambda}$ integral, $\mathbf{\Lambda}=\{\lambda_\alpha\}$. Inserting our expression for the Δt step propagator Eq. (13), we find

$$U(\mathbf{Q}_f,\mathbf{Q}_i,t)=\int d\mathbf{\Lambda}_0\prod_{k=1}^{n-1}\int d\mathbf{Q}_k d\mathbf{\Lambda}_k \exp\left[\sum_{k=0}^{n-1} -i\mathbf{\Lambda}_k\cdot(\mathbf{Q}_{k+1}-\mathbf{Q}_k)+\Delta t H(\mathbf{Q}_k,\mathbf{\Lambda}_k)\right], \quad (14a)$$

with

$$H(\mathbf{Q}_k,\mathbf{\Lambda}_k)=\sum_{\alpha>\beta} H_{\alpha\beta}[Q_{\alpha,k};\lambda_{\alpha,k}-\lambda_{\beta,k}], \quad (14b)$$

where we have introduced the notations $d\mathbf{Q}_k=\Pi_\alpha\, dQ_{\alpha,k}$ and $d\mathbf{\Lambda}_k=\Pi_\alpha(d\lambda_{\alpha,k}/2\pi)$. We are now in a position to take the continuous time limit. Writing $\mathbf{Q}_{k+1}-\mathbf{Q}_k=\Delta t\dot{\mathbf{Q}}$, which is valid because the charge in any node changes only slightly over the time scale Δt, the action of this discrete path integral has the form $S=\Delta t\Sigma_{k=1}^{n} S_k$, which goes over into a time integral in the continuous limit. Using the standard path integral notation $\int\mathcal{D}\mathbf{Q}\mathcal{D}\mathbf{\Lambda}=\int d\mathbf{\Lambda}_0\Pi_{k=1}^{n-1}\int d\mathbf{Q}_k d\mathbf{\Lambda}_k$, and invoking the symmetry $H_{\alpha\beta}(\lambda_\alpha-\lambda_\beta)=H_{\beta\alpha}(\lambda_\beta-\lambda_\alpha)$ we recover Eq. (3). The only explicit constraint on the path integral comes with the charge configurations at the start and finish, $\mathbf{Q}_i$ and $\mathbf{Q}_f$. We also note that $H_{\alpha\beta}$ depends on any external parameters such as voltages or chemical potentials driving the charge $\mathbf{Q}$.

In the simplest case of one charge and counting variable, the form of the path integral is the same as the (Euclidian time) path integral representation of a quantum mechanical propagator in phase space with position coordinate Q and momentum coordinate λ.[32] The differences with the quantum version are that the propagator evolves probability distributions, not amplitudes (similarly to Ref. 25), as well as the fact that the "Hamiltonian" $H=(1/2)\Sigma_{\alpha\beta}H_{\alpha\beta}(\mathbf{Q},\lambda_\alpha-\lambda_\beta)$ is not really a Hamiltonian, but rather a current cumulant generating function and, therefore, is not Hermitian in general. Even so, because of the similarity we shall refer to H as the Hamiltonian from now on.

B. Absorbed charges, boundary conditions, and correlation functions

A useful special case occurs when one has absorbed charges. These are charges that vanish into (or are injected from) absorbing nodes without altering the system dynamics. In mesoscopics, for example, the absorbing nodes are metallic reservoirs. Formally, we divide the charges into those that are conserved and those that are absorbed: $\mathbf{Q}=\{\mathbf{Q}^c,\mathbf{Q}^a\}$, where the subset of absorbed charges $\mathbf{Q}^a=\{Q_\alpha^a\}$ does not appear in $H_{\alpha\beta}$. We do the same for the corresponding counting variables: $\mathbf{\Lambda}=\{\mathbf{\Lambda}^c,\mathbf{\Lambda}^a\}$. Because $H_{\alpha\beta}$ does not depend on $\mathbf{Q}^a$, these charges may be integrated out by integrating the action by parts,

$$i\int_0^t dt'\mathbf{\Lambda}^a\cdot\dot{\mathbf{Q}}^a=-i\int_0^t dt'\mathbf{Q}^a\cdot\dot{\mathbf{\Lambda}}^a+i(\mathbf{\Lambda}_f^a\cdot\mathbf{Q}_f^a-\mathbf{\Lambda}_i^a\cdot\mathbf{Q}_i^a), \quad (15)$$

and then functionally integrating over $\mathbf{Q}^a$ to obtain $\delta(\dot{\mathbf{\Lambda}}^a)$, where δ is a functional delta function. This immediately constrains the $\mathbf{\Lambda}^a$ to be constants of motion so the functional integration over $\mathbf{\Lambda}^a$ becomes a normal integration, $\mathcal{D}\mathbf{\Lambda}^a\to d\mathbf{\Lambda}^a$. The absorbed kinetic terms in the action may then be integrated to obtain

$$U(\mathbf{Q}_f,\mathbf{Q}_i,t)=\int d\mathbf{\Lambda}^a\int\mathcal{D}\mathbf{Q}^c\mathcal{D}\mathbf{\Lambda}^c\exp\{S(\mathbf{Q},\mathbf{\Lambda})\}, \quad (16a)$$

$$S(\mathbf{Q},\mathbf{\Lambda})=\int_0^t dt'\left[-i\mathbf{\Lambda}^c\cdot\dot{\mathbf{Q}}^c+(1/2)\sum_{\alpha\beta}H_{\alpha\beta}(\lambda_\alpha-\lambda_\beta)\right]-i\mathbf{\Lambda}^a\cdot(\mathbf{Q}_f^a-\mathbf{Q}_i^a). \quad (16b)$$

Often one is interested in the probability to transmit some amount of charge through each of the absorbing nodes. By applying a Fourier transform to Eq. (16a) with respect to $\mathbf{Q}^a(t)-\mathbf{Q}^a(0)$ we remove the last term in Eq. (16b) and obtain the path integral representation for the characteristic function Z which generates current moments at every absorbing node

$$Z(\mathbf{\Lambda}^a)=\int \mathcal{D}\mathbf{Q}^c\mathcal{D}\mathbf{\Lambda}^c \exp\{S(\mathbf{Q},\mathbf{\Lambda})\}, \tag{17a}$$

$$S(\mathbf{Q},\mathbf{\Lambda})=\int_0^t dt'\left[-i\mathbf{\Lambda}^c\cdot\dot{\mathbf{Q}}^c+(1/2)\sum_{\alpha\beta}H_{\alpha\beta}(\lambda_\alpha-\lambda_\beta)\right]. \tag{17b}$$

Note that the counting variables $\mathbf{\Lambda}^a$ enter the action (17b) only as a set of constant parameters. The initial condition in the path integral (17) is given by the initial charge states $\mathbf{Q}^c(0)$. There is a choice of the final condition: By fixing the final $\mathbf{Q}^c(t)$ one obtains the distribution of the conserved charge subject to this constraint, while by fixing $\mathbf{\Lambda}^c(t)$ the corresponding characteristic function is obtained. The choice of $\mathbf{\Lambda}^c(t)=0$ in Eq. (17) gives the characteristic function of the absorbed charge under the condition that the conserved charge is not being monitored, i.e., the final charge state is integrated over. Therefore, $\ln Z$ becomes the generator of the FCS, defining the charge cumulants at the absorbing node,

$$\langle\langle[Q_\alpha^a(t)-Q_\alpha^a(0)]^n\rangle\rangle=\left.\frac{\partial^n \ln Z}{(\partial i\lambda_\alpha^a)^n}\right|_{\mathbf{\Lambda}^a=0}. \tag{18}$$

In the long time limit, this quantity is proportional to time, independent of the details of the boundary conditions.

Alternatively, in the short time limit one may calculate irreducible correlation functions of absorbed and conserved current fluctuations, $\mathbf{I}=\dot{\mathbf{Q}}$. These correlation functions can be obtained by extending the time integral in (3b) to infinity, introducing sources[32] in the action, $S\to S+i\int dt\ \chi(t)\cdot\mathbf{I}(t)$, and applying functional derivatives with respect to χ. Repeating the steps leading to Eqs. (17), we find that variables λ_α in the Hamiltonian in Eq. (17b) have to be shifted $\lambda_\alpha\to\lambda_\alpha+\chi_\alpha$. Then, the irreducible current correlation function is given by

$$\langle\langle I_{\alpha_1}(t_1)\cdots I_{\alpha_n}(t_n)\rangle\rangle=\left.\frac{\delta^n \ln Z[\chi]}{\delta i\chi_{\alpha_1}(t_1)\cdots\delta i\chi_{\alpha_n}(t_n)}\right|_{\chi=0}. \tag{19}$$

With these correlation functions, one may calculate, for example, the frequency dependence of current cumulants.[33]

C. The saddle point approximation

If the Hamiltonian has some dimensionless large prefactor, then the path integral (3) may be evaluated using the saddle point approximation, which is justified below. At the saddle point, (where the first variation of the action vanishes), we can write equations of motion analogous to the Hamiltonian equations of classical mechanics:

$$i\dot{\mathbf{Q}}^c=\frac{\partial}{\partial\mathbf{\Lambda}^c}H(\mathbf{Q}^c,\mathbf{\Lambda}),\quad i\dot{\mathbf{\Lambda}}^c=-\frac{\partial}{\partial\mathbf{Q}^c}H(\mathbf{Q}^c,\mathbf{\Lambda}), \tag{20}$$

where $H(\mathbf{Q}^c,\mathbf{\Lambda})=(1/2)\Sigma_{\alpha\beta}H_{\alpha\beta}(\mathbf{Q}^c;\lambda_\alpha-\lambda_\beta)$. There may be many saddle point solutions in general, and one has to sum over all of them. Equations (20) are solved subject to the temporal boundary conditions and generally describe the relaxation of the conserved charges from the initial state to a stationary state $\{\overline{\mathbf{Q}^c},\overline{\mathbf{\Lambda}^c}\}$ on a time scale given by τ_C, the dynamical time scale of the nodes. These stationary coordinates are functions of any external parameters as well as the (constant) absorbed counting variables $\mathbf{\Lambda}^a$. In the saddle point approximation, the action takes the form

$S=S_{sp}+S_{\mathrm{fluc}}$.[7] The term S_{sp} is the contribution to the action from the solution of the Eqs. (20), which describes the evolution of the system from the initial to the final state. The term S_{fluc} describes fluctuations around the saddle point and is suppressed compared to the saddle-point contribution, if the Hamiltonian has a large prefactor (in analogy to the $\hbar$-expansion of quantum mechanics). Physically, the validity condition for the saddle point approximation is that there should be many (transporting) charge carriers in the nodes. For times longer than the charge relaxation time of the node, the dominant contribution is from the stationary state only, where the saddle-point part of the action is simply linear in time:

$$S_{sp}(\overline{\mathbf{Q}},\overline{\mathbf{\Lambda}}) = tH(\overline{\mathbf{Q}},\overline{\mathbf{\Lambda}}), \quad t \gg \tau_C. \tag{21}$$

The linear time dependence of Eq. (21) indicates that the dynamics are Markovian on a long time scale. It is the fact that the contribution S_{sp} emerges in a dominant way which makes the approach given here a powerful tool to analyze the counting statistics of transmitted charge.

We now discuss the large parameter that justifies the saddle point approximation. The boundary conditions on the charge in the absorbing nodes fix a (dimensionless) charge scale of the system, γ. All charges in the network are scaled accordingly, $\mathbf{Q}\to\gamma\mathbf{Q}$. We make the assumption that there is a one parameter scaling of the Hamiltonian, $H\to\gamma H$. The time is also scaled by τ_C, the time scale of charge relaxation in the nodes. The dimensionless action is now $S=\gamma\int_0^{t/\tau_C}dt'$ $\times(-i\dot{Q}\lambda+\tau_C H)$. The saddle point action is proportional to $\gamma t/\tau_C$, while the fluctuation contribution will be of order t/τ_C. We note that the parameter γ is related to (though not necessarily the same as) the separation of time scales, τ_C/τ_0, needed to derive the path integral. For the mesoscopic conductors considered in the example section V B of this paper, the charge scale is set by the maximum number of semiclassical states on the cavity involved in transport, $\gamma=\Delta\mu N_F\gg 1$, the bias times the density of states at the Fermi level. On the other hand, for the chaotic cavity, $\tau_C/\tau_0=\gamma/(G_L+G_R)$, where $G_{L,R}\gg 1$ are the dimensionless conductances of the left and right point contact.

D. Relation to the master equation and Doi–Peliti technique

The evolution operator $U(\mathbf{Q},\mathbf{Q}',t)$ may be interpreted as a Green function of a differential equation which determines the propagation in time of an initial probability distribution $\Gamma(\mathbf{Q})$. In the theory of stochastic processes, such a differential equation is called a master equation. A natural question that arises is the relationship of the formalism presented here to other approaches to stochastic problems.

The most general type of Markovian master equation for discrete states and discrete time is of the form

$$\Gamma_n(t_{k+1}) = \sum_m P_{nm}(t_{k+1},t_k)\Gamma_m(t_k), \tag{22}$$

where $\Gamma_m(t_k)$ is the probability to be in state m at time t_k and P_{nm} is the transition probability from state m to state n. The state is described by a vector $n=(n_1,\ldots,n_N)$ whose components are the charges n_α of each node α. The Markovian assumption implies that $t_{k+1}-t_k=\Delta t$ is greater than the correlation time, τ_0. If we further assume that the probability to make a transition to another state is small, $P_{nm}\ll 1$ for $n\neq m$, so that the transition probability is only linear in Δt, a transition rate $W_{nm}=P_{nm}/\Delta t$ may be defined. It then follows that we may write a differential master equation,

$$\dot{\Gamma}_n(t) = \sum_m [W_{nm}\Gamma_m(t) - W_{mn}\Gamma_n(t)]. \tag{23}$$

Equation (23) is the starting point for the Doi–Peliti technique,[24] where one formally maps the space of physical states to the Fock space of states $|n\rangle=(a_1^\dagger)^{n_1}\cdots(a_N^\dagger)^{n_N}|0\rangle$, where n is the number of charges. The entire state of the system is expressed by a vector $|\Psi\rangle=\Sigma_n\Gamma_n|n\rangle$ which weights the states $|n\rangle$ with their probabilities Γ_n. Thus, the master equation (23) may be interpreted as a

many-body Schrödinger equation where the rates W_{mn} are incorporated into a Hamiltonian in a second-quantized form. One may then write a coherent-state path integral over the variables a, and $a^{\dagger}$ for this many-body quantum system and perform perturbation expansions along with the renormalization group.[25] This procedure eventually involves taking the continuum limit so the discrete charge states become continuous.

Let us now consider how our formalism is related to the master equation or the Doi–Peliti technique. According to the results of Sec. II, our stochastic path integral, Eq. (3) solves the continuum variable version of Eq. (22) with the transition probabilities given by the one step propagator $U(\mathbf{Q},\mathbf{Q}',\Delta t)$. *In general, the transition probabilities are neither small nor linear in time* for $\Delta t > \tau_0$. It is instructive nevertheless to consider the special case of processes where $H\tau_0 \ll 1$, when we can expand the one-step propagator (13) to first order in Δt,

$$U(\mathbf{Q},\mathbf{Q}',\Delta t) \approx \delta(\mathbf{Q}-\mathbf{Q}') + \Delta t \int d\mathbf{\Lambda} e^{-i\mathbf{\Lambda}\cdot(\mathbf{Q}-\mathbf{Q}')} H(\mathbf{Q}',\mathbf{\Lambda}). \tag{24}$$

Defining the Fourier transform of the generating function as $\tilde{H}(\mathbf{Q},\mathbf{Q}')$, the differential equation governing the evolution of a probability distribution of charges $\Gamma(\mathbf{Q})$ is then

$$\dot{\Gamma}(\mathbf{Q},t) = \int d\mathbf{Q}' \tilde{H}(\mathbf{Q},\mathbf{Q}')\Gamma(\mathbf{Q}',t). \tag{25}$$

Comparison with the continuous version of the master equation (23),

$$\dot{\Gamma}(\mathbf{Q},t) = \int d\mathbf{Q}' [W(\mathbf{Q},\mathbf{Q}')\Gamma(\mathbf{Q}',t) - W(\mathbf{Q}',\mathbf{Q})\Gamma(\mathbf{Q},t)], \tag{26}$$

indicates that $\tilde{H}$ is related to W. The Hamiltonian may be expressed in terms of the transition kernel[34] as,

$$H(\mathbf{Q}',\mathbf{\Lambda}) = \int d\mathbf{Q} [e^{i(\mathbf{Q}-\mathbf{Q}')\cdot\mathbf{\Lambda}} - 1] W(\mathbf{Q},\mathbf{Q}'), \tag{27}$$

where the normalization of probability is expressed by $H(\mathbf{Q}',0)=0$. Equation (27) is an important result, because it allows the conversion of the master equation (26) into the stochastic path integral (3).

We would like to stress that our formalism is not simply equivalent to the differential master equation (26) (and, therefore, the Doi–Peliti technique), but that it allows the treatment of a complementary class of problems. Our formalism assumes effectively continuous charge, and thus cannot resolve effects due to the discreteness of charge on the nodes. Such effects are present in the master equation (23). In contrast, the differential master equation assumption, $H\tau_0 \ll 1$ (which simply states that transition probabilities are small in the time interval τ_0) is not required. Our formalism is especially important when this is not the case, i.e., $H\tau_0 \sim 1$.

This is illustrated by the simple example from mesoscopics of two metallic reservoirs connected by a single electron barrier with hopping probability p and bias $\Delta\mu$ at zero temperature. For a time interval Δt larger than the correlation time $\tau_0 = \hbar/\Delta\mu$ (the time scale for an electron wavepacket to transverse the barrier), $\Delta t/\tau_0$ electrons approach the barrier and either are transmitted or reflected. Mathematically, this is a classical binomial process with the generator

$$S = (\Delta t/\tau_0)\ln[1 + p(e^{ie\lambda} - 1)]. \tag{28}$$

As this action is the starting point of many mesoscopic implementations of the formalism, it is an important example. Since the action is proportional to the large parameter $\Delta t/\tau_0 > 1$, for $p \sim 1$ the expansion of $\exp(S)$ to first order in Δt is strictly forbidden, effectively not allowing a first order differential master equation. Only in the limit $p \ll 1$, (i.e., when Eq. (28) describes a Poissonian process) may the logarithm be expanded to first order. This suggests that Eq. (26) describes the

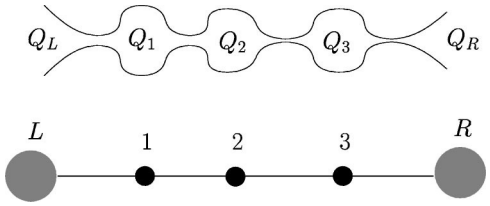

FIG. 2. A one-dimensional lattice of nodes connected on both ends to absorbing reservoirs. This situation could represent a series of mesoscopic chaotic cavities connected by quantum point contacts.

slow dynamics of systems whose fast transitions are Poissonian in nature. A more general type of dynamics such as the binomial distribution may only be found using the continuous charge state master equation in discrete time (22).

III. THE FIELD THEORY

From the stochastic network, Fig. 1, it is straightforward to go to spatially continuous systems as the spacing between the nodes is taken to zero. The goal is to introduce a Hamiltonian functional $h(\rho,\lambda)$ whose arguments are the charge density ρ and the counting field functions λ, that are themselves functions of space and time. We may then replace $(1/2)\Sigma_{\alpha,\beta}H_{\alpha,\beta}\rightarrow\int dz h(\rho,\lambda)$. Our description is local, so in the model each node is only connected to its nearest neighbors. We first derive the one-dimensional field theory with one charge species in detail, and then generalize to multiple dimensions and charge species.

Consider a series of identical, equidistant nodes separated by a distance Δz. This nodal chain could represent a chain of chaotic cavities, Fig. 2, in a mesoscopic context.[35,36] The sum over α and β becomes a sum over each node in space connected to its neighbors. The action for this arrangement is

$$S=\int_0^t dt'\sum_\alpha\{-\lambda_\alpha\dot{Q}_\alpha+H(Q_\alpha,Q_{\alpha-1};\lambda_\alpha-\lambda_{\alpha-1})\},\tag{29}$$

where for simplicity we have chosen real counting variables, $i\lambda_\alpha\rightarrow\lambda_\alpha$. The imaginary counting variables will be restored at the end of the section. The only constraint made on H is that probability is conserved, $H(\lambda_\alpha-\lambda_{\alpha-1})=0$ for $\lambda_\alpha=\lambda_{\alpha-1}$. We now derive a lattice field theory by formally expanding H in $\lambda_\alpha-\lambda_{\alpha-1}$ and $Q_\alpha-Q_{\alpha-1}$. Only differences of the counting variables will appear in the series expansion, while we must keep the full Q dependence of the Hamiltonian. If there are $N\gg1$ nodes in the lattice, for fixed boundary conditions the difference between adjacent variables, $\lambda_\alpha-\lambda_{\alpha-1}$ and $Q_\alpha-Q_{\alpha-1}$ will be of order $1/N$, and therefore, provides a good expansion parameter. The expansion of the Hamiltonian (29) to second order in the difference variables gives

$$H=\frac{\partial H}{\partial\lambda_\alpha}(\lambda_\alpha-\lambda_{\alpha-1})+\frac{1}{2}\frac{\partial^2H}{\partial\lambda_\alpha^2}(\lambda_\alpha-\lambda_{\alpha-1})^2+\frac{\partial^2H}{\partial Q_\alpha\partial\lambda_\alpha}(Q_\alpha-Q_{\alpha-1})(\lambda_\alpha-\lambda_{\alpha-1}),\tag{30}$$

where the expansion coefficients are evaluated at $\lambda_\alpha=\lambda_{\alpha-1}$ and $Q_\alpha=Q_{\alpha-1}$ and are functions of $Q_{\alpha-1}$. Terms involving only differences of $Q_\alpha-Q_{\alpha-1}$ are zero because $H(\lambda_\alpha-\lambda_{\alpha-1})=0$ for $\lambda_\alpha=\lambda_{\alpha-1}$. All terms in Eq. (30) need explanation. First, the expression $\partial H/\partial\lambda_\alpha$ is the local current at zero bias (because the charges in adjacent nodes are equal) which will usually be zero. There may be circumstances where this term should be kept,[37] but we do not consider them here. The term $\partial^2H/\partial Q_\alpha\partial\lambda_\alpha=-G(Q_{\alpha-1})$ is the linear response of the current to a charge difference. Hence, G is the generalized conductance[38] of the connector between nodes α and $\alpha-1$. $\partial^2H/\partial\lambda_\alpha^2=C(Q_{\alpha-1})$ is the current noise through the same connector because H is the generator of current cumulants.

We are now in a position to take the continuum limit by replacing the node index α with a coordinate z, introducing the fields $Q(z),\lambda(z)$, and making the expansions

$$\lambda_\alpha - \lambda_{\alpha-1} \to \lambda' \Delta z + (1/2)\lambda''(\Delta z)^2 + \mathcal{O}(\Delta z)^3, \tag{31a}$$

$$Q_\alpha - Q_{\alpha-1} \to Q' \Delta z + (1/2)Q''(\Delta z)^2 + \mathcal{O}(\Delta z)^3. \tag{31b}$$

The action may now be written in terms of intensive fields by scaling away Δz,

$$H \to h(\rho,\lambda)\Delta z, \quad Q_\alpha \to \rho(z)\Delta z, \quad G_\alpha(\Delta z)^2 \to D(\rho), \quad C_\alpha \Delta z \to F(\rho), \tag{32}$$

and taking the limit $\Sigma_\alpha H \to \int dz h(\rho,\lambda)$. One may check that expanding the Hamiltonian to higher than second order in Δz will result in terms suppressed by powers of $\Delta z/L$ and consequently vanish as $\Delta z \to 0$. This scaling argument for the field theory is analogous to Van Kampen's size expansion.[39] Though the lattice spacing Δz does not appear in the continuum limit, it provides a physical cutoff for any ultra-violet divergences that might appear in a loop expansion.

These considerations leave the one-dimensional action as

$$S = -\int_0^t dt' \int_0^L dz[\lambda\dot{\rho} + D\rho'\lambda' - \tfrac{1}{2}F(\lambda')^2]. \tag{33}$$

Here D is the local diffusion constant and F is the local noise density which are discussed in detail below. It is very important that these two functionals D, F are all that is needed to calculate current statistics. Classical field equations may be obtained by taking functional derivatives of the action with respect to the charge and counting fields: $\delta S/\delta\rho(z) = \delta S/\delta\lambda(z) = 0$ to obtain the equations of motion,

$$\dot{\lambda} = -\frac{1}{2}\frac{\delta F}{\delta\rho}(\lambda')^2 - D\lambda'', \quad \dot{\rho} = [-F\lambda' + D\rho']'. \tag{34}$$

From the charge equation, one can see immediately that the term inside the derivative may be interpreted as a current density so that local charge conservation is guaranteed. We have to solve these coupled differential equations subject to the boundary conditions

$$\rho(t,0) = \rho_L(t), \quad \rho(t,L) = \rho_R(t), \quad \lambda(t,0) = \lambda_L(t), \quad \lambda(t,L) = \lambda_R(t), \tag{35}$$

where $\rho_L(t)$, $\rho_R(t)$, $\lambda_L(t)$, and $\lambda_R(t)$ are arbitrary time dependent functions. Functions $\rho_L(t)$ and $\rho_R(t)$ are the charge densities at the far left and right end of the system which may be externally controlled. Functions $\lambda_L(t)$ and $\lambda_R(t)$ are the counting variables of the absorbed charges at the far left and right end which count the current that passes them.

Once Eqs. (34) are solved subject to the boundary conditions (35), the solutions $\rho(z,t)$ and $\lambda(z,t)$ should be substituted back into the action (33) and integrated over time and space. The resulting function, $S_{sp}[\rho_L(t),\rho_R(t),\lambda_L(t),\lambda_R(t),t,L]$ is the generating function for time-dependent cumulants of the current distribution. Often, the relevant experimental quantities are the stationary cumulants. These are given by neglecting the time dependence, finding static solutions, $\dot{\rho} = \dot{\lambda} = 0$, and imposing static boundary conditions. Similarly to Sec. II D, we can also introduce sources $\int dtdz\chi(z,t)\rho(z,t)$ and calculate density correlation functions.

To estimate the contribution of the fluctuations to the action, it is useful to define dimensionless variables. The boundary conditions ρ_L, and ρ_R provide the charge density scale ρ_0 in the problem, so we define $\rho(z) = \rho_0 f(z)$, where $f \sim 1$ is an occupation. We furthermore rescale $z \to Lz$, and $t \to \tau_D t$, where $\tau_D = L^2/D$ is the diffusion time, thus obtaining

$$S = -L\rho_0 \int_0^t dt' \int_0^1 dz' \left[\lambda\dot{f} + f'\lambda' - \frac{F}{2D\rho_0}(\lambda')^2\right]. \tag{36}$$

We assume that the combination $F/D\rho_0$ is of order 1. From Eq. (36), the dimensionless large parameter is $\gamma = \rho_0 L \gg 1$, i.e., the number of transporting charge carriers. As in Sec. II C, the saddle point contribution is of order $\gamma t/\tau_D$, while the fluctuation contribution is of order t/τ_D.

Repeating this derivation in multiple dimensions with N charge species $\rho=\{\rho_i(\mathbf{r})\}$ and counting fields $\mathbf{\Lambda}=\{\lambda_i(\mathbf{r})\}$, $i=1,\ldots,N$ yields the action

$$S=-\int_0^t dt'\int_\Omega d\mathbf{r}[\mathbf{\Lambda}\dot{\rho}+\nabla\mathbf{\Lambda}\hat{D}\nabla\rho-(1/2)\nabla\mathbf{\Lambda}\hat{F}\nabla\mathbf{\Lambda}], \tag{37}$$

where tensor notation is used and we have introduced $\hat{F}_{ij}=\partial_{\lambda_i}\partial_{\lambda_j}h$ and $\hat{D}_{ij}=-\partial_{\rho_i}\partial_{\lambda_j}h$ as general matrix functionals of the field vector ρ and coordinate $\mathbf{r}$ which should be interpreted as noise and diffusion matrices. If the medium is isotropic, then the vector gradients simply form a dot product. It should be emphasized that the vectors appearing are vectors of different species of charge fields, as all node delimitation has been accounted for in the spatial integration. The functional integral now runs over all field configurations that obey the imposed boundary conditions at the surface $\partial\Omega$. Classical field equations may be formally obtained by taking functional derivatives of the action with respect to the charge and counting fields as in the one-dimensional (1D) case.

As in any field theory, symmetries of the action play an important role because they lead to conserved quantities. We first note that the Hamiltonian $h(\rho,\nabla\rho,\nabla\mathbf{\Lambda})$ is a functional of $\nabla\mathbf{\Lambda}$ alone with no $\mathbf{\Lambda}$ dependence. This symmetry is analogous to gauge invariance, and leads to the equation of motion

$$\dot{\rho}+\nabla\cdot\mathbf{j}=0,\quad \mathbf{j}=-\hat{D}\nabla\rho+\hat{F}\nabla\mathbf{\Lambda}, \tag{38}$$

which can be interpreted as conservation of the conditional current $\mathbf{j}$. The next symmetry is related to the invariance under a shift in the space and time coordinates $\{\delta\mathbf{r},\delta t\}$. This symmetry leads to equations analogous to the conservation of the local energy/momentum tensor.[40] We do not explicitly give this quantity because it is rather cumbersome in the general case. However, for the stationary limit (where $\dot{\rho}$ and $\dot{\lambda}$ vanish) and for symmetric diffusion and noise tensors, the one charge species conservation law is relatively simple and is given by

$$\sum_m \nabla_m T_{mn}=0,\quad T_{mn}=j_m(\nabla_n\lambda)-(\nabla_n\rho)(\hat{D}\nabla\lambda)_m-h\delta_{mn}. \tag{39}$$

For the special case of a one-dimensional geometry, the Hamiltonian itself is the conserved quantity (see Sec. V A).

In the continuum limit, all terms of higher order in Λ are suppressed so that the action is quadratic in the Λ variables. This fact may be viewed as a consequence of the central limit theorem and confirms the observation made by Nagaev that local noise in the mesoscopic diffusive wire (see Sec. V A) is Gaussian.[19] To further clarify the physical meaning of D and F, and also to make connection with previous work,[32] we restore the complex variables, $\Lambda\to i\Lambda$, and make a Hubbard–Stratonovich transformation by introducing an auxiliary vector field ν,

$$\exp\{-(1/2)\nabla\mathbf{\Lambda}\hat{F}\nabla\mathbf{\Lambda}\}=(\det\hat{F})^{-1/2}\int\mathcal{D}\nu\exp\{-(1/2)\nu\hat{F}^{-1}\nu+i\nu\nabla\mathbf{\Lambda}\}. \tag{40}$$

We may then integrate out the Λ variables, taking account of the boundary terms to obtain,

$$U=\exp\left\{\int_0^t dt'\int_{\partial\Omega}d\mathbf{s}\cdot(i\Lambda^a\mathbf{J})\right\}\int\mathcal{D}\rho\mathcal{D}\nu\delta(\dot{\rho}+\nabla\cdot\mathbf{J})(\det\hat{F})^{-1/2}\exp\left\{-\frac{1}{2}\int_0^t dt'\int_\Omega d\mathbf{r}'\,\nu\hat{F}^{-1}\nu\right\}, \tag{41}$$

where the δ above is a functional delta function, imposing the Langevin equation

$$\dot{\rho}+\nabla\cdot\mathbf{J}=0, \tag{42a}$$

$$\mathbf{J} = -\hat{D}\nabla\rho + \nu, \tag{42b}$$

with a current noise source ν, whose correlator[41] is given by

$$\langle \nu(\mathbf{r},t)\nu(\mathbf{r}',t')\rangle = \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\hat{F}(\rho). \tag{42c}$$

J may be interpreted as the physical current density [not to be confused with the conditional current density (38)] so that local current conservation is guaranteed, and the $(\det \hat{F})^{-1/2}$ serves to normalize the ν probability distribution. The role of the boundary term is to count the current **J** flowing out of the boundary with the counting variable Λ^a, which serves as a Lagrange multiplier. This formula gives an immediate translation between the Langevin approach and full counting statistics, a connection not previously known. The algorithm is as follows:

(1) Given a Langevin equation of the form (42), write the average of the boundary term with source Λ^a as a path integral (41) over noise and density fields;[42]
(2) introduce an auxiliary field Λ that takes on the value Λ^a at the boundaries and represents the delta function in Eq. (41) imposing current conservation (42a) in Fourier form;
(3) integrate out the Gaussian noise to obtain an action of the form of Eq. (37);
(4) find where the first variation of the action is zero and solve the equations of motion subject to the boundary conditions;
(5) insert the solutions back into the action, and do the space and time integrals. The answer is the current cumulant generating function.

IV. PERTURBATION THEORY

We have shown in Sec. II C that a large number of participating elementary charges justifies the saddle point approximation for the generator of counting statistics. While the generator may sometimes be found in closed form,[7] in general, it has no compact expression and the cumulants should be found separately at every order. This may be done by expanding $S_{sp}(Q,\lambda,\chi)$ as a series in χ and solving the saddle point equations to a given order in χ directly. However, there is another approach for evaluating the higher cumulants, the cascade diagrammatics representing higher-order cumulants in terms of the lower ones. It has been introduced by Nagaev in the context of mesoscopic charge statistics in the diffusive wire[19] and later extended to the chaotic cavity,[20] but without proof. The basic idea is that lower order cumulants mix in to yield corrections to the bare fluctuations of higher order cumulants. This method was used successfully in Ref. 43 to explain the recent experiment of Ref. 44. In this section, we demonstrate that these rules follow naturally from the stochastic path integral in the same way as Feynman diagrams follow from the quantum mechanical functional integral. In Sec. IV C we present another (simpler) method for computing cumulants based completely on differential operators obtained from the Hamiltonian equations of motion. In Sec. IV D we generalize the cascade diagrammatics to an arbitrary network, and to the case of time-dependent correlators.

A. The principle of minimal correlations

To motivate the cascade diagrammatics, we refer to a specific physical system (see the inset of Fig. 8), the mesoscopic chaotic cavity.[1] For the purposes of this section, the cavity is a conserving node carrying charge Q, the electronic reservoirs correspond to the left and right are absorbing nodes, and the two point contacts are the connectors described by Hamiltonians H_L, H_R (see Fig. 3). Although a detailed description of this system is given in Sec. V B, we would like to mention that the mesoscopic cavity is described by an electron distribution function f, which is fluctuating around its mean value, f_0. The actual electrical charge in the cavity Q and the occupation f are related via the large parameter γ through $Q=\gamma(f-f_0)$, where $\gamma=\Delta\mu N_F \gg 1$ (the density of states at the Fermi energy N_F times the bias $\Delta\mu$) is the maximum possible number of electrons on the cavity which contribute to the transport (see Sec. II C).

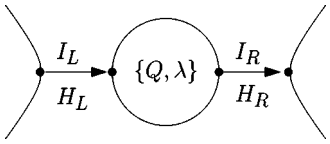

FIG. 3. Network representing a chaotic cavity. The state of the internal node is described by the variable Q, the charge on the cavity. The statistics of the connectors are characterized by the two generating functions $H_{L,R}$.

The cascade approach builds on the principle of minimal correlations developed in Ref. 18: The point contacts create bare noise $\langle\langle \tilde{I}_L^2\rangle\rangle = \partial^2 H_L/(\partial i\lambda_L)^2$, and $\langle\langle \tilde{I}_R^2\rangle\rangle = \partial^2 H_R/(\partial i\lambda_R)^2$ with no correlation, $\langle\langle \tilde{I}_L \tilde{I}_R\rangle\rangle = 0$ [see Eq. (5)]. However, for times longer than the average dwell time of electrons in the cavity, the current conservation requirement imposes "minimal correlations" on the fluctuations of the physical currents I_L and I_R, which can be expressed in the form of the Langevin equations,

$$I_L = \tilde{I}_L - G_L Q, \quad I_R = \tilde{I}_R + G_R Q, \tag{43}$$

where $\tilde{I}_{L,R}$ are now the sources of bare noise, $G_{L,R}$ are the generalized conductances of the left and right point contact, and Q is the fluctuating charge in the cavity. Current conservation of the physical currents, $I_L = I_R = I$, can now be used to obtain

$$I = \frac{G_R \tilde{I}_L + G_L \tilde{I}_R}{G_L + G_R}, \quad Q = \frac{\tilde{I}_L - \tilde{I}_R}{G_L + G_R}. \tag{44}$$

Combining powers of I and Q and averaging over the bare noise, we obtain the minimal correlation result for arbitrary cumulants $\langle\langle Q^k I^l\rangle\rangle_m$. In particular, using $\langle\langle \tilde{I}_L \tilde{I}_R\rangle\rangle = 0$, we find the second cumulant of current is[17,18]

$$\langle\langle I^2\rangle\rangle = \langle\langle I^2\rangle\rangle_m = \frac{G_R^2 \langle\langle \tilde{I}_L^2\rangle\rangle + G_L^2 \langle\langle \tilde{I}_R^2\rangle\rangle}{(G_L + G_R)^2}, \tag{45}$$

where the subscript m denotes the minimal correlation result. We stress that the bare correlators $\langle\langle \tilde{I}_{L,R}^2\rangle\rangle$ are fully determined by the average occupation function f_0 of the cavity.

This example demonstrates that a simple redefinition of the current fluctuations makes it straightforward to find the noise. Therefore, it came as a surprise[45] that the minimal correlation approach is not sufficient to correctly obtain higher-order cumulants of current. The reason for the failure of the minimal correlation approach has been found recently by Nagaev,[19] who showed that from the third order cumulant on, there are "cascade corrections" to the minimal correlation result, which may be interpreted as "noise of noise." For example, the third cumulant of current through the mesoscopic cavity,[20]

$$\langle\langle I^3\rangle\rangle = \langle\langle I^3\rangle\rangle_m + 3\langle\langle IQ\rangle\rangle_m \frac{\partial}{\partial Q} \langle\langle I^2\rangle\rangle_m, \tag{46}$$

contains a contribution from fluctuations of the charge in the cavity that couples back into the current fluctuations. The factor of 3 comes from the fact that there are 3 independent currents that the charge fluctuation may be correlated with. For higher cumulants, there will be more cascade corrections that may be represented in a diagrammatic form.[19,20]

B. Derivation of diagrammatic rules

We now present a derivation of these diagrammatic rules for a single node attached between two absorbing nodes. Generalizations to an arbitrary network will subsequently be given in Sec.

IV D. As we have shown in Sec. II C, the charge scale imposed by the boundary conditions, γ, gives a dimensionless large parameter which justifies the saddle point approximation of the path integral, so that fluctuations around the saddle point are suppressed by $1/\gamma$. In the diagrammatic language, we will show that loop diagrams are suppressed by the same factor $1/\gamma$. The diagrammatic approach given here is based on perturbation theory originally developed in quantum mechanics.[29]

Consider the path integral expression of the generating function for the charge absorbed in the left (L) and right (R) node:

$$Z(\chi_L,\chi_R)=\int \mathcal{D}Q\mathcal{D}\lambda\ \exp\left\{\int_0^t dt'[-i\dot{Q}\lambda+H(Q,\lambda,\chi_L,\chi_R)]\right\}, \tag{47}$$

where $H=H_L(Q,\lambda-\chi_L)+H_R(Q,\chi_R-\lambda)$. The perturbation theory is formulated as follows. First, the external counting variables are set to zero, $\chi_L=\chi_R=0$. The Hamiltonian $H\to H_L(Q,\lambda)+H_R(Q,-\lambda)$ has a stationary saddle point located at $\{Q_0,\lambda_0\}$ that we wish to define as the origin of coordinates. The probability distributions of transferred charge are normalized, so

$$\partial_Q^n H_{L,R}(Q,\lambda)|_{\lambda=0}=0, \quad \forall\, n. \tag{48}$$

In particular, $\partial_Q H_L(\lambda)|_{\lambda=0}=\partial_Q H_R(\lambda)|_{\lambda=0}=0$, and therefore $\lambda_0=0$. Next, $\partial_{i\lambda}H(\lambda)|_{\lambda=0}=\langle I_L(Q)\rangle-\langle I_R(Q)\rangle=0$, since H_L and H_R are the generators of the left and right current respectively. Therefore, Q_0 is fixed as the charge in the node such that left and right connector currents are equal on average. The stability of the saddle point is guaranteed by the fact that the bare noise correlators, $\langle\langle\tilde{I}^2_{L,R}\rangle\rangle$, are positive. The derivatives $\partial_{i\lambda}\partial_Q H_L=-G_L$, $\partial_{i\lambda}\partial_Q H_R=-G_R$ define the generalized conductance of each connector, where the current flows from left to right in both connectors.

The principle of minimal correlation plays an important role in the cascade diagrammatics. We will show that this principle is equivalent to exploiting certain freedoms in the path integral in order to postpone the cascade corrections to third and higher order cumulants. In the long-time limit, $t\gg\tau_C$ (where $1/\tau_C=G_L+G_R$ is the relaxation rate of the charge in the node), the absorbed current is conserved, $I_R=I_L$. Therefore, the current through the node can be defined as weighted average of the left and right connector currents $I=(1-v)I_L+vI_R$, where v is an arbitrary constant. The corresponding counting variable χ is introduced by substituting $\chi_R=v\chi$ and $\chi_L=(v-1)\chi$. Consider now the second derivative

$$\left.\frac{\partial^2 H}{\partial\, i\chi\,\partial Q}\right|_{\chi=0}=(v-1)G_L+vG_R. \tag{49}$$

We may set it to zero by fixing $v=G_L/(G_L+G_R)$. This is equivalent to imposing conservation of current fluctuations as in Eq. (44). If we consider further the derivative

$$\left.\frac{\partial^2 H}{\partial\, i\lambda\,\partial Q}\right|_{\chi=0}=-(G_L+G_R), \tag{50}$$

we have the freedom to scale λ to make the right hand side of Eq. (50) equal to -1 [this scaling only alters the χ independent prefactor of Eq. (47)]. The Hamiltonian takes the new form

$$H=H_L\left(Q,\frac{G_R\chi+\lambda}{G_L+G_R}\right)+H_R\left(Q,\frac{G_L\chi-\lambda}{G_L+G_R}\right). \tag{51}$$

We refer to these new variables as minimal correlation coordinates and will see that they simplify the diagrammatic expansion.

Define $\delta Q(t)=Q(t)-Q_0$ and $\delta\lambda(t)=\lambda(t)-\lambda_0$. If we expand the Hamiltonian in a power series in χ, δQ, and $\delta\lambda$, the terms linear in δQ and $\delta\lambda$ vanish at the saddle point, as well as the $(\delta Q)^2$ coefficient by Eq. (48) with $n=2$. As argued above, in the minimal correlation coordinates, $\partial_{i\lambda}\partial_Q H(Q_0,\lambda_0)=-1$. With these transformations, we may split the action S as

$$S = S_0 + \int_0^t dt' V(t'), \quad S_0 = -i \int_0^t dt' \delta\lambda(\tau_C \delta\dot{Q} + \delta Q), \tag{52}$$

where V represents the rest of the H power series and will be treated perturbatively. It should be emphasized that V is a general nonlinear function of $\delta\lambda$, so unlike most quantum examples, the full momentum dependence must be kept.

In order to formulate the perturbation theory, we add two sources, J and K to the action, $S \to S + \int dt'[J\delta Q + iK\delta\lambda]$, so that any average of a function of the variables $\delta Q, \delta\lambda$ may be evaluated by taking functional derivatives with respect to the sources J, and K, and then setting the sources to zero. In particular, for the generating function we can write

$$\begin{aligned} Z(\chi) &= \int \mathcal{D}Q\mathcal{D}\lambda \, \exp\left\{ \int_0^t dt' V(\delta Q, \delta\lambda, \chi) \right\} \exp\left\{ S_0 + \int_0^t dt'[J\delta Q + iK\delta\lambda] \right\} \Bigg|_{J,K=0} \\ &= \exp\left\{ \int_0^t dt' V\left(\frac{\delta}{\delta J}, \frac{\delta}{\delta iK}, \chi \right) \right\} \int \mathcal{D}Q\mathcal{D}\lambda \, \exp\left\{ S_0 + \int_0^t dt'[J\delta Q + iK\delta\lambda] \right\} \Bigg|_{J,K=0}. \end{aligned} \tag{53}$$

Using S_0. from Eq. (52) we evaluate the integral over Q and λ and obtain

$$Z(\chi) = \exp\left\{ \int_0^t dt' V\left(\frac{\delta}{\delta J}, \frac{\delta}{\delta iK}, \chi \right) \right\} W(J,K) \Bigg|_{J,K=0}, \tag{54}$$

where the functional $W(J,K)$ is

$$W(J,K) = \exp\left\{ \int \int_0^t dt' dt'' J(t') D(t',t'') K(t'') \right\}. \tag{55}$$

The operator $D = (\tau_C \partial_t + 1)^{-1}$ is the retarded propagator, and may be found explicitly by inverting the kernel in frequency space,

$$D(t,t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-t')}}{-i\tau_C\omega + 1} = \tau_C^{-1} \Theta(t-t') \exp[-(t-t')/\tau_C]. \tag{56}$$

It describes the relaxation of the charge $Q(t)$ to the stationary state Q_0 with the rate $1/\tau_C = G_L + G_R$.

Expanding the exponential in Eq. (54) and taking the $t \gg \tau_C$ limit, we arrive at the following expression for the nth current cumulant

$$\langle\langle I^n \rangle\rangle = t^{-1} \frac{\delta^n}{\delta(i\chi)^n} \sum_{m=1}^{\infty} \frac{1}{m!} \left[\int_0^t dt' V\left(\frac{\delta}{\delta J}, \frac{\delta}{\delta iK}, \chi \right) \right]^m W(J,K) \Bigg|_{\substack{\chi = J = K = 0 \\ \text{connected}}}. \tag{57}$$

According to the linked cluster expansion,[32] by considering $\ln Z(\chi)$ rather than $Z(\chi)$, we have eliminated all disconnected terms. In order to compare with the results of Ref. 20, we introduce a new notation by defining

$$\partial_Q^j \langle\langle Q^k I^l \rangle\rangle_m \equiv \partial_Q^j \partial_{i\lambda}^k \partial_{i\chi}^l V(Q_0, \lambda_0, \chi = 0). \tag{58}$$

Here $\langle\langle Q^k I^l \rangle\rangle_m$ is the irreducible correlator expressed in terms of the noise sources, i.e., the minimal correlation cumulant. In this notation, the expansion of V in a Taylor series of all variables takes the form:

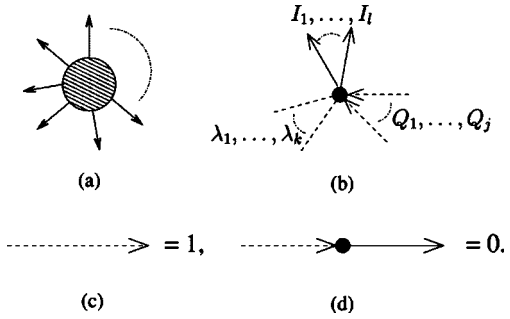

FIG. 4. (a) An n-point current cumulant. (b) The vertex connecting l external lines with j internal Q lines and k internal λ lines. (c) The propagator connecting λ to Q, equal to 1 in the stationary limit. (d) The vanishing vertex $\partial_Q\langle I\rangle$ in minimal correlation coordinates.

$$V(\delta Q, \delta\lambda, \chi) = \sum_{j,k,l} \frac{1}{j!\,k!\,l!} \partial_Q^j \langle\langle Q^k I^l\rangle\rangle_m [\delta Q(t)]^j [i\delta\lambda(t)]^k [i\chi]^l. \tag{59}$$

Inserting the expansion Eq. (59) into the formula for the current cumulants Eq. (57) gives the formal solution to the problem. From the form of $W(J,K)$ and V, we can immediately read off the diagrammatic rules with the internal lines given by the propagators (56), and the expansion coefficients $\partial_Q^j\langle\langle Q^k I^l\rangle\rangle_m$ playing the role of vertices.

The following simplifications can be done before the rules are finally formulated. First, it is straightforward to see that loop diagrams are suppressed by powers of γ^{-1}. Indeed, according to our single-parameter scaling assumption, the action (52) has a large prefactor γ, which can be explicitly displayed, $S \to \gamma S$, by rescaling the charge, $Q \to \gamma Q$. Then it becomes clear that each propagator D, represented by an internal line, comes with a factor of γ^{-1}. Each vertex comes from V and therefore has a factor of γ. If a diagram has I internal lines, E external legs, V vertices and L loops, it will come with a total γ power of $V-I$. Furthermore, Euler's formula tells us that $V+L-I=1$. Therefore, diagrams with no loops ("tree" diagrams) come with a power of γ, while loop diagrams are suppressed by the number of loops, γ^{1-L}. From now on we will concentrate on tree-level diagrams, since they represent current cumulants at the level of the saddle-point approximation.

Second, in the long time limit, $t \gg \tau_C$, each propagator (56) integrated over time gives 1. As a result, since every vertex is connected to at least one other vertex, all the time integrals together simply give a factor of t, and the time dependence cancels on the right hand side of the Eq. (57). There are no time integrals in the vertices and the propagators just give a factor of 1 as in Ref. 20. We are now able to formulate the diagrammatic rules for high-order current cumulants:

(1) The nth order cumulant $\langle\langle I^n\rangle\rangle$ is a connected n-point function of n external legs I represented by solid arrows [see Fig. 4(a)];
(2) the external legs must be connected by using vertices [see Fig. 4(b)] and linking internal dashed lines to internal dashed arrows;
(3) the vertices $\partial_Q^j\langle\langle I^l Q^k\rangle\rangle_m$ are represented by a circle with l external legs, k internal outgoing dashed lines, and j internal incoming dashed arrows [see Fig. 4(b)].
(4) Multiply each diagram by the number of inequivalent permutations (NIP).

Formally, the vertices $\partial_Q^j\langle\langle I^l Q^k\rangle\rangle_m$ are the expansion coefficients in (59). However, it is important to note that they can also be easily evaluated by solving the Langevin equations (43) and expressing the minimal correlation cumulants $\langle\langle I^l Q^k\rangle\rangle_m$ in terms of cumulants of the noise sources, $\langle\langle \tilde{I}_L^{l+k}\rangle\rangle$ and $\langle\langle \tilde{I}_R^{l+k}\rangle\rangle$. Some vertices are zero, $\partial^p H/\partial Q^p(Q_0,\lambda_0)|_{\chi=0}=0$ because of probability conservation, but other may or may not be zero depending on the physical system. Here, the advantage of the minimal correlation coordinates is made clear: the vertex $\partial_Q\langle\langle I\rangle\rangle_m=0$, and therefore any diagram that contains this vertex is zero [see Fig. 4(d)].

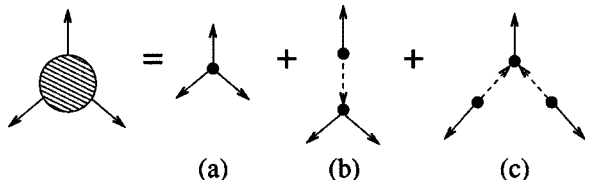

FIG. 5. Tree level contributions to the third cumulant of transmitted current.

To obtain the overall prefactor of a diagram, one can write out all the numerical constants and count the number of different ways of producing the same diagram.[32] For example, there is the $n!$ from the χ derivatives, the $1/m!$ from the Taylor series of e^V, a binomial coefficient from expanding V^m, and the $1/(j!k!l!)$ from every vertex with $j+k+l$ attachments for the different lines. To compensate these factors, we have to do the combinatorics of the number of equivalent terms: Interchange the vertices, find the number of different placements of lines on a vertex, etc. Often, the number of permutations of the n external legs will cancel the $m!$, and the $j!k!l!$ number of permutations of the internal legs attaching to the vertex will cancel that factor arising from the Taylor expansion.

Rather than making this expansion, there is a simpler method which exploits these cancellations given by counting the number of inequivalent permutations of the diagram (NIP). The NIP of the diagram is defined by how many ways the external legs of the diagram may be relabeled, such that the diagram is not topologically equivalent under deformation of the external legs. In other words, a diagram with n external legs has $n!$ ways of labeling them. If this diagram with a given labeling of the legs may be topologically deformed to give the diagram back with a different labeling, these two sets of labelings are equivalent permutations. If we write out all the different labelings the external legs can have, and cross out every labeling that is an equivalent permutation of another, then the number of labelings that remain is the NIP. This number is most easily found by dividing $n!$ by the number of equivalent permutations of the diagram. The number of equivalent permutations of the diagram is also called the symmetry factor of the diagram.

We illustrate these two approaches with the third cumulant, see Fig. 5. With the simplifications discussed above, these diagrams may be written as

$$\langle\langle I^3\rangle\rangle = \langle\langle I^3\rangle\rangle_m + 3\langle\langle IQ\rangle\rangle_m \frac{\partial}{\partial Q}\langle\langle I^2\rangle\rangle_m + 3\langle\langle IQ\rangle\rangle_m^2 \frac{\partial^2}{\partial Q^2}\langle\langle I\rangle\rangle_m. \tag{60}$$

Note that diagram (c) does not appear in Ref. 20, because it happens to vanish for the chaotic cavity [see also Eq. (46)]. Referring to the formula (57), the contributions in Eq. (60) are from $m=1,2,3$ respectively. Each diagram must have a χ^3 term in the expansion. We first show the combinatorial method to obtain the prefactor: Diagram (a) has a factor of $1/3!$ from the number of permutations of the χ variables, canceling the $3!$ from the χ derivatives. Diagram (b) has a factor of $1/2!$ from the number of permutations of the χ variables, a factor of $1/2!$ from the Taylor series of the exponential, a factor of 2 from the binomial expansion of V^2, and the $3!$ from the χ derivatives, leaving a factor of 3. Diagram (c) has a factor of $1/3!$ from the Taylor series of the exponential, a factor of 3 from the binomial expansion of V^3, a factor of $1/2!$ from the number of permutations of the δQ variables, a factor of 2 from the functional derivatives acting on W, and the $3!$ from the χ derivatives, leaving a factor of 3. The NIP is simpler to derive: We divide the number of permutations of the external legs, $m!$, by the number of equivalent permutation of the elements of the diagram that leave it unchanged. The number of equivalent permutations of diagrams (a,b,c) are $3!,2!,2!$, leaving the overall factors 1, 3, 3.

The computation of these diagrammatic contributions is best understood by a little practice on some examples. Consider three of the diagrams that contribute to the fourth cumulant drawn in Fig. 6. The diagrams symbolically represents the combinations:

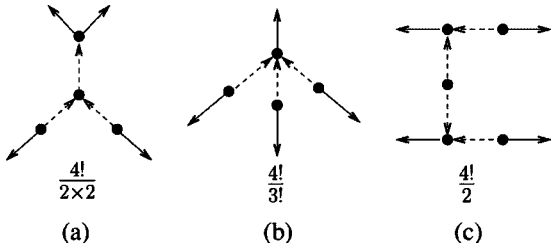

FIG. 6. Three examples of diagrams contributing to the fourth cumulant.

$$(a) = \frac{\partial}{\partial Q}\langle\langle I^2\rangle\rangle_m \frac{\partial^2}{\partial Q^2}\langle\langle Q\rangle\rangle_m \langle\langle IQ\rangle\rangle_m^2, \tag{61a}$$

$$(b) = \frac{\partial^3}{\partial Q^3}\langle\langle I\rangle\rangle_m \langle\langle IQ\rangle\rangle_m^3, \tag{61b}$$

$$(c) = \langle\langle Q^2\rangle\rangle_m \left(\frac{\partial^2}{\partial Q^2}\langle\langle I\rangle\rangle_m\right)^2 \langle\langle IQ\rangle\rangle_m^2. \tag{61c}$$

To figure out the numerical prefactors, we divide 4! (4 is the number of external legs) by the symmetry factor of the diagram. We first consider the symmetry factor of (a): The upper two legs may be flipped, and the lower two legs may be independently flipped where the dotted arrows join without altering the topology of the diagram. Therefore, the symmetry factor is $2\times 2=4$, and the NIP is $4!/4=6$. Moving on to diagram (b), the three lower legs may be permuted amongst themselves to give a symmetry factor 3!, and therefore, the NIP is $4!/3!=4$. Finally, diagram (c) may be flipped about its center for a symmetry factor of 2, giving a NIP of $4!/2=12$.

C. Operator approach

In the stationary limit, $t \gg \tau_C$, the action takes the form $S=tH(Q,\lambda,\chi)$ so that the evaluation of the cumulant generating function reduces to finding the stationary point of the Hamiltonian H as a function of the variables λ and Q. This can be done by solving the equations $\partial_Q H=0$ and $\partial_\lambda H=0$. The generating function is then obtained by substituting the solutions $\{\bar{Q},\bar{\lambda}\}$ into the Hamiltonian. In the previous section we have shown that this problem can be solved using path integral methods, and the solution can be represented diagrammatically. In the next section we will exploit the full strength of the path integral formalism in order to generalize the diagrammatics to an arbitrary network, and for the case of time-dependent charges. However, in the stationary limit, the conceptual simplicity of the problem of finding the stationary point of the function H indicates that there should exist a simple iterative procedure for evaluating the cumulants up to a given order. In this section we use classical mechanics methods to prove that this is indeed the case.

We first make the variable transformation $i\lambda\to\lambda$, and $i\chi\to\chi$, so that the Hamiltonian becomes a real function. For $\chi=0$ the saddle point is located at $\{Q_0,\lambda_0\}$. For nonzero χ the saddle point moves to a new position $\{\bar{Q},\bar{\lambda}\}$, which depends on χ, and the Hamiltonian $H(\bar{Q},\bar{\lambda},\chi)$ becomes the generator of cumulants of the current,

$$\langle\langle I^n\rangle\rangle = d^n H(\bar{Q},\bar{\lambda},\chi)/d\chi^n|_{\chi=0}\,. \tag{62}$$

By expressing the total χ derivative in terms of partial derivatives, the average current can be written as

$$\langle I\rangle = (\partial_\chi + Q'\partial_Q + \lambda'\partial_\lambda)H\,(Q,\lambda,\chi)\big|_{\{\chi=0,Q_0,\lambda_0\}}, \tag{63}$$

where $Q'=dQ/d\chi, \lambda'=d\lambda/d\chi$ are χ dependent. We wish to eliminate the functions Q' and λ' and to express the cumulant in terms of the partial derivatives of H. This is done by applying a total derivative to the equations of motion: $[\partial_Q H]'=[\partial_\lambda H]'=0$ and leads to two equations for Q' and λ' which may be solved,

$$Q' = \frac{\{\partial_\lambda H, \partial_\chi H\}}{\{\partial_Q H, \partial_\lambda H\}}, \quad \lambda' = -\frac{\{\partial_Q H, \partial_\chi H\}}{\{\partial_Q H, \partial_\lambda H\}}, \tag{64}$$

where $\{A,B\}$ is the Poisson bracket, defined as $\{A,B\}=\partial_\lambda A\,\partial_Q B-\partial_Q A\,\partial_\lambda B$. The solutions have to be inserted into the Eq. (63).

The advantage of this representation is clear: Now the right hand side of the Eq. (63) (before taking the $\chi=0$ saddle point) depends only on variables λ, Q, and χ. Therefore, we can apply the procedure again in order to express the high-order cumulant in terms of partial derivatives. This procedure solves the problem by giving a single operator,

$$\mathrm{D} = \partial_\chi + \frac{\{\partial_\lambda H, \partial_\chi H\}\partial_Q - \{\partial_Q H, \partial_\chi H\}\partial_\lambda}{\{\partial_Q H, \partial_\lambda H\}}, \tag{65}$$

which, being applied n times to a given Hamiltonian H and evaluating the resulting expression at the $\chi=0$ saddle point, gives cumulants of current:

$$\langle\langle I^n\rangle\rangle = \mathrm{D}^n H\,(Q,\lambda,\chi)\big|_{\{\chi=0,Q_0,\lambda_0\}}. \tag{66}$$

This approach is obviously more simple compared to the diagrammatic method, since in the diagrammatics, after drawing all of the diagrams, they have to be evaluated individually by taking many partial derivatives of the Hamiltonian and evaluating them at the $\chi=0$ saddle point. With this new approach, given the Hamiltonian H, the operator D may be constructed (65) and with a mathematical program, an arbitrary cumulant may be easily computed (66).

It is easy to see the importance of the minimal correlation coordinates in this solution. After applying D several times, the derivative quotient rule generates a large number of denominators, $\{\partial_Q H, \partial_\lambda H\}=(\partial_Q\partial_\lambda H)(\partial_\lambda\partial_Q H)-(\partial_Q\partial_Q H)(\partial_\lambda\partial_\lambda H)$. At $\chi=0$, as we argued previously, $\partial_Q\partial_Q H=0$, and it is possible to change coordinates so that $\partial_Q\partial_\lambda H=-1$. As a result, the denominator in (66) is equal to 1, which greatly simplifies the expansion. Finally, we would like to stress that the operator approach, introduced in this section for the one node case, can be easily generalized to a network.

D. Network cascade diagrammatics: Correlation functions

Consider now a general network. In the Sec. IV B, we saw that the dominant contribution to Eq. (47) arises from tree-level diagrams. On time scales $t \gg \tau_C$, the time dependence drops out, and the current cumulants are static. We now generalize the diagrammatic rules presented in the Sec. IV B to investigate time- and node-dependent correlation functions of conserved and absorbed charges, Eq. (19). To define the network, we must arbitrarily label the current flow, yielding a directed network. By doing so we fix the signs of the elements $H_{\alpha\beta}=-H_{\beta\alpha}$ of the Hamiltonian. In particular, the elements of the generalized conductance matrix $\hat{G}$,

$$G_{\alpha\beta} = \frac{\partial^2 H}{\partial(i\lambda_\alpha)\,\partial Q_\beta} \tag{67}$$

(evaluated at $\mathbf{Q}=\mathbf{Q}_0, \mathbf{\Lambda}=0$) are negative or positive depending on the chosen direction. If we segregate absorbing (a) and conserving (c) nodes, the conductance matrix $\hat{G}$ may be put in block form. Two of them, the blocks $\hat{G}_{cc}$ (real symmetric) and $\hat{G}_{ac}$ will be relevant. This gives us the necessary tool to define the generalized minimal correlation coordinates. We consider the frequency dependent response by letting the evolution time extent to infinity, and introduce the time

Fourier transform of the variables $\{\mathbf{Q}^c,\mathbf{\Lambda}^c,\chi^c,\chi^a\}$, where the vector $\{\chi^c,\chi^a\}$ is a time-dependent source term introduced to produce correlation functions of the conserved and absorbed currents [see Eq. (19)].

Following the steps of Sec. IV B, we again split the action into two parts, $S=S_0+\int dtV$, where

$$S_0 = i\int dt[-\mathbf{\Lambda}^c\dot{\mathbf{Q}}^c + \mathbf{\Lambda}^c\hat{G}_{cc}\mathbf{Q}^c + (\chi^c\hat{G}_{cc}+\chi^a\hat{G}_{ac})\mathbf{Q}^c]$$
$$= i\int\int \frac{d\omega d\omega'}{2\pi}[\mathbf{\Lambda}^c(i\omega'+\hat{G}_{cc})\mathbf{Q}^c + (\chi^c\hat{G}_{cc}+\chi^a\hat{G}_{ac})\mathbf{Q}^c]\delta(\omega+\omega'), \tag{68}$$

and where we have dropped the δ in front of the variables for simplicity. As in Sec. IV B, the generalized minimal correlation coordinates are defined by shifting and rescaling the $\mathbf{\Lambda}^c$ variables in order to eliminate the χ variables in Eq. (68). However, because χ is now a vector, the proportionality factor must be a frequency dependent matrix,

$$\mathbf{\Lambda}^c(\omega)\rightarrow\hat{D}^\dagger(\omega)[\mathbf{\Lambda}^c(\omega)+\hat{G}^\dagger_{cc}\chi^c(\omega)+\hat{G}^\dagger_{ca}\chi^a(\omega)]. \tag{69}$$

Here $\hat{D}(\omega)$ is the matrix network propagator,

$$\hat{D}(\omega) = -(i\omega\hat{E}+\hat{G}_{cc})^{-1}, \tag{70}$$

and $\hat{E}$ is the identity matrix. It is straightforward to verify that after the shift, the functional $\int dtV$ becomes the generator of cumulants of minimal correlation currents, i.e., of the currents which are solutions of the Langevin equations:

$$I^c_\alpha = -i\omega Q^c_\alpha = -i\omega\sum_{\beta\gamma} D_{\alpha\beta}(\omega)\tilde{I}_{\beta\gamma}, \tag{71a}$$

$$I^a_\alpha = \sum_{\beta\gamma\alpha'} G_{\alpha\alpha'}D_{\alpha'\beta}(\omega)\tilde{I}_{\beta\gamma}+\sum_\gamma \tilde{I}_{\alpha\gamma}, \tag{71b}$$

where $\tilde{I}_{\alpha\beta}$ are the bare noise sources as defined in Eq. (5). We finally rescale $\chi^c(\omega)\rightarrow\chi^c(\omega)/(i\omega)$ in order to replace conserved currents with charges, $\mathbf{I}^c\rightarrow\mathbf{Q}^c$.

The total action now acquires the following form

$$S = (2\pi i)^{-1}\int d\omega\mathbf{\Lambda}^c(-\omega)\mathbf{Q}^c(\omega)+\int dtV[\mathbf{Q}^c,\hat{D}^\dagger(\mathbf{\Lambda}^c+\chi^c)+\hat{D}^\dagger\hat{G}^\dagger_{ca}\chi^a,\chi^a], \tag{72}$$

where the simplified form of the $\mathbf{\Lambda}$ argument of V follows after composing the various transformations. Following the plan of the previous section, we replace the charge and counting variables $\{\mathbf{Q}(\omega),\mathbf{\Lambda}(\omega)\}$ by functional derivatives with respect to the charge and counting sources $\{\mathbf{J}(\omega),\mathbf{K}(\omega)\}$, and take the V term outside of the functional integral. The functional integrals may now be performed to obtain

$$W(\mathbf{J},\mathbf{K}) = \exp\left\{\int\int\frac{d\omega d\omega'}{2\pi}\mathbf{J}(\omega')\mathbf{K}(\omega)\delta(\omega+\omega')\right\}. \tag{73}$$

The perturbation V must now be expanded in a Taylor series with respect to all variables. The time dependence only appears through the variables themselves, so the expansion coefficients will be time independent, with the exception of the propagator $D_{\alpha\beta}(\omega)$ multiplying the counting variables.

$$V=\sum_{\{i_\alpha,j_\alpha,k_\alpha,l_\alpha\}=0}^{\infty}\frac{\delta^{j_1+\cdots+j_n}}{\delta(Q_1^c)^{j_1}\cdots\delta(Q_n^c)^{j_n}}\langle\langle(I_1^a)^{l_1}\cdots(I_r^a)^{l_r}(Q_1^c)^{i_1}\cdots(Q_q^c)^{i_q}(Q_1^c)^{k_1}\cdots(Q_p^c)^{k_p}\rangle\rangle_m$$
$$\times\frac{(\chi_1^a)^{l_1}}{l_1!}\cdots\frac{(\chi_r^a)^{l_r}}{l_r!}\times\frac{(\chi_1^c)^{i_1}}{i_1!}\cdots\frac{(\chi_r^c)^{i_q}}{i_q!}\times\frac{\lambda_1^{k_1}}{k_1!}\cdots\frac{\lambda_p^{k_p}}{k_p!}\times\frac{(Q_1^c)^{j_1}}{j_1!}\cdots\frac{(Q_n^c)^{j_n}}{j_n!}. \tag{74}$$

As in the one node case, the vertices $\delta_{Q_\alpha^c}\langle I_\beta^a\rangle$ vanish. We note again that the notation chosen for the expansion coefficients in Eq. (74) connects the formalism described here with the Langevin equation point of view. The minimal correlation cumulant $\langle\langle\cdots\rangle\rangle_m$ may be calculated either by the expansion procedure described by Eqs. (72) and (74), or by expressing the physical currents and charges in terms of the current source cumulants by solving the Langevin equations for currents and charges, given by Eq. (71).

The nth order irreducible correlator $\langle\langle I_1^a(\omega_1)\cdots Q_n^c(\omega_n)\rangle\rangle$ may be expressed as a tree-level diagram with n external lines representing absorbed currents I_α^a and conserved charges Q_α^c. Every vertex is local in time, so if there are p legs at a vertex, each is assigned an independent frequency, while the time integral imposes overall frequency conservation, $\delta(\Sigma_i\,\omega_i)$. The cascade rules are generalized as follows:

(1) Every vertex represents the object

$$\delta_{Q_1^c(\omega_1)}\cdots\delta_{Q_l^c(\omega_l)}\langle\langle I_{l+1}^a(\omega_{l+1})\cdots Q_n^c(\omega_n)\rangle\rangle_m,$$

which is multiplied by a δ-function conserving overall frequency, $\delta(\Sigma_{i=1}^n\,\omega_i)$;
(2) the minimal correlation cumulants $\langle\langle I_{l+1}^a(\omega_{l+1})\cdots Q_n^c(\omega_n)\rangle\rangle_m$ may be evaluated by expressing them in terms of cumulants of sources $\langle\langle\tilde{I}_{\alpha\beta}^n\rangle\rangle$ via the solutions (71) of the Langevin equations, or by Eq. (74) if the Hamiltonian is known;
(3) the internal dashed arrow goes from $Q_\alpha^c(\omega)$ to $\delta_{Q_\alpha^c(\omega)}$. It conserves the node index α and the frequency ω;[46]
(4) external lines for absorbed currents and conserved charges originate from $I_\alpha^a(\omega)$ or $Q_\alpha^c(\omega)$ of the vertexes. They conserve the node index and the frequency;
(5) sum over all internal node indices, and integrate over all internal frequencies to remove all but one of the frequency delta functions;
(6) the result has to be multiplied by the total number of inequivalent permutations.

The cascade rules are easily extended to the field theory (see Sec. III). The functional analog to the inverse conductance matrix is the operator

$$\hat{G}^{-1}(\mathbf{r}-\mathbf{r}')\equiv\frac{\delta^2 h}{\delta\lambda(\mathbf{r})\delta\rho(\mathbf{r}')}=-\,\delta(\mathbf{r}-\mathbf{r}')\,\nabla\,\hat{D}\,\nabla\,. \tag{75}$$

The diffusion propagator $(i\omega+\hat{G}^{-1})^{-1}$ can be used to solve the Langevin equations (42) for the density $\rho(\omega,\mathbf{r})$ and current $I(\omega)$ in order to evaluate minimal correlation cumulants. We would like to stress that these cumulants are limited to second order only, because in the diffusion limit the noise sources are Gaussian. The summation over node indices is replaced with an integration over the coordinate $\mathbf{r}$.

V. APPLICATIONS

The formalism presented above is intentionally abstract and general. This is to facilitate maximum applicability and not to tie it to a particular field. However, it is important to give concrete examples. For this reason, we give a detailed treatment of two problems. As a first problem, we consider the saddle-point equations of the 1D field theories for D and F being arbitrary functions of the density ρ [see Eq. (33)]. We apply the results of this analysis to the transport in a diffusive mesoscopic wire at zero temperature, rederive the FCS generating function of the transmitted charge obtained in Refs. 8 and 10, and give new results. We also prove the

conjecture made in Ref. 22 that the current noise of the diffusive symmetric exclusion process at half-filling is Gaussian, i.e., all high-order cumulants of transmitted charge vanish. In the end of the Sec. V A we generalize our results to multi-dimensional diffusion models and prove the universality of their transport statistics. As a second problem, we address the statistics of charge fluctuations in a mesoscopic chaotic cavity. We explicitly find the probability distributions for different physical configurations.

A. FCS for one-dimensional field theories. The mesoscopic diffusive wire

Before demonstrating our solution for the FCS of the mesoscopic diffusive wire specifically, we first consider the general 1D field theory with the action (33). In the stationary limit, $\dot{\rho}=\dot{\lambda}=0$ the action can be written as

$$S = t\int_0^L dz\left[- D\rho'\lambda' + \frac{1}{2}F(\lambda')^2 \right]. \tag{76}$$

The stationary saddle-point equations

$$(F\lambda' - D\rho')' = 0, \quad 2D\lambda'' + \frac{\delta F}{\delta \rho}(\lambda')^2 = 0, \tag{77}$$

can be partially integrated leading to the following two equations:

$$D\rho' = \pm\sqrt{\mathcal{I}^2 - 2\mathcal{H}F}, \tag{78a}$$

$$\lambda' = 2\mathcal{H}/(\mathcal{I} - D\rho'). \tag{78b}$$

The two integration constants $\mathcal{I}=-D\rho'+F\lambda'$ and $\mathcal{H}=-D\rho'\lambda'+(F/2)(\lambda')^2$ are the conserved (conditional) current and the Hamiltonian density, respectively. These conservation laws follow from the symmetries of our 1*D* field theory [see Eqs. (38) and (39) and the surrounding discussion]. Thus we obtain the following result for the action (76),

$$S = tL\mathcal{H}. \tag{79}$$

Equations (78) and (79) represent the formal solution of the FCS problem for 1D diffusion models with $D(\rho)$ and $F(\rho)$ being arbitrary functions of ρ. The following procedure has to be done in order to obtain the cumulant generating function $S(\chi)$ of the transmitted charge:

(1) The differential equation (78a) has to be solved for $\rho(z)$ with the boundary conditions $\rho(z)|_{z=0}=\rho_L$ and $\rho(z)|_{z=L}=\rho_R$. The constant $\mathcal{I}$ should be expressed through the constants ρ_L, ρ_R, and $\mathcal{H}$;
(2) next, $\rho(z)$ is substituted into Eq. (78b) which is integrated to obtain $\lambda(z)$ with the boundary conditions $\lambda_L=0$ and $\lambda_R=\chi$;
(3) finally, using the solution for $\lambda(z)$ the constant $\mathcal{H}$ is expressed in terms of ρ_L, ρ_R, χ, and substituted into the action (79).

We note that by expressing $\mathcal{H}$ and χ in terms of $\mathcal{I}$, we may also formally obtain the logarithm of the current distribution,

$$\ln P(I) = S(\mathcal{I}) - t\mathcal{I}\chi(\mathcal{I}), \quad \mathcal{I}\to I, \tag{80}$$

as a result of the stationary phase approximation for the integral $P(I)=\int d\chi \exp[S(\chi)-tI\chi]$ and because $\partial\mathcal{H}/\partial\chi=\mathcal{I}/L$.

As an example of the 1D field theory, we consider the FCS of the electron charge transmitted through the mesoscopic diffusive wire. When the chemical potential difference $\Delta\mu=\mu_L-\mu_R>0$ is applied to the wire, the electrons flow from the left lead to the right lead with the average current

$I_0 = e^{-1} G \Delta\mu$, where G is the conductance of the wire. The elastic electron scattering causes nonequilibrium fluctuations of the current. At zero temperature, and for noninteracting electrons (the cold electron regime), the zero-frequency current noise power has been found[15,47,48] to be equal to $\langle\langle I^2 \rangle\rangle = (1/3) e I_0$, i.e., the noise is suppressed compared to the Poissonian value. The suppression factor $1/3$ was shown to be universal,[49,50] i.e., it does not depend on the character of the disorder or on the shape of the wire. The FCS of the transmitted charge has been studied in Refs. 8 and 10 using quantum-mechanical methods, and recently in Ref. 22 using a classical method with the following result for the generating function of cumulants of the dimensionless charge Q/e:

$$S(\chi) = (tI_0/e) \operatorname{arcsinh}^2[\sqrt{\exp(\chi) - 1}]. \tag{81}$$

Here we will rederive this result using our classical method.

On the classical level, the electrons in the diffusive wire are described by the distribution function $f(z)$. Under transport conditions (and at zero temperature), this distribution $f(z)$ varies from $f_L = 1$ in the left lead to $f_R = 0$ in the right lead. Starting from the Langevin equation[32] as described in Sec. III or, alternatively, taking the continuum limit for the series of mesoscopic cavities,[36] we arrive at the action (76) with the form[51]

$$S = (tI_0/e) \int_{-1/2}^{1/2} dz [- f' \lambda' + f(1 - f)(\lambda')^2], \tag{82}$$

where we have rescaled the coordinate z, $\rho(z)$ has been replaced with the distribution $f(z)$, and where $D = 1$, and $F = 2f(1-f)$ up to the overall constant I_0/e. This form of F is quite general for fermionic systems. It originates from the Pauli blocking factors, i.e., the transition probability is proportional to the probability that the initial state is populated times the probability that the final state is empty.[15] Applying now the procedure described in the beginning of this section, we solve the saddle-point equations and find the fields f and λ,

$$f(z, \chi) = \frac{1}{2} \left[1 - \frac{\sinh(2\alpha z)}{\sinh \alpha} \right], \tag{83a}$$

$$\lambda(z, \chi) = 2 \operatorname{arctanh}[\tanh(\alpha/2) \tanh(\alpha z)], \tag{83b}$$

$$\alpha = \operatorname{arcsinh}[\sqrt{\exp(\chi) - 1}], \tag{83c}$$

where $\mathcal{H} = \alpha^2$, so that according to the Eq. (79) we immediately obtain the result (81).

The logarithm of the current distribution $\ln[P(I)]$ can be now found from Eq. (80). We obtain the following result:

$$\ln[P(I)] = - (tI_0/e)[2\alpha \coth \alpha \ln(\cosh \alpha) - \alpha^2], \tag{84}$$

where α has to be expressed in terms of $\mathcal{I} = I/I_0$ by solving the equation

$$\alpha \coth \alpha = I/I_0. \tag{85}$$

The last equation has real positive solutions, $0 < \alpha < \infty$, for $I > I_0$, and pure imaginary solutions $\alpha = i\beta$ with $0 < \beta < \pi/2$, for $I < I_0$. The distribution $P(I)$ is strongly asymmetric around the average current $I = I_0$ (see Fig. 7). It has the following asymptotics: $\ln P = -(tI_0/e)[\mathcal{I}^2 - (2 \ln 2)\mathcal{I}]$, for $\mathcal{I} = I/I_0 \gg 1$, i.e., P has a Gaussian tail, and $\ln P = -(\pi^2/4)(tI_0/e)$, for $I = 0$.

We also plot the conditional electron occupation $f(z, I)$, Eq. (83a), for different values of the normalized current I/I_0. There are several interesting points to stress. (i) For large currents, $I > I_0$, the function f drops mostly at the ends of the wire, while for small currents, $I < I_0$, the drop of f is mostly concentrated in the center of the wire. This effect has a simple explanation. At the end points of the wire, $z = \pm 1/2$, the occupation $f(z)$ is fixed independent of the particular value of the current I. On the other hand, its derivative takes the value $f' = -\mathcal{I} = -I/I_0$ at $z = \pm 1/2$, which can be

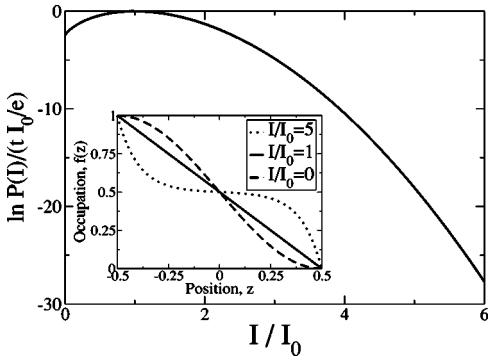

FIG. 7. The logarithm of the distribution of the current through a mesoscopic diffusive wire as a function of the ratio I/I_0 of the current to its average value I_0. The distribution is strongly asymmetric, with the Gaussian tale at $I \gg I_0$. Inset: The electron occupation f inside the wire as a function of the rescaled coordinate z, under the condition that the average current $I=I_0$, no current $I=0$, and large current $I=5I_0$ has been measured.

easily verified using Eqs. (83a) and (85). As a result, $f(z)$ deviates from its linear behavior, $f(z) = 1/2 - z$, characteristic of the average value of current, $\mathcal{I}=1$. The actual reason for this effect is that according to Eq. (42b) the total current $\mathcal{I}=-f'+\nu$ contains a contribution from the source of noise, ν. The greatest contribution is concentrated at the center of the wire, where the noise power $F=2f(1-f)$ has its maximum, while it vanishes at the ends of the wire. Since the current $\mathcal{I}$ is conserved, f' has to be redistributed in such a way as to partially compensate the effect of the source ν. (ii) Fluctuations of f are strongly suppressed at the ends of the wire, which is imposed by the boundary conditions, and at the center of the wire, as a result of the discrete symmetry, $\{z \to -z; f \to 1-f\}$. (iii) Eq. (85) has additional solutions with $\beta > \pi/2$. These solutions are not physical however, since f becomes negative or larger than 1 leading to $I<0$, which is impossible at $T=0$.

Returning to the saddle-point equations (77), we note that if $\delta F/\delta\rho = 0$ for a particular density ρ_0, then the fields $\rho(z)=\rho_0$, and $\lambda(z)=\chi z/L$ solve these equations. The fluctuations of the current become Gaussian with the noise power $\langle\langle I^2\rangle\rangle = F(\rho_0)/L$. This generalizes and proves the conjecture made in Ref. 22 that the noise of the diffusive symmetric exclusion process is Gaussian at half-filling, $f=1/2$.

As a final remark we note that the whole class of multi-dimensional field theories,

$$S = t\int_{\Omega} d\mathbf{r}[-\nabla\lambda\,\hat{D}\,\nabla\rho + (1/2)\,\nabla\lambda\,\hat{F}\,\nabla\lambda], \tag{86}$$

with $\hat{D}=D(\rho)\hat{T}$, $\hat{F}=F(\rho)\hat{T}$, and $\hat{T}$ being an arbitrary constant symmetric tensor,[52] bear the same kind of the universality as the shot noise in diffusive conductors discussed above (see Refs. 49 and 50). The reason is that the field theory with the action (86) can be mapped on the 1D theory with the action (76) by making use of the parameterization

$$\rho(\mathbf{r}) = \rho[\varphi(\mathbf{r})], \quad \lambda(\mathbf{r}) = \lambda[\varphi(\mathbf{r})], \tag{87}$$

where the function $\varphi(\mathbf{r})$ satisfies the equation

$$\nabla\cdot[\hat{T}\,\nabla\,\varphi(\mathbf{r})] = 0. \tag{88}$$

Using Eqs. (77) for ρ and λ as functions of φ, it is straightforward to verify that the fields $\rho(\mathbf{r})$ and $\lambda(\mathbf{r})$ given by (87) and (88) satisfy the saddle-point equations for the action (86). One of the equations is the conservation of current:

$$\mathbf{j} = -\hat{D}\nabla\rho + \hat{F}\nabla\lambda = \mathcal{I}\hat{T}\nabla\varphi. \tag{89}$$

Since the 1D Hamiltonian density is conserved, the action takes the following form

$$S = t\mathcal{G}\mathcal{H}, \tag{90}$$

where the constant $\mathcal{G}$ depends only on the geometry of the boundary $\partial\Omega$ by Eq. (88):

$$\mathcal{G} = \int_{\Omega} d\mathbf{r}\,\nabla\varphi\hat{T}\nabla\varphi = \int_{\partial\Omega} d\mathbf{s}\cdot\varphi\hat{T}\nabla\varphi. \tag{91}$$

Consider now a two-terminal diffusive wire, so that the surface $\partial\Omega$ consists of the left $\partial\Omega_L$ and right $\partial\Omega_R$ contact surfaces, and the open surface $\partial\Omega_0$ with no current through it. We choose the boundary conditions for φ to be

$$\varphi(\mathbf{r})_{\partial\Omega_L} = 0, \quad \varphi(\mathbf{r})_{\partial\Omega_R} = 1, \quad d\mathbf{s}\cdot\hat{T}\nabla\varphi(\mathbf{r})_{\partial\Omega_0} = 0, \tag{92}$$

so that $\rho(\mathbf{r})|_{\partial\Omega_L} = \rho_L$, $\rho(\mathbf{r})|_{\partial\Omega_R} = \rho_R$, $\lambda(\mathbf{r})|_{\partial\Omega_L} = 0$, $\lambda(\mathbf{r})|_{\partial\Omega_R} = \chi$, and $d\mathbf{s}\cdot\mathbf{j}(\mathbf{r})|_{\partial\Omega_0} = 0$. Then $\mathcal{H}$ becomes a function of ρ_L, ρ_R, and χ, and the action is the generator of the cumulants of the transmitted charge. If instead, $\mathcal{H}$ and χ are expressed in terms of $\mathcal{I}$ (as above for the 1D theory), then one obtains the logarithm of the distribution of the current, $\ln[P(I)] = S(I) - tI\chi(I)$, where $I = \mathcal{G}\mathcal{I}$, according to Eqs. (89), (91), and (92). The constant $\mathcal{G}$ may be interpreted as a "geometrical conductance" of a wire. In particular, in the "ohmic" regime, i.e., when D is independent of ρ, we have $I_0 = \mathcal{I}(\chi)|_{\chi=0} = D(\rho_L - \rho_R)$, and therefore $\mathcal{G} = I_0/[D(\rho_L - \rho_R)]$. In this case, the ratio S/I_0 does not contain $\mathcal{G}$ and becomes fully universal, proving also the universality of the result (81) as a special case.

To summarize, we have proven the universality of the FCS of the transmitted charge for a two-terminal multi-dimensional generalized wire described by the action (86) with the noise tensor $F(\rho)\hat{T}$, being an arbitrary function of the charge density ρ, and with the constant diffusion tensor $D\hat{T}$. The universality means that the FCS depends neither on the shape of the conductor, nor on its dimensionality.[53] The FCS of a mesoscopic wire given by Eq. (81) is a particular example of universal FCS. In the more general case, when $\hat{D}$ is a function of ρ, the FCS depends on the geometry through only one parameter $\mathcal{G}$, the geometrical conductance given by Eq. (91).

B. Charge fluctuations in a chaotic cavity

As another example of the applicability of the stochastic path integral approach, we now consider transport through a chaotic cavity. This problem is often investigated in mesoscopic physics because of its simplicity and conceptual clarity. A cavity consists of a large conducting island of irregular shape that is connected to two metallic leads through quantum point contacts (see inset of Fig. 8). The distinctive property of the chaotic cavity separating it from diffusive conductors is that the conductance is determined solely by the ballistic point contacts. The chaotic cavity itself may be either disordered or ballistic. Chaotic cavities can be described by a semiclassical theory if the point contacts have conductances much larger than e^2/h. The statistics of current flow through the cavity have been addressed using various methods. The zero-frequency noise power has been calculated using random matrix theory[54] and the minimal correlation principle.[18] The higher order current cumulants have been obtained in Refs. 7 and 20. The results are in complete agreement with random matrix theory.

In this section we will address another type of statistics. In a typical experimental setup, the cavity is connected to the electrical circuit not only through the leads, but also through nearby metallic gates via the electrostatic interaction. Observing potential fluctuations at these additional gates gives direct insight into the statistics of charge on the cavity. The noise power of the charge fluctuations in this system has been calculated in Ref. 55. The full statistics have been recently

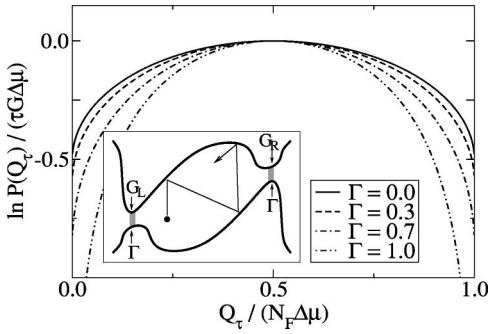

FIG. 8. The logarithm of the distribution of charge Q_τ in a symmetric cavity, $G_L=G_R$, averaged over measurement time τ in the long time limit $\tau \gg \tau_D$ and at zero temperature. The results are presented for several transparencies Γ of the point contacts. It is clearly seen that the tails of the distribution grow in the tunneling limit $\Gamma \ll 1$. The distribution is symmetric, i.e., odd cumulants vanish.

addressed using a random matrix theory.[56] Here, we rederive these results using the stochastic path integral, show new results on the temperature dependence of these statistics, and also investigate the instantaneous fluctuation statistics.

In a semiclassical approach, both leads L,R and the cavity are described by electron distribution functions f_L, f_R, and f. The Fermi functions in the leads $f_\alpha = f_F(E-\mu_\alpha)$ are characterized by their chemical potential μ_α and their temperature T. The chaotic electron motion inside the cavity makes the cavity distribution function $f(E,t)$ isotropic and position independent. Only its energy dependence must be retained. From now on we set the electron charge to one, $e=1$. Then the charge Q in the cavity is given in terms of the electron distribution function and density of states N_F as $Q=N_F\int dEf$. The average value of charge is determined by the low-energy cutoff of the integral and is not relevant for the present discussion. The charge and electrostatic potential of the cavity are related by a geometrical capacitance C_g. In the following, we restrict ourselves to the case $C_g \gg e^2 N_F$ which describes complete screening of the charge in the cavity. A more general discussion can be found in Ref. 56. To analyze the time evolution of the charge, we note that if the size of the cavity is smaller than the electron–electron and electron–phonon scattering length, every electron entering the cavity at a certain energy leaves it at the same energy. The single electron energy is thus conserved and we can formulate a current conservation law separately for each energy interval dE,

$$N_F \dot{f}(E,t) = J_L(E,t) + J_R(E,t), \tag{93}$$

where J_α denote ingoing particle currents per energy interval dE in the left and right contacts. These currents are described by binomial processes with the cumulant generating function given by[5]

$$H_\alpha(f, i\lambda_\alpha)dE = \Gamma^{-1} G_\alpha dE \, \ln[1 + \Gamma f_\alpha (1-f)(e^{i\lambda_\alpha}-1) + \Gamma f(1-f_\alpha)(e^{-i\lambda_\alpha}-1)], \tag{94}$$

where we have introduced the conductances of the point contacts G_α, $\alpha = L,R$, and their transparency Γ.

The quantity of interest is the total number of electrons in the cavity averaged over the measurement time τ,

$$Q_\tau = (N_F/\tau)\int_0^\tau dt \int dEf(E,t). \tag{95}$$

We first consider the long time limit, $\tau \gg \tau_D$, where $\tau_D = N_F/(G_L+G_R)$ is the average dwell time of an electron in the cavity. In this limit, the action is stationary with respect to the variables f and λ,

$$S = \tau \int dE[H(f,i\lambda) + i(N_F/\tau)\chi f], \quad H = H_L + H_R, \tag{96}$$

where the external variable χ generates the statistics of the desired quantity Q_τ.

At zero temperature $T=0$, the variables λ and f are independent of the energy E, and the integration in Eq. (96) amounts to a multiplication by $\Delta\mu=\mu_L-\mu_R$. Evaluating the Fourier transform of the characteristic function $Z(i\chi)$,

$$Z(i\chi) = (2\pi)^{-1} \int dQ d\lambda \, \exp(S), \tag{97}$$

we express the full probability distribution $P(Q_\tau)$ of charge on the cavity as an integral

$$P(Q_\tau) = (2\pi)^{-1} \int d\lambda \, \exp[\tau\Delta\mu H(f,i\lambda)], \quad f = Q_\tau/(N_F\Delta\mu). \tag{98}$$

This integral will be calculated in the saddle-point approximation. For the tunneling limit $\Gamma \ll 1$ and for open point contacts $\Gamma=1$ we obtain

$$\ln P(Q_\tau)_{\Gamma\ll 1} = -\tau G\Delta\mu[\sqrt{f(1-f_0)} - \sqrt{f_0(1-f)}]^2, \tag{99a}$$

$$\ln P(Q_\tau)_{\Gamma=1} = \tau G\Delta\mu\left[f_0 \ln\left(\frac{f}{f_0}\right) + (1-f_0)\ln\left(\frac{1-f}{1-f_0}\right)\right], \tag{99b}$$

where $G=G_L+G_R$, and where we have introduced the average distribution function $f_0=G_L/(G_L+G_R)$ in the cavity. We summarize that the results (99) have been obtained under the conditions $T=0$, $\tau \gg \tau_D$, and for $\Gamma \ll 1$ and $\Gamma=1$. These results can be easily generalized to the case of a multi-terminal cavity.

Although the general case of an arbitrary transparency Γ has been also solved analytically, the final expression for the charge distribution is too lengthy to be presented here. The Fig. 8 shows the distribution $P(Q_\tau)$ at zero temperature for various transparencies Γ of the point contacts. The cavity is taken to be symmetric $G_L=G_R$. It is clearly seen that the tails of the distribution grow towards the tunneling limit.

At finite temperature, further analytical progress can be made by considering the first few cumulants of the charge Q_τ. The integral (96) for the cumulant generating function has to be evaluated at the saddle point. For $\chi=0$ the solution of the saddle-point equations $\partial S/\partial\lambda=0$ and $\partial S/\partial f=0$ are simply given by $\lambda=0$ and $f=f_0$, where $f_0=(G_Lf_L+G_Rf_R)/(G_L+G_R)$ is the average electron distribution function in the cavity. From the diagrammatic technique discussed in Sec. IV we derive analytical expressions for the first few cumulants. The second cumulant has been obtained in Ref. 55. As an example, we present here the result for the third cumulant for the case of open point contacts, $\Gamma=1$:

$$\langle\langle Q_\tau^3\rangle\rangle = -\frac{2\tau_D^3}{\tau^2}\frac{G_LG_R(G_L-G_R)}{(G_L+G_R)^2}\left[\Delta\mu + 3\frac{\Delta\mu - k_BT\sinh(\Delta\mu/k_BT)}{\cosh(\Delta\mu/k_BT)-1}\right]. \tag{100}$$

The first few cumulants are plotted in Fig. 9 as a function of the dimensionless bias $\Delta\mu/k_BT$. Note that the fourth cumulant may change its sign as one goes from a symmetric cavity ($\beta=0$) to an asymmetric cavity ($\beta=0.9$).

So far we have considered the time of measurement τ longer than the dwell time τ_D. Next we consider the opposite limit $\tau \ll \tau_D$ (but still larger than $\tau_0=\hbar/\Delta\mu$) and study the instantaneous fluctuations of the charge Q in the cavity at zero temperature, $T=0$. For this purpose we will use the stochastic path integral (3) for the propagator $U(Q_f,Q_i,t)$ of the cavity charge. The distribution $P(Q)$ of instantaneous fluctuations can be obtained by taking the $t\to\infty$ limit of the propagator $U(Q_f,Q_i,t)$ and setting $Q_f=Q$. We note that in the long time limit, $t \gg \tau_D$, the initial state Q_i

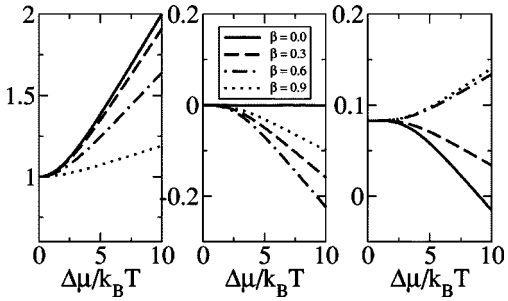

FIG. 9. Cumulants of the charge inside a chaotic cavity, $\langle\langle Q_\tau^n\rangle\rangle$, $n=2,3,4$ (in arbitrary units) as functions of the dimensionless potential difference $\Delta\mu/k_BT$. The parameter $\beta=(G_L-G_R)/(G_L+G_R)$ characterizes the asymmetry of the cavity.

relaxes to the stationary state $\overline{Q}$, and as a result the saddle-point expression of the propagator $U=\exp(S_{sp})$ factorizes according to $S_{sp}=S_0(\overline{Q})+S_i(Q_i)+S_f(Q_f)$. Here the stationary contribution to the action is zero, $S_0=0$, since there is no charge accumulation on a long time scale. We will show that the initial state contribution vanishes, $S_i=0$, so the system looses its memory about the initial state. Thus we obtain $\ln P(Q)=S_f(Q)$.

We now focus on the case of a cavity with two tunneling contacts ($\Gamma\ll 1$). Using the Hamiltonians in Eq. (94), and replacing the counting variable $\lambda\to i\lambda$, we write the action as

$$S=G\Delta\mu\int dt[\tau_D\lambda\dot{f}+h_s(\lambda,f)], \tag{101a}$$

$$h_s=(1-f_0)f(e^{\lambda}-1)+f_0(1-f)(e^{-\lambda}-1), \tag{101b}$$

where h_s is the scaled Hamiltonian. The saddle point equations take the following form

$$\tau_D\dot{f}=-(1-f_0)fe^{\lambda}+f_0(1-f)e^{-\lambda}, \tag{102a}$$

$$\tau_D\dot{\lambda}=\sinh(\lambda)+(1-2f_0)[\cosh(\lambda)-1]. \tag{102b}$$

The solution of the Eq. (102b) for λ reads

$$\lambda(t)=\ln\left[\frac{1+Af_0\exp(t/\tau_D)}{1-A(1-f_0)\exp(t/\tau_D)}\right], \tag{103}$$

where A is the integration constant.

To show that the initial contribution to the action S_i is zero, we note that independent of the constant A, the absolute value of λ is a growing function with the stationary state given by $\overline{\lambda}=0$ at $t=-\infty$. This means that starting from early times $t_0\to-\infty$, the solutions are $\lambda(t)=0$ and $f(t)-f_0=[f(t_0)-f_0]\exp[-(t-t_0)/\tau_D]$. They describe the relaxation of the initial state $f(t_0)$ to the stationary state $\overline{f}=f_0$. Substituting these solutions to Eqs. (101) we immediately find that $S_i=0$.

After making this point we skip the rest of the details and present the final result for $\ln P(Q)=S_f(Q)$:

$$\ln P(Q)_{\Gamma\ll 1}=-\tau_DG\Delta\mu\left[f\ln\left(\frac{f}{f_0}\right)+(1-f)\ln\left(\frac{1-f}{1-f_0}\right)\right], \tag{104}$$

which can now be compared to the results (99). The cumulant generating function for the distribution (104) is given by $S(\chi)=\tau_DG\Delta\mu\ln[1+f_0(e^{\chi}-1)]$. Note that $\tau_DG\Delta\mu=N_F\Delta\mu$ is the total number of the semi-classical states in the cavity which participate in transport. Therefore the distribution (104) can be interpreted as being a result of uncorrelated binomial fluctuations of the

Fermi occupations of each semi-classical state. We would like to mention that the same result can be obtained by solving the stationary master equation.

VI. CONCLUSIONS

We have put forth a stochastic path integral formulation of fluctuation statistics in networks. The mathematical building blocks of the theory are (1) the probability distributions of transport processes through the connectors, (2) a continuity equation linking the connector currents to the charge accumulation in nodes (charge conservation), and (3) a separation of time scales between nodal dynamics and connector fluctuations. The relevant action of the path integral is derived from these considerations and is related to the probability of (charge conserving) paths in phase space. The dominant contribution to the statistics comes from the saddle point approximation to the path integral, and the generating function for the interacting system is simply the action at the saddle point. Fluctuations are suppressed by the number of transporting elementary charges in the network. We have considered the continuum limit to obtain a field theory, and mapped it onto a Langevin equation with Gaussian noise. Cascade diagrammatic rules were found in agreement with Nagaev for the one node case, and extended to general current correlation functions in an arbitrary network. Applications to the current statistics of the diffusive wire and fluctuation statistics of the charge inside a mesoscopic cavity were also discussed. As the building blocks of the theory are classical probability theory, the potential application of this formalism is very broad and applicable to any field where fluctuations are important, including mesoscopics, biology, economics, fluid and chemical dynamics.

Note added. After this paper was submitted for publication, the authors learned of previous related work by Bertini *et al.*[57] Although they did not consider transport statistics, they did consider the probability to manifest a given macroscopic fluctuation of the particle density in diffusive lattice gas models and arrive at the action Eq. (33). However, the Gaussian nature of the local fluctuations was assumed *a priori*. We thank B. Derrida for bringing these papers to our attention.

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Fragile $\mathcal{PT}$-symmetry in a solvable model

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One of the simplest pseudo-Hermitian models with real spectrum (viz., square-well on a real interval $\mathcal{I}$ of coordinates) is re-examined. A $\mathcal{PT}$-symmetric complex deformation $\mathcal{C}$ of $\mathcal{I}$ is introduced and shown tractable via an innovated approach to matching conditions. The result is surprising: An *arbitrarily small* deformation $\mathcal{I} \to \mathcal{C}$ implies a sudden collapse (i.e., the spontaneous $\mathcal{PT}$-symmetry breaking) of virtually *all* the spectrum (i.e., up to its low-energy part). © *2004 American Institute of Physics.* [DOI: 10.1063/1.1803928]

I. NON-HERMITIAN HAMILTONIANS AND THEIR SPECTRA

Thirty-five years ago, Bender and Wu[1] published an extremely exciting discovery that certain bound-state problems may be much better understood when one drops the "obligatory" Hermiticity assumption $H=H^\dagger$ and admits that a coupling constant $g>0$ in Schrödinger equation

$$H(g)|\psi_n(g)\rangle = E_n(g)|\psi_n(g)\rangle, \quad n=0,1,\ldots \tag{1}$$

is analytically continued to a complex value $g \in \mathbb{C}$. In this perspective Bender and Wu worked, for definiteness, with the quartic anharmonic-oscillator Hamiltonians

$$H(g) = H^{(4)}(g) = \hat{p}^2 + f^2\hat{x}^2 + g\,\hat{x}^4, \tag{2}$$

and demonstrated that the separate (though, in general, complex) spectra $\{E_n(g)\}$ may *all* be interpreted as the sets of an intersection of *all* the Riemann sheets of a *single* analytic function $\mathbb{E}^{(4)}(g)$ with a corresponding "line" of a constant g. Many years later, similar observations were made and verified for the cubic model

$$H(g) = H^{(3)}(g) = \hat{p}^2 + f^2\hat{x}^2 + i\,g\,\hat{x}^3 \tag{3}$$

(see Ref. 2 for more details), etc. In all of these models, the costs of the generalization $H \neq H^\dagger$ proved much lower than expected. For all the nonzero couplings $g \neq 0$, all of their complex "exceptional points" (EP)[3] proved well separated in the complex plane of g for both Eqs. (2) and (3).

A new important development of the subject emerged cca six years ago when Bender and Boettcher published their letter.[4] Having extended their attention to the whole class of the power-law models

$$H(g) = H^{(2+\delta)}(g) = \hat{p}^2 + f^2\hat{x}^2 + g\,\hat{x}^2\,(i\hat{x})^\delta, \quad \delta>0, \quad g>0 \tag{4}$$

[reproducing the above special cases (2) and (3) at $\delta=2$ and $\delta=1$, respectively], they summarized several existing perturbative and numerical experiments (for illustration one could cite, e.g., Refs. 5–7), complemented them by numerous new WKB arguments and conjectured that after one introduces a suitable Hilbert space, *all* the Hamiltonians (4) (with, for simplicity, $f=0$) will possess the *purely real* (and discrete and, from below, bounded, i.e., "observable-like") spectra, in spite of their *manifestly* non-Hermitian origin.

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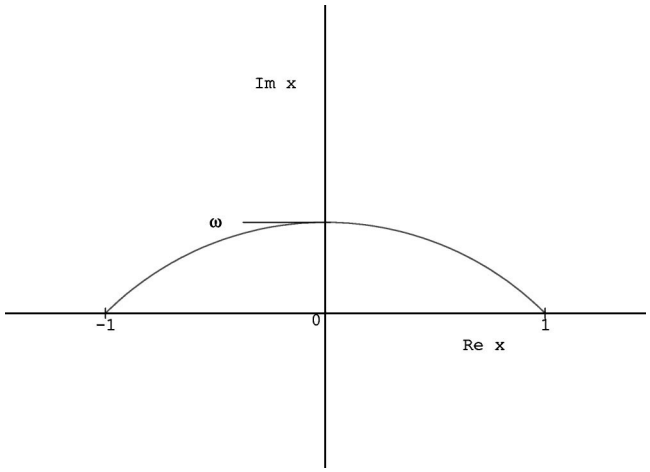

FIG. 1. Integration path $\mathcal{C}$ with an upwards deformation $\omega>0$.

For the pioneering conjecture of this type, several rigorous proofs [cf., e.g., the Fourier-transformation results[7] for Eq. (2) at $g<0$, or the manifest reality of perturbative energies after re-summation for Eq. (3) at the real g[5]] were already available and many other had only to come [cf., for illustration, proofs in the difficult case of Eq. (3) in Ref. 8]. Nevertheless, the core of the message delivered by Bender and Boettcher lied in the emphasis attributed to the parity-plus-complex-conjugation symmetry (conveniently called $\mathcal{PT}$-symmetry) of their sample non-Hermitian Hamiltonians $H^{(2+\delta)}(g)$ with real spectra. This inspired an extensive subsequent study of the structure of the relationship between the reality of the spectrum and the $\mathcal{PT}$-symmetry of the underlying non-Hermitian Hamiltonian.[9]

We intend to contribute to the latter effort by the description of an exactly solvable example which exhibits a rather counterintuitive enhanced sensitivity to a very small change of its coordinate domain. We shall start from an overall review of the state of the art in Sec. II where we emphasize the theoretical importance as well as some practical weaknesses of the pseudo-Hermitian constraint imposed upon the non-Hermiticity of the Hamiltonians.

In Sec. III we return to the study of quantitative characteristics of the specific, differential-equation models where the current and robust property of Hermiticity $H=H^{\dagger}$ is being replaced by the $\mathcal{PT}$-symmetry which may be fragile.[10,11] We restrict our attention to the most elementary non-Hermitian square-well model (of Ref. 12, with real spectrum) and extend its scope slightly by the replacement of its usual domain (viz., a finite interval $\mathcal{I}$) by a broken line (or by any other smoothly deformed curve $\mathcal{C}$—cf. Fig. 1) in the complex plane of coordinates.

Our main mathematical results are presented in Sec. IV where our new method of solving the matching conditions is shown applicable to an explicit qualitative description of the structure of the bound states in the broken-path regime. We explain in detail how our "moving-lattice" method decisively facilitates the global analysis of the matching conditions.

Our key physical message is finally formulated in Sec. V emphasizing that our innovative geometric interpretation of the matching conditions offers the rigorous proof that in our example, an arbitrarily small imaginary shift $0\to i\omega$ of the matching point causes a non-perturbative, *sudden* complexification of *all* the high-energy part of the spectrum. In the currently accepted terminology this means that the vast majority of the wave functions encounters a spontaneous breakdown of *their* $\mathcal{PT}$-symmetry. We shall conclude in Sec. VI that this symmetry is *manifestly* fragile in our particular model.

II. $\mathcal{PT}$-SYMMETRY

A. Variational picture

In the early stages of study of $\mathcal{PT}$-symmetric quantum mechanics people tried to understand the complexified Schrödinger Hamiltonians of the type (4) as models on the real line, with a pair

of the real and imaginary potentials of a definite behavior with respect to the parity $\mathcal{P}$. Along these lines one arrives at an introduction of the two harmonic-oscillator-type bases $\{|n^{(\pm)}\rangle\}$ (with definite, fixed parities $^{(\pm)}$) and transforms the $\mathcal{PT}$-symmetric differential Schrödinger equations $H|\psi\rangle = E|\psi\rangle$ with a pre-selected normalization of $|\psi\rangle = \Sigma_n\ (|n^{(+)}\rangle\psi_n^{(+)} + i|n^{(-)}\rangle\psi_n^{(-)})$ into the variational-like real and partitioned matrix problems containing arrays $\vec{\psi}^{(\pm)}$ of the real wave function components $\psi_n^{(\pm)}$,

$$\begin{pmatrix} A & -C \\ C^T & D \end{pmatrix}\begin{pmatrix} \vec{\psi}^{(+)} \\ \vec{\psi}^{(-)} \end{pmatrix} = E\begin{pmatrix} \vec{\psi}^{(+)} \\ \vec{\psi}^{(-)} \end{pmatrix}. \tag{5}$$

The infinite-dimensional submatrices $A=A^T$ and $D=D^T$ are real and symmetric but the spectrum itself need not be real at all.[13] These considerations inspired Mostafazadeh who conjectured, in a series of papers,[14] that the Bender's and Boettcher's $\mathcal{PT}$-symmetric quantum mechanics should be classified as a mere special case of the more universal pseudo-Hermitian quantum mechanics, the origins and foundations of which might be traced back to Dirac *et al.*[15] In such an overall setting, he proposed to weaken the $\mathcal{PT}$ symmetry of the Hamiltonians to their mere pseudo-Hermiticity

$$H^\dagger = \eta H \eta^{-1}, \quad \eta = \eta^\dagger, \tag{6}$$

where we may set, in our particular example (5),

$$\eta = \eta_P = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \eta_P^{-1}. \tag{7}$$

In the light of the well known[16] huge ambiguity of the assignment of the "metric" η to any given pseudo-Hermitian Hamiltonian $H \neq H^\dagger$, Mostafazadeh also proposed that the "natural" choices with the indeterminate parity-like metric operators [like $\eta_{\mathcal{P}}$ in Eq. (7)] should be *all* replaced by *any* (i.e., very often, nondiagonal and strongly Hamiltonian-dependent) positive definite alternative $\eta_+ > 0$. In parallel to Mostafazadeh, similar conclusions have been reached in Refs. 17 and 18 defining, in the present language, the particular positive definite metrics $\eta_+ = \mathcal{PQ}$ and $\eta_+ = \mathcal{CP}$ using the additional symmetry generators $\mathcal{Q}$ and $\mathcal{C}$ of quasi-parity and charge, respectively.

The latter procedure enables us to call all the similar non-Hermitian Hamiltonians H "quasi-Hermitian" because, in accord with the Ref. 16, the positivity of $\eta_+ > 0$ suppresses many interpretation difficulties and leaves the quasi-norm $\|\varphi\| = \sqrt{\langle\varphi|\,\eta_+|\varphi\rangle}$ real and nondegenerate. This makes the corresponding Hamiltonians compatible with their standard quantum-mechanical probabilistic tractability.[19]

B. Square-well illustration

One of the main sources of inspiration for the selection of potentials in Schrödinger equations (say, in the Coulombic form) is the principle of correspondence which allows us to extend and transfer to quantum mechanics the experimental experience gained during centuries in the common, macroscopic world. A counterintuitive character of many quantum phenomena allows us to search for some new and unusual Schrödinger equations, e.g., by a complexification of their axes of coordinates $\mathbb{R} \to \mathcal{C}$.[4] Alternatively, we may obtain manifestly $\mathcal{PT}$-symmetric equations

$$\left[-\frac{d^2}{dx^2} + V(x) + iW(x) \right]\psi(x) = E\psi(x) \tag{8}$$

by staying on the real line and "deforming" the shapes of $V(x) = +V(-x)$ and $W(x) = -W(-x)$. Samples of both these approaches may be found, e.g., in Ref. 10 (considering mainly the asymptotically power-law potentials) or Ref. 20 (paying attention to some exponentially confining forces) or Ref.12 (where an even steeper, infinitely deep square well has been complexified) or Ref. 21 (where the mathematical properties have been discussed for the next-step models with delta-functions mimicking the "infinitely thin" square wells).

The square-well model represents a reasonable phenomenological compromise exhibiting, as a bonus, an important merit of exact solvability. We shall pick up it in what follows, interpreting the infinitely deep real part of the potential

$$V(x)=\begin{cases}+\infty\\0\\+\infty\end{cases}\quad\text{for}\quad\begin{cases}x>1\\-1<x<1\\x<-1\end{cases}\tag{9}$$

as a requirement that all the wave functions vanish at $x=\pm 1$. We break the Hermiticity of our Hamiltonian by adding the imaginary and $\mathcal{PT}$-symmetric finite interaction term with coupling $Z>0$,

$$W(x)=\begin{cases}+Z,\\-Z\end{cases}\quad\text{for}\quad\begin{cases}\text{Re } x<0\\\text{Re } x>0.\end{cases}\tag{10}$$

Once we assume that the interval of the coordinates x remains purely real, the spectrum of energies $E_n=E_n(Z)$ proves discrete and real at all $Z<Z_{\text{critical}}\approx 4.48$ (cf. Ref. 22). It smoothly converges towards the well known square-well energy levels $E_n(0)=(n+1)^2\pi^2/4$ in the Hermitian limit $Z\to 0$.

In an extension of the above square-well model we shall now assume that the interval of the coordinates x will be deformed to complex plane, to a suitable curve $\mathcal{C}$ of integration of our complexified Schrödinger equation. More rigorously, we reinterpret our original differential Eq. (8) with nonanalytic potential $W(x)$ as two individual equations, each of which is only defined on the respective half-plane of x with $Re x>0$ and $Re x<0$. Both of them contain a constant, safely analytic potential, but their solutions must be matched at a point where the curve $\mathcal{C}$ intersects the boundary of the two domains. The corresponding generalized, $\mathcal{PT}$-symmetric (i.e., left-right–symmetric) curve $\mathcal{C}$ is sampled in Fig. 1.

III. EXACT SOLVABILITY OF THE NEW MODEL

Once we define our potential (10) in the whole complex plane of $x\in\mathbb{C}$, solutions $\psi(x)$ will be analytic in both its half-planes. The only distinctive feature of our present generalization $(-1,1)=\mathcal{I}\to\mathcal{C}$ lies in the requirement of the matching of the left and right branches $\psi_{\mp}(x)$ of our full wave function $\psi(x)$ at a point $x_0=i\omega$ on the imaginary axis. This enables us to postulate the matching rules

$$\psi_-(i\omega)=\psi_+(i\omega)=1,\quad \partial_x\psi_-(i\omega)=\partial_x\psi_+(i\omega)=iA\tag{11}$$

in terms of an auxiliary real parameter $A\in(-\infty,\infty)$.

A. Re-parametrization of the matching conditions

As long as our potentials V and W are constant almost everywhere, the general solution of our differential Schrödinger equation (8) may be put equal to a sum of the hyperbolic sine and cosine. The left and right solutions $\psi_{\mp}(x)$ are different, having to vanish at the different boundary points $x\to\mp 1$,

$$\psi_-(x)=R_-\sinh\kappa^*(1+x),\quad \psi_+(x)=R_+\sinh\kappa(1-x).\tag{12}$$

With $\kappa=s-it$, the values of the two free real parameters s and t will be determined by the differentiation in Eq. (8),

$$E=t^2-s^2,\quad Z=2\,st.\tag{13}$$

As long as a change of the sign of κ would influence just the (arbitrary) sign of the overall normalization coefficients $R_{\pm}$, we conveniently restrict our attention to the quadrant of $s>0$ and $t>0$ (note that we fixed the sign of $Z>0$ in advance). The insertion of the right and left solutions

(12) in the matching conditions (11) gives the following complex (and transcendental) algebraic equations,

$$L\ \sinh\ \kappa^{*}(1+i\omega)=R\ \sinh\ \kappa(1-i\omega)=1,$$

$$\kappa^{*}L\ \cosh\ \kappa^{*}(1+i\omega)=-\kappa\ R\ \cosh\ \kappa(1-i\omega)=iA.$$

Their solution is our main task. In the first step, we can get rid of the redundant constants by taking the ratios,

$$\kappa^{*}\ \mathrm{cotanh}\ \kappa^{*}(1+i\omega)=-\kappa\ \mathrm{cotanh}\ \kappa(1-i\omega)=iA. \tag{14}$$

The former equal sign is trivial while the latter one represents a complex equation which defines the real parameter A *and* inter-relates the two real and positive parameters s and t in addition. As long as we have $Z=2st$, this should determine all their admissible values.

Changing our notation and putting $\omega=\tan\ \varphi$ with $\varphi\in(-\pi/2,\pi/2)$, let us now introduce two auxiliary linear functions $S=S(s,t)$ and $T=T(s,t)$ defined by the elementary two-dimensional rotation

$$\begin{pmatrix} S \\ T \end{pmatrix}=\begin{pmatrix} \cos\ \varphi & -\sin\ \varphi \\ \sin\ \varphi & \cos\ \varphi \end{pmatrix}\begin{pmatrix} s \\ t \end{pmatrix} \tag{15}$$

where the angle of the rotation measures also the upward shift of the matching point in the complex plane of our complex coordinates. In this notation we may re-write our matching constraint (14) in the form

$$A\ \sinh\left(\frac{S}{\cos\ \varphi}-i\frac{T}{\cos\ \varphi}\right)=(t+is)\cosh\left(\frac{S}{\cos\ \varphi}-i\frac{T}{\cos\ \varphi}\right) \tag{16}$$

which admits a facilitated separation of its real and imaginary part. The value of A drops out of their ratio which may be further re-arranged to represent our matching condition in the most compact real form

$$s\ \sinh\left(\frac{2S}{\cos\ \varphi}\right)=-t\ \sin\left(\frac{2T}{\cos\ \varphi}\right). \tag{17}$$

In the limit $\varphi\to 0$ the latter equation coincides with the $\omega=0$ prescription of Ref. 12. At the generalized $\omega\neq 0$ the replacement of s and t by S and T via Eq. (15) converts our new and more complicated matching formula (17) into its final form

$$\tau=\sigma\frac{\omega+\varrho(\tau)\sinh\ \sigma}{1-\varrho(\tau)\omega\ \sinh\ \sigma},\quad \omega=\tan\ \varphi, \tag{18}$$

where we abbreviated $\sigma=2S/\cos\ \varphi$, $\tau=2T/\cos\ \varphi$ and $\varrho=\varrho(\tau)=-1/\sin\ \tau$. This equation is an implicit definition of a certain set of curves $\tau=\Theta(\sigma)$ in the $\sigma-\tau$ plane. In principle, the knowledge of these curves would enable us to find all their intersections $(\sigma_k,\ \tau_k)$, $k=0,1,\ldots$ with our original constraint $t=Z/(2s)$.

B. The lattice-moving method of solving Eq. (18)

Our present key idea is that the function $\varrho=\varrho(\tau)$ is periodic, i.e., it remains constant on a discrete lattice $\mathcal{L}$ of its argument τ. In this spirit we shall split the real axis of τ into intervals of the length 2π numbered by an integer k. Then we introduce the second variable $p=\pm 1$ marking the right and the left half of each of these intervals, respectively. This guarantees that at a fixed p the sign of the sine function remains the same and equal to $-p$. Finally, due to the symmetry of each of the sine-shaped curves we split the half-intervals in the quarter-intervals marked by another index $q=\pm 1$,

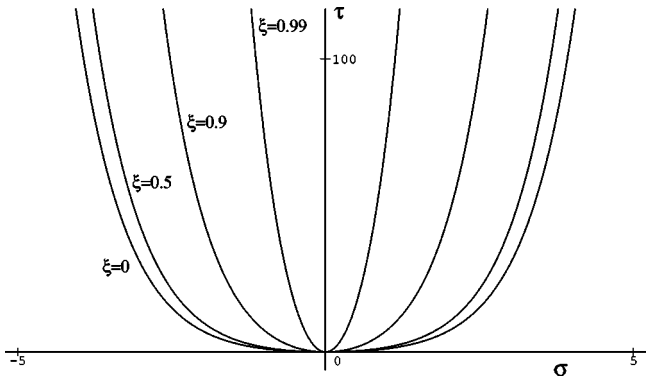

FIG. 2. The lattice-dependent curve (22) with $p=+1$ at a few ξ.

$$\tau=(2k+1)\pi+p\frac{\pi}{2}+q\frac{\pi}{2}\xi\equiv\tau_{(k,q)}(p,\xi),\quad \xi=\xi(\tau)\in(0,1). \tag{19}$$

As a consequence, our parameters $\varrho(\tau)$ become represented by the functions which are independent of k and q,

$$\Omega(p,\xi)=-\frac{1}{\sin\,\tau_{(k,q)}(p,\xi)}=+\frac{p}{\cos(\pi\xi/2)}. \tag{20}$$

The parameters ϱ remain constant over all the lattices $\mathcal{L}_{(p_0,\xi_0)}$ of points $\tau_{(k,q)}(p_0,\xi_0)$ where the sign p_0 and the parameter ξ_0 are temporarily fixed.

1. Verification: Straight-path solution re-visited

At $\omega=0$ and $\mathcal{C}=\mathcal{I}$, the use of the limiting, simplified version

$$\tau=\varrho(\tau)\sigma\,\sinh\,\sigma,\quad \omega=0 \tag{21}$$

of our matching condition (18) leads to an enormous simplification of the construction performed in Ref. 12. There, severe difficulties originated from a strong and pronounced τ-dependence of the factor $\varrho=\varrho(\tau)$ which is a very quickly changing function of its argument τ. In our present setting, the discretization (19) enables us to fix the value of $\varrho=\Omega$ by reducing our attention from all the values of τ to their lattices $\mathcal{L}_{(p,\xi)}$. Treating them separately, one at a time, we only have to keep in mind the overall range of our real constants $\Omega(p,\xi)=p|\Omega(p,\xi)|=p\Omega(+1,\xi)\notin(-1,1)$. This enables us to re-parametrize the matching condition (21),

$$\tau=\tau_{(k,q)}(p,\xi)=\Omega(p,\xi)\sigma\,\sinh\,\sigma,\quad p,\xi=fixed. \tag{22}$$

In the new language, the graph of the function $\Omega\,\sigma\,\sinh\,\sigma$ is a parabolic curve which is oriented up or down at the respective $p=+1$ and $p=-1$. As long as we are interested in the positive $\tau>0$, we may discard $p=-1$ and fix $\tau=\tau_{(k,q)}(+1,\xi)>0$ and $\varrho(\tau)=\Omega(p,\xi)=\Omega(+1,\xi)\geqslant 1$. The curves $\tau=\Omega(+1,\xi)\sigma\,\sinh\,\sigma\equiv\Theta_\xi(\sigma)$ then shrink in proportion to the growth of ξ, proceeding from their broadest $\xi=0$ version (where $|\Omega|=1$) via the narrowing parabolic curves until the degenerate single and upwards-oriented half-line in the limit $\xi\to 1$, i.e., $\Omega\to\infty$. This is illustrated in Fig. 2 where the unlimited shrinking of the curves is sampled at $\xi=0,0.5,0.9$, and $\xi=0.99$.

When we zoom out a stripe of $\tau=\tau_{(k,q)}(p,\xi)$ at a fixed $k=30$ in Fig. 2, we get Fig. 3. In Fig. 3 the variations of τ are determined solely by the changes of ξ and q which are sampled by a few horizontal lines. As long as the right-hand-side function $\Theta_\xi(\sigma)$ depends on both σ and ξ, Eq. (22) will be satisfied *only* at the points of intersection of each particular ξ-marked horizontal line with another particular, ξ-assigned parabolic curve. In this manner the points of intersection $(\sigma_{\xi_m},\tau_{\xi_m})$

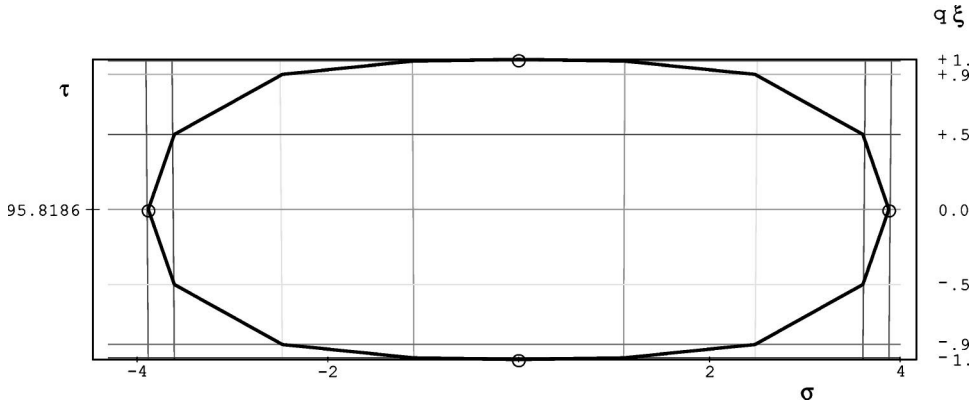

FIG. 3. The oval-shaped matching constraint $\tau=\Theta(\sigma)$ in its ξ-discretization at $\omega=0$ and $k=30$.

in Fig. 3 sample the graphical solution of the matching condition (22). As long as we choose a fairly large stripe number $k=30$, the parabolas of Fig. 2 are represented by the almost straight and almost vertical lines in Fig. 3. This makes the identification of all the intersections particularly easy. We see that the points of intersection form the horizontally prolate ovals, each of which being confined within its $k=k_0$ and $p=+1$ stripe, and not exceeding the interior of the "maximal," $|\Omega|=1$ parabola. It is obvious that the horizontal lines (= lattices of τ) as well as the more or less vertical parabolas move smoothly with the growth of ξ. The resulting picture reproduces precisely our old graphical proof[12] of the existence of solutions at $\omega=0$. Our present new discretization method appears to offer a feasible extension of this proof and analysis to $\omega\neq 0$.

IV. BOUND STATES AT $\omega\neq 0$ IN GRAPHICAL REPRESENTATION

Once we wish to determine the spectrum of the square-well energies $E_n=t_n^2-s_n^2$ at any $\omega\neq 0$, we have to find all the real values of $s=s_n$ and $t=t_n$ which satisfy *both* the constant-coupling constraint (13) *and* the matching condition (17). In the first step, let us re-express the former elementary hyperbolic-curve correlation $Z=2st$ in the new variables σ and τ.

A. The *Z*-dependent hyperbolic-curve constraint

Rotation (15) implies that under the assumption $\omega>0$ we have $\tau>0$ while the sign of σ may be both positive and negative. Alternatively, the choice of $\omega<0$ would imply that we must keep $\sigma>0$ while the sign of τ is allowed to vary. This means that one of the two hyperbolas defined by the rule $Z=2st$ may be discarded immediately. Of course, in our innovated notation we must describe these hyperbolas by the slightly less transparent rotated quadratic equation

$$\tau^2+2\tau\sigma\frac{\cos 2\varphi}{\sin 2\varphi}-\sigma^2-\frac{4Z}{\sin 2\varphi\,\cos^2\varphi}=0. \tag{23}$$

At $\omega=\tan\varphi>0$ it is easy to select the correct branch defined by the formula

$$\tau=\Xi(\sigma)=\frac{1}{2}\left(\omega-\frac{1}{\omega}\right)\sigma+\frac{1}{2}\sqrt{\left(\omega+\frac{1}{\omega}\right)^2\sigma^2+4X^2},\quad X^2=\frac{4Z}{\sin 2\varphi\,\cos^2\varphi}. \tag{24}$$

In parallel, at $\omega=\tan\varphi=-\tilde{\omega}<0$ we must use the *different* formula

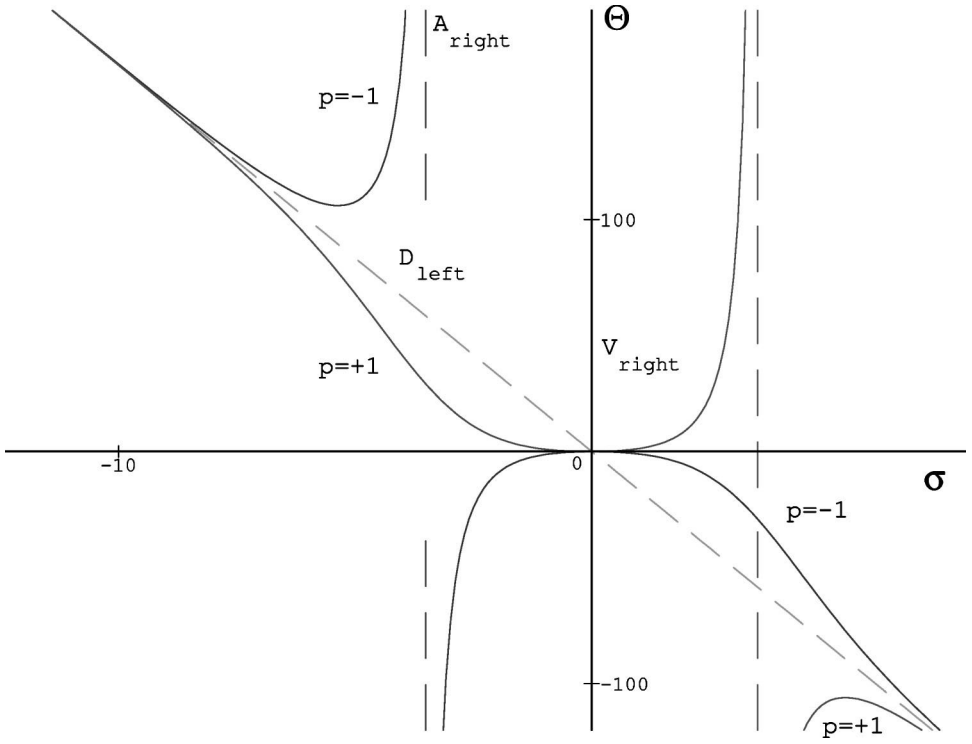

FIG. 4. Two lattice-dependent functions $\tau=\Theta_{(p,0)}(\sigma)$ at $\omega=0.06$.

$$\sigma=\Upsilon(\tau)=\frac{1}{2}\left(\frac{1}{\omega}-\omega\right)\tau+\frac{1}{2}\sqrt{\left(\omega+\frac{1}{\omega}\right)^2\tau^2+4Y^2},\quad Y^2=\frac{-4Z}{\sin 2\varphi\,\cos^2\varphi}. \tag{25}$$

In other words, we must treat the up and down shifts $i\omega$ of the matching point separately, reflecting the fact that we already broke the symmetry between the half-planes of coordinates $x\in\mathbb{C}$ by having chosen the positive coupling $Z>0$ in advance.

B. The second, matching constraint

The application of the lattice-shifting technique of Sec. III B may be extended to both the positive and negative ω. The variable $\tau=\tau_{(k,q)}(p,\xi)$ remains represented by the same function of the interval selector k, of the two sign-variables $q=\pm1$ and $p=\pm1$ and of the continuous ξ varying in the compact interval $(0,1)$.

1. Moving lattices

Let us now select $\omega>0$ and keep the two auxiliary variables p and ξ fixed. This restricts the range of our variable τ to the lattice $\mathcal{L}=\mathcal{L}(p,\xi)$ where the function $\Omega=\Omega(p,\xi)=p/\cos(\pi\xi/2)$ remains constant. This leads to a decisive simplification of our matching condition (18),

$$\tau=\Theta_{(p,\xi)}(\sigma)=\sigma\frac{\omega+\Omega\,\sinh\,\sigma}{1-\Omega\,\omega\,\sinh\,\sigma},\quad p,\xi=fixed. \tag{26}$$

A typical graph of the function $\Theta_{(p,\xi)}(\sigma)$ at both $p=\pm1$ and at the minimal $\xi=0$ and/or $|\Omega|=1$ is displayed in Fig. 4. With respect to the growth of the lattice-characterizing parameter ξ from 0 to 1 it is trivial to see from Eq. (26) that

- at $p=+1$ and $\sigma>0$, the right branch of the well-shaped curve $\Theta_{(+1,\xi)}(\sigma)>0$ is bounded by its perpendicular asymptote at $\sigma_\infty(\xi)=\text{arcsinh}(1/[\omega\Omega(+1,\xi)])$. With the growth of ξ and Ω it inadvertently moves to the left and in the limit of $\xi\to 1$ it coincides with the vertical half-axis $V_{\text{right}}(\sigma_\infty(1)=0)$;
- in parallel, the left branch of the same well moves upwards and coincides with its diagonal asymptote D_{left} in the same limit, $\lim_{\xi\to 1}\Theta_{(+1,\xi)}(\sigma)=-\sigma/\omega$;
- at $p=-1$ and $\sigma<-\sigma_\infty(\xi)<0$, there exists another hyperbolic well sampled in Fig. 4, with definition $\tau=\Theta_{(-1,\xi)}(\sigma)$ and asymptotes D_{left} and (ξ-dependent) A_{right}. With the growth of ξ this well moves downwards and to the right and coincides with the wedge formed by D_{left} and V_{right} at $\xi=1$.

This geometric picture has several consequences. The most important one is that at the minimal $\xi=0$ the curves of Fig. 4 contain the initial points of all the ovals of the solutions in the manner indicated by the $\xi=0$ point in Fig. 3 above. With the growth of ξ the similar oval-shaped curves are then being formed at any ω.

2. Four families of half-ovals

In a continuing description of the structure of solutions of Eq. (26) we must distinguish between the positive and negative σ. For $\sigma\geqslant 0$, the analysis is simpler since the ovals (or rather half-ovals) as sampled in Fig. 3 at $\omega=0$ can solely exist in the stripes with $p=+1$. With the growth of ξ they open their two $q=\pm 1$ branches to the left until they attain their maximal width and reach the boundaries of their stripes on the vertical axis V_{right} in the limit $\xi\to 1$.

At $\sigma<0$ we have to parallel the above half-ovals by their $p=+1$ partners which start to open to the right at the leftmost curve with $\xi=0$. They end their growth at $\xi=1$ while touching the boundaries of their $p=+1$ stripes on the diagonal D_{left}.

In contrast to our above $\omega=0$ exercise in Sec. III B 1, the choice of $\sigma<0$ admits the existence of another family of the half-ovals within the $D_{\text{left}}-V_{\text{right}}$ wedge. Of course, they can only exist within the stripes where $p=-1$ and in the domain of the sufficiently large $\tau\gtrsim\tau_0$ (i.e., at $k\geqslant k_{\text{minimal}}$) where they can originate on the curve $\tau=\Theta_{(-1,0)}(\sigma)\geqslant\tau_0$. In this domain they form the two subfamilies again, depending on whether they originated on the left or right branch of the $\xi=0$ curve.

3. Two patterns of gluing the half-ovals

With the growth of ξ, the left half-ovals within the wedge $D_{\text{left}}-V_{\text{right}}$ open to the left, ending their growth at $\xi=1$ in the intersections of the boundaries of their $p=-1$ stripes with the left diagonal straight line D_{left}. At these points these half-ovals meet their $p=+1$ partners so that in contrast to the $\omega=0$ pattern (with a series of the separated and closed ovals—cf. their picture in Ref. 12), the resulting locus of the solutions forms a wavy, sine-like-shaped line which oscillates to the left and right and moves up to the left along the diagonal D_{left}. As long as this curve remains confined between its two envelopes $\Theta_{(\pm 1,0)}(\sigma)$, the asymptotic decrease of the amplitude of this wobbling is exponential. A schematic example of such a wavy curve appears in Fig. 5.

In the same range of the sufficiently large τ, the second, similar wavy pattern is formed along the axis V_{right}. In exactly the same manner it results from the gluing of the right $p=-1$ half-ovals which open to the right and reach the line V_{right} where they find a continuation in the above-mentioned $p=+1$ half-ovals at $\sigma>0$. In contradistinction to the previous case, the amplitude of the wobbling is asymptotically constant. Still, this fact alone is sufficient to exclude this branch from further consideration because the $Z=2st$ constraint is asymptotically a hyperbola with asymptotes at the angles $\varphi=\arctan\omega$ and $\varphi'=\arctan\omega-\pi/2$ with respect to the axis V_{right}.

In all the remaining domain of the not too large values of τ, just smooth perturbations ocur of the $\omega=0$ pattern of disconnected ovals. At $\omega>0$ the height of the ovals exceeds the height of a single stripe. This is consistent with the fact that an inner part of the ovals lies within the $D_{\text{left}}-V_{\text{right}}$ wedge and must belong, therefore, to a $p=-1$ stripe. This also does not contradict to the steady decrease of the minimum of the graph of the curve $\Theta_{(-1,\xi)}(\sigma)$ since with the growth of ξ the

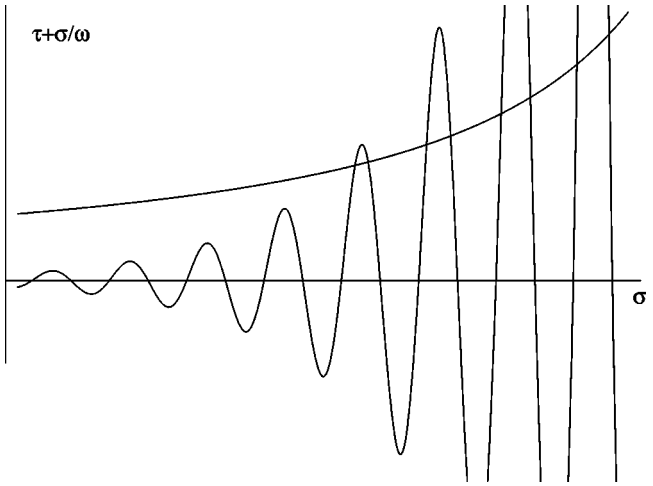

FIG. 5. Damped oscillations of $\Theta(\sigma)$ vs constraint $2st=Z$.

solutions of Eq. (26) start to exist in the lower and lower $p=-1$ stripes within the wedge. In this way, the resulting loci of solutions of Eq. (26) are allowed to form the separate ovals in a fully consistent manner, indeed.

V. ENERGIES

The ultimate goal of our considerations is achieved. We clarified that an optimal strategy of the determination of all the parameters $s=s_n$ and $t=t_n$ in the bound-state formula $E_n=t_n^2-s_n^2$, $n=0,1,\ldots$ is based on a suitable change of variables $(s,t)\to(\sigma,\tau)$ which merely re-scales and rotates the original hyperbolic constraint $Z=2st$ and re-expresses all the real deformed-path square-well energies by the "rotated" formula

$$E=E_n(Z,\varphi)=\tfrac{1}{4}\,[(\tau_n^2-\sigma_n^2)\cos 2\varphi-2\,\sigma_n\tau_n\sin 2\varphi]\cos^2\varphi. \tag{27}$$

This leads to a vital simplification of the matching of wave functions. In the real $\sigma-\tau$ plane, the construction of all the physical bound states (if any) is reduced to an identification of all the admissible parameters (σ_n,τ_n) with all the intersections of a certain pair of curves. One of them is the elementary Z-dependent hyperbola (the smooth curve in Fig. 5). A sufficiently transparent graphical representation of the shape of the second one is more difficult and required in fact the greater portion of our previous text. This curve is sampled by its quickly oscillating asymptotic part in Fig. 5.

A. A comment on asymmetry between $\omega>0$ and $\omega<0$

We mainly paid attention to the positive values of the shift $\omega>0$ pertaining to the generic form of the family of the hyperbolae given by Eq. (24). They are sampled by the smoother curve in Fig. 5. The figure also illustrates a generic pattern of the intersection of these hyperbolas with half-oval families confined within areas specified by their envelope curves exemplified in Fig. 4.

We did not notice in Sec. IV B 1 that after reflection of Fig. 4 with respect to the origin of coordinates σ and τ, its $p=-1$ and $p=+1$ envelope curves are mapped upon each other. This simplifies marginally the construction and follows from the invariance of Eq. (26) *on the lattices* since the simultaneous replacements $\tau\to-\tau$ and $\sigma\to-\sigma$ are equivalent to $\Omega\to-\Omega$ while the latter change of sign merely means that we have to transform $p\to-p$.

We did not deduce, *ibidem*, that another simultaneous sign-change of $\sigma\to-\sigma$ and $\omega\to-\omega$ preserves the form of the original, lattice-independent matching condition (18). This is more important because at the negative $\omega=-\tilde{\omega}<0$ we would be forced to replace the most complicated

pattern of Fig. 4 (where we always employ the positive $\tilde{\omega}=|\omega|$) by its left-right-reflected copy complemented by the corresponding correct hyperbolic branch of curve $Z=2st$ in its alternative form (25). After the left-right mirroring transform it enables us to simplify the situation by returning to the original Fig. 4 complemented by the trivially modified reflected hyperbola

$$\sigma=\Sigma(\tau)=\frac{1}{2}\left(\frac{1}{\tilde{\omega}}-\tilde{\omega}\right)\tau-\frac{1}{2}\sqrt{\left(\tilde{\omega}+\frac{1}{\tilde{\omega}}\right)^2\tau^2+4Y^2},\quad Y^2=\frac{+4Z}{\sin 2\tilde{\varphi}\cos^2\tilde{\varphi}}. \tag{28}$$

Hence, all what we have derived at the positive ω may *immediately* be transferred to the case where ω is negative, *without* changing the half-oval curves and with the mere addition of the second branch (28) of the hyperbola. In Fig. 5 this would just mean a replacement of the upper hyperbola by its minus-sign partner. Of course, such an extension of the whole picture is essentially trivial and it need not be discussed separately at all.

B. The breakdown of $\mathcal{PT}$ symmetry at high energies

Our construction of a closed form of the bound states is transparent and, undoubtedly, potentially useful. For the straight path $\mathcal{C}$ with $\omega=\varphi=0$ and for all the values of $Z>0$ which are not too large, the square-well model already found interesting applications in the study of the spontaneous $\mathcal{PT}$-symmetry breaking at the sufficiently large Z.[22] An even more important role of this model seems to have emerged within the supersymmetric quantum mechanics.[23] In all these and similar applications, our present results simply mean that all the changes caused by a shift of a small size $|\omega|$ remain smooth if and only if we do not move to the very high energies.

In contrast to that, an introduction of *any* nonvanishing shift ω changes the high-energy region completely and abruptly. In place of infinitely many real and positive energies $E_n(Z)$, $n=0,1,\ldots$ which formed the complete spectrum at $\omega=0$, the choice of *any* $\omega=\tan\varphi\neq 0$ makes the number of the real intersections (σ_n,τ_n) *finite*, $n=0,1,\ldots,n_{\max}(Z,\varphi)$ with a certain maximal real energy at $n_{\max}(Z,\varphi)<\infty$. The mathematical foundation of this conclusion is almost trivial: Up to a finite number of exceptions, the energies may only be generated by the intersections in the domain of the large $\tau\gg 1$ where both the Z-dependent hyperbolas with $\omega>0$ and $\omega=-|\omega|<0$ have almost the same asymptotic representation,

$$\tau=-\frac{1}{|\omega|}\sigma\mp\frac{|X^2|}{(|\omega|+1/|\omega|)\sigma}+\mathcal{O}(\sigma^{-3}),\quad \text{sign }\omega=\pm 1,\quad \sigma\ll -1. \tag{29}$$

This means that both of them share the dominant term (representing just the straight line of their common asymptote D_{left}) and approach this asymptote at an inverse-power rate from above or below, respectively (the former case is illustrated in Fig. 5 displaying just the deviation from the asymptote).

The same asymptote D_{left} is further shared by both the upper and lower envelopes $\Theta_{(\mp 1,0)}\times(\sigma)$ of the second, quickly wobbling curve. Nevertheless, from definition (26) we easily derive their leading-order asymptotic form

$$\tau=-\frac{1}{|\omega|}\sigma\mp\frac{|\omega|+1/|\omega|}{\sinh\sigma}+\mathcal{O}(\sinh^{-2}\sigma),\quad \text{sign }\omega=\pm 1,\quad \sigma\ll -1. \tag{30}$$

This implies that the *quick, exponential* decrease of *both* the envelopes in Eq. (30) *guarantees* that the wobbling line cannot have *any* real intersections with *neither* of the two hyperbolic Z-dependent curves (29) with their too slow, power-law rate of approach to the asymptote. This is illustrated in Fig. 5 as a key message of the whole construction and implies that the number of the real energies remains finite at *any* nonvanishing $\omega\neq 0$ and Z. In the other words, infinitely many real energies which existed at $\omega=0$ become "lost" and "dissolved" in complex conjugate pairs. This occurs precisely at the moment when (say, in Fig. 5) the intersecting Z-dependent hyperbola moves (say, due to a slight increase of Z) to the top of a particular half-oval (there, the two energies merge at a "Bender–Wu singularity"[1] or "exceptional point"[3]) and, in the next stage,

TABLE I. Cardinalities $N^{(\text{real})}$ and $N^{(\text{complex})}$ of the square-well energies E with Im $E=0$ and Im $E\neq 0$, respectively.

ω	Z	$N^{(\text{real})}$	$N^{(\text{complex})}$	Comment
0	0	∞	0	Hermitian case
0	$0<Z<4.475\ldots$	∞	0	$\mathcal{PT}$-symmetric case of Ref. 12
0	$4.475\ldots<Z<12.8015\ldots$	∞	2	$\mathcal{PT}$-symmetry broken Ref. 22
0	$Z_N<Z<Z_{N+1}$	∞	2N	$\mathcal{PT}$-symm. br. at $E<E_{\text{crit}}(N)$
$\neq 0$	$\neq 0$	finite	∞	$\mathcal{PT}$-symm. br. at $E>E_{\text{crit}}(Z,\omega)$
$\neq 0$	0	∞	0	new $\mathcal{PT}$-symmetric case

separates from the half-oval completely (Ref. 22 studied this type of a pairwise complexification of the square-well energies at $\omega=0$ in more detail).

The disappearance of the real intersections of the two curves in Fig. 5 occurs at any $Z\neq 0$ and implies that the $\mathcal{PT}$ symmetry of our wave functions becomes broken at all the sufficiently large energies. In the other words, our initial choice of the form of the wave functions does not suddenly represent *all* the possible bound-state solutions. In a way discussed in full detail in our previous $\omega=0$ study[22] this means that all the "missing" bound states must be sought in a certain more-parametric and manifestly $\mathcal{PT}$-symmetry-breaking form.

The only exception in encountered at $Z=0$ where the message offered by Fig. 5 is different because in the limit $Z\to 0$ the upper hyperbolic curve moves down and coincides *strictly* with the horizontal axis. This forces us to return to the very origin of our present construction and repeat all its steps under the new explicit postulate that $t=0$. In this case, the kind reader may easily verify that the $Z=0$ result *proves* in fact *independent* of the value of ω so that all the repeated $Z=0$ and $\omega\neq 0$ (i.e., non-Hermitian though still $\mathcal{PT}$-symmetric) construction returns us back to the energies which *coincide* with the well known Hermitian square-well spectrum.

VI. SUMMARY

All our results are summarized in Table I which may be read, first of all, as an advertisement of our almost involuntary discovery of an extremely elementary and transparent new $\mathcal{PT}$-symmetric model with real energies (cf. the last line). On a more general level, the main item in the review Table I (viz., its last but one line) warns against all the noncritical intuition which might prove misleading in the realm of $\mathcal{PT}$ symmetric models. In this sense, our results may be perceived as a nonnumerical complement to numerical experiments of paper[10] where several "not entirely smooth" potentials clearly inclined towards a spontaneous $\mathcal{PT}$-symmetry breakdown at high energies.

On this background we believe that in the nearest future, attention will be re-attracted to the real role of non-analyticity in the $\mathcal{PT}$ symmetric potentials and models, with inspiration by our present rigorous proof that any nonvanishing shift of ω at $Z\neq 0$ *makes* the $\mathcal{PT}$-symmetry of our square-well model *suddenly* to break down. This breakdown involves infinitely many levels at once, i.e., it occurs in a way which seems characteristic for virtually all the exactly solvable *analytic* models.[11,24] At the same time, the discontinuity of the breakdown might reflect its *nonanalytic* origin, contrasting with the robust survival of the reality of spectra under path-deformations in many not too strongly singular analytic potentials.[25]

We have seen that the square-well model is exceptional in representing a solvable laboratory which seems to lie on a very boundary between "robust" and "fragile" models with $\mathcal{PT}$-symmetry. In this sense, our present key message is encouraging since the geometric language of our innovated "moving-lattice" method proved extremely efficient and seems productive. Its former aspect becomes clear when we compare the $\omega=0$ discussion here and in Ref. 12, while its second property is still to be verified in the future.

ACKNOWLEDGMENTS

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Extremal covariant positive operator valued measures

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We consider the convex set of positive operator valued measures (POVM) which are covariant under a finite dimensional unitary projective representation of a group. We derive a general characterization for the extremal points, and provide bounds for the ranks of the corresponding POVM densities, also relating extremality to uniqueness and stability of optimized measurements. Examples of applications are given. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1806262]

I. INTRODUCTION

An essential step in the design of the new quantum information technology[1] is to assess the ultimate precision limits achievable by quantum measurements in extracting information from physical systems. For example, the security analysis of a quantum cryptographic protocol[2] is based on the evaluation of the limits posed in principle by the quantum laws to any possible eavesdropping strategy. A general method to establish such limits is to optimize a quantum measurement according to a suitable criterion, and this is the general objective of the so-called *quantum estimation theory*.[3,4] Different criteria can be adopted for optimizing the measurement, the choice of a particular one depending on the particular problem at hand. Moreover, many different optimization problems often share the same form, e.g., they resort to the maximization of a concave function on the set of the possible measurements. We remind that measurements form a convex set, the convex combination corresponding to the random choice between two different apparatuses. Since a concave function attains its maximum in an extremal point, it is clear that the optimization problem is strictly connected to the problem of characterizing the extremal points of the convex set.

The quantum measurements interesting in most applications are *covariant*[4] with respect to a group of physical transformations. In a purely statistical description of a quantum measurement in terms of the outcome probability only—i.e., without considering the state-reduction—the measurement is completely described by a positive operator valued measure (POVM) on its probability space. In terms of POVM's, "group covariant" means that there is an action of the transformation group on the probability space which maps events into events, in such a way that when the measured system is transformed according to a group transformation, the probability of a given event becomes the probability of the transformed event. Such a scenario naturally occurs in the estimation of an unknown group transformation performed on a known input state, e.g., in the estimation of an unknown unitary transformation,[5,6] in the measurement of a phase shift in the radiation field,[4,7] or in the estimation of rotations on a system of spins.[8] A first technique for characterizing extremal covariant POVM's and quantum operations has been presented in Ref. 9

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inspired by the method for characterizing extremal correlation matrices of Ref. 10, in particular, classification of extremal POVM's has been presented for the case of trivial stability group, i.e., when the only transformation which leaves the input state unchanged is the identity. Here we solve the characterization problem for extremal covariant POVM's in the general case of nontrivial stability group, providing a simple criterion for extremality in Theorem 1 in terms of minimality of the support of the *seed* of the POVM, presenting iff conditions for extremality in Theorem 3, and providing bounds for the rank of extremal POVM's [in the following we will define the rank of a POVM as the rank of its respective density: see Eq. (6) for its definition]. We show that, contrarily to the usual credo, the optimal covariant POVM can have rank larger than one. Indeed, there are group representations for which covariant POVM cannot have unit rank, since this would violate a general bound for the rank of the POVM in relation to dimensions and multiplicity of the invariant subspaces of the group. In the present paper we adopt the maximum likelihood optimality criterion, which, however, as we will show, is formally equivalent to the solution of the optimization problem in a very large class of optimality criteria. Other issues of practical interest that we address are the uniqueness and the stability of the optimal covariant POVM. The whole derivation is given for finite dimensional Hilbert spaces: as we will show in a simple example, it can be generalized to infinite dimensions, however, at the price of making the theory much more technical.

The paper is organized as follows. After introducing covariant POVM's and their convex structure in Sec. II, the main group theoretical tools that will be used for the characterization of covariant POVM's are presented in Sec. III. In Sec. IV we give a characterization of extremal covariant POVM's in finite dimension with a general stability group, deriving an algebraic extremality criterion, along with a general bound for the rank of the extremal POVM's in terms of the dimensions of the invariant subspaces of the group and of the stability subgroup. Properties of extremal POVM's in relation with optimization problems are analyzed in Sec. V, where also the issues of uniqueness and stability of the optimal covariant POVM's are addressed. Finally, examples of application of the theory to estimation of rotation, state, phase shift, etc., are given in Sec. VI, providing extremal POVM's with a nontrivial stability group and giving examples of optimization problems with solution consisting of extremal POVM with rank greater than one.

II. CONVEX STRUCTURE OF COVARIANT POVM'S

The general description of the statistics of a measurement is given in terms of a probability space $\mathcal{X}$—the set of all possible measurement *outcomes*—equipped with a σ-algebra $\sigma(\mathcal{X})$ of subsets $\mathsf{B}\subseteq\mathcal{X}$ and with a probability measure p on $\sigma(\mathcal{X})$. Each subset $\mathsf{B}\in\sigma(\mathcal{X})$ describes the event "the outcome x belongs to B" and the statistics of the measurement is fully specified by the probability measure p, which associates to any event B its probability $p(\mathsf{B})$.

In quantum mechanics the probability $p(\mathsf{B})$ is given by the Born rule,

$$p(\mathsf{B}) \doteq \mathrm{Tr}[\rho P(\mathsf{B})], \tag{1}$$

where ρ is a density operator (i.e., a positive semidefinite operator with unit trace) on the Hilbert space $\mathcal{H}$ of the measured system, representing its state, whereas P is the POVM of the apparatus, giving the probability measure p for every given state ρ of the quantum system. Mathematically a POVM $P:\sigma(\mathcal{X})\to\mathcal{B}(\mathcal{H})$ is a *positive operator valued measure* on $\sigma(\mathcal{X})$, namely it satisfies the following defining properties:

$$0 \leqslant P(\mathsf{B}) \leqslant I \quad \forall\, \mathsf{B}\in\sigma(\mathcal{X}), \tag{2}$$

$$P(\cup_{i=1}^{\infty}\mathsf{B}_i) = \sum_{i=1}^{\infty} P(\mathsf{B}_i) \quad \forall\, \{\mathsf{B}_i\} \text{ disjoint}, \tag{3}$$

$$P(\mathfrak{X}) = I. \tag{4}$$

Notice that the set of POVM's for $\sigma(\mathfrak{X})$ is a convex set, namely, if P_1 and P_2 are POVM's for $\sigma(\mathfrak{X})$, then also $\lambda P_1 + (1-\lambda)P_2$ is a POVM for $\sigma(\mathfrak{X})$ for any $0 \leqslant \lambda \leqslant 1$. The measurement described by the POVM $\lambda P_1 + (1-\lambda)P_2$ corresponds to randomly choosing between two different measuring apparatuses described by the POVM's P_1 and P_2, respectively. The extremal points of such convex set of POVM's—the so-called *extremal POVM's*—correspond to measurements that cannot result from a random choice between different measuring apparatuses.

In the following we will focus attention to the case of probability space $\mathfrak{X}$ given by the quotient $\mathbf{G}/\mathbf{G}_0$ of a compact Lie group $\mathbf{G}$ with respect to a subgroup $\mathbf{G}_0$. Physically, this situation arises when the POVM is designed to estimate a state in the group-orbit $\{U_g \rho U_g^\dagger | g \in \mathbf{G}\}$ of a given state ρ, with the group $\mathbf{G}$ acting on the Hilbert space $\mathcal{H}$ of a quantum system via the unitary projective representation $\mathsf{R}(\mathbf{G}) \doteq \{U_g | g \in \mathbf{G}\}$. In such a case, in fact, the probability space of the POVM is exactly $\mathfrak{X} = \mathbf{G}/\mathbf{G}_0$, and $\mathbf{G}_0 = \{h \in \mathbf{G} | U_h \rho U_h^\dagger = \rho\}$ is the stability group of ρ, whence the points of the orbit are in one-to-one correspondence with the elements of $\mathfrak{X} = \mathbf{G}/\mathbf{G}_0$. Notice that in the following the fact that the representation is projective is inconsequential, whence there will be no need for reminding.

An important class of measurements with $\mathfrak{X} = \mathbf{G}/\mathbf{G}_0$ is described by the *covariant* POVM's,[4] namely those POVM's which enjoy the property

$$P(g\mathsf{B}) = U_g P(\mathsf{B}) U_g^\dagger \quad \forall\, \mathsf{B} \in \sigma(\mathfrak{X}), \quad \forall\, g \in \mathbf{G}, \tag{5}$$

where $g\mathsf{B} \doteq \{gx | x \in \mathsf{B}\}$. Any POVM P in this class is absolutely continuous with respect to the measure $\mathrm{d}x$ induced on $\mathfrak{X}$ by the normalized Haar measure $\mathrm{d}g$ on the group $\mathbf{G}$, and admits an operator density M, namely

$$M : \mathfrak{X} \to \mathcal{B}(\mathcal{H}), \quad P(\mathsf{B}) = \int_{\mathsf{B}} \mathrm{d}x\, M(x). \tag{6}$$

For a covariant POVM, the operator density has the form[4]

$$M(x) = U_{g(x)} \Xi U_{g(x)}^\dagger, \tag{7}$$

where $g(x) \in \mathbf{G}$ is any element in the equivalence class $x \in \mathfrak{X} = \mathbf{G}/\mathrm{G}_0$, and Ξ is an Hermitian operator satisfying the constraints

$$\Xi \geqslant 0, \quad \int_{\mathbf{G}} \mathrm{d}g\, U_g \Xi U_g^\dagger = I, \tag{8}$$

$$[\Xi, U_h] = 0 \quad \forall\, h \in \mathbf{G}_0. \tag{9}$$

The operator Ξ is usually referred to as the *seed* of the covariant POVM.[11]

Notice that the constraints (8) are needed for positivity and normalization of the probability density, whereas identity (9) guarantees that $M(x) = U_{g(x)} \Xi U_{g(x)}^\dagger$ does not depend on the particular element $g(x)$ in the equivalence class x. It is easy to see that the constraints (8) and (9) still define a convex set C, namely, for any $\Xi_1, \Xi_2 \in \mathsf{C}$ and for any $0 \leqslant \lambda \leqslant 1$ one has $\lambda \Xi_1 + (1-\lambda)\Xi_2 \in \mathsf{C}$. Precisely, the convex set C is the intersection of the cone of positive semidefinite operators with the two affine hyperplanes given by identity (9) and by the normalization condition in Eq. (8). Since a covariant POVM is completely specified by its seed Ξ as in Eq. (7), the classification of the the extremal covariant POVM's resorts to the classification of the extremal points in the convex set C.

III. GROUP THEORETIC TOOLS

Let $\mathbf{G}$ be a compact Lie group, with invariant Haar measure $\mathrm{d}g$ normalized as $\int_{\mathbf{G}}\mathrm{d}g=1$, and consider a unitary representation $\mathsf{R}(\mathbf{G})=\{U_g|g\in\mathbf{G}\}$ on a finite dimensional Hilbert space $\mathcal{H}$. Then $\mathcal{H}$ is decomposed as direct sum of orthogonal irreducible subspaces as follows:

$$\mathcal{H}=\bigoplus_{\mu\in\mathsf{S}}\bigoplus_{i=1}^{m_\mu}\mathcal{H}_i^{(\mu)}, \tag{10}$$

S denoting the collection of equivalence classes of irreducible components of the representation, the classes being labeled by the greek index μ, whereas the italic index i numbers equivalent representations in the same class. Let $T_{ij}^{(\mu)}:\mathcal{H}_j^{(\mu)}\to\mathcal{H}_i^{(\mu)}$ denote invariant isomorphisms connecting the irreducible representations of the equivalence class μ of dimension d_μ, namely for any $i,j=1,\ldots,m_\mu$ $T_{ij}^{(\mu)}:\mathcal{H}_j^{(\mu)}\to\mathcal{H}_i^{(\mu)}$ is an invertible operator satisfying the identity

$$U_gT_{ij}^{(\mu)}U_g^\dagger=T_{ij}^{(\mu)},\quad\forall\, g\in\mathbf{G}. \tag{11}$$

Consistently with this notation $T_{ii}^{(\mu)}$ will denote the projection operator on $\mathcal{H}_i^{(\mu)}$. Since all subspaces $\mathcal{H}_i^{(\mu)}$ are isomorphic, we can equivalently write

$$\bigoplus_{i=1}^{m_\mu}\mathcal{H}_i^{(\mu)}\equiv\mathcal{H}_\mu\otimes\mathcal{M}_\mu, \tag{12}$$

where $\mathcal{H}_\mu$ denotes the *representation space*, i.e., an abstract d_μ-dimensional subspace where a representation of the class μ acts, while $\mathcal{M}_\mu$ denotes the *multiplicity space*, i.e., a m_μ-dimensional space which is unaffected by the action of the group. In this way, the decomposition (10) can be written in the Wedderburn's form,[12]

$$\mathcal{H}=\bigoplus_{\mu\in\mathsf{S}}\mathcal{H}_\mu\otimes\mathcal{M}_\mu. \tag{13}$$

Due to Schur lemmas, an operator O in the commutant of the representation $\mathsf{R}(\mathbf{G})$ can be decomposed as follows:[13]

$$O=\sum_\mu\sum_{i,j=1}^{m_\mu}\frac{\mathrm{Tr}[T_{ji}^{(\mu)}O]}{d_\mu}T_{ij}^{(\mu)}, \tag{14}$$

whereas, in terms of the decomposition (13) one has

$$O=\oplus_{\mu\in\mathsf{S}}(I_\mu\otimes O_\mu), \tag{15}$$

I_μ denoting the identity on the representation space $\mathcal{H}_\mu$, and $O_\mu\in\mathcal{B}(\mathcal{M}_\mu)$ being a suitable set of operators on the multiplicity spaces $\mathcal{M}_\mu$.

In this paper we will consider covariant POVM's with $\mathcal{X}=\mathbf{G}/\mathbf{G}_0$ where both $\mathbf{G}$ and $\mathbf{G}_0$ are compact Lie groups, represented on the Hilbert space $\mathcal{H}$ by the unitary representations $\mathsf{R}(\mathbf{G})=\{U_g|g\in\mathbf{G}\}$ and $\mathsf{R}(\mathbf{G}_0)=\{U_h|h\in\mathbf{G}_0\}$. We will denote with S and S_0 the equivalence classes of irreducible representations of $\mathsf{R}(\mathbf{G})$ and $\mathsf{R}(\mathbf{G}_0)$, respectively. The constraints (8) and (9) can be rewritten in a remarkably simple form using the decompositions of $\mathcal{H}$ in irreducible subspaces under the action of $\mathbf{G}$ and $\mathbf{G}_0$. In fact, due to the invariance of the Haar measure $\mathrm{d}g$, the integral in (8) belongs to the commutant of $\mathsf{R}(\mathbf{G})$. Rewriting the constraint (8) by using (14), one obtains easily,

$$\mathrm{Tr}[T_{ij}^{(\mu)}\Xi]=d_\mu\delta_{ij},\quad\forall\,\mu\in\mathsf{S},\quad\forall\, i,j=1,\ldots,m_\mu. \tag{16}$$

Moreover, according to (8) and (9), the operator Ξ must be a positive semidefinite operator in the commutant of $R(\mathbf{G}_0)$ (9), then we have

$$\Xi = \oplus_{\nu \in \mathsf{S}_0} (I_\nu \otimes X_\nu^\dagger X_\nu), \tag{17}$$

where X_ν is an operator on the multiplicity subspace $\mathcal{M}_\nu$.

IV. EXTREMAL COVARIANT POVM'S WITH A NONTRIVIAL STABILITY GROUP

In this section we will classify the extremal points of the convex set C of covariant seeds, namely the convex set of operators that satisfy both conditions (8) and (9). For the characterization of the extremal points of a convex set we will use the well-known method of perturbations. We will say that the operator $\Theta \in \mathcal{B}(\mathcal{H})$ is a "perturbation" of a given $\Xi \in \mathsf{C}$ if and only if there exists an $\epsilon > 0$ such that $\Xi + t\Theta \in \mathsf{C}$ for any $t \in [-\epsilon, \epsilon]$. With such definition one has that an operator Ξ is extremal if and only if its unique perturbation is the trivial one, namely if Θ is a perturbation of Ξ then $\Theta = 0$.

Let us start with a simple lemma which is useful for the characterization of the perturbations of a given seed Ξ.

Lemma 1: Let $\Xi \in \mathcal{B}(\mathcal{H})$ be a positive semidefinite operator. Then, for any Hermitian $\Theta \in \mathcal{B}(\mathcal{H})$ the condition

$$\exists \epsilon > 0: \quad \forall\, t \in [-\epsilon, \epsilon]\ \Xi + t\Theta \geqslant 0 \tag{18}$$

is equivalent to

$$\mathsf{Supp}(\Theta) \subseteq \mathsf{Supp}(\Xi). \tag{19}$$

Proof: Suppose that the condition (18) holds. Then for any $|\phi\rangle \in \mathsf{Ker}(\Xi)$ one necessarily has $\langle\phi|\Theta|\phi\rangle = 0$. Therefore, for any vector $|\psi\rangle \in \mathcal{H}$ one has

$$|\langle\psi|\Theta|\phi\rangle| = \frac{1}{t}|\langle\psi|(\Xi + t\Theta)|\phi\rangle| \leqslant \frac{1}{t}\sqrt{\langle\psi|(\Xi + t\Theta)|\psi\rangle\langle\phi|(\Xi + t\Theta)|\phi\rangle} = 0.$$

Hence $\mathsf{Ker}(\Xi) \subseteq \mathsf{Ker}(\Theta)$, implying that $\mathsf{Supp}(\Theta) \subseteq \mathsf{Supp}(\Xi)$. Conversely, suppose that (19) holds. Let us denote by λ the smallest nonzero eigenvalue of Ξ and by $\|\Theta\|$ the norm of Θ, then condition (18) holds with $\epsilon = \lambda / \|\Theta\|$. ■

Using the previous lemma we can state that an Hermitian operator Θ is a perturbation for a given seed Ξ if and only if the following conditions are satisfied:

$$\mathsf{Supp}(\Theta) \subseteq \mathsf{Supp}(\Xi), \tag{20}$$

$$\mathrm{Tr}[\Theta T_{ij}^{(\mu)}] = 0 \quad \forall\, \mu \in \mathsf{S}, \quad \forall\, i,j = 1, \ldots, m_\mu, \tag{21}$$

$$[\Theta, U_h] = 0 \quad \forall\, h \in \mathbf{G}_0 \tag{22}$$

[conditions (21) and (22) follow directly from the normalization constraints (16) and (17)].

This set of conditions leads to an interesting property of extremal seeds.

Theorem 1: *Ξ is an extremal point of C if and only if for any $\zeta \in \mathsf{C}$ one has*

$$\mathsf{Supp}(\zeta) \subseteq \mathsf{Supp}(\Xi) \Rightarrow \zeta = \Xi. \tag{23}$$

Proof: To prove necessity it is sufficient to define $\Theta \doteq \Xi - \zeta$ and note that it is a perturbation of Ξ. In fact, Θ is in the commutant of $\mathsf{R}(\mathbf{G}_0)$, $\mathsf{Supp}(\Theta) \subseteq \Xi$, and $\mathrm{Tr}[\Theta T_{ij}^{\mu}] = 0\ \forall \mu \in \mathsf{S}$, $\forall i, j = 1, \ldots, m_\mu$. But, since Ξ is extremal, then Θ must be zero.

Vice versa, assume (23). If Θ is a perturbation for Ξ, then there exists some $t \neq 0$ such that $\zeta \doteq \Xi + t\Theta \in \mathsf{C}$. But a perturbation must satisfy (19), then $\mathsf{Supp}(\zeta) \subseteq \mathsf{Supp}(\Xi)$. Using (23) it is then clear that $\Theta = t^{-1}(\zeta - \Xi) = 0$. ■

The proposition tells us that extremal seeds have "minimal support," in the sense that there is no element $\zeta \in \mathsf{C}$ with $\mathsf{Supp}(\zeta) \subseteq \mathsf{Supp}(\Xi)$ which is different from Ξ.

Theorem 2: *Let be* $\Xi \in \mathsf{C}$. *Write* Ξ *in the form* (17). *Then an operator* Θ *is a perturbation of* Ξ *if and only if*

$$\mathrm{Tr}[\Theta T_{ij}^{(\mu)}] = 0 \quad \forall\, \mu \in \mathsf{S}, \quad \forall\, i,j = 1, \ldots, m_\mu \tag{24}$$

and Θ *can be written as follows:*

$$\Theta = \oplus_{\nu \in \mathsf{S}_0} (I_\nu \otimes X_\nu^\dagger A_\nu X_\nu), \tag{25}$$

with $X_\nu \in \mathcal{B}(\mathcal{M}_\nu)$ *and* $A_\nu \in \mathcal{B}(\mathsf{Rng}(X_\nu))$ *Hermitian* $\forall\, \nu \in \mathsf{S}_0$.

Proof: Suppose Θ is a perturbation. Condition (21) is the same as (24). Due to the condition (22), Θ must be an Hermitian operator in the commutant of $\mathsf{R}(\mathbf{G}_0)$, then we can write it in the block form $\Theta = \oplus_{\nu \in \mathsf{S}_0} (I_\nu \otimes O_\nu)$, with each $O_\nu \in \mathcal{B}(\mathcal{M}_\nu)$ Hermitian. Moreover, condition (20) along with (17) imply that each operator O_ν must have $\mathsf{Supp}(O_\nu) \subseteq \mathsf{Supp}(X_\nu^\dagger X_\nu) = \mathsf{Supp}(X_\nu)$. Using the singular value decomposition $X_\nu = \sum_{i=1}^{r_\nu} \lambda_i^{(\nu)} |w_i^{(\nu)}\rangle\langle v_i^\nu|$ [$\{|v_i^\nu\rangle\}$ and $\{|w_i^{(\nu)}\rangle\}$ are orthonormal bases for $\mathsf{Supp}(X_\nu)$ and $\mathsf{Rng}(X_\nu)$, respectively] one can see that any Hermitian operator O_ν with $\mathsf{Supp}(O_\nu) \subseteq \mathsf{Supp}(X_\nu)$ admit the decomposition $O_\nu = X_\nu^\dagger A_\nu X_\nu$, with A_ν Hermitian operator in $\mathcal{B}(\mathsf{Rng}(X_\nu))$. Conversely, if both conditions (24) and (25) hold, then conditions (20)–(22) are obviously fulfilled. ■

Theorem 3: *Let* P_ν *be the projection operator onto the subspace* $\mathcal{H}_\nu \otimes \mathcal{M}_\nu \subseteq \mathcal{H}$ *corresponding to the class* $\nu \in \mathsf{S}_0$. *An operator* $\Xi \in \mathsf{C}$ *written in the form* $\Xi = \oplus_{\nu \in \mathsf{S}_0} (I_\nu \otimes X_\nu^\dagger X_\nu)$ *is extremal if and only if*

$$\oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu)) = \mathsf{Span}\{F_{ij}^{(\mu)} | \mu \in \mathsf{S},\ i,j = 1, \ldots, m_\mu\}, \tag{26}$$

where

$$F_{ij}^{(\mu)} \doteq \oplus_{\nu \in \mathsf{S}_0} X_\nu \, \mathrm{Tr}_{\mathcal{H}_\nu}[P_\nu T_{ij}^{(\mu)} P_\nu] X_\nu^\dagger.$$

Proof: Using the characterization of Theorem 2, we know that Ξ is extremal if and only if for any operator Θ satisfying (24) and (25) one has $\Theta = 0$. Let us take Θ in the form (25), and rewrite the direct sum as an ordinary sum

$$\Theta = \sum_{\nu \in \mathsf{S}_0} P_\nu (I_\nu \otimes X_\nu^\dagger A_\nu X_\nu) P_\nu, \tag{27}$$

using the projectors P_ν onto $\mathcal{H}_\nu \otimes \mathcal{M}_\nu$. Using invariance of trace under cyclic permutations, we can write

$$\mathrm{Tr}[\Theta T_{ij}^{(\mu)}] = \sum_{\nu \in \mathsf{S}_0} \mathrm{Tr}[(I_\nu \otimes A_\nu)(I_\nu \otimes X_\nu) P_\nu T_{ij}^{(\mu)} P_\nu (I_\nu \otimes X_\nu^\dagger)] = \sum_{\nu \in \mathsf{S}_0} \mathrm{Tr}[A_\nu X_\nu \mathrm{Tr}_{\mathcal{H}_\nu}[P_\nu T_{ij}^{(\mu)} P_\nu] X_\nu^\dagger]. \tag{28}$$

Define the space $\mathcal{R} \doteq \oplus_{\nu \in \mathsf{S}_0} \mathsf{Rng}(X_\nu)$ and denote as $\oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu))$ the linear space of operators acting on $\mathcal{R}$ which are block diagonal on the subspaces $\mathsf{Rng}(X_\nu)$, $\nu \in \mathsf{S}_0$. Then, the extremality condition for Ξ becomes: for any Hermitian operator $A \in \oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu))$ one has

$$\mathrm{Tr}[A F_{ij}^{(\mu)}] = 0 \ \ \forall\, \mu \in \mathsf{S}, \quad \forall\, i,j = 1, \ldots, m_\mu \Rightarrow A = 0. \tag{29}$$

In terms of the Hilbert–Schmidt product $(A,B) \doteq \mathrm{Tr}[A^\dagger B]$ this condition says that the unique Hermitian operator $A \in \oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu))$ which is orthogonal to the whole set of operators $\mathsf{F} \doteq \{F_{ij}^{(\mu)} | \mu \in \mathsf{S},\ i,j = 1, \ldots, m_\mu\}$ is the null operator. Orthogonality to the set F is equivalent to orthogonality to the set of Hermitian operators $\mathsf{F}' = \{(F_{ij}^{(\mu)} + F_{ji}^{(\mu)}), i(F_{ij}^{(\mu)} - F_{ji}^{(\mu)}) | \mu \in \mathsf{S},\ i,j = 1, \ldots, m_\mu\}$. Such orthogonality holds if and only if F' is a spanning set for the real space of Hermitian operators in $\oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu))$. Nevertheless, using the Cartesian decomposition we see that any complex block operator $O \in \oplus_{\nu \in \mathsf{S}_0} \mathcal{B}(\mathsf{Rng}(X_\nu))$ can be written as a sum of two Hermitian

ones, whence the extremality condition is equivalent to $\mathsf{Span}(\mathsf{F}') = \oplus_{\nu\in\mathsf{S}_0}\mathcal{B}(\mathsf{Rng}(X_\nu)$. Finally, the observation $\mathsf{Span}(\mathsf{F}') = \mathsf{Span}(\mathrm{F})$ completes the proof. ■

Notice that for trivial stability group $\mathbf{G}_0 = \{e\}$ (e denotes the identity element), we recover the characterization of Ref. 9: there, one has indeed a single equivalence class $\overline{\nu}$ in S_0 with one-dimensional representation space $\mathcal{H}_{\overline{\nu}}$ so that the whole Hilbert space $\mathcal{H}$ is isomorphic to the multiplicity space $\mathcal{M}_{\overline{\nu}}$ and the extremality condition (26) reduces to $\mathsf{Span}\{XT_{ij}^{(\mu)}X^\dagger \,|\, \mu\in\mathsf{S},\ i,j = 1,\ldots,m_\mu\} = \mathcal{B}(\mathsf{Rng}(X))$.

Corollary 1: Any rank-one seed is extremal.

Proof: Let Ξ be a rank-one seed. In this case there is only one class ν_0 in the decomposition (17) of Ξ (otherwise Ξ could not have unit rank), and the space $\mathcal{B}(\mathsf{Rng}(X_{\nu_0}))$ to be spanned is one dimensional, whence the condition (26) is always satisfied. ■

An alternative proof of Corollary 1 follows by observing that any rank-one element of the cone D of positive semidefinite operators is necessarily extremal for such cone: since the convex set C is a subset of D, a rank-one seed $\Xi\in\mathsf{C}$ is necessarily an extreme point of C.

Corollary 2: Let $\Xi\in\mathsf{C}$ be an extremal seed and write it in the form $\Xi = \oplus_{\nu\in\mathsf{S}_0}(I_\nu\otimes X_\nu^\dagger X_\nu)$. Define $r_\nu \doteq \mathrm{rank}(X_\nu)$. Then

$$\sum_{\nu\in\mathsf{S}_0} r_\nu^2 \leqslant \sum_{\mu\in\mathsf{S}} m_\mu^2. \tag{30}$$

Proof: This relation follows directly from the extremality condition by noting that the left-hand side is the dimension of the complex linear space of block operators $\oplus_{\nu\in\mathsf{S}_0}\mathcal{B}(\mathsf{Rng}(X_\nu))$, while the right-hand side is the cardinality of the spanning set $\mathsf{F} = \{F_{ij}^{(\mu)} \,|\, \mu\in\mathsf{S},\ i,j = 1,\ldots,m_\mu\}$. ■

In Sec. VI we will see an explicit example of extremal POVM which achieves this bound.

V. EXTREMAL POVM'S AND OPTIMIZATION PROBLEMS

A crucial step in a quantum estimation approach is the optimization of the estimation strategy for a given figure of merit. This consists in finding the POVM which maximizes some linear (more generally concave) functional $\mathcal{F}$—e.g., the average fidelity of the estimated state with the true one. Then, the convex structure of the set of POVM's plays a fundamental role in this problem, since, due to concavity of $\mathcal{F}$, one can restrict the optimization procedure to the extremal POVM's only.

In the covariant case, the problem resorts to optimize the state estimation in the orbit $\{U_g\rho U_g^\dagger \,|\, g\in\mathbf{G}\} \simeq \mathbf{G}/\mathbf{G}_0$ of a given state ρ under the action of a group $\mathbf{G}$, $\mathbf{G}_0$ being the stability group of ρ. The optimization typically is the maximization of a linear functional corresponding to the average value of a positive function $f(x,x_*)$, where the average is taken over all the couples (x,x_*) of measured and true values x, $x_*\in\mathcal{X}\doteq\mathbf{G}/\mathbf{G}_0$, respectively. The joint probability density $p(x,x_*)$ is connected to the conditional density $p(x\,|\,x_*)$ given by the Born rule via Bayes, assuming an *a priori* probability distribution of the true value x_*. In the covariant problem the function f enjoys the invariance property $f(gx,gx_*) = f(x,x_*)\ \forall g\in\mathbf{G}$, and is taken as a decreasing function of the distance $|x-x_*|$ of the measured value x from the true one x_*. In the case of compact $\mathbf{G}$ one can assume a uniform *a priori* distribution for x_* values, so that the functional corresponding to the average can be written as follows:

$$\mathcal{F}_\rho[\Xi] = \int_{\mathbf{G}} \mathrm{d}g \int_{\mathbf{G}} \mathrm{d}g_*\, f(gx_0,g_*x_0)\mathrm{Tr}[U_{g_*}\rho U_{g_*}^\dagger U_g \Xi U_g^\dagger] \tag{31}$$

$$= \int_{\mathbf{G}} \mathrm{d}g\, f(x_0,gx_0)\mathrm{Tr}[U_g\rho U_g^\dagger \Xi], \tag{32}$$

where x_0 is the equivalence class containing the identity. In the following, we will consider as the prototype optimization problem the maximization of the likelihood functional[3,4]

$$\mathcal{L}_\rho[\Xi] \doteq \mathrm{Tr}[\rho\Xi], \tag{33}$$

corresponding to the choice $f(x,x_*)=\delta(x-x_*)$ in Eq. (31). Maximizing $\mathcal{L}_\rho[\Xi]$ means maximizing the probability density that the measured value x coincides with the true value x_*. For such estimation strategy the optimization problem has a remarkably simple form, enabling a general treatment for a large class of group representations.[13] Moreover, the solution of the maximum likelihood is formally equivalent to the solution of any optimization problem with a positive (which, a part from an additive constant, means bounded from below) summable function $f(x,x_*)$. Indeed, we can define the map

$$\mathcal{M}(\rho) = k^{-1}\int_{\mathbf{G}} \mathrm{d}g\, f(x_0,gx_0)U_g\rho U_g^\dagger, \tag{34}$$

where $k=\int_{\mathbf{G}}\mathrm{d}g\, f(x_0,gx_0)$. This map is completely positive, unital and trace preserving, and, in particular, $\mathcal{M}(\rho)$ is a state. With this definition, we have

$$\mathcal{F}_\rho[\Xi] = k\mathcal{L}_{\mathcal{M}(\rho)}[\Xi], \tag{35}$$

whence the maximization of $\mathcal{F}_\rho$ is equivalent to the maximization of the likelihood for the transformed state $\mathcal{M}(\rho)$.

Essentially all optimal covariant measurements known in the literature are represented by rank-one operators. The rank-one assumption often provides a useful instrument for simplifying calculations. Nevertheless, as we will show in the following, the occurrence of POVM's with rank grater than one is unavoidable in some relevant situations.

Proposition 1: For any $\Xi\in\mathsf{C}$,

$$\mathrm{rank}[\Xi] \geqslant \max_{\mu\in\mathsf{S}}\left(\frac{m_\mu}{d_\mu}\right). \tag{36}$$

Proof: Let us decompose $\mathcal{H}$ into irreducible subspaces for the representation $\mathsf{R}(\mathbf{G})$ of $\mathbf{G}$ as follows:

$$\mathcal{H} = \oplus_{\mu\in\mathsf{S}}\oplus_{i=1}^{m_\mu}\mathcal{H}_i^{(\mu)}. \tag{37}$$

Take an orthonormal basis $\mathsf{B}_i^{(\mu)}=\{|(\mu,i),n\rangle\,|\,n=1,\ldots,d_\mu\}$ for each subspace $\mathcal{H}_i^{(\mu)}$ in such a way that $|(\mu,i),n\rangle = T_{ij}^{(\mu)}|(\mu,j),n\rangle$ for any n, $T_{ij}^{(\mu)}:\mathcal{H}_j\to\mathcal{H}_i$ being the invariant isomorphism which intertwines the equivalent representations (μ,i) and (μ,j). Diagonalize Ξ as

$$\Xi = \sum_{k=1}^{\mathrm{rank}(\Xi)} |\eta_k\rangle\langle\eta_k| \tag{38}$$

and write

$$|\eta_k\rangle = \sum_{\mu\in\mathsf{S}}\sum_{i=1}^{m_\mu}\sum_{n=1}^{d_\mu} c^k_{(\mu,i),n}|(\mu,i),n\rangle. \tag{39}$$

Since $\langle\eta_k|T_{ij}^{(\mu)}|\eta_k\rangle=\sum_{n=1}^{d_\mu}c^{k*}_{(\mu,i),n}c^k_{(\mu,j),n}$, the normalization constraints (16) become

$$\sum_{k=1}^{\mathrm{rank}(\Xi)}\sum_{n=1}^{d_\mu} c^{k*}_{(\mu,i),n}c^k_{(\mu,j),n} = d_\mu\delta_{ij}. \tag{40}$$

This relation implies that for any $\mu\in\mathsf{S}$ the vectors $\{\mathbf{c}_{(\mu,i)}\,|\,i=1,\ldots,m_\mu\}$ defined by $(\mathbf{c}_{(\mu,i)})_{k,n}\doteq c^k_{(\mu,i),n}$ are orthogonal: since they are m_μ orthogonal vectors in a linear space whose dimension is $d_\mu\times\mathrm{rank}(\Xi)$, it follows that $m_\mu\leqslant d_\mu\times\mathrm{rank}(\Xi)$, hence $\mathrm{rank}(\Xi)\geqslant m_\mu/d_\mu\ \forall\,\mu\in\mathsf{S}$. ■

Summarizing, every times $m_\mu > d_\mu$ for some class $\mu \in \mathsf{S}$, a covariant POVM cannot be represented by a rank-one seed, due to the normalization constraints.

The previous proposition exhibits a structural reason for which, in the presence of equivalent representations, the set C of covariant seeds may contain only elements with rank greater than one. On the other hand, in the following we will discuss the occurrence of covariant POVM's with rank greater than one in explicit optimization problems, independently of the presence of equivalent representations.

Proposition 2: Let Ξ be an extremal point of C. *Denote by P the projector onto* $\mathsf{Supp}(\Xi)$, *and let* $r \doteq \mathrm{rank}(P)$. *Then Ξ is the unique seed which maximizes the likelihood for the state* $\rho = P/r$.

Proof: First, we need to prove that Ξ commutes with the representation $\mathsf{R}(\mathbf{H}_0) \doteq \{U_k | k \in \mathbf{H}_0\}$, where $\mathbf{H}_0$ is the stability group of ρ. Define the group average

$$\xi \doteq \frac{\int_{\mathbf{H}_0} \mathrm{d}h\, U_h \Xi U_h^\dagger}{\int_{\mathbf{H}_0} \mathrm{d}h}. \tag{41}$$

Since $\mathsf{R}(\mathbf{H}_0)$ is the stability group of the projector onto $\mathsf{Supp}(\Xi)$, clearly $\mathsf{Supp}(\Xi)$ is invariant under $\mathsf{R}(\mathbf{H}_0)$, whence ξ satisfies $\mathsf{Supp}(\xi) \subseteq \mathsf{Supp}(\Xi)$. Moreover, using the invariance of the Haar measure it is easy to see that ξ commutes with $\mathsf{R}(\mathbf{H}_0)$. Finally, ξ is an element of C. In fact, it is positive semidefinite, satisfies (16) and commutes with $\mathsf{R}(\mathbf{G}_0)$, which is by definition a subset of $\mathsf{R}(\mathbf{H}_0)$. Since Ξ is extremal, using Theorem 1 we can conclude that $\Xi = \xi$, whence Ξ commutes with $\mathsf{R}(\mathbf{H}_0)$.

Let us prove now optimality. For any arbitrary seed $\zeta \in \mathsf{C}$, the following bound holds:

$$\mathcal{L}_\rho[\zeta] = \mathrm{Tr}[\rho\zeta] = \frac{\mathrm{Tr}[P\zeta]}{r} \leqslant \frac{\mathrm{Tr}[\zeta]}{r} = \frac{\dim(\mathcal{H})}{r}, \tag{42}$$

where the last equality follows from the normalization constraints (16). Clearly Ξ achieves the bound, whence it is optimal. Notice that the inequality $\mathrm{Tr}[P\zeta] \leqslant \mathrm{Tr}[\zeta]$ becomes equality if and only if $\mathsf{Supp}(\zeta) \subseteq \mathsf{Supp}(\Xi)$, then using Theorem 1 we can see that Ξ represents the unique optimal POVM. ■

Consider now a density matrix σ with support in the orthogonal complement of $\mathsf{Supp}(\Xi)$, and consider the randomization

$$\rho = (1-\alpha)\frac{P}{r} + \alpha\sigma, \tag{43}$$

with $0 \leqslant \alpha \leqslant 1$. In the following we prove that, for sufficiently small $\alpha > 0$, Ξ is still optimal for the maximum likelihood strategy. In other words, the extremal POVM represented by Ξ is stable under randomization, and the same measuring apparatus can be used for a larger class of mixed states.

Proposition 3: Consider the randomized state ρ in (43) and denote by $\overline{q}$ the maximum eigenvalue of σ. If $\alpha < 1/(1+r\overline{q})$, then Ξ is the unique seed which maximizes the likelihood for the state ρ.

Proof: First, notice that Ξ commutes with the representation $\mathsf{R}(\mathbf{H}_0)$ of the stability group of ρ. This follows from the observation that the condition $\alpha < 1/(1+r\overline{q})$ implies that $(1-\alpha)/r$ is strictly the largest eigenvalue of ρ. Then, P is the projector on the eigenspace with maximum eigenvalue of ρ, while, for any $h \in \mathbf{G}$, $P_h \doteq U_h P U_h^\dagger$ is the projector on the eigenspace with maximum eigenvalue of $\rho_h \doteq U_h \rho U_h^\dagger$. If $h \in \mathbf{H}_0$ then it must be $\rho_h = \rho$, and, necessarily, $P_h = P$. Therefore $\mathbf{H}_0$ is a subgroup of the stability group of P. But Ξ commutes with the representation of the stability group of P, as proven in Proposition 2, then it commutes also with $\mathsf{R}(\mathbf{H}_0)$.

Now we prove optimality of Ξ. Let us denote by Q the projection onto $\mathsf{Supp}(\sigma)$. The following bound holds for any $\zeta \in \mathsf{C}$:

$$\mathcal{L}_\rho[\zeta] = \frac{(1-\alpha)}{r}\,\mathrm{Tr}[P\zeta] + \alpha\,\mathrm{Tr}[\sigma\zeta] \tag{44}$$

$$\leqslant \frac{(1-\alpha)}{r}\,\mathrm{Tr}[P\zeta] + \alpha\overline{q}\,\mathrm{Tr}[Q\zeta] \tag{45}$$

$$\leqslant \frac{(1-\alpha)}{r}\,\mathrm{Tr}[(P+Q)\zeta] \tag{46}$$

$$\leqslant \frac{(1-\alpha)}{r}\,\mathrm{Tr}[\zeta] = \frac{(1-\alpha)}{r}\,\dim(\mathcal{H}). \tag{47}$$

This bound is achieved by Ξ, proving its optimality. Notice that Ξ is the unique optimal seed. In fact, equality in (46) is attained if and only if $\mathrm{Tr}[Q\zeta]=0$, namely when $\mathsf{Supp}(Q)\subseteq\mathsf{Ker}(\zeta)$, while in (47) equality is attained if and only if $\mathsf{Supp}(\zeta)\subseteq\mathsf{Supp}(P)\oplus\mathsf{Supp}(Q)$. Therefore the bound is achieved if and only if $\mathsf{Supp}(\zeta)\subseteq\mathsf{Supp}(P)=\mathsf{Supp}(\Xi)$, implying $\zeta=\Xi$. ■

VI. EXAMPLES

A. Extremal POVM's with a nontrivial stability group

Example 1: Consider the group of rotations, represented in a $(2j+1)$-dimensional Hilbert space $\mathcal{H}_j$ by the irreducible representation $R_{\mathbf{n},\varphi} \doteq e^{i\varphi\mathbf{n}\cdot\mathbf{j}}$, where φ is an angle, $\mathbf{n}$ is a unit vector, and $\mathbf{j}\doteq(j_x,j_y,j_z)$ is the angular momentum operator. In this case a covariant estimation in the orbit of a pure state $|\psi\rangle$ generally may involve a nontrivial stability group. This is actually the case when $|\psi\rangle \doteq |jm\rangle_{\mathbf{n_0}}$, is an eigenvector of $\mathbf{n_0}\cdot\mathbf{j}$ for some unit vector $\mathbf{n_0}$. Clearly in such case the stability group $\mathbf{G}_0$ consists of rotations around $\mathbf{n_0}$, and the state estimation in the orbit reduces to the estimation of a rotated direction $\mathbf{n}'$. The same situation arises for any state ρ mixture of eigenvectors of $\mathbf{n_0}\cdot\mathbf{j}$. Without loss of generality, let us take $\mathbf{n_0}$ as the direction of the z axis, and write $\rho=\Sigma_{m=-j}^{j} p_m |jm\rangle\langle jm|$ with $p_m \geqslant 0\ \forall m$. Let us denote by P the projector onto $\mathsf{Supp}(\rho)$, and take $\overline{m}$ such that $p_{\overline{m}}=\max_m\{p_m\}$. Then, since

$$\mathrm{Tr}[\rho\zeta] \leqslant p_{\overline{m}}\,\mathrm{Tr}[P\Xi] \leqslant p_{\overline{m}}\,\mathrm{Tr}[\Xi] = p_{\overline{m}}(2j+1),$$

one has that $\Xi=(2j+1)|j\overline{m}\rangle\langle j\overline{m}|$ is the optimal POVM. Notice that such POVM commutes with the stability group $\mathsf{R}(\mathbf{G}_0)$ and is extremal, as a consequence of Corollary 1.

Example 2: Consider the group $\mathbb{SU}(d)$ of unitary $d\times d$ matrices with unit determinant, acting on the space $\mathcal{H}\doteq\mathbb{C}^d$. It is easy to see that each vector $|\psi\rangle\in\mathcal{H}$ has a nontrivial stability group $\mathbf{G}_0\equiv\mathbb{U}(d-1)$. In fact, by introducing an orthonormal basis $\mathsf{B}_\perp\doteq\{|n\rangle\,|\,n=1,\ldots,d-1\}$ for the orthogonal complement $\mathcal{H}^\perp$ of the line $\mathsf{Span}\{|\psi\rangle\}$, and the basis $\mathsf{B}\doteq|\psi\rangle\cup\mathsf{B}_\perp$ for $\mathcal{H}$, the stability group $\mathbf{G}_0$ consists on matrices of the form

$$U_h = \begin{pmatrix} \omega_h & \mathbf{0} \\ \mathbf{0} & V_h \end{pmatrix}, \tag{48}$$

where $\omega_h\in\mathbb{C}$, $|\omega_h|=1$, and V_h is a unitary $(d-1)\times(d-1)$ matrix with $\mathrm{Det}(V_h)=\omega_h^*$. Let us consider now the tensor representation $\mathsf{R}(\mathbf{G})=\{U_g^{\otimes 2}\,|\,U_g\in\mathbb{SU}(d)\}$ on the space $\mathcal{H}^{\otimes 2}$. This representation has two irreducible subspaces, the symmetric and the antisymmetric ones $\mathcal{H}_+$ and $\mathcal{H}_-$, with dimensions $d_+=d(d+1)/2$ and $d_-=d(d-1)/2$, respectively. Denote by P_+ and P_- the projectors on $\mathcal{H}_+$ and $\mathcal{H}_-$. Let us apply the representation $\mathsf{R}(\mathbf{G})$ on the state $|\psi\rangle^{\otimes 2}\in\mathcal{H}^{\otimes 2}$. Clearly the stability group is the same $\mathbf{G}_0$ as before, and it is represented by $\mathsf{R}(\mathbf{G}_0)=\{U_h^{\otimes 2}\,|\,h\in\mathbf{G}_0\}$. It is easy to see that

$\mathsf{R}(\mathbf{G}_0)$ contains five irreducible components, carried by the subspaces $\mathcal{H}_1=\mathsf{Span}\{|\psi\rangle^{\otimes 2}\}$, $\mathcal{H}_2=\mathsf{Span}\{|\psi\rangle\}\otimes\mathcal{H}^{\perp}$, $\mathcal{H}_3=\mathcal{H}^{\perp}\otimes\mathsf{Span}\{|\psi\rangle\}$, $\mathcal{H}_4=P_+(\mathcal{H}^{\perp\otimes 2})$, and $\mathcal{H}_5=P_-(\mathcal{H}^{\perp\otimes 2})$. Notice that $\mathcal{H}_2$ and $\mathcal{H}_3$ carry equivalent representations, corresponding to a two-dimensional multiplicity space. An example of extremal POVM is given by

$$\Xi=\frac{d(d+1)}{2}|\psi\rangle\langle\psi|^{\otimes 2}\oplus\frac{d}{d-2}P_-QP_-,$$

where Q is the projection on $\mathcal{H}^{\perp\otimes 2}$. Since the two summands are proportional to $|\psi\rangle\langle\psi|^{\otimes 2}$ and P_-QP_-, which are the projectors on $\mathcal{H}_1$ and $\mathcal{H}_5$, respectively, then Ξ belongs to the commutant of $\mathsf{R}(\mathbf{G}_0)=\{U_h^{\otimes 2}|h\in\mathbf{G}_0\}$. Notice that the subspaces $\mathcal{H}_1$ and $\mathcal{H}_5$ have multiplicities $m_1=m_5=1$, corresponding to one-dimensional multiplicity spaces $\mathcal{M}_1\equiv\mathcal{M}_5\equiv\mathbb{C}$ (whence the partial traces over $\mathcal{H}_{1,5}$ will be c numbers). Moreover, using the fact that $\mathrm{Tr}_{\mathcal{H}_1}[P_+]=1$, $\mathrm{Tr}_{\mathcal{H}_1}[P_-]=0$, $\mathrm{Tr}_{\mathcal{H}_5}[P_+]=0$, $\mathrm{Tr}_{\mathcal{H}_5}[P_-]=(d-1)(d-2)/2$ one can check extremality using the condition (26). Let us observe that in this example we have $r_1=r_5=1$ and $m_+=m_-=1$, where r_1 and r_5 are defined as in Corollary 2, while m_+ and m_- are the multiplicities of the two irreducible representations of $\mathsf{R}(\mathbf{G})$. Then the bound of (30) is saturated. Finally, we remark that this POVM is optimal for discriminating states in the orbit of $|\psi\rangle^{\otimes 2}$,[13] in the orbit of $\rho=(1/r)(|\psi\rangle\langle\psi|^{\otimes 2}+P_-QP_-)$ where $r=1+[(d-1)(d-2)/2]$ because of Proposition 2, and also in the orbit of any randomization $\rho'=(1-\alpha)\rho+\alpha\sigma$ where σ is density matrix with $\mathsf{Supp}(\sigma)\subseteq\mathsf{Ker}(P)$, and $\alpha<1/(1+r)$, because of Proposition 3.

B. Extremal POVM's with rank greater than one

Example 1: Consider the Abelian group $\mathbf{G}=\mathbb{U}(1)$ of phase shifts, acting in the space $\mathcal{H}=\mathbb{C}^d$ by the representation $\mathsf{R}(\mathbf{G})=\{U(\varphi)=\exp(i\varphi N)|\ \varphi\in[-\pi,\pi]\}$, where the generator N is given by $N=\sum_{n=0}^{d-1}n|n\rangle\langle n|$ for some orthonormal basis $\{|n\rangle|n=0,1,\ldots,d-1\}$. The stability group $\mathbf{G}_0$ may be either the whole $\mathbb{U}(1)$ (for ρ diagonal on the eigenstates of the generator), or a discrete subgroup $\mathbf{G}_0=\mathbb{Z}_k$ for some integer k, including the case $k=1$ of trivial stability group. We exclude the degenerate case $\mathbf{G}_0=\mathbb{U}(1)$ of shift invariant states. The parameter space $\mathfrak{X}=\mathbb{U}(1)/\mathbb{Z}_k$ will be a circle, parametrized by an angle $\theta\in[-\pi,\pi]$, and the action of a group element $g(\varphi)\in\mathbf{G}$ on an element $\theta\in\mathfrak{X}$ will be given by $g(\varphi)\theta=\theta+k\varphi$.

Due to constraint (16), a seed Ξ is represented in the eigenbasis of the generator by a correlation matrix, namely by a positive semidefinite matrix with unit diagonal entries. Vice versa, any correlation matrix corresponds to a seed in the case of trivial stability group $\mathbf{G}_0$. In Ref. 10 one can find a constructive method which provides extremal correlation matrices with rank $r>1$: here we show that any of such matrices can be viewed as the optimal seed for the estimation problem in the orbit of a particular state. Let us choose as optimality criterion the maximization of the average value of a positive summable function $f:\mathfrak{X}\times\mathfrak{X}\to\mathbb{R}_+$ depending only on the difference $\theta-\theta_*$ between the measured and the true value. Suppose ρ a state with stability group $\mathbf{G}_0=\mathbb{Z}_k$. As we noted at the beginning of Sec. V, the maximization of $\mathsf{F}_\rho[\Xi]$—the average value of $f(\theta-\theta_*)$—corresponds to the maximization of the likelihood $\mathcal{L}_{\mathcal{M}(\rho)}[\Xi]$ for the transformed state $\mathcal{M}(\rho)=f_0^{-1}\int_{-\pi}^{\pi}(\mathrm{d}\varphi/2\pi)f(-k\varphi)U_\varphi\rho U_\varphi^\dagger$ [from Eq. (34)]. Notice that the map $\mathcal{M}$ is trivially covariant—i.e., $\mathcal{M}(U_\phi\rho U_\phi^\dagger)=U_\phi\mathcal{M}(\rho)U_\phi^\dagger$—since the group is Abelian. For simplicity here we require that the map $\mathcal{M}$ is invertible, whence also $\mathcal{M}^{-1}$ is covariant and trace preserving (but generally not positive). Covariance of $\mathcal{M}$ implies that the stability group of $\mathcal{M}(\rho)$ contains the stability group of ρ, and covariance of $\mathcal{M}^{-1}$ implies the reverse inclusion, whence the stability group is not changed by the maps.

Let us take now an extremal correlation matrix Ξ with $\mathrm{rank}(\Xi)=r\geqslant 1$ and denote by P the projector onto $\mathsf{Rng}(\Xi)$. Using Proposition 2, we can see that Ξ commutes with the representation $\mathsf{R}(\mathbf{H}_0)$, where $\mathbf{H}_0$ is the stability group of P. Call λ the modulus of the minimum eigenvalue of $\mathcal{M}^{-1}(P/r)$, then

$$\rho = \frac{\lambda}{1+d\lambda} I + \frac{1}{1+d\lambda} \mathcal{M}^{-1}(P/r)$$

is a density operator. Notice that the stability group $\mathbf{G}_0$ of ρ is the same stability group of $\mathcal{M}^{-1}(P)$, which coincides with $\mathbf{H}_0$, the stability group of P. Therefore Ξ commutes with the representation $\mathsf{R}(\mathbf{G}_0)$. It is easy to show that Ξ is the unique seed commuting with $\mathsf{R}(\mathbf{G}_0)$ which is also optimal for the estimation of states in the orbit of ρ. In fact, for any ζ in the convex set C of the seeds with stability group $\mathbf{G}_0$, we have

$$\mathsf{F}_\rho[\zeta] = f_0 \operatorname{Tr}[\zeta \mathcal{M}(\rho)] = f_0\left(\frac{\lambda}{1+d\lambda} \operatorname{Tr}[\zeta] + \frac{1}{r(1+d\lambda)} \operatorname{Tr}[\zeta P] \right) \leqslant f_0\left(\frac{d}{r}\right)\left(\frac{1+r\lambda}{1+d\lambda}\right).$$

This bound is achieved choosing $\zeta = \Xi$, moreover, as in Proposition 2, we can observe that the functional $\operatorname{Tr}[\zeta P]$ with $\zeta \in \mathsf{C}$ is maximum if and only if $\zeta = \Xi$, then the maximum is unique.

Example 2: We provide now an example with a noncompact group represented in an infinite dimensional Hilbert space. This example is out of the general treatment of the present paper—which considers only finite dimensions—and is given only with the purpose of showing that our results could be generalized to infinite dimensions, however at the price of much more technical proofs.

Take $\mathcal{H}$ as the Fock space, and consider the projective representationon $\mathcal{H}$ of the group of translations on the complex plane $\mathbb{C}$ in terms of the Weyl–Heisenberg operators $\mathsf{R}(\mathbf{G}) = \{D(\alpha) = e^{\alpha a^\dagger - \bar{\alpha} a} | \alpha \in \mathbb{C}\}$, where $[a, a^\dagger] = 1$. Here we will consider the twofold tensor representation $\{D(\alpha)^{\otimes 2} | \alpha \in \mathbb{C}\}$ on $\mathcal{H}^{\otimes 2}$. Using the unitary operator $V = e^{(\pi/4)(a_1 a_2^\dagger - a_1^\dagger a_2)}$, one can write $D(\alpha)^{\otimes 2} = V(D(\sqrt{2}\alpha) \otimes I) V^\dagger$ and see that the irreducible subspaces of this representation are $\mathcal{H}_n = V(\mathcal{H} \otimes \mathsf{Span}\{|\phi_n\rangle\})$, where $\{|\phi_n\rangle | n = 1, 2, \ldots, \infty\}$ is any orthonormal basis for $\mathcal{H}$. All these subspaces carry equivalent representations, the isomorphism between $\mathcal{H}_m$ and $\mathcal{H}_n$ being

$$T_{mn} = V(I \otimes |\phi_m\rangle\langle\phi_n|) V^\dagger. \tag{49}$$

In terms of these isomorphisms, the normalization constraints (16) for a seed operator become[13]

$$\operatorname{Tr}[T_{mn} \zeta] = 2 \delta_{mn}. \tag{50}$$

Notice that the number 2 in this formula has nothing to do with the dimension of $\mathcal{H}_n$ which is infinite: in the noncompact case the dimensions are replaced by positive numbers depending only on the equivalence class of representations. In principle, since the space $\mathcal{H}^{\otimes 2}$ is infinite dimensional, there is the possibility of extremal covariant POVM's with an infinite rank. Actually we can provide the remarkable example

$$\Xi = 2V(|0\rangle\langle 0| \otimes I) V^\dagger, \tag{51}$$

where $|0\rangle$ is the vacuum state of the Fock basis $\{|m\rangle | a^\dagger a |m\rangle = m |m\rangle\}$. The corresponding POVM can be realized by averaging the outcomes of two independent measurements with $\Xi_1 = |0\rangle\langle 0| \otimes I$ and $\Xi_2 = I \otimes |0\rangle\langle 0|$,[13] which in quantum optics correspond to two heterodyne measurements.[14]

We can observe that Ξ maximizes the likelihood functional for any state of the form $\rho = V(|0\rangle\langle 0| \otimes \sigma) V^\dagger$, where $\sigma = \sum_{n=0}^\infty p_n |\phi_n\rangle\langle\phi_n|$, is a mixed state with $p_n > 0 \, \forall \, n$. In fact, for any seed ζ, one has the bound

$$\begin{aligned} \operatorname{Tr}[V(|0\rangle\langle 0| \otimes \sigma) V^\dagger \zeta] &= \sum_{n=0}^\infty p_n \operatorname{Tr}[V(|0\rangle\langle 0| \otimes |\phi_n\rangle\langle\phi_n|) V^\dagger \zeta] \\ &\leqslant \sum_{n=0}^\infty p_n \operatorname{Tr}[V(I \otimes |\phi_n\rangle\langle\phi_n|) V^\dagger \zeta] = \sum_n p_n \operatorname{Tr}[T_{nn} \zeta] = 2, \end{aligned} \tag{52}$$

and since Ξ achieves the bound (52), it is optimal. Moreover Ξ is the unique optimal seed. In fact,

the equality in (52) is achieved if and only if $\mathrm{Tr}[V(|0\rangle\langle 0|\otimes|\phi_n\rangle\langle\phi_n|)V^\dagger\zeta]=\mathrm{Tr}[V(I\otimes|\phi_n\rangle\times\langle\phi_n|)V^\dagger\zeta]$ for any n: by expanding the identity on the Fock basis, the positivity of ζ implies $\langle m|\langle\phi_n|V^\dagger\zeta V|m\rangle|\phi_n\rangle=0$ for any $m\neq 0$. Hence the unique nonzero diagonal elements of ζ are on the vectors $V|0\rangle|\phi_n\rangle$. On the other hand, the positivity of ζ along with the normalization constraint $\mathrm{Tr}[T_{mn}\zeta]=0\ \forall m\neq n$ imply that all the off diagonal elements of ζ are zero. Hence $\zeta=2V\Sigma_{n=1}^{\infty}(|0\rangle\times\langle 0|\otimes|\phi_n\rangle\langle\phi_n|)V^\dagger=2V(|0\rangle\langle 0|\otimes I)V^\dagger=\Xi$. The fact that Ξ is the unique optimal seed ensures that it is also extremal, otherwise there would be two different seeds which are equally optimal. Notice that Ξ is extremal also according to our characterization (26).

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A new geometrical look at gravity coupled with Yang–Mills fields

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A new geometrical framework for tetrad-affine formulation of gravity, pure or coupled with Yang–Mills fields, is proposed. After analyzing the geometrical properties of the new mathematical setting, field equations are deduced from a variational principle in the Poincaré–Cartan formalism. A generalized Noether Theorem is stated and classical relationship between symmetries and conserved quantities are recovered in the newer scheme. Some explicit examples are given. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1806536]

I. INTRODUCTION

In recent papers,[1,2] we developed a geometrical framework for the description of Lagrangian field theories depending on the derivatives of the fields, only through their antisymmetric combinations.

For example, for Yang–Mills theories,[3–7] where one can interpret the dynamical field A as a connection on a suitable principal fiber bundle, and the strength field F as the associated curvature, only the antisymmetric part of the gradient of A is involved in the construction of F; in this case, the approach outlined in Refs. 1 and 2 allows to cut away the "inessential" coordinates from the geometrical construction, so getting some important results: Taking care from the beginning only of the physical degrees of freedom of the theory, regularizing Yang–Mills Lagrangians and obtaining a simpler action of gauge transformations on the "derivatives" of the dynamical field A.

The aim of this paper is to extend the mathematical machinery to gravity, in a tetrad-affine formulation.

The mathematical arena we chose to formulate our theory is the gauge natural bundle framework for gravity (see, for example, Refs. 8–13). Dynamical fields are metric connections (*a priori* not necessarily torsion-free) and pseudo-orthonormal tetrads. More precisely, metric connections are viewed as principal connections on the structure bundle $[P, M, \pi, \mathrm{SO}(1,3)]$ over the space–time manifold M, while tetrads turn out to be sections of a suitable associated bundle, locally diffeomorphic to the co-frames bundle.

The resulting geometrical framework automatically embodies the Lorentz invariance of the theory; here, in fact, tetrads are truly gauge natural objects, subject to the transformations of the structure bundle P. Moreover, the use of the gauge natural bundle framework also avoids the necessity of assuming the existence of a globally defined tetrad field.

Following the lines traced in Refs. 1 and 2, we construct a new affine bundle over the configuration space of the theory, by changing the standard definition of jet-equivalence.

In the resulting mathematical setting, we describe a class of interaction between the gravitational and the Yang–Mills fields, including minimal coupling, in the Poincaré–Cartan formalism.

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This is achieved by adopting as preferred coordinates in the new space directly the components of the curvature and torsion tensor fields, thereby gauging away all unphysical degrees of freedom.

The paper is organized as follows. In Sec. II, we construct the new bundle as an appropriate quotient space of the standard jet-bundle. In order to implement a variational calculus, we extend to the newly defined space some classical geometrical structures of jet-bundle theory. For simplicity, we develop in detail the purely gravitational case only. The geometrical setting suitable for describing coupled gravitational and Yang–Mills fields is easily obtained joining together the present geometrical framework with the one proposed in Refs. 1 and 2. The argument is entirely straightforward and is left to the reader.

In Sec. III, we define the Poincaré–Cartan form associated with a Lagrangian on the new bundle. We derive the field equations from a variational principle. Both purely gravitational and coupled with Yang–Mills fields cases are explicitly worked out.

In Sec. IV, making use of the Poincaré–Cartan formalism, we state a generalized Nöther Theorem and investigate the relationships between symmetries and conserved currents in the newer scheme. We analyze explicitly the coupled gravitational Yang–Mills Lagrangian in curved space–time and get the conserved quantities related to gauge and diffeomorphism invariance.

The supersymmetric extension of this formalism and the description of the interaction with spinor fields are, at the moment, under investigation and will form the subject of a future work.

II. THE GEOMETRICAL FRAMEWORK

A mathematical scenario suitable for globally describing gravity in the tetrad formalism is the gauge natural bundle framework, where the structure bundle of the theory is a principal fiber bundle $[P,M,\pi,\mathrm{SO}(1,3)]$ over space–time M (see, for example, Refs. 8–12 and references therein).

In this context, denoting by $L(M)$ the frame bundle over M, a tetrad field turns out to be a section of a $GL(4,\Re)$ bundle $\mathcal{E}$, which is the bundle associated with $P\times L(M)$ through the left action

$$\lambda:(\mathrm{SO}(1,3)\times GL(4,\Re))\times GL(4,\Re)\to GL(4,\Re),\quad \lambda(\Lambda,J;X)=\Lambda\cdot X\cdot J^{-1}.$$

Accordingly, local fibered coordinates on $\mathcal{E}\to M$ are functions of the kind x^i, e_i^μ $(i,\mu=1,\ldots,4)$ undergoing the transformation laws

$$\overline{x^j}=\overline{x^j}(x^i),\quad \overline{e_j^\mu}=e_i^\sigma\Lambda^\mu{}_\sigma(x)\frac{\partial x^i}{\partial\overline{x^j}}, \tag{2.1}$$

where $\Lambda^\mu{}_\sigma(x)\in\mathrm{SO}(1,3)$, $\forall x\in M$.

The assignment of a tetrad field $x\to e^\mu(x)=e_i^\mu(x)dx^i$ allows to define a metric over M by setting $g:=\eta_{\mu\nu}e^\mu\otimes e^\nu(g_{ij}:=\eta_{\mu\nu}e_i^\mu e_j^\nu)$, with $\eta:=\mathrm{diag}(-1,1,1,1)$. By construction, g is invariant under transformations (2.1).

In this way, the structure bundle $[P,M,\pi,\mathrm{SO}(1,3)]$ becomes the bundle of orthonormal frames associated with the metric g: For each tetrad e there is an isomorphism between P and $\mathrm{SO}(M,g)$.

Therefore, the quotient bundle $\mathcal{C}:=J_1P/\mathrm{SO}(1,3)$ of principal connections over the structure bundle P is naturally identified with the bundle of g-metric compatible linear connections over M.

As is well known, every connection one-form on P may be expressed locally as

$$\omega(x,\Lambda)=\omega^\mu{}_\nu(x,\Lambda)\otimes\underline{\mathrm{u}}_\mu{}^\nu:=[\Lambda^\mu{}_\sigma\Lambda_\nu{}^\gamma\omega_i{}^\sigma{}_\gamma(x)dx^i-\Lambda_\nu{}^\eta d\Lambda^\mu{}_\eta]\otimes\underline{\mathrm{u}}_\mu{}^\nu, \tag{2.2}$$

where $\omega_i{}^\mu{}_\nu(x)$ are the connection coefficients, $\underline{\mathrm{u}}_\mu{}^\nu$ denote a basis of the Lie algebra $\mathfrak{so}(1,3)$ of SO(1, 3), and $\Lambda_\mu{}^\eta:=(\Lambda^{-1})^\eta{}_\mu$. In view of this, we can put on $\mathcal{C}$ local coordinates of the form x^i, $\omega_i{}^{\mu\nu}(:=\omega_i{}^\mu{}_\sigma\eta^{\sigma\nu})$ with $\mu<\nu$.

Because of the above identification, given a (local) tetrad field $e_i^\mu(x)dx^i$ the transformations (2.1) can be viewed as changes of (local) sections $e^\nu \to \overline{e^\mu} = \Lambda^\mu{}_\nu(x)e^\nu$ of $P \to M$. The latter induce associated changes of (local) trivialization of P itself, in turn yielding corresponding coordinate transformations in $\mathcal{C}$ of the form

$$\overline{x^i} = \overline{x^i}(x^j), \quad \overline{\omega_i}^{\mu\nu} = \Lambda^\mu{}_\sigma(x)\Lambda^\nu{}_\gamma(x)\frac{\partial x^j}{\partial \overline{x^i}}\omega_j{}^{\sigma\gamma} - \Lambda_\sigma{}^\eta(x)\frac{\partial \Lambda^\mu{}_\eta(x)}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^i}}\eta^{\sigma\nu}, \tag{2.3}$$

where $\omega_j{}^{\sigma\gamma} := -\omega_j{}^{\gamma\sigma}$ whenever $\sigma > \gamma$.

Now, let us consider the fibered product $\mathcal{E} \times_M \mathcal{C}$ ($\mathcal{E}\times\mathcal{C}$ for short) over M, between the bundles $\mathcal{E}$ and $\mathcal{C}$.

We apply to the study of the bundle $\mathcal{E}\times\mathcal{C} \to M$ and its sections the whole geometrical machinery developed in Refs. 1 and 2. Referring systematically to Refs. 1 and 2 for proofs, comments and notations, we outline here the main results, especially useful for the present purposes.

First of all, let $J_1(\mathcal{E}\times\mathcal{C}, M)$ be the first jet-bundle associated with $\mathcal{E}\times\mathcal{C} \to M$, referred to jet-coordinates x^i, e_i^μ, $\omega_i{}^{\mu\nu}$, $e_{ij}^\mu (\simeq \partial e_i^\mu / \partial x^j)$, $\omega_{ij}{}^{\mu\nu} (\simeq \partial \omega_i{}^{\mu\nu} / \partial x^j)$. The latter are subject to the transformation laws (2.1) and (2.3) together with

$$\overline{e}_{jk}^\mu = e_{ih}^\sigma \frac{\partial x^h}{\partial \overline{x^k}}\Lambda^\mu{}_\sigma \frac{\partial x^i}{\partial \overline{x^j}} + e_i^\sigma \frac{\partial \Lambda^\mu{}_\sigma}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^k}}\frac{\partial x^i}{\partial \overline{x^j}} + e_i^\sigma \Lambda^\mu{}_\sigma \frac{\partial^2 x^i}{\partial \overline{x^k}\partial \overline{x^j}} \tag{2.4a}$$

and

$$\begin{aligned}\overline{\omega}_{ik}{}^{\mu\nu} = {} & \Lambda^\mu{}_\sigma\Lambda^\nu{}_\gamma \frac{\partial x^j}{\partial \overline{x^i}}\frac{\partial x^h}{\partial \overline{x^k}}\omega_{jh}{}^{\sigma\gamma} + \frac{\partial \Lambda^\mu{}_\sigma}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^k}}\Lambda^\nu{}_\gamma \frac{\partial x^j}{\partial \overline{x^i}}\omega_j{}^{\sigma\gamma} + \Lambda^\mu{}_\sigma \frac{\partial \Lambda^\nu{}_\gamma}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^k}}\frac{\partial x^j}{\partial \overline{x^i}}\omega_j{}^{\sigma\gamma} \\ & + \Lambda^\mu{}_\sigma\Lambda^\nu{}_\gamma \frac{\partial^2 x^j}{\partial \overline{x^k}\partial \overline{x^i}}\omega_j{}^{\sigma\gamma} + - \frac{\partial \Lambda_\sigma{}^\eta}{\partial x^s}\frac{\partial x^s}{\partial \overline{x^k}}\frac{\partial \Lambda^\mu{}_\eta}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^i}}\eta^{\sigma\nu} - \Lambda_\sigma{}^\eta \frac{\partial^2 \Lambda^\mu{}_\eta}{\partial x^s \partial x^h}\frac{\partial x^s}{\partial \overline{x^k}}\frac{\partial x^h}{\partial \overline{x^i}}\eta^{\sigma\nu} \\ & - \Lambda_\sigma{}^\eta \frac{\partial \Lambda^\mu{}_\eta}{\partial x^h}\frac{\partial^2 x^h}{\partial \overline{x^k}\partial \overline{x^i}}\eta^{\sigma\nu}.\end{aligned} \tag{2.4b}$$

Following the main idea of Refs. 1 and 2, we introduce the following equivalence relation on the bundle $J_1(\mathcal{E}\times\mathcal{C}, M)$: Given two points $z = (x^i, e_i^\mu, \omega_i{}^{\mu\nu}, e_{ij}^\mu, \omega_{ij}{}^{\mu\nu})$ and $\hat{z} = (\hat{x}^i, \hat{e}_i^\mu, \hat{\omega}_i{}^{\mu\nu}, \hat{e}_{ij}^\mu, \hat{\omega}_{ij}{}^{\mu\nu}) \in J_1(\mathcal{E}\times\mathcal{C}, M)$, we set $z \sim \hat{z} \Leftrightarrow x^i = \hat{x}^i$, $e_i^\mu = \hat{e}_i^\mu$, $\omega_i{}^{\mu\nu} = \hat{\omega}_i{}^{\mu\nu}$, and $(e_{ij}^\mu - e_{ji}^\mu) = (\hat{e}_{ij}^\mu - \hat{e}_{ji}^\mu)$, $(\omega_{ij}{}^{\mu\nu} - \omega_{ji}{}^{\mu\nu}) = (\hat{\omega}_{ij}{}^{\mu\nu} - \hat{\omega}_{ji}{}^{\mu\nu})$ (the geometrical meaning of the above equivalence relation is explained in Ref. 2).

Transformation laws (2.1), (2.3), (2.4a), and (2.4b) ensure that the above equivalence relation is independent of the choice of local coordinates and, therefore, geometrically significant.

We denote by $\mathcal{J}(\mathcal{E}\times\mathcal{C})$ the quotient space $J_1(\mathcal{E}\times\mathcal{C}, M)/\sim$ and by $\rho : J_1(\mathcal{E}\times\mathcal{C}, M) \to \mathcal{J}(\mathcal{E}\times\mathcal{C})$ the corresponding canonical projection. We may refer $J_1(\mathcal{E}\times\mathcal{C}, M)$ to local $\mathcal{J}$-coordinates x^i, e_i^μ, $\omega_i{}^{\mu\nu}$, $E_{ij}^\mu := \frac{1}{2}(e_{ij}^\mu - e_{ji}^\mu)$, $\Omega_{ij}{}^{\mu\nu} := \frac{1}{2}(\omega_{ij}{}^{\mu\nu} - \omega_{ji}{}^{\mu\nu})$ $(i<j)$, whose transformation laws are given by Eqs. (2.1) and (2.3) together with

$$\overline{E}_{jk}^\mu = E_{ih}^\sigma \Lambda^\mu{}_\sigma \frac{\partial x^h}{\partial \overline{x^k}}\frac{\partial x^i}{\partial \overline{x^j}} + \frac{1}{2}e_i^\sigma \frac{\partial \Lambda^\mu{}_\sigma}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^k}}\frac{\partial x^i}{\partial \overline{x^j}} - \frac{1}{2}e_i^\sigma \frac{\partial \Lambda^\mu{}_\sigma}{\partial x^h}\frac{\partial x^h}{\partial \overline{x^j}}\frac{\partial x^i}{\partial \overline{x^k}} \tag{2.5a}$$

and

$$\overline{\Omega}_{ik}{}^{\mu\nu} = \Lambda^{\mu}{}_{\sigma}\Lambda^{\nu}{}_{\gamma}\frac{\partial x^j}{\partial \overline{x}^i}\frac{\partial x^h}{\partial \overline{x}^k}\Omega_{jh}{}^{\sigma\gamma} + \frac{1}{2}\frac{\partial \Lambda^{\mu}{}_{\sigma}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^k}\Lambda^{\nu}{}_{\gamma}\frac{\partial x^j}{\partial \overline{x}^i}\omega_j{}^{\sigma\gamma} - \frac{1}{2}\frac{\partial \Lambda^{\mu}{}_{\sigma}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^i}\Lambda^{\nu}{}_{\gamma}\frac{\partial x^j}{\partial \overline{x}^k}\omega_j{}^{\sigma\gamma}$$
$$+ \frac{1}{2}\Lambda^{\mu}{}_{\sigma}\frac{\partial \Lambda^{\nu}{}_{\gamma}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^k}\frac{\partial x^j}{\partial \overline{x}^i}\omega_j{}^{\sigma\gamma} - \frac{1}{2}\Lambda^{\mu}{}_{\sigma}\frac{\partial \Lambda^{\nu}{}_{\gamma}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^i}\frac{\partial x^j}{\partial \overline{x}^k}\omega_j{}^{\sigma\gamma} - \frac{1}{2}\frac{\partial \Lambda_{\sigma}{}^{\eta}}{\partial x^s}\frac{\partial x^s}{\partial \overline{x}^k}\frac{\partial \Lambda^{\mu}{}_{\eta}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^i}\eta^{\sigma\nu}$$
$$+ \frac{1}{2}\frac{\partial \Lambda_{\sigma}{}^{\eta}}{\partial x^s}\frac{\partial x^s}{\partial \overline{x}^i}\frac{\partial \Lambda^{\mu}{}_{\eta}}{\partial x^h}\frac{\partial x^h}{\partial \overline{x}^k}\eta^{\sigma\nu}, \tag{2.5b}$$

with the identifications $E^{\mu}_{ij}=-E^{\mu}_{ji}$ and $\Omega_{ij}{}^{\mu\nu}=-\Omega_{ji}{}^{\mu\nu}$ (implicitly understood) whenever $i>j$.

Still following Refs. 1 and 2, we may endow the affine bundle $\mathcal{J}(\mathcal{E}\times\mathcal{C})\to\mathcal{E}\times\mathcal{C}$ with the following geometrical structures, reproducing some standard results of jet-bundle geometry in $\mathcal{J}(\mathcal{E}\times\mathcal{C})$:

• *$\mathcal{J}$-extension of sections*. Given a (local) section $\sigma: M\to\mathcal{E}\times\mathcal{C}$, we define its *$\mathcal{J}$-extension* $\mathcal{J}\sigma: M\to\mathcal{J}(\mathcal{E}\times\mathcal{C})$ as $\mathcal{J}\sigma := \rho\circ j_1\sigma$, $j_1\sigma: M\to j_1(\mathcal{E}\times\mathcal{C}, M)$ denoting the standard first jet-extension of σ.

Any section $\gamma: M\to\mathcal{J}(\mathcal{E}\times\mathcal{C})$ is said *holonomic* if there exists a section $\sigma: M\to\mathcal{E}\times\mathcal{C}$ such that $\gamma=\mathcal{J}\sigma$. Every holonomic section γ is then expressed locally as $\gamma: x\to\big(x^i, e^{\mu}_i(x), \omega_i{}^{\mu\nu}(x), E^{\mu}_{ij}(x) = \frac{1}{2}(\partial e^{\mu}_i(x)/\partial x^j - \partial e^{\mu}_j(x)/\partial x^i), \Omega_{ij}{}^{\mu\nu}(x) = \frac{1}{2}(\partial\omega_i{}^{\mu\nu}(x)/\partial x^j - \partial\omega_j{}^{\mu\nu}(x)/\partial x^i)\big)$.

• *Contact forms*. We may introduce in $\mathcal{J}(\mathcal{E}\times\mathcal{C})$ the concept of contact form by defining the following two-forms

$$\theta^{\mu} := de^{\mu}_j\wedge dx^j + E^{\mu}_{ij}dx^i\wedge dx^j, \quad \theta^{\mu\nu} := d\omega_j{}^{\mu\nu}\wedge dx^j + \Omega_{ij}{}^{\mu\nu}dx^i\wedge dx^j, \quad \mu,\nu = 1,\ldots,4. \tag{2.6}$$

It is easily seen that the behavior of the two-forms (2.6) under changes of coordinates (2.1), (2.3), and (2.5) is given by the equations

$$\overline{\theta^{\mu}} := d\overline{e}^{\mu}_j\wedge d\overline{x}^j + \overline{E}^{\mu}_{ij}d\overline{x}^i\wedge d\overline{x}^j = \Lambda^{\mu}_{\sigma}\theta^{\sigma} \tag{2.7a}$$

and

$$\overline{\theta^{\mu\nu}} := d\overline{\omega}^{\mu\nu}_j\wedge d\overline{x}^j + \overline{\Omega}^{\mu\nu}_{ij}d\overline{x}^i\wedge d\overline{x}^j = \Lambda^{\mu}_{\sigma}\Lambda^{\nu}_{\gamma}\theta^{\sigma\gamma}, \tag{2.7b}$$

showing the invariance of the module generated locally by the two-forms (2.6). The bundle spanned locally by the forms (2.6) is called *contact bundle* over $\mathcal{J}(\mathcal{E}\times\mathcal{C})$ and it is denoted by $\mathcal{C}(\mathcal{J}(\mathcal{E}\times\mathcal{C}))$; every section $\eta: \mathcal{J}(\mathcal{E}\times\mathcal{C})\to\mathcal{C}(\mathcal{J}(\mathcal{E}\times\mathcal{C}))$ is called a *contact two-form* on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$. As it happens for standard jet-bundles, the contact forms (2.6) characterize the holonomic sections of $\mathcal{J}(\mathcal{E}\times\mathcal{C})\to M$, namely

Proposition 2.1: A section $\gamma: M\to\mathcal{J}(\mathcal{E}\times\mathcal{C})$ is holonomic if and only if $\gamma^*(\theta^{\mu})=0$ and $\gamma^*(\theta^{\mu\nu})=0\ \forall\,\mu,\nu=1,\ldots,4$.

• *$\mathcal{J}$-prolongation of morphisms*. We want to construct a sort of $\mathcal{J}$-prolongation for bundle morphisms Φ of $\mathcal{E}\times\mathcal{C}$

$$\begin{array}{ccc} \mathcal{E}\times\mathcal{C} & \xrightarrow{\ \Phi\ } & \mathcal{E}\times\mathcal{C} \\ \downarrow & & \downarrow \\ M & \xrightarrow{\ \chi\ } & M \end{array}$$

projecting to diffeomorphisms χ of M. As we shall see, this is possible for a particular family of bundle morphisms only, but general enough for our purposes.

Once again borrowing from Ref. 1, we start by singling out those bundle morphisms (Φ,χ) whose ordinary jet-prolongations $j_1\Phi$ on $J_1(\mathcal{E}\times\mathcal{C}, M)$ satisfy the requirement

$$\rho \circ j_1\Phi(w_1) = \rho \circ j_1\Phi(\omega_2) \quad \forall\, w_1, w_2 \in \rho^{-1}(z), \tag{2.8}$$

for any $z \in \mathcal{J}(\mathcal{E}\times\mathcal{C})$. In a local chart, we may repeat the same arguments stated in Ref. 1 and end up with the conclusion that the most general bundle morphism (ϕ, χ) satisfying the ansatz (2.8) has necessarily the local form

$$y^i = \chi^i(x),$$

$$b_i^\nu = \Phi_i^\nu(x,e,\omega) = \Gamma_\mu^\nu(x)\frac{\partial x^r}{\partial y^i}e_r^\mu + \Gamma_{\gamma\eta}^\mu(x)\frac{\partial x^r}{\partial y^i}\omega_r{}^{\gamma\eta} + f_i^\nu(x), \tag{2.9}$$

$$\eta_i{}^{\nu\gamma} = \Phi_i{}^{\nu\gamma}(x,e,\omega) = \Gamma_\mu^{\nu\gamma}(x)\frac{\partial x^r}{\partial y^i}e_r^\mu + \Gamma_{\mu\sigma}^{\nu\gamma}(x)\frac{\partial x^r}{\partial y^i}\omega_r{}^{\mu\sigma} + f_i{}^{\nu\gamma}(x),$$

where $\Gamma_\mu^\nu(x)$, $\Gamma_{\gamma\eta}^\nu(x)$, $\Gamma_\mu^{\nu\gamma}(x)$, $\Gamma_{\mu\sigma}^{\nu\gamma}(x)$, $f_i^\nu(x)$, and $f_i{}^{\nu\gamma}(x)$ are arbitrary local functions on M (with $\Gamma_{\gamma\eta}^\nu = -\Gamma_{\eta\gamma}^\nu$ and $\Gamma_{\mu\sigma}^{\nu\gamma} = -\Gamma_{\sigma\mu}^{\nu\gamma}$). Moreover, a direct calculation shows that the characterization (2.9) is invariant under changes of coordinates (2.1) and (2.3), and then geometrically well set. Indeed, it is easily seen that the formal expressions (2.9) transform as

$$\overline{y^i} = \overline{\chi}^i(\overline{x}),$$

$$\overline{b_i^\nu} = \overline{\Gamma}_\mu^\nu(\overline{x})\frac{\partial \overline{x^r}}{\partial \overline{y^i}}\overline{e_r^\mu} + \overline{\Gamma}_{\gamma\eta}^\nu(\overline{x})\frac{\partial \overline{x^r}}{\partial \overline{y^i}}\overline{\omega_r}^{\gamma\eta} + \overline{f_i^\nu}(\overline{x}),$$

$$\overline{\eta_i}^{\nu\gamma} = \overline{\Gamma}_\mu^{\nu\gamma}(\overline{x})\frac{\partial \overline{x^r}}{\partial \overline{y^i}}\overline{e_r^\mu} + \overline{\Gamma}_{\mu\sigma}^{\nu\gamma}(\overline{x})\frac{\partial \overline{x^r}}{\partial \overline{y^i}}\overline{\omega_r}^{\mu\sigma} + \overline{f_i}^{\nu\gamma}(\overline{x}),$$

where

$$\overline{\Gamma}_\mu^\nu(\overline{x}) := \Gamma^\lambda_{\eta|x(\overline{x})}\Lambda^\nu{}_{\lambda|\chi(x(\overline{x}))}\Lambda_\mu{}^\eta{}_{|\overline{x}},$$

$$\overline{\Gamma}_{\gamma\eta}^\nu(\overline{x}) := \Gamma^\sigma_{\mu\rho|x(\overline{x})}\Lambda^\nu{}_{\sigma|\chi(x(\overline{x}))}\Lambda_\eta{}^\rho{}_{|\overline{x}}\Lambda_\gamma{}^\mu{}_{|\overline{x}},$$

$$\overline{f_i^\nu}(\overline{x}) := \frac{\partial x^j}{\partial \overline{x^i}}f^\lambda_{j|x(\overline{x})}\Lambda^\nu{}_{\lambda|\chi(x(\overline{x}))} - \Lambda^\nu{}_{\sigma|\chi(x(\overline{x}))}\Gamma^\sigma_{\gamma\lambda|x(\overline{x})}\Lambda^\rho{}_{\mu|\overline{x}}\frac{\partial \Lambda_\rho{}^\gamma}{\partial \overline{x^k}}{}_{|\overline{x}}\frac{\partial \overline{x^k}}{\partial \overline{y^i}}\eta^{\mu\lambda},$$

$$\overline{\Gamma}_\mu^{\nu\gamma}(\overline{x}) := \Gamma^{\lambda\tau}_{\sigma\ |x(\overline{x})}\Lambda^\nu{}_{\lambda|\chi(x(\overline{x}))}\Lambda^\gamma{}_{\tau|\chi(x(\overline{x}))}\Lambda_\mu{}^\sigma{}_{|\overline{x}},$$

$$\overline{\Gamma}_{\mu\sigma}^{\nu\gamma}(\overline{x}) := \Lambda^\nu{}_{\rho|\chi(x(\overline{x}))}\Lambda^\gamma{}_{\eta|\chi(x(\overline{x}))}\Gamma^{\rho\eta}_{\beta\alpha|x(\overline{x})}\Lambda_\mu{}^\beta{}_{|\overline{x}}\Lambda_\sigma{}^\alpha{}_{|\overline{x}},$$

and

$$\overline{f_i}^{\nu\gamma}(\overline{x}) := \Lambda^\nu{}_{\rho|\chi(x(\overline{x}))}\Lambda^\gamma{}_{\eta|\chi(x(\overline{x}))}\left[-\Gamma^{\rho\eta}_{\beta\alpha|x(\overline{x})}\frac{\partial \overline{x^h}}{\partial \overline{y^i}}\Lambda^\mu{}_{\sigma|\overline{x}}\frac{\partial \Lambda_\mu{}^\beta}{\partial \overline{x^h}}{}_{|\overline{x}}\eta^{\sigma\alpha} + \frac{\partial x^j}{\partial \overline{x^i}}f_j{}^{\rho\eta}\right]$$
$$-\Lambda_\sigma{}^\mu{}_{|\chi(x(\overline{x}))}\frac{\partial \Lambda^\nu{}_\mu}{\partial x^h}{}_{|\chi(x(\overline{x}))}\frac{\partial x^h}{\partial \overline{x^j}}\eta^{\sigma\gamma},$$

thus proving the required invariance.

Condition (2.8) being satisfied, given any bundle morphism (2.9) we may define its

$\mathcal{J}$-prolongation $\mathcal{J}\Phi:\mathcal{J}(\mathcal{E}\times\mathcal{C})\to\mathcal{J}(\mathcal{E}\times\mathcal{C})$ as

$$\mathcal{J}\Phi(z) \coloneqq \rho\circ j_1\Phi(w) \quad \forall\, w\in\rho^{-1}(z), z\in\mathcal{J}(\mathcal{E}\times\mathcal{C})$$

In local coordinates, the explicit expression of $\mathcal{J}\Phi$ is given by (see Ref. 1 for details)

$$\mathcal{J}\Phi:\begin{cases} y^i=\chi^i(x) \\ b_i^\nu=\Gamma_\mu^\nu(x)\dfrac{\partial x^r}{\partial y^i}e_r^\mu+\Gamma_{\gamma\eta}^\nu(x)\dfrac{\partial x^r}{\partial y^i}\omega_r{}^{\gamma\eta}+f_i^\nu(x) \\ \eta_i^{\nu\gamma}=\Gamma_\mu^{\nu\gamma}(x)\dfrac{\partial x^r}{\partial y^i}e_r^\mu+\Gamma_{\mu\sigma}^{\nu\gamma}(x)\dfrac{\partial x^r}{\partial y^i}\omega_r{}^{\mu\sigma}+f_i{}^{\nu\gamma}(x) \\ B_{ij}^\nu=(\Gamma_\mu^\nu E_{ks}^\mu+\Gamma_{\sigma\gamma}^\nu\Omega_{ks}^{\sigma\gamma})\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^s}{\partial y^j}+\dfrac{1}{2}\Bigg[\dfrac{\partial\Gamma_\mu^\nu}{\partial x^k}\left(\dfrac{\partial x^k}{\partial y^j}\dfrac{\partial x^r}{\partial y^i}-\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^r}{\partial y^j}\right)e_r^\mu \\ \quad+\dfrac{\partial\Gamma_{\sigma\gamma}^\nu}{\partial x^k}\left(\dfrac{\partial x^k}{\partial y^j}\dfrac{\partial x^r}{\partial y^i}-\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^r}{\partial y^j}\right)\omega_r{}^{\sigma\gamma}+\dfrac{\partial f_i^\nu}{\partial x^k}\dfrac{\partial x^k}{\partial y^j}-\dfrac{\partial f_j^\nu}{\partial x^k}\dfrac{\partial x^k}{\partial y^i}\Bigg] \\ \Delta_{ij}{}^{\nu\gamma}=(\Gamma_\mu^{\nu\gamma}E_{ks}^\mu+\Gamma_{\mu\sigma}^{\nu\gamma}\Omega_{ks}{}^{\mu\sigma})\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^s}{\partial y^j}+\dfrac{1}{2}\Bigg[\dfrac{\partial\Gamma_{\mu\sigma}^{\nu\gamma}}{\partial x^k}\left(\dfrac{\partial x^k}{\partial y^j}\dfrac{\partial x^r}{\partial y^i}-\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^r}{\partial y^j}\right)\omega_r{}^{\mu\sigma} \\ \quad+\dfrac{\partial\Gamma_\mu^{\nu\gamma}}{\partial x^k}\left(\dfrac{\partial x^k}{\partial y^j}\dfrac{\partial x^r}{\partial y^i}-\dfrac{\partial x^k}{\partial y^i}\dfrac{\partial x^r}{\partial y^j}\right)e_r^\mu+\dfrac{\partial f_i{}^{\nu\gamma}}{\partial x^k}\dfrac{\partial x^k}{\partial y^j}-\dfrac{\partial f_j{}^{\nu\gamma}}{\partial x^k}\dfrac{\partial x^k}{\partial y^i}\Bigg] \end{cases}.$$

As it happens for standard jet-prolongations in ordinary jet-bundles,[16] $\mathcal{J}$-prolongations are characterized by the property of preserving contact forms and $\mathcal{J}$-extensions. More precisely we have

Proposition 2.2: A bundle automorphism (Ψ,χ) *of* $\mathcal{J}(\mathcal{E}\times\mathcal{C})\to M$ *satisfies* $\Psi^*(\eta)\in Span\{\theta^\sigma,\theta^{\sigma\nu};\ \sigma,\nu=1,\dots,4\}\,\forall\,\eta\in Span\{\theta^\sigma,\theta^{\sigma\nu};\ \sigma,\nu=1,\dots,4\}\Leftrightarrow\Psi=\mathcal{J}\Phi$ *for some bundle morphism* (Φ,χ) *of* $\mathcal{E}\times\mathcal{C}\to M$.

Proposition 2.3: Given a bundle automorphism (Ψ,χ) *of* $\mathcal{J}(\mathcal{E}\times\mathcal{C})\to M$, *one has* $\Psi\circ\mathcal{J}\sigma\circ\chi^{-1}$ *is a* $\mathcal{J}$*-extension for every section* $\sigma:\mathcal{E}\times\mathcal{C}\to M\Leftrightarrow\Psi=\mathcal{J}\Phi$ *for some bundle morphism* (Φ,χ) *of* $\mathcal{E}\times\mathcal{C}\to M$.

The proofs of the above Propositions are strictly analogous to the corresponding ones given in Ref. 1 and will be omitted.

• *$\mathcal{J}$-prolongation of vector fields*. As made for bundle morphisms, we want to define a sort of $\mathcal{J}$-prolongation for vector fields X on $\mathcal{E}\times\mathcal{C}$, projecting to M.

To this end, still following Ref. 1, we first single out those vector fields X on $\mathcal{E}\times\mathcal{C}$, projecting to M, whose first jet-prolongations $J_1(X)$ on $J_1(\mathcal{E}\times\mathcal{C},M)$ pass to the quotient $\mathcal{J}(\mathcal{E}\times\mathcal{C})$.

Indeed, given any such vector field X, it is well defined the *$\mathcal{J}$-prolongation* $\mathcal{J}(X):\mathcal{J}(\mathcal{E}\times\mathcal{C})\to T\mathcal{J}(\mathcal{E}\times\mathcal{C})$ as

$$\mathcal{J}(X)(z) \coloneqq \rho_{*\rho^{-1}(z)}(j_1(X)) \quad \forall\, z\in\mathcal{J}(\mathcal{E}\times\mathcal{C}), \tag{2.10}$$

amounting to taking the standard first jet-prolongation $J_1(X)$ and to projecting it on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$.

Proceeding as in Ref. 1, we may conclude that the most general vector field satisfying the required ansatz is expressed locally as

$$X=\epsilon^i(x)\frac{\partial}{\partial x^i}+\left(-\frac{\partial\epsilon^k}{\partial x^q}e_k^\mu+D_\nu^\mu(x)e_q^\mu+D_{\gamma\sigma}^\mu(x)\omega_q{}^{\gamma\sigma}+G_q^\mu(x)\right)\frac{\partial}{\partial e_q^\mu}+\sum_{\mu<\nu}\left(-\frac{\partial\epsilon^k}{\partial x^q}\omega_k{}^{\mu\nu}+D_\sigma^{\mu\nu}(x)e_q^\sigma\right.$$
$$\left.+D_{\gamma\sigma}^{\mu\nu}(x)\omega_q{}^{\gamma\sigma}+G_q{}^{\mu\nu}(x)\right)\frac{\partial}{\partial\omega_q{}^{\mu\nu}}, \tag{2.11}$$

where $\epsilon^i(x)$, $D_\nu^\mu(x)$, $D_{\gamma\sigma}^\mu(x)$, $G_q^\mu(x)$, $D_\sigma^{\mu\nu}(x)$, $D_{\gamma\sigma}^{\mu\nu}(x)$, and $G_q{}^{\mu\nu}(x)$ are arbitrary local functions on M (with $D_{\gamma\sigma}^\mu=-D_{\sigma\gamma}^\mu$ and $D_{\gamma\sigma}^{\mu\nu}=-D_{\sigma\gamma}^{\mu\nu}$). A straightforward check shows that the representations (2.11)

are invariant under changes of coordinates (2.1) and (2.3). In fact, it is easily seen that they undergo the transformation law

$$X = \overline{\epsilon}^i \frac{\partial}{\partial \overline{x}^i} + \left(- \frac{\partial \overline{\epsilon}^k}{\partial \overline{x}^q} \overline{e}_k^\mu + \overline{D}_\nu^\mu \overline{e}_q^\nu + \overline{D}_{\gamma\sigma}^\mu \overline{\omega}_q{}^{\gamma\sigma} + \overline{G}_q^\mu \right) \frac{\partial}{\partial \overline{e}_q^\mu} + \sum_{\mu<\nu} \left(- \frac{\partial \overline{\epsilon}^k}{\partial \overline{x}^q} \overline{\omega}_k{}^{\mu\nu} + \overline{D}_\sigma^{\mu\nu} \overline{e}_q^\sigma + \overline{D}_{\gamma\sigma}^{\mu\nu} \overline{\omega}_q{}^{\gamma\sigma} + \overline{G}_q{}^{\mu\nu} \right) \frac{\partial}{\partial \overline{\omega}_q{}^{\mu\nu}},$$

where

$$\overline{\epsilon}^i := \epsilon^k \frac{\partial \overline{x}^i}{\partial x^k},$$

$$\overline{D}_\nu^\mu := D_\rho^\eta \Lambda_\nu{}^\rho \Lambda^\mu{}_\eta + \Lambda_\nu{}^\eta \epsilon^i \frac{\partial \Lambda^\mu{}_\eta}{\partial x^i},$$

$$\overline{D}_{\gamma\sigma}^\mu := D_{\xi\nu}^\eta \Lambda^\mu{}_\eta \Lambda_\gamma{}^\xi \Lambda_\sigma{}^\nu,$$

$$\overline{G}_q^\mu := G_j^\nu \frac{\partial x^j}{\partial \overline{x}^q} \Lambda^\mu{}_\nu - D_{\gamma\sigma}^\eta \Lambda^\xi{}_\nu \frac{\partial \Lambda_\xi{}^\gamma}{\partial \overline{x}^q} \eta^{\nu\sigma} \Lambda^\mu{}_\eta,$$

$$\overline{D}_\sigma^{\mu\nu} := D_\eta^{\alpha\beta} \Lambda_\sigma{}^\eta \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta,$$

$$\overline{D}_{\gamma\sigma}^{\mu\nu} := \left[\xi^i \frac{\partial (\Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta)}{\partial x^i} + \Lambda^\mu{}_\rho \Lambda^\nu{}_\eta D_{\alpha\beta}^{\rho\eta} \right] \Lambda_\gamma{}^\alpha \Lambda_\sigma{}^\beta,$$

and

$$\overline{G}_q{}^{\mu\nu} := G_j{}^{\alpha\beta} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \frac{\partial x^j}{\partial \overline{x}^q} - \xi^i \frac{\partial}{\partial x^i} \left(\Lambda_\rho{}^\eta \frac{\partial \Lambda^\mu{}_\eta}{\partial \overline{x}^q} \eta^{\rho\nu} \right) - \frac{\partial \overline{\xi}^h}{\partial \overline{x}^q} \Lambda_\rho{}^\eta \frac{\partial \Lambda^\mu{}_\eta}{\partial \overline{x}^h} \eta^{\rho\nu} - \left[\xi^i \frac{\partial (\Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta)}{\partial x^i} + \Lambda^\mu{}_\rho \Lambda^\nu{}_\eta D_{\alpha\beta}^{\rho\eta} \right] \Lambda^\lambda{}_\gamma \frac{\partial \Lambda_\lambda{}^\alpha}{\partial \overline{x}^q} \eta^{\gamma\beta}.$$

Still referring to Ref. 1 for details, in local coordinates we have the explicit expression

$$\mathcal{J}(X) = \epsilon^i \frac{\partial}{\partial x^i} + \left(- \frac{\partial \epsilon^k}{\partial x^q} e_k^\mu + D_\nu^\mu e_q^\nu + D_{\gamma\sigma}^\mu \omega_q{}^{\gamma\sigma} + G_q^\mu \right) \frac{\partial}{\partial e_q^\mu} + \sum_{\mu<\nu} \left(- \frac{\partial \epsilon^k}{\partial x^q} \omega_k{}^{\mu\nu} + D_\sigma^{\mu\nu} e_q^\sigma + D_{\gamma\sigma}^{\mu\nu} \omega_q{}^{\gamma\sigma} + G_q{}^{\mu\nu} \right) \frac{\partial}{\partial \omega_q{}^{\mu\nu}} + \sum_{i<j} h_{ij}^\mu \frac{\partial}{\partial E_{ij}^\mu} + \sum_{\mu<\nu} \sum_{i<j} h_{ij}{}^{\mu\nu} \frac{\partial}{\partial \Omega_{ij}{}^{\mu\nu}}, \tag{2.12}$$

where

$$h_{ij}^\mu := \frac{1}{2} \left(\frac{\partial D_\nu^\mu}{\partial x^j} e_i^\nu - \frac{\partial D_\nu^\mu}{\partial x^i} e_j^\nu + \frac{\partial D_{\sigma\gamma}^\mu}{\partial x^j} \omega_i{}^{\sigma\gamma} - \frac{\partial D_{\sigma\gamma}^\mu}{\partial x^i} \omega_j{}^{\sigma\gamma} + \frac{\partial G_i^\mu}{\partial x^j} - \frac{\partial G_j^\mu}{\partial x^i} \right) + D_\nu^\mu E_{ij}^\nu + D_{\sigma\gamma}^\mu \Omega_{ij}{}^{\sigma\gamma} + \left(E_{ki}^\mu \frac{\partial \epsilon^k}{\partial x^j} - E_{kj}^\mu \frac{\partial \epsilon^k}{\partial x^i} \right),$$

and

$$h_{ij}{}^{\mu\nu} := \frac{1}{2}\left(\frac{\partial D_\sigma^{\mu\nu}}{\partial x^j} e_i^\sigma - \frac{\partial D_\sigma^{\mu\nu}}{\partial x^i} e_j^\sigma + \frac{\partial D_{\gamma\sigma}^{\mu\nu}}{\partial x^j} \omega_i{}^{\gamma\sigma} - \frac{\partial D_{\gamma\sigma}^{\mu\nu}}{\partial x^i} \omega_j{}^{\gamma\sigma} + \frac{\partial G_i{}^{\mu\nu}}{\partial x^j} - \frac{\partial G_j{}^{\mu\nu}}{\partial x^i} \right) + D_\sigma^{\mu\nu} E_{ij}^\sigma + D_{\sigma\gamma}^{\mu\nu} \Omega_{ij}{}^{\sigma\gamma}$$
$$+ \left(\Omega_{ki}{}^{\mu\nu} \frac{\partial \epsilon^k}{\partial x^j} - \Omega_{kj}{}^{\mu\nu} \frac{\partial \epsilon^k}{\partial x^i} \right).$$

According to ordinary jet-prolongations,[16] $\mathcal{J}$-prolongations (2.10) are characterized by preserving contact forms and are a Lie algebra. More specifically, we have the following (see Ref. 1 for proofs).

Proposition 2.4: Let $\pi: \mathcal{J}(\mathcal{E}\times\mathcal{C}) \to \mathcal{E}\times\mathcal{C}$ denote the natural projection. Given a vector field Y on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$, projectable on $\mathcal{E}\times\mathcal{C}$, such that its projection $X(z) := \pi_{*\pi^{-1}(z)}(Y)$ $(\forall z \in \mathcal{E}\times\mathcal{C})$ defines a vector field on $\mathcal{E}\times\mathcal{C}$ of the form (2.11), then

$$Y = \mathcal{J}(X) \Leftrightarrow L_Y\theta^\mu, L_Y\theta^{\mu\nu} \in Span\{\theta^\sigma, \theta^{\sigma\mu}; \sigma, \mu = 1, \ldots, 4\}$$

Corollary 2.1: The $\mathcal{J}$-prolongations (2.10) from a Lie algebra.

For later use, we introduce new fibered coordinates on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$ of the form

$$x^i = x^i, \quad e_i^\mu = e_i^\mu, \quad \omega_i{}^{\mu\nu} = \omega_i{}^{\mu\nu}, \quad T_{ij}^\mu := 2E_{ji}^\mu + \omega_i{}^\mu{}_\nu e_j^\nu - \omega_j{}^\mu{}_\nu e_i^\nu \tag{2.13a}$$

and

$$R_{ij}{}^{\mu\nu} := 2\Omega_{ji}{}^{\mu\nu} + \tfrac{1}{2}(\omega_i{}^\mu{}_\lambda \omega_j{}^{\lambda\nu} - \omega_j{}^\mu{}_\lambda \omega_i{}^{\lambda\nu} - \omega_i{}^\nu{}_\lambda \omega_j{}^{\lambda\mu} + \omega_j{}^\nu{}_\lambda \omega_i{}^{\lambda\mu}), \tag{2.13b}$$

where $\omega_i{}^\mu{}_\nu := \omega_i{}^{\mu\sigma}\eta_{\sigma\nu}$. The idea is to take the components of the torsion tensor $T^\mu = de^\mu + \omega^\mu{}_\nu \wedge e^\nu$ and the curvature tensor $R^{\mu\nu} = d\omega^{\mu\nu} + \omega^\mu{}_\lambda \wedge \omega^{\lambda\nu}$ as $\mathcal{J}$-coordinates.

Taking Eqs. (2.1), (2.3), and (2.5) into account, it is a straightforward matter to verify the validity of the expected transformation laws

$$\overline{T}_{ij}^\mu = T_{hk}^\sigma \Lambda^\mu{}_\sigma \frac{\partial x^h}{\partial \overline{x}^i} \frac{\partial x^k}{\partial \overline{x}^j} \quad \text{and } \overline{R}_{ij}{}^{\mu\nu} = R_{hk}{}^{\sigma\gamma} \Lambda^\mu{}_\sigma \Lambda^\nu{}_\gamma \frac{\partial x^h}{\partial \overline{x}^i} \frac{\partial x^k}{\partial \overline{x}^j}. \tag{2.14}$$

Now, we define the following two-forms on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$

$$T^\mu := \tfrac{1}{2} T_{ij}^\mu dx^i \wedge dx^j \quad \text{and } R^{\mu\nu} := \tfrac{1}{2} R_{ij}{}^{\mu\nu} dx^i \wedge dx^j, \tag{2.15}$$

henceforth referred to as the *torsion* and the *curvature* two-forms on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$, respectively. In view of Eqs. (2.14), the latter undergo the transformation laws

$$\overline{T} = T^\sigma \Lambda^\mu{}_\sigma \quad \text{and } \overline{R}^{\mu\nu} = R^{\sigma\gamma} \Lambda^\mu{}_\sigma \Lambda^\nu{}_\gamma \tag{2.16}$$

showing the invariance of the module locally generated by the forms (2.15).

We conclude this section by introducing suitable bases of the tangent and cotangent bundles $T\mathcal{J}(\mathcal{E}\times\mathcal{C})$ and $T^*\mathcal{J}(\mathcal{E}\times\mathcal{C})$, respectively, which will be useful in the subsequent discussion. To this end, we preliminarily define the forms

$$\tau_i^\mu := de_i^\mu + \omega_j{}^\mu{}_\nu e_i^\nu dx^j \quad \text{and } \rho_i{}^{\mu\nu} := d\omega_i{}^{\mu\nu} + \tfrac{1}{2}(\omega_j{}^\mu{}_\lambda \omega_i{}^{\lambda\nu} - \omega_j{}^\nu{}_\lambda \omega_i{}^{\lambda\mu}) dx^j.$$

Then we choose the 1-forms

$$Dx^i := dx^i, \ \tau_i^\mu, \ \rho_i{}^{\mu\nu}, \ DT_{ij}^\mu := dT_{ij}^\mu + \omega_k{}^\mu{}_\lambda T_{ij}^\lambda dx^k \tag{2.17a}$$

and

$$DR_{ij}{}^{\mu\nu} := dR_{ij}{}^{\mu\nu} + \omega_k{}^\mu{}_\lambda R_{ij}{}^{\lambda\nu} dx^k - \omega_k{}^{\lambda\nu} R_{ij}{}^\mu{}_\lambda dx^k, \tag{2.17b}$$

as a local basis of $T^*\mathcal{J}(\mathcal{E}\times\mathcal{C})$; the vectors

$$\frac{D}{Dx^k} := \frac{\partial}{\partial x^k} - \omega_k{}^\mu{}_\nu e_i^\nu \frac{\partial}{\partial e_i^\mu} - \frac{1}{2}\omega_k{}^\mu{}_\lambda \omega_i{}^{\lambda\nu} \frac{\partial}{\partial \omega_i{}^{\mu\nu}} - \frac{1}{2}\omega_k{}^\mu{}_\lambda T_{ij}^\lambda \frac{\partial}{\partial T_{ij}^\mu}$$
$$+ \frac{1}{4}(-\omega_k{}^\mu{}_\lambda R_{ij}{}^{\lambda\nu} + \omega_k{}^{\lambda\nu} R_{ij}{}^\mu{}_\lambda) \frac{\partial}{\partial R_{ij}{}^{\mu\nu}}, \quad \frac{D}{De_i^\mu} := \frac{\partial}{\partial e_i^\mu}, \tag{2.18a}$$

$$\frac{D}{D\omega_i{}^{\mu\nu}} := \frac{\partial}{\partial \omega_i{}^{\mu\nu}}, \quad \frac{D}{DT_{ij}^\mu} := \frac{\partial}{\partial T_{ij}^\mu}, \quad \frac{D}{DR_{ij}{}^{\mu\nu}} := \frac{\partial}{\partial R_{ij}{}^{\mu\nu}},$$

form the local dual basis of $T\mathcal{J}(\mathcal{E}\times\mathcal{C})$.

We also notice that, if we set

$$\tau^\mu := \tau_i^\mu \wedge dx^i \text{ and } \rho^{\mu\nu} := \rho_i{}^{\mu\nu} \wedge dx^i, \tag{2.19}$$

then we can represent the contact forms as

$$\theta^\mu = \tau^\mu - T^\mu \quad \text{and} \quad \theta^{\mu\nu} = \rho^{\mu\nu} - R^{\mu\nu}. \tag{2.20}$$

III. THE FIELD EQUATIONS

In this section we shall derive the field equations of the theory from a variational principle.

To this end, we notice that a Lagrangian on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$ is a horizontal four-form, locally expressed in terms of the coordinates (2.13) as

$$L = \mathcal{L}(x, e, \omega, T, R)ds, \tag{3.1}$$

with $ds := dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^4$ and $\mathcal{L}$ is a scalar density.

Borrowing from Refs. 1 and 2, we associate with any Lagrangian (3.1) a corresponding Poincaré–Cartan four-form on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$, locally described as

$$\Theta_L := \mathcal{L}ds - \tfrac{1}{2}\theta^\mu \wedge P_\mu - \tfrac{1}{4}\theta^{\mu\nu} \wedge P_{\mu\nu}, \tag{3.2}$$

where $P_\mu := (\partial\mathcal{L}/\partial T_{ij}^\mu)ds_{ij}$ and $P_{\mu\nu} := (\partial\mathcal{L}/\partial R_{ij}{}^{\mu\nu})ds_{ij}$ (with $ds_{ij} := \partial/\partial x^i \rfloor \partial/\partial x^j \rfloor ds$).

To every Lagrangian L we associate the action functional

$$A_L(\sigma) := \int_D \mathcal{J}\sigma^*(L) = \int_D \mathcal{J}\sigma^*(\Theta_L),$$

$\forall$ section $\sigma: D \subset M \to \mathcal{E}\times\mathcal{C}$, D compact domain.

Now, let Φ_ξ be a one-parameter group of $\mathcal{J}$-prolongable diffeomorphisms (2.9) on $\mathcal{E}\times\mathcal{C}$, projecting (for simplicity) on the identity map of M. Let X denote the infinitesimal generator of Φ_ξ; it follows that X is a $\mathcal{J}$-prolongable vector field (2.11) on $\mathcal{E}\times\mathcal{C}$, vertical with respect to the fibration $\mathcal{E}\times\mathcal{C}\to M$.

Given a section $\sigma: M \to \mathcal{E}\times\mathcal{C}$, we can deform it along X by setting $\sigma_\xi := \Phi_\xi \circ \sigma$; then we have $\mathcal{J}\sigma_\xi = \mathcal{J}(\Phi_\xi \circ \sigma) = \mathcal{J}\Phi_\xi \circ \mathcal{J}\sigma$.

We call *first variation* of A_L at σ in the direction X, the expression

$$\frac{\delta A_L}{\delta X}(\sigma) := \frac{d}{d\xi}\int_D \mathcal{J}\sigma_\xi^* \Theta_{L|_{\xi=0}} = \int_D \mathcal{J}\sigma^*(\mathcal{J}(X) \rfloor d\Theta_L) + \int_{\partial D} \mathcal{J}\sigma^*(\mathcal{J}(X) \rfloor \Theta_L). \tag{3.3}$$

In connection with this, a section σ is said *critical* if $\delta A_L/\delta X(\sigma) = 0$ for all compact domains D and all deformations $\mathcal{J}\sigma_\xi$ constant on the boundary ∂D. Due to this last condition at the boundary, it follows that a section σ is critical if and only if the equation

$$\mathcal{J}\sigma^*(\mathcal{J}(X)\rfloor d\Theta_L)=0 \tag{3.4}$$

holds true, for all $\mathcal{J}$-prolongable vector fields X.

In order to develop the calculations about Eq. (3.4), let us introduce the following differential operators acting on tensor-valued forms on $\mathcal{J}(\mathcal{E}\times\mathcal{C})$:

$$D\eta^\mu = d\eta^\mu + \omega_i{}^\mu{}_\nu dx^i\wedge\eta^\nu, \tag{3.5a}$$

$$D\eta_\mu = d\eta_\mu - \omega_i{}^\nu{}_\mu dx^i\wedge\eta_\nu, \tag{3.5b}$$

$$D\eta^\mu{}_\nu = d\eta^\mu{}_\nu + \omega_i{}^\mu{}_\lambda dx^i\wedge\eta^\lambda{}_\nu - \omega_i{}^\lambda{}_\nu dx^i\wedge\eta^\mu{}_\lambda, \tag{3.5c}$$

$$D\eta_\nu{}^\mu = d\eta_\nu{}^\mu - \omega_i{}^\lambda{}_\nu dx^i\wedge\eta_\lambda{}^\mu + \omega_i{}^\mu{}_\lambda dx^i\wedge\eta_\nu{}^\lambda. \tag{3.5d}$$

Making use of the bases (2.17) and taking Eqs. (2.20) and (3.5) as well as the identities $D\tau^\mu = \rho_j{}^{\mu\nu}\eta_{\nu\sigma}e_i^\sigma\wedge dx^j\wedge dx^i$, $D\rho^{\mu\nu}=0$, $(\partial\mathcal{L}/\partial T_{ij}^\mu)ds=\frac{1}{2}dx^j\wedge dx^i\wedge P_\mu$ and $(\partial\mathcal{L}/\partial R_{ij}{}^{\mu\nu})ds=\frac{1}{2}dx^j\wedge dx^i\wedge P_{\mu\nu}$ into account (we notice that the identities $D\tau^\mu=\rho_j{}^{\mu\nu}\eta_{\nu\sigma}e_i^\sigma\wedge dx^j$ and $D\rho^{\mu\nu}=0$ are nothing but a restatement of the Bianchi identities in the present geometrical setting), it is easily seen that

$$d\Theta_L = D\Theta_L = (D\mathcal{L}/De_i^\mu)\tau_i^\mu\wedge ds + \tfrac{1}{2}(D\mathcal{L}/D\omega_i{}^{\mu\nu})\rho_i{}^{\mu\nu}\wedge ds - (D\mathcal{L}/DT_{ji}^\mu)e_j^\sigma\eta_{\sigma\nu}\rho_i{}^{\mu\nu}\wedge ds - \tfrac{1}{2}\theta^\mu\wedge DP_\mu - \tfrac{1}{4}\theta^{\mu\nu}\wedge DP_{\mu\nu}.$$

Choosing infinitesimal deformations X of the special form

$$X = G_i^\mu(x)\frac{D}{De_i^\mu} + \frac{1}{2}G_i{}^{\mu\nu}(x)\frac{D}{D\omega_i{}^{\mu\nu}},$$

for simplicity, we have then

$$\mathcal{J}(X)\rfloor D\Theta_L = \frac{D\mathcal{L}}{De_i^\mu}G_i^\mu ds + \frac{1}{2}\frac{D\mathcal{L}}{D\omega_i{}^{\mu\nu}}G_i{}^{\mu\nu}ds - \frac{1}{2}G_i^{\mu\nu}\left(\frac{D\mathcal{L}}{DT_{ji}^\mu}e_j^\sigma\eta_{\sigma\nu} - \frac{D\mathcal{L}}{DT_{ji}^\nu}e_j^\sigma\eta_{\sigma\mu}\right)ds + \\ - \frac{1}{2}G_i^\mu dx^i\wedge DP_\mu - \frac{1}{4}G_i{}^{\mu\nu}dx^i\wedge DP_{\mu\nu} - \frac{1}{2}\theta^\mu\wedge\mathcal{J}(X)\rfloor DP_\mu - \frac{1}{4}\theta^{\mu\nu}\wedge\mathcal{J}(X)\rfloor DP_{\mu\nu}. \tag{3.6}$$

Pulling-back Eq. (3.6) through $\mathcal{J}\sigma$, we obtain the expression

$$\mathcal{J}\sigma^*(\mathcal{J}(X)\rfloor D\Theta_L) = G_i^\mu(x)\mathcal{J}\sigma^*\left(\frac{D\mathcal{L}}{De_i^\mu}ds - \frac{1}{2}dx^i\wedge DP_\mu\right) + \frac{1}{2}G_i{}^{\mu\nu}(x)\mathcal{J}\sigma^*\left(\frac{D\mathcal{L}}{D\omega_i{}^{\mu\nu}}ds - \frac{D\mathcal{L}}{DT_{ji}^\mu}e_j^\sigma\eta_{\sigma\nu}ds + \frac{D\mathcal{L}}{DT_{ji}^\nu}e_j^\sigma\eta_{\sigma\mu}ds - \frac{1}{2}dx^i\wedge DP_{\mu\nu}\right).$$

Due to the arbitrariness of X, by imposing the requirement (3.4), we get two sets of final equations

$$\mathcal{J}\sigma^*\left(\frac{D\mathcal{L}}{De_i^\mu} - D_k\frac{D\mathcal{L}}{DT_{ki}^\mu}\right)=0, \tag{3.7a}$$

$$\mathcal{J}\sigma^*\left(\frac{D\mathcal{L}}{D\omega_i{}^{\mu\nu}} - \frac{D\mathcal{L}}{DT_{ji}^\mu}e_j^\sigma\eta_{\sigma\nu} + \frac{D\mathcal{L}}{DT_{ji}^\nu}e_j^\sigma\eta_{\sigma\mu} - D_k\frac{D\mathcal{L}}{DR_{ki}{}^{\mu\nu}}\right)=0, \tag{3.7b}$$

representing the actual field equations of the theory.

In particular, if we consider the purely gravitational Lagrangian

$$L = \tfrac{1}{2} e_i^{\mu} dx^i \wedge e_j^{\nu} dx^j \wedge R^{\lambda\rho} \epsilon_{\mu\nu\lambda\rho} := \mathcal{L} ds, \tag{3.8}$$

where $\mathcal{L} := \frac{1}{4} e_i^{\mu} e_j^{\nu} R_{k\ell}{}^{\lambda\rho} \epsilon^{ijkl} \epsilon_{\mu\nu\lambda\rho}$, Eqs. (3.7) yield

$$\tfrac{1}{2} e_j^{\nu} R_{kl}{}^{\sigma\lambda} \epsilon^{ijkl} \epsilon_{\mu\nu\sigma\lambda} = 0, \tag{3.9a}$$

$$-2 D_k(e_p^{\sigma}) e_q^{\lambda} \epsilon^{pqki} \epsilon_{\sigma\lambda\mu\nu} = 0, \tag{3.9b}$$

where $D_k(e_p^{\sigma}) = \partial e_p^{\sigma} / \partial x^k + \omega_k{}^{\sigma}{}_{\lambda} e_p^{\lambda}$.

As is well known, (provided that $\det(e_i^{\mu}) \neq 0$) the theory described by Eqs. (3.9) is on-shell equivalent to Einstein's theory in empty space.

Joining together the present mathematical setting with that proposed in Refs. 1 and 2, we can develop a new geometrical approach to the combined theory of gravitational and Yang–Mills fields.

To this end, let $Q \to M$ be a principal fiber bundle over space–time, with structural group a semisimple Lie group G.

Principal connections of $Q \to M$ are additional dynamical fields; the latter may be represented as sections of the affine bundle $J_1 Q/G \to M$ (the space of principal connections), referred to local coordinates x^i, a_i^A, $A = 1, \ldots, r = \dim G$ (see Refs. 1 and 2 for more details).

The extended configuration space of the theory is the fibered product $\mathcal{E} \times_M \mathcal{C} \times_M J_1 Q/G$ ($\mathcal{E} \times \mathcal{C} \times J_1 Q/G$ for short) over M.

The construction of the associated quotient space $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$ follows the lines illustrated in Refs. 1 and 2 and in the present paper too. Then, once again referring to Refs. 1 and 2 for comments and details, we recall that we can choose the components of the curvature tensor F_{ij}^A of the connection as $\mathcal{J}$-coordinates (together with T_{ij}^{μ} and $R_{ij}{}^{\mu\nu}$) on $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$ [More precisely, if $A_{ij}^A \left(\simeq \frac{1}{2}(\partial a_i^A / \partial x^j - \partial a_j^A / \partial x^i)\right)$ are $\mathcal{J}$-coordinates on $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$, then we have $F_{ij}^A := 2A_{ji}^A + a_j^B a_i^C C_{CB}^A$, C_{CB}^A being the structure coefficients of the Lie algebra of the group G.]

There are r further contact two-forms on $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$, expressed as

$$\theta^A := da_i^A \wedge dx^i + A_{ij}^A dx^i \wedge dx^j = \Phi^A - F^A,$$

where $F^A := \frac{1}{2} F_{ij}^A dx^i \wedge dx^j$, $\Phi^A := \Phi_i^A \wedge dx^i$ with $\Phi_i^A := da_i^A + \frac{1}{2} a_i^B a_j^C C_{CB}^A dx^j$.

Also, we complete the bases (2.17) and (2.18) to local bases of $T\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$ and $T^* \mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$, respectively, by introducing the vectors

$$\frac{D}{Dx^k} := \frac{\partial}{\partial x^k} - \omega_k{}^{\mu}{}_{\nu} e_i^{\nu} \frac{\partial}{\partial e_i^{\mu}} - \frac{1}{2} \omega_k{}^{\mu}{}_{\lambda} T_{ij}^{\lambda} \frac{\partial}{\partial T_{ij}^{\mu}} - \frac{1}{2} \omega_k{}^{\mu}{}_{\lambda} \omega_i{}^{\lambda\nu} \frac{\partial}{\partial \omega_i{}^{\mu\nu}} + \frac{1}{4} (-\omega_k{}^{\mu}{}_{\lambda} R_{ij}{}^{\lambda\nu} + \omega_k{}^{\lambda\nu} R_{ij}{}^{\mu}{}_{\lambda}) \frac{\partial}{\partial R_{ij}{}^{\mu\nu}}$$
$$+ \frac{1}{2} a_k^B a_i^C C_{CB}^A \frac{\partial}{\partial a_i^A} - \frac{1}{2} F_{ij}^B a_k^C C_{CB}^A \frac{\partial}{\partial F_{ij}^A}, \quad \frac{D}{Da_i^A} := \frac{\partial}{\partial a_i^A}, \quad \frac{D}{DF_{ij}^A} := \frac{\partial}{\partial F_{ij}^A},$$

and the forms

$$\Phi_i^A, \quad DF_{ij}^A := dF_{ij}^A + F_{ij}^B a_k^C C_{CB}^A dx^k.$$

The latter are consistent with the definition of the covariant differential operator D, acting on tensorial forms on $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$ as

$$D\eta^A := d\eta^A + a_k^B dx^k \wedge \eta^C C_{BC}^A,$$

$$D\eta_A := d\eta_A - a_k^B dx^k \wedge \eta_C C_{BA}^C.$$

For the present case, a Lagrangian is then a horizontal four-form on $\mathcal{J}(\mathcal{E} \times \mathcal{C} \times J_1 Q/G)$, locally expressed as

$$L = \mathcal{L}(x,e,\omega,a,T,R,F)ds.$$

The corresponding Poincaré–Cartan form is given by

$$\Theta_L = \mathcal{L}ds - \tfrac{1}{2}\theta^{\mu} \wedge P_{\mu} - \tfrac{1}{4}\theta^{\mu\nu} \wedge P_{\mu\nu} - \tfrac{1}{2}\theta^{A} \wedge P_{A},$$

where $P_A := (\partial\mathcal{L}/\partial F^A_{ij})ds_{ij}$, and the ansatz

$$\mathcal{J}\sigma * (\mathcal{J}(X) \rfloor d\Theta_L) = 0,$$

for all $\mathcal{J}$-prolongable vector fields X on $\mathcal{E}\times\mathcal{C}\times J_1Q/G$, yields field equation of the form (3.7) together with (see Refs. 1 and 2)

$$\mathcal{J}\sigma * \left(\frac{\partial\mathcal{L}}{\partial a^A_i} - D_k \frac{\partial\mathcal{L}}{\partial F^A_{ki}} \right) = 0. \tag{3.10}$$

More in detail, in the theory of interacting gravitational and free Yang–Mills fields, the Lagrangian L is the sum of the purely gravitational Lagrangian (3.8) and of the free Yang–Mills one. Therefore, in the present geometrical framework, we have explicitly

$$L = \mathcal{L}ds := (\tfrac{1}{4}e^{\mu}_i e^{\nu}_j R_{kl}{}^{\lambda\rho}\varepsilon^{ijkl}\varepsilon_{\mu\nu\lambda\rho} - \tfrac{1}{4}F^A_{ij}F^B_{pq}\gamma_{AB}\eta^{\mu\nu}e^p_{\mu}e^i_{\nu}\eta^{\lambda\sigma}e^q_{\lambda}e^j_{\sigma}e)ds, \tag{3.11}$$

where $e := \det(e^{\mu}_i)$, e^i_{μ} denotes the inverse matrix of e^{μ}_i and γ_{AB} indicates the adjoint-invariant metric of the Lie algebra $\mathfrak{G}$ of the Lie group G.

Inserting expression (3.11) in Eqs. (3.7) and (3.10) as well as taking the identities $\partial e^j_{\nu}/\partial e^{\mu}_i = -e^j_{\mu}e^i_{\nu}$ and $\partial e/\partial e^{\mu}_i = ee^i_{\mu}$ into account, we get the final equations

$$\tfrac{1}{2}e^{\nu}_j R_{kl}{}^{\sigma\lambda}\varepsilon^{ijkl}\varepsilon_{\mu\nu\sigma\lambda} = -(F^{Ai}_j F^j_{Ak}e^k_{\mu} - \tfrac{1}{4}F^A_{jk}F^{jk}_A e^i_{\mu})e, \tag{3.12a}$$

$$-2D_k(e^{\sigma}_p)e^{\lambda}_q\epsilon^{pqki}\epsilon_{\sigma\lambda\mu\nu} = 0, \tag{3.12b}$$

$$D_k(F^{ik}_A e) = 0, \tag{3.12c}$$

where $F^{ij}_A := F^B_{kh}\gamma_{BA}\eta^{\mu\nu}e^k_{\mu}e^i_{\nu}\eta^{\sigma\lambda}e^h_{\sigma}e^j_{\lambda}$ and $D_k(F^{ik}_A e) = \partial(F^{ik}_A e)/\partial x^k - a^B_k(F^{ik}_C e)C^C_{BA}$.

In the right side of Eq. (3.12a) we recover the energy-momentum tensor $T^i_{\mu} := F^{Ai}_j F^j_{Ak}e^k_{\mu} - \frac{1}{4}F^A_{jk}F^{jk}_A e^i_{\mu}$ of the Yang–Mills field.

It is worth noticing that all the restrictions about the vector fields $\mathcal{J}(X)$ in Eq. (3.4) may be removed. In fact, it is easily seen that Eq. (3.4) automatically implies

$$\mathcal{J}\sigma * (X \rfloor d\Theta_L) = 0, \quad \forall\, X \in D^1(\mathcal{J}(\mathcal{E}\times\mathcal{C}\times J_1Q/G)). \tag{3.13}$$

As pointed out in Ref. 1, this remark plays an important role in the study of the relationships between Nöther vector fields and infinitesimal dynamical symmetries. This topic will be dealt with in the next Section.

IV. SYMMETRIES AND NOETHER THEOREM

The Poincaré–Cartan representation (3.13) of the field equations turns out to be especially useful in the study of symmetries and conserved quantities. To see this point, let us introduce the following[14,15]

Definition 4.1: A vector field Z on $\mathcal{J}(\mathcal{E}\times\mathcal{C}\times J_1Q/G)$ is called a generalized infinitesimal Lagrangian symmetry *if it satisfies the requirement*

$$L_Z(\mathcal{L}ds) = d\alpha, \tag{4.1}$$

for some $(m-1)$-form α on $\mathcal{J}(\mathcal{E}\times\mathcal{C}\times J_1Q/G)$.

Definition 4.1 extends the usual notion of Lagrangian symmetry. In fact, if the vector field Z satisfies $L_Z(\mathcal{L}ds)=0$ and projects to M, then we have

$$\mathcal{L} = \det\left|\frac{\partial \chi_s^i}{\partial x^j}\right| \mathcal{L}\circ\Psi_s \quad \forall\, s,$$

(Ψ_s,χ_s) denoting the flow of Z.

Definition 4.2: A vector field Z on $\mathcal{J}(\mathcal{E}\times\mathcal{C}\times J_1Q/G)$ is called a Noether vector field *if it satisfies the following condition*

$$L_Z\Theta_L = \omega + d\alpha, \tag{4.2}$$

where ω is a m-form belonging to the ideal generated by the contact forms and α is any $(m-1)$-form on $\mathcal{J}(E)$.

As above, if Z satisfies the trivial case $L_Z\Theta_L=0$ and projects to M, then Z is an infinitesimal dynamical symmetry. Indeed, in such a circumstance, denoting again by (Ψ_s,χ_s) the flow of Z, it is a straightforward matter to see that $\Psi_s^*\circ\mathcal{J}\sigma\circ\chi_{-s}^*$ is a critical section if $\mathcal{J}\sigma$ does.

Directly from Proposition 2.4 we derive

Proposition 4.1: If a generalized infinitesimal Lagrangian symmetry Z is a $\mathcal{J}$-prolongation of some vector field (2.11) *on $\mathcal{E}\times\mathcal{C}\times J_1Q/G$, then it is a Noether vector field.*

Also, we have

Proposition 4.2: If a Noether vector field Z is a $\mathcal{J}$-prolongation of some vector field (2.11) *on $\mathcal{E}\times\mathcal{C}\times J_1Q/G$, then it is an infinitesimal dynamical symmetry*. (See Ref. 1 for proofs.)

We can associate with any Noether vector field Z a corresponding conserved current, so restating a sort of Noether theorem in the present geometrical setting. In fact, given Z satisfying Eq. (4.2) and a critical section $\sigma: M\to\mathcal{E}\times\mathcal{C}\times J_1Q/G$, Eqs. (3.13) and (4.2) imply

$$d\mathcal{J}\sigma^*(Z\rfloor\Theta_L-\alpha) = \mathcal{J}\sigma^*(\omega - Z\rfloor d\Theta_L) = 0,$$

showing that the current $\mathcal{J}\sigma^*(Z\rfloor\Theta_L-\alpha)$ is conserved on shell.

As an example, let us consider once again the Lagrangian (3.11), expressing gravity coupled with a Yang–Mills field; the associated Poincaré–Cartan form is

$$\Theta_L = \mathcal{L}ds - \tfrac{1}{4}\theta^{\mu\nu}\wedge e_i^\sigma e_j^\lambda \varepsilon^{ijpq}\varepsilon_{\sigma\lambda\mu\nu}ds_{pq} + \tfrac{1}{2}\theta^A\wedge F_A^{ij}eds_{ij}.$$

As it is well known, diffeomorphisms, Lorentz transformations (for tetrad and connection) and gauge transformations (for the Yang–Mills field) are dynamical symmetries of the theory. We want to restate these results in the newer scheme.

To start with, let $Y=\xi^i(\partial/\partial x^i)$ be the generator of a (local) one parameter group of diffeomorphisms of M. The vector field Y may be "lifted" to vector fields X on $\mathcal{E}\times\mathcal{C}\times J_1Q/G$, by setting locally

$$X = \xi^i\frac{\partial}{\partial x^i} - \frac{\partial\xi^k}{\partial x^q}e_k^\mu\frac{\partial}{\partial e_q^\mu} - \frac{1}{2}\frac{\partial\xi^k}{\partial x^q}\omega_k{}^{\mu\nu}\frac{\partial}{\partial\omega_q{}^{\mu\nu}} - \frac{\partial\xi^k}{\partial x^q}a_k^A\frac{\partial}{\partial a_q^A}. \tag{4.3}$$

We stress that the procedure is not covariant but strictly depends on the local coordinates in which we are working. In any case, we show that vector fields having a local representation (4.3) are Noether vector fields and infinitesimal dynamical symmetries.

To this end, recalling Eq. (2.11), we notice that vector fields (4.3) are $\mathcal{J}$-prolongable; in connection with this, making use of Eq. (2.12), we easily get the local expression

$$\mathcal{J}(X) = \xi^i \frac{\partial}{\partial x^i} - \frac{\partial \xi^k}{\partial x^q} e_k^\mu \frac{\partial}{\partial e_q^\mu} - \frac{1}{2} \frac{\partial \xi^k}{\partial x^q} \omega_k{}^{\mu\nu} \frac{\partial}{\partial \omega_q{}^{\mu\nu}} - \frac{\partial \xi^k}{\partial x^q} a_k^A \frac{\partial}{\partial a_q^A} + T_{jk}^\mu \frac{\partial \xi^k}{\partial x^i} \frac{\partial}{\partial T_{ij}^\mu} + \frac{1}{2} R_{jk}{}^{\mu\nu} \frac{\partial \xi^k}{\partial x^i} \frac{\partial}{\partial R_{ij}{}^{\mu\nu}} + F_{jk}^A \frac{\partial \xi^k}{\partial x^i} \frac{\partial}{\partial F_{ij}^A}, \tag{4.4}$$

for their $\mathcal{J}$-prolongations on $\mathcal{J}(\mathcal{E}\times\mathcal{C}\times J_1 Q/G)$.

We prove now that the fields $\mathcal{J}(X)$ are infinitesimal Lagrangian symmetry. To do this, it is convenient to work in new "tetrad" coordinates on $\mathcal{E}\times\mathcal{C}\times J_1 Q/G$ of the form [of course, the coordinate transformation (4.5) is thought in the invariant region of $\mathcal{E}\times\mathcal{C}\times J_1 Q/G$ in which one has $e \neq 0$]

$$x^i,\ e_i^\mu, \quad \omega_\sigma{}^{\mu\nu} := \omega_i^{\mu\nu} e_\sigma^i, \quad a_\sigma^A := a_i^A e_\sigma^i,$$

$$T_{\sigma\lambda}^\mu := T_{ij}^\mu e_\sigma^i e_\lambda^j, \quad R_{\sigma\lambda}{}^{\mu\nu} := R_{ij}{}^{\mu\nu} e_\sigma^i e_\lambda^j, \quad F_{\sigma\lambda}^A := F_{ij}^A e_\sigma^i e_\lambda^j. \tag{4.5}$$

In these coordinates the vector field $\mathcal{J}(X)$ assumes the simpler expression

$$\mathcal{J}(X) = \xi^i \frac{\partial}{\partial x^i} - \frac{\partial \xi^k}{\partial x^q} e_k^\mu \frac{\partial}{\partial e_q^\mu},$$

while the Lagrangian is locally described as

$$L = \mathcal{L}ds = (R_{\mu\nu}{}^{\mu\nu} e - \tfrac{1}{4} F_{\mu\nu}^A F_A^{\mu\nu} e) ds,$$

where $F_A^{\mu\nu} := F_{\sigma\lambda}^B \eta^{\sigma\mu} \eta^{\lambda\nu} \gamma_{BA}$.

It is then a straightforward matter to verify that

$$L_{\mathcal{J}(X)}(\mathcal{L}ds) = \mathcal{J}(X)(\mathcal{L})ds + \mathcal{L}d(\mathcal{J}(X) \rfloor ds) = -\frac{\partial \xi^k}{\partial x^k}\mathcal{L}ds + \frac{\partial \xi^k}{\partial x^k}\mathcal{L}ds = 0.$$

Therefore, from Propositions 4.1 and 4.2, we conclude that the vector fields $\mathcal{J}(X)$ are Noether vector fields and thus infinitesimal dynamical symmetries.

There are no (nontrivial) conserved quantities arising from the fields (4.4). In fact, a direct calculation shows that the inner product $\mathcal{J}(X) \rfloor \Theta_L$ consists in an exact term plus a term vanishing identically when pulled-back under critical section.

Another family of Noether vector fields and infinitesimal dynamical symmetries is given by infinitesimal gauge transformations for the Yang–Mills field.

The latter may be represented by vector fields X on $\mathcal{E}\times\mathcal{C}\times J_1 Q/G$ of the form

$$X = D_i b^A \frac{\partial}{\partial a_i^A}, \tag{4.6}$$

where $b^A = b^A(x) \in F(M)$ and $D_i b^A = \partial b^A/\partial x^i + b^C a_i^B C_{BC}^A$.

As above, vector fields (4.6) are $\mathcal{J}$-prolongable and their $\mathcal{J}$-prolongations $\mathcal{J}(X)$ on $\mathcal{E}\times\mathcal{C}\times J_1 Q/G$ are locally expressed as

$$\mathcal{J}(X) = D_i b^A \frac{\partial}{\partial a_i^A} + \frac{1}{2} b^C F_{ij}^B C_{BC}^A \frac{\partial}{\partial F_{ij}^A}. \tag{4.7}$$

The latter are infinitesimal Lagrangian symmetries, indeed one has

$$L_{\mathcal{J}(X)}(\mathcal{L}ds) = L_{\mathcal{J}(X)}(-\tfrac{1}{4} F_{ij}^A F_A^{ij} e ds) = -\tfrac{1}{2} b^B F_{ij}^C C_{CB}^A F_A^{ij} e ds = 0. \tag{4.8}$$

The vanishing of (4.8) is due to the relation $\gamma_{AB} C_{CD}^A = \gamma_{A[B} C_{CD]}^A$, consequence of the adjoint-invariance of the metric γ.

Once again, it follows that the vector fields (4.7) are Noether vector fields and infinitesimal dynamical symmetries of the theory. Moreover, if σ is a critical section, then the quantities

$$\mathcal{Q} = \mathcal{J}\sigma * (\mathcal{J}(X) \rfloor \Theta_L) = D_i b^A(x) F_A^{ij}(x) ds_j,$$

are the conserved Noether currents, associated with the fields (4.7).

To introduce the third and last example, let us consider a tensor-valued function $A^\mu{}_\nu(x) \in \mathfrak{GD}(1,3)$, $\forall x \in M$. Through any such an $A^\mu{}_\nu$, we can define the following vector field on $\mathcal{E} \times \mathcal{C} \times J_1 Q/G$

$$X = A^\gamma{}_\sigma e_q^\sigma \frac{\partial}{\partial e_q^\gamma} - \frac{1}{2} D_q A^{\mu\nu} \frac{\partial}{\partial \omega_q{}^{\mu\nu}}, \tag{4.9}$$

where $D_q A^{\mu\nu} = \partial A^{\mu\nu}/\partial x^q + \omega_q{}^\mu{}_\sigma A^{\sigma\nu} - \omega_q{}^\sigma{}_\nu A^\mu{}_\sigma$. We notice that expressions (4.9) are covariant, in the sense that, under changes of coordinates, they undergo the transformation law

$$X = \overline{A}^\gamma{}_\sigma \overline{e}_q^\sigma \frac{\partial}{\partial \overline{e}_q^\gamma} - \frac{1}{2} D_q \overline{A}^{\mu\nu} \frac{\partial}{\partial \overline{\omega}_q{}^{\mu\nu}},$$

with $\overline{A}^\nu{}_\lambda = \Lambda^\nu{}_\mu A^\mu{}_\sigma \Lambda_\lambda{}^\sigma$.

Taking Eqs. (2.11) and (2.12) into account, it is easily seen that vector fields (4.9) are $\mathcal{J}$-prolongable and their $\mathcal{J}$-prolongations are locally described as

$$\mathcal{J}(X) = A^\gamma{}_\sigma e_q^\sigma \frac{\partial}{\partial e_q^\gamma} - \frac{1}{2} D_q A^{\mu\nu} \frac{\partial}{\partial \omega_q{}^{\mu\nu}} + \frac{1}{2} A^\mu{}_\sigma T_{ij}^\sigma \frac{\partial}{\partial T_{ij}^\mu} + \frac{1}{2} A^\mu{}_\sigma R_{ij}{}^{\sigma\nu} \frac{\partial}{\partial R_{ij}{}^{\mu\nu}}. \tag{4.10}$$

As made for the previous cases, we show that vector fields (4.10) are infinitesimal Lagrangian symmetries. To do this, it is again convenient working in the coordinates (4.5), in which the fields (4.10) have local expression

$$\begin{aligned}\mathcal{J}(X) = {} & A^\gamma{}_\sigma e_q^\sigma \frac{\partial}{\partial e_q^\gamma} - \frac{1}{2}\left[D_q A^{\mu\nu} e_\sigma^q + A^\gamma{}_\sigma \omega_\gamma{}^{\mu\nu}\right] \frac{\partial}{\partial \omega_\sigma{}^{\mu\nu}} - A^\gamma{}_\mu a_\gamma^A \frac{\partial}{\partial a_\mu^A} + \frac{1}{2}\left[A^\mu{}_\sigma T_{\lambda\rho}^\sigma - 2A^\gamma{}_\lambda T_{\gamma\rho}^\mu\right] \frac{\partial}{\partial T_{\lambda\rho}^\mu} \\ & + \frac{1}{2}\left[A^\mu{}_\gamma R_{\sigma\lambda}{}^{\gamma\nu} - A^\gamma{}_\sigma R_{\gamma\lambda}{}^{\mu\nu}\right] \frac{\partial}{\partial R_{\sigma\lambda}{}^{\mu\nu}} - A^\gamma{}_\mu F_{\gamma\nu}^A \frac{\partial}{\partial F_{\mu\nu}^A}.\end{aligned}$$

Using the latter, it is a straightforward matter to verify that the identity

$$L_{\mathcal{J}(X)}(\mathcal{L} ds) = A^\mu{}_\mu \mathcal{L} ds + A^{\mu\lambda} F_{\mu\nu}^A F_{\lambda\sigma}^B \eta^{\nu\sigma} \gamma_{AB} e ds = 0$$

holds true, because of the skew-symmetry of $A^{\mu\nu}$ and the symmetry of $F_{\mu\nu}^A F_{\lambda\sigma}^B \eta^{\nu\sigma} \gamma_{AB}$.

As above, the conclusion follows that the fields (4.10) are infinitesimal dynamical symmetries and that, denoting by σ a critical section, the quantities

$$\mathcal{Q} = \mathcal{J}\sigma * (\mathcal{J}(X) \rfloor \Theta_L) = -\tfrac{1}{2} D_t A^{\alpha\beta}(x) e_i^\mu(x) e_j^\nu(x) \epsilon^{ijpt} \epsilon_{\mu\nu\alpha\beta} ds_p,$$

are the corresponding conserved Noether currents.

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Hyperbolic Kac Moody algebras and Einstein billiards

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We identify the hyperbolic Kac Moody algebras for which there exists a Lagrangian of gravity, dilatons, and p-forms which produces a billiard that can be identified with their fundamental Weyl chamber. Because of the invariance of the billiard upon toroidal dimensional reduction, the list of admissible algebras is determined by the existence of a Lagrangian in three space–time dimensions, where a systematic analysis can be carried out since only zero-forms are involved. We provide all highest dimensional parent Lagrangians with their full spectrum of p-forms and dilaton couplings. We confirm, in particular, that for the rank 10 hyperbolic algebra, $CE_{10}=A_{15}^{(2)\wedge}$, also known as the dual of $B_8^{\wedge\wedge}$, the maximally oxidized Lagrangian is nine-dimensional and involves besides gravity, 2 dilatons, a 2-form, a 1-form, and a 0-form. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1806537]

I. INTRODUCTION

It has been shown recently that the dynamics of the gravitational scale factors becomes equivalent, in the vicinity of a spacelike singularity, to that of a relativistic particle moving freely on an hyperbolic billiard and bouncing on its walls.[1–6] A criterion for the gravitational dynamics to be chaotic is that the billiard has a finite volume. This in turn stems from the remarkable property that the billiard can be identified with the fundamental Weyl chamber of an hyperbolic Kac Moody algebra. Some of these algebras are well known: in particular, the famous hyperbolic algebras [$E_{10}=E_8^{\wedge\wedge}$, $BE_{10}=B_8^{\wedge\wedge}$, $DE_{10}=D_8^{\wedge\wedge}$, $AE_n=A_{n-2}^{\wedge\wedge}$; more generally, the names here given to the algebras are taken from Refs. 12 and 13; in the table of the Dynkin diagrams given in Ref. 13, the name $D_{r+1}^{(2)}$ should be replaced by $D_{r+1}^{(2)\wedge}$] E_{10}, BE_{10}, DE_{10} (Refs. 8–10) are related to strings, supergravities, and M-theory; the $AE_n, n<10$ (Ref. 7) emerge from pure gravity in various dimensions and more generally, the algebras that are overextensions of finite dimensional simple Lie algebras[11,12]—also twisted overextensions[13]—are associated with gravitational models that reduce to G/H coset models upon toroidal dimensional reduction to $D=3$. Several other hyperbolic algebras also appear in the billiard analysis of $D=4$ and $D=5$ spatially homogeneous cosmological models.[14] This kind of analysis has attracted a lot of interest recently in connection with U-dualities[15] and hidden symmetries of M-theory.[16–21]

The purpose of this paper is twofold: first we select all hyperbolic Kac Moody algebras for which a billiard description exists and then we explicitly construct all Lagrangians describing gravity coupled to dilatons and p-forms producing these billiards.

We are able to give exhaustive results because (i) the hyperbolic algebras are all known and classified (note however six missing cases in Ref. 22, two with rank 3, two with rank 4, and two with rank 5; their Dynkin diagrams are displayed at the end of the paper),[22] and (ii) only the finite number of algebras with rank r between 3 and 10 are relevant in this context. Note that there are infinitely many hyperbolic algebras of rank two and that there exists no hyperbolic algebra of rank $r>10$. The analysis is considerably simplified because of the invariance of the billiard under

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toroidal dimensional reduction to dimensions $D \geqslant 3$. Indeed, as explained in Ref. 12, the billiard region stays the same, but a symmetry wall in D dimensions may become an electric or magnetic p-form wall in a lower dimension. The invariance under dimensional reduction implies in particular that the selection of algebras with a billiard description can be performed by analyzing Lagrangians in $D=3$ dimensions.

Simplifications in $D=3$ occur because only 0-forms are present: indeed, via appropriate dualizations, all p-forms can be reduced to 0-forms. To be concrete, for the hyperbolic algebras of real rank r between 3 and 6, we first try to reproduce their Dynkin diagram with a set of r dominant walls comprising one symmetry wall $(\beta^2-\beta^1)$ and $(r-1)$ scalar walls. If this can be done, we still have to check that the remaining walls are subdominant i.e., that they can be written as linear combinations of the dominant ones with positive coefficients. In particular, this analysis requires that any dominant set necessarily involves one magnetic wall and $(r-2)$ electric walls. Note that our search for gravitational Lagrangians in $D=3$ is systematic although no symmetry is required. To deal with the hyperbolic algebras of ranks 7–10, it is actually not necessary to first reduce to three dimensions: the overextensions of finite simple Lie algebras have already been associated with billiards of some Lagrangians and for the remaining four algebras, the rules we have found in the previous cases allow to straightforwardly construct the Lagrangian in the maximal oxidation dimension.

We then analyze which three-dimensional system admits parents in higher dimensions and construct the Lagrangian in the maximal oxidation dimension. In order to do so, we take an algebra in the previous list and we determine successively the maximal space–time dimension, the dilaton number, the p-form content, and the dilaton couplings:

(1) One considers the Dynkin diagram of the selected algebra and looks at the length of its "A-chain" (an "A-chain" of length k is a chain of k vertices with norm squared equal to 2 and simply laced), starting with the symmetry root. Our analysis produces the following oxidation rule: if the A-chain has length k, the theory can be oxidized up to

   (a) $D_{\max}=k+2$, if the next connected root has a norm squared smaller than 2;
   (b) $D_{\max}=k+1$, if the next connected root has a norm squared greater than 2.
   This generalizes the oxidation rule by Refs. 23–26, obtained by group theoretical arguments applied to coset models.

(2) For given space dimension $d=D-1$ and rank r of the algebra, the number of dilatons is given by $N=r-d$ because the dominant walls are required to be r independent linear forms in the d scale factors $\{\beta^1,\ldots,\beta^d\}$ and the N dilatons.
(3) Because it is known how the p-form walls connect to the A-chain,[12] one can read on the Dynkin diagram which p-forms [or their dual $(d-p-1)$-forms] appear in the maximal oxidation dimension.
(4) The dilaton couplings of the p-forms are computed from the norms and scalar products of the walls which have to generate the Cartan matrix of the hyperbolic algebra. This means in particular that, even if the nature of the walls changes during the oxidation procedure, their norms and scalar products remain unchanged. Note also that in all dimensions $D>3$ the subdominant conditions are always satisfied.

As a by-product of our analysis, we note that, for each billiard identifiable as the fundamental Weyl chamber of an hyperbolic algebra, the positive linear combinations of the dominant walls representing the subdominant ones only contain integer coefficients. Hence, the dominant walls of the Lagrangian correspond to the simple roots of the hyperbolic algebra, while the subdominant ones correspond to nonsimple positive roots. The gravitational theory does not give all the positive roots; even the three-dimensional scalar Lagrangians do not describe coset spaces in general. Nevertheless, the reflections relative to the simple roots generate the Weyl group of the hyperbolic algebra; this group in turn gives an access to other positive roots and suggests that a Lagrangian capable to produce these roots via billiard walls needs more exotic fields than just p-forms.

Our analysis is linked with the important physical problem of hidden symmetries of gravita-

tional theories. Furthermore, as recalled above, the hyperbolic character of the underlying Kac Moody algebra has crucial consequences on the dynamical features of the physical systems under consideration as it is linked to chaos and the BKL behavior.[1] As these properties are discussed at length in the literature, we shall not repeat them here and refer the interested reader to Refs. 11 and 27–29 for hidden symmetries and Refs. 5 and 7 for chaotic behavior.

Our paper is organized as follows: The general framework of our analysis is outlined in the first section: the form of the searched for gravitational Lagrangians is recalled, together with the list of their walls and the metric used to build the Cartan matrix. In the next four sections, we deal with hyperbolic algebras of rank 3–6. First, in $D=3$ space–time dimensions, we compute the three-dimensional dilaton couplings needed to reproduce the Dynkin diagram and check the status of the subdominant walls. This is how we select the admissible algebras. Next, for each of them, we determine which Lagrangian can be oxidized and we produce it in the maximal oxidation dimension. The 18 hyperbolic algebras of ranks 7–10 are reviewed in the last section; as explained before, they are singled out for special treatment because 14 of them are overextensions of finite dimensional simple Lie algebras and the remaining 4 are dual to the overtextension $B_n^{\wedge\wedge}$ (with $n=5,6,7,8$). We explicitly write down the $D_{\max}=9$ Lagrangian system obtained previously in Ref. 30, the billiard of which is the fundamental Weyl chamber of the algebra CE_{10}. Among the four hyperbolic algebras of rank 10, CE_{10} is special because, unlike E_{10}, BE_{10}, and DE_{10}, it does not stem from supergravities. Finally, we close our paper with some conclusions.

II. GENERAL FRAMEWORK

The billiard analysis refers to the dynamics, in the vicinity of a spacelike singularity, of a gravitational model described by the Lagrangian (compared to the notations of Ref. 12, we have put a factor of 2 in the exponents of the dilaton couplings; this way, a factor $1/2$ will be removed in front of the dilatonic part of the p-form walls)

$$\mathcal{L}_D = {}^{(D)}R \star \mathbb{1} - \sum_\alpha \star d\phi^\alpha \wedge d\phi^\alpha - \frac{1}{2}\sum_p e^{2\lambda^{(p)}(\phi)} \star F^{(p+1)} \wedge F^{(p+1)}, \quad D \geqslant 3, \tag{2.1}$$

where $\lambda^{(p)}(\phi)=\Sigma_\alpha \lambda_\alpha^{(p)}\phi^\alpha$ and $\star\mathbb{1}=\sqrt{|{}^{(D)}g|}\, dx^0\wedge\cdots\wedge dx^{D-1}$. The dilatons are denoted by ϕ^α ($\alpha=1,\ldots,N$); their kinetic terms are normalized with a weight 1 with respect to the Ricci scalar. The Einstein metric has Lorentz signature $(-,+,\ldots,+)$; its determinant is ${}^{(D)}g$. The integer $p\geqslant 0$ labels the various p-forms $A^{(p)}$ present in the theory, with field strengths $F^{(p+1)}=dA^{(p)}$. If there are several p-form gauge fields with the same form degree p, we will use different letters $A^{(p)}, B^{(p)},\ldots$, to distinguish them.

The rules for computing the billiards have been given in details in Refs. 6, 7, and 12 to which we refer the reader. We here recall the essential tools that are used throughout the paper.

A. The walls

The walls bounding the billiard have different origins: some arise from the Einstein–Hilbert action and involve only the scale factors β^i ($i=1,\ldots,d$), introduced through the Iwasawa decomposition of the space metric. They are

(1) the symmetry walls

$$w_{ij}^S(\beta) = \beta^j - \beta^i, \quad i<j, \tag{2.2}$$

and

(2) the curvature walls

$$w^G_{i;jk}(\beta) = 2\beta^i + \sum_{\ell \neq i,j,k} \beta^\ell, \quad i \neq j, i \neq k, j \neq k. \tag{2.3}$$

The others come from the energy densities of the p-forms; they depend on the scale factors and the dilatons and are

(3) the electric walls

$$w^{E(p)}_{i_1 \cdots i_p}(\beta, \phi) = \beta^{i_1} + \cdots + \beta^{i_p} + \sum_\alpha \lambda^{(p)}_\alpha \, \phi^\alpha, \quad i_1 < \cdots < i_p \tag{2.4}$$

and

(4) the magnetic walls

$$w^{M(p)}_{i_1 \cdots i_{d-p-1}}(\beta, \phi) = \beta^{i_1} + \cdots + \beta^{i_{d-p-1}} - \sum_\alpha \lambda^{(p)}_\alpha \, \phi^\alpha, \quad i_1 < \cdots < i_{d-p-1}. \tag{2.5}$$

Notice that upon the change of ϕ^α into $-\phi^\alpha$, the electric walls of a p-form become the magnetic walls of its dual $(d-p-1)$-form and vice versa.

The region of hyperbolic space where the particle motion takes place is defined through the inequalties $w^S_{ij} \geqslant 0$, $w^G_{i;jk} \geqslant 0$, $w^{E(p)}_{i_1 \cdots i_p} \geqslant 0$, and $w^{M(p)}_{i_1 \cdots i_{d-p-1}} \geqslant 0$; in fact, these inequalities follow from a simpler subset, namely

$$\beta^1 \leqslant \beta^2 \cdots \leqslant \beta^d, \quad w^G_{1;23} \geqslant 0, \quad w^E_{1 \cdots p} \geqslant 0, \quad w^M_{1 \cdots (d-p-1)} \geqslant 0, \tag{2.6}$$

which may still be redundant. The walls forming the minimal set needed to define completely the billiard are called "dominant"; the others are referred to as subdominant. More precisely, a wall is called subdominant if it can be expressed as a linear combination with positive coefficients of the dominant ones.

B. The metric

Given two walls $w(\beta, \phi) = w_i \, \beta^i + w_\alpha \, \phi^\alpha = w_\mu \, \beta^\mu$ and $w'(\beta, \phi) = w'_i \beta^i + w'_\alpha \phi^\alpha = w'_\mu \beta^\mu$—the $\beta^\mu (\mu = 1, \ldots, d, 1+d, \ldots, N+d)$ here denote scale factors β^i $(i = 1, \ldots, d)$ and dilatons, $\beta^{\alpha+d} = \phi^\alpha$—their scalar product is defined as

$$(w|w') = G^{\mu\nu} \, w_\mu \, w'_\nu = \sum_i (w_i \, w'_i) - \frac{1}{d-1} \left(\sum_i w_i \right) \left(\sum_j w'_j \right) + \sum_\alpha (w_\alpha \, w'_\alpha). \tag{2.7}$$

The metric $G^{\mu\nu}$ is the inverse of the Lorentzian metric $G_{\mu\nu}$ defining the kinetic term of the scale factors and dilatons; as shown in (2.7), it depends explicitly on the spatial dimension d. Notice that a symmetry wall has a norm squared equal to 2. Furthermore, the p-form electric wall $w^E_{1 \cdots p}$ is orthogonal to all symmetry walls except one, namely, $w^S_{p,p+1} = \beta^{p+1} - \beta^p$; the corresponding scalar product is equal to -1.

Let $\{w_B = w_B(\beta, \phi), B = 1, \ldots, r\}$ denote a set of dominant walls. The enclosed billiard volume is finite if the scalar products are such that the $r \times r$ matrix

$$A_{BC} = 2 \frac{(w_B|w_C)}{(w_B|w_B)} \tag{2.8}$$

is the generalized Cartan matrix of an hyperbolic Kac Moody algebra of rank r.

III. RANK 3 HYPERBOLIC ALGEBRAS

A. $D=3$

In space dimension $d=2$, one has a single symmetry wall, namely,

$$\alpha_1 = \beta^2 - \beta^1 \tag{3.1}$$

and $N=r-d=3-2=1$ dilaton denoted as ϕ. It is obvious that only a 0-form magnetic wall can be connected to the symmetry wall, say

$$\alpha_2 = \beta^1 - \lambda\phi. \tag{3.2}$$

Let us show that the last dominant wall has to be an electric one denoted by

$$\alpha_3 = \lambda'\phi. \tag{3.3}$$

Indeed, had one taken for dominant the magnetic wall $\tilde{\alpha}_3=\beta^1-\lambda'\phi$ instead of (3.3), then, its corresponding electric wall, which is precisely $\alpha_3=\lambda'\phi$, would be dominant too because of the impossibility to write it as a linear combination with positive coefficients of the other three α_1, α_2, and $\tilde{\alpha}_3$.

Using the metric (2.7) adapted to $d=2$, we build the matrix

$$A_{ij} = 2\frac{(\alpha_i|\alpha_j)}{(\alpha_i|\alpha_i)} \tag{3.4}$$

and obtain

$$A = \begin{pmatrix} 2 & -1 & 0 \\ -\dfrac{2}{\lambda^2} & 2 & -2\dfrac{\lambda'}{\lambda} \\ 0 & -2\dfrac{\lambda}{\lambda'} & 2 \end{pmatrix}, \tag{3.5}$$

which has to be identified with the generalized Cartan matrix of an hyperbolic Kac Moody algebra of rank 3. Because ϕ can be changed into $-\phi$, λ and λ' can be chosen positive.

Since in such a matrix (i) the nonzero off-diagonal entries are negative integers and (ii) not any finite or affine Lie algebra of rank 2 has an off-diagonal negative integer <-4, one immediately infers from the expression of A_{21} in (3.5) that the allowed values for λ are

$$\lambda \in \{\sqrt{2}, 1, \sqrt{2/3}, 1/2\}. \tag{3.6}$$

Being a symmetry wall, α_1 has norm squared equal to 2; α_2 has norm squared $\lambda^2 \leqslant 2$, so that, if the Dynkin diagram has an arrow between α_1 and α_2, this arrow must be directed towards α_2. Once the value of λ has been fixed, one needs to find λ' such that both $2\lambda'/\lambda$ and $2\lambda/\lambda'$ are positive integers: this leaves $\lambda=\lambda'/2, \lambda', 2\lambda'$. These values are further constrained by the condition that the subdominant walls $\tilde{\alpha}_2=\lambda\phi$ and $\tilde{\alpha}_3=\beta^1-\lambda'\phi$, stay really behind the others, i.e., that there exist $k>0$ and $\ell \geqslant 0$ such that

$$\tilde{\alpha}_2 = k\alpha_3 \Rightarrow \lambda/\lambda' = k, \tag{3.7}$$

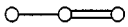
$$\tilde{\alpha}_3 = \alpha_2 + \ell\alpha_3 \Rightarrow \lambda/\lambda' = \ell + 1, \tag{3.8}$$

which implies $k=\ell+1 \geqslant 1$. Hence, the subdominant conditions require

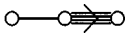
$$\lambda' = \lambda \quad \text{or} \quad \lambda' = \lambda/2. \tag{3.9}$$

Let us summarize the 8 different possibilities for the pairs (λ, λ') that lead to Cartan matrices and draw the corresponding Dynkin diagrams:

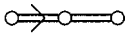
(i) for $\lambda = \sqrt{2}$ and $\lambda' = \sqrt{2}$, the Dynkin diagram describes the overextension $A_1^{\wedge\wedge}$

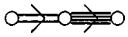
3-1 

and for $\lambda = \sqrt{2}$ and $\lambda' = 1/\sqrt{2}$, the Dynkin diagram corresponds to the twisted overextension[13] $A_2^{(2)\wedge}$

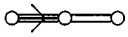
3-2 

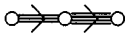
(ii) $\lambda = 1$; the two possibilities are $\lambda' = 1$ and $\lambda' = 1/2$. The Dynkin diagrams are, respectively;

3-3 

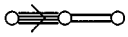
3-4 

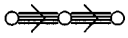
(iii) $\lambda = \sqrt{2/3}$; the two possibilities are $\lambda' = \sqrt{2/3}$ and $\lambda' = 1/\sqrt{6}$ with Dynkin diagrams given by

3-5 

3-6 

(iv) $\lambda = 1/2$; the two possibilities are $\lambda' = 1/2$ and $\lambda' = 1/4$. The Dynkin diagrams are, respectively,

3-7 

3-8 

Comments:

(1) When $\lambda' = \lambda$, α_2 and α_3 have to be assigned to a single scalar field; when $\lambda' \neq \lambda$, two scalars are needed in the three-dimensional Lagrangian.
(2) The algebra (3-8) is missing in Table 2 of Ref. 22. The subalgebra obtained when removing the first or the last root is the affine $A_2^{(2)}$; the removal of the middle root gives $A_1 \times A_1$ so that this algebra satisfies indeed the criterion of hyperbolicity.
(3) Remark that none of the 8 algebras above is strictly hyperbolic. (A strictly hyperbolic algebra is such that upon removal of a simple root, only finite Lie algebras are left behind.) The latter are listed in Table 1 of Ref. 22.

B. $D=4$

The four-dimensional Lagrangian will have no dilaton in it since $N = r - d = 0$; hence, if such a Lagrangian exists, it cannot stem from a higher dimensional parent and $D_{\max} = 4$. When looking at the algebras of rank 3 selected above, one sees that only (3-1) and (3-2) have an A-chain of length $k = 2$ and allow, *a priori*, a second symmetry wall. One starts with

$$\alpha_1 = \beta^3 - \beta^2 \quad \text{and} \quad \alpha_2 = \beta^2 - \beta^1. \tag{3.10}$$

The third root may only contain β^1 and can be associated with

(1) The curvature wall $\alpha_3 = 2\beta^1$ in the case of four-dimensional pure gravity. The Dynkin diagram bears number (3-1) above and is the overextension $A_1^{\wedge\wedge}$.
(2) The electric/magnetic wall of a 1-form: $\alpha_3 = \beta^1$. This case leads to diagram (3-2) which belongs to the twisted overextension $A_2^{(2)\wedge}$.

One sees immediately that the regions of hyperbolic space delimited by both sets of walls coincide; the difference is entirely due to the normalization of the third wall which is thus responsible for the emergence of two distinct Cartan matrices.

IV. RANK 4 HYPERBOLIC ALGEBRAS

A. $D=3$

In order to reproduce through walls the four roots of such an algebra, besides the scale factors β^1 and β^2, one needs $N=2$ dilatons; they will be denoted as $\phi^1 = \phi, \phi^2 = \varphi$. There is one symmetry wall, i.e., $\alpha_1 = \beta^2 - \beta^1$ and, *a priori*, two choices can be made for the next three dominant walls: either (i) one takes one magnetic wall and two electric ones or (ii) one takes one electric wall and two magnetic ones. We will start with case (i) and show later how case (ii) is eliminated on account of the subdominant conditions.

1. One magnetic wall and two electric ones

The dominant walls are thus the symmetry wall

$$\alpha_1 = \beta^2 - \beta^1, \tag{4.1}$$

the magnetic wall, written as (this ansatz represents no loss of generality because starting from the more general expression $\alpha_2 = \beta^1 - \lambda\phi + \mu\varphi$, one can redefine the dilatons via an orthogonal transformation—leaving the dilaton Lagrangian invariant—to get the simpler expression used above)

$$\alpha_2 = \beta^1 - \lambda\phi \tag{4.2}$$

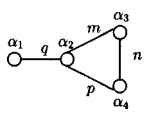
and the two electric ones

$$\alpha_3 = \lambda'\phi - \mu'\varphi, \tag{4.3}$$

respectively,

$$\alpha_4 = \lambda''\phi + \mu''\varphi. \tag{4.4}$$

As before, the signs have already been distributed to account for the negative signs of the off-diagonal Cartan matrix elements when allowing the parameters to be either all $\geqslant 0$ or all $\leqslant 0$; that they can further be chosen positive is due to the possibility to change ϕ^α into $-\phi^\alpha$. The general structure of the Dynkin diagram is therefore the following:



where we have not drawn the arrows and q, m, n, p are integers which count the number of lines joining two vertices.

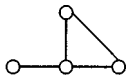
What are the possible values that can be assigned to q, m, n, and p? Since this diagram has to become the Dynkin diagram of an hyperbolic algebra, the maximal value of each of these integers is 3, because there is no finite or affine algebra of rank 3 with off-diagonal Cartan matrix elements

smaller than −3. Another point is that if there were an arrow between α_1 and α_2 it necessarily points towards α_2: one has indeed $(\alpha_1,\alpha_2)=-1$, $(\alpha_1,\alpha_1)=2$ (it is a symmetry wall), $(\alpha_2,\alpha_2)=\lambda^2$ and $A_{21}=-2/\lambda^2$ can only be $-1,-2$ or -3. We may also state that if A_{ij} is neither 0 nor −1 then $A_{ji}=-1$, because this is a common property of all finite or affine algebras of rank 3. Taking all these restrictions into account, one has to consider three different situations characterized, respectively, by (i) m, n, p are all different from zero, (ii) $n=0$ and m, p are not zero, (iii) $p=0$ and n, m are not zero.

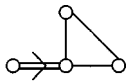
(i) If m, n, and p are all nonzero, then they must all be equal to 1 because, upon removal of the root α_1, one obtains a triangular diagram; now, in the set of the finite or affine algebras, there is only one such triangular Dynkin diagram and it is simply laced. That leaves, *a priori*, three cases labeled by the values $q=1,2,3$. The corresponding dilaton couplings are

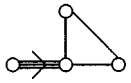
$$\lambda=\sqrt{\frac{2}{q}};\quad \lambda'=\frac{1}{\sqrt{2q}};\quad \mu'=\sqrt{\frac{3}{2q}};\quad \lambda''=\frac{1}{\sqrt{2q}};\quad \mu''=\sqrt{\frac{3}{2q}}. \tag{4.5}$$

The Dynkin diagrams corresponding to $q=1$, 2, and 3, are respectively,

4-1 

which is the overextension $A_1^{\wedge\wedge}$ and

4-2 

4-3 

The subdominant conditions are satisfied in all cases; let us show this explicitly. With the couplings in (4.5), the dominant walls other than the symmetry wall read

$$\alpha_2=\beta^1-2\frac{\phi}{\sqrt{2q}},\quad \alpha_3=\frac{\phi}{\sqrt{2q}}-\varphi\sqrt{\frac{3}{2q}},\quad \alpha_4=\frac{\phi}{\sqrt{2q}}+\varphi\sqrt{\frac{3}{2q}}. \tag{4.6}$$

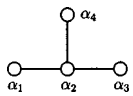
The corresponding subdominant ones are

$$\tilde{\alpha}_2=2\frac{\phi}{\sqrt{2q}},\quad \tilde{\alpha}_3=\beta^1-\frac{\phi}{\sqrt{2q}}+\varphi\sqrt{\frac{3}{2q}},\quad \tilde{\alpha}_4=\beta^1-\frac{\phi}{\sqrt{2q}}-\varphi\sqrt{\frac{3}{2q}} \tag{4.7}$$

and they obey

$$\tilde{\alpha}_2=\alpha_3+\alpha_4,\quad \tilde{\alpha}_3=\alpha_2+\alpha_4,\quad \tilde{\alpha}_4=\alpha_2+\alpha_3. \tag{4.8}$$

(ii) If $n=0$ and m, p are not zero, the structure of the Dynkin diagram is the following:



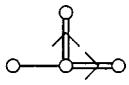
Comparison with the similar graphs of Ref. 22 impose (i) $m=p=2$, (ii) $q=1$ or $q=2$, and (iii) an arrow pointing from α_2 to α_3 and another arrow from α_2 to α_4. Accordingly, the dilaton couplings producing them are given by

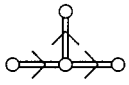
$$\lambda=\sqrt{\frac{2}{q}};\quad \lambda'=\frac{1}{\sqrt{2q}};\quad \mu'=\frac{1}{\sqrt{2q}};\quad \lambda''=\frac{1}{\sqrt{2q}};\quad \mu''=\frac{1}{\sqrt{2q}}. \tag{4.9}$$

TABLE I. Possible couplings.

	λ	λ'	μ'
1	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$
2.a	$\sqrt{2}$	$1/\sqrt{2}$	$\sqrt{3/2}$
2.b	$\sqrt{2}$	$1/\sqrt{2}$	$1/\sqrt{2}$
2.c	$\sqrt{2}$	$1/\sqrt{2}$	$1/\sqrt{6}$
3	1	1	1
4.a	1	1/2	$\sqrt{3}/2$
4.b	1	1/2	1/2
4.c	1	1/2	$1/\sqrt{12}$
5	$\sqrt{2/3}$	$\sqrt{2/3}$	$\sqrt{2/3}$
6.a	$\sqrt{2/3}$	$1/\sqrt{6}$	$1/\sqrt{2}$
6.b	$\sqrt{2/3}$	$1/\sqrt{6}$	$1/\sqrt{6}$
6.c	$\sqrt{2/3}$	$1/\sqrt{6}$	$1/\sqrt{18}$

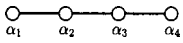
The Dynkin diagrams corresponding to $q=1$ and 2, are, respectively,

4-4 

4-5 

Again, the subdominant conditions are fulfilled: indeed, one gets $\tilde{\alpha}_2=\alpha_3+\alpha_4$, $\tilde{\alpha}_3=\alpha_2+\alpha_4$, $\tilde{\alpha}_4=\alpha_2+\alpha_3$.

(iii) If $p=0$ and n, m are not zero, the structure of the Dynkin diagram is the following:



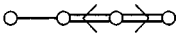
The dominant walls now simplify as

$$\alpha_1=\beta^2-\beta^1, \quad \alpha_2=\beta^1-\lambda\phi, \quad \alpha_3=\lambda'\phi-\mu'\varphi, \quad \alpha_4=\mu''\varphi. \tag{4.10}$$

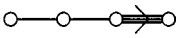
We want the corresponding magnetic and electric walls to be effectively subdominant: this is indeed satisfied when (1) λ and therefore λ' are positive; (2) $\lambda'/\lambda\leqslant 1$ (that is $\lambda'/\lambda=1$ or $\lambda'/\lambda=1/2$), and (3) $\mu'/\mu''\geqslant\lambda'/\lambda$. Accordingly, the remaining possibilities for λ, λ', and μ' are, *a priori*, those given in Table I.

The different values for μ' correspond to distinct admissible values for A_{32}. Finally, for the values of μ'', we again meet two cases depending on which of A_{34} or A_{43} is equal to -1. In each case, one has still to check the subdominant conditions.

(1) The two possibilities lead to a Cartan matrix: either $\mu''=2\sqrt{2}$ or $\mu''=\sqrt{2}$. The former case is ruled out because the subdominant conditions cannot be satisfied. The Dynkin diagram of the remaining case describes the twisted overextension $D_3^{(2)\wedge}$,

4-6 

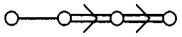
(2a) Either $\mu''=\sqrt{2/3}$ or $\mu''=\sqrt{6}$; both lead to hyperbolic algebras which correspond, respectively, to the overextension $G_2^{\wedge\wedge}$,

4-7 

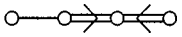
and to the twisted overextension $D_4^{(3)\wedge}$,

4-8 

(2b) Either $\mu''=\sqrt{1/2}$ or $\mu''=\sqrt{2}$; the Dynkin diagrams correspond respectively to the twisted overextension $A_4^{(2)\wedge}$,

4-9 

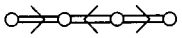
and to the overextension $C_2^{\wedge\wedge}$,

4-10 

(2c) Only the value $\mu''=2/\sqrt{6}$ is compatible with the subdominant conditions. The corresponding algebra is given by

4-11 

(3) Here again, only the value $\mu''=1$ can be retained on account of the subdominant conditions. This leads to

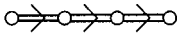
4-12 

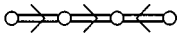
(4a) Either $\mu''=\sqrt{3}$ or $\mu''=1/\sqrt{3}$; both values are admissible. They lead to

4-13 

4-14 

(4b) Either $\mu''=1/2$ or $\mu''=1$; both values are allowed and they give, respectively,

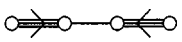
4-15 

4-16 

(4c) Does not correspond to any hyperbolic algebra.

(5) Only the value $\mu''=\sqrt{2/3}$ is compatible with the subdominant conditions but again there is no corresponding hyperbolic algebra.

(6a) Only the first of the 2 values $\mu''=\sqrt{2}$ and $\mu''=\sqrt{2}/3$ leads to an hyperbolic algebra, which is

4-17 

(6b) and (6c) do not give a hyperbolic algebra.

2. One electric wall and two magnetic ones

This case can be eliminated on account of the subdominant conditions. Indeed, without loss of generality, one may choose the parametrization of the dominant walls such that the electric wall takes a simple form, i.e., such that

$$\alpha_1 = \beta^2 - \beta^1,$$

$$\alpha_2 = \beta^1 - \lambda\phi - \mu\varphi,$$

$$\alpha_3 = \beta^1 - \lambda'\phi + \mu'\varphi,$$

$$\alpha_4 = \lambda''\phi. \tag{4.11}$$

Being assumed subdominant, the electric walls associated with α_2 and α_3, namely $\tilde{\alpha}_2 = \lambda\phi + \mu\varphi$ and $\tilde{\alpha}_3 = \lambda'\phi - \mu'\varphi$ need be proportional to α_4; this happens only when $\mu = \mu' = 0$, but then (4.11) does no longer define a rank four root system.

B. $D > 3$

Our aim is now to determine which of the 17 algebras selected in the previous section admit Lagrangians in higher space–time dimensions and to provide the maximal oxidation dimension and the p-forms content with its characteristic features. By considering each Dynkin diagram and looking at the length of the A-chain starting from the symmetry root α_1, we establish the following "empirical" oxidation rule: if the A-chain has length k one can oxidize the spatial dimension up to (i) $d = k+1$ if the norm squared of the next connected root is smaller than 2 and up (ii) to $d = k$ if the norm squared of the next connected root is greater than 2. In particular, the subdominant conditions are always satisfied. Explicitly,

(1) Diagram (4-1) is the overextension $A_2^{\wedge\wedge}$. We know from Ref. 12 that it corresponds to pure gravity in $D_{\max} = 5$.

(2) Diagrams (4-2) and (4-3) have an A-chain of length 1; the three-dimensional theory cannot be oxidized.

(3) Diagram (4-4): $D_{\max} = 4$. The walls are given by

$$\alpha_1 = \beta^3 - \beta^2, \quad \alpha_2 = \beta^2 - \beta^1, \tag{4.12}$$

$$\alpha_3 = \beta^1 - \phi/\sqrt{2}, \quad \alpha_4 = \beta^1 + \phi/\sqrt{2}. \tag{4.13}$$

The last two are the electric and magnetic dominant walls of a one-form coupled to the dilaton. One sees immediately that $\tilde{\alpha}_3 = \alpha_4$ and $\tilde{\alpha}_4 = \alpha_3$.

(4) Diagram (4-5): the three-dimensional Lagrangian has no parent in $D > 3$.

(5) Diagram (4-6) is the twisted overextension $D_3^{(2)\wedge}$. The 3D Lagrangian cannot be oxidized the reason being that $\|\alpha_3\|^2 > 2$.

(6) Diagram (4-7) is the overextension $G_2^{\wedge\wedge}$. We know from Ref. 12 that the theory can be oxidized up to $D_{\max} = 5$ where the Lagrangian is that of the Einstein–Maxwell system.

(7) Diagram (4-8) describes $D_4^{(3)\wedge}$. The A-chain has length $k = 3$ and the next connected root is longer than $\sqrt{2}$. The maximal oxidation dimension is $D_{\max} = 4$ and the dominant walls are given by

$$\alpha_1 = \beta^3 - \beta^2, \quad \alpha_2 = \beta^2 - \beta^1, \tag{4.14}$$

$$\alpha_3 = \beta^1 - \sqrt{3/2}\phi, \quad \alpha_4 = \sqrt{6}\phi. \tag{4.15}$$

The root α_3 is the electric wall of a 1-form, α_4 is the electric wall of a 0-form. One easily checks that the subdominant magnetic walls satisfy

$$\tilde{\alpha}_3 = \beta^1 + \sqrt{3/2}\phi = \alpha_3 + \alpha_4, \tag{4.16}$$

$$\tilde{\alpha}_4 = \beta^1 + \beta^2 - \sqrt{6}\phi = 2\alpha_3 + \alpha_2. \tag{4.17}$$

(8) Diagram (4-9) represents $A_4^{(2)\wedge}$. $D_{\max}=4$. Its billiard realization requires

$$\alpha_1=\beta^3-\beta^2,\quad \alpha_2=\beta^2-\beta^1, \tag{4.18}$$

$$\alpha_3=\beta^1-\sqrt{1/2}\phi,\quad \alpha_4=\sqrt{1/2}\phi. \tag{4.19}$$

The last two are again the electric walls of a 1-form and a zero-form; only the dilaton couplings differ from the previous ones. The subdominant conditions are fulfilled: indeed, one obtains $\tilde{\alpha}_3=\alpha_3+2\alpha_4$ and $\tilde{\alpha}_4=2\alpha_3+\alpha_4+\alpha_2$.

(9) Diagram (4-10) is the overextension $C_2^{\wedge\wedge}$. We know from Ref. 12 that the theory can be oxidized up to $D_{\max}=4$.

(10) Diagram (4-11) has $D_{\max}=4$ and

$$\alpha_1=\beta^3-\beta^2,\quad \alpha_2=\beta^2-\beta^1, \tag{4.20}$$

$$\alpha_3=\beta^1-\sqrt{1/6}\phi,\quad \alpha_4=\sqrt{2/3}\phi. \tag{4.21}$$

It has the same form content as (4-8) and (4-9) but the dilaton couplings are still different. Again, the subdominant conditions are fulfilled: $\tilde{\alpha}_3=\alpha_3+\alpha_4$ and $\tilde{\alpha}_4=2\alpha_3+\alpha_2$.

(11) Diagrams (4-12) to (4-17): their 3D Lagrangians cannot be oxidized because there is a unique root of norm squared equal to 2.

Comments:

(a) The subdominant conditions are indeed always fulfilled in $D>3$ and only positive integer coefficients enter the linear combinations.

(b) In case (4-4), α_3 and α_4 are the electric and magnetic walls of the same one-form. In the other cases, they are respectively assigned to a single one-form and a single zero-form. The root multiplicity being one, there is no room for various p-forms with identical couplings.

V. RANK 5 HYPERBOLIC ALGEBRAS

A. $D=3$

The three-dimensional Lagrangians need $N=r-d=3$ dilatons ($\phi^1=\phi,\phi^2=\varphi,\phi^3=\psi$); there are two scale factors and one symmetry wall $\alpha_1=\beta^2-\beta^1$. In order to reproduce the other four simple roots of the algebra in terms of dominant walls, one has *a priori* three different cases to consider: indeed, the set of dominant walls can comprise (i) one magnetic wall and three electric ones, (ii) two electric walls and two magnetic ones and (iii) one electric wall and three magnetic ones. Only the first possibility will survive because as soon as the set of dominant walls contains more than one magnetic wall, one can show that the corresponding electric walls cannot fulfill the subdominant conditions. Although the proof is a straightforward generalization of the one given in Sec. IV A, we will provide it at the end of this section.

1. One magnetic wall and three electric ones

As in the previous sections, we use the freedom to redefine dilatons through an orthogonal transformation and choose the parametrization of the dominant walls such that

$$\alpha_1=\beta^2-\beta^1, \tag{5.1}$$

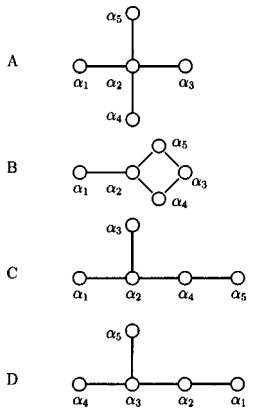
$$\alpha_2=\beta^1-\lambda\phi, \tag{5.2}$$

$$\alpha_3=\lambda'\phi-\mu'\varphi, \tag{5.3}$$

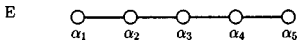
$$\alpha_4 = \lambda''\phi + \mu''\varphi - \nu''\psi, \tag{5.4}$$

$$\alpha_5 = \lambda'''\phi + \mu'''\varphi + \nu'''\psi. \tag{5.5}$$

One sees immediately that the symmetry root α_1 is only linked to the magnetic root α_2 while α_2 can further be connected to one, two or three roots. According to (Ref. 22), five different structures for the Dynkin diagrams can be encountered; we classify them below according to the total number of roots connected to α_2; this number is 4 in case A, 3 in cases B and C, 2 in cases D and E.



Note that C and D simply differ by the assignment of the symmetry root.



Case A: This case may be discarded. Indeed, there are in fact two hyperbolic algebras with a Dynkin diagram of that shape: one of them has a long and four short roots, while the other one has one short and four long roots. Either one cannot find couplings that reproduce their Cartan matrix or it is the subdominant condition that is violated. More concretely:

(A1) Consider first the case for which $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ correspond to the short roots and α_5 is the long root. Then, according to (Ref. 22), one needs

$$\|\alpha_1\|^2 = \|\alpha_2\|^2 = \|\alpha_3\|^2 = \|\alpha_4\|^2 = 2, \quad \text{and} \quad \|\alpha_5\|^2 = 4. \tag{5.6}$$

These conditions are immediately translated into

$$\lambda^2 = 2, \quad \lambda'^2 + \mu'^2 = 2, \quad \lambda''^2 + \mu''^2 + \nu''^2 = 2, \quad \lambda'''^2 + \mu'''^2 + \nu'''^2 = 4. \tag{5.7}$$

Hence $\lambda = \sqrt{2}$. From the shape of the diagram or equivalently from the elements of the Cartan matrix, one infers successively

(1) $A_{23} = -1 = -\lambda\lambda'$ which gives $\lambda' = 1/\sqrt{2}$ and $\mu' = \sqrt{3/2}$;
(2) $A_{24} = -1 = -\lambda\lambda''$ and $A_{34} = 0 = \lambda'\lambda'' - \mu'\mu''$ which gives $\lambda'' = 1/\sqrt{2}$, $\mu'' = 1/\sqrt{6}$ and $\nu'' = 2/\sqrt{3}$;
(3) $A_{25} = -2 = -\lambda\lambda'''$ which gives $\lambda''' = \sqrt{2}$;
(4) $A_{35} = 0 = \lambda'\lambda''' - \mu'\mu'''$ which gives $\mu''' = \sqrt{2/3}$ and, using the norm of α_5, $\nu''' = 2/\sqrt{3}$.

Notice that the condition $A_{45} = 0 = \lambda''\lambda''' + \mu''\mu''' - \nu''\nu'''$ is identically satisfied.

In summary, in order to fit the Dynkin diagram displayed in A (with simple lines between α_2 and $\alpha_1, \alpha_3, \alpha_4$ and a double line between α_2 and α_5 oriented towards α_2), besides the symmetry wall, we need the following set of dominant walls:

$$\alpha_2 = \beta^1 - \sqrt{2}\phi, \quad \alpha_4 = \frac{\phi}{\sqrt{2}} + \frac{\varphi}{\sqrt{6}} - \frac{2\psi}{\sqrt{3}}, \tag{5.8}$$

$$\alpha_3 = \frac{\phi}{\sqrt{2}} - \sqrt{\frac{3}{2}}\varphi, \quad \alpha_5 = \sqrt{2}\phi + \sqrt{\frac{2}{3}}\varphi + \frac{2\psi}{\sqrt{3}}. \tag{5.9}$$

It is now easy to verify, for instance, that $\tilde{\alpha}_3 = \beta^1 - (\phi/\sqrt{2}) + \sqrt{\frac{3}{2}}\varphi$, cannot be written as a positive linear combination of the $\alpha_i, i = 2, \ldots, 5$. Accordingly, on account of the subdominant conditions, this case has to be rejected.

(A2) There is another possibility producing the same diagram as in (A1) above where the symmetry wall α_1 now plays the role of the long root: their norms are

$$\|\alpha_1\|^2 = 2 \quad \text{and} \quad \|\alpha_2\|^2 = \|\alpha_3\|^2 = \|\alpha_4\|^2 = \|\alpha_5\|^2 = 1, \tag{5.10}$$

but the equations giving the couplings analogous to Eq. (1)–(4) above have no solution.

(A3) In the third case, there is a short and four long roots with norms

$$\|\alpha_1\|^2 = \|\alpha_2\|^2 = \|\alpha_3\|^2 = \|\alpha_4\|^2 = 2 \quad \text{and} \quad \|\alpha_5\|^2 = 1. \tag{5.11}$$

One can solve the equations for the couplings and write the following set of billiard walls: the symmetry wall $\alpha_1 = \beta^2 - \beta^1$ and

$$\alpha_2 = \beta^1 - \sqrt{2}\phi, \quad \alpha_4 = \frac{\phi}{\sqrt{2}} + \frac{\varphi}{\sqrt{6}} - \frac{2\psi}{\sqrt{3}}, \tag{5.12}$$

$$\alpha_3 = \frac{\phi}{\sqrt{2}} - \sqrt{\frac{3}{2}}\varphi, \quad \alpha_5 = \frac{\phi}{\sqrt{2}} + \frac{\varphi}{\sqrt{6}} + \frac{\psi}{\sqrt{3}}. \tag{5.13}$$

However, like in case (A1) above, one sees immediately that $\tilde{\alpha}_3 = \beta^1 - (\phi/\sqrt{2}) + (3\varphi/\sqrt{6})$, for instance, is not subdominant; that is the reason why we discard this possibility.

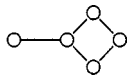
Cases B: There are three hyperbolic algebras with a Dynkin diagram of this shape.

(B1) The first one admits the following couplings:

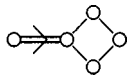
$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\tfrac{3}{2}};$$

$$\lambda'' = 0; \quad \mu'' = \sqrt{\tfrac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = \frac{1}{\sqrt{2}}; \quad \mu''' = \frac{1}{\sqrt{6}}; \quad \nu''' = \frac{2}{\sqrt{3}} \tag{5.14}$$

and is the overextension $A_3^{\wedge\wedge}$

5-1 

(B2) The second one has the following Dynkin diagram:

5-2 

and the following set of dilaton couplings:

$$\lambda = 1; \lambda' = \tfrac{1}{2}; \quad \mu' = \frac{\sqrt{3}}{2};$$

$$\lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{3}}; \quad \nu'' = \frac{\sqrt{2}}{\sqrt{3}}; \quad \lambda''' = \tfrac{1}{2}; \quad \mu''' = \frac{1}{2\sqrt{3}}; \quad \nu''' = \frac{\sqrt{2}}{\sqrt{3}}. \tag{5.15}$$

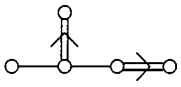
(B3) The diagram of the third one is the same as (5-2) but with the reversed arrow; this is impossible since in the present context the norms are required to satisfy $\|\alpha_1\|^2 \geqslant \|\alpha_2\|^2$.

Case C: In order to generate this kind of structure, one needs $\lambda''' = \mu''' = 0$ and $\lambda'\lambda'' = \mu'\mu''$. Next, from the subdominant condition for $\tilde{\alpha}_3$, we deduce that A_{32} can be -2 or -3 but since we want hyperbolic algebras, only the value $A_{32} = -2$ can be retained. Therefore $A_{23} = -1$ and $\lambda = \sqrt{2}$, $\lambda' = \lambda'' = 1/\sqrt{2}$, $\mu' = 1/\sqrt{2}$, $\mu'' = 1/\sqrt{2}$, and $\nu'' = 1$. *A priori*, one might still have $\nu''' = 2, 1, \sqrt{2}$ but only one value is compatible with the magnetic wall $\tilde{\alpha}_5$ being subdominant, namely $\nu''' = 1$. Accordingly, the couplings need to be defined as

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \frac{1}{\sqrt{2}};$$

$$\lambda'' = \frac{1}{\sqrt{2}}; \quad \mu'' = \frac{1}{\sqrt{2}}; \quad \nu'' = 1; \quad \lambda''' = 0; \quad \mu''' = 0; \quad \nu''' = 1. \tag{5.16}$$

and the Dynkin diagram is the following:

5-3 

Case D: Dynkin diagrams of this shape can only be recovered with

$$\lambda'' = \lambda''' = 0 \quad \text{and either} \quad \lambda = \sqrt{2} \quad \text{or} \quad \lambda = 1. \tag{5.17}$$

(D.1) $\lambda = \sqrt{2}$.

All hyperbolic diagrams of that type have in their Cartan matrix $A_{34} = A_{43} = -1$ which means that $\|\alpha_3\|^2 = \|\alpha_4\|^2$. Two additional cases must be considered depending on which of α_2 or α_5 has a norm equal to the norm of α_3:

(1) In case (D.1.1) we assume that the norms of α_3, α_4, and α_5 are equal.
(2) In case (D.1.2) we assume that the norms of α_2, α_3, and α_4 are equal.

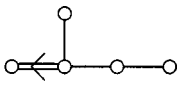
The subdominant conditions here simply reduce to $A_{23} = -1$.

(D.1.1) Again two hyperbolic algebras correspond to this case. For the first one, the billiard walls are built out of the following couplings:

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}};$$

$$\lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{1}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = \sqrt{\frac{2}{3}}; \quad \nu''' = \frac{2}{\sqrt{3}} \tag{5.18}$$

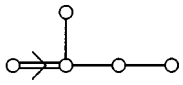
and the Dynkin diagram is that of the overextension $B_3^{\wedge\wedge}$,

5-4 

One can produce a billiard for the second one using the same couplings as in (5.18) except for

$$\lambda'' = 0; \quad \mu'' = 2\sqrt{\frac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}. \tag{5.19}$$

The Dynkin diagram here describes the twisted overextension $A_5^{(2)\wedge}$,

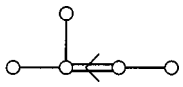
5-5 

(D.1.2) Here also, two hyperbolic algebras correspond to this case but one is eliminated on account of the subdominant conditions. For the remaining one, the couplings are

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \frac{1}{\sqrt{2}};$$

$$\lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{2}}; \quad \nu'' = \frac{1}{\sqrt{2}}; \quad \lambda''' = 0; \quad \mu''' = \frac{1}{\sqrt{2}}; \quad \nu''' = \frac{1}{\sqrt{2}} \tag{5.20}$$

and the Dynkin diagram is

5-6 

(D.2) $\lambda = 1$.

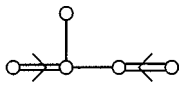
In Table 2 of Ref. 22, there are two hyperbolic algebras with a Dynkin diagram of this shape. Both are admissible for our present purpose:

(D.2.1) The first one has couplings given by

$$\lambda = 1; \quad \lambda' = \frac{1}{2}; \quad \mu' = \frac{\sqrt{3}}{2};$$

$$\lambda'' = 0; \quad \mu'' = \frac{2}{\sqrt{3}}; \quad \nu'' = \sqrt{\frac{2}{3}}; \quad \lambda''' = 0; \quad \mu''' = \frac{1}{\sqrt{3}}; \quad \nu''' = \sqrt{\frac{2}{3}} \tag{5.21}$$

and corresponds to

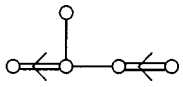
5-7 

(D.2.2) The second one requires

$$\lambda = 1; \quad \lambda' = \frac{1}{2}; \quad \mu' = \frac{\sqrt{3}}{2};$$

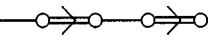
$$\lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{3}}; \quad \nu'' = \frac{1}{\sqrt{6}}; \quad \lambda''' = 0; \quad \mu''' = \frac{1}{\sqrt{3}}; \quad \nu''' = \sqrt{\frac{2}{3}} \tag{5.22}$$

and has the following diagram:

5-8 

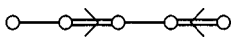
Case E: Table 2 of Ref. 22 displays two hyperbolic algebras of rank 5 which are duals of each other and have linear diagrams. Only one of these two can be associated to a billiard the walls of which correspond to (E.1) $\lambda = \sqrt{2}$, $\lambda'' = \lambda''' = \mu''' = 0$ and all other dilaton couplings equal to $1/\sqrt{2}$.

Its Dynkin diagram is the twisted overextension $A_6^{(2)\wedge}$ and is given by

5-9 

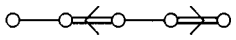
There are however two more hyperbolic algebras with such linear Dynkin diagrams; they are missing in Ref. 22 but perfectly relevant in the present context:

(E.2) the first one is the overextension $C_3^{\wedge\wedge}$,

5-10 

whose couplings are equal to the previous ones except $\nu'''=\sqrt{2}$.

(E.3) The second one is the dual of $C_3^{\wedge\wedge}$ known as the twisted overextension $D_4^{(2)\wedge}$; its Dynkin diagram corresponds to the previous one with reversed arrows

5-11 

and the dilaton couplings are such that $\lambda=\lambda'=\mu'=\mu''=\nu''=\nu'''=\sqrt{2}$ while $\lambda''=\lambda'''=\mu'''=0$.

2. Two or more magnetic walls

That these cases may be discarded will be proved on a particular case but the argument can be easily generalized. Suppose the dominant set comprises two magnetic walls and two electric ones, we can always choose the parametrization such that

$$\alpha_1=\beta^2-\beta^1,$$

$$\alpha_2=\beta^1-\lambda\phi-\mu\varphi-\nu\psi,$$

$$\alpha_3=\beta^1-\lambda'\phi-\mu'\varphi+\nu'\psi,$$

$$\alpha_4=\lambda''\phi+\mu''\varphi,$$

$$\alpha_5=\lambda'''\phi. \tag{5.23}$$

Being assumed subdominant, the electric walls $\tilde{\alpha}_2=\lambda\phi+\mu\varphi+\nu\psi$ and $\tilde{\alpha}_3=\lambda'\phi+\mu'\varphi-\nu'\psi$, independent of β^1, must be written as positive linear combinations of α_4 and α_5 only; this requires $\nu=\nu'=0$ but then (5.23) can no longer describe a rank five root system.

The same argument remains of course valid for more magnetic walls.

B. *D*>3

The empirical oxidation rule set up in the previous sections also holds for the rank 5 algebras:

(1) Diagram (5-1) is the Dynkin diagram of the overextension $A_3^{\wedge\wedge}$. The Lagrangian is that of pure gravity in $D_{\max}=6$.
(2) Diagram (5-2): the three-dimensional Lagrangian cannot be oxidized because of the norm of α_2.
(3) Diagram (5-3): The Lagrangian can be oxidized twice, up to $D_{\max}=5$. The dominant walls are the three symmetry walls $\alpha_1=\beta^4-\beta^3$, $\alpha_2=\beta^3-\beta^2$, $\alpha_3=\beta^2-\beta^1$ and the electric wall of a 1-form

$$\alpha_4=\beta^1-\sqrt{1/3}\phi \tag{5.24}$$

and its magnetic wall

$$\alpha_5=\beta^1+\beta^2+\sqrt{1/3}\phi. \tag{5.25}$$

Obviously, $\tilde{\alpha}_4=\alpha_5$ and $\tilde{\alpha}_5=\alpha_4$.

(4) Diagram (5-4) represents $B_3^{\wedge\wedge}$. The maximally oxidized Lagrangian is six-dimensional. The dominant walls are here the four symmetry walls $\alpha_1=\beta^5-\beta^4$, $\alpha_2=\beta^4-\beta^3$, $\alpha_3=\beta^3-\beta^2$, $\alpha_4=\beta^2-\beta^1$, and

$$\alpha_5=\beta^1+\beta^2, \tag{5.26}$$

which is the electric or magnetic wall of a self-dual 2-form: obviously $\tilde{\alpha}_5=\alpha_5$.

(5) Diagram (5-5) is the twisted overextension $A_5^{(2)\wedge}$. Here, $D_{\max}=4$ and besides the symmetry walls $\alpha_1=\beta^3-\beta^2$ and $\alpha_2=\beta^2-\beta^1$, one finds

$$\alpha_3=\beta^1-\sqrt{3/2}\phi, \tag{5.27}$$

$$\alpha_4=\sqrt{2/3}\phi-2/\sqrt{3}\varphi, \tag{5.28}$$

$$\alpha_5=2\sqrt{2/3}\varphi+2/\sqrt{3}\psi, \tag{5.29}$$

which are the electric walls, respectively, of a one-form and two 0-forms. One easily checks that $\tilde{\alpha}_3=\alpha_3+\alpha_4+\alpha_5$, $\tilde{\alpha}_4=\alpha_2+2\alpha_3+\alpha_5$, and $\tilde{\alpha}_5=\alpha_2+2\alpha_3+\alpha_4$.

(6) Diagram (5-6): $D_{\max}=4$ and one needs $\alpha_1=\beta^3-\beta^2$, $\alpha_2=\beta^2-\beta^1$, and

$$\alpha_3=\beta^1-\sqrt{1/2}\phi, \tag{5.30}$$

$$\alpha_4=\sqrt{1/2}\phi-\sqrt{1/2}\varphi, \tag{5.31}$$

$$\alpha_5=\sqrt{1/2}\phi+\sqrt{1/2}\varphi. \tag{5.32}$$

The form-field content is the same as the previous one but the dilaton couplings are different. Moreover: $\tilde{\alpha}_3=\alpha_3+\alpha_4+\alpha_5$, $\tilde{\alpha}_4=\alpha_2+2\alpha_3+\alpha_5$, and $\tilde{\alpha}_5=\alpha_2+2\alpha_3+\alpha_4$.

(7) Diagrams (5-7) and (5-8): their 3D Lagrangians cannot be further oxidized because of the norm of α_2.

(8) Diagram (5-9) describes $A_6^{(2)\wedge}$. Here, $D_{\max}=4$. One obtains the billiard with $\alpha_1=\beta^3-\beta^2$, $\alpha_2=\beta^2-\beta^1$, and

$$\alpha_3=\beta^1-\sqrt{1/2}\phi, \tag{5.33}$$

$$\alpha_4=\sqrt{1/2}\phi-\sqrt{1/2}\varphi, \tag{5.34}$$

$$\alpha_5=\sqrt{1/2}\varphi. \tag{5.35}$$

One draws the same conclusion as for (5-6) and (5-9) above. Here again: $\tilde{\alpha}_3=\alpha_3+\alpha_4+\alpha_5$, $\tilde{\alpha}_4=\alpha_2+2\alpha_3+\alpha_4+2\alpha_5$, and $\tilde{\alpha}_5=\alpha_2+2\alpha_3+2\alpha_4+\alpha_5$.

(9) Diagram (5-10) is the overextension $C_3^{\wedge\wedge}$; the maximal oxidation dimension is $D_{\max}=4$ and the corresponding Lagrangian can be found in Ref. 12.

(10) Diagram (5-11) is the twisted overextension $D_4^{(2)\wedge}$. No Lagrangian exists in higher dimensions.

Comment:

The results of this section show again that the subdominant conditions play an important role in three dimensions where they effectively contribute to the elimination of several Dynkin diagrams. However, once they are satisfied in three dimensions, they are always fulfilled in all dimensions where a Lagrangian exists and only integers enter the linear combinations.

VI. RANK 6 HYPERBOLIC ALGEBRAS

A. $D=3$

The number of dilatons in the three-dimensional Lagrangian is equal to $N=4$: we denote them by $\phi^1=\phi, \phi^2=\varphi, \phi^3=\psi, \phi^4=\chi$. A straightforward generalization of the argument used in the previous sections implies that a single configuration for the set of dominant walls has to be considered. It comprises one magnetic wall and four electric ones.

After allowed simplifications, the dominant walls are parametrized according to

$$\alpha_1 = \beta^2 - \beta^1, \tag{6.1}$$

$$\alpha_2 = \beta^1 - \lambda\phi, \tag{6.2}$$

$$\alpha_3 = \lambda'\phi - \mu'\varphi, \tag{6.3}$$

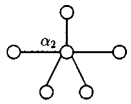
$$\alpha_4 = \lambda''\phi + \mu''\varphi - \nu''\psi, \tag{6.4}$$

$$\alpha_5 = \lambda'''\phi + \mu'''\varphi + \nu'''\psi - \rho'''\chi, \tag{6.5}$$

$$\alpha_6 = \lambda''''\phi + \mu''''\varphi + \nu''''\psi + \rho''''\chi. \tag{6.6}$$

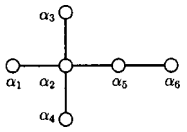
The structure of the Dynkin diagrams is therefore displayed in one of the cases labeled A–E below, depending on the number of vertices connected to α_2. When necessary, further subclasses are introduced according to the number of vertices linked to α_3.

Case A: The central vertex is labeled α_2 and is connected to the five other vertices:

A 

There is a single hyperbolic algebra of this type in Ref. 22; one can solve the equations for the dilaton couplings, but the subdominant walls are not expressible as positive linear combinations of the dominant ones.

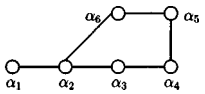
Case B: The root α_2 is connected to four vertices:

B 

There are three hyperbolic algebras with that kind of Dynkin diagram but none of them can be retained: indeed, couplings exist but the subdominant conditions cannot be fulfilled.

Case C: α_2 has three links.

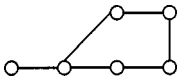
One has first the loop diagram

C.1 

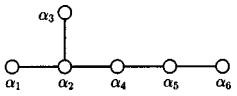
One hyperbolic algebra has such a Dynkin diagram, namely, the overextension $A_4^{\wedge\wedge}$. As we already know from Ref. 6, the searched for three-dimensional Lagrangian coincides with the toroidal dimensional reduction of the seven-dimensional Einstein–Hilbert Lagrangian. The dilaton couplings are given by

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$
$$\nu''' = \frac{\sqrt{3}}{2}; \quad \rho''' = \frac{\sqrt{5}}{2}; \quad \lambda'''' = \frac{1}{\sqrt{2}}; \quad \mu'''' = \frac{1}{\sqrt{6}}; \quad \nu'''' = \frac{1}{2\sqrt{3}}; \quad \rho'''' = \frac{\sqrt{5}}{2} \tag{6.7}$$

and its Dynkin diagram is

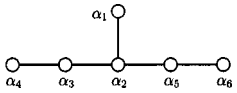
6-1 

Next comes the tree diagram

C.2 

Two hyperbolic algebras have a Dynkin diagram of this shape; but they cannot be associated with billiards again because of the impossibility to satisfy the subdominant conditions.

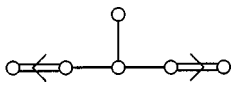
One also has to allow a relabeling of the vertices according to

C.3 

There are five hyperbolic algebras of that type; but for only one of them can one fulfill all conditions. The dilaton couplings are given by

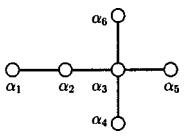
$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{1}{\sqrt{3}}; \quad \lambda''' = \frac{1}{\sqrt{2}}; \quad \mu''' = \frac{1}{\sqrt{6}};$$
$$\nu''' = \frac{1}{\sqrt{3}}; \quad \rho''' = 1; \quad \lambda'''' = 0; \quad \alpha'''' = 0; \quad \beta'''' = 0; \quad \rho'''' = 1 \tag{6.8}$$

and its Dynkin diagram is the following

6-2 

Cases D are characterized by the fact that α_2 has two links:

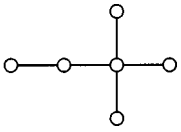
(D.1). Corresponds further to α_3 having four links

D.1 

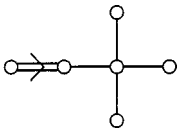
Three diagrams of (Ref. 22) fit in this shape; only two of them are realized through billiards. The couplings of the first one are given by

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}} = \mu'''; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = 0;$$
$$\nu''' = \frac{1}{\sqrt{3}}; \quad \rho''' = 1; \quad \lambda'''' = 0; \quad \mu'''' = \sqrt{\frac{2}{3}}; \quad \nu'''' = \frac{1}{\sqrt{3}}; \quad \rho'''' = 1, \tag{6.9}$$

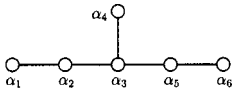
they provide the Dynkin diagram which is $D_4^{\wedge\wedge}$:

6-3 

For the second one, $\lambda = 1$ and all the other couplings are those given in (6.9) divided by $\sqrt{2}$. They lead to the following diagram:

6-4 

Case (D.2) corresponds to α_3 having three connections

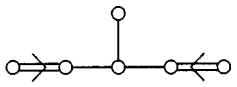
D.2 

and differs from (C.3) above by the assignment of the symmetry root. There are 4 Dynkin diagrams representing hyperbolic algebras of this type and they all admit a billiard.

(D.2.1) The couplings are

$$\lambda = 1; \quad \lambda' = \frac{1}{2}; \quad \mu' = \frac{\sqrt{3}}{2}; \quad \lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{3}}; \quad \nu'' = \sqrt{\frac{2}{3}}; \quad \lambda''' = 0; \quad \mu''' = \frac{1}{\sqrt{3}};$$
$$\nu''' = \frac{1}{\sqrt{6}}; \quad \rho''' = \frac{1}{\sqrt{2}}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = \sqrt{2}, \tag{6.10}$$

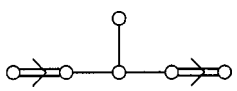
and the Dynkin diagram corresponds to

6-5 

(D.2.2) The couplings are the same as in (6.10) above except ρ'''' which reads

$$\rho'''' = 1/\sqrt{2}. \tag{6.11}$$

The Dynkin diagram is

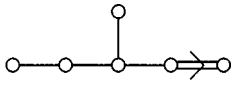
6-6 

(D.2.3) The dilaton couplings are given by

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = \sqrt{\frac{2}{3}};$$

$$\nu''' = \frac{1}{\sqrt{3}}; \quad \rho''' = 1; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = 1 \tag{6.12}$$

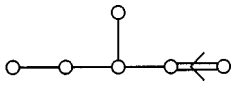
they provide the Dynkin diagram of $B_4^{\wedge\wedge}$,

6-7 

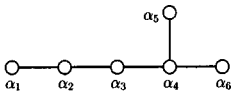
(D.2.4) The couplings are the same as in (6.12) except

$$\rho'''' = 2 \tag{6.13}$$

and the algebra is $A_7^{(2)\wedge}$,

6-8 

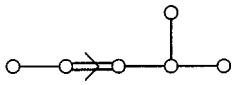
Case D.3 describes the general structure below in which α_2 and α_3 have two links while α_4 is connected three times

D.3 

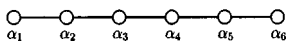
There are two hyperbolic algebras of that type but only one satisfies all billiard conditions. Its nonzero couplings are

$$\lambda = \sqrt{2} \quad \text{and} \quad \lambda' = \mu' = \mu'' = \nu'' = \nu''' = \rho''' = \rho'''' = 1/\sqrt{2}. \tag{6.14}$$

The Dynkin diagram is

6-9 

Case E: This set provides all linear diagrams. There are seven hyperbolic algebras of this kind and all of them are admissible

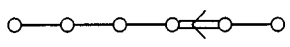
E 

(E.1) has the following couplings:

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$

$$\nu''' = \sqrt{3}; \quad \rho''' = 1; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = 2, \tag{6.15}$$

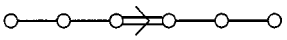
and its Dynkin diagram belongs to $E_6^{(2)\wedge}$,

6-10 

(E.2) corresponds to

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{1}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$
$$\nu''' = \frac{\sqrt{3}}{2}; \quad \rho''' = \frac{1}{2}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = 1, \tag{6.16}$$

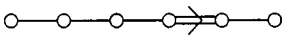
and its algebra is associated with

6-11 

(E.3) The walls are defined through the following set of parameters:

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \sqrt{\frac{3}{2}}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{\frac{2}{3}}; \quad \nu'' = \frac{2}{\sqrt{3}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$
$$\nu''' = \frac{\sqrt{3}}{2}; \quad \rho''' = \frac{1}{2}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = 1, \tag{6.17}$$

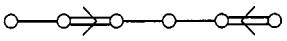
and the algebra is $F_4^{\wedge\wedge}$,

6-12 

(E.4) has the following couplings:

$$\lambda = \sqrt{2}; \quad \lambda' = \frac{1}{\sqrt{2}}; \quad \mu' = \frac{1}{\sqrt{2}}; \quad \lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{2}}; \quad \nu'' = \frac{1}{\sqrt{2}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$
$$\nu''' = \frac{1}{\sqrt{2}}; \quad \rho''' = \frac{1}{\sqrt{2}}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = \sqrt{2} \tag{6.18}$$

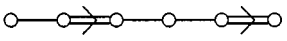
and its diagram corresponds to $C_4^{\wedge\wedge}$,

6-13 

(E.5) has the same couplings as those given in (6.18) except

$$\rho'''' = \frac{1}{\sqrt{2}}. \tag{6.19}$$

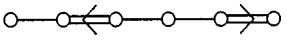
Its diagram corresponds to $A_8^{(2)\wedge}$,

6-14 

(E.6) is characterized by

$$\lambda = \sqrt{2}; \quad \lambda' = \sqrt{2}; \quad \mu' = \sqrt{2}; \quad \lambda'' = 0; \quad \mu'' = \sqrt{2}; \quad \nu'' = \sqrt{2}; \quad \lambda''' = 0; \quad \mu''' = 0;$$
$$\nu''' = \sqrt{2}; \quad \rho''' = \sqrt{2}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = \sqrt{2} \tag{6.20}$$

and its diagram describes $D_5^{(2)\wedge}$,

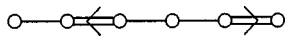
6-15 

(E.7) is the last one of this rank; its couplings are

$$\lambda = 1; \quad \lambda' = \frac{1}{2}; \quad \mu' = \frac{\sqrt{3}}{2}; \quad \lambda'' = 0; \quad \mu'' = \frac{1}{\sqrt{3}}; \quad \nu'' = \sqrt{\frac{2}{3}}; \quad \lambda''' = 0; \quad \mu''' = 0;$$

$$\nu''' = \frac{\sqrt{3}}{2\sqrt{2}}; \quad \rho''' = \frac{1}{2\sqrt{2}}; \quad \lambda'''' = 0; \quad \mu'''' = 0; \quad \nu'''' = 0; \quad \rho'''' = \frac{1}{\sqrt{2}} \tag{6.21}$$

and its diagram gives $A_8^{(2)\prime\wedge}$,

6-15 

B. $D>3$

Our next task is again to study which of the 16 algebras admitting a three-dimensional billiard model allow in addition a higher dimensional Lagrangian description.

(1) Diagram (6-1) is the overextension $A_4^{\wedge\wedge}$. The maximal oxidation dimension is $D_{\max}=7$, where the Lagrangian describes pure gravity.[7]

(2) Diagram (6-2): Here, $D_{\max}=5$. The dominant walls are the symmetry walls $\alpha_1=\beta^4-\beta^3$, $\alpha_2=\beta^3-\beta^2$, $\alpha_3=\beta^2-\beta^1$, and

$$\alpha_4 = \beta^1 - 1/\sqrt{3}\phi, \tag{6.22}$$

$$\alpha_5 = \beta^1 + \beta^2 + 1/\sqrt{3}\phi - \psi, \tag{6.23}$$

$$\alpha_6 = \psi. \tag{6.24}$$

These are respectively the electric walls of a one-form, a two-form and a zero-form. One easily checks that $\tilde{\alpha}_4=\alpha_5+\alpha_6$, $\tilde{\alpha}_5=\alpha_4+\alpha_6$ and $\tilde{\alpha}_6=\alpha_2+\alpha_3+\alpha_4+\alpha_5$.

(3) Diagram (6-3) is the overextension $D_4^{\wedge\wedge}$; its 3D version can be oxidized up to $D_{\max}=6$ and the Lagrangian is written in Refs. 11 and 12.

(4) Diagrams (6-4), (6-5), and (6-6): their Lagrangians have no higher dimensional parent.

(5) Diagram (6-7) is the overextension $B_4^{\wedge\wedge}$. Remark that since the diagram has a fork one can oxidize in two different ways, both lead to $D_{\max}=6$. The Lagrangians can again be found in Refs. 11 and 12.

(6) Diagram (6-8) is the twisted overextension $A_7^{(2)\wedge}$. $D_{\max}=6$. The dominant walls are the symmetry walls $\alpha_1=\beta^5-\beta^4$, $\alpha_2=\beta^4-\beta^3$, $\alpha_3=\beta^3-\beta^2$, and $\alpha_4=\beta^2-\beta^1$, and

$$\alpha_5 = \beta^1 + \beta^2 - \phi, \tag{6.25}$$

$$\alpha_6 = 2\phi, \tag{6.26}$$

which are the electric walls of a 2-form and a zero-form. Their respective magnetic walls are subdominant; indeed one finds

$$\tilde{\alpha}_5 = \beta^1 + \beta^2 + \phi = \alpha_5 + \alpha_6, \tag{6.27}$$

$$\tilde{\alpha}_6 = \beta^1 + \beta^2 + \beta^3 + \beta^4 - 2\phi = 2\alpha_5 + \alpha_4 + 2\alpha_3 + \alpha_2. \tag{6.28}$$

(7) Diagram (6-9): $D_{\max}=4$. The wall system reads $\alpha_1=\beta^3-\beta^2$, $\alpha_2=\beta^2-\beta^1$ and

$$\alpha_3 = \beta^1 - 1/\sqrt{2}\phi, \tag{6.29}$$

$$\alpha_4 = 1/\sqrt{2}(\phi - \psi), \tag{6.30}$$

$$\alpha_5 = 1/\sqrt{2}(\psi - \chi), \tag{6.31}$$

$$\alpha_6 = 1/\sqrt{2}(\psi + \chi); \tag{6.32}$$

the last four are the electric walls of a 1-form and three zero-forms. The subdominant condition is fulfilled: indeed, one finds $\tilde{\alpha}_3 = \alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$, $\tilde{\alpha}_4 = \alpha_2 + 2\alpha_3 + \alpha_4 + \alpha_5 + \alpha_6$, $\tilde{\alpha}_5 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_6$, $\tilde{\alpha}_6 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5$.

(8) Diagram (6-10) is the twisted overextension $E_6^{(2)\wedge}$. The oxidation rule gives the maximal dimension $D_{\max} = 5$. The walls other than the symmetry ones are

$$\alpha_4 = \beta^1 - 2/\sqrt{3}\phi, \tag{6.33}$$

$$\alpha_5 = \sqrt{3}\phi - \varphi, \tag{6.34}$$

$$\alpha_6 = 2\varphi. \tag{6.35}$$

One checks that $\tilde{\alpha}_4 = \alpha_3 + 2\alpha_4 + 2\alpha_5 + \alpha_6$, $\tilde{\alpha}_5 = \alpha_2 + 2\alpha_3 + 3\alpha_4 + \alpha_5 + \alpha_6$, $\tilde{\alpha}_6 = \alpha_2 + 2\alpha_3 + 3\alpha_4 + 2\alpha_5$.

(9) Diagram (6-11): A Lagrangian exists in $D_{\max} = 5$ which produces besides the symmetry walls

$$\alpha_4 = \beta^1 - 1/\sqrt{3}\phi, \tag{6.36}$$

$$\alpha_5 = \sqrt{3}/2\phi - 1/2\varphi, \tag{6.37}$$

$$\alpha_6 = \varphi. \tag{6.38}$$

The subdominant conditions read $\tilde{\alpha}_4 = \alpha_3 + 2\alpha_4 + 2\alpha_5 + \alpha_6$, $\tilde{\alpha}_5 = \alpha_2 + 2\alpha_3 + 3\alpha_4 + \alpha_5 + \alpha_6$, and $\tilde{\alpha}_6 = \alpha_2 + 2\alpha_3 + 3\alpha_4 + 2\alpha_5$.

(10) Diagram (6-12) is the overextension $F_4^{\wedge\wedge}$; the maximally oxidized theory is six-dimensional and contains the metric, one dilaton, one zero-form, and a one-form.[11,12]

(11) Diagram (6-13) is the overextension $C_4^{\wedge\wedge}$.[11] This is the last one of its series: remember that the $C_n^{\wedge\wedge}$ algebras are hyperbolic only for $n \leqslant 4$. The maximal oxidation dimension is $D_{\max} = 4$; besides the symmetry walls, the other dominant ones are

$$\alpha_3 = \beta^1 - 1/\sqrt{2}\phi, \tag{6.39}$$

$$\alpha_4 = 1/\sqrt{2}(\phi - \varphi), \tag{6.40}$$

$$\alpha_5 = 1/\sqrt{2}(\varphi - \psi), \tag{6.41}$$

$$\alpha_6 = \sqrt{2}\psi. \tag{6.42}$$

The subdominant conditions are satisfied, they read $\tilde{\alpha}_3 = \alpha_3 + 2\alpha_4 + 2\alpha_5 + \alpha_6$, $\tilde{\alpha}_4 = \alpha_2 + 2\alpha_3 + \alpha_4 + 2\alpha_5 + \alpha_6$, $\tilde{\alpha}_5 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$, $\tilde{\alpha}_6 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + 2\alpha_5$.

(12) Diagram (6-14) is the twisted overextension $A_8^{(2)\wedge}$. There is no higher dimensional theory.

(13) Diagram (6-15) represents $D_5^{(2)\wedge}$. In $D_{\max} = 4$, the dominant walls other than the symmetry ones are given by

$$\alpha_3 = \beta^1 - 1/\sqrt{2}\phi, \tag{6.43}$$

$$\alpha_4 = 1/\sqrt{2}(\phi - \varphi), \tag{6.44}$$

$$\alpha_5 = 1/\sqrt{2}(\varphi - \psi), \tag{6.45}$$

$$\alpha_6 = 1/\sqrt{2}\psi. \tag{6.46}$$

One obtains easily the following expressions $\tilde{\alpha}_3 = \alpha_3 + 2\alpha_4 + 2\alpha_5 + \alpha_6$, $\tilde{\alpha}_4 = \alpha_2 + 2\alpha_3 + \alpha_4 + 2\alpha_5 + 2\alpha_6$, $\tilde{\alpha}_5 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + 2\alpha_6$, $\tilde{\alpha}_6 = \alpha_2 + 2\alpha_3 + 2\alpha_4 + 2\alpha_5 + \alpha_6$.

(14) Diagram (6-16) describes $A_8^{(2)\prime\wedge}$; it cannot be associated to a billiard in $D > 3$.

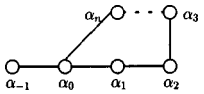
Comment:

Here again, in $D > 3$, the subdominant conditions are always satisfied; it is only in $D = 3$ that their role is crucial in the selection of the admissible algebras. Hence, they do not add any constraint in the oxidation construction.

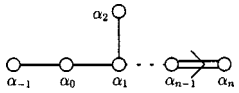
VII. RANK 7, 8, 9, AND 10 HYPERBOLIC ALGEBRAS

These hyperbolic algebras fall into two classes: the first one comprises all algebras of rank $7 \leqslant r \leqslant 10$ that are overextensions of the following finite simple Lie algebras $A_n, B_n, D_n, E_6, E_7, E_8$. They are

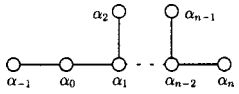
$A_n^{\wedge\wedge}$ $(n = 5,6,7)$,



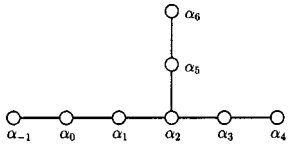
$B_n^{\wedge\wedge}$ $(n = 5,6,7,8)$,



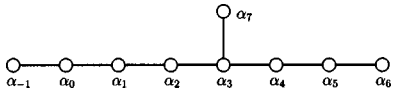
$D_n^{\wedge\wedge}$ $(n = 5,6,7,8)$,



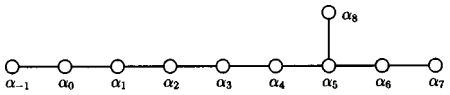
$E_6^{\wedge\wedge}$,



$E_7^{\wedge\wedge}$,

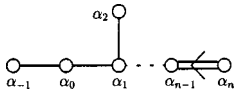


$E_8^{\wedge\wedge}$,



In the second class, one finds the four duals of the $B_n^{\wedge\wedge}$ $(n=5,6,7,8)$, i.e., the algebras known as $CE_{n+2}=A_{2n-1}^{(2)\wedge}$,

$$CE_{n+2} = A_{2n-1}^{(2)\wedge},$$



A. Overextensions of finite simple Lie algebras

The algebras of the first class have already been encountered as billiards of some three-dimensional G/H coset theories as explained in Ref. 12 to which we refer for more information. Those of rank 10, E_{10}, BE_{10}, and DE_{10} have been found[8] to describe the billiards of the seven string theories, M, IIA, IIB, I, HO, HE and the closed bosonic string in 10 dimensions. More precisely, these theories split into three separate blocks which correspond to three distinct billiards: namely, $\mathcal{B}_2=\{M, IIA, IIB\}$ leads to E_{10}, $\mathcal{B}_1=\{I, HO, HE\}$ corresponds to BE_{10}, and $\mathcal{B}_0=\{D=10$ closed bosonic string$\}$ gives DE_{10}.

For sake of completeness, we here simply recall the maximal spacetime dimensions and the specific p-forms menus producing the billiards.

(1) $A_n^{\wedge\wedge}$ $(n=5,6,7)$: the Lagrangian is that of pure gravity in $D_{\max}=n+3$.
(2) $B_n^{\wedge\wedge}$ $(n=5,6,7,8)$: the maximally oxidized Lagrangian lives in $D_{\max}=n+2$, where it comprises a dilaton, a 1-form coupled to the dilaton with coupling equal to $\lambda^{(1)}(\phi)=\phi/\sqrt{d-1}$ and a 2-form coupled to the dilaton with coupling equal to $\lambda^{(2)}(\phi)=2\phi/\sqrt{d-1}$.
(3) $D_n^{\wedge\wedge}$ $(n=5,6,7,8)$: a Lagrangian exists in $D_{\max}=n+2$ and comprises a dilaton and a 2-form coupled to the dilaton with coupling equal to $\lambda^{(2)}(\phi)=2\phi/\sqrt{d-1}$.
(4) $E_6^{\wedge\wedge}$: the maximal oxidation dimension is $D_{\max}=8$. The Lagrangian has a dilaton, a 0-form with coupling $\lambda^{(0)}(\phi)=\phi\sqrt{2}$ and a 3-form with coupling $\lambda^{(3)}(\phi)=-\phi/\sqrt{2}$.
(5) $E_7^{\wedge\wedge}$: the maximal space–time dimension is $D_{\max}=10$. The Lagrangian describes gravity and a 4-form: it is a truncation of type IIB supergravity.
(6) $E_8^{\wedge\wedge}$: $D_{\max}=11$. The Lagrangian describes gravity coupled to a 3-form; it is the bosonic sector of eleven dimensional supergravity.

B. The algebras $CE_{n+2}=A_{2n-1}^{(2)\wedge}$

The Weyl chamber of the algebras CE_{n+2} $(n=5,6,7,8)$, which are dual to $B_n^{\wedge\wedge}$, allows a billiard realization in maximal dimension $D_{\max}=n+1=d+1$. The field content of the theory is the following: there are two dilatons, ϕ and φ, a 0-form coupled to the dilatons through

$$\lambda^{(0)}(\phi) = 2\sqrt{\frac{(d-1)}{d}}\phi - \frac{2}{\sqrt{d}}\varphi, \tag{7.1}$$

a one form with dilaton couplings

$$\lambda^{(1)}(\phi) = -\sqrt{\frac{d}{(d-1)}}\ \phi \tag{7.2}$$

and a 2-form with the following couplings

$$\lambda^{(2)}(\phi) = -\frac{2}{\sqrt{d(d-1)}}\phi - \frac{2}{\sqrt{d}}\varphi. \tag{7.3}$$

In particular, the Lagrangian in $D_{\max}=9$ producing the billiard identifiable as the fundamental Weyl chamber of CE_{10} corresponds to $n=8=d$ and is explicitly given by[30]

$$\mathcal{L}_9 = {}^{(9)}R * \mathbb{1} - \star d\phi \wedge d\phi - \star d\varphi \wedge d\varphi - \tfrac{1}{2}\, e^{(2\phi\sqrt{7/2}-\varphi\sqrt{2})} \star F^{(1)} \wedge F^{(1)} - \tfrac{1}{2} e^{-4\phi\sqrt{2/7}} \star F^{(2)} \wedge F^{(2)} - \tfrac{1}{2}\, e^{-(\phi\sqrt{2/7}+\varphi\sqrt{2})} \star F^{(3)} \wedge F^{(3)}. \tag{7.4}$$

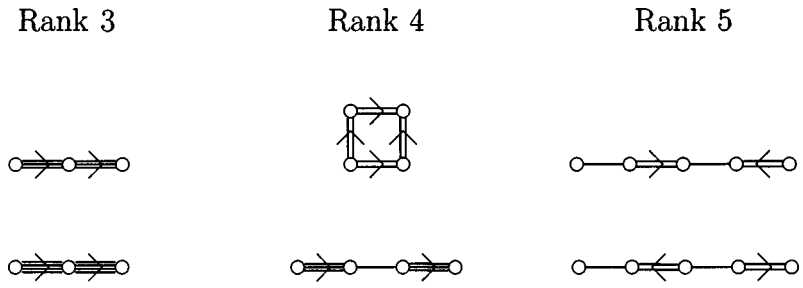
CE_{10} is the fourth hyperbolic algebra of rank 10; contrary to the other three cited above, which belong to the class of the overtextensions of finite simple Lie algebras, its Lagrangian (7.4) does not stem from string theories.

VIII. CONCLUSIONS

In this paper we have presented all Lagrangian systems in which gravity, dilatons and p-forms combine in such a way as to produce a billiard that can be identified with the Weyl chamber of a given hyperbolic Kac Moody algebra. Exhaustive results have been systematically obtained by first constructing Lagrangians in three space–time dimensions, at least for the algebras of rank $r \leqslant 6$. We insist on the fact that our three-dimensional Lagrangians are not assumed to realize a coset theory. We also have solved the oxidation problem and provided the Lagrangians in the maximal space time dimension with their p-forms content and specific dilaton couplings. It turns out that the subdominant conditions play no role in the oxidation analysis. The positive integer coefficients that appear when expressing the subdominant walls in terms of the dominant ones in the maximal oxidation dimension have been systematically worked out.

IX. MORE HYPERBOLIC ALGEBRAS

For completeness, we draw hereafter the Dynkin diagrams of 6 hyperbolic algebras missing in Ref. 22. This raises their total number to 142, in agreement with Ref. 31.



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Lifshits tails for random smooth magnetic vortices

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We study the density of states of the Pauli Hamiltonian with a Poisson random distribution of smooth finite-width vortices and we obtain classical bounds for the Lifshits tails for them. These Hamiltonians are smooth approximations to the self-adjoint extensions of the Aharonov–Bohm Hamiltonian. In this case because pairs of impurities are coupled by the magnetic field we cannot use the Laplace characteristic functional. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The following formal Hamiltonian may be used to represent a system of magnetic vortices distributed randomly in a two-dimensional domain:

$$H=\frac{1}{2m}\left(\mathbf{p}-\sum_{i=1}^{N}\alpha\frac{\mathbf{k}\times(\mathbf{r}-\mathbf{r}_i)}{(\mathbf{r}-\mathbf{r}_i)^2}\right)^2+\sum_{i=1}^{N}\pi\frac{\beta}{m}\delta^2(\mathbf{r}-\mathbf{r}_i). \tag{1.1}$$

It is known experimentally[1,2] that magnetic vortices may appear in two-dimensional electron gas layers on top of superconductivity materials when the external magnetic field penetrates the sample at some points in the form of isolated random flux tubes. Suppression of the Hall conductivity has been observed in these cases.

Numerical calculations using perturbation theory have been carried out in Refs. 3–5. For the operator considered in (1.1), with a repulsive delta function and the assumption that $\alpha\in\left[-\frac{1}{2},\frac{1}{2}\right]$, numerical calculations for the case $\beta=|\alpha|$, have shown that[4] if α is small, the density of states of this operator exhibits Landau oscillations, while for α close to $\frac{1}{2}$, no such oscillations are observed, indeed the density of states increases monotonically and there is a Lifshits tail at the bottom of the spectrum ($E=0$). It has been proposed[5] that this model may explain some features of the integer quantum Hall effect.

The integrated density of states and the existence of Lifshits tails for random Schrödinger operators of the type $-\Delta+V_\omega$, where V_ω is a random scalar potential, have been the object of extensive study in mathematical physics (see Refs. 6–8 for the basic theory and results). Recently there has been much interest in the study of their generalization to random Schrödinger operators with magnetic field

$$H(\mathbf{A},V_\omega)=(\mathbf{p}+\mathbf{A}_\omega)^2+V_\omega. \tag{1.2}$$

The case of nonrandom magnetic field was studied in, for example, Refs. 9–13 while other papers have proved results for Lifshits tails for operators where the magnetic field is random.[14–16]

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Nakamura[14] has studied the case where $\mathbf{A}_\omega$ is random, $V_\omega=0$ and the magnetic field $\mathbf{B}_\omega=\nabla\times\mathbf{A}_\omega$ is almost surely uniformly bounded on $\mathbb{R}^d$, $d\geqslant 2$. He obtained the following result for the Lifshits tails of the integrated density of states $N(\lambda)$:

$$\limsup_{\lambda\downarrow 0}\frac{\ln(-\ln N(\lambda))}{\ln\lambda}\leqslant -\frac{d}{2}. \tag{1.3}$$

Ueki[15] considered the case when $\mathbf{A}_\omega$ and V_ω are independent, and V_ω is Gaussian. He obtained

$$\lim_{\lambda\to-\infty}\frac{\ln N(\lambda)}{\lambda^2}=-\frac{1}{2\gamma(0)}, \tag{1.4}$$

where γ is the covariance of V_ω. In Ref. 16, the operator considered is the Pauli operator $(\mathbf{p}-\mathbf{A}_\omega)^2\pm(g/2)\mathbf{k}\cdot\mathbf{B}_\omega$, where $g>2$ is the anomalous magnetic moment, and $\mathbf{k}\cdot\mathbf{B}_\omega$ is a Gaussian field. In this case

$$\lim_{\lambda\to-\infty}\frac{\ln N(\lambda)}{\lambda^2}=-\frac{2}{(g-2)^2\gamma(0)}, \tag{1.5}$$

where γ is the covariance of $\mathbf{k}\cdot\mathbf{B}_\omega$.

In this paper we study the Pauli Hamiltonian for a Poisson random distribution of smooth finite-width Aharonov–Bohm vortices. These vortices are based on smooth approximations to the self-adjoint extensions of the Aharonov–Bohm Hamiltonian analyzed in Ref. 17, with the added condition that cutoffs are introduced to ensure that the vector potential is summable.

With probability one, the spectrum of this operator is the whole real line. We obtain classical bounds for the asymptotic behavior of the integrated density of states at the bottom of the spectrum. The analysis follows the method of Ref. 6 for a random Schrödinger operator with a Poisson distributed random potential. However the expression for the potential is not simply a sum over all the atoms of the Poisson distribution, but contains also cross-terms. For this reason, we cannot use the Laplace characteristic functional and have to proceed by a direct method. The cases mentioned above for random magnetic fields are different from the present one, since in this case $\mathbf{B}_\omega$ is neither bounded nor Gaussian.

II. THE MODEL

The Aharonov–Bohm (AB) Hamiltonian[18] is formally given by

$$H^{AB}=(\mathbf{p}+\mathbf{A})^2, \tag{2.1}$$

where

$$\mathbf{A}(\mathbf{r})=\alpha\frac{\mathbf{k}\times\mathbf{r}}{r^2}.$$

This Hamiltonian is not essentially self-adjoint, but has a four-parameter family of self-adjoint extensions,[19,20] which reduces to a two-parameter family if only those self-adjoint extensions that commute with the angular momentum operator are considered.

In Ref. 17, finite-width approximations to the self-adjoint extensions of the AB Hamiltonian were studied. Let $\tilde{a}:\mathbb{R}\mapsto\mathbb{R}$ be a smooth, monotonic nondecreasing function with $\tilde{a}(r)=0$ for $r\leqslant 0$ and $\tilde{a}(r)=1$ for $r\leqslant 1$. Let $\tilde{b}(r)=(1/r)(d/dr)\tilde{a}(r)$. Then $\tilde{b}$ has support only in [0, 1], and $\int_0^\infty\tilde{b}(r)r\,dr=1$. Let $\alpha\notin\mathbb{Z}$, and write $|\alpha|=N+\delta$, where $N\in\mathbb{N}_0$ and $0<\delta<1$. We take

$$\mathbf{A}_\rho(\mathbf{r})=\alpha\frac{\hat{\mathbf{k}}\times\mathbf{r}}{r^2}\tilde{a}\left(\frac{r-\rho}{\rho^5}\right) \tag{2.2}$$

for $\rho>0$ and $\mathbf{B}_\rho=\mathrm{curl}\,\mathbf{A}_\rho$. Then

$$\hat{\mathbf{k}} \cdot \mathbf{B}_\rho(\mathbf{r}) = \alpha\left(1 - \frac{\rho}{r}\right)\rho^{-10}\tilde{b}\left(\frac{r-\rho}{\rho^5}\right). \tag{2.3}$$

Let

$$H_\rho = (i\nabla + \mathbf{A}_\rho)^2 + \frac{\beta}{\alpha}\hat{\mathbf{k}} \cdot \mathbf{B}_\rho. \tag{2.4}$$

β may be identified with $-\frac{1}{2}g\alpha$, where g is the anomalous magnetic moment. In Ref. 17 it was shown that only two one-parameter subfamilies of self-adjoint extensions of the Aharonov–Bohm Hamiltonian can be approximated as $\rho \to 0$, in the norm resolvent sense, by such Pauli operators. For the operator H_ρ in $L^2(\mathbb{R}^2)$ to be a smooth approximation an element of the one of these one-parameter families of self-adjoint extensions, β must depend on ρ, for small ρ, in one of the following ways:

$$\text{(a) } \beta(\alpha,\rho) \simeq -|\alpha|\left(1 - \frac{2\delta}{|\alpha|}\nu\rho^{2\delta}\right), \tag{2.5}$$

$$\text{(b) } \beta(\alpha,\rho) \simeq (|\alpha| - 2(N+1))\left(1 - \frac{2(1-\delta)}{2(N+1) - |\alpha|}\nu\rho^{2(1-\delta)}\right), \tag{2.6}$$

for some constant ν satisfying $-\infty < \nu \leqslant \infty$.

We note here that

(1) $\lim_{\rho\to 0} \beta \leqslant -|\alpha|$;

(2) if we suppose that $\hat{\mathbf{k}}\cdot\mathbf{B}_\rho(\mathbf{r})$ has a maximum point at r_0, then it is easy to see that for small ρ the inequality

$$\hat{\mathbf{k}} \cdot \mathbf{B}_\rho(r_0) > \frac{a(r_0)}{r_0^2}, \tag{2.7}$$

is satisfied.

Motivated by the above discussion, we shall consider the following Hamiltonian in $L^2(\mathbb{R}^2)$

$$H = (i\nabla + \mathbf{A}(\mathbf{r} - \mathbf{r}_1))^2 + \frac{\beta}{\alpha}\hat{\mathbf{k}} \cdot \mathbf{B}(\mathbf{r} - \mathbf{r}_1), \tag{2.8}$$

where

$$\mathbf{A}(\mathbf{r}) = \alpha\frac{\hat{\mathbf{k}} \times \mathbf{r}}{r^2}a(r) \text{ and } \mathbf{B} = \operatorname{curl}\mathbf{A}. \tag{2.9}$$

We shall assume that $\beta \leqslant -|\alpha|$ and that $a:\mathbb{R}\mapsto\mathbb{R}$ is of class C_0^4 with $a(r)=0$ for $r\leqslant 0$. Note that $\operatorname{div}\mathbf{A}=0$ and we have $\hat{\mathbf{k}}\cdot\mathbf{B}(\mathbf{r})=\alpha\, b(r)$ where $b(r)=(1/r)(d/dr)a(r)$. We assume also that at a maximum point r_0 of b,

$$b_0 := b(r_0) > \frac{a(r_0)}{r_0^2}. \tag{2.10}$$

So far we have considered a smooth magnetic vortex centered at $\mathbf{r}_1$. Let $\mathbf{r}_i \in \mathbb{R}^2$, where $i \in \mathbb{N}$, be distributed with a Poisson distribution in $\mathbb{R}^2$. Then the Pauli Hamiltonian H_ω in $L^2(\mathbb{R}^2)$ for an infinite set of Poisson distributed smooth vortices is as follows:

$$H_\omega = \left(i\nabla + \sum_{i=1}^{\infty} \mathbf{A}(\mathbf{r}-\mathbf{r}_i) \right)^2 + \frac{\beta}{\alpha}\hat{\mathbf{k}} \cdot \sum_{i=1}^{\infty} \mathbf{B}(\mathbf{r}-\mathbf{r}_i). \tag{2.11}$$

We can use an adaptation of the usual argument to show that with probability one the spectrum of this operator is $\mathbb{R}$. We need to show that with nonzero probability the spectrum of H_ω contains arbitrarily large negative numbers (cf. Theorem 5.34 of Ref. 6). Since $\operatorname{div} \mathbf{A}=0$,

$$\langle \psi, \mathbf{A}(\cdot - \mathbf{r}_i) \cdot \nabla \psi \rangle = -\langle \mathbf{A}(\cdot - \mathbf{r}_i) \cdot \nabla \psi, \psi \rangle. \tag{2.12}$$

Therefore if ψ is real valued

$$\langle \psi, \mathbf{A}(\cdot - \mathbf{r}_i) \cdot \nabla \psi \rangle = 0 \tag{2.13}$$

and thus

$$\langle \psi, H_\omega \psi \rangle = \langle \psi, (-\Delta + V)\psi \rangle, \tag{2.14}$$

where

$$V(\mathbf{r}) = \frac{\beta}{\alpha}\hat{\mathbf{k}} \cdot \sum_{i=1}^{\infty} \mathbf{B}(\mathbf{r}-\mathbf{r}_i) + \left| \sum_{i=1}^{\infty} \mathbf{A}(\mathbf{r}-\mathbf{r}_i) \right|^2 = \beta \sum_{i=1}^{\infty} b(|\mathbf{r}-\mathbf{r}_i|) + \alpha^2 \left| \sum_{i=1}^{\infty} \mathbf{D}(\mathbf{r}-\mathbf{r}_i) \right|^2, \tag{2.15}$$

with

$$\mathbf{D}(\mathbf{r}) = \frac{a(|\mathbf{r}|)}{|\mathbf{r}|^2}\mathbf{r}.$$

Consider what happens at the origin if n Poisson points are placed symmetrically on a circle of radius r_0 centered at the origin so that $\Sigma_{i=1}^{n}\mathbf{r}_i=0$, while all the others are located very far from the origin. Then

$$V(\mathbf{0}) = \beta \sum_{i=1}^{n} b(|\mathbf{r}_i|) + \alpha^2 \left| \sum_{i=1}^{n} \mathbf{D}(\mathbf{r}_i) \right|^2 = \beta n b(r_0) + \alpha^2 \frac{a^2(r_0)}{r_0^4} \left| \sum_{i=1}^{n} \mathbf{r}_i \right|^2 = -n|\beta| b_0. \tag{2.16}$$

Thus by this configuration we can produce an arbitrarily deep well and by varying this configuration slightly we can do this with nonzero probability.

III. LIFSHITS TAILS

In this section we prove upper and lower bounds on the integrated density of states $N(\lambda)$ as $\lambda \to -\infty$. Our result is as follows:

Theorem: *Let the Hamiltonian H_ω be as defined in Sec. II. Then,*

$$\limsup_{\lambda \to -\infty} \ln N(\lambda) \leqslant -\frac{|\lambda|}{|\beta| b_0} \ln|\lambda| \tag{3.1}$$

and

$$\liminf_{\lambda \to -\infty} \ln N(\lambda) \geqslant -\frac{|\lambda|}{c_1 |\beta| b_0} \ln|\lambda|, \tag{3.2}$$

where

$$c_1 = \frac{6}{11}\left[1 - \frac{|\alpha|}{|\beta|}\left(1 - \frac{8}{3}\frac{a(r_0)}{b_0 r_0^2} + \frac{22}{9}\frac{a^2(r_0)}{{b_0}^2 r_0^4} \right)^{1/2} \right]. \tag{3.3}$$

Proof: The upper bound is straightforward. Applying the diamagnetic inequality (see for example, Theorem 15.7 of Ref. 22), we have

$$\mathrm{Tr}(\exp(-tH_{\omega,\Lambda})) \leqslant \mathrm{Tr}(\exp(-tH'_{\omega,\Lambda})), \tag{3.4}$$

where $H'_\omega = -\Delta + \beta\Sigma_{i=1}^{\infty} b(|\mathbf{r}-\mathbf{r}_i|)$, and the operators $H_{\omega,\Lambda}$ and $H'_{\omega,\Lambda}$ are, respectively, H_ω and H'_ω restricted to some finite domain Λ with Dirichlet boundary conditions.

If $\tilde{N}$ is the Laplace transform of N then from the corresponding bounds for the nonmagnetic case we get (see, for example, Theorems 5.18 and 9.1 of Ref. 6),

$$\tilde{N}(t) \leqslant \frac{1}{4\pi t}\exp(2\pi\rho r_0 e^{|\beta|b_0 t})(1+o(1)) \tag{3.5}$$

as $t\to\infty$ and (3.1) follows by a Tauberian argument.

As mentioned earlier, because the magnetic field couples pairs of impurities, the lower bound requires much more work. From Theorem 9.5 of Ref. 6 we have the following lower bound for $\tilde{N}(t)$:

$$\tilde{N}(t) \geqslant \frac{1}{\Lambda_\psi}\mathbb{E}[\exp(-t\langle\psi, H_\omega\psi\rangle)] \tag{3.6}$$

for any ψ which has unit norm and compact support, and is in the quadratic form domain of H_ω. This simply means that it is in the form domain of the Laplacian operator. Here $\Lambda_\psi = |\mathrm{supp}\ \psi|$. If ψ is real valued, we have from (2.14)

$$\mathbb{E}[\exp(-t\langle\psi, H_\omega\psi\rangle)] = e^{-t\langle\psi,-\Delta\psi\rangle}\mathbb{E}[e^{-t\langle\psi,V\psi\rangle}]. \tag{3.7}$$

Since the first term in (2.15) is nonpositive, the problem may be treated in a similar way to that of an attractive Poisson potential.[21] The crucial difference in the subsequent discussion is that, because of the second term on the r.h.s. of (2.15), we cannot calculate the expectation of $\exp(-t\langle\psi, V\psi\rangle)$ using the Laplace characteristic functional (Sec. 1.C of Ref. 6). So proceeding in a direct fashion, since a and b have compact support:

$$\mathbb{E}[e^{-t\langle\psi,V\psi\rangle}] = e^{-\rho|\Lambda|}\sum_{N=0}^{\infty}\frac{\rho^N}{N!}I_N(\psi,t), \tag{3.8}$$

where

$$I_N(\psi,t) = \int_{\Lambda^N} \mathrm{d}^2\mathbf{r}_1\cdots\mathrm{d}^2\mathbf{r}_N \exp\left(-t\int \mathrm{d}^2\mathbf{r}\, V_N(\mathbf{r}_1-\mathbf{r},\ldots,\mathbf{r}_N-\mathbf{r};1)|\psi(\mathbf{r})|^2\right) \tag{3.9}$$

and

$$V_N(\mathbf{r}_1,\ldots\mathbf{r}_N;s) = \frac{\beta}{\alpha}\hat{\mathbf{k}}\cdot\sum_{i=1}^{N}\mathbf{B}(\mathbf{r}_i) + s\alpha^2\left|\sum_{i=1}^{N}\mathbf{D}(\mathbf{r}_i)\right|^2. \tag{3.10}$$

Without loss of generality we can take Λ to be a disk of radius L centred at the origin. From (3.6)–(3.8) we obtain

$$\tilde{N}(t) \geqslant \frac{1}{\Lambda_\psi}e^{-t\langle\psi,-\Delta\psi\rangle}e^{-\rho|\Lambda|}\sum_{N=0}^{\infty}\frac{\rho^N}{N!}I_N(\psi,t). \tag{3.11}$$

For $t>0$ let the function $\phi(\mathbf{r}) = \phi_t(r)$ be defined by

$$\phi_t(r) = \begin{cases} N_t\sigma(t)e^{-(1/2)\sigma^2(t)r^2}, & 0 \leqslant r \leqslant 1 - \dfrac{1}{\sigma(t)}, \\ N_t\sigma^2(t)\exp\left(-\dfrac{1}{2}(\sigma(t)-1)^2\right)(1-r), & 1 - \dfrac{1}{\sigma(t)} < r \leqslant 1, \\ 0, & r > 1, \end{cases} \tag{3.12}$$

where $\sigma(t) = \exp(\exp(\xi t))$ for some $\xi < c_1|\beta|b_0$ and the constants N_t are such that $\|\phi_t\|_2 = 1$. The function ϕ_t is circularly symmetric with support in the unit ball centered at the origin. We shall explain the choice of this function later. Take

$$\psi_t(\mathbf{r}) = \frac{1}{R(t)}\phi\left(\frac{\mathbf{r}}{R(t)}\right),$$

where $R(t)$ is a function of t to be determined later. We shall write ϕ, ψ, and R rather than ϕ_t, ψ_t, and $R(t)$ to make the notation less cumbersome and we shall also use the notation

$$\sigma_1^2 := \int_0^1 \phi'^2(r) r dr \text{ and } \sigma_2^2 := \int_0^1 \phi^2(r) r^3 dr. \tag{3.13}$$

We have

$$\Lambda_\psi = \pi R^2, \tag{3.14}$$

$$\langle \psi, -\Delta\psi \rangle = R^{-2}\sigma_1^2, \tag{3.15}$$

and

$$I_N(\psi,t) = \int_{\Lambda^N} \mathrm{d}^2\mathbf{r}_1 \cdots \mathrm{d}^2\mathbf{r}_N \exp\left(-t\int_{r\leqslant 1} \mathrm{d}^2\mathbf{r} V_N(\mathbf{r}_1 - R\mathbf{r}, \ldots, \mathbf{r}_N - R\mathbf{r}; 1)|\phi(\mathbf{r})|^2\right). \tag{3.16}$$

Taking one term in (3.11) we get

$$\tilde{N}(t) \geqslant \frac{e^{-\rho|\Lambda|}}{N!\,\pi R^2} e^{-\sigma_1^2 t/R^2} I_N(\psi,t). \tag{3.17}$$

As usual we shall be making R small and using the Laplace approximation theorem to estimate $I_N(\psi,t)$ for large t. Now $-V_N(\mathbf{r}_1, \ldots, \mathbf{r}_N; 1)$ has maximum equal to $|\beta|Nb_0$. This maximum is attained when b is at a maximum, and the second term in (3.10) is zero, that is when $\mathbf{r}_1, \ldots, \mathbf{r}_N$ lie on a circle of radius r_0 centered at the origin so that $\Sigma_{i=1}^N \mathbf{r}_i = \mathbf{0}$. However there are a large number of these configurations for large N and this makes the second derivative at these points singular. Because it is difficult to estimate $I_N(\psi,t)$ for large t and N we find a lower bound by taking $N = 3n$ for some $n \in \mathbb{N}$. See the remark at the end of the proof for a justification of this choice. Using

$$(x_1 + \cdots + x_r)^2 \leqslant r(x_1^2 + \cdots + x_r^2), \tag{3.18}$$

we find that

$$\begin{aligned} \left|\sum_{i=1}^{3n} \mathbf{D}(\mathbf{r}_i)\right|^2 &\leqslant (|\mathbf{D}(\mathbf{r}_1) + \mathbf{D}(\mathbf{r}_2) + \mathbf{D}(\mathbf{r}_3)| + \cdots + |\mathbf{D}(\mathbf{r}_{3n-2}) + \mathbf{D}(\mathbf{r}_{3n-1}) + \mathbf{D}(\mathbf{r}_{3n})|)^2 \\ &\leqslant n(|\mathbf{D}(\mathbf{r}_1) + \mathbf{D}(\mathbf{r}_2) + \mathbf{D}(\mathbf{r}_3)|^2 + \cdots + |\mathbf{D}(\mathbf{r}_{3n-2}) + \mathbf{D}(\mathbf{r}_{3n-1}) + \mathbf{D}(\mathbf{r}_{3n})|^2). \end{aligned} \tag{3.19}$$

Therefore

$$V_{3n}(\mathbf{r}_1 - R\mathbf{r}, \ldots, \mathbf{r}_{3n} - R\mathbf{r}; s) \leqslant \sum_{i=1}^{n} V_3(\mathbf{r}_{3i-2} - R\mathbf{r}, \mathbf{r}_{3i-1} - R\mathbf{r}, \mathbf{r}_{3i} - R\mathbf{r}; sn). \tag{3.20}$$

Substituting this into (3.16) gives

$$I_{3n}(\psi, t) \geqslant [\overline{I_3}(n, \phi, t)]^n, \tag{3.21}$$

where

$$\overline{I_3}(n, \phi, t) = \int_{\Lambda^3} \mathrm{d}^2\mathbf{r}_1 \mathrm{d}^2\mathbf{r}_2 \mathrm{d}^2\mathbf{r}_3 \exp\left(- t \int_{r \leqslant 1} \mathrm{d}^2\mathbf{r} V_3(\mathbf{r}_1 - R\mathbf{r}, \mathbf{r}_2 - R\mathbf{r}, \mathbf{r}_3 - R\mathbf{r}; n) |\phi(\mathbf{r})|^2 \right). \tag{3.22}$$

Therefore (3.17) implies that

$$\widetilde{N}(t) \geqslant \frac{e^{-\rho|\Lambda|}}{(3n)!\,\pi R^2} e^{-\sigma_1^2 t/R^2} [\overline{I_3}(n, \phi, t)]^n. \tag{3.23}$$

Now we use the Laplace approximation theorem to estimate $\overline{I_3}(n, \phi, t)$ for large t. As explained earlier, $-V_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; n)$ attains its maximum when $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are equally spaced on a circle of radius r_0 centered at the origin.

Using the rotational symmetry of $V_3(\cdot; n)$ and ϕ we can integrate over the orientation of $\mathbf{r}_1$ to get

$$\overline{I_3}(n, \phi, t) = 2\pi \int_0^L r_1 \mathrm{d}r_1 \int_{\Lambda^2} \mathrm{d}^2\mathbf{r}_2 \mathrm{d}^2\mathbf{r}_3 \exp\left(- t \int_{r \leqslant 1} \mathrm{d}^2\mathbf{r} V_3(r_1\mathbf{i} - R\mathbf{r}, \mathbf{r}_2 - R\mathbf{r}, \mathbf{r}_3 - R\mathbf{r}; n) \cdot |\phi(\mathbf{r})|^2 \right). \tag{3.24}$$

$-V_3(r_1\mathbf{i}, \mathbf{r}_2, \mathbf{r}_3; n)$ is at a maximum when $r_1 = r_0$, $\mathbf{r}_2 = \tilde{\mathbf{r}}_2 := r_0(-\frac{1}{2}\mathbf{i} + \frac{1}{2}\sqrt{3}\mathbf{j})$ and $\mathbf{r}_3 = \tilde{\mathbf{r}}_3 := r_0(-\frac{1}{2}\mathbf{i} - \frac{1}{2}\sqrt{3}\mathbf{j})$. Therefore we make the transformations $r_1 \to r_0 + r_1$, $\mathbf{r}_2 \to \tilde{\mathbf{r}}_2 + \mathbf{r}_2$ and $\mathbf{r}_3 \to \tilde{\mathbf{r}}_3 + \mathbf{r}_3$ which gives

$$\overline{I_3}(n, \phi, t) = 2\pi \int_{-r_0}^{L - r_0} \mathrm{d}r_1 (r_0 + r_1) \int_{\Lambda - \tilde{\mathbf{r}}_2} \mathrm{d}^2\mathbf{r}_2 \int_{\Lambda - \tilde{\mathbf{r}}_3} \mathrm{d}^2\mathbf{r}_3 \exp\left(- t \int_{r \leqslant 1} \mathrm{d}^2\mathbf{r} V_3((r_0 + r_1)\mathbf{i} - R\mathbf{r}, \tilde{\mathbf{r}}_2 + \mathbf{r}_2 - R\mathbf{r}, \tilde{\mathbf{r}}_3 + \mathbf{r}_3 - R\mathbf{r}; n) |\phi(\mathbf{r})|^2 \right). \tag{3.25}$$

Now, from Taylor's theorem, we know that

$$f(\mathbf{x} + \mathbf{x}') = f(\mathbf{x}) + \mathbf{x}' \cdot \nabla f(\mathbf{x}) + \tfrac{1}{2}(\mathbf{x}' \cdot \nabla)^2 f(\mathbf{x}) + \tfrac{1}{6}(\mathbf{x}' \cdot \nabla)^3 f(\mathbf{x} + \zeta\mathbf{x}'), \tag{3.26}$$

where $\zeta \in (0, 1)$. Let us apply this to the function $V_3(\cdot; n)$, taking $\mathbf{x} = (r_0\mathbf{i}, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3)$, and $\mathbf{x}' = (r_1\mathbf{i} - R\mathbf{r}, \mathbf{r}_2 - R\mathbf{r}, \mathbf{r}_3 - R\mathbf{r})$.

First, we have that

$$V_3(r_0\mathbf{i}, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3; n) = 3\beta b_0, \tag{3.27}$$

where $b_0 = b(r_0)$ and

$$\nabla V_3(r_0\mathbf{i}, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3; n) = \mathbf{0}, \tag{3.28}$$

because the function has a minimum at that point. In the next term,

$$((r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r})\cdot\nabla)^2V_3(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3;n)$$
$$=\langle((r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r}),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r})\rangle, \tag{3.29}$$

where the 6×6 matrix $D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)$ is given in the Appendix. We can write (3.29) as a sum of four terms:

$$\langle(r_1\mathbf{i},\mathbf{r}_2,\mathbf{r}_3),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(r_1\mathbf{i},\mathbf{r}_2,\mathbf{r}_3)\rangle+R^2\langle(\mathbf{r},\mathbf{r},\mathbf{r}),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(\mathbf{r},\mathbf{r},\mathbf{r})\rangle$$
$$+R\langle(r_1\mathbf{i},\mathbf{r}_2,\mathbf{r}_3),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(\mathbf{r},\mathbf{r},\mathbf{r})\rangle+R\langle(\mathbf{r},\mathbf{r},\mathbf{r})D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3),(r_1\mathbf{i},\mathbf{r}_2,\mathbf{r}_3)\rangle. \tag{3.30}$$

The first term in (3.30) is independent of $\mathbf{r}$ and it is equal to

$$\langle(r_1,\mathbf{r}_2,\mathbf{r}_3),D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(r_1,\mathbf{r}_2,\mathbf{r}_3)\rangle, \tag{3.31}$$

where $D'_{2,n}(\mathbf{r}',\mathbf{r}'',\mathbf{r}''')$ is the 5×5 matrix obtained by deleting from $D_{2,n}(\mathbf{r}',\mathbf{r}'',\mathbf{r}''')$ all the terms involving derivatives with respect to the second component of $\mathbf{r}'$. This is another step needed to account for the symmetry inherent in maximizing the integrand in (3.22).

For the second term, writing $\mathbf{r}=(x,y)$ and using

$$\int_{r\leqslant1}\mathrm{d}^2\mathbf{r}\,x^2|\phi(\mathbf{r})|^2=\int_{r\leqslant1}\mathrm{d}^2\mathbf{r}\,y^2|\phi(\mathbf{r})|^2=\frac{1}{2}\sigma_2^2, \tag{3.32}$$

we have that

$$\int_{r\leqslant1}\mathrm{d}^2\mathbf{r}\langle(\mathbf{r},\mathbf{r},\mathbf{r}),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(\mathbf{r},\mathbf{r},\mathbf{r})\rangle|\phi(\mathbf{r})|^2=2C_1\sigma_2^2, \tag{3.33}$$

where

$$C_1=\frac{3}{4}b''(r_0)+\alpha^2n\left(\frac{9}{4}b_0^2-6b_0\frac{a(r_0)}{r_0^2}+\frac{11}{2}\frac{a^2(r_0)}{r_0^4}\right). \tag{3.34}$$

Note that all the terms in the integrand of (3.33) are even or odd in $\mathbf{r}$ and only the even terms give a nonzero result. The contribution from the last two terms in (3.30) is zero since, for example,

$$\int_{r\leqslant1}\mathrm{d}^2\mathbf{r}\langle(r_1\mathbf{i},\mathbf{r}_2,\mathbf{r}_3),D_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(\mathbf{r},\mathbf{r},\mathbf{r})\rangle|\phi(\mathbf{r})|^2 \tag{3.35}$$

vanishes because integrand is odd in $\mathbf{r}$.

For the third order term, we have that

$$|((r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r})\cdot\nabla)^3V_3\ ((r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)+\zeta(r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r}));n)|$$
$$\leqslant[\max(|r_1|,\|\mathbf{r}_2\|,\|\mathbf{r}_3\|)+R\|\mathbf{r}\|]^3|D_{3,n}((r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)+\zeta(r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r}))|, \tag{3.36}$$

where

$$D_{3,n}(\mathbf{x})=\sum_{i,j,k=1}^{6}\frac{\partial^3V_3(\mathbf{x};n)}{\partial x_i\partial x_j\partial x_k},$$

and $\|\mathbf{r}\|\leqslant1$ because the integration in the exponential in (3.22) is carried out over the unit disk.

Also, the above assumptions on the functions a and b imply that their derivatives are uniformly bounded, so that

$$|D_{3,n}((r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)+\zeta(r_1\mathbf{i}-R\mathbf{r},\mathbf{r}_2-R\mathbf{r},\mathbf{r}_3-R\mathbf{r}))|\leqslant nC_2, \tag{3.37}$$

where the constant C_2 does not depend on n or R.

This gives

$$\overline{I_3}(n,\phi,t) \geqslant 2\pi e^{3t|\beta|b_0}\exp(-tC_1\sigma_2^2R^2)\int_{-r_0}^{L-r_0} dr_1(r_0+r_1)\int_{\Lambda-\tilde{\mathbf{r}}_2} d^2\mathbf{r}_2\int_{\Lambda-\tilde{\mathbf{r}}_3} d^2\mathbf{r}_3$$
$$\times\exp\left(-\frac{t}{2}\langle(r_1,\mathbf{r}_2,\mathbf{r}_3),D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)(r_1,\mathbf{r}_2,\mathbf{r}_3)\rangle - tnC_2[\max(|r_1|,\|\mathbf{r}_2\|,\|\mathbf{r}_3\|)+R]^3\right). \tag{3.38}$$

Now we perform the following transformation

$$(\rho_1,\boldsymbol{\rho}_2,\boldsymbol{\rho}_3) = \frac{t^{1/2}}{\sqrt{2}}[D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)]^{1/2}(r_1,\mathbf{r}_2,\mathbf{r}_3) \tag{3.39}$$

and afterwards restrict the domain of integration to B_η, a hypercube in 5 dimensions of side $2t^{1/2}\eta$ around 0.

Letting $D_n=\det[D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)]$, after the transformation (3.39), we get

$$\overline{I_3}(n,\phi,t) \geqslant \frac{2^{7/2}\pi}{D_n^{1/2}}t^{-(5/2)}e^{3t|\beta|b_0}\exp(-tC_1\sigma_2^2R^2 - tnC_2[\sqrt{10}\eta\|[D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)]^{-(1/2)}\|+R]^3)$$
$$\times\int_{B_\eta} d\rho_1 d^2\boldsymbol{\rho}_2 d^2\boldsymbol{\rho}_3(r_0+\sqrt{2}t^{-1/2}([D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)]^{-(1/2)}(\rho_1,\boldsymbol{\rho}_2,\boldsymbol{\rho}_3))_1)e^{-(\rho_1,\boldsymbol{\rho}_2,\boldsymbol{\rho}_3)^2}, \tag{3.40}$$

where $(\mathbf{x})_1$ denotes the first component of $\mathbf{x}$.

The second term in the integrand in (3.40) is odd, and so its integral over a symmetric domain is zero. We further define

$$\tilde{C}_1 = |\alpha|\left(9b_0^2 - 24b_0\frac{a(r_0)}{r_0^2} + 22\frac{a^2(r_0)}{r_0^4}\right)^{1/2} \tag{3.41}$$

so that $C_1=\frac{3}{4}b''(r_0)+\frac{1}{4}\tilde{C}_1^2n$. There exist positive constants C_4, C_5, C_6, and C_7 such that

$$D_n^{-(1/2)} \geqslant C_4n^{-(5/2)}, \tag{3.42}$$

$$\sqrt{10}\|[D'_{2,n}(r_0\mathbf{i},\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)]^{-(1/2)}\| \leqslant C_5n^{-(1/2)} \tag{3.43}$$

and

$$\int_{B_\eta} d\rho_1 d^2\boldsymbol{\rho}_2 d^2\boldsymbol{\rho}_3 e^{-(\rho_1,\boldsymbol{\rho}_2,\boldsymbol{\rho}_3)^2} \geqslant \pi^{5/2}(1-C_6e^{C_7t\eta^2}). \tag{3.44}$$

Putting together what we have obtained so far and substituting into (3.23), we get

$$\tilde{N}(t) \geqslant e^{-\rho|\Lambda|}\frac{K_3^nt^{-(5/2)n}}{n^{(11/2)n}R^2}(1-C_6e^{-C_7t\eta^2})^n\exp\left(\left(3|\beta|b_0n - \frac{\sigma_1^2}{R^2} - \frac{1}{4}\tilde{C}_1^2\sigma_2^2R^2n^2\right.\right.$$
$$\left.\left. - \frac{3}{4}b''(r_0)\sigma_2^2R^2n - C_2C_5n^{1/2}\right)t\right), \tag{3.45}$$

where $K_3=(8\sqrt{2}/27)\pi^{5/2}\rho^3r_0C_4$. We would like to make the term in n^2 in the exponential, $\frac{1}{4}\tilde{C}_1^2\sigma_2^2R^2n^2$, small by letting $R\to 0$. However in doing this we make the term σ_1^2/R^2 large. Therefore we minimize the sum of the two terms by taking $R=\sqrt{2/\tilde{C}_1}(\sigma_1/\sigma_2)^{1/2}n^{-(1/2)}$. Note that in the nonmagnetic case the corresponding term is of order n and not n^2. To maximize the right-hand

side of (3.45) we take n as a function of t. We shall also write R in terms of n, and hence in terms of t so that $R \to 0$ as $t \to \infty$. Therefore we write

$$n(t) = \frac{K_3^{2/11}}{e} t^{-(5/11)} (1 - C_6 e^{-C_7 t \eta^2})^{2/11} \exp\left(\frac{2t}{11} (3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2) \right), \tag{3.46}$$

so that

$$R(t) = \sqrt{\frac{2e}{\tilde{C}_1}} \left(\frac{\sigma_1}{\sigma_2} \right)^{1/2} K_3^{-(1/11)} t^{5/22} (1 - C_6 e^{-C_7 t \eta^2})^{-(1/11)} \exp\left(- \frac{t}{11} (3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2) \right) \tag{3.47}$$

as $t \to \infty$.

Then we have that there exists t_0 independent of ϕ such that

$$\begin{aligned} \tilde{N}(t) \geqslant \frac{e^{-\rho|\Lambda|}}{2} \tilde{C}_1 \frac{\sigma_2}{\sigma_1} \exp\Bigg(& \frac{11}{2e} \frac{K_3^{2/11}}{t^{5/11}} (1 - C_6 e^{-C_7 t \eta^2})^{2/11} \exp\left(\frac{2t}{11} (3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2) \right) \\ & - \frac{C_2 C_5}{\sqrt{e}} K_3^{1/11} t^{17/22} (1 - C_6 e^{-C_7 t \eta^2})^{1/11} \exp\left(\frac{t}{11} (3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2) \right) - \frac{3}{2\tilde{C}_1} b''(r_0) \sigma_1 \sigma_2 t \Bigg) \end{aligned} \tag{3.48}$$

for $t > t_0$. The last two terms are subdominant. Clearly, the above is meaningful only if

$$3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2 > 0. \tag{3.49}$$

First of all, we note that by the Heisenberg Uncertainty Principle, $\sigma_1 \sigma_2$ cannot be made smaller than 1. However we have defined ϕ so that $\sigma_1 \sigma_2 \to 1$ as $t \to \infty$. This explains our choice of ϕ in (3.12). So then as $t \to \infty$,

$$\tfrac{2}{11} (3|\beta| b_0 - \tilde{C}_1 \sigma_1 \sigma_2) \to c_1 |\beta| b_0, \tag{3.50}$$

where c_1 was defined in (3.3).

Now, the fact that $|\beta| > |\alpha|$ together with assumption (2.10) which implies that

$$\frac{8}{3} \frac{a(r_0)}{b_0 r_0^2} - \frac{22}{9} \frac{a^2(r_0)}{{b_0}^2 r_0^4} > 0, \tag{3.51}$$

ensures that (3.49) is true. This gives us as $t \to \infty$

$$\tilde{N}(t) \geqslant \frac{e^{-\rho|\Lambda|}}{2} \tilde{C}_1 \frac{\sigma_2}{\sigma_1} \exp\left(\frac{11}{2e} {K_3}^{2/11} t^{-(5/11)} (1 - C_6 e^{-C_7 t \delta^2})^{2/11} \exp(c_1 |\beta| b_0 t) \right). \tag{3.52}$$

Furthermore, as $t \to \infty$,

$$\frac{\sigma_2}{\sigma_1} = \frac{1}{\sigma^2(t)} (1 + o(1)), \tag{3.53}$$

so that

$$\ln \tilde{N}(t) \geqslant \frac{11}{2e} {K_3}^{2/11} t^{-(5/11)} \exp(c_1 |\beta| b_0 t)(1 + o(1)) \tag{3.54}$$

as $t \to \infty$ or

$$\liminf_{t\to\infty} t^{5/11}\exp(-c_1|\beta|b_0 t)\ln \tilde{N}(t) \geqslant \frac{11}{2e}K_3^{2/11}. \tag{3.55}$$

From this we can use a Tauberian argument (Theorem 9.7 of Ref. 6) to obtain (3.2). □

Remark 1: In the above calculation, we have been working with the choice $N=3n$ which, after applying the inequality (3.18), leads us to work with $V_3(\cdot;n)$. This choice demands some justification.

We note first of all that working with $V_m(\mathbf{r}_1,\ldots,\mathbf{r}_m;n)$ for $m>1$ ensures that we can exploit the fact the second term in (3.10) is zero for a certain configuration of $\mathbf{r}_1,\ldots,\mathbf{r}_m$, so that the maximum value of $-V_m(\mathbf{r}_1,\ldots,\mathbf{r}_m;n)$ is $m|\beta|b_0$ (as in (3.27)).

If we apply inequality (3.18) directly to N, leading us to work with $V_1(\mathbf{r};n)$, the corresponding maximum value will be less than the expected $|\beta|b_0$, so that we get a worse lower bound.

For the case $m=2$ (i.e., choosing $N=2n$), we find that the expression corresponding to the l.h.s. of (3.49) is of the order $2|\beta|b_0-2\sqrt{2}|\alpha|b_0\sigma_1\sigma_2$. As noted earlier, the Heisenberg Uncertainty Principle forbids $\sigma_1\sigma_2<1$, so the method does not work in this case.

For $m>3$, we find that we do not get any improvement over the case $m=3$. For example, for the case $m=4$, the expression corresponding to the l.h.s. of (3.49) is

$$4|\beta|b_0-4|\alpha|b_0\sigma_1\sigma_2\left(1-\frac{2a(r_0)}{b_0 r_0^2}\right)^{1/2} \tag{3.56}$$

while for the case $m=5$, it is again of the order $5|\beta|b_0-5|\alpha|b_0\sigma_1\sigma_2$. This explains why we have chosen to work with the case $m=3$.

Remark 2: We have hitherto assumed that $\beta\leqslant-|\alpha|$. We note, however, that because of (3.51), there exists $\varepsilon>0$ such that (3.49) is true when $\beta<-|\alpha|+\varepsilon$. In this case, $c_1|\beta|b_0$ is not of order b_0 for large b_0.

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APPENDIX

Let $(\mathbf{r}_1,\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)=\left(r_0\mathbf{i},r_0\left(-\frac{1}{2}\mathbf{i}+\frac{1}{2}\sqrt{3}\mathbf{j}\right),r_0\left(-\frac{1}{2}\mathbf{i}-\frac{1}{2}\sqrt{3}\mathbf{j}\right)\right)$. Then $D_{2,n}(\mathbf{r}_1,\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_3)=B+2\alpha^2 nA$, where

$$B=\begin{pmatrix} b''(r_0) & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{1}{4}b''(r_0) & \frac{\sqrt{3}}{4}b''(r_0) & 0 & 0\\ 0 & 0 & \frac{\sqrt{3}}{4}b''(r_0) & \frac{3}{4}b''(r_0) & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{1}{4}b''(r_0) & -\frac{\sqrt{3}}{4}b''(r_0)\\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{4}b''(r_0) & \frac{3}{4}b''(r_0) \end{pmatrix} \tag{A1}$$

and the matrix A is symmetric and its entries a_{ij} are given by

$$a_{11}=\left(b_0-\frac{a(r_0)}{r_0^2}\right)^2, \tag{A2}$$

$$a_{12}=0, \tag{A3}$$

$$a_{13} = \left(b_0 - \frac{a(r_0)}{r_0^2} \right) \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right), \tag{A4}$$

$$a_{14} = \left(b_0 - \frac{a(r_0)}{r_0^2} \right) \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right), \tag{A5}$$

$$a_{15} = a_{13}, \tag{A6}$$

$$a_{16} = - a_{14}, \tag{A7}$$

$$a_{22} = \left(\frac{a(r_0)}{r_0^2} \right)^2, \tag{A8}$$

$$a_{23} = \frac{a(r_0)}{r_0^2} \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right), \tag{A9}$$

$$a_{24} = \frac{a(r_0)}{r_0^2} \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right), \tag{A10}$$

$$a_{25} = - a_{23}, \tag{A11}$$

$$a_{26} = - a_{24}, \tag{A12}$$

$$a_{33} = \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right)^2 + \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right)^2, \tag{A13}$$

$$a_{34} = \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right) \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) + \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right), \tag{A14}$$

$$a_{35} = \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right)^2 - \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right)^2, \tag{A15}$$

$$a_{36} = \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right) \left(\frac{\sqrt{3}}{4} b_0 - \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) + \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right), \tag{A16}$$

$$a_{44} = \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right)^2 + \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right)^2, \tag{A17}$$

$$a_{45} = \left(\frac{1}{4} b_0 - \frac{a(r_0)}{r_0^2} \right) \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) - \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right) \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right), \tag{A18}$$

$$a_{46} = - \left(- \frac{\sqrt{3}}{4} b_0 + \frac{\sqrt{3} a(r_0)}{2 r_0^2} \right)^2 + \left(\frac{3}{4} b_0 - \frac{a(r_0)}{2 r_0^2} \right)^2, \tag{A19}$$

$$a_{55} = a_{33}, \tag{A20}$$

$$a_{56} = -a_{34}, \tag{A21}$$

$$a_{66} = a_{44}. \tag{A22}$$

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Coherent solutions for relativistic vectorial fields

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Approximate interacting localized solutions of a vectorial massive nonlinear equation are obtained by using the asymptotic perturbation (AP) method, based on Fourier expansion and spatio-temporal rescaling. The amplitude slow modulation of Fourier modes is described by a system of nonlinear evolution equations solvable via an appropriate change of variables. Various types of localized solutions (dromions, lumps, ring solitons, and breathers) as well as multiple soliton and instanton solutions can be explicitly constructed and their interaction is completely elastic, because they pass through each other and preserve their shape, the only change being a phase shift. © *2004 American Institute of Physics*.
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I. INTRODUCTION

Many methods are available for obtaining nontrivial solutions of nonlinear partial differential equations. We cite, for example, the bilinear method, inverse scattering transformation, symmetry reductions, Backlund and Darboux transformations, etc.[1–3] The most important solutions are the celebrated solitons, i.e., exponentially stable localized solutions of integrable (exact solutions) or nonintegrable nonlinear equations (exact or approximate solutions) in $1+1$ dimensions. In the past 30 years, solitons have been extensively applied in many natural sciences and especially in almost all fields of physics such as plasma physics, optics, fluid mechanics, and so on.[4,5]

In $2+1$ dimensions, there are many nonlinear equations integrable by the inverse scattering method such as the Davey–Stewartson (DS) equation, Kadomtsev–Petviashvili (KP) equation. A new type of coherent (exponentially localized in all directions) solution (dromion) driven by straight line solitons has been found in some cases, for example for the so called DS-I equation.[6–11]

Moreover, it has been demonstrated that dromions exist as approximate solutions in the particular case of ion acoustic waves in an unmagnetized or magnetized plasma and electron acoustic waves.[12–14] Each dromion propagates with its own group velocity and during a collision maintains its shape, because a phase shift is the only change. They are solutions of a *C*-integrable (solvable via an appropriate change of variables) nonlinear partial differential system of equations describing N-interacting waves $(N>1)$ for modulated amplitudes $\Psi_j=\Psi_j(\xi,\eta,\tau)$, $j=1,\ldots,N$.

In this paper, we seek approximate localized solutions for the following nonlinear equation for a massive vectorial field,

$$(\partial_\mu\partial^\mu + M^2)A^\nu + a|A_\mu|^2A^\nu = 0, \tag{1.1}$$

where $A^\nu=(A^0,\underline{A})$, $\partial_\mu\partial^\mu=\partial_t^2-\nabla^2$, M and a are parameter and $|A_\mu|^2=A^\mu A^*_\mu$.

We consider the interaction and eventually the collisions among coherent solutions with different velocities that are not close to each other and use the asymptotic reduction (AP) method[15,16] based on the spatio-temporal rescaling

$$\xi^\mu = \varepsilon^2 x^\mu, \tag{1.2}$$

where

$$\xi^{\mu} = (\xi^0, \underline{\xi}), \quad x^{\mu} = (x^0, \underline{x}), \tag{1.3}$$

with $\xi^0 = \tau$ and $x^0 = t$. The small positive nondimensional parameter ε is artificially introduced to serve as bookkeeping device and will be set equal to unity in the final analysis. The reduction method focuses on a solution that is small and is close to a superposition of N several dispersive waves, with different group velocities.

In the linear limit the solution is

$$\sum_{j=1}^{N} C_j^{\nu} \exp(-is_j), \quad s_j = k_{j,\mu} x^{\mu} = \omega_j t - \underline{K}_j \,.\, \underline{x}, \quad j = 1, \ldots, N, \; N > 1, \tag{1.4}$$

where C_j^{ν} are the complex amplitudes, $\underline{K}_j \equiv (K_{1,j}, K_{2,j}, K_{3,j})$ the wave vectors and the (circular) frequency ω_j is furnished by the dispersion relation $\omega_j = \omega_j(\underline{K}_j)$. The amplitudes of these N nonresonant dispersive waves (constant in the linear limit) are slowly modulated by the non linear term of the vectorial massive nonlinear Eq. (1.1).

In Sec. II we derive a model system of equations for the slow modulation of the Fourier modes amplitudes and, subsequently, in Sec. III we show that it is *C*-integrable. The Cauchy problem is resolved, just by quadratures, and explicit nontrivial solutions are constructed. In Sec. IV, we demonstrate the existence of dromions which preserve their shape during collisions, the only change being a phase shift. Moreover, other coherent solutions (line solitons, multilump solutions, ring solitons, instanton solutions, and breathers) are derived. Conclusion and final considerations are reserved for the last section.

II. DERIVATION OF THE MODEL SYSTEM

It is well known that the linearized version of Eq. (1.1),

$$(\partial_{\mu}\partial^{\mu} + M^2) A^{\nu} = 0, \tag{2.1}$$

is satisfied by Fourier modes with constant amplitudes,

$$A_j^{\nu} \approx C_j^{\nu} \exp i(\underline{K}_j \,.\, \underline{X} - \omega_j t) = C_j^{\nu} \exp(-ik_{j,\mu} x^{\mu}), \tag{2.2}$$

if the following dispersion relation is verified:

$$\omega_j^2 = K_j^2 + M^2. \tag{2.3}$$

The group velocity $\underline{U}_j$ (the speed with which a wave packet peaked at that Fourier mode would move) is

$$\underline{U}_j = \frac{d\omega_j}{d\underline{K}_j} = \frac{\underline{K}_j}{\omega_j}. \tag{2.4}$$

In the following we consider a superposition of N dispersive waves, characterized by different values of the wave vector $\underline{K}_j$ and by group velocities not close to each other. Weak nonlinearity induces a slow variation of the amplitudes of these dispersive waves and the AP method derives the nonlinear system of equations for the Fourier modes amplitudes modulation, obviously in appropriate "slow" and "coarse-grained" variables defined by Eq. (1.2). Since the amplitude of Fourier modes are not constant, higher order harmonics appear and in order to construct an approximate solution that is small of order ε and that is close in the limit of small ε to the linear solution (2.2), we introduce the asymptotic Fourier expansion

$$A^{\nu}(x) = \sum_{\underline{n}=-\infty}^{\infty} \exp\left(i\sum_{j=1}^{N} n_j s_j \right) \varepsilon^{\gamma_{\underline{n}}} \psi_{\underline{n}}^{\nu}(\xi;\varepsilon), \tag{2.5}$$

where the index $\underline{n}$ stands for the set $\{n_j; j=1, 2, \ldots, N\}$, s_j is given in Eq. (1.4) and summation is limited only to terms with n_j odds (note that the only nonlinear term present in Eq. (1.1) is cubic). The functions, $\psi_{\underline{n}}^{\nu}(\xi, \eta, \tau, \varepsilon)$ depend parametrically on ε and we assume that their limit for $\varepsilon \to 0$ exists and is finite. We moreover assume that there hold the conditions

$$\gamma_{\underline{n}} = \gamma_{-\underline{n}}, \tag{2.6}$$

$$\gamma_{\underline{n}} = \sum_{j=1}^{N} |n_j|, \text{ otherwise}. \tag{2.7}$$

This implies that we obtain the main amplitudes if one of the indices n_j has unit modulus and all the others vanish. We use the following notations:

$$\psi_{\underline{n}}(\xi, \varepsilon \to 0) = \Psi_j(\xi), \text{ if } n_j = 1 \text{ and } n_m = 0 \text{ for } j \neq m, \tag{2.8a}$$

$$\psi_{\underline{n}}(\xi, \varepsilon \to 0) = \Phi_j(\xi), \text{ if } n_j = -1 \text{ and } n_m = 0 \text{ for } j \neq m. \tag{2.8b}$$

Taking into account (2.6) and (2.8), the Fourier expansion (2.5) can be written more explicitly in the following form:

$$\begin{aligned} A^{\nu}(x) = &\sum_{j=1}^{N} [\exp(is_j)\Psi_j(\xi) + \varepsilon^2 \exp(3is_j)\Psi_{3,j}(\xi) + \text{c.c.}] + \sum_{j=1}^{N} [\exp(-is_j)\Phi_j(\xi) \\ &+ \varepsilon^2 \exp(-3is_j)\Psi_{-3,j}(\xi) + \text{c.c.}] + O(\varepsilon^4), \end{aligned} \tag{2.9}$$

where c.c. stands for complex conjugate.

Substituting (2.9) in Eq. (1.1) and considering the different equations obtained for every harmonic and for a fixed order of approximation in ε, we obtain for $n_j=1$, $n_m=0$, if $j \neq m$, to the order of ε^3, the following system of equations for the modulated amplitudes:

$$(-2ik_{\mu}\partial^{\mu})\Psi_j^{\nu} + a\sum_{m=1}^{N} [(\Psi_{\mu,m}\Psi_m^{*\mu} + \Phi_{\mu,m}\Phi_m^{*\mu})\Psi_j^{\nu} + \Phi_m^{\nu}\Phi_m^{*\mu}\Psi_{\mu,j}] = 0, \tag{2.10}$$

and $n_j=-1$, $n_m=0$, if $j \neq m$, to the order of ε^3,

$$(2ik_{\mu}\partial^{\mu})\Phi_j^{\nu} + a\sum_{m=1}^{N} [(\Phi_{\mu,m}\Phi_m^{*\mu} + \Psi_{\mu,m}\Psi_m^{*\mu})\Phi_j^{\nu} + \Psi_m^{\nu}\Psi_m^{*\mu}\Phi_{\mu,j}] = 0. \tag{2.11}$$

The validity of the approximate solution should be expected to be restricted on bounded intervals of the τ-variable and on time-scale $t=O(1/\varepsilon^2)$. If one wishes to study solutions on intervals such that $\tau=O(1/\varepsilon)$, then the higher terms will in general affect the solution and must be included.

III. INTEGRABILITY OF THE MODEL SYSTEM OF EQUATIONS

The system of nonlinear equations (2.10) and (2.11) is *C*-integrable by means of an appropriate transformation of the dependent variables. We set

$$\Psi_j^{\nu}(\xi) = \rho_j^{\nu}(\xi)\exp[i\vartheta_j^{\nu}(\xi)], \quad \Phi_j^{\nu}(\xi) = \chi_j^{\nu}(\xi)\exp[i\varphi_j^{\nu}(\xi)], \quad j = 1, \ldots N, \tag{3.1}$$

with $\rho_j^{\nu}=\rho_j^{\nu}(\xi)$, $\chi_j^{\nu}=\chi_j^{\nu}(\xi)>0$ and $\vartheta_j^{\nu}=\vartheta_j^{\nu}(\xi)$, $\varphi_j^{\nu}=\varphi_j^{\nu}(\xi)$ real functions. Then Eqs. (2.10) and (2.11) yield

$$\rho^{\nu}_{j,\tau}(\xi) + \underline{U}_j \,.\, \nabla\, \rho^{\nu}_j(\xi) = 0, \tag{3.2}$$

$$\chi^{\nu}_{j,\tau}(\xi) + \underline{U}_j \,.\, \nabla\, \chi^{\nu}_j(\xi) = 0, \tag{3.3}$$

$$(\vartheta_{j,\tau}(\xi) + \underline{U}_j \,.\, \nabla\, \vartheta^{\nu}_j(\xi))\rho^{\nu}_j + \frac{a}{2\omega_j}\sum_{m=1}^{N}[(\rho_{\mu,m}\rho^{\mu}_m + \chi_{\mu,m}\chi^{\mu}_m)\rho^{\nu}_j + \chi^{\nu}_m\chi^{\mu}_m\rho_{\mu,j}] = 0, \tag{3.4}$$

$$(\varphi_{j,\tau} + \underline{U}_j \,.\, \nabla\, \varphi^{\nu}_j)\chi^{\nu}_j - \frac{a}{2\omega_j}\sum_{m=1}^{N}[(\chi_{\mu,m}\chi^{\mu}_m + \rho_{\mu,m}\rho^{\mu}_m)\chi^{\nu}_j + \rho^{\nu}_m\rho^{\mu}_m\chi_{\mu,j}] = 0. \tag{3.5}$$

A suitable solution for the Cauchy problem of (3.2) and (3.3) reads

$$\rho^{\nu}_j = \rho^{\nu}_j(\alpha_{\mu,j}\xi^{\mu}),\ \chi^{\nu}_j = \chi^{\nu}_j(\beta_{\mu,j}\xi^{\mu}), \tag{3.6}$$

where $\alpha^{\nu}_{\mu,j}=(\alpha^{\nu}_{0,j},\underline{\alpha}^{\nu}_j)$, $\beta^{\nu}_{\mu,j}=(\beta^{\nu}_{0,j},\underline{\beta}^{\nu}_j)$, the $8N$ real functions $\rho_j(\underline{\alpha}^{\nu}_j\cdot\underline{\xi})$, $\chi_j(\underline{\beta}^{\nu}_j\cdot\underline{\xi})$ which represent the initial shape can be chosen arbitrarily and $\alpha^{\nu}_{\mu,j},\beta^{\nu}_{\mu,j}$ are real constants which satisfy the relation

$$\alpha^{\nu}_{0,j} + \underline{\alpha}^{\nu}_j\underline{U} = 0, \quad \beta^{\nu}_{0,j} + \underline{\beta}^{\nu}_j\underline{U} = 0. \tag{3.7}$$

A suitable solution of (3.4) and (3.5) is

$$\vartheta^{\nu}_j = \delta_j(\tilde{\alpha}^{\nu}_{\mu,j}\xi^{\mu}) - \frac{a}{2\omega_j}\sum_{m=1}^{N}\int_0^{\tau}\frac{(\chi^{\nu}_m(\lambda)\chi^{\mu}_m(\lambda)\rho_{\mu,j}(\lambda))}{\rho^{\nu}_j(\lambda)}d\tilde{\tau} - \frac{a}{2\omega_j}\sum_{m=1}^{N}\int_0^{\tau}(\rho_{\mu,m}(\lambda)\rho^{\mu}_m(\lambda) + \chi_{\mu,m}(\lambda)\chi^{\mu}_m(\lambda))d\tilde{\tau}, \tag{3.8a}$$

where

$$f(\lambda) = f(\underline{\xi} - \underline{U}_j\cdot(\tau-\tilde{\tau}),\tilde{\tau}), \tag{3.8b}$$

and

$$\varphi^{\nu}_j = \tilde{\delta}_j(\tilde{\beta}^{\nu}_{\mu,j}\xi^{\mu}) + \frac{a}{2\omega_j}\sum_{m=1}^{N}\int_0^{\tau}\frac{(\rho^{\nu}_m(\lambda)\rho^{\mu}_m(\lambda)\chi_{\mu,j}(\lambda))}{\chi^{\nu}_j(\lambda)}d\tilde{\tau} + \frac{a}{2\omega_j}\sum_{m=1}^{N}\int_0^{\tau}(\chi_{\mu,m}(\lambda)\chi^{\mu}_m(\lambda) + \rho_{\mu,m}(\lambda)\rho^{\mu}_m(\lambda))d\tilde{\tau}, \tag{3.9}$$

where the $8N$ functions $\delta^{\nu}_j(\underline{\alpha}^{\nu}_j\cdot\underline{\xi})$, $\tilde{\delta}^{\nu}_j(\underline{\alpha}^{\nu}_j\cdot\underline{\xi})$ are fixed by the initial data and

$$\tilde{\alpha}^{\nu}_{0,j} + \underline{\tilde{\alpha}}^{\nu}_j\cdot\underline{U}_j = 0, \quad \tilde{\beta}^{\nu}_{0,j} + \underline{\tilde{\beta}}^{\nu}_j\cdot\underline{U}_j = 0. \tag{3.10}$$

The approximate solution for the massive vector field Eq. (1.1) is

$$A^{\nu} = 2\varepsilon\sum_{j=1}^{N}\rho^{\nu}_j\cos(\vartheta^{\nu}_j + k_{j,\mu}\xi^{\mu}) + 2\varepsilon\sum_{j=1}^{N}\chi^{\nu}_j\cos(\varphi^{\nu}_j - k_{j,\mu}\xi^{\mu}) + O(\varepsilon^3). \tag{3.11}$$

The corrections of order ε^3 to the approximate solution depend on higher harmonics and can be easily calculated from results obtained in Sec. II.

IV. EXACT SOLUTIONS FOR THE *C*-INTEGRABLE MODEL EQUATION

A. Nonlinear wave

The most simple solution of the system (2.10) and (2.11) is the plane wave

$$\chi_j^\nu = \tilde{C}_j^\nu = \text{const}, \quad \vartheta_j^\nu = -\tilde{k}_{\mu,j}^\nu \xi^\mu, \tag{4.1a}$$

$$\rho_j^\nu = C_j^\nu = \text{const}, \quad \varphi_j^\nu = -\hat{k}_{\mu,j}^\nu \xi^\mu, \tag{4.1b}$$

$$\hat{k}_{\mu,j}^\nu = (\hat{\omega}_j^\nu, \underline{K}_j), \quad \tilde{k}_{\mu,j}^\nu = (\tilde{\omega}_j^\nu, \underline{K}_j), \tag{4.1c}$$

where the amplitudes and phases are connected according to the dispersion relation

$$\tilde{\omega}_j = \underline{U}_j \cdot \underset{-}{\tilde{K}}_j + \frac{a}{2\omega_j} \sum_{m=1}^{N} \left(\frac{\tilde{C}_m^\nu \tilde{C}_m^\mu C_{\mu,j}}{C_j^\nu} + C_{\mu,m} C_m^\mu + \tilde{C}_{\mu,m} \tilde{C}_m^\mu \right), \tag{4.2a}$$

$$\hat{\omega}_j = \underline{U}_j \cdot \underset{-}{\tilde{K}}_j - \frac{a}{2\omega_j} \sum_{m=1}^{N} \left(\frac{C_m^\nu C_m^\mu \tilde{C}_{\mu,j}}{\tilde{C}_j^\nu} + \tilde{C}_{\mu,m} \tilde{C}_m^\mu + C_{\mu,m} C_m^\mu \right). \tag{4.2b}$$

B. Solitons

The *C*-integrable nature of the system (2.10) and (2.11) implies the existence of more interesting solutions. It is possible the existence of *N* solitons which interact each other preserving their shapes and propagate with the relative group velocity $\underline{U}_j$ **(**see (2.4)**)**. These *N* solitons have fixed speeds but arbitrary shapes:

$$\rho_j^\nu = \frac{2C_j^\nu}{ch(2C_j^\nu(\alpha_{\mu,j}^\nu \xi^\mu))}, \quad \chi_j^\nu = \frac{2\tilde{C}_j^\nu}{ch(2\tilde{C}_j^\nu(\beta_{\mu,j}^\nu \xi^\mu))}, \tag{4.3a}$$

$$\delta_j^\nu = 0 \text{ for } j = 1, \ldots, N, \tag{4.3b}$$

where $\alpha_{\mu,j}^\nu$, $\beta_{\mu,j}^\nu$ are given by (3.7), C_j^ν, $\tilde{C}_j^\nu$ for $j=1, \ldots, N$, are real constants of order ε, and the phases ϑ_j^ν, φ_j^ν are given by (3.8)–(3.9).

Substituting (4.3) in (3.7) we obtain the approximate solution good to the order of ε. Each soliton advances with a constant velocity (the group velocity) before and after collisions. Only the phase is changed during collisions owing to the presence of the other solitons.

For example, if for the initial conditions we choose $N=2$ and

$$A^\nu(\underline{x},0) = 4\sum_{j=1}^{2} \frac{C_j^\nu}{ch(2C_j^\nu(\underline{\alpha}_j^\nu \cdot (\underline{x} - \underline{x}_{0,j}^\nu)))} \cos(\underline{K}_j \cdot \underline{x}), \tag{4.4}$$

where the initial positions are $x_{0,1}^\nu$, $x_{0,2}^\nu$, then the approximate solution good to the order of ε is given by

$$A^\nu(\underline{x},t) = 4\sum_{j=1}^{2} \frac{C_j^\nu \cos(k_{\mu,j} x^\mu + \vartheta_j^\nu)}{ch(2C_j^\nu(\alpha_{\mu,j} \cdot (x^\mu - x_{0,j}^\mu)))}. \tag{4.5}$$

C. Dromions

It is well known that dromions have been found in many $(2+1)$-dimensional equations integrable by the inverse scattering method and usually are driven by two or more nonparallel straight-line "ghost" solitons. The localized wave packet is located at the intersection of two line-solitons of the mean field and the lump travels along the tracks. In the DS-I system dromion solutions are driven by two perpendicular line "ghost" solitons, while in the Kadomtsev–Petviashvili equation the dromion solutions are driven by nonperpendicular line "ghost" solitons. In the last case dromions exist only for some suitable potentials of the field. Recently dromions solutions driven by curved and straight-line solitons have been found for some nonlinear equations in $2+1$ dimensions.[9]

The existence of localized solutions is possible also for *C*-integrable systems, because dromion solutions are not exclusive characteristics of equations integrable by the inverse scattering method.

A particular solution of the model system (2.10) and (2.11) is given by

$$\rho_j^\nu = C_j^\nu \exp(-B_j^\nu|\underline{\xi} - \underline{U}_j\tau|), \quad \chi_j^\nu = 0,\ \varphi_j^\nu = 0, \tag{4.6}$$

$$\delta_j^\nu = 0 \text{ for } j = 1,2,\ldots,N, \tag{4.7}$$

where B_j^ν, C_j^ν are real constants (note that the functions ρ_j^ν 4.6(a) are localized) and ϑ_j^ν is given by Eq. (3.5).

Substituting the solution (4.6) in Eq. (3.7) and taking $N=2$ we obtain for two dromions with different shapes and amplitudes the approximate solution

$$A^\nu(\underline{x},t) = 2\sum_{j=1}^{2} C_j^\nu \exp(-B_j^\nu|\underline{\xi} - \underline{U}_j\tau|)\cos(k_{\mu,j}x^\mu + \vartheta_j^\nu). \tag{4.8}$$

In Fig. 1 we show a collision between two dromions: the initial condition is shown in Fig. 1(a), then the two dromions collide [Fig. 1(b)] and then separate [Fig. 1(c)]. We can see that dromions preserve their shapes but with a phase shift.

D. Lumps

It is well known that in high dimension, in addition to the dromion solutions, other interesting localized solutions, formed by rational functions, are the multiple lumps. Obviously, there are many possible choices in order to obtain multilump solutions. For instance, we take

$$\rho_j^\nu = \frac{B_j^\nu}{C_j^\nu + D_j^\nu|\underline{\xi} - \underline{U}_j\tau|^2}, \quad \chi_j^\nu = 0,\ \varphi_j^\nu = 0, \tag{4.9a}$$

$$\delta_j^\nu = 0 \text{ for } j = 1,\ldots,N, \tag{4.9b}$$

where B_j^ν, C_j^ν, and D_j^ν are arbitrary real constants and ϑ_j^ν is given by Eq. (3.5).

E. Ring solitons

The multiple ring solitons are solutions that are not equal to zero at some closed curves and decay exponentially away from the closed curves. A possible selection is

$$\rho_j^\nu = C_j^\nu \exp(-B_j^\nu f_j^\nu(R_j)), \quad \chi_j^\nu = 0,\ \varphi_j^\nu = 0, \tag{4.10a}$$

$$\delta_j^\nu = 0 \text{ for } j = 1,\ldots,N, \tag{4.10b}$$

ϑ_j^ν given by Eq. (3.5) and

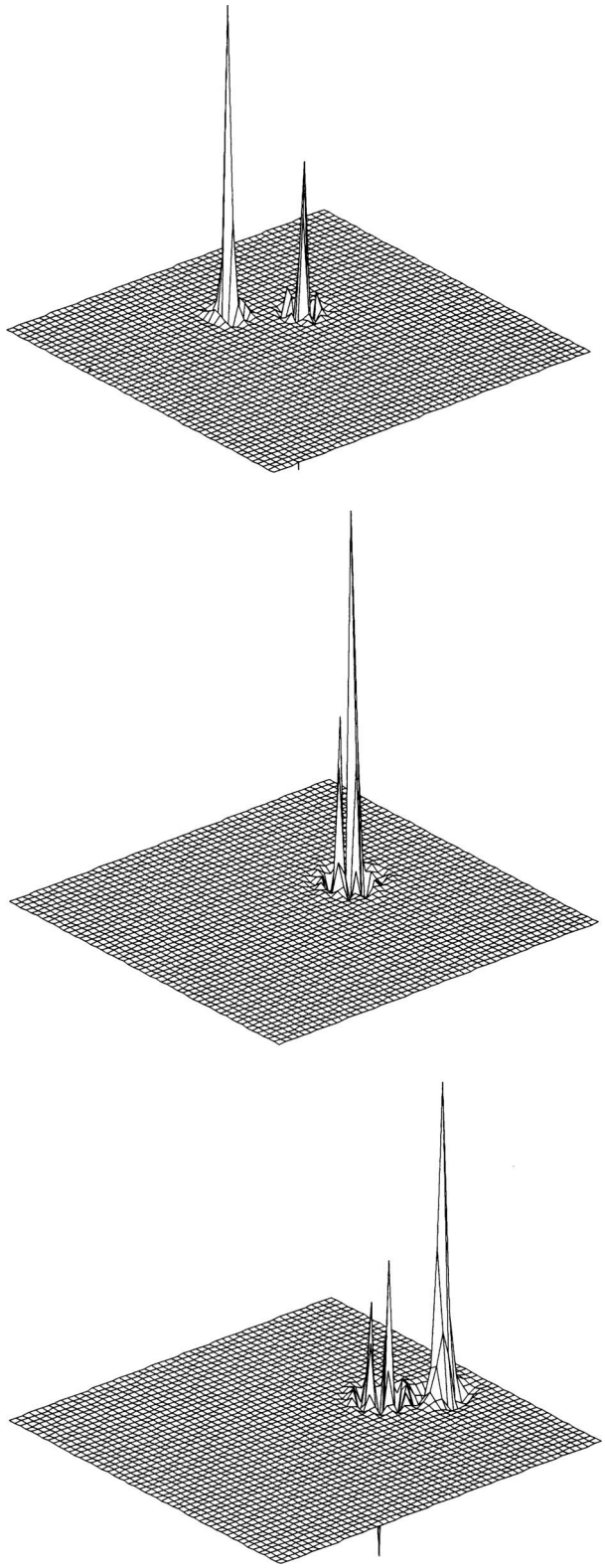

FIG. 1. Evolution plots of two dromions with different shapes and amplitudes ($A_1=2.0$, $A_2=2.5$, $B_1=0.01$, $B_2=0.01$, $K_{1,1}=1.3$, $K_{2,1}=1.2$, $K_{1,2}=0.8$, $K_{2,2}=0.7$). The initial condition is represented in (a), then the two dromions undergo a collision (b) and separate (c).

$$R_j = |\underline{\xi} - \underline{U}_j \tau|, \tag{4.10c}$$

$$f_j^\nu(R_j) = (R_j - R_{0,j}^\nu)^2, \tag{4.10d}$$

with C_j^ν, B_j^ν, and $R_{0,j}^\nu$ as arbitrary constants.

F. Instantons

If we choose a decaying function of time, we obtain also multiple instanton solutions, for example,

$$\rho_j^\nu = C_j^\nu \exp(\underline{\alpha}_j^\nu \cdot \underline{\xi} - \lambda_j^\nu \tau), \quad \chi_j^\nu = 0, \quad \varphi_j^\nu = 0, \tag{4.11a}$$

$$\delta_j^\nu = 0 \text{ for } j = 1, \ldots, N, \tag{4.11b}$$

with ϑ_j^ν given by Eq. (3.5), C_j^ν, $\underline{\alpha}_j^\nu$ arbitrary constants and

$$\lambda_j^\nu = \underline{\alpha}_j^\nu \cdot \underline{U}_j. \tag{4.11c}$$

G. Moving breatherlike structures

Finally, if we choose some types of periodic functions of time in the above mentioned solutions, then we obtain breathers. For example, we take

$$\rho_j^\nu = C_j^\nu \cos(\underline{\alpha}_j^\nu \cdot \underline{\xi} - \Omega_j^\nu t)\exp[-B_j^\nu |\underline{\xi} - \underline{U}_j \tau|], \quad \chi_j^\nu = 0, \quad \varphi_j^\nu = 0, \tag{4.12a}$$

$$\delta_j^\nu = 0 \text{ for } j = 1, \ldots, N, \tag{4.12b}$$

with ϑ_j^ν given by Eq. (3.5), B_j^ν, C_j^ν, $\underline{\alpha}_j^\nu$ arbitrary constants and

$$\Omega_j^\nu = \underline{\alpha}_j^\nu \cdot \underline{U}_j. \tag{4.12c}$$

V. CONCLUSION

We have found approximate analytical solutions for the vectorial massive nonlinear equation (1.1). Appropriately coarse-grained and slow variables have been introduced and a model system of equations for the amplitudes modulation of Fourier modes has been derived by means of the AP method.

The model system is *C*-integrable and with appropriate nontrivial initial conditions we can obtain multiple localized solutions (dromions, solitons, lumps, ring solitons, breathers, instantons) moving with different and not close to each other velocities. The richness of the solitons types is obviously a consequence of the high dimensions of the nonlinear equations.

This topic will be further investigated with the derivation of the model equation for other nonlinear waves and of the model equations for the interactions among phase resonant waves. Moreover, it will be worthy to study further the behavior of the solutions, and in particular of the dromions, beyond the leading order in the expansion parameter ε.

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Avoiding superluminal propagation of higher spin waves via projectors onto W^2 invariant subspaces

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We propose to describe higher spins as invariant subspaces of the Casimir operators of the Poincaré Group, P^2, and the squared Pauli–Lubanski operator, W^2, in a properly chosen representation, $\psi(\mathbf{p})$ (in momentum space), of the Homogeneous Lorentz Group. The resulting equation of motion for any field with $s \neq 0$ is then just a specific combination of the respective covariant projectors. We couple minimally electromagnetism to this equation and show that the corresponding wave fronts of the classical solutions propagate causally. Furthermore, for $(s,0)\oplus(0,s)$ representations, the formalism predicts the correct gyromagnetic factor, $g_s=1/s$. The advocated method allows us to describe any higher spin without auxiliary conditions and by one covariant matrix equation alone. This master equation is only quadratic in the momenta and its dimensionality is that of $\psi(\mathbf{p})$. We prove that the suggested master equation avoids the Velo–Zwanziger problem of superluminal propagation of higher spin waves and points toward a consistent description of higher spin quantum fields. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1794843]

I. INTRODUCTION

The field theoretical description of interacting particles with spin >1 is a long standing problem. The interaction of a spin $\frac{3}{2}$ Rarita–Schwinger (RS) field minimally coupled to an external electromagnetic field was shown to be inconsistent more than 40 years ago.[1] Later on, Velo and Zwanziger observed superluminal propagation of the RS wave front in the presence of a minimally coupled electromagnetic field[2] and also studied the conditions under which the Proca field interacting with an external electromagnetic field propagates causally.[3] After these works many authors have addressed the above problem from different perspectives and for different interactions[4] and the general feeling seems to be that it is not possible to construct a consistent quantum theory for massive particles with $s>1$.

At several decades of distance in looking afresh onto the equations of motion can lead to a different understanding of this fundamental problem. Weinberg emphasizes in his textbook on quantum field theory[5] that the equation of motion satisfied by the Dirac field is nothing but the record about the way how one puts together the two irreducible representations, $(1/2,0)$, and $(0,1/2)$, of the proper orthochronous Lorentz group to form a field that transforms invariantly under parity. In a wider understanding, this means that the equations of motion satisfied by a field are just a consequence of the properties of the representations of the Homogeneous Lorentz Group (HLG) chosen by us to accommodate the field and the discrete symmetries we require to be realized in this space. Closely related arguments can be found, among others, in Refs. 6–9.

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More recently, Refs. 10 and 11 studied covariant projectors onto invariant subspaces of the squared Pauli–Lubanski operator in the representation space of the four-vector–spinor and showed that the associated equations are free from the Velo–Zwanziger problem. The corresponding projectors for the $(s,0)\oplus(0,s)$ representation space were studied in Ref. 12 where it was shown that under minimal coupling a particle in this representation has the correct value for the spin gyromagnetic factor, $g_s=1/s$, thus proving Belinfante's conjecture[13] from 1953.

In this work we explore the projectors onto the invariant subspaces of the Poincaré Casimir operators, the squared four-momentum and the squared Pauli–Lubanski operator, for any s, and study the propagation of the corresponding wave fronts along the lines of Refs. 2 and 3. The paper is organized as follows. In the next section we recall in brief a current description of higher spins and its relation to the Poincaré group. In Sec. III we suggest describing higher spins as invariant subspaces of the Poincaré Casimirs. In Sec. IV we show that particles within this framework propagate causally in the presence of an electromagnetic field, thus avoiding the classical Velo–Zwanziger problem. In this paper we close with a brief summary.

II. CURRENT DESCRIPTION OF FIELDS AND ITS RELATION TO POINCARÉ GROUP REPRESENTATIONS

The primary classification of elementary systems is usually done by identifying them (up to form factors) with the irreducible representations (irreps) of the Poincaré group (PG). If so, then one necessarily has to consider particles as invariant spaces of the Casimir operators of this group—the squared four-momentum P^2, on the one side, and the squared Pauli–Lubanski operator W^2, on the other side and label them by their respective eigenvalues, p^2, and $-p^2s(s+1)$, as $|p^2,s(s+1)\rangle$. Further quantum numbers can be associated with the Casimir invariants of the underlying Homogeneous Lorentz Group (HLG), $SO(1,3)$, and are approached by the reduction chain $PG\supset SO(1,3)$. For finite dimensional representations, the Casimir invariants of $SO(1,3)$ are frequently expressed in terms of two $SU(2)$ Casimirs, in turn denoted by $\mathbf{S}_L^2$, and $\mathbf{S}_R^2$, of $SU(2)_L\otimes SU(2)_R$, a group that is locally isomorphic to $SL(2,C)$, the universal covering of HLG. The two additional quantum labels gained in this manner are the well known left- and right-handed "angular momenta," s_L, and s_R, respectively. Therefore, a covariant state labeling can be introduced as $|p^2,s(s+1);s_L,s_R\rangle$, with $s=|s_L-s_R|,\ldots,s_L+s_R$. In so doing one encounters essentially two types of finite dimensional HLG representations.

(1) The first ones contain just one W^2 invariant subspace, and correspond to the case when one of the s_L, s_R labels vanishes [i.e., either $(s_L,0)$, or $(0,s_R)$], and $s_R=s_L$. In such a case, $s_{L/R}(s_{L/R}+1)=s(s+1)$, equals the $[-(1/m^2)W^2]$ eigenvalue in the space under consideration [see Eq. (20)] and W^2– and $\mathbf{S}_{L/R}^2$ invariant spaces coincide. Irreps of the above type are suggestive of replacing W^2– by $SU(2)$ spin labels.

As long as the basic fields in physics are precisely of the above type [the Dirac field is $(1/2,0)\oplus(0,1/2)$, the electromagnetic field strength tensor is $(1,0)\oplus(0,1)$, and scalars are just $(0,0)$] identifying Poincaré labels with $SU(2)$ spins works out without any harm.

(2) The second ones are HLG irreps containing several W^2 invariant subspaces. In this case, both s_L and s_R are nonvanishing, and the irreps are of the type (s_L,s_R) with $s_L\neq 0$, and $s_R\neq 0$. Examples are the vector- and tensor-gauge fields, $(1/2,1/2)$ and $(1,1)$, respectively. In the rest frame, $W^2=-(1/m^2)\ \mathbf{S}^2$ hence W^2 and $\mathbf{S}^2$ invariant subspaces coincide. However, beyond the rest frame, in flight, W^2 and $\mathbf{S}^2$ invariant subspaces are no longer identical, a situation caused by the property of the boost to mix up SU(2) spins differing by one unit.

Often, Lorentz representations that contain as building blocks irreps of the second type, appear attractive for the description of higher spins, the classical examples being the totally symmetric K rank Lorentz tensors with Dirac spinor components, generically denoted by $\psi_{\mu_1\cdots\mu_K}$. They are exploited for the description of fields that have been labeled in the rest frame by the highest spin $J=K+1/2$. The separation between Lorentz and spinor indices inherent to such

tensors makes them especially appealing for the construction of covariant fermion–boson vertices. However, one has to face the problem of how to pick up the favored degrees of freedom and exclude interference with the unwanted ones. It seems inevitable to return back to the Poincaré invariants, if one wishes to distinguish all the degrees of freedom contained in $\psi_{\mu_1\cdots\mu_K}$ in a covariant and transitionally invariant fashion. Yet, for one reason or the other, this is not the path tenaciously pursued by the theory. Rather, one still prefers to stay within the elaborated scheme of substituting W^2 by $SU(2)$ labels, but, yes, modify the latter scheme to account for the new situation in introducing constraints, considered as appropriate.

To be specific, in order to select out of ψ_μ **(**a field belonging to $[(1/2,0)\oplus(0,1/2)]\otimes(1/2,1/2)$**)** the W^2 invariant subspace that relates to spin $3/2$ at rest, one requires

$$(i\partial^\mu\gamma_\mu - m)\psi_\nu = 0,$$

$$\partial^\mu\psi_\mu = 0,$$

$$\gamma^\mu\psi_\mu = 0. \tag{1}$$

Exploiting constraints (some times termed to as auxiliary, or, supplementary, conditions) in place of W^2 quantum numbers brings the advantage of remaining within the framework of equations linear in the momenta, and to work with four-dimensional Dirac spinors. However, these advantages reveal themselves as deceptive at the moment one has to face grave worries about the compatibility of constraints and dynamics. Recall that the constraints change upon gauging and one has to make sure that the modification is preserved in time by the equation of motion and the latter does not violate causality. Notice that covariance alone is indeed a necessary but not a sufficient condition for special relativity. For example, space-like intervals are doubtlessly covariant objects, but they are unacceptable for the description of *free* physical fields as they prescribe the particle to violate causality during propagation. Precisely a flaw of that very type was revealed by Velo and Zwanziger in Ref. 2 regarding the $\gamma^\mu\psi_\mu=0$ constraint onto the four-vector spinor. Velo and Zwanziger showed that the above constraint triggers acausal propagation of Rarita–Schwinger particles crossing an electromagnetic field.

In the present article we shall avoid the previous inconsistencies in developing a different view on the form and content of wave equations for higher spins. Namely, we take the position that the equation of motion for whatever free particle has to be (i) a function of P^2 and W^2, the Casimir invariants of the Poincaré group, (ii) operates immediate, i.e., without any supplementary constraints, on the HLG representation chosen to embed the field as one of its covariant sectors.[16]

Within this context, there are two primordial equations of motion to be satisfied by any field. One of them searches for P^2 invariant subspaces. It is nothing more but the Klein–Gordon equation. The other one secures in addition invariance under pseudo-rotations and pins-down W^2 invariant subspaces by means of appropriately constructed covariant projectors. It is that very latter type of equations on which we focus attention here. For the sake of self-sufficiency of the presentation, the subsequent section opens with a brief review of the basics of space–time symmetries.

III. COVARIANT WAVE EQUATIONS FOR HIGHER SPINS FROM W^2 INVARIANT SUBSPACES

A. Basics of space–time transformations

A general Poincaré transformation in space–time can be written in the factorized form

$$g(b,\Lambda) = T(b)\Lambda, \tag{2}$$

where $T(b)=g(b,E)$ (E denotes the unit matrix) is a translation and $\Lambda=g(0,\Lambda)$ is a proper Lorentz transformation. In the standard convention, the generators of the translation group in $1+3$ time–space dimensions, $\mathcal{T}_{1,3}$, are P_μ in $T(b)$, which are commuting,

$$[P_\mu, P_\nu] = 0. \tag{3}$$

The HLG transformation in coordinate space,

$$x'_\mu = \Lambda_\mu{}^\nu \quad x_\nu, \quad \Lambda_{\mu\nu} = \exp\left[-\frac{i}{2}\theta^{\mu\nu} L_{\mu\nu} \right], \quad L_{\mu\nu} = X_\mu P_\nu - X_\nu P_\mu, \tag{4}$$

induces the following transformation for a field $\psi(x)$,

$$\psi'(x) = \exp\left[-\frac{i}{2}\theta^{\mu\nu} M_{\mu\nu} \right] \psi(\Lambda^{-1} x). \tag{5}$$

Here, $\theta^{\mu\nu}$are continuous parameters, while the $n \times n$ matrices $M_{\mu\nu}$ represent a totally antisymmetric 2nd rank Lorentz tensor. They are the generators of the homogeneous Lorentz group in the representation space of interest, and satisfy the commutation relations of the associated algebra:

$$[M_{\mu\nu}, M_{\alpha\beta}] = -i(g_{\mu\alpha} M_{\nu\beta} - g_{\mu\beta} M_{\nu\alpha} + g_{\nu\beta} M_{\mu\alpha} - g_{\nu\alpha} M_{\mu\beta}). \tag{6}$$

Their commutators with the generators of the translation group read as

$$[P_\mu, M_{\alpha\beta}] = i(g_{\mu\alpha} P_\beta - g_{\mu\beta} P_\alpha), \tag{7}$$

where $g_{\mu\nu}$=diag$(1,-1,-1,-1)$ is the metric tensor. The $M_{\mu\nu}$ generators consist of

$$M_{\mu\nu} = L_{\mu\nu} + S_{\mu\nu}, \quad [L_{\mu\nu}, S_{\mu\nu}] = 0, \tag{8}$$

where $L_{\mu\nu}$ and $S_{\mu\nu}$ in turn generate rotations in external coordinate- and internal representation spaces. The generators of boosts $(\mathcal{K}_x, \mathcal{K}_y, \mathcal{K}_z)$ and rotations (J_x, J_y, J_z) are related to $M_{\mu\nu}$ via

$$\mathcal{K}_i = M_{0i}, \quad J_i = \frac{1}{2}\epsilon_{ijk} M_{jk}, \tag{9}$$

respectively.

B. Pauli Lubanski vector and associated Casimir invariant

The Pauli–Lubanski (PL) vector is now defined as

$$W_\mu = \frac{1}{2}\epsilon_{\mu\nu\alpha\beta} M^{\nu\alpha} P^\beta, \tag{10}$$

where $\epsilon_{0123}=1$. This operator can be shown to satisfy the commutators

$$[W_\alpha, M_{\mu\nu}] = i(g_{\alpha\mu} W_\nu - g_{\alpha\nu} W_\mu), \quad [W_\alpha, P_\mu] = 0, \tag{11}$$

i.e., it transforms as a four-vector under Lorentz transformations. The remarkable point is that the external coordinate part of $M_{\mu\nu}$, namely the "orbital" momentum $L_{\mu\nu}$, does not contribute to W_μ due to the anti-symmetric Levi-Civita tensor. As a result, W_μ restricts to

$$W_\mu = \frac{1}{2}\epsilon_{\mu\nu\rho\tau} S^{\nu\rho} P^\tau, \tag{12}$$

and its square (in covariant form) is calculated to be

$$W^2 = -\frac{1}{2} S_{\mu\nu} S^{\mu\nu} P^2 + G^2, \quad G_\mu := S_{\mu\nu} P^\nu. \tag{13}$$

The operators $S_{\mu\nu}$ act exclusively in the internal spin space and commute like

$$[S_{\mu\nu},S_{\alpha\beta}] = -i(g_{\mu\alpha}S_{\nu\beta} - g_{\mu\beta}S_{\nu\alpha} + g_{\nu\beta}S_{\mu\alpha} - g_{\nu\alpha}S_{\mu\beta}). \tag{14}$$

As long as Eq. (14) has same form as Eq. (6), one may view $S_{\mu\nu}$ as generators of Lorentz transformations in the intrinsic space. However, in contrast to Eq. (7), $S_{\mu\nu}$ *commute* with the operators of translations,

$$[P_\alpha,S_{\mu\nu}] = 0. \tag{15}$$

In effect, one does not find precisely Poincaré transformations in the internal space but rather a contracted form of them. Hereafter we will refer to the group generated by $S_{\mu\nu}$ as the "Internal Homogeneous Lorentz Group" ($\mathcal{I}$HLG) to distinguish it from the HLG spanned by $M_{\mu\nu}$. In summary, one can write down generators of boosts and rotations in the internal space as

$$K_i = S_{0i}, \quad S_i = \frac{1}{2}\epsilon_{ijk}S_{jk}. \tag{16}$$

The internal HLG has by itself two Casimir invariants, in turn given by $C_1 = 1/4 S_{\mu\nu}S^{\mu\nu}$, and $C_2 = S_{\mu\nu}\tilde{S}^{\mu\nu}$, with $\tilde{S}_{\mu\nu} = \epsilon_{\mu\nu\rho\tau}S^{\rho\tau}$. In terms of **K**, and **S** one finds

$$C_1 = \frac{1}{2}(\mathbf{S}^2 - \mathbf{K}^2), \quad C_2 = i\mathbf{S}\cdot\mathbf{K}. \tag{17}$$

The latter equation allows us to cast W^2 into the form

$$W^2 = -2C_1P^2 + G^2. \tag{18}$$

For irreps of the type $(s,0)\oplus(0,s)$ where $K_i = \mp iS_i$, one finds the insightful relation[11]

$$G^2 = -W^2. \tag{19}$$

The insertion of Eq. (19) into Eq. (18) amounts to

$$W^2 = -\mathbf{S}^2P^2. \tag{20}$$

The latter relation explains the privileged position of $(s,0)\oplus(0,s)$ states to carry a unique SU(2) spin both at rest [where W^2 any way reduces to $-\mathbf{S}^2\,m^2$ in accord with Eq. (20)] and in flight. However, for all the other types of Lorentz representations, $W^2 \neq G^2$ and the $[-(1/m^2)W^2]$ labels for particles in flight do not have the interpretation of ordinary $SU(2)$ spin. In the following we label W^2 invariant subspaces by s but in general without any reference to SU(2) spin.

C. Covariant projectors onto W^2 invariant subspaces

To begin with, we recall that the interpretation of elementary systems as Poincaré group irreducible representations requires any field to transform invariantly under the action of both P^2 and W^2. In the following we work with massive fields. The former invariance leads to the Klein–Gordon equation for any arbitrary field,

$$(P^2 - m^2)\psi(\mathbf{p}) = 0. \tag{21}$$

Invariance under the action of W^2 results in the new condition

$$\Pi^s(\mathbf{p})\psi(\mathbf{p}) = \psi(\mathbf{p}), \tag{22}$$

where $\Pi^s(\mathbf{p})$ stands for an appropriately constructed covariant projector onto the $(-p^2s(s+1))$ invariant subspace of W^2 in $\psi(\mathbf{p})$. To be specific, for the case of the four-vector spinor, such projectors have been presented in Ref. 10. In general, equations of the type (22) are equivalent to

$$[W^2 + P^2 s(s+1)]\psi(\mathbf{p}) = 0. \tag{23}$$

Next, it is necessary to account for the mass shell condition in Eq. (21). For this purpose, we sum up Eqs. (23) and (21), weighted by $1/s$ and $(-s)$, respectively, to obtain

$$\left[\frac{1}{s}W^2 + sP^2 + m^2\right]\psi(\mathbf{p}) = 0, \tag{24}$$

and cast the latter equation into the explicitly covariant form

$$[t_{\mu\nu}P^\mu P^\nu - m^2]\psi(\mathbf{p}) = 0. \tag{25}$$

Here $t_{\mu\nu}$ stands for

$$t_{\mu\nu} = \frac{1}{s}(2C_1 g_{\mu\nu} - S_{\alpha\nu}S^\alpha{}_\mu) - s\, g_{\mu\nu};$$

C_1 denotes the first Casimir in Eq. (17) and $S^{\beta\rho}$ are the $\mathcal{I}$HLG generators in the particular representation chosen for $\psi(\mathbf{p})$. Their construction as solutions of the algebra of the Lorentz group for the representation space under consideration is straightforward.[7,9,10]

Using now the gauge principle for electromagnetism in this equation, we obtain

$$\left[\left(\frac{1}{s}(2C_1 g_{\mu\nu} - S_{\alpha\nu}S^\alpha{}_\mu) - s\, g_{\mu\nu}\right)\pi^\mu\ \pi^\nu - m^2\right]\psi(\mathbf{p}) = 0, \tag{26}$$

with $\pi^\mu = P^\mu + eA^\mu$, and e denoting the charge of the field $\psi(\mathbf{p})$. Notice that Eq. (26) is a covariant matrix equation that operates in the vector space of the dimensionality of $\psi(\mathbf{p})$. For example, when $\psi(\mathbf{p})$ stands for the four-vector-spinor, W^2 is represented by a 16×16 matrix. For the sake of illustration, here we bring the Lagrangian density for the lowest Rarita–Schwinger representation. It reads as

$$\mathcal{L}(x) = \overline{\psi}(x)t_{\mu\nu}\ \pi^\mu\ \pi^\nu\ \psi(x) - m^2\overline{\psi}(x)\psi(x), \tag{27}$$

where $\overline{\psi}(x) = \psi^\dagger(x)(\gamma^0 \otimes g)$ where g is the matrix of the metric tensor. The definition of $\overline{\psi}(x)$ has to be performed for each representation individually. When applied to the Dirac representation $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$, Eq. (26) also has the great advantage to yield the correct value of the gyromagnetic factor, $g_s = 2$. This is not fortuitous but reflects the general property of our master equation (26) to predict the correct value for the gyromagnetic ratio as $g_s = 1/s$ for fields in $(s,0)\oplus(0,s)$. Had we used instead Eq. (23) alone, we would have found the problematic case of $g_s = 1/s(s+1)$.

With respect to $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$, Eq. (24) is nothing more than the Klein–Gordon equation for each field component. This is due to the fact that the squared Pauli–Lubanski vector for all $(s,0)\oplus(0,s)$ fields is just $-s(s+1)P^2\mathbf{1}_{(2s+1)\times(2s+1)}$. The W^2 Casimir invariant identifies only the spin content and remains indifferent to the discrete C, P, or, T properties of the representation of interest. Recall that one has different options to stick together, say, $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$ depending on whether one wants $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$ to diagonalize the parity, $\gamma^0\mathcal{R}$ or, the charge conjugation, $i\gamma_2 K$, operator. For parity eigenstates one ends up with the standard Dirac equation, while for C-parity states one finds again the Dirac equation but with a Majorana mass term, respectively. Notice however that, under gauging, this equation gives the right magnetic properties for $(s,0)\oplus(0,s)$ fields. This means that solutions to Dirac equation are solutions to Eq. (26) although the converse is not necessarily true since our equation specifies just the value of the spin.

For product representation spaces of the type $\psi_{\mu_1\mu_2\ldots\mu_K}$, the most interesting representation space for applications in hadron physics, the situation is different provided, one is tracking the highest spin. As long as the highest spins are nondegenerate, there is no confusion with parity doubling, as would be the case for the lower spins. For these reasons, Eq. (26) has its major merits

with respect to the highest spins in the representations. Next we study wave front propagation of particles described by means of Eq. (26) along the line of Refs. 2 and 3.

IV. AVOIDING SUPERLUMINAL PROPAGATION OF HIGHER SPIN WAVES

Wave propagation is associated with a hyperbolic system of partial differential equations.[14] For such a class of differential equations the initial value problem can be posed on a class of surfaces ("space-like" surfaces with respect to the equation of motion). The equations possess solutions with wave fronts traveling along rays at finite velocities. At any point on the surface, the rays form a cone that is entirely determined by the coefficients of the highest derivatives in the equation of motion.[14] The wave front can be characterized by $n^\mu=(n^0,\mathbf{n})$, the vectors normal to the characteristic surface. The system of equations is hyperbolic if n^0 is real for any $\mathbf{n}$. To find the normal vectors it is sufficient to first replace in the highest derivatives of the equation of motion P_μ by n_μ and then calculate the determinant $D(n)$ (so called "characteristic determinant"[3]) of the matrix given by the corresponding coefficients.

A. Wave front propagation of the Klein–Gordon, Dirac, and Rarita–Schwinger equations

In cases when the coupling to external fields is carried by the lower derivatives in the equation of motion, such as, say, the Klein–Gordon equation, the ray cones for interacting and free fields coincide. Indeed, in the latter case and under minimal coupling one finds

$$[\pi^\mu\pi_\mu - m^2]\psi(\mathbf{p}) = [P^\mu P_\mu + e(P^\mu A_\mu + A^\mu P_\mu) + e^2 A^\mu A_\mu - m^2]\psi(\mathbf{p}) = 0. \tag{28}$$

The vanishing of the characteristic determinant in this case yields

$$D(n) = \mathrm{Det}(n^2) = n^2 = 0, \tag{29}$$

which has real n^0 for any $\mathbf{n}$. The same is true for Dirac particles, though not as obvious. As is well known, a Dirac particle coupled minimally to the electromagnetic field is described by

$$[\gamma^\mu(P_\mu + eA_\mu) - m]\psi(\mathbf{p}) = 0. \tag{30}$$

Now, the resulting characteristic determinant is found to be the square of Eq. (29),

$$D(n) = \mathrm{Det}(\gamma^\mu n_\mu) = (n^2)^2. \tag{31}$$

The vanishing of this determinant results once again into a ray cone that coincides with the light cone.

The wave front propagation of the solution of the Rarita–Schwinger set of equations was studied in great detail in Ref. 2. To understand the essence of the latter work recall that Eqs. (1) or the analogous equation in the interacting case can be derived from a Lagrangian, a method suggested by Fierz and Pauli.[15] Within the latter framework not all the Euler–Lagrange equations appear as genuine equations of motion, meaning that some of them may not involve time derivatives, a property that qualifies them only as constraints onto the fields. Precisely this is the case for the Rarita–Schwinger framework discussed in Sec. II. As a consequence, any surface in space–time is a characteristic surface.[14] The Rarita–Schwinger system of coupled equations turns to be equivalent to a system of hyperbolic equations supplemented by constraints that are conserved in time. In this case, the wave fronts of the constrained system are no longer given by the characteristic determinant of the Euler-Lagrange equations. Rather, it is necessary to find the genuine equation of motion, i.e., the one which (i) contains all the higher order derivatives needed for the complete characterization of the system, and (ii) preserves the constraints in time. Finding such an equation in general introduces, in addition to the derivatives already present in the system of coupled equations, also new ones which as a rule spoil causal propagation, a result due to Refs. 2 and 3.

B. Wave front propagation of W^2 invariant subspaces

In the present work we suggested an alternative formalism to the Rarita–Schwinger framework. Our proposal was to pin down the degrees of freedom of interest by means of Eq. (26). This equation was build upon the covariant projector onto the W^2 invariant vector spaces in the representation under consideration, and did not invoke any supplementary conditions. In this concern, it is worth remarking that the formalism does not deal with the whole representation space but only with one of its W^2 invariant subspaces. Below we prove that equations of the latter type do not suffer the Velo–Zwanziger problem upon gauging.

First, we have to check that for all the degrees of freedom of $\psi(\mathbf{p})$, the second order time-derivatives enter Eq. (26) with nonvanishing coefficients. This can be done in full generality in momentum space where

$$t_{00} = \frac{1}{s}(2C_1 g_{00} - S_{\alpha 0} S^{\alpha}{}_{0}) - s g_{00} = \mathbf{1}. \tag{32}$$

Therefore, for all W^2 invariant subspaces, the time derivative of each field component in Eq. (26) does not vanish. This equation will be hyperbolic if the solutions n^0 to $D(n)=0$ are real for any $\mathbf{n}$. In this case we must solve

$$\mathrm{Det}\left[-\frac{1}{s} W^2(n) - s\, n^2 \right] = 0. \tag{33}$$

In order to demonstrate that (26) is a hyperbolic equation in the HLG representation space chosen for $\psi(\mathbf{p})$ here we exploit decomposition of the latter into invariant subspaces of W^2.

The most transparent representation of W^2 is obtained in the basis of $\mathbf{p}$-dependent W^2 eigenstates where W^2 is block diagonal and equal to

$$W^2(P) = -P^2\ \mathrm{Diag}[s_1(s_1+1)\mathbf{1}_{s_1}, s_2(s_2+1)\mathbf{1}_{s_2}, \ldots, s_N(s_N+1)\mathbf{1}_{s_N}]. \tag{34}$$

Here $\{s_1, s_2, \ldots, s_N\}$ label the different eigensubspaces of W^2 (one of them being s) in the representation of interest, while $\mathbf{1}_{s_j}$ denotes the unit matrix of dimensionality $(2s_j+1)\times(2s_j+1)$. Notice that the dimensionality, (d), of the representation space $\psi(\mathbf{p})$ relates to the W^2 quantum numbers via $d=\Sigma_i\, m_i(2s_i+1)$, where m_i is the multiplicity of s_i. The latter accounts for possible degeneracies of the W^2 invariant subspaces in $\psi(\mathbf{p})$ with respect to further symmetries such as, one of the discrete space–time symmetries.

The determinant (33) is calculated as

$$\mathrm{Det}\left[-\frac{1}{s} W^2(n) - s\, n^2 \right] = \prod_{k=0}^{N} \left(n^2 \left(\frac{s_k(s_k+1)}{s} - s \right) \right)^{2s_k+1}. \tag{35}$$

As long as for the integer/half-integer s under consideration, there are no positive integers and half-integers s_k satisfying

$$\frac{s_k(s_k+1)}{s} - s = 0, \tag{36}$$

the roots of the characteristic determinant are $n^2=0$. Thus the solutions have n^0 real for any $\mathbf{n}$, and Eq. (26) is a set of hyperbolic equations for the $\psi(\mathbf{p})$ components. The characteristic surfaces are the same for free and interacting particles, and the ray cone coincides with the light cone. In other words, the wave front propagation of W^2 invariant subspaces is free from the Velo–Zwanziger problem.

V. CONCLUSIONS AND PERSPECTIVES

In the present article we advocate the idea to consider higher spins as invariant subspaces of the Casimir operators of the Poincaré group, the squared four-momentum and the squared Pauli–Lubanski vector, in a properly chosen representation of the HLG, $\psi(\mathbf{p})$. In executing the idea we demonstrated that any higher spin is described in terms of one covariant matrix equation that (i) is determined exclusively by the HLG generators in $\psi(\mathbf{p})$, (ii) is of the dimensionality of $\psi(\mathbf{p})$, and (iii) is always of second order in the momenta. We gauged this equation minimally and found the resulting particle propagation to be causal, thus avoiding the classical Velo–Zwanziger problem. Moreover, for the single spin valued $(s,0)\oplus(0,s)$ representations, our master equation (26) has the great advantage to predict the correct value for the gyromagnetic ratio, $g_s=1/s$, thus proving Belinfante's conjecture[13] from 1953.

The development of a calculation scheme for interacting particles of higher spins from the perspective of the present work is underway.

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Finite size effects in thermal field theory

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We consider a neutral self-interacting massive scalar field defined in a d-dimensional Euclidean space. Assuming thermal equilibrium, we discuss the one-loop perturbative renormalization of this theory in the presence of rigid boundary surfaces (two parallel hyperplanes), which break translational symmetry. In order to identify the singular parts of the one-loop two-point and four-point Schwinger functions, we use a combination of dimensional and zeta-function analytic regularization procedures. The infinities which occur in both the regularized one-loop two-point and four-point Schwinger functions fall into two distinct classes: local divergences that could be renormalized with the introduction of the usual bulk counterterms, and surface divergences that demand counterterms concentrated on the boundaries. We present the detailed form of the surface divergences and discuss different strategies that one can assume to solve the problem of the surface divergences. We also briefly mention how to overcome the difficulties generated by infrared divergences in the case of Neumann–Neumann boundary conditions. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1808485]

I. INTRODUCTION

The Casimir effect is the manifestation of the zero-point energy of the quantized electromagnetic field, in the presence of metallic plates.[1] A very simple calculation predicts that in a four-dimensional space–time, uncharged perfectly conducting parallel plates should attract each other with a force per unit area $F(L) \propto 1/L^4$, where L is the distance between the plates. Extensive reviews of this subject can be found in Refs. 2–6. As stressed by Milloni *et al.*,[7] a brief argument showing that the zero-point energy associated with the quantized electromagnetic field must have a physical meaning was already given by Einstein and Stern.[8] These authors noted that a zero-point energy seems necessary in order to avoid a first-order quantum correction to β^{-1} in the classical limit $\beta \gg \omega$ in Planck's expression for the average energy of an oscillator in equilibrium with radiation at temperature β^{-1}.

Although the vacuum energies of different physical configurations are formally divergent, their diference can be finite. In the case of a free scalar field, interacting only with boundary surfaces, the Casimir approach can be summarized as follows: first a complete set of modes solutions of the Klein–Gordon equation satisfying appropriate boundary conditions, and their respective eigenfrequencies are presented. Next, the divergent zero-point energy is regularized by the introduction of an ultraviolet cutoff. Finally, the polar part of the regularized energy is removed using a renormalization procedure. This procedure was first discussed by Fierz[9] a long time ago, followed by Boyer[10] and also by Svaiter and Svaiter[11,12] In these two last references, an attempt to clarify the relation between the cutoff method and analytic regularization procedures in Casimir effect has been developed. In particular, in these papers an analytic regularization procedure was interpreted as a cutoff method, and using a mixed cutoff in the regularized zero-point energy, it was possible to unify these two methods both in two- and three-dimensional space–

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times. Further, a general proof was given that when the introduction of an exponential cutoff yields an analytic function with a pole at the origin, then the analytic regularization using the zeta function (or a generalization for the zeta function) is equivalent to the application of a cutoff with the subtraction of the singular part at the origin.[13,14] More recently, Fulling offered an interesting discussion with regard to the problems in the renormalization program devised to find the renormalized vacuum stress tensor in different field theories.[15]

It is important to point out that these results are valid at one-loop level and one is dealing with free fields only. It is clear that the formalism must be generalized to take into account the case of self-interacting fields. Although higher-loop corrections to the Casimir effect seem beyond experimental reach today, theoretically such corrections are certainly of interest. Nevertheless, with the exception for some few papers, only global issues have been discussed in the study of radiative corrections to the Casimir effect. One such exception is the discussion presented by Robaschik *et al.*[16] With this scenario in mind, it is natural to ask the important question: how to implement the perturbative renormalization algorithm, assuming the presence of rigid boundaries (hard walls), using the standard weak-coupling perturbative expansion in quantum field theory, that is, how to implement the one-loop perturbative renormalization of a self-interacting scalar theory, assuming boundary conditions which do break translational symmetry. Our aim when studying these issues is linked to the following question: does the infrared problem have a solution in theories where translational invariance is broken? Note that temperature effects can solve the infrared problem in some models in quantum field theory;[17] for a recent treatment in non-abelian gauge theories at high temperature, and the infrared problem, see for example, Ref. 18. Also, in massless scalar $\lambda\varphi^4$ theory, if thermal equilibrium with a reservoir is assumed, the infrared problem can be solved after a ressumation procedure. The standard is to use the Dyson–Schwinger equation to write a nonperturbative version of the self-energy gap equation, or to use the composite operator formalism.[19–21]

We would like to call the attention of the reader that there are some disagreements in the literature as to implementing the one-loop perturbative renormalization in finite size systems when translational invariance is broken. In the one-loop approximation, Albuquerque *et al.*[22] found that the mass counterterm depends on the size of the compact dimension in the $\lambda\varphi^4$ theory. Also, Malbouisson *et al.*[23] assumed a self-interacting scalar field confined between two infinite parallel plates, and using the techniques developed by Ananos *et al.*[21] these authors did not find any surface counterterm in the $\lambda\varphi^4$ theory at finite temperature. Furthermore, they were able to define temperature and size-dependent mass and coupling constant terms in systems where translational invariance is broken.

The purpose of this paper is to present a detailed calculation of the one-loop renormalization of the $\lambda\varphi^4$ theory at finite temperature, assuming that one of the spatial coordinates is confined to a finite interval. Since this assumption is not sufficient to explicitly breaking the translational symmetry, we will further introduce boundary surfaces where the field satisfies appropriate boundary conditions. In this situation, the breaking of the translational invariance of the theory is ensured. This paper is a natural continuation of the papers of Fosco and Svaiter[24] and also Caicedo and Svaiter.[25] Our aim is to further the understanding of the renormalization procedure in systems at finite temperature where there is a break of translational symmetry. We will discuss the Dirichlet–Dirichlet (DD) and also the Neumann–Neumann (NN) boundary conditions. For the Dirichlet–Dirichlet boundary conditions, the model is free of infrared divergences. In the Neumann–Neumann boundary conditions case, infrared divergences associated with zero modes will appear for bare massless fields. We show that there is no clear meaning for a thermal- or size-dependent mass in such situations. Consequently, a resummation procedure cannot be used to solve the infrared problem in the case of Neumann–Neumann boundary conditions.

The organization of the paper is the following: in Sec. II we sketch the general formalism of the theory, deriving the one-loop two-point and four-point functions. In Sec. III we use two different analytic regularization procedures, i.e., dimensional regularization and zeta-function analytic regularization, to identify the polar contributions that appear in the expressions of the one-loop two-point and four-point Schwinger functions. In Sec. IV we renormalize the four-point

Schwinger function and the problem for the infrared divergences is raised. In the conclusions we will discuss alternative solutions for the problem of the surfaces counterterms. In this paper we use $\hbar = c = k_B = 1$.

II. GENERAL FORMALISM AND THE FINITE TEMPERATURE GENERATING FUNCTIONAL OF SCHWINGER FUNCTIONS

The static properties of finite temperature field theory can be derived from the partition function.[26] To obtain the partition function the starting point is the Feynman, Matheus, and Salam approach.[27] Thus, let us consider the generating functional of (complete) Green's functions for a self-interacting scalar field theory defined in a flat d-dimensional Euclidean space $Z(h)$, given by

$$Z(h) = \int [\mathrm{d}\varphi] \exp\left(- S[\varphi] + \int \mathrm{d}^d x \; h(x)\varphi(x) \right), \tag{1}$$

where $[\mathrm{d}\varphi]$ is a translational invariant measure [formally given by $[\mathrm{d}\varphi] = \Pi_{x \in R^d} \mathrm{d}\varphi(x)$] and $S[\varphi]$ is the classical action associated with the scalar field. The quantity $Z(h)$ can be regarded as the functional integral representation for the imaginary time evolution operator $\langle \varphi_2 | U(t_2, t_1) | \varphi_1 \rangle$, with boundary conditions $\varphi(t_1, \vec{x}) = \varphi_1(\vec{x})$ and $\varphi(t_2, \vec{x}) = \varphi_2(\vec{x})$ which gives the transition amplitude from the initial state $|\varphi_1\rangle$ to a final state $|\varphi_2\rangle$ in the presence of some scalar source of compact support. As usual, the generating functional of the connected correlation functions shall be given by $W(h) = \ln Z(h)$. In a free scalar theory, $Z(h)$ as well as $W(h)$ can be calculated exactly. Regarding the Lagrangian density, we assume that

$$\mathcal{L}(\varphi, \partial\varphi) = \frac{1}{2}(\partial\varphi)^2 + \frac{1}{2} m_0^2 \varphi^2 + \frac{1}{4!} \lambda_0 \varphi^4, \tag{2}$$

where m_0 is the bare mass and λ_0 is the bare coupling constant of the model. We are also assuming $m_0^2 \geqslant 0$ and also $\lambda_0 > 0$. The Euclidean n-point correlation functions, i.e., the n-point Schwinger functions are given by the expectation value with respect to the weight $\exp(-S(\varphi))$, defined as

$$G^{(n)}(x_1, x_2, \ldots, x_n) = \frac{1}{Z(h)} \left. \frac{\delta^n Z(h)}{\delta h(x_1) \cdots \delta h(x_n)} \right|_{h=0}. \tag{3}$$

The n-point connected correlation functions $G_c^{(n)}(x_1, x_2, \ldots, x_n)$ are given by

$$G_c^{(n)}(x_1, x_2, \ldots, x_n) = \frac{1}{Z(h)} \left. \frac{\delta^n W(h)}{\delta h(x_1) \cdots \delta h(x_n)} \right|_{h=0}. \tag{4}$$

Finally, the generating functional of connected one-particle irreducible correlation functions (the effective action) is introduced by performing a Legendre transformation on $W(h)$,

$$\Gamma(\varphi_0) = - W(h) + \int \mathrm{d}^d x \; \varphi_0(x) h(x). \tag{5}$$

Let us define the proper vertices $\Gamma^{(n)}(x_1, \ldots, x_n)$ as

$$\Gamma^{(n)}(x_1, \ldots, x_n) = \left. \frac{\delta^n \Gamma(\varphi_0)}{\delta\varphi_0(x_1) \cdots \delta\varphi_0(x_n)} \right|_{\varphi_0 = 0}, \tag{6}$$

where the normalized vacuum expectation value of the field $\varphi_0(x)$ is given by

$$\varphi_0(x) = \frac{\delta W}{\delta h(x)}. \tag{7}$$

It is clear that in the case of a single scalar field, for a zero normalized vacuum expectation value of the field $\varphi_0(x)$, the effective action may be represented as a functional power series around the value $\varphi_0 = 0$, with the form

$$\Gamma(\varphi_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \mathrm{d}^d x_1 \cdots \mathrm{d}^d x_n \, \Gamma^{(n)}(x_1, \ldots, x_n) \varphi_0(x_1) \cdots \varphi_0(x_n). \tag{8}$$

If the bare coupling constant vanishes, i.e., $\lambda_0 = 0$, the generating functional of all n-point Schwinger functions $Z(h)$ can be calculated exactly, since we have to evaluate only Gaussian integrals. After some manipulations we obtain that the Gaussian generating functional $Z_0(h)$ is given by

$$Z_0(h) = \exp\left(\frac{1}{2} \int \mathrm{d}^d x \int \mathrm{d}^d y \; h(x) G_0^{(2)}(x - y, m_0) h(y) \right), \tag{9}$$

where the two-point Schwinger function (the inverse kernel) satisfies

$$(-\Delta_x + m_0^2) G_0^{(2)}(x - y, m_0) = \delta^d(x - y). \tag{10}$$

In this situation, the free Euclidean field is a Gaussian random variable defined by its two-point correlation function

$$G_0^{(2)}(x - y, m_0) = \langle x | (-\Delta + m_0^2)^{-1} | y \rangle, \tag{11}$$

and the two-point Schwinger function has a well-known Fourier representation given by

$$G_0^{(2)}(x - y, m_0) = \frac{1}{(2\pi)^d} \int \mathrm{d}^d p \frac{e^{ip(x-y)}}{(p^2 + m_0^2)}. \tag{12}$$

In the next section we will show that the two-point function $G_0^{(2)}(x-y, m_0)$ can be expressed in terms of the modified Bessel function of the third kind or Macdonald's function $K_\mu(x)$. At present, we are not interested in evaluating the two-point Schwinger function, but only in the analysis of the behavior of $G_0^{(2)}(x-y, m_0)$ in a given ϵ neighborhood. Let us assume that $m|x-y| \ll 1$; in this case, for $d \geqslant 3$ we can use that $G_0^{(2)}(x-y, m_0^2) \approx G_0^{(2)}(x-y, m_0^2 = 0) = |x-y|^{-(d-2)}$. For $d=2$, the mass parameter cannot be eliminated from the denominator and we have the following short distance behavior: $G_0^{(2)}(x-y, m_0^2) \propto \ln(m|x-y|)$. It is well known that a massless two-dimensional scalar field theory is not consistent, once the model has severe infrared divergences. There are different proposals to circumvent this problem; we only mention some of them. For instance, one may violate the positivity of the state vector space; another attempt is to restrict the test functions of the theory, and finally one can introduce a cutoff in the definition of the positive and negative Wightman functions. It is clear that such cutoff procedure is equivalent to introducing a box to regulate the theory in the infrared. Later, we will discuss other strategies to solve the problem of the infrared divergences in scalar theories at finite temperature.

Coming back to the generating functional of all Schwinger functions, for $\lambda_0 \neq 0$ it is not possible to find a closed exact expression for the partition function, and a perturbative expansion is mandatory. Let us then assume the weak-coupling perturbative expansion of the theory. It is important to point out that the partition function can be defined in arbitrary geometries, and classical boundary conditions must be implemented in the two-point Schwinger function, restricting the space of functions that appear in the functional integrals. If we want to include thermal effects, and assuming thermal equilibrium, from the Feynman, Matheus, and Salam formula we have

$$\langle\varphi_b|e^{-iH(t_f-t_i)}|\varphi_a\rangle=\int_{\varphi(t_i)=\varphi_a}^{\varphi(t_f)=\varphi_b}\exp\left(i\int_{t_i}^{t_f}dt\int d^{d-1}x\ \mathcal{L}(\varphi,\partial\varphi)\right),\tag{13}$$

where we have to assume that $t_f-t_i=-i\beta$ and also set $\varphi_a=\varphi_b$, and the sum over all φ_a must be performed in order to produce the trace. The partition function $\mathrm{Tr}[e^{-\beta H}]$ is given by

$$\mathrm{Tr}[e^{-\beta H}]=\int_{\text{periodic}}[d\varphi]\exp\left(i\int_{ti}^{t_i-i\beta}dt\int d^{d-1}x\ \mathcal{L}(\varphi,\partial\varphi)\right),\tag{14}$$

where the integration over the fields satisfying $\varphi(t_i-i\beta,\vec{x})=\varphi(t,\vec{x})$. Since the time integration must range from some value t_i to $t_i-i\beta$, let $t_i=0$ and set the contour along the negative imaginary axis from 0 to $-i\beta$. Thus, $t=-i\tau$, where $0\leqslant\tau\leqslant\beta$, and we have

$$Z(h)|_{h=0}=\int_{\text{periodic}}[d\varphi]\exp\left(\int_0^{\beta}d\tau\int d^{d-1}x\ \mathcal{L}(\varphi,\partial\varphi)\right).\tag{15}$$

To generate the n-point Schwinger functions we need to couple the field with an external source. We will assume that the system is confined between two parallel hyperplates (which we call the Casimir configuration), localized at $z=0$ and $z=L$, and we are using Cartesian coordinates $x^{\mu}=(\vec{r},z)$, where $\vec{r}$ is a $(d-1)$ dimensional vector perpendicular to the $\vec{z}$ vector. Note that since we assume thermal equilibrium with a reservoir, we have periodicity in the first coordinate and $0\leqslant r_1\leqslant\beta$. See, for example, Ref. 28, or for a complete review of quantum field theory at thermal equilibrium, see for example, Ref. 29. The choice of Dirichlet–Dirichlet boundary conditions means that the scalar field satisfies

$$\varphi(\vec{r},z)|_{z=0}=\varphi(\vec{r},z)|_{z=L},\tag{16}$$

and Neumann–Neumann boundary conditions means that

$$\frac{\partial}{\partial z}\varphi(\vec{r},z)|_{z=0}=\frac{\partial}{\partial z}\varphi(\vec{r},z)|_{z=L}.\tag{17}$$

In the next section we will discuss the perturbative renormalization at the one-loop level of the field theory in the presence of rigid boundaries. The great interest of this matter is when systems contain macroscopic structures, how is it possible to implement the renormalization program? We will examine how the weak-coupling perturbative expansion and the renormalization program can be implemented. In order to identify the singular part of the one-loop two-point Schwinger function, we use a combination of dimensional and zeta-function analytic regularization procedures. We also present the detailed form of the surface divergences. Note that due to our choice (two-parallel hyperplates), the region outside the boundaries is the union of two-simple connected domains. The renormalization of the field theory in such exterior regions must be carried out along the same lines as for the interior region. For simplicity we are considering only the interior region.

III. THE REGULARIZED ONE-LOOP TWO AND FOUR-POINT SCHWINGER FUNCTIONS

The aim of this section is to reshape a well-known result, adding finite temperature effects to the problem. In order to implement the renormalization program in a scalar field theory where we assume Dirichlet–Dirichlet or Neumann–Neumann boundary conditions on rigid surfaces one must introduce surface counterterms. To write the full renormalized action for the theory with rigid boundaries we need two regulators: the first one is the usual ϵ that is introduced in the dimensional regularization procedure and the second one which we call η, represents the distance to a boundary. Accordingly we will show that the full renormalized action must be given by

$$S(\varphi)=\int_0^L \mathrm{d}z\int \mathrm{d}^{d-1}r\left(\frac{A(\epsilon)}{2}(\partial_\mu\varphi)^2+\frac{B(\epsilon)}{2}\varphi^2+\frac{C(\epsilon)}{4!}\varphi^4\right)+\int \mathrm{d}^{d-1}r(c_1(\eta)\varphi^2(\vec{r},0)+c_2(\eta)\varphi^2(\vec{r},L))$$
$$+\int \mathrm{d}^{d-1}r(c_3(\eta)\varphi^4(\vec{r},0)+c_4(\eta)\varphi^4(\vec{r},L)), \tag{18}$$

where $A(\epsilon)$, $B(\epsilon)$, and $C(\epsilon)$ are the usual coefficients for the bulk counterterms and the coefficients $c_i(\eta)$, $i=1,\ldots,4$, which depend on the boundary conditions for the field, are the coefficients for the surface counterterms. As usual, all of these coefficients must be calculated order by order in perturbation theory. Note that we are interested in systems that are invariant under translation along directions parallel to the plates, which implies that the full momentum is not conserved. For such conditions, a more convenient representation for the n-point Schwinger functions to implement the perturbative renormalization is a mixed $(\vec{p},z)$ representation. Careless one-loop perturbation theory leads to ultraviolet counterterms that depend on the distance between the plates or also to the absence of surface counterterms.[22,23]

In a straightforward way, in the Matsubara formalism all the Feynman rules are the same as in the zero temperature case, except that the momentum-space integrals over the zeroth component is replaced by a sum over discrete frequencies. For the case of boson fields we must perform the replacement

$$\int \frac{\mathrm{d}^d p}{(2\pi)^d}f(p)\to\frac{1}{\beta}\sum_n\int\frac{\mathrm{d}^{d-1}p}{(2\pi)^{d-1}}f\left(\frac{2n\pi}{\beta},\vec{p}\right), \tag{19}$$

where we are using the following notation: $(\int \mathrm{d}^{d-1}r=\int_0^\beta \mathrm{d}r_1\int \mathrm{d}^{d-2}r)$.

We begin the study of the interacting theory by building the one-loop correction $(G_1^{(2)}(\lambda_0,x,x'))$ to the bare two-point Schwinger function $G_0^{(2)}(x,x')$, for both the DD and NN boundary conditions. Using the Feynman rules we have that $G_1^{(2)}(\lambda_0,\vec{r}_1,z_1,\vec{r}_2,z_2)$ can be written as

$$G_1^{(2)}(\lambda_0,\vec{r}_1,z_1,\vec{r}_2,z_2)=\frac{\lambda_0}{2}\int \mathrm{d}^{d-1}r\int_0^L \mathrm{d}z\; G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{0},z)G_0^{(2)}(\vec{r}-\vec{r}_2,z,z_2). \tag{20}$$

Even though the functions $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$ and $G_0^{(2)}(\vec{r}_2-\vec{r}_3,z_2,z_3)$ are singular at coincident points $(\vec{r}_1=\vec{r}_2,\ z_1=z_2)$ and $(\vec{r}_2=\vec{r}_3,\ z_2=z_3)$, the singularities are integrable for points outside the plates. It is worth mentioning that the most simple way to take into account the boundary is to implement the boundary conditions through the explicit form of the free two-point Schwinger function $G_0^{(2)}(x-y,m_0)$. A straightforward substitution yields the order λ_0 correction to the bare two-point Schwinger function in the one-loop approximation for the case of Dirichlet–Dirichlet boundary conditions. Using the Feynman rules, $G_2^{(4)}(\lambda_0,x_1,x_2,x_3,x_4)$, i.e., the $O(\lambda_0^2)$ correction to the bare one-loop four-point Schwinger function, is given by

$$G_2^{(4)}(\lambda_0,\vec{r}_1,z_1,\vec{r}_2,z_2,\vec{r}_3,z_3,\vec{r}_4,z_4)=\frac{\lambda_0^2}{2}\int \mathrm{d}^{d-1}r\int \mathrm{d}^{d-1}r'\int_0^L \mathrm{d}z\int_0^L \mathrm{d}z' G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)$$
$$\times(G_0^{(2)}(\vec{r}-\vec{r}',z,z'))^2G_0^{(2)}(\vec{r}'-\vec{r}_3,z',z_3)G_0^{(2)}(\vec{r}'-\vec{r}_4,z',z_4). \tag{21}$$

Note that we supress the m_0 term in each expression. Again, all G_0's are singular at coincident points, but the singularities are integrable for points outside the plates, except for $G_0^{(2)}(\vec{r}-\vec{r}',z,z')$. Having in mind the above discussion, in this section we will study the following expressions:

$$\frac{\lambda_0}{2}\int \mathrm{d}^{d-1}r\int_0^L \mathrm{d}z(G_0^{(2)}(\vec{0},z)) \tag{22}$$

and

$$\frac{\lambda_0^2}{2}\int \mathrm{d}^{d-1}r \int \mathrm{d}^{d-1}r' \int_0^L \mathrm{d}z \int_0^L \mathrm{d}z' (G_0^{(2)}(\vec{r}-\vec{r}',z,z'))^2. \tag{23}$$

Let us first study $\frac{1}{2}G_0^{(2)}(\vec{0},z) \equiv I(z,m_0,L,\beta,d)$, and define the following quantities: $1/b=2/\beta$, $L=a$ and finally the dimensionless coupling constant $g=\mu^{4-d}\lambda_0$. Therefore, the argument in the integral defined in Eq. (22) , $I(z,m_0,a,b,d)$ can be written as

$$I(z,m_0,a,b,d) = \frac{g}{2(2\pi)^{d-2}ab}\sum_{n=-\infty}^{\infty}\sum_{n'=1}^{\infty}\sin^2\left(\frac{n'\pi z}{a}\right)\int \mathrm{d}^{d-2}p \frac{1}{\left(\vec{p}^2+\left(\frac{n'\pi}{a}\right)^2+\left(\frac{n\pi}{b}\right)^2++m_0^2\right)}. \tag{24}$$

There are two points that we would like to stress. First to perform analytic regularizations we must introduce a parameter μ with dimension of mass in order to have dimensionless quantities raised to a complex power. Second, the generalization for the case of Neumann boundary conditions is straightforward, although in this case infrared divergences associated with the $n=0$ mode will appear in the case of massless scalar field. To circumvent this situation, we must have a finite Euclidean volume to regularize the model in the infrared, or trying to implement a resummation to generate a thermal mass. We will return to this point later.

Using trigonometric identities, it is convenient to write the amputated one-loop two-point Schwinger in two parts. The first comprises the contributions that do not depend on the distance to the boundary, and the second the contributions that do depend on this distance. Therefore, the quantity $I(z,m_0,a,b,d)$ can be split in two parts $T_1(m_0,a,b,d)$ and $T_2(z,m_0,a,b,d)$, i.e.,

$$I(z,m_0,a,b,d) = T_1(m_0,a,b,d) + T_2(z,m_0,a,b,d). \tag{25}$$

The first quantity $T_1(m_0,a,b,d)$, independent on the distance to the boundaries can be expressed in the following way:

$$T_1(m_0,a,b,d) = I_0(m_0,a,b,d) + I_1(m_0,a,b,d) + I_2(m_0,a,b,d), \tag{26}$$

where each term is given, respectively, by

$$I_0(m_0,a,b,d) = -\frac{g}{16(2\pi)^{d-2}ab}\int \mathrm{d}^{d-2}p \frac{1}{(\vec{p}^2+m_0^2)}, \tag{27}$$

$$I_1(m_0,a,b,d) = \frac{g}{8(2\pi)^{d-2}ab}\sum_{n=1}^{\infty}\int \mathrm{d}^{d-2}p \frac{1}{\left(\vec{p}^2+m_0^2+\left(\frac{n\pi}{a}\right)^2\right)}, \tag{28}$$

and finally

$$I_2(m_0,a,b,d) = \frac{g}{4(2\pi)^{d-2}ab}\sum_{n,n'=1}^{\infty}\int \mathrm{d}^{d-2}p \frac{1}{\left(\vec{p}^2+\left(\frac{n\pi}{a}\right)^2+\left(\frac{n'\pi}{b}\right)^2+m_0^2\right)}. \tag{29}$$

The contribution that depends on the distance to the boundaries given by $T_2(z,m_0,a,b,d)$, can be split in the following way:

$$T_2(z,m_0,a,b,d) = I_3(z,m_0,b,d) + I_4(z,m_0,a,b,d) + I_5(z,m_0,b,d) + I_6(z,m_0,a,b,d). \tag{30}$$

Each term contributing to $T_2(z,m_0,a,b,d)$ is given, respectively, by

$$I_3(z,m_0,b,d)=\frac{g}{2b}h(d)\int_{m_0}^{\infty}\mathrm{d}v(v^2-m_0^2)^{(d-4)/2}\exp(-2vz), \tag{31}$$

$$I_4(z,m_0,a,b,d)=\frac{g}{2b}h(d)\int_{m_0}^{\infty}\mathrm{d}v(v^2-m_0^2)^{(d-4)/2}(\coth av-1)\cosh 2vz, \tag{32}$$

$$I_5(z,m_0,b,d)=\frac{g}{b}h(d)\sum_{n=1}^{\infty}\int_{m_0}^{\infty}\mathrm{d}v\left(v^2-m_0^2-\left(\frac{n\pi}{b}\right)^2\right)^{(d-4)/2}\exp(-2vz), \tag{33}$$

and finally

$$I_6(z,m_0,a,b,d)=\frac{g}{b}h(d)\sum_{n=1}^{\infty}\int_{\alpha}^{\infty}\mathrm{d}v\left(v^2-m_0^2-\left(\frac{n\pi}{b}\right)^2\right)^{(d-4)/2}(\coth av-1)\cosh 2vz. \tag{34}$$

In the above expression the quantity α is given by

$$\alpha=\left(m_0^2+\left(\frac{n\pi}{b}\right)^2\right)^{1/2}, \tag{35}$$

and $h(d)$, that appears in Eqs. (31)–(34) is an entire function given by

$$h(d)=\frac{1}{4(4\pi)^{(d-2)/2}}\frac{1}{\Gamma\left(\frac{d-2}{2}\right)}. \tag{36}$$

Let us investigate each contribution in detail. Using dimensional regularization we obtain for $I_0(m_0,d)$ the following expression:

$$I_0(m_0,a,b,d)=-\frac{g}{16ab(2\sqrt{\pi})^{d-2}}\Gamma\left(2-\frac{d}{2}\right)(m_0^2)^{(d/2)-2}. \tag{37}$$

An analytic expression for the gamma function $\Gamma(z)$, defined in the whole complex plane, can be found and in the neighborhood of a pole $z=-n$ $(n=0,1,2,\ldots)$ the gamma function has the representation

$$\Gamma(z)=\frac{(-1)^n}{n!}\frac{1}{(z+n)}+\Omega(z+n), \tag{38}$$

with regular part $\Omega(z+n)$. Using that $4-d=\epsilon$ and the duplication formula for the gamma function $\Gamma(z)$ we have

$$I_0\,(m_0,a,b,d)\big|_{d=4}=-\frac{g}{16\pi\,ab}\frac{1}{m_0^{\epsilon}}\left(\frac{1}{\epsilon}+\Omega(\epsilon)\right). \tag{39}$$

Here one may adopt different renormalization schemes. We can choose the minimal subtraction (MS) scheme, in which we eliminate only the pole term $1/\epsilon$ in the dimensionally regularized expression for the Schwinger functions. Another choice is the modified minimal subtraction (MS) scheme, where we eliminate not only the pole term $1/\epsilon$ but also the regular part around the pole. Note that in the minimal subtraction scheme the counterterms acquire the simplest expression, while the renormalized Schwinger functions have more complicated expressions. Let us analyze the second expression, given by $I_1(m_0,a,b,d)$. Using dimensional regularization it is possible to show that

$$I_1(m_0,a,b,d)=\frac{g}{8(2\sqrt{\pi})^{d-2}ab}\Gamma\left(2-\frac{d}{2}\right)\sum_{n=1}^{\infty}\frac{1}{\left(m_0^2+\left(\frac{n\pi}{a}\right)^2\right)^{2-(d/2)}}. \tag{40}$$

We note that to extract a finite result from $I_1(m_0,a,b,d)$ we still have to use the analytic extension of the Epstein–Hurwitz zeta function. A direct calculation gives

$$I_1(m_0,a,b,d)=-\frac{g}{8ab}m_0^{d-4}\frac{\sqrt{\pi}}{(2\sqrt{\pi})^{d-1}}\Gamma\left(2-\frac{d}{2}\right)+\frac{gm_0^{d-3}}{8b}\frac{1}{(2\pi)^{d-1}}$$
$$\times\left(\Gamma\left(\frac{3-d}{2}\right)+4\sum_{n=1}^{\infty}(am_0n)^{(3-d)/2}K_{(3-d)/2}(2m_0na)\right). \tag{41}$$

The first term in the above equation is a polar part and the second one is finite. Assuming the minimal subtraction scheme, $I_1(m_0,a,b,d)$ becomes finite. The next term that we must analyze is $I_2(m_0,a,b,d)$ defined by

$$I_2(m_0,a,b,d)=\frac{g}{4ab}\frac{1}{(2\pi)^{d-2}}\sum_{n,n'=1}^{\infty}\int \mathrm{d}^{d-2}p\frac{1}{\left(\vec{p}^2+\left(\frac{n\pi}{a}\right)^2+\left(\frac{n'\pi}{b}\right)^2+m_0^2\right)}. \tag{42}$$

The contribution given by the above equation is a part of the amputated one-loop two-point Schwinger function that does not depend on the distance to the boundaries, and in the renormalization procedure it will require only a usual bulk counterterm. The form of the counterterm is given by the principal part of the Laurent expansion of Eq. (42) around some d, which must be given by the analytic extension of the Epstein zeta function in the complex d plane. The structure of the divergences of the Epstein zeta function is well known in the literature.[30–33] Since the polar structure of the above equation can be found in the literature, we will focus only on the position-dependent divergent part given by $T_2(z,m_0,a,b,d)$. We are now in position to discuss the behavior of $I_3(z,m_0,b,d)$, $I_4(z,m_0,a,b,d)$, $I_5(z,m_0,b,d)$ and finally $I_6(z,m_0,a,b,d)$.

Let us first analyze $I_3(z,m_0,b,d)$. Using the following integral representation of the modified Bessel functions of third kind, or Macdonald's functions $K_\nu(x)$,[34]

$$\int_u^{\infty}(x^2-u^2)^{\nu-1}e^{-\mu x}\,\mathrm{d}x=\frac{1}{\sqrt{\pi}}\left(\frac{2u}{\mu}\right)^{(\nu-1/2)}\Gamma(\nu)K_{\nu-1/2}(u\mu), \tag{43}$$

which is valid for $u>0$, $\mathrm{Re}(\mu)>0$ and $\mathrm{Re}(\nu)>0$, we see that $I_3(z,m_0,a,b,d)$ can be written in terms of these functions. A simple substitution gives

$$I_3(z,m_0,a,b,d)=\frac{2}{b}\frac{h(d)}{(2\sqrt{\pi})^{d-1}}\left(\frac{m_0}{z}\right)^{(d-3)/2}K_{(d-3/2)}(2m_0z). \tag{44}$$

Using a asymptoptic formula for the Bessel function, $I_3(z,m_0,a,b,d)$ is given by

$$I_3(z,m_0,a,b,d)=\frac{2}{b}\frac{h(d)}{(2\sqrt{\pi})^{d-1}}\frac{\Gamma\left(\frac{d-3}{2}\right)}{z^{d-3}}. \tag{45}$$

We can see that we have a divergent behavior as $z\to 0$, which demands a surface counterterm. Let us show that the other terms also contain surface divergences, and study $I_4(z,m_0,a,b,d)$. To advance in the calculations, we must extend the binomial series for both positive or negative integral exponents, written in the form

$$(1+x)^k = \sum_{n=0}^{\infty} C_n^k x^n. \tag{46}$$

First, it is possible to show that the binomial expansion holds for any real exponent α, $|x|<1$ and $\alpha \epsilon R$, i.e.,

$$(1+x)^\alpha = \sum_{n=0}^{\infty} C_\alpha^n x^n, \tag{47}$$

where C_α^n are the generalization of the binomial coefficients. Since we are using dimensional regularization, it is possible to extend the binomial expansion when both the exponent α as well the variable x assume complex values. For this purpose we use the following theorem.

For any complex exponent α and any complex z in $|z|<1$, the binomial series

$$\sum_{n=0}^{\infty} C_\alpha^n z^n = 1 + C_\alpha^1 z + \cdots + C_\alpha^n z^n + \cdots \tag{48}$$

converges and has for sum the principal value of the power $(1+z)^\alpha$, where the principal value of the power b^a is given by the number uniquely defined by the formula $b^a = \exp(a \ln b)$, where a and b denotes any complex numbers, with $b \neq 0$ as the only condition, and $\ln b$ is given its principal value. Going back to $I_4(z,m_0,a,b,d)$, using the generalization of the binomial theorem, let us define $C^{(1)}(d,k) = \frac{1}{2} h(d)(-1)^k C_{(d-4)/2}^k$ to obtain

$$I_4(z,m_0,a,b,d) = \frac{g}{a^{d-3} b} \sum_{k=0}^{\infty} C^{(1)}(d,k)(m_0 a)^{2k} \int_{m_0 a}^{\infty} u^{d-4-2k} (\coth u - 1) \cosh\left(\frac{2uz}{a}\right). \tag{49}$$

Let us use the following integral representation of the gamma function:

$$\int_0^\infty \mathrm{d}t\, t^{\mu-1} e^{-\nu t} = \frac{1}{\nu^\mu} \Gamma(\mu), \quad \mathrm{Re}(\mu) > 0, \quad \mathrm{Re}(\nu) > 0, \tag{50}$$

and also the following integral representation of the product of the gamma function times the Hurwitz zeta function,

$$\int_0^\infty \mathrm{d}t\, t^{\mu-1} e^{-\alpha t} (\coth t - 1) = 2^{1-\mu} \Gamma(\mu) \zeta\left(\mu, \frac{\alpha}{2} + 1\right), \quad \mathrm{Re}(\alpha) > 0, \quad \mathrm{Re}(\mu) > 1, \tag{51}$$

where $\zeta(s,u)$ is the Hurwitz zeta function defined by[34]

$$\zeta(s,u) = \sum_{n=0}^{\infty} \frac{1}{(n+u)^s}, \quad \mathrm{Re}(s) > 1, \quad u \neq 0, -1, -2, \ldots. \tag{52}$$

It is not difficult to show that $I_4(z,m_0,a,b,d)$ contains surface divergences at $z=0$ and also $z=a$. For more details, see, for example, Ref. 35. The other expression that we must study is $I_5(z,m_0,a,b,d)$. Using an integral representation of the Bessel function of third kind we have

$$I_5(z,m_0,a,b,d) = \frac{1}{b} \frac{1}{(2\sqrt{\pi})^{d-1}} \sum_{n=1}^{\infty} \left(\frac{\alpha}{z}\right)^{(d-3)/2} K_{(d-3)/2}(2\alpha z). \tag{53}$$

Using an asymptotic representation of the Bessel function it is posssible to present also the singular behavior near $z=0$. Let us finally investigate $I_6(z,m_0,a,b,d)$. A simple calculation for the massless case gives

$$I6\,(z,m_0,a,b,d)|_{m=0}=\frac{1}{a^{d-3}b}\sum_{k=0}^{\infty}C^{(2)}(d,k)\left(\frac{a}{b}\right)^{2k}\sum_{n=1}^{\infty}n^{2k}\int_{n\pi a/b}^{\infty}\mathrm{d}u\;u^{d-4-2k}(\coth u-1)\cosh\left(\frac{2uz}{a}\right), \tag{54}$$

where $C^{(2)}(d,k)=h(d)(-1)^kC^k_{(d-4)/2}\pi^{2k}$ is an entire function in the complex d plane. The integral that appears in Eq. (54) cannot be evaluated explicity in terms of well-known functions. Nevertheless it is possible to write Eq. (54) in a convenient way where the structure of the divergences near the plate when $y\to b$ appear. Clearly for details see Ref. 35. In the next section we will investigate the singularities of the four-point Schwinger function.

IV. THE FOUR-POINT SCHWINGER FUNCTION IN THE ONE-LOOP APPROXIMATION

We now turn our attention to the four-point Schwinger function in the one-loop approximation. For simplicity we shall study only the zero temperature case. In this section we are following the discussion developed in Ref. 25. Introducing new variables as $u_{\pm}\equiv z\pm z'$, and also $(\vec{\rho}=\vec{r}-\vec{r}')$, the zero-temperature two-point Schwinger function in the tree-level $G_0^{(2)}(\vec{\rho},z,z')$ can be split into

$$G_0^{(2)}(\vec{\rho},z,z')=G_+^{(2)}(\vec{\rho},u_+)+G_-^{(2)}(\vec{\rho},u_-), \tag{55}$$

where we are defining $A_n(a,m_0,d,\vec{\rho})$ by

$$A_n(a,m_0,d,\vec{\rho})=\frac{1}{(2\pi)^{d-1}}\int\mathrm{d}^{d-1}p\frac{e^{i\vec{p}\cdot\vec{\rho}}}{\left(\vec{p}^2+\left(\frac{n\pi}{a}\right)^2+m_0^2\right)}, \tag{56}$$

and so $G_{\pm}^{(2)}(\vec{\rho},u_{\pm})$ can be expressed as

$$G_{\pm}^{(2)}(\vec{\rho},u_{\pm})=\mp\frac{1}{a}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi u_{\pm}}{a}\right)A_n(a,m_0,d,\vec{\rho}). \tag{57}$$

Before proceeding, let us present a explicit formula for the free two-point Schwinger function $G_{\pm}^{(2)}(\rho,u_{\pm})$ in terms of Bessel functions. Let us define an analytic function $f(d)$ by

$$f(d)=\frac{1}{\sqrt{\pi}(2\pi)^{(d-1)/2}}\frac{\Gamma\left(\frac{d-2}{2}\right)}{\Gamma\left(\frac{d-3}{2}\right)}. \tag{58}$$

Strictly speaking, it is possible to show that we can write $G_{\pm}^{(2)}(\rho,u_{\pm})$ in terms of the Bessel function of the third kind. To this end, we use the standard formula

$$\frac{1}{(2\pi)^d}\int\mathrm{d}^dr\;F(r)e^{i\vec{k}\cdot\vec{r}}=\frac{1}{\sqrt{\pi}(2\pi)^{d/2}}\frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d-2}{2}\right)}\int_0^{\infty}F(r)r^{d/2}J_{(d-3)/2}(kr)\mathrm{d}r, \tag{59}$$

which leads us to

$$G_{\pm}^{(2)}(\rho,u_{\pm})=\mp\frac{f(d)}{\rho^{(d-3)/2}a}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi u_{\pm}}{a}\right)\int_0^{\infty}\mathrm{d}p\frac{p^{(d-1)/2}}{\left(p^2+\left(\frac{n\pi}{L}\right)^2+m_0^2\right)}J_{(d-3)/2}(p\rho), \tag{60}$$

where $J_{\nu}(x)$ is the Bessel function of the first kind of order ν. The integral in Eq. (60) can be calculated by using the result[34]

$$\int_0^\infty \mathrm{d}x \frac{x^{\nu+1} J_\nu(ax)}{(x^2+b^2)} = b^\nu K_\nu(ab), \tag{61}$$

implying that it is possible to write $G_\pm^{(2)}(\rho, u_\pm)$ as

$$G_\pm^{(2)}(\rho,u_\pm) = \mp \frac{f(d)}{\rho^{(d-3)/2} a} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi u_\pm}{a}\right)\left(\left(\frac{n\pi}{a}\right)^2 + m_0^2\right)^{(d-3)/4} K_{(d-3)/2}\left(\rho\sqrt{m_0^2+\left(\frac{n\pi}{a}\right)^2}\right). \tag{62}$$

Using Eq. (55) and the above formula, the explicit expression for the two-point Schwinger function in a generic d-dimensional Euclidean space confined between two flat parallel hyperplanes, where we assume Dirichlet–Dirichlet boundary conditions is given. It is difficult to use the above expressions for $G_\pm^{(2)}(\rho, u_\pm)$ to investigate the analytic structure of the four-point function for both the bulk and near the boundaries. Nevertheless, it is clear that the divergences of the four-point function in the one-loop approximation appear at coincident points and therefore the singular behavior is encoded in the polar part of $M(\lambda_0, a, m, d)$ given by

$$M(\lambda_0,a,m_0,d) = g^2 \int \mathrm{d}^{d-1}r \int \mathrm{d}^{d-1}r' \int_0^a \mathrm{d}z \int_0^a \mathrm{d}z' F(\vec{r},\vec{r}',z,z')(G_0^{(2)}(\vec{r}-\vec{r}',z,z'))^2. \tag{63}$$

It is easy to show that $G_2^{(4)}(\lambda_0, a, m_0, d)_{\mathrm{amp}}$ is given by

$$G_2^{(4)}(\lambda_0,a,m_0,d)_{\mathrm{amp}} = \frac{g^2}{2(2\pi)^{2d-2}} \int \mathrm{d}^{d-1}r \int \mathrm{d}^{d-1}r' \int \mathrm{d}^{d-1}k \int \mathrm{d}^{d-1}q \times \sum_{n=1}^{\infty} \frac{e^{i\vec{\rho}\cdot(\vec{q}-\vec{k})}}{\left(\vec{q}^2+\left(\frac{n\pi}{a}\right)^2+m_0^2\right)\left(\vec{k}^2+\left(\frac{n\pi}{a}\right)^2+m_0^2\right)}, \tag{64}$$

where $F(\vec{r},\vec{r}',z,z')$ is a regular function. As with the one-loop two-point function, it is not difficult to realize that the above equation has two kinds of singularities, those coming from the bulk and those arising from the behavior near the surface. As before, the behavior in the bulk is similar to the thermal field theory case and consequently we will discuss only the singularities arising from the boundaries. This can be done studying the polar part of $\tilde{M}(\lambda_0, a, m_0, d)$ given by

$$\tilde{M}(\lambda,a,m_0,d) = \frac{g^2}{2}\int_0^a \mathrm{d}z \int_0^a \mathrm{d}z' \mathcal{F}(z,z')(G_0^{(2)}(\vec{0},z,z'))^2, \tag{65}$$

where $\mathcal{F}(z,z')$ is a regular function. Now, we recall that the form of $G_\pm^{(2)}(\rho,u_\pm)|_{\rho=0}$ is given by

$$G_\pm^{(2)}(\rho,u_\pm)|_{\rho=0} = \mp \frac{1}{(2\pi)^{d-1}a} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi u_\pm}{a}\right) \int \mathrm{d}^{d-1}p \frac{1}{\left(\vec{p}^2+m_0^2+\left(\frac{n\pi}{a}\right)^2\right)}, \tag{66}$$

where it is not difficult to show that

$$G_\pm^{(2)}(\rho,u_\pm)|_{\rho=0} = \mp\left(-\frac{1}{2a}A_0(\rho,L,m_0)|_{\rho=0} + f_2\left(a,m_0,d,\frac{u_\pm}{2}\right)\right). \tag{67}$$

In the above definition we are making use of the auxiliary function $f_2(a,d,m_0,z)$ given by

$$f_2(a,m_0,d,z)=\frac{1}{2(2\pi)^{d-1}}\int \mathrm{d}^{d-1}p\,\frac{1}{\sqrt{\vec{p}^2+m_0^2}}\,\frac{\cosh((a-2z)\sqrt{\vec{p}^2+m_0^2})}{\sinh(a\sqrt{\vec{p}^2+m_0^2})}. \tag{68}$$

Note that the amputated one-loop two-point Schwinger function can be decomposed in a translational invariant part and a translational invariance breaking part, given exactly by $f_2(a,m_0,d,z)$. When we sum to find the free propagator, we end up with the following expression:

$$G_0^{(2)}(\rho,z,z')|_{\rho=0}=f_2\left(a,m_0,d,\frac{u_-}{2}\right)-f_2\left(a,m_0,d,\frac{u_+}{2}\right). \tag{69}$$

For the sake of simplicity, we will discuss only the massless case once the singularities of the massive case have the same structure as in the massless one. The function $f_2(a,m_0,d,u_+/2)$ is nonsingular in the bulk, i.e., in the interior of the interval $[0,a]$, while $f_2(a,m_0,d,u_-/2)$ has a singularity along the line $z=z'$. Indeed, closer inspection shows that for $0\leqslant z,z'\leqslant a$ the only singularities are those at $u_+=0$, $u_+=2a$ and also $u_-=0$. The former two are genuinely boundary singularities (the two conditions imply $z,z'\to 0$ or $z,z'\to a$), while the last comes from $z=z'$ in the whole domain and is just the standard bulk singularity. In fact, using the structure of the two-point function and showing just those terms from which singularities might arise, one finds that the counterterms for $\tilde{M}$ are given by

$$-\,\mathrm{pole}\int_0^a \mathrm{d}z\int_0^a \mathrm{d}z'\left[\frac{C_1}{(z+z')^{d-2}}+\frac{C_2}{(2a-z-z')^{d-2}}+\frac{C_3}{(z-z')^{d-2}}+\cdots\right]^2, \tag{70}$$

where C_i, $i=1,\ldots,3$ are regular functions that do not depend on z or z'. From this discussion it is clear that in order to render the field theory finite, we must introduce surface terms in the action. This is a general statement. For any fields that satisfy boundary conditions that break the translational invariance it suffices to introduce surface counterterms in the action, in addition to the usual bulk counterterms, to render the theory finite in the ultraviolet.[36–38] Now we are able to discuss whether in the Casimir configuration the infrared problems can be solved for the case of Neumann boundary conditions. For the case of massless $(\lambda\varphi^4)_d$ theory at finite temperature, the infrared problem can be solved after a resummation procedure.[17–20,39] The key point for the solution of the infrared problem is to use the Dyson–Schwinger equation to rewrite the self-energy gap equation. Simple inspection of Eq. (24) show us that it is not possible to implement such scheme in a situation where there is a break of translational invariance.

A different possibility to approach the infrared problem is to single out the zero mode component of the field, treating the nonzero modes perturbatively and treating the zero mode exactly. This is a standard procedure in high-temperature field theory, where by means of the dimensional reduction idea, we relate the thermal Schwinger functions in a d-dimensional Euclidean space to zero temperature Schwinger functions in a $(d-1)$ dimensional Euclidean space.[40–42] In this situation we have a dimensionally reduced effective theory. The key point in this construction is the fact that the leading infrared behavior of any field theory at high temperature in a d-dimensional Euclidean space is governed by the zero frequency Matsubara mode.

V. DISCUSSIONS AND CONCLUSIONS

In this paper we are interested in the analysis of the important questions of perturbative expansion and renormalization program in quantum field theory with boundary conditions that break translation symmetry, assuming that the system is in equilibrium with a reservoir at temperature β^{-1}. Specifically, the purpose of this paper is to study the renormalization procedure up to one-loop level in the $(\lambda\varphi^4)_d$ theory at finite temperature assuming that the scalar field satisfies Dirichlet–Dirichlet or Neumann–Neumann boundary conditions on two parallel hyperplates.

We first obtained the regularized one-loop diagrams associated with scalar field defined in the Casimir configuration in a d-dimensional Euclidean space. We obtained a well-known result concerning surface divergences that appear in the one-loop two-point and four-point Schwinger

functions as a consequence of the uncertainty principle. There are at least three different possible solutions to eliminate these divergences. The first one is to take into account that real materials have imperfect conductivity at high frequencies. As was stressed by many authors, the infinities that appear in renormalized values of local observables for the ideal conductor (or perfect mirror) represent a breakdown of the perfect-conductor approximation. A wavelength cutoff corresponding to the finite plasma frequency must be included. The second one is to substitute classical boundary conditions by classical potentials; for previous papers using this idea see, for example, Refs. 43–45. A localized boundary with some cutoff can also be used to replace the potential. Nevertheless, it is necessary to renormalize the potential.[25] The third one regards a quantum mechanical treatment of the boundary conditions. A fruitful approach to avoid surface divergences, discussed by Kennedy *et al.*[46] is to treat the boundary as a quantum mechanical object. This approach was developed by Ford and Svaiter[47] to produce finite values for the renormalized $\langle\varphi^2\rangle$ and other quantities that diverge as one approaches the classical boundary.

Consequently, we have two main distinct directions for future investigations. The first is related to the infrared divergences of our model. Infrared divergences of massless thermal field theory arise from the zero frequency Matsubara modes, so we construct an effective $(d-1)$ dimensional theory by integrating out the nonstatic modes and therefore the zero frequency Matsubara modes which are responsible for infrared divergences can be treated separately. The second direction is related to the surface divergences. In the Euclidean formalism for field theory, one may imagine that our simplified model of rigid boundaries is a good approximation only for points in the bulk; for points close to the surfaces however, our approximation is no longer acurate and a model taking into account at least thermal fluctuations of the boundaries must be developed.[48] In other words, a fundamental understanding of the perturbative renormalization algorithm in the standard weak-coupling perturbative expansion of an Euclidean field in the presence of fluctuating boundaries is desired. This interesting situation of thermal fluctuating boundaries is under the investigation by the authors.

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On a conjecture of Givental

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These brief notes record our puzzles and findings surrounding Givental's recent conjecture which expresses higher genus Gromov–Witten invariants in terms of the genus-0 data. We limit our considerations to the case of a complex projective line, whose Gromov–Witten invariants are well-known and easy to compute. We make some simple checks supporting his conjecture. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1808486]

I. BRIEF SUMMARY

These notes are brief sketches of our troubles and findings surrounding a work of Givental.[5]

Let $\mathcal{F}_g$ be the generating function in the small phase space for genus-g Gromov–Witten (GW) invariants of a manifold X with a semisimple Frobenius structure on $H^*(X,\mathbb{Q})$. Then, Givental's conjecture, whose equivariant counterpart he has proved,[5] is

$$e^{\Sigma_{g\geq 2}\lambda^{g-1}\mathcal{F}_g(t)} = \left[e^{(\lambda/2)\Sigma_{k,l\geq 0}\Sigma_{i,j} V_{kl}^{ij}\sqrt{\Delta_i}\sqrt{\Delta j}\partial_{q_k^i}\partial_{q_l^j}} \prod_j \tau(\lambda\Delta_j;\{q_n^j\}) \right]\Bigg|_{q_n^j=T_n^j}, \tag{1}$$

where $i,j=1,\ldots,\dim H^*(X,\mathbb{Q})$; τ is the KdV tau-function governing the intersection theory on the Deligne–Mumford space $\overline{\mathcal{M}}_{g,n}$; and V_{kl}^{ij},Δ_j, and T_n^j are functions of the small phase space coordinates $t\in H^*(X,\mathbb{Q})$ and are defined by solutions to the flat-section equations associated with the genus-0 Frobenius structure of $H^*(X,\mathbb{Q})$.[5] This remarkable conjecture organizes the higher genus GW invariants in terms of the genus-0 data and the τ function for a point. The motivation for our work lies in verifying the conjecture for $X=\mathbb{P}^1$, which is the simplest example with a semisimple Frobenius structure on its cohomology ring and whose GW invariants can be easily computed.

We have obtained two particular solutions to the flat-section equations (5), an analytic one encoding the two-point descendant GW invariants of $\mathbb{P}^1$ and a recursive one corresponding to Givental's fundamental solution. According to Givental, both of these two solutions are supposed to yield the same data V_{kl}^{ij},Δ_j, and T_n^j. Unfortunately, we were not able to produce the desired information using our-analytic solutions, but the recursive solutions do lead to sensible quantities which we need. Combined with an expansion scheme which allows us to verify the conjecture at each order in λ, we thus use our recursive solutions to check the conjecture (1) for $\mathbb{P}^1$ up to order λ^2. Already at this order, we need to expand the differential operators in (1) up to λ^6 and need to consider up to genus-3 free energy in the τ functions, and the computations quickly become cumbersome with increasing order. We have managed to re-express the conjecture for this case into a form which resembles the Hirota-bilinear relations, but at this point, we have no insights into a general proof. It is nevertheless curious how the numbers work out, and we hope that our results would provide a humble support for Givental's master equation.

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Many confusions still remain—for instance, the discrepancy between our analytic and recursive solutions. As mentioned above, Givental's conjecture for $\mathbb{P}^1$ can be rewritten in a form which resembles the Hirota-bilinear relations for the KdV hierarchies [see (32)]. It would thus be interesting to speculate a possible relation between his conjecture and the conjectural Toda hierarchy for $\mathbb{P}^1$.

We have organized our notes as follows: in Sec. II, we review the canonical coordinates for $\mathbb{P}^1$, to be followed by our solutions to the flat-section equations in Sec. III. We conclude by presenting our checks in Sec. IV.

II. CANONICAL COORDINATES FOR $\mathbb{P}^1$.

We here review the canonical coordinates $\{u_\pm\}$ for $\mathbb{P}^1$.[1,2,4] Recall that a Frobenius structure on $H^*(\mathbb{P}^1,\mathbb{Q})$ carries a flat pseudo-Riemannian metric $\langle\cdot,\cdot\rangle$ defined by the Poincaré intersection pairing. The canonical coordinates are defined by the property that they form the basis of idempotents of the quantum cup product, denoted in the present note by $\circ$. The flat metric $\langle\cdot,\cdot\rangle$ is diagonal in the canonical coordinates, and following Givental's notation, we define $\Delta_\pm := 1/\langle\partial_{u_\pm},\partial_{u_\pm}\rangle$.

Let $\{t^\alpha\}, \alpha \in \{0,1\}$ be the flat coordinates of the metric and let $\partial_\alpha := \partial/\partial t^\alpha$. The quantum cohomology of $\mathbb{P}^1$ is

$$\partial_0 \circ \partial_\alpha = \partial_\alpha \quad \text{and} \quad \partial_1 \circ \partial_1 = e^{t^1}\partial_0.$$

The eigenvalues and eigenvectors of $\partial_1\circ$ are

$$\pm e^{t^1/2} \quad \text{and } (\pm e^{t^1/4}\partial_0 + e^{-t^1/4}\partial_1),$$

respectively. So, we have

$$(\pm e^{t^1/4}\partial_0 + e^{-t^1/4}\partial_1)\circ(\pm e^{t^1/4}\partial_0 + e^{-t^1/4}\partial_1) = \pm 2\, e^{t^1/4}(\pm e^{t^1/4}\partial_0 + e^{-t^1/4}\partial_1),$$

which implies that

$$\frac{\partial}{\partial_{u_\pm}} = \frac{\partial_0 \pm e^{-t^1/2}\partial_1}{2},$$

such that

$$\partial_{u_\pm}\circ\partial_{u_\pm} = \partial_{u_\pm} \quad \text{and } \partial_{u_\pm}\circ\partial_{u_\mp} = 0.$$

We can solve for $u_\pm$ up to constants as

$$u_\pm = t^0 \pm 2\, e^{t^1/2}. \tag{2}$$

To compute $\Delta_\pm$, note that

$$\frac{1}{\Delta_\pm} := \langle\partial_{u_\pm},\partial_{u_\pm}\rangle = \pm\frac{1}{2e^{t^1/2}}.$$

The two bases are related by

$$\partial_0 = \partial_{u_+} + \partial_{u_-} \quad \text{and } \partial_1 = e^{t^1/2}(\partial_{u_+} - \partial_{u_-}).$$

Define an orthonormal basis by $f_i = \Delta_i^{1/2}\partial/\partial u_i$. Then the transition matrix Ψ from $\{\partial/\partial t_\alpha\}$ to $\{f_i\}$ is given by

$$\Psi_{\alpha}^{\ i} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-t^1/4} & -i\, e^{-t^1/4} \\ e^{t^1/4} & i\, e^{t^1/4} \end{pmatrix} = \begin{pmatrix} \Delta_+^{-1/2} & \Delta_-^{-1/2} \\ \frac{1}{2}\Delta_+^{1/2} & \frac{1}{2}\Delta_-^{1/2} \end{pmatrix}, \tag{3}$$

such that

$$\frac{\partial}{\partial t_\alpha} = \sum_i \Psi_{\alpha}^{\ i} f_i.$$

We will also need the inverse of (3):

$$(\Psi^{-1})_i^{\ \alpha} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{t^1/4} & e^{-t^1/4} \\ i\, e^{t^1/4} & -i\, e^{-t^1/4} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\Delta_+^{1/2} & \Delta_+^{-1/2} \\ \frac{1}{2}\Delta_-^{1/2} & \Delta_-^{-1/2} \end{pmatrix}. \tag{4}$$

III. SOLUTIONS TO THE FLAT-SECTION EQUATIONS

The relevant data V_{kl}^{ij}, Δ_j, and T_n^j are extracted from the solutions to the flat-section equations of the genus-0 Frobenius structure for $H^*(\mathbb{P}^1, \mathbb{Q})$. We here find two particular solutions. The analytic solution correctly encodes the two-point descendant GW invariants, while the recursive solution is used in the next section to verify Givental's conjecture.

A. Analytic solution

The genus-0 free energy for $\mathbb{P}^1$ is

$$\mathcal{F}_0 = \tfrac{1}{2}(t^0)^2 t^1 + e^{t^1}.$$

Flat sections S_α of $TH^*(\mathbb{P}^1, \mathbb{Q})$ satisfy the equations

$$z\, \partial_\alpha S_\beta = \mathcal{F}_{\alpha\beta\mu} g^{\mu\nu} S_\nu, \tag{5}$$

where $z \neq 0$ is an arbitrary parameter and $\mathcal{F}_{\alpha\beta\mu} := \partial^3 \mathcal{F} / \partial t^\alpha \partial t^\beta \partial t^\mu$. The only nonvanishing components of $\mathcal{F}_{\alpha\beta\mu}$ are

$$\mathcal{F}_{001} = 1 \quad \text{and } \mathcal{F}_{111} = e^{t^1}.$$

Hence, we find that the general solutions to the flat-section equations (5) are

$$S_0 = e^{t^0/z}[c_1 I_0(2\, e^{t^1/2}/z) - c_2 K_0(2\, e^{t^1/2}/z)] \tag{6}$$

and

$$S_1 = e^{t^0/z} e^{t^1/2}[c_1 I_1(2e^{t^1/2}/z) + c_2 K_1(2e^{t^1/2}/z)],$$

where $I_n(x)$ and $K_n(x)$ are modified Bessel functions, and c_i are integration constants which may depend on z.

We would now like to find two particular solutions corresponding to the following Givental's expression:

$$S_{\alpha\beta}(z) = g_{\alpha\beta} + \sum_{n\geqslant 0,(n,d)\neq(0,0)} \frac{1}{n!} \left\langle \phi_\alpha \cdot \frac{\phi_\beta}{z - \psi} \cdot (t^0\phi_0 + t^1\phi_1)^n \right\rangle_d, \tag{7}$$

where $S_{\alpha\beta}$ denotes the αth component of the βth solution. Here, $\{\phi_\alpha\}$ is a homogeneous basis of $H^*(\mathbb{P}^1, \mathbb{Q})$, $g_{\alpha\beta}$ is the intersection paring $\int_{\mathbb{P}^1} \phi_\alpha \cup \phi_\beta$ and $\psi \in H^2(\overline{M}_{0,n+2}(\mathbb{P}^1, d), \mathbb{Q})$ is the first Chern class of the universal cotangent line bundle over the moduli space $\overline{M}_{0,n+2}(\mathbb{P}^1, d)$. In order to find the particular solutions, we compare our general solution (6) with the 0th components of $S_{0\beta}$

in (7) *at the origin of the phase space*. The two-point functions appearing in (7) have been computed at the origin in Ref. 6 and have the following forms:

$$S_{00}\big|_{t^\alpha=0} = -\sum_{m=1}^{\infty} \frac{1}{z^{2m+1}} \frac{2d_m}{(m!)^2}, \quad \text{where } d_m = \sum_{k=1}^{m} 1/k, \tag{8}$$

and

$$S_{01}\big|_{t^\alpha=0} = 1 + \sum_{m=1}^{\infty} \frac{1}{z^{2m}} \frac{1}{(m!)^2}. \tag{9}$$

Using the standard expansion of the modified Bessel function K_0, we can evaluate (6) at the origin of the phase space to be

$$c_1 I_0\left(\frac{2}{z}\right) - c_2 K_0\left(\frac{2}{z}\right) = c_1 I_0\left(\frac{2}{z}\right) - c_2\left[-(-\log(z) + \gamma_E) I_0\left(\frac{2}{z}\right) + \sum_{m=1} \frac{c_m}{z^{2m}(m!)^2}\right], \tag{10}$$

where γ_E is Euler's constant. Now matching (10) with (8) gives

$$c_1 = -c_2 \log(1/z) - c_2 \gamma_E \quad \text{and } c_2 = \frac{2}{z},$$

while noticing that (9) is precisely the expansion of $I_0(2/z)$ and demanding that our general solution coincides with (9) at the origin yields

$$c_1 = 1 \quad \text{and } c_2 = 0.$$

To recapitulate, we have found

$$S_{00} = -\frac{2e^{t^0/z}}{z}\left[(\gamma_E - \log(z)) I_0\left(\frac{2e^{t^1/2}}{z}\right) + K_0\left(\frac{2e^{t^1/2}}{z}\right)\right],$$

$$S_{10} = \frac{2e^{t^0/z}e^{t^1/2}}{z}\left[K_1\left(\frac{2e^{t^1/2}}{z}\right) - (\gamma_E - \log(z)) I_1\left(\frac{2e^{t^1/2}}{z}\right)\right],$$

$$S_{01} = e^{t^0/z} I_0\left(\frac{2e^{t^1/2}}{z}\right),$$

$$S_{11} = e^{t^0/z}e^{t^1/2} I_1\left(\frac{2e^{t^1/2}}{z}\right).$$

We have checked that these solutions correctly reproduce the corresponding descendant Gromov–Witten invariants obtained in Ref. 6.

If the inverse transition matrix in (4) is used to relate the matrix elements S^i_α to $S_{\alpha\beta}$ as $S^i_\alpha = S_{\alpha\beta}((\psi^{-1})^t)^\beta_j \delta^{ji}$, then we should have

$$S^\pm_\alpha = \sqrt{\pm 2} e^{t^1/4}\left(\frac{1}{2} S_{\alpha 0} \pm \frac{e^{-t^1/2}}{2} S_{\alpha 1}\right). \tag{11}$$

B. Recursive solution

In Refs. 4 and 5, Givental has shown that near a semisimple point, the flat-section equations (5) have a fundamental solution given by

$$S^i_\alpha = \Psi^j_\alpha (R_0 + zR_1 + z^2R_2 + \cdots + z^nR_n + \cdots)_{jk}[\exp(U/z)]^{ki},$$

where $R_n = (R_n)_{jk}, R_0 = \delta_{jk}$ and U is the diagonal matrix of canonical coordinates. The matrix R_1 satisfies the relations

$$\Psi^{-1}\frac{\partial \Psi}{\partial t^1} = \left[\frac{\partial U}{\partial t^1}, R_1\right] \tag{12}$$

and

$$\left[\frac{\partial R_1}{\partial t^1} + \Psi^{-1}\left(\frac{\partial \Psi}{\partial t^1}\right)R_1\right]_{\pm\pm} = 0, \tag{13}$$

which we use to find its expression. From the transition matrix given in (3) we see that

$$\Psi^{-1}\frac{\partial \Psi}{\partial t^1} = \frac{1}{4}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},$$

while taking the $(+-)$ component of the relation (12) gives

$$\frac{i}{4} = \frac{\partial U_{++}}{\partial t^1}(R_1)_{+-} - (R_1)_{+-}\frac{\partial U_{--}}{\partial t^1} = 2e^{t^1/2}(R_1)_{+-},$$

where in the last step we have used the definition (2) of canonical coordinates. We therefore have

$$(R_1)_{+-} = \frac{i}{8}e^{-t^1/2},$$

and similarly considering the $(-+)$ component of (12) gives

$$(R_1)_{-+} = \frac{i}{8}e^{-t^1/2}.$$

The diagonal components of R_1 can be obtained from (13), which implies that

$$\frac{\partial (R_1)_{++}}{\partial t^1} = (R_1)_{+-}\frac{\partial U_{--}}{\partial t^1}(R_1)_{-+} - \frac{\partial U_{++}}{\partial t^1}(R_1)_{+-}(R_1)_{-+} = \frac{\exp(-t^1/2)}{32} = -\frac{\partial (R_1)_{--}}{\partial t^1}.$$

Hence, $(R_1)_{++} = -\exp(-t^1/2)/16 = -(R_1)_{--}$ and the matrix R_1 can be written as

$$(R_1)_{jk} = \frac{1}{16}e^{-t^1/2}\begin{pmatrix} -1 & 2i \\ 2i & 1 \end{pmatrix}. \tag{14}$$

In general, the matrices R_n satisfy the recursion relations[4]

$$(\mathrm{d} + \Psi^{-1}\,\mathrm{d}\Psi)R_n = [\mathrm{d}U, R_{n+1}],$$

which, for our case, imply the following set of equations:

$$\frac{\partial R_n}{\partial t^0} = 0, \tag{15}$$

$$\frac{\partial (R_n)_{++}}{\partial t^1} = -\frac{i}{4}(R_n)_{-+}, \tag{16}$$

$$(R_{n+1})_{-+} = -\frac{1}{2}e^{-t^1/2}\left[\frac{\partial (R_n)_{-+}}{\partial t^1} - \frac{i}{4}(R_n)_{++}\right], \tag{17}$$

$$\frac{\partial (R_n)_{--}}{\partial t^1} = \frac{i}{4}(R_n)_{+-}, \tag{18}$$

$$(R_{n+1})_{+-} = \frac{1}{2}e^{-t^1/2}\left[\frac{\partial (R_n)_{+-}}{\partial t^1} + \frac{i}{4}(R_n)_{--}\right]. \tag{19}$$

Lemma 3.1: *For $n \geqslant 1$, the matrices R_n in the fundamental solution are given by*

$$(R_n)_{ij} = \frac{(-1)^n}{(2n-1)}\frac{\alpha_n}{2^n}e^{-nt^1/2}\begin{pmatrix} -1 & (-1)^{n+1}2n\ i \\ 2n\ i & (-1)^{n+1} \end{pmatrix}, \tag{20}$$

where

$$\alpha_n = (-1)^n \frac{1}{8^n n!}\prod_{\ell=1}^{n}(2\ell-1)^2, \quad \alpha_0 = 1.$$

These solutions satisfy the unitarity condition,

$$\mathbf{R}(z)\mathbf{R}^t(-z) := (1 + zR_1 + z^2R_2 + \cdots + z^nR_n + \cdots)(1 - zR_1^t + z^2R_2^t + \cdots + (-1)^n z^n R_n^t + \cdots) = 1,$$

and the homogeneity condition and, thus, are unique.

Proof: For $n=1, \alpha_1=-1/8$ and (20) is equal to the correct solution (14). The proof now follows by an induction on n. Assume that (20) holds true up to and including $n=m$. Using the fact that

$$\alpha_{m+1} = -\frac{(2m+1)^2}{8(m+1)}\alpha_m,$$

we can show that R_{m+1} in (20) satisfies the relations (16)–(19) as well as (15).

To check unitarity, consider the z^k-term $P_k := \Sigma_{\ell=0}^{k}(-1)^\ell R_{k-\ell}R_\ell^t$ in $\mathbf{R}(z)\mathbf{R}^t(-z) = \Sigma_{k=0} P_k z^k$. As shown by Givental, the equations satisfied by the matrices R_n imply that the off-diagonal entries of P_k vanish. As a result, combined with the antisymmetry of P_k for odd k, we see that P_k vanishes for k odd. Hence, we only need to show that for our solution, P_k vanishes for all positive even k as well. To this end, we note that Givental has also deduced from the equation $\mathrm{d}P_k + [\Psi^{-1}\,\mathrm{d}\Psi, P_k] = [\mathrm{d}U, P_{k+1}]$ that the diagonal entries of P_k are constant. The expansion of P_{2k} is

$$P_{2k} = R_{2k} + R_{2k}^t + \cdots,$$

where the remaining terms are products of R_ℓ, for $\ell < 2k$. Now, we proceed inductively. We first note that R_1 and R_2 given in (20) satisfy the condition $P_2=0$, and assume that R_ℓ's in (20) for $\ell < 2k$ satisfy $P_\ell = 0$. Then, since the off-diagonal entries of P_n vanish for all n, the expansion of P_{2k} is of the form

$$P_{2k} = A\ e^{-2k\ t^1/2} + B,$$

where A is a constant diagonal matrix resulting from substituting our solution (20) and B is a possible diagonal matrix of integration constants for R_{2k}. But, since the diagonal entries of P_n are constant for all n, we know that $A=0$. We finally choose the integration constants to be zero so that $B=0$, yielding $P_{2k}=0$. Hence, the matrices in our solution (20) satisfy the unitarity condition and are manifestly homogeneous. It then follows by the proposition in Ref. 5 that our solutions R_n are unique. □

Let $\mathbf{R} := (R_0 + zR_1 + z^2R_2 + \cdots + z^nR_n + \cdots)$. Then, we can use the matrices R_n from Lemma 3.1 to find

$$S_0^{+} = (\mathbf{R}_{++} - i\,\mathbf{R}_{-+})\frac{\exp(u_+/z)}{\sqrt{\Delta_+}} = \left[1 + \sum_{n=1}^{\infty}\frac{\alpha_n}{2^n}\exp\left(\frac{-nt^1}{2}\right)(-z)^n\right]\frac{\exp(u_+/z)}{\sqrt{\Delta_+}}, \tag{21}$$

$$S_0^{-} = (\mathbf{R}_{--} + i\,\mathbf{R}_{+-})\frac{\exp(u_-/z)}{\sqrt{\Delta_-}} = \left[1 + \sum_{n=1}^{\infty}(-1)^n\frac{\alpha_n}{2^n}\exp\left(\frac{-nt^1}{2}\right)(-z)^n\right]\frac{\exp(u_-/z)}{\sqrt{\Delta_-}}, \tag{22}$$

$$S_1^{+} = (\mathbf{R}_{++} + i\,\mathbf{R}_{-+})\frac{\sqrt{\Delta_+}}{2}\exp(u_+/z) = \left[1 - \sum_{n=1}^{\infty}\frac{(2n+1)}{(2n-1)}\frac{\alpha_n}{2^n}\exp\left(\frac{-nt^1}{2}\right)(-z)^n\right]\frac{\sqrt{\Delta_+}}{2}\exp(u_+/z), \tag{23}$$

$$S_1^{-} = (\mathbf{R}_{--} - i\,\mathbf{R}_{+-})\frac{\sqrt{\Delta_-}}{2}\exp(u_-/z) = \left[1 - \sum_{n=1}^{\infty}(-1)^n\frac{(2n+1)}{(2n-1)}\frac{\alpha_n}{2^n}\exp\left(\frac{-nt^1}{2}\right)(-z)^n\right]\frac{\sqrt{\Delta_-}}{2}\exp(u_-/z). \tag{24}$$

Using the above expressions for $S_\alpha{}^i(z)$, we can also find $V^{ij}(z,w)$, which is given by the expression

$$V^{ij}(z,w) := \frac{1}{z+w}[S_\mu{}^i(w)]^t[g^{\mu\nu}][S_\nu{}^j(z)].$$

If we define

$$A_{p,q} := \frac{(4p\ q-1)}{(2p-1)(2q-1)}\frac{\alpha_p\alpha_q}{2^{p+q}}e^{[-(p+q)t^1/2]}$$

and

$$B_{p,q} := \frac{2(p-q)}{(2p-1)(2q-1)}\frac{\alpha_p\alpha_q}{2^{p+q}}e^{[-(p+q)t^1/2]},$$

then after some algebraic manipulations we obtain

$$V^{++}(z,w) = e^{u_+/w+u_+/z}\left\{\frac{1}{z+w} + \sum_{k,l=0}^{\infty}\left[\sum_{n=0}^{k}(-1)^n A_{l+n+1,k-n}\right](-1)^{k+l}w^k z^l\right\},$$

$$V^{--}(z,w) = e^{u_-/w+u_-/z}\left\{\frac{1}{z+w} - \sum_{k,l=0}^{\infty}\left[(-1)^{k+l}\sum_{n=0}^{k}(-1)^n A_{l+n+1,k-n}\right](-1)^{k+l}w^k z^l\right\}, \tag{25}$$

$$V^{+-}(z,w) = e^{u_+/w+u_-/z}\left\{\sum_{k,l=0}^{\infty}\left[i(-1)^l\sum_{n=0}^{k}B_{l+n+1,k-n}\right](-1)^{k+l}w^k z^l\right\},$$

$$V^{-+}(z,w) = e^{u_-/w+u_+/z}\left\{\sum_{k,l=0}^{\infty}\left[i(-1)^k\sum_{n=0}^{k}B_{l+n+1,k-n}\right](-1)^{k+l}w^k z^l\right\}. \tag{26}$$

C. A puzzle

Incidentally, we note that in the asymptotic limit $z \to 0$,

$$S_0{}^+ = \Re\left[\sqrt{\frac{2\pi}{z}}e^{t^0/z}I_0\left(\frac{2e^{t^1/2}}{z}\right)\right]$$

and

$$S_0{}^- = -i\sqrt{\frac{2}{\pi z}}e^{t^0/z}K_0\left(\frac{2e^{t^1/2}}{z}\right)$$

reproduce the expansions in (21) and (22). This is in contrast to what was expected from the discussion leading to (11). Despaired of matching the two expressions, it seems to us that the analytic correlation functions obtained in Sec. III A do not encode the right information that appear in Givental's conjecture. In the following section, we will use the recursive solutions from Sec. III B to check Givental's conjectural formula at low genera.

IV. CHECKS OF THE CONJECTURE AT LOW GENERA

The T_n^i that appear in Givental's formula (1) are defined by the equations[5]

$$S_0{}^\pm := \left[1 - \sum_{n=0}^{\infty} T_n^\pm (-z)^{n-1}\right]\frac{\exp(u_\pm/z)}{\sqrt{\Delta_\pm}}.$$

From the computations of $S_0{}^+$ and $S_0{}^-$ in (21) and (22), respectively, one can extract T_n^i to be

$$T_n^+ = \begin{cases} 0, & n = 0,1, \\ -\dfrac{\alpha_{n-1}}{2^{n-1}}\exp\left[\dfrac{-(n-1)t^1}{2}\right], & n \geqslant 2, \end{cases}$$

$$T_n^- = \begin{cases} 0, & n = 0,1, \\ -(-1)^{n-1}\dfrac{\alpha_{n-1}}{2^{n-1}}\exp\left[\dfrac{-(n-1)t^1}{2}\right], & n \geqslant 2. \end{cases}$$

Notice that

$$T_n^- = (-1)^{n-1}T_n^+. \tag{27}$$

The functions V_{kl}^{ij} are defined by the expansion[5]

$$V^{ij}(z,w) = e^{u^i/w + u^j/z}\left[\frac{\delta^{ij}}{z+w} + \sum_{k,l=0}^{\infty}(-1)^{k+l}V_{kl}^{ij}w^k z^l\right],$$

and from (25) and (26) we see that

$$V_{kl}^{++} = \sum_{n=0}^{k}(-1)^n A_{l+n+1,k-n} = \sum_{n=0}^{k}\frac{(-1)^n(4(l+n+1)(k-n)-1)}{(2l+2n+1)(2k-2n-1)}T_{l+n+2}^+ T_{k-n+1}^+,$$

$$V_{kl}^{+-} = i(-1)^l\sum_{n=0}^{k}B_{l+n+1,k-n} = i(-1)^l\sum_{n=0}^{k}\frac{2(l+2n+1-k)}{(2l+2n+1)(2k-2n-1)}T_{l+n+2}^+ T_{k-n+1}^+.$$

There seems to be a misprint in the original formula for V_{kl}^{ij} in Ref. 5, i.e., we believe that w and z should be exchanged, as in our expression here.

Now, the τ function for the intersection theory on the Deligne–Mumford moduli space $\overline{\mathcal{M}}_{g,n}$ of stable curves is defined by

$$\tau(\lambda;\{q_k\}) = \exp\left(\sum_{g=0}^{\infty} \lambda^{g-1}\mathcal{F}_g^{\mathrm{pt}}(\{q_k\})\right)$$

and has the following nice scaling invariance: consider the scaling of the phase-space variables q_k given by

$$q_k \mapsto s^{k-1}q_k \tag{28}$$

for some constant s. Then, since a nonvanishing intersection number $\langle \tau_{k_1}\cdots\tau_{k_n}\rangle$ must satisfy

$$\sum_{i=1}^{n}(k_i-1) = \dim(\overline{\mathcal{M}}_{g,n}) - n = 3g-3,$$

we see that under the transformation (28), the genus-g generating function $\mathcal{F}_g^{\mathrm{pt}}$ must behave as

$$\mathcal{F}_g^{\mathrm{pt}}(\{s^{k-1}q_k\}) = (s^3)^{g-1}\mathcal{F}_g^{\mathrm{pt}}(\{q_k\}).$$

Hence, upon scaling the "string coupling constant" λ to $s^{-3}\lambda$, we see that

$$\tau(s^{-3}\lambda;\{s^{k-1}q_k\}) = \tau(\lambda;\{q_k\}). \tag{29}$$

Now, consider the function

$$F(\{q_n^+\},\{q_n^-\}) := [e^{(\lambda/2)\Sigma_{k,l\geq 0}\Sigma_{i,j\in\{\pm\}}V_{kl}^{ij}\sqrt{\Delta_i}\sqrt{\Delta_j}\partial_{q_k^i}\partial_{q_l^j}}\tau(\lambda\Delta_+;\{q_n^+\})\tau(\lambda\Delta_-;\{q_n^-\})]. \tag{30}$$

Then, since the Gromov–Witten potentials of $\mathbb{P}^1$ for $g\geq 2$ all vanish, Givental's conjectural formula for $\mathbb{P}^1$ is

$$F(\{T_n^+\},\{T_n^-\}) = 1,$$

where it is understood that one sets $q_k^i = T_k^i$ after taking the derivatives with respect to q_k^i. Since T_n^+ and T_n^- are related by (27), let us rescale $q_k^- \mapsto (-1)^{k-1}q_k^-$ in (30). Then, since $\Delta_+ = -\Delta_-$, we observe from (29) that

$$F(\{T_n^+\},\{T_n^-\}) = \left\{\exp\left[\frac{\lambda}{2}\Delta_+\sum_{k,l\geq 0}\left(V_{kl}^{++}\partial_{q_k^+}\partial_{q_l^+} + i(-1)^{l-1}V_{kl}^{+-}\partial_{q_k^+}\partial_{q_l^-} + i(-1)^{k-1}V_{kl}^{-+}\partial_{q_k^-}\partial_{q_l^+}\right.\right.\right.$$
$$\left.\left.\left. - (-1)^{k+l}V_{kl}^{--}\partial_{q_k^-}\partial_{q_l^-}\right)\right]\tau(\lambda\Delta_+;\{q_n^+\})\tau(\lambda\Delta_+;\{q_n^-\})\right\}\Bigg|_{q_n^+,q_n^-=T_n^+}.$$

But, the V_{kl}^{ij} satisfy the relations $V_{kl}^{--} = -(-1)^{k+l}V_{kl}^{++}$ and $V_{kl}^{+-} = V_{lk}^{-+}$, so

$$F(\{T_n^+\},\{T_n^-\}) = \left\{\exp\left[\frac{\lambda}{2}\Delta_+\sum_{k,l\geq 0}\left(V_{kl}^{++}(\partial_{q_k^+}\partial_{q_l^+} + \partial_{q_k^-}\partial_{q_l^-})\right.\right.\right.$$
$$\left.\left.\left. + 2i(-1)^{l-1}V_{kl}^{+-}\partial_{q_k^+}\partial_{q_l^-}\right)\right]\tau(\lambda\Delta_+;\{q_n^+\})\tau(\lambda\Delta_+;\{q_n^-\})\right\}\Bigg|_{q_n^+,q_n^-=T_n^+}. \tag{31}$$

Now, consider the following transformations of the variables:

$$q_k^+ = x_k + y_k \quad \text{and } q_k^- = x_k - y_k,$$

so that

$$\partial_{q_k^+} = \tfrac{1}{2}(\partial_{x_k} + \partial_{y_k}) \quad \text{and } \partial_{q_k^-} = \tfrac{1}{2}(\partial_{x_k} - \partial_{y_k}).$$

Then, in these new coordinates, (31) becomes

$$F(\{T_n^+\},\{T_n^-\}) = G(\{T_n^+\},\{0\}),$$

where the new function $G(\{x_k\},\{y_k\})$ is defined by

$$G(\{x_n\},\{y_n\}) = \exp\left[\frac{\lambda}{4}\Delta_+ \sum_{k,l\geqslant 0}(V_{kl}\partial_{x_k}\partial_{x_l} + W_{kl}\partial_{y_k}\partial_{y_l})\right]\tau(\lambda\Delta_+;\{x_n+y_n\})\tau(\lambda\Delta_+;\{x_n-y_n\}), \quad (32)$$

where

$$V_{kl} \coloneqq V_{kl}^{++} + i(-1)^{l-1}V_{kl}^{+-},$$

$$W_{kl} \coloneqq V_{kl}^{++} - i(-1)^{l-1}V_{kl}^{+-}.$$

Here, we have simplified the expression by noting that the mixed derivative terms cancel because of the identity $V_{kl}^{+-}=(-1)^{k-1}V_{lk}^{+-}$.

Remark: The conjecture expressed in terms of (32), i.e., that $G(\{T_k^+\},\{0\})=1$, is now in a form which resembles the Hirota bilinear relations, which might be indicating some kind of an integrable hierarchy, perhaps of Toda type.

Because the tau functions are exponential functions, upon acting on them by the differential operators, we can factor them out in the expression of $G(\{x_k\},\{y_k\})$. We thus define the following.

Definition 4.1: *$P(\lambda\Delta_+,\{x_k\},\{y_k\})$ is a formal power series in the variables $\lambda\Delta_+,\{x_k\}$ and $\{y_k\}$ such that*

$$G(\{x_k\},\{y_k\}) = P(\lambda\Delta_+,\{x_k\},\{y_k\})\tau(\lambda\Delta_+,\{x_k+y_k\})\tau(\lambda\Delta_+,\{x_k-y_k\}).$$

Hence, Givental's conjecture for $\mathbb{P}^1$ can be restated as follows.

Conjecture 4.2 (Givental): *The generating function $G(\{T_k^+\},\{0\})$ is equal to one, or equivalently*

$$P(\lambda\Delta_+,\{T_k^+\},\{0\}) = \frac{1}{\tau(\lambda\Delta_+,\{T_k^+\})^2}. \quad (33)$$

This conjecture can be verified order by order in λ. This procedure is possible because when $q_0=q_1=0$, only a finite number of terms in the free energies and their derivatives are nonvanishing. In particular, the genus-0 and genus-1 free energies vanish when $q_0=q_1=0$.

Let us check (33) up to order λ^2, for which we need to consider up to λ^6 expansions in the differential operators acting on the τ functions. Let $h=\lambda\Delta_+$. The low-genus free energies for a point target space can be easily computed using the KdV hierarchy and topological axioms; they can also be verified using Faber's program.[3] The terms relevant to our computation are

$$\begin{aligned}\frac{\mathcal{F}_0^{\mathrm{pt}}}{h} + \mathcal{F}_1^{\mathrm{pt}} + h\mathcal{F}_2^{\mathrm{pt}} = \frac{1}{h}\Bigg[&\frac{(q_0)^3}{3!} + \frac{(q_0)^3q_1}{3!} + 2!\,\frac{(q_0)^3(q_1)^2}{3!\,2!} + 3!\,\frac{(q_0)^3(q_1)^3}{3!\,3!} + \frac{(q_0)^4q_2}{4!}\\ &+ 3\frac{(q_0)^4q_1q_2}{4!} + 12\frac{(q_0)^4(q_1)^2q_2}{4!\,2!} + \frac{(q_0)^5q_3}{5!} + 4\frac{(q_0)^5q_1q_3}{5!} + 6\frac{(q_0)^5(q_2)^2}{5!\,2!}\\ &+ 30\frac{(q_0)^5q_1(q_2)^2}{5!\,2!} + \frac{(q_0)^6q_4}{6!} + 10\frac{(q_0)^6q_2q_3}{6!} + 90\frac{(q_0)^6(q_2)^3}{6!\,3!} + \cdots\Bigg] + \Bigg[\frac{1}{24}q_1\\ &+ \frac{1}{24}\frac{(q_1)^2}{2!} + \frac{1}{12}\frac{(q_1)^3}{3!} + \frac{1}{4}\frac{(q_1)^4}{4!} + \frac{1}{24}q_0q_2 + \frac{1}{12}q_0q_1q_2 + \frac{1}{4}\frac{q_0(q_1)^2q_2}{2!}\\ &+ \frac{q_0(q_1)^3q_2}{3!} + \frac{1}{6}\frac{(q_0)^2(q_2)^2}{2!\,2!} + \frac{2}{3}\frac{(q_0)^2q_1(q_2)^2}{2!\,2!} + \frac{10}{3}\frac{(q_0)^2(q_1)^2(q_2)^2}{2!\,2!\,2!}\end{aligned}$$

$$+\frac{1}{24}\frac{(q_0)^2q_3}{2!}+\frac{1}{8}\frac{(q_0)^2q_1q_3}{2!}+\frac{1}{2}\frac{(q_0)^2(q_1)^2q_3}{2!\,2!}+\frac{7}{24}\frac{(q_0)^3q_2q_3}{3!}$$
$$+\frac{35}{24}\frac{(q_0)^3q_1q_2q_3}{3!}+2\frac{(q_0)^3(q_2)^3}{3!\,3!}+12\frac{(q_0)^3q_1(q_2)^3}{3!\,3!}+\frac{1}{24}\frac{(q_0)^3q_4}{3!}+\frac{1}{6}\frac{(q_0)^3q_1q_4}{3!}$$
$$+48\frac{(q_0)^4(q_2)^4}{4!\,4!}+\frac{59}{12}\frac{(q_0)^4(q_2)^2q_3}{4!\,2!}+\frac{7}{12}\frac{(q_0)^4(q_3)^2}{4!\,2!}+\frac{11}{24}\frac{(q_0)^4q_2q_4}{4!}$$
$$+\frac{1}{24}\frac{(q_0)^4q_5}{4!}+\cdots\Bigg]+h\Bigg[\frac{7}{240}\frac{(q_2)^3}{3!}+\frac{29}{5760}q_2q_3+\frac{1}{1152}q_4+\frac{7}{48}\frac{q_1(q_2)^3}{3!}$$
$$+\frac{7}{8}\frac{(q_1)^2(q_2)^3}{2!\,3!}+\frac{29}{1440}q_1q_2q_3+\frac{29}{288}\frac{(q_1)^2q_2q_3}{2!}+\frac{1}{384}q_1q_4+\frac{1}{96}\frac{(q_1)^2q_4}{2!}$$
$$+\frac{7}{12}\frac{q_0(q_2)^4}{4!}+\frac{49}{12}\frac{q_0q_1(q_2)^4}{4!}+\frac{5}{72}\frac{q_0(q_2)^2q_3}{2!}+\frac{5}{12}\frac{q_0q_1(q_2)^2q_3}{2!}$$
$$+\frac{29}{2880}\frac{q_0(q_3)^2}{2!}+\frac{29}{576}\frac{q_0q_1(q_3)^2}{2!}+\frac{11}{1440}q_0q_2q_4+\frac{11}{288}q_0q_1q_2q_4+\frac{1}{1152}q_0q_5$$
$$+\frac{1}{288}q_0q_1q_5+\frac{245}{12}\frac{(q_0)^2(q_2)^5}{2!\,5!}+\frac{11}{6}\frac{(q_0)^2(q_2)^3q_3}{2!\,3!}+\frac{109}{576}\frac{(q_0)^2q_2(q_3)^2}{2!\,2!}$$
$$+\frac{17}{960}\frac{(q_0)^2q_3q_4}{2!}+\frac{7}{48}\frac{(q_0)^2(q_2)^2q_4}{2!\,2!}+\frac{1}{90}\frac{(q_0)^2q_2q_5}{2!}+\frac{1}{1152}\frac{(q_0)^2q_6}{2!}+\cdots\Bigg].$$

This expression gives the necessary expansion of $\tau(\lambda\Delta_+;\{x_k\pm y_k\})$ for our consideration, and upon evaluating $G(\{T_k^+\},\{0\})$, we find

$$P(h,\{T_k^+\},\{0\})=1-\frac{17}{2\,359\,296}e^{-3t^1/2}h+\frac{41\,045}{695\,784\,701\,952}e^{-3t^1}h^2+\mathcal{O}(h^3). \tag{34}$$

At this order, the expansion of the right-hand side of (33) is

$$\tau(h,\{T_k^+\})^{-2}=1-2\mathcal{F}_2^{\mathrm{pt}}h+2[(\mathcal{F}_2^{\mathrm{pt}})^2-\mathcal{F}_3^{\mathrm{pt}}]h^2+\mathcal{O}(h^3).$$

At $q_n=T_n^+,\forall n$, the genus-2 free energy is precisely given by

$$\mathcal{F}_2^{\mathrm{pt}}=\frac{1}{1152}T_4+\frac{29}{5760}T_3T_2+\frac{7}{240}\frac{T_2^3}{3!}=\frac{17}{4\,718\,592}e^{-3t^1/2},$$

and the genus-3 free energy is

$$\mathcal{F}_3^{\mathrm{pt}}=\frac{1}{82\,944}T_7+\frac{77}{414\,720}T_2T_6+\frac{503}{1\,451\,520}T_3T_5+\frac{17}{11\,520}(T_2)^2T_5+\frac{607}{2\,903\,040}(T_4)^2$$
$$+\frac{1121}{241\,920}T_2T_3T_4+\frac{53}{6912}(T_2)^3T_4+\frac{583}{580\,608}(T_3)^3+\frac{205}{13\,824}(T_2)^2(T_3)^2+\frac{193}{6912}(T_2)^4T_3$$
$$+\frac{245}{20\,736}(T_2)^6=-\frac{656\,431}{22\,265\,110\,462\,464}e^{-3t^1}.$$

Thus, we have

$$\tau(h,\{T_k^+\})^{-2}=1-\frac{17}{2\,359\,296}e^{-3t^1/2}h+\frac{41\,045}{695\,784\,701\,952}e^{-3t^1}h^2+\mathcal{O}(h^3),$$

which agrees with our computation of $P(\lambda,\{T_k^+\},\{0\})$ in (34).

It would be very interesting if one could actually prove Givental's conjecture, but even our particular example remains elusive and verifying its validity to all orders seems intractable using our method.

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Space–time slices and surfaces of revolution

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Under certain conditions, a $(1+1)$-dimensional slice $\hat{g}$ of a spherically symmetric black hole space–time can be equivariantly embedded in $(2+1)$-dimensional Minkowski space. The embedding depends on a real parameter that corresponds physically to the surface gravity κ of the black hole horizon. Under conditions that turn out to be closely related, a real surface that possesses rotational symmetry can be equivariantly embedded in three-dimensional Euclidean space. The embedding does not obviously depend on a parameter. However, the Gaussian curvature is given by a simple formula: If the metric is written $g=\phi(r)^{-1}\,\mathrm{d}r^2+\phi(r)\mathrm{d}\theta^2$, then $K_g=-\frac{1}{2}\phi''(r)$. This note shows that metrics g and $\hat{g}$ occur in dual pairs, and that the embeddings described above are orthogonal facets of a single phenomenon. In particular, the metrics and their respective embeddings differ by a Wick rotation that preserves the ambient symmetry. Consequently, the embedding of g depends on a real parameter. The ambient space is not smooth, and κ is inversely proportional to the cone angle at the axis of rotation. Further, the Gaussian curvature of $\hat{g}$ is given by a simple formula that seems not to be widely known. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1808487]

I. INTRODUCTION

The most concrete way to study a surface is (when possible) to embed it isometrically in a flat three-dimensional space. Isometric embedding "realizes" the abstract surface, and is useful for developing geometric intuition.[1] Naturally, the signature of the surface metric is related to the signature of the ambient metric. For example, a "space–time slice" of signature $(1+1)$ cannot be isometrically embedded in $\mathbf{R}^3$; instead, one might seek an embedding into the Minkowski space $\mathbf{R}^{2+1}$.

If an abstract surface has symmetry, it is natural to seek an embedding in which the intrinsic symmetry is realized by a symmetry of the ambient space. When this occurs, the embedding is said to be *equivariant* (with respect to the actions of the abstract symmetry groups).

This paper originates with two families of equivariant isometric embeddings. The first realizes slices of certain spherically symmetric static space–times as surfaces in Minkowski space $\mathbf{R}^{2+1}$, see Refs. 7 and 10. (These papers were in turn inspired by earlier work[3,4,6,9,11,12] involving higher-dimensional embeddings into flat space.) The second is a "symplectic" description of (classical) surfaces of revolution, see Ref. 8. Each family of metrics has continuous symmetry: time translation and rotation, respectively.

These two families of metrics are equivariantly related by "Wick rotation," in a sense made precise below. The relationship is roughly analogous to the duality between conjugate minimal surfaces: For each suitable space–time slice, there is a "dual" surface of revolution, and a single equivariant embedding into $\mathbf{C}^3$ that interpolates the embeddings of the respective surfaces into flat (real) three-dimensional spaces. The resulting one-parameter family of metrics on the abstract surface interpolates metrics of different signatures, so unlike the situation for minimal surfaces, the interpolating metrics are not mutually isometric (even locally).

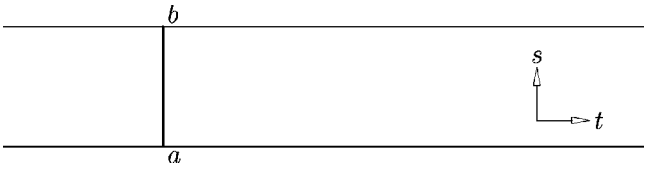

FIG. 1. The domain of an intrinsic metric.

Geometric properties of one family have consequences for the other family.

(i) The Gaussian curvature of a space–time slice is given by an extremely simple formula.
(ii) The surface gravity of a black hole horizon has a geometric interpretation as angular defect of a cone singularity. In particular, the metrics studied in Ref. 8 are instances of a one-parameter family of (possibly singular) metrics that are "smoothly embedded" in a (flat) singular ambient space.

Organization: In Sec. II we introduce the abstract surfaces under consideration; fixed points are removed for simplicity, and the intrinsic "Wick rotation" is described as a discrete symmetry. In Sec. III, we equip the ambient space $\mathbf{C}^3$ with coordinates, an action of the additive complex group, and an appropriate (flat) indefinite metric. Section IV describes the interpolating embedding, a map from $\mathbf{C}\times\mathbf{R}$ to $\mathbf{C}^3$. The equivariant embeddings of space–time slices and surfaces of revolution are the restrictions of this embedding to $i\mathbf{R}\times\mathbf{R}$ and $\mathbf{R}\times\mathbf{R}$. In Sec. V, we address "boundary" questions of smoothness and embeddability.

II. INTRINSIC METRICS

We take the mathematical point of view that a "metric" comprises a metric tensor and a parameter domain (or manifold). Thus, a metric can be two-dimensional, compact, connected, oriented, etc.

Consider an oriented two-dimensional metric that admits a free, isometric action of the additive group $\mathbf{R}$. The interpretation of the symmetry depends on the signature: In Lorentz signature, the action should be viewed as time translation of a $(1+1)$-dimensional slice of a static space–time. In Riemannian signature, the action is something like a rotation about an axis, except that fixed points have been removed and the resulting metric lifted to its universal cover.

The existence of useful coordinate systems is independent of the metric signature, so for the moment we work with a Riemannian metric g.

A. Isothermal parameters

Away from fixed points of the action, existence of isothermal parameters is elementary: Construct nets of curves by taking orbits of the action and the associated g-orthogonal family. Clearly these curves are coordinate curves in which the metric is diagonal and the group action is a coordinate translation. A change of variable in the direction transverse to the action ensures that the diagonal metric components are equal; see Ref. 8 for details.

More precisely, our metric may be regarded as living on the planar domain $D:=\mathbf{R}\times(a,b)$ with coordinates (t,s), and with $\mathbf{R}$ acting by translation in t, Fig. 1. After changing s if necessary, there exists a smooth function $\varphi:(a,b)\to\mathbf{R}$ such that

$$g=\varphi(s)(\mathrm{d}t^2+\mathrm{d}s^2). \tag{2.1}$$

B. Action-angle coordinates

An additional change of transverse coordinate expresses the metric in *action-angle* (or *symplectic*) form

$$g = \phi(r)\mathrm{d}t^2 + \frac{1}{\phi(r)}\mathrm{d}r^2. \tag{2.2}$$

Indeed, set

$$r = \int^s \varphi(\zeta)\mathrm{d}\zeta, \quad \phi(r) = \varphi(s). \tag{2.3}$$

The integral equation defines r as a function of s (up to an additive constant) on each interval where φ is nonvanishing, and the resulting coordinate is easily shown to satisfy (2.2). The additive constant amounts to translation of the interval (a,b), and is geometrically harmless.

Given a nonvanishing function $\phi:(a,b)\to\mathbf{R}$, the equations

$$s = \int^r \frac{\mathrm{d}\zeta}{\phi(\zeta)}, \quad \varphi(s) = \phi(r), \tag{2.4}$$

define a translation-invariant, isothermal metric on D that satisfies (2.1). These constructions are inverse to each other up to isometry of g and domain translation of ϕ. In other words, an isometry class of g corresponds to a function ϕ that is unique up to translation in the domain. For reasons originating in symplectic geometry, this correspondence is called the *momentum construction*, and the function ϕ is called the *momentum profile* of g.

C. Elementary metric geometry

In action-angle coordinates, the arc length element along a generator, and the area form, are

$$\mathrm{d}\sigma = \frac{\mathrm{d}r}{\sqrt{\phi(r)}}, \quad \mathrm{d}A = \mathrm{d}r\ \mathrm{d}t. \tag{2.5}$$

The second formula highlights the geometric significance of the coordinate r: In a region of surface defined by the inequalities $c_1 \leqslant t \leqslant c_2$, the change in r is proportional to the enclosed surface area. On a surface of revolution where the t-interval $[0,2\pi]$ corresponds to one full turn, $2\pi r$ measures zonal area.

The Killing field $\mathrm{d}/\mathrm{d}t$ that generates the group action has squared length $\phi(r)$. This formula is meaningful even for metrics of Lorentz signature: The symmetry is time translation. For a Riemannian metric embedded as a surface of revolution in $\mathbf{R}^3$, one full turn of the surface is a t interval of length 2π, and $\sqrt{\phi(r)}$ is the Euclidean radius of the surface at r.

D. Gaussian curvature

The interplay between action-angle and isothermal (i.e., holomorphic) coordinates on a surface of revolution leads to a remarkable formula for the Gaussian curvature, see Ref. 8,

$$K = -\tfrac{1}{2}\phi''(r).$$

On the Lorentzian side, direct calculation shows that the Gaussian curvature of a space–time slice is

$$K = \tfrac{1}{2}\phi''(r).$$

In both signatures

$$K = -\tfrac{1}{2}g_{tt}''(r). \tag{2.6}$$

From the standpoint of constructing metrics of specified (e.g., constant) curvature, action-angle coordinates have the substantial advantage that the Gaussian curvature is a *linear* function of

the profile. Further, as we shall see, metrics presented in this form are explicitly embeddable in a flat ambient space.

E. Complexification

Regard t as a *complex* coordinate. The complex-valued tensor,

$$g_{\mathbf{C}} = \phi(r)\mathrm{d}t^2 + \frac{1}{\phi(r)}\mathrm{d}r^2,$$

on $\mathbf{C}\times(a,b)$ is real valued on $\mathbf{R}\times(a,b)$, where it is positive–definite, and on $i\mathbf{R}\times(a,b)$, where it has Lorentz signature. *Intrinsic Wick rotation* is the transformation $t\mapsto it$, under which g corresponds to

$$\hat{g} = -\phi(r)\mathrm{d}t^2 + \frac{1}{\phi(r)}\mathrm{d}r^2. \tag{2.7}$$

We assume from now on that the additive group $\mathbf{C}$ acts by translation in t. Since t is determined by the group action, while r is characterized by (2.2), the duality $g\leftrightarrow\hat{g}$ (which is defined using coordinates) actually depends only on $g_{\mathbf{C}}$. The metric $\hat{g}$ is the space–time slice associated to the surface of revolution g.

F. An example

Consider the momentum profile $\phi(r)=1-r^2$ on $(-1,1)$. By (2.4),

$$s = \int_0^r \frac{\mathrm{d}\zeta}{1-\zeta^2} = \frac{1}{2}\log\left|\frac{1+r}{1-r}\right|,$$

or $r=\tanh s$ and $\varphi(s)=\operatorname{sech}^2 s$. The arc length element and function are

$$\mathrm{d}\sigma = \frac{\mathrm{d}r}{\sqrt{1-r^2}}, \quad \sigma = \arcsin r, \quad \text{or } r=\sin\sigma.$$

If this metric is embedded isometrically in $\mathbf{R}^3$, the radius at r is $\sqrt{\phi(r)}=\sqrt{1-r^2}=\cos\sigma$. As should be clear, we are looking at the round metric of unit radius on a sphere, a fact that is confirmed (at least circumstantially) by the fact that the Gaussian curvature is $-\frac{1}{2}\phi''(r)=1$. The dual space–time slice is

$$\hat{g} = \frac{\mathrm{d}r^2}{1-r^2} - (1-r^2)\mathrm{d}t^2,$$

a portion of the well-known de Sitter metric, which embeds in $\mathbf{R}^{2+1}$ as (part of) a hyperboloid of one sheet. Figure 2 depicts the images at the same scale. The coordinate curves on the hyperboloid are not those of embedding coordinates. These classic embeddings are presented here to illuminate similarity; a formal relationship is developed below.

III. THE AMBIENT SPACE

Consider the ambient space $\mathbf{C}^3=\{(T,X,Y)\}$, and write $T=T_1+iT_2$, etc. Endow $\mathbf{C}^3$ with the flat metric

$$E = \mathrm{Re}(\mathrm{d}T^2+\mathrm{d}X^2+\mathrm{d}Y^2) = (\mathrm{d}T_1^2+\mathrm{d}X_1^2+\mathrm{d}Y_1^2) - (\mathrm{d}T_2^2+\mathrm{d}X_2^2+\mathrm{d}Y_2^2).$$

Euclidean space is identified with the totally real slice $\mathbf{R}^3\subset\mathbf{C}^3$, while Minkowski space is the three-dimensional subspace $i\mathbf{R}\times\mathbf{R}^2=\mathbf{R}^{2+1}$ defined by the equations $T_1=X_2=Y_2=0$. The *ambient Wick rotation* is the map $\mathsf{W}:(T,X,Y)\mapsto(iT,X,Y)$, which carries $\mathbf{R}^3$ to $\mathbf{R}^{2+1}$.

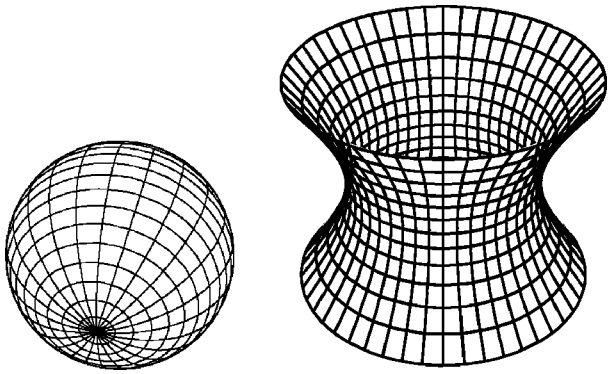

FIG. 2. Riemannian and Lorentzian embeddings of $\phi(r)=1-r^2$.

The ambient symmetry group that realizes the intrinsic symmetries of our surface metrics is the additive complex group acting as "(complex) rotation about the Y axis,"

$$\mathsf{R}_\theta(T,X,Y) = (X\sin\theta + T\cos\theta, X\cos\theta - T\sin\theta, Y). \tag{3.1}$$

A short calculation gives

$$\mathsf{W}^{-1}\mathsf{R}_{i\theta}\mathsf{W}(T,X,Y) = (X\sinh\theta + T\cosh\theta, X\cosh\theta + T\sinh\theta, Y).$$

This formula hints at the close relationship between rotations of Euclidean space and boosts of Minkowski space.

Henceforth, the ambient space is essentially $\mathbf{C}^2\times\mathbf{R}\subset\mathbf{C}^3$. In fact, the embeddings of primary interest take values in $\mathbf{C}\times\mathbf{R}\times\mathbf{R}$; only T is "really" complex. However, Eq. (3.1) shows that continuous interpolation of embeddings requires consideration of $\mathbf{C}^2=\mathbf{R}^{2,2}$.

Cylindrical coordinates: The *complex cylindrical coordinates* mappings $\Phi^\pm:\mathbf{C}^2\to\mathbf{C}^2$ are defined by

$$(T,X) = \Phi^+(\rho,\psi) = e^\rho(\sin\psi,\cos\psi),$$

$$(T,X) = \Phi^-(\rho,\psi) = ie^\rho(\cos\psi,-\sin\psi). \tag{3.2}$$

Two mappings are required to cover a dense open set in $\mathbf{C}^2$, see below. The ambient group action is coordinate translation,

$$\mathsf{R}_\theta\Phi^\pm(\rho,\psi) = \Phi^\pm(\rho,\psi+\theta).$$

The metric quadratic form $Q=t_1^2+x_1^2-t_2^2-x_2^2$ partitions $\mathbf{C}^2$ into sets of spacelike (for which Q is positive), timelike (for which Q is negative), and lightlike vectors. Each of these sets is a union of rays into the origin, so understanding these sets amounts to understanding the way each intersects the unit sphere $S^3=\{t_1^2+x_1^2+t_2^2+x_2^2=1\}$. The lightlike cone intersects the sphere in a real 2-torus whose complement consists of two linked solid tori. The real cones over these solid tori are the sets of spacelike and timelike vectors, and the mapping $(T,X)\mapsto(iX,-iT)$ (among others) involutively exchanges these sets. The image of Φ^+ is the set of spacelike vectors, so the image of Φ^- is the set of timelike vectors.

The pullback tensors $(\Phi^\pm)^*E$ express the metric E "in cylindrical coordinates,"

$$(\Phi^\pm)^*E = \pm e^{2\rho}(\mathrm{d}\psi^2+\mathrm{d}\rho^2) + \mathrm{d}Y^2. \tag{3.3}$$

It is straightforward to verify that the restrictions to the real three-dimensional ambient slices of interest satisfy

$$E^3 = e^{2\rho}(\mathrm{d}\psi^2 + \mathrm{d}\rho^2) + \mathrm{d}Y^2,$$

$$E^{2+1} = e^{2\rho}(-\mathrm{d}\psi^2 + \mathrm{d}\rho^2) + \mathrm{d}Y^2.$$

To check the second equation, it is necessary to use both cylindrical coordinate regions.

An equivariant embedding of a surface is one for which (intrinsic) t-translation is induced by ψ-translation in cylindrical coordinates.

IV. EMBEDDINGS

Fix a real constant $\kappa > 0$, let $\phi:(a,b)\to\mathbf{R}$ be a positive profile satisfying $|\phi'| \leqslant 2\kappa$, and let g be the metric on $\mathbf{C}\times(a,b)$ as in (2.2). The functions

$$T = \frac{1}{\kappa}\sqrt{\phi(r)}\sin(\kappa t), \qquad X = \frac{1}{\kappa}\sqrt{\phi(r)}\cos(\kappa t), \qquad Y = \int^r \sqrt{\frac{1}{\phi(\zeta)}\left[1 - \left(\frac{1}{2\kappa}\phi'(\zeta)\right)^2\right]}\,\mathrm{d}\zeta, \tag{4.1}$$

define a mapping $f:\mathbf{C}\times(a,b)\to\mathbf{C}^3$. (The function Y, which depends only on r, is well-defined up to an additive constant, which alters the mapping by an ambient translation.) Not incidentally, Y is real valued. To see that f is an isometric embedding of g into $(\mathbf{C}^3, E)$, use cylindrical coordinates,

$$\mathrm{d}\psi = \kappa\,\mathrm{d}t, \quad \mathrm{d}\rho = \frac{\phi'(r)}{2\phi(r)}\mathrm{d}r, \quad \mathrm{d}Y = \sqrt{\frac{1}{\phi(r)}\left[1 - \left(\frac{1}{2\kappa}\phi'(r)\right)^2\right]}\mathrm{d}r$$

so the pullback of E by f is

$$f^*E = e^{2\rho}(\mathrm{d}\psi^2 + \mathrm{d}\rho^2) + \mathrm{d}Y^2 = \frac{\phi(r)}{\kappa^2}\left(\kappa^2\mathrm{d}t^2 + \frac{\phi'(r)^2}{4\phi(r)^2}\mathrm{d}r^2\right) + \mathrm{d}Y^2 = \phi(r)\mathrm{d}t^2 + \frac{1}{\phi(r)}\mathrm{d}r^2 = g.$$

Observe that the embedding "decouples" in complex cylindrical coordinates, ψ is a function of t alone, while ρ and Y are functions of r alone. Since the ambient and intrinsic group actions are translations in ψ and t, respectively, equivariance of f is obvious.

A. Negative profiles

The embedding (4.1) was introduced under the condition that $\phi > 0$. If $\phi < 0$ on an interval, the wish that Y be real valued imposes the condition $|\phi'| \geqslant 2\kappa$. In this situation, we are led to define

$$T = \frac{1}{\kappa}\sqrt{-\phi(r)}\cos(\kappa t), \qquad X = -\frac{1}{\kappa}\sqrt{-\phi(r)}\sin(\kappa t), \qquad Y = \int^r \sqrt{\frac{1}{\phi(\zeta)}\left[1 - \left(\frac{1}{2\kappa}\phi'(\zeta)\right)^2\right]}\,\mathrm{d}\zeta. \tag{4.2}$$

The formal expression of this mapping in terms of the cylindrical coordinate mapping Φ^- is identical to that of (4.1) with respect to Φ^+. In particular, Eq. (4.2) defines an equivariant isometric embedding of the metric

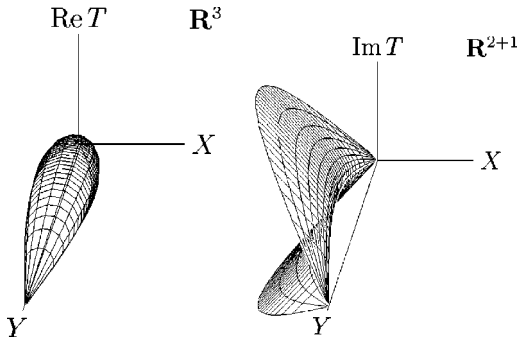

FIG. 3. A surface of revolution and the dual space–time slice.

$$g = \frac{1}{\phi(r)}\mathrm{d}r^2 + \phi(r)\mathrm{d}t^2, \quad \phi < 0,$$

into $\mathbf{C}^3$. Since $\phi<0$ but t is imaginary, the intrinsic coordinates have "switched roles," r is timelike and t is spacelike.

B. The Schwarzschild–de Sitter metric

The metrics associated to the positive portion of the profile $\phi(r)=1-(2/r)-(r^2/100)$ are depicted in Fig. 3. The X and Y axes are the real axes of the complex coordinate directions. The space–time slice that results is part of the Schwarzschild–de Sitter metric.

Each surface intersects the (X,Y) plane in the curve whose parametrization may be read off Eq. (4.1); the respective surfaces are swept out as this curve is acted on by a real or imaginary coordinate translation in ψ.

V. FIXED POINTS AND HORIZONS

In the preceding section we omitted points at which $\phi=0$, including fixed points of the group action and null lines in the ambient space. In this section, we investigate issues related to boundary conditions.

A. Riemannian signature

In the Riemannian situation, the profile is non-negative, $\sqrt{\phi(r)}$ is the length of the Killing field generating the group action, and a t interval of length $2\pi/\kappa$ corresponds to one full turn of the image surface. Consequently, the action has a fixed point at each zero of ϕ. To understand the significance of κ, we look more closely at the geometry of g near a fixed point.

Without loss of generality, we transform such that $\phi(0)=0$, and $\phi>0$ in some interval to the right of 0. The Taylor expansion is

$$\phi(r) = \phi'(0)r + o(r) \quad \text{near } r = 0.$$

Let θ be the cone angle at the vertex. Because the area element of g is $\mathrm{d}A=\mathrm{d}r\,\mathrm{d}t$, the portion of surface $0\leqslant r\leqslant\varepsilon$ has area $2\pi\varepsilon/\kappa$. The boundary curve $\{r=\varepsilon\}$ has circumference $2\pi\sqrt{\phi(\varepsilon)}/\kappa$. By elementary geometry, the cone angle is

$$\theta = \lim_{\varepsilon\to 0}\frac{\text{circumference}^2}{2\cdot\text{area}} = \frac{\pi}{\kappa}\phi'(0).$$

Since the image of the embedding is smooth at a fixed point iff $\theta=2\pi$, smoothness is equivalent to $\phi'(0)=2\kappa$. A similar argument holds if ϕ is positive to the left of 0: The embedding is smooth

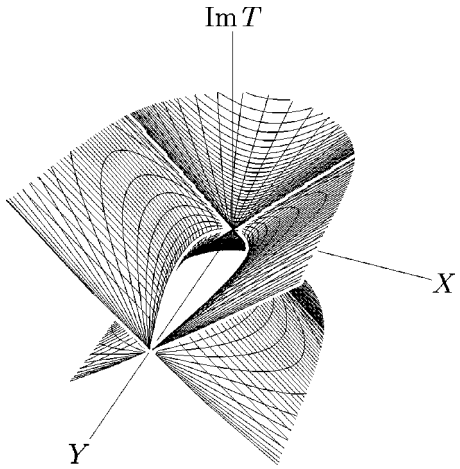

FIG. 4. Extension of the Schwarzschild–de Sitter embedding.

iff $\phi'(0)=-2\kappa$. Generally, $\phi'(0)$ is a measure of angular defect (also known as point curvature) at a fixed point.[2]

In Ref. 8, the value $\kappa=1$ was used tacitly. If $\kappa\neq 1$, it is appropriate to view the embedding (4.1) as taking values not in $\mathbf{R}^3$, but in a space that is flat away from the Y axis and has cone angle $2\pi/\kappa$ along the Y axis. If $|\phi'|=2$ at a zero of the profile, the embedding meets the Y axis perpendicularly; the intrinsic and ambient metric singularities have the same total angle.

B. Lorentz signature

Provided the radicand in the definition of Y is non-negative, the embedding of a space–time slice extends to intervals on which ϕ achieves negative values. Geometrically, a zero of the profile must map to a null line in $\mathbf{R}^{2+1}$, and the image of the embedding can cross from the spacelike portion of $\mathbf{R}^{2+1}$ to the timelike portion, see Fig. 4.

A *horizon* of an embedding is a curve in $\mathbf{R}^{2+1}$ along which the image is null. Intrinsically, a horizon comes from a zero of ϕ, where the space–time slice degenerates. A glance at (4.1) shows that the embedding is smooth at a horizon only if $|\phi'|=2\kappa$ and $\phi''<0$. There are two horizons in Fig. 4: one in the foreground (a cosmological horizon), and one containing the origin (the black hole horizon).

C. Embeddability criteria

Engman[5] studied momentum profiles and their associated surfaces of revolution, and characterized embeddability in terms of bounds on the total curvature of a disk centered at a fixed point. His bounds naturally have a space–time analogue, though a satisfactory topological interpretation is lacking due to noncompactness.

The portion of metric associated to a profile ϕ embeds iff the coordinate function Y in (4.1) is real valued. Non-negativity of the radicand is an obvious necessary condition, and is sufficient if the profile is (say) real analytic at each zero. If a metric associated to ϕ embeds, then at each point of the momentum interval one of the following conditions holds:

(i) $\phi>0$ and $|\phi'|\leqslant 2\kappa$,
(ii) $\phi<0$ and $|\phi'|\geqslant 2\kappa$,
(iii) $\phi=0$, $|\phi'|=2\kappa$.

In the Riemannian situation, the profile must be non-negative, and the metric embeds iff $|\phi'| \leqslant 2\kappa$. To obtain bounds on the total curvature of a disk, assume without loss of generality that $\kappa = 1$ (so that the ambient space is smooth), $\phi(0) = 0$, and $\phi'(0) = 2$. For $r_1 > 0$, the total curvature of the disk $D = \{0 \leqslant r \leqslant r_1\}$ is

$$\int_D K \, \mathrm{d}A = -\pi \int_0^{r_1} \phi''(r) \mathrm{d}r = \pi(2 - \phi'(r_1)).$$

We read off at once that the metric embeds iff the total curvature of an arbitrary disk (centered at the fixed point) is between 0 and 4π. A similar analysis holds for profiles that are positive to the left of a zero.

The upper bound is topologically significant: By the Gauss–Bonnet theorem, a surface of revolution generated by a profile that vanishes twice has total curvature 4π, even if the surface is not smooth at a fixed point. There are two ways the upper bound can be achieved by a profile satisfying $\phi(0) = 0$ and $\phi'(0) = 2$: The profile can become too steep (downward), or vanish at some $r_1 > 0$. In either case, ϕ no longer defines an embedding.

The space–time situation is analogous to an extent: There is an embeddability criterion in terms of total curvature, which has the expected sign change from the Riemannian case. Because the symmetry group is noncompact, we must speak of curvature *per unit time*. Further, it is meaningful to speak of embeddings defined by negative profiles, so there are two cases to consider. As above, we assume ϕ is a profile satisfying $\phi(0) = 0$ and $\phi'(0) = \pm 2\kappa$, and that ϕ is nonvanishing between 0 and r_1 for some $r_1 > 0$.

If $\phi > 0$, embeddability is equivalent to the pointwise inequality $|\phi'| \leqslant 2\kappa$. Integrating the curvature form $K \, \mathrm{d}A$ over a t interval of length 1 and the r interval $[0, r_1]$, we find that the total curvature per unit time is nonpositive, but no less than -4π, in every neighborhood of the horizon $r = 0$.

If $\phi < 0$, embeddability is equivalent to the bounds $|\phi'| \geqslant 2\kappa$. By an entirely analogous argument, the total curvature over $[0, r_1]$ is either $\geqslant 2\pi$ or is nonpositive. However, total curvature is a continuous function of r_1, and since the total curvature vanishes in the limit as $r_1 \to 0$, the first bound cannot hold for arbitrary r_1.

We conclude that embeddability of a piece of space–time metric associated to a negative profile implies that the metric has nonpositive total curvature in every neighborhood of the horizon, regardless of the sign of the profile. In an interval where the profile is positive, the total curvature is no smaller than -4π, while if the profile is negative, there is no *a priori* lower bound on the total curvature.

Nonpositivity of the total curvature implies the observation made in Ref. 7, if $\phi'(0) = 2\kappa \neq 0$ then the metric embeds in a neighborhood of the horizon if $\phi'' < 0$.

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On the resolvent and spectral functions of a second order differential operator with a regular singularity

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We consider the resolvent of a second order differential operator with a regular singularity, admitting a family of self-adjoint extensions. We find that the asymptotic expansion for the resolvent in the general case presents unusual powers of λ which depend on the singularity. The consequences for the pole structure of the ζ function, and for the small-t asymptotic expansion of the heat kernel, are also discussed. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1809257]

I. INTRODUCTION

It is well known that in quantum field theory under external conditions, quantities like vacuum energies and effective actions, which describe the influence of boundaries or external fields on the physical system, are generically divergent and require a renormalization to get a physical meaning.

In this context, a powerful and elegant regularization scheme to deal with these problems is based on the use of the ζ function[1,2] or the heat kernel (for recent reviews see, for example, Refs. 3–7) associated to the relevant differential operators appearing in the quadratic part of the actions. In this way, ground state energies, heat-kernel coefficients, functional determinants, and partition functions for quantum fields can be given in terms of the corresponding ζ function, where the ultraviolet divergent pieces of the one-loop contributions are encoded as poles of its holomorphic extension.

Thus, it is of major interest in Physics to determine the singularity structure of ζ functions associated with these physical models.

In particular,[8] for an elliptic boundary value problem in a ν-dimensional compact manifold with boundary, described by a differential operator A of order ω, with smooth coefficients and a ray of minimal growth, defined on a domain of functions subject to local boundary conditions, the ζ function

$$\zeta_A(s) := \mathrm{Tr}\{A^{-s}\} \tag{1.1}$$

has a meromorphic extension to the complex s plane whose singularities are isolated simple poles at $s=(\nu-j)/\omega$, with $j=0,1,2,\ldots$.

In the case of positive definite operators, the ζ function is related, via Mellin transform, to the trace of the heat kernel of the problem, and the pole structure of $\zeta_A(s)$ determines the small-t asymptotic expansion of this trace,[8,9]

$$\mathrm{Tr}\{e^{-tA}\} \sim \sum_{j=0}^{\infty} a_j(A) t^{(j-\nu)/\omega}, \tag{1.2}$$

where the coefficients are related to the residues by

$$a_j(A) = \mathrm{Res}|_{s=(\nu-j)/\omega}\, \Gamma(s)\zeta_A(s). \tag{1.3}$$

For operators of the form $-\partial_x^2+V(x)$ with a singular potential $V(x)$ asymptotic to κ/x^2 as $x\to 0$, this expansion is substantially different. If $\kappa \geqslant 3/4$, the operator is essentially self-adjoint. This case has been treated in Refs. 10–12, where log terms are found, as well as terms with coefficients which are distributions concentrated at the singular point $x=0$. For the case $\kappa > -1/4$, the Friedrichs extension has been treated in Ref. 13 for operators in $\mathbf{L_2}(0,1)$, and in Ref. 14 for operators in $\mathbf{L_2}(\mathbf{R}^+)$, making use of the scale invariance of the operator domain and explicit representations of the resolvent. Moreover, as a particular case of a manifold with an isolated conic singularity, Ref. 15 gave a description of the boundary behavior of the Friedrichs heat kernel which does not make use of the resolvent, and showed via boundary maps how it can be used to construct the heat kernel for other self-adjoint extensions of these operators, showing explicitly the first two terms in the asymptotic expansion of the trace of their difference.

On the other hand, Ref. 16 gave the pole structure of the ζ function of a second order differential operator defined on the (noncompact) half-line $\mathbf{R}^+$, having a singular zeroth order term $V(x)=\kappa\, x^{-2}+x^2$. It showed that, for a certain range of real values of κ, this operator admits nontrivial self-adjoint extensions in $\mathbf{L_2}(\mathbf{R}^+)$, for which the associated ζ function (given by an integral representation) presents isolated simple poles which (in general) do not lie at $s=(1-j)/2$ for $j=0,1,\ldots$ [as would be the case for a regular $V(x)$], and can even take irrational values.

A similar structure has been noticed in Ref. 17 for the singularities of the ζ and η functions of a system of first order differential operators with a singular zeroth order term $\sim g\, x^{-1}$, which also admits a family of self-adjoint extensions for real g taking values in a certain range. It has been shown that, in the general case, the asymptotic expansion of the resolvent contains g-dependent powers of λ which make the ζ and η functions to present poles lying at points which depend on the singularity, with residues depending on the self-adjoint extension.

Let us mention that singular potentials $\sim 1/x^2$ have been considered in the description of several physical systems, like the Calogero model,[16,18–20] conformal invariant quantum mechanical models[21–23] and, more recently, the dynamics of quantum particles in the asymptotic near-horizon region of black-holes.[24–28] The self-adjoint extensions of these operators have also been considered in Ref. 29. Moreover, singular superpotentials has been considered as possible agents of supersymmetry breaking in models of supersymmetric quantum mechanics.[30–32]

It is the aim of the present paper to analyze the behavior of the resolvent, the ζ function and the trace of the heat kernel of a second order differential operator with a regular singularity in a compact segment, $D_x=-\partial_x^2+g(g-1)x^{-2}$, for those values of g for which it admits a family of self-adjoint extensions.

Following the scheme developed in Ref. 17, we will show that the asymptotic expansion for the resolvent in the general case presents powers of λ which depend on the singularity, and can even take irrational values. The consequence of this behavior on the corresponding ζ function is the presence of simple poles lying at points which also depend on the singularity, with residues depending on the self-adjoint extension considered.

We first construct the resolvents for two particular extensions, for which the boundary condition at the singular point $x=0$ is invariant under the scaling $x\to c\,x$. The resolvent expansion for these special extensions displays the usual powers, leading to the usual poles for the ζ function (and the usual structure for the asymptotic expansion of the heat-kernel trace).

The resolvents of the remaining extensions are convex linear combinations of these special extensions, but the coefficients in the convex combination depend on the eigenvalue parameter λ. This dependence leads to unusual powers in the resolvent expansion, and hence to unusual poles for the zeta function (and unusual powers in the asymptotic expansion of the heat-kernel trace).

These self-adjoint extensions are not invariant under the scaling $x \to c\,x$. As $c \to 0$ they tend (at least formally) to one of the invariant extensions, and as $c \to \infty$ they tend to the other. As $c \to 0$ the residues at the anomalous poles tend to zero, whereas as $c \to \infty$ these residues become infinite. The way these residues depend on the boundary condition is explained by a scaling argument in Sec. VII.

The structure of the paper is as follows: In Sec. II we define the operator and determine its self-adjoint extensions for $\frac{1}{2} < g < \frac{3}{2}$, and in Sec. III we study their spectra. In Sec. IV we construct the resolvent for a general extension as a linear combination of the resolvent of two limiting cases, and in Sec. V we consider the traces of these operators. The asymptotic expansions of these traces, evaluated in Sec. VI, are used in Sec. VII to construct the associated ζ function and study its singularities, as well as the small-t asymptotic expansion of the heat-kernel trace. The special case $g = \frac{1}{2}$ is considered in Appendix A.

II. THE OPERATOR AND ITS SELF-ADJOINT EXTENSIONS

Let us consider the differential operator,

$$D_x = -\frac{d^2}{dx^2} + \frac{g(g-1)}{x^2}, \tag{2.1}$$

with $g \in \mathbb{R}$, defined on a domain of smooth functions with compact support in a segment, $\mathcal{D}(D) = C_0^\infty(0,1)$. It can be easily seen that D_x so defined is symmetric.

The adjoint operator D_x^*, which is the maximal extension of D_x, is defined on the domain $\mathcal{D}(D_x^*)$ of functions $\phi(x) \in \mathbf{L_2}(0,1)$, having a locally sumable second derivative and such that

$$D_x\phi(x) = -\phi''(x) + \frac{g(g-1)}{x^2}\phi(x) = f(x) \in \mathbf{L_2}(0,1). \tag{2.2}$$

Lemma 2.1: If $\phi(x) \in \mathcal{D}(D_x^*)$ *and* $\frac{1}{2} < g < \frac{3}{2}$, *then* (the case $g = \frac{1}{2}$ will be considered separately, in Appendix A)

$$\left| \phi(x) - \left(\frac{C_1[\phi]x^g + C_2[\phi]x^{1-g}}{\sqrt{2g-1}} \right) \right| \leqslant \frac{\|D_x\phi(x)\|}{(3/2-g)\sqrt{2g+1}} x^{3/2} \tag{2.3}$$

and

$$\left| \phi'(x) - \left(\frac{gC_1[\phi]x^{g-1} + (1-g)C_2[\phi]x^{-g}}{\sqrt{2g-1}} \right) \right| \leqslant \frac{3/2\|D_x\phi(x)\|}{(3/2-g)\sqrt{2g+1}} x^{1/2} \tag{2.4}$$

for some constants $C_1[\phi]$ *and* $C_2[\phi]$, *where* $\|\cdot\|$ *is the* $\mathbf{L_2}$ *norm.*

Proof: Let us write $\phi(x) = x^g u(x)$. Then, Eq. (2.2) implies

$$u'(x) = K_2 x^{-2g} - x^{-2g}\int_0^x y^g f(y)\mathrm{d}y,$$

$$u(x) = K_1 + \frac{K_2}{1-2g}x^{1-2g} - \int_0^x y^{-2g}\int_0^y z^g f(z)\mathrm{d}z\ \mathrm{d}y, \tag{2.5}$$

for some constants K_1 and K_2. Now, taking into account that

$$\left| \int_0^x y^g f(y) dy \right| \leqslant \frac{x^{g+1/2}}{\sqrt{2g+1}} \|f\|,$$

$$\left| \int_0^x y^{-2g} \int_0^y z^g f(z) \mathrm{dz}\ \mathrm{dy} \right| \leqslant \frac{x^{3/2-g}}{(3/2-g)\sqrt{2g+1}} \|f\|, \tag{2.6}$$

we immediately get Eqs. (2.3) and (2.4).

Lemma 2.2: Let $\phi(x), \psi(x) \in \mathcal{D}(D^*)$ *and* $\frac{1}{2} < g < \frac{3}{2}$. *Then*

$$(D_x\psi, \phi) - (\psi, D_x\phi) = \{C_1[\psi]^* C_2[\phi] - C_2[\psi]^* C_1[\phi]\} + \{\psi(1)^* \phi'(1) - \psi'(1)^* \phi(1)\}. \tag{2.7}$$

Proof: From Eq. (2.2) one easily obtains

$$(D_x\psi, \phi) - (\psi, D_x\phi) = \lim_{\varepsilon \to 0^+} \int_\varepsilon^1 \partial_x \{\psi(x)^* \phi'(x) - \psi'(x)^* \phi(x)\} \mathrm{dx}, \tag{2.8}$$

from which, taking into account the results in Lemma 2.1, Eq. (2.7) follows directly.

Now, if $\psi(x)$ in Eq. (2.7) belongs to the domain of the closure of D_x, $\overline{D_x} = (D_x^*)^*$,

$$\psi(x) \in \mathcal{D}(\overline{D_x}) \subset \mathcal{D}(D_x^*), \tag{2.9}$$

then the right-hand side of Eq. (2.7) must vanish for any $\phi(x) \in \mathcal{D}(D_x^*)$. Therefore

$$C_1[\psi] = C_2[\psi] = \psi(1) = \psi'(1) = 0. \tag{2.10}$$

On the other hand, if $\psi(x), \phi(x)$ belong to the domain of a symmetric extension of D_x [contained in $\mathcal{D}(D_x^*)$], the right-hand side of Eq. (2.7) must also vanish.

Thus, the closed extensions of D_x correspond to the subspaces of $\mathbb{C}^4$ under the map $\Phi \to (C_1[\Phi], C_2[\Phi], \phi(1), \phi'(1))$, and the self-adjoint extensions correspond to those subspaces $S \subset \mathbb{C}^4$ such that $S = S^\perp$, with the orthogonal complement taken in the sense of the symplectic form on the right-hand side of Eq. (2.7).

For definiteness, in the following we will consider self-adjoint extensions satisfying the local boundary condition:

$$\phi(1) = 0. \tag{2.11}$$

Each such extension is determined by a condition of the form

$$\alpha C_1[\Phi] + \beta C_2[\Phi] = 0, \tag{2.12}$$

with $\alpha, \beta \in \mathbb{R}$, and $\alpha^2 + \beta^2 = 1$. We denote this extension by $D_x^{(\alpha,\beta)}$.

III. THE SPECTRUM

In order to determine the spectrum of the self-adjoint extensions of D_x for $\frac{1}{2} < g < \frac{3}{2}$, we need the solutions of

$$(D_x - \lambda)\phi_\lambda(x) = 0, \tag{3.1}$$

satisfying the boundary conditions in Eqs. (2.11) and (2.12).

The general solution of the homogeneous equation for $\lambda = 0$ is

$$\phi_0(x) = \frac{1}{\sqrt{2g-1}} (C_1 x^g + C_2 x^{1-g}), \tag{3.2}$$

and the boundary conditions in Eqs. (2.11) and (2.12) imply that

$$C_1 + C_2 = 0, \quad \alpha C_1 + \beta C_2 = 0. \tag{3.3}$$

Consequently, there are no zero modes except for the self-adjoint extension characterized by $\alpha = \beta = 1/\sqrt{2}$.

For $\lambda \neq 0$, the solutions of Eq. (3.1) are of the form

$$\phi(x) = \frac{C_1}{\sqrt{2g-1}} \frac{\Gamma(\frac{1}{2}+g)}{2^{1/2-g}\mu^{g-1/2}} \sqrt{x} J_{g-1/2}(\mu x) + \frac{C_2}{\sqrt{2g-1}} \frac{\Gamma(\frac{3}{2}-g)}{2^{g-1/2}\mu^{1/2-g}} \sqrt{x} J_{1/2-g}(\mu x), \tag{3.4}$$

where $\mu = +\sqrt{\lambda}$, and the μ-dependent coefficients have been introduced for later convenience.

Taking into account that

$$J_\nu(z) = z^\nu \left\{ \frac{1}{2^\nu \Gamma(1+\nu)} + O(z^2) \right\}, \tag{3.5}$$

we get from Eqs. (2.3) and (2.12),

$$\alpha\, C_1 + \beta\, C_2 = 0. \tag{3.6}$$

On the other hand, the condition in Eq. (2.11) implies

$$\phi(1) = \frac{C_1}{\sqrt{2g-1}} \frac{\Gamma(\frac{1}{2}+g)}{2^{1/2-g}\mu^{g-1/2}} J_{g-1/2}(\mu) + \frac{C_2}{\sqrt{2g-1}} \frac{\Gamma(\frac{3}{2}-g)}{2^{g-1/2}\mu^{1/2-g}} J_{1/2-g}(\mu) = 0. \tag{3.7}$$

For $\alpha = 0$, Eq. (3.6) implies $C_2 = 0$ (Dirichlet boundary conditions at the origin). Therefore, $\phi(1) = 0 \Rightarrow J_{g-1/2}(\mu) = 0$. Thus, the spectrum of this self-adjoint extension is positive and nondegenerate, with the eigenvalues of $D_x^D := D_x^{(0,1)}$ given by

$$\lambda_n = j_{g-1/2,n}^2, \quad n = 1, 2, \ldots, \tag{3.8}$$

where $j_{\nu,n}$ is the nth positive zero of the Bessel function $J_\nu(z)$. [Let us recall that large zeros of $j_{\nu,}(\lambda)$ have the asymptotic expansion

$$j_{\nu,n} \simeq \gamma - \frac{4\nu^2 - 1}{8\gamma} + O\left(\frac{1}{\gamma}\right)^3, \tag{3.9}$$

with $\gamma = \left[n + (\nu/2) - \frac{1}{4}\right]\pi$.]

For $\alpha \neq 0$, from Eqs. (3.6) and (3.7) we easily get the following transcendental equation for the eigenvalues of $D_x^{(\alpha,\beta)}$:

$$F(\mu) := \mu^{2g-1} \frac{J_{1/2-g}(\mu)}{J_{g-1/2}(\mu)} = \rho(\alpha, \beta), \tag{3.10}$$

where we have defined

$$\rho(\alpha, \beta) := \frac{\beta}{\alpha} \frac{2^{2g-1}\Gamma(\frac{1}{2}+g)}{\Gamma(\frac{3}{2}-g)}. \tag{3.11}$$

For the positive eigenvalues $\lambda = \mu^2$, both sides in Eq. (3.10) have been plotted in Fig. 1, for particular values of $\rho(\alpha, \beta)$ and g.

Moreover, if $\beta/\alpha > 1 \Rightarrow \rho(\alpha, \beta) > \rho(\alpha, \alpha)$, and the extension $D_x^{(\alpha,\beta)}$ has a negative eigenvalue. Indeed, if $\lambda_- = (i\mu)^2 < 0$, then

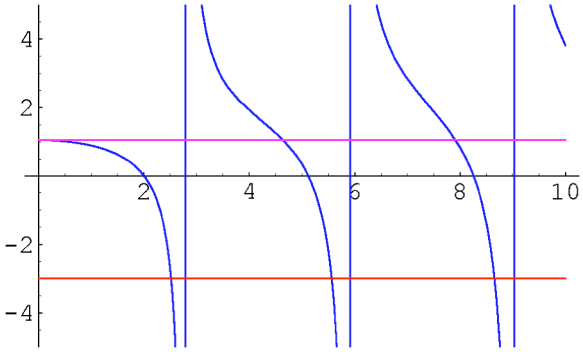

FIG. 1. Plot for $F(\mu)$, $\rho(\alpha,\beta)=-3$ and $\rho(\alpha,\alpha)$, with $g=3/4$.

$$F(i\mu)=\mu^{2g-1}\frac{I_{1/2-g}(\mu)}{I_{g-1/2}(\mu)}=2^{2g-1}\frac{\Gamma(\frac{1}{2}+g)}{\Gamma(\frac{3}{2}-g)}\left\{1+\frac{(2g-1)\mu^2}{(3-2g)(1+2g)}+O(\mu^4)\right\}, \tag{3.12}$$

where $I_\nu(\mu)$ is the modified Bessel function. For a plot, see Fig. 2. (It can be seen that this negative eigenvalue goes to $-\infty$ as $\alpha\to 0$, while the corresponding eigenfunction tends to concentrate tends to concentrate on the singularity at $x=0$. See also Ref. 33.)

Notice that the spectrum is always nondegenerate, and there is a positive eigenvalue between each pair of consecutive squared zeros of $J_{g-1/2}(\lambda)$. Therefore, from Eq. (3.9) we get $\lambda_n=\pi^2\, n^2+O(n)$.

In particular, for the $\beta=0$ extension (which we call the "N-extension"), $D_x^N:=D_x^{(1,0)}$, it can be seen from Eq. (3.10) that the eigenvalues are given by

$$\lambda_n=j_{1/2-g,n}^2, \quad n=1,2,\ldots, \tag{3.13}$$

where $j_{1/2-g,n}^2$ are the positive zeros of $J_{1/2-g}(\mu)$.

IV. THE RESOLVENT

In this section we will construct the resolvent of D_x,

$$G(\lambda)=(D_x-\lambda)^{-1}, \tag{4.1}$$

for its different self-adjoint extensions when $\frac{1}{2}<g<\frac{3}{2}$.

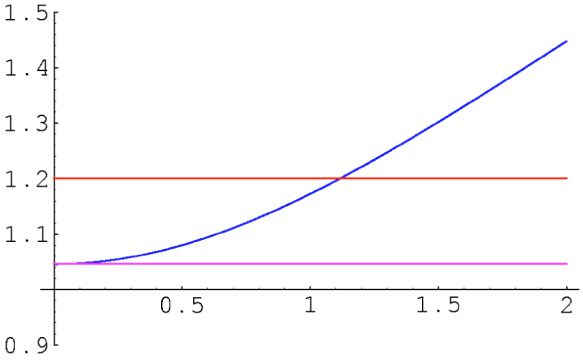

FIG. 2. Plot for $F(i\,\mu)$, $\rho(\alpha,\beta)=1.2$ and $\rho(\alpha,\alpha)$, with $g=3/4$.

We will first consider the two limiting cases in Eq. (2.12), namely the "*D*-extension," for which $\alpha=0\Rightarrow C_2[\phi]=0$, and the "*N*-extension," with $\beta=0\Rightarrow C_1[\phi]=0$. The resolvent for a general self-adjoint extension will be later evaluated as a linear combination of those obtained for these two limiting cases.

For the kernel of the resolvent we have

$$(D_x-\mu^2)G(x,y;\mu^2)=\delta(x-y), \tag{4.2}$$

where $\mu^2=\lambda$, with $-\pi/2<\arg(\mu)\leqslant\pi/2$.

To proceed, we need some particular solutions of the homogeneous equation (3.1). Then, let us define

$$L^D(x,\mu)=\sqrt{x}J_{g-1/2}(\mu x),$$

$$L^N(x,\mu)=\sqrt{x}J_{1/2-g}(\mu x),$$

$$R(x,\mu)=\sqrt{x}(J_{1/2-g}(\mu)J_{g-1/2}(\mu x)-J_{g-1/2}(\mu)J_{1/2-g}(\mu x)). \tag{4.3}$$

Notice that $R(1,\mu)=0$.

We will also need the Wronskians,

$$W[L^D(x,\mu),R(x,\mu)]=\frac{2\cos(g\pi)}{\pi}J_{g-1/2}(\mu)=\frac{1}{\gamma_D(\mu)},$$

$$W[L^N(x,\mu),R(x,\mu)]=\frac{2\cos(g\pi)}{\pi}J_{1/2-g}(\mu)=\frac{1}{\gamma_N(\mu)}, \tag{4.4}$$

which vanish only at the zeros of $J_\nu(\mu)$, for $\nu=\pm\left(g-\frac{1}{2}\right)$.

A. The resolvent for the *D*-extension

In this case, the function

$$\phi(x)=\int_0^1 G_D(x,y;\mu^2)f(y)\mathrm{d}y \tag{4.5}$$

must satisfy $\phi(1)=0$ and $C_2[\phi]=0$, for any function $f(x)\in\mathbf{L_2}(0,1)$.

This requires that

$$G_D(x,y;\mu^2)=\gamma_D(\mu)\times\begin{cases}L^D(x,\mu)R(y,\mu) & \text{for } x\leqslant y,\\ R(x,\mu)L^D(y,\mu) & \text{for } x\geqslant y.\end{cases} \tag{4.6}$$

The fact that the boundary conditions are satisfied, as well as $(D_x-\mu^2)\phi(x)=f(x)$, can be straightforwardly verified from Eqs. (4.3) and (4.4).

Indeed, from Eqs. (4.5), (4.6), (4.3), and (4.4), one gets

$$\phi(x)=\frac{C_1^D[\phi]}{\sqrt{2g-1}}x^g+O(x^{3/2}), \tag{4.7}$$

with

$$C_1^D[\phi]=\frac{\pi\mu^{g-1/2}\sqrt{2g-1}}{2^{1/2+g}\cos(g\pi)J_{g-1/2}(\mu)\Gamma(\frac{1}{2}+g)}\int_0^1 R(y,\mu)f(y)\mathrm{d}y, \tag{4.8}$$

for μ not a zero of $J_{g-1/2}(\mu)$.

Notice that $C_1^D[\phi] \neq 0$ if the integral on the right-hand side of Eq. (4.8) is nonvanishing.

B. The resolvent for the *N*-extension

In this case, the function

$$\phi(x) = \int_0^1 G_N(x,y;\mu^2) f(y) \mathrm{d}y \tag{4.9}$$

must satisfy $\phi(1)=0$ and $C_1[\phi]=0$, for any function $f(x) \in \mathbf{L_2}(0,1)$.

This requires that

$$G_N(x,y;\mu^2) = \gamma_N(\mu) \times \begin{cases} L^N(x,\mu) R(y,\mu) & \text{for } x \leqslant y, \\ R(x,\mu) L^N(y,\mu) & \text{for } x \geqslant y. \end{cases} \tag{4.10}$$

These boundary conditions, as well as the fact that $(D_x - \mu^2)\phi(x) = f(x)$, can be straightforwardly verified from Eqs. (4.3) and (4.4).

In this case, from Eqs. (4.9), (4.10), (4.3), and (4.4), one gets

$$\phi(x) = \frac{C_2^N[\phi]}{\sqrt{2g-1}} x^{1-g} + O(x^{3/2}), \tag{4.11}$$

with

$$C_2^N[\phi] = \frac{\pi \mu^{1/2-g} \sqrt{2g-1}}{2^{3/2-g} \cos(g\pi) J_{1/2-g}(\mu) \Gamma(\frac{3}{2}-g)} \int_0^1 R(y,\mu) f(y) \mathrm{d}y, \tag{4.12}$$

for μ not a zero of $J_{1/2-g}(\mu)$.

Notice that $C_2^N[\phi] \neq 0$ if the integral on the right-hand side of Eq. (4.12) [the same integral as the one appearing in the *D*-extension, Eq. (4.8)] is nonvanishing.

C. The resolvent for a general self-adjoint extension of D_x

For the general case, we can adjust the boundary conditions

$$\phi(1) = 0, \quad \alpha C_1[\phi] + \beta C_2[\phi] = 0, \quad \alpha, \beta \neq 0, \tag{4.13}$$

for

$$\phi(x) = \int_0^1 G(x,y;\lambda) f(y) \mathrm{d}y, \tag{4.14}$$

for any $f(x) \in \mathbf{L_2}(0,1)$, by taking a linear combination of the resolvent for the limiting cases,

$$G(x,y;\lambda) = [1 - \tau(\lambda)] G_D(x,y;\lambda) + \tau(\lambda) G_N(x,y;\lambda). \tag{4.15}$$

Since the boundary condition at $x=1$ is automatically fulfilled, one must just impose

$$\alpha[1 - \tau(\lambda)] C_1^D[\phi] + \beta \tau(\lambda) C_2^N[\phi] = 0. \tag{4.16}$$

Notice that, in view of Eqs. (4.8), (4.12), and (3.10),

$$\alpha C_1^D[\phi] - \beta C_2^N[\phi] = 0, \tag{4.17}$$

precisely when $\lambda = \mu^2$ is an eigenvalue of $D_x^{(\alpha,\beta)}$. Therefore, from Eq. (4.16) we get the resolvent of $D_x^{(\alpha,\beta)}$ by setting

$$\tau(\mu^2)=\frac{\alpha C_1^D[\phi]}{\alpha C_1^D[\phi]-\beta C_2^N[\phi]}=\frac{1}{1-\rho(\alpha,\beta)\mu^{1-2g}\dfrac{J_{g-1/2}(\mu)}{J_{1/2-g}(\mu)}}, \tag{4.18}$$

for μ not a zero of $J_{1/2-g}(\mu)$.

V. THE TRACE OF THE RESOLVENT

It follows from Eq. (4.15) that the resolvent of a general self-adjoint extension of D_x can be expressed in terms of the resolvents of the two limiting cases, $G_D(\lambda)$ and $G_N(\lambda)$. Moreover, since the eigenvalues of any extension grow as n^2 (see Sec. III), these resolvents are trace class operators.

Then, we have

$$\mathrm{Tr}\{G(\lambda)\}=\mathrm{Tr}\{G_D(\lambda)\}-\tau(\lambda)[\mathrm{Tr}\{G_D(\lambda)\}-\mathrm{Tr}\{G_N(\lambda)\}]. \tag{5.1}$$

From Eqs. (4.6) and (4.10) we straightforwardly get (see Appendix B for the details)

$$\mathrm{Tr}\{G_D(\mu^2)\}=\int_0^1 \mathrm{tr}\{G_D(x,x;\mu^2)\}\mathrm{d}x=\frac{J_{1/2+g}(\mu)}{2\mu J_{g-1/2}(\mu)}=\frac{2g-1}{4\mu^2}-\frac{J'_{g-1/2}(\mu)}{2\mu J_{g-1/2}(\mu)} \tag{5.2}$$

and

$$\mathrm{Tr}\{G_N(\mu^2)\}=\int_0^1 \mathrm{tr}\{G_N(x,x;\mu^2)\}\mathrm{d}x=\frac{J_{3/2-g}(\mu)}{2\mu J_{1/2-g}(\mu)}=-\frac{2g-1}{4\mu^2}-\frac{J'_{1/2-g}(\mu)}{2\mu J_{1/2-g}(\mu)}, \tag{5.3}$$

where we have taken into account that

$$J_{\nu+1}(z)=\frac{\nu}{z}J_\nu(z)-J'_\nu(z). \tag{5.4}$$

Finally, we get

$$\mathrm{Tr}\{G(\mu^2)\}=\left\{\frac{2g-1}{4\mu^2}-\frac{J'_{g-1/2}(\mu)}{2\mu J_{g-1/2}(\mu)}\right\}-\tau(\mu^2)\left\{\frac{2g-1}{2\mu^2}-\frac{1}{2\mu}\left(\frac{J'_{g-1/2}(\mu)}{J_{g-1/2}(\mu)}-\frac{J'_{1/2-g}(\mu)}{J_{1/2-g}(\mu)}\right)\right\}. \tag{5.5}$$

VI. ASYMPTOTIC EXPANSION FOR THE TRACE OF THE RESOLVENT

Using the Hankel asymptotic expansion for Bessel functions[34] (see Appendix C), we get for the first term on the right-hand side of Eq. (5.5),

$$\mathrm{Tr}\{G_D(\mu^2)\}\sim\sum_{k=1}^{\infty}\frac{A_k(g,\sigma)}{\mu^k}=\frac{i\sigma}{2\mu}+\frac{g}{2\mu^2}-\frac{i\sigma g(g-1)}{4\mu^3}+\frac{g(g-1)}{4\mu^4}+O(\mu^{-5}), \tag{6.1}$$

where $\sigma=1$ for $\Im(\mu)>0$, and $\sigma=-1$ for $\Im(\mu)<0$. The coefficients in this series can be straightforwardly evaluated from Eqs. (C8) and (C19). Notice that $A_k(g,-1)=A_k(g,1)^*$, since $A_{2k}(g,1)$ is real and $A_{2k+1}(g,1)$ is pure imaginary.

Similarly, from (C22) we simply get for the second factor in the second term on the right-hand side of Eq. (5.5),

$$\mathrm{Tr}\{G_D(\mu^2)-G_N(\mu^2)\}\sim\frac{2g-1}{2\mu^2}. \tag{6.2}$$

Finally, taking into account Eq. (C12), we have

$$\tau(\mu^2) \sim \frac{1}{1 - e^{\sigma i\pi(g-1/2)}\rho(\alpha,\beta)\mu^{1-2g}} \sim \sum_{k=0}^{\infty} (e^{\sigma i\pi(g-1/2)}\rho(\alpha,\beta)\mu^{1-2g})^k, \tag{6.3}$$

where $\sigma=1$ ($\sigma=-1$) corresponds to $\Im(\mu)>0$ ($\Im(\mu)<0$).

Notice the appearance of g-dependent powers of μ in this asymptotic expansion.

VII. THE ζ FUNCTION AND THE TRACE OF THE HEAT KERNEL

The ζ function for a general self-adjoint extension of D_x is defined, for $\Re(s)>1/2$, as

$$\zeta(s) = -\frac{1}{2\pi i}\oint_C \lambda^{-s}\,\mathrm{Tr}\{\mathrm{G}(\lambda)\}\mathrm{d}\lambda, \tag{7.1}$$

where the curve $\mathcal{C}$ encircles counterclockwise the spectrum of the operator, keeping to the left of the origin. According to Eq. (5.1), we have

$$\zeta(s) = \zeta^D(s) + \frac{1}{2\pi i}\oint_C \lambda^{-s}\tau(\lambda)\mathrm{Tr}\{\mathrm{G}_D(\lambda) - G_N(\lambda)\}\mathrm{d}\lambda, \tag{7.2}$$

where $\zeta^D(s)$ is the ζ function for the D-extension.

Since, according to the discussion in Sec. III, D_x^D has a positive spectrum, and the self-adjoint extension $D_x^{(\alpha,\beta)}$ has at most one negative eigenvalue, we can write

$$\zeta^{(\alpha,\beta)}(s) = \zeta^D(s) + \Theta(s) - \frac{1}{2\pi i}\int_{-i\infty+0}^{i\infty+0} \lambda^{-s}\tau(\lambda)\mathrm{Tr}\{G_D(\lambda) - G_N(\lambda)\}\mathrm{d}\lambda, \tag{7.3}$$

where $\Theta(s)=\lambda_-^{-s}$ if there is a negative eigenvalue, and vanishes otherwise.

We can also write

$$\zeta^{(\alpha,\beta)}(s) = \frac{e^{-i(\pi/2)s}}{\pi}\int_1^{\infty} \mu^{1-2s}\,\mathrm{Tr}\{G((e^{i(\pi/4)}\mu)^2)\}\mathrm{d}\mu + \frac{e^{i(\pi/2)s}}{\pi}\int_1^{\infty} \mu^{1-2s}\,\mathrm{Tr}\{G((e^{-i(\pi/4)}\mu)^2)\}\mathrm{d}\mu + h_1(s), \tag{7.4}$$

where $h_1(s)$ is an entire function. [The cut of the complex plane has been chosen to lie on the left half-plane. So, a negative real number can be written as $\lambda_-=e^{i\theta}|\lambda_-|$, where θ can take the value $+\pi$ or $-\pi$, depending on the position of the cut. In any case, $\Theta(s)=\lambda_-^{-s}=e^{-is\theta}|\lambda_-|^{-s}$ is an entire function, and the value of θ has no effects on the singular part of the ζ function.] Therefore, in order to determine the poles of $\zeta^{(\alpha,\beta)}(s)$, we can subtract and add a partial sum of the asymptotic expansion obtained in the preceding section to $\mathrm{Tr}\{G(\lambda)\}$ in the integrands on the right-hand side of Eq. (7.4).

In so doing, we get for the D-extension and for a real $s>1/2$,

$$\begin{aligned}\zeta^D(s) &= \frac{1}{\pi}\sum_{\sigma=\pm1}\int_1^{\infty} e^{-i\sigma(\pi/2)s}\mu^{1-2s}\left\{\sum_{k=1}^{N} e^{-i\sigma(\pi/4)k}A_k(g,\sigma)\mu^{-k}\right\}\mathrm{d}\mu + h_2(s)\\ &= \frac{1}{\pi}\sum_{k=1}^{N}\frac{\Re\{e^{-i(\pi/2)(s+k/2)}A_k(g,1)\}}{s-(1-k/2)} + h_2(s),\end{aligned} \tag{7.5}$$

where $h_2(s)$ is holomorphic in the open half-plane $\Re(s)>(1-N)/2$.

Consequently, the meromorphic extension of $\zeta^D(s)$ presents simple poles at

$$s = 1 - k/2 \quad \text{for } k = 1,2,3,\ldots, \tag{7.6}$$

with residues

$$\text{Res } \zeta^D(s)_{s=1-k/2} = -\frac{1}{\pi}\Re\{iA_k(g,1)\}, \tag{7.7}$$

where the coefficients $A_k(g,1)$ are given in Eq. (6.1). Notice that these residues vanish for even k.

In particular, for $s=1/2$ ($k=1$) one gets

$$\text{Res } \zeta^D(s)\,|_{s=1/2} = -\frac{1}{\pi}\Re\{iA_1(g,1)\} = \frac{1}{2\pi}. \tag{7.8}$$

This is the unique pole present in $\zeta^D(s)$ for the $g=1$ case, where there is no singularity in the 0th order coefficient of D_x.

For a general self-adjoint extension $D_x^{(\alpha,\beta)}$, we must also consider the singularities coming from the asymptotic expansion of $\tau(\lambda)\text{Tr}\{G_D(\lambda)-G_N(\lambda)\}$ in Eq. (5.1), given in Eqs. (6.2) and (6.3).

From Eq. (7.3), and taking into account Eq. (7.4), for real $s>1/2$ we can write

$$\zeta^{(\alpha,\beta)}(s)-\zeta^D(s) = h_3(s) - \frac{2g-1}{2\pi}\sum_{\sigma=\pm1} e^{-i\sigma(\pi/2)(s+1)}\int_1^\infty \mu^{-1-2s}\left\{\sum_{k=0}^{N}(e^{i\sigma(\pi/2)(g-1/2)}\rho(\alpha,\beta)\mu^{1-2g})^k\right\}\mathrm{d}\mu$$

$$= -\left(\frac{2g-1}{2\pi}\right)\sum_{k=0}^{N}\frac{1}{s-(\frac{1}{2}-g)k}\Re\{e^{i(\pi/2)((g-1/2)k-s-1)}\rho(\alpha,\beta)^k\} + h_3(s), \tag{7.9}$$

where $h_3(s)$ is holomorphic for $\Re(s)>(\frac{1}{2}-g)(N+1)$.

Therefore, $(\zeta^{(\alpha,\beta)}(s)-\zeta^D(s))$ has a meromorphic extension which presents simple poles located at negative g-dependent positions,

$$s = -(g-\tfrac{1}{2})k \quad \text{for } k=1,2,\ldots, \tag{7.10}$$

with residues which depend on the self-adjoint extension given by

$$\text{Res}\{\zeta^{(\alpha,\beta)}(s)-\zeta^D(s)\}\,|_{s=(1/2-g)k} = -\left(\frac{2g-1}{2\pi}\right)\rho(\alpha,\beta)^k\sin\left[\frac{\pi}{2}(2g-1)k\right]. \tag{7.11}$$

Notice that these poles are irrational for irrational values of g. Moreover, the residues vanish for the "N-extension" ($\rho(\alpha,0)=0$), and have a singular limit for $\alpha\to0$.

In particular, these poles for the $g=1$ case (for which there are no singularity in the zeroth order term of D_x) are negative half-integers, since in this case the residues vanish for even k.

It is interesting to notice that the poles in Eq. (7.10) are also poles of the ζ function of the corresponding self-adjoint extension of the operator $-\partial_x^2+g(g-1)x^{-2}+x^2$ in $\mathbf{L}_2(\mathbb{R}^+)$ considered in Ref. 16, with exactly the same residues, as can be easily verified.

Let us remark that when $\alpha\neq0$ the residue of $\zeta^{(\alpha,\beta)}$ at $s=-(g-\frac{1}{2})k$ is a constant times $(\beta/\alpha)^k$. This is consistent with the behavior of D_x under the scaling isometry $Tu(x)=c^{1/2}u(cx)$ taking $\mathbf{L_2}(0,1)\to\mathbf{L_2}(0,1/c)$. The extension $D_x^{(\alpha,\beta)}$ is unitarily equivalent to the operator $(1/c^2)\dot{D}_x^{(\alpha',\beta')}$ similarly defined on $\mathbf{L_2}(0,1/c)$, with $\alpha'=c^{-g}\alpha$ and $\beta'=c^{g-1}\beta$,

$$T\,D_x^{(\alpha,\beta)} = \frac{1}{c^2}\dot{D}_x^{(\alpha',\beta')}\,T. \tag{7.12}$$

Notice that only for the extensions with $\alpha=0$ or $\beta=0$ the boundary condition at the singular point $x=0$, Eq. (2.12), is left invariant by this scaling.

Therefore, we have for the ζ function of the scaled problem

$$\dot{\zeta}^{(\alpha',\beta')}(s) = c^{-2s}\zeta^{(\alpha,\beta)}(s), \tag{7.13}$$

and for the residues

$$\text{Res}\,\{\zeta^{(\alpha',\beta')}(s)\}\,|_{s=(1/2-g)k} = c^{(2g-1)k}\,\text{Res}\,\{\zeta^{(\alpha,\beta)}(s)\}\,|_{s=(1/2-g)k}. \tag{7.14}$$

The factor $c^{(2\,g-1)k}$ exactly cancels the effect the change in the boundary condition at the singularity has on $\rho(\alpha,\beta)$,

$$\rho(\alpha,\beta)^k = c^{(1-2g)k}\rho(\alpha',\beta')^k. \tag{7.15}$$

Then, the difference between the intervals $(0,1)$ and $(0,1/c)$ has no effect on the structure of these residues, which presumably are determined locally in a neighborhood of $x=0$.

In this way we conclude that, for a general self-adjoint extension, the presence of poles in the ζ function located at g-dependent positions is a consequence of the singular behavior ($\sim x^{-2}$) of the zeroth order term in D_x near the origin, together with a scaling noninvariant boundary condition at the singularity.

Finally, let us remark that the relation between the ζ function and the trace of the heat kernel of $D_x^{(\alpha,\beta)}$,

$$\zeta^{(\alpha,\beta)}(s) = \frac{1}{\Gamma(s)}\int_0^1 t^{s-1}\,\text{Tr}\{e^{-tD_x^{(\alpha,\beta)}}\}\,dt + H(s), \tag{7.16}$$

where $H(s)$ is an entire function, straightforwardly lead to the following small-t asymptotic expansion:

$$\text{Tr}\{e^{-tD_x^{(\alpha,\beta)}} - e^{-tD_x^{D}}\} \sim \left(g-\frac{1}{2}\right) - \sum_{k=1}^{\infty}\left\{\Gamma\left(\left[\frac{1}{2}-g\right]k\right)\frac{2g-1}{2\pi}\rho(\alpha,\beta)^k \sin\left[\frac{\pi}{2}(2g-1)k\right]\right\}t^{(g-1/2)k}. \tag{7.17}$$

The first term on the right-hand side, coming from Eq. (6.2) and the first term in the asymptotic expansion of $\tau(\lambda)$ in Eq. (6.3), coincides with the result reported in Ref. 15. Notice also the g-dependent powers of t appearing in the asymptotic series on the right-hand side of Eq. (7.17) for any general self-adjoint extension [except for the "N-extension," for which $\rho(\alpha,0)=0$]. In particular, the first term in this series reduces to

$$-\frac{\beta}{\alpha}\frac{2^{2g-1}}{\Gamma(\frac{1}{2}-g)}t^{g-1/2}. \tag{7.18}$$

This power of t also coincides with the result quoted in Ref. 15, but we find a different coefficient.

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APPENDIX A: THE CASE $g=1/2$

The case $g=1/2$, for which the differential operator D_x takes the form

$$D_x = -\frac{d^2}{dx^2} - \frac{1}{4\,x^2}, \tag{A1}$$

requires a separate consideration which we briefly present in this appendix.

Along the same lines as in the proof of Lemma 2.1, it is straightforward to show that, if $\phi(x) \in \mathcal{D}(D_x^*)$, then

$$|\phi(x) - (C_1[\phi]\sqrt{x} + C_2[\phi]\sqrt{x}\,\log x)| \leqslant \frac{\|D_x\phi(x)\|}{\sqrt{2}}x^{3/2} \tag{A2}$$

and

$$\left|\phi'(x) - \left[\frac{1}{2}C_1[\phi]x^{-1/2} + C_2[\phi]\left(x^{-1/2} + \frac{1}{2}x^{-1/2}\,\log x\right)\right]\right| \leqslant \frac{3}{2\sqrt{2}}\|D_x\phi(x)\|x^{1/2} \tag{A3}$$

for some constants $C_1[\phi]$ and $C_2[\phi]$, where $\|\cdot\|$ stands for the $\mathbf{L_2}$ norm.

Therefore, it is easy to see that Eq. (2.7) is also valid in the present case, and the self-adjoint extensions of D_x correspond again to those subspaces $S\subset\mathbb{C}^4$ such that $S=S^{\perp}$, with the orthogonal complement taken in the sense of the symplectic form on the right-hand side of Eq. (2.7).

If, in addition, we select the Dirichlet condition at $x=1$, $\phi(1)=0$, the remaining self-adjoint extensions of D_x correspond to a one-parameter family characterized by Eq. (2.12), $D_x^{(\alpha,\beta)}$.

There exists a particular self-adjoint extension for which $C_2[\phi]=0$, namely $D_x^D := D_x^{(0,1)}$, such that the functions in its domain behave near the origin as

$$\phi(x) = C_1[\phi]\sqrt{x} + O(x^{3/2}). \tag{A4}$$

The eigenfunction of D_x^D corresponding to the eigenvalue λ is given by

$$\phi(x) = C_1[\phi]\sqrt{x}J_0(\mu x), \tag{A5}$$

where $\lambda=\mu^2$ and μ is a (positive) zero of $J_0(\mu)$.

For an arbitrary self-adjoint extension $D_x^{(\alpha,\beta)}$ with $\alpha\neq 0$, the eigenfunction corresponding to the eigenvalue $\lambda=\mu^2$ is given by

$$\phi(x) = \{C_1[\phi] - C_2[\phi](\log\,\mu - \log\,2 + \gamma)\}\sqrt{x}J_0(\mu x) + \frac{\pi}{2}C_2[\phi]\sqrt{x}N_0(\mu x), \tag{A6}$$

where $C_1[\phi]$, $C_2[\phi]$ are constrained by Eq. (2.12). The condition $\phi(1)=0$ leads to the equation

$$(\theta - \log\,\mu)J_0(\mu) + \frac{\pi}{2}N_0(\mu) = 0, \tag{A7}$$

where $\theta=-\beta/\alpha+\log 2-\gamma$, which determines the spectrum of $D_x^{(\alpha,\beta)}$. Notice that there are no negative eigenvalues.

In order to determine the kernels of the resolvents $\mathcal{G}^D(\mu^2) := (D_x^D-\mu^2)^{-1}$ and $\mathcal{G}^{(\alpha,\beta)}(\mu^2) := (D_x^{(\alpha,\beta)}-\mu^2)^{-1}$, we define

$$\mathcal{L}^D(x;\mu) = \sqrt{x}J_0(\mu x),$$

$$\mathcal{L}^{(\alpha,\beta)}(x;\mu) = \sqrt{x}\left\{(\theta - \log\,\mu)J_0(\mu x) + \frac{\pi}{2}N_0(\mu x)\right\},$$

$$\mathcal{R}(x;\mu) = \sqrt{x}\{N_0(\mu)J_0(\mu x) - J_0(\mu)N_0(\mu x)\}, \tag{A8}$$

to get

$$\mathcal{G}^D(x,y;\mu^2) = \frac{1}{W[\mathcal{L}^D(x;\mu),\mathcal{R}(x;\mu)]}\times\begin{cases}\mathcal{L}^D(x;\mu)\mathcal{R}(y;\mu), & x\leqslant y,\\ \mathcal{L}^D(y;\mu)\mathcal{R}(x;\mu), & x\geqslant y,\end{cases} \tag{A9}$$

and

$$\mathcal{G}^{(\alpha,\beta)}(x,y;\mu^2)=\frac{1}{W[\mathcal{L}^{(\alpha,\beta)}(x;\mu),\mathcal{R}(x;\mu)]}\times\begin{cases}\mathcal{L}^{(\alpha,\beta)}(x;\mu)\mathcal{R}(y;\mu), & x\leqslant y,\\ \mathcal{L}^{(\alpha,\beta)}(y;\mu)\mathcal{R}(x;\mu), & x\geqslant y,\end{cases} \tag{A10}$$

where the Wronskians can be easily computed from (A8),

$$W[\mathcal{L}^{D}(x;\mu),\mathcal{R}(x;\mu)]=\frac{2}{\pi}J_0(\mu),$$

$$W[\mathcal{L}^{(\alpha,\beta)}(x;\mu),\mathcal{R}(x;\mu)]=\frac{2}{\pi}(\theta-\log\,\mu)J_0(\mu)+N_0(\mu). \tag{A11}$$

From Eq. (3.9), it can be seen that both $\mathcal{G}^{D}(\lambda)$ and $\mathcal{G}^{(\alpha,\beta)}(\lambda)$ are trace class operators.

Now, taking into account that[34,35]

$$\int x\,Z_1(0,x)Z_2(0,x)\mathrm{d}x=\frac{x^2}{2}\{Z_1(0,x)Z_2(0,x)+Z_1(1,x)Z_2(1,x)\}, \tag{A12}$$

where $Z_{1,2}(\nu,x)=J_\nu(x)$ or $N_\nu(x)$, the traces of the resolvents can be readily computed to get

$$\mathrm{Tr}\{\mathcal{G}^{D}(\mu^2)\}=\int_0^1\mathcal{G}^{D}(x,x;\mu^2)\mathrm{d}x=\frac{1}{2\mu}\frac{J_1(\mu)}{J_0(\mu)},$$

$$\mathrm{Tr}(\mathcal{G}^{(\alpha,\beta)(\mu^2)})=\int_0^1\mathcal{G}^{(\alpha,\beta)}(x,x;\mu^2)\mathrm{d}x=\frac{1}{2\mu}\frac{\frac{2}{\pi}(\theta-\log\,\mu)J_1(\mu)+N_1(\mu)}{\frac{2}{\pi}(\theta-\log\,\mu)J_0(\mu)+N_0(\mu)}. \tag{A13}$$

From Eqs. (C6) and (C7) one straightforwardly gets the same asymptotic expansion for these two traces,

$$\begin{aligned}\mathrm{Tr}\{\mathcal{G}^{D}(\mu^2)\}&\sim\frac{e^{i\sigma(\pi/2)}}{2\mu}\left(\frac{P(1,\mu)-i\sigma\,Q(1,\mu)}{P(0,\mu)-i\sigma\,Q(0,\mu)}\right)\\&\sim\mathrm{Tr}(\mathcal{G}^{(\alpha,\beta)}(\mu^2))\sim\sum_{k=1}^{\infty}\frac{A_k(1/2,\sigma)}{\mu^k}=\frac{i\,\sigma}{2\mu}+\frac{1}{4\,\mu^2}+\frac{i\,\sigma}{16\mu^3}-\frac{1}{16\,\mu^4}+O(\mu^{-5}),\end{aligned} \tag{A14}$$

where $\sigma=+1\ (-1)$ for $\Im(\mu)>0\ (\Im(\mu)<0)$.

Notice that the asymptotic series in Eq. (A14) coincides with the right-hand side of Eq. (6.1) evaluated at $g=1/2$. Therefore, from Eq. (7.5) one concludes that, in the present case, $\zeta^{(\alpha,\beta)}(s)$ has simple poles only at $s=1-k/2$, for $k=1,2,3,\ldots$, with residues given by

$$\mathrm{Res}\ \zeta^{D}(s)\,|_{s=1-k/2}=-\frac{1}{\pi}\Re\{iA_k(1/2,1)\} \tag{A15}$$

(vanishing for even k) for all the self-adjoint extensions of D_x.

So, in contrast to the case of $1/2<g<3/2$, the pole structure of the ζ function for $g=1/2$ is independent of the self-adjoint extension considered and does not differ from the usual one.

APPENDIX B: EVALUATION OF THE TRACES OF THE RESOLVENTS

In this appendix we briefly describe the evaluation of the traces appearing in Sec. V.

From Eq. (4.6) we get for the kernel of $G_D(\lambda)$ on the diagonal

$$G_D(x,x;\mu^2) = \gamma_D x\{J_{1/2-g}(\mu)J_{g-1/2}(\mu\, x)^2 - J_{g-1/2}(\mu)J_{g-1/2}(\mu\, x)J_{1/2-g}(\mu)\}. \tag{B1}$$

Therefore, in order to evaluate its trace it is sufficient to know the primitives[35,36]

$$\int xJ_\nu^2(\mu\, x)\mathrm{d}x = \frac{x^2}{2}\{J_\nu(x\,\mu)^2 - J_{\nu-1}(x\,\mu)J_{\nu+1}(x\,\mu)\} \tag{B2}$$

and

$$\int xJ_\nu(\mu\, x)J_{-\nu}(\mu\, x)\mathrm{d}x = \frac{-\nu^2}{\mu^2\Gamma(1-\nu)\Gamma(1+\nu)}\left[{}_1F_2(\{-1/2\},\{-\nu,\nu\},-x^2\mu^2) - 1\right], \tag{B3}$$

where

$$\begin{aligned}{}_1F_2(\{-1/2\},\{-\nu,\nu\},-x^2\mu^2) = -\frac{\pi x^2\mu^2\csc(\pi\nu)}{4\nu}&\{J_{-1-\nu}(x\,\mu)J_{-1+\nu}(x\,\mu) + 2\,J_{-\nu}(x\,\mu)J_\nu(x\,\mu)\\ &+ J_{1-\nu}(x\,\mu)J_{1+\nu}(x\,\mu)\}.\end{aligned} \tag{B4}$$

These primitives, together with the relation

$$J_{\nu-1}(z) + J_{\nu+1}(z) = \frac{2\nu}{z}J_\nu(z), \tag{B5}$$

necessary to simplify the intermediate results, straightforwardly lead to Eq. (5.2).

Similarly, for the kernel of $G_N(\lambda)$ on the diagonal we have

$$G_N(x,x;\mu^2) = \gamma_N\, x\{-J_{g-1/2}(\mu)J_{1/2-g}(\mu\, x)^2 + J_{1/2-g}(\mu)J_{1/2-g}(\mu\, x)J_{g-1/2}(\mu\, x)\}. \tag{B6}$$

The same argument as before leads to Eq. (5.3).

APPENDIX C: THE HANKEL EXPANSION

To develop an asymptotic expansion for the trace of the resolvent we employ the Hankel asymptotic expansion for the Bessel functions which, for completeness, we briefly describe in this appendix.

For $|z|\to\infty$, with ν fixed and $|\arg z| < \pi$, we have[34]

$$J_\nu(z) \sim \left(\frac{2}{\pi\, z}\right)^{1/2}\{P(\nu,z)\cos\,\chi(\nu,z) - Q(\nu,z)\sin\,\chi(\nu,z)\} \tag{C1}$$

and

$$N_\nu(z) \sim \left(\frac{2}{\pi\, z}\right)^{1/2}\{P(\nu,z)\sin\,\chi(\nu,z) + Q(\nu,z)\cos\,\chi(\nu,z)\}, \tag{C2}$$

where

$$\chi(\nu,z) = z - \left(\frac{\nu}{2} + \frac{1}{4}\right)\pi, \tag{C3}$$

$$P(\nu,z) \sim \sum_{k=0}^{\infty}\frac{(-1)^k\,\Gamma(\frac{1}{2}+\nu+2k)}{(2k)!\,\Gamma(\frac{1}{2}+\nu-2k)}\frac{1}{(2z)^{2k}}, \tag{C4}$$

and

$$Q(\nu,z) \sim \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(\frac{1}{2}+\nu+2k+1)}{(2k+1)!\,\Gamma(\frac{1}{2}+\nu-2k-1)} \frac{1}{(2z)^{2k+1}}. \tag{C5}$$

Moreover, $P(-\nu,z)=P(\nu,z)$ and $Q(-\nu,z)=Q(\nu,z)$, since these functions depend only on ν^2 (see Ref. 34, p. 364).

Therefore,

$$J_\nu(z) \sim \frac{e^{-i\sigma z}\, e^{i\sigma\pi[(\nu/2)+1/4]}}{\sqrt{2\pi z}} \{P(\nu,z) - i\sigma\, Q(\nu,z)\}, \tag{C6}$$

where $\sigma=1$ for z in the upper open half-plane and $\sigma=-1$ for z in the lower open half-plane.

Similarly,

$$N_\nu(z) \sim i\sigma \frac{e^{-i\sigma z}\, e^{i\sigma\pi[(\nu/2)+1/4]}}{\sqrt{2\pi z}} \{P(\nu,z) - i\sigma\, Q(\nu,z)\}, \tag{C7}$$

with $\sigma=1$ if $\Im(z)>0$ and $\sigma=-1$ for $\Im(z)<0$.

In these equations,

$$P(\nu,z) - i\sigma\, Q(\nu,z) \sim \sum_{k=0}^{\infty} \langle \nu,k\rangle \left(\frac{-i\sigma}{2z}\right)^k, \tag{C8}$$

where the coefficients

$$\langle \nu,k\rangle = \frac{\Gamma(\frac{1}{2}+\nu+k)}{k!\,\Gamma(\frac{1}{2}+\nu-k)} = \langle -\nu,k\rangle \tag{C9}$$

are the Hankel symbols.

For the quotient of two Bessel functions we have

$$\frac{J_{\nu_1}(z)}{J_{\nu_2}(z)} \sim e^{i\sigma(\pi/2)(\nu_1-\nu_2)} \frac{P(\nu_1,z) - i\sigma\, Q(\nu_1,z)}{P(\nu_2,z) - i\sigma\, Q(\nu_2,z)}, \tag{C10}$$

where $\sigma=1$ for $\Im(z)>0$ and $\sigma=-1$ for $\Im(z)<0$. The coefficients of this asymptotic expansion can be easily obtained, to any order, from Eq. (C8),

$$\frac{P(\nu_1,z) \pm i\, Q(\nu_1,z)}{P(\nu_2,z) \pm i\, Q(\nu_2,z)} \sim 1 + (\langle \nu_1,1\rangle - \langle \nu_2,1\rangle)\left(\frac{\pm i}{2z}\right) + O\left(\frac{1}{z^2}\right). \tag{C11}$$

In particular,

$$\frac{J_{1/2-g}(z)}{J_{g-1/2}(z)} \sim e^{i\sigma\pi(1/2-g)} \frac{P(\frac{1}{2}-g,z) - i\sigma\, Q(\frac{1}{2}-g,z)}{P(g-\frac{1}{2},z) - i\sigma\, Q(g-\frac{1}{2},z)} = e^{i\sigma\pi(1/2-g)}, \tag{C12}$$

since $P(\nu,z)$ and $Q(\nu,z)$ are even in ν.

Similarly, the derivative of the Bessel function has the following asymptotic expansion[34] for $|\arg z|<\pi$:

$$J'_\nu(z) \sim -\frac{2}{\sqrt{2\pi z}} \{R(\nu,z)\sin\,\chi(\nu,z) + S(\nu,z)\cos\,\chi(\nu,z)\} \tag{C13}$$

and

$$N'_\nu(z) \sim \frac{2}{\sqrt{2\pi z}}\{R(\nu,z)\cos\,\chi(\nu,z) - S(\nu,z)\sin\,\chi(\nu,z)\}, \tag{C14}$$

where

$$R(\nu,z) \sim \sum_{k=0}^{\infty}(-1)^k \frac{\nu^2+(2k)^2-1/4}{\nu^2-(2k-1/2)^2}\frac{\langle \nu,2k\rangle}{(2z)^{2k}} \tag{C15}$$

and

$$S(\nu,z) \sim \sum_{k=0}^{\infty}(-1)^k \frac{\nu^2+(2k+1)^2-1/4}{\nu^2-(2k+1-1/2)^2}\frac{\langle \nu,2k+1\rangle}{(2z)^{2k+1}}. \tag{C16}$$

Then,

$$J'_\nu(z) \sim \mp i\frac{e^{\mp iz}\,e^{\pm i\pi[(\nu/2)+1/4]}}{\sqrt{2\pi z}}\{R(\nu,z) \mp i\,S(\nu,z)\}, \tag{C17}$$

where the upper sign is valid for $\Im(\lambda)>0$, and the lower one for $\Im(\lambda)<0$. We have also

$$R(\nu,z) \pm i\,S(\nu,z) = P(\nu,z) \pm i\,Q(\nu,z) + T_\pm(\nu,z), \tag{C18}$$

with

$$T_\pm(\nu,z) \sim \sum_{k=1}^{\infty}(2k-1)\langle \nu,k-1\rangle\left(\frac{\pm i}{2z}\right)^k. \tag{C19}$$

Therefore, we get

$$\frac{J'_\nu(z)}{J_\nu(z)} \sim \mp i\left\{1+\frac{T_\mp(\nu,z)}{P(\nu,z)\mp iQ(\nu,z)}\right\}, \tag{C20}$$

where the upper sign is valid for $\Im(\lambda)>0$, and the lower one for $\Im(\lambda)<0$. The coefficients of the asymptotic expansion on the right-hand side of Eq. (C20) can be easily obtained from Eqs. (C8) and (C19),

$$\frac{T_\pm(\nu,z)}{P(\nu,z)\pm iQ(\nu,z)} = \left(\frac{\pm i}{2z}\right) + O\left(\frac{1}{z^2}\right). \tag{C21}$$

Finally, since the Hankel symbols are even in ν [see Eq. (C9)], from Eqs. (C8), (C19), and (C20) we have

$$\frac{J'_\nu(z)}{J_\nu(z)} \sim \frac{J'_{-\nu}(z)}{J_{-\nu}(z)}. \tag{C22}$$

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Deformations of loop algebras and integrable systems: hierarchies of integrable equations

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Using special quasigraded Lie algebras, that could be viewed as deformations of loop algebras, we obtain new hierarchies of integrable nonlinear equations admitting zero-curvature representations. In particular, we obtain integrable hierarchies that generalize the Heisenberg magnet, Landau–Lifshitz, and anisotropic chiral field hierarchies. We also obtain a new type of $so(3)$ anisotropic chiral field equation along with its higher rank generalization. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1804229]

I. INTRODUCTION

It is known that integrability of equations of $1+1$ field theory and condensed matter physics is based on the possibility to represent them in the form of the so-called zero-curvature equations:[1–3]

$$\frac{\partial U(x,t,\lambda)}{\partial t} - \frac{\partial V(x,t,\lambda)}{\partial x} + [U(x,t,\lambda), V(x,t,\lambda)] = 0, \tag{1}$$

where U, V are the matrix-valued functions, depending on the dynamical variables (fields), their derivatives with respect to the "space" coordinate x and an additional complex parameter λ usually called "spectral."

The most convenient interpretation of zero-curvature equations, that has arisen independently in Refs. 4 and 5 for the case of the rational dependence of $U-V$ pair on λ, is to consider them as a consistency condition for a set of a commuting Hamiltonian flows on the dual space to some infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ of matrix-valued function of λ written in the Euler–Arnold (generalized Lax) form

$$\frac{\partial L(\lambda)}{\partial t_l} = ad^*_{\nabla I_l(L(\lambda))} L(\lambda), \quad \frac{\partial L(\lambda)}{\partial t_k} = ad^*_{\nabla I_k(L(\lambda))} L(\lambda), \tag{2}$$

where $L(\lambda) \in \tilde{\mathfrak{g}}^*$ is the generic element of the dual space, $\nabla I_k(L(\lambda)) \in \tilde{\mathfrak{g}}$ is the algebra-valued gradient of $I_k(L(\lambda))$, and the "Hamiltonians" $I_k(L(\lambda)), I_l(L(\lambda))$ belong to the set of mutually commuting with respect to the natural Lie–Poisson bracket functions on $\tilde{\mathfrak{g}}^*$. Consistency condition of Eqs. (2) coincides with Eq. (1), where $U \equiv \nabla I_k$, $V \equiv \nabla I_l$, $x \equiv t_k$, $t \equiv t_l$ for some fixed indices k and l. Requiring Eq. (1) to be true for all degrees of spectral parameter λ we obtain a self-consistent system of differential equations in the dynamical variables—coordinate functions on $\tilde{\mathfrak{g}}^*$. In this way we obtain a lot of equations in partial derivatives that are labeled by the two commuting Hamiltonians I_k and I_l. The set of such equations with different l and fixed k (i.e., with fixed space variable $x \equiv t_k$) constitutes so-called *integrable hierarchy*.[3]

Hence, in order to construct integrable hierarchies in the framework of the described earlier approach it is necessary to construct infinite family of commuting Hamiltonians on the dual space

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to some infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ of the algebra-valued functions of one complex variable λ. From the fact that not for arbitrary dependence of U, V on λ corresponding Eq. (1) have nontrivial solutions,[6] it follows that not for all algebras $\tilde{\mathfrak{g}}$ this program could be realized. That is why very special Lie algebras $\tilde{\mathfrak{g}}$ admitting some algorithm of construction of infinite set of mutually commuting functions on $\tilde{\mathfrak{g}}^*$ are required in this approach. The most powerful of such algorithms is the famous Kostant–Adler scheme.[7,8] In particular, it is known[2,4,5,9] that applying it to the graded loop algebras $L(\mathfrak{g})=\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$ it is possible to obtain almost all known integrable equations.

The main purpose of the present paper is to extend applications of the approach of Refs. 4 and 5 to construction of integrable differential equations in order to obtain new hierarchies of integrable differential equations in partial derivatives. For this purpose we construct a new class of infinite-dimensional Lie algebras to which the Kostant–Adler scheme may be applied. Contrary to the loop algebras they are not graded but possess a weaker property of a *quasigradation*. Constructed quasigraded Lie algebras are *continuous multiparametric deformations* of the graded loop algebras $L(\mathfrak{g})$. Matrix elements of a certain matrice A serve for the parameters of the deformation. We denote the corresponding infinite-dimensional Lie algebras by $\tilde{\mathfrak{g}}_A$. We study the properties of the obtained algebras $\tilde{\mathfrak{g}}_A$ in detail. We construct their coadjoint representations and infinite sets of coadjoint invariants $\{I_k^m\}$. Restricting these invariants onto subspaces $(\tilde{\mathfrak{g}}_A^{\pm})^*$, where $\tilde{\mathfrak{g}}_A=\tilde{\mathfrak{g}}_A^+ + \tilde{\mathfrak{g}}_A^-$, we obtain two infinite sets of polynomial functions $\{I_k^{m\pm}\}$. From the framework of the Kostant–Adler scheme it follows that the functions $\{I_k^{m\pm}\}$ mutually commute inside each set: $\{I_k^{m\pm}, I_l^{n\pm}\}=0$, where $\{,\}$ is the standard Lie–Poisson bracket on $\tilde{\mathfrak{g}}_A$. In such a way we obtain two sets of integrable equations: the first set is generated by pairs of the Hamiltonians $\{I_k^{m+}\}$ and $\{I_l^{n+}\}$ and associated with the Lie algebra $\tilde{\mathfrak{g}}_A^+$ and the second set is associated with the Lie algebra $\tilde{\mathfrak{g}}_A^-$ and pairs of the Hamiltonians $\{I_k^{m-}\}$ and $\{I_l^{n-}\}$. Besides, like in the case of the ordinary loop algebras,[2] the scope of the Kostant–Adler (K–A) scheme can be extended, proving that $\{I_k^{m\pm}, I_l^{n\mp}\}=0$. This fact permits us to consider the third type of integrable equations generated by the Hamiltonians $\{I_k^{m\pm}\}$ and $\{I_l^{n\mp}\}$ and associated with the whole Lie algebra $\tilde{\mathfrak{g}}_A$. Although this set of equations contains in itself sets of equations connected with $\tilde{\mathfrak{g}}_A^{\pm}$, the last two are completely self-contained and could be considered separately. Hence, in the result, using the triple $(\tilde{\mathfrak{g}}_A, \tilde{\mathfrak{g}}_A^-, \tilde{\mathfrak{g}}_A^+)$ we obtain three types of integrable hierarchies: two "small" hierachies associated with $\tilde{\mathfrak{g}}_A^{\pm}$ and "large" hierarchy associated with $\tilde{\mathfrak{g}}_A$.

We show that for all the types of hierarchies their structure depends on the matrix of deformation A which play the role of the anisotropy tensor. There are two substantially different cases. The first case is connected with the nondegenerate matrices A. In this case the hierarchies connected with the algebras $\tilde{\mathfrak{g}}_A^+$ and $\tilde{\mathfrak{g}}_A^-$ are equivalent and yield integrable hierarchies that could be viewed as an "anisotropic deformation" of the generalized Heisenberg magnet hierarchy or a matrix generalization of the Landau–Lifshitz hierarchy. Large hierarchy connected with the whole algebra $\tilde{\mathfrak{g}}_A$ gives in case of the nondegenerate matrices A a new type of anisotropic chiral field equation. The second case is connected with the degenerated matrices A. In this case the hierarchies corresponding to the algebras $\tilde{\mathfrak{g}}_A^{\pm}$ cease to be equivalent. Moreover in the case of hierarchies associated with the algebras $\tilde{\mathfrak{g}}_A^+$ an additional reduction appears. Multiparametric character of the algebra $\tilde{\mathfrak{g}}_A$ gives us a new possibility to perform reduction procedure. Manipulating by these parameters (matrix elements of the matrix A) we can, in some cases, substantially simplify corresponding U-operator and reduce the number of its independent components. In the present paper we illustrate this by the simplest example of the minimally degenerated matrices A. In this case the integrable hierarchy, that corresponds to the algebra $\tilde{\mathfrak{g}}_A^+$ and $\mathfrak{g}=so(n)$, is a vector generalization of the Landau–Lifshitz hierarchy. Ordinary Landau–Lifshitz hierarchy corresponds to the case $\mathfrak{g}=so(4)$, $A=\mathrm{diag}(a_1,a_2,a_3,0)$. The large hierarchy connected with the whole algebra $\tilde{\mathfrak{g}}_A$ gives us in this degenerated case "coupled" generalized Landau–Lifshitz and generalized anisotropic chiral field hierarchies.

The structure of the present paper is the following: in the second section we introduce algebras $\tilde{\mathfrak{g}}_A$ and describe their properties, in the third section we describe infinite-dimensional Hamiltonian

systems on the algebras $\tilde{\mathfrak{g}}_A^{\pm}$ and $\tilde{\mathfrak{g}}_A$ possessing infinite sets of mutually commuting integrals. In the fourth section we consider the corresponding hierarchies of integrable equations admitting zero-curvature representations.

II. K–A ADMISSIBLE QUASIGRADED LIE ALGEBRAS

In this section we describe a new class of infinite-dimensional Lie algebras $\tilde{\mathfrak{g}}$ that could be used to generate classical integrable systems. These algebras satisfy the following integrability requirements (IR):

- (IR1) they possess an infinite number of algebraically independent invariants of coadjoint representation;
- (IR2) they are decomposable into the direct sum of two subalgebras: $\tilde{\mathfrak{g}}=\tilde{\mathfrak{g}}^{-}+\tilde{\mathfrak{g}}^{+}$; and
- (IR3) subalgebras $\tilde{\mathfrak{g}}^{+}$, $\tilde{\mathfrak{g}}^{-}$ possess infinite set of embedded ideals $\mathcal{J}_{\pm n}$ of finite codimensions.

A. General construction

Definition 1: Infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ *is called* $\mathbb{Z}$*-quasigraded of type* (p,q)[10] *if it admits the decomposition*

$$\tilde{\mathfrak{g}}=\sum_{j\in\mathbb{Z}}\mathfrak{g}_j, \quad \textit{such that } [\mathfrak{g}_i,\mathfrak{g}_j]\subset\sum_{k=-p}^{q}\mathfrak{g}_{i+j+k}.$$

The following proposition holds true.[16]

Proposition 1: Let $\tilde{\mathfrak{g}}$ *be* $\mathbb{Z}$*-quasi graded of type* $(0,1)$, *or* $(1,0)$. *Then* $\tilde{\mathfrak{g}}$ *satisfies conditions* (*IR2*) *and* (*IR3*).

So our aim in this section will be a construction of $\mathbb{Z}$-quasi graded algebras of type $(0,1)$. For this purpose we will deform Lie algebraic structure in loop algebras. We will introduce into $L(\mathfrak{g})=\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$ new Lie bracket

$$[X\otimes p(\lambda),Y\otimes q(\lambda)]_F=[X,Y]\otimes p(\lambda)q(\lambda)-F(X,Y)\otimes\lambda p(\lambda)q(\lambda), \tag{3}$$

where $X,Y\in\mathfrak{g}$, $p(\lambda),q(\lambda)\in Pol(\lambda,\lambda^{-1})$, $[,]$ in the right-hand side of this identity denotes ordinary Lie bracket in $\mathfrak{g}$ and map $F:\mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ is skew. It is evident by the very construction that the Lie algebras with the so defined bracket are $\mathbb{Z}$-quasi graded Lie algebras of type $(0,1)$ with the quasigrading being defined in the standard way by degrees of the spectral parameter λ.

The following propositions answer the question when bracket (3) satisfies the Jacobi identity.

Proposition 2: For bracket (3) to satisfy the Jacobi identities the cochain F should satisfy the following two requirements:

$$(J1)\quad \sum_{c.p.\{i,j,k\}}([F(X_i,X_j),X_k]+[F(X_i,X_j),X_k])=0,$$

$$(J2)\quad \sum_{c.p.\{i,j,k\}}F(F(X_i,X_j),X_k)=0.$$

In the case of classical matrix Lie algebras it is possible to give an explicit construction of large (multiparametric) family of cochains F, that satisfy conditions $(J1)-(J2)$. Let $\mathfrak{g}$ be hereafter a classical matrix Lie algebra of the type $gl(n)$, $so(n)$, and $sp(n)$ over the field of the complex or real numbers. We will realize algebra $so(n)$ as algebra of skew-symmetric matrices: $so(n)=\{X\in gl(n)|X=-X^{\mathsf{T}}\}$ and algebra $sp(n)$ as the following matrix algebra: $sp(n)=\{X\in gl(n)|X=sX^{\mathsf{T}}s\}$, where n is an even number, $s\in so(n)$ and $s^2=-1$.

The following proposition holds true.

Proposition 3: Let $\mathfrak{g}$ *be a classical matrix Lie algebra over the field* $\mathbb{K}$ *of complex or real numbers. Let us define the numerical* ($\mathbb{K}$*-valued*) $n\times n$ *matrix A of the following type*:

(1) *A is arbitrary for $\mathfrak{g}=gl(n)$;*
(2) *$A=A^{\mathsf{T}}$ for $\mathfrak{g}=so(n)$;* and
(3) *$A=-sA^{\mathsf{T}}s$ for $\mathfrak{g}=sp(n)$.*

Then maps $F_A:\mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ of the form $F_A(X,Y)=XAY-YAX$ are correctly defined skew symmetric maps that satisfy conditions (J1)–(J2).

Remark 1: Cocycle F_A defines a second Lie bracket in the finite dimensional Lie algebras $\mathfrak{g}$, that is compatible with the standard one. This fact was noticed in Ref. 11 and was used to construct compatible Poisson brackets on the finite-dimensional Lie algebras $\mathfrak{g}$. The idea to use the same cocycle to generate infinite-dimensional Lie algebras with Kostant–Adler decomposition was proposed in Ref. 12 as a natural generalization of semi-geometric construction of Refs. 13–16 of special quasigraded Lie algebras on the higher genus curves.

Definition 2: We will denote Lie bracket in the space $\mathfrak{g}$, defined by the cocycle F_A by $[,]_A$ and the corresponding finite-dimensional Lie algebra by $\mathfrak{g}_A$. We will denote infinite-dimensional space $\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$ with the Lie bracket given by (3) *and cocycle F_A by $\widetilde{\mathfrak{g}}_A$.*

Lie bracket in the algebra $\widetilde{\mathfrak{g}}_A$ will have the following form:

$$[X(\lambda),Y(\lambda)]_{F_A}=[X(\lambda),Y(\lambda)]-\lambda[X(\lambda),Y(\lambda)]_A, \tag{4}$$

where $X(\lambda),Y(\lambda)\in L(\mathfrak{g})=\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$, $A(\lambda)\equiv 1-\lambda A$, and we extend brackets $[,]$ and $[,]_A$ from Lie algebra $\mathfrak{g}$ to Lie algebra of $\mathfrak{g}$-valued functions $L(\mathfrak{g})$ in a natural way. This bracket can be also written in the more compact form as follows:

$$[X(\lambda),Y(\lambda)]_{F_A}\equiv[X(\lambda),Y(\lambda)]_{A(\lambda)}=X(\lambda)A(\lambda)Y(\lambda)-Y(\lambda)A(\lambda)X(\lambda). \tag{5}$$

Now we can introduce the convenient bases in the algebras $\widetilde{\mathfrak{g}}_A$. Due to the fact that we are dealing with matrix Lie algebras $\mathfrak{g}$, we will denote their basic elements as X_{ij}. For example, for the case $\mathfrak{g}=gl(n)$ we will have that $X_{ij}=I_{ij}$, where $(I_{ij})_{ab}=\delta_{ai}\delta_{bj}$ for the case $\mathfrak{g}=so(n)$ we will have that $X_{ij}=I_{ij}-I_{ji}$ etc. Let $X_{ij}^m\equiv X_{ij}\otimes\lambda^m$ be the natural basis in $\widetilde{\mathfrak{g}}_A$. Commutation relations (4) in this basis have the following form:

$$[X_{ij}^r,X_{kl}^m]_{F_A}=\sum_{p,q}C_{ij,kl}^{pq}X_{pq}^{r+m}-\sum_{p,q}C_{ij,kl}^{pq}(A)X_{pq}^{r+m+1}, \tag{6}$$

where $C_{ij,kl}^{pq}$ and $C_{ij,kl}^{pq}(A)$ are the structure constants of the Lie algebras $\mathfrak{g}$ and $\mathfrak{g}_A$, respectively.

Remark 2: Algebras $\widetilde{\mathfrak{g}}_A$ can be realized also in the space of special matrix valued functions of λ with an ordinary Lie bracket $[,]$. In particular in the case of the diagonal matrices A they can be realized as the special quasigraded Lie algebras on the higher genus curves (see Refs. 13–16). They can be also realized as *special quasigraded subalgebras* of $gl(n)$-loop algebras, which contrary to the graded subalgebras of loop algebras are not isomorphic to the corresponding loop algebras. Nevertheless we consider realization in the space $\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$ with the "deformed" bracket to be the most convenient.

Remark 3: Contrary to the case of loop algebras our algebras $\widetilde{\mathfrak{g}}_A$ admit only one type of decomposition $\widetilde{\mathfrak{g}}_A=\widetilde{\mathfrak{g}}_A^+ + \widetilde{\mathfrak{g}}_A^-$ compatible with quasigrading, where the subalgebras $\widetilde{\mathfrak{g}}_A^{\pm}$ are defined in the natural way

$$\widetilde{\mathfrak{g}}_A^+=\mathrm{Span}_{\mathbb{K}}\{X_{ij}^m|m\geqslant 0\},\quad \widetilde{\mathfrak{g}}_A^-=\mathrm{Span}_{\mathbb{K}}\{X_{ij}^m|m<0\}. \tag{7}$$

The following proposition holds true.

Proposition 4: Let $\det A\neq 0$ then the algebra $\widetilde{\mathfrak{g}}_{A^{-1}}^-$ is isomorphic to the algebra $\widetilde{\mathfrak{g}}_A^+$.

Proof: This follows from the substitution of variables in the algebra $\widetilde{\mathfrak{g}}_A$: $\widetilde{X^{-n}}=A^{-1/2}X^{n-1}A^{-1/2}$, which maps generators of $\widetilde{\mathfrak{g}}_A^+$ into the generators of $\widetilde{\mathfrak{g}}_{A^{-1}}^-$.

Let us consider several examples of the algebra $\widetilde{\mathfrak{g}}_A$:

Example 1: Let $\mathfrak{g}=so(4)$ and matrix A be diagonal: $A=\mathrm{diag}(a_1,a_2,a_3,a_4)$. In this case commutation relations will be more simple if we introduce standard basis in $so(4)$ algebra. Putting

$X_k^n \equiv \epsilon_{ijk} X_{ij}^n$, $Y_k^m \equiv X_{i4}^m$ where $i,j,k \in 1,3$ we obtain the following commutation relations for the $\widetilde{so(4)_A}$:

$$[X_i^r, X_j^s] = \epsilon_{ijk} X_k^{r+s} - \epsilon_{ijk} a_k X_k^{r+s+1}, \tag{8a}$$

$$[X_i^r, Y_j^r] = \epsilon_{ijk} Y_k^{r+s} - \epsilon_{ijk} a_j Y_k^{r+s+1}, \tag{8b}$$

$$[Y_i^r, Y_j^s] = \epsilon_{ijk} X_k^{r+s} - a_4 \epsilon_{ijk} X_k^{r+s+1}. \tag{8c}$$

In the case when $a_4 = 0$ this algebra coincides with anisotropic affine algebra discovered in Ref. 17 (see also Ref. 18) in the connection with the integrability of Landau–Lifshitz equations.

B. Coadjoint representation and its invariants

In this subsection we define dual spaces, coadjoint representations and their invariants for the Lie algebras $\tilde{\mathfrak{g}}_A$. Let us at first explicitly describe the dual space $\tilde{\mathfrak{g}}_A^*$ of $\tilde{\mathfrak{g}}_A$. For this purpose we will define the pairing between $\tilde{\mathfrak{g}}_A$ and $\tilde{\mathfrak{g}}_A^*$ in the following standard way:

$$\langle X, L \rangle = \mathrm{res}_{\lambda=0} \mathrm{Tr}\,(X(\lambda) L(\lambda)). \tag{9}$$

The generic element of the dual space $L(\lambda) \in \tilde{\mathfrak{g}}_A^*$ is written as follows:

$$L(\lambda) = \sum_{k \in Z} \sum_{i,j=1,n} l_{ij}^{(k)} \lambda^{-(k+1)} X_{ij}^*. \tag{10}$$

The following proposition holds true:[12]

Proposition 5: The coadjoint action of the algebra $\tilde{\mathfrak{g}}_A$ on the dual space $\tilde{\mathfrak{g}}_A^*$ has the form

$$ad^*_{X(\lambda)} \circ L(\lambda) = A(\lambda) X(\lambda) L(\lambda) - L(\lambda) X(\lambda) A(\lambda), \tag{11}$$

where $X(\lambda), Y(\lambda) \in \tilde{\mathfrak{g}}_A$, $L(\lambda) \in \tilde{\mathfrak{g}}_A^*$.

Remark 4: Note that linear spaces $\tilde{\mathfrak{g}}_A$ and $\tilde{\mathfrak{g}}_A^*$ do not coincide as $\tilde{\mathfrak{g}}_A$-modules. Moreover, rigorously speaking, they also do not coincide as linear spaces because $\tilde{\mathfrak{g}}_A^*$ contains formal power series, and $\tilde{\mathfrak{g}}_A$, by the very definition, consists of the Loran polynomials.

Proposition 5 has the following important corollary.

Corollary 1: Let $L(\lambda)$ be the generic element of $\tilde{\mathfrak{g}}_A^*$. Then the functions

$$I_k^m(L(\lambda)) = \frac{1}{m} \mathrm{res}_{\lambda=0} \lambda^{-(k+1)} \mathrm{Tr}\,(L(\lambda) A(\lambda)^{-1})^m \tag{12}$$

are invariants of the coadjoint representation of $\tilde{\mathfrak{g}}_A$.

Remark 5: Matrix $A(\lambda)^{-1} \equiv (1 - \lambda A)^{-1}$ has to be understood as a power series in λ in the neighborhood of 0 or ∞: $A(\lambda)^{-1} = (1 + A\lambda + A^2\lambda^2 + \cdots)$ or $A(\lambda)^{-1} = -(A^{-1}\lambda^{-1} + A^{-2}\lambda^{-2} + \cdots)$.

Remark 6: We will also use invariants of the Lie algebras $\widetilde{so(2n)_A}$ of the form

$$P_k(L(\lambda)) = \mathrm{res}_{\lambda=0} \lambda^{-(k+1)} Pf(L(\lambda)). \tag{13}$$

They can be expressed as functions of the invariants introduced in corollary 1.

C. Lie–Poisson structure

Let us define the Poisson structures in the space $\tilde{\mathfrak{g}}_A^*$ using the defined earlier pairing $\langle , \rangle$. It defines Lie–Poisson (Kirillov–Kostant) bracket on $P(\tilde{\mathfrak{g}}_A^*)$ in the following standard way:

$$\{F(L(\lambda)), G(L(\lambda))\} = \langle L(\lambda), [\nabla F(L(\lambda)), \nabla G(L(\lambda))]_{A(\lambda)} \rangle, \tag{14}$$

where $\nabla F(L(\lambda)) = \Sigma_{k \in Z} \Sigma_{i,j=1}^n [\partial F / \partial l_{ij}^{(k)}] X_{ij}^k$, $\nabla G(L) = \Sigma_{m \in Z} \Sigma_{k,l=1}^n [\partial G(\lambda) / \partial l_{kl}^{(m)}] X_{kl}^m$.

From corollary 1 and standard arguments follows the next statement.

Proposition 6: Functions $I_k^m(L(\lambda))$ are central for the Lie–Poisson bracket (14).

Let us explicitly calculate Poisson bracket (14). It is easy to show that for the coordinate functions $l_{ij}^{(m)}$ these brackets will have the following form:

$$\{l_{ij}^{(n)}, l_{kl}^{(m)}\} = \sum_{p,q} C_{ij,kl}^{pq} l_{pq}^{(n+m)} - \sum_{p,q} C_{ij,kl}^{pq}(A) l_{pq}^{(n+m+1)}. \tag{15}$$

It is evident that this bracket determines in the space of linear functions $\{l_{ij}^{(n)}\}$ a structure of the Lie algebra isomorphic to $\tilde{\mathfrak{g}}_A$. That is why the corresponding Poisson algebra possesses decomposition into direct sum of two Poisson subalgebras or, in other words, subspaces $(\tilde{\mathfrak{g}}_A^{\pm})^*$ are Poisson.

III. INFINITE-DIMENSIONAL HAMILTONIAN SYSTEMS VIA K–A ADMISSIBLE LIE ALGEBRAS

In the previous section we have constructed infinite-dimensional Lie algebras $\tilde{\mathfrak{g}}_A$ that have a decomposition into direct sum of two subalgebras and possess an infinite set of invariants of coadjoint representation, i.e., admit so-called the Kostant–Adler scheme. In this section we apply the Kostant–Adler scheme and its extension to $\tilde{\mathfrak{g}}_A$ in order to construct an infinite set of mutually commuting (with respect to the natural Lie–Poisson bracket) functions on $\tilde{\mathfrak{g}}_A^{\pm}$ and $\tilde{\mathfrak{g}}_A$ and obtain a "deformed" Lax representation for the corresponding Hamiltonian equations.

A. Integrable Hamiltonian systems connected with algebras $\tilde{\mathfrak{g}}_A^{\pm}$

Let $L^{\mp}(\lambda) \equiv \Sigma_{i,j=1,n} L_{ij}^{\mp}(\lambda) X_{ji} = \Sigma_{k \in \mathbb{Z}_{\pm}} \Sigma_{i,j=1,n} l_{ij}^{(k)} \lambda^{-(k+1)} X_{ji}$ be the generic elements of the spaces $(\tilde{\mathfrak{g}}_A^{\pm})^*$. Let us consider restriction of the invariant functions $\{I_k^m(L(\lambda))\}$ onto these subspaces. Note, that although Poisson subspaces $(\tilde{\mathfrak{g}}_A^{\pm})^*$ are infinite dimensional, all functions $\{I_k^m(L^{\pm}(\lambda))\}$ are polynomials, i.e., after restriction to $(\tilde{\mathfrak{g}}_A^{\pm})^*$ no infinite sums appear in their explicit expressions. Corresponding Hamiltonian equations are written as

$$\frac{\partial L_{ij}^{\mp}(\lambda)}{\partial t_k^m} = \{L_{ij}^{\mp}(\lambda), I_k^m(L^{\mp}(\lambda))\}. \tag{16}$$

The following important theorem holds true.

Theorem 1: (*i*) *Time flows defined by Eq. (16) mutually commute.* (*ii*) *Euler–Arnold equations (16) are written in the deformed Lax form*

$$\frac{\partial L^{\mp}(\lambda)}{\partial t_k^m} = A(\lambda) M_k^m(\lambda) L^{\mp}(\lambda) - L^{\mp}(\lambda) M_k^m(\lambda) A(\lambda), \tag{17}$$

where $M_k^m(\lambda) = \nabla I_k^m(L^{\mp}(\lambda)) \equiv \Sigma_{s \in \mathbb{Z}_{\pm}} \Sigma_{i,j=1}^n [\partial I_k^m / \partial l_{ij}^{(s)}] X_{ij}^s$ *is an algebra-valued gradient of* $I_k^m(L^{\mp}(\lambda))$. (*iii*) *Functions* $I_l^n(L^{\pm})$ *are constant along all times* $t_k^{m\pm}$: $[\partial I_l^n(L^{\pm}) / \partial t_k^{m\pm}] = 0$.

Proof of the theorem follows from the general framework of the Kostant–Adler scheme.[8]

Remark 7: Using earlier mentioned realizations of $\tilde{\mathfrak{g}}_A$ deformed Lax equations could be rewritten in the forms of the standard Lax equations, but in this case corresponding $L-M$ pairs will be more complicated and we prefer to work with the Lax equations in the "deformed" form (17).

B. Integrable Hamiltonian systems connected with algebras $\tilde{\mathfrak{g}}_A$

Let us now extend our phase space from $(\tilde{\mathfrak{g}}_A^{\pm})^*$ to the whole space $\tilde{\mathfrak{g}}_A^*$ and extend corresponding Hamiltonian flows. In other words, let us consider the same Hamiltonians as functions on the extended phase space. Corresponding Hamiltonian equations are written in the standard way

$$\frac{\partial L_{ij}(\lambda)}{\partial_k^{m\mp} t} = \{L_{ij}(\lambda), I_k^m(L^{\mp}(\lambda))\}. \tag{18}$$

Note, that on the extended phase space there are two types of the Hamiltonian flows: "positive" flows defined by the Hamiltonians $I_k^m(L^+(\lambda))$ and "negative" flows defined by the Hamiltonians $I_l^n(L^-(\lambda))$. A remarkable fact is positive time flows commute with negative ones. The following analog of theorem 1 holds true.

Theorem 2: *The time flows defined by Eq. (18) commute for all times* t_k^{m+}, t_l^{n-}.

(*ii*) *Euler–Arnold equations (18) could be written in the deformed Lax form*

$$\frac{\partial L(\lambda)}{\partial t_k^{m\mp}} = A(\lambda) M_k^{m\mp}(\lambda) L(\lambda) - L(\lambda) M_k^{m\mp}(\lambda) A(\lambda), \tag{19}$$

where $M_k^{m\mp}(\lambda) = \nabla I_k^m(L^{\mp}(\lambda)) \equiv \Sigma_{s\in\mathbb{Z}_\pm} \Sigma_{i,j=1}^n [\partial I_k^m / \partial l_{ij}^{(s)}] X_{ij}^s$.

(*iii*) *The functions* $I_q^p(L^{\pm})$ *are constant along all times* $t_k^{m\pm}$ *and* $t_l^{n\mp}$.

Proof of this theorem is analogous to the proof of the corresponding theorem for the case of the loop algebras (see Ref. 4, and references therein).

Remark 8: Note that theorem 2 does not follow directly from the Kostant–Adler scheme[8] because commutativity of the time flows (18) implies commutativity of the corresponding Hamiltonians $I_k^m(L^{\pm}(\lambda)), I_l^n(L^{\mp}(\lambda))$ with respect to the initial Lie–Poisson bracket on $\tilde{\mathfrak{g}}_A^*$ (commutativity of these functions with respect to the r-matrix bracket $\{,\}_0$ (see Ref. 8) follows trivially from theorem 1).

In this section we have obtained Hamiltonian systems of the Euler–Arnold type on the special infinite-dimensional Lie algebras posessing infinite number of the commuting integrals of motion. These Hamiltonian systems, despite being infinite-dimensional are "mechanical" because they are described by ordinary differential equations. Nevertheless we can consider our dynamical variables $l_{ij}^{(p)}$ to be functions of all time variables $t_k^{m\pm}$ and using the commutativity of all time flows obtain differential identities on functions $l_{ij}^{(p)}(t_k^{m\pm})$, that coincide with the wanted integrable equations in partial derivatives. For this purpose in the next section we will derive an analog of zero-curvature equations.

IV. DEFORMED ZERO CURVATURE EQUATIONS

In this section we will obtain zero curvature-type equations as compatibility conditions for the set of the commutative Hamiltonian flows constructed in the previous section.

The following theorem holds true.

Theorem 3: *Let infinite-dimensional Lie algebras* $\tilde{\mathfrak{g}}_A$, $\tilde{\mathfrak{g}}_A^{\pm}$, *their dual spaces and polynomial Hamiltonians* $I_k^m(L^{\pm}(\lambda))$, $I_l^n(L^{\pm}(\lambda))$ *on them be defined as in previous sections. Then algebra-valued gradients of these functions satisfy the deformed zero-curvature equations*

$$\frac{\partial \nabla I_k^m(L^{\pm}(\lambda))}{\partial t_l^{n\pm}} - \frac{\partial \nabla I_l^n(L^{\pm}(\lambda))}{\partial t_k^{m\pm}} + [\nabla I_k^m(L^{\pm}(\lambda)), \nabla I_l^n(L^{\pm}(\lambda))]_{A(\lambda)} = 0, \tag{20}$$

$$\frac{\partial \nabla I_k^m(L^{\pm}(\lambda))}{\partial t_l^{n\mp}} - \frac{\partial \nabla I_l^n(L^{\mp}(\lambda))}{\partial t_k^{m\pm}} + [\nabla I_k^m(L^{\pm}(\lambda)), \nabla I_l^n(L^{\mp}(\lambda))]_{A(\lambda)} = 0. \tag{21}$$

Proof of this theorem is analogous to the proof of the analogous theorem of Ref. 16.

Remark 9: Using earlier mentioned realizations of $\tilde{\mathfrak{g}}_A$ deformed zero-curvature equations can be rewritten in the form of the standard zero-curvature equations, but in this case corresponding $U-V$ pairs will be more complicated and we will work with zero-curvature equations in the deformed form (20) and (21).

Theorem 3 provides us with an infinite number of $\tilde{\mathfrak{g}}_A^{\pm}$-valued $U-V$ pairs that satisfy zero curvature-type equations. The latter are nonlinear equations in the partial derivatives on the dynamical variables—matrix elements of the matrices $L^{\pm}(\lambda)$. In the terminology of Ref. 3 equations

generated by the infinite set of $U-V$ pairs are called "integrable in the kinematic sense." In the next subsections we will consider the simplest examples of such integrable equations and their hierarchies. We distinguish three types of hierarchies connected with the algebras $\tilde{\mathfrak{g}}_A^{\pm}$ and $\tilde{\mathfrak{g}}_A$. For the case of integrable hierarchies connected with $\tilde{\mathfrak{g}}_A^{\pm}$ we should consider only Eq. (20) while considering hierarchies connected with $\tilde{\mathfrak{g}}_A$ we should consider both Eqs. (20) and (21), which reflects the fact, that we have in this case both positive and negative flows.

Now we will explain in more detail the technique of obtaining integrable equations in partial derivatives starting from zero-curvature equations. Let us at first note that in the described approach no space variable x is *a priori* singled out: all times $t_k^{m\pm}$ are equivalent. Fixation of the space flow is equivalent to the fixation of integrable hierarchy. For this purpose one should fix Hamiltonians that generate x-flow. For the case of integrable systems, connected with algebras $\tilde{\mathfrak{g}}_A^*$ this choice yields fixation of dynamical variables. In more detail, for the dynamical variables in this case serve the matrix elements of $U \equiv \nabla I_k^m(L^{\mp}(\lambda))$, where Hamiltonian $I_k^m(L^{\mp}(\lambda))$ is chosen to generate an x-flow. Using zero-curvature conditions one can express matrix elements of all other matrix gradients $\nabla I_l^n(L^{\mp}(\lambda))$ via these dynamical variables and their derivatives with respect to the space coordinate. Substituting these expressions back to zero-curvature condition we obtain the wanted equation in partial derivatives on the matrix elements of $\nabla I_k^m(L^{\mp}(\lambda))$.

For the case of integrable systems associated with the whole algebras $\tilde{\mathfrak{g}}_A$ there are two types of Hamiltonians and two types of flows. That is why in this case the number of independent dynamical variables may be doubled: their role is played by matrix elements of $\nabla I_k^m(L^+(\lambda))$and $\nabla I_l^n(L^-(\lambda))$ that generate evolution with respect to x_+ and x_- correspondingly.

V. INTEGRABLE HIERARCHIES ASSOCIATED WITH ALGEBRAS $\tilde{\mathfrak{g}}_A^-$

In this section we will obtain integrable hierarchies of differential equations in partial derivatives, admitting a zero curvature type representation (20) with the values in $\tilde{\mathfrak{g}}_A^-$.

Let us consider dual space $(\tilde{\mathfrak{g}}_A^-)^*$. Its generic element has the following form:

$$L^+(\lambda) = \sum_{k<0} \sum_{i,j=1,n} l_{ij}^{(k)} \lambda^{-(k+1)} X_{ji} = L^{(-1)} + L^{(-2)} + \lambda^2 L^{(-3)} + \lambda^3 L^{(-4)} + \cdots, \tag{22}$$

where $L^{(-k)} \equiv \Sigma_{i,j=1,n} l_{ij}^{(-k)} X_{ji}$. Let us now calculate the Hamiltonians $I_k^m(L^+(\lambda))$. In order for the Hamiltonians $I_k^m(L^+(\lambda))$ to be polynomials we have to expand expression $A(\lambda)^{-1}$ in the power series in the neighborhood of zero: $A(\lambda)^{-1} = 1 + A\lambda + A^2\lambda^2 + \cdots$. From the results of the previous section it follows that the matrix gradients of Hamiltonians $I_k^m(L^+(\lambda))$ satisfy deformed zero-curvature Eq. (20). We will be interested in the two simplest Hamiltonians of the set $I_k^2(L^+(\lambda))$. By the direct calculations we obtain for them the following expressions:

$$I_0^2(L^+(\lambda)) = 1/2 \operatorname{Tr}(L^{(-1)})^2, \quad I_1^2(L^+(\lambda)) = \operatorname{Tr}(A(L^{(-1)})^2) + \operatorname{Tr}(L^{(-1)}L^{(-2)}). \tag{23}$$

The corresponding matrix gradients are

$$\nabla I_0^2(L^+(\lambda)) = L^{(-1)}\lambda^{-1}, \quad \nabla I_1^2(L^+(\lambda)) = L^{(-1)}\lambda^{-2} + ((AL^{(-1)} + L^{(-1)}A) + L^{(-2)})\lambda^{-1}. \tag{24}$$

As it follows from the earlier work, in order to fix integrable hierarchy we should choose the Hamiltonian, that generates x-flow. We will take for such the Hamiltonian function $I_0^2(L^+(\lambda))$, putting $t_0^{2+} \equiv x$, $\nabla I_0^2(L^+(\lambda)) \equiv U(x,\lambda)$, $\nabla I_k^m(L^+(\lambda)) \equiv V_k^m(x,\lambda), m,k>0$ as the basic $U-V$ pairs that generate this hierarchy. In this case the role of the dynamical variables is played by the matrix elements of the matrix $L^{(-1)}$.

A. Matrix generalization of the Landau–Lifshitz equation

In this subsection we will obtain an explicit form of the simplest equation of the earlier described hierarchy. For this purpose we have to choose a Hamiltonian that generates "time" flow

in the simplest possible way. We take for such Hamiltonian the function $I_1^2(L^+(\lambda))$, i.e., $t \equiv t_1^{2+}$. In the result we obtain that zero-curvature Eq. (20) is equivalent to the following λ-independent equations:

$$\frac{\partial L}{\partial t} - \frac{\partial M}{\partial x} = [L, M]_A, \tag{25a}$$

$$\frac{\partial L}{\partial x} = [L, M], \tag{25b}$$

where $L \equiv L^{(-1)}, M \equiv L^{(-2)} + (AL^{(-1)} + L^{(-1)}A)$.

In order to obtain equations in partial derivatives on the dynamical variables—matrix elements of the matrix L it is necessary to solve Eq. (25b), i.e., to express M via L and L_x and then substitute this expression into Eq. (25a). We will illustrate this procedure on the simplest, but most interesting example and show that corresponding equation coincides with matrix generalization of the Landau–Lifshitz equation.

Let $\mathfrak{g} = gl(n)$, $so(2n)$, or $sp(n)$. In this case in order to solve Eq. (25b), i.e., in order to obtain instead of two Eqs. (25a) and (25b) one matrix equation in partial derivatives it is necessary to impose additional constraint on the matrix L[15] (a similar situation holds for the Heisenberg magnet hierarchies associated with the higher rank algebras[19,20]). We will chose the simplest G-invariant form of such matrix constraint

$$L^2 = -\tfrac{1}{4}E, \tag{26}$$

where E is a unit matrix. This constraint means that L belongs to the degenerated coadjoint orbits of G of the following type: $Gl(n)/GL(p) \times GL(q)$, $SO(2n)/Gl(n)$, or $SP(n)/GL(n)$.

On this orbit we may solve Eq. (25b) in the next way

$$M = -\left[L, \frac{\partial L}{\partial x}\right] + M', \text{ where } M' \in \ker ad_L.$$

Ambiguity connected with the existence of $\ker ad_L$ is removed by the requirement that the constraint (26) is consistent with Eqs. (25a) and (25b). The following proposition is true.

Proposition 7: Let $M' = 1/2(AL + LA)$. *Then the constraint (26) is consistent with Eqs. (25a) and (25b), i.e.,* $(\partial L^2/\partial x)|_{L^2=-(1/4)E} = 0$ *and* $(\partial L^2/\partial t)_{L^2=-(1/4)E} = 0$.

Proposition is proved by direct verification.

The resulting equation acquires the following form:

$$\frac{\partial L}{\partial t} = -\left[L, \frac{\partial^2 L}{\partial x^2}\right] + \frac{1}{2}\frac{\partial}{\partial x}(AL + LA) - \left[L, \left[L, \frac{\partial L}{\partial x}\right]\right]_A + \frac{1}{2}[L, AL + LA]_A, \tag{27}$$

where $L^2 = -\frac{1}{4}E$. This equation is an "anisotropic" generalization of the Heisenberg magnet equation. Let us also show that it coincides with matrix generalization of the Landau–Lifshitz equation. In order to do this we will consider the following example.

Example 2: Let $\mathfrak{g} = so(4)$, $\mathrm{Tr}\, A = 0$ and matrix L satisfy G-invariant constraint (26). In this case it is easy to show that matrix S can be written in the form

$$L = \begin{pmatrix} 0 & -s_3 & s_2 & s_1 \\ s_3 & 0 & -s_1 & s_2 \\ -s_2 & s_1 & 0 & s_3 \\ -s_1 & -s_2 & -s_3 & 0 \end{pmatrix},$$

where three-component vector $\boldsymbol{s}$ belongs to $S^2 = SO(3)/SO(2) = SO(4)/SO(3) \times SO(2)$:

$$\langle \boldsymbol{s},\boldsymbol{s}\rangle = 1/4.$$

As a result of the special form of matrix L, the second and third items of the right-hand side of Eq. (27) conceal and it could be rewritten as equation for the vector $\boldsymbol{s}$ as follows:

$$\frac{\partial \boldsymbol{s}}{\partial t} = \left[\boldsymbol{s} \times \frac{\partial^2 \boldsymbol{s}}{\partial x^2}\right] + [\boldsymbol{s} \times J(\boldsymbol{s})],$$

where $J=1/4(\hat{A}^2-2a_4\hat{A})$, $\hat{A}=\mathrm{diag}(a_1,a_2,a_3)$. This is the famous Landau–Lifshitz equation.

In such a way we have obtained that the case $\mathfrak{g}=so(4)$ in Eq. (27) corresponds to the Landau–Lifshitz equation. Hence, Eq. (27) could be indeed considered as a direct matrix generalization of the Landau–Lifshitz equation.

B. Other equations from the hierarchy. Anisotropic chiral field equations

In this subsection we will show that the hierarchy of differential equations associated with $\widetilde{\mathfrak{g}}_A^-$ include [except Eqs. (25a) and (25b)] other interesting equations. In order to obtain such equations we have to choose other Hamiltonians that generate time flows. For this purpose, we will consider also Hamiltonians $P(L^+(\lambda))$. We will be interested in the simplest Hamiltonian of this power series, namely in $P_0(L^+(\lambda))$. Direct calculation gives

$$P_0(L^+(\lambda)) = P(L^{(-1)}), \tag{28}$$

where $P(L)\equiv\det(L)$ if $\mathfrak{g}=gl(n)$ or $\mathfrak{g}=sp(n)$, $P(L)\equiv\mathrm{Pf}(L)$ if $\mathfrak{g}=so(n)$ and n is even. Its matrix gradient has the following form:

$$\nabla P_0(L^+(\lambda)) = \sum_{i,j=1}^{n} \frac{\partial P(L^{(-1)})}{\partial l_{ij}^{(-1)}} X_{ij}\lambda^{-1}. \tag{29}$$

The corresponding zero-curvature condition yields the following λ-independent equation:

$$\frac{\partial L}{\partial \tau} - \frac{\partial M}{\partial x} = -[L,M]_A, \tag{30}$$

where $L\equiv L^{(-1)}$, $M\equiv\nabla P$ and we have used that $[L,M]=0$ due to the G-invariance of P. Equation (30) is, in some sense, the higher rank generalization of the ordinary $so(3)$-anisotropic chiral field equation. In order to show this we consider the following example.

Example 3: Let $\mathfrak{g}=so(4)$. The corresponding Lax operator $L\in so(4)$ has the form

$$L = \sum_{1\leqslant i<j\leqslant 3} l_{ij}X_{ij} + \sum_{1\leqslant i\leqslant 3} l_{ij}X_{i4} \equiv \sum_{1\leqslant k\leqslant 3} l_k^+ X_k + \sum_{1\leqslant k\leqslant 3} l_k^- Y_k,$$

where $X_k\equiv\epsilon_{ijk}X_{ij}$, $Y_k\equiv X_{k4}$, $l_k^+\equiv\epsilon_{ijk}l_{ij}$, $l_k^-\equiv l_{k4}$. Introducing the vectors $l^+=\Sigma_{1\leqslant k\leqslant 3}l_k^+X_k$, $l^-=\Sigma_{1\leqslant k\leqslant 3}l_k^-Y_k$, $L\equiv l^++l^-$ we obtain for our Hamiltonians the following expressions:

$$I_0^2(L) = 1/2((l^+,l^+)+(l^-,l^-)), \quad P_0^2(L) = (l^+,l^-).$$

The corresponding matrix gradients are easily calculated to be the following:

$$\nabla I_0^2(L) \equiv \lambda^{-1}L, \quad \nabla P_0^2(L) \equiv \lambda^{-1}M = \lambda^{-1}\left(\sum_{1\leqslant k\leqslant 3} l_k^- X_k + \sum_{1\leqslant k\leqslant 3} l_k^+ Y_k\right). \tag{31}$$

Let us hereafter assume that matrix $A\in\mathrm{Symm}(4)$ is diagonal: $A=\mathrm{diag}(a_1,a_2,a_3,a_4)$. By direct calculation, using commutation relations

$$[X_i,X_j]_A = \epsilon_{ijk}a_kX_k, \quad [X_i,Y_j]_A = \epsilon_{ijk}a_jY_k, \quad [Y_i,Y_j]_A = a_4\epsilon_{ijk}X_k, \tag{32}$$

we obtain the following differential equations for components of vectors $l^\pm$:

$$\frac{\partial l_i^+}{\partial \tau} - \frac{\partial l_i^-}{\partial x} = a_i \epsilon_{ijk} l_j^+ l_k^- + a_4 \epsilon_{ijk} l_j^+ l_k^-, \quad \frac{\partial l_i^-}{\partial \tau} - \frac{\partial l_i^+}{\partial x} = \epsilon_{ijk} l_j^+ a_k l_k^+ - \epsilon_{ijk} l_j^- a_k l_k^-. \tag{33}$$

Introducing vectors u, v with the components $u_i = l_i^+ + l_i^-$, $v_i = l_i^+ - l_i^-$ and new "light-cone" coordinates $\xi \equiv \tau - x$, $\eta \equiv \tau + x$ we can rewrite Eqs. (33) in the following form:

$$\frac{\partial u_i}{\partial \xi} = 1/2(-a_i \epsilon_{ijk} u_j v_k - a_4 \epsilon_{ijk} u_j v_k + \epsilon_{ijk} u_j a_k v_k + \epsilon_{ijk} v_j a_k u_k),$$

$$\frac{\partial v_i}{\partial \eta} = 1/2(-a_i \epsilon_{ijk} u_j v_k - a_4 \epsilon_{ijk} u_j v_k - \epsilon_{ijk} u_j a_k v_k - \epsilon_{ijk} v_j a_k u_k).$$

Taking into account that $\epsilon_{ijk}(a_i + a_j + a_k) \equiv (a_1 + a_2 + a_3)\epsilon_{ijk}$ and putting for simplicity $\mathrm{Tr}\, A \equiv a_1 + a_2 + a_3 + a_4 = 0$ we obtain that the last equations are written as follows:

$$\frac{\partial u_i}{\partial \xi} = \epsilon_{ijk} u_j a_k v_k, \quad \frac{\partial v_i}{\partial \eta} = \epsilon_{ijk} a_j u_j v_k \tag{34}$$

or, introducing matrix $\hat{A} = \mathrm{diag}(a_1, a_2, a_3)$ we can rewrite Eqs. (24) in vector form

$$\frac{\partial u}{\partial \xi} = [u \times \hat{A}(v)], \quad \frac{\partial v}{\partial \eta} = [\hat{A}(u) \times v]. \tag{35}$$

Equations (35) are the standard anisotropic $so(3)$-chiral field equations[21] (see also Refs. 18 and 22, and references therein). They satisfy two second order constraints

$$(\boldsymbol{u}, \boldsymbol{u}) = c_1, \quad (\boldsymbol{v}, \boldsymbol{v}) = c_2. \tag{36}$$

that follow from the constancy of the Hamiltonians $I_0^2(L)$ and $P_0^2(L)$ along all time flows.

Remark 10: Considered earlier $so(4)$-example is very special. Resulting decomposition of Eq. (30) in a pair of Eqs. (35) is a consequence of the fact that the algebra $so(4)$ is decomposed into the direct sum of two $so(3)$ subalgebras. That is why, in the general case, Eq. (30) could not be transformed into the simple form of Eqs. (35).

VI. INTEGRABLE HIERARCHIES ASSOCIATED WITH ALGEBRAS $\widetilde{\mathfrak{g}}_A^+$

In this section we consider integrable hierarchies admitting the deformed zero-curvature representation with $U-V$ pairs taking the value in the algebra $\widetilde{\mathfrak{g}}_A^+$. The generic element of the dual space $(\widetilde{\mathfrak{g}}_A^+)^*$ has the following form:

$$L^-(\lambda) = \sum_{k \geqslant 0} \sum_{i,j=1,n} l_{ij}^{(k)} \lambda^{-(k+1)} X_{ji} = \lambda^{-1} L^{(0)} + \lambda^{-2} L^{(1)} + \lambda^{-3} L^{(2)} + \cdots, \tag{37}$$

where $L^{(k)} \equiv \Sigma_{i,j=1,n} l_{ij}^{(k)} X_{ji}$. Contrary to the case of the algebra $\widetilde{\mathfrak{g}}_A^-$ the structure of the hierarchy will strongly depend on the form of the matrix A. There will be two essentially different cases: the case that corresponds to the nondegenerated matrices A and the case that corresponds to the degenerated matrices A. We begin with the first case.

A. Hierarchies connected with the nondegenerated matrices *A*

Let us consider Hamiltonians $I_k^m(L^-(\lambda))$ in case $\det A \neq 0$. In order for these Hamiltonians to be well-defined we have to expand expression $A(\lambda)^{-1}$ in the power series in the neighborhood of infinity: $A(\lambda)^{-1} = -(A^{-1}\lambda^{-1} + A^{-2}\lambda^{-2} + A^{-3}\lambda^{-3} + \cdots)$. In this case all functions $I_k^m(L^-(\lambda))$ are polynomials in the dynamical variables $l_{ij}^{(k)}$. Hence, as it follows from the results of the previous sections,

their matrix gradients satisfy deformed zero-curvature Eq. (20). Let us consider corresponding Hamiltonians. For the first two Hamiltonians of the set $I_k^2(L^-(\lambda))$ we obtain the following expressions:

$$I_{-4}^2(L^-(\lambda)) = \tfrac{1}{2}\,\mathrm{Tr}\,(A^{-1}L^{(0)})^2, \quad I_{-5}^2(L^+(\lambda)) = \mathrm{Tr}\,(A^{-1}(A^{-1}L^{(0)})^2) + \mathrm{Tr}\,(A^{-1}L^{(0)}A^{-1}L^{(1)}).$$

Their matrix gradients are

$$\nabla I_{-4}^2(L^-(\lambda)) = A^{-1}L^{(0)}A^{-1}, \quad \nabla I_{-5}^2(L^-(\lambda)) = A^{-1}(L^{(0)}\lambda + ((A^{-1}L^{(0)} + L^{(0)}A^{-1}) + L^{(1)}))A^{-1}. \quad (38)$$

By direct calculation it is easy to show that corresponding zero-curvature Eq. (20) after substitution: $L^{(-1)}=A^{-1/2}L^{(0)}A^{-1/2}$, $M=A^{-1/2}(L^{(1)}+(A^{-1}L^{(0)}+L^{(0)}A^{-1}))A^{-1/2}$ coincide with Eqs. (25) with matrix A replaced by the matrix A^{-1}. Hence, $U-V$ pair (38) gives differential equations equivalent to Eqs. (25). Corresponding hierarchies will also be equivalent. This equivalence is a consequence of the fact that in the case of the nondegenerated matrices A algebras $\tilde{\mathfrak{g}}_A^+$ and $\tilde{\mathfrak{g}}_{A^{-1}}^-$ are isomorphic. We will use these Lax pairs and the corresponding Hamiltonians in the next subsections, in particular, considering integrable equations connected with the whole algebra $\tilde{\mathfrak{g}}_A$.

B. Hierarchies connected with the degenerated matrices *A*

In this subsection we will consider integrable hierarchy connected with the algebras $\tilde{\mathfrak{g}}_A^+$ and degenerated matrices A. We will restrict ourselves to the consideration of the case of the "minimal" degeneracy of A, i.e., when rank $A=n-1$ and the case of the algebras $\mathfrak{g}=so(n)$. We will show that simplest of the corresponding hierarchies coincide with the vector generalization of the Landau–Lifshitz hierarchy.

Let us now consider the corresponding hierachies in details. Without the loss of the generosity we will put $A=\mathrm{diag}(A',0)$, where $A'\in \mathrm{Symm}(n-1)$. Let us consider commuting second order integrals (Hamiltonians), that generate our hierarchies. For this purpose we will consider block-diagonal nondegenerate matrices $\mathcal{A}$ of the type: $\mathcal{A}=A+aI$, where A is the earlier described matrix, $I=\mathrm{diag}(0,0,\ldots,0,1)$. By the very definition $A=\lim_{a\to 0}\mathcal{A}$. We will consider commuting integrals of the systems connected with $\tilde{\mathfrak{g}}_A^+$ and obtain the corresponding commuting integrals on $\tilde{\mathfrak{g}}_A^+$ as a limiting case of the commuting integrals on $\tilde{\mathfrak{g}}_{\mathcal{A}}^+$. Commuting integrals of the series $I^r(L^-(\lambda))$ contain expression $\mathcal{A}^{-1}$ and in the limit $a\to 0$ should be regularized in the appropriate way. For example, in order to regularize the simplest integral of the series $I^2(L^-(\lambda))$ we have to multiply it by a. Taking into account that $\mathcal{A}^{-1}=A^{-1}+a^{-1}I$ we obtain its explicit form

$$I_{-4}^{2'}(L^-(\lambda)) = \lim_{a\to 0} aI_{-4}^2(L^-(\lambda)) = 1/2\ \mathrm{Tr}\,(IL^{(0)}A^{-1}L^{(0)}).$$

Here, without abuse of notation we introduce the following: $A^{-1}\equiv \mathrm{diag}((A')^{-1},0)$.

Matrix gradient of $I_{-4}^{2'}$ has the form $\nabla I_{-4}^{2'}=-(IL^{(0)}A^{-1}+A^{-1}L^{(0)}I)$. As it was explained above fixation of the integrable hierarchy is equivalent to fixation of the U operator that generate space flow. We will take matrix $\nabla I_{-4}^{2'}$ for such the U-operator. This is the simplest possible choice that provides integrable hierarchy with the minimal number of dynamical variables equal to $(n-1)$. In the next subsections we will show that this hierarchy coincides with the generalized Landau–Lifshitz hierarchy.

C. Simplest equation of the generalized Landau–Lifshitz hierarchy

In order to choose one of the equations from the fixed hierarchy, i.e., when U operator is fixed we have to choose second operator in $U-V$ pair that generates time flow. In this subsection we consider the case when $V\equiv \nabla I_{-5}^{2'}$, where the "regularized" Hamiltonian $I_{-5}^{2'}$ is defined as follows:

$$I_{-5}^{2'}(L^-(\lambda)) = \lim_{a\to 0}(aI_{-5}^2(L^-(\lambda)) - 2I_{-4}^2(L^-(\lambda))).$$

Direct calculation gives its following explicit form:

$$I_{-5}^{2'}(L^-(\lambda)) = -(\mathrm{Tr}(IL^{(1)}A^{-1}L^{(0)}) + \mathrm{Tr}(IL^{(0)}A^{-1}L^{(1)})) + 1/2\ \mathrm{Tr}\,(A^{-1}L^{(0)}A^{-1}L^{(0)}) - \mathrm{Tr}(A^{-2}L^{(0)}IL^{(0)}).$$

In the case of the diagonal matrices $A' = \mathrm{diag}(a_1, a_2, \ldots, a_{n-1})$ Hamiltonians $I_{-4}^{2'}$ and $I_{-5}^{2'}$ acquire the following coordinate form:

$$I_{-4}^{2'}(L^-(\lambda)) = \sum_{i<n}\frac{(l_{in}^{(0)})^2}{a_i}, \quad I_{-5}^{2'}(L^-(\lambda)) = \sum_{i<n}\left(2\frac{l_{in}^{(1)}l_{in}^{(0)}}{a_i} + \frac{(l_{in}^{(0)})^2}{a_i^2}\right) - \sum_{0<i<j<n}\frac{(l_{ij}^{(0)})^2}{a_ia_j}.$$

Corresponding matrix gradients are written as follows:

$$\nabla I_{-4}^{2'} = 2\sum_{i<n}\frac{l_{in}^{(0)}}{a_i}X_{in}, \quad \nabla I_{-5}^{2'} = 2\lambda\sum_{i<n}\frac{l_{in}^{(0)}}{a_i}X_{in} - 2\sum_{i<j<n}\frac{l_{ij}^{(0)}}{a_ia_j}X_{ij} + 2\sum_{i<n}\left(\frac{l_{in}^{(1)}}{a_i} + \frac{l_{in}^{(0)}}{a_i^2}\right)X_{in}.$$

Dividing both matrix gradients by two (it is equivalent to the rescaling of the corresponding time variables) and introducing the following notations: $m_i^{(1)} = l_{in}^{(1)} + [l_{in}^{(0)}/a_i]$, we obtain that for the chosen $U-V$ pair deformed zero-curvature equation is equivalent to the following system of differential equations:

$$\frac{\partial l_{in}^{(0)}}{\partial t} - \frac{\partial m_i^{(1)}}{\partial x} = \sum_{k=1}^{n-1}\frac{l_{ik}^{(0)}l_{kn}^{(0)}}{a_k^2}, \tag{39}$$

$$\frac{\partial l_{in}^{(0)}}{\partial x} = \sum_{k=1}^{n-1}\frac{l_{ik}^{(0)}l_{kn}^{(0)}}{a_k}, \tag{40}$$

$$\frac{\partial l_{ij}^{(0)}}{\partial x} = m_i^{(1)}l_{jn}^{(0)} - m_j^{(1)}l_{in}^{(0)}. \tag{41}$$

In order to obtain differential equation in partial derivatives in the dynamical variables $l_{jn}^{(0)}$ we have to express $m_i^{(1)}$ and $l_{ij}^{(0)}$ via $l_{jn}^{(0)}$ and their derivatives. Using this and Eq. (40) it is easy to deduce that

$$l_{ij}^{(0)} = \frac{\partial l_{in}^{(0)}}{\partial x}l_{jn}^{(0)} - \frac{\partial l_{jn}^{(0)}}{\partial x}l_{in}^{(0)}, \tag{42}$$

$$m_i^{(1)} = \frac{\partial^2 l_{in}^{(0)}}{\partial x^2} + c_2(L^{(0)})l_{in}^{(0)}, \tag{43}$$

where $c_2(L^{(0)})$ is some scalar function of the dynamical variables $l_{in}^{(0)}$. In order to determine its explicit form we will use that Hamiltonians $I_{-4}^{2'}$ and $I_{-5}^{2'}$ are constant along all the flows. For convenience we will hereafter put $I_{-4}^{2'} = \mathrm{const}_1 = 1$, $I_{-5}^{2'} = \mathrm{const}_2 = 0$. Introducing the vector $(\boldsymbol{l})_i = l_{in}^{(0)}/a_i$ we obtain $c_2(\boldsymbol{l}) = 1/2(\boldsymbol{l},\boldsymbol{l}) + 3/2((\partial\boldsymbol{l}/\partial x), A'(\partial\boldsymbol{l}/\partial x))$. Using Eq. (42) it is easy to deduce that:

$$\sum_{k=1}^{n-1}[l_{ik}^{(0)}l_{kn}^{(0)}/a_ia_k^2] = -1/2[\partial(\boldsymbol{l},\boldsymbol{l})/\partial x](\boldsymbol{l})_i + (\boldsymbol{l},\boldsymbol{l})[\partial(\boldsymbol{l})_i/\partial x].$$

In the result we obtain the following differential equation in partial derivatives:

$$\frac{\partial \boldsymbol{l}}{\partial t}=\frac{\partial}{\partial x}\left(\frac{\partial^2 \boldsymbol{l}}{\partial x^2}+3/2\left(\frac{\partial \boldsymbol{l}}{\partial x},A'\frac{\partial \boldsymbol{l}}{\partial x}\right)\boldsymbol{l}\right)+3/2(\boldsymbol{l},\boldsymbol{l})\frac{\partial \boldsymbol{l}}{\partial x}. \tag{44}$$

In new notations: $\boldsymbol{s}=(A')^{1/2}\boldsymbol{l}$, $J\equiv(A')^{-1}$ we obtain that constraint $(\boldsymbol{l},A'\boldsymbol{l})=1$ passes to the standard constraint $(\boldsymbol{s},\boldsymbol{s})=1$ and Eq. (44) passes to the higher Landau–Lifshitz equation

$$\frac{\partial \boldsymbol{s}}{\partial t}=\frac{\partial}{\partial x}\left(\frac{\partial^2 \boldsymbol{s}}{\partial x^2}+3/2\left(\frac{\partial \boldsymbol{s}}{\partial x},\frac{\partial \boldsymbol{s}}{\partial x}\right)\boldsymbol{s}\right)+3/2(\boldsymbol{s},J\boldsymbol{s})\frac{\partial \boldsymbol{s}}{\partial x}. \tag{45}$$

In the case $n=4$ this equation is the higher equation of the Landau–Lifshitz hierarchy.[18] For $n>4$ this equation was obtained also in Ref. 23 using the technique of "dressing" and the embedding of a special realization of the algebra $\widetilde{so(n)}_A^+$ into algebra $so(n)((\lambda))$ of formal power series.

D. Landau–Lifshitz equation

In this subsection we will consider another equation from the earlier introduced generalized Landau–Lifshitz hierarchy. In such a way we will obtain the ordinary Landau–Lifshitz equation and show that although there is direct vector generalization of the Landau–Lifshitz hierarchy, but it does not contain vector generalization of the Landau–Lifshitz (L–L) equation.

In order to obtain a precise analog of L−L equation we have to find out Hamiltonian that generates a "correct" time flow. This will be the simplest Hamiltonian of the series

$$P(L^-(\lambda))\equiv Pf(\lambda^{-1}L^{(0)}+\lambda^{-2}L^{(1)}+\lambda^{-3}L^{(3)}+\cdots). \tag{46}$$

Due to the fact that pfaffian exists only for the orthogonal matrices in the spaces of even dimensions there arise the natural condition $n=2N$. By direct calculation we obtain: $P_{-N}(L^-(\lambda))\equiv Pf(L^{(0)})$. Its matrix gradient is written as follows:

$$\nabla P_{-N}(L^-(\lambda))=\sum_{i<n}\frac{\partial Pf(L^{(0)})}{\partial l_{in}^{(0)}}X_{in}+\sum_{i,j<n}\frac{\partial Pf(L^{(0)})}{\partial l_{ij}^{(0)}}X_{ij}. \tag{47}$$

Let us consider the corresponding zero-curvature equations

$$\frac{\partial\,\nabla I_{-4}^{2'}(L^-(\lambda))}{\partial\tau}-\frac{\partial\,\nabla P_{-N}(L^-(\lambda))}{\partial x}+[\nabla I_{-4}'^{2}(L^-(\lambda)),\ \nabla P_{-N}(L^-(\lambda))]_{A(\lambda)}=0.$$

Taking into account, that $[X_{in},X_{jn}]_A=0$, and $\Sigma_{i=1}^{n-1}[\partial P_{-N}(L^-(\lambda))/\partial l_{ij}^{(0)}]l_{in}^{(0)}=0$, we obtain that $[\nabla I_{-4}^{2'}(L^-(\lambda)),\nabla P_{-N}(L^-(\lambda))]_A=0$ and the corresponding zero-curvature type equation is reduced to the spectral parameter-independent form

$$\frac{\partial\,\nabla I_{-4}^{2'}(L^{(0)})}{\partial\tau}-\frac{\partial\,\nabla P_{-N}(L^{(0)})}{\partial x}+[\nabla I_{-4}^{2'}(L^{(0)}),\ \nabla P_{-N}(L^{(0)})]=0. \tag{48}$$

Before making a more detailed analysis of Eq. (48) in the case of general n, we will consider $n=4$ example in order to obtain the ordinary Landau–Lifshitz equation.

Example 4: Let $\mathfrak{g}=so(4)$. Taking into account Z_2 grading of $so(4)$: $so(4)=so(3)+\mathbb{R}^3$ and denoting projection of $\nabla P_{-N}(L^-(\lambda))$ onto subalgebra $so(3)\subset so(4)$ by $\nabla_+P_{-N}(L^-(\lambda))$ and projection onto subspace $\mathbb{R}^3\subset so(4)$ by $\nabla_-P_{-N}(L^-(\lambda))$ we obtain that Eq. (48) is rewritten as follows:

$$\frac{\partial\,\nabla I_{-4}^{2'}(L^{(0)})}{\partial\tau}=-[\nabla I_{-4}^{2'}(L^{(0)}),\quad \nabla_+P_{-4}(L^{(0)})]+\frac{\partial\nabla_-P_{-4}(L^{(0)})}{\partial x}, \tag{49}$$

$$\frac{\partial \nabla_+ P_{-4}(L^{(0)})}{\partial x} = [\nabla I^{2'}_{-4}(L^{(0)}), \nabla_- P_{-4}(L^{(0)})]. \tag{50}$$

Introducing notations: $l_i = l^{(0)}_{i4}$, $m_i = \epsilon_{ijk} l^{(0)}_{jk}$, $Y_i = X_{i4}$, $X_k = \epsilon_{ijk} X_{jk}$ $(i,j,k<4)$ we obtain

$$\nabla I^{2'}_{-4}(L^{(0)}) = \sum_{i=1}^{3} a_i^{-1} l_i Y_i, \quad \nabla_+ P_{-4}(L^{(0)}) = \sum_{i=1}^{3} l_i X_i, \quad \nabla_- P_{-4}(L^{(0)}) = \sum_{i=1}^{3} m_i Y_i.$$

Substituting this expression into Eqs. (49) and introducing in the evident manner vectors $\boldsymbol{l}$, $\boldsymbol{m}$, and matrix $J \equiv \mathrm{diag}(a_1^{-1}, a_2^{-1}, a_3^{-1})$ we obtain the following equations:

$$J\frac{\partial \boldsymbol{l}}{\partial \tau} = -[J\boldsymbol{l} \times \boldsymbol{l}] + \frac{\partial \boldsymbol{m}}{\partial x}, \tag{51a}$$

$$\frac{\partial \boldsymbol{l}}{\partial x} = [J\boldsymbol{l}, \boldsymbol{m}]. \tag{51b}$$

Due to the fact that all Hamiltonians are constant along all time flows, vectors $\boldsymbol{m}$ and $\boldsymbol{l}$ are subjected to the conditions: $I^{2'}_{-4} = (J\boldsymbol{l}, \boldsymbol{l}) = c_2$, $P_{-4} = (\boldsymbol{m}, \boldsymbol{l}) = c_1$. For the sake of simplicity we will hereafter put $c_2 = 1$, $c_1 = 0$. Using these constraints and Eq. (51b) we obtain for the vector $\boldsymbol{m}$ the explicit expression: $\boldsymbol{m} = -[\boldsymbol{l}, (\partial \boldsymbol{l}/\partial x)]$. Substituting this expression into Eq. (51a) we obtain the following equation:

$$J\frac{\partial \boldsymbol{l}}{\partial \tau} = -\left[\boldsymbol{l}, \frac{\partial^2 \boldsymbol{l}}{\partial x^2}\right] - [J\boldsymbol{l} \times \boldsymbol{l}]. \tag{52}$$

Introducing variables: $\boldsymbol{s} = J^{1/2}\boldsymbol{l}$, $t = -(\det J)^{1/2}\tau$ we can write Eq. (52) as follows:

$$\frac{\partial \boldsymbol{s}}{\partial t} = \left[\boldsymbol{s}, \frac{\partial^2 \boldsymbol{s}}{\partial x^2}\right] + [J\boldsymbol{s} \times \boldsymbol{s}], \text{where } (\boldsymbol{s}, \boldsymbol{s}) = 1. \tag{53}$$

It is easy to see, that Eq. (53) coincides with the standard *Landau–Lifshitz equation*.

Let us now consider Eq. (48) in the case of $n>4$. The next theorem is true.

Theorem 4: *In the case $n>4$ hierarchy of the vector Eq. (45) contains no nontrivial analog of the Landau–Lifshitz equation.*

Proof: Let us show, that the Hamiltonian flows that generate time flow of L–L equations are trivial for the case $n>4$. In order to do this it is enough to show that the V operator (i.e., matrix gradient of the corresponding Hamiltonian) is trivial. But this follows from the definition of the pfaffian: $P_{-N}(L^{(0)}) = \Sigma_{i_1, i_2, \ldots, i_{2N} \leqslant n} \epsilon_{i_1 i_2 i_3 \cdots i_{2N}} l^{(0)}_{i_1 i_2} l^{(0)}_{i_3 i_4} \cdots l^{(0)}_{i_{2N-1} i_{2N}}$ and Eq. (42). Indeed, substituting expression $l^{(0)}_{ij} = [\partial l^{(0)}_{in}/\partial x] l^{(0)}_{jn} - [\partial l^{(0)}_{jn}/\partial x] l^{(0)}_{in}$ in the explicit expression of $\nabla P_{-N}(L^{(0)})$ and taking into account skew symmetry of the tensor $\epsilon_{i_1 i_2 i_3 \cdots i_{2N}}$, we obtain that for the case when $\nabla P_{-N}(L^{(0)})$ is a polynomial in $L^{(0)}$ of the degree exceeding one, i.e., when $n = 2N > 4$, $\nabla P_{-N}(L^{(0)})$ turns identically zero.

The theorem is proved.

VII. INTEGRABLE HIERARCHIES ASSOCIATED WITH ALGEBRAS $\widetilde{\mathfrak{g}}_A$

In this section we will obtain the simplest equations of integrable hierarchies associated with algebras $\widetilde{\mathfrak{g}}_A$. We will again distinguish two types of hierarchies—those connected with degenerated and those connected with nondegenerated matrices A.

A. Hierarchy connected with nondegenerated matrices *A*

Let us consider the second order Hamiltonians $I^2_k(L^+(\lambda))$and $I^2_l(L^-(\lambda))$. For the first Hamiltonians of these sets we have (see previous sections) the following expressions:

$$I_0^2(L^+(\lambda)) = 1/2\ \mathrm{Tr}\,(L^{(-1)})^2, \quad I_{-4}^2(L^-(\lambda)) = 1/2\ \mathrm{Tr}\,(A^{-1}L^{(0)}A^{-1}L^{(0)}). \tag{54}$$

The corresponding matrix gradients are

$$\nabla I_0^2(L^+(\lambda)) = L^{(-1)}\lambda^{-1}, \quad \nabla I_{-4}^2(L^-(\lambda)) = A^{-1}L^{(0)}A^{-1}. \tag{55}$$

As it follows from the results of Sec. III B Hamiltonians $I_k^2(L^+(\lambda))$ and $I_l^2(L^-(\lambda))$, considered as functions on $\widetilde{\mathfrak{g}}_A^*$ commute with respect to the usual Lie-Poisson bracket on $\widetilde{\mathfrak{g}}_A^*$. Hence, their matrix gradients satisfy deformed zero-curvature equations

$$\frac{\partial\ \nabla I_0^2(L^+(\lambda))}{\partial x_-} - \frac{\partial\ \nabla I_{-4}^2(L^-(\lambda))}{\partial x_+} + [\nabla I_0^2(L^+(\lambda)),\ \nabla I_{-4}^2(L^-(\lambda))]_{A(\lambda)} = 0. \tag{56}$$

A direct calculation gives us λ independent form of Eqs. (56):

$$\frac{\partial U}{\partial x_+} = [U,V]_A, \quad \frac{\partial V}{\partial x_-} = [U,V], \tag{57}$$

where $V \equiv L^{(-1)}$, $U \equiv A^{-1}L^{(0)}A^{-1}$. We consider Eqs. (57) to be the new examples of *anisotropic chiral field equations*. They go together with natural constraints

$$\mathrm{Tr}(UA)^r = \mathrm{const}_r^-, \quad \mathrm{Tr}(V)^r = \mathrm{const}_r^+, r \in \overline{1,n} \tag{58}$$

that follows from the fact that Hamiltonians $I_0^r(L^+(\lambda))$ and $I_{-r-2}^r(L^-(\lambda))$ are constant along all time flows: $I_0^r(L^+(\lambda)) = \mathrm{const}_r^+$, $I_{-r-2}^r(L^-(\lambda)) = \mathrm{const}_r^-$.

Remark 11: Note, that in order to obtain usual "isotropic"chiral field equations we have to put $A_{ij} \to a\delta_{ij}$ not $A_{ij} \to 0$. This is explained by the fact that a standard Lax pair generating isotropic chiral field equations depends not on $\lambda^{\pm 1}$ but on $(\lambda \pm a)^{-1}$.

Example 5: Let $\mathfrak{g} = so(3)$, $A = \mathrm{diag}(a_1, a_2, a_3)$. In this case we can consider elements of $U, V \in g^* \simeq so(3)$ as vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^3$ and rewrite Eqs. (57) in the following form:

$$\frac{\partial \boldsymbol{u}}{\partial x_+} = A([\boldsymbol{u} \times \boldsymbol{v}]), \quad \frac{\partial \boldsymbol{v}}{\partial x_-} = [\boldsymbol{u} \times \boldsymbol{v}], \tag{59}$$

where matrix A acts on $\boldsymbol{u} = \Sigma_{i=1,3} u_k X_k$ as on a vector in $\mathbb{R}^3$: $A(\boldsymbol{u}) = \Sigma_{i=1,3} a_k u_k X_k$. Constraints (58) that correspond to the two second order Hamiltonians $I_0^2(L^+(\lambda))$ are written as follows: $(\boldsymbol{u}, A^{-1}\boldsymbol{u}) = \mathrm{const}^-$, $(\boldsymbol{v}, \boldsymbol{v}) = \mathrm{const}^+$.

Using Eqs. (59) it is easy to deduce that there exists vector-potential $\boldsymbol{\phi}$ such that $\boldsymbol{u} = A(\partial\boldsymbol{\phi}/\partial x_-), \boldsymbol{v} = (\partial\boldsymbol{\phi}/\partial x_+)$. In the result we obtain that Eqs. (59) are equivalent to the following equation:

$$\frac{\partial^2 \boldsymbol{\phi}}{\partial x_+ \partial x_-} = -\left[\frac{\partial \boldsymbol{\phi}}{\partial x_+} \times A\left(\frac{\partial \boldsymbol{\phi}}{\partial x_-}\right)\right]. \tag{60}$$

B. Hierarchies connected with the degenerated matrices *A*

Let us consider the simplest equation of the hierarchy associated with the degenerated matrices A. In this case, like in the case of hierarchies associated with Lie algebras $\widetilde{\mathfrak{g}}_A^+$ degeneration of A will lead to the "reduction" i.e., decreasing the number of independent "fields" in the corresponding system of equations in partial derivatives. We will again restrict ourselves to the simplest case of rank $A = n-1$.

Let us consider the second order Hamiltonians $I_0^2(L^+(\lambda))$ and $I_{-4}^{2'}(L^-(\lambda))$. They have (see previous sections) the following form:

$$I_0^2(L^+(\lambda)) = 1/2\ \mathrm{Tr}\,(L^{(-1)})^2, \quad I_{-4}^{2'}(L^-(\lambda)) = -\,\mathrm{Tr}\,(IL^{(0)}A^{-1}L^{(0)}). \tag{61}$$

The corresponding matrix gradients are

$$\nabla I_0^2(L^+(\lambda)) = L^{(-1)}\lambda^{-1}, \quad \nabla I_{-4}^{2'}(L^-(\lambda)) = -\,(IL^{(0)}A^{-1} + A^{-1}L^{(0)}I). \tag{62}$$

Here, as in the previous section, without abuse of notation we introduce the following: $A^{-1} = \mathrm{diag}((A')^{-1}, 0)$ where $A = \mathrm{diag}(A', 0)$ and matrix A' is nondegenerate.

The Hamiltonians $I_0^2(L^+(\lambda))$ and $I_{-4}^{2'}(L^-(\lambda))$, considered as functions on $\tilde{\mathfrak{g}}_A^*$ commute with respect to the usual Lie–Poison bracket on $\tilde{\mathfrak{g}}_A^*$. Corresponding zero-curvature condition

$$\frac{\partial\, \nabla I_0^2(L^+(\lambda))}{\partial x_-} - \frac{\partial\, \nabla I_{-4}^{2'}(L^-(\lambda))}{\partial x_+} + [\nabla I_0^2(L^+(\lambda)),\ \nabla I_{-4}^{2'}(L^-(\lambda))]_{A(\lambda)} = 0$$

yields the following λ-independent equations:

$$\frac{\partial V}{\partial x_-} = [U_-, V], \quad \frac{\partial U_-}{\partial x_+} = [U_-, V]_A, \tag{63}$$

where $U_- \equiv (IL^{(0)}A^{-1} + A^{-1}L^{(0)}I)$, $V \equiv L^{(-1)}$. Note, that although Eqs. (63) look very similar to Eqs. (57) they do not coincide: matrix-valued functions U and U_- have a different number of independent components.

Let us now consider the most interesting case $\mathfrak{g} = so(n)$ and rewrite Eqs. (63) in a more simple way. Let us take into consideration the following Z_2 grading of $so(n)$: $so(n) = so(n)_0 + so(n)_1 \equiv so(n-1) + \mathbb{R}^{n-1}$. We will denote the part of the matrix valued function V, that belongs to the subalgebra $so(n-1)$ of the earlier decomposition by V_+ and the part that belongs to $\mathbb{R}^{n-1}$ by V_- (note that by the definition U_- belong to $\mathbb{R}^{n-1}$). In the result we obtain that Eqs. (63) are equivalent to the following three equations:

$$\frac{\partial V_+}{\partial x_-} = [U_-, V_-], \quad \frac{\partial V_-}{\partial x_-} = [U_-, V_+], \quad \frac{\partial U_-}{\partial x_+} = [U_-, V_+]_A. \tag{64}$$

Introducing in the evident manner vectors $\boldsymbol{u}_-$ and $\boldsymbol{v}_-$ that correspond to the matrices U_- and V_- we may rewrite these equations as follows:

$$\frac{\partial V_+}{\partial x_-} = \boldsymbol{u}_- \wedge \boldsymbol{v}_-, \quad \frac{\partial \boldsymbol{v}_-}{\partial x_-} = -\,V_+(\boldsymbol{u}_-), \quad \frac{\partial \boldsymbol{u}}{\partial x_+} = -\,V_+A'(\boldsymbol{u}_-). \tag{65}$$

This is a system of differential equations in partial derivatives on the $n(n-1)/2 + (n-1)$ independent functions—components of vectors $\boldsymbol{u}_-$ and $\boldsymbol{v}_-$ and matrix V_+. Comparing with Eqs. (56) we see that we have reduced our system on $(n-1)(n-2)/2$ functional degrees of freedom. In the case $n=4$ system (64) admit further reduction.

Example 6: Let $\mathfrak{g} = so(4)$. In this case, introducing instead of $so(3)$-valued matrix V_+ vector $\boldsymbol{v}_+ \in \mathbb{R}^3$ we may rewrite all Eqs. (64) in the vector form:

$$\frac{\partial \boldsymbol{v}_+}{\partial x_-} = [\boldsymbol{u}_- \times \boldsymbol{v}_-], \quad \frac{\partial \boldsymbol{v}_-}{\partial x_-} = [\boldsymbol{u}_- \times \boldsymbol{v}_+], \tag{66}$$

$$\frac{\partial \boldsymbol{u}_-}{\partial x_+} = [A'(\boldsymbol{u}_-) \times \boldsymbol{v}_+], \tag{67}$$

where $\boldsymbol{u} \times \boldsymbol{v}$ denote ordinary vector product of two vectors $\boldsymbol{u}$, $\boldsymbol{v}$. These equations satisfy three second order constraints

$$(\boldsymbol{u}_-, A'\boldsymbol{u}_-) = \text{const}^-, \quad (\boldsymbol{v}_+, \boldsymbol{v}_-) = \text{const}_1^+, \quad (\boldsymbol{v}_+, \boldsymbol{v}_+) + (\boldsymbol{v}_-, \boldsymbol{v}_-) = \text{const}_2^+, \tag{68}$$

that follows from the constancy of functions $I_{-4}^{2'}(L^-(\lambda))$, $P_0(L^+(\lambda))$, $I_0^2(L^+(\lambda))$ along all flows.

Taking into account definition of the vectors $\boldsymbol{v}_+$ and explicit form of the isomorphism $so(4) \simeq so(3)+so(3)$ we may put $\boldsymbol{v}_+ = \pm \boldsymbol{v}_-$ [evidently such reduction is well agreed with Eqs. (66)]. In the result we obtain the system of two vector equations that after replacement of variables $\boldsymbol{u} = A'^{1/2}(\boldsymbol{u}_-)$, $\boldsymbol{v} \equiv \boldsymbol{v}_-$ pass to the standard anisotropic chiral field Eqs. (35).

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Moduli of quantum Riemannian geometries on ⩽4 points

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We classify parallelizable noncommutative manifold structures on finite sets of small size in the general formalism of framed quantum manifolds and vielbeins introduced previously [S. Majid, Commun. Math. Phys. **225**, 131 (2002)]. The full moduli space is found for ⩽3 points, and a restricted moduli space for 4 points. Generalized Levi–Cività connections and their curvatures are found for a variety of models including models of a discrete torus. The topological part of the moduli space is found for ⩽9 points based on the known atlas of regular graphs. We also remark on aspects of quantum gravity in this approach. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1804231]

I. INTRODUCTION

There has been a lot of interest over the years[1–8] in the specific application of noncommutative geometry[9] to the commutative algebra of functions on a finite set Σ (usually a finite group) in which the differential forms do not commute with functions. This provides a systematic way of handling geometry on finite lattices which, at the level of cohomology, electromagnetism, and Yang–Mills theory has already proven interesting and computable. Notably, Ref. 8 contains the moduli of $U(1)$-Yang–Mills on the permutation group S_3 while Ref. 7 quantizes $U(1)$-Yang–Mills theory on the finite group $\mathbb{Z}_2\times\mathbb{Z}_2$.

In this paper we want systematically to extend this theory to the gravitational case. Some first steps are in Ref. 10, to which the present paper is a sequel. It was shown there that finite groups have indeed a natural Riemannian geometry in a vielbein and frame-bundle formalism[11] which was worked out in detail for S_3 (it turns out to have Ricci essentially proportional to the metric, i.e., an "Einstein manifold"). Similarly, the alternating group A_4 was considered in Ref. 12 and has an essentially unique invariant metric with 4-bein and an associated spin connection with nonzero curvature but with Ricci=0, i.e., solves the vacuum Einstein equations. Hence the system of equations for a framed quantum Riemannian manifold is already known to have interesting nontrivial solutions. However, for quantum gravity (or classical but finite gravity) we need a better understanding of the moduli spaces of *all* metrics, connections, etc. and this is what we study now on small sets. Once one has this, one can in principle begin to quantize this moduli space in a path integral approach, i.e., quantum gravity.

Section II starts with a brief account of the formalism for algebras which we then rapidly specialize to the case $\mathbb{C}(\Sigma)$, the algebra of functions in a finite set. That the theory is a specialization of a functorial construction that is formulated for general algebras ensures that it is not *ad hoc* (indeed, this same theory can be specialized to classical geometry and to q-deformed geometry for other choices of algebra[13]). Following Ref. 10, we find that for finite sets Σ the classification of "differential forms" or exterior algebras of parallelizable type reduces to the classification of finite regular graphs with vertices Σ and a fixed number n arrows from every vertex. New results are Theorem 2.1 showing in detail that the calculus is then inner, and Theorem 2.2 for the construction of two-forms. Both are needed in the paper. Further ingredients in the formalism are

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a choice of n-beins and a frame group G (in our case a finite group) acting on the vector space spanned by them. This gives the moduli of "quantum framed manifold" structures on Σ. After this, one may look for a compatible connection ∇, find the Riemann curvature and from this the Ricci tensor and Ricci scalar. In this way we set up the theory that we are going to explore for small numbers of points.

In Sec. III A we analyze the case $\Sigma=\{x,y\}$ of two points and frame groups S_2,S_3 acting on an einbein e_1 parametrized by a function Θ. We find that for each einbein there is a natural generalized Levi–Cività connection

$$\nabla(fe_1)=\mathrm{d}f\otimes e_1+2f\langle\Theta\rangle e_1\otimes e_1$$

for any function f, where $\langle\ \rangle$ is the average value over the two points. This has zero Riemannian curvature, which emerges as a typical feature on two points. In our spin connection approach we find also the moduli of spin connections; for S_2 framing we have a unique spin connection underlying ∇. For S_3 we find a larger moduli of spin connections, with gauge curvature, underlying the Riemannian geometry itself (all giving the same ∇).

In Sec. III B we similarly cover the case $\Sigma=\{x,y,z\}$ of three points and frame groups S_2,S_3 acting on a zweibein. The zweibein moduli space is itself nontrivial as an algebraic variety but we show how to put a generic point into a canonical form, and then study spin connections for a fixed zweibein. A general feature for three points emerges, namely that in all our models the Ricci scalar vanishes, but the Riemann and Ricci tensors themselves generically do not. For S_2 we have a linear constraint on the zweibein to admit a connection, after which there is a one-parameter family of connections. For S_3 there is no constraint on the zweibein and an eight-dimensional moduli of connections.

The canonical form for the vielbeins obtained in our analysis of 2 and 3 points in Sec. III is one where (after linear transformations), one may restrict to vielbeins which have only a scalar Θ_a associated to each edge. In Sec. IV we proceed to restrict attention to this canonical form, now for four point sets. Physically, the modulus of the vielbein assigns a "length" to each edge, while the natural connectivity for 4 points is that of $\mathbb{Z}_2\times\mathbb{Z}_2$ (interpreted as a discrete model of a torus), which we consider in Secs. IV A–IV C; we consider various frame groups, among them an interesting choice (Sec. IV B) is a frame group $\mathbb{Z}_4$ of "quarter rotations" again as a discrete model of a torus; we find the most general connection, its Riemann and Ricci curvatures, etc. This model has the feature (Theorem 4.4) that a fully metric compatible spin connection is determined uniquely by the zweibein, but with the latter further constrained. By contrast, our weaker "skew metric compatible" or cotorsion free condition admits further parameters a,b with the zweibein relatively unconstrained. We also see what happens if one takes too big a calculus on the frame group, namely additional unphysical modes emerge which do not, however, enter into the covariant derivative. This seems to us an important lesson for finite manifold-building by these methods. Section IV D completes the picture by covering the alternative connectivity of 4 points joined in a tetrahedron, which is more like a sphere. Here with $\mathbb{Z}_3$ frame group of "one-third" rotations we find an unusual but interesting calculus, moduli, etc., without classical analogue.

Later, in Sec. V we make some first remarks on the quantum theory, including a look at the discrete torus model on $\mathbb{Z}_2\times\mathbb{Z}_2$. Mainly, we find what we show on this model to be a reasonable unitarity or *-structure on the system which is needed to reduce the functional integrals to real variables. We do not try to do the integrals themselves, which would be beyond the scope of our current analysis.

Finally, Sec. VI return to a more qualitative account of all bidirectional framed geometries up to 9 points, deduced from the known atlas of graphs.[14] This covers the connectivity or topological aspect of the vielbein moduli space. At this level a vielbein amounts to a coloring of the graph into n-colors. For each such vielbein, there are further continuous degrees of freedom for matrices e_a labeled according to the coloring a (as seen in detail in Sec. III). If we ignore these then we have in principle a "combinatorial quantum gravity" in which one sums over all such colorings.

Let us note that "geometry" on finite sets in some form or other has a long pedigree. Common to all approaches is the basic data of "differentials" as defined by directed edges between vertices

(a "digraph" or quiver). Such objects are used in representation theory for quivers formed on Dynkin diagrams. One also considers in that context some kind of "vector bundles" with vector spaces over each vertex albeit of varying dimension. Similarly in physics as well as in simplicial cohomology one may "approximate" a manifold by a finite triangulation and work on that. From the algebraic point of view one does not actually need bidirectional edges, e.g., every poset defines a connectivity graph and differential calculus with $x\to y$ if $x<y$ (albeit not a parallelizable one if it is finite). This would be relevant to modeling Lorentzian manifolds[15] with $x\to y$ modeling a time-like path from x to y. Hence the deeper notions of vielbeins and Riemannian geometry that we develop on such data potentially have several applications.

II. PRELIMINARIES: FORMALISM OF QUANTUM RIEMANNIAN MANIFOLDS

Here we briefly recall the formalism of Ref. 10. To tie in with the general theory we start with a brief recap over general algebras in Sec. II A. Then in Sec. II B we specialize to the finite set case in more detail than outlined in Ref. 10. We cover here only the parallelizable case where the frame bundle algebra has a trivial tensor product form. There is a still more general theory where the bundle is nontrivial, see Ref. 10, but this needs much more machinery and we do not cover it here. It would be needed for finite posets, for example.

A. Over general algebras

Let M be a unital algebra. We equip M with a differential structure in the sense $(\Omega^1(M),\mathrm{d})$, where $\Omega^1(M)$ is an $M-M$ bimodule, and $\mathrm{d}:M\to\Omega^1(M)$. This is a notion common to all approaches to noncommutative geometry including Ref. 9. We also need $\Omega^2(M)$ or (in principle) higher $\Omega^k(M)$ with $\mathrm{d}^2=0$, for which we can take the maximal prolongation of $\Omega^1(M)$ or any of its quotients.

In this context we define a (left) *vielbein* or V-bein as a collection $\{e_a\}$ forming an M-basis of one-forms $e_a\in\Omega^1(M)$, i.e., $\Omega^1(M)\cong M\otimes V$ where $V=\mathrm{span}\{e_a\}$. One can also think equivalently of the V-bein as a map $e:V\to\Omega^1(M)$ as in Ref. 10 if we regard V as a fixed abstract vector space. Given a vielbein we deduce operators $\rho_a^b,\partial^a:M\to M$ where

$$e_a f=\sum_b \rho_a^b(f)e_b,\quad \mathrm{d}f=\sum_a(\partial^a f)e_a,\quad \forall\, f\in M \tag{1}$$

as an expression of the bimodule and exterior derivative structure.

Next, we assume that we actually have an A-vielbein, i.e., we require V to be an A-comodule under a Hopf algebra A. There is also a more general theory with A merely a coalgebra, i.e., this is not a critical assumption. We fix a left-covariant differential structure $\Omega^1(A)$ on the fiber of the frame bundle. Like Lie groups, quantum groups are always parallelizable and hence $\Omega^1(A)=A\otimes\Lambda^1$ for some space of invariant one-forms Λ^1. This is a quotient of the augmentation ideal A_+ of A (classically it means the functions that vanish at the group identity), i.e., $\Lambda^1=A_+/Q_A$ for some left ideal $Q_A\subseteq A_+$. We call $\Lambda^{1*}\subset H_+$ the associated "quantum tangent space," where we suppose Λ^1 is finite dimensional and H a Hopf algebra dually paired with A (it plays the role classically of the enveloping algebra of the Lie algebra of the frame group). We will be interested only in the bicovariant case as in Ref. 10 where one knows from the Woronowicz theory[16] that Λ^1 is Ad-stable or that Λ^{1*} inherits Ad as a "quantum Lie bracket." When A is coquasitriangular one knows that Λ^{1*} is in fact a braided-Lie algebra.[17] However, neither assumption is critical for the geometry.

We let $\{f^i\}$ be a basis of Λ^{1*} and we denote by $\triangleright$ its left action inherited from the left action of H on V corresponding to the coaction of A. It is only this action which is needed in the formulas below. In this basis a spin connection means a collection of one-forms $\{A_i\}$. Its torsion tensor corresponds to

$$\mathrm{d}e_a + \sum_i A_i \wedge f^i \triangleright e_a \tag{2}$$

and we are interested in torsion-free connections. We also (optionally) impose a regularity or "differentiability" condition linking $\Omega^2(M)$ and $\Omega^1(A)$, namely

$$\sum_{ij} A_i \wedge A_j \langle f^i f^j, q\rangle = 0 \quad \forall\, q \in Q_A. \tag{3}$$

This ensures that the component two-forms $\{F_i\}$ of the curvature of the spin connection, namely

$$F_i = \mathrm{d}A_i + \sum_{jk} c_i^{jk} A_j \wedge A_k \tag{4}$$

have a proper geometrical interpretation as a curvature two-form with values in Λ^{1*}. Here $c_i^{jk} = \langle e_i, f^j f^k\rangle$ are structure constants of the product of H projected to Λ^{1*} (where $\{e_i\}$ is a dual basis of Λ^1).

For metrics we specialize to the case $g = \Sigma_{a,b}\ \eta^{ab} e_a \otimes_M e_b$ where $\eta \in V \otimes V$ is a nondegenerate H-invariant "local metric." This is not the most general setup up in Refs. 11 and 10, where one can consider g an arbitrary (but nondegenerate) two-form. In our case the cotorsion-free condition, which is the natural generalization of Levi–Cività metric compatibility in Refs. 11 and 10, is vanishing of

$$\mathrm{d}e_a + \sum_i S^{-1}(f^i) \triangleright e_a \wedge A_i \tag{5}$$

where S denotes the antipode of H.

Finally, we specialize to the case of $\Omega^2(M)$ constructed from an H-equivariant projection $\pi: V \otimes V \to V \otimes V$ according to the scheme indicated in Ref. 10. From the above, we know that $\Omega^1(M) \otimes_M \Omega^1(M) \cong M \otimes V \otimes V$ allowing us to define surjections

$$\Omega^1(M) \underset{M}{\otimes} \Omega^1(M) \to \Omega^2(M),$$

where we quotient out $M \otimes \ker \pi$. In fact we define Λ as a quadratic algebra on V with relations $\ker \pi$, and $\Omega(M) \cong M \otimes \Lambda$. Such a scheme imposes constraints on π. In this setting there is a canonical lift

$$i: \Omega^2(M) \hookrightarrow \Omega^1(M) \underset{M}{\otimes} \Omega^1(M), \quad i(e_a \wedge e_b) = \pi(e_a \otimes e_b). \tag{6}$$

Finally, we let $i(F_i) = \Sigma_{a,b}\ i(F_i)^{ab} e_a \otimes_M e_b$ define the components in the V-bein basis of the lifted F_i. Then

$$\mathrm{Ricci} = \sum_{i,a,b} i(F_i)^{ab} e_b \underset{M}{\otimes} f^i \triangleright e_a. \tag{7}$$

The full Riemann curvature of the connection and the covariant derivative acting on one-forms are

$$\mathrm{Riemann}(\alpha) = \sum_{i,a} \alpha^a F_i \underset{M}{\otimes} f^i \triangleright e_a, \quad \nabla\, \alpha = \sum_a \mathrm{d}\alpha^a \underset{M}{\otimes} e_a - \sum_{i,a} \alpha^a A_i \underset{M}{\otimes} f^i \triangleright e_a \tag{8}$$

where $\alpha = \Sigma_a\ \alpha^a e_a$. The derivation of these local formulas from a more abstract theory is in Ref. 10, in an equivalent comodule notation.

B. Over finite sets

We now specialize the above to the case $M = \mathbb{C}(\Sigma)$ where Σ is a finite set and $H = \mathbb{C}(G)$ where G is a finite group. In this case the possible $\Omega^1(\Sigma)$ are given by subsets

$$E \subset \Sigma \times \Sigma - \text{diagonal}$$

of "allowed directions." This is already known from Ref. 9 and E is the same as the structure of a quiver or digraph with vertex set Σ and the notation $x \to y$ whenever $(x,y) \in E$. In the geometrical examples we typically expect E symmetric or "bidirectional," i.e., for every edge $x \to y$ there is an edge $x \leftarrow y$, but we do not assume this in general. Explicitly,

$$\Omega^1(\Sigma) = \text{span}\{\, \delta_x \otimes \delta y | x \to y\}, \quad \mathrm{d}f = \sum_{y \in F_x} (f(y) - f(x)) \delta_x \otimes \delta_y; \quad F_x = \{\, y | x \to y\}.$$

Note also that the k-fold product

$$\Omega^1(\Sigma) \underset{M}{\otimes} \cdots \underset{M}{\otimes} \Omega^1(\Sigma) = \text{span}\{\, \delta_x \otimes \delta_{x_1} \otimes \cdots \otimes \delta_{x_k} | x \to x_1 \to x_2 \to \cdots \to x_k\},$$

i.e., the linear span of the set of k-arcs. The bimodule structures are the pointwise ones for products from the extreme left and right.

As explained in Ref. 10 a vielbein in this setting is possible *iff* E fibers over Σ, i.e., F_x have cardinality n (say), independent of x. In this case an n-bein is the specification of invertible $n \times n$ matrices $e_{\cdot x,\cdot}$ for each $x \in \Sigma$. Here e_{axy} has indices $a \in 1, \ldots, n$ and $y \in F_x$. We write the inverses as e_a^{-1xy} with

$$\sum_{y \in F_x} e_a^{-1xy} e_{bxy} = \delta_{a,b}, \quad \sum_a e_a^{-1xy} e_{axy'} = \delta^y_{y'}. \tag{9}$$

In this case the operators (1) are

$$\rho^b_a(f)(x) = \sum_{y \in F_x} e_b^{-1xy} f(y) e_{axy}, \quad (\partial^a f)(x) = \sum_{y \in F_x} (f(y) - f(x)) e_a^{-1xy}. \tag{10}$$

A calculus on an algebra M is inner if there is a one-form θ with $\mathrm{d}f = [\theta, f]$ for $f \in M$.

Theorem 2.1: *cf. Ref. 10. A finite set calculus equipped with a vielbein is inner,*

$$\theta = \sum_a \Theta_a e_a, \quad \Theta_a(x) = \sum_{y \in F_x} e_a^{-1xy}.$$

Moreover, the maximal prolongation exterior algebra $\Omega(\Sigma)$ *has likewise* $\mathrm{d} = [\theta, \}$ (*graded anticommutator) and is generated by* $\mathbb{C}(\Sigma)$ *and the quadratic algebra on the* $\{e_a\}$ *with relations*

$$\sum_{y \in F_{x,z}} \sum_{a,b} e_a^{-1xy} e_b^{-1yz} e_a \wedge e_b = 0, \quad \forall\, (x,z) \notin E \cup \text{diag}; \quad F_{x,z} = \{\, y | x \to y \to z\}.$$

Proof: We define θ as stated. Then the explicit formulas (10) allow one to verify that $\mathrm{d}f = [\theta, f]$ for any function f, as required. The maximal prolongation of the Ω^1 is defined as the tensor algebra over $M = \mathbb{C}(\Sigma)$ modulo the relations in degree 2 imposed by extending d as a superderivation with $\mathrm{d}^2 = 0$. More precisely, we lift any one-form to the universal differential calculus over $\mathbb{C}(\Sigma)$, apply the universal exterior derivative there, and then project down to Ω^2. That this should be well-defined defines the minimal relations in degree 2 (which are the only ones imposed in the maximal prolongation). In our case a basis of the kernel of the projection to Ω^1 is given by $\delta_x \mathrm{d} \delta_z = 0$ whenever $(x,z) \notin E \cup \text{diag}$, so we require for each such (x,z) the relation

$$\mathrm{d}\delta_x \wedge \mathrm{d}\delta_z = 0.$$

We compute

$$\mathrm{d}\delta_x = \sum_a \sum_{y\in F_\cdot} (\delta_x(y) - \delta_x) e_a^{-1\cdot y} e_a = \sum_a (e_a^{-1\cdot x} - \delta_x \Theta_a(x)) e_a,$$

where $\cdot$ denotes a functional dependence on points in Σ and we adopt the convention that $e_a^{-1wx} = 0 = e_{awx}$ if $x \notin F_w$. Note also that

$$\sum_a e_a^{-1\cdot x} \rho_a^c(f) = \sum_{y\in F_\cdot} \sum_a e_a^{-1\cdot x} e_c^{-1\cdot y} f(y) e_{\cdot y} = f(x) e_c^{-1\cdot x}$$

by (10) and (9). The latter also implies that $\Sigma_a \Theta_a(x) e_{axy} = 1$ if $y \in F_x$. Hence

$$\begin{aligned}
\mathrm{d}\delta_x \wedge \mathrm{d}\delta_z &= \sum_{a,b,c} e_a^{-1\cdot x} \rho_a^c(e_b^{-1\cdot z}) e_c \wedge e_b - \sum_{a,b,c} e_a^{-1\cdot x} \Theta_b(z) \rho_a^c(\delta_z) e_c \wedge e_b - \sum_{a,b,c} \delta_x \Theta_a(x) \rho_a^c(e_b^{-1\cdot z}) e_c \wedge e_b \\
&\quad + \sum_{a,b,c} \delta_x \Theta_a(x) \Theta_b(z) \rho_a^c(\delta_z) e_c \wedge e_b \\
&= \sum_{b,c} e_c^{-1\cdot x} e_b^{-1xz} e_c \wedge e_b - \sum_{b,c} \delta_z(x) \Theta_b(z) e_c^{-1\cdot z} e_c \wedge e_b - \delta_x \sum_{b,c} \sum_{y\in F_x} e_c^{-1xy} e_b^{-1yz} e_c \wedge e_b \\
&\quad + \delta_x \sum_{a,b,c} \Theta_a(x) \Theta_b(z) e_{axz} e_c^{-1xz} e_c \wedge e_b.
\end{aligned}$$

The first and last terms vanish for $(x,z) \notin E$ and the second term for $x \neq z$. Hence in this case we obtain precisely the relation stated from the remaining third term. This completes the proof of the result mentioned in Ref. 10.

It is then a computation to write

$$e_a = \sum_{(x,y)\in E} e_{axy} \delta_x \mathrm{d}\delta_y = \sum_{y\in F_\cdot} e_{a\cdot y} \mathrm{d}\delta_y$$

and obtain $\mathrm{d}e_a = \theta e_a + e_a \theta$. Note that the compatibility of d with the relations (1) for all f more or less requires this relation since applying d to (1) gives $(\mathrm{d}e_a - \{\theta, e_a\}) f = \rho_a^b(f)(\mathrm{d}e_b - \{\theta, e_b\})$ after using (1) and that the calculus is inner. □

We note in passing that by similar computations the maximal prolongation has

$$\begin{aligned}
\theta \wedge \theta = \sum_{a,b} \Theta_a e_a \Theta_b e_b &= \sum_{a,b,c} \Theta_a \sum_{y\in F_\cdot} e_c^{-1\cdot y} \Theta_b(y) e_{a\cdot y} e_c \wedge e_b \\
&= \sum_{b,c} \sum_{y\in F_\cdot} e_c^{-1\cdot y} \Theta_b(y) e_c \wedge e_b = \sum_{a,b} \sum_{\cdot\to y\to z} e_a^{-1\cdot y} e_b^{-1yz} e_a \wedge e_b
\end{aligned}$$

which [in view of the relations for $\Omega^2(\Sigma)$] has contributions only from $z = \cdot$ and $\cdot \to z$. This is not necessarily zero, i.e., θ is not necessarily closed [rather, $\mathrm{d}\theta = 2\theta \wedge \theta$ so that $\alpha = -2\theta$ is always a zero curvature $U(1)$ connection].

We also require for a G-covariant vielbein that $V = \mathrm{span}\{e_a\}$ is a G module. The above constructions are all G-covariant under these local transformations of V. To define more general exterior algebras $\Omega(\Sigma)$ we let $\pi: V \otimes V \to V \otimes V$ be a G-equivariant projection operator, with components defined by $\pi_x(e_a \otimes e_b) = \Sigma_{c,d} \pi_{ab}^{cd} e_c \otimes e_d$. We define operators

$$\pi_{x,z}: \mathbb{C}F_{x,z} \to \mathbb{C}F_{x,z}, \quad \pi_{x,z}{}^{y}{}_{y'} = \sum_{a,b,c,d} \pi_{ab}^{cd} e_a^{-1xy} e_b^{-1yz} e_{cxy'} e_{dy'z} \tag{11}$$

on the space spanned by 2-arcs with fixed endpoints x, z.

Theorem 2.2: *π defines an exterior algebra with $\mathrm{d}^2 = 0$ as a quotient of the tensor algebra on V by the quadratic relations*

$$\ker \pi = 0$$

iff

$$\text{(i)}\quad \sum_{a,b,c,d} \pi_{ab}^{cd} e_a^{-1xy} e_b^{-1yz} e_{cxy'} e_{dy'z'} = 0, \quad \forall\, z \neq z';\quad y \in F_{x,z},\quad y' \in F_{x,z'}$$

$$\text{(ii)}\quad \sum_{y \in F_{x,z}} \pi_{x,z}{}^{y}{}_{y'} = 0, \quad \forall\, (x,z) \notin E \cup \mathrm{diag},\quad y' \in F_{x,z}.$$

Proof: We identify $\Omega^1(\Sigma) \otimes_M \Omega^1(\Sigma)$ with $\mathbb{C}(\Sigma) \otimes V \otimes V$ via the vielbein so that π induces left-module projection operators on this. These are, therefore, given by projection matrices π_x on the space spanned by the 2-arcs from x, for each x. Their components are

$$\pi^{yz}_{x_{y'z'}} = \sum_{a,b,c,d} \pi_{ab}^{cd} e_a^{-1xy} e_b^{-1yz} e_{cxy'} e_{dy'z'}.$$

We require that these are also right module maps, which is the condition (i) stated. It means that $\pi^{yz}_{x_{y'z'}} = \pi_{x,z}{}^{y}{}_{y'} \delta_z^{z'}$ for a family of projections $\pi_{x,z}$ for each fixed x, z. These are the operators (11). As explained in Ref. 10 there is then a condition on the family of projectors to ensure that the quotient $\Omega^1(\Sigma) \otimes_M \Omega^1(\Sigma) \to \Omega^2(\Sigma)$ factors through the maximal prolongation, namely the condition (ii). This is necessary and sufficient for the relations in $\Omega^2(\Sigma)$ defined by $\ker \pi$ to be compatible with the extension of d to two-forms via the graded Leibniz rule. □

The maximal prolongation in Theorem 2.1 can be viewed as given by a generalization of this construction in which the projection π is allowed to vary from point to point. The more specific construction in Theorem 2.2 is necessarily a quotient of it by further relations.

Finally, we fix an Ad-stable subset $\mathcal{C} \subset G$ with $e \notin \mathcal{C}$ (e here the group identity), e.g., a nontrivial conjugacy class. These describe the bicovariant calculi $\Omega^1(G)$ in the Woronowicz theory.[16] The space of invariant forms Λ^1 in $\Omega^1(G)$ has basis $\{e_i \,|\, i \in \mathcal{C}\}$. The dual basis of Λ^{1*} is $\{f^i\}$ with $f^i = i - e$. The torsion and cotorsion equations then have the same forms (2) and (5), with $Si = i^{-1}$ the group algebra antipode. The regularity condition now reads

$$\sum_{ij=q} A_i \wedge A_j = 0, \quad \forall\, q \notin \mathcal{C} \cup \{e\}. \tag{12}$$

This is empty if we chose the universal calculus on G (where $\mathcal{C} = G - \{e\}$), but in general it is a quadratic constraint. The curvature form is then

$$F_i = \mathrm{d}A_i + \sum_{jk=i} A_j \wedge A_k - \left\{ A_i, \sum_j A_j \right\}. \tag{13}$$

The formulas for the Ricci and Riemann tensors and ∇ have the same form (8).

III. MODULI OF GEOMETRIES ON TWO OR THREE POINTS

In this section we describe the moduli space of possible vielbeins and metrics on two or three points, and moduli of spin connections and their curvature for some points in the moduli of vielbeins with respect to frame group S_2 or S_3.

More precisely, the moduli of possible vielbeins is in the first place labeled by two natural numbers $m = |\Sigma|$ and n a fixed number of arcs from each point. For each m, n, the combinatorial part of the moduli space consists of determining all possible quiver structures with no self-arcs, i.e., all $E \subseteq \Sigma \times \Sigma - \mathrm{diag}$ with F_x of cardinality n at each $x \in \Sigma$. We interpret it as finding all possible parallelizable $\Omega^1(\Sigma)$ with n-dimensional cotangent space. Note that $\overline{E}$ where we flip the entries of E defines another calculus $\overline{\Omega^1}(\Sigma)$ and in the asymmetric case one could (although we do not do it here) demand this to also be parallelizable, with an associated number $\overline{n}$. There is a corresponding moduli of geometries built on this arrow-reversed calculus.

For $m = 2$ or $\Sigma = \{x, y\}$ there is only one possibility, namely $n = 1$ and the quiver

$$x \leftrightarrow y$$

up to relabelings. This is the universal calculus on Σ where E is as large as possible.

For $m=3$ or $\Sigma=\{x,y,z\}$ there are two cases for $n=1$, namely

$$\begin{array}{ccc} x & \to & y \\ & \searrow\ \swarrow & \\ & z & \end{array}, \quad x \leftrightarrow y \leftarrow z$$

up to relabelings. These are asymmetric. For $n=2$ there is only one possibility, the universal calculus on Σ again, which is always symmetric. It is given by

$$\begin{array}{ccc} x & \leftrightarrow & y \\ & \searrow\ \swarrow & \\ & z & \end{array}.$$

Next, for our projection matrix π to define $\Omega^2(\Sigma)$ we make the "naïve" choice

$$\pi = \tfrac{1}{2}(\mathrm{id} - \tau), \tag{14}$$

where τ is the usual "flip" operator on the tensor product, i.e., we assume the basic one-forms anticommute. This seems to give reasonable results for $n=2$ and a small number of points (in general it would be too restrictive). For $n=1$ we choose $\pi=1$ (the choice $\pi=0$ is also allowed but not very interesting). More generally, we should determine all possible equivariant $\pi: V\otimes V\to V\otimes V$ for choice of frame group G and a representation V of dimension n. The representation theory of G then dictates the possible equivariant projection matrices $\pi: V\otimes V\to V\otimes V$. This is the representation theoretic part of the moduli space. In our case, we take symmetric groups S_2, S_3 appropriate to a our small number of points. For $n=1$, V has to be trivial (we denote this by $\mathbb{C}$) or the sign representation given by $(-1)^{l(g)}$ where l is the length function. For $n=2$ we have $V=\mathbb{C}\oplus\mathrm{sign}$, $V=\mathrm{sign}\oplus\mathrm{sign}$ or, in the case of S_3 also its two-dimensional representation. In all three cases $V\otimes V=\mathbb{C}\oplus\mathrm{sign}\oplus V$ and the "naïve" π (14) projects out all but the sign representation here (cf. in classical geometry the top form transforms by the determinant under a linear transformation). The invariant local metric η up to a normalization is also classified by representation theory and we take it as the generator of the natural trivial representation in the decomposition of $V\otimes V$.

Fixing all the above quasi-combinatorial data, we have a moduli space

$$\mathrm{Vielbeins}_{m,n,E,\pi} = \{e_{a,x,y}\}/\mathrm{GL}_n \tag{15}$$

consisting of m $n\times n$ invertible matrices subject to the constraints in Theorem 2.2. We divide by an overall GL_n acting on the left and corresponding to a change of basis of V. We arrive at a certain algebraic variety which we shall describe first.

Finally, for a fixed vielbein and the above data, we look at the moduli of spin connections for η. This last part requires us to fix a differential structure on G. For S_2 the only choice is the universal calculus $\Omega^1(S_2)$. For S_3 there is the universal calculus and the calculus corresponding to the two-cycles conjugacy class. The remaining conjugacy class does not give a reasonable geometry of S_3 (it is not connected) and does not appear to give interesting results, so we omit it. In all cases we assume that the action of G on V is not trivial when restricted to the braided-Lie algebra generators f^i. Otherwise, they would act as zero, the Riemann curvature would be automatically zero and ∇ would be just given by d for any spin connection. So we omit this uninteresting case in our analysis.

The case $\pi=0$ is trivial and we deal with it here. In this case $\Omega^1(\Sigma)$ is the top degree so that there is no constraint on the $\{e_{axy}\}$ other than being invertible, i.e.,

$$\mathrm{Vielbeins}_{m,n,E,0} = (GL_n)^{m-1}.$$

Similarly the torsion, cotorsion and regularity conditions are empty and any collection of one-forms $\{A_i\}$ are trivially a spin connection, with zero curvature.

A. Two points

For $\Sigma=\{x,y\}$ the only choice is the universal calculus as explained above, which has $n=1$, i.e., we look for a 1-bein e_1. We write

$$e_1=\alpha\delta_x\otimes\delta_y+\beta\delta_y\otimes\delta_x;\quad e_{1xy}=\alpha,\quad e_{1yx}=\beta,\quad \alpha,\beta\neq 0.$$

The partial derivatives and commutation relations are

$$e_1 f=\overline{f}e_1,\quad \partial^1 f=(\overline{f}-f)\Theta;\quad \Theta(x)=\alpha^{-1},\quad \Theta(y)=\beta^{-1};$$

$$\overline{f}(x)=f(y),\quad \overline{f}(y)=f(x).$$

The generating one-form and exterior derivative are

$$\theta=\Theta e_1,\quad \mathrm{d}f=(\overline{f}-f)\theta.$$

For $\Omega^2(\Sigma)$ we have only one nontrivial possibility, namely $\pi=1$, which gives the maximal prolongation with no relations in the exterior algebra (it is the universal exterior algebra on Σ). The conditions in Theorem 2.2 are empty as the assumptions are never satisfied. Here $\Lambda=\mathbb{C}[e_1]$ and each $\Omega^k(\Sigma)$ is one-dimensional over $\mathbb{C}(\Sigma)$. The exterior derivatives are defined by the graded-Leibniz rule and

$$\mathrm{d}e_1=(\Theta+\overline{\Theta})e_1^2.$$

Proposition 3.1: For any Θ *the dimensions* p_i of H^i *are* $1:0:0:\ldots$. *Here*

$$H^0=\mathbb{C}.1,\quad H^i=\{0\};\quad i\geqslant 1.$$

Proof: First of all we show explicitly that, in accordance with Theorem 2.2, $\mathrm{d}^2=0$.

$$\mathrm{d}(\mathrm{d}f)=\mathrm{d}(\Theta(\overline{f}-f)e_1)=(\Theta\overline{\Theta}(f-\overline{f})+\Theta\overline{\Theta}(\overline{f}-f))e_1^2=0.$$

The functions f such that $df=0$ are the constant ones so the nullspace of d acting on $\mathbb{C}(\Sigma)$ is one-dimensional (and therefore, $p_0=1$). Since the dimension of $\Omega^1(\Sigma)=2$ this means that the image of d in $\Omega^1(\Sigma)$ is one-dimensional. If $\omega=fe_1$ is a one-form, $\mathrm{d}\omega=0$ if and only if $f\overline{\Theta}+f\overline{\Theta}=0$, or $f=\Theta(\delta_x-\delta_y)$ which implies that the nullspace of d contained in $\Omega^1(\Sigma)$ is one-dimensional. Then, $p_1=1-1=0$. In turn, the image of d in $\Omega^2(\Sigma)$ is one-dimensional, and so $p_2=1-1=0$ and so forth. □

Since we are working modulo an overall change of basis including normalization, only $\alpha^{-1}\beta$ is significant, so

$$\mathrm{Vielbeins}_{2,1,\mathrm{univ},1}=\mathbb{C}^*.$$

Next we look at spin connections. For group G we assume a symmetric group acting in the only nontrivial possibility, the sign representation on e_1. Thus $f^i\triangleright e_1=0$ if the permutation i is even and $f^i\triangleright e_1=-2e_1$ if i is odd. For S_2 we have only the universal calculus, hence only one f^i where $i=(12)$. We write $A=ae_1$ for a function a. Then the torsion-free condition becomes

$$\Theta+\overline{\Theta}-2a=0,$$

which is also the cotorsion-free condition, while the regularity condition is empty. Hence for each one-bein there is a unique spin connection

$$a = \frac{\alpha + \beta}{2\alpha\beta} = \frac{\Theta + \overline{\Theta}}{2},$$

which is a constant function. Its curvature is

$$F = \mathrm{d}A - 2A^2 = 0,$$

which means that the Riemann tensor is also zero. The covariant derivative is

$$\nabla(fe_1) = \mathrm{d}f \otimes e_1 + f(\Theta + \overline{\Theta})e_1 \otimes e_1. \tag{16}$$

For S_3 with its three-dimensional (two-cycles) calculus we have $f^i \triangleright e_1 = -2e_1$ and writing the three components functions a_1, a_2, a_3 of the spin connections in directions (12), (23), and (13), the torsion and cotorsion conditions for any fixed one-bein become

$$\Theta + \overline{\Theta} - 2(a_1 + a_2 + a_3) = 0$$

while the regularity (which does not depend on the representation) is

$$a_1\overline{a_2} + a_2\overline{a_3} + a_3\overline{a_1} = 0.$$

There are different classes of solutions including a two-dimensional part of the moduli space of spin connections for a generic one-bein. The curvature is

$$F_i = (a_i - \overline{a_i})(\overline{\Theta} - \Theta)e_1 \wedge e_1$$

and is typically nonzero if the factor $(\overline{\Theta} - \Theta)(x) = (\alpha - \beta/)\alpha\beta$ is nonzero. On the other hand, we find (16) again, with zero Riemann curvature.

For S_3 with its five-dimensional (universal) calculus, a spin connection consists of components b_1, b_2 in the three-cycles directions which are unconstrained, and a_1, a_2, a_3 in the two-cycles directions, with the single linear equation

$$\Theta + \overline{\Theta} - 2(a_1 + a_2 + a_3) = 0$$

for vanishing of torsion and cotorsion. The regularity condition is empty. So here the moduli space of connections is linear for each vielbein. There is typically curvature at the frame bundle level but again the Riemann curvature vanishes since ∇ is still given by (16).

We conclude for 2 points that increasing the frame braided Lie algebra allows more spin connections but these do not enter into the Riemannian geometry itself. Instead, we find a unique generalized Levi–Cività type covariant derivative (16) for each einbein, and it has zero Riemannian curvature.

B. Three points

For $\Sigma = \{x, y, z\}$ there are two fibrations for $n=1$ and one for $n=2$ as explained above.

For $n=1$ a vielbein means three invertible numbers $\{e_{\cdot x}\}, \{e_{\cdot y}\}, \{e_{\cdot z}\}$. However, both types of fibrations for $n=1$ imply $\pi=0$ as the only solution. This is forced by the conditions in Theorem 2.2 as follows. For the triangular fibration the 2-arcs are

$$x \to y \to z, \quad y \to z \to x, \quad z \to x \to y$$

but then condition (ii) requires $\pi_{x,z}{}^{y}{}_{y'} = 0$, which implies $\pi = 0$. For the case of the other fibration the two-arcs are

$$z \to x \to y, \quad x \to y \to x, \quad y \to x \to y.$$

In this case condition (ii) requires $\pi_{z,y}{}^{x}{}_{x'} = 0$ and hence $\pi = 0$. Hence for $n=1$ only the trivial case $\pi = 0$ already covered in general above is allowed.

For $n=2$ we have only one fibration, which is the universal $\Omega^1(\Sigma)$. Then a vielbein means in the first place three invertible matrices

$$e_{\cdot x\cdot}=X,\quad e_{\cdot y\cdot}=Y,\quad e_{\cdot z\cdot}=Z.$$

Because of the cyclic nature of the graph, we label the columns of X as y,z, of Y as z,x and of Z as x,y. There are two types of two-arcs, namely

$$x\to y\to z,\quad x\to z\to y,\quad y\to x\to z,\quad y\to z\to x,\quad z\to x\to y,\quad z\to y\to x$$

or

$$x\to y\to x,\quad x\to z\to x,\quad y\to x\to y,\quad y\to z\to y,\quad z\to x\to y,\quad z\to y\to x.$$

Finally, we take the "naive" form (14) for π. The condition (ii) in Theorem 2.2 is empty because $\Omega^1(\Sigma)$ is universal. Condition (i) gives equations of the form

$$0=\pi^{xyz}_{xy'z'}=\tfrac{1}{2}(e_1^{-1xy}e_2^{-1yz}-e_2^{-1xy}e_1^{-1yz})(e_{1xy'}e_{2y'z'}-e_{2xy'}e_{1y'z'})$$

for $z'\neq z$ and $x\to y'\to z'$. Similarly for other 2-arcs in place of $x\to y\to z$. The allowed cases are vanishing of

$$\pi^{xyz}_{xzy},\quad \pi^{xyz}_{xyx},\quad \pi^{xyx}_{xzy},\quad \pi^{xzx}_{xyz},\quad \pi^{xzx}_{xzy},\quad \pi^{xzy}_{xyz},\quad \pi^{xyx}_{xyz},\quad \pi^{xzy}_{xyx},\quad \pi^{xyz}_{xzx},\quad \pi^{xzy}_{xzx}$$

and the cyclic rotations of (xyz). Finally, keeping in mind the factorization in the formula for π, we define

$$f(x,y,z)=X_{1y}Y_{2z}-X_{2y}Y_{1z}=X_{11}Y_{21}-X_{21}Y_{11},$$

$$f(x,y,x)=X_{1y}Y_{2x}-X_{2y}Y_{1x}=X_{11}Y_{22}-X_{21}Y_{12},$$

etc. Here the first two entries of f determine the matrices used, while the second two entries of f label the indices on the matrices. Similarly, we define $\overline{f}(x,y,z)$, etc. in the same way but with X^{-t}, Y^{-t}, Z^{-t} the inverse-transposed matrices. With these notations we see that

$$\mathrm{Vielbeins}_{3,2,\mathrm{univ,flip}}$$

is the variety consisting of three invertible matrices X,Y,Z subject to the relations

$$0=\overline{f}(x,y,z)f(x,z,y),\quad 0=\overline{f}(x,y,z)f(x,y,x),\quad 0=\overline{f}(x,y,x)f(x,z,y),$$

$$0=\overline{f}(x,z,x)f(x,y,z),\quad 0=\overline{f}(x,z,x)f(x,z,y),\quad 0=f(x,y,z)\overline{f}(x,z,y),$$

$$0=f(x,y,z)\overline{f}(x,y,x),\quad 0=f(x,y,x)\overline{f}(x,z,y),$$

$$0=f(x,z,x)\overline{f}(x,y,z),\quad 0=f(x,z,x)(x,z,y),$$

and their cyclic rotations of (xyz), and modulo an overall GL_2.

In principle this could have several cases depending on which factor vanishes in each case. One special case is

$$f(x,y,z)=0,\quad f(x,z,y)=0,\quad \overline{f}(x,y,z)=0,\quad \overline{f}(x,z,y)=0,$$

and its cyclic rotations. These equations reduce to

$$X_{21}Y_{11}=X_{11}Y_{21},\quad Y_{12}X_{22}=X_{12}Y_{22},\quad X_{11}Z_{21}=Z_{11}X_{21},\quad X_{22}Z_{12}=X_{12}Z_{22}.$$

Up to an overall GL_2, this component of the moduli space of vielbeins has the general solution

$$X=\begin{pmatrix}\alpha_1 & 0\\ 0 & \alpha_2\end{pmatrix},\quad Y=\begin{pmatrix}\beta_1 & 0\\ 0 & \beta_2\end{pmatrix},\quad Z=\begin{pmatrix}\gamma_1 & 0\\ 0 & \gamma_2\end{pmatrix}$$

modulo a remaining $\mathbb{C}^*\times\mathbb{C}^*$ (e.g., up to GL_n one can assume $\alpha_1=\alpha_2=1$). We have

$$\Theta_a(x)=\alpha_a^{-1},\quad \Theta_a(y)=\beta_a^{-1},\quad \Theta_a(z)=\gamma_a^{-1}$$

and

$$e_a f=R_a(f)e_a,\quad \partial^a f=(R_a(f)-f)\Theta_a,$$

where we identify Σ with $\mathbb{Z}_3$ and use its addition law according to the conventions above to define $R_a(f)=f(()+a)$. For the exterior algebra, by our choice of π, the exterior algebra relations are $e_1\wedge e_2=-e_2\wedge e_1$ and $e_1^2=e_2^2=0$. We are finally ready to look at compatible spin connections, which we do for groups S_2 and then S_3, with their natural nontrivial representations and calculi. Note that since we have already chosen a diagonal form of the vielbein moduli space, different actions are not all equivalent.

Proposition 3.2: For any values of Θ_1,Θ_2 the dimensions p_i of H^i are $1:2:1$. *Here*

$$H^0=\mathbb{C}.1,\quad H^1=\mathbb{C}.\langle-\Theta_1\delta_y e_1+\Theta_2\delta_z e_2,-\Theta_1\delta_x e_1+\Theta_2\delta_y e_2\rangle,\quad H^2=\mathbb{C}.e_1\wedge e_2.$$

Proof: Since in this case $R_2=R_1^{-1}$ we have

$$\mathrm{d}(\mathrm{d}f)=(\Theta_1R_1\Theta_2-\Theta_2R_2\Theta_1)(R_1R_2f-f)=0,\ \forall\ f\in\mathbb{C}[\Sigma]$$

and d is cohomological. By observing that $\mathrm{d}f=0$ if and only if f is constant, we have $p_0=1$ and the dimension of the image of d in $\Omega^1(\Sigma)$ (which is itself of dimension 6) is 2. If $\omega=fe_1+ge_2$ is a one form, then $\mathrm{d}\omega=0$ if and only if $(-\Theta_2\overline{\partial^2}f+f\overline{\partial^1}\Theta_2+\Theta_1\overline{\partial^1}g-g\overline{\partial^2}\Theta_1)=0$. This equation admits a four-dimensional space of solutions, therefore $p_1=4-2=2$. Moreover the image of d in the two-forms is of dimension 2, and given that d sends every two-form to zero, one obtains $p_2=3-2=1$. H^1 is spanned by $\langle-\Theta_1\delta_y e_1+\Theta_2\delta_z e_2,-\Theta_1\delta_x e_1+\Theta_2\delta_y e_2\rangle$, and $H^2=\mathbb{C}.e_1\wedge e_2$. □

For S_2 with its universal calculus, we choose the natural action of $i=(12)$ of $V=\mathrm{span}\{e_1,e_2\}$ that flips the basis vectors (hence by orientation reversal of the frame). The invariant metric here is

$$\eta=e_1\otimes e_1+e_2\otimes e_2$$

and the action of the braided-Lie algebra generator of S_2 is $f^i\triangleright e_1=e_2-e_1$ and $f^i\triangleright e_2=e_1-e_2$. Let us denote by $\overline{\partial^i}\equiv R_i-\mathrm{id}$ the usual finite difference on the group $\mathbb{Z}_3$, and $\langle\ \rangle$ denotes the average value over the three points.

Proposition 3.3: For 3 points, two-dimensional cotangent space and S_2 frame group, existence of a torsion free cotorsion free connection requires the zweibein to obey

$$\Theta_1+R_1\Theta_2=\langle\Theta_1+\Theta_2\rangle.$$

In this case there is a one-parameter family of connections of the form

$$A=(\Theta_1-\lambda)e_1+(-R_2\Theta_1+\lambda)e_2$$

for an arbitrary constant λ. *The covariant derivative is*

$$\nabla e_1=-\nabla e_2=((\Theta_1-\lambda)e_1+(-R_2\Theta_1+\lambda)e_2)\otimes(e_1-e_2).$$

Its Riemannian and Ricci curvatures are

$$\text{Riemann}(e_1) = -\text{Riemann}(e_2) = \rho e_1 \wedge e_2 \otimes (e_2 - e_1), \quad \text{Ricci} = \frac{\rho}{2}(e_1 + e_2) \otimes (e_1 - e_2),$$

where

$$\rho = (2\lambda - \langle \Theta_1 + \Theta_2 \rangle)\overline{\partial}^2 \Theta_1.$$

The Ricci scalar vanishes identically.

Proof: Writing a spin connection $A = ae_1 + be_2$, the torsion and cotorsion equations reduce to

$$\overline{\partial}^1 \Theta_2 = \overline{\partial}^2 \Theta_1 = -(a + b) = R_2(a) + R_1(b)$$

and there is no regularity condition since the calculus on S_2 is universal. The third of these equations has solution $b = -R_2(a)$ since $(\mathrm{id} + R_1)$ is invertible on $\mathbb{Z}_3$. The full system for a vielbein and spin connection then reduces to invertibility of the Θ_i values, the stated constraint on the zweibein, and

$$a = \Theta_1 - \lambda, \quad b = -R_2\Theta_1 + \lambda$$

for an arbitrary constant λ. A straightforward computation then gives the curvature as

$$F = \mathrm{d}A - A^2 = \rho e_1 \wedge e_2$$

for ρ as stated, which Riemann curvature as the action of F. One may also compute this directly from the covariant derivative stated. Finally, for the antisymmetrization projector that we use, the lifting map i is

$$i(e_1 \wedge e_2) = \tfrac{1}{2}(e_1 \otimes e_2 - e_2 \otimes e_1). \tag{17}$$

Using this to lift the two-form values of the Riemann tensor and contracting as in (7) we obtain the Ricci tensor as stated. Its further contraction by the inverse metric is then zero. □

We see among other things that Θ_2 is determined up to a constant from Θ_1, i.e., not every zweibein is allowed. On the other hand, for a generic allowed zweibein we have zero full curvature for a unique spin connection in the family, given by $\lambda = \frac{1}{2}\langle \Theta_1 + \Theta_2 \rangle$. Otherwise the curvatures are nonzero.

For S_3 with its standard two-dimensional irreducible representation and 2-cycles calculus, we have now $i = (12), (23), (13)$ (as i ranges 1,2,3) with the above flip action of (12) extended to a permutation of $e_1, e_2, e_3 \equiv -e_1 - e_2$. The invariant metric is

$$\eta = e_1 \otimes e_1 + e_2 \otimes e_2 + \tfrac{1}{2}(e_1 \otimes e_2 + e_2 \otimes e_1)$$

and the action of S_3 on the vielbein is

$$f^1 \triangleright e_1 = e_2 - e_1, \quad f^2 \triangleright e_1 = 0, \quad f^3 \triangleright e_1 = -2e_1 - e_2,$$

$$f^1 \triangleright e_2 = e_1 - e_2, \quad f^2 \triangleright e_2 = -e_1 - 2e_2, \quad f^3 \triangleright e_2 = 0.$$

Proposition 3.4: For 3 points, two-dimensional cotangent space and S_3 frame group, the zweibein is unconstrained and the torsion free cotorsion free connections are of the form

$$A_i = a_i e_1 + b_i e_2; \quad a_1 = a, \quad b_1 = b,$$

$$a_2 = \tfrac{1}{2}(\overline{\Theta}_1 - a), \quad b_2 = R_2\overline{\Theta}_1 + b, \quad a_3 = R_1\overline{\Theta}_2 + a, \quad b_3 = \tfrac{1}{2}(\overline{\Theta}_2 - b)$$

for arbitrary functions a, b and constants λ, μ. Here $\overline{\Theta}_1 \equiv \Theta_1 - \lambda$ and $\overline{\Theta}_2 \equiv \Theta_2 - \mu$ are notations. For a regular connection we would need in addition:

$$aR_1b_2 - bR_2a_2 + a_3R_1b - b_3R_2a + a_2R_1b_3 - b_2R_2a_3 = 0,$$

$$a_2R_1b - b_2R_2a + aR_1b_3 - bR_2a_3 + a_3R_1b_2 - b_3R_2a = 0.$$

The covariant derivative for the connection is

$$\nabla e_1 = (3a + 2R_1\overline{\Theta}_2)e_1 \otimes e_1 + R_1\overline{\Theta}_2 e_1 \otimes e_2 + \overline{\Theta}_2 e_2 \otimes e_1 + \tfrac{1}{2}(\overline{\Theta}_2 - 3b)e_2 \otimes e_2,$$

$$\nabla e_2 = \tfrac{1}{2}(\overline{\Theta}_1 - 3a)e_1 \otimes e_1 + \overline{\Theta}_2 e_1 \otimes e_2 + R_2\overline{\Theta}_1 e_2 \otimes e_1 + (3b + 2R_2\overline{\Theta}_1)e_2 \otimes e_2.$$

Proof: The torsion equations for a spin connection with components a_i, b_i are

$$\overline{\partial}^1\Theta_2 + a_1 + b_1 + 2b_3 - a_3 = 0, \quad -\overline{\partial}^2\Theta_1 - a_1 - b_1 + b_2 - 2a_2 = 0$$

and the cotorsion equations

$$\overline{\partial}^1\Theta_2 - (R_2a_1 + R_1b_1 - R_2a_3 + 2R_1b_3) = 0,$$

$$-\overline{\partial}^2\Theta_1 + R_1b_1 + R_2a_1 - R_1b_2 + 2R_2a_2 = 0.$$

By combining these equations and using similar methods as in the previous S_2 examples, one finds that their general solution is of the form:

$$\Theta_1 = 2a_2 + a_1 + \lambda, \quad R_1(\Theta_2) = a_3 - a_1 + \mu,$$

$$b_1 + 2b_3 = R_2(a_3 - a_1), \quad 2b_3 + b_2 = R_2(2a_2 + a_3)$$

for some constants λ, μ. This means that for a fixed vielbein and constants μ, λ the equations for a connection are solved as stated. One then writes out the covariant derivative and the optional regularity condition. □

We can see here (and also in our previous examples) why full metric compatibility $\nabla\eta = 0$ is too strong in finite noncommutative geometry (which is why we need our weaker cotorsion-free condition):

Proposition 3.5: The covariant derivatives above do not fully preserve the metric unless $a = b = 0$ *and* $\Theta_1 = \lambda, \Theta_2 = \mu$ *are constant.*

Proof: We compute

$$\begin{aligned}\nabla\eta = {} & \left(\frac{9}{2}a + 4R_1\overline{\Theta}_2 + \frac{\overline{\Theta}_1}{2}\right)e_1 \otimes e_1 \otimes e_1 + (2R_1\overline{\Theta}_2 + \overline{\Theta}_1)e_1 \otimes e_1 \otimes e_2 + (2R_1\overline{\Theta}_2 + \overline{\Theta}_1)e_1 \otimes e_2 \otimes e_1 \\ & + (2\overline{\Theta}_2 + R_2\overline{\Theta}_1)e_2 \otimes e_1 \otimes e_1 + (2\overline{\Theta}_1 + R_1\overline{\Theta}_2)e_1 \otimes e_2 \otimes e_2 + (\overline{\Theta}_2 + 2R_2\overline{\Theta}_1)e_2 \otimes e_1 \otimes e_2 + (\overline{\Theta}_2 \\ & + 2R_2\overline{\Theta}_1)e_2 \otimes e_2 \otimes e_1 + \left(\frac{9}{2}b + 4R_2\overline{\Theta}_1 + \frac{\overline{\Theta}_2}{2}\right)e_2 \otimes e_2 \otimes e_2.\end{aligned}$$

For this to be zero forces $a = b = \overline{\Theta}_1 = \overline{\Theta}_2 = 0$ which translates as stated since λ, μ are arbitrary. □

One may proceed to compute the curvatures, etc., for a general solution. Here we present the results for the special case where the zweibein is constant with $\Theta_1 = \lambda$, $\Theta_2 = \mu$ say, but the a, b are artibrary, i.e., the flat background but not flat spin connection case.

Proposition 3.6: For constant zweibein but a, b *arbitrary, the Riemann and Ricci curvatures take the form*

$$\text{Riemann}(e_1) = (3\partial^2 a - \partial^1 b)e_1 \wedge e_2 \otimes e_1 - 2\partial^1 b e_1 \wedge e_2 \otimes e_2,$$

$$\text{Riemann}(e_2) = -\partial^2 a e_1 \wedge e_2 \otimes e_1 + 3\partial^1 b e_1 \wedge e_2 \otimes e_2,$$

$$\text{Ricci} = -\tfrac{3}{4}\partial^2 a e_1 \otimes e_1 + \tfrac{3}{2}\partial^1 b e_1 \otimes e_2 - \tfrac{1}{2}(3\partial^2 a - \partial^1 b)e_2 \otimes e_1 + \partial^1 b e_2 \otimes e_2.$$

The Ricci scalar vanishes identically. The regularity condition is

$$aR_1(b) = 0.$$

Proof: We compute the gauge curvature of the spin connection as

$$F_1 = (\mu\overline{\partial}^2 a + \lambda\overline{\partial}^1 b)e_1 \wedge e_2,$$

$$F_2 = -\left(\frac{1}{2}\mu\overline{\partial}^2 a - \lambda\overline{\partial}^1 b\right)e_1 \wedge e_2,$$

$$F_3 = -(-\mu\overline{\partial}^2 a + \lambda\overline{\partial}^1 b)e_1 \wedge e_2.$$

Its action on the zweibein then determines the Riemann curvature as stated, using (8). We recall that $\partial^i = \Theta_i\overline{\partial}^i$ is the geometrical partial derivative defined by d and we revert to this. We use the same lifting map as in Proposition 3.1 and (7) to find

$$\text{Ricci} = \frac{1}{2}\begin{pmatrix} F_2 - F_1 & F_1 + 2F_2 \\ -F_1 - 2F_3 & F_1 - F_3 \end{pmatrix}$$

in the e_i basis. This gives the result stated. Finally, note that the inverse of the matrix in η is

$$\eta^{-1} = \frac{4}{3}\begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix}$$

in the dual basis and it is this which we use to contract against the Ricci tensor to obtain the Ricci scalar. Independently of the details of F_i, we have this as $\frac{2}{3}(F_2 - F_1 + F_1 - F_3 - \frac{1}{2}(F_1 + 2F_2 - F_1 - 2F_3)) = 0$, i.e., vanishes identically. □

The general case may be worked out in the same way: The formulas for the F_i are rather more complicated functions of the $a, b, \lambda, \mu, \Theta_i$, but the other steps follow the same pattern. In particular, the Ricci tensor has the same asymmetric form and the Ricci scalar vanishes in general. We see that with 3 points, the conditions with frame group S_2 are a little strong and constrain the zweibein, while with S_3 there are an abundance of spin connections compatible with any zweibein, namely a, b arbitrary (and two further parameters which one might fix, for example, by $\lambda = \langle\Theta_1\rangle$ and $\mu = \langle\Theta_2\rangle$) and that in all cases with three points, the Ricci scalar vanishes. Note that we have not covered it here, but one has a similar picture for S_3 with its universal calculus; then there are five one-forms A_i for the spin connection with linear equations for the torsion and cotorsion that prescribe the derivatives of Θ_1, Θ_2 in terms of the fields, and an empty equation for regularity.

IV. GEOMETRIES ON FOUR POINTS

For four points we will not be fully general as above but restrict to the more interesting class of models featuring already in our analysis for 2,3 points. First of all, we shall focus on the case of all arrows bidirectional, i.e., a symmetric subset E to define the calculus. This means for four points that we have (a) the square connectivity which is a two-dimensional calculus or (b) the universal or three-dimensional calculus. We look mainly at the former since it has a clear geometrical interpretation as the connectivity of a torus, namely in Secs. IV A–IV C. Indeed, this is

the natural calculus for the group $\mathbb{Z}_2\times\mathbb{Z}_2$ viewed as a discrete model of a torus. Section IV D covers the alternative of the universal calculus on the basis which has the connectivity of a tetrahedron or discrete model of a sphere.

Next, rather than the full analysis, we shall restrict attention to the diagonal vielbeins given by scalars attached to the edges as we deduced up to equivalence for the 3 points case above. These scalars are our remaining continuous degrees of freedom and allow our square to "pulse" by stretching or contracting edges. Such a restricted class is interesting for any fixed combinatorics. On the other hand, we will have more choices for the frame group and its calculus, still giving several models.

A. Discrete torus as base space

Thus, in this section, and the next two, we write the vertices as $\Sigma=\{(0,0),(1,0),(0,1),(1,1)\}$, using an additive group notation.

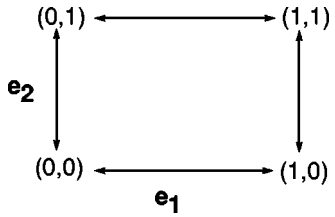
Over each point we have a fiber

$$F_{(0,0)}=\{(1,0),(0,1)\},\quad F_{(1,0)}=\{(0,0),(1,1)\},\quad F_{(0,1)}=\{(0,0),(1,1)\},\quad F_{(1,1)}=\{(1,0),(0,1)\}$$

of order 2. We fix the connectivity by identifying these fibers by vielbeins of the diagonal form

$$e_{1,x,y}=\Theta_1^{-1}(x)\delta_{y-x,(1,0)},\quad e_{2,x,y}=\Theta_2^{-1}(x)\delta_{y-x,(0,1)}$$

for any two points $x,y\in\Sigma$. This is the natural vielbeinon $\mathbb{Z}_2\times\mathbb{Z}_2$ with additional continuous nowhere-zero functional parameters Θ_i. We have the picture



From each point in the lattice it is possible to move in two directions, which correspond to the vectors e_1 and e_2. Here e_1 translates adding the element $(1,0)$ of $\mathbb{Z}_2\times\mathbb{Z}_2$, and e_2 corresponds to moving by adding $(0,1)$. We define the translation operators acting on the functions f as

$$(R_1f)(x)=f(x+(1,0)),\quad (R_2f)(x)=f(x+(0,1))$$

and obtain the partial derivatives

$$\partial^1 f(x)=(f(x+(1,0))-f(x))\Theta_1,\quad \partial^2 f(x)=(f(x+(0,1))-f(x))\Theta_2$$

and commutation relations [which define the right multiplication on $\Omega^1(\Sigma)$, left multiplication being the obvious one] as:

$$e_1f=R_1(f)e_1,\quad e_2f=R_2(f)e_2$$

for all functions f. This has the same form as we found up to GL_2 for three points in the preceding section and completes our description of Ω^1 and its $\mathbb{C}(\mathbb{Z}_2\times\mathbb{Z}_2)$-basis $\{e_1,e_2\}$.

Next we fix the projector π as the naive antisymmetrizer (14) on the e_a basis, again as we took in Sec. III B for three points. We check that for four points it obeys the condition needed in Theorem 2.2 to define the two-forms Ω^2. Thus, labeling the points as x,y,z,t where we start at $(0,0)$ and go around the square clockwise, we have the possible 2 arcs of two different forms:

$$x\to y\to z,\quad y\to z\to t,$$

$$x\to t\to z,\quad y\to x\to t,$$

$$z \to t \to x, \quad t \to x \to y,$$

$$z \to y \to x, \quad t \to z \to y,$$

or

$$x \to y \to x, \quad y \to z \to y,$$

$$z \to y \to z, \quad x \to t \to x,$$

$$y \to x \to y, \quad z \to t \to z,$$

$$t \to x \to t, \quad t \to z \to t.$$

To check out condition (i) in Theorem 2.2 we will consider the two-arcs leaving from x, the starting point being irrelevant in the reasoning which follows. This implies that we have to verify the vanishing of $\pi^{yx}_{xyz}, \pi^{tx}_{xyz}, \pi^{yz}_{xyx}, \pi^{yz}_{xtx}$. Now, in general

$$\pi^{yz}_{x_{y'z'}} = (e_1^{-1xy} e_2^{-1yz} - e_2^{-1xy} e_1^{-1yz})(e_{1xy'} e_{2y'z} - e_{2xy'} e_{1y'z'})$$

and replacing in this expression the actual form of the arc, we establish that

$$\pi^{yx}_{xyz}, \quad \pi^{tx}_{xyz}, \quad \pi^{yz}_{xyx}, \quad \pi^{yz}_{xtx}$$

are zero. (We obtain a similar result swapping upper and lower indices.) The second constraint of Theorem 2.2 is not trivially satisfied in this case. The conditions $\pi_{x,z}{}^{y}{}_{t} + \pi_{x,z}{}^{t}{}_{t} = 0$ and $\pi_{x,z}{}^{y}{}_{y} + \pi_{x,z}{}^{t}{}_{y} = 0$ both give

$$\Theta_1 R_1 \Theta_2 = \Theta_2 R_2 \Theta_1, \quad \text{i.e.,} \quad \partial_1 \Theta_2 - \partial_2 \Theta_1 = 0. \tag{18}$$

Finally, we will take as a metric the element $\eta = e_1 \otimes e_1 + e_2 \otimes e_2$ and we will take the lifting (17) which is the natural choice for the antisymmetrizer projector. The exterior differentials of the base elements are

$$\mathrm{d}e_1 = \overline{\partial}^1 \Theta_2 e_1 \wedge e_2, \quad \mathrm{d}e_2 = -\overline{\partial}^2 \Theta_1 e_1 \wedge e_2,$$

where we recall that $\overline{\partial^a} = \Theta_a^{-1} \partial^a = R_a - \mathrm{id}$ are the usual group finite differences.

Proposition 4.1: For generic values of Θ_1, Θ_2 the dimensions p_i of H^i are 1:2:1. Here

$$H^0 = \mathbb{C}.1, H^1 = \langle (\Theta_2(y)\delta_t + \Theta_2(z)\delta_z)e_1, (\Theta_2(z)\delta_x + \Theta_2(y)\delta_t)e_2 \rangle, \quad H^2 = \mathbb{C}\,.\, e_1 \wedge e_2.$$

Proof:

$$\mathrm{d}(\mathrm{d}f) = (\Theta_1 R_1 \Theta_2 - \Theta_2 R_2 \Theta_1)(R_1 R_2 f - f) e_1 \wedge e_2 = 0, \ \forall\, f \in \mathbb{C}[\Sigma]$$

which is zero due to the constraint we imposed on the Θs. In the usual way, $p_0 = 1$, and the dimension of the image of d in $\Omega^1(\Sigma)$ (itself of dimension 8) is 3. A one form $fe_1 + ge_2$ is in the nullspace of d if and only if it satisfies $(-\Theta_2 \overline{\partial^2} f + f \overline{\partial^1} \Theta_2 + \Theta_1 \overline{\partial^1} g - g \overline{\partial^2} \Theta_1) = 0$; it is easy to find that the solution space of this equation has, for generic values of Θ_i satisfying (18), dimension 5 (and therefore, $p_1 = 5 - 3 = 2$). This, in turn, implies the image of d inside $\Omega^2(\Sigma)$ is three-dimensional. Then, $p_2 = 4 - 3 = 1$. For generic values of Θ, $e_1 \wedge e_2$ is not in the image of d, and gives a representative for H^2. □

For the remaining aspects of the geometry we fix the frame group and its calculus. Then we can solve for the connections, curvature, etc. Even with all of the above choices, we have several models.

B. Torus model with $\mathbb{Z}_4 \subset SO(2)$ frame group

Here we think of the additive group $\mathbb{Z}_4=\{\overline{0},\overline{1},\overline{2},\overline{3}\}$ as a discrete model of SO(2), i.e., 90-degree notations. This is in keeping with our discrete model of a torus. We have on $\mathbb{Z}_4$ either the three-dimensional universal calculus or the natural two-dimensional calculus given by a square.

1. 3D calculus on $\mathbb{Z}_4$

We choose the three-dimensional (universal) calculus defined on Z_4 by $\{\overline{1},\overline{2},\overline{3}\}$. This corresponds to $f^{\overline{1}},f^{\overline{2}},f^{\overline{3}}$ acting as the corresponding rotation of the vielbein vectors e_1 and e_2, minus the identity, that is

$$f^{\overline{1}} \triangleright e_1 = e_2 - e_1, \quad f^{\overline{1}} \triangleright e_2 = -e_1 - e_2,$$

$$f^{\overline{2}} \triangleright e_1 = -2e_1, \quad f^{\overline{2}} \triangleright e_2 = -2e_2,$$

$$f^{\overline{3}} \triangleright e_1 = -e_1 - e_2, \quad f^{\overline{3}} \triangleright e_2 = e_1 - e_2.$$

Proposition 4.2: The moduli space of torsion free cotorsion free connections on the quantum Riemannian manifold above is given by

$$A_1 = \alpha e_1 + \beta e_2,$$

$$A_2 = \frac{1}{2}(-\alpha+\beta-\gamma-\delta-\overline{\partial}^2\Theta_1)e_1 + \frac{1}{2}(-\alpha-\beta+\gamma-\delta-\overline{\partial}^1\Theta_2)e_2,$$

$$A_3 = \gamma e_1 + \delta e_2$$

for four functions $\alpha,\beta,\gamma,\delta$ subject to the linear constraint

$$(R_1+R_2)a = 0, \quad (R_1+R_2)b = 0,$$

where $a=\gamma-\alpha$ and $b=\beta-\delta$. The corresponding covariant derivative is

$$\nabla e_1 = (b-\overline{\partial}^2\Theta_1)e_1\otimes e_1 + ae_1\otimes e_2 + (a-\overline{\partial}^1\Theta_2)e_2\otimes e_1 - be_2\otimes e_2,$$

$$\nabla e_2 = -ae_1\otimes e_1 + (b-\overline{\partial}^2\Theta_1)e_1\otimes e_2 + be_2\otimes e_1 + (a-\overline{\partial}^1\Theta_2)e_2\otimes e_2.$$

Proof: We want the connection to be torsion free, i.e., it has to satisfy the following two linear equations:

$$A_1^1 + A_1^2 + 2A_2^2 - A_3^1 + A_3^2 = -\overline{\partial}^1\Theta_2,$$

$$-A_1^1 + A_1^2 - 2A_2^1 - A_3^1 - A_3^2 = \overline{\partial}^2\Theta_1,$$

from which we obtain the general solution above, without constraints on $\alpha,\beta,\gamma,\delta$. In conformity to what we have done so far, we also demand that the cotorsion of the connection be zero. Notice that, differently from the previous cases investigated in this paper, the elements of the fiber group $\mathbb{Z}_4$ are not of order 2, which implies that the action of S on the f^is is not trivial; we have in fact $S^{-1}(f^1)=f^3, S^{-1}(f^2)=f^2, S^{-1}(f^3)=f^1$, and the zero-cotorsion condition can be put down as

$$-R_1A_1^2 + R_2A_1^1 - 2R_1A_2^2 - R_2A_3^1 - R_1A_3^2 = -\overline{\partial}^1\Theta_2,$$

$$R_1A_1^2 + R_2A_1^1 + 2R_2A_2^1 - R_1A_3^2 + R_2A_3^1 = \overline{\partial}^2\Theta_1.$$

The requirement on the cotorsion translates into the constraint $(R_1+R_2)a=(R_1+R_2)b=0$, where a,b are defined in the statement of the proposition. The regularity condition is empty, because the calculus on $\mathbb{Z}_4$ is the universal one. We then compute the covariant derivative using (8). □

Note that the covariant derivative depends only on a,b so these parametrize the "physical" or effective moduli space, which is, therefore, four-dimensional: Two functions on $\mathbb{Z}_2\times\mathbb{Z}_2$ modulo the linear constraint. One may check that the torsion is indeed zero, which is to say $\nabla\wedge e_1=\mathrm{d}e_1$ and $\nabla\wedge e_2=\mathrm{d}e_2$. The cotorsion condition means that ∇ respects η in a skew sense, as one may also directly verify evaluating the cotorsion of the metric (when the torsion is null)

$$\Gamma\eta = (\nabla\wedge\mathrm{id} - \mathrm{id}\wedge\nabla)(e_1\otimes e_1 + e_2\otimes e_2) = 0,$$

where

$$(\nabla\wedge\mathrm{id})\eta = \overline{\partial}^1\Theta_2 e_1\wedge e_2\otimes e_1 - \overline{\partial}^2\Theta_1 e_1\wedge e_2\otimes e_2$$

and

$$(\mathrm{id}\wedge\nabla)\eta = (-(R_1+R_2)a + \overline{\partial}^1\Theta_2)e_1\wedge e_2\otimes e_1 - ((R_1+R_2)b + \overline{\partial}^2\Theta_1)e_1\wedge e_2\otimes e_2$$

(later on we will consider $\nabla\eta=0$ in the usual full sense).

Proposition 4.3: The Ricci scalar for the covariant derivative above is

$$R = \partial^2 a + \overline{\partial}^1\Theta_2 R_2 a - 2aR_2 a + \partial^1 b + \overline{\partial}^2\Theta_1 R_1 b - 2bR_1 b$$

Proof: From the action of the f^i we can then compute the Riemann curvature using the general theory in Sec. II, finding now

$$\mathrm{Riemann}(e_1) = (-F_1 - 2F_2 - F_3)\otimes e_1 + (F_1 - F_3)\otimes e_2,$$

$$\mathrm{Riemann}(e_2) = (-F_1 + F_3)\otimes e_1 + (-F_1 - 2F_2 - F_3)\otimes e_2.$$

In the same way the Ricci tensor is

$$\mathrm{Ricci} = \tfrac{1}{2}((F_1 - F_3)e_1\otimes e_1 + (F_1 + 2F_2 + F_3)e_1\otimes e_2 - (F_1 + 2F_2 + F_3)e_2\otimes e_1 + (F_1 - F_3)e_2\otimes e_2),$$

where we identify the two-forms F_i with their scalar coefficients as multiples of the top form $e_1\wedge e_2$. Taking the trace in a standard way, the Ricci scalar is $R=F_1-F_3$ (this and the other component $F_1+2F_2+F_3$ occur also in the Riemann tensor so we see that the Ricci tensor vanishes if and only if the entire Riemann tensor does). We can compute F_1,F_2,F_3 by means of

$$F_1 = \mathrm{d}A_1 + A_2\wedge A_3 + A_3\wedge A_2 - 2A_1\wedge A_1 - A_2\wedge A_1 - A_1\wedge A_2 - A_3\wedge A_1 - A_1\wedge A_3,$$

$$F_2 = \mathrm{d}A_2 + A_1\wedge A_1 + A_3\wedge A_3 - A_1\wedge A_2 - A_2\wedge A_1 - 2A_2\wedge A_2 - A_3\wedge A_2 - A_2\wedge A_3,$$

$$F_3 = \mathrm{d}A_3 + A_2\wedge A_1 + A_1\wedge A_2 - A_3\wedge A_1 - A_1\wedge A_3 - A_3\wedge A_2 - A_2\wedge A_3 - 2A_3\wedge A_3,$$

as inferred from (13) where

$$\mathrm{d}A_1 = (-\Theta_2\overline{\partial}^2\alpha + \alpha\overline{\partial}^1\Theta_2 + \Theta_1\overline{\partial}^1\beta - \beta\overline{\partial}^2\Theta_1)e_1\wedge e_2,$$

$$\mathrm{d}A_2 = \frac{1}{2}(\Theta_1\overline{\partial}^1(-\alpha-\beta+\gamma-\delta) + \Theta_2\overline{\partial}^2(\alpha-\beta+\gamma+\delta) + \overline{\partial}^1\Theta_2(-\alpha+\beta-\gamma-\delta+2\Theta_1) + \overline{\partial}^2\Theta_1(\alpha + \beta-\gamma+\delta-2\Theta_2))e_1\wedge e_2,$$

$$\mathrm{d}A_3 = (-\Theta_2\overline{\partial}^2\gamma + \gamma\overline{\partial}^1\Theta_2 + \Theta_1\overline{\partial}^1\delta - \delta\overline{\partial}^2\Theta_1)e_1\wedge e_2,$$

and

$$A_1\wedge A_1 = \alpha R_1\beta - \beta R_2\alpha,$$

$$A_1\wedge A_2 = \frac{\alpha}{2}(-R_1\alpha - R_1\beta + R_1\gamma - R_1\delta + \overline{\partial}^1\Theta_2) + \frac{\beta}{2}(R_2\alpha - R_2\beta + R_2\gamma + R_2\delta - \overline{\partial}^2\Theta_1),$$

etc. The detailed form of the curvature two-form is

$$\begin{aligned}F_1 = {}& -\partial^2\alpha + \partial^1\beta + \alpha\left(-R_1\beta - R_1\delta - R_2\alpha + R_2\gamma + \frac{\overline{\partial}^1\Theta_2}{2}\right) + \beta\left(R_2\alpha + R_2\gamma + R_2\beta - R_2\delta - \frac{\overline{\partial}^2\Theta_1}{2}\right)\\ &+ \gamma\left(-R_1\delta - R_1\beta - R_1\alpha + R_1\gamma + \frac{\overline{\partial}^1\Theta_2}{2}\right) + \delta\left(R_1\beta - R_1\delta + R_2\gamma + R_2\alpha - \frac{\overline{\partial}^2\Theta_1}{2}\right) + \frac{\overline{\partial}^2\Theta_1}{2}R_1(\beta\\ &- \delta) - \frac{\overline{\partial}^1\Theta_2}{2}R_2(\alpha - \gamma),\end{aligned}$$

$$\begin{aligned}F_2 = {}& \frac{1}{2}\partial^1(-\alpha - \beta + \gamma - \delta) + \frac{1}{2}\partial^2(\alpha - \beta + \gamma + \delta) + \frac{\overline{\partial}^1\Theta_2}{2}(-R_2(\beta - \delta) - \alpha + \beta - \gamma - \delta)\\ &+ \frac{\overline{\partial}^2\Theta_1}{2}(-R_1(\alpha - \gamma) + \alpha + \beta - \gamma + \delta) + \frac{\alpha}{2}(3R_1\beta - R_2(\beta - \delta) - \overline{\partial}^2\Theta_1 + R_1\delta) + \frac{\beta}{2}(-3R_2\alpha\\ &+ R_1(\alpha - \gamma) - \overline{\partial}^1\Theta_2 - R_2\gamma) + \frac{\gamma}{2}(3R_1\delta + R_2(\beta - \delta) + \overline{\partial}^2\Theta_1 + R_1\beta) + \frac{\delta}{2}(-3R_2\gamma - R_1a\\ &+ \overline{\partial}^1\Theta_2 - R_2\alpha),\end{aligned}$$

$$\begin{aligned}F_3 = {}& -\partial^2\gamma + \partial^1\delta + \frac{\overline{\partial}^1\Theta_2}{2}R_2(\alpha - \gamma) - \frac{\overline{\partial}^2\Theta_1}{2}R_1(\beta - \delta) + \alpha\left(-R_1\delta - R_1\alpha + R_1\gamma - R_1\beta + \frac{\overline{\partial}^1\Theta_2}{2}\right)\\ &+ \beta\left(R_2\alpha + R_2\gamma + R_1\beta - R_1\delta - \frac{\overline{\partial}^2\Theta_1}{2}\right) + \gamma\left(-R_1\delta + R_1\alpha - R_1\gamma + \frac{\overline{\partial}^1\Theta_2}{2} - R_1\beta\right)\\ &+ \delta\left(R_2\gamma + R_2\alpha + R_2\beta - R_2\delta - \frac{\overline{\partial}^2\Theta_1}{2}\right),\end{aligned}$$

from which we compute the Ricci curvature, etc. as above, and write in terms of a, b. □

It is useful to observe that it is not mandatory to compute the curvature two-form in order to get hold of the Riemann tensor. One could also[10] use the formula $\mathrm{Riemann}(e_1) = ((\mathrm{id}\wedge\nabla) - (\mathrm{d}\otimes\mathrm{id}))\circ\nabla(e_1)$ and similarly for e_2, which provides a useful check. Either way, the Riemann tensor turns out to have the form

$$\mathrm{Riemann}(e_1) = \rho e_1\wedge e_2\otimes e_1 + Re_1\wedge e_2\otimes e_2, \quad \mathrm{Riemann}(e_2) = -Re_1\wedge e_2\otimes e_1 + \rho e_1\wedge e_2\otimes e_2$$

with

$$\rho = \partial^2 b - \partial^1 a + 2bR_1a - 2aR_2b - \overline{\partial}^2\Theta_1R_1a + \overline{\partial}^1\Theta_2R_2b$$

and R the Ricci scalar computed above. We see in particular that $a=b=0$ is a natural point in the effective moduli space where the Ricci tensor (and the entire curvature) is zero.

Next we consider full metric compatibility as opposed to the weaker cotorsion condition.

Theorem 4.4: *The metric η satisfies the equation $\nabla\eta=0$, if and only if*

$$a=\overline{\partial}^1\Theta_2,\quad b=\overline{\partial}^2\Theta_1,\quad \overline{\partial}^2(\overline{\partial}^1\Theta_2)=0,\quad \overline{\partial}^1(\overline{\partial}^2\Theta_1)=0.$$

The Ricci scalar is given by

$$R=-(\overline{\partial}^1\Theta_2)^2-(\overline{\partial}^2\Theta_1)^2.$$

Proof: We only need to state explicitly the equality $\nabla\eta=0$, as in

$$\nabla(e_1\otimes e_1+e_2\otimes e_2)=2((b-\overline{\partial}^2\Theta_1)e_1\otimes e_1\otimes e_1+(a-\overline{\partial}^1\Theta_2)e_2\otimes e_1\otimes e_1+(b-\overline{\partial}^2\Theta_1)e_1\otimes e_2\otimes e_2+(a-\overline{\partial}^1\Theta_2)e_2\otimes e_2\otimes e_2)=0$$

the solution to the above equation is $a=\overline{\partial^1}\Theta_2$, $b=\overline{\partial^2}\Theta_1$. The kernel constraint on a,b then requires the constraint on the vielbein. □

We see that not every vielbein admits a strictly metric compatible condition—in general we need our weaker cotorsion-free condition. However, when it does so, the covariant derivative is uniquely determined as in classical Riemannian geometry.

2. 2D calculus on $\mathbb{Z}_4$

We also consider the two-dimensional (2D) calculus on $\mathbb{Z}_4$, defined by $\{\overline{1},\overline{3}\}$ with $f^{\overline{1}}$ and $f^{\overline{3}}$, acting as before. Our interesting result is that the geometric content is the same as the universal calculus above except that some redundant modes in the universal case are not present, but replaced by a quadratic regularity condition.

Proposition 4.5: With the above specification for the action, the moduli space of torsion free, cotorsion free connections is given by

$$A_1=\left(-\alpha-\frac{\overline{\partial}^2\Theta_1}{2}\right)e_1+\left(\beta-\frac{\overline{\partial}^1\Theta_2}{2}\right)e_2,$$

$$A_3=\left(\beta-\frac{\overline{\partial}^2\Theta_1}{2}\right)e_1+\left(\alpha-\frac{\overline{\partial}^1\Theta_2}{2}\right)e_2,$$

with the conditions

$$(R_1+R_2)a=0,\quad (R_1+R_2)b=0,$$

where $a=\alpha+\beta$ and $b=\beta-\alpha$. In terms of a,b the covariant derivative ∇ is as before, in Proposition 4.1, and the regularity condition reads

$$\overline{\partial}^2\Theta_1\overline{\partial}^2a-\overline{\partial}^1\Theta_2\overline{\partial}^1b=0.$$

Proof: Here the parameters α,β are not the same as in the previous section (but related to them). We solve the zero torsion condition

$$A_1^1+A_1^2-A_3^1+A_3^2=-\overline{\partial}^1\Theta_2,$$

$$-A_1^1+A_1^2-A_3^1-A_3^2=\overline{\partial}^2\Theta_1,$$

which gives the solution above in terms of α,β or the combinations a,b, but free of any constraint on the a,b. Next we require the connection to have zero cotorsion:

$$-R_1A_1^2-R_1A_3^2-R_2A_1^1+R_2A_3^1=-\overline{\partial}^1\Theta_2,$$

$$-R_1A_1^2+R_1A_3^2+R_2A_1^1+R_2A_3^1=\overline{\partial}^2\Theta_1,$$

and obtain the constraint $(R_1+R_2)a=(R_1+R_2)b=0$. We then compute the covariant derivative using the action of f^1, f^3. The regularity condition in this case is given by

$$A_1\wedge A_1+A_3\wedge A_3=0.$$

□

Corollary 4.6: The Riemann and Ricci tensors corresponding to the connection above have the form (in terms of a and b) as in Proposition 4.2.

Proof: This follows since the Riemann and Ricci tensors are determined by ∇ which has the same form. It is also instructive (but a different computation) to compute them directly; as usual from the definition of the curvature

$$F_1=\mathrm{d}A_1-2A_1\wedge A_1-A_3\wedge A_1-A_1\wedge A_3,$$

$$F_3=\mathrm{d}A_3-A_1\wedge A_3-A_3\wedge A_1-2A_3\wedge A_3,$$

we compute the expression for the Riemann tensor:

$$\mathrm{Riemann}(e_1)=(-F_1-F_3)\otimes e_1+(F_1-F_3)\otimes e_2,$$

$$\mathrm{Riemann}(e_2)=(-F_1+F_3)\otimes e_1+(-F_1-F_3)\otimes e_2,$$

inserting the actual form of F_1 and F_3 and the regularity condition.

The Ricci tensor is

$$\mathrm{Ricci}=\frac{1}{2}((F_1-F_3)e_1\otimes e_1+(F_1+F_3)e_1\otimes e_2+(-F_1-F_3)e_2\otimes e_1+(F_1-F_3)e_2\otimes e_2).$$

□

If we want Ricci flatness, we must force $F_1=F_3=0$. Note that if the Ricci is null, so is the Riemann tensor.

The condition for the metric compatibility is the same as in Theorem 4.4.

Proposition 4.7: The metric η satisfies the equation $\nabla\eta=0$, if and only if

$$a=\overline{\partial}^1\Theta_2,\quad b=\overline{\partial}^2\Theta_1,\quad \overline{\partial}^2(\overline{\partial}^1\Theta_2)=0,\quad \overline{\partial}^1(\overline{\partial}^2\Theta_1)=0.$$

The regularity condition holds and the Riemann and Ricci tensors are as in Theorem 4.4.

Proof: We impose the condition $\nabla\eta=0$, which has the same shape as in the previous case. We then check that the regularity condition in Proposition 4.1 indeed holds for these a, b. □

We conclude that moving to the 2D calculus on $\mathbb{Z}_4$ gives essentially the same Riemannian geometry as using the universal (3D) calculus but without some of the superfluous modes that we found there. Instead, these are replaced by a regularity condition. This gives us some insight into the "correct" choice of calculus for the frame group and what happens if one chooses one that is too big.

C. Torus model with translations $\mathbb{Z}_2\times\mathbb{Z}_2$ as frame group

We take now the frame group to be $\mathbb{Z}_2\times\mathbb{Z}_2$ acting by "translation" on our base space which we recall is also the group $\mathbb{Z}_2\times\mathbb{Z}_2$. We write the frame group elements as $\overline{00},\overline{01},\overline{10},\overline{11}$, say. As before, we have two choices for the calculus on the frame group.

1. 3D calculus on $\mathbb{Z}_2\times\mathbb{Z}_2$

This is the universal calculus defined by $\{\overline{10},\overline{10},\overline{11}\}$. The corresponding f's act by

$$f^{\overline{10}}\triangleright e_1=-2e_1,\quad f^{\overline{10}}\triangleright e_2=0,$$

$$f^{\overline{01}}\triangleright e_1=0,\quad f^{\overline{01}}\triangleright e_2=-2e_2,$$

$$f^{\overline{11}}\triangleright e_1=-2e_1,\quad f^{\overline{11}}\triangleright e_2=-2e_2.$$

Proposition 4.8: The moduli space of torsion free, cotorsion free connections is given by

$$A_{10}=\alpha e_1-\left(\delta+\frac{\overline{\partial}^1\Theta_2}{2}\right)e_2,$$

$$A_{01}=-\left(\gamma+\frac{\overline{\partial}^2\Theta_1}{2}\right)e_1+\beta e_2,$$

$$A_{11}=\gamma e_1+\delta e_2.$$

We set $a=\alpha+\gamma$, $b=\beta+\delta$. The covariant derivative corresponding to this connection is

$$\nabla e_1=2ae_1\otimes e_1-\overline{\partial}^1\Theta_2 e_2\otimes e_1,\quad \nabla e_2=-\overline{\partial}^2\Theta_1 e_1\otimes e_2+2be_2\otimes e_2.$$

Proof: We solve the torsion condition

$$2A_{10}^2+2A_{11}^2=-\overline{\partial}^1\Theta_2,\quad -2A_{01}^1-2A_{11}^1=\overline{\partial}^2\Theta_1$$

and the zero cotorsion condition

$$-2R_1A_{10}^2-2R_1A_{11}^2=-\overline{\partial}^1\Theta_2,\quad 2R_2A_{01}^1+2R_2A_{11}^1=\overline{\partial}^2\Theta_1;$$

then we work out the covariant derivative using (8). □

There is no regularity condition for the universal calculus on the frame group (because there is no element different from the identity which lies outside the subset defining the calculus).

Proposition 4.9: The Riemann and Ricci tensors corresponding to the above connection are

$$\text{Riemann}(e_1)=-2\left(-\partial^2 a+\overline{\partial}^1\Theta_2(\Theta_1-R_2a)+\frac{\overline{\partial}^1\Theta_2\overline{\partial}^2\Theta_1}{2}\right)e_1\wedge e_2\otimes e_1,$$

$$\text{Riemann}(e_2)=-2\left(\overline{\partial}^2\Theta_1(R_1b-\Theta_2)+\partial^1 b-\frac{\overline{\partial}^2\Theta_1\overline{\partial}^1\Theta_2}{2}\right)e_1\wedge e_2\otimes e_2,$$

$$\text{Ricci}=\left(-\partial^2 a+\overline{\partial}^1\Theta_2(\Theta_1-R_2a)+\frac{\overline{\partial}^1\Theta_2\overline{\partial}^2\Theta_1}{2}\right)e_1\otimes e_2$$
$$-\left(\overline{\partial}^2\Theta_1(R_1b-\Theta_2)+\partial^1 b-\frac{\overline{\partial}^2\Theta_1\overline{\partial}^1\Theta_2}{2}\right)e_2\otimes e_1.$$

Proof: We have

$$F_{10}=\mathrm{d}A_{10}+A_{01}\wedge A_{11}+A_{11}\wedge A_{01}-2A_{10}\wedge A_{10}-A_{10}\wedge A_{01}-A_{01}\wedge A_{10}-A_{10}\wedge A_{11}-A_{11}\wedge A_{10},$$

$$F_{01}=\mathrm{d}A_{01}+A_{10}\wedge A_{11}+A_{11}\wedge A_{10}-A_{10}\wedge A_{01}-A_{01}\wedge A_{10}-2A_{01}\wedge A_{01}-A_{01}\wedge A_{11}-A_{11}\wedge A_{01},$$

$$F_{11} = \mathrm{d}A_{11} + A_{10}\wedge A_{01} + A_{01}\wedge A_{10} - A_{11}\wedge A_{10} - A_{10}\wedge A_{11} - A_{11}\wedge A_{01} - A_{01}\wedge A_{11},$$

and

$$\mathrm{Riemann}(e_1) = -2(F_{10}+F_{11})\otimes e_1, \quad \mathrm{Riemann}(e_2) = -2(F_{01}+F_{11})\otimes e_2.$$

The same result is obtained by $\mathrm{Riemann}(e_a) = ((\mathrm{id}\wedge\nabla) - (\mathrm{d}\otimes\mathrm{id}))\circ\nabla(e_a)$. □

Proposition 4.10: The condition $\nabla\eta = 0$ is satisfied if and only if $\alpha = -\gamma$ and $\beta = -\delta$ and $\overline{\partial^1}\Theta_2 = \overline{\partial^2}\Theta_1 = 0$. In this case, both the Riemann and the Ricci tensor are zero.

Proof: The first part of the proposition is easily proved by computing

$$\nabla(e_1\otimes e_1 + e_2\otimes e_2) = 4ae_1\otimes e_1\otimes e_1 - 2\overline{\partial^1}\Theta_2 e_2\otimes e_1\otimes e_1 - 2\overline{\partial^2}\Theta_1 e_1\otimes e_2\otimes e_2 + 4be_2\otimes e_2\otimes e_2$$
$$= 0$$

which means $a = b = \overline{\partial^1}\Theta_2 = \overline{\partial^2}\Theta_1 = 0$ have; this implies that the Riemann and the Ricci tensor are both zero. □

2. 2D calculus on $\mathbb{Z}_2\times\mathbb{Z}_2$

The calculus on the fiber will be defined now by $\{\overline{10}, \overline{01}\}$

Proposition 4.11: The moduli space of torsion free, cotorsion free connections is given by

$$A_{10} = \alpha e_1 - \frac{\partial^1\Theta_2}{2}e_2,$$

$$A_{01} = -\frac{\partial^2\Theta_1}{2}e_1 + \beta e_2.$$

We set $a = \alpha$, $b = \beta$ (as in the case before but with $\gamma = \delta = 0$), then the covariant derivative has the same form as in Proposition 4.8. The regularity condition is

$$a\overline{\partial^1}b - b\overline{\partial^2}a = 0.$$

Proof: We solve the torsion equations

$$2A^2_{10} = -\overline{\partial^1}\Theta_2, \quad -2A^1_{01} = \overline{\partial^2}\Theta_1$$

and the cotorsion equations

$$-2R_1A^2_{10} = -\overline{\partial^1}\Theta_2, \quad 2R_2A^1_{01} = \overline{\partial^2}\Theta_1.$$

The regularity condition is, in this case, $A_{10}\wedge A_{01} + A_{01}\wedge A_{10} = 0$, which comes out as $aR_1b - bR_2a = 0$, which can be written as stated. □

Corollary 4.12: The Riemann and Ricci tensors are (as functions of a, b) as in Proposition 4.9.

Proof: This follows from ∇ but can also be computed directly as useful check; the curvature two form corresponding to the regular connection above, is given by

$$F_{10} = \left(-\Theta_2\overline{\partial^2}a + \overline{\partial^1}\Theta_2(\Theta_1 - R_2a) + \frac{\overline{\partial^1}\Theta_2\overline{\partial^2}\Theta_1}{2}\right)e_1\wedge e_2,$$

$$F_{01} = \left(\overline{\partial^2}\Theta_1(R_1b - \Theta_2) + \Theta_1\overline{\partial^1}b - \frac{\overline{\partial^2}\Theta_1\overline{\partial^1}\Theta_2}{2}\right)e_1\wedge e_2,$$

computed from the expression for F (regularity condition applied)

$$F_{10} = \mathrm{d}A_{10} - 2A_{10} \wedge A_{10},$$

$$F_{01} = \mathrm{d}A_{01} - 2A_{01} \wedge A_{01},$$

the Ricci tensor is $F_{01}e_1 \otimes e_2 - F_{10}e_2 \otimes e_1$, Riemann is given by $\mathrm{Riemann}(e_1) = -2F_{10} \otimes e_1$, $\mathrm{Riemann}(e_2) = -2F_{01} \otimes e_2$. □

Finally, the only connection fulfilling the condition

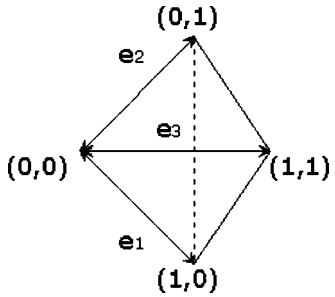
$$\nabla\eta = \nabla(e_1 \otimes e_1 + e_2 \otimes e_2) = -4ae_1 \otimes e_1 \otimes e_1 + 2be_2 \otimes e_2 \otimes e_2 + \overline{\partial}^1\Theta_2(e_1 \otimes e_2 \otimes e_1 + e_1 \otimes e_1 \otimes e_2) - 2\overline{\partial}^2\Theta_1 e_1 \otimes e_2 \otimes e_2 = 0$$

is, in this case, the null connection.

We see again the same phenomenon as in Sec. IV B; working with the "correct" 2D calculus rather than the universal 3D eliminates redundant fields that do not enter into the Riemannian geometry, trading them for an optional regularity condition.

D. Discrete sphere base with $\mathbb{Z}_3 \subset \mathbf{SO(2)}$ frame group

As the main alternative to the above models, we look at the case of the universal calculus on the 4 points of our base space, which has the connectivity of a tetrahedron or discrete model of a sphere:



Our results are rather unusual, probably due to the small number of points in the model. As a projector we are led to π defined by

$$\pi(e_a \otimes e_b) = i(e_a \wedge e_b) = \begin{cases} 0 & a \neq b \\ \frac{1}{3}(e_1 \otimes e_1 + e_2 \otimes e_2 \otimes e_3 \otimes e_3) & a = b. \end{cases}$$

This means that Ω^2 has the relations

$$e_1^2 = e_2^2 = e_3^2 \equiv \mathrm{Top}, \quad e_a \wedge e_b = 0, \quad \forall\, a \neq b.$$

This projector obeys the compatibility condition (i) of Theorem 2.2 as follows. We are required to list all the two-arcs contained in the graph. Naming the vertices as x, y, z, t (starting from (0,0) and going clockwise) the possible two arcs from x are

$$x \to y \to x, \quad x \to y \to z, \quad x \to y \to t,$$

$$x \to z \to x, \quad x \to z \to y, \quad x \to z \to t,$$

$$x \to t \to x, \quad x \to t \to y, \quad x \to t \to z.$$

Now we have to make sure all the possible expression of the form

$$\pi^{yz}_{xyx}, \pi^{yt}_{xyx}, \pi^{zy}_{xyx}, \pi^{zt}_{xyx}, \ldots$$

(60 of them in total) vanish, which happens to be the case. Note that we just considered the two arcs departing from x, since the choice of "start point" is immaterial here due to the symmetry of the graph. The second condition of Theorem 2.2 is empty in the case, because the calculus on Σ is the universal one. $\Omega^2(\Sigma)$ The action of the external derivative on the vielbein elements e_a is computed from Theorem 2.1 and is

$$\mathrm{d}e_1 = (\Theta_1 + R_1\Theta_1)\mathrm{Top} \equiv \tilde{\Theta}_1\mathrm{Top}, \quad \mathrm{d}e_2 = (\Theta_2 + R_2\Theta_2)\mathrm{Top} \equiv \tilde{\Theta}_2\mathrm{Top},$$

$$\mathrm{d}e_3 = (\Theta_3 + R_3\Theta_3)\mathrm{Top} \equiv \tilde{\Theta}_3\mathrm{Top}.$$

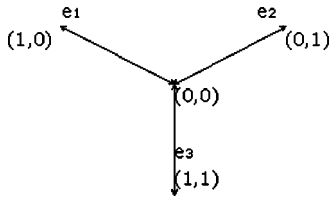
Next, we take $\mathbb{Z}_3=\{\overline{0},\overline{1},\overline{2}\}$ as a frame group, with calculus defined by $\{\overline{1},\overline{2}\}$. $\overline{f^1},\overline{f^2}$ will act on e_1,e_2,e_3 as $e_1\to e_3\to e_2\to e_1$ (notice that the definition of the projector is invariant under this action), or

$$\overline{f^1}\triangleright e_1 = e_3 - e_1, \quad \overline{f^2}\triangleright e_1 = e_2 - e_1,$$

$$\overline{f^1}\triangleright e_2 = e_1 - e_2, \quad \overline{f^2}\triangleright e_2 = e_3 - e_2,$$

$$\overline{f^1}\triangleright e_3 = e_2 - e_3, \quad \overline{f^2}\triangleright e_3 = e_1 - e_3$$

[it is an anticlockwise rotation in the picture below, which is the tetrahedron from the viewpoint of the vertex $(0,0)$]



Proposition 4.13: The moduli space of torsion free connections is 16-dimensional, given by 6 functional parameters $\alpha_1,\ldots,\alpha_3,\beta_1,\ldots,\beta_3$ with two independent equations given by

$$\tilde{\Theta}_1 + \alpha_3 - \alpha_1 - \beta_1 + \beta_2 = 0$$

and cyclic permutations. The additional conditions for zero-cotorsion are the two independent equations given by

$$\overline{\partial^1}(\alpha_1 + \beta_1) - \overline{\partial^2}\alpha_2 - \overline{\partial^3}\beta_3 - \alpha_2 + \alpha_3 + \beta_2 - \beta_3 = 0$$

and cyclic permutations.

Proof: Firstly, we write down the zero torsion conditions, but with a notation of the form

$$A^1_1 = \alpha_1, \quad A^2_1 = \alpha_2, \quad A^3_1 = \alpha_3, \quad A^1_2 = \beta_1, \quad A^2_2 = \beta_2, \quad A^3_2 = \beta_3$$

to underline a symmetry of the theory with respect to cyclical permutations in the upper indexes of the A^j_i (as usual, the lower index refers to the frame group directions). The vanishing of the cotorsion corresponds to

$$\tilde{\Theta}_1 + R_2\alpha_2 - R_1\alpha_1 + R_3\beta_3 - R_1\beta_1 = 0$$

and cyclic permutations. Combining the torsion and cotorsion equations we obtain the equations as stated. □

The covariant derivative shows the same rotational symmetry. In fact,

$$\nabla e_1 = (\omega + \tilde{\omega}) \otimes e_1 - \omega \otimes e_2 - \tilde{\omega} \otimes e_3,$$

$$\omega = \sum_a \alpha_a e_a, \quad \tilde{\omega} = \sum_a \beta_a e_a$$

and ∇e_2 and ∇e_3 can be found by cyclical rotations of ∇e_1.

Proposition 4.14: The Riemann tensor corresponding to the connection above is

$$\mathrm{Riemann}(e_1) = -(\rho + \tilde{\rho})\,\mathrm{Top} \otimes e_1 + \tilde{\rho}\,\mathrm{Top} \otimes e_2 + \rho \mathrm{Top} \otimes e_3$$

[$\mathrm{Riemann}(e_2), \mathrm{Riemann}(e_3)$ *can be found by cyclical rotation] where*

$$\rho = \partial^1 \alpha_1 + \alpha_1 \tilde{\Theta}_1 + \beta_1 R_1(\beta_1 - \alpha_1) - \alpha_1 R_1(2\alpha_1 + \beta_1) + cycl\,.\,,$$

$$\tilde{\rho} = \partial^1 \beta_1 + \beta_1 \tilde{\Theta}_1 + \alpha_1 R_1(\alpha_1 - \beta_1) - \beta_1 R_1(2\beta_1 + \alpha_1) + cycl\,.\,,$$

and the Ricci scalar, $R = -(\rho + \tilde{\rho})$.

Proof: Riemann tensor is obtained in the usual way from the curvature components F_i; the expression for Ricci then comes out as

$$\mathrm{Ricci} = \frac{1}{3}[-(F_1 + F_2)e_1 \otimes e_1 + F_2 e_1 \otimes e_2 + F_1 e_1 \otimes e_3 + F_1 e_2 \otimes e_1 - (F_1 + F_2)e_2 \otimes e_2 + F_2 e_2 \otimes e_3$$
$$+ F_2 e_3 \otimes e_1 + F_1 e_3 \otimes e_2 - (F_1 + F_2)e_3 \otimes e_3]$$

[from which the Ricci scalar $R = -(F_1 + F_2)$]. The curvature two-form is

$$F_1 = \mathrm{d}A_1 + A_2 \wedge A_2 - 2A_1 \wedge A_1 - A_2 \wedge A_1 - A_1 \wedge A_2,$$

$$F_2 = \mathrm{d}A_2 + A_1 \wedge A_1 - A_1 \wedge A_2 - A_2 \wedge A_1 - 2A_2 \wedge A_2$$

and similarly for the other components. □

We know that the moduli space of connections has two functional parameters, which we see here is reflected in the two physical curvature parameters $\rho, \tilde{\rho}$. This model is obviously far from classical, but we see that it has several reasonable features including a cyclic symmetry and a degree 2 top form, i.e., a nonclassical "surface."

V. REMARKS ON THE QUANTUM THEORY

So far we have solved only the classical geometry, which could form the basis for classical equations of motion for gravity and matter in a classical background. For quantum theory at least in a path integral approach one must integrate over all such moduli with respect to an action weighting. Here quantum gravity, in particular, diverges badly. The advantage of working only on a finite number of points as we have done above is that now such functional integrals become finite dimensional integrals, which may still diverge but which are surely much more tractable. Such integrals for gauge theory on S_3 are discussed in Ref. 8 and carried to fruition for Yang–Mills on $\mathbb{Z}_2 \times \mathbb{Z}_2$ in Ref. 7, where the theory was found to be divergent but renormalizable. Here we make some first remarks about how to extend this in principle to the gravitational case. The new ingredient, not yet covered, is the correct "unitarity" or reality condition on the spin connection, which we now propose.

Thus, until now we could have worked above over a generic field, but now we work over $\mathbb{C}$ and specify reality or "unitarity" conditions which should be expected for a physical interpretation. This cuts down our moduli still further and also reduces us to integration over real variables in our finite setting. To do this, we note that $\mathbb{C}(\Sigma)$ is a *-algebra with * given by pointwise complex

conjugation. We extend this to inner calculi with the assumption $\theta^*=\theta$ so that * anticommutes with d (other conventions are also possible). For models based on groups and conjugacy classes with elements of order 2 this is naturally implemented by $e_a^*=e_a$ (more generally, $e_{a^{-1}}$), as in Refs. 6–8. For the models based on $\mathbb{Z}_2\times\mathbb{Z}_2$ connectivity in Sec. IV we take $e_a^*=e_a$. We likewise, and more importantly, take

$$\theta^* = \theta,$$

which ensures that $\mathrm{d}=[\theta,\ \}$ behaves as usual for a * structure in the differential graded algebra (so d graded-commutes with *). In terms of field components this translates to

$$\overline{\Theta_a(x)} = R_a\Theta_a(x).$$

This is consistent with our model in Sec. IV, for example, where the condition (18) on Θ in Sec. VI A for a two-form projector is invariant under *.

Next, we consider the spin connection components. For a unitary action for the braided-Lie algebra generators f^i we would take $A_i^*=A_i$. What is a unitary action is motivated from Hopf algebra theory where for the action of a Hopf *-algebra one would require $(f^i\triangleright e_a)^*=S^{-1}(f^{i^*})\triangleright e_a^*$, where in our case $Sf^i=f^{i^{-1}}$ is inversion in the frame group algebra. The *-structure on the braided-Lie algebra generators is not so clear, but if we assumed that $f^{i*}=f^{i^{-1}}$ as for elements in a group algebra, these two inverses cancel and we would be led to require $(f^i\triangleright e_a)^*=f^i\triangleright e_a$. This indeed holds for the actions in the present paper, particularly those in Sec. IV, since these are obtained from permutations. Next, if the generators are unitary in this sense, we want the frame group connection to be "antihermitian" so we propose here

$$A_i^* = A_{i^{-1}}$$

for the component one-forms. This has the reasonable consequence that applying * to the torsion equations gives the cotorsion equations, i.e., these are related by complex conjugation in the unitary version of the theory. This is desirable as it suggests that imposing the unitarity condition on the moduli space of torison and cotorsion free connections is not so likely to give no solutions. This too is borne out when we look closely at the moduli of connections on our $\mathbb{Z}_2\times\mathbb{Z}_2$ in Proposition 4.2 or 4.5. We concentrate on the second of these as the more physical model with modes a,b.

Proposition 5.1: The reality condition in the moduli of torsion free and cotorsion free connections on the discrete torus in Proposition 4.5 is $\overline{a}=R_2a$, $\overline{b}=R_1b$. *The regularity condition is invariant under conjugation and the Ricci scalar in Proposition 4.5 is real up to a "total divergence" given by* $\overline{\partial^1},\overline{\partial^2}$.

Proof: From the above, we deduce from Proposition 4.5 and the reality condition on the Θ_a that $\overline{\alpha}=-R_1\beta$, $\overline{\beta}=R_2\alpha$ which translates as stated given that the functions a,b reverse sign under R_1R_2. The latter also means that $R_1(\overline{\partial^2}a)=\overline{\partial^2}(-R_2a)=\overline{\partial^2}a$, and similarly $\overline{\partial^1}b$ is R_2-invariant. Since $(\overline{\partial^2}\Theta_1)^*=R_1(\overline{\partial^2}\Theta_1)$, and similarly with R_2 for $\overline{\partial^1}\Theta_2$, we see that the regularity condition is invariant under *. We then compute

$$\begin{aligned}\overline{R} &= R_1(\partial^1 b+\overline{\partial}^2\Theta_1R_1b)+R_2(\partial^1a+\overline{\partial}^1\Theta_2R_2a)-2bR_1b-2aR_2a\\ &= R+\overline{\partial}^1(\partial^1b+\overline{\partial}^2\Theta_1R_1b)+\overline{\partial}^2(\partial^2a+\overline{\partial}^1\Theta_2R_2a),\end{aligned}$$

where $(\partial^1b)^*=(R_1\Theta_1)\partial^1R_1b=R_1(\partial^1b)$, and similarly for ∂^2a. □

The reduced moduli space with full metric compatibility in Proposition 4.7 is also consistent with this *-structure, i.e., our reality condition holds for a,b given by Θ_a as stated there. Moreover, the stated condition on the Θ_a required for this reduces simply to a,b real.

After that, for quantum gravity one should presumably take as action $S=\Sigma_{x\in\Sigma}R(x)$ using the Ricci scalar curvature; we are not in a position to deduce field equations by a variational principle, so this is an assumption of one way to make sense of the quantum theory. To see how this works

we again look at our discrete torus model on 4 points. We already know from Sec. III that for 2 or 3 points the Ricci scalar vanishes in all our models, so this model would be the first with nontrivial Ricci scalar. From the above Propostition 5.1 we see that the action S is real. Moreover, our fields a,b, etc. are functions on the four points but so highly constrained as to be fully determined each by a single complex number, which we denote A,B. Here

$$A = a(0,0) = -a(0,0), \quad \overline{A} = a(0,1) = -a(1,0),$$

$$B = b(0,0) = -b(1,1), \quad \overline{B} = b(1,0) = -b(0,1).$$

Note that the Ricci scalar splits up into two terms

$$R = R_B + R_A; \quad R_B = \partial^1 b + \overline{\partial}^2 \theta_1 R_1 b - 2bR_1 b = R_2 \theta_1 \overline{b} - \theta_1 b - 2b\overline{b}$$

and the similar expression for R_A with $1,2$ interchanged. Writing

$$\Theta = \Theta_1(0,0), \quad \overline{\Theta} = \Theta_1(1,0), \quad \tilde{\Theta} = \Theta_1(0,1), \quad \overline{\tilde{\Theta}} = \Theta_1(1,1)$$

we find

$$S = S_B + S_A; \quad S_B = -8B\overline{B} + 2B(\overline{\tilde{\Theta}} - \Theta) + 2\overline{B}(\tilde{\Theta} - \overline{\Theta}),$$

where we compute R_B at the four points in terms of our new variables and add up. Similarly for the A field and Θ_2. If we restrict to the full metric compatibility in Theorem 4.4 then the action is just $S_B = -4B^2$ and the dynamical variables are $\Theta, \tilde{\Theta}$ constrained such that $B = \tilde{\Theta} - \overline{\Theta}$ is real. Again similarly for the A system.

Finally, we make a polar decomposition of the fields as

$$B = \lambda e^{\imath\phi}, \quad \Theta = \mu e^{\imath\psi}, \quad \tilde{\Theta} = \tilde{\mu} e^{i\tilde{\psi}}$$

in terms of real positive $\lambda, \mu, \tilde{\mu}$ and angles $\phi, \psi, \tilde{\psi}$. In terms of these, we find

$$S_B = -8\lambda^2 + 4\lambda\tilde{\mu}\cos(\phi - \tilde{\psi}) - 4\lambda\mu\cos(\phi + \psi)$$

with similar results for the A system. Then "quantum gravity" is reduced to integrals over these real variables. There remains the constraint (18) as well as the optional regularity condition to be imposed on the moduli in Proposition 4.5. These both cross-couple the A and B systems making even this simplest model nontrivial.

It is not our scope to consider the quantum theory in detail here, particularly since the geometries in this paper are low dimensonal, where one does not expect very dynamical quantum gravity; for a compact surface in two-dimensions the integral of the classical Ricci scalar is a constant by the Gauss–Bonnet theorem. For a classical torus this should be zero, so we see that the discrete torus model already exhibits nonstandard behavior, the meaning of which remains to be understood. It also remains to identify physical observables to be computed by such functional integral methods. However, our low-dimensional example does indicate the possibility of reasonable unitarity constraints and illustrate how a quantum gravity theory might proceed in principle.

VI. COMBINATORICS OF GEOMETRIES UP TO NINE POINTS

For higher numbers of points we do not attempt a detailed classification but rather we overview the range of possibilities with a view to picking out the most interesting ones.

In the first place, we now limit ourselves to the more interesting case of symmetric ("bidirectional") differential calculi. These are just graphs with no self-edges and no more than one edge between vertices. For a fibration with fiber size n, these are the so-called n-regular graphs. There is no classification theory for n-regular graphs (e.g., any n-regular simplicial approximation of a

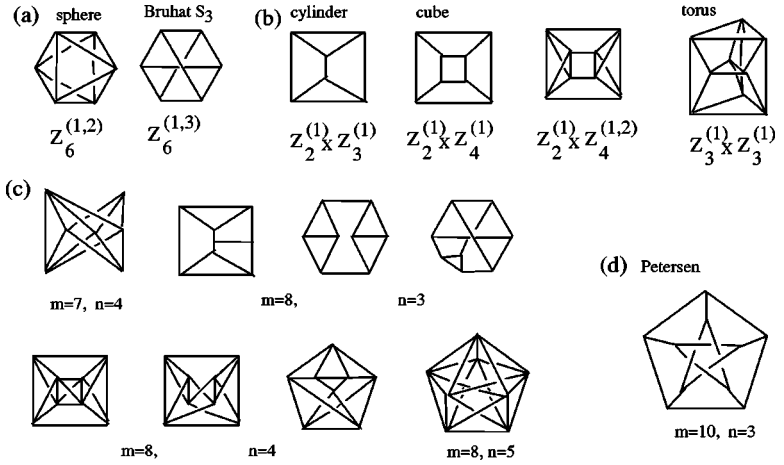


FIG. 1. (a) Examples of circulant graphs; (b) all products of circulants up to $m=9$; (c) graphs up to $m=8$ not circulants or products of them; (d) Petersen graph at $m=10$.

manifold gives one) but small ones are listed in Ref. 14. From there we see that there is a reasonable number for $m\leqslant 8$ after which the number grows rapidly. We deal only with connected graphs.

Note also for any m that here are none for $n=1$ (except $m=2$). For $n=2$ there is just the m-gon for all m. This is the differential calculus on $\mathbb{Z}_m$ with $\mathcal{C}=\{-1,1\}$. For $n=m-1$ there is exactly the universal calculus or totally connected graph. We observe that the m-gon and universal calculi are members of a "circulant graph" family $\mathbb{Z}_m^{1,p,q,\cdots}$ where $p,q,\ldots$ are distinct integers modulo m. They correspond to the calculus on $\mathbb{Z}_m$ with $\mathcal{C}=\{\pm 1,\pm p,\pm q,\ldots\}$ where we only have p if $2p=0$ mod m, etc. The direct product of circulants with $\mathcal{C}_1,\mathcal{C}_2$ means with $\mathcal{C}=(\mathcal{C}_1,0)\cup(0,\mathcal{C}_2)$ (as for the product of any groups equipped with differential structures, see Ref. 10). An example of a circulant is in Fig. 1. Note also the "handshaking lemma" in graph theory that nm has to be even. Then we have the following list of connected graphs which is complete up to $m=8$:

For $m=2$ we have only the universal calculus at $n=1$.

For $m=3$ we have only the universal calculus which equals the 3-gon calculus at $n=2$.

For $m=4$ we have only the 4-gon at $n=2$, which can also be viewed as $\mathbb{Z}_2^{(1)}\times\mathbb{Z}_2^{(1)}$ (i.e., with the direct product calculus where $\mathcal{C}=\{(0,1),(1,0)\}$), and the universal calculus at $n=3$.

For $m=5$ we have only the 5-gon at $n=2$ and the universal at $n=4$.

For $m=6$ we have only the 6-gon at $n=2$ and two choices at $n=3$. These are the circulant $\mathbb{Z}_6^{(1,3)}$, which is also the graph for the S_3 calculus with its two-cycles conjugacy class, and the circulant $\mathbb{Z}_2^{(1)}\times\mathbb{Z}_3^{(1)}$. At $n=4$ we have only the circulant $\mathbb{Z}_6^{(1,2)}$, which is a triangulation of the sphere and is also the graph for S_3 with a left-covariant calculus. See Figs. 1(a) and 1(b). At $n=5$ we just have the universal one. Note that the three-cycles calculus on S_3 is not connected so does not appear in this list.

For $m=7$ we have only the 7-gon at $n=2$, none at $n=3,5$ and two choices at $n=4$. One is the circulant $\mathbb{Z}_7^{(1,2)}$ and the other is shown in Fig. 1(c). At $n=6$ we just have the universal one.

For $m=8$ we have the 8-gon at $n=2$ and five at $n=3$. One of these is the cube, which is $\mathbb{Z}_2^{(1)}\times\mathbb{Z}_2^{(1)}\times\mathbb{Z}_2^{(1)}$. It can also be viewed as $\mathbb{Z}_2^{(1)}\times\mathbb{Z}_4^{(1)}$. Another is the circulant $\mathbb{Z}_8^{(1,4)}$. See Fig. 1(b). The remaining three are as in Fig. 1(c). At $n=4$ there are six, namely the circulants $\mathbb{Z}_8^{(1,2)}$ and $\mathbb{Z}_8^{(1,3)}$, and $\mathbb{Z}_2^{(1)}\times\mathbb{Z}_4^{(1,2)}$ and the remaining three in Fig. 1(c). At $n=5$ there are three, namely the circulants $\mathbb{Z}_8^{(1,2,4)}$ and $\mathbb{Z}_8^{(1,3,4)}$ and the remaining one in Fig. 1(c). At $n=6$ we have only the circulant $\mathbb{Z}_8^{(1,2,3)}$. At $n=7$ we just have the universal calculus.

For $m=9$ there is the 9-gon at $n=2$, none at $n=3$ and already sixteen at $n=4$, of which three are groups, namely the circulants $\mathbb{Z}_9^{(1,3)}$, $\mathbb{Z}_9^{(1,4)}$ and a simplicial torus [see Fig. 1(b)], which is $\mathbb{Z}_3^{(1)}\times\mathbb{Z}_3^{(1)}$. There are none at $n=5$ and three at $n=6$ of which two are circulants on $\mathbb{Z}_9$, and so forth.

Figure 1(d) also shows an important $m=10$ graph with $n=3$ which is a $\mathbb{Z}_2$ quotient of the dodecahedron and can be thought of as a discrete $\mathbb{RP}^2$.

At the qualitative or "topological" level of this section, we can immediately present a discrete moduli space of combinatorial solutions for vielbeins. Namely, for any E that fibers over Σ with $|F_x|=n$, an n-bein is provided by any choice of bijections $s_x:\{1,\dots,n\}\to F_x$ by

$$e_{axy}=\delta_{s_x(a),y}=e_a^{-1xy},\quad e_a=\sum_x \delta_x \mathrm{d}\delta_{s_x(a)} \tag{19}$$

giving

$$e_a f=f(s_\cdot(b))e_a,\quad (\partial^a f)(x)=f(s_x(a))-f(x). \tag{20}$$

Here $s_\cdot(a)$ is a function on Σ (with $\cdot$ denoting the functional dependence). Pictorially, we label all one-arcs arbitrarily by $\{1,\dots,n\}$ and $s_x(a)$ is the endpoint of the arc labeled a from x. The element θ and the relations of the maximal prolongation are

$$\theta=\sum_a e_a,\quad \sum_{\substack{a\ b\\ x\to\to z}} e_a\wedge e_b=0,\quad \forall\, x\neq z, x\not\to z. \tag{21}$$

The corresponding projectors are

$$\pi(e_a\otimes e_b)=e_a\otimes e_b-\sum_x \frac{\delta_x}{|F_{x,z}|}\sum_{\substack{c\ d\\ x\to\to z}} e_c\otimes e_d;\quad \text{where } x\overset{a\ \ b}{\to\to} z \tag{22}$$

and have a functional dependence. Since the wedge product is given by setting to zero the elements of the tensor product which are in the kernel of this projector, we have the lift $i:\Omega^2\to\Omega^1\otimes\Omega^1$ given by the same formula. These formulas are for general left-parallelizable calculi. In our bidirectional case each arc really means two arrows since we can move along it in either direction. In this case the combinatorial data $\{s_x(a)\}$ for this class of vielbeins is a bicoloring of the graph, with two colors $a\in\{1,\dots,n\}$ for each arc, namely one for each arrow. Moveover, we can follow the colored arrows from vertex to vertex and in this way the doubled-up graph (in which each arc is a pair of arrows going in opposite directions) is decomposed into colored loops. The loops of each color need not be connected.

For the framed geometry one must also choose a frame group G acting on the vector space V spanned by the vielbeins, a calculus on the group given by an Ad-stable subset, and projectors π. For the combinatorial solutions above it is natural to take $G=S_n$ acting by permuting the colors, i.e., $g\triangleright e_a=e_{g(a)}$ for a permutation g. We can then take (for example) the universal differential calculus on S_n where $i\in S_n-\{e\}$ so that there is no regularity condition to solve when we use the braided-Lie algebra with basis $\{f^i\}$. Then the torsion and cotorsion equations for A_i are linear and hence determined by linear algebra. More generally, our choice of frame group and associated structures have to be chosen according to what geometry we want to model. I.e., for each choice of regular graph for the "topology" of the finite set, we have further choices for the actual geometry we want to model. We have already seen how this goes for a small number of points; there are progressively more choices as the number of points increases.

Finally, putting together all the considerations in the paper, we arrive at a first impression of "quantum gravity" in our finite geometry approach. Let us discuss this in a fixed n dimensions, say. As in our examples in Sec. IV, we focus for the sake of discussion on the case of bidirectional graphs and vielbein of the form

$$e_{axy}=\Theta_a(x)^{-1}\delta_{s_x(a),y},$$

where we are allowed to vary each edge in the combinatorial vielbein discussed above by continuous degree of freedom Θ_a. Then for the partition function of this part of quantum gravity one should sum over all remaining topological variables, i.e., all numbers m of points, all n-regular

graphs (so the cotangent bundle is n-dimensional) with the variable m vertices, and all colorings s_a of them into loops (see above); then for each of those (and associated choices of frame group) we integrate over the moduli spaces for the continuous degrees of freedom Θ_a of the vielbein and the spin connection, weighted with some action such as the Einstein–Hilbert one. For example we have at this point the real integrals $\mathrm{d}\lambda, \mathrm{d}\phi, \mathrm{d}\mu, \mathrm{d}\tilde{\mu}, \mathrm{d}\psi, \mathrm{d}\tilde{\psi}$ with the action in Sec. V as a small piece of such a quantum gravity in two-dimensions, in the sector consisting of 4 points with square connectivity and coloring according to $\mathbb{Z}_2^{(1)} \times \mathbb{Z}_2^{(1)}$. Note carefully that our approach is intrinsically a quantum gravity theory in which differential structures (which go into the graph) are summed over as well as more familiar modes.

We are now ready to observe a new kind of duality which is suggested by our sketch of quantum gravity: The sum over all n-regular graphs (n fixed) with variable numbers m of points, which is the main combinatorial part of our theory in n-dimensions, is the same as in the Feynman diagram rules for a scalar theory in flat space with Φ^n-interaction terms. There the graph edges correspond to propagating fields and each vertex is an interaction, i.e., the interpretation is entirely different. The weights for each graph are also somewhat different, but in the Feynman rules one again identifies the loops in the graph (each contributes a momentum integral). One could, therefore, speculate that some flat space quantum field theory with Feynman rules could be equivalent to finite quantum gravity with some action, which would be a novel and somewhat unexpected duality between gravity and elementary particles. These remarks are of course speculative at the moment but may be an interesting direction for further study.

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Nonintegrability of nonhomogeneous nonlinear lattices

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We study the integrability of nonlinear lattices with nonhomogeneous polynomial potentials. We prove a nonintegrability theorem for these dynamical systems. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1806260]

I. INTRODUCTION

The integrability or nonintegrability of a given Hamiltonian system is one of the most fundamental and important issues in characterizing the dynamics of its solutions. Ziglin's theorem[1,2] provides a powerful method to prove the nonintegrability of a given Hamiltonian system. In addition to Ziglin's original example, the Ziglin's theorem has been successfully applied to several Hamiltonian systems with a small number of degrees of freedom to prove the nonexistence of an additional first integral: some homogeneous potential systems,[3] the three-particle Fermi–Pasta–Ulam (FPU) lattice,[4] and the Hénon–Heiles system.[5,6]

Nonlinear lattices are simple Hamiltonian systems with a large number of degrees of freedom, which have been of great physical interest in connection with the dynamical foundation of the statistical mechanics. Their dynamical behavior has been extensively studied since the numerical experiments by Fermi, Pasta, and Ulam on the relaxation process toward equilibrium in one-dimensional nonlinear lattices.[7] It has been believed that nonlinear lattice models are in general nonintegrable, except for some integrable models such as the Toda lattice.[8] However, there are only a few nonlinear lattice models that have been proved to be nonintegrable: homogeneous interaction potential lattices with the fixed-end boundary condition[9,10] and the FPU-β lattice, which has quadratic and quartic interaction potentials, with the fixed-end boundary condition.[11] For these lattice models, the nonintegrability has been proved in a strong sense that no additional analytic first integral exists in the complex phase space.

In the present paper, we consider a more general class of nonlinear lattice models described by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N} [U(q_i) + V(q_i - q_{i-1})], \tag{1}$$

which is defined on the complex symplectic manifold $\mathcal{M} = \mathbf{C}^{2N} = \{(q_1, \ldots, q_N, p_1, \ldots, p_N)\}$. We assume the periodic boundary condition, i.e., $q_0 = q_N$. The on-site potential U and the nearest neighbor interaction potential V are of the forms

$$U(X) = \sum_{k=2}^{2m} \frac{\mu_k}{k} X^k, \tag{2}$$

$$V(X) = \sum_{k=2}^{2m} \frac{\kappa_k}{k} X^k, \tag{3}$$

where $\mu_k \in \mathbf{R}$ and $\kappa_k \in \mathbf{R}$ are the real constants. We assume $\mu_k = 0$ for odd k so that the on-site potential $U(X)$ may have the symmetry $U(X) = U(-X)$. The purpose of the present paper is to give rigorous results on the nonintegrability of the nonlinear lattices described by Eq. (1). For this purpose, we derive a reduced Hamiltonian system for the system (1), which describes the dynamics on a low-dimensional invariant manifold, and apply a version of the Ziglin's theorem derived by Yoshida[12] to the reduced system. We prove a nonintegrability theorem for the nonlinear lattices described by Eq. (1).

The present paper is organized as follows. In Sec. II, we review the Ziglin's theorem in the case of generic two-dimensional systems. In Sec. III, we review known results on the application of Ziglin's theorem to nonhomogeneous potential systems. In Sec. IV, we relate the nonintegrability of the reduced system with that of the original full system. The reduced Hamiltonian system of (1) is derived and the main theorem is given in Sec. V.

II. ZIGLIN'S THEOREM

The aim of this section is to give a brief review of Ziglin's theorem.[1] Consider the two-dimensional Hamiltonian system

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + \Phi(x,y) \tag{4}$$

with an analytic potential function $\Phi(x,y)$ in the complex phase space $\mathbf{C}^4 = \{(x,y,p_x,p_y)\}$. The solutions of this system are functions of complex time $t \in \mathbf{C}$. Assume that there exists a straight-line solution of the form

$$x(t) = 0, \quad y(t) = \varphi(t). \tag{5}$$

The solution $\varphi(t)$ satisfies the differential equation

$$\frac{\mathrm{d}^2\varphi}{\mathrm{d}t^2} + \Phi_y(0,\varphi) = 0, \tag{6}$$

where $\Phi_y = \partial\Phi/\partial y$. This equation has the integral

$$\frac{1}{2}\left(\frac{\mathrm{d}\varphi}{\mathrm{d}t}\right)^2 + \Phi(0,\varphi) = h, \tag{7}$$

where $h \in \mathbf{R}$ is a constant corresponding to the energy. The function $\varphi(t)$ is determined as the inverse function of

$$t = \int_{\varphi_0}^{\varphi} \mathrm{d}w/\sqrt{P(w)}, \tag{8}$$

with

$$P(w) = 2[h - \Phi(0,w)], \tag{9}$$

where the integral (8) is taken along a path of integration starting from an initial point φ_0 to the end point φ in the w plane. The value φ determined as a function of t gives the solution $\varphi(t)$.

The function $z=\sqrt{P(w)}$ defines a Riemann surface $\mathcal{R}$ and the roots of $P(w)=0$ give the branch points. Let γ be an arbitrary closed path encircling some of the branch points. The value T_γ of integral (8) given by

$$T_\gamma = \oint_\gamma \mathrm{d}w/\sqrt{P(w)} \tag{10}$$

does not vanish in general and T_γ gives a period of the function $\varphi(t)$. The period T_γ depends only on the homotopy class $[\gamma]$ of γ on $\mathcal{R}$.

Now we consider variational equations along the solution $\varphi(t)$. The variational equations for x and y directions are decoupled because the existence of solution (5) implies that $\Phi_{xy}(0,\varphi(t))=0$ holds identically. Let ξ be the variation in the x direction. The equation for ξ is called the normal variational equation (NVE) and given by

$$\frac{\mathrm{d}^2\xi}{\mathrm{d}t^2} + \Phi_{xx}(0,\varphi(t))\xi = 0. \tag{11}$$

Let us consider a set $\{\gamma\}$ of closed paths, which share a common base point $w_0=\varphi(t_0)$ on $\mathcal{R}$. Since $\mathcal{R}$ is parametrized by $t\in\mathbf{C}$, a closed path γ corresponds to a path in the t plane. In what follows, the analytic continuation along a closed path γ in $\mathcal{R}$ is considered as the analytic continuation along the corresponding path in the t plane. A 2×2 symplectic matrix $g(\gamma)\in \mathrm{SL}(2,\mathbf{C})$ called a monodromy matrix is defined for each closed path γ. The monodromy matrix $g(\gamma)$ describes the time evolution of a system of fundamental solutions of Eq. (11) along γ, i.e., $g(\gamma)$ is defined as the matrix such that

$$(\xi_1(t+T_\gamma),\xi_2(t+T_\gamma)) = (\xi_1(t),\xi_2(t))\cdot g(\gamma), \tag{12}$$

where $\{\xi_1,\xi_2\}$ is a system of fundamental solutions of the NVE. The monodromy matrix $g(\gamma)$ depends only on the homotopy class $[\gamma]$ of γ on $\mathcal{R}$. The set of all monodromy matrices forms a group G called the monodromy group.

Definition: A monodromy matrix $g\in G$ is said to be nonresonant if the eigenvalues $\{\rho,\rho^{-1}\}$ of g satisfy that $\rho^n\neq 1$ for any nonzero integer n.

Let $H^{-1}(h)$ be the energy surface defined by $H^{-1}(h)=\{(x,y,p_x,p_y)\in\mathbf{C}^4 \,|\, H(x,y,p_x,p_y)=h\}$. We define a point set Γ_h by $\Gamma_h=\{(0,\varphi(t),0,\dot{\varphi}(t))\in H^{-1}(h)\,|\,t\in\mathbf{C}\}$. Ziglin's theorem[1] can be stated as follows in our situation.

Theorem 1: *Suppose that system (4) has an integral $f(x,y,p_x,p_y)=$const, which is analytic in a neighborhood of Γ_h and functionally independent of H. If there exists a nonresonant monodromy matrix $g_1\in G$, then any monodromy matrix $g_2\in G$ satisfies that either (i) g_2 commutes with g_1, or (ii)* $\mathrm{tr}\, g_2=0$.

III. APPLICATION OF ZIGLIN'S THEOREM TO POLYNOMIAL POTENTIAL SYSTEMS

A. Monodromy group for homogeneous potential systems

We briefly review some known results on the monodromy matrices of NVE for a homogeneous potential system (for detail, see Ref. 3). Consider the Hamiltonian system (4) with a homogeneous potential of degree $2m\geqslant 4$, which has the straight-line solution of the form (5). The equation for $\varphi(t)$ and the NVE can be written as

$$\frac{\mathrm{d}^2\varphi}{\mathrm{d}t^2} + \alpha_{2m}\varphi^{2m-1} = 0 \tag{13}$$

and

$$\frac{d^2\xi}{dt^2} + \beta_{2m}\varphi(t)^{2m-2}\xi = 0, \tag{14}$$

where α_{2m} and β_{2m} are real constants and we assume $\alpha_{2m} > 0$. We define a parameter λ_{2m} as

$$\lambda_{2m} = \frac{\beta_{2m}}{\alpha_{2m}}. \tag{15}$$

In this case, the function $P(w)$ in Eq. (8) is given by

$$P(w) = 2\left[h - \left(\frac{\alpha_{2m}}{2m}\right)w^{2m}\right], \tag{16}$$

and the branch points $\hat{s}_k$, $k=0,1,\ldots,2m-1$ in the Riemann surface $\mathcal{R}$ defined by $z=\sqrt{P(w)}$ are located at

$$\hat{s}_k = \left(\frac{2mh}{\alpha_{2m}}\right)^{1/2m} \exp\left[i\frac{\pi k}{m}\right]. \tag{17}$$

We define two closed paths $\hat{\gamma}_1$ and $\hat{\gamma}_2$ in $\mathcal{R}$ as follows: $\hat{\gamma}_1$ is a counterclockwise circuit encircling two branch points $\hat{s}_0$ and $\hat{s}_m$, which defines the real period; $\hat{\gamma}_2$ is a counter-clockwise circuit encircling $\hat{s}_1$ and $\hat{s}_{m+1}$. A common base point w_0 is taken between $w=0$ and $\hat{s}_0$ on the real w axis. It is known that the NVE (14) is transformed into the Gauss hypergeometric equation by the change of the independent variable from t to $z=(\alpha_{2mh}/2mh)[\varphi(t)]^{2m}$.[3] This fact enables us to obtain explicit expressions for the two monodromy matrices $\hat{g}_1$ and $\hat{g}_2$, which associate with $\hat{\gamma}_1$ and $\hat{\gamma}_2$, respectively, as follows:[12]

$$\hat{g}_1 = \begin{pmatrix} -1 & -BC \\ A & ABC-1 \end{pmatrix}^2, \tag{18}$$

$$\hat{g}_2 = \begin{pmatrix} -1-\Omega AB & -B(ABC+\Omega AB+\Omega^{-1}C) \\ \Omega A & ABC+\Omega AB-1 \end{pmatrix}^2, \tag{19}$$

where

$$A = 1-\Omega^{-1}e^{-i2\pi a}, \quad B = 1-\Omega^{-1}e^{-i2\pi b}, \quad C = 2\Omega/(\Omega-1), \tag{20}$$

and

$$\Omega = e^{i\pi/m}, \quad a+b = 1/2-1/2m, \quad ab = -\lambda_{2m}/4m. \tag{21}$$

In the homogeneous potential case, the monodromy matrices do not depend on the energy h as seen in Eqs. (18) and (19). A simple computation shows that

$$\mathrm{tr}\,\hat{g}_1 = \mathrm{tr}\,\hat{g}_2 = F_{2m}(\lambda_{2m}), \tag{22}$$

where the function $F_{2m}(\lambda_{2m})$ is defined by

$$F_{2m}(\lambda_{2m}) = \frac{4}{\sin^2(\pi/2m)}\cos^2\left[(\pi/2m)\sqrt{(m-1)^2+4m\lambda_{2m}}\right] - 2. \tag{23}$$

It can be confirmed that $\hat{g}_1$ and $\hat{g}_2$ commute, i.e., the commutator $[\hat{g}_1,\hat{g}_2]=0$, if and only if λ_{2m} has values such that $F_{2m}(\lambda_{2m})=\pm 2$. In addition, we can show that $F_{2m}(\lambda_{2m})>2$ when λ_{2m} is in the region S_{2m} defined by

$$S_{2m} = \{\lambda \in \mathbf{R} | \lambda < 0 \text{ or } 1 < \lambda < 2m-1 \text{ or } 2m+2 < \lambda < 6m-2 \text{ or } \cdots \text{ or } j(j-1)m + j < \lambda < j(j+1)m - j \text{ or } \cdots\}. \tag{24}$$

B. Nonintegrability theorem for nonhomogeneous potential systems

Consider the nonhomogeneous Hamiltonian system

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \sum_{k=2}^{2m} \Phi_k(x,y), \tag{25}$$

where $\Phi_k(x,y)$ is the homogeneous part of degree k, and assume that the system has the straight-line solution of the form (5). The equation for $\varphi(t)$ can be written in the form

$$\frac{d^2\varphi}{dt^2} + W'(\varphi) = 0, \tag{26}$$

where we introduced an effective potential function $W(X)$ defined by

$$W(X) = \sum_{k=2}^{2m} \frac{\alpha_k}{k} X^k. \tag{27}$$

The NVE can be written in the form

$$\frac{d^2\xi}{dt^2} + \left[\sum_{k=2}^{2m} \beta_k \varphi(t)^{k-2}\right]\xi = 0. \tag{28}$$

In Eqs. (27) and (28), α_k and β_k represent the real constants, and we assume that $\alpha_2 > 0$ and $\alpha_{2m} > 0$.

The function $P(w)$ in Eq. (8) is given by

$$P(w) = 2[h - W(w)]. \tag{29}$$

There are h-dependent branch points s_k, $k=0,1,\ldots,2m-1$ in the Riemann surface $\mathcal{R}$ such that $s_k/\hat{s}_k \to 1$ in the limit $h \to \infty$, where $\hat{s}_k$ is the branch point of the homogeneous system given by Eq. (17). In what follows, we assume that the branch points $s_0, s_1, \ldots, s_{2m-1}$ differ from each other for any $h > 0$, i.e., the algebraic equation $W(X) - h = 0$ has $2m$ distinct roots for any $h > 0$. Since any branch point s_k does not collide with the others as h varies under this assumption, we can define the following two closed paths $\gamma_1(h)$ and $\gamma_2(h)$, which deform continuously as h varies: $\gamma_1(h)$ is a counterclockwise circuit encircling only two branch points s_0 and s_m on the real w axis; $\gamma_2(h)$ is a counterclockwise circuit encircling only s_1 and s_{m+1}. A common base point w_0 is taken between $w=0$ and s_0 on the real w axis.

Let $g_1(h)$ and $g_2(h)$ be the two monodromy matrices associated with $\gamma_1(h)$ and $\gamma_2(h)$, respectively. These monodromy matrices depend on h. The elements of $g_1(h)$ and $g_2(h)$ are analytic functions of h in the interval $(0,\infty)$, since s_k, $k=0,1,\ldots,2m-1$ are analytic functions of h due to the assumption that $W(X)-h=0$ has $2m$ distinct roots for any $h>0$. When the potential is nonhomogeneous, there is no analytical method to calculate the monodromy matrices. However, Yoshida pointed out in Ref. 12 that they can be evaluated in the limits $h \to 0$ and $h \to \infty$.

In the limit $h \to \infty$, the highest order terms of φ become dominant in Eqs. (26) and (28). Therefore, $g_1(h)$ and $g_2(h)$ converges to the monodromy matrices $\hat{g}_1$ and $\hat{g}_2$ of the homogeneous system of degree $2m$, respectively, which are given by Eqs. (18) and (19). We have

$$\lim_{h\to\infty} \operatorname{tr} g_1(h) = \lim_{h\to\infty} \operatorname{tr} g_2(h) = F_{2m}(\lambda_{2m}) \tag{30}$$

and

$$\lim_{h\to\infty}[g_1(h),g_2(h)]=[\hat{g}_1,\hat{g}_2]. \tag{31}$$

In the opposite limit $h\to 0$, the lowest order terms of φ become dominant in Eqs. (26) and (28): the NVE (28) tends to that of the homogeneous system of degree 2. The assumption on the roots of $W(X)-h=0$ implies that only two branch points s_0 and s_m are real numbers for any $h>0$. These two real branch points approach those of the homogeneous system of degree 2, which are given by $w=\pm(2h/\alpha_2)^{1/2}$, in the limit $h\to 0$. Therefore, $g_1(h)$ converges to the monodromy matrix of the homogeneous system of degree 2 that corresponds to the real period and we have

$$\lim_{h\to 0}\operatorname{tr} g_1(h)=2\cos[2\pi\sqrt{\lambda_2}], \tag{32}$$

where $\lambda_2=\beta_2/\alpha_2$.

Based on the above arguments, Yoshida obtained the following useful theorem.[12] To state the theorem, we define a point set of a straight line solution $\Gamma_h=\{(0,\varphi(t),0,\dot{\varphi}(t))\in H^{-1}(h)\,|\,t\in\mathbf{C}\}$ and a family of the straight line solutions $\{\Gamma_h\}_{h_0,\varepsilon}=\{\Gamma_h\in\mathbf{C}^4\,|\,h\in U_\varepsilon(h_0)=(h_0-\varepsilon,h_0+\varepsilon)\}$, where $h_0\in(0,\infty)$ is an arbitrary fixed energy value and ε is a small positive real number.

Theorem 2: *Suppose that* $m\geqslant 2$, $\alpha_2>0$, $\alpha_{2m}>0$, *and the algebraic equation* $W(X)-h=0$ *has* $2m$ *distinct roots for any* $h>0$. *If* $\lambda_{2m}=\beta_{2m}/\alpha_{2m}$ *is a value such that* $F_{2m}(\lambda_{2m})\notin\{0,\pm 2,2\cos[2\pi\sqrt{\lambda_2}]\}$, *then for any* $h_0>0$ *and any* $\varepsilon>0$ *the system (25) cannot have an additional integral, which is analytic and functionally independent of H in a connected neighborhood of* $\{\Gamma_h\}_{h_0,\varepsilon}$.

Proof: We consider the monodromy matrices $g_1(h)$ and $g_2(h)$ defined in the above. The components of $g_1(h)$ and $g_2(h)$ are analytic functions of h in the whole interval $(0,\infty)$. From Eqs. (30) and (32), in the limits $h\to 0$ and $h\to\infty$, we know $\operatorname{tr} g_1(0)=2\cos[2\pi\sqrt{\lambda_2}]$ and $\operatorname{tr} g_1(\infty)=\operatorname{tr} g_2(\infty)=F_{2m}(\lambda_{2m})$.

Since $g_1(h)$ is an analytic function of h in the whole interval $(0,\infty)$, the condition $F_{2m}(\lambda_{2m})\neq 2\cos[2\pi\sqrt{\lambda_2}]$ implies that $\operatorname{tr} g_1(h)$ actually changes as h varies. Therefore, there exists a dense subset S of the interval $(0,\infty)$ such that $g_1(h)$ is nonresonant for any $h\in S$. Assume that there exists an additional integral in a neighborhood of $\{\Gamma_h\}_{h_0,\varepsilon}$. It follows from Theorem 1 that either $[g_1(h),g_2(h)]=0$ or $\operatorname{tr} g_2(h)=0$ holds for any fixed $h\in S\cap U_\varepsilon(h_0)$.

Assume that $[g_1(\bar{h}),g_2(\bar{h})]\neq 0$ for some $\bar{h}\in S\cap U_\varepsilon(h_0)$. Because of the continuity of $[g_1(h),g_2(h)]$ with respect to h, $[g_1(h),g_2(h)]\neq 0$ holds in some neighborhood $U'(\bar{h})\subseteq U_\varepsilon(h_0)$ of $\bar{h}$. Thus, $\operatorname{tr} g_2(h)=0$ holds for any $h\in S'$, where S' is defined by $S'=S\cap U'(\bar{h})$. Since $\operatorname{tr} g_2(h)$ is an analytic function of h and $\operatorname{tr} g_2(h)=0$ holds in the dense subset S' of $U'(\bar{h})$, it follows that $\operatorname{tr} g_2(h)=0$ holds identically over the whole interval $(0,\infty)$. This contradicts the assumption $\operatorname{tr} g_2(\infty)=F_{2m}(\lambda_{2m})\neq 0$. On the other hand, if we assume that $\operatorname{tr} g_2(\bar{h})\neq 0$ for some $\bar{h}\in S\cap U_\varepsilon(h_0)$, then it follows that $[g_1(h),g_2(h)]=0$ holds for any $h\in S''$, where S'' is a dense subset of some neighborhood of $\bar{h}$, by a similar argument to the above. Since $[g_1(h),g_2(h)]$ is an analytic function of h and $[g_1(h),g_2(h)]=0$ holds in the dense subset S'', it follows that $[g_1(h),g_2(h)]=0$ holds identically over the whole interval $(0,\infty)$. Thus, we have $\lim_{h\to\infty}[g_1(h),g_2(h)]=0$. The commutator is given by $[\hat{g}_1,\hat{g}_2]$ in the limit $h\to\infty$ from Eq. (31). Therefore, $F_{2m}(\lambda_{2m})=\pm 2$ follows from $\lim_{h\to\infty}[g_1(h),g_2(h)]=0$. This contradicts the assumption $F_{2m}(\lambda_{2m})\neq\pm 2$. From the above arguments, the nonexistence of an additional integral, which is analytic and functionally independent of H in a connected neighborhood of $\{\Gamma_h\}_{h_0,\varepsilon}$, has been proven. ■

Remark: A condition to guarantee the analyticity of $g_1(h)$ and $g_2(h)$ was not included in the original statement of this theorem in Ref. 12. As a sufficient condition, we added the nondegeneracy condition on the roots of $W(X)-h=0$.

IV. REDUCED HAMILTONIAN SYSTEM ON LOW-DIMENSIONAL INVARIANT MANIFOLD AND NONINTEGRABILITY

In this section we give a lemma, which relates the nonintegrability of a reduced system on a low-dimensional invariant manifold and that of the full system. Consider the Hamiltonian system of $n+2$ degrees of freedom,

$$H(q_1,\ldots,q_{n+2},p_1,\ldots,p_{n+2}), \tag{33}$$

which is defined on the complex symplectic manifold $\mathcal{N}=\mathbf{C}^{2(n+2)}$. Suppose that the Hamiltonian system (33) has a four-dimensional invariant manifold $\mathcal{I}$ defined by

$$\mathcal{I}=\{(q_1,\ldots,q_{n+2},p_1,\ldots,p_{n+2})\in \mathbf{C}^{2(n+2)} | q_i=p_i=0, i=1,2,\ldots,n\}, \tag{34}$$

and the vector field restricted to $\mathcal{I}$ is associated with the Hamiltonian $\tilde{H}(q_{n+1},q_{n+2},p_{n+1},p_{n+2})$, which we call the *reduced Hamiltonian*. The reduced Hamiltonian $\tilde{H}$ is related to the original Hamiltonian H as

$$\tilde{H}(q_{n+1},q_{n+2},p_{n+1},p_{n+2})=H(0,\ldots,0,q_{n+1},q_{n+2},0,\ldots,0,p_{n+1},p_{n+2}). \tag{35}$$

Let Γ_h be a straight line solution of the reduced Hamiltonian system. We denote its family by $\{\Gamma_h\}$. Then, we have the following lemma.

Lemma 1: Suppose that the reduced Hamiltonian system (35) is nonintegrable, in the sense that there does not exist an additional integral which is analytic and functionally independent of $\tilde{H}$ in a connected neighborhood of $\{\Gamma_h\}$ in $\mathcal{I}$. Then, the full Hamiltonian system (33) cannot have a set of $n+2$ analytic integrals $f_1=H,f_2,\ldots,f_{n+2}$ defined in a connected neighborhood U of $\{\Gamma_h\}$ in $\mathcal{N}$, such that

(C1) The 1-forms $\mathrm{d}f_i, i=1,2,\ldots,n+2$ are linearly independent over a dense open set $D\subseteq U$ such that $D\cap\mathcal{I}\neq\phi$.

(C2) They form an involutive set: the Poisson brackets for any pair of f_i and f_j vanish, i.e., $\{f_i,f_j\}=0, i,j=1,2,\ldots,n+2$.

Proof: Suppose that there exists a set of $n+2$ integrals satisfying the conditions (C1) and (C2). Let $\tilde{f}_i$ defined by $\tilde{f}_i(q_{n+1},q_{n+2},p_{n+1},p_{n+2})=f_i(0,\ldots,0,q_{n+1},q_{n+2},0,\ldots,0,p_{n+1},p_{n+2})$. Since $\mathcal{I}$ is the invariant manifold, each $\tilde{f}_i$ is an integral of the reduced system (35) in $\mathcal{I}\cap U$. The nonexistence of an additional integral, which is functionally independent of $\tilde{H}$ in $\mathcal{I}\cap U$, implies that $\tilde{f}_i$ and $\tilde{H}$ are functionally dependent in $\mathcal{I}\cap U$. Then, $\tilde{f}_i$ is a function of $\tilde{H}$ only, i.e., $\tilde{f}_i=\Psi_i(\tilde{H})$ with some analytic function Ψ_i. Therefore, except for the Hamiltonian $f_1=H$, we can assume that $f_i=0$ over $\mathcal{I}\cap U$ for $i=2,3,\ldots,n+2$. In fact, if $\tilde{f}_i\neq 0$, then we can use $f_i-\Psi_i(H)$ as an integral instead of f_i.

There is a point $x\in D\cap\mathcal{I}$ such that $\mathrm{d}f_i$, $i=1,2,\ldots,N$ are linearly independent at x. Let U_x be a neighborhood of x in $\mathcal{N}$. Since f_i is an analytic function of $(q_1,\ldots,q_{n+2},p_1,\ldots,p_{n+2})$, we can expand f_i for $i=2,3,\ldots,n+2$ in U_x as

$$f_i=\sum_{|\boldsymbol{\nu}|=1}^{\infty} f_{\boldsymbol{\nu}}^{(i)}(q_{n+1},q_{n+2},p_{n+1},p_{n+2})q_1^{\nu_1}\cdots q_n^{\nu_n}p_1^{\nu_{n+1}}\cdots p_n^{\nu_{2n}}, \tag{36}$$

where ν_j, $j=1,\ldots,2n$ are non-negative integers, $\boldsymbol{\nu}$ is the multi-index $\boldsymbol{\nu}=(\nu_1,\ldots,\nu_{2n}), |\boldsymbol{\nu}|=\nu_1+\nu_2+\cdots+\nu_{2n}$, and $f_{\boldsymbol{\nu}}^{(i)}$ is an analytic function of $(q_{n+1},q_{n+2},p_{n+1},p_{n+2})$, and we used the fact $\tilde{f}_i=0$.

A simple calculation using Eq. (36) shows that the 1-form $\mathrm{d}f_i$ at x is of the form

$$\mathrm{d}f_i=\sum_{j=1}^{n}[a_j^{(i)}(x)\mathrm{d}q_j+a_{n+j}^{(i)}(x)\mathrm{d}p_j], \tag{37}$$

for $i=2,3,\ldots,n+2$. In Eq. (37), $a_j^{(i)}$ is given by $f_{\boldsymbol{\nu}}^{(i)}$ with the multi-index $\boldsymbol{\nu}$ such that its kth component is $\nu_k=\delta_{jk}$, where δ_{jk} is the Kronecker's delta. Note that $\mathrm{d}f_i$ does not include the terms

of $\mathrm{d}q_i$ and $\mathrm{d}p_i$, $i=n+1,n+2$. Let L_x be a subspace of the tangent space $T_x\mathcal{N}$ at the point x defined by $L_x=\mathrm{span}\{\partial/\partial q_1,\ldots,\partial/\partial q_n,\partial/\partial p_1,\ldots,\partial/\partial p_n\}$ and L_x^* be the dual space of L_x defined by $L_x^*=\mathrm{span}\{\mathrm{d}q_1,\ldots,\mathrm{d}q_n,\mathrm{d}p_1,\ldots,\mathrm{d}p_n\}$. Equation (37) shows that $\mathrm{d}f_i\in L_x^*$ for $i=2,3,\ldots,n+2$. In addition, we define a subspace $L_{f,x}=\{v\in L_x|\mathrm{d}f_i(v)=0,\ i=2,3,\ldots,n+2\}\subseteq L_x$. Since the 1-forms $\mathrm{d}f_i$, $i=2,3,\ldots,n+2$ are linearly independent at x, the dimension of $L_{f,x}$ is obtained as $\dim L_{f,x}=\dim L_x-(n+1)=n-1$.

Let I be the isomorphism between the cotangent bundle $T^*\mathcal{N}$ and the tangent bundle $T\mathcal{N}$, which maps a 1-form to the associated Hamiltonian vector field. From Eq. (36), the Hamiltonian vector fields $I\,\mathrm{d}f_i$, $i=2,3,\ldots,n+2$ associated with the Hamiltonian f_i are obtained at x as follows:

$$I\,\mathrm{d}f_i=\sum_{j=1}^{n}\left[b_j^{(i)}(x)\frac{\partial}{\partial q_j}+b_{n+j}^{(i)}(x)\frac{\partial}{\partial p_j}\right], \tag{38}$$

where $b_j^{(i)}=a_{n+j}^{(i)}$, $b_{n+j}^{(i)}=-a_j^{(i)}$, $j=1,2,\ldots,n$. The condition (C2) implies that $\mathrm{d}f_i(I\,\mathrm{d}f_j)=0$, $i,j,=2,3,\ldots,n+2$ and thus $I\,\mathrm{d}f_j\in L_{f,x}$, $j,=2,3,\ldots,n+2$. Since the map I is nondegenerate, the $n+1$ vectors $I\,\mathrm{d}f_j$, $j=2,3,\ldots,n+2$ are linearly independent. This implies $\dim L_{f,x}\geqslant n+1$ and we get a contradiction. Therefore, there cannot exist a set of $n+2$ integrals satisfying the two conditions (C1) and (C2). ■

V. NONINTEGRABILITY THEOREM FOR NONLINEAR LATTICES

A. Invariant manifold and reduced Hamiltonian

Consider the lattice Hamiltonian (1) with the polynomial potential functions (2) and (3) in $\mathcal{M}=\mathbf{C}^{2N}$. Suppose that the on-site potential $U(X)$ has the symmetry $U(X)=U(-X)$, that is, $\mu_k=0$ for odd k. In the following arguments, we employ the periodic boundary condition and assume the lattice size N to be a multiple of four, i.e.,

$$q_0=q_N,\quad q_{N+1}=q_1,\quad N=4n\ (n\in\mathbf{N}). \tag{39}$$

The equations of motion read

$$\frac{\mathrm{d}^2q_i}{\mathrm{d}t^2}+U'(q_i)-V'(q_{i+1}-q_i)+V'(q_i-q_{i-1})=0,\quad i=1,2,\ldots,N. \tag{40}$$

We define the canonical transformation $(q_1,\ldots,q_N,p_1\ldots,p_N)\mapsto(Q_0,\ldots,Q_{N-1},P_0,\ldots,P_{N-1})$ as follows:

$$q_i=\sum_{k=0}^{N-1}Q_k\left[\sin\left(\frac{2\pi k}{N}i\right)+\cos\left(\frac{2\pi k}{N}i\right)\right], \tag{41}$$

$$p_i=\frac{1}{N}\sum_{k=0}^{N-1}P_k\left[\sin\left(\frac{2\pi k}{N}i\right)+\cos\left(\frac{2\pi k}{N}i\right)\right], \tag{42}$$

where $i=1,2,\ldots,N$. This new variables Q_k and P_k are called the normal mode coordinates. Then, as for the invariant manifold, we have the following.

Proposition 1: Suppose that $U(X)$ has the symmetry $U(X)=U(-X)$ and $N=4n$ $(n\in\mathbf{N})$. *Nonlinear lattice* (1) *with the periodic boundary condition has the four-dimensional invariant manifold* $\mathcal{I}_1$ *defined by*

$$\mathcal{I}_1=\{(Q_0,\ldots,Q_{N-1},P_0,\ldots,P_{N-1})\in\mathbf{C}^{2N}|Q_k=P_k=0,\ k\neq N/4,N/2\}. \tag{43}$$

Moreover, the reduced Hamiltonian $\tilde{H}_1$, *which determines the vector field on* $\mathcal{I}_1$, *is given by*

$$\tilde{H}_1 = \frac{1}{2N}(p_x^2 + p_y^2) + \frac{N}{2}[U(x-y) + U(x+y)] + \frac{N}{4}[V(2(x+y)) + V(2(y-x)) + 2V(-2y)], \quad (44)$$

where $(x, y, p_x, p_y) = (Q_{N/4}, Q_{N/2}, P_{N/4}, P_{N/2})$.

Proof: From Eqs. (41) and (42), any point in $\mathcal{I}_1$ is expressed in the original $(\mathbf{q}, \mathbf{p})$ coordinates as follows:

$$\begin{aligned} q_{4k+1} &= -q_{4k+2} = Q_{N/4} - Q_{N/2}, \quad p_{4k+1} = -p_{4k+2} = \frac{1}{N}(P_{N/4} - P_{N/2}), \\ -q_{4k+3} &= q_{4k+4} = Q_{N/4} + Q_{N/2}, \quad -p_{4k+3} = p_{4k+4} = \frac{1}{N}(P_{N/4} + P_{N/2}), \end{aligned} \quad (45)$$

where $k = 0, 1, \ldots, N/4 - 1$. Let $\mathcal{I}_1'$ be the submanifold of $\mathcal{M}$ defined by

$$\begin{aligned} \mathcal{I}_1' = \{(q_1, \ldots, q_N, p_1, \ldots, p_N) \in \mathbf{C}^{2N} | & q_{4k+1} = -q_{4k+2} = q_1, \quad q_{4k+3} = -q_{4k+4} = q_3, \\ & p_{4k+1} = -p_{4k+2} = p_1, \quad p_{4k+3} = -p_{4k+4} = p_3, \quad k = 0, 1, \ldots, N/4 - 1\}. \end{aligned} \quad (46)$$

The submanifold $\mathcal{I}_1'$ is identical with $\mathcal{I}_1$. Then, in order to show that $\mathcal{I}_1$ is an invariant manifold, it is enough to show that $\mathcal{I}_1'$ is invariant under the flow associated with Hamiltonian (1). Since $U(X) = U(-X)$, it can be easily checked that for any initial point on $\mathcal{I}_1'$ the solution to Eqs. (40) with the periodic boundary condition is of the form

$$q_{4k+1}(t) = -q_{4k+2}(t) = \psi_1(t), \quad q_{4k+3}(t) = -q_{4k+4}(t) = \psi_2(t), \quad k = 0, 1, \ldots, N/4 - 1, \quad (47)$$

where ψ_1 and ψ_2 are the solutions of the set of differential equations

$$\frac{\mathrm{d}^2\psi_1}{\mathrm{d}t^2} + U'(\psi_1) - V'(-2\psi_1) + V'(\psi_1 + \psi_2) = 0, \quad (48)$$

$$\frac{\mathrm{d}^2\psi_2}{\mathrm{d}t^2} + U'(\psi_2) - V'(-2\psi_2) + V'(\psi_1 + \psi_2) = 0. \quad (49)$$

Since the solution (47) is contained in $\mathcal{I}_1'$ for any t, $\mathcal{I}_1'$, or $\mathcal{I}_1$ is an invariant manifold. The reduced Hamiltonian (44) is obtained by substituting Eq. (45) into the original Hamiltonian (1) and rewriting $(Q_{N/4}, Q_{N/2}, P_{N/4}, P_{N/2})$ by (x, y, p_x, p_y). ■

Remark: It is not assumed that the potential functions $U(X)$ and $V(X)$ are polynomials in the proof of Proposition 1.

The reduced Hamiltonian system (44) with the potentials (2) and (3) has a straight line solution of the form $x(t) = 0$, $y(t) = \varphi(t)$. The solution φ satisfies the differential equation

$$\frac{\mathrm{d}^2\varphi}{\mathrm{d}t^2} + \sum_{r=1}^{m} (\mu_{2r} + 2^{2r}\kappa_{2r})\varphi^{2r-1} = 0, \quad (50)$$

with the integral

$$\frac{1}{2}\left(\frac{\mathrm{d}\varphi}{\mathrm{d}t}\right)^2 + W_1(\varphi) = h, \quad (51)$$

where the effective potential function $W_1(X)$ is defined by

$$W_1(X) = \sum_{r=1}^{m} \frac{1}{2r}(\mu_{2r} + 2^{2r}\kappa_{2r})X^{2r}. \tag{52}$$

In Eq. (51), h can be regarded as the single particle energy and is related to the energy H of the whole system (1) as $h=H/N$. As for the NVE, we have

$$\frac{\mathrm{d}^2\xi}{\mathrm{d}t^2} + \left[\sum_{k=2}^{2m}(k-1)(\mu_k + 2^{k-1}\kappa_k)\varphi(t)^{k-2}\right]\xi = 0. \tag{53}$$

From Eqs. (50) and (53), parameters λ_2 and λ_{2m} are determined as

$$\lambda_2 = \frac{\mu_2 + 2\kappa_2}{\mu_2 + 4\kappa_2}, \quad \lambda_{2m} = (2m-1)\frac{\mu_{2m} + 2^{2m-1}\kappa_{2m}}{\mu_{2m} + 2^{2m}\kappa_{2m}}. \tag{54}$$

B. Main theorem

The straight line solution φ defines a point set $\Gamma_{1,h}=\{(q_1,\ldots,q_N,p_1,\ldots,p_N)\in H^{-1}(Nh)\,|\,q_i=(-1)^i\varphi(t),\ p_i=(-1)^i\dot{\varphi}(t),\ t\in\mathbf{C},\ i=1,2,\ldots,N\}\subseteq\mathcal{M}=\mathbf{C}^{2N}$. In addition, we define a family of $\Gamma_{1,h}$ by $\{\Gamma_{1,h}\}_{h_0,\varepsilon}=\{\Gamma_{1,h}\in\mathcal{M}\,|\,h\in(h_0-\varepsilon,h_0+\varepsilon)\}$, where $h_0\in(0,\infty)$ and ε is a small positive real number. Then, our theorem is stated as follows.

Theorem 3: *Suppose that $m\geqslant 2$ and $N=4n$ ($n\in\mathbf{N}$). Further, suppose that parameters in the potentials μ_k, κ_k, $k=2,3,\ldots,2m$ have values such that (i) $\mu_k=0$ for odd k, (ii) the inequalities $\min\{\mu_2+2\kappa_2,\mu_2+4\kappa_2\}>0$, $\mu_{2m}\geqslant 0$, and $\kappa_{2m}>0$ hold, and (iii) the algebraic equation $W_1(X)-h=0$ has $2m$ distinct roots for any $h>0$. Then, for any $h_0>0$ and any $\varepsilon>0$, reduced system (44) cannot have an additional integral, which is analytic and functionally independent of $\tilde{H}_1$, in a connected neighborhood of $\{\Gamma_{1,h}\}_{h_0,\varepsilon}$ in $\mathcal{I}_1$. Moreover, periodic nonlinear lattice (1) with potential functions (2) and (3) is nonintegrable in the following sense: for any $h_0>0$ and any $\varepsilon>0$, in a connected neighborhood $U_{\mathcal{M}}$ of $\{\Gamma_{1,h}\}_{h_0,\varepsilon}$ in $\mathcal{M}$, there does not exist an involutive set of N analytic integrals $f_1=H,f_2,\ldots,f_N$ such that there is a point in $U_{\mathcal{M}}\cap\mathcal{I}_1$ at which $\mathrm{d}f_i$, $i=1,\ldots,N$ are linearly independent.*

Proof: Consider the invariant manifold $\mathcal{I}_1$ and the reduced Hamiltonian system $\tilde{H}_1$. Equation (50) shows that $\alpha_2=\mu_2+4\kappa_2$ and $\alpha_{2m}=\mu_{2m}+2^{2m}\kappa_{2m}$. It follows from the assumptions in (ii) that $\alpha_2>0$ and $\alpha_{2m}>0$. From Eq. (54), the parameter λ_{2m} is rewritten as

$$\lambda_{2m} = (2m-1)\left[1 - \frac{2^{2m-1}}{(\mu_{2m}/\kappa_{2m}) + 2^{2m}}\right]. \tag{55}$$

Since $m\geqslant 2$ and $\mu_{2m}/\kappa_{2m}\geqslant 0$, we see that $1<(2m-1)/2\leqslant\lambda_{2m}<2m-1$ and thus λ_{2m} is in the region S_{2m} defined by Eq. (24). This implies $F_{2m}(\lambda_{2m})>2$. It follows from the assumption $\min\{\mu_2+2\kappa_2,\mu_2+4\kappa_2\}>0$ that $\lambda_2>0$ and $2\cos[2\pi\sqrt{\lambda_2}]\leqslant 2$. Therefore, $F_{2m}(\lambda_{2m})\notin\{0,\pm 2,2\cos[2\pi\sqrt{\lambda_2}]\}$. From Theorem 2, the reduced Hamiltonian system (44) cannot have an additional integral, which is analytic and functionally independent of $\tilde{H}_1$ in a connected neighborhood of $\{\Gamma_{1,h}\}_{h_0,\varepsilon}$ in $\mathcal{I}_1$. Then, the hypotheses of Lemma 1 are satisfied and hence Theorem 3 has been proven. ■

C. Application to small *m* cases

We apply Theorem 3 to some cases of small m. For these cases, we can give explicit conditions on the parameters μ_k and κ_k such that $W_1(X)-h=0$ has $2m$ distinct roots for any $h>0$. If we introduce a new variable $Y=X^2$, we have the algebraic equation

$$\mathcal{F}_m(Y) = \sum_{r=1}^{m} A_r Y^r - h = 0, \tag{56}$$

instead of the equation $W_1(X)-h=0$, where A_r is defined by

$$A_r = \frac{1}{2r}(\mu_{2r} + 2^{2r}\kappa_{2r}). \tag{57}$$

The equation $W_1(X)-h=0$ has $2m$ distinct roots for any $h>0$ if and only if $\mathcal{F}_m(Y)=0$ has m distinct roots for any $h>0$. In what follows, we consider the cases of $m=2$, 3, and 4.

Corollary 1: Suppose that $m=2$ and $N=4n$ $(n \in \mathbf{N})$. If parameters μ_k, κ_k, $k=2,3,4$ satisfy that $\min\{\mu_2+2\kappa_2, \mu_2+4\kappa_2\}>0$, $\mu_4 \geqslant 0$, $\kappa_4>0$, and $\mu_3=0$, then periodic nonlinear lattice (1) with potential functions (2) and (3) is nonintegrable in the sense of Theorem 3.

Proof: The discriminant $D(\mathcal{F}_2)$ of the polynomial $\mathcal{F}_2$ is calculated as

$$D(\mathcal{F}_2) = A_1^{\,2} + 4A_2 h. \tag{58}$$

Since $A_1>0$ and $A_2>0$, $D(\mathcal{F}_2)>0$ holds for any $h>0$. This implies that $\mathcal{F}_2(Y)=0$ has two distinct roots for any $h>0$. Therefore, the hypotheses of Theorem 3 are satisfied and the corollary has been proven. ■

The FPU lattice corresponds to the case of $\mu_2=\mu_3=\mu_4=0$. Corollary 1 shows that if $\kappa_2, \kappa_4>0$ then the FPU lattice is nonintegrable.

Corollary 2: Suppose that $m=3$ and $N=4n$ $(n \in \mathbf{N})$. If parameters μ_k, κ_k, $k=2,3,\ldots,6$ satisfy that $\min\{\mu_2+2\kappa_2, \mu_2+4\kappa_2\}>0$, $\mu_6 \geqslant 0$, $\kappa_6>0$, $\mu_3=\mu_5=0$, and $-\sqrt{3A_1A_3}<A_2\leqslant 2\sqrt{A_1A_3}$, then periodic nonlinear lattice (1) with potential functions (2) and (3) is nonintegrable in the sense of Theorem 3.

Proof: The discriminant $D(\mathcal{F}_3)$ is calculated as

$$D(\mathcal{F}_3) = -27A_3^{\,2}h^2 + 2A_2(2A_2^{\,2} - 9A_1A_3)h + A_1^{\,2}(A_2^{\,2} - 4A_1A_3). \tag{59}$$

If $D(\mathcal{F}_3)\neq 0$ holds for any $h>0$, then $\mathcal{F}_3(Y)=0$ has three distinct roots for any $h>0$. The discriminant $D(\mathcal{F}_3)$ is simply a quadratic function of h. In Eq. (59), $A_1>0$ and $A_3>0$ because of the assumptions $\mu_2+4\kappa_2>0$, $\mu_6\geqslant 0$, and $\kappa_6>0$. It is easily confirmed that $D(\mathcal{F}_3)<0$ holds for any $h>0$ if $A_1, A_3>0$ and $-\sqrt{3A_1A_3}<A_2\leqslant 2\sqrt{A_1A_3}$. Then, the hypotheses of Theorem 3 are satisfied and the Corollary has been proven. ■

Corollary 3: Suppose that $m=4$ and $N=4n$ $(n \in \mathbf{N})$. If parameters μ_k, κ_k, $k=2,3,\ldots,8$ satisfy that $\min\{\mu_2+2\kappa_2, \mu_2+4\kappa_2\}>0$, $\mu_8\geqslant 0$, $\kappa_8>0$, $\mu_3=\mu_5=\mu_7=0$, and $108A_1^{\,2}A_4^{\,2}+27(A_3^{\,2} - 4A_2A_4)A_1A_3+(32A_2A_4-9A_3^{\,2})A_2^{\,2}>0$, then periodic nonlinear lattice (1) with potential functions (2) and (3) is nonintegrable in the sense of Theorem 3.

Proof: Since $\mathcal{F}_4(Y)$ is a quartic function with $A_1, A_4>0$, it has two distinct real roots and a pair of two complex conjugate roots for $h>0$ if $\mathcal{F}_4(Y)$ is a unimodal function on the real Y axis for $h=0$, i.e., if $\mathrm{d}\mathcal{F}_4(Y)/\mathrm{d}Y=0$ has only one real root. The derivative $\mathrm{d}\mathcal{F}_4(Y)/\mathrm{d}Y$ is a cubic function and the discriminant of $\mathrm{d}\mathcal{F}_4(Y)/\mathrm{d}Y$ is given by

$$D(\mathrm{d}\mathcal{F}_4/\mathrm{d}Y) = -4[108A_1^{\,2}A_4^{\,2} + 27(A_3^{\,2} - 4A_2A_4)A_1A_3 + (32A_2A_4 - 9A_3^{\,2})A_2^{\,2}]. \tag{60}$$

The equation $\mathrm{d}\mathcal{F}_4(Y)/\mathrm{d}Y=0$ has only one real root when $D(\mathrm{d}\mathcal{F}_4/\mathrm{d}Y)<0$. Since $D(\mathrm{d}\mathcal{F}_4/\mathrm{d}Y)<0$ holds from the assumption, it follows that $\mathcal{F}_4(Y)=0$ has four distinct roots for any $h>0$. Then, the hypotheses of Theorem 3 are satisfied and the corollary has been proven. ■

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The invariant charges of the Nambu–Goto string and canonical quantization

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It is shown that the algebra of diffeomorphism-invariant charges of the Nambu–Goto string cannot be quantized in the framework of canonical quantization. The argument is shown to be independent of the dimension of the underlying Minkowski space. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The action of the Nambu–Goto string is a generalization of the reparametrization-invariant action of the relativistic particle in d-dimensional Minkowski space, where instead of a point-particle, a one-dimensional extended object (a string) is considered. Correspondingly, the solutions of the equations of motion are surfaces swept out by the string in space–time (called world-sheets) which are extremal with respect to the Minkowski metric. The parametrization of these surfaces is not fixed by the equations of motion, and, hence, a change of the parametrization corresponds to a symmetry transformation which does not change the physical state of the system. Therefore, the Nambu–Goto string is a system with gauge group given by the diffeomorphisms of a surface. As such, it provides an interesting model to study the fundamental problem of quantizing a system with gauge freedom given by the diffeomorphism group.

For closed strings, the world-sheet is tube-shaped. It was shown especially in this case that the Nambu–Goto string can be treated as an integrable system and that its integrals of motion can be constructed from a suitably defined monodromy.[1] These integrals of motion are functionals on the world-sheet which are invariant under arbitrary reparametrizations (gauge transformations) and as such are observable quantities. They form a graded Poisson algebra,[2,3] the Poisson algebra of invariant charges, and were shown to be complete in the sense that, up to translations in the direction of its total energy-momentum vector, the string can be reconstructed from the knowledge of the invariant charges and the infinitesimal generators of boosts.[4] In this scheme, the constraints which are present in the system enter as a condition on the representation of the algebra, and—along with conditions regarding Hermiticity and positivity of the energy—distinguish its physically meaningful representations.

The algebra of invariant charges provides the starting point of the algebraic quantization of the Nambu–Goto string.[1] This scheme is based on the idea that the correspondence principle should be applied to physically meaningful quantities only, which in a theory with gauge freedom means that it is applicable only to gauge-invariant observables. In this spirit, the graded Poisson algebra of invariant charges of the Nambu–Goto string is quantized by application of the correspondence principle, replacing the Poisson brackets by commutators and allowing for particular (observable) quantum corrections which are restricted by demanding structural similarity of the classical and the quantum algebra. So far, it does not seem at all likely that in this scheme an obstruction regarding the dimension d of the underlying Minkowski space should appear (other than $d>2$). In contrast to this, the canonical quantization of the Nambu–Goto string is consistent only in certain critical dimensions. Here, the correspondence principle is assumed to hold for the Fourier modes

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of some particular parametrization, i.e., for quantities which are not observable. It leads to the well-known construction of Fock space which contains the physically relevant states as a subspace.

In this paper, which is an exposition of results gained some years ago,[5] it is shown that canonical quantization does not yield a representation of the algebra of invariant charges. After a short exposition of known results regarding the algebraic approach to the quantization of the Nambu–Goto string[2,3,6] in the following two sections, the fourth section contains an investigation of the canonical quantization and its application to the algebra of invariant charges. It is shown that unobservable anomalies arise in the defining relations of the algebra in $3+1$ dimensions. In Sec. V it is then shown that the problem cannot be cured by adjusting the dimension of the underlying Minkowski space.

II. THE POISSON ALGEBRA OF INVARIANTS

In the Hamiltonian formalism, the fact that the world-sheet is independent of the particular parametrization chosen to describe it becomes manifest in the appearance of two primary constraints which are the infinitesimal generators of gauge transformations (reparametrizations). The canonical momenta p_μ and positions x_μ, $\mu=0,\ldots,d-1$ are not independent of each other, and the canonical Hamilton function vanishes. Following Dirac's treatment of systems with constraints, a total Hamiltonian H_T is introduced which is a linear combination of the two primary constraints with two Lagrangian multipliers α and β. Here, we specialize to the case where α and β do not depend on the original degrees of freedom x_μ and p_μ. The dynamics of the string is thus governed by the gauge freedom only, and fixing the two Lagrangian multipliers corresponds to fixing a gauge. It follows that integrals of motion of H_T are gauge-invariant quantities, i.e., invariant charges which do not depend on the parametrization. In Ref. 1 it was shown that by treating the string as an integrable system, such invariant charges arise as (symmetric polynomials of) the eigenvalues of a monodromy matrix of a system of linear differential equations whose compatibility condition (a "zero curvature condition") is equivalent to the equations of motion of the string.

It is convenient to express the equations of motion as well as the constraints in terms of left and right movers $u^\pm_\mu(\tau,\sigma)=p_\mu(\tau,\sigma)\pm(1/2\pi\alpha')\partial_\sigma x_\mu(\tau,\sigma)$, $\mu=0,\ldots,d-1$, where $1/2\pi\alpha'$ is the string tension. Here, a foliation is chosen such that $\partial_\tau x_\mu(\tau,\sigma)$ is a timelike vector and $\partial_\sigma x_\mu(\tau,\sigma)$ is spacelike, $\sigma\in[0,\omega(\tau))$, where $\omega(\tau)$ is the period of the string's parametrization (as a function of σ at fixed τ). The constraints are then equivalent to demanding that $u^\pm$ be lightlike. With left and right movers, an invariant charge is given by the following explicit expression,

$$\begin{aligned}\mathcal{Z}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma) &\overset{\text{def}}{=} \mathcal{R}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma)+\mathcal{R}^\pm_{\mu_2\cdots\mu_N\mu_1}(\tau,\sigma)+\cdots+\mathcal{R}^\pm_{\mu_N\mu_1\cdots\mu_{N-1}}(\tau,\sigma)\\ &=\int_\sigma^{\sigma+\omega(\tau)} d\sigma' u^\pm_{\mu_1}(\tau,\sigma')\mathcal{R}^\pm_{\mu_2\cdots\mu_N}(\tau,\sigma'),\end{aligned}\tag{1}$$

where

$$\mathcal{R}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma)=\int_\sigma^{\sigma+\omega(\tau)} d\sigma_1\mu^\pm_{\mu_1}(\tau,\sigma_1)\int_\sigma^{\sigma_1} d\sigma_2 u^\pm_{\mu_2}(\tau,\sigma_2)\cdots\int_\sigma^{\sigma_{N-1}} d\sigma_N u^\pm_{\mu_N}(\tau,\sigma_N).\tag{2}$$

From the equations of motion of the monodromy matrices (see Ref. 3), one finds

$$\partial_\sigma\mathcal{R}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma)=u^\pm_{\mu_1}(\tau,\sigma)\mathcal{R}^\pm_{\mu_2\cdots\mu_N}(\tau,\sigma)-\mathcal{R}^\pm_{\mu_1\cdots\mu_{N-1}}(\tau,\sigma)u^\pm_{\mu_N}(\tau,\sigma),$$

$$\partial_\tau\mathcal{R}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma)=(\alpha\pm\beta)(\tau,\sigma)\partial_\sigma\mathcal{R}^\pm_{\mu_1\cdots\mu_N}(\tau,\sigma),\tag{3}$$

such that, indeed,

$$\partial_\sigma \mathcal{Z}^{\pm}_{\mu_1\cdots\mu_N}(\tau,\sigma) = \partial_\tau \mathcal{Z}^{\pm}_{\mu_1\cdots\mu_N}(\tau,\sigma) = 0. \tag{4}$$

Another way to express the fact that the functionals $\mathcal{Z}$ are gauge invariant is that they Poisson-commute with the total Hamiltonian, $\{\mathcal{Z}^{\pm}_{\mu_1\cdots\mu_N}, H_T\}_0 = 0$. Here, the Poisson bracket is derived from the canonical Poisson bracket $\{x_\mu, p_\nu\}_0$, such that (for fixed τ, where w.l.o.g. $\omega(\tau) = 2\pi$ and with the periodic δ-distribution $\delta_{2\pi}$),

$$\{u^{\pm}_\mu(\tau,\sigma), u^{\pm}_\nu(\tau,\sigma')\}_0 = \pm\frac{1}{2\pi\alpha'} 2\eta_{\mu\nu}\partial_\sigma\delta_{2\pi}(\sigma-\sigma'), \quad \text{all others } 0. \tag{5}$$

The invariant charges form a Poisson algebra with respect to this bracket.[2,3] From the knowledge of the invariants, together with the generators of boosts, the string can be reconstructed up to translations in the direction of its total energy-momentum vector and, in this sense, the invariant charges are complete.[4] (The ambiguity is due to the fact that the construction of the $\mathcal{Z}$ relies only on $\partial_\sigma x$, not on x itself. If the string splits into different parts or if two strings collide,[7] an absolute position, the splitting or meeting point, enters.)

Let us now turn to an exposition of the structure of the Poisson algebra of invariant charges.[6] An invariant charge $\mathcal{Z}_{\mu_1\cdots\mu_N}$ can be split into a sum of so-called homogeneous invariants $\mathcal{Z}^{(K)}_{\mu_1\cdots\mu_N}$ of order $K=1,\ldots,N$, which arise from powers of the logarithm of the monodromy matrices[2,3] and are themselves invariant under arbitrary reparametrizations,

$$\mathcal{Z}^{\pm}_{\mu_1\cdots\mu_N} = \sum_{K=1}^{N} \mathcal{Z}^{\pm(K)}_{\mu_1\cdots\mu_N}.$$

The only invariant charge of order $K=1$ is the total momentum, $\mathcal{Z}^{-(1)}_\mu = \mathcal{Z}^{+(1)}_\mu = \oint d\sigma_1 u^{\pm}_\mu(\tau,\sigma_1) = \mathcal{P}_\mu$. It is the only invariant charge which is an element of both the algebra built from left movers and the one built from right movers, and it Poisson-commutes with all (homogeneous) invariant charges. In what follows, only massive strings will be considered, where $\mathcal{P}^2 = \mathfrak{m}^2$, and we pass to the rest frame of the string where $\mathcal{P}_\mu = (\mathfrak{m},0,\ldots,0)$, $\mathfrak{m}>0$. By (5), the algebra built from left movers and the one built from right movers Poisson-commute with one another, and their structure constants differ only by signs. It is therefore sufficient to analyze the right mover part (referred to as $\mathfrak{h}$) only. Analogous results then hold also for the left mover part. The algebra $\mathfrak{h}$ is graded under the action of the Poisson bracket $\{\cdot,\cdot\}$ which, compared to the canonical one, is rescaled by a factor $2\pi\alpha'$,

$$\mathfrak{h} = \bigoplus_{\ell=0}^{\infty} \mathfrak{V}^\ell(\mathfrak{h}), \quad \{\mathfrak{V}^{\ell_1},\mathfrak{V}^{\ell_2}\} \subset \mathfrak{V}^{\ell_1+\ell_2}, \quad \mathfrak{V}^{\ell_1}\cdot\mathfrak{V}^{\ell_2} \subset \mathfrak{V}^{\ell_1+\ell_2+1}, \quad \ell = N-K-1, \tag{6}$$

where each $\mathfrak{V}^\ell$ is finite dimensional as a vector space. A parity operator is defined on $\mathfrak{h}$ which assigns positive (negative) parity to an invariant which contains an even (odd) number of spacelike indices. Each $\mathfrak{V}^\ell$ splits up into a direct sum of a space with even ($\mathfrak{V}^\ell_+$) or odd ($\mathfrak{V}^\ell_-$) parity (one of which may be trivial). The vector space $\mathfrak{V}^0$ is $(d-1)$-dimensional and forms a subalgebra isomorphic to the Lie algebra $\mathrm{so}(d-1)$, the Lie algebra of the stabilizer group of $\mathcal{P}_\mu$. All vector spaces $\mathfrak{V}^\ell_\pm$ are invariant under the Poisson action of $\mathfrak{V}^0$, and, therefore, each of them carries a linear representation of $\mathrm{so}(d-1)$ and can be decomposed into a direct sum of isotypical components (corresponding to different spins and parities).

By a well-scrutinized conjecture, which has been proved for $d=3$ up to degree $\ell=7$, any invariant charge can be expressed as a polynomial in certain standard invariants, and the number of standard invariants in each level $\mathfrak{V}^\ell$ is known. It was shown, however, in Refs. 2 and 3 that some invariant charges, the so-called exceptional elements, cannot be expressed in terms of *Poisson brackets* of standard invariants of lower degrees. Moreover, a major complication in the investigation of $\mathfrak{h}$ is that taking a Poisson bracket of two standard invariants, one in general obtains not only a standard invariant, but, additionally, a linear combination of *products* of other standard invariants, whence the standard invariants do not form a Lie algebra. In fact, it was

shown that there is no algebraic basis which would render $\mathfrak{h}$ as the enveloping algebra of a *Lie* algebra.[2,3] Instead, it is necessary to generate $\mathfrak{h}$ by (multiple) Poisson brackets *as well as* by products of a set of generating invariant charges. The generating invariant charges do not freely generate $\mathfrak{h}$, and relations (other than those given by antisymmetry and the Jacobi identity) between (multiple) Poisson brackets and products persist. Their number at given degree ℓ is equal to $m_\ell - n_\ell$, where n_ℓ is the number of standard invariants in $\mathfrak{V}^\ell$ and m_ℓ is the number of Hall-basis elements in $\mathfrak{V}^\ell$ which can be built from standard invariants of lower degree than ℓ, see Ref. 6. (A Hall-basis contains only such Poisson brackets as cannot be transformed into each other by antisymmetry or by the Jacobi identity.)

In what follows, $d=4$ spacetime dimensions are considered and some of the structural insight gained in Ref. 6 is reproduced. The set of generating invariants in $d=4$ is given by $3+14$ invariants from $\mathfrak{V}^0$ and $\mathfrak{V}^1$, respectively, which generate a subalgebra $\mathfrak{U}$ of $\mathfrak{h}$, together with the (modified) exceptional elements $B_0^{(\ell)}$, $\ell=1,3,5,\ldots$, which form an Abelian subalgebra of $\mathfrak{h}$, and act semidirectly on $\mathfrak{U}$. In the present investigation only $\ell\leqslant 2$ will be considered, where these claims were proved rigorously. Employing an angular momentum (or rather a spin) basis $\{e_0, e_\pm=(1/\sqrt{2})(e_1\pm ie_2), e_3\}$ in $\mathbb{R}^4$, we obtain the following generating invariants for the vector space basis of $\mathfrak{V}^0$:

$$J_{1,1}=\frac{-1}{4\mathfrak{m}}(i\mathcal{Z}^{(2)}_{0+3}-i\mathcal{Z}^{(2)}_{03+}),\quad J_{1,0}=\frac{-1}{4\mathfrak{m}}(i\mathcal{Z}^{(2)}_{0+-}-i\mathcal{Z}^{(2)}_{0-+}),\quad J_{1,-1}=\frac{-1}{4\mathfrak{m}}(i\mathcal{Z}^{(2)}_{0-3}-i\mathcal{Z}^{(2)}_{03-}).$$

As a vector space, $\mathfrak{V}^1$ is spanned by

$$(J_1^2)_0,\ B_0^{(1)},\ S_1 \text{ and } (J_1^2)_2,\ T_2,\ S_2,$$

which are multiplets of so(3) with spin $J=0$, 1, and 2, respectively, with the 14 generating invariants given by

$$B_0^{(1)}=\mathcal{Z}^{(2)}_{0-0+}+\frac{1}{2}\mathcal{Z}^{(2)}_{0303},$$

$$T_2=\{T_{2,m}|m=-2,\ldots,2\} \text{ with } T_{2,-2}=\frac{1}{2}\mathcal{Z}^{(2)}_{00--},$$

$$S_2=\{S_{2,m}|m=-2,\ldots,2\} \text{ with } S_{2,-2}=i\mathcal{Z}^{(2)}_{03--}, \tag{7}$$

$$S_1=\{S_{1,m}|m=-1,\ldots,1\} \text{ with } S_{1,-1}=\mathcal{Z}^{(2)}_{0+--}-\mathcal{Z}^{(2)}_{0-33},$$

$$\text{with } i\{J_{1,\pm1},X_{j,m}\}=\pm\frac{1}{\sqrt{2}}\sqrt{(j\pm m+1)(j\mp m)}X_{j,m\pm1},$$

and where

$$(X_{j_1}\cdot Y_{j_2})_{j,m}=\underbrace{\sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2}}_{m_1+m_2=m}\langle j,m|j_1,m_1;j_2,m_2\rangle X_{j_1,m_1}\cdot Y_{j_2,m_2}.$$

Here, the Clebsch–Gordan coefficients $\langle j,m|j_1,m_1;j_2,m_2\rangle$ are defined with conventions of Condon and Shortley. The action of $J_{1,1}$ respects the parity, the tensor rank N, as well as the order K, and, hence, the basis elements with higher magnetic numbers than $m=-J$ are indeed again invariants of the same parity, tensor rank $N=4$ and order $K=2$, whose explicit form can be calculated

using (5) (or the closed formulas for Poisson brackets of invariant charges given in Refs. 2 and 3). Complex conjugation yields an involution on the algebra, and the phases of the generating invariants are chosen such that for $m=0$ they are real, $X^*_{j,m}=(-1)^m X_{j,-m}$.

The vector space basis of $\mathfrak{V}^2$ is again given by products and Poisson brackets of the above generating invariant charges. By (6), such Poisson brackets can only be single brackets built from elements of $\mathfrak{V}^1$. The number of standard invariants in $\mathfrak{V}^1$ being 14, $\frac{1}{2}\cdot 14\cdot 13=91$ such brackets can be formed, if the antisymmetry of the bracket is taken into account (no dependences from the Jacobi identity arise, since no multiple brackets appear). The number of standard invariants in $\mathfrak{V}^2$ being 40, 51 algebraic relations between these brackets persist, which by the above remarks will also involve products of generators. They were given in Ref. 6 and are reproduced in Appendix A. The relations, which are real, are organized in nine multiplets, and it follows that only nine relations are truly independent, while the others can be produced by the action of $\mathfrak{V}^0$.

III. ALGEBRAIC QUANTIZATION BY CORRESPONDENCE

The basic idea of the algebraic approach is that the correspondence principle is physically meaningful only for *observable* (i.e., gauge-invariant) quantities. Since it provides an alternative to the canonical quantization scheme of the Nambu–Goto string, the general idea is reproduced here, cf. Ref. 6. The classical Poisson algebra with commutative multiplication is to be deformed into an associative algebra, where Poisson brackets are replaced by commutators and certain quantum corrections are admitted, which are restricted by demanding structural similarity of the classical and the quantum algebra (see below). In particular, it is required that the number of independent relations should not be changed. In principle, this quantization scheme is applicable in arbitrary dimensions, but the calculations used in this paper have been performed in $1+3$ dimensions. In a first step, it is assumed that (dimensionless) quantum generators $\hat{\mathfrak{Y}}_1$, $\hat{\mathfrak{T}}_2$, $\hat{\mathfrak{S}}_2$, $\hat{\mathfrak{S}}_1$, $\hat{\mathfrak{B}}_0{}^{(\ell)}$, $\ell=1,3,\ldots$, exist which correspond to the classical ones (when scaled by factors $(\hbar/2\pi\alpha')^{\ell+1}$). The quantum version of a classical relation at order ℓ is then obtained as follows:

(i) Replace each rescaled Poisson bracket by a commutator $[\cdot,\cdot]$ (multiplied with a factor $2\pi\alpha'/i\hbar$) without changing the order of the bracket's entries. The action of $\mathfrak{V}^0$ on higher levels $\mathfrak{V}^\ell$ remaining the same, this replacement can be done for the full multiplet. Replace the multiplication by anticommutators $\{\cdot,\cdot\}$ (multiplied with a factor $\frac{1}{2}$).

(ii) By construction, the resulting relation consists of (anti-)commutators of the dimensionless generators, multiplied by a global factor $(\hbar/2\pi\alpha')^{(\ell+1)}$. Now quantum corrections are admitted which have the same spin and parity as the relation under consideration but are of lower degree. They enter the relation multiplied by an appropriate positive power of $\hbar$ as well as with parameters which respect the reality property of the relation and are restricted by the structural similarity conditions (see below).

As an example, we consider the classical relation with $J^P=1^-$ involving $B_0^{(1)}$,

$$\{B_0^{(1)},S_1\}_1=-i6\sqrt{\frac{2}{5}}\{T_2,S_2\}_1+2\sqrt{\frac{3}{5}}\{T_2,S_1\}_1-24\sqrt{\frac{3}{5}}(J_1\cdot S_2)_1+i12\sqrt{2}(J_1\cdot S_1)_1,$$

where Poisson brackets and products are multiplets of spin $J=1$ as given in formulas (A1) and (A2) in Appendix A. This relation is replaced by

$$[\hat{\mathfrak{B}}_0^{(1)},\hat{\mathfrak{S}}_1]_1=-i6\sqrt{\frac{2}{5}}[\hat{\mathfrak{T}}_2,\hat{\mathfrak{S}}_2]_1+2\sqrt{\frac{3}{5}}[\hat{\mathfrak{T}}_2,\hat{\mathfrak{S}}_1]_1-i12\sqrt{\frac{3}{5}}\{\hat{\mathfrak{Y}}_1,\hat{\mathfrak{S}}_2\}_1-6\sqrt{2}\{\hat{\mathfrak{Y}}_1,\hat{\mathfrak{S}}_1\}_1+id\hat{\mathfrak{S}}_1$$

with a real (in fact, rational) parameter d and multiplets of (anti-)commutators with spin $J=1$. Note that in quantum relations, $\{\cdot,\cdot\}$ denotes the anticommutator, not the Poisson bracket. Let us now consider the requirement of structural similarity of the classical and the quantized algebra which puts restrictions on these parameters. In order to compare two relations, they have to be brought into some standard form, and the multiplication now being noncommutative, it is clear

that in doing so, one may pick up correction terms of lower order, for instance (see Ref. 6),

$$\{\{A_{j_1},B_{j_2}\}_j,C_{j_3}\}_J=\sum_k(-)^{k+j_2+j_3}\sqrt{(2j+1)(2k+1)}\cdot\left((-)^{j+1}\begin{Bmatrix}j_2 & j_1 & j\\ j_3 & J & k\end{Bmatrix}[[\mathbf{A_{j_1}},\mathbf{C_{j_3}}]_\mathbf{k},\mathbf{B_{j_2}}]_\mathbf{J}\right.$$
$$\left.+\begin{Bmatrix}j_1 & j_2 & j\\ j_3 & J & k\end{Bmatrix}\{\{B_{j_2},C_{j_3}\}_k,A_{j_1}\}_J\right)$$

with $6j$-symbols $\{:::\}$ (the correction term is printed in boldface letters). By this mechanism, new dependences between these lower order correction terms may arise, which do not possess a classical analog. It has been shown explicitly up to the fifth degree[6,8] that these dependences can be trivially fulfilled or can be reduced to old dependences by fixing the parameters in the quantum relations in a suitable way. In $\ell=2$, all but one (which appears in the relation with $J^P=1^+$) have been shown to be trivial. The elements of the quantized algebra are again referred to as observables.

In Refs. 9 and 10 it was shown that a quantization which is consistent with the relations found so far is possible to all orders ℓ, provided that certain hypotheses concerning the classical algebra (as sketched in the preceding section) are true. There, an *a posteriori* approach was pursued, namely to use an explicit infinite dimensional embedding Lie algebra whose elements are not necessarily invariant under reparametrizations, but which is distinguished by the fact that, restricted to its reparametrization invariant elements, it provides a concrete realization of the quantum algebra of observables found in Ref. 6.

IV. CANONICAL QUANTIZATION

The canonical quantization of the Nambu–Goto string is by far more popular than the approach described above. Its virtue is that it is much simpler. On the other hand, it has some undesirable features, for instance, to name but two, the appearance of a critical dimension and the impossibility to fully implement the constraints. While the general theory of strings has by now evolved into an elaborate theory in its own right and has moved away from the original Nambu–Goto action, it is still worthwhile to consider the fundamental question whether, in the presence of the alternative approach of algebraic quantization, the canonical quantization scheme is apt to capture the reparametrization invariance of the Nambu–Goto string. It is the aim of the following sections to show that the Fourier modes of an arbitrary parametrization do not provide a suitable starting point for the quantization of the algebra of invariant charges.

A. Classical Fourier modes

In order to fix the notation, the well-known decomposition of left and right movers $u_\mu^\pm$, $\mu=0,\ldots,d-1$, into Fourier modes is reproduced here,

$$u_\mu^-(\tau,\sigma)=p_\mu(\tau,\sigma)-\frac{1}{2\pi\alpha'}\partial_\sigma x_\mu(\tau,\sigma)=\frac{\mathcal{P}_\mu}{2\pi}+\frac{\mathfrak{m}}{2\pi}\sum_{n>0}(\alpha_\mu^n(\tau)e^{in\sigma}+\alpha_\mu^{-n}(\tau)e^{-in\sigma})$$
$$u_\mu^+(\tau,\sigma)=p_\mu(\tau,\sigma)+\frac{1}{2\pi\alpha'}\partial_\sigma x_\mu(\tau,\sigma)=\frac{\mathcal{P}_\mu}{2\pi}+\frac{\mathfrak{m}}{2\pi}\sum_{n>0}(\beta_\mu^n(\tau)e^{-in\sigma}+\beta_\mu^{-n}(\tau)e^{in\sigma}), \tag{8}$$

with $(\alpha_\mu^{-n})^*=\alpha_\mu^n$ and $(\beta_\mu^{-n})^*=\beta_\mu^n$. The zero modes α_μ^0 and β_μ^0 are equal to $\mathcal{P}_\mu/\mathfrak{m}$, since the positions' zero mode is independent of σ and hence vanishes in $\partial_\sigma x$. Note that in the conformal gauge, where $2\pi\alpha' p(\tau,\sigma)=\partial_\tau x(\tau,\sigma)$, the components' dependence on τ is given as follows:

$$\alpha_\mu^{\pm n}(\tau)=\alpha_\mu^{\pm n}e^{\mp in\tau}\text{ and }\beta_\mu^{\pm n}(\tau)=\beta_\mu^{\pm n}e^{\mp in\tau}. \tag{9}$$

In what follows, the dependence on τ is suppressed, and we write $\alpha_\mu^{\pm n}$ for $\alpha_\mu^{\pm n}(\tau)$. With conventions as above, we find the following (un-rescaled) Poisson brackets,

$$\{\alpha_\mu^m, \alpha_\nu^{-n}\}_0 = -\frac{4\pi}{2\pi\alpha'\mathfrak{m}^2} in\,\eta_{\mu\nu}\delta_{m,n} \quad \text{and} \quad \{\beta_\mu^m, \beta_\nu^{-n}\}_0 = -\frac{4\pi}{2\pi\alpha'\mathfrak{m}^2} in\,\eta_{\mu\nu}\delta_{m,n}, \tag{10}$$

all others 0. It is important to bear in mind that, apart from the zero mode $\mathcal{P}_\mu/\mathfrak{m}$, the Fourier coefficients depend on the chosen parametrization. Nonetheless, it is of course possible that certain polynomials in the coefficients are independent of the parametrization. Prominent examples are the generators of the Poincaré group. Moreover, as was analyzed in Ref. 4 and further elaborated in Ref. 11, the *classical* invariant charges $\mathcal{Z}$ can be expressed as polynomials of Fourier modes: Inserting the decomposition (8) in (1), we find (for the left mover part of the algebra, and likewise for the right mover part)

$$\begin{aligned}\mathcal{Z}_{\mu_1\cdots\mu_N} &= \frac{\mathfrak{m}^N}{(2\pi)^N}\sum_{n_1=-\infty}^{\infty}\cdots\sum_{n_N=-\infty}^{\infty}\alpha_{\mu_1}^{n_1}\cdots\alpha_{\mu_N}^{n_N}\oint d\sigma_1 e^{in_1\sigma_1}\int_{\sigma_1}^{\sigma_1+2\pi} d\sigma_2 e^{in_2\sigma_2}\cdots\int_{\sigma_1}^{\sigma_{N-1}} d\sigma_N e^{in_N\sigma_N}\\ &= \frac{\mathfrak{m}^N}{(2\pi)^N}\sum_{n_1=-\infty}^{\infty}\cdots\sum_{n_N=-\infty}^{\infty}\alpha_{\mu_1}^{n_1}\cdots\alpha_{\mu_N}^{n_N}\sum_{K=1}^{N}\frac{(2\pi)^K}{(K-1)!}\left(\frac{1}{i}\right)^{N-K} C^{[K,N]}_{n_1\cdots n_N},\end{aligned}$$

where, by (4), the starting point of the last integration is irrelevant, and where, without loss of generality, $\omega(\tau)=2\pi$. Following Ref. 11, the iterated integrals are replaced by a sum over combinatorial factors $C^{[K,N]}_{n_1\cdots n_N}$ with the following properties:

(i) cyclic symmetry in $n_1,\ldots,n_N$

(ii) recursion relation:

$$C^{[K,N]}_{n_1\cdots n_N} = \frac{1}{n_N}\left(C^{[K,N-1]}_{n_1\cdots n_{N-2}n_{N-1}+n_N} - C^{[K,N-1]}_{n_1+n_N n_2\cdots n_{N-1}}\right) \text{ for } n_N\neq 0,$$

(iii)

$$C^{[N,N]}_{n_1\cdots n_N} = \delta_{n_1,0}\cdots\delta_{n_N,0} \text{ and } C^{[K,N]}_{0\cdots 0} = \delta_{K,N}.$$

Due to the recursion relation, the combinatorial coefficients are in general linear combinations of products of Kronecker symbols (with rational coefficients). It follows from the definitions that the Fourier decomposition of homogeneous invariants is given as follows,

$$\mathcal{Z}^{(K)}_{\mu_1\cdots\mu_N} = \frac{\mathfrak{m}^N}{(2\pi)^{N-K}}\frac{1}{(K-1)!}\left(\frac{1}{i}\right)^{N-K}\sum_{n_1=-\infty}^{\infty}\cdots\sum_{n_N=-\infty}^{\infty}\alpha_{\mu_1}^{n_1}\cdots\alpha_{\mu_N}^{n_N}C^{[K,N]}_{n_1\cdots n_N}. \tag{11}$$

It is important to note that the degree $\ell=N-K-1$ of the homogeneous invariant can be determined only by the inverse power of the factor 2π (minus 1), while its tensor rank N is encoded in the power of the mass $\mathfrak{m}$. The rest system is implemented by requesting that $\alpha_\mu^{n=0}=\delta_{\mu,0}$.

The reader is assumed to be familiar with the canonical approach and hence it is only mentioned that the decomposition of left and right movers into Fourier modes leads to the following decomposition of the constraints:

$$0\approx\pi\alpha'(u^-)^2 =: \sum_{n=-\infty}^{\infty}\overline{L^n}e^{in\sigma}, \quad 0\approx\pi\alpha'(u^+)^2 =: \sum_{n=-\infty}^{\infty}L^{-n}e^{in\sigma},$$

where L^n and $\overline{L^n}$ are generators of (two copies of) the Witt algebra.

B. Normal ordering of the invariant charges

In the canonical quantization procedure, the correspondence principle is applied to the (nonobservable) Fourier modes. They are replaced by operators on Fock space, with positive modes corresponding to annihilation operators, and negative modes corresponding to creation operators (such that in the conformal gauge, $e^{-in\tau}$, $n>0$, belongs to an annihilation operator). Zero modes correspond to multiples of the identity and normal ordering is used to define monomials of operators. The Poisson brackets (10) are replaced by commutators $(1/i\hbar)[\cdot,\cdot]$, such that

$$[\alpha_\mu^m,\alpha_\nu^{-n}]=\hbar\frac{4\pi}{2\pi\alpha'\mathfrak{m}^2}n\,\eta_{\mu\nu}\delta_{m,n}\quad\text{and}\quad[\beta_\mu^m,\beta_\nu^{-n}]=\hbar\frac{4\pi}{2\pi\alpha'\mathfrak{m}^2}n\,\eta_{\mu\nu}\delta_{m,n},\tag{12}$$

all others 0. The consequences of this quantization procedure for the Witt algebra are well known. It yields a *nontrivial* central extension of it, the so-called Virasoro algebra, and, due to the appearance of the central charge, it is not possible to define the physical subspace of the Fock space as the kernel of all generators $:L^n:$ and $:\overline{L^n}:$, but only of those with $n\geqslant -1$ (alternatively of those with $n\leqslant 1$). For later use, the explicit form of a generator with $n>0$ is reproduced here,

$$:\overline{L^n}:=\frac{\alpha'}{2}\mathfrak{m}\mathcal{P}\cdot\alpha^n+\frac{\alpha'}{4}\mathfrak{m}^2\sum_{m=1}^{n-1}\alpha^m\cdot\alpha^{n-m}+\frac{\alpha'}{2}\mathfrak{m}^2\sum_{m=1}^{\infty}\alpha^{-m}\cdot\alpha^{n+m},\tag{13}$$

the dot $\cdot$ denoting Lorentz products. Application of the canonical quantization procedure to a homogeneous invariant charge $\mathcal{Z}^{(K)}_{\mu_1\cdots\mu_N}$ as in (11) renders a normally ordered counterpart

$$:\mathcal{Z}^{(K)}_{\mu_1\cdots\mu_N}:=\frac{\mathfrak{m}^N}{(2\pi)^{N-K}}\frac{(-i)^{N-K}}{(K-1)!}\sum_{n_1=-\infty}^{\infty}\cdots\sum_{n_N=-\infty}^{\infty}:\alpha_{\mu_1}^{n_1}\cdots\alpha_{\mu_N}^{n_N}C^{[K,N]}_{n_1\cdots n_N}:.\tag{14}$$

The combinatorial factors are to be calculated in such a manner that after evaluation of the Kronecker symbols no indices with relative signs (for instance, n_1-n_2 with n_1, $n_2>0$) arise in order to simplify the distinction between positive, negative and zero modes, and lengthy calculations then yield homogeneous invariant charges expressed in terms of annihilation and creation operators (for those needed in what follows, see Appendix B).

In this section, the dimension of the underlying space–time has so far been arbitrary. For an attempt to quantize the algebra of observables canonically, let us again specialize to $1+3$ dimensions and proceed as follows: in a first step, the normally ordered quantum analogs of the classical generators J_1, T_2, S_2, S_1 and $B_0^{(\ell)}$ are calculated by application of formula (14). Next, we consider the zeroth level $\mathfrak{V}^0$ as well as the action of $\mathfrak{V}^0$ on the other levels $\mathfrak{V}^\ell$, where the rescaled Poisson brackets are replaced by commutators multiplied by $2\pi\alpha'/i\hbar$. By Appendix B, we find for the generators of $\mathfrak{V}^0$:

$$:J_{1,-1}:=-\frac{\mathfrak{m}^2}{4\pi}\sum_{n=1}^{\infty}\frac{1}{n}(\alpha_-^{-n}\alpha_3^n-\alpha_3^{-n}\alpha_-^n),\quad:J_{1,0}:=-\frac{\mathfrak{m}^2}{4\pi}\sum_{n=1}^{\infty}\frac{1}{n}(\alpha_+^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_+^n),$$

$$:J_{1,+1}:=-\frac{\mathfrak{m}^2}{4\pi}\sum_{n=1}^{\infty}\frac{1}{n}(\alpha_+^{-n}\alpha_3^n-\alpha_3^{-n}\alpha_+^n).$$

Obviously, commutators of the form

$$[\alpha_\mu^{-n}\alpha_\nu^n,\ \text{:polynomial in }\alpha\text{'s:}],\quad n>0,$$

can only yield normally ordered terms, and we may conclude that the action of $J_{1,m}$ remains unchanged. Therefore, $\mathfrak{V}^0$ as well as the multiplet structure of $\mathfrak{V}^\ell$ is not affected by the quantization prescription. Regarding the quantum relations in higher degrees ℓ, one now proceeds as follows. Write all terms of the classical relation (in terms of the appropriate multiplets) on the left

hand side of an equation. Replace all generators by their normally ordered counterparts, and the rescaled Poisson brackets and products as described in Sec. III. The commutators are then evaluated by application of the derivation rule. Finally, all resulting terms are brought into normal order. From the classical relation it follows that in leading order the result is 0, but from the process of reordering, quantum corrections may arise.

Explicitly, the relations which form the starting point of the calculations are the following:

$$J^P=4^-: \quad \frac{2\pi\alpha'}{\hbar}[:T_2:,:S_2:]_4 = 0 + \text{anomalies},$$

$$J^P=3^+\ (i): \quad \frac{2\pi\alpha'}{\hbar}[:T_2:,:T_2:]_3 + i\frac{2\pi\alpha'}{\hbar}[:S_2:,:S_1:]_3 + 16(:J_1:^3)_3 = 0 + \text{anomalies},$$

$$(ii): \quad \frac{2\pi\alpha'}{\hbar}[:S_2:,:S_2:]_3 - i2\frac{2\pi\alpha'}{\hbar}[:S_2:,:S_1:]_3 - 4\{:J_1:,:T_2:\}_3 - 48(:J_1:^3)_3 = 0 + \text{anomalies},$$

$$J^P=3^-: \quad \frac{2\pi\alpha'}{\hbar}[:T_2:,:S_2:]_3 - i\frac{2\pi\alpha'}{\hbar}[:T_2:,:S_1:]_3 + 4\{:J_1:,:S_2:\}_3 = 0 + \text{anomalies},$$

$$J^P=2^-: \quad \frac{2\pi\alpha'}{\hbar}[:T_2:,:S_2:]_2 + \frac{i}{3}\sqrt{\frac{7}{2}}\frac{2\pi\alpha'}{\hbar}[:T_2:,:S_1:]_2 - \frac{2}{3}\sqrt{14}\{:J_1:,:S_2:\}_2 = 0 + \text{anomalies},$$

$$J^P=1^+: \quad \frac{2\pi\alpha'}{\hbar}[:S_2:,:S_2:]_1 + i\sqrt{\frac{2}{3}}\frac{2\pi\alpha'}{\hbar}[:S_2:,:S_1:]_1 + \frac{1}{6}\sqrt{5}\frac{2\pi\alpha'}{\hbar}[:S_1:,:S_1:]_1 - 8\sqrt{\frac{2}{3}}\{:J_1:,:T_2:\}_1$$
$$- 16\sqrt{\frac{2}{15}}\{:J_1:,(:J_1:^2)_0\}_1 + \frac{\hbar^2}{(2\pi\alpha')^2}\, f\,\sqrt{10}:J_1: = 0 + \text{anomalies},$$

and for the action of $:B_0^{(1)}:$,

$$J^P=2^+: \quad \frac{2\pi\alpha'}{\hbar}[:B_0^{(1)}:,:T_2:]_2 - i\sqrt{6}\frac{2\pi\alpha'}{\hbar}[:S_2:,:S_1:]_2 = 0 + \text{anomalies},$$

$$J^P=1^-: \quad \frac{2\pi\alpha'}{\hbar}[:B_0^{(1)}:,:S_1:]_1 + i6\sqrt{\frac{2}{5}}\frac{2\pi\alpha'}{\hbar}[:T_2:,:S_2:]_1 - 2\sqrt{\frac{3}{5}}\frac{2\pi\alpha'}{\hbar}[:T_2:,:S_1:]_1$$
$$+ 12i\sqrt{\frac{3}{5}}\{:J_1:,:S_2:\}_1 + 6\sqrt{2}\{:J_1:,:S_1:\}_1 = 0 + \text{anomalies},$$

$$J^P=2^-: \quad \frac{2\pi\alpha'}{\hbar}[:B_0^{(1)}:,:S_2:]_2 + i2\sqrt{\frac{2}{3}}\frac{2\pi\alpha'}{\hbar}[:T_2:,:S_1:]_2 - i2\sqrt{\frac{2}{3}}\{:J_1:,:S_2:\}_2 - i6\{:J_1:,:S_1:\}_2$$
$$= 0 + \text{anomalies}.$$

Note that (as in the case of algebraic quantization) there is no need to use an anticommutator if the coupling to spin J in a product $(:J_1:^n)_J$ is unique.

The *observable* quantum correction $+(\hbar^2/(2\pi\alpha')^2)f\sqrt{10}:J_1:$, found in Ref. 6 for the relation with $J^P=1^+$, was added to the left hand side of the equation (in normally ordered form) in order to simplify the comparison with the algebraically quantized relations: if they were reproduced in the canonical approach, all right hand sides would be identically 0 (with the parameter f fixed). However, as we shall see below, we will find anomalies which destroy the algebraic structure of the algebra $\mathfrak{h}$. What is worse, the anomalies neither possess reparametrization-invariant classical counterparts, nor can they be written in terms of Virasoro generators.

C. Anomalies for $\ell=2$

Let us start with some general considerations as to which anomalies are to be expected in the relations in $\mathfrak{V}^2$. First we note that commutators $[:\mathcal{Z}^{(2)}_{\mu_1\ldots\mu_4}:,:\mathcal{Z}^{(2)}_{\nu_1\ldots\nu_4}:]$ yield at most $2+2-1$

annihilation operators and as many creation operators. Likewise, we find at most three annihilation and three creation operators in products $\mathfrak{m}^{-1}{:}\mathcal{Z}^{(2)}_{0\mu_1\mu_2}{::}\mathcal{Z}^{(2)}_{\nu_1\ldots\nu_4}{:}$ and $\mathfrak{m}^{-3}{:}\mathcal{Z}^{(2)}_{0\mu_1\mu_2}{::}\mathcal{Z}^{(2)}_{0\nu_1\nu_2}{::}\mathcal{Z}^{(2)}_{0\rho_1\rho_2}{:}$, respectively (see Appendix B). Now, reordering terms with at most three annihilation and three creation operators, we derive a quantum correction consisting of at most two annihilation and two creation operators, and reordering such terms finally yields quantum corrections consisting of at most one annihilation and one creation operator. The expressions possess the following physical units:

Order	Units ($\ell=2$)
leading (=0)	$\dfrac{2\pi\alpha'}{\hbar}\dfrac{\mathfrak{m}^8}{(2\pi)^4}\dfrac{\hbar 2\pi}{2\pi\alpha'\mathfrak{m}^2}=\dfrac{\mathfrak{m}^6}{(2\pi)^3}$
first reordering	$\dfrac{\mathfrak{m}^6}{(2\pi)^3}\dfrac{\hbar 2\pi}{2\pi\alpha'\mathfrak{m}^2}=\dfrac{\mathfrak{m}^4}{(2\pi)^2}\dfrac{\hbar}{2\pi\alpha'}$
second reordering	$\dfrac{\mathfrak{m}^4}{(2\pi)^2}\dfrac{\hbar}{2\pi\alpha'}\dfrac{\hbar 2\pi}{2\pi\alpha'\mathfrak{m}^2}=\dfrac{\mathfrak{m}^2}{2\pi}\dfrac{\hbar^2}{(2\pi\alpha')^2}$

which makes sense as $\mathfrak{m}^4/(2\pi)^2$ is the unit of an element of $\mathfrak{V}^1$, and $\mathfrak{m}^2/(2\pi)$ is that of an element of $\mathfrak{V}^0$. By the canoncial commutation relations (12), either two spacelike or two timelike indices are contracted, whence the parity is unchanged by reorderings. The anomalies will again arise as multiplets of so(3), such that it suffices to calculate the anomalies for fixed magnetic quantum number $m=-J$. In fact, the possible anomalies for each relation can be predicted. For example, the only possible quantum correction with $m=-4$ would be $\alpha_-^{(\cdot)}\alpha_-^{(\cdot)}\alpha_-^{(\cdot)}\alpha_-^{(\cdot)}$, which, however, has positive parity P and hence cannot appear in the relation with $J^P=4^-$. While many of the possible anomalies arise somewhere in the course of the calculation, most of them cancel and only some remain in the end.

The calculations are performed for fixed but arbitrary summation indices and, at intermediate steps, involve several thousand terms. (The convergence problem of the infinite series of operators is ignored, since the sole purpose of this investigation is the comparison with the ordinary canonical approach, where these questions likewise do not play a role.) It is therefore necessary to use computer algebra, and the program package MATHEMATICA was employed (for an explanation of the devised routines, see Ref. 5). In the course of the calculation, some simplifications have to be done by hand, such as

$$-\sum_{n_1,n_2>0}\frac{3}{n_1n_2}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}+\sum_{n_1,n_2>0}\frac{4}{n_1(n_1+n_2)}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}+\sum_{n_1,n_2>0}\frac{2}{n_2(n_1+n_2)}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}$$
$$=\sum_{n_1,n_2>0}\frac{-n_1+n_2}{n_1n_2(n_1+n_2)}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}=0,$$

or

$$\sum_{n_1,n_2>0}\frac{1}{n_1n_2}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}=\sum_{n_1,n_2>0}\frac{2}{n_1(n_1+n_2)}\alpha_\mu^{-n_1-n_2}\alpha_\nu^{n_1}\alpha_\nu^{n_2}.$$

In order to check the manipulations, it was calculated that indeed, the leading order terms in the relations yield 0. The results of the calculation are

J^P	Anomalies for $m=-J$
4^-	0
3^+ (i)	$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{-8}{nm}(\alpha_-^{-n}\alpha_-^{-m}\alpha_-^m\alpha_3^n-\alpha_3^{-n}\alpha_-^{-m}\alpha_-^m\alpha_-^n)$
(ii)	$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{20}{nm}(\alpha_-^{-n}\alpha_-^{-m}\alpha_-^m\alpha_3^n-\alpha_3^{-n}\alpha_-^{-m}\alpha_-^m\alpha_-^n)$
3^-	$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4i}{nm}(2\alpha_0^{-n}\alpha_-^{-m}\alpha_-^m\alpha_-^n-2\alpha_-^{-n}\alpha_-^{-m}\alpha_-^m\alpha_0^n+\alpha_-^{-n}\alpha_-^{-m}\alpha_-^{n+m}-\alpha_-^{-n-m}\alpha_-^n\alpha_-^m)$
2^-	0
1^+	$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\frac{1}{\sqrt{10}}\frac{80}{3}\left(\sum_{n>0}\frac{1}{n^2}(\alpha_3^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_3^n)+\sum_{n,m>0}\frac{1}{(n+m)^2}(\alpha_3^{-n-m}\alpha_-^{n+m}-\alpha_-^{-n-m}\alpha_3^{n+m})\right)$

and similar results were found for the relations involving $B_0^{(1)}$ (see Appendix C). In addition to the anomalies given above, the following term appeared in the relation with $J^P=1^+$ for $m=-1$,

$$\frac{\hbar^2}{(2\pi\alpha')^2}\frac{\mathfrak{m}^2}{2\pi}\frac{1}{\sqrt{10}}\frac{64}{3}\sum_{n>0}\frac{1}{n}(\alpha_3^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_3^n),$$

whence we deduce that $f=-128/30$. Note that this is not consistent with the result found later by the method presented in Ref. 10.

The anomalies in the relation with $J^P=1^+$ can be rewritten in the following way. Since there are $n-1$ possibilities to write $\mathbb{N}\ni n>0$ as a sum of two natural numbers $n_i>0$, the following identity holds:

$$\sum_{n_1,n_2>0}\frac{1}{(n_1+n_2)^2}X_{(n_1+n_2)}=\sum_{n>0}\frac{n-1}{n^2}X_n,$$

and the anomalies for $J^P=1^+$ can be simplified to yield

$$\begin{aligned}&\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\left(\sum_{n>0}\frac{1}{n^2}(\alpha_3^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_3^n)+\sum_{n>0}\left(\frac{1}{n}-\frac{1}{n^2}\right)(\alpha_3^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_3^n)\right)\\&\quad=\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n>0}\frac{1}{n}(\alpha_3^{-n}\alpha_-^n-\alpha_-^{-n}\alpha_3^n)=\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{\pi}:J_{1,-1}:.\end{aligned}\tag{15}$$

At first sight, this is surprising, since after once reordering an expression in $\mathfrak{V}^2$ we would not expect an element of $\mathfrak{V}^0$ to arise (but rather one of $\mathfrak{V}^1$). However, as was remarked in Sec. IV A, the tensor rank of an expression in terms of annihilation and creation operators (or Fourier components) is given by the power of $\mathfrak{m}$ in the expression, while the corresponding degree ℓ is given only by the negative power of 2π in the expression minus 1 (which is correctly given here by $\ell=2-1$). We should therefore not think of the above expression as an element of $\mathfrak{V}^0$, but rather as

an anomaly with $\ell=1$, accidentally having a similar form as $J_{1,-1}\in\mathfrak{V}^0$. It is illustrative to explicitly retrace how this term arises.

Remark 1: The term (15) is part of the following commutator:

$$\frac{2\pi\alpha'}{\hbar}[:\mathcal{Z}^{(2)}_{0-++}:,:\mathcal{Z}^{(2)}_{03--}:], \tag{16}$$

which appears in the relation with $J^P=1^+$, $m=-1$.

Proof: First note that by (7) this commutator appears in $[S_2,S_1]_{1,-1}$ and, hence, is indeed part of the relation under consideration. Now, in the homogeneous invariants $:\mathcal{Z}^{(2)}_{\mu_1\cdots\mu_4}:$, terms of the following form appear,

$$\frac{\mathfrak{m}^4}{(2\pi)^2}\delta_{\mu_1,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1(n_1+n_2)}(\alpha^{-n_1-n_2}_{\mu_2}\alpha^{n_1}_{\mu_4}\alpha^{n_2}_{\mu_3}+\alpha^{-n_1}_{\mu_4}\alpha^{-n_2}_{\mu_3}\alpha^{n_1+n_2}_{\mu_2}),$$

such that a commutator $(2\pi\alpha'/\hbar)[:\mathcal{Z}^{(2)}_{\mu_1\cdots\mu_4}:,:\mathcal{Z}^{(2)}_{\nu_1\cdots\nu_4}:]$ yields (among other terms)

$$\frac{\mathfrak{m}^8}{(2\pi)^4}\frac{2\pi\alpha'}{\hbar}\sum_{n_1,n_2>0}\sum_{m_1,m_2>0}\frac{1}{n_1(n_1+n_2)m_1(m_1+m_2)}\alpha^{-n_1-n_2}_{\mu_2}\alpha^{n_1}_{\mu_4}[\alpha^{n_2}_{\mu_3},\alpha^{-m_1}_{\nu_4}]\alpha^{-m_2}_{\nu_3}\alpha^{m_1+m_2}_{\nu_2}$$

$$=\frac{2\mathfrak{m}^6}{(2\pi)^3}\sum_{n_1,n_2>0}\sum_{m_2>0}\frac{\eta_{\mu_3\nu_4}}{n_1(n_1+n_2)(n_2+m_2)}\alpha^{-n_1-n_2}_{\mu_2}\alpha^{n_1}_{\mu_4}\alpha^{-m_2}_{\nu_3}\alpha^{n_2+m_2}_{\nu_2}.$$

Hence from (16) we find the contribution

$$-\frac{\mathfrak{m}^6}{4\pi^3}\sum_{n_1,n_2,m_2>0}\frac{1}{n_1(n_1+n_2)(n_2+m_2)}\alpha^{-n_1-n_2}_{-}\alpha^{n_1}_{+}\alpha^{-m_2}_{-}\alpha^{n_2+m_2}_{3},$$

which by normal ordering yields the anomaly

$$-\frac{\mathfrak{m}^6}{4\pi^3}\sum_{n_1,n_2,m_2>0}\frac{1}{n_1(n_1+n_2)(n_2+m_2)}[\alpha^{n_1}_{+},\alpha^{-m_2}_{-}]\alpha^{-n_1-n_2}_{-}\alpha^{n_2+m_2}_{3}$$

$$=\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{\pi^2}\sum_{n_1,n_2>0}\frac{1}{(n_1+n_2)^2}\alpha^{-n_1-n_2}_{-}\alpha^{n_1+n_2}_{3}$$

and in the same manner we find

$$-\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{\pi^2}\sum_{n_1,n_2>0}\frac{1}{(n_1+n_2)^2}\alpha^{-n_1-n_2}_{3}\alpha^{n_1+n_2}_{-}.$$

■

Let us now turn to an interpretation of the anomalies.

D. Unobservability of the anomalies

First we note that in the conformal gauge (9) the anomalies are independent of τ. However, no invariant charges $\mathcal{Z}_{\ldots}$ correspond to the anomalies, and it can even be shown directly that the anomalies do not in general correspond to classical functionals on the world-sheet which are

invariant under changes of the parametrization. To see this, we rewrite the anomalies in a more compact manner as multiplets of so(3). To that end, the following operators are defined:

$$(i)\ :R_1: = \{:R_{1,-1}:,:R_{1,0}:,:R_{1,1}:\} \overset{\text{def}}{=} \{:R_{0-}:,:R_{03}:,-:R_{0+}:\},\ \text{with}$$

$$\mathcal{M}_{\mu\nu} = x_\mu \mathcal{P}_\nu - x_\nu \mathcal{P}_\mu + \frac{2\pi\alpha'}{2i} \underbrace{\frac{\mathfrak{m}^2}{2\pi} \sum_{n>0} \frac{1}{n} (\alpha_\mu^{-n}\alpha_\nu^n - \alpha_\nu^{-n}\alpha_\mu^n}_{:R_{\mu\nu}:} + \beta_\mu^{-n}\beta_\nu^n - \beta_\nu^{-n}\beta_\mu^n).$$

$$(ii)\ :A_{2,m}: = \frac{\mathfrak{m}^2}{2\pi} \sum_{n>0} \frac{1}{n} (\alpha_1^{-n}\alpha_1^n)_{2,m} = \frac{\mathfrak{m}^2}{2\pi} \sum_{n>0} \frac{1}{n} \underbrace{\sum_{m_1,m_2=-1}^{1}}_{m_1+m_2=m} \langle 2,m|1,m_1;1,m_2\rangle \alpha_{1,m_1}^{-n}\alpha_{1,m_2}^n$$

$$\text{with } \alpha_{1,-1}^{\pm n} = \alpha_-^{\pm n},\ \alpha_{1,0}^{\pm n} = \alpha_3^{\pm n} \text{ and } \alpha_{1,1}^{\pm n} = -\alpha_+^{\pm n}.$$

$:A_{2,m}:$ is symmetric in the coordinate indices, since for the Clebsch–Gordan coefficients we have $\langle 2,\pm 1|1,\pm 1;1,0\rangle = \langle 2,\pm 1|1,0;1,\pm 1\rangle$ and $\langle 2,0|1,-1;1,1\rangle = \langle 2,0|1,1;1,-1\rangle$.

An elementary calculation now shows that the anomalies can be written as follows:

J^P	Anomalies
4^-	0
3^- (i)	$\frac{\hbar}{2\pi\alpha'} 8\{:J_1:,:A_2:\}_3$
(ii)	$-\frac{\hbar}{2\pi\alpha'} 20\{:J_1:,:A_2:\}_3$
3^-	$\frac{\hbar}{2\pi\alpha'} 4i\{:R_1:,:A_2:\}_3 +$ "more"
2^-	0
1^+	$\frac{\hbar}{2\pi\alpha'} \frac{1}{\sqrt{10}} \frac{80}{3} \frac{\mathfrak{m}^2}{\pi} :J_1:$

with anticommutators $\{\cdot,\cdot\}_{j,m}$ again coupled to spin j and magnetic quantum number m, and where (still) $f=-128/30$. Here, the term "more" in a relation indicates that further anomalous terms appear which involve mixed summation indices such as $n+m$ and for which no further simplification has been found. Similarly, for the relations involving $B_0^{(1)}$,

J^P	Anomalies
2^+	$-\frac{\hbar}{2\pi\alpha'}4\sqrt{6}\{:J_1:,:A_2:\}_2$
2^-	$-\frac{\hbar}{2\pi\alpha'}2\sqrt{6}\mathrm{i}\{:R_1:,:A_2:\}_2+$ "more"
1^-	$-\frac{\hbar}{2\pi\alpha'}12\sqrt{\frac{3}{5}}\{:R_1:,:A_2:\}_1+$ "more" $+\frac{\hbar^2}{(2\pi\alpha')^2}12:R_1:$

where the anomaly of second order in the relation with $J^P=1^-$ appears when the normally ordered anomaly term is written as the anticommutator $\{:R_1:,:A_2:\}_1$.

We are now prepared to state the main result of the present investigation.

Remark 2: The classical symmetric monomials $A_{2,m}$ which correspond to the products $:A_{2,m}:$ are not observable.

Proof: Consider a left mover u_μ which is written in terms of classical Fourier modes (8) and split it into its negative, positive, and null modes,

$$u_\mu(\sigma)=\frac{\mathfrak{m}}{2\pi}\sum_{n>0}\alpha_\mu^n e^{in\sigma}+\frac{\mathfrak{m}}{2\pi}\sum_{n>0}\alpha_\mu^{-n}e^{-in\sigma}+\frac{\mathfrak{m}}{2\pi}\alpha_\mu^0=:u_\mu^p(\sigma)+u_\mu^n(\sigma)+u_\mu^0,$$

and calculate the following integral, which is symmetrized in the coordinate indices μ and ν,

$$\begin{aligned}I(\mu,\nu)&=\int_0^{2\pi}d\sigma_1 u_{(\mu}(\sigma_1)\int_0^{\sigma_1}d\sigma_2(u_{\nu)}^p(\sigma_2)-u_{\nu)}^n(\sigma_2))\\&=\frac{\mathfrak{m}^2}{4\pi^2}\int_0^{2\pi}d\sigma_1\sum_{n_1=-\infty}^{\infty}e^{in_1\sigma_1}\alpha_{(\mu}^{n_1}\left(\sum_{n_2>0}\alpha_{\nu)}^{n_2}\frac{e^{in_2\sigma_1}-1}{in_2}-\sum_{n_2>0}\alpha_{\nu)}^{-n_2}\frac{e^{-in_2\sigma_1}-1}{-in_2}\right)\\&=\frac{\mathfrak{m}^2}{4\pi^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2>0}\alpha_{(\mu}^{n_1}\alpha_{\nu)}^{n_2}\frac{1}{in_2}2\pi(\delta_{n_1+n_2,0}-\delta_{n_1,0})\\&\quad+\frac{\mathfrak{m}^2}{4\pi^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2>0}\alpha_{(\mu}^{n_1}\alpha_{\nu)}^{-n_2}\frac{1}{in_2}2\pi(\delta_{n_1-n_2,0}-\delta_{n_1,0})\\&=\frac{\mathfrak{m}^2}{2\pi}\frac{2}{i}\sum_{n_2>0}\frac{1}{n_2}\alpha_{(\mu}^{-n_2}\alpha_{\nu)}^{n_2}-\underbrace{\frac{\mathfrak{m}^2}{4\pi^2}\frac{2\pi}{i}\sum_{n_2>0}\frac{1}{n_2}(\alpha_{(\mu}^0\alpha_{\nu)}^{n_2}+\alpha_{(\mu}^0\alpha_{\nu)}^{-n_2})}_{\circledast}.\end{aligned}$$

For μ and ν spacelike, the term $\circledast$ vanishes in the rest system and, hence, the products $:A_{2,m}:$ (which contain spacelike indices only) are linear combinations of integrals of the form $I(\mu,\nu)$. Now consider a change of parametrization $\sigma\to\hat{\sigma}$. Then the integral over u_ν is invariant:

$$\int_{\sigma_0}^{\sigma} d\sigma_1[u_\nu^p(\sigma_1)+u_\nu^n(\sigma_1)+u_\nu^0]=\int_{\sigma_0}^{\sigma} d\sigma_1 u_\nu(\sigma_1)=\int_{\hat\sigma_0}^{\hat\sigma} d\hat\sigma_1\hat u_\nu(\hat\sigma_1)=\int_{\hat\sigma_0}^{\hat\sigma} d\hat\sigma_1[\hat u_\nu^p(\hat\sigma_1)+\hat u_\nu^n(\hat\sigma_1)+u_\nu^0].$$

Here, we have used that the zero modes α_ν^0 are independent of the parametrization. Note that the splitting of $\hat u$ into positive and negative modes has to be done with respect to the new parametrization. In contrast to this, the difference of positive and negative modes does not in general possess the correct behavior under reparametrizations,

$$\int_{\sigma_0}^{\sigma} d\sigma_1[u_\nu^p(\sigma_1)-u_\nu^n(\sigma_1)]\overset{\text{i.g.}}{\neq}\int_{\hat\sigma_0}^{\hat\sigma} d\hat\sigma_1[\hat u_\nu^p(\hat\sigma_1)-\hat u_\nu^n(\hat\sigma_1)]. \tag{17}$$

To see this, consider the following counter example. Given a left mover with

$$u_0(\sigma)=1,\ \text{hence}\ u_0^p(\sigma)=u_0^n(\sigma)=0,$$

the left hand side of (17) is zero, while this is not true in general for the right hand side. Consider the reparametrization $\sigma\to\hat\sigma$ with $\sigma=f(\hat\sigma)$, where

$$e^{i\sigma}=\frac{e^{i\hat\sigma}-w}{\overline{w}e^{i\hat\sigma}-1}\ \text{with fixed}\ w,\ |w|<1,\ w=|w|e^{i\chi}.$$

In more technical terms, consider the unit disk $\subset\mathbb{C}$, whose boundary corresponds to the string. Then the above defines an automorphism of the disk which maps the boundary of the disk to itself, while respecting its orientation. Therefore, it does indeed define a parametrization. Obviously, we have

$$d\sigma=(1-|w|^2)\frac{d\hat\sigma}{(1-\overline{w}e^{i\hat\sigma})(1-we^{-i\hat\sigma})},$$

and, hence, the transformed $\hat u_0(\hat\sigma)$ is given as

$$\hat u_0(\hat\sigma)=u_0(f(\hat\sigma))\frac{df(\hat\sigma)}{d\hat\sigma}=\frac{1-|w|^2}{(1-\overline{w}e^{i\hat\sigma})(1-we^{-i\hat\sigma})}.$$

In particular, the zero mode $\hat u_0^0(\hat\sigma)=u_0^0(\sigma)=1$ is invariant, while for positive and negative modes an explicit calculation yields

$$\hat u_0^p(\hat\sigma)=(1-|w|^2)\sum_{l\geqslant 1}\left(\sum_{n\geqslant 0}|w|^{2n}\right)|w|^l e^{-il\chi}e^{il\hat\sigma},$$

$$\hat u_0^n(\hat\sigma)=(1-|w|^2)\sum_{l\leqslant -1}\left(\sum_{n\geqslant |l|}|w|^{2n}\right)|w|^l e^{-il\chi}e^{il\hat\sigma}.$$

We may thus conclude that while the left hand side of (17) is zero, the right hand side yields

$$\int_{\hat\sigma_0}^{\hat\sigma} d\hat\sigma_1[\hat u_0^p(\hat\sigma_1)-\hat u_0^n(\hat\sigma_1)]=(1-|w|^2)\sum_{l\geqslant 1}\left(\sum_{n\geqslant 0}|w|^{2n}|w|^l e^{-il\chi}\frac{e^{il\hat\sigma}-e^{il\hat\sigma_0}}{il}\right.$$
$$\left.-\sum_{n\geqslant l}|w|^{2n}|w|^{-l}e^{il\chi}\frac{e^{-il\hat\sigma}-e^{-il\hat\sigma_0}}{-il}\right)\neq 0$$

for general $\hat\sigma\neq\hat\sigma_0+2\pi$. Therefore, the products $A_{2,m}$ are not invariant under general reparametrizations. ■

An alternative proof of the above remark is to show that the *classical* monomial corresponding to an anomaly does not Poisson-commute with the generators of the Witt algebra. For instance, for the Poisson bracket of $A_{2,-2}=(\mathfrak{m}^2/2\pi)\Sigma(1/n)\alpha_-^{-n}\alpha_-^n$ and $\overline{L^l}$, $l\geqslant 2$, we find the following term,

$$-\sum_{m=1}^{l-1}\alpha_-^m\alpha_-^{l-m},$$

and similarly for $l\leqslant -2$. Since the anomalies cannot be written as functions of the constraints, they do not even vanish weakly (on the physical subspace) and we may conclude that not even in this sense, the invariant charges in $3+1$ dimensions can be represented as a subalgebra of the polynomial algebra of normally ordered annihilation and creation operators.

To conclude, it is emphasized that the anomalies are not multiples of the identity, and, therefore, canonical quantization does not merely yield a central extension of the algebra of invariant charges.

V. ANOMALIES APPEAR IN ANY DIMENSION

The calculations in the preceding section were performed in a $d=3+1$ dimensional background. A natural objection would be to claim that in some critical dimension, the problem could be absent. This, however, is not the case.

From the relation in $d=3+1$ with $J^P=2^+$ involving the exceptional element $B_0^{(1)}$, we can deduce that in arbitrary dimensions d, commutators of normally ordered invariant charges will in general yield anomalies which do not correspond to classical reparametrization-invariant quantities. This follows directly from the fact that the relation under consideration for, say, $m=-2$ can also be read independently of the dimension d as follows:

$$\tfrac{1}{2}[:\mathcal{Z}^{(2)}_{0-0+}:+\tfrac{1}{2}:\mathcal{Z}^{(2)}_{0303}:,:\mathcal{Z}^{(2)}_{00--}:]-[:\mathcal{Z}^{(2)}_{0-33}:,:\mathcal{Z}^{(2)}_{0+--}:]+[:\mathcal{Z}^{(2)}_{0+--}:,:\mathcal{Z}^{(2)}_{0-33}:]-2[:\mathcal{Z}^{(2)}_{03--}:,:\mathcal{Z}^{(2)}_{0-3+}:]$$

$$=-\frac{\hbar}{2\pi\alpha'}8\left(\frac{\sqrt{2}}{4m}\{i:\mathcal{Z}^{(2)}_{0-3}:-i:\mathcal{Z}^{(2)}_{03-}:,X\}-\frac{1}{2m}\{i:\mathcal{Z}^{(2)}_{0+-}:-i:\mathcal{Z}^{(2)}_{0-+}:,Y\}\right),$$

with

$$X=\frac{\mathfrak{m}^2}{2\pi}\frac{1}{\sqrt{2}}\sum_{n>0}\frac{1}{n}(\alpha_-^{-n}\alpha_3^n+\alpha_3^{-n}\alpha_-^n),\quad Y=\frac{\mathfrak{m}^2}{2\pi}\sum_{n>0}\frac{1}{n}\alpha_-^{-n}\alpha_-^n,$$

and where the basis e_0, $e_\pm=(1/\sqrt{2})(e_1\pm ie_2)$, $e_3,\ldots,e_{d-1}$ is chosen in d-dimensional Minkowski space.

Although the above may not be one of the defining relations in d dimensions, its classical counterpart (where the commutators are again replaced by Poisson brackets and the right hand side is set to 0) is an identity in the Poisson algebra of invariant charges for arbitrary dimension d. The proof of Remark 2 being independent of the dimension of the underlying space, we deduce that the right hand side of the above still is not observable. Neither is it a function of the Virasoro generators, and hence the algebra of normally ordered invariant charges is no subalgebra of the normally ordered polynomials in annhihilation and creation operators, not even on the physical subspace and independently of the dimension d.

It is instructive to consider this result also from the following different point of view.

Remark 3: Consider the commutator of a normally ordered invariant charge $:\mathcal{Z}^{(2)}_{\mu_1\cdots\mu_4}:$ with a Virasoro generator $:\overline{L^n}:$, $n>0$. Then from the terms in $:\overline{L^n}:$ which involve two annihilation operators, we find anomalies of the following form:

$$A(i_1,i_2,i_3,i_4)=\eta_{\mu_{i_1}\mu_{i_2}}\sum_{n_1=1}^{n-1}(\alpha^{n-n_1}_{\mu_{i_3}}\alpha^{n_1}_{\mu_{i_4}}+\alpha^{n_1}_{\mu_{i_3}}\alpha^{n-n_1}_{\mu_{i_4}}),\tag{18}$$

$$A(i_1,i_2,i_3)=\eta_{\mu_{i_1}\mu_{i_2}}\frac{n}{2}(n-1)\alpha^n_{\mu_{i_3}}.\tag{19}$$

Proof: The claim follows from Appendix B by simple calculations. Anomalies of the form (18) arise from normal ordering expressions such as

$$\sum_{m_1,m_2>0}\frac{1}{m_1m_2}\sum_{n_1=1}^{n-1}\sum_{\nu=0}^{d-1}[\alpha_\nu^{n-n_1},\alpha_{\mu_{i_1}}^{-m_1}]\alpha^{n_1\nu}\alpha_{\mu_{i_2}}^{-m_2}\alpha_{\mu_{i_3}}^{m_2}\alpha_{\mu_{i_4}}^{m_1}$$

$$+\sum_{m_1,m_2>0}\frac{1}{m_1m_2}\sum_{n_1=1}^{n-1}\sum_{\nu=0}^{d-1}[\alpha_\nu^{n-n_1},\alpha_{\mu_{i_2}}^{-m_2}]\alpha^{n_1\nu}\alpha_{\mu_{i_1}}^{-m_1}\alpha_{\mu_{i_3}}^{m_2}\alpha_{\mu_{i_4}}^{m_1}.$$

Likewise, anomalies of the form (19) arise from normal ordering of expressions

$$\sum_{m_1,m_2>0}\frac{1}{m_1(m_1+m_2)}\sum_{n_1=1}^{n-1}\sum_{\nu=0}^{d-1}\alpha^{n_1\nu}[\alpha_\nu^{n-n_1},\alpha_{\mu_{i_1}}^{-m_1}\alpha_{\mu_{i_2}}^{-m_2}]\alpha_{\mu_{i_3}}^{m_1+m_2}$$

as well as

$$\sum_{m_1,m_2>0}\frac{1}{m_1m_2}\sum_{n_1=1}^{n-1}\sum_{\nu=0}^{d-1}\alpha^{n_1\nu}[\alpha_\nu^{n-n_1},\alpha_{\mu_{i_1}}^{-m_1}\alpha_{\mu_{i_2}}^{-m_2}]\alpha_{\mu_{i_3}}^{m_1+m_2}.$$

Here, the anomalies turn out to be independent of n_1 such that the sum $\Sigma_{n_1=1}^{n-1}$ yields the factor $\frac{1}{2}n(n-1)$. ■

No other anomalies appear, since one needs at least three operators which are not multiples of the identity and at least two creation operators in order to find nontrivial contributions. The leading order of the commutator is 0, as it corresponds to the classical result (the invariant charges Poisson-commute with the generators of the Witt algebra). From Appendix B one calculates that the complete set of anomalies is given by

$$A(1,2,3,4)-A(1,3,4,2)-A(1,3,2,4)+A(1,4,3,2)+A(2,3,4,1)$$

$$-A(2,4,3,1)-A(2,4,1,3)+A(3,4,1,2)$$

and

$$-(\delta_{\mu_1,0}A(2,3,4)+\delta_{\mu_1,0}A(4,3,2)+\delta_{\mu_2,0}A(3,4,1)+\delta_{\mu_2,0}A(1,4,3)+\delta_{\mu_3,0}A(4,1,2)$$

$$+\delta_{\mu_3,0}A(2,1,4)+\delta_{\mu_4,0}A(1,2,3)+\delta_{\mu_4,0}A(3,2,1))$$

$$+(\delta_{\mu_1,0}A(2,4,3)+\delta_{\mu_2,0}A(1,3,4)+\delta_{\mu_3,0}A(2,4,1)+\delta_{\mu_4,0}A(1,3,2)).$$

These anomalies do not vanish in any particular dimension of the underlying Minkowski space. Neither are they functions of the Virasoro generators and hence they do not vanish on the physical subspace. To see that they furthermore do not in general correspond to classical observables, we consider the following example in d dimensions with canonical basis $e_0,\ldots,e_{d-1}$:

$$[:\overline{L}^m:,:\mathcal{Z}_{0011}:],\ m\geqslant 2.$$

Here, a simple calculation shows that the anomalies are proportional to

$$2\sum_{n=1}^{m-1}(\alpha_1^{m-n}\alpha_1^n-\alpha_0^{m-n}\alpha_0^n) \text{ and } m(m-1)(\alpha_0^m-\alpha_1^m), \tag{20}$$

such that the Poisson bracket of $\overline{L^l}$ with the *classical* momomials corresponding to (20) yields terms of the form

$$2\sum_{n=1}^{m-1}((m-n)(\alpha_1^n\alpha_1^{l+m-n}-\alpha_0^n\alpha_0^{l+m-n})+n(\alpha_1^{m-n}\alpha_1^{l+m}-\alpha_0^{m-n}\alpha_0^{l+m}))$$

and

$$-m^2(m-1)(\alpha_1^{l+m}-\alpha_0^{l+m}).$$

It follows that the normally ordered invariants do not commute with the generators of the Virasoro algebra, and that, again, the anomalies which arise are neither themselves invariant nor do they vanish on the physical subspace. Again, they are not simply multiples of the identity, and, in fact, for invariants of higher tensor rank may even be polynomials in annihilation and creation operators of arbitrary rank. Hence, the question of whether canonical quantization encodes the geometric content of the Nambu–Goto string has to be answered in the negative.

Similar problems occur when the gauge is fixed to the light-cone gauge. One of the reasons for the necessity of a critical dimension in the canonical approach is that in this gauge, the generators of the Poincaré group only close as a Lie algebra (at least weakly) in $d=26$. Calculating the action of these generators on invariant charges we also find anomalies which, however, contrary to those arising in a commutator of two generators, do not vanish in some critical dimension. Hence, the canonically quantized invariant charges no longer transform covariantly in this approach. For details, see Ref. 5.

The results presented here show that the canonical approach and the algebraic quantization are inequivalent. This means, in particular, that the usual Fock space does not yield a suitable representation of the algebra of invariant charges. Lately, a representation providing an alternative to the Fock space construction was proposed in Ref. 12.

To conclude, some comments on the relation between the algebra of the invariant charges and the so-called DDF operators[13] seem to be appropriate. Since the latter commute with all Virasoro generators (in the conformal gauge), they are sometimes considered to provide a "canonical algebra of invariant quantities." However, the crucial point is that the *construction rules* for a genuine invariant quantity must be gauge-independent. This requirement is met by the algebra of invariant charges: regardless of whether one starts from a conformal or from some other parametrization, the rules for the construction of the algebra of invariant charges are the same (and the charges are invariant under arbitrary reparametrizations). In contrast to this, the construction of the DDF operators relies on choosing the conformal gauge, and, hence, by the above criterion, the DDF operators are not genuinely invariant.

Note added. In the meantime, a construction of classical DDF-like operators independent of a particular gauge has been given and it was shown that the classical invariant charges can be written as functionals of these operators.[14] One main difficulty in using these operators as a starting point for quantization is to show that Lorentz symmetry can be kept after quantization.

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APPENDIX A: THE CLASSICAL RELATIONS AT $\ell=2$

$$
\begin{aligned}
J^P=4^-:&\quad 0=\{T_2,S_2\}_4,\\
J^P=3^+:&\quad 0=\{T_2,S_2\}_3+i\{S_2,S_1\}_3-i16(J_1^3)_3,\\
&\quad 0=\{S_2,S_2\}_3-i2\{S_2,S_1\}_3+i8(J_1\cdot T_2)_3+i48(J_1^3)_3,\\
J^P=3^-:&\quad 0=\{T_2,S_2\}_3-i\{T_2,S_1\}_3-i8(J_1\cdot S_2)_3,\\
J^P=2^-:&\quad 0=\{T_2,S_2\}_2+\frac{i}{3}\sqrt{\frac{7}{2}}\{T_2,S_1\}_2+i\frac{4}{3}\sqrt{14}(J_1\cdot S_2)_2,\\
J^P=1^+:&\quad 0=\{S_2,S_2\}_1+i\sqrt{\frac{2}{3}}\{S_2,S_1\}_1+\frac{1}{6}\sqrt{5}\{S_1\cdot S_1\}_1\\
&\qquad +i16\sqrt{\frac{2}{3}}(J_1\cdot T_2)_1+i32\sqrt{\frac{2}{15}}(J_1\cdot(J_1^2)_0)_1.
\end{aligned}
$$

Action of the exceptional element $B_0^{(1)}$:

$$
\begin{aligned}
J^P=2^+:&\quad \{B_0^{(1)},T_2\}_2=i\sqrt{6}\{S_2,S_1\}_2,\\
J^P=2^-:&\quad \{B_0^{(1)},S_2\}_2=-i2\sqrt{\frac{2}{3}}\{T_2,S_1\}_2-i4\sqrt{\frac{2}{3}}(J_1\cdot S_2)_2+12(J_1\cdot S_1)_2,\\
J^P=1^-:&\quad \{B_0^{(1)},S_1\}_1=-i6\sqrt{\frac{2}{5}}\{T_2,S_2\}_1+2\sqrt{\frac{3}{5}}\{T_2,S_1\}_1-24\sqrt{\frac{3}{5}}(J_1\cdot S_2)_1\\
&\qquad +i12\sqrt{2}(J_1\cdot S_1)_1.
\end{aligned}
$$

Here,

$$
\{X_{j_1},Y_{j_2}\}_{j,m}=\underbrace{\sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2}}_{m_1+m_2=m}\langle j,m|j_1,m_1;j_2,m_2\rangle\{X_{j_1,m_1},Y_{j_2,m_2}\},
\tag{A1}
$$

$$
(X_{j_1}\cdot Y_{j_2})_{j,m}=\underbrace{\sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2}}_{m_1+m_2=m}\langle j,m|j_1,m_1;j_2,m_2\rangle X_{j_1,m_1}\cdot Y_{j_2,m_2}.
\tag{A2}
$$

APPENDIX B: NORMALLY ORDERED ALGEBRA ELEMENTS

$$
:\mathcal{Z}_{0ij}^{(2)}:=\frac{\mathfrak{m}^3}{2\pi}\frac{1}{i}\sum_{n>0}\frac{1}{n}(\alpha_i^{-n}\alpha_j^n-\alpha_j^{-n}\alpha_i^n),
$$

$$
\begin{aligned}
:\mathcal{Z}_{\mu_1\mu_2\mu_3\mu_4}^{(2)}:=\frac{\mathfrak{m}^4}{4\pi^2}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1n_2}&(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_2}^{-n_2}\alpha_{\mu_3}^{n_2}\alpha_{\mu_4}^{n_1}-\alpha_{\mu_1}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_4}^{n_2}\alpha_{\mu_2}^{n_1}-\alpha_{\mu_1}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_2}^{n_2}\alpha_{\mu_4}^{n_1}\\
&+\alpha_{\mu_1}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_3}^{n_2}\alpha_{\mu_2}^{n_1}+\alpha_{\mu_2}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_4}^{n_2}\alpha_{\mu_1}^{n_1}-\alpha_{\mu_2}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_3}^{n_2}\alpha_{\mu_1}^{n_1}-\alpha_{\mu_2}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_1}^{n_2}\alpha_{\mu_3}^{n_1}\\
&+\alpha_{\mu_3}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_1}^{n_2}\alpha_{\mu_2}^{n_1})
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_1,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1(n_1+n_2)}(\alpha_{\mu_2}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_4}^{n_1+n_2}+\alpha_{\mu_4}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_2}^{n_1+n_2}+\alpha_{\mu_2}^{-n_1-n_2}\alpha_{\mu_4}^{n_1}\alpha_{\mu_3}^{n_2}\\
&+\alpha_{\mu_4}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_3}^{n_2})\\
&- \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_2,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1(n_1+n_2)}(\alpha_{\mu_3}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_1}^{n_1+n_2}+\alpha_{\mu_1}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_3}^{n_1+n_2}+\alpha_{\mu_3}^{-n_1-n_2}\alpha_{\mu_1}^{n_1}\alpha_{\mu_4}^{n_2}\\
&+\alpha_{\mu_1}^{-n_1-n_2}\alpha_{\mu_3}^{n_1}\alpha_{\mu_4}^{n_2})\\
&- \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_3,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1(n_1+n_2)}(\alpha_{\mu_4}^{-n_1}\alpha_{\mu_1}^{-n_2}\alpha_{\mu_2}^{n_1+n_2}+\alpha_{\mu_2}^{-n_1}\alpha_{\mu_1}^{-n_2}\alpha_{\mu_4}^{n_1+n_2}+\alpha_{\mu_2}^{-n_1-n_2}\alpha_{\mu_4}^{n_1}\alpha_{\mu_1}^{n_2}\\
&+\alpha_{\mu_4}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_1}^{n_2})\\
&- \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_4,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1(n_1+n_2)}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_2}^{-n_2}\alpha_{\mu_3}^{n_1+n_2}+\alpha_{\mu_3}^{-n_1}\alpha_{\mu_2}^{-n_2}\alpha_{\mu_1}^{n_1+n_2}+\alpha_{\mu_1}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_3}^{n_2}\\
&+\alpha_{\mu_3}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_1}^{n_2})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_1,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1n_2}(\alpha_{\mu_2}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_3}^{n_1+n_2}+\alpha_{\mu_3}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_4}^{n_2})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_2,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1n_2}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_4}^{n_1+n_2}+\alpha_{\mu_4}^{-n_1-n_2}\alpha_{\mu_1}^{n_1}\alpha_{\mu_3}^{n_2})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_3,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1n_2}(\alpha_{\mu_2}^{-n_1}\alpha_{\mu_4}^{-n_2}\alpha_{\mu_1}^{n_1+n_2}+\alpha_{\mu_1}^{-n_1-n_2}\alpha_{\mu_2}^{n_1}\alpha_{\mu_4}^{n_2})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_4,0}\sum_{n_1>0}\sum_{n_2>0}\frac{1}{n_1n_2}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_3}^{-n_2}\alpha_{\mu_2}^{n_1+n_2}+\alpha_{\mu_2}^{-n_1-n_2}\alpha_{\mu_1}^{n_1}\alpha_{\mu_3}^{n_2})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_1,0}\delta_{\mu_2,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_3}^{-n_1}\alpha_{\mu_4}^{n_1}+\alpha_{\mu_4}^{-n_1}\alpha_{\mu_3}^{n_1})\\
&- 2\frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_1,0}\delta_{\mu_3,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_2}^{-n_1}\alpha_{\mu_4}^{n_1}+\alpha_{\mu_4}^{-n_1}\alpha_{\mu_2}^{n_1})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_1,0}\delta_{\mu_4,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_2}^{-n_1}\alpha_{\mu_3}^{n_1}+\alpha_{\mu_3}^{-n_1}\alpha_{\mu_2}^{n_1})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_2,0}\delta_{\mu_3,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_4}^{n_1}+\alpha_{\mu_4}^{-n_1}\alpha_{\mu_1}^{n_1})\\
&- 2\frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_2,0}\delta_{\mu_4,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_3}^{n_1}+\alpha_{\mu_3}^{-n_1}\alpha_{\mu_1}^{n_1})\\
&+ \frac{\mathfrak{m}^4}{4\pi^2}\delta_{\mu_3,0}\delta_{\mu_4,0}\sum_{n_1>0}\frac{1}{n_1^2}(\alpha_{\mu_1}^{-n_1}\alpha_{\mu_2}^{n_1}+\alpha_{\mu_2}^{-n_1}\alpha_{\mu_1}^{n_1}).
\end{aligned}
$$

APPENDIX C: THE ANOMALIES FOR THE RELATIONS INVOLVING $B_0^{(1)}$

J^P — Anomalies with $m=-J$

2^+

$$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4}{nm}(2\alpha_-^{-n}\alpha_+^{-m}\alpha_-^m\alpha_-^n-2\alpha_-^{-n}\alpha_-^{-m}\alpha_+^m\alpha_-^n+\alpha_3^{-n}\alpha_3^{-m}\alpha_-^m\alpha_-^n-\alpha_-^{-n}\alpha_-^{-m}\alpha_3^m\alpha_3^n)$$

2^-

$$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4i}{nm}(2\alpha_-^{-n}\alpha_3^{-m}\alpha_0^m\alpha_-^n-2\alpha_-^{-n}\alpha_0^{-m}\alpha_3^m\alpha_-^n+\alpha_0^{-n}\alpha_-^{-m}\alpha_3^m\alpha_-^n-\alpha_-^{-n}\alpha_-^{-m}\alpha_3^m\alpha_0^n$$
$$+\alpha_0^{-n}\alpha_3^{-m}\alpha_-^m\alpha_-^n-\alpha_-^{-n}\alpha_3^{-m}\alpha_-^m\alpha_0^n)$$
$$+\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4i}{n(n+m)}(-2\alpha_3^{-n}\alpha_-^{-m}\alpha_-^{n+m}+2\alpha_-^{-n-m}\alpha_3^n\alpha_-^m+\alpha_-^{-n}\alpha_-^{-m}\alpha_3^{n+m}$$
$$-\alpha_3^{-n-m}\alpha_-^n\alpha_-^m+\alpha_-^{-n}\alpha_3^{-m}\alpha_-^{n+m}-\alpha_-^{-n-m}\alpha_-^n\alpha_3^m)$$

1^-

$$\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4}{nm}\frac{3}{5}(6\alpha_0^{-n}\alpha_-^{-m}\alpha_-^m\alpha_+^n-6\alpha_+^{-n}\alpha_-^{-m}\alpha_-^m\alpha_0^n+3\alpha_0^{-n}\alpha_-^{-m}\alpha_3^m\alpha_3^n-3\alpha_3^{-n}\alpha_-^{-m}\alpha_3^m\alpha_0^n$$
$$+3\alpha_0^{-n}\alpha_3^{-m}\alpha_-^m\alpha_3^n-3\alpha_3^{-n}\alpha_3^{-m}\alpha_-^m\alpha_0^n-2\alpha_0^{-n}\alpha_3^{-m}\alpha_3^m\alpha_-^n+2\alpha_-^{-n}\alpha_3^{-m}\alpha_3^m\alpha_0^n+\alpha_0^{-n}\alpha_-^{-m}\alpha_+^m\alpha_-^n$$
$$-\alpha_-^{-n}\alpha_-^{-m}\alpha_+^m\alpha_0^n+\alpha_0^{-n}\alpha_+^{-m}\alpha_-^m\alpha_-^n-\alpha_-^{-n}\alpha_+^{-m}\alpha_-^m\alpha_0^n)$$
$$+\frac{\hbar}{2\pi\alpha'}\frac{\mathfrak{m}^4}{(2\pi)^2}\sum_{n,m>0}\frac{4}{n(n+m)}\frac{3}{5}(6\alpha_+^{-n}\alpha_-^{-m}\alpha_-^{n+m}-6\alpha_-^{-n-m}\alpha_+^n\alpha_-^m+3\alpha_3^{-n}\alpha_3^{-m}\alpha_-^{n+m}$$
$$-3\alpha_-^{-n-m}\alpha_3^n\alpha_3^m+3\alpha_3^{-n}\alpha_-^{-m}\alpha_3^{n+m}-3\alpha_3^{-n-m}\alpha_3^n\alpha_-^m-2\alpha_-^{-n}\alpha_3^{-m}\alpha_3^{n+m}+2\alpha_3^{-n-m}\alpha_-^n\alpha_3^m$$
$$+\alpha_-^{-n}\alpha_+^{-m}\alpha_-^{n+m}-\alpha_-^{-n-m}\alpha_-^n\alpha_+^m+\alpha_-^{-n}\alpha_-^{-m}\alpha_+^{n+m}-\alpha_+^{-n-m}\alpha_-^n\alpha_-^m)$$

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A technique to identify solvable dynamical systems, and another solvable extension of the goldfish many-body problem

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We take advantage of the simple approach, recently discussed, which associates to (solvable) matrix equations (solvable) dynamical systems interpretable as (interesting) many-body problems, possibly involving auxiliary dependent variables in addition to those identifying the positions of the moving particles. Starting from a solvable matrix evolution equation, we obtain the corresponding many-body model and note that in one case the auxiliary variables can be altogether eliminated, obtaining thereby an (also Hamiltonian) extension of the "goldfish" model. The solvability of this novel model, and of its *isochronous* variant, is exhibited. A related, as well *solvable*, model, is also introduced, as well as its *isochronous* variant. Finally, the small oscillations of the *isochronous* models around their equilibrium configurations are investigated, and from their isochronicity certain diophantine relations are evinced. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND SOME RESULTS

Recently we discussed a simple approach which associates to (solvable) matrix equations (solvable) dynamical systems, generally interpretable as (interesting) many-body problems, possibly involving auxiliary dependent variables in addition to those identifying the positions of the moving particles.[16,17] In this paper we apply the same approach to a new (namely, not previously considered in this context), but again *solvable*, matrix evolution equation, and we thereby obtain a novel class of *solvable* many-body models, generally involving auxiliary variables.[16] We then note that in one case the auxiliary variables can be altogether eliminated, obtaining thereby a novel *solvable* extension, see (7) and its *isochronous* variant (10), of the "goldfish" many-body problem.[13,8,14,15] In this section we outline the main findings concerning these models, and in Sec. II we prove them. In Sec. III we introduce an alternative approach, which leads to the identification of another *solvable* model, also endowed with an *isochronous* variant. In Sec. IV we focus on the (obviously *isochronous*) behavior of these two *isochronous* models around their equilibrium configurations, and we thereby obtain, as a purely mathematical by-product, certain *diophantine* results (including a conjecture that we test numerically but we have been so far unable to prove). Since the equilibrium configuration of the first *isochronous* model—the one which provides a generalized version of the goldfish N-body problem—turns out to coincide with the (complex) zeros x_n of the generalized Laguerre polynomial $L_N^{(-2N-1)}(x)$ the first class of *diophantine* relations involves these zeros. The second class involves less exotic numbers. Some additional remarks are proffered in Sec. V. A more detailed analysis of the behavior of this extended "goldfish" model, including the explicit display of its solution in the three cases with only one, only two and only three particles, will be presented in a separate paper.[19]

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The starting point of the treatment is the *solvable* matrix evolution equation

$$\ddot{U} = a(\dot{U}U + U\dot{U}). \tag{1}$$

Here the $N \otimes N$ matrix $U \equiv U(t)$ is the dependent variable, the independent variable t ("time") is *real* and superimposed dots indicate derivatives with respect to it; a indicates a *scalar* constant, which might of course be eliminated by a trivial rescaling of the dependent or independent variables, although we prefer not to do so in order to keep track of the contributions coming from the (nonlinear) right-hand side of this matrix evolution equation, (1), and also to maintain open the option to set a to zero, going thereby back to the standard goldfish many-body problem and related results.[16,17,13]

It is easily seen that the *general* solution of this matrix evolution equation, (1), reads

$$U(t) = a^{-1}[\cos(At) - BA^{-1}\sin(At)]^{-1}[A\sin(At) + B\cos(At)], \tag{2a}$$

where A and B are two arbitrary *constant* $N \otimes N$ matrices. In terms of the initial-value problem for the matrix evolution equation (1) clearly (2a) entails

$$U(0) = a^{-1}B, \quad \dot{U}(0) = a^{-1}(A^2 + B^2), \tag{2b}$$

and these two matrix equations can be inverted to yield

$$A^2 = -a^2[U(0)]^2 + a\dot{U}(0), \quad B = aU(0). \tag{2c}$$

Note that the explicit expression (2a) entails that the matrix $U(t)$ is actually a function of the matrix A^2 rather than A.

As shown in Sec. II, the *solvable* many-body problem related to the *solvable* matrix evolution equation (1) is characterized by the following Newtonian equations of motion:

$$\ddot{z}_n = 2a\dot{z}_n z_n - 2\sum_{m=1, m\neq n}^{N} (z_n - z_m)M_{nm}M_{mn}, \tag{3a}$$

$$(z_n - z_m)\dot{M}_{nm} + 2(\dot{z}_n - \dot{z}_m)M_{nm} = a(z_n^2 - z_m^2)M_{nm} + \sum_{\ell=1;\ell\neq n,m}^{N} (z_n + z_m - 2z_\ell)M_{n\ell}M_{\ell m} - (z_n - z_m)M_{nm}(F_n - F_m), \quad n \neq m. \tag{3b}$$

The N coordinates $z_n \equiv z_n(t)$ denote the positions of the N moving particles, the $N(N-1)$ "auxiliary variables" $M_{nm} \equiv M_{nm}(t)$ evolve according to the system of $N(N-1)$ first-order ODEs (3b), and the N "source terms" F_n can be assigned as arbitrary functions of time, or even of the other dependent variables z_m and $M_{m\ell}$ without spoiling the solvable character of the model. Here and throughout indices like n, m, ℓ range from 1 to N unless otherwise indicated.

An interesting redefinition of the auxiliary variables obtains by setting

$$M_{nm} = (z_n - z_m)^{-1}(\dot{z}_n\dot{z}_m)^{1/2}u_{nm} \tag{4}$$

(as already mentioned in Ref. 16 this assignment is suggested by the form of the Lax matrix introduced in Ref. 7). The equations of motion (3) of the many-body model take thereby the form

$$\ddot{z}_n = 2a\dot{z}_n z_n + 2\sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m}{z_n - z_m}u_{nm}u_{mn}, \tag{5a}$$

$$\dot{u}_{nm} + \frac{\dot{z}_n - \dot{z}_m}{z_n - z_m} u_{nm}(1 - u_{nm}u_{mn}) = -\sum_{\ell=1;\ell\neq n,m}^{N} \dot{z}_\ell \left[\frac{u_{n\ell}(u_{\ell m} + u_{nm}u_{\ell n})}{z_n - z_\ell} + \frac{u_{\ell m}(u_{n\ell} + u_{nm}u_{m\ell})}{z_m - z_\ell} \right]$$

$$- u_{nm}(F_n - F_m), \quad n \neq m. \tag{5b}$$

Here the auxiliary variables are of course the $N(N-1)$ quantities $u_{nm}(t)$; and note that, while the (Newtonian) equations of motion (5a) that characterize the evolution of the "particle coordinates" $z_n(t)$ follow straightforwardly from (3a) via (4), to obtain the equations (5b) that characterize the evolution of the auxiliary variables $u_{nm}(t)$ from (5b) one must use, in addition to (4), the equations of motion (5a). It is now clear that, for $F_n=0$ (or, equivalently, for $F_n=F$), the $N(N-1)$ evolution equations (5b) admit the (special) solution

$$u_{nm} = -1, \quad n \neq m, \tag{6}$$

entailing that the Newtonian equations of motion (5a) become then

$$\ddot{z}_n = 2a\dot{z}_n z_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m}. \tag{7}$$

For $a=0$ these equations of motion coincide with those of the standard "goldfish" model (see Refs. 13, 8, 14, 15, and 17 and the literature quoted there); for $a\neq 0$ they characterize a novel *solvable* extension of the goldfish many-body problem.

Before discussing the solvability of this model, (7), let us note its Hamiltonian character (see Ref. 14 and the literature quoted there). Indeed the Hamiltonian

$$H = \sum_{n=1}^{N} \left\{ -\frac{a}{s} z_n^2 + \exp(sp_n) \prod_{m=1,m\neq n}^{N} (z_n - z_m)^{-1} \right\}, \tag{8a}$$

where s is an arbitrary (nonvanishing) constant, yields the Hamiltonian equations

$$\dot{z}_n = \frac{\partial H}{\partial p_n} = s\exp(sp_n) \prod_{m=1,m\neq n}^{N} (z_n - z_m)^{-1}, \tag{8b}$$

$$\dot{p}_n = -\frac{\partial H}{\partial z_n} = \frac{1}{s}\left\{ 2az_n + \sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n + \dot{z}_m}{z_n - z_m} \right\}. \tag{8c}$$

Note that to write more neatly the second set of these Hamiltonian equations, (8c), we used the first, (8b). It is then obvious that t-differentiation of (the logarithm of) the first set of Hamiltonian equations (8b), yields, via the second set (8c), just the Newtonian equations of motion (7), demonstrating thereby their Hamiltonian character.

The solution of the initial-value problem for this many-body model, (7), is given by the following result (proven in Sec. II): the coordinates $z_n(t)$ are the N eigenvalues of the $N\otimes N$ matrix (2a) with

$$(A^2)_{nm} = -\delta_{nm}a^2 z_n^2(0) + a[\dot{z}_n(0)\dot{z}_m(0)]^{1/2}, \quad B_{nm} = \delta_{nm}az_n(0). \tag{9}$$

Here δ_{nm} is the standard Kronecker symbol, $\delta_{nm}=1$ if $n=m$, $\delta_{nm}=0$ if $n\neq m$. These formulas indicate that the $N\otimes N$ matrix B is diagonal, while the $N\otimes N$ matrix A^2 is the sum of a diagonal matrix and a dyadic matrix.

Via the standard trick (outlined at the end of this section; for more detailed and general treatments see, for instance, Refs. 10, 12, and 14) the following variant of the model (7) is obtained:

$$\ddot{z}_n - 3i\omega\dot{z}_n - 2\omega^2 z_n = 2a(\dot{z}_n - i\omega z_n)z_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m - i\omega(\dot{z}_n z_m + \dot{z}_m z_n) - \omega^2 z_n z_m}{z_n - z_m}. \tag{10}$$

Here and throughout ω is a *real* (for definiteness, *positive*) constant, and because of the way this ω-modified system is obtained from (7) *all* its nonsingular solutions are completely periodic with period,

$$T = \frac{2\pi}{\omega}, \tag{11}$$

or with an integer multiple of this basic period. Indeed the solutions $z_n(t)$ of these equations of motion, (10), are the N eigenvalues of the ω-modified matrix $\tilde{U}(t)$ defined as follows:

$$\tilde{U}(t) = \exp(i\omega t)U(\tau), \quad \tau = \frac{\exp(i\omega t) - 1}{i\omega}, \tag{12a}$$

where the matrix $U(\tau)$ is defined by (2a) (of course with t replaced by τ), but now with

$$\tilde{U}(0) = a^{-1}B, \quad \dot{\tilde{U}}(0) = a^{-1}(A^2 + B^2) + i\omega\tilde{U}(0), \tag{12b}$$

entailing

$$A^2 = -a^2[\tilde{U}(0)]^2 + a\dot{\tilde{U}}(0) - ia\omega\tilde{U}(0), \quad B = a\tilde{U}(0). \tag{12c}$$

In terms of the initial-value data for the model (10) these expressions read

$$(A^2)_{nm} = -\delta_{nm}a^2 z_n^2(0) + a\{[\dot{z}_n(0) - i\omega z_n(0)][\dot{z}_m(0) - i\omega z_m(0)]\}^{1/2},$$

$$B_{nm} = \delta_{nm}a z_n(0). \tag{12d}$$

Note that the assertion made above about the complete periodicity of *all* the nonsingular solutions of the system (10) is implied by the assertion made now about the solution of this system, since it is clear that the matrix $\tilde{U}$ is periodic in the time variable t with period T, see (11), (12a), and (2a). This incidentally allows to consider this generalized goldfish model, (10), as describing an assembly of "nonlinear harmonic oscillators."[18] The behavior of this system in the neighborhood of its equilibrium configuration is discussed in Sec. IV.

Finally let us emphasize that the solutions $z_n(t)$ of the generalized goldfish model (10) are necessarily *complex* (for *positive* ω, $\omega > 0$) and that these equations of motion can be reformulated as *real* and *covariant* equations describing the motion in the (horizontal) plane of N particles the positions of which there are identified by the *real* two-vectors $\vec{r}_n$ related to the *complex* numbers z_n by the standard[11,12,16] relations

$$z_n = x_n + iy_n, \quad a = a_x - ia_y, \tag{13a}$$

$$\vec{r}_n = (x_n, y_n, 0), \quad \vec{a} = (a_x, a_y, 0), \quad \hat{k} = (0,0,1), \tag{13b}$$

which entail that the equations of motion (10) read then as follows:

$$\ddot{\vec{r}}_n - 3\omega\hat{k}\wedge\dot{\vec{r}}_n - 2\omega^2\vec{r}_n = 2[\dot{\vec{r}}_n(\vec{a}\cdot\vec{r}_n) + \vec{r}_n(\vec{a}\cdot\dot{\vec{r}}_n) - \vec{a}(\dot{\vec{r}}_n\cdot\vec{r}_n)] - 2\omega\hat{k}\wedge[2\vec{r}_n(\vec{a}\cdot\vec{r}_n) - \vec{a}r_n^2]$$
$$+ 2\sum_{m=1,m\neq n}^{N} r_{nm}^{-2}\{\dot{\vec{r}}_n(\dot{\vec{r}}_m\cdot\vec{r}_{nm}) + \dot{\vec{r}}_m(\dot{\vec{r}}_n\cdot\vec{r}_{nm}) - \vec{r}_{nm}(\dot{\vec{r}}_n\cdot\dot{\vec{r}}_m) - \omega\hat{k}\wedge[\dot{\vec{r}}_n(\vec{r}_m\cdot\vec{r}_{nm})$$
$$+ \dot{\vec{r}}_m(\vec{r}_n\cdot\vec{r}_{nm}) - \vec{r}_n([\dot{\vec{r}}_n+\dot{\vec{r}}_m]\cdot\vec{r}_m) + \vec{r}_m([\dot{\vec{r}}_n+\dot{\vec{r}}_m]\cdot\vec{r}_m)] + \omega^2[\vec{r}_n r_m^2 - \vec{r}_m r_n^2]\}, \tag{13c}$$

where we use the short-hand notation $\vec{r}_{nm}\equiv\vec{r}_n-\vec{r}_m$ entailing $r_{nm}^2=r_n^2+r_m^2-2\vec{r}_n\cdot\vec{r}_m$. This equation is covariant [thanks to the definition (13) of a; note the minus sign there], but it is not rotation-invariant because the constant two-vector $\vec{a}$ identifies a preferred direction in the plane.

Before closing this section let us, for completeness, outline how the *isochronous* model (10) is obtained from (7), which to this end we rewrite here in the following (merely notationally) modified guise:

$$\zeta_n'' = 2a\zeta_n'\zeta_n + 2\sum_{m=1,m\neq n}^{N}\frac{\zeta_n'\zeta_m'}{\zeta_n-\zeta_m}, \tag{14}$$

where $\zeta_n\equiv\zeta_n(\tau)$ and appended primes indicate of course differentiations with respect to the (*complex*, see immediately below) independent variable τ. We then set

$$z_n(t) = \exp(i\omega t)\zeta_n(\tau),\quad \tau = \frac{\exp(i\omega t)}{i\omega}. \tag{15}$$

And it is then easily verified that (14) implies (10).

II. SOLUTION TECHNIQUE

The point of departure of our treatment is the $N\otimes N$ matrix equation (1). We then introduce the parametrization of the $N\otimes N$ matrix $U(t)$ in terms of its N eigenvalues $z_n(t)$ and of its diagonalizing $N\otimes N$ matrix $R(t)$,

$$U = RZR^{-1}, \tag{16a}$$

$$Z = \mathrm{diag}[z_n]. \tag{16b}$$

But before proceeding to obtain the evolution equations implied by (1) for the diagonal matrix $Z(t)$ and for the diagonalizing matrix $R(t)$, or rather (see below) for the matrix $M(t)$ defined in terms of $R(t)$ by the formula

$$M = R^{-1}\dot{R}, \tag{17}$$

let us note that the formulas (16) define the matrix R only up to multiplication from the right by an *arbitrary* diagonal matrix, say

$$D = \mathrm{diag}[d_n], \tag{18}$$

since replacing in (16a) R with

$$\tilde{R} = RD \tag{19}$$

is clearly of no consequence. The corresponding "gauge transformation" of the matrix M,

$$\tilde{M} = \tilde{R}^{-1}\dot{\tilde{R}} = D^{-1}MD + D^{-1}\dot{D}, \tag{20a}$$

namely

$$\tilde{M}_{nn} = M_{nn} + \frac{\dot{d}_n}{d_n}, \tag{20b}$$

$$\tilde{M}_{nm} = d_n^{-1} M_{nm} d_m, \quad n \neq m, \tag{20c}$$

entails that in our parametrization of the $N \otimes N$ matrix $U(t)$ [via (16) with (17)] the N^2 matrix elements of this matrix get replaced by the N elements $z_n(t)$ of the diagonal matrix $Z(t)$ [namely by the N eigenvalues of the matrix $U(t)$: see (16)] and by the $N(N-1)$ off-diagonal elements $M_{nm}(t)$ (with $n \neq m$) of the $N \otimes N$ matrix $M(t)$, while the N diagonal elements $M_{nn}(t)$ can be arbitrarily adjusted by choosing appropriately the elements $d_n(t)$ of the diagonal matrix $D(t)$, see (20b) [of course, up to a corresponding adjustment of the corresponding off-diagonal elements, see (20c)].

Differentiation of (16a) with respect to the independent variable t yields, using (17),

$$\dot{U} = R\{\dot{Z} + [M,Z]\}R^{-1}, \tag{21a}$$

$$\ddot{U} = R\{\ddot{Z} + [\dot{M},Z] + 2[M,\dot{Z}] + [M,[M,Z]]\}R^{-1}. \tag{21b}$$

Here and throughout we use of course the standard notation $[X,Y] \equiv XY - YX$ for the commutator of two matrices.

The treatment in this section has been up to now identical to that of Ref. 16 (it is reported here to make this paper self-contained). We now insert these formulas, (16) and (21), in the matrix evolution equation (1) and we thereby obtain the $N \otimes N$ matrix evolution equation,

$$\ddot{Z} + [\dot{M},Z] + 2[M,\dot{Z}] + [M,[M,Z]] = a\{(\dot{Z} + [M,Z])Z + Z(\dot{Z} + [M,Z])\}, \tag{22}$$

namely, by separating the diagonal and off-diagonal terms, precisely the system (3), where we made the notational assignment

$$M_{nn} \equiv F_n \tag{23}$$

and, consistently with the observation made above, we retain the freedom to assign arbitrarily these N quantities F_n.

All the other findings reported in Sec. I follow sufficiently straightforwardly not to require additional elaboration here.

Of course alternative assignments, different from (4), could be made.[16] For instance the introduction of the new auxiliary variables $g_{nm}(t)$ in place of $M_{nm}(t)$ via the natural position[16]

$$M_{nm} = (z_n - z_m)^{-2} g_{nm}, \quad n \neq m, \tag{24}$$

transforms the equations of motion (3) into

$$\ddot{z}_n = 2a\dot{z}_n z_n - 2\sum_{m=1, m\neq n}^{N} \frac{g_{nm}g_{mn}}{(z_n - z_m)^3}, \tag{25a}$$

$$\dot{g}_{nm} - a(z_n + z_m)g_{nm} = -\sum_{\ell=1;\ell\neq n,m}^{N} g_{n\ell}g_{\ell m}[(z_n - z_\ell)^{-2} - (z_m - z_\ell)^{-2}] - g_{nm}(F_n - F_m), \quad n \neq m. \tag{25b}$$

But, for $a \neq 0$, there is no choice of the arbitrarily assignable quantities F_n that is consistent with getting rid of the auxiliary variables g_{nm} (in the sense of making them time independent).

Before ending this section we like to reiterate[16] that the approach presented here is not altogether new, see, for instance, the following papers: Refs. 4, 25, 20, 26–29, 23, 5, 6, 22, 24, 3, 2, and 17.

III. AN ALTERNATIVE APPROACH

In this section we describe an alternative approach (see, for instance, Sec. 2.3 of Ref. 14). Let $\psi(z,t)$ be a monic polynomial of degree N in the (complex) variable z, and let us denote with $c_m(t)$ its coefficients and with $z_n(t)$ its zeros [which will be eventually identified with the coordinates of the particles evolving according to the Newtonian equations of motion (7)]:

$$\psi(z,t)=\prod_{n=1}^{N}[z-z_n(t)]=z^N+\sum_{m=1}^{N}c_m(t)z^{N-m}. \tag{26}$$

Note that this formula implies the relation

$$c_1(t)=-\sum_{n=1}^{N}z_n(t). \tag{27}$$

We now recall the relations [that obtain by logarithmic differentiation of the representation of $\psi(z,t)$ via its zeros, see (26); or see the Eqs. (2.3.2–8, 11) of Ref. 14],

$$\psi_t(z,t)=-\psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\dot{z}_n(t), \tag{28}$$

that clearly implies [via (27)]

$$z\psi_t(z,t)-\dot{c}_1(t)\psi(z,t)=\psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\{-z_n(t)\dot{z}_n(t)\} \tag{29a}$$

and

$$\psi_{tt}(z,t)=\psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{-\ddot{z}_n(t)+2\sum_{m=1,m\neq n}^{N}\frac{\dot{z}_n(t)\dot{z}_m(t)}{z_n(t)-z_m(t)}\right\}. \tag{29b}$$

Here and below subscripted variables denote of course partial differentiations.

It is clear from these formulas, (29), that the equations of motion (7) imply that the polynomial (26) satisfy the PDE

$$\psi_{tt}(z,t)-2a[z\psi_t(z,t)-\dot{c}_1(t)\psi(z,t)]=0, \tag{30}$$

and clearly this PDE, via the (second) relation (26), entails the system of ODEs,

$$\ddot{c}_m-2a\dot{c}_{m+1}+2a\dot{c}_1c_m=0, \tag{31a}$$

supplemented with the "boundary conditions"

$$c_0=1,\ \ c_{N+1}=0. \tag{31b}$$

Note that (31a) is trivially satisfied for $m=0$ [see (31b)], and that it can be integrated once for $m=1$ yielding

$$c_2=\frac{1}{2}c_1^2+\frac{1}{2a}(\dot{c}_1+C), \tag{32}$$

where C is an integration constant. Insertion of this expression of c_2 in (31a) with $m=2$ yields

$$\dot{c}_3 = \left(\frac{1}{2a}\right)^2 \dddot{c}_1 + \frac{\ddot{c}_1 c_1 + 2\dot{c}_1^2 + C\dot{c}_1}{2a} + \frac{1}{2}\dot{c}_1 c_1^2, \tag{33}$$

the right-hand side of which is however not an exact differential. Alternatively one could start from $m=N$ [which yields, see (34), the Schrödinger-type linear equation

$$\ddot{c}_N + 2a\dot{c}_1 c_N = 0, \tag{34}$$

with $c_N(t)$ playing the role of eigenfunction and $\dot{c}_1(t)$ playing the role of "potential"] and work all the way down by solving sequentially (but only formally) the series of second-order, nonhomogeneous, linear ODEs for $c_m(t)$ with $m=N-1, N-2, \ldots$, arriving in the end, for $m=1$, to a highly nonlinear (integrodifferential) equation for $c_1(t)$.

Clearly the fact that the system (31) is *solvable* is far from trivial. It is obviously implied by the results described above, since the coefficients $c_m(t)$ can be explicitly written in terms of the zeros $z_n(t)$ (see, for instance, Sec. 2.3.1 of Ref. 14); in particular (26) and (16) clearly entail the relations

$$c_1(t) = -\,\mathrm{trace}[U(t)], \quad c_N(t) = (-)^N \det[U(t)] \tag{35}$$

with the $N \otimes N$ matrix $U(t)$ evolving according to (2a).

The *isochronous* variant of this system, (31), can be obtained by first rewriting it in the following guise:

$$\gamma_m'' - 2a\gamma_{m+1}' + 2a\gamma_1'\gamma_m = 0, \quad \gamma_0 = 1, \quad \gamma_{N+1} = 0 \tag{36}$$

with $\gamma_m \equiv \gamma_m(\tau)$, and by then setting

$$c_m(t) = \exp(im\omega t)\,\gamma_m(\tau), \quad \tau = \frac{\exp(i\omega t) - 1}{i\omega}. \tag{37}$$

It reads

$$\ddot{c}_m - i(2m+1)\omega\dot{c}_m - m(m+1)\omega^2 c_m - 2a[\dot{c}_{m+1} - i(m+1)\omega c_{m+1}] + 2a[\dot{c}_1 - i\omega c_1]c_m = 0,$$

$$c_0 = 1, \quad c_{N+1} = 0. \tag{38}$$

Again, the *isochronous* character of the *general* solution of this system, implied by our treatment, is a nontrivial finding (up to the observation that all true mathematical results are indeed trivial).

A detailed discussion of the behavior of these *solvable* systems of ODEs, (31) and (38), as well as (7) and (10), for small values of N is postponed to a separate paper.[19] In the next section we consider the behavior of the *isochronous* models, (10) and (38), in the neighborhood of their equilibrium configurations.

IV. EQUILIBRIUM CONFIGURATIONS OF THE ISOCHRONOUS MODELS, SMALL OSCILLATIONS AND DIOPHANTINE RELATIONS

In this section we discuss the equilibrium configuration of the two (clearly related) *isochronous* models characterized by the equations of motion (10) and (38), as well as the behavior of these systems in the neighborhood of their equilibrium configurations. In this manner we also obtain some results for "remarkable matrices," following an approach already employed in the past in analogous contexts, see for instance Refs. 1, 9, and 14 and the references cited there.

The equilibrium configuration

$$z_n(t) = \overline{z_n},\ \ \dot{z}_n(t) = 0 \tag{39a}$$

of the system (10) is clearly characterized by the following system of N algebraic equations which determine (up to permutations) the N unknowns $\overline{z_n}$:

$$1 = i\left(\frac{a}{\omega}\right)\overline{z_n} + \sum_{m=1,m\neq n}^{N} \frac{\overline{z_m}}{\overline{z_n} - \overline{z_m}}. \tag{39b}$$

This suggests setting

$$\overline{z_n} = \left(\frac{i\omega}{2a}\right)x_n. \tag{40}$$

This notation is convenient to make contact with other results; the reader should of course note that the numbers x_n introduced here have nothing to do with the real parts of the quantities z_n, see (13). Indeed these N numbers x_n need not be real; they satisfy the N algebraic equations

$$x_n = -2 + 2\sum_{m=1,m\neq n}^{N} \frac{x_m}{x_n - x_m}, \tag{41a}$$

or equivalently

$$x_n = -2N + 2\sum_{m=1,m\neq n}^{N} \frac{x_n}{x_n - x_m}, \tag{41b}$$

and can therefore be identified as the N zeros of the generalized Laguerre polynomial $L_N^{(-2N-1)}(x)$,

$$L_N^{(-2N-1)}(x_n) = 0. \tag{41c}$$

[Let us provide, for completeness, a proof of this result (not new, see Refs. 1 and 9 and the literature quoted there). The (conveniently normalized) generalized Laguerre polynomial

$$(-)^N N! L_N^{(-2N-1)}(x) \equiv \chi(x) = \sum_{m=0}^{N} \frac{(N+m)!x^{N-m}}{(N-m)!m!} \tag{42}$$

is characterized by the ODE

$$x\chi''(x) - (x+2N)\chi'(x) + N\chi(x) = 0, \tag{43}$$

while its representation via its zeros,

$$\chi(x) = \prod_{n=1}^{N}(x - x_n) \tag{44a}$$

entails clearly [by logarithmic differentiation; or see the Eqs. (7), (12), and (13) of Sec. 2.3.2 of Ref. 14]

$$\chi'(x) = \chi(x)\sum_{n=1}^{N}(x - x_n)^{-1}, \tag{44b}$$

$$x\chi'(x) - N\chi(x) = \chi(x)\sum_{n=1}^{N}(x - x_n)^{-1}x_n, \tag{44c}$$

$$x\chi''(x) = \chi(x)\sum_{n=1}^{N}(x-x_n)^{-1}2\sum_{m=1,m\neq n}^{N}(x_n-x_m)^{-1}x_n, \tag{44d}$$

where the appended primes denote of course differentiations. It is then clear that the insertion of these three formulas in (43) entails (41b).

Let us now consider the behavior of our *isochronous* system (10) in the neighborhood of its equilibrium configuration. To this end we set

$$z_n(t) = \overline{z_n} + \varepsilon w_n(t), \tag{45}$$

and we then insert this assignment in the equations of motion (10) treating ε as a small parameter. We thus get the *linearized* equations of motion

$$\ddot{w}_n - 3i\omega\dot{w}_n - 2\omega^2 w_n = 2a\overline{z_n}(\dot{w}_n - 2i\omega w_n) + 2\sum_{m=1,m\neq n}^{N}\left[\frac{-i\omega(\overline{z_m}\dot{w}_n + \overline{z_n}\dot{w}_m)}{\overline{z_n}-\overline{z_m}} + \frac{\omega^2(\overline{z_m^2}w_n - \overline{z_n^2}w_m)}{(\overline{z_n}-\overline{z_m})^2}\right], \tag{46a}$$

namely

$$\underline{\ddot{w}} + i\omega\underline{\Gamma}\underline{\dot{w}} + \omega^2\underline{\Lambda}\underline{w} = 0. \tag{46b}$$

Here and throughout this section, to underline the vector and matrix character of our formulas, N-vectors are denoted by *lower* case *underlined* letters, hence $\underline{w} \equiv \underline{w}(t)$ denotes the N-vector of components $w_n \equiv w_n(t)$, and likewise $N \otimes N$ matrices are denoted by *upper* case *underlined* letters. In particular the two (constant) matrices $\underline{\Gamma}$ and $\underline{\Lambda}$ are defined (componentwise) as follows, via (40), in terms of the N zeros x_n of the generalized Laguerre polynomial $L_N^{(-2N-1)}(x)$:

$$\Gamma_{nm} = -\delta_{nm} + (1-\delta_{nm})\frac{2x_n}{x_n - x_m}, \tag{47a}$$

$$\Lambda_{nm} = -\delta_{nm}2\left[1 + x_n + \sum_{\ell=1,\ell\neq n}^{N}\frac{x_\ell^2}{(x_n - x_\ell)^2}\right] + (1-\delta_{nm})\frac{2x_n^2}{(x_n - x_m)^2}. \tag{47b}$$

Note that to simplify the expression of the diagonal part of the matrix $\underline{\Gamma}$ we used (41a). For an analogous simplification of the expression of the diagonal part of the matrix $\underline{\Lambda}$ see, in the Appendix, (A8) with (A2).

The *general* solution of the linear evolution equations (46), is provided by the formula

$$\underline{w}(t) = \sum_{k=1}^{2N} a_k \exp(i\lambda_k\omega t)\underline{v}^{(k)}, \tag{48}$$

where the $2N$ constants a_k are arbitrary [to be determined, in the context of the initial-value problem, from the $2N$ initial data $w_n(0)$ and $\dot{w}_n(0)$], while the $2N$ numbers λ_k, respectively, the corresponding N-vectors $\underline{v}^{(k)}$, are the eigenvalues, respectively, the eigenvectors, of the following (generalized) N-vector eigenvalue equation [see (46b)]:

$$-\lambda_k^2\underline{v}^{(k)} - \lambda_k\underline{\Gamma}\underline{v}^{(k)} + \underline{\Lambda}\underline{v}^{(k)} = 0, \quad k = 1, \ldots, 2N. \tag{49}$$

Hence the numbers λ_k are the $2N$ roots of the following equation (polynomial of degree $2N$) in λ:

$$\det[\lambda^2\underline{1} + \lambda\underline{\Gamma} - \underline{\Lambda}] = 0. \tag{50}$$

Here and throughout $\underline{1}$ denotes of course the $N \otimes N$ unit matrix, $(\underline{1})_{nm} = \delta_{nm}$.

But we already know, from our previous treatment, that the solutions of the *isochronous* model (10) are *completely periodic* with period T, see (11). [Actually solutions with a (larger)

period which is an integer multiple of T can also emerge, due to the exchange of the identity of the eigenvalues of the matrix $U(t)$, see (12), through the motion; and some exceptional singular solutions also exist, in which two or more particles collide at some finite time; but neither one of these two phenomena can occur for the *small* oscillations around the equilibrium configuration considered here.] The same periodicity property must therefore characterize the behavior (48) in the neighborhood of the equilibrium configuration of this system. We thus arrive at the following *diophantine* finding: *the* $2N$ *numbers* λ_k *are all integers*. In fact, motivated by this finding and by some numerical checks, we make the following conjecture.

Conjecture: *Let the two* $N \otimes N$ *matrices* $\underline{\Gamma}$ *and* $\underline{\Lambda}$ *be defined by (47), in terms of the* N *zeros* x_n *of the generalized Laguerre polynomial* $L_N^{(-2N-1)}(x)$, *namely the polynomial of degree* N *characterized by the ODE (43); then*

$$\det[\lambda^2 \underline{1} + \lambda \underline{\Gamma} - \underline{\Lambda}] = \prod_{k=1}^{N} [(\lambda - 2k)(\lambda + 2k - 1)]. \tag{51}$$

It stands to reason that a route to prove this result emerge from the approach (based on generalized Lagrangean interpolation and yielding finite-dimensional representations of the differential operator[14]) employed in Refs. 1 and 9 to obtain analogous results; an outline of this approach, which seems to indicate some progress in this direction, is provided in the Appendix, but unfortunately it does not quite allow to prove the above conjecture, of the validity of which we are nevertheless quite certain, on the basis of numerical checks, see below.

Indeed a related *diophantine* conjecture—more explicit hence more suitable for numerical checks—is provided below, in the context of the investigation of the behavior of the *isochronous* system (38) in the neighborhood of its equilibrium configuration,

$$c_m(t) = \overline{c_m} = \left(\frac{i\omega}{2a}\right)^m \frac{(N+m)!}{(N-m)!m!}. \tag{52}$$

The fact that this formula provides a time-independent solution of (38) can be easily verified, as well as its consistency with (42) and (40).

To study the behavior of the system (38) in the neighborhood of this equilibrium configuration, (52), we now set

$$c_m(t) = \overline{c_m} + \varepsilon \left(\frac{i\omega}{2a}\right)^m \eta_m(t), \tag{53}$$

and by treating ε as a small parameter we obtain the following *linearized* system for the time evolution of the quantities $\eta_m(t)$:

$$\ddot{\eta}_m - i(2m+1)\omega \dot{\eta}_m + [N(N+1) - m(m+1)]\omega^2 \eta_m - i\omega \dot{\eta}_{m+1}$$
$$- (m+1)\omega^2 \eta_{m+1} + \frac{(N+m)!}{(N-m)!m!}[i\omega \dot{\eta}_1 + \omega^2 \eta_1] = 0,$$

$$\eta_0 = 0, \ \eta_{N+1} = 0, \tag{54a}$$

namely

$$\ddot{\underline{\eta}} + i\omega \underline{C}\, \dot{\underline{\eta}} + \omega^2 \underline{L}\, \underline{\eta} = 0, \tag{54b}$$

where the two matrices $\underline{C}$ and $\underline{L}$ are defined (componentwise) as follows:

$$C_{nm} = -\delta_{nm}(2n+1) - \delta_{n+1,m} + \delta_{1m}\frac{(N+n)!}{(N-n)!n!}, \tag{55a}$$

$$L_{nm} = \delta_{nm}[N(N+1) - n(n+1)] - \delta_{n+1,m}(n+1) + \delta_{1m}\frac{(N+n)!}{(N-n)!n!}. \tag{55b}$$

The *general* solution of this system of linear equations reads

$$\underline{\eta}(t) = \sum_{k=1}^{2N} b_k \exp(i\lambda_k \omega t)\underline{w}^{(k)}, \tag{56}$$

where the $2N$ constants b_k are arbitrary [to be determined, in the context of the initial-value problem, from the $2N$ initial data $\eta_n(0)$ and $\dot{\eta}_n(0)$], while the $2N$ numbers λ_k, respectively, the corresponding N-vectors $\underline{w}^{(k)}$, are the eigenvalues, respectively, the eigenvectors, of the following (generalized) matrix eigenvalue equation [see (54b)]:

$$-\lambda_k^2 \underline{w}^{(k)} - \lambda_k \underline{C}\,\underline{w}^{(k)} + \underline{L}\,\underline{w}^{(k)} = 0, \quad k = 1, \ldots, 2N. \tag{57}$$

Hence the numbers λ_k are the $2N$ roots of the following equation (polynomial of degree $2N$) in λ:

$$\det[\lambda^2 \underline{1} + \lambda \underline{C} - \underline{L}] = 0. \tag{58}$$

But obviously these numbers coincide with those defined above, see (50). We may therefore assert with certainty that they are *all* integers, and the Conjecture made above can now be reformulated to read

$$\det[\lambda^2 \underline{1} + \lambda \underline{C} - \underline{L}] = \prod_{k=1}^{N} [(\lambda - 2k)(\lambda + 2k - 1)]. \tag{59}$$

An even more explicit reformulation of this *diophantine* assertion can be made by taking advantage of the expressions (55) and noting that they entail that $\lambda = 2$ is certainly a root of (58) because the first line of the determinant of order N in the left-hand side of (58) and (59) is proportional to $\lambda - 2$. It reads [after factoring out the $(\lambda - 2)$ factor]

$$\begin{vmatrix} \lambda - 1 + N(N+1) & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ g_2 & f_2 & h_2 & 0 & 0 & 0 & 0 & 0 \\ g_3 & 0 & f_3 & h_3 & 0 & 0 & 0 & 0 \\ \vdots & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ g_n & 0 & 0 & 0 & f_n & h_n & 0 & 0 \\ \vdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \mathbf{0} \\ g_{N-1} & 0 & 0 & 0 & 0 & 0 & f_{N-1} & h_{N-1} \\ g_N & 0 & 0 & 0 & 0 & 0 & 0 & f_N \end{vmatrix} = \left[\prod_{k=2}^{N} (\lambda - 2k)\right]\left[\prod_{j=1}^{N} (\lambda + 2j - 1)\right] \tag{60a}$$

where

$$f_n = (\lambda - n + N)(\lambda - n - N - 1), \tag{60b}$$

$$g_n = \frac{(N+n)!}{(N-n)!n!}(\lambda - 1), \tag{60c}$$

$$h_n = n + 1 - \lambda. \tag{60d}$$

Examples of the (true) *diophantine* relations entailed, for increasing values of N, by this formula follow:

$$\begin{vmatrix} \lambda+5 & -1 \\ 12(\lambda-1) & \lambda(\lambda-5) \end{vmatrix} = (\lambda-4)(\lambda+1)(\lambda+3) = \lambda^3 - 13\lambda - 12, \tag{61}$$

$$\begin{vmatrix} \lambda+11 & -1 & 0 \\ 60(\lambda-1) & (\lambda+1)(\lambda-6) & 3-\lambda \\ 120(\lambda-1) & 0 & \lambda(\lambda-7) \end{vmatrix}$$
$$= (\lambda-4)(\lambda-6)(\lambda+1)(\lambda+3)(\lambda+5)$$
$$= (\lambda-7)(\lambda-6)\lambda(\lambda+1)(\lambda+11) + 60(\lambda-1)[(\lambda-7)\lambda + 2(\lambda-3)]$$
$$= (\lambda-7)(\lambda-6)\lambda(\lambda+1)(\lambda+11) + 60(\lambda-6)(\lambda-1)(\lambda+1)$$
$$= 120(\lambda-3)(\lambda-1) + (\lambda-7)\lambda[(\lambda-6)(\lambda+1)(\lambda+11) + 60(\lambda-1)]$$
$$= \lambda^5 - \lambda^4 - 43\lambda^3 + \lambda^2 + 402\lambda + 360, \tag{62}$$

$$\begin{vmatrix} \lambda+19 & -1 & 0 & 0 \\ 180(\lambda-1) & (\lambda+2)(\lambda-7) & 3-\lambda & 0 \\ 840(\lambda-1) & 0 & (\lambda+1)(\lambda-8) & 4-\lambda \\ 1680(\lambda-1) & 0 & 0 & \lambda(\lambda-9) \end{vmatrix}$$
$$= (\lambda-4)(\lambda-6)(\lambda-8)(\lambda+1)(\lambda+3)(\lambda+5)(\lambda+7)$$
$$= (\lambda-8)(\lambda+1)[(\lambda-9)(\lambda-7)\lambda(\lambda+2)(\lambda+19) - 60(\lambda-1)(3\lambda^2 - 13\lambda - 42)]$$
$$= (\lambda-4)[1680(\lambda-3)(\lambda-1) + (\lambda-9)\lambda(\lambda^4 + 11\lambda^3 + 9\lambda^2 - 179\lambda - 1522)]$$
$$= \lambda^7 - 2\lambda^6 - 98\lambda^5 + 100\lambda^4 + 2809\lambda^3 - 98\lambda^2 - 22\,872\lambda - 20\,160, \tag{63}$$

$$\begin{vmatrix} \lambda+29 & -1 & 0 & 0 & 0 \\ 420(\lambda-1) & (\lambda+3)(\lambda-8) & 3-\lambda & 0 & 0 \\ 3360(\lambda-1) & 0 & (\lambda+2)(\lambda-9) & 4-\lambda & 0 \\ 15\,120(\lambda-1) & 0 & 0 & (\lambda+1)(\lambda-10) & 5-\lambda \\ 30\,240(\lambda-1) & 0 & 0 & 0 & \lambda(\lambda-11) \end{vmatrix}$$
$$= (\lambda-4)(\lambda-6)(\lambda-8)(\lambda-10)(\lambda+1)(\lambda+3)(\lambda+5)(\lambda+7)(\lambda+9)$$
$$= (\lambda-10)(\lambda-8)(\lambda+1)(\lambda+3)[(\lambda-11)(\lambda-9)(\lambda+2)(\lambda+29) - 420(\lambda-1)\lambda(\lambda^2 - 5\lambda - 18)]$$
$$= (\lambda-4)[-30\,240(\lambda-5)(\lambda-3)(\lambda-1)$$
$$+ (\lambda-11)\lambda(\lambda^6 + 12\lambda^5 - 50\lambda^4 - 900\lambda^3 + 229\lambda^2 + 888\lambda + 120\,780)]$$
$$= \lambda^9 - 3\lambda^8 - 186\lambda^7 + 378\lambda^6 + 11\,529\lambda^5$$
$$- 11\,907\lambda^4 - 275\,584\lambda^3 + 11\,532\lambda^2 + 2\,078\,640\lambda + 1\,814\,400. \tag{64}$$

In these equations we also reported the expressions that are obtained when the determinants are computed by expanding via the first, or the last, line, which only contain two nonvanishing terms and yield relations that also have a nontrivial diophantine character.

The determinant appearing in the left-hand side of (60a) can be somewhat simplified, without changing its value, by performing the similarity transformation that corresponds to multiplying its element in the line n and the column m by the factor g_m/g_n, see (60c). Thereby (60) gets replaced by

$$\begin{vmatrix} \lambda-1+N(N+1) & -\frac{(N+2)(N-1)}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ N(N+1)(\lambda-1) & f_2 & \tilde{h}_2 & 0 & 0 & 0 & 0 & 0 \\ N(N+1)(\lambda-1) & 0 & f_3 & \tilde{h}_3 & 0 & 0 & 0 & 0 \\ \vdots & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ N(N+1)(\lambda-1) & 0 & 0 & 0 & f_n & \tilde{h}_n & 0 & 0 \\ \vdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \mathbf{0} \\ N(N+1)(\lambda-1) & 0 & 0 & 0 & 0 & 0 & f_{N-1} & \tilde{h}_{N-1} \\ N(N+1)(\lambda-1) & 0 & 0 & 0 & 0 & 0 & 0 & f_N \end{vmatrix} = \left[\prod_{k=2}^{N}(\lambda-2k)\right]\left[\prod_{j=1}^{N}(\lambda+2j-1)\right], \tag{65a}$$

where f_n is of course always defined by (60b) and

$$\tilde{h}_n = \frac{(N+n+1)(N-n)(n+1-\lambda)}{n+1}. \tag{65b}$$

Another version of this formula is obtained by subtracting, in the determinant which appears in the left-hand side of (65a), from every line (except the first two) the line above it,

$$\begin{vmatrix} \lambda-1+N(N+1) & -\frac{(N+2)(N-1)}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ N(N+1)(\lambda-1) & f_2 & \tilde{h}_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -f_2 & \tilde{f}_3 & \tilde{h}_3 & 0 & 0 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \ddots & \ddots & \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 0 & 0 & -f_{n-1} & \tilde{f}_n & \tilde{h}_n & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \ddots & \mathbf{0} \\ 0 & 0 & 0 & 0 & 0 & -f_{N-2} & \tilde{f}_{N-1} & \tilde{h}_{N-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & -f_{N-1} & \tilde{f}_N \end{vmatrix} = \left[\prod_{k=2}^{N}(\lambda-2k)\right]\left[\prod_{j=1}^{N}(\lambda+2j-1)\right], \tag{66a}$$

where f_n, respectively, $\tilde{h}_n$ continues of course to be defined by (60b), respectively, (65b) while

$$\tilde{f}_n = f_n - \tilde{h}_{n-1} = (\lambda-2n)\left(\lambda-n+\frac{N(N+1)}{n}\right). \tag{66b}$$

Since clearly [see (60b) and (66b)]

$$f_{N-1} = \tilde{f}_N = (\lambda+1)(\lambda-2N), \tag{66c}$$

we identify from this formulation, (66), two additional roots of the original determinant [in addition to $\lambda=2$, see (59)], namely $\lambda=-1$ and $\lambda=2N$, since the last line of the determinant in the left-hand side of (66a) vanishes for these values of λ, see (66c).

As example, let us exhibit (66) for $N=5$,

$$\begin{vmatrix} \lambda+29 & -14 & 0 & 0 & 0 \\ 30(\lambda-1) & (\lambda-8)(\lambda+3) & -8(\lambda-3) & 0 & 0 \\ 0 & -(\lambda-8)(\lambda+3) & (\lambda-6)(\lambda+7) & -\frac{9}{2}(\lambda-4) & 0 \\ 0 & 0 & -(\lambda-9)(\lambda+2) & (\lambda-8)\left(\lambda+\frac{7}{2}\right) & -2(\lambda-5) \\ 0 & 0 & 0 & -1 & 1 \end{vmatrix}$$
$$= (\lambda-4)(\lambda-6)(\lambda-8)(\lambda+3)(\lambda+5)(\lambda+7)(\lambda+9), \tag{67}$$

where we eliminated from the last line, and of course from the right-hand side, the factor $(\lambda-10)(\lambda+1)$.

Let us end this section by mentioning that an analogous discussion could be made for the *nonisochronous* cases (7) [namely, (10) with $\omega=0$] and (31) [namely, (38) with $\omega=0$]. In those cases *any* configuration is an equilibrium one, since particles with vanishing initial velocities do not move. But the mathematical implications of the behavior of these models near their equilibrium configuration are not so interesting: indeed a treatment analogous to that made above leads merely to the rather trivial identity

$$\begin{vmatrix} z+c_1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_2 & z & -1 & 0 & 0 & 0 & 0 & 0 \\ c_3 & 0 & z & -1 & 0 & 0 & 0 & 0 \\ \vdots & \mathbf{0} & \ddots & \ddots & \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ c_n & 0 & 0 & 0 & z & -1 & 0 & 0 \\ \vdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \ddots & \ddots & \ddots & 0 \\ c_{N-1} & 0 & 0 & 0 & 0 & 0 & z & -1 \\ c_N & 0 & 0 & 0 & 0 & 0 & 0 & z \end{vmatrix} = z^N + \sum_{m=1}^{N} c_m z^{N-m}, \tag{68}$$

valid for any arbitrary set of N numbers c_n.

V. OUTLOOK

Recently, via an approach analogous to that described in Sec. III, a model remarkably similar to that considered in this paper has been investigated by Gomez-Ullate, Hone, and Sommacal.[21] The equations of motions of their model, in its "many-body problem" formulation, read

$$\ddot{z}_n = 2(1-N)z_n^3 + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m + z_n^4}{z_n - z_m}, \tag{69}$$

and those of the model related to it via the approach of Sec. III read

$$\ddot{c}_m + (m+1)(m+2)c_{m+2} - 2c_2c_m = 0, \tag{70a}$$

with the "boundary conditions"

$$c_0 = 1, \quad c_{N+1} = 0. \tag{70b}$$

Via the simple change of dependent variables,

$$z_n = b\tilde{z}_n, \; b = \left(\frac{a}{1-N}\right)^{1/2}, \tag{71}$$

the equations of motion (69) can be recast in the form

$$\ddot{\tilde{z}}_n = 2a\tilde{z}_n^3 + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{\tilde{z}}_n\dot{\tilde{z}}_m + b^2\tilde{z}_n^4}{\tilde{z}_n - \tilde{z}_m}, \tag{72}$$

demonstrating that they are indeed rather similar to (7). Likewise, via the simple change of dependent variables,

$$c_{2m} = \frac{(-a)^m \tilde{c}_m}{(2m)!}, \tag{73}$$

the evolution equations (70a) (with even m; note that they are decoupled from those for odd m) become

$$\ddot{\tilde{c}}_m - 2a\tilde{c}_{m+1} + 2a\tilde{c}_1\tilde{c}_m = 0, \tag{74}$$

which are remarkably similar to the evolution equations (31a). However, in contrast to the systems treated in this paper, (7) and (31), which are *solvable*, as explained above, for *all* values of the positive integer N, the systems (69) and (70), or equivalently (72) and (74), have been shown to be *solvable* only for $N<4$; moreover, for $N=3$ their solution generally involves transcendental (more precisely, elliptic) functions of the time variable, as well as algebraic functions of such elliptic functions (typically roots of N-degree polynomials the coefficients of which evolve in time as elliptic functions), in contrast to the solution of the models treated in this paper, which clearly only involve, for all values of N, algebraic functions of elementary (more precisely, exponential, or equivalently trigonometric) functions of the time variable [again, typically, via roots of N-degree polynomials the coefficients of which evolve exponentially, or equivalently trigonometrically, in the time variable, see (2a)].

APPENDIX

Let the two $N\otimes N$ matrices $\underline{X}$ and $\underline{D}$ be defined, in terms of the N, *a priori* arbitrary, numbers x_n, as follows:

$$\underline{X} = \mathrm{diag}[x_n],\ X_{nm} = \delta_{nm}x_n, \tag{A1}$$

$$D_{nm} = \delta_{nm}d_n + (1-\delta_{nm})(x_n - x_m)^{-1}, \tag{A2a}$$

$$d_n = \sum_{\ell=1,\ell\neq n}^{N} (x_n - x_\ell)^{-1}. \tag{A2b}$$

[Beware, this nondiagonal matrix $\underline{D}$ has nothing to do with the diagonal matrix D of Sec. II, see (18)–(20).] It is then known [see Eq. (2.4.1–5d) of Ref. 14] that

$$(\underline{D}^2)_{nm} = \delta_{nm}\left[d_n^2 - \sum_{\ell=1,\ell\neq n}^{N} (x_n - x_\ell)^{-2}\right] + (1-\delta_{nm})2[d_n(x_n - x_m)^{-1} - (x_n - x_m)^{-2}], \tag{A3}$$

and that the following result (Corollary 2.4.1–3 of Ref. 14) holds: *if for the differential operator*

$$\hat{A} = \sum_k a_k(x)\left(\frac{d}{dx}\right)^k \tag{A4a}$$

there holds the equation

$$\hat{A}f(x) = 0 \tag{A4b}$$

with $f(x)$ a polynomial in x of degree less than N, then the $N\otimes N$ matrix

$$\underline{A} = \sum_k a_k(\underline{X})\underline{D}^k \tag{A5a}$$

has vanishing determinant,

$$\det[\underline{A}] = 0. \tag{A5b}$$

Assume now that the N numbers x_n coincide with the N zeros of the generalized Laguerre polynomial $L_N^{(-2N-1)}(x)$. There holds then the following relations:

$$d_n = \frac{1}{2} + \frac{N}{x_n}, \tag{A6a}$$

$$x_n^2 \sum_{\ell=1,\ell\neq n}^{N} (x_n - x_\ell)^{-2} = -\frac{1}{12}(x_n^2 + 4N^2 - 8N), \tag{A6b}$$

$$\sum_{\ell=1,\ell\neq n}^{N} x_\ell^2 (x_n - x_\ell)^{-2} = -\frac{1}{12}(x_n^2 + 12x_n + 4N^2 + 4N + 12) \tag{A6c}$$

[the first coincides with (41b) via (A2b), the second and third can be easily obtained from the first, or, more directly, from Eq. (4.2c) of Ref. 1, via (41a) and (41b)].

Using these formulas we see [from (47a), via (A1), (A2), and (A6a)] that

$$\underline{\Gamma} = 2\underline{X}\underline{D} - \underline{X} - (1+2N)\underline{1}, \tag{A7}$$

and likewise [from (47b), via (A1), (A2), and (A6)] that

$$\underline{\Lambda} = -\underline{X}^2\underline{D}^2 + (\underline{X} + 2N)\underline{X}\underline{D} - N\underline{X}. \tag{A8}$$

Hence (50) reads now

$$\det\{\underline{X}^2\underline{D}^2 - [\underline{X} + 2(N-\lambda)]\underline{X}\underline{D} + (N-\lambda)\underline{X} + [\lambda^2 - (1+2N)\lambda]\underline{1}\} = 0. \tag{A9}$$

Therefore if, for some value of λ, the ODE

$$x^2 f''(x) - [x + 2(N-\lambda)]xf'(x) + [(N-\lambda)x + \lambda^2 - (1+2N)\lambda]f(x) = 0 \tag{A10}$$

were satisfied by a polynomial in x of degree less than N, we could assert that that same value of λ satisfies the determinantal equation (A9). But unfortunately, as it can be easily shown, for no value of λ this ODE is satisfied by a polynomial of degree less than N [for certain values of λ it is satisfied by a polynomial $f(x)$ of degree no less than N; for instance for $N=1$ and $\lambda=0$ this equation is satisfied by the polynomial $f(x)=x+2$ of degree 1]. We must therefore conclude (much to our surprise) that this approach does not (seem to) allow us to prove the conjecture proffered above.

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An algebraic Birkhoff decomposition for the continuous renormalization group

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This paper aims at presenting the first steps towards a formulation of the Exact Renormalization Group Equation in the Hopf algebra setting of Connes and Kreimer. It mostly deals with some algebraic preliminaries allowing us to formulate perturbative renormalization within the theory of differential equations. The relation between renormalization, formulated as a change of boundary condition for a differential equation, and an algebraic Birkhoff decomposition for rooted trees is explicited. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1794366]

I. INTRODUCTION

During the last five decades, renormalization group theory has proven to be a major discovery in theoretical physics whose applications range from high energy physics, its original birthplace,[19] to statistical physics and dynamical systems, thanks to the work of Wilson.[16] Originally proposed as a computational device in quantum field theory allowing to compare physical theories defined at different energy scales, it finally turned out to have a deep conceptual significance. Indeed, it is known since more than twenty years that renormalization group arguments allow to define the theory in the sense that one can construct a finite renormalized quantum field theory by asking it to fulfil a differential equation known as the Exact Renormalization Group Equation.[20]

On the other side, renormalization recently triggered a couple of mathematical works[4] that focused on algebraic aspects of the subtraction procedure and of the resulting renormalization group invariance. While these works mostly focus on the BPHZ procedure formulated within the minimal subtraction procedure in dimensional regularization (see, for instance, Ref. 17 for an application to the renormalization of the wave function), it is obvious that the framework proposed by Connes and Kreimer is versatile enough to encompass the ERGE.

This paper aims at presenting the first steps towards a formulation of the ERGE in the Hopf algebra setting. It mostly deals with some algebraic preliminaries allowing to formulate perturbative renormalization within the theory of differential equations.

In the first part, we present some general results on rooted trees and their interpretation as a coefficients of formal power series of nonlinear operators, in analogy with the theory developed in numerical analysis under the name of B-series.[2,10] In the second part, we explicit the relation between renormalization, formulated as a change of boundary condition for a differential equation, and an algebraic Birkhoff decomposition for rooted trees.

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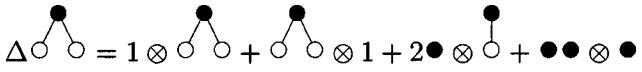


FIG. 1. Example of coproduct.

While this paper mostly presents some elementary facts, a more thorough survey involving the precise relation between trees and Feynman diagrams and their use as computational tools for effective actions will be the subject of a forthcoming publication.

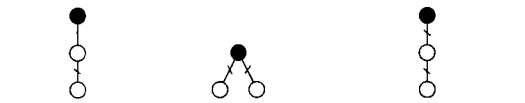
II. TREES AND POWER SERIES OF NONLINEAR OPERATORS

This section presents the algebraic tools for the interpretation of the continuous renormalization group in term of Birkhoff decomposition. We introduce the well-known Hopf algebra H of rooted trees to generate formal power series of (nonlinear) operators. Recalling the isomorphism between the group of characters of H and series with nonzero constant term, we focus on two particular series: The geometrical series $f_{\phi_1}[X]$ and the exponential series $f_{\phi_e}[X]$.

A. The Hopf algebra of rooted trees

Most of the material is detailed in Refs. 9 and 7 and refers to the original work Ref. 4. A rooted tree is a distinguished vertex, the *root*, together with a set of vertices and nonintersecting oriented lines. Any vertex has one and only one incoming line, except the root which has only outgoing lines. The *fertility* of a vertex is the number of its outgoing lines, its *length* is the number of lines of the (unique) path that joins it to the root. Two rooted trees are isomorphic if the number of vertices with given length and fertility is the same for all possible choices of lengths and fertilities. Symbols T, one for each isomorphism class, together with a unit 1 corresponding to the empty tree generate a complex commutative algebra H with disjoint union as a product.

A *simple cut* c of a tree T is a (nonempty) subset of its lines (selected for deletions) such that the path from the root to any other vertex includes at most one line of c. Deleting the cut lines produces $\mathrm{Card}(c)+1$ subtrees: The *trunk* $R_c(T)$ which contains the original root and the set $P_c(T)$ of the pruned branches. The set of simple cuts of T is written $C(T)$.



Definition II.1: H is a Hopf algebra with counit $\epsilon=0$ *except* $\epsilon(1)=1$, *the antipode*

$$S: \quad \bullet \mapsto \quad -\bullet$$

$$T \mapsto \quad -T - \sum_{c\in C(T)} - S(P_c(T))R_c(T) \tag{1}$$

and the coproduct

$$\Delta(T) = T\otimes 1 + 1\otimes T + \sum_{c\in C(T)} P_c(T)\otimes R_c(T), \quad \Delta(1) = 1\otimes 1. \tag{2}$$

(See Fig. 1.)

Among the common quantities associated to a tree T, we use the *symmetry factor* S_T which is the number of isomorphic trees that can be generated by permutation of the branches, the number of vertices $|T|$ (including the root) and the *depth* which is the maximum length of the vertices of T. The number of vertices is a natural graduation which makes H a graded connected Hopf algebra.[15]

The dual H^* (i.e., the set of linear applications from an Hopf algebra H to $\mathbb{C}$) is an algebra with the convolution product $*$

$$f * g(a) \doteq \langle f \otimes g, \Delta a \rangle, \tag{3}$$

for $f, g \in H^*, a \in H$ and $\langle , \rangle$ the duality pairing. For those f in H^* for which the transposition of the multiplication m of H takes its values in $H^* \otimes H^*$, one writes $\Delta(f) \doteq {}^t m(f)$, i.e.,

$$\Delta f(a \otimes b) = f(ab) \; \forall \; a, b \in H. \tag{4}$$

A *derivation* is an element δ of H^* satisfying

$$\Delta \delta = \delta \otimes \epsilon + \epsilon \otimes \delta. \tag{5}$$

The algebra generated by the derivations and ϵ is an Hopf algebra[15] H_* for the product (3) and coproduct (4) (antipode, unit and counit are obtained by transposition of antipode and unit of H). A *character* ϕ (algebra morphism from H to $\mathbb{C}$) is a grouplike element of H_*

$$\Delta \phi = \phi \otimes \phi. \tag{6}$$

Characters with product (3) and unity ϵ form a group G. The inverse is given by the antipode

$$\phi^{-1} = \phi \circ S. \tag{7}$$

When H is graded, with degree $|.|$, derivations are called *infinitesimal characters* because

$$e^{\delta} \doteq \sum_{n=0}^{+\infty} \frac{\delta^n}{n!} \tag{8}$$

(well defined since $\delta^n(a)$ vanishes as soon as $n > |a|$) is grouplike.[9] The correspondence between characters and infinitesimal characters is one to one:

$$\ln \phi \doteq \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n} (\phi - \epsilon)^n, \phi \in G, \tag{9}$$

is a derivation satisfying $e^{\ln \phi} = \phi$. [Identify

$$\Delta(\ln \phi) = \sum_{n=1,p=0}^{n=+\infty,p=n} \frac{(-1)^{p+1}}{n} C_p^n \phi^p \otimes \phi^p \quad \text{to } \ln xy = \sum_{n=1,p=0}^{n=+\infty,p=n} \frac{(-1)^{p+1}}{n} C_p^n x^p y^p, \quad x, y \in \mathbb{R},$$

$$\ln \phi \otimes \epsilon + \epsilon \otimes \ln \phi = \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n} (\phi^n \otimes \epsilon + \epsilon \otimes \phi^n) \quad \text{to } \ln x + \ln y = \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n} (x^n + y^n).$$

Developing $e^{\ln \phi}(a)$ in $\tilde{\phi} \doteq \phi - \epsilon$, terms in $\tilde{\phi}^p$ cancel by combinatoric for $2 \leqslant p \leqslant |a|$. For $p > |a|, \tilde{\phi}^p(a)$ vanishes because for graded connected Hopf algebra[9] $\Delta(a) = a \otimes 1 + 1 \otimes a + \Sigma a' \otimes a''$ with $|a'|, |a''| < |a|$.] Similarly $\ln e^{\delta}$ coincides with δ. The set of infinitesimal characters is linearly spanned by derivations Z^T that cancel everywhere but on a given generator

$$Z^T(T') \doteq 0 \text{ for any } T' \neq T, \quad Z^T(T) \doteq 1, \quad Z^T(1) = 0. \tag{10}$$

B. Power series of operators

Let $\mathcal{E}$ be a Banach vector space with norm $\|.\|, \mathcal{S}(\mathcal{E})$ the set of smooth applications from $\mathcal{E}$ to $\mathcal{E}$ and $\mathcal{L}_n^s(\mathcal{E})$ the set of n-linear symmetric applications from $\mathcal{E}^n$ to $\mathcal{E}$. Take $X \in \mathcal{S}(\mathcal{E})$. For any $x \in \mathcal{E}$, there exists an infinite sequence of smooth

$$X_x^{[n]} \in \mathcal{L}_n^s(\mathcal{E}), \tag{11}$$

such that for any y in the neighborhood of x

$$X(x+y) = X(x) + X'_x(y) + \cdots + \frac{1}{n!}X_x^{[n]}(y,\ldots,y) + \mathcal{O}(\|y\|^{n+1}). \tag{12}$$

For instance when the norm is associated to real coordinates over a base e_μ, X is a collection of smooth functions X^μ with derivatives $X^\mu_{,\nu\ldots}$ and (summing on repeated indices)

$$X'_x(y) = X^\mu_{,\nu}(x)y^\nu e_\mu, \quad X''_x(y_1,y_2) \doteq X^\mu_{,\nu\rho}(x)y_1^\nu y_2^\rho e_\mu. \tag{13}$$

Here we intend to work with a coordinate free notation and we view $X^{[n]}$ as an element of $\mathcal{L}_n^s(\mathcal{S}(\mathcal{E}))$

$$X^{[n]}(X_1,X_2,\ldots,X_n): \quad \mathcal{E} \to \mathcal{E} \tag{14}$$

$$x \mapsto X_x^{[n]}(X_1(x),X_2(x),\ldots,X_n(x)). \tag{15}$$

One defines a formal power series in $\hbar$ by Taylor expanding X around the identity

$$X(x+\hbar Y(x)) = X(x) + \hbar X'(Y)(x) + \frac{\hbar^2}{2}X''(Y,Y)(x) + \cdots, \tag{16}$$

with $Y \in \mathcal{S}(\mathcal{E})$. When $Y=X$, (16) can be written in a nice graphic way by using rooted trees. Explicitly one defines

$$X^{\bullet} \doteq X \quad , \quad X^{\overset{\bullet}{\circ}} \doteq X'(X) \tag{17}$$

$$X^{\overset{\bullet}{\circ}\circ} \doteq \frac{1}{2}X''(X,X) \quad , \quad X^{\overset{\bullet}{\circ}\circ\circ} \doteq \frac{1}{3!}X'''(X,X,X) \tag{18}$$

so that (16) writes

$$X(\mathbb{I}+\hbar X) = X^{\bullet} + \hbar X^{\overset{\bullet}{\circ}} + \hbar^2 X^{\overset{\bullet}{\circ}\circ} + \hbar^3 X^{\overset{\bullet}{\circ}\circ\circ} + \ldots \tag{19}$$

Formally there is no reason to limit to trees of depth 1 and one associates to any T the operator recursively defined by

$$X^T \doteq \frac{1}{\prod \theta_i!}X^{[n]}(\underbrace{X^{T_1},X^{T_1},\ldots}_{\theta_1 \text{ times}},\underbrace{X^{T_2},\ldots}_{\theta_2 \text{ times}},\ldots,\underbrace{X^{T_m},\ldots}_{\theta_m \text{ times}}). \tag{20}$$

$$X^1 = \mathbb{I} \tag{21}$$

where the T_i's are the subtrees of T obtained by promoting as roots the vertices of T of length 1 and $n=\Sigma_{i=1}^m \theta_i$ is the fertility of the root of T. For instance

$$X^{\overset{\bullet}{\circ}\overset{\bullet}{\circ}\circ} = \frac{1}{8}X''(X'(X''(X,X)),X'(X''(X,X))). \tag{22}$$

Note that the numerical factor in X^T is $1/S_T$. In the following, we use the shorthand notation

$$X^T = \frac{1}{\prod \theta_i!} X^{[n]}(X_i^{\theta_i}). \tag{23}$$

When X is a linear operator, $X^T=0$ as soon as $n>1$. The following construction, inspired from the theory of Butcher group,[10] is mostly interesting for nonlinear operators and provide a generalization of Taylor expansion (19) by associating to any smooth X a formal power serie $f[X]$

$$f[X] \doteq \sum_T f_T X^T \hbar^{|T|}, \tag{24}$$

where f_T are complex numbers and the sum runs over all generators (including unit 1).

The set $\mathcal{G}$ of series with $f_1=1$ is in one to one correspondence with the characters of H. Moreover $\mathcal{G}$ with the composition of series

$$f \circ g[X] = \sum_T f_T X^T \left(\sum_{T'} g_{T'} X^{T'} \hbar^{|T'|} \right) \hbar^{|T|}, \tag{25}$$

is a group, isomorphic to G^{op}, the opposite of the group of characters of H. That $\mathcal{G}$ is a group is known from the theory of Butcher group. However, by using the Hopf algebraic structure of trees we present a proof of the isomorphism

$$G^{op} \sim \mathcal{G}, \tag{26}$$

that does not require to compute explicitly the coefficients of the product series (25), as this is done in Ref. 10 for instance. The main tool for our proof is a slight adaptation to our component free notation of Caley's relation[3] between differentials and trees. It appears indeed that the differentials of the X^T's are easily computed in a graphic way. In the simplest cases this is immediate from definition (20), for instance

$$X^{\bullet\prime}(X^{\curlywedge}) = X^{\curlyvee} \text{ and } X^{\bullet\prime\prime}(X^{\curlywedge}, X^{\curlywedge}) = 2X^{\curlywedge\!\curlywedge}. \tag{27}$$

The differentiation process consists in grafting on a tree as many trees as the order of derivation, with a suitable numerical ponderation reflecting the symmetry of the argument.

Lemma II.2: For any trees $T, T_1, \ldots, T_l$ and integers $\beta_1, \ldots \beta_l$

$$X^{T[k]}(\underbrace{X^{T_1}, X^{T_1}, \ldots}_{\beta_1 \text{ times}}, \ldots, \underbrace{X^{T_l}, X^{T_l}, \ldots}_{\beta_l \text{ times}}) = \prod \beta_i ! \sum_{\tilde{T}} n(\tilde{T}; T, \prod T_i^{\beta_i}) X^{\tilde{T}}, \tag{28}$$

where $k \doteq \Sigma_{i=1}^l \beta_i$ and $n(\tilde{T}; T, \Pi T_i^{\beta_i})$ is the number of simple cut c of $\tilde{T}$ such that

$$R_c(\tilde{T}) = T \text{ and } P_c(\tilde{T}) = \Pi T_i^{\beta_i}. \tag{29}$$

Proof: Let $X \in \mathcal{S}(\mathcal{E}), x \in \mathcal{E}$ and $y \doteq y_1 + \ldots + y_J$ in a neighborhood of x. For any collection $\{z_i\}_{i \in [1,n]}$ of elements of $\mathcal{E}$,

$$X_{x+y}^{[n]}(z_i) = \sum_{\beta=0}^{+\infty} \sum_{[\beta_j]=\beta} \frac{1}{\prod \beta_j!} X_x^{[n+\beta]}(y_j^{\beta_j}, z_i), \tag{30}$$

where the second sum runs on all the configurations of the β_j's such that $\Sigma_{i=1}^J \beta_j = \beta$ and we use notation similar as (23). This formula can be obtained by comparing

$$X(x+y+z) = X(x+y) + \sum_{n=1}^{+\infty} \sum_{[\alpha_i]=n} \frac{1}{\prod \alpha_i!} X^{[n]}_{x+y}(z_i^{\alpha_i}), \tag{31}$$

where $z=z_1+\cdots+z_n$ is in a neighborhood of $x+y$, to

$$X(x+y+z) = X(x) + \sum_{n=1}^{+\infty} \sum_{[\beta_j,\alpha_i]=n} \frac{1}{\prod \beta_j ! \prod \alpha_i!} X^{[n]}_{x}(y_j^{\beta_j}, z_i^{\alpha_i}). \tag{32}$$

Choosing all $\alpha_i=1$, the term $X^{[n]}_{x+y}(z_i)$ in (30) is identified to the sum of terms of (31) that are linear in each z_i. For instance

$$X'_{x+y_1+y_2}(z_1) = X'_x(z_1) + X''_x(z_1,y_1) + X''_x(z_1,y_2) + X'''_x(z_1,y_1,y_2) + \tfrac{1}{2}X'''_x(z_1,y_1,y_1) + \tfrac{1}{2}X'''_x(z_1,y_2,y_2) + \cdots.$$

Then

$$X^T(x+y) = \frac{1}{\prod \theta_i!} X^{[n]}_{x+y}(X_i^{\theta_i}(x+y)) \tag{33}$$

$$= \frac{1}{\prod \theta_i!} \sum_{\beta=0}^{+\infty} \sum_{[\beta_j]=\beta} \frac{1}{\prod \beta_j!} X^{[n+\beta]}_{x}(y_j^{\beta_j}, X_i^{\theta_i}(x+y)). \tag{34}$$

Inserting

$$X_i(x+y) = X_i(x) + \sum_{r=1}^{+\infty} \sum_{[\beta'_j]=r} \frac{1}{\prod \beta'_j!} X^{[r]}_{ix}(y_j^{\beta'_j}), \tag{35}$$

and choosing $\{y_j\}$ of cardinality $J=k$, one identifies $X_x^{T[k]}(y_j)$ as the terms of (34) linear in each y_j, namely those appearing with either β_j or $\beta'_j=1$. Explicitly, for a tree T with depth 1,

$$X^{T'}(X^{\tilde{T}_1}) = \frac{1}{n!} X^{[n+1]}_x(X^{\tilde{T}_1}, X^n) + \frac{1}{(n-1)!} X^{[n]}_x(X'(X^{\tilde{T}_1}), X^{n-1}) = \sum_{\tilde{T}} n(\tilde{T}; T, \tilde{T}_1) X^{\tilde{T}},$$

for any $\tilde{T}_1$. For instance, with notations (13)

$$X^{\bullet\!\!\diagup\!\!\diagdown'}(X^\bullet) = \tfrac{1}{2}(X^\mu_{,\nu\rho} X^\nu X^\rho)_{,\delta} X^\delta e_\mu = \tfrac{1}{2} X^\mu_{,\nu\rho\delta} X^\nu X^\rho X^\delta e_\mu + \tfrac{1}{2} X^\mu_{,\nu\rho} X^\nu_{,\delta} X^\rho X^\delta e_\mu + \tfrac{1}{2} X^\mu_{,\nu\rho} X^\nu X^\rho_{,\delta} X^\delta e_\mu \tag{36}$$

$$= 3X^{\bullet\!\!\diagup\!\!\diagdown} + X^{\bullet\!\!\diagup\!\!\diagdown\!\!\diagup} \tag{37}$$

Similarly for any k and distinct T_j's one obtains

$$X^{T[k]}(X^{\tilde{T}_1}, \ldots, X^{\tilde{T}_k}) = \sum_{\tilde{T}} n(\tilde{T}; T, \Pi\tilde{T}_j) X^{\tilde{T}}. \tag{38}$$

When some of the $\tilde{T}_j$'s are identic, the extra factor $1/\beta_j!$ is absorbed by the definition of $\tilde{T}$ but such terms have to be identified as part of

$$\frac{1}{\beta_j!} X^{T[\beta_j]}(\tilde{X}_j^{\beta_j}). \tag{39}$$

Hence the lemma for any T of depth 1. The final result is obtained recursively on the depth of T.■

Proposition II.3: $\mathcal{G}$ is a group, isomorphic to G^{op}.

Proof: Since $\mathcal{G}$ is in bijection with G, we just have to show that

$$\sum_T \phi(T) X^T \left(\sum_{T'} \psi(T') X^{T'} \hbar^{|T'|} \right) \hbar^{|T|} = \sum_T (\psi * \phi)(T) X^T \hbar^{|T|}, \tag{40}$$

for any $\phi, \psi \in G$. In the l.h.s. ϕ is evaluated on generators only. By (2) and (3) one checks that the same is true for the r.h.s. Moreover both sides are linear in ϕ so this is enough to work with the infinitesimal character

$$\phi = Z^{T_0}, \tag{41}$$

for a fixed T_0. Note that a similar simplification is not available for ψ since $P_c(T)$ may not be a single generator. Then r.h.s. of (40) reduces to

$$X^{T_0} \hbar^{|T_0|} + \sum_T \sum_{c \in \tilde{C}(T)} \psi(P_c(T)) X^T \hbar^{|T|}, \tag{42}$$

where $\tilde{C}(T)$ is the set of simple cuts of T such that $R_c(T) = T_0$. The l.h.s. of (40) developed thanks to (19) writes

$$X^{T_0} \hbar^{|T_0|} + \sum_{T_1} \psi(T_1) X^{T_0{}'}(X^{T_1}) \hbar^{|T_0|+|T_1|} + \cdots + \sum_{\{T_i^{\beta_i}\}} \frac{\Pi \psi(T_i)^{\beta_i}}{\Pi \beta_i!} X^{T_0{}^{[n]}}(T_i^{\beta_i}) \hbar^{\Sigma_i |T_i|} + \cdots, \tag{43}$$

where sums run over generators distinct from 1 and we use a similar notation as in (23). Thanks to lemma II.2, (43) = (42). ■

Thanks to this isomorphism one can easily compute some interesting series. Let us write

$$f_\phi[X], \tag{44}$$

the formal power series associated to a character ϕ by the isomorphism II.3. We define the *exponential series* as the one corresponding to the character

$$\phi_e \doteq e^{Z \bullet}, \tag{45}$$

defined by (8) and (10). Since (see Ref. 4 for the definition of the factorial $T!$ of a tree)

$$\phi_e(T) = \frac{1}{T!}, \tag{46}$$

the exponential series writes

$$f_{\phi_e}[X] = \sum_T \frac{1}{T!} \hbar^{|T|} X^T. \tag{47}$$

Another nice example is the *geometrical series*

$$(\mathbb{I} - \hbar X)^{-1} = f_{\phi_1}[X] = \sum_T \hbar^{|T|} X^T, \tag{48}$$

obtained by noting that the constant character

$$\phi_1 : T \mapsto 1 \quad \forall\, T, \tag{49}$$

is the inverse of the character $T \mapsto 0$ except $1 \mapsto 1, \bullet \mapsto -1$.

III. FIXED POINT EQUATION AND ALGEBRAIC BIRKHOFF DECOMPOSITION

The geometrical and exponential series (47) and (48) are interesting to solve a fixed point equation. In particular if we view a fixed point equation as the integral form of a differential

equation then the change of initial condition (corresponding to the change of the constant in the fixed point equation) is coded into the group G_2 of characters of the Hopf algebra of decorated rooted trees. Namely if $\phi \in G_2$ represents the solution for initial condition x_0 and $\phi_+ \in G_2$ corresponds to the solution for initial condition x_1, then the decomposition

$$\phi_+ = \phi_- * \phi, \tag{50}$$

turns out to define an *algebraic Birkhoff decomposition* (see definition III.1) similar as the one introduced by Connes and Kreimer in their seminal paper Ref. 4.

Using trees to solve fixed point and differential equations is at the heart of the theory of *B*-series (see Ref. 1 for a nice overview of such applications). However, to the knowledge of the authors, the interpretation in terms of Birkhoff decomposition is not found in the literature.

A. Change of initial conditions in fixed point equations

Let us start by the fixed point equation

$$x = x_0 + \hbar X(x), \tag{51}$$

where $X \in \mathcal{S}(\mathcal{E})$, $\hbar$ is small and $x_0 \in \mathcal{E}$. (51) is formally solved by writing

$$x = (\mathbb{I} - \hbar X)^{-1}(x_0), \tag{52}$$

that is to say, thanks to (48)

$$x = f_{\phi_1}[X](x_0) = \sum_T \hbar^{|T|} X^T(x_0). \tag{53}$$

This is the same series as the one found by recursively developing $x = x_0 + \hbar X(x_0 + \hbar X(X_0 + \cdots))$.

Consider now a curve $x : \mathbb{R} \to \mathcal{E}$ given by

$$x(t) = x_0 + \hbar \int_{t_0}^{t} X(x(u))du, \tag{54}$$

for some $X \in \mathcal{S}(\mathcal{E})$. This is the integral form of the differential equation

$$\frac{dx}{dt} = \hbar X(x), \quad x(t_0) = x_0. \tag{55}$$

By recursively developing

$$x(t) = x_0 + \hbar \int_{t_0}^{t} X\left(x_0 + \hbar \int_{t_0}^{t_1} X\left(x_0 + \int_{t_0}^{t_2} \cdots\right) dt_2\right) dt_1, \tag{56}$$

one finds[1]

$$x(t) = \sum_T \frac{1}{T!}(t - t_0)^{|T|} \hbar^{|T|} X^T(x_0), \tag{57}$$

that is to say, according to (47)

$$x(t) = f_{\phi_e}[X_0](x_0), \tag{58}$$

where

$$X_0 \doteq (t - t_0)X. \tag{59}$$

One may be tempted to solve (55) formally by writing

$$x(t) = e^{\hbar X_0}(x_0). \tag{60}$$

The genuine definition of the exponential of an operator ($\exp(X) = \mathbb{I} + X + (1/2)X \circ X + \cdots$) is not compatible with (58). However, *defining*

$$e^{\hbar X_0} \doteq f_{\phi_e}[X_0], \tag{61}$$

ensures that (58) equals (60). In other terms rooted trees provide a definition of the exponential of a (nonlinear) operator which is compatible with the resolution of fixed point equations.

The same differential equation can be directly solved in its integral form (54) by considering the Banach vector space $\mathcal{E}'$ of curves in $\mathcal{E}$ and the operator $\chi \in \mathcal{S}(\mathcal{E}')$ defined by

$$\chi(x):t \mapsto \int_{t_0}^{t} X(x(u))du. \tag{62}$$

Considering x_0 as the curve $t \mapsto x_0$, (54) reads as the fixed point equation

$$x = x_0 + \hbar\chi(x), \tag{63}$$

whose formal solution is given by (53)

$$x = (\mathbb{I} - \hbar\chi)^{-1}(x_0) = f_{\phi_1}[\chi](x_0). \tag{64}$$

Trees are especially useful to deal with change of initial condition. Let us fix

$$x(t_1) = x_1, \tag{65}$$

for a given $x_1 \in \mathcal{E}$ and $t_1 \neq t$. Solution (58) becomes

$$x(t) = f_{\phi_e}[X_1](x_1), \tag{66}$$

where

$$X_1 \doteq (t - t_1)X. \tag{67}$$

In order to keep a trace of the solution with an initial condition at t_0, let us write (66) for $t = t_0$,

$$x_0 = f_{\phi_e}[X_1 - X_0](x_1), \tag{68}$$

which, inserted into (58)

$$x(t) = f_{\phi_e}[X_0] \circ f_{\phi_e}[X_1 - X_0](x_1), \tag{69}$$

and compared to (66) yields

$$f_{\phi_e}[X_1] = f_{\phi_e}[X_0] \circ f_{\phi_e}[X_1 - X_0]. \tag{70}$$

A similar decomposition can be found for the integral form (54) of the differential equation. The solution for initial condition (67) is

$$x = f_{\phi_1}[\zeta](x_1), \tag{71}$$

with

$$\zeta(x):t \mapsto \int_{t_1}^{t} X(x(u))du. \tag{72}$$

Factorizing

$$(\mathbb{I} - \hbar\zeta)^{-1} = (\mathbb{I} - \hbar\chi)^{-1} \circ (\mathbb{I} - \hbar\xi)^{-1} \tag{73}$$

where we define

$$\hbar\xi \doteq \mathbb{I} - (\mathbb{I} - \hbar\zeta) \circ (\mathbb{I} - \hbar\chi)^{-1}, \tag{74}$$

yields by (48)

$$f_{\phi_1}[\zeta] = f_{\phi_1}[\chi] \circ f_{\phi_1}[\xi]. \tag{75}$$

Both (70) and (75) involves a unique character ϕ_1 or ϕ_e and three distinct operators χ, ζ, ξ, or $X_0, X_1, X_1 - X_0$. To fix notations we now focus on the decomposition of geometrical series (75) but the following is also true for exponential series. In order to take advantage of the isomorphism (26) one needs a series involving the same operator. This can be obtained by considering the group G_2 of characters of the Hopf algebra H_2 of *decorated rooted trees*, i.e., trees whose vertices carry a decoration chosen in a set of cardinality two, in our case of interest either a bullet or a square. To any generator $\mathcal{T}$ of H_2, one associates $Y^{\mathcal{T}} \in \mathcal{S}(\mathcal{E}')$ defined in a similar manner as in (20) with the extra rule that bullets are associated to ξ and squares to ζ. For instance

$$Y^{\blacksquare} = \zeta, \quad Y^{\bullet} = \xi, \tag{76}$$

$$Y^{\begin{smallmatrix}\blacksquare\\ \diagup\ \diagdown\\ \bullet\quad\bullet\end{smallmatrix}} = \zeta''(\xi, \xi). \tag{77}$$

Let $\mathcal{G}_2$ be the group of power series $\mathbb{I} + \Sigma_{\mathcal{T}} f_{\mathcal{T}} Y^{\mathcal{T}}$. A straightforward adaptation of proposition II.3 shows that

$$\mathcal{G}_2 \, G_2^{op}. \tag{78}$$

Let us define two characters of H_2

$$\phi_-(\mathcal{T}) \doteq \begin{cases} \phi_1(\mathcal{T}) \text{ if } \mathcal{T} \in H_{\bullet} \\ 0 \text{ if } \mathcal{T} \notin H_{\bullet}, \end{cases} \qquad \phi_+(\mathcal{T}) \doteq \begin{cases} \phi_1(\mathcal{T}) \text{ if } \mathcal{T} \in H_{\blacksquare} \\ 0 \text{ if } \mathcal{T} \notin H_{\blacksquare}, \end{cases} \tag{79}$$

where $H_{\bullet}$ is the set of trees decorated with bullets only and $H_{\blacksquare}$ those decorated by square only. Then

$$f_{\phi_1}[\zeta] = f_{\phi_+}[Y], \quad f_{\phi_1}[\xi] = f_{\phi_-}[Y], \tag{80}$$

are both elements of G_2^{op}. By (75) and (78)

$$f_{\phi_1}[\chi] = f_{\phi}[Y], \tag{81}$$

for the character $\phi \in G_2$ given by (remembering (49), ϕ_-^{-1} vanishes on all generators of H_2 except $\phi_-^{-1}(1) = 1, \phi_-^{-1}(\bullet) = -1$; by (3) one obtains

$$\phi(\mathcal{T}) = \begin{cases} 1 & \text{for } \mathcal{T} \in H_{\blacksquare} \\ -1 & \text{for } \mathcal{T} = \bullet \\ -n_{\mathcal{T}} & \text{otherwise,} \end{cases} \tag{82}$$

where $n_{\mathcal{T}} = 1$ if there is a simple cut such that $R_c(\mathcal{T}) \in H_{\blacksquare}$ and $P_c(\mathcal{T}) = \bullet, n_{\mathcal{T}} = 0$ otherwise)

$$\phi = \phi_-^{-1} * \phi_+. \tag{83}$$

(75) can be written with a unique operator Y and three characters

$$f_{\phi_+}[Y] = f_\phi \circ f_{\phi_-}[Y]. \tag{84}$$

(70) can be written as well, by associating bullet to $X_1 - X_0$, square to X_1 and defining $\phi_\pm$ according to ϕ_e instead of ϕ_1.

(83) is the announced equation (50), establishing that the change of initial condition in a fixed point equation is coded into the group of characters of the algebra of decorated rooted trees. In next section, we show that (83) [or equivalently (84) by identifying characters and series] allows to define a so-called algebraic Birkhoff decomposition.

B. Algebraic Birkhoff decomposition

A decomposition of the same kind as (83) appears in renormalization of quantum field theory with minimal subtraction scheme and dimensional regularization.[4] The bare theory gives rise to a loop

$$\gamma(z) \in G_F, \quad z \in \mathcal{C}, \tag{85}$$

where $\mathcal{C} \in \mathbb{C}$ is a small circle around the dimension D of space time and G_F is the group of characters of the Hopf algebra of Feynman diagrams H_F. The renormalized theory is the evaluation at $z=D$ of the holomorphic part γ_+ of the *Birkhoff decomposition* of γ. To give a similar interpretation to our decomposition (83), we need to adapt to rooted trees some of the tools of Ref. 4 initially developed for Feynman diagrams.

An important feature is the commutative algebra $\mathcal{A}$ of smooth functions meromorphic inside $\mathcal{C}$ with pole only at D. Also important are the subalgebras $\mathcal{A}_+ \subset \mathcal{A}$ of functions holomorphic inside $\mathcal{C}$, and $\mathcal{A}_- \subset \mathcal{A}$ the subalgebra of polynomial in $1/(z-D)$ without constant term. There exists a projection

$$p_-: \mathcal{A} \to \mathcal{A}_-, \tag{86}$$

parallel to $\mathcal{A}_+$, i.e.

$$\text{Ker } p_- = \mathcal{A}_+. \tag{87}$$

Feynman rules (ponderated by a suitable mass factor) yields an algebra homomorphism

$$U: H_F \to \mathcal{A}. \tag{88}$$

The counterterms are given by the algebra homomorphism

$$C(X) \doteq -p_-\Big(U(X) + \sum C(X')U(X'')\Big), \tag{89}$$

where

$$\Delta(X) = X \otimes 1 + 1 \otimes X + \sum X' \otimes X'', \quad X \in \tilde{H}_F \doteq \text{Ker } \epsilon, \tag{90}$$

while the renormalized theory is given by the homomorphism

$$R(X) = (C * U)(X). \tag{91}$$

One checks that

$$C(\tilde{H}_F) \subset \mathcal{A}_-, \quad R(\tilde{H}_F) \subset \mathcal{A}_+. \tag{92}$$

Equation (91) viewed as an equality between algebra homomorphisms

$$C * U = R, \tag{93}$$

is called the *algebraic Birkhoff decomposition* of U. Such a terminology is justified by considering the G_F-valued loops

$$\gamma(z) \doteq \chi_z \circ U, \quad \gamma_-(z) = \chi_z \circ C, \quad \gamma_+(z) = \chi_z \circ R, \tag{94}$$

where

$$\chi_z(f) \doteq f(z) \quad \forall f \in \mathcal{A}. \tag{95}$$

Indeed (91) indicates that

$$\gamma_+(z) = \gamma_-(z)\gamma(z) \quad \forall z \in \mathcal{C}, \tag{96}$$

for the pointwise product in G. One then shows that (96) is precisely the Birkhoff decomposition of γ. Namely, viewing $\mathcal{C}$ as a subset of the Riemann sphere $\mathbb{C}P_1$, γ_- extends to a G_F-valued holomorphic maps on $\mathcal{C}_-$ (the component of the complement of $\mathcal{C}$ containing ∞) with $\gamma_-(\infty)=0$ while γ_+ extends to G_F-valued holomorphic maps on $\mathcal{C}_+$ (the other component of the complement of $\mathcal{C}$). The reader is invited to consult Ref. 4 for a precise definition of the Birkhoff decomposition and its link to the Riemann–Hilbert problem. Let us simply recall that the replacement of γ by γ_+ is a natural principle to extract a finite value from the singular expression $\gamma(z)$.

The use of the algebra of meromorphic functions on $\mathcal{C}$ is intimately linked to dimensional regularization scheme. In the framework of the continuous renormalization group, there is no pole given by the dimension of space–time. However, given a decomposition of algebra homomorphisms such as (93), satisfying conditions (92), it still makes sense to talk of Birkhoff decomposition, but in the following algebraic sense (taken from Refs. 15 or 12).

Definition III.1: Let H be a commutative Hopf algebra, $\mathcal{A}$ a commutative algebra with a projection p_- on a subalgebra $\mathcal{A}_-$. An algebra homomorphism $\gamma: H \to \mathcal{A}$ has an algebraic Birkhoff decomposition if there exists two algebras homomorphisms γ_+, γ_- from H to $\mathcal{A}$ such that

$$\gamma_+ = \gamma_- * \gamma, \tag{97}$$

where $*$ is the convolution product (3) *and*

$$p_+\gamma_+ = \gamma_+, \quad p_-\gamma_- = \gamma_-, \tag{98}$$

where p_+ is the projection on

$$\mathcal{A}_+ = \mathrm{Ker}\, p_-. \tag{99}$$

To interpret (83) and (84) as an algebraic Birkhoff decomposition one may be first tempted to consider the algebra of polynomials in $Y^{\mathcal{T}}$ as the equivalent in the continuous renormalization framework of the meromorphic functions. As well characters may be understood as the equivalent of the homomorphisms defined by Feynman rules: In the same way that U, C, R map a Feynman diagram to a meromorphic function, characters map a decorated rooted tree to a monomial in $Y^{\mathcal{T}}$,

$$\Phi(\mathcal{T}) \doteq \phi(\mathcal{T})Y^{\mathcal{T}}, \quad \Phi_\pm(\mathcal{T}) \doteq \phi_\pm(\mathcal{T})Y^{\mathcal{T}}. \tag{100}$$

Unfortunately $\Phi, \Phi_\pm$ do not define an algebraic Birkhoff decomposition. For instance (see the proof of proposition III.2 for the computation of ϕ)

$$\Phi_+(\ \bullet^{\,1}\ ) \ = \ 0 \tag{101}$$

$$(\Phi_- * \Phi)(\ \blacksquare\!\!\circ\ ) \ = \ \langle \Phi_- \otimes \Phi, 1 \otimes \ \blacksquare\!\!\circ\ + \ \blacksquare\!\!\circ\ \otimes 1 + \bullet \otimes \blacksquare \rangle \tag{102}$$

$$= \ -Y \ \blacksquare\!\!\circ\ + Y^{\circ} Y^{\blacksquare}. \tag{103}$$

A solution would be to define the product of monomials so that (103) vanishes,

$$Y^{\blacksquare} Y^{\circ} = Y \ \blacksquare\!\!\circ \tag{104}$$

but such a product would not be commutative. However, by considering the (commutative) formal product of decorations, it appears that the sum (ponderated by the numerical coefficient) of the products of decorations in (103) vanishes (i.e., $-\circ\blacksquare+\circ\blacksquare=0$). Consequently we propose a Birkhoff decomposition with value on the the algebra $\mathcal{A}$ of decorations, that is to say the free unital algebra generated by square and bullet

$$\mathcal{A} = \overline{\{1, \bullet, \blacksquare\}}. \tag{105}$$

For $\mathcal{A}_-$ we choose the unital subalgebra of $\mathcal{A}$ generated by the bullet

$$\mathcal{A}_- = \overline{\{1, \bullet\}}. \tag{106}$$

We note p_- the projection $\mathcal{A} \to \mathcal{A}_-$

$$p_-(1) = 1, \quad p_-(\bullet) = \bullet, \quad p_-(\blacksquare) = 0, \tag{107}$$

extended to all $\mathcal{A}$ by algebra homomorphism

$$p_-(\bullet^n \blacksquare^m + \bullet^{n'} \blacksquare^{m'}) = \bullet^n + \bullet^{n'}. \tag{108}$$

$\mathcal{A}_+$ and p_+ are defined by (99). Let Γ be the algebra homorphism $H_2 \to \mathcal{A}$

$$\Gamma(1) = 1, \quad \Gamma(\mathcal{T}) = \bullet^{|\mathcal{T}|_\circ} \blacksquare^{|\mathcal{T}|_\square} \tag{109}$$

where $|\mathcal{T}|_\circ$ is the number of bullets of $\mathcal{T}$ and $|\mathcal{T}|_\square$ is the number of squares. Γ just "counts the decorations," for instance

$$\Gamma(\ \blacksquare\!\!\circ\!\!\circ\ ) = \bullet^3 \blacksquare. \tag{110}$$

Finally we define three algebra homomorphisms from H_2 to $\mathcal{A}$,

$$\gamma(\mathcal{T}) = \phi(T)\Gamma(T), \quad \gamma_\pm(\mathcal{T}) = \phi_\pm(T)\Gamma(T). \tag{111}$$

Proposition III.2: $\gamma_+ = \gamma_- * \gamma$ is an algebraic Birkhoff decomposition.

Proof: Let $\overline{H_\bullet}$ be the algebra of trees with bullets only (and similarly $\overline{H_\blacksquare}$). Then

$$\gamma_-(\mathcal{T}) = \begin{cases} \bullet^{|\mathcal{T}|_\circ} & \text{for } \mathcal{T} \in \overline{H_\bullet} \\ 0 & \text{otherwise}, \end{cases} \qquad \gamma_+(\mathcal{T}) = \begin{cases} \blacksquare^{|\mathcal{T}|_\square} & \text{for } \mathcal{T} \in \overline{H_\blacksquare} \\ 0 & \text{otherwise}, \end{cases} \tag{112}$$

so that (98) is satisfied, as well as (99) by construction. By algebra homomorphism, (97) has to be checked only on generators. Let us first note that

$$\gamma(\mathcal{T}) = \begin{cases} \blacksquare^{|\mathcal{T}|_\square} & \text{for } \mathcal{T} \in H_\blacksquare \\ -\bullet & \text{for } \mathcal{T} = \bullet \\ -n_{\mathcal{T}} \bullet^{|\mathcal{T}|_\circ} \blacksquare^{|\mathcal{T}|_\square} & \text{otherwise} \end{cases} \tag{113}$$

where $n_{\mathcal{T}}$ is defined in (82). Second, for any $\mathcal{T} \neq 1$

$$(\gamma_- * \gamma)(\mathcal{T}) = \gamma(\mathcal{T}) + \gamma_-(\mathcal{T}) + \sum_{c \in C(\mathcal{T})} \gamma_-(P_c(\mathcal{T}))\,\gamma(R_c(\mathcal{T})). \tag{114}$$

This is then not difficult to check (97) for $\mathcal{T} \in H_\bullet$ or $\mathcal{T} \in H_\blacksquare$.

For $\mathcal{T} \notin H_\bullet \cup H_\blacksquare$,

$$(\gamma_- * \gamma)(\mathcal{T}) = -\,n_{\mathcal{T}}\,\bullet^{|\mathcal{T}|_\bullet}\blacksquare^{|\mathcal{T}|_\square} + \sum_{c \in C(\mathcal{T})} \gamma_-(P_c(\mathcal{T}))\,\gamma(R_c(\mathcal{T})). \tag{115}$$

Assume $n_{\mathcal{T}}=0$. Then (115) is nonzero only if there is at least either a simple cut c such that

$$P_c(\mathcal{T}) \in \overline{H_\bullet} \text{ and } R_c(\mathcal{T}) \in H_\blacksquare, \tag{116}$$

or a simple cut $\tilde{c}$ with

$$P_{\tilde{c}}(\mathcal{T}) \in \overline{H_\bullet} \text{ and } n_{R_{\tilde{c}}(\mathcal{T})} \neq 0. \tag{117}$$

Assume there exists a simple cut c for which $P_c(\mathcal{T})$ is a single tree. Then there exist a $\tilde{c}$ in which $R_{\tilde{c}}(\mathcal{T})$ is the subtree of $\mathcal{T}$ consisting in $R_c(\mathcal{T})$ and the root of $P_c(\mathcal{T})$ while $P_{\tilde{c}}(\mathcal{T})$ is the union of all the subtrees of $P_c(\mathcal{T})$ obtained by promoting as roots the vertices of length 1 ($P_{\tilde{c}}(\mathcal{T}) \neq \emptyset$ because $n_{\mathcal{T}}=0$). The simple cut c contributes to (115) with a factor

$$\bullet^{|P_c(\mathcal{T})|}\blacksquare^{|R_c(\mathcal{T})|}, \tag{118}$$

whereas $\tilde{c}$ contributes with a factor

$$\bullet^{|P_{\tilde{c}}(\mathcal{T})|}(-\bullet\blacksquare^{|R_{\tilde{c}}(\mathcal{T})|_\square}). \tag{119}$$

This is easy to observe that (118) $=-$ (119). The same is true if $P_c(\mathcal{T})$ is a product of m trees, the only difference being that the contribution of c is canceled by the sum of the contributions of the m $\tilde{c}$ obtained by grafting alternatively to $R_c(\mathcal{T})$ each of the roots of $P_c(\mathcal{T})$. Also, starting from a $\tilde{c}$, one would similarly notice that its contribution is canceled by a c so that, finally, (115) vanishes for any $\mathcal{T} \notin H_\blacksquare \cup H_\bullet$ with $n_{\mathcal{T}}=0$. Hence (97).

The same procedure applies when $n_{\mathcal{T}} \neq 0$. The term of (115) in $\gamma(\mathcal{T})$ is cancelled by the sum of the $n_{\mathcal{T}}$ terms corresponding to the simple cuts with $P_c(\mathcal{T})=\bullet$. ■

As announced in (50), we have shown that the change of initial condition in a fixed point equation does correspond to the algebraic Birkhoff decomposition of the algebra morphisms associated by (111) to the characters encoding the solutions. By convention we say that γ_+ is the positive part of the algebraic $\mathcal{A}$-valued Birkhoff decomposition of γ.

C. Continuous renormalization group

Birkhoff decomposition has been introduced in renormalization of quantum field theory by Connes and Kreimer in the framework of minimal subtraction scheme and dimensional regularization. Our algebraic Birkhoff decomposition (83) has an interpretation in the framework of the continuous renormalization group of Wilson[23] (see also Ref. 18 for a nice introduction). The latest describes the evolution of the parameters of a quantum field theory under a change of the observation scale. When the rescaling is parametrized by a continuous quantity, say the energy, the evolution is governed by flow equation

$$\Lambda \frac{\partial}{\partial \Lambda} S = \beta(\Lambda, S), \tag{120}$$

in which $\Lambda \in \mathbb{R}^{*+}$ is the scale and $S=S(\Lambda)$ implements the parameters (mainly S is a functional of the fields and their coupling constants). The initial conditions are encoded by the knowledge of $S_0 \doteq S(\Lambda_0)$ at a given scale Λ_0. A typical example of continuous renormalization group equations (120) are Polchinski's equations[20] which gives $\beta(\Lambda, S)$ for a theory with an infrared (IR) cutoff.

Let us consider the most general context by simply assuming that the theory is described by a smooth operator S

$$S{:}\Lambda \mapsto S(\Lambda) \in \mathcal{E},$$

where $\mathcal{E} \doteq \mathcal{S}(\mathcal{H})$ and $\mathcal{H}$ is the (infinite dimensional) vector space spanned by vectors labeled with the parameters of the theory. A scale transformation

$$\Lambda \to \Lambda^s,$$

with $s \in \mathbb{R}^{*+}$ induces the transformation[14]

$$S(\Lambda) \to S(\Lambda^s) = s^{\Delta} S(\Lambda)$$

where $\Delta \in \mathcal{E}$ is the diagonal matrix whose coefficients are the dimensions of the parameters. We define the dimensionless quantities $x(\Lambda) \in \mathcal{E}$ and $t \in \mathbb{R}$,

$$S(\Lambda) = \Lambda^{\Delta} x(\Lambda), \quad t \doteq \ln\left(\frac{\Delta}{\mu}\right),$$

where μ is a parameter of the theory with same dimension as Λ. Then (120) yields

$$\Lambda \frac{\partial x}{\partial \Lambda} = -\Delta x + \Lambda^{-\Delta} \beta(\Lambda, \Lambda^{\Delta} x). \tag{121}$$

By dimensional analysis, β is transforming homogeneously under change of scale,

$$\beta(\Lambda, \Lambda^{\Delta} x) = \Lambda^{\Delta} \beta(1, x), \tag{122}$$

so that, writing $\hbar X(x) \doteq \beta(1, x)$ and $D = -\Delta$,

$$\frac{\partial x}{\partial t} = Dx + \hbar X(x), \tag{123}$$

whose integral form, with initial condition $x_0 = \Lambda_0^D S_0$, is

$$x(t) = e^{(t-t_0)D} x_0 + \hbar \int_{t_0}^{t} e^{(t-u)D} X(x(u)) du. \tag{124}$$

Viewing x as an element of $\mathcal{E}'$, Banach vector space of applications from $\mathbb{R}^{*+}$ to $\mathcal{E}$, we define

$$\tilde{x}_0 \in \mathcal{E}' : t \mapsto e^{(t-t_0)D} x_0, \tag{125}$$

and $\chi \in \mathcal{S}(\mathcal{E}')$,

$$\chi(x) : t \mapsto \int_{t_0}^{t} e^{(t-u)D} X(x(u)) du \quad \forall\, x \in \mathcal{E}' \tag{126}$$

so that (124) reads as the fixed point equation

$$x = \tilde{x}_0 + \hbar \chi(x). \tag{127}$$

In the context of Wilson's continuous renormalization group, Λ_0 is interpreted as an ultraviolet (UV) cutoff and one is interested in the limits of very high energy scale, i.e., $t_0 \to +\infty$. However $\tilde{x}_0$ is already ill-defined since

$$e^{(t-t_0)D}x_0 \begin{cases} \text{converges on } \mathcal{H}^+ \\ \text{is constantly zero on } \mathcal{H}^0 \\ \text{diverges on } \mathcal{H}^-, \end{cases} \quad \text{as } t_0 \to +\infty \tag{128}$$

where $\mathcal{H}^+, \mathcal{H}^0, \mathcal{H}^- \subset \mathcal{H}$ are the proper subspaces of D corresponding to positive, zero and negative eigenvalues (the corresponding parameters are called *relevant, marginal* and *irrelevant*). χ as well is ill defined, even in the relevant sector. A solution to ensure the finiteness of $x(t)$ at high scale consists in fixing the initial conditions for the irrelevant sector at scale t_1 (equivalently: At scale Λ_1) distinct from t_0. Namely one imposes the mixed boundary conditions

$$x_R \doteq P\tilde{x}_1 + (\mathbb{I} - P)\tilde{x}_0, \tag{129}$$

where P is the orthogonal projection from $\mathcal{H}$ to $\mathcal{H}^-$ and

$$\tilde{x}_1 \in \mathcal{E}' : t \mapsto e^{(t-t_1)D}x_1. \tag{130}$$

Defining

$$\rho(x) : t \mapsto \int_{t_1}^{t} e^{(t-u)D}X(x(u))du \tag{131}$$

and

$$\zeta \doteq P\rho + (\mathbb{I} - P)\chi, \tag{132}$$

allows us to write (127) with initial condition x_R

$$x(t) = x_R + \hbar\zeta(x). \tag{133}$$

This is a well-known result that $x(t)$ computed with mixed boundary condition, namely

$$x(t) = f_{\phi_1}[\zeta](x_R) \tag{134}$$

remains finite at high energy scale and does not depend on x_0. Trees have already been used to prove this result (see Refs. 11, 8, and 21, for instance). To be complete we propose here a simple proof taking advantage of the Hopf algebraic structure.

Proposition III.3: $\lim_{t_0 \to +\infty} f_{\phi_1}[\zeta](x_R)$ *is finite order by order and does not depend on* x_0.

Proof: The idea is to use decorated trees in a similar way as (76) except that the rule now is

$$Y^{\bullet} = \zeta_1 \doteq P_\rho, \quad Y^{\blacksquare} = \zeta_2 \doteq (\mathbb{I} - P)\chi. \tag{135}$$

Then

$$\zeta \; \overset{\bullet}{\circ} \; = \; (\zeta_1 + \zeta_2)'(\zeta_1 + \zeta_2) \tag{136}$$

$$= (\zeta_1)'(\zeta_1) + (\zeta_1)'(\zeta_2) + (\zeta_2)'(\zeta_1) + (\zeta_2)'(\zeta_2) \tag{137}$$

$$= \; Y \; \overset{\bullet}{\circ} \; + Y \; \overset{\bullet}{\square} \; + Y \; \overset{\blacksquare}{\circ} \; + Y \; \overset{\blacksquare}{\square} \tag{138}$$

$$= \sum_{\mathcal{T} \in \left\{ \begin{array}{c} \bullet \\ \circ \end{array} \right\}_2} Y^{\mathcal{T}} \tag{139}$$

where $\{T\}_2$ is the set of all decorated trees obtained by decoration of the vertices of $T \in H$, e.g.,

$$\{\bullet\}_2 = \{\bullet, \blacksquare\}. \tag{140}$$

It is not difficult to check that the same is true for any $T \in H$,

$$\zeta^T = \sum_{\mathcal{T} \in \{T\}_2} Y^{\mathcal{T}}. \tag{141}$$

Thus

$$f_{\phi_1}[\zeta] = \sum_{\mathcal{T} \in H_2} Y^{\mathcal{T}}. \tag{142}$$

Since

$$\lim_{t_0 \to +\infty} Y^1(x_R) = \lim_{t_0 \to +\infty} x_R = \tilde{x}_1, \tag{143}$$

and $Y^{\bullet}$ does not depend on t_0 then

$$\lim_{t_0 \to +\infty} Y^{\bullet}(x_R) = Y^{\bullet}(\tilde{x}_1). \tag{144}$$

Similarly for any $\mathcal{T} \in H_{\bullet}$, $\lim_{t_0 \to +\infty} Y^{\mathcal{T}}(x_R)$ is both x_0 and t_0 independent. In the same way

$$\lim_{t_0 \to +\infty} Y^{\blacksquare}(x_R) = \lim_{t_0 \to +\infty} (\mathbb{I} - P) \int_{t_0}^{t} e^{(t-u)D} X(\tilde{x}_1(u)) du, \tag{145}$$

is finite because X is smooth. Similarly for any $\mathcal{T} \in H_{\blacksquare}$. For $\mathcal{T}$ decorated with both bullets and squares, combination of (144) and (145) ensures that $Y^{\mathcal{T}}$ is finite and x_0 independent. ■

Now, using decorated rooted trees with the rule (76), one identifies $f_{\phi_1}[\zeta](x_R) = f_{\phi_+}[Y](x_R)$ as the renormalized theory, $f_{\phi_1}[\chi](x_R) = f_{\phi}[Y](x_R)$ as the bare theory and the counterterms are given by $f_{\phi_-}[Y](x_R)$. By proposition III.2 one finally obtains the main result of this paper:

The bare and renormalized theories define two algebra morphisms γ and γ_+ between the Hopf algebra of decorated rooted trees and the free algebra $\mathcal{A}$ of decorations. γ_+ is the positive part of the algebraic $\mathcal{A}$-valued Birkhoff decomposition of γ.

IV. OUTLOOK AND CONCLUSION

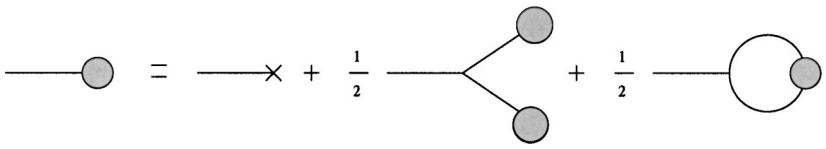
As a nice application for the tools developed above in the resolution of fixed point equation, let us mention Schwinger–Dyson equations. The latest (see Ref. 13 as well as Ref. 5 for a pedagogical account) form a system of nonlinear implicit functional differential equations analogous to the exact renormalization group equation in many respects. They are best formulated as an equation for the functional derivative of the connected generating functional $W[j]$

$$\left((\Box_x + m^2) \frac{\delta}{\delta J(x)} - V' \left(\frac{\delta}{\delta J(x)} \right) + J(x) \right) e^{W[J]} = 0, \tag{146}$$

for a Euclidian scalar field theory with interacting potential $V(\phi)$. In the simplest case of a $\lambda \phi^3$ theory, the equation reads

$$\frac{\delta W}{\delta J(x)} = \int dy\ K(x,y)J(y) + \frac{\lambda}{2}\int dy\ K(x,y)\left(\frac{\delta W}{\delta J(y)}\right)^2 + \frac{\lambda}{2}\int dy\ K(x,y)\frac{\delta^2 W}{\delta J(y)^2}, \qquad (147)$$

where $K(x,y)$ is the kernel of the free propagator. They are best captured by a diagrammatic expression,



that can be used recursively to generate the full Feynamn diagram expansion. Beyond ordinary convention of QFT, note that the cross stands for an insertion of the source J.

For our purpose, it is rewritten as a fixed point equation for the classical field $\phi(x) = \delta W / \delta J(x)$

$$\phi = \phi_0 + \lambda\ F_1(\phi) + \lambda\ F_2(\phi), \qquad (148)$$

where ϕ_0 is the classical field in the absence of interaction. The functions F_i are in one-to-one correspondence with the diagrams appearing above. This equation can be solved perturbatively in powers of λ by a recursive procedure. The order n term can be easily expressed as a sum over trees with n vertices which are decorated with the 2 diagrams of (147). These are trees that are drawn on the Feynman diagram and that retrace the ways a given Feynman diagram can be obtained through an iteration of the Schwinger–Dyson equations.

While the correspondence between Feynman diagrams and trees is in general complicated, if one restricts to the classical level, the Schwinger–Dyson degenerates because only F_1 survives. Accordingly, they reduce to the classical equation of motion so that the previous tree expansion is nothing but the tree level Feynman diagram expansion. Finally, a Legendre transformation from $W[j]$ to $\Gamma[\phi]$ allows to formulate an equation for $\delta\Gamma / \delta\phi(x)$.

A more precise treatment of Schwinger–Dyson equations within the Hopf algebraic framework of rooted trees will be developped in some future work. As a (temporary) conclusion, let us recall that we have presented the first algebraic steps towards an adaption of Connes–Kreimer work to the ERGE. As in the BPHZ procedure with minimal subtraction scheme in dimensional regularization, renormalized and bare theories are linked inside a Birkhoff decomposition. In the BPHZ framework, renormalization corresponds to the projection of meromorphic functions (with pole only at dimension of space time) on their holomorphic part. Continuous renormalization appears as a projection on one decoration. Whether the algebra of decorations is an artefact—hiding deeper connection with the Rieman–Hilbert problem—or is truly meaningful is not perfectly clear at the moment. Hopefully this might be clarified by revisiting our algebraic Birkhoff decomposition within the more general framework of Rota–Baxter equation (see Ref. 6 for nice and recent development on this topic).

Finally, it appears that the Birkhoff decomposition, which plays a major role in the theory of integrable systems, provides a relation between the latter and renormalization theory.[22] This could have important consequences for actual computations in renormalization by using the full power of complete integrability.

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Asymptotic quasinormal frequencies for black holes in nonasymptotically flat space–times

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The exact computation of asymptotic quasinormal frequencies is a technical problem which involves the analytic continuation of a Schrödinger-type equation to the complex plane and then performing a method of monodromy matching at several poles in the plane. While this method was successfully used in asymptotically flat space–time, as applied to both the Schwarzschild and Reissner–Nordstrøm solutions, its extension to nonasymptotically flat space–times has not been achieved yet. In this work it is shown how to extend the method to this case, with the explicit analysis of Schwarzschild–de Sitter and large Schwarzschild–anti–de Sitter black holes, both in four dimensions. We obtain, for the first time, analytic expressions for the asymptotic quasinormal frequencies of these black hole space–times, and our results match previous numerical calculations with great accuracy. We also list some results concerning the general classification of asymptotic quasinormal frequencies in *d*-dimensional space–times. © *2004 American Institute of Physics.*
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I. INTRODUCTION

A long time has passed since research first focused on analyzing the linear stability of four dimensional black hole solutions in general relativity.[1,2] However, it was not until very recent times that this stability problem was addressed within a *d*-dimensional setting.[3–5] These papers tried to be as exhaustive as possible, studying in detail the perturbation theory of spherically symmetric black holes in *d* dimensions and allowing for the possibilities of both charge and a background cosmological constant. Having thus acquired a list of stable black hole solutions, the next question to address within this problem are quasinormal modes—the damped oscillations which describe the return to the initial configuration, after the onset of a linear perturbation (see Refs. 6 and 7 for reviews).

Besides their natural role in the perturbation theory of general relativity, quasinormal modes have recently been the focus of much attention following suggestions that they could have a role to play in the quest for a theory of quantum gravity.[8,9] The idea is to look at those special modes

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which are infinitely damped, and thus do not radiate. It was suggested in Ref. 8 that an application of Bohr's correspondence principle to these asymptotic quasinormal frequencies could yield new information about quantum gravity, in particular on the quantization of area at a black hole event horizon. It was further suggested in Ref. 9 that asymptotic quasinormal frequencies could help fix certain parameters in loop quantum gravity. Both these suggestions lie deeply on the fact that the real part of the asymptotic quasinormal frequencies is given by the logarithm of an integer number, a fact that was analytically shown to be true, for Schwarzschild black holes in d-dimensional space–time, in Refs. 10 and 11. A question of particular relevance that immediately follows is whether the suggestions in Refs. 8 and 9 are universal or are only applicable to the Schwarzschild solution. Given the mentioned analysis of Refs. 3 and 5, one has at hand all the required information to address this problem and compute asymptotic quasinormal frequencies of d-dimensional black holes. A preliminary clue is already present in Ref. 11, where the analysis of the four-dimensional Reissner–Nordstrøm solution yielded a negative answer: the asymptotic quasinormal frequencies obeyed a complicated relation which did not seem to have the required form. While extending this result to both the d-dimensional and the extremal Reissner–Nordstrøm solutions did not pose great obstacles,[12] an extension of the analytical techniques in Ref. 11 to nonasymptotically flat space–times proves to be a greater challenge. It is the goal of this paper to carry out an extension of the techniques in Ref. 11 to nonasymptotically flat space–times, with the explicit analysis of Schwarzschild–de Sitter and large Schwarzschild–anti–de Sitter black holes, both in four dimensions. The detailed study of these solutions in d-dimensions will appear elsewhere,[12] including charged solutions in asymptotically de Sitter and asymptotically anti–de Sitter space–times, as well as an analysis of the implications of our results on what concerns the proposals of Refs. 8 and 9, dealing with the application of quasinormal modes to quantum gravity.

It is important to stress that even if the ideas in Refs. 8 and 9 turn out not to be universal, it is still the case that quasinormal frequencies will most likely have a role to play in the quest for a theory of quantum gravity. Indeed, quasinormal frequencies can also be regarded as the poles in the black hole greybody factors which play a pivotal role in the study of Hawking radiation. Furthermore, the monodromy technique introduced in Ref. 11 to analytically compute asymptotic quasinormal frequencies was later extended, in Ref. 13, so that it can also be used in the computation of asymptotic greybody factors. It was first suggested in Ref. 13 that the results obtained for these asymptotic greybody factors could be of helpin identifying the dual conformal field theory which microscopically describes the black hole, and these ideas have been taken one step forward with the recent work of Ref. 14. It remains to be seen how much asymptotic quasinormal modes and greybody factors can help in understanding quantum gravity.

Let us conclude this introduction with some generics concerning quasinormal frequencies (we refer the reader to the upcoming[12] for a full list of conventions and details). Later, in Sec. II, we shall compute asymptotic quasinormal frequencies for a Schwarzschild–de Sitter black hole in four-dimensional space–time. Our results will also be shown to match earlier numerical computations with great accuracy. In Sec. III, we shall study large Schwarzschild–anti–de Sitter black holes in four dimensions, and analytically compute their asymptotic quasinormal frequencies. Again, our results match earlier numerical computations to great accuracy. We end with some comments concerning the general classification of asymptotic quasinormal frequencies in d-dimensional space–times.[12]

For a four-dimensional Schwarzschild black hole, one has the asymptotic quasinormal frequencies

$$\lim_{n\to+\infty}\omega_n \sim [\text{offset}] + in[\text{gap}] + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right),$$

where the real part of the offset is the frequency of the emitted radiation, and the gap are the quantized increments in the inverse relaxation time. Here, the gap is given by the surface gravity. One can try to extend this analysis to more general situations and also include space–times with two horizons, but then generic results become much harder to obtain.[15–18] We shall take the time

dependence for the perturbation to be $e^{i\omega t}$, so that $\mathbb{I}\mathrm{m}(\omega)>0$ for stable solutions. There is also a reflection symmetry $\omega\leftrightarrow-\overline{\omega}$ which changes the sign of $\mathbb{R}\mathrm{e}(\omega)$. In this case, our quasinormal mode conventions are the following (see Ref. 12 for a full list of conventions in d dimensions). The perturbation master equations of Refs. 3 and 5 can be cast in a Schrödinger-type form as

$$-\frac{\mathrm{d}^2\Phi_\omega}{\mathrm{d}x^2}(x)+V(x)\Phi_\omega(x)=\omega^2\Phi_\omega(x), \tag{1.1}$$

where the potential will vary according to the specific case at hand. The boundary conditions are the usual: incoming waves at the black hole horizon and outgoing waves at infinity (or at the cosmological horizon, for the asymptotically de Sitter case). (For the asymptotically anti–de Sitter situation things will be different.) These can be written as

$$\Phi_\omega(x)\sim e^{i\omega x} \text{ as } x\to-\infty,$$

$$\Phi_\omega(x)\sim e^{-i\omega x} \text{ as } x\to+\infty,$$

where x is the tortoise coordinate. Indeed, if the metric is chosen as $g=-f(r)\mathrm{d}t\otimes\mathrm{d}t+f(r)^{-1}\,\mathrm{d}r\otimes\mathrm{d}r+r^2\,\mathrm{d}\Omega_2^2$, with parameters $M=\boldsymbol{\mu}$ for the black hole mass and $\Lambda=3\boldsymbol{\lambda}$ for the background cosmological constant, then at any (event or cosmological) horizon, $f(R_H)=0$. One can expand near the horizon $f(r)\simeq(r-R_H)f'(R_H)+\cdots$, and it follows for the tortoise,

$$x\equiv\int\frac{\mathrm{d}r}{f(r)}\simeq\int\frac{\mathrm{d}r}{(r-R_H)f'(R_H)}=\frac{1}{f'(R_H)}\log(r-R_H)\equiv\frac{1}{2k_H}\log(r-R_H)\equiv\frac{1}{4\pi T_H}\log(r-R_H),$$

locally near the chosen horizon. Here k_H is the surface gravity and T_H is the Hawking temperature.

II. ASYMPTOTICALLY DE SITTER SPACE–TIMES

Reference 5 discusses the stability of black holes in asymptotically de Sitter (dS) space–times to tensor, vector, and scalar-type perturbations of the metric and the electromagnetic field. For black holes without charge, which is the case we shall focus on, tensor and vector-type perturbations are stable in any dimension. Scalar-type perturbations are stable up to dimension six but there is no proof of stability in dimension $d\geqslant 7$. As we shall work in four dimensions, we are guaranteed a stable solution. Quantization in dS space was first addressed in Ref. 19. These authors found that the cosmological event horizon is stable, but also that there is an isotropic background of thermal radiation. Analysis of the wave equation in dS space also led to the natural boundary conditions on quasinormal modes: incoming waves at the black hole horizon and outgoing waves at the cosmological horizon. The Schwarzschild dS solution in dimension $d=4$ has parameters $\boldsymbol{\mu}$ and $\boldsymbol{\lambda}>0$, with metric

$$f(r)=1-\frac{2\boldsymbol{\mu}}{r}-\boldsymbol{\lambda}r^2.$$

The potentials to be used in the master equation (1.1), describing the evolution of scalar, electromagnetic and gravitational fields, can be followed through the Klein–Gordon, Maxwell, and Einstein equations, respectively. They will necessarily depend on the specific field under consideration and are as follows. For scalar perturbations[20]

$$V_s(r)=f(r)\left(\frac{\ell(\ell+1)}{r^2}+\frac{2\boldsymbol{\mu}}{r^3}-2\boldsymbol{\lambda}\right), \tag{2.1}$$

while for electromagnetic perturbations[21]

$$V_{\mathrm{em}}(r) = f(r)\left(\frac{\ell(\ell+1)}{r^2}\right). \tag{2.2}$$

The gravitational perturbations decompose into two sets, the odd and the even parity one.[21] For the odd parity perturbations one has (these are the vector-type gravitational perturbations)

$$V_{\mathrm{odd}}(r) = f(r)\left(\frac{\ell(\ell+1)}{r^2} - \frac{6\boldsymbol{\mu}}{r^3}\right), \tag{2.3}$$

while for the even parity perturbations (these are the scalar-type gravitational perturbations),

$$V_{\mathrm{even}}(r) = \frac{2f(r)}{r^3}\frac{9\boldsymbol{\mu}^3 + 3a^2\boldsymbol{\mu}r^2 + a^2(1+a)r^3 + 3\boldsymbol{\mu}^2(3ar - 3\boldsymbol{\lambda}r^3)}{(3\boldsymbol{\mu} + ar)^2}, \tag{2.4}$$

where $a=\frac{1}{2}(\ell(\ell+1)-2)$. In all cases, we have denoted by ℓ the angular momentum quantum number, which yields the multipolarity of the field. These are the potentials we shall use in the following.

To simplify the calculation, we choose the radius of the black hole to be our length unit. The radius of the cosmological horizon will then be an adimensional quantity $R>1$. In this case, it is easily seen that the warp factor must be of the form

$$f(r) = 1 - \frac{2\boldsymbol{\mu}}{r} - \boldsymbol{\lambda}r^2 = -\frac{\boldsymbol{\lambda}(r-1)(r-R)(r+R+1)}{r},$$

and consequently the black hole's parameters will be given in our units by

$$\boldsymbol{\lambda} = \frac{1}{R^2+R+1},$$

$$\boldsymbol{\mu} = \frac{R^2+R}{2(R^2+R+1)}.$$

The (complex) tortoise coordinate which vanishes at the origin is

$$x = \int \frac{\mathrm{d}r}{f(r)} = \frac{1}{2k_H}\log(1-r) + \frac{1}{2k_C}\log\left(1-\frac{r}{R}\right) + \frac{1}{2k_F}\log\left(1+\frac{r}{R+1}\right),$$

where

$$k_H = \frac{1}{2}f'(1) = \frac{(R-1)(R+2)}{2(R^2+R+1)},$$

$$k_C = \frac{1}{2}f'(R) = -\frac{(R-1)(2R+1)}{2R(R^2+R+1)},$$

$$k_F = \frac{1}{2}f'(-R-1) = \frac{(R+2)(2R+1)}{2(R+1)(R^2+R+1)},$$

are the surface gravities at the black hole horizon $r=1$, the cosmological horizon $r=R$, and the fictitious horizon $r=-R-1$. Notice that we take the surface gravity at the cosmological horizon to be negative.

As in Ref. 11, we notice that although x has a ramification point at each horizon, $\mathbb{R}\mathrm{e}(x)$ is well defined and we can look at the Stokes line $\mathbb{R}\mathrm{e}(x)=0$. Since $x(0)=0$, this curve contains the origin and its singular points are given by

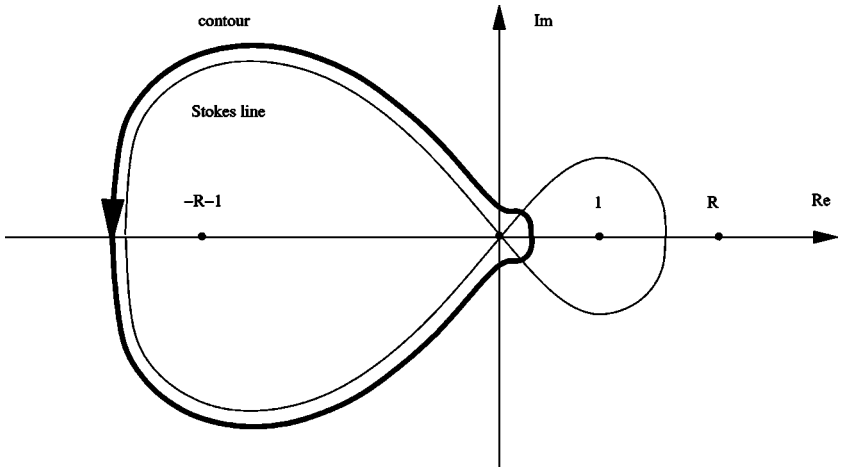

FIG. 1. Stokes line for the Schwarzschild dS black hole, along with the chosen contour for monodromy matching.

$$\frac{dx}{dr} = 0 \;\Leftrightarrow\; \frac{1}{f(r)} = 0 \Leftrightarrow r = 0.$$

For $r \sim 0$ one has $f(r) \sim (-2\mu/r)$ and hence

$$x \sim -\int \frac{r\,dr}{2\mu} = -\frac{r^2}{4\mu}.$$

Consequently the Stokes line is given by $r = \rho e^{\pm(i\pi/4)}$, $\rho \in \mathbb{R}$ in a neighborhood of the origin. On the other hand, for $r \sim \infty$ one has $f(r) \sim -\Lambda r^2$, and thus

$$x \sim -\int \frac{dr}{\Lambda r^2} = x_0 + \frac{1}{\Lambda r}.$$

Notice that in particular x has no monodromy at infinity, and hence

$$\frac{1}{k_H} + \frac{1}{k_C} + \frac{1}{k_F} = 0.$$

Thus we can choose the three ramification lines of x to cancel each other off, and x_0 is well defined. Using the expression for x with an appropriate choice of ramification line in each logarithm, one can compute the real part of x_0, which is not zero. Therefore the Stokes line cannot extend all the way to infinity and the four lines starting out at the origin must thus connect among themselves. Studying the behavior of $\mathbb{R}\mathrm{e}(x)$ near the horizons, it is not hard to guess that the Stokes line is as indicated in Fig. 1. This guess is moreover verified by a numerical computation of the same Stokes line, indicated in Fig. 2.

Since for $r \sim 0$ the presence of the cosmological constant is irrelevant, we expect the potential to behave as in the Schwarzschild black hole, and this is indeed the case,

$$V \sim \frac{j^2 - 1}{4x^2},$$

where $j = 0$ for scalar fields and scalar-type gravitational perturbations, $j = 1$ for electromagnetic perturbations, and $j = 2$ for vector-type gravitational perturbations. Correspondingly, for $x \sim 0$ the complexified solution of the Schrödinger-type equation is of the form

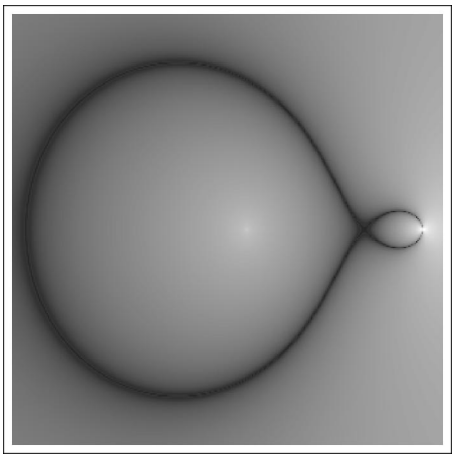

FIG. 2. Numerical calculation of the Stokes line for the Schwarzschild dS black hole.

$$\Phi(x) \sim A_+\sqrt{2\pi\omega x}J_{j/2}(\omega x) + A_-\sqrt{2\pi\omega x}J_{-j/2}(\omega x),$$

where J_ν represents a Bessel function of the first kind and $A_\pm$ are (complex) integration constants.

For the asymptotic quasinormal modes one has $\mathbb{I}\mathrm{m}(\omega) \gg \mathbb{R}\mathrm{e}(\omega)$, and hence ω is approximately purely imaginary. Consequently in a neighborhood of the origin one has $\omega x \in \mathbb{R}^+$ for $r=\rho e^{i\pi/4}$, $\rho \in \mathbb{R}$, and $\omega x \in \mathbb{R}^-$ for $r=\rho e^{-i\pi/4}$, $\rho \in \mathbb{R}$. From the asymptotic expansion

$$J_\nu(z) = \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right),\ z \gg 1,$$

we see that

$$\Phi(x) \sim 2A_+\cos(\omega x - \alpha_+) + 2A_-\cos(\omega x - \alpha_-) = (A_+e^{-i\alpha_+} + A_-e^{-i\alpha_-})e^{i\omega x} + (A_+e^{i\alpha_+} + A_-e^{i\alpha_-})e^{-i\omega x},$$

for $r=\rho e^{i\pi/4}$, $\rho \in \mathbb{R}^-$, where

$$\alpha_\pm = \frac{\pi}{4}(1 \pm j).$$

For $z \sim 0$ one has the expansion

$$J_\nu(z) = z^\nu w(z),$$

where $w(z)$ is an even holomorphic function. Consequently, as one rotates from $r=\rho e^{i\pi/4}$, $\rho \in \mathbb{R}^-$ to $r=\rho e^{-i\pi/4}$, $\rho \in \mathbb{R}^-$, one has

$$\sqrt{2\pi e^{3\pi i}\omega x}J_{\pm j/2}(e^{3\pi i}\omega x) = e^{(3\pi i/2)(1\pm j)}\sqrt{2\pi\omega x}J_{\pm j/2}(\omega x) \sim 2e^{6i\alpha_\pm}\cos(\omega x - \alpha_\pm)$$

and hence

$$\begin{aligned}\Phi(x) &\sim 2A_+e^{6i\alpha_+}\cos(-\omega x - \alpha_+) + 2A_-e^{6i\alpha_-}\cos(-\omega x - \alpha_-)\\ &= (A_+e^{7i\alpha_+} + A_-e^{7i\alpha_-})e^{i\omega x} + (A_+e^{5i\alpha_+} + A_-e^{5i\alpha_-})e^{-i\omega x},\end{aligned}$$

for $r=\rho e^{-i\pi/4}$, $\rho \in \mathbb{R}^-$. As one would expect, this completely parallels the computation for the Schwarzschild solution in Ref. 11. Next we compute the monodromy of the solution at infinity. For $r \sim \infty$ we have

$$V_s \sim 2\boldsymbol{\lambda}^2 r^2 \sim \frac{2}{(x-x_0)^2} = \frac{3^2-1}{4(x-x_0)^2},$$

$$V_{\text{em}} \sim V_{\text{odd}} \sim -\boldsymbol{\lambda}\ell(\ell+1),$$

$$V_{\text{even}} \sim -\boldsymbol{\lambda}\left[\ell(\ell+1) - \frac{18\boldsymbol{\mu}^2\boldsymbol{\lambda}}{a^2}\right].$$

Consequently, either

$$\Phi(x) \sim B_+\sqrt{2\pi\omega(x-x_0)}J_{3/2}(\omega(x-x_0)) + B_-\sqrt{2\pi\omega(x-x_0)}J_{-3/2}(\omega(x-x_0))$$

or (here $\tilde{\omega}^2=\omega^2+\boldsymbol{\lambda}\ell(\ell+1)$ for the electromagnetic and odd parity perturbations, and $\tilde{\omega}^2=\omega^2+\boldsymbol{\lambda}[\ell(\ell+1)-18\mu^2\lambda/a^2]$ for the even parity perturbations)

$$\Phi(x) \sim B_+e^{i\tilde{\omega}(x-x_0)} + B_-e^{-i\tilde{\omega}(x-x_0)}$$

for $r\sim\infty$; in any case, Φ is holomorphic and hence the monodromy of Φ at infinity is equal to one. If Φ corresponds to a quasinormal mode, its monodromy around $r=1$ must be the same as the monodromy of $e^{i\omega x}$, that is, $e^{i\omega(2\pi i/2k_H)}=e^{-\pi\omega/k_H}$. Similarly, its monodromy around $r=R$ must be the same as the monodromy of $e^{-i\omega x}$, that is, $e^{\pi\omega/k_C}$. Since the only other singularities of Φ are at the origin and at $r=-R-1$, it is then clear that the monodromy of Φ around the contour depicted in the figure must be

$$\frac{1}{e^{-(\pi\omega/k_H)+(\pi\omega/k_C)}} = e^{(\pi\omega/k_H)-(\pi\omega/k_C)}.$$

The monodromy of $e^{\pm i\omega}$ around the contour is $e^{\pm i\omega(2\pi i/2k_F)}=e^{\mp\pi\omega/k_F}$. As one goes around the contour the coefficient of $e^{i\omega x}$ in the asymptotic expansion of Φ gets multiplied by

$$\frac{A_+e^{7i\alpha_+}+A_-e^{7i\alpha_-}}{A_+e^{-i\alpha_+}+A_-e^{-i\alpha_-}}.$$

For this term to have the required monodromy we must impose

$$\frac{A_+e^{7i\alpha_+}+A_-e^{7i\alpha_-}}{A_+e^{-i\alpha_+}+A_-e^{-i\alpha_-}}e^{-\pi\omega/k_F} = e^{(\pi\omega/k_H)-(\pi\omega/k_C)} \Leftrightarrow \frac{A_+e^{7i\alpha_+}+A_-e^{7i\alpha_-}}{A_+e^{-i\alpha+}+A_-e^{-i\alpha_-}} = e^{-2\pi\omega/k_C}.$$

Similarly, for the term in $e^{-i\omega x}$ we get the condition

$$\frac{A_+e^{5i\alpha_+}+A_-e^{5i\alpha_-}}{A_+e^{i\alpha_+}+A_-e^{i\alpha_-}}e^{-\pi\omega/k_F} = e^{(\pi\omega/k_H)-(\pi\omega/k_C)} \Leftrightarrow \frac{A_+e^{5i\alpha_+}+A_-e^{5i\alpha_-}}{A_+e^{i\alpha_+}+A_-e^{i\alpha_-}} = e^{2\pi\omega/k_H}.$$

The condition for these equations to have nontrivial solutions (A_+,A_-) is then

$$\begin{vmatrix} e^{7i\alpha_+}-e^{-2\pi\omega/k_C}e^{-i\alpha_+} & e^{7i\alpha_-}-e^{-2\pi\omega/k_C}e^{-i\alpha_-} \\ e^{5i\alpha_+}-e^{2\pi\omega/k_H}e^{i\alpha_+} & e^{5i\alpha_-}-e^{2\pi\omega/k_H}e^{i\alpha_-} \end{vmatrix} = 0 \Leftrightarrow \begin{vmatrix} \sin\left(4\alpha_+-\frac{i\pi\omega}{k_C}\right) & \sin\left(4\alpha_--\frac{i\pi\omega}{k_C}\right) \\ \sin\left(2\alpha_++\frac{i\pi\omega}{k_H}\right) & \sin\left(2\alpha_-+\frac{i\pi\omega}{k_H}\right) \end{vmatrix} = 0.$$

As in the Schwarzschild case, this equation is automatically satisfied for $j=0$. This is to be expected, as for $j=0$ the Bessel functions $J_{\pm j/2}$ coincide and do not form a basis for the space of solutions of the Schrödinger-type equation near the origin. As in Ref. 11, we consider this equation for j nonzero and take the limit as $j\to 0$. This amounts to writing the equation as a power series in j and equating to zero the first nonvanishing coefficient, which in this case is the coefficient of the linear part. Thus, we just have to require that the derivative of the determinant above with respect to j be zero for $j=0$. This amounts to

$$\begin{vmatrix} \pi\cos\left(\pi-\frac{i\pi\omega}{k_C}\right) & -\pi\cos\left(\pi-\frac{i\pi\omega}{k_C}\right) \\ \sin\left(\frac{\pi}{2}+\frac{i\pi\omega}{k_H}\right) & \sin\left(\frac{\pi}{2}+\frac{i\pi\omega}{k_H}\right) \end{vmatrix} + \begin{vmatrix} \sin\left(\pi-\frac{i\pi\omega}{k_C}\right) & \sin\left(\pi-\frac{i\pi\omega}{k_C}\right) \\ \frac{\pi}{2}\cos\left(\frac{\pi}{2}+\frac{i\pi\omega}{k_H}\right) & -\frac{\pi}{2}\cos\left(\frac{\pi}{2}+\frac{i\pi\omega}{k_H}\right) \end{vmatrix} = 0,$$

from where we obtain our final result as

$$\cosh\left(\frac{\pi\omega}{k_H}-\frac{\pi\omega}{k_C}\right)+3\cosh\left(\frac{\pi\omega}{k_H}+\frac{\pi\omega}{k_C}\right)=0. \tag{2.5}$$

Notice that if ω is a solution of this equation then so is $-\overline{\omega}$, as must be the case with quasinormal modes.

To recover the Schwarzschild quasinormal frequencies we first write out the equation as

$$e^{(\pi\omega/k_H)-(\pi\omega/k_C)}+e^{-(\pi\omega/k_H)+(\pi\omega/k_C)}+3e^{(\pi\omega/k_H)+(\pi\omega/k_C)}+3e^{-(\pi\omega/k_H)-(\pi\omega/k_C)}=0,$$

and next take the limit as $R\to\infty$, in which $k_H\to\frac{1}{2}$ and $k_C\to 0^-$. If we assume that $\mathbb{R}\mathrm{e}(\omega)>0$, we see that the two middle terms are exponentially small, and hence the equation reduces to

$$e^{\pi\omega/k_H}+3e^{-\pi\omega/k_H}=0\Leftrightarrow e^{4\pi\omega}=-3,$$

which is exactly the equation obtained in Refs. 10 and 11. Therefore, the Schwarzschild black hole is not a singular limit of the Schwarzschild dS black hole as far as the quasinormal modes are concerned, unlike what happens with the Reissner–Nordstrøm black hole solution. The reason for this is clear from the monodromy calculation: whereas the structure of the tortoise near the singularity $r=0$ in the Reissner–Nordstrøm solution depends crucially on whether the charge is zero or not, in the Schwarzschild dS case it does not depend on $\boldsymbol{\lambda}$. Thus, as $R\to+\infty$, the cosmological horizon approaches the point at infinity and the contour approaches the contour used in Ref. 11.

For $j=1$ one has $\alpha_+=\pi/2$, $\alpha_-=0$ and hence the condition for the quasinormal frequencies is

$$\begin{vmatrix} -\sin\left(\frac{i\pi\omega}{k_C}\right) & -\sin\left(\frac{i\pi\omega}{k_C}\right) \\ -\sin\left(\frac{i\pi\omega}{k_H}\right) & \sin\left(\frac{i\pi\omega}{k_H}\right) \end{vmatrix} = 0\Leftrightarrow \sin\left(\frac{i\pi\omega}{k_C}\right)\sin\left(\frac{i\pi\omega}{k_H}\right)=0,$$

with the solutions

$$\omega=ink_H \quad \text{or} \quad \omega=ink_C \quad (n\in\mathbb{N}).$$

Again, as $R\to\infty$ one obtains the Schwarzschild result, $\omega=ni/2$. Finally, for $j=2$ one has $2\alpha_\pm=(\pi/2)\pm\pi$, $4\alpha_\pm=\pi\pm 2\pi$, and consequently the quasinormal frequencies are the same as in the $j=0$ case, for which $2\alpha_\pm=\pi/2$, $4\alpha_\pm=\pi$.

Let us now review the literature concerning asymptotic quasinormal frequencies in the Schwarzschild dS space–time, so that we can compare our results to what has been previously accomplished on this subject. First of all, it is possible to prove, without computing explicitly the quasinormal frequencies, that $j=0$ and $j=2$ perturbations must have the same quasinormal spectra,[22] and so this is a consistency check on our results. For Schwarzschild dS, early results on quasinormal modes were studied in Ref. 23, without great emphasis on the asymptotic case. The first analytical results in $d=4$ were derived in the near-extremal situation, where event and cosmological horizons are nearly coincident,[24] but the approximation used therein is not expected to hold in the asymptotic limit, at least on what concerns the real part of the asymptotic frequencies. Further approximations were studied in Ref. 25, in a limit where the black hole mass is much smaller than the space–time radius of curvature, but focusing explicitly on the time *dependent* transient situation. An attempt at an analytic solution for the asymptotic quasinormal frequencies,

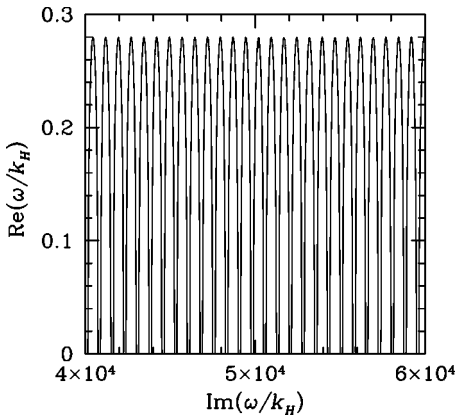

FIG. 3. Real versus imaginary part of quasinormal frequencies for the nearly extremal Schwarzschild dS solution.

using the monodromy technique of Ref. 11, was done in Ref. 26. However, an erroneous identification of the relevant contours led these authors to an incorrect result (see also Ref. 27, where other arguments were given trying to explain the failure of Ref. 26 to reproduce available numerical data). Perhaps the most thorough analytical work on Schwarzschild dS asymptotic quasinormal frequencies to date is the one in Ref. 18. These authors find that because there are two different surface gravities, there are also two sets of solutions for $\mathbb{I}\mathrm{m}(\omega)$ when the horizons are *widely* spaced, namely $\mathbb{I}\mathrm{m}(\omega)$ equally spaced with spacing equal to k_H or $\mathbb{I}\mathrm{m}(\omega)$ equally spaced with spacing equal to k_C. It was further claimed in Ref. 18 that this lack of consensus on quasinormal frequencies was due to the fact that there is no global definition of temperature in this space–time. Our results appear to confirm this expectation: in the limit where the cosmological radius goes to infinity, and one recovers the Schwarzschild modes, we found the spacing to be equal to k_H. In the limit where the black hole radius is very small, (2.5) yields modes with spacing equal to k_C (notice that this formula does not depend on the choice of units).

Besides the mentioned works, there are also numerical results available, and this is where our comparisons prove to be most conclusive. In Ref. 28 the asymptotic quasinormal frequencies for electromagnetic and gravitational perturbations of nearly extremal Schwarzschild dS space–times were studied. It turned out that, for gravitational perturbations, the real part of the asymptotic quasinormal frequencies has an oscillatory behavior as plotted against its imaginary part. We plot the same figure as in Ref. 28, using our final result (2.5), in Fig. 3. This figure corresponds to the roots of (2.5) for a near extremal black hole with $k_H = 10^{-3}$, and should be compared to Fig. 4 in Ref. 28 which refers to the same value of k_H. One immediately observes agreement to large accuracy: first, the oscillation period is exactly the same. Second, the value of $\max(\mathbb{R}\mathrm{e}(\omega))$ in Ref. 28 is of the same order as our maximum, but always larger than it, as it must be since our value refers to the asymptotic regime only. Moreover, and on what concerns $j=1$ electromagnetic perturbations, the numerical data in Ref. 28 is very clear and indicates that the real part of the asymptotic quasinormal frequencies should vanish, and this is precisely what we have obtained. Further numerical results have recently been obtained in Ref. 29, this time around without any near extremality constraints. Again, for the gravitational perturbations, the real part of the asymptotic quasinormal frequencies was found to have an oscillatory behavior. Also, for electromagnetic perturbations, the real part of the asymptotic quasinormal frequencies was found to vanish. Our analytical results still agree very well with the numerics: we are able to reproduce the basic features of Fig. 2 in Ref. 29, with the exception that we also find modes with a zero real part. This should not be cause for concern as it is known to be highly difficult to numerically obtain modes with a vanishing real part. On what concerns the $j=1$ perturbations of Ref. 29, we obtain exactly what they have found.

III. ASYMPTOTICALLY ANTI–DE SITTER SPACE–TIMES

Reference 5 discusses the stability of black holes in asymptotically anti–de Sitter (AdS) space–times to tensor, vector and scalar perturbations of the metric and the electromagnetic field. For black holes without charge, which is the case we shall focus on, tensor and vector perturbations are stable in any dimension. Scalar perturbations are stable in dimension four but there is no proof of stability in dimension $d \geqslant 5$. As we shall work in four dimensions, we are guaranteed a stable solution. Quantization of scalar field in AdS was first addressed in Ref. 30. An important theme concerned boundary conditions: because AdS light rays can reach spatial infinity and return to the origin in finite time, as measured by the observer at the origin, one could expect for reflecting boundary conditions at the AdS walls. However, these walls are at timelike spatial infinity. As it turns out, the sensible boundary conditions to impose on quasinormal modes include the usual incoming waves at the black hole horizon and then vanishing of the fields at infinity (i.e., at the boundary of AdS). The Schwarzschild AdS solution in dimension $d=4$ has parameters $\boldsymbol{\mu}$ and $\boldsymbol{\lambda} < 0$, with metric

$$f(r) = 1 - \frac{2\boldsymbol{\mu}}{r} - \boldsymbol{\lambda} r^2 = 1 - \frac{2\boldsymbol{\mu}}{r} + |\boldsymbol{\lambda}| r^2.$$

The potentials to be used in the master equation (1.1) are the same as before. Also, in the following we shall focus on scalar field perturbations.

Again, to simplify the calculation we choose the radius of the black hole to be our length unit. The length scale determined by the cosmological constant will then be an adimensional quantity R, with $\boldsymbol{\lambda} = -1/R^2$. It is then easily seen that the warp factor must be of the form

$$f(r) = 1 - \frac{2\boldsymbol{\mu}}{r} - \boldsymbol{\lambda} r^2 = \frac{(r-1)(r^2 + r + 1 + R^2)}{R^2 r}$$

and consequently the black hole mass will be given in our units by

$$\boldsymbol{\mu} = \frac{1 + R^2}{2R^2}.$$

Moreover, one can compute

$$f(r) = \frac{(r-1)(r-\gamma)(r-\overline{\gamma})}{R^2 r},$$

where

$$\gamma = -\frac{1}{2} + \frac{i}{2}\sqrt{4R^2 + 3}.$$

For simplicity, we shall consider quasinormal modes for large black holes only, in which $R \ll 1$. This serves our purpose of illustrating how the techniques in Ref. 11 are generalized for asymptotically AdS space–times, whereas the full case is carefully analyzed in Ref. 12. For these large black holes we have, approximately,

$$\gamma = e^{i(2\pi/3)} = \sqrt[3]{1}, \quad \overline{\gamma} = \gamma^2,$$

and consequently

$$\frac{1}{f(r)} = \frac{R^2}{3}\left(\frac{1}{r-1} + \frac{\overline{\gamma}}{r-\gamma} + \frac{\gamma}{r-\overline{\gamma}}\right).$$

The (complex) tortoise coordinate which vanishes at the origin is therefore

$$x = \int \frac{\mathrm{d}r}{f(r)} = \frac{R^2}{3}(\log(1-r) + \overline{\gamma}\log(1-\overline{\gamma}r) + \gamma\log(1-\gamma r)).$$

We now wish to examine the Stokes line, i.e., the curve $\mathbb{I}\mathrm{m}(\omega x)=0$. However, this time around, the expression of the tortoise makes it clear that $\mathbb{I}\mathrm{m}(\omega x)$ is a multivalued function. To bypass this problem, we choose a particular branch and simply trace out the curve shifting the ramification lines so that it never hits them. Note that the behavior of $e^{\pm i\omega x}$ will still be oscillatory along the curve. Again the Stokes line has a unique singular point at the origin, where four lines meet, as

$$\omega x \sim -\int \frac{\omega r\,\mathrm{d}r}{2\boldsymbol{\mu}} = -\frac{\omega r^2}{4\boldsymbol{\mu}}$$

for $r\sim 0$. To understand its behavior near the singularities, we notice that following our procedure, the curve

$$\mathbb{I}\mathrm{m}(\alpha\log(z)) = 0$$

is the curve

$$\alpha\log(z) = \rho \;\Leftrightarrow\; z = e^{\xi\rho}e^{i\eta\rho}$$

[with $\alpha=1/(\xi+i\eta)$ and $\rho\in\mathbb{R}$ a parameter]. This is a spiral that approaches the singularity $z=0$, except in the case where $\xi=0$, i.e., when α is purely imaginary. Therefore, generically one expects the Stokes line to hit all three singularities, and hence the fourth line starting out at the origin must extend all the way to infinity. For $r\sim\infty$ we have

$$x \sim \int \frac{R^2\,\mathrm{d}r}{r^2} = x_0 - \frac{R^2}{r}.$$

In particular, x has no monodromy at infinity, as can also be seen from its expression and the fact that

$$1+\gamma+\gamma^2 = 0.$$

We can therefore choose the three ramification lines of x to cancel each other off, making x_0 well defined. (There are however three nonequivalent ways of doing this, leading to three possible values of x at infinity: x_0, $\overline{x_0}$, and $-|x_0|$. The second choice leads to the quasinormal frequencies $-\overline{\omega}$, where ω are the quasinormal frequencies obtained by choosing x_0; the third choice leads to no solutions.) Using the expression for x with appropriate choice of ramification line in each logarithm, one then obtains

$$x_0 = \frac{2\pi\sqrt{3}R^2}{9}e^{-i\pi/3}.$$

Therefore we must have

$$\omega x_0 \in \mathbb{R} \;\Leftrightarrow\; \omega = \zeta e^{i\pi/3}\ (\zeta\in\mathbb{R}^+).$$

For such a value of ω and our choice of ramification lines, it is easily seen that ωx is real for $r=\rho e^{i\pi/3}$, $\rho\in(-1,+\infty)$. On the other hand, near the origin the Stokes line is given by

$$\mathbb{I}\mathrm{m}(-e^{i\pi/3}r^2) = 0 \;\Leftrightarrow\; r = \rho e^{-i\pi/6} \quad \text{or} \quad r = \rho e^{i\pi/3}\ (\rho\in\mathbb{R}).$$

Consequently, it is not hard to guess that the Stokes line is as depicted in Fig. 4. We have verified this guess with a numerical computation of the same Stokes line, and this is indicated in Fig. 5. It should be noted that due to the ramification lines (which can be readily identified in the figure) the spirals at the singularities are not so clearly depicted in the numerical result.

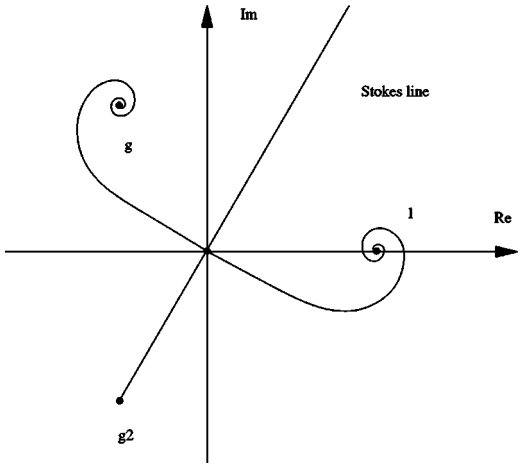

FIG. 4. Stokes line for the Schwarzschild AdS black hole.

Now, for $r\sim\infty$ we have

$$V_s \sim 2\lambda^2 r^2 \sim \frac{2}{(x-x_0)^2} = \frac{3^2-1}{4(x-x_0)^2}.$$

Consequently,

$$\Phi(x) \sim B_+\sqrt{2\pi\omega(x-x_0)}\; J_{3/2}(\omega(x-x_0)) + B_-\sqrt{2\pi\omega(x-x_0)}\; J_{-3/2}(\omega(x-x_0))$$

for $r\sim\infty$. The boundary condition $\Phi=0$ at $r=\infty$ requires that $B_-=0$. Hence,

$$\Phi(x) \sim B_+\sqrt{2\pi\omega(x-x_0)}\; J_{3/2}(\omega(x-x_0)),$$

for $r\sim\infty$. Now, and as in the Schwarzschild dS case, for $r\sim 0$ the presence of the cosmological constant is irrelevant, and the potential behaves as in the Schwarzschild black hole,

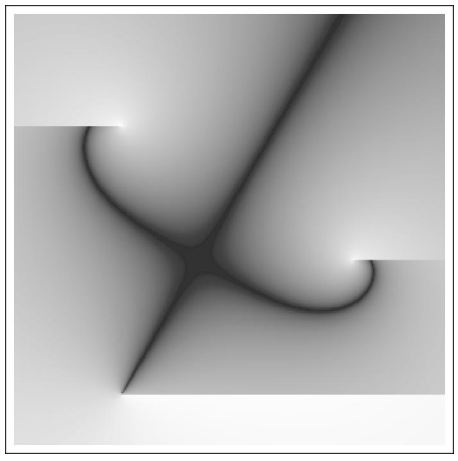

FIG. 5. Numerical calculation of the Stokes line for the Schwarzschild AdS black hole.

$$V_s \sim \frac{j^2-1}{4x^2},$$

where $j=0$ for scalar field perturbations. Correspondingly, for $x\sim 0$ the complexified solution of the Schrödinger-type equation is of the form

$$\Phi(x) \sim A_+\sqrt{2\pi\omega x}\, J_{j/2}(\omega x) + A_-\sqrt{2\pi\omega x}\, J_{-j/2}(\omega x),$$

where $A_\pm$ are (complex) integration constants. One has $\omega x \in \mathbb{R}^+$ for $r=\rho e^{i\pi/3}$, $\rho\in\mathbb{R}$, and $\omega x\in\mathbb{R}^-$ for $r=\rho e^{-i\pi/6}$, $\rho\in\mathbb{R}$. From the asymptotic expansion for $J_\nu(z)$, with $z\gg 1$, we see that

$$\begin{aligned}\Phi(x) &\sim 2A_+\cos(\omega x-\alpha_+) + 2A_-\cos(\omega x-\alpha_-)\\ &= (A_+e^{-i\alpha_+}+A_-e^{-i\alpha_-})e^{i\omega x} + (A_+e^{i\alpha_+}+A_-e^{i\alpha_-})e^{-i\omega x},\end{aligned}$$

for $r=\rho e^{i\pi/3}$, $\rho\in\mathbb{R}^+$, where

$$\alpha_\pm = \frac{\pi}{4}(1\pm j).$$

The same expansion yields

$$\Phi(x) \sim B_+e^{-i\beta_+}e^{i\omega(x-x_0)} + B_+e^{i\beta_+}e^{-i\omega(x-x_0)} = -B_+e^{-i\omega x_0}e^{i\omega x} - B_+e^{i\omega x_0}e^{-i\omega x}$$

in the same limit, since

$$\beta_+ = \frac{\pi}{4}(1+3) = \pi.$$

We conclude that A_+, A_- must satisfy

$$(A_+e^{-i\alpha_+}+A_-e^{-i\alpha_-})e^{i\omega x_0} = (A_+e^{i\alpha_+}+A_-e^{i\alpha_-})e^{-i\omega x_0}.$$

Again for $z\sim 0$, one has the expansion

$$J_\nu(z) = z^\nu w(z),$$

where $w(z)$ is an even holomorphic function. Consequently, as one rotates from $r=\rho e^{i\pi/3}$, $\rho\in\mathbb{R}^-$ to $r=\rho e^{-i\pi/6}$, $\rho\in\mathbb{R}^+$ one has

$$\sqrt{2\pi e^{-\pi i}\omega x}\, J_{\pm j/2}(e^{-\pi i}\omega x) = e^{(-\pi i/2)(1\pm j)}\sqrt{2\pi\omega x}\, J_{\pm j/2}(\omega x) \sim 2e^{-2i\alpha_\pm}\cos(\omega x-\alpha_\pm)$$

and hence

$$\begin{aligned}\Phi(x) &\sim 2A_+e^{-2i\alpha_+}\cos(-\omega x-\alpha_+) + 2A_-e^{-2i\alpha_-}\cos(-\omega x-\alpha_-)\\ &= (A_+e^{-i\alpha_+}+A_-e^{-i\alpha_-})e^{i\omega x} + (A_+e^{-3i\alpha_+}+A_-e^{-3i\alpha_-})e^{-i\omega x},\end{aligned}$$

for $r=\rho e^{-i\pi/6}$, $\rho\in\mathbb{R}^+$. This form of the solution can be propagated along the corresponding branch of the Stokes line which approaches the event horizon, and where we know that $\Phi(x)$ must behave as $e^{i\omega x}$. Consequently we obtain the second condition on A_+, A_- as

$$A_+e^{-3i\alpha_+} + A_-e^{-3i\alpha_-} = 0.$$

The two conditions on these coefficients can only have nontrivial solutions if and only if

$$\begin{vmatrix} e^{-3i\alpha_+} & e^{-3i\alpha_-} \\ e^{-i\alpha_+}e^{i\omega x_0} - e^{i\alpha_+}e^{-i\omega x_0} & e^{-i\alpha_-}e^{i\omega x_0} - e^{i\alpha_-}e^{-i\omega x_0}\end{vmatrix} = 0 \quad\Leftrightarrow\quad \begin{vmatrix} e^{-3i\alpha_+} & e^{-3i\alpha_-} \\ \sin(\alpha_+-\omega x_0) & \sin(\alpha_--\omega x_0)\end{vmatrix} = 0.$$

Again, this equation is automatically satisfied for $j=0$. We must thus consider j nonzero and then take the limit as $j\to 0$. This amounts to writing the equation as a power series in j and equating to

zero the first nonvanishing coefficient, which in this case is the coefficient of the linear part. Thus we just have to require that the derivative of the determinant above with respect to j be zero for $j=0$. This is

$$\begin{vmatrix} -\frac{3i\pi}{4}e^{-3i\pi/4} & \frac{3i\pi}{4}e^{-3i\pi/4} \\ \sin\left(\frac{\pi}{4}-\omega x_0\right) & \sin\left(\frac{\pi}{4}-\omega x_0\right) \end{vmatrix} + \begin{vmatrix} e^{-3i\pi/4} & e^{-3i\pi/4} \\ \frac{\pi}{4}\cos\left(\frac{\pi}{4}-\omega x_0\right) & -\frac{\pi}{4}\cos\left(\frac{\pi}{4}-\omega x_0\right) \end{vmatrix} = 0$$

from where we obtain our final result as

$$\tan\left(\frac{\pi}{4}-\omega x_0\right)=\frac{i}{3} \quad \Leftrightarrow \quad \omega x_0=\frac{\pi}{4}-\arctan\left(\frac{i}{3}\right)+n\pi (n\in\mathbb{N}). \tag{3.1}$$

If one makes use of the notation $\omega=[\text{offset}]+n[\text{gap}]$ (which is slightly different from the one in the Introduction), it is simple to obtain the numerical values

$$[\text{offset}]=\frac{\frac{\pi}{4}-\arctan\left(\frac{i}{3}\right)}{R^2\left(\frac{\sqrt{3}\pi}{9}-\frac{i\pi}{3}\right)}=\frac{1}{R^2}(0.572\,975+0.419\,193i)$$

and

$$[\text{gap}]=\frac{9}{4\sqrt{3}R^2}+\frac{9i}{4R^2}=\frac{1}{R^2}(1.299\,04+2.25i),$$

in complete agreement with available numerical results, as we shall see in the following (recall that we have taken the radius of the black hole horizon as our length unit).

We now need to review the literature concerning the calculation of asymptotic quasinormal frequencies in the Schwarzschild AdS space–time, in order to compare our results to earlier work done on this subject. Quasinormal modes of Schwarzschild AdS black holes were addressed in Refs. 31, 20, and 32, having a direct interpretation in terms of the dual conformal field theory, as large static AdS black holes correspond to conformal field theory thermal states. However, for what concerns us in this paper, only the first modes were computed in Refs. 31 and 20. Due to the AdS/CFT correspondence, this work sparked a series of investigations on AdS asymptotic quasinormal frequencies, which naturally concentrated on the five-dimensional case (see, e.g., Refs. 33–36). For the case that concerns us in here, $d=4$, the first numerical results for the asymptotic quasinormal frequencies were published in Ref. 37. These authors found that scalar perturbations are isospectral with both odd and even parity gravitational perturbations, and they also found the existence of modes with purely imaginary frequency. Later, an extensive study of asymptotic quasinormal frequencies for Schwarzschild AdS black holes in $d=4$ was done in Ref. 38, and numerically produced a number which exactly matches our analytical prediction. While the authors of Ref. 38 found that the real part of the frequency mode increases with the overtone number, n, in what seems to be a characteristic particular to AdS space, they also found that, for the large black holes which we have studied in the present paper, the offset is

$$[\text{offset}]=\frac{1}{R^2}(0.578+0.420i),$$

and the gap is

$$[\text{gap}] = \frac{1}{R^2}(1.299 + 2.250i),$$

in complete and precise agreement with our analytical results.

IV. FUTURE DIRECTIONS

Having opened the way for an extension of the monodromy technique introduced in Ref. 11 to the case of nonasymptotically flat space–times, and having at hand the full list of potentials for both gravitational and electromagnetic perturbations of d-dimensional black holes,[3,5] one can now proceed and compute asymptotic quasinormal modes for d-dimensional black holes. This is done in Ref. 12. The relevance of this calculation towards quantum gravity is dual: on the one hand, one would like to test if the ideas in Refs. 8 and 9 are universal. A positive answer would have great consequences in the theoretical development of both loop quantum gravity and string theory. On the other hand, the computation of these asymptotic quasinormal frequencies will open the way to the calculation of asymptotic greybody factors for d-dimensional black holes which, as we have alluded at previously, may have a deeper role to play on the road to quantum gravity than the quasinormal frequencies. Indeed, it is expected that these greybody factors may yield clues on dual string theoretic microscopic descriptions of black holes, at high energies.[13,14] These are themes to which we shall return in future publications.

For the moment, let us conclude with some comments on the upcoming results.[12] Besides generalizing the present results to d dimensions (and removing the large black hole constraint in the AdS case), we also show how to include charge in this nonasymptotically flat situation. In what respects the charged solutions, we have also generalized the computation of asymptotic quasinormal frequencies in the four-dimensional Reissner–Nordstrøm solution of Ref. 11, to d dimensions, with the following result:

$$e^{\beta_H^+\omega} + (1 + 2\cos(\pi j)) + (2 + 2\cos(\pi j))e^{-\beta_H^-\omega} = 0,$$

where the $\beta_H^\pm$ are the inverse temperatures at the outer and the inner horizons, and

$$j = \frac{d-3}{2d-5}.$$

This formula is valid in any dimension and for any type of gravitational or electromagnetic perturbation. In the case of the extremal Reissner–Nordstrøm solution, where mass equals charge, we have found that the asymptotic frequencies are solutions of the expression

$$\omega = \frac{d-3}{d-2}\left(\frac{d-3}{4\pi R_H}\right)\log\left(\frac{\sin\left(\frac{5\pi j}{2}\right)}{\sin\left(\frac{\pi j}{2}\right)}\right),$$

where R_H is the radius of the extremal horizon and j is as before. We have also found solutions for normal modes in d-dimensional pure AdS space, and solutions for quasinormal modes in pure dS space, for particular values of the dimension. A complete list of all these results will appear in Ref. 12.

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Composite systems and the role of the complex numbers in quantum mechanics

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An axiomatic approach to the mathematical formalism of quantum mechanics, based upon a certain concept of conditional probability, has been proposed in two recent papers by the author. It leads to Jordan operator algebras and thus comes rather close to the standard Hilbert space model of quantum mechanics, but still includes the so-called exceptional Jordan algebras, for which a Hilbert space representation does not exist. This approach is now extended by defining a mathematical model of composite systems. Such a model is required for the study of the joint distribution of two quantum observables. A very general type of observables (not only the real-valued observables corresponding to the self-adjoint operators) is considered. The joint distribution is defined, using the concept of conditional probability, and exhibits a certain dependence on the succession of the observations which is different from the classical case and unknown so far in quantum mechanics. Finally, it turns out that, at least in the finite-dimensional case, a really satisfying model of the composite system exists only if each single system is modeled by a complex Jordan matrix algebra (or a direct sum), and the model then becomes the tensor product. This provides some reasoning why the exceptional Jordan algebras can be ruled out, why quantum mechanics needs the complex numbers and the complex Hilbert space, and why the tensor product is the right choice for the model of a composite system.
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I. INTRODUCTION

An axiomatic approach to the mathematical formalism of quantum mechanics, based upon a certain concept of conditional probability and some interpretable postulates concerning these conditional probabilities, has recently been presented by the author.[10,11] It leads to Jordan operator algebras and thus comes rather close to the standard Hilbert space model of quantum mechanics, but still includes the so-called exceptional Jordan algebras, for which a Hilbert space representation does not exist.

This approach is extended by proposing a mathematical model of composite systems. The combination of two systems to a single one is equally important for modeling physical as well as stochastic systems, e.g., for the definition of a joint distribution of two random variables. For this purpose, classical probability theory contains the concept of product σ-algebras, and quantum mechanics uses the Hilbert space tensor product.

The proposed model renders possible the study of joint distributions of a very general type of quantum observables (usually, only real-valued observables corresponding to self-adjoint operators are considered). The joint distributions are defined using the concept of the conditional probabilities, thus differ from those considered by other authors,[5,12,13] and exhibit a certain dependence on the succession of the observations which is different from the classical case and unknown so far in quantum mechanics. The goal to become able to define a unique joint distribution for a pair of quantum observables satisfying a certain compatibility criterion is the major motiva-

tion for the proposed model of a composite system, which thus differs from the algebraic concepts[6,16] and from other concepts[1,8,9] where only product distributions are considered and the uniqueness of the joint distribution is not addressed.

Finally, it turns out that, at least in the finite-dimensional case, a model of the composite system that satisfies all the postulates from Refs. 10 and 11 exists only if each single system is modeled by a complex Jordan matrix algebra (or a direct sum), and the model then becomes the tensor product. This rules out not only the exceptional octonion, but also the real and quaternion Jordan matrix algebras and may be a reason why quantum mechanics needs the complex numbers and the complex Hilbert space. Moreover, this provides some reasoning why the tensor product is the right choice for modeling composite systems.

Beyond that, this may have some impact on quantum information and quantum computing where a certain phenomenon of composite quantum systems, the so-called *entanglement*, plays a major role, but this is out of the scope of the present paper.

Section II of the paper provides a brief survey of the author's recently presented approach,[10,11] which is then extended in Sec. III by defining the postulates for a mathematical model of a composite system. After studying the joint distributions in Sec. IV, the paper addresses the questions whether and when the postulates can be fulfilled and whether they determine a unique mathematical model (Secs. V and VI); currently, only the finite-dimensional case can be resolved and, for this purpose, Jordan matrix algebras are considered. Some still open issues are summarized in the conclusions.

II. NON-BOOLEAN PROBABILITIES

An *orthospace*[10] is a set $\mathcal{E}$ with distinguished elements 0 and $\mathbb{I}$, an orthogonality relation $\perp$, and a partial binary operation + such that for $D,E,F\in\mathcal{E}$:

(OS1) $E\perp F\Rightarrow F\perp E$,
(OS2) $E+F$ is defined for $E\perp F$, and $E+F=F+E$,
(OS3) $D\perp E, D\perp F, E\perp F\Rightarrow D\perp E+F, F\perp D+E$ and $D+(E+F)=(D+E)+F$,
(OS4) $0\perp E$ and $E+0=E$ for all $E\in\mathcal{E}$,
(OS5) For every $E\in\mathcal{E}$ there exists a unique $E'\in\mathcal{E}$ such that $E\perp E'$ and $E+E'=\mathbb{I}$,
(OS6) $E\perp F'\Leftrightarrow$ There exists a $D\in\mathcal{E}$ such that $E\perp D$ and $E+D=F$.

Then $0'=\mathbb{I}$ and $E''=E$ for $E\in\mathcal{E}$. A further relation $\prec$ is defined on $\mathcal{E}$ via $E\prec F:\Leftrightarrow E\perp F'\Leftrightarrow\mathcal{E}$ containing an element D such that $D\perp E$ and $F=E+D(E,F\in\mathcal{E})$. A *state* is a map $\mu:\mathcal{E}\rightarrow[0,1]$ such that $\mu(\mathbb{I})=1$ and $\mu(E+F)=\mu(E)+\mu(F)$ for all orthogonal pairs $E,F\in\mathcal{E}$. Then $\mu(0)=0$, and μ is additive for each finite family of pairwise orthogonal elements in $\mathcal{E}$. (OS6) ensures that $\mu(E)\leqslant\mu(F)$ for $E\prec F$. If μ is a state and $E\in\mathcal{E}$ with $\mu(E)>0$ and if ν is another state such that $\nu(F)=\mu(F)/\mu(E)$ holds for all $F\in\mathcal{E}$ with $F\prec E$, then ν is called a *conditional probability* of μ under E.

A *σ-orthospace* is an orthospace $\mathcal{E}$ such that $\Sigma_{n=1}^{\infty}E_n$ is defined in $\mathcal{E}$ for every sequence of mutually orthogonal events E_n, and a state μ is *σ-additive* if $\mu(\Sigma_{n=1}^{\infty}E_n)=\Sigma_{n=1}^{\infty}\mu(E_n)$. A σ-UCP *space* is a σ-orthospace $\mathcal{E}$ satisfying the following two axioms:[11]

(UC1) *If $E,F\in\mathcal{E}$ and $E\neq F$, then there is a σ-additive state μ with $\mu(E)\neq\mu(F)$.*
(UC2) *For each σ-additive state μ and $E\in\mathcal{E}$ with $\mu(E)>0$, there exists one and only one σ-additive conditional probability μ_E of μ under E.*

With a σ-UCP space $\mathcal{E}$, there is a σ-additive state μ with $\mu(E)=1$ for each element $E\neq 0,D$ in (OS6) becomes unique, the relation $\prec$ is antisymmetric (but still not an order relation), and we have $E\perp E\Leftrightarrow E\perp\mathbb{I}\Leftrightarrow E=0(E\in\mathcal{E})$.

The elements $E\in\mathcal{E}$ are interpreted as *events* and will be called so in the following. The (only partially defined) operation + is interpreted as the *or* connection of mutually exclusive events, E' is the *negation* of E. For a σ-additive state μ, the interpretation of the real number $\mu(E)$ is that of the *probability* of the event E in the state μ, and $\mu_E(F)$ is the probability of the event F in the state

μ after the event E has been observed. Using the same terminology as in mathematical probability theory, we will also write $\mu(F|E)$ for $\mu_E(F)$ in the sequel. If $\mu(E)=1$, then $\mu_E=\mu$ and $\mu(F|E)=\mu(F)$ for all $F\in\mathcal{E}$.

If $\mu(F|E)$ does not depend on μ for two events E,F with $E\neq 0$, we say that F is *statistically predictable* under E and denote the state-independent conditional probability by $\mathbb{P}(F|E)$. We then have that F is statistically predictable under E with $\mathbb{P}(F|E)=\lambda$ if and only if $\mu(F)=\lambda$ holds for every σ-additive state μ with $\mu(E)=1$. Cases with $0<\mathbb{P}(F|E)<1$ are a particular non-Boolean phenomenon playing a major role within quantum measurement.[10]

An *observable* is a σ-homomorphism X from another σ-orthospace $\mathcal{F}$ to $\mathcal{E}$. If μ is a σ-additive state on $\mathcal{E}$, a σ-additive state μ^X is defined on $\mathcal{F}$ via $\mu^X(F):=\mu(X(F))$; μ^X is called the distribution of X under μ.

The classical σ-algebras and particularly the system $\mathcal{B}$ of Borel-measurable sets in $\mathbb{R}$ are σ-orthospaces. If $\mathcal{F}=\mathcal{B}$, the observable $X:\mathcal{B}\to\mathcal{E}$ is called a *real-valued* or $\mathbb{R}$*-valued* observable on $\mathcal{E}$, although it is a map from $\mathcal{B}$ to $\mathcal{E}$. The reason is that we want to keep the notation in line with what is called a real-valued classical random variable. The *expectation value* of a real-valued observable X in a σ-additive state μ on $\mathcal{E}$ is defined as $\mathrm{Exp}_\mu(X):=\int t\,\mathrm{d}\mu^X$, and X is *bounded* if

$$\|X\|:=\inf\{r\geqslant 0|X([-r,r])=\mathbb{I}\}$$

is finite ($\inf\varnothing=\infty$). Now let $O_b(\mathcal{E},\mathbb{R})$ denote the set of all bounded $\mathbb{R}$-valued observables on $\mathcal{E}$. An observable $\chi_E\in O_b(\mathcal{E},\mathbb{R})$ is allocated to each $E\in\mathcal{E}$ via ($B\in\mathcal{B}$),

$$\chi_E(B):=\begin{cases} E & \text{for } 1\in B \text{ and } 0\notin B,\\ E' & \text{for } 1\notin B \text{ and } 0\in B,\\ 0 & \text{for } 1\notin B \text{ and } 0\notin B,\\ \mathbb{I} & \text{for } 1\in B \text{ and } 0\in B.\end{cases}$$

With a real-valued observable X and a measurable function $f:\mathbb{R}\to\mathbb{R}$, another real-valued observable Y is defined via $Y(B):=X(f^{-1}(B))$ for $B\in\mathcal{B}$; Y is denoted by $f(X)$ in the sequel. Then $\chi_{X(B)}=I_B(X)$, where B is any Borel set and I_B is the indicator function with $I_B(t)=1$ for $t\in B$ and $I_B(t)=0$ for $t\notin B$.

$O_b(\mathcal{E},\mathbb{R})$ forms a pre-JB algebra (i.e., its completion is a JB algebra[7]) if the following three axioms hold in the σ-UCP space $\mathcal{E}$:[11]

(A1) $\mu(E|F)\mu(F)+\mu(E'|F')\mu(F')=\mu(F|E)\mu(E)+\mu(F'|E')\mu(E')$ *for all events* E *and* F *and all* σ*-additive states* μ *on* $\mathcal{E}$.

(A2) *For each pair of events* E *and* F *there is a bounded real-valued observable* $U_E(F)$ *such that* $\mu(F|E)\mu(E)=\mathrm{Exp}_\mu(U_E(F))$ *for every* σ*-additive state* μ *on* $\mathcal{E}$.

(A3) *For each pair of bounded real-valued observables* X *and* Y *there is one and only one bounded real-valued observable* $X+Y$ *such that* $\mathrm{Exp}_\mu(X+Y)=\mathrm{Exp}_\mu(X)+\mathrm{Exp}_\mu(Y)$ *for every* σ*-additive state* μ *on* $\mathcal{E}$.

The addition operation on $O_b(\mathcal{E},\mathbb{R})$ is given by (A3), the generally nonassociative multiplication operation $\circ$ can be derived from (A1) and (A2). The relation $\prec$ then becomes an order relation and coincides with the usual order relation $\leqslant$ on JB algebras if, as it is often done later on, $E\in\mathcal{E}$ and $\chi_E\in O_b(\mathcal{E},\mathbb{R})$ are identified with each other.

III. POSTULATES FOR A MODEL OF A COMPOSITE SYSTEM

A model of a composite system consisting of two single systems each modeled by the σ-UCP spaces $\mathcal{E}$ and $\mathcal{F}$, respectively, should be a σ-UCP space $\mathcal{C}$ with at least the following property:

(C1) There is a map $\otimes:\mathcal{E}\times\mathcal{F}\to\mathcal{C}$ such that $0\otimes F=E\otimes 0=0$ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$, $\mathbb{I}\otimes\mathbb{I}=\mathbb{I}$, and $E_1\otimes F_1\perp E_2\otimes F_2$ whenever $E_1\perp E_2$ or $F_1\perp F_2$ ($E_1,E_2\in\mathcal{E}$ and $F_1,F_2\in\mathcal{F}$). Moreover,

$\Sigma(E_k \otimes F) = (\Sigma E_k) \otimes F$ for every sequence of mutually orthogonal events E_k in $\mathcal{E}$ and every event F in $\mathcal{F}$, and $\Sigma(E \otimes F_k) = E \otimes (\Sigma F_k)$ for every sequence of mutually orthogonal events F_k in $\mathcal{F}$ and every event E in $\mathcal{E}$.

A particular role is played by the state-independent conditional probabilities, and we shall now see that they are multiplicative on $\mathcal{C}$.

Proposition 3.1: Assume that $\mathcal{E}$ and $\mathcal{F}$ are σ-UCP spaces and that $\mathcal{C}$ is a σ-UCP space such that (C1) holds. If $E \in \mathcal{E}$ is statistically predictable under $D (0 \neq D \in \mathcal{E})$ and $F \in \mathcal{F}$ is statistically predictable under $G (0 \neq G \in \mathcal{F})$, then $E \otimes F$ is statistically predictable under $D \otimes G$ with $\mathbb{P}(E \otimes F | D \otimes G) = \mathbb{P}(E|D)\mathbb{P}(F|G)$.

Proof: Let ρ be a σ-additive state on $\mathcal{C}$ with $\rho(D \otimes G) = 1$. Then $\rho(D \otimes \mathbb{I}) = 1 = \rho(\mathbb{I} \otimes G)$. We now define σ-additive states μ_1 and μ_2 on $\mathcal{E}$ via $\mu_1(C) := \rho(C \otimes G)$ and $\mu_2(C) := \rho(C \otimes \mathbb{I})$ for $C \in \mathcal{E}$. Since $\mu_1(D) = 1 = \mu_2(D)$ and since E is statistically predictable under D, we get $\mathbb{P}(E|D) = \mu_1(E) = \rho(E \otimes G) = \mu_2(E) = \rho(E \otimes \mathbb{I})$ and $\mathbb{P}(E'|D) = \mu_1(E') = \rho(E' \otimes G) = \mu_2(E') = \rho(E' \otimes \mathbb{I})$.

If $\mathbb{P}(E|D) > 0$, we define a σ-additive state ν on $\mathcal{F}$ via $\nu(H) := \rho(E \otimes H)/\mathbb{P}(E|D)$ for $H \in \mathcal{F}$. Then $\nu(G) = 1$ and $\mathbb{P}(F|G) = \nu(F) = \rho(E \otimes F)/\mathbb{P}(E|D)$.

If $\mathbb{P}(E|D) = 0$, then $\mathbb{P}(E'|D) = 1$ and we consider the σ-additive states ν_1 and ν_2 on $\mathcal{F}$ defined via $\nu_1(H) := \rho(E' \otimes H)$ and $\nu_2(H) := \rho(\mathbb{I} \otimes H)$ for $H \in \mathcal{F}$. Thus $\nu_1(G) = 1 = \nu_2(G)$ and $\mathbb{P}(F|G) = \nu_1(F) = \rho(E' \otimes F) = \nu_2(F) = \rho(\mathbb{I} \otimes F)$. Hence $\rho(E \otimes F) = \rho(\mathbb{I} \otimes F) - \rho(E' \otimes F) = 0$.

We thus get that $E \otimes F$ is statistically predictable under $D \otimes G$ with $\mathbb{P}(E \otimes F | D \otimes G) = \mathbb{P}(E|D)\mathbb{P}(F|G)$. □

With a further σ-UCP space $\mathcal{D}$ and two observables $X: \mathcal{E} \to \mathcal{D}$ and $Y: \mathcal{F} \to \mathcal{D}$, a σ-additive state ν on $\mathcal{C}$ is called a *joint distribution* of (X, Y) under the σ-additive state μ on $\mathcal{D}$, if

$$\nu(E \otimes F) = \mu(X(E))\mu(Y(F)|X(E))$$

for all $E \in \mathcal{E}$ and $F \in \mathcal{F}$. This definition of a joint distribution is rather naturally based upon the concept of conditional probabilities and differs from the joint distributions considered by other authors.[5,12,13] Gudder[5] defines a joint distribution via $\mu(X(E) \wedge Y(F))$, which coincides with the above one when the lattice operation $\wedge$ exists and $X(E)$ and $Y(F)$ commute for all E, F.

Generally, the right-hand side of the above equation is additive only in F, but not in E, and a necessary condition for the existence of the joint distribution is that it is additive in E as well. We shall discuss this later on. Moreover, beyond that, the existence and the uniqueness of the joint distribution require the following second postulate on $\mathcal{C}$:

(C2) For every σ-additive bistate ρ on $\mathcal{E} \times \mathcal{F}$, there exists one and only one σ-additive state ω on $\mathcal{C}$ with $\rho(E, F) = \omega(E \otimes F)$ for $E \in \mathcal{E}$ and $F \in \mathcal{F}$.

Here, a *bistate* is a map $\rho: \mathcal{E} \times \mathcal{F} \to [0, 1]$ with $\rho(\mathbb{I}, \mathbb{I}) = 1, \rho(E_1 + E_2, F) = \rho(E_1, F) + \rho(E_2, F)$ and $\rho(E, F_1 + F_2) = \rho(E, F_1) + \rho(E, F_2)$ for all $E, E_1, E_2 \in \mathcal{E}$ with $E_1 \perp E_2$ and $F, F_1, F_2 \in \mathcal{F}$ with $F_1 \perp F_2$. A bistate is σ-additive if it is σ-additive in each component with the other component fixed.

A *stochastically independent coupling* $\mu \otimes \nu$ of the σ-additive states μ on $\mathcal{E}$ and ν on $\mathcal{F}$ is a σ-additive state $\mu \otimes \nu$ on $\mathcal{C}$ with $(\mu \otimes \nu)(E \otimes F) = \mu(E)\nu(F)$ for $E \in \mathcal{E}$ and $F \in \mathcal{F}$. It immediately follows from (C2) that a unique stochastically independent coupling $\mu \otimes \nu$ exists by applying (C2) to the bistate $\rho(E, F) := \mu(E)\nu(F)$ for $E \in \mathcal{E}$ and $F \in \mathcal{F}$. Other authors,[1,8,9] when defining a model for a composite system, consider only these product states and no bistates and do not address the uniqueness of the coupled state.

When (C2) holds, the following proposition now provides the reverse of Proposition 3.1. Note that $E \otimes F$ is statistically predictable under $D \otimes G$ with $\mathbb{P}(E \otimes F | D \otimes G) = 0$ for any F and G in $\mathcal{F}$ if E and D are orthogonal in $\mathcal{E}$ (and for any D and E in $\mathcal{E}$ if F and G are orthogonal in $\mathcal{F}$).

Proposition 3.2: Assume that $\mathcal{E}$ and $\mathcal{F}$ are σ-UCP spaces and that $\mathcal{C}$ is a σ-UCP space such that (C1) and (C2) hold. Let $E \otimes F$ be statistically predictable under $D \otimes G$ for the events $D, E \in \mathcal{E}$ and $F, G \in \mathcal{F} (D \neq 0, G \neq 0)$.

If $\mathbb{P}(E \otimes F | D \otimes G) > 0$, then E is statistically predictable under D and F is statistically predictable under G with $\mathbb{P}(E \otimes F | D \otimes G) = \mathbb{P}(E|D)\mathbb{P}(F|G)$.

If $\mathbb{P}(E\otimes F|D\otimes G)=0$, *then* E *is statistically predictable under* D *with* $\mathbb{P}(E|D)=0$ *or* F *is statistically predictable under* G *with* $\mathbb{P}(F|G)=0$.

Proof: Let μ be any σ-additive state on $\mathcal{E}$ with $\mu(D)=1$ and ν any σ-additive state on $\mathcal{F}$ with $\nu(G)=1$. Then $(\mu\otimes\nu)(D\otimes G)=1$ and $\lambda:=\mathbb{P}(E\otimes F|D\otimes G)=(\mu\otimes\nu)(E\otimes F)=\mu(E)\nu(F)$.

$\lambda>0$: Then $\mu(E)\neq 0\neq\nu(F)$. Since $\mu(E)=\lambda/\nu(F)$ holds for all σ-additive states μ on $\mathcal{E}$ with $\mu(D)=1$ and ν fixed, we get that E is statistically predictable under D with $\mathbb{P}(E|D)=\lambda/\nu(F)\neq 0$. Now $\nu(F)=\lambda/\mathbb{P}(E|D)$ for all σ-additive states ν on $\mathcal{F}$ with $\nu(G)=1$. Thus F is statistically predictable under G with $\mathbb{P}(F|G)=\lambda/\mathbb{P}(E|D)$.

$\lambda=0$: If $\mu(E)=0=\nu(F)$ for all μ,ν with $\mu(D)=1=\nu(G)$, then $\mathbb{P}(E|D)=0=\mathbb{P}(F|G)$. If $\mu(E)>0$ for some μ with $\mu(D)=1$, then $\nu(F)=0$ for all ν with $\nu(G)=1$, i.e., $\mathbb{P}(F|G)=0$. If $\nu(F)>0$ for some ν with $\nu(G)=1$, then $\mu(E)=0$ for all μ with $\mu(D)=1$, i.e., $\mathbb{P}(E|D)=0$. □

An event $D\neq 0$ in a σ-UCP space $\mathcal{E}$ is called an *atom* if $0<E<D$ for an event E in $\mathcal{E}$ implies that either $E=0$ or $E=D$. Then all events in $\mathcal{E}$ are statistically predictable under D. Vice versa, if all events in $\mathcal{E}$ are statistically predictable under an event D, D must be an atom. To see this, assume that an event $0<E<D$ exists with $0\neq E\neq D$. Then there is an event $F\neq 0$ with $E\perp F$ and $D=E+F$, and there are σ-additive states μ and ν with $\mu(E)=1$ and $\nu(F)=1$. Hence $\mu(E|D)=1$ and $\nu(E|D)=0$ such that E cannot be statistically predictable under D.

Proposition 3.3: Assume that $\mathcal{E}$ *and* $\mathcal{F}$ *are* σ*-UCP spaces and that* $\mathcal{C}$ *is a* σ*-UCP space such that (C1) and (C2) hold. If* $D\in\mathcal{E}$ *and* $G\in\mathcal{F}$ *are atoms, then* $D\otimes G$ *is an atom in* $\mathcal{C}$.

Proof: Let $D\in\mathcal{E}$ and $G\in\mathcal{F}$ be atoms. From Proposition 3.1 we get that $E\otimes F$ is statistically predictable under $D\otimes G$ for every $E\in\mathcal{E}$ and $F\in\mathcal{F}$. A σ-additive bistate ρ on $\mathcal{E}\times\mathcal{F}$ is defined via $\rho(E,F):=\mathbb{P}(E\otimes F|D\otimes G)$, and there is a unique σ-additive state ω on $\mathcal{C}$ with $\omega(E\otimes F)=\rho(E,F)$ for $E\in\mathcal{E}$ and $F\in\mathcal{F}$.

Now let μ be a σ-additive state on $\mathcal{C}$ with $\mu(D\otimes G)=1$. Then $\mu(E\otimes F)=\mathbb{P}(E\otimes F|D\otimes G)=\rho(E,F)$ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$. Therefore $\mu=\omega$, and every event C in $\mathcal{C}$ is statistically predictable under $D\otimes G$ with $\mathbb{P}(C|D\otimes G)=\omega(C)$. Thus $D\otimes G$ is an atom in $\mathcal{C}$. □

IV. JOINT DISTRIBUTIONS OF QUANTUM OBSERVABLES

Note that the product σ-algebra $\mathcal{C}=\mathcal{B}\otimes\mathcal{B}$ which is identical with the Borel measurable subsets of $\mathbb{R}^2$ satisfies (C1) and (C2) for $\mathcal{E}=\mathcal{F}=\mathcal{B}$. Therefore, the joint distribution of two real-valued observables, if it exists, is a probability distribution on $\mathbb{R}^2$.

In classical probability theory, a joint distribution of a family of random variables always exists. In the σ-UCP space model, however, many different cases are possible, and the joint distribution of (X,Y) may exist while the one of (Y,X) does not.

Let $\mathcal{E},\mathcal{F},\mathcal{C}$ be σ-UCP spaces such that $\mathcal{C}$ satisfies (C1) and (C2) for $\mathcal{E}$ and $\mathcal{F}$. With a fourth σ-UCP space $\mathcal{D}$ and two observables $X:\mathcal{E}\to\mathcal{D}$ and $Y:\mathcal{F}\to\mathcal{D}$, we write

$$X\underset{\mu}{\to}Y,\quad \text{if the joint distribution } \mu^{(X,Y)} \text{ of } (X,Y) \text{ under the } \sigma\text{-additive state } \mu \text{ on } \mathcal{D} \text{ exists on } \mathcal{C},$$

$$X\underset{\mu}{\leftrightarrow}Y,\quad \text{if } X\underset{\mu}{\to}Y \text{ as well as } Y\underset{\mu}{\to}X \ (X \text{ and } Y \text{ are then called } \textit{compatible under } \mu),$$

$$X\to Y,\quad \text{if } X\underset{\mu}{\to}Y \text{ holds for all states } \mu \text{ on } \mathcal{D}, \text{ and}$$

$$X\leftrightarrow Y,\quad \text{if } X\to Y \text{ as well as } Y\to X \ (X \text{ and } Y \text{ are then called } \textit{compatible}).$$

We have

$$X\underset{\mu}{\to}Y\Rightarrow\chi_{X(E)}\underset{\mu}{\to}\chi_{Y(F)} \text{ for all } E\in\mathcal{E} \text{ and } F\in\mathcal{F},$$

and with two events E and F in the σ-UCP space $\mathcal{D}$, we have

$$\chi_E \underset{\mu}{\rightarrow} \chi_F \Leftrightarrow \mu(F) = \mu(F|E)\mu(E) + \mu(F|E')\mu(E')$$

(μ a σ-additive state on $\mathcal{D}$). Two events E and F are said to be compatible (compatible under μ), if χ_E and χ_F are compatible (compatible under μ).

In classical probability theory, the joint distributions $\mu^{(X,Y)}$ and $\mu^{(Y,X)}$ are connected via $\mu^{(X,Y)}(E\otimes F)=\mu^{(Y,X)}(F\otimes E)$, which is equivalent to $\mu(X(E))\mu(Y(F)|X(E))=\mu(Y(F))\times\mu(X(E)|Y(F))$. It is axiom (A1) that ensures this property for the σ-UCP spaces as well.

Lemma 4.1: Let E and F be events in a σ-UCP space $\mathcal{D}$ that satisfies (A1). They are equivalent for a σ-additive state μ on $\mathcal{D}$:

(i) *E and F are compatible under* μ,
(ii) $\mu(E)\mu(F|E)=\mu(F)\mu(E|F)$, $\mu(E)\mu(F'|E)=\mu(F')\mu(E|F')$, *and* $\mu(E')\mu(F|E')=\mu(F)\mu(E'|F)$.

Proof: First we assume (ii). Then $\mu(F|E)\mu(E)+\mu(F|E')\mu(E')=\mu(E|F)\mu(F)+\mu(E'|F)\mu(F)=\mu(F)$ and $\mu(E|F)\mu(F)+\mu(E|F')\mu(F')=\mu(F|E)\mu(E)+\mu(F'|E)\mu(E)=\mu(E)$. Note that (A1) is not needed here for the proof of the implication (ii) $\Rightarrow$ (i).

We now assume (i). Then $\mu(E)=\mu(E|F)\mu(F)+\mu(E|F')\mu(F')$ and $\mu(F)=\mu(F|E)\mu(E)+\mu(F|E')\mu(E')$. Hence

$$\begin{aligned}\mu(E'|F')\mu(F') &= (1-\mu(E|F'))\mu(F')\\ &= \mu(F')-\mu(E)+\mu(E|F)\mu(F) = 1-\mu(F)-\mu(E)+\mu(E|F)\mu(F)\end{aligned}$$

and

$$\begin{aligned}\mu(F'|E')\mu(E') &= (1-\mu(F|E'))\mu(E')\\ &= \mu(E')-\mu(F)+\mu(F|E)\mu(E) = 1-\mu(E)-\mu(F)+\mu(F|E)\mu(E).\end{aligned}$$

Thus, by forming the difference of these two identities and then by (A1),

$$\mu(E|F)\mu(F)-\mu(F|E)\mu(E)=\mu(E'|F')\mu(F')-\mu(F'|E')\mu(E')=\mu(F|E)\mu(E)-\mu(E|F)\mu(F),$$

i.e.,

$$\mu(E)\mu(F|E)=\mu(F)\mu(E|F).$$

Since the compatibility of E and F under μ implies the one of E and F' as well as of E' and F, the other two equations of (ii) follow in the same way. □

Theorem 4.2: *Let $\mathcal{E},\mathcal{F},\mathcal{C}$ be σ-UCP spaces such that $\mathcal{C}$ satisfies (C1) and (C2) for $\mathcal{E}$ and $\mathcal{F}$. Let $\mathcal{D}$ be a fourth σ-UCP space where (A1) holds, μ a σ-additive state on $\mathcal{D}$ and let $X:\mathcal{E}\rightarrow\mathcal{D}$ and $Y:\mathcal{F}\rightarrow\mathcal{D}$ be observables. If $X(E)$ and $Y(F)$ are compatible under μ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$, then the joint distributions $\mu^{(X,Y)}$ on $\mathcal{C}$ and $\mu^{(Y,X)}$ on $\overline{\mathcal{C}}$ (which is similar to $\mathcal{C}$, but with exchanged roles of $\mathcal{E}$ and $\mathcal{F}$) exist and satisfy $\mu^{(X,Y)}(E\otimes F)=\mu^{(Y,X)}(F\otimes E)$.*

Proof: From Lemma 4.1 we get that $\mu(X(E)|Y(F))\mu(Y(F))=\mu(Y(F)|X(E))\mu(X(E))$ for $E\in\mathcal{E}$ and $F\in\mathcal{F}$. This then implies (1) the σ-additivity in E with F fixed as well as in F with E fixed, (2) the existence of both the joint distributions, and (3) the identity $\mu^{(X,Y)}(E\otimes F)=\mu^{(Y,X)}(F\otimes E)$. □

We now assume that $\mathcal{E}=\mathcal{F}=\mathcal{B}$ ($\mathcal{B}$ is the system of the Borel sets in $\mathbb{R}$) and that $\mathcal{D}$ is a standard quantum logic, i.e., the system of the closed linear subspaces of a Hilbert space $\mathcal{H}$ or, equivalently, the system of the orthogonal projectors on $\mathcal{H}$. Then $\mu(E|F)=\mathrm{Exp}_\mu(FEF)/\mu(F)$ for $E,F\in\mathcal{D}$.[10]

Therefore, $F\rightarrow E$ holds if and only if $E=FEF+F'EF'$, which is equivalent to $EF=FE$. Thus, $F\rightarrow E, E\rightarrow F$ and $E\leftrightarrow F$ are equivalent to each other and to the standard quantum-mechanical concept of compatibility in this case. Moreover, $X\rightarrow Y, Y\rightarrow X, X\leftrightarrow Y$, and $[X,Y]=0$ become

equivalent for real-valued observables X and Y. Here the observable which is a spectral measure is identified with the corresponding operator, and the observables χ_E, χ_F are identified with the events E, F.

However, the situation is different when the joint distribution exists only under a single σ-additive state μ. We have $F \underset{\mu}{\rightarrow} E$ if and only if

$$\mu(E) = \mathrm{Exp}_\mu(FEF + F'EF') = \mathrm{Exp}_\mu(2FEF + E - EF - FE)$$

or, equivalently,

$$\mathrm{Exp}_\mu(FEF) = \mathrm{Exp}_\mu(EF + FE)/2,$$

which is not symmetrical in E and F. An example can easily be constructed by using two nonorthogonal vectors $\eta, \xi \in \mathcal{H}$ with $\|\eta\| = 1 = \|\xi\|$ and choosing $E = |\eta\rangle\langle\eta|, F = |\xi\rangle\langle\xi|$, and $\mu(D) = \langle\eta|D\eta\rangle$; then $E \underset{\mu}{\rightarrow} F$, but not $F \underset{\mu}{\rightarrow} E$. Moreover, the above equivalence immediately implies that all pairs of events are compatible under the trace state if $\mathcal{H}$ has a finite dimension, which distinguishes the trace among other states.

If X and Y are real-valued observables, $\mu^{(X,Y)}$ is the joint distribution of two subsequent observations (measurements) of X and Y, where X is observed (measured) first and Y second. That $\mu^{(X,Y)}$ may exist while $\mu^{(Y,X)}$ does not exist, shows that the time order of observations (measurements) plays a more significant role with the non-Boolean probabilities than with the classical probabilities. Quantum probabilities are non-Boolean, which is the origin of many typical quantum phenomena.[10]

The classical concept of stochastic independence can now be extended to the general case of observables $X: \mathcal{E} \rightarrow \mathcal{D}$ and $Y: \mathcal{F} \rightarrow \mathcal{D}$ ($\mathcal{E}, \mathcal{F}, \mathcal{D}$ σ-UCP spaces) in the following obvious way: X and Y are *independent under* μ if $\mu(X(E)) = \mu(X(E)|Y(F))$ holds for $\mu(Y(F)) > 0$ and $\mu(Y(F)) = \mu(Y(F)|X(E))$ holds for $\mu(X(E)) > 0$ ($E \in \mathcal{E}$ and $F \in \mathcal{F}$). Note that this implies $X(E) \underset{\mu}{\leftrightarrow} Y(F)$ for $E \in \mathcal{E}, F \in \mathcal{F}$ and, if the assumptions of Theorem 4.2 hold, the joint distributions exist with

$$\mu^{(X,Y)}(E \otimes F) = \mu^X(E)\mu^Y(F) = \mu^{(Y,X)}(F \otimes E).$$

When (A1), (A2), and (A3) hold, two events E and F in $\mathcal{E}$ are independent under μ if and only if they are compatible under μ and the identity $\mathrm{Exp}_\mu(E \circ F) = \mu(E)\mu(F)$ holds for the product $E \circ F$ in $O_b(\mathcal{E}, \mathbb{R})$. For two independent real-valued observables we then get $\mathrm{Exp}_\mu(X \circ Y) = \mathrm{Exp}_\mu(X)\mathrm{Exp}_\mu(Y)$ and $\mathrm{Var}_\mu(X+Y) = \mathrm{Var}_\mu(X) + \mathrm{Var}_\mu(Y)$. The first equation follows since the bounded real-valued observables can be approximated by linear combinations of events in $O_b(\mathcal{E}, \mathbb{R})$; the second equation follows from the first one. Using the Chebychev inequality, the weak *law of large numbers* can now be proved under the same assumptions and in the same way as with classical probabilities, but only for the bounded observables.

In classical probability theory, the law of large numbers provides the link between probabilities and relative frequencies as well as between expectation values and statistical averages. In quantum theory, the law of large numbers gets an additional significance since the convergence towards a constant observable also means that large systems become asymptotically classical.

V. JORDAN MATRIX ALGEBRAS

We shall now study the question whether a σ-UCP space $\mathcal{C}$ satisfying (C1) and (C2) exists for given σ-UCP spaces $\mathcal{E}$ and $\mathcal{F}$. Unfortunately, a general answer cannot be given at present, and we have to restrict to the case when $\mathcal{E}, \mathcal{F}$ as well as $\mathcal{C}$ satisfy (A1), (A2), and (A3) and $O_b(\mathcal{E}, \mathbb{R})$ as well as $O_b(\mathcal{F}, \mathbb{R})$ are finite dimensional. Then $O_b(\mathcal{E}, \mathbb{R}), O_b(\mathcal{F}, \mathbb{R})$ and, as we shall see later on, $O_b(\mathcal{C}, \mathbb{R})$ as well are finite-dimensional formally real Jordan algebras and are direct sums of real, complex, quaternion or octonion Jordan matrix algebras.[7]

Let $\mathbb{H}$ denote the noncommutative field of quaternions and $\mathbb{O}$ the noncommutative and nonassociative field of octonions (Cayley numbers). For $K = \mathbb{R}, \mathbb{C}, \mathbb{H}$ or $\mathbb{O}$, $M_n(K)$ is the algebra of $n \times n$-matrices over K and $H_n(K)$ the algebra of the Hermitian elements of $M_n(K)$ equipped with the Jordan product. Then $H_n(K)$ with $K = \mathbb{R}, \mathbb{C}, \mathbb{H}$ is a Jordan algebra for all positive integers n, $H_n(\mathbb{O})$

is a Jordan algebra if and only if $n \leqslant 3$ (Ref. 7). These are the real, complex, quaternion, and octonion Jordan matrix algebras. The real dimension of $H_n(K)$ is $n+kn(n-1)/2$ where k is the real dimension of K, i.e., $k=1$ for $K=\mathbb{R}, k=2$ for $K=\mathbb{C}, k=4$ for $K=\mathbb{H}$, and $k=8$ for $K=\mathbb{O}$.

Let $J_n(K)$ denote the system of idempotent elements in $H_n(K); J_n(K)$ with $n \neq 2$ and $K \neq \mathbb{O}$ as well as $J_3(\mathbb{O})$ are UCP spaces[10] and satisfy (A1), (A2), and (A3). Note that σ-additivity need not be distinguished from finite additivity, due to the finite dimension, and that $\mathcal{O}_b(J_n(K), \mathbb{R}) = H_n(K)$ by identifying the Hermitian matrices with their spectral measures.

Theorem 5.1: *Assume $\mathcal{E}=J_n(K)$ and $\mathcal{F}=J_m(K)$ with $K=\mathbb{R}, \mathbb{C}, \mathbb{H}$ and $m, n \geqslant 3$, or with $K=\mathbb{O}$ and $m=n=3$. Then a σ-UCP space $\mathcal{C}$ satisfying (C1) and (C2) as well as (A1), (A2), and (A3) exists if and only if $K=\mathbb{C}$.*

I*n this case, (C1) and (C2) are fulfilled with $\mathcal{C}=J_{mn}(\mathbb{C})$ and $E \otimes F \in J_{mn}(\mathbb{C})$ being the Kronecker product of $E \in J_n(\mathbb{C})$ and $F \in J_m(\mathbb{C})$.*

The proof of Theorem 5.1 will be broken into a series of lemmas. First note that the tensor product $M_n(\mathbb{C}) \otimes M_m(\mathbb{C})$ can be identified with $M_{mn}(\mathbb{C})$ via the Kronecker product,

$$X \otimes Y = \begin{pmatrix} x_{11}Y & \cdots & x_{1n}Y \\ \vdots & \ddots & \vdots \\ x_{n1}Y & \cdots & x_{nn}Y \end{pmatrix},$$

for $X \in M_n(\mathbb{C})$ and $Y \in M_m(\mathbb{C})$. Then $E \otimes F \in J_{mn}(\mathbb{C})$ for $E \in J_n(\mathbb{C}), F \in J_m(\mathbb{C})$.

The real-linear spaces $H_n(\mathbb{C}) \otimes H_m(\mathbb{C})$ and $H_{mn}(\mathbb{C})$ coincide, and $H_{mn}(\mathbb{C})$ is the real-linear hull of the $E \otimes F \in J_{mn}(\mathbb{C})$ with $E \in J_n(\mathbb{C})$ and $F \in J_m(\mathbb{C})$. Note that this does not hold for the real Jordan matrix algebras.

Lemma 5.2: $\mathcal{C}=J_{mn}(\mathbb{C})$ with $E \otimes F$ being the Kronecker product fulfills (C1) and (C2) for $\mathcal{E} = J_n(\mathbb{C})$ and $\mathcal{F}=J_m(\mathbb{C}), n, m \geqslant 3$.

Proof: (C1) is obviously fulfilled, and we prove (C2). Let ρ be a bistate on $J_n(\mathbb{C}) \times J_m(\mathbb{C})$. By Gleason's theorem,[4] there is one and only one positive matrix $T_F \in H_n(\mathbb{C})$ for every $F \in J_m(\mathbb{C})$ such that $\rho(E,F)=\mathrm{tr}(ET_F)$ for all $E \in J_n(\mathbb{C})$. The map $F \to T_F$ is then orthogonally additive in F and, for each positive matrix $X \in H_n(\mathbb{C})$, we again apply Gleason's theorem, this time to the map $F \to \mathrm{tr}(XT_F)$ on $J_m(\mathbb{C})$, such that there is one and only one positive matrix $S_X \in H_m(\mathbb{C})$ with $\mathrm{tr}(XT_F))=\mathrm{tr}(S_XF)$. Since every matrix in $H_n(\mathbb{C})$ is the difference of two positive matrices, we can assume that an $S_X \in H_m(\mathbb{C})$ with $\mathrm{tr}(XT_F))=\mathrm{tr}(S_XF)$ exists for every $X \in H_n(\mathbb{C})$. The map $X \to S_X$ is real-linear, and the map $H_n(\mathbb{C}) \times H_m(\mathbb{C}) \ni (X,Y) \to \mathrm{tr}(S_XY)$ is a bilinear extension of ρ. Therefore, there exists a real-linear functional ω on the real-linear tensor product $H_n(\mathbb{C}) \otimes H_m(\mathbb{C}) = H_{mn}(\mathbb{C})$ such that $\omega(X \otimes Y)=\mathrm{tr}(S_XY)$ for $X \in H_n(\mathbb{C})$ and $Y \in H_m(\mathbb{C})$. Hence $\rho(E,F)=\omega(E \otimes F)$, and ω is positive as well as uniquely determined since $H_{mn}(\mathbb{C})$ is the real-linear hull of the $E \otimes F \in J_{mn}(\mathbb{C})$ with $E \in J_n(\mathbb{C})$ and $F \in J_m(\mathbb{C})$. The restriction of ω to $\mathcal{C}=J_{mn}(\mathbb{C})$ provides the desired state. □

We now assume that $\mathcal{E}, \mathcal{F}, \mathcal{C}$ are σ-UCP spaces where (A1), (A2), and (A3) hold, that $\mathcal{O}_b(\mathcal{E}, \mathbb{R})$ and $\mathcal{O}_b(\mathcal{F}, \mathbb{R})$ are finite-dimensional and that $\mathcal{C}$ satisfies (C1) and (C2) for $\mathcal{E}$ and $\mathcal{F}$. Note that χ_E and E as well as $\chi_{E \otimes F}$ and $E \otimes F$ are not distinguished in the sequel.

On $\mathcal{O}_b(\mathcal{C}, \mathbb{R})$, we consider the weak topology induced by those linear functionals φ which have the shape $\varphi(X)=s\,\mathrm{Exp}_\mu(X) - t\,\mathrm{Exp}_\nu(X)$ with σ-additive states μ, ν on $\mathcal{C}, s, t \in \mathbb{R}$.

Lemma 5.3: $\mathcal{O}_b(\mathcal{C}, \mathbb{R})$ is the weakly closed linear hull of $\{E \otimes F : E \in \mathcal{E}, F \in \mathcal{F}\}$.

Proof: We assume that the weakly closed linear hull of $\{E \otimes F : E \in \mathcal{E}, F \in \mathcal{F}\}$ does not coincide with $\mathcal{O}_b(\mathcal{C}, \mathbb{R})$. Then there is a linear functional $\varphi \neq 0$ on $\mathcal{O}_b(\mathcal{C}, \mathbb{R})$, having the above shape with σ-additive states μ, ν on $\mathcal{C}, s, t \in \mathbb{R}$, such that $\varphi(E \otimes F)=0$ for $E \in \mathcal{E}, F \in \mathcal{F}$. Then $s=t \neq 0$, since $\varphi(\mathbb{I} \otimes \mathbb{I})=0$ and $\varphi \neq 0$. Since the restrictions of μ and ν to $\{E \otimes F : E \in \mathcal{E}, F \in \mathcal{F}\}$ provide identical bistates on $\mathcal{E} \times \mathcal{F}$, μ and ν must coincide on $\mathcal{C}$, contradicting $\varphi \neq 0$. Note that $\mathcal{O}_b(\mathcal{C}, \mathbb{R})$ is the linear hull of $\mathcal{C}$.[11] □

Lemma 5.4: For every bistate ρ on $\mathcal{E} \times \mathcal{F}$, there is a unique linear functional φ_ρ on the linear tensor product $\mathcal{O}_b(\mathcal{E}, \mathbb{R}) \otimes \mathcal{O}_b(\mathcal{F}, \mathbb{R})$ such that $\rho(E,F)=\varphi_\rho(E \otimes F)$ for $E \in \mathcal{E}, F \in \mathcal{F}$.

Proof: For $E \in \mathcal{E}$ with $\rho(E, \mathbb{I}) > 0$ define a state ρ_E on $\mathcal{F}$ via $\rho_E(F) := \rho(E,F)/\rho(E, \mathbb{I})$. Let $\hat{\rho}_E$ be

its linear extension to $\mathcal{O}_b(\mathcal{F},\mathbb{R})$, i.e., $\hat{\rho}_E(Y)$ is the expectation value of the observable X in the state $\hat{\rho}_E$. Define $\hat{\rho}_E := 0$ for $\rho(E,\mathbb{I})=0$. Since $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ is the linear hull of $\mathcal{E}$,[11] we can choose a basis $E_1,\ldots,E_n$ of $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ such that $E_1,\ldots,E_n \in \mathcal{E}$. Every $X \in \mathcal{O}_b(\mathcal{E},\mathbb{R})$ then has the shape $X=t_1E_1 + \cdots + t_nE_n$ with unique numbers $t_1,\ldots,t_n \in \mathbb{R}$, and we define a bilinear functional φ_0 via

$$\varphi_0(X,Y) := \sum_{k=1}^{n} t_k \rho(E_k,\mathbb{I})\hat{\rho}_{E_k}(Y)$$

for $X \in \mathcal{O}_b(\mathcal{E},\mathbb{R})$ and $Y \in \mathcal{O}_b(\mathcal{F},\mathbb{R})$. Hence, there is a linear functional φ_ρ on $\mathcal{O}_b(\mathcal{E},\mathbb{R}) \otimes \mathcal{O}_b(\mathcal{F},\mathbb{R})$ with $\varphi_\rho(X\otimes Y)=\varphi_0(X,Y)$. Then $\varphi_\rho(E_k\otimes F)=\rho(E_k,F)$ for $F \in \mathcal{F}$.

For $F \in \mathcal{F}$ with $\rho(\mathbb{I},F)>0$ define a state ρ^F on $\mathcal{E}$ via $\rho^F(E) := \rho(E,F)/\rho(\mathbb{I},F)$. Let $\hat{\rho}^F$ be its linear extension to $\mathcal{O}_b(\mathcal{E},\mathbb{R})$. Define $\hat{\rho}^F := 0$ for $\rho(\mathbb{I},F)=0$. The maps $X \to \rho(\mathbb{I},F)\hat{\rho}^F(X)$ and $X \to \varphi_\rho(X\otimes F)$ are linear functionals on $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ coinciding on the basis $E_1,\ldots,E_n$ and therefore being identical. Hence $\varphi_\rho(E\otimes F)=\rho(E,F)$ for all $E \in \mathcal{E}$ and $F \in \mathcal{F}$.

Since $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ is the linear hull of $\mathcal{E}$ and $\mathcal{O}_b(\mathcal{F},\mathbb{R})$ is the linear hull of $\mathcal{F}$, $\mathcal{O}_b(\mathcal{E},\mathbb{R}) \otimes \mathcal{O}_b(\mathcal{F},\mathbb{R})$ is generated by $\{E\otimes F : E \in \mathcal{E}, F \in \mathcal{F}\}$, which implies the uniqueness of φ_ρ. □

Lemma 5.5: Every linear functional ρ on the linear tensor product $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ has the shape $\rho=\alpha\rho_+ - \beta\rho_-$ with $\alpha,\beta \geqslant 0$ such that the maps $\mathcal{E}\times\mathcal{F} \ni (E,F) \to \rho_\pm(E\otimes F)$ are bistates.

Proof: For $X,Y \in \mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$, we define $X \leqslant Y :\Leftrightarrow (\varphi\otimes\psi)(X) \leqslant (\varphi\otimes\psi)(Y)$ for all positive linear functionals φ on $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ and ψ on $\mathcal{O}_b(\mathcal{F},\mathbb{R})$.

Since every linear functional on $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ or $\mathcal{O}_b(\mathcal{F},\mathbb{R})$ is the difference of two positive functionals, the dual space of $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ is generated by the $\varphi\otimes\psi$ with positive functionals φ on $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ and ψ on $\mathcal{O}_b(\mathcal{F},\mathbb{R})$. Therefore, $X \leqslant 0$ and $0 \leqslant X$ holds if and only if $X=0$ such that $\leqslant$ becomes an order relation.

Now let $X \in \mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$. Then X has the shape

$$X = \sum_{k=1}^{n} t_k E_k \otimes F_k$$

with $k \in \mathbb{N}, E_1,\ldots,E_n \in \mathcal{E}, F_1,\ldots,F_n \in \mathcal{F}$ and $t_1,\ldots,t_n \in \mathbb{R}$. Hence $|(\varphi\otimes\psi)(X)| \leqslant \Sigma|t_k|(\varphi\otimes\psi)(\mathbb{I}\otimes\mathbb{I})$ for positive functionals φ on $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ and ψ on $\mathcal{O}_b(\mathcal{F},\mathbb{R})$, i.e., $-\Sigma|t_k|\mathbb{I}\otimes\mathbb{I} \leqslant X \leqslant \Sigma|t_k|\mathbb{I}\otimes\mathbb{I}$. Obviously, $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ is Archimedian and thus an order unit space[7] with the order unit $\mathbb{I}\otimes\mathbb{I}$.

Therefore,[7] every linear functional ρ on $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ has the shape $\rho=\rho_+-\rho_-$ with positive linear functionals ρ_+ and ρ_-. Then, either $\rho_\pm=0$ or the maps $\mathcal{E}\times\mathcal{F} \ni (E,F) \to \rho_\pm(E\otimes F)/\rho_\pm(\mathbb{I}\otimes\mathbb{I})$ are bistates. □

Lemma 5.6: $\dim \mathcal{O}_b(\mathcal{C},\mathbb{R}) = \dim \mathcal{O}_b(\mathcal{E},\mathbb{R}) \dim \mathcal{O}_b(\mathcal{F},\mathbb{R})$.

Proof: We prove that there is a linear bijection Φ from the linear tensor product $\mathcal{O}_b(\mathcal{E},\mathbb{R}) \otimes \mathcal{O}_b(\mathcal{F},\mathbb{R})$ onto $\mathcal{O}_b(\mathcal{C},\mathbb{R})$. Every element Z of $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ has the shape

$$\sum_{k=1}^{n} t_k E_k \otimes F_k$$

with $E_1,\ldots,E_n \in \mathcal{E}, F_1,\ldots,F_n \in \mathcal{F}$ and $t_k \in \mathbb{R}$, and we allocate to Z the element $\Phi(Z)$ of $\mathcal{O}_b(\mathcal{C},\mathbb{R})$, having the same shape in $\mathcal{O}_b(\mathcal{C},\mathbb{R})$. Note that the same notation $E\otimes F$ is used here for two different objects, one lying in $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$ and the other one in $\mathcal{C}\subseteq\mathcal{O}_b(\mathcal{C},\mathbb{R})$. In $\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})$,

$$\sum_{k=1}^{n} t_k E_k \otimes F_k = 0$$

holds if and only if (use Lemma 5.4 and Lemma 5.5)

$$\sum_{k=1}^{n} t_k \rho(E_k, F_k) = 0$$

for every bistate ρ on $\mathcal{E}\times\mathcal{F}$. By (C2), this is equivalent to

$$\sum_{k=1}^{n} t_k \mu(E_k \otimes F_k) = 0$$

for every σ-additive state μ on $\mathcal{C}$, i.e., to

$$\sum_{k=1}^{n} t_k E_k \otimes F_k = 0$$

in $\mathcal{O}_b(\mathcal{C},\mathbb{R})$. Therefore $\Phi:\mathcal{O}_b(\mathcal{E},\mathbb{R})\otimes\mathcal{O}_b(\mathcal{F},\mathbb{R})\to\mathcal{O}_b(\mathcal{C},\mathbb{R})$ is a well-defined and injective linear map. The range of Φ has a finite dimension, is closed then and thus, by Lemma 5.3, Φ is surjective as well. □

The *center* of a Jordan algebra $\mathcal{A}$ is the set of those elements of $\mathcal{A}$ that operator-commute with every element of $\mathcal{A}$, and $\mathcal{A}$ is called a *factor* if its center consists of the scalar multiples of the identity $\mathbb{I}$ alone. The finite-dimensional JB factors are the Jordan matrix algebras over $\mathbb{R},\mathbb{C},\mathbb{H}$ or $\mathbb{O}$.

In the sequel, we shall need the so-called *Jordan triple product*[7] $\{\ ,\ ,\ \}$, which is defined as follows for three elements X,Y,Z in a Jordan algebra: $\{X,Y,Z\} := X\circ(Y\circ Z) - Y\circ(Z\circ X) + Z\circ(X\circ Y)$.

If E and F are atoms in a finite-dimensional JB factor $\mathcal{A}$, there is an atom D which is orthogonal neither with E nor with F. If E and F are not orthogonal, choose $D=E$ or $D=F$. If E and F are orthogonal, they must be *strongly connected* and hence $\{E,\mathcal{A},F\}\neq\{0\}$.[7] Since $\mathcal{A}$ is generated by its atoms, there is an atom D with $0\neq\{E,D,F\}=E\circ(F\circ D)-D\circ(E\circ F)+F\circ(E\circ D)$ $=E\circ(F\circ D)+F\circ(E\circ D)$, and since E and F operator-commute, $E\circ(F\circ D)=F\circ(E\circ D)$, such that $F\circ D\neq 0\neq E\circ D$.

Lemma 5.7: If $\mathcal{O}_b(\mathcal{E},\mathbb{R})$ and $\mathcal{O}_b(\mathcal{F},\mathbb{R})$ are factors, then $\mathcal{O}_b(\mathcal{C},\mathbb{R})$ is a factor.

Proof: $\mathcal{O}_b(\mathcal{C},\mathbb{R})$ is a factor if and only if 0 and $\mathbb{I}\otimes\mathbb{I}$ are the only idempotent elements in its center. Assume that H is an idempotent element in the center, and let $E\in\mathcal{E}$ and $F\in\mathcal{F}$ be atoms. Then (see Ref.7)

$$E\otimes F = \{H,E\otimes F,H\} + \{H',E\otimes F,H'\}$$

and $\{H,E\otimes F,H\}$ as well as $\{H',E\otimes F,H'\}$ are idempotent ($H'=\mathbb{I}\otimes\mathbb{I}-H$). Since $E\otimes F$ is an atom (Proposition 3.3), one of these two idempotent elements must equal 0 and the other one must equal $E\otimes F$, i.e., either $E\otimes F\leqslant H$ or $E\otimes F\leqslant H'$. Both cases are symmetric, and we assume $E\otimes F\leqslant H$.

Now let $D_o\in\mathcal{E}$ and $G_o\in\mathcal{F}$ be atoms such that $\mathbb{P}(E|D_o)\neq 0$ and $\mathbb{P}(F|G_o)\neq 0$. Then again either $D_o\otimes G_o\leqslant H$ or $D_o\otimes G_o\leqslant H'$. From Proposition 3.1 we get $\mathbb{P}(E\otimes F|D_o\otimes G_o)\neq 0$, i.e., $\{D_o\otimes G_o,E\otimes F,D_o\otimes G_o\}\neq 0$, which excludes $D_o\otimes G_o\leqslant H'$ such that $D_o\otimes G_o\leqslant H$.

Now let $D\in\mathcal{E}$ and $G\in\mathcal{F}$ be any atoms. Then there exists an atom $D_o\in\mathcal{E}$ which is orthogonal with neither E nor D, and there is an atom $G_o\in\mathcal{F}$ which is orthogonal with neither F nor G. Then $\mathbb{P}(E|D_o)\neq 0\neq\mathbb{P}(D_o|D)$ and $\mathbb{P}(F|G_o)\neq 0\neq\mathbb{P}(G_o|G)$. Applying the above, we get first $D_o\otimes G_o\leqslant H$ and then $D\otimes G\leqslant H$ (by exchanging E,F with D_o,G_o and D_o,G_o with D,G).

Now let $D_1,\ldots,D_n\in\mathcal{E}$ and $G_1,\ldots,G_m\in\mathcal{F}$ be pairwise orthogonal atoms in $\mathcal{E}$ and $\mathcal{F}$, respectively, with $\mathbb{I}=\Sigma D_j$ and $\mathbb{I}=\Sigma G_k$. Then $\mathbb{I}\otimes\mathbb{I}=\Sigma\Sigma D_j\otimes G_k\leqslant H$ and therefore $\mathbb{I}\otimes\mathbb{I}=H$. □

Proof of Theorem 5.1: $\mathcal{E}=J_n(K)$ and $\mathcal{F}=J_m(K)$ with $K=\mathbb{R},\mathbb{C},\mathbb{H}$, or $\mathbb{O}, m,n\geqslant 3$, and $m=n=3$ if $K=\mathbb{O}$. Assume that a UCP space $\mathcal{C}$ satisfying (C1) and (C2) as well as (A1), (A2), and (A3) exists with $\mathcal{O}_b(\mathcal{C},\mathbb{R})$ being finite-dimensional. By Lemmas 5.6, 5.7 and Proposition 3.3, $\mathcal{O}_b(\mathcal{C},\mathbb{R})$ is a JB factor with $\dim\mathcal{O}_b(\mathcal{C},\mathbb{R})=\dim H_n(K)\dim H_m(K)$ and the identity in $\mathcal{O}_b(\mathcal{C},\mathbb{R})$ is the sum of the mn pairwise orthogonal atoms $E_j\otimes F_k$, where $E_1,\ldots,E_n$ are orthogonal atoms in $\mathcal{E}$ the sum of which is $\mathbb{I}$, and $F_1,\ldots,F_m$ are orthogonal atoms in $\mathcal{F}$ the sum of which is $\mathbb{I}$. Therefore $\mathcal{O}_b(\mathcal{C},\mathbb{R})$

$=H_{mn}(K_0)$ with $K_0=\mathbb{R},\mathbb{C}$ or $\mathbb{H}$; $K_0=\mathbb{O}$ is not possible since $mn\geqslant 9$ and $H_{mn}(\mathbb{O})$ is a Jordan algebra only if $mn=3$.

Case 1: $K=\mathbb{R}$. Then $\dim \mathcal{O}_b(\mathcal{C},\mathbb{R})=\dim H_n(\mathbb{R})\dim H_m(\mathbb{R})=m(m+1)n(n+1)/4$. On the other hand, $\dim \mathcal{O}_b(\mathcal{C},\mathbb{R})$ must equal $\dim H_{mn}(K_0)$ which is $mn(mn+1)/2$ for $K_0=\mathbb{R}, m^2n^2$ for $K_0=\mathbb{C}$, and $mn(2mn-1)$ for $K_0=\mathbb{H}$, i.e., $(m+1)(n+1)=2(mn+1), 4mn$, or $8mn-4$, but all these three cases are impossible since $(m+1)(n+1)<2(mn+1)\leqslant 4mn\leqslant 8mn-4$ for $m,n\geqslant 3$.

Case 2: $K=\mathbb{C}$. See Lemma 3.2.

Case 3: $K=\mathbb{H}$. Then $\dim \mathcal{O}_b(\mathcal{C},\mathbb{R})=m(2m-1)n(2n-1)$ which must equal $mn(mn+1)/2$ for $K_0=\mathbb{R}, m^2n^2$ for $K_0=\mathbb{C}$, and $mn(2mn-1)$ for $K_0=\mathbb{H}$, i.e., $(2m-1)(2n-1)=(mn+1)/2, mn$ or $2mn-1$, which is impossible since $(2m-1)(2n-1)>2mn-1\geqslant mn\geqslant (mn+1)/2$.

Case 4: $K=\mathbb{O}$. Then $\mathcal{E}=\mathcal{F}=J_3(\mathbb{O})$, $\dim \mathcal{O}_b(\mathcal{C},\mathbb{R})=27^2\neq 45,81,153$ which are the dimensions of $H_9(\mathbb{R}), H_9(\mathbb{C}), H_9(\mathbb{H})$. □

VI. NONUNIQUENESS OF THE MODEL

We now turn to the question whether the postulates for a model of a composite system uniquely determine such a model, and we first define with mathematical rigor what uniqueness here means.

Let $\mathcal{E}$ and $\mathcal{F}$ be two σ-UCP spaces, and let $\mathcal{C}_1,\otimes_1$ and $\mathcal{C}_2,\otimes_2$ be two models for a composite system consisting of $\mathcal{E}$ and $\mathcal{F}$ such that the axioms (C1) and (C2) are fulfilled. The two models are isomorphic if there is an isomorphism Π between the two σ-UCP spaces $\mathcal{C}_1$ and $\mathcal{C}_2$ with $\Pi(E\otimes_1 F)=\Pi(E)\otimes_2\Pi(F)$ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$.

We shall now see that there are two nonisomorphic models for $\mathcal{E}=J_n(\mathbb{C})$ and $\mathcal{F}=J_m(\mathbb{C}), n,m\geqslant 3$. The first one is $\mathcal{C}_1:=J_{mn}(\mathbb{C})$ with $\otimes_1$ being the Kronecker product (Lemma 5.2). The second one $\mathcal{C}_2:=\mathcal{C}_1=J_{mn}(\mathbb{C})$, but $\otimes_2$ is now defined differently from $\otimes_1$ in the following way: $E\otimes_2 F:=E\otimes_1 F^t$, where F^t is the transposed matrix of the matrix F.

The second model $\mathcal{C}_2,\otimes_2$ satisfies the axioms (C1) and (C2) as well; (C1) follows from the fact that the map $F\to F^t$ is an isomorphism of $\mathcal{F}=J_m(\mathbb{C})$, and (C2) can be seen in the following way. If ρ is a bistate on $\mathcal{E}\times\mathcal{F}$, define another bistate ρ' by $\rho'(E,F):=\rho(E,F^t)$. From Lemma 5.2 we get that there is a state ω' on $J_{mn}(\mathbb{C})$ with $\omega'(E\otimes_1 F)=\rho'(E,F)$ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$. Then $\rho(E,F)=\rho'(E,F^t)=\omega'(E\otimes_1 F^t)=\omega'(E\otimes_2 F)$ such that ω' is the desired state extending ρ on $\mathcal{C}_2$ with $\otimes_2$. It is unique since $H_{mn}(\mathbb{C})$ is the real-linear hull of the $E\otimes_2 F\in J_{mn}(\mathbb{C})$ with $E\in J_n(\mathbb{C})$ and $F\in J_m(\mathbb{C})$.

If $\mathcal{C}_1$ with $\otimes_1$ and $\mathcal{C}_2$ with $\otimes_2$ were isomorphic, there would be an automorphism Π of $J_{mn}(\mathbb{C})$ with $\Pi(E\otimes_1 F)=\Pi(E)\otimes_2\Pi(F)=\Pi(E)\otimes_1(\Pi(F))^t$ for all $E\in\mathcal{E}$ and $F\in\mathcal{F}$. Then, Π would have a unique extension to an automorphism of $H_{mn}(\mathbb{C})$ which would have a unique complex-linear extension Π' to $M_{mn}(\mathbb{C})$. The latter extension would be either multiplicative or antimultiplicative,[7] i.e., either $\Pi'(AB)=\Pi'(A)\Pi'(B)$ for all matrices A,B in $M_{mn}(\mathbb{C})$ or $\Pi'(AB)=\Pi'(B)\Pi'(A)$ for all A,B in $M_{mn}(\mathbb{C})$. However, both cases are impossible since the restriction of Π' to $M_n(\mathbb{C})\otimes\mathbb{I}$ is the identity map and is multiplicative while the restriction of Π' to $\mathbb{I}\otimes M_m(\mathbb{C})$ is the matrix transposition which is antimultiplicative.

Therefore, the two models $\mathcal{C}_1$ with $\otimes_1$ and $\mathcal{C}_2$ with $\otimes_2$ are not isomorphic. The same kind of nonuniqueness occurs with those tensor products that have been considered by other authors.[1,8,9]

VII. CONCLUSIONS

The conditional probabilities considered in the σ-UCP space model take us directly to the definition of joint distributions in Sec. III. The Hilbert space formalism of quantum mechanics itself does not give such a clear answer to the question what a joint distribution could be, and different solutions, all distinct from the above one, have therefore been proposed (e.g., by Urbanik[12,13] or Gudder[5,12]). A new phenomenon of the joint distributions defined in Sec. III is that the joint distribution of (X,Y) under a given state may exist while the one of (Y,X) does not. Time order of observations (measurements) plays a more significant role here than in classical probability theory.

Moreover, the consideration of joint distributions not only for real-valued observables, but for a very general type of observables has immediately provided the postulates for a mathematical model of a composite quantum system. This model is in line with product σ-algebras used in classical probability theory as well as with the Hilbert space tensor product used in quantum-mechanics—at least in the finite-dimensional case.

The UCP space modeling the combined system [e.g., $J_{mn}(\mathbb{C})$ for the single systems $J_m(\mathbb{C})$ and $J_n(\mathbb{C})$] contains atoms that do not have the shape $E \otimes F$ with atoms E and F in the UCP spaces modeling the single systems. This means that maximum information on the combined system is not the same as maximum information on each single system, which is a well-known and widely discussed quantum feature called *entanglement*.[14] It originates from the underlying non-Boolean event structure and distinguishes quantum mechanics from classical physics and classical probability theory, both using Boolean event structures. Quantum entanglement has been regaining interest during the past 10 years because of its role in the theories of quantum information and quantum computing.

Theorem 5.2 distinguishes the complex Jordan matrix algebras not only from the exceptional octonion one, but also from the real and quaternion ones. This might be a reason why quantum mechanics needs the complex numbers and the complex Hilbert space. There are other ways of distinguishing the complex case from the real one and the other cases by features either of the underlying state space[2,3] or of the underlying orthomodular space.[15] Such features can mathematically be described, but are physically or statistically less plausible.

Theorem 5.2 covers the finite-dimensional case. The infinite-dimensional case, including the type II and type III JBW factors,[7] still needs further study. If it turns out that the existence of a satisfactory model of a composite system requires the complex numbers in the infinite-dimensional cases as well, we would get a complete axiomatic characterization of the quantum mechanical standard model which uses only the complex Hilbert space.

Furthermore, the combination of only two single systems to a composite system has been regarded. The extension to a finite number of systems is straightforward, but an extension to an arbitrary number of systems may be required. Note that product σ-algebras of an infinite (countable as well as noncountable) number of σ-algebras are used in mathematical probability theory for the study of stochastic processes.

Another open issue is the question whether σ-UCP spaces exist that do not stem from Jordan operator algebras; so far all known examples do, and thus satisfy the axioms (A1), (A2), and (A3). Or are these axioms automatically fulfilled by every σ-UCP space and redundant therefore? Finite UCP spaces are the finite Boolean algebras, but do UCP spaces exist that contain only a finite number of events and at least one pair of incompatible events?

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On spherically symmetric solutions with horizon in model with multicomponent anisotropic fluid

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A family of spherically symmetric solutions in the model with m-component multicomponent anisotropic fluid is considered. The metric of the solution depends on parameters $q_s>0$, $s=1,\ldots,m$, relating radial pressures and the densities and contains $(n-1)m$ parameters corresponding to Ricci-flat "internal space" metrics and obeying certain $m(m-1)/2$ ("orthogonality") relations. For $q_s=1$ (for all s) and certain equations of state ($p_i^s=\pm\rho^s$) the metric coincides with the metric of intersecting black brane solution in the model with antisymmetric forms. A family of solutions with (regular) horizon corresponding to natural numbers $q_s=1,2,\ldots$ is singled out. Certain examples of "generalized simulation" of intersecting M-branes in $D=11$ supergravity are considered. The post-Newtonian parameters β and γ corresponding to the four-dimensional section of the metric are calculated. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1812357]

I. INTRODUCTION

This paper is devoted to spherically symmetric solutions with a horizon in the multidimensional model with multicomponent anisotropic fluid defined on product manifolds $\mathbf{R}\times M_0\times\cdots\times M_n$. These solutions in certain cases may simulate black brane solutions[1–3] (for a review on p-brane solutions see Ref. 4 and references therein).

We remind that p-brane solutions (e.g., black brane ones) usually appear in the models with antisymmetric forms and scalar fields (see also Refs. 5–15). Cosmological and spherically symmetric solutions with p-branes are usually obtained by the reduction of the field equations to the Lagrange equations corresponding to Toda-type systems.[14] An analogous reduction for the models with multicomponent "perfect" fluid was done earlier in Refs. 16 and 17.

For cosmological models with antisymmetric forms without scalar fields any p-brane is equivalent to a multicomponent anisotropic perfect fluid with the equations of state:

$$p_i=-\rho, \quad \text{or } p_i=\rho, \tag{1.1}$$

when the manifold M_i belongs or does not belong to the brane world-volume, respectively (here p_i is the pressure in M_i and ρ is the density, see Sec. II).

In this paper we find a new family of exact spherically symmetric solutions in the model with m-component anisotropic fluid for the following equations of state (see Appendix for more familiar form of equations of state):

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$$p_r^s = -\rho^s(2q_s-1)^{-1}, \quad p_0^s = \rho^s(2q_s-1)^{-1}, \tag{1.2}$$

and

$$p_i^s = \left(1-\frac{2U_i^s}{d_i}\right)\rho^s \Big/ (2q_s-1), \tag{1.3}$$

$i>1$, $s=1,\dots,m$, where for sth component: ρ^s is a density, p_r^s is a radial pressure, p_i^s is a pressure in M_i, $i=2,\dots,n$. Here parameters U_i^s $(i>1)$ and the parameters $q_s=U_1^s>0$ obey the following "orthogonality" relations (see also Sec. II below)

$$B_{sl}=0, \quad s\neq l, \tag{1.4}$$

where

$$B_{sl} \equiv \sum_{i=1}^{n}\frac{U_i^s U_i^l}{d_i} + \frac{1}{2-D}\left(\sum_{i=1}^{n} U_i^s\right)\left(\sum_{j=1}^{n} U_j^l\right), \tag{1.5}$$

$q_s\neq 1/2$; and $s,l=1,\dots,m$. The manifold M_0 is d_0-dimensional sphere in our case and p_0^s is the pressure in the tangent direction.

The one-component case was considered earlier in Ref. 1. For the special case with $q_s=1$ see Refs. 2 and 3 (for one-component and multicomponent case, respectively).

The paper is organized as follows. In Sec. II the model with multicomponent (anisotropic or "perfect") fluid is formulated. In Sec. III a subclass of spherically symmetric solutions (generalizing solutions from Ref. 3) is presented and solutions with (regular) horizon corresponding to integer q_s are singled out. Section IV deals with certain examples of two-component solutions in dimension $D=11$ containing for $q_s=1$ intersecting $M2\cap M2$, $M2\cap M5$, and $M5\cap M5$ black brane metrics. In Sec. V the post-Newtonian parameters for the four-dimensional section of the metric are calculated. In the Appendix a class of general spherically symmetric solutions in the model under consideration is presented.

II. THE MODEL

Here, we consider a family of spherically symmetric solutions to Einstein equations with a multicomponent anisotropic fluid matter source

$$R_N^M - \tfrac{1}{2}\delta_N^M R = kT_N^M \tag{2.1}$$

defined on the manifold

$$M = \underset{\text{radial variables}}{\mathbf{R}} \times \underset{\text{spherical variables}}{(M_0=S^{d_0})} \times \underset{\text{time}}{(M_1=\mathbf{R})} \times M_2 \times \cdots \times M_n, \tag{2.2}$$

with the block-diagonal metrics

$$ds^2 = e^{2\gamma(u)}\,du^2 + \sum_{i=0}^{n} e^{2X^i(u)} h^{(i)}_{m_i n_i}\,dy^{m_i}\,dy^{n_i}. \tag{2.3}$$

Here $\mathbf{R}=(a,b)$ is interval. The manifold M_i with the metric $h^{(i)}$, $i=1,2,\dots,n$, is the Ricci-fiat space of dimension d_i:

$$R_{m_i n_i}[h^{(i)}]=0, \tag{2.4}$$

and $h^{(0)}$ is standard metric on the unit sphere S^{d_0},

$$R_{m_0 n_0}[h^{(0)}] = (d_0-1)h^{(0)}_{m_0 n_0}, \tag{2.5}$$

u is radial variable, κ is the multidimensional gravitational constant, $d_1=1$ and $h^{(1)}=-dt\otimes dt$.

The energy-momentum tensor is adopted in the following form:

$$T_N^M = \sum_{s=1}^{m} T_N^{(s)M}, \tag{2.6}$$

where

$$T_N^{(s)M} = \mathrm{diag}(-(2q_s-1)^{-1}\rho^s, (2q_s-1)^{-1}\rho^s \delta_{k_0}^{m_0}, -\rho^s, p_2^s \delta_{k_2}^{m_2}, \ldots, p_n^s \delta_{k_n}^{m_n}), \tag{2.7}$$

$q_s > 0$ and $q_s \neq 1/2$. The pressures p_i^s and the density ρ^s obey the relations (1.3) with constants U_i^s, $i > 1$.

The "conservation law" equations

$$\nabla_M T_N^{(s)M} = 0 \tag{2.8}$$

are assumed to be valid for all s.

In what follows we set $\kappa = 1$ for simplicity.

III. EXACT SOLUTIONS

Let us define

$$1°, \quad U_0^s = 0, \tag{3.1}$$

$$2°, \quad U_1^s = q_s, \tag{3.2}$$

$$3°, \quad (U^s, U^l) = U_i^s G^{ij} U_j^l, \tag{3.3}$$

where $U^s = (U_i^s)$ is $(n+1)$-dimensional vector and

$$G^{ij} = \frac{\delta^{ij}}{d_i} + \frac{1}{2-D} \tag{3.4}$$

are components of the matrix inverse to the matrix of the minisuperspace metric[18,19]

$$(G_{ij}) = (\mathrm{d}_i \delta_{ij} - \mathrm{d}_i \mathrm{d}_j), \tag{3.5}$$

$i, j = 0, \ldots, n$, and $D = 1 + \Sigma_{i=0}^n d_i$ is the total dimension.

In our case the scalar products (3.3) are given by relations

$$(U^s, U^l) = B_{kl} \tag{3.6}$$

with B_{kl} from (1.5) and hence due to (1.4) vectors U^s are mutually orthogonal, i.e.,

$$(U^s, U^l) = 0, \quad s \neq l. \tag{3.7}$$

It is proved in the Appendix that the relation 1° implies

$$(U^s, U^s) > 0, \tag{3.8}$$

for all s.

For the equations of state (1.2) and (1.3) with parameters obeying (1.4) we have obtained the following spherically symmetric solutions to the Einstein equations (2.1) (see Appendix),

$$\mathrm{d}s^2 = J_0 \left(\frac{\mathrm{d}r^2}{1 - \dfrac{2\mu}{r^d}} + r^2 \, \mathrm{d}\Omega_{d_0}^2 \right) - J_1 \left(1 - \frac{2\mu}{r^d} \right) \mathrm{d}t^2 + \sum_{i=2}^{n} J_i h_{m_i n_i}^{(i)} \, \mathrm{d}y^{m_i} \, \mathrm{d}y^{n_i}, \tag{3.9}$$

$$\rho^s = \frac{(2q_s-1)(\mathrm{d}q_s)^2 P_s(P_s+2\mu)(1-2\mu r^{-d})^{q_s-1}}{2(U^s,U^s)\left(\prod_{s=1}^{m} H_s\right)^2 J_0 r^{2d_0}}, \tag{3.10}$$

by methods similar to obtaining p-brane solutions.[14] Here $d=d_0-1$, $\mathrm{d}\Omega_{d_0}^2=h^{(0)}_{m_0n_0}\,\mathrm{d}y^{m_0}\,\mathrm{d}y^{n_0}$ is spherical element, the metric factors

$$J_i = \prod_{s=1}^{m} H_s^{-2U^{si}/(U^s,U^s)}, \tag{3.11}$$

$$H_s = 1 + \frac{P_s}{2\mu}\left[1-\left(1-\frac{2\mu}{r^d}\right)^{q_s}\right]; \tag{3.12}$$

$P>0$, $\mu>0$ are constants and

$$U^{si} = G^{ij}U_j^s = \frac{U_i^s}{d_i} + \frac{1}{2-D}\sum_{j=0}^{n} U_j^s. \tag{3.13}$$

Using (3.13) and $U_0^s=0$ we get

$$U^{s0} = \frac{1}{2-D}\sum_{j=0}^{n} U_j^s \tag{3.14}$$

and hence one can rewrite (3.9) as follows:

$$\mathrm{d}s^2 = J_0\left[\frac{\mathrm{d}r^2}{1-\dfrac{2\mu}{r^d}} + r^2\,\mathrm{d}\Omega_{d_0}^2 - \left(\prod_{s=1}^{m} H_s^{-2q_s/(U^s,U^s)}\right)\left(1-\frac{2\mu}{r^d}\right)\mathrm{d}t^2 + \sum_{i=2}^{n}\left(\prod_{s=1}^{m} H_s^{-2U_i^s/(d_i(U^s,U^s))}\right)h^{(i)}_{m_in_i}\,\mathrm{d}y^{m_i}\,\mathrm{d}y^{n_i}\right]. \tag{3.15}$$

These solutions are the special case of general solutions spherically symmetric solutions obtained in the Appendix by the method suggested in Ref. 17.

Black holes for natural q_s: For natural

$$q_s = 1,2,\ldots, \tag{3.16}$$

the metric has a horizon at $r^d=2\mu=r_h^2$. Indeed, for these values of q_s the functions $H_s(r)>0$ are smooth in the interval $(r_*,+\infty)$ for some $r_*<r_h$. For odd $q_s=2m_s+1$ (for all s) one gets $r_*=0$.

A global structure of the black hole solutions corresponding to these values of q_s will be a subject of a separate publication.

It was shown in Ref. 1 that in the one-component case for $2U^{s0}\neq -1$ and $0<q_s<1$ one obtains singularity at $r^d\to 2\mu$.

Remark: For noninteger $q_s>1$ the function $H_s(r)$ have a nonanalytical behavior in the vicinity of $r^d=2\mu$. In this case one may conject that the limit $r^d\to 2\mu$ corresponds to the singularity (in the general case) but here a separate investigation is needed.

IV. EXAMPLES: GENERALIZED SIMULATION OF INTERSECTING BLACK BRANES

The solutions with a horizon from the preceding section allows us to simulate the intersecting black brane solutions[4] in the model with antisymmetric form without scalar fields[2] when all $q_s=1$.

These solutions may also be generalized to the case of general natural $q_s \in \mathbf{N}$. In this case the parameters U_i^s and the pressures have the following form:

$$U_i^s = q_s d_i, \quad p_i^s = -\rho^s, \quad i \in I_s,$$

$$0, \quad (2q_s - 1)^{-1}\rho^s, \quad i \notin I_s. \tag{4.1}$$

Here $I_s=\{i_1,\ldots,i_k\} \in \{1,\ldots n\}$ is the index set[4] corresponding to the "brane" submanifold $M_{i_1} \times \cdots \times M_{i_k}$.

The "orthogonality" relations (1.4) lead us to the following dimension of intersection of brane submanifolds:[4]

$$d(I_s \cap I_l) = \frac{d(I_s)d(I_l)}{D-2}, \quad s \neq l, \tag{4.2}$$

where $d(I_s)=\Sigma_{i\in I_s} d_i$ is dimension of p-brane world volume.

Remark: The set of Diophantus equations (4.2) was solved explicitly in Ref. 20 for so-called "flower" Ansatz from Ref. 21. The solution in this case takes place for infinite number of dimensions $D=6,10,11,14,18,20,26,27,\ldots$, etc.

As an example, here we consider a "generalized simulation" of intersecting $M2\cap M5$, $M2\cap M2$ and $M5\cap M5$ black branes in $D=11$ supergravity. In what follows functions H_s, $s=1,2$, are defined in (3.12).

(a) For an analog of intersecting $M2\cap M5$ branes the metric reads

$$\mathrm{d}s^2 = H_1^{1/(3q_1)} H_2^{2/(3q_2)} \left[\frac{\mathrm{d}r^2}{1-2\mu/r^d} + r^2 \mathrm{d}\Omega_{d_0}^2 - H_1^{-1/q_1} H_2^{-1/q_2} \left\{ \left(1 - \frac{2\mu}{r^d}\right) \mathrm{d}t^2 + \mathrm{d}y^{m_2}\, \mathrm{d}y^{m_2} \right\} \right.$$
$$\left. + H_2^{-1/q_2} h^{(3)}_{m_3 n_3}\, \mathrm{d}y^{m_3}\, \mathrm{d}y^{n_3} + H_1^{-1/q_1}\, \mathrm{d}y^{m_4}\, \mathrm{d}y^{m_4} + h^{(5)}_{m_5 n_5}\, \mathrm{d}y^{m_5}\, \mathrm{d}y^{n_5} \right], \tag{4.3}$$

where $M2$-brane includes three one-dimensional: M_2, M_4 and the time manifold M_1; and $M5$-brane includes M_1, M_2, $M_3 (d_3=4)$.

(b) An analog of two electrical $M2$ branes intersecting on the time manifold has the following metric

$$\mathrm{d}s^2 = H_1^{1/(3q_1)} H_2^{1/(3q_2)} \left[\frac{\mathrm{d}r^2}{1-2\mu/r^d} + r^2\, \mathrm{d}\Omega_{d_0}^2 - H_1^{-1/q_1} H_2^{-1/q_2} \left(1 - \frac{2\mu}{r^d}\right) \mathrm{d}t^2 + H_1^{-1/q_1} h^{(2)}_{m_2 n_2}\, \mathrm{d}y^{m_2}\, \mathrm{d}y^{n_2} \right.$$
$$\left. + H_2^{-1/q_2} h^{(3)}_{m_3 n_3}\, \mathrm{d}y^{m_3}\, \mathrm{d}y^{n_3} + h^{(4)}_{m_4 n_4}\, \mathrm{d}y^{m_4} \mathrm{d}y^{n_4} \right], \tag{4.4}$$

where $d_2=d_3=2$.

(c) For an analog of two intersecting $M5$ branes the dimension of intersection is 4 and the metric reads

$$\mathrm{d}s^2 = H_1^{2/(3q_1)} H_2^{2/(3q_2)} \left[\frac{\mathrm{d}r^2}{1-2\mu/r} + r^2\, \mathrm{d}\Omega_2^2 - H_1^{-1/q_1} H_2^{-1/q_2} \left\{ \left(1 - \frac{2\mu}{r}\right) \mathrm{d}t^2 + h^{(2)}_{m_2 n_2}\, \mathrm{d}y^{m_2}\, \mathrm{d}y^{n_2} \right\} \right.$$
$$\left. + H_1^{-1/q_1} h^{(3)}_{m_3 n_3}\, \mathrm{d}y^{m_3}\, \mathrm{d}y^{n_3} + H_2^{-1/q_2} h^{(4)}_{m_4 n_4}\, \mathrm{d}y^{m_4}\, \mathrm{d}y^{n_4} \right]. \tag{4.5}$$

Here $d_0=d_3=d_4=2$ and $d_2=3$.

For the density of the sth component we get in any of these three cases

$$\rho^s = \frac{(2q_s - 1)\mathrm{d}^2 P_s (P_s + 2\mu)(1 - 2\mu r^{-d})^{q_s^{-1}}}{4(H_1 H_2)^2 J_0 r^{2d_0}}, \tag{4.6}$$

where

$$J_0 = \prod_{s=1}^{2} H_s^{d(I_s)/(9q_s)} \tag{4.7}$$

and $d(I_s) = 3, 6$ for $M2$, $M5$ branes, respectively.

V. PHYSICAL PARAMETERS

A. Gravitational mass and PPN parameters

Here we set $d_0 = 2$ ($d = 1$). Let us consider the four-dimensional space–time section of the metric (3.15). Introducing a new radial variable by the relation

$$r = R\left(1 + \frac{\mu}{2R}\right)^2, \tag{5.1}$$

we rewrite the 4-section in the following form:

$$\mathrm{d}s^2_{(4)} = \left(\prod_{s=1}^{m} H^{-2U^{s0}/(U^s, U^s)}\right)\left[-\left(\prod_{s=1}^{m} H_s^{-2q_s/(U^s, U^s)}\right)\left(\frac{1 - \dfrac{\mu}{2R}}{1 + \dfrac{\mu}{2R}}\right)^2 \mathrm{d}t^2 + \left(1 + \frac{\mu}{2R}\right)^4 \delta_{ij}\, \mathrm{d}x^i\, \mathrm{d}x^j\right], \tag{5.2}$$

$i, j = 1, 2, 3$. Here $R^2 = \delta_{ij} x^i x^j$.

The parametrized post-Newtonian (Eddington) parameters are defined by the well-known relations

$$g_{00}^{(4)} = -(1 - 2V + 2\beta V^2) + O(V^3), \tag{5.3}$$

$$g_{ij}^{(4)} = \delta_{ij}(1 + 2\gamma V) + O(V^2), \tag{5.4}$$

$i, j = 1, 2, 3$. Here

$$V = \frac{GM}{R} \tag{5.5}$$

is the Newtonian potential, M is the gravitational mass and G is the gravitational constant.

From (5.2)–(5.4) we obtain

$$GM = \mu + \sum_{s=1}^{m} \frac{P_s q_s (q_s + U^{s0})}{(U^s, U^s)} \tag{5.6}$$

and

$$\beta - 1 = \sum_{s=1}^{m} \frac{|A_s|}{(GM)^2}(q_s + 2U^{s0}), \tag{5.7}$$

$$\gamma - 1 = -\sum_{s=1}^{m} \frac{P_s q_s}{(U^s, U^s) GM} (q_s + U^{s0}), \tag{5.8}$$

where

$$|A_s| = \tfrac{1}{2} q_s^2 P_s (P_s + 2\mu)/(U^s, U^s) \tag{5.9}$$

(see Appendix) or, equivalently,

$$P_s = -\mu + \sqrt{\mu^2 + 2|A_s|(U^s, U^s) q_s^{-2}} > 0. \tag{5.10}$$

For fixed U_i^s the parameter $\beta - 1$ is proportional to the ratio of two quantities: the weighted sum of multicomponent anisotropic fluid density parameters $|A_s|$ and the gravitational radius squared $(GM)^2$.

B. Hawking temperature

The Hawking temperature of the black hole may be calculated using the well-known relation[22]

$$T_H = \frac{1}{4\pi\sqrt{-g_{tt} g_{rr}}} \frac{d(-g_{tt})}{\mathrm{d}r}_{\text{horizon}}. \tag{5.11}$$

We get

$$T_H = \frac{d}{4\pi (2\mu)^{1/d}} \prod_{s=1}^{m} \left(1 + \frac{P_s}{2\mu}\right)^{-q_s/(U^s, U^s)}. \tag{5.12}$$

Here all q_s are natural numbers.

For any of $D = 11$ metrics from Sec. IV the Hawking temperature reads

$$T_H = \frac{d}{4\pi (2\mu)^{1/d}} \prod_{s=1}^{2} \left(1 + \frac{P_s}{2\mu}\right)^{-1/(2q_s)}.$$

.

VI. CONCLUSIONS

In this paper, using the methods developed earlier for obtaining perfect fluid and p-brane solutions, we have considered a family of spherically symmetric solutions in the model with m-component anisotropic fluid when the equations of state (1.2)–(1.4) are imposed. The metric of any solution contains $(n-1)$ Ricci-flat "internal" space metrics and depends upon a set of parameters U_i^s, $i > 1$.

For $q_s = 1$ (for all s) and certain equations of state (with $p_i^s = \pm \rho^s$) the metric of the solution coincides with that of intersecting black brane solution in the model with antisymmetric forms without dilatons.[3] For natural numbers $q_s = 1, 2, \ldots$, we have obtained a family of solutions with regular horizon.

Here we have considered three examples of solutions with horizon, that simulate (by fluids) binary intersecting $M2$ and $M5$ black branes in $D = 11$ supergravity.

We have also calculated (for possible estimations of observable effects of extra dimensions) the post-Newtonian parameters β and γ corresponding to the four-dimensional section of the metric and the Hawking temperature as well.

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APPENDIX A: LAGRANGE REPRESENTATION

It is more convenient for finding of exact solutions, to write the stress-energy tensor in cosmological-type form,

$$(T_N^{(s)M}) = \mathrm{diag}(-\hat{\rho}^s, \hat{p}_0^s \delta_{k_0}^{m_0}, \hat{p}_1^s \delta_{k_1}^{m_1}, \ldots, \hat{p}_n^s \delta_{k_n}^{m_n}), \tag{A1}$$

where $\hat{\rho}^s$ and $\hat{p}_i^s$ are "effective" density and pressures of sth component, respectively, depending upon the radial variable u and the physical density ρ^s and pressures p_i^s are related to the effective ("hat") ones by formulas

$$\rho^s = -\hat{p}_1^s, \quad p_r^s = -\hat{\rho}^s, \quad p_i^s = \hat{p}_i^s \quad (i \neq 1), \tag{A2}$$

$s = 1, \ldots, m$.

The equations of state may be written in the following form:

$$\hat{p}_i = \left(1 - \frac{2U_i^s}{d_i}\right)\hat{\rho}^s, \tag{A3}$$

where U_i^s are constants, $i = 0, 1, \ldots, n$. It follows from (A2) and (A3), and $U_1^s = q_s$ that

$$\rho^s = (2q_s - 1)\hat{\rho}^s. \tag{A4}$$

The "conservation law" equations $\nabla_M T_N^{(s)M} = 0$ may be written, due to relations (2.3) and (A1) in the following form:

$$\dot{\hat{\rho}}^s + \sum_{i=0}^{n} \mathrm{d}_i \dot{X}^i (\hat{\rho}^s + \hat{p}_i^s) = 0. \tag{A5}$$

Using the equation of state (A3) we get

$$\hat{\rho}^s = -A_s e^{2U_i^s X^i - 2\gamma_0}, \tag{A6}$$

where $\gamma_0(X) = \Sigma_{i=0}^n \mathrm{d}_i X^i$ and A_s are constants.

The Einstein equations (2.1) with the relations (A3) and (A6) imposed are equivalent to the Lagrange equations for the Lagrangian,

$$L = \tfrac{1}{2} e^{-\gamma + \gamma_0(X)} G_{ij} \dot{X}^i \dot{X}^j - e^{\gamma - \gamma_0(X)} V, \tag{A7}$$

where

$$V = \tfrac{1}{2} d_0 (d_0 - 1) \exp(2U_i^0 X^i) + A_s \exp(2U_i^s X^i) \tag{A8}$$

is the potential and the components of the minisupermetric G_{ij} are defined in (3.5),

$$U_i^0 X^i = -X^0 + \gamma_0(X), \quad U_i^0 = \delta_i^0 + d_i, \tag{A9}$$

$i = 0, \ldots, n$ (for the cosmological case see Refs. 16 and 17).

For $\gamma = \gamma_0(X)$, i.e., when the harmonic time gauge is considered, we get the set of Lagrange equations for the Lagrangian,

$$L = \tfrac{1}{2} G_{ij} \dot{X}^i \dot{X}^j - V, \tag{A10}$$

with the zero-energy constraint imposed,

$$E = \tfrac{1}{2} G_{ij} \dot{X}^i \dot{X}^j + V = 0. \tag{A11}$$

It follows from the restriction $U_0^s = 0$ that

$$(U^0, U^s) \equiv U_i^0 G^{ij} U_j^s = 0. \tag{A12}$$

Indeed, the contravariant components $U^{0i} = G^{ij} U_j^0$ are the following ones:

$$U^{0i} = -\frac{\delta_0^i}{d_0}. \tag{A13}$$

Then we get $(U^0, U^s) = U^{0i} U_i^s = -U_0^s / d_0 = 0$. In what follows we also use the formula

$$(U^0, U^0) = \frac{1}{d_0} - 1 < 0 \tag{A14}$$

for $d_0 > 1$.

Now we prove that $(U^s, U^s) > 0$ for all $s > 0$. Indeed, minisupermetric has the signature $(-, +, \ldots, +)$,[18,19] vector U^0 is timelike and orthogonal to any vector $U^s \neq 0$. Hence any vector U^s is spacelike.

APPENDIX B: GENERAL SPHERICALLY SYMMETRIC SOLUTIONS

When the orthogonality relations (A12) and (3.7) are satisfied the Euler–Lagrange equations for the Lagrangian (A10) with the potential (A8) have the following solutions (see relations from Ref. 17 adopted for our case):

$$X^i(u) = -\sum_{\alpha=0}^{m} \frac{U^{\alpha i}}{(U^\alpha, U^\alpha)} \ln |f_\alpha(u - u_\alpha)| + c^i u + \overline{c}^i, \tag{B1}$$

where u_α are integration constants; and vectors $c = (c^i)$ and $\overline{c} = (\overline{c}^i)$ are dually orthogonal to covectors $U^\alpha = (U_i^\alpha)$, i.e., they satisfy the linear constraint relations

$$U^0(c) = U_i^0 c^i = -c^0 + \sum_{j=0}^{n} \mathrm{d}_j c^j = 0, \tag{B2}$$

$$U^0(\overline{c}) = U_i^0 \overline{c}^i = -\overline{c}^0 + \sum_{j=0}^{n} \mathrm{d}_j \overline{c}^j = 0, \tag{B3}$$

$$U^s(c) = U_i^s c^i = 0, \tag{B4}$$

$$U^s(\overline{c}) = U_i^s \overline{c}^i = 0. \tag{B5}$$

Here

$$f_\alpha(\tau) = R_\alpha \frac{\sinh(\sqrt{C_\alpha}\tau)}{\sqrt{C_\alpha}}, \quad C_\alpha > 0, \quad \eta_\alpha = +1,$$

$$R_\alpha \frac{\cosh(\sqrt{C_\alpha}\tau)}{\sqrt{C_\alpha}}, \quad C_\alpha > 0, \quad \eta_\alpha = -1,$$

$$R_\alpha \frac{\sin(\sqrt{|C_\alpha|}\tau)}{\sqrt{|C_\alpha|}}, \quad C_\alpha < 0, \quad \eta_\alpha = +1,$$

$$R_\alpha \tau, \quad C_\alpha = 0, \quad \eta_\alpha = +1, \tag{B6}$$

$\alpha = 0, \ldots, m$; where $R_0 = d_0 - 1$, $\eta_0 = 1$, $R_s = \sqrt{2|A_s|(U^s, U^s)}$, $\eta_s = -\text{sign } A_s$ $(s = 1, \ldots, m)$.

The zero-energy constraint, corresponding to the solution (B1) reads

$$E = \frac{1}{2}\sum_{\alpha=0}^{m} \frac{C_\alpha}{(U^\alpha, U^\alpha)} + \frac{1}{2} G_{ij} c^i c^j = 0. \tag{B7}$$

Special solutions: The (weak) horizon condition (i.e., infinite time of propagation of light for $u \to +\infty$) leads us to the following integration constants:

$$\overline{c^i} = 0, \tag{B8}$$

$$c^i = \overline{\mu} \sum_{\alpha=0}^{m} \frac{U_1^\alpha U^{\alpha i}}{(U^\alpha, U^\alpha)} - \overline{\mu}\delta_1^i, \tag{B9}$$

$$C_\alpha = (U_1^\alpha)^2 \overline{\mu}^2, \tag{B10}$$

where $\overline{\mu} > 0$, $\alpha = 0, \ldots, m$. For analogous choice of parameters in the p-brane case see Refs. 13, 14, and 4.

We also introduce a new radial variable $r = r(u)$ by relations

$$\exp(-2\overline{\mu} u) = 1 - \frac{2\mu}{r^d}, \quad \mu = \overline{\mu} d > 0, \quad d = d_0 - 1, \tag{B11}$$

and set $u_s < 0$ and $A_s < 0$ for all s and also $u_0 = 0$.

The relations of the Appendix imply the formulas (3.9) and (3.10) for the solution from Sec. III with

$$H_s = \exp(-\overline{\mu} q_s u) f_s(u - u_s), \quad A_s = -\frac{(dq_s)^2}{2(U^s, U^s)} P_s(P_s + 2\mu), \tag{B12}$$

$P_s > 0$.

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On the Treves theorem for the Ablowitz–Kaup–Newell–Segur equation

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According to a theorem of Treves, the conserved functionals of the Ablowitz, Kaup, Newell, and Segur (AKNS) equation vanish on all pairs of formal Laurent series $(\tilde{q},\tilde{r})$ of a specified form, both of them with a pole of the first order. We propose a new and very simple proof for this statement, based on the theory of Bäcklund transformations; using the same method, we prove that the AKNS conserved functionals vanish on other pairs of Laurent series. The spirit is the same as in our previous paper on the Treves theorem for the Korteweg–de Vries hierarchy, with some nontrivial technical differences. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND PRELIMINARIES

Some recent works of Treves (see Refs. 10 and 11, and references therein) have introduced, in the words of Dickey,[2] a "fresh idea" in the sector of integrable evolutionary PDEs [Korteweg–de Vries (KdV), nonlinear Schrödinger, etc.]. The discovery of Treves is that all the conserved functionals of these equations vanish when they are evaluated on certain formal Laurent series (intending the integrals which appear in the functionals as loop integrals in $\mathbb{C}$ around zero).

To be more specific, let us consider the KdV equation $q_t = q_{xxx} - 12qq_x$, and the functionals $h = h(q)$ which are integrals of polynomials in q and its x derivatives; for any such functional to be conserved by the KdV equation, it is necessary and sufficient[10] that $h(\tilde{q}) = 0$ for all formal Laurent series with complex coefficients of the form $\tilde{q} = 1/x^2 + \tilde{q}_0 + \Sigma_{k=2}^{+\infty} \tilde{q}_k x^k$. Now, let us pass to the coupled equations

$$q_t = \tfrac{1}{2} q_{xx} - q^2 r, \quad r_t = -\tfrac{1}{2} r_{xx} + q r^2, \tag{1.1}$$

which have been considered in Ref. 11; as well known, these become the nonlinear Schrödinger equation $iq_\tau = (1/2)q_{xx} - |q|^2 q$ if r is the complex conjugate of q and $\tau := it$; if q, r are regarded as independent, the pair (1.1) is usually called the AKNS equation after Ablowitz, Kaup, Newell, and Segur (see Ref. 8, and references therein), a terminology which we also use in this paper.

Let us consider the functionals $h(q,r)$ which are integrals of polynomials in q, r and their x derivatives; for any such functional to be conserved by Eq. (1.1), it is necessary[11] that $h(\tilde{q},\tilde{r}) = 0$ for all pairs of Laurent series $\tilde{q} = e^{\varphi}(1/x + \alpha + \beta x + \Sigma_{k=2}^{+\infty} \tilde{\chi}_k x^k)$, $\tilde{r} = e^{-\varphi}(1/x - \alpha + \beta x + \Sigma_{k=2}^{+\infty} \tilde{\rho}_k x^k)$ (with $\varphi, \alpha, \beta, \tilde{\chi}_k, \tilde{\rho}_k \in \mathbb{C}$); differently from the KdV case, the sufficiency of this condition has been conjectured but not proved in Ref. 11.

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The proofs in the original papers of Treves are based on a long and highly technical analysis, where a central role is played by the recurrence relations for some standard basis of conserved functionals. A simple alternative proof of the necessary condition for the KdV, and an analogue of this result for the Boussinesq equation, were obtained by Dickey[2] using the dressing method for the Lax operator. Another proof of necessity for the KdV was proposed in a paper of ours,[7] where we employed the invariance of the KdV conserved functionals under the (auto)-Bäcklund transformation. The relation between Refs. 2 and 7 has been very recently discussed in Ref. 3, where the extension of the Bäcklund method to the Boussinesq and the other GD hierarchies has also been sketched.

In the present paper the Bäcklund invariance of the conserved functionals will be used in relation to the AKNS, to get a new proof of the Treves theorem for this equation. Using this idea we will show that the AKNS conserved functionals vanish on other nontrivial pairs of Laurent series, in particular for those of the form $\tilde{q}=e^{\varphi}(2/x^2+\alpha+\beta x+\Sigma_{k=2}^{+\infty}\tilde{\chi}_k x^k)$, $\tilde{r}=e^{-\varphi}(1+\beta x^3+\Sigma_{k=4}^{+\infty}\tilde{\rho}_k x^k)$.

Both for the pairs $(\tilde{q},\tilde{r})$ considered by Treves and for the ones in the above variant, our proof is very simple and conceptually similar to the argument of Ref. 7 for the KdV: in fact, we show that any $(\tilde{q},\tilde{r})$ as before is the Bäcklund transform of a pair (q,r) of holomorphic series (with no negative powers of x), on which every functional of polynomial type is zero for trivial reasons.

In comparison with our previous analysis of the KdV case, the AKNS is a bit more difficult regarding the precise definition of the Bäcklund transformation; in fact, even though this transformation for the AKNS is known in the literature,[1,9] its usual formulation involves rational maps that would cause some troubles in the present framework; for this reason, in this paper we give a different presentation which is more implicit but involves only polynomial mappings.

Let us describe the organization of the paper. In the rest of this Introduction, we generalize for our present needs the language of differential algebras and formal variational calculus already employed in Ref. 7; the AKNS equation and the space of its conserved functionals are described formally within this framework. In Sec. II we state precisely the Treves theorem for the AKNS (Proposition 2.1) and our variant of it mentioned before (Proposition 2.2). In Sec. III we introduce the Bäcklund transformation and state the invariance under it of the AKNS conserved functionals, in a way suitable for our purposes; in Sec. IV we use it to prove Propositions 2.1 and 2.2.

Two Appendixes have been added to review the matrix Lax formalism *à la* Drinfeld–Sokolov, and its relation to Bäcklund transformations, for certain classes of integrable systems and especially for the AKNS; the aim is, essentially, to justify the slightly nonstandard presentation of the Bäcklund machinery employed in this work.

All vector spaces considered in this paper are over $\mathbb{C}$. As anticipated, hereafter we summarize some concepts from differential algebra and from the formal variational calculus of Gelfand–Dickey,[4] including their applications to the AKNS theory.

Differential algebras: By a differential algebra, we mean an associative algebra (commutative or not) equipped with a derivation, i.e., with a linear map of the algebra into itself having the Leibnitz property with respect to the product. We do not require the algebra to possess a unity; if this exists, one easily proves that it is annihilated by the derivation. A morphism of differential algebras is an algebraic morphism respecting the derivations.

A differential algebra is typically written as $(\mathcal{Q},\partial_x)$; the subscript x attached to the derivation is also used to denote its action on the elements q of the algebra, so $\partial_x\colon \mathcal{Q}\to\mathcal{Q}$, $q\mapsto q_x$.

We write $\mathcal{Q}_x$ for the image of ∂_x; if $q,p\in\mathcal{Q}$ and $p=q_x$, sometimes we say that q is a primitive of p. The quotient vector space

$$\int \mathcal{Q} := \mathcal{Q}/\mathcal{Q}_x = \{q+\mathcal{Q}_x | q\in\mathcal{Q}\} \tag{1.2}$$

is called the *space of integrals* of $\mathcal{Q}$. The corresponding quotient map is denoted with

$$\int : \mathcal{Q} \to \int \mathcal{Q}, \quad q \mapsto \int q := q + \mathcal{Q}_x, \tag{1.3}$$

and we call $\int q$ the integral of q; of course $\int q_x = 0$ for each q. Let $\mathcal{S}$ be any subset of $\mathcal{Q}$; we write

$$\int \mathcal{S} := \{s + \mathcal{Q}_x | s \in \mathcal{S}\} \subset \int \mathcal{Q}, \tag{1.4}$$

and note that the restriction of (1.3) is a map $\mathcal{S} \to \int \mathcal{S}, s \mapsto \int s$.

Sometimes, it is necessary to specify the dependence from the differential algebra $\mathcal{Q}$ of the previous operations of integration: in this case we write $\int^{\mathcal{Q}}$ for the map (1.3) or its restriction to $\mathcal{S}$, and $\int^{>\mathcal{Q}} \mathcal{S}$ for the set (1.4).

A differential subalgebra of a differential algebra $(\mathcal{Q}, \partial_x)$ is a subalgebra $\mathcal{P} \subset \mathcal{Q}$ closed under ∂_x; of course, the differential subalgebra $\mathcal{P}$ with the restricted map $\partial_x \restriction \mathcal{P} \equiv \partial_x$ is itself a differential algebra. In this situation, one must distinguish between two kinds of integration, the first one intrinsic for the differential algebra $(\mathcal{P}, \partial_x)$, and the second one relative to $\mathcal{Q}$. In the first case, we introduce as usual the quotient space and the quotient map

$$\int \mathcal{P} := \mathcal{P}/\mathcal{P}_x, \quad \int : \mathcal{P} \mapsto \int \mathcal{P}, \quad p \mapsto \int p := p + \mathcal{P}_x; \tag{1.5}$$

in the second case, we consider the space and the map

$$\int^{\mathcal{Q}} \mathcal{P} := \{p + \mathcal{Q}_x | p \in \mathcal{P}\} \subset \int \mathcal{Q}, \quad \int^{\mathcal{Q}} : \mathcal{P} \mapsto \int^{\mathcal{Q}} \mathcal{P}, \quad p \mapsto \int^{\mathcal{Q}} p := p + \mathcal{Q}_x. \tag{1.6}$$

One easily checks the existence of a unique map

$$\psi: \int \mathcal{P} \to \int^{\mathcal{Q}} \mathcal{P} \text{ such that } \psi\left(\int p\right) = \int^{\mathcal{Q}} p \quad \forall\, p \in \mathcal{P}. \tag{1.7}$$

The map ψ is linear and furthermore, it is injective if and only if

$$\mathcal{P} \cap \mathcal{Q}_x = \mathcal{P}_x. \tag{1.8}$$

If condition (1.8) holds, we will say that $\mathcal{P}$ is a *strict differential subalgebra* of $\mathcal{Q}$. [Of course, for any differential subalgebra $\mathcal{P}$ it is $\mathcal{P} \cap \mathcal{Q}_x \supset P_x$; Eq. (1.8) means that any element of $\mathcal{P}$ with a primitive in $\mathcal{Q}$ also has a primitive in $\mathcal{P}$.]

Throughout the paper, the term *ideal* is employed with the usual sense; a *differential ideal* of a differential algebra is an ideal closed under the derivation.

Gelfand–Dickey differential algebra in any number γ of generators: This is the commutative differential algebra

$$\mathfrak{F} := \mathbb{C}[\xi_1, \ldots \xi_\gamma, \xi_{1,x}, \ldots, \xi_{\gamma,x}, \ldots]_0, \tag{1.9}$$

made of complex polynomials in infinitely many indeterminates $\xi_s, \xi_{s,x}, \xi_{s,xx}, \ldots$ $(s = 1, \ldots, \gamma)$, without free term (the absence of this is indicated by the subscript 0); $\mathfrak{F}$ is equipped with the unique derivation $\partial_x \equiv \cdot_x$ such that

$$(\xi_s)_x = \xi_{s,x}, \quad (\xi_{s,x})_x = \xi_{s,xx}, \quad \ldots\ . \tag{1.10}$$

We write F, G, etc., for the elements of $\mathfrak{F}$. (For example, $F := \xi_{1,x}^2 \xi_{2,xx}$, $G := 3\xi_{1,x}\xi_2 \in \mathfrak{F}$; $FG = 3\xi_{1,x}^3 \xi_2 \xi_{2,xx}$.)

For the elements of $\int \mathfrak{F} = \mathfrak{F}/\mathfrak{F}_x$, which have the form $f = \int F$ $(F \in \mathfrak{F})$, the general denomination of "integrals" is of course available; however, in this case the name *functionals* is more standard.

The Gelfand–Dickey algebra $\mathfrak{F}$ can be represented in terms of transformations on any commutative differential algebra $(\mathcal{Q},\partial_x)$, in the following way. Let us consider the Cartesian product $\times^\gamma\mathcal{Q}\equiv\mathcal{Q}^\gamma$; then, any $F\in\mathfrak{F}$ induces a map

$$F(\,)\colon\ \mathcal{Q}^\gamma\to\mathcal{Q},\ \ (q_1,\ldots,q_\gamma)\mapsto F(q_1,\ldots,q_\gamma), \tag{1.11}$$

where $F(q_1,\ldots,q_\gamma)$ is obtained from the expression of the polynomial F replacing ξ_s with q_s, $\xi_{s,x}$ with $q_{s,x}$, etc.

It is important to distinguish the elements of $\mathfrak{F}$ from the maps on $\mathcal{Q}^\gamma$: this is the reason why the symbol of the map in (1.11) contains parentheses. (In Ref. 7, for the same reason we used bold symbols for the elements of $\mathfrak{F}$, and nonbold notations for the maps on $\mathcal{Q}$; in the present framework, the proliferation of bold symbols would be excessive.) We note that

$$F(\,)\in\mathrm{Pol}(\mathcal{Q}^\gamma,\mathcal{Q}), \tag{1.12}$$

where $\mathrm{Pol}(\mathcal{X},\mathcal{Y})$ are the polynomial maps[7] between any two vector spaces $\mathcal{X},\mathcal{Y}$ and $\mathcal{Q}^\gamma$ is regarded as a vector space with the product structure. $\mathrm{Pol}(\mathcal{Q}^\gamma,\mathcal{Q})$ is a commutative algebra with the pointwise product, and a differential algebra with the unique derivation $\partial_x\colon\ P(\,)\mapsto P_x(\,)$ such that $P_x(q):=P(q)_x$ for all $P(\,)$. The correspondence

$$\mathfrak{F}\to\mathrm{Pol}(\mathcal{Q}^\gamma,\mathcal{Q}),\ \ F\mapsto F(\,) \tag{1.13}$$

is a morphism of differential algebras. It also induces a linear map

$$\int\mathfrak{F}\to\mathrm{Pol}\left(\mathcal{Q}^\gamma,\int\mathcal{Q}\right),\ \ f\mapsto f(\,) \tag{1.14}$$

in the following way: if $f=\int F$, then

$$f(\,)\colon\ \mathcal{Q}^\gamma\to\int\mathcal{Q},\ \ (q_1,\ldots,q_\gamma)\mapsto f(q_1,\ldots,q_\gamma):=\int F(q_1,\ldots,q_\gamma). \tag{1.15}$$

The maps (1.11) and (1.15) will be called the *representations* on $\mathcal{Q}$ of F and f, respectively.

Vector fields and Lie derivatives: We consider again the Gelfand–Dickey differential algebra (1.9). In this framework, by a vector field we simply mean a family

$$X=(X_1,\ldots,X_\gamma)\in\mathfrak{F}^\gamma \tag{1.16}$$

[this is represented as map $X(\,)=(X_1(\,),\ldots,X_\gamma(\,))\in\mathrm{Pol}(\mathcal{Q}^\gamma,\mathcal{Q}^\gamma)$ on any commutative differential algebra $\mathcal{Q}$]. The Lie derivative on $\mathfrak{F}$ induced by X is the unique derivation

$$\mathcal{L}_X\colon\ \mathfrak{F}\to\mathfrak{F}\ \text{ such that }\mathcal{L}_X\partial_x=\partial_x\mathcal{L}_X,\ \ \mathcal{L}_X\xi_s=X_s\ \ (s=1,\ldots,\gamma); \tag{1.17}$$

the corresponding Lie derivative on $\int\mathfrak{F}$ is the unique map

$$\mathcal{L}_X\colon\ \int\mathfrak{F}\to\int\mathfrak{F}\ \text{ such that }\ \mathcal{L}_X\int\ =\int\mathcal{L}_X; \tag{1.18}$$

of course this map is linear. The set of *conserved functionals* of a vector field X is

$$\mathfrak{I}_X:=\left\{h\in\int\mathfrak{F}\,|\,\mathcal{L}_Xh=0\right\}; \tag{1.19}$$

this is a vector subspace of $\int\mathfrak{F}$.

The AKNS theory and its conserved functionals (Ref. 8): This is a theory in $\gamma=2$ components. For our purposes, it is necessary to formulate it in the language of formal variational calculus; so, we introduce the Gelfand–Dickey algebra

$$\mathfrak{F} := \mathbb{C}[\xi, \eta, \xi_x, \eta_x, \dots]_0 \tag{1.20}$$

with generators $\xi_1 \equiv \xi, \xi_2 \equiv \eta$. The AKNS vector field is

$$X_{\mathrm{AKNS}} \equiv X := (\tfrac{1}{2}\xi_{xx} - \xi^2\eta, -\tfrac{1}{2}\eta_{xx} + \xi\eta^2) \in \mathfrak{F}^2. \tag{1.21}$$

The space of conserved functionals

$$\mathfrak{Z}_{X_{\mathrm{AKNS}}} \equiv \mathfrak{Z} \tag{1.22}$$

is known to be of infinite dimension, a remarkable property placing this vector field within the realm of integrable systems. In the Appendixes A and B we will review the Lax formalism to obtain the conserved functionals of this vector field and of similar systems. This approach gives a basis $(h_i)_{i=1,2,\dots}$ for $\mathfrak{Z}$, derived from the "fundamental invariants" of the Lax operator: the first elements are

$$h_1 := \tfrac{1}{2}\int \xi\eta, \quad h_2 := \tfrac{1}{4}\int \xi_x\eta, \quad h_3 := -\tfrac{1}{8}\int (\xi^2\eta^2 + \xi_x\eta_x), \quad h_4 := \tfrac{1}{16}\int (-3\eta^2\xi\xi_x + \xi_x\eta_{xx}). \tag{1.23}$$

II. THE TREVES THEOREM (AND SOME VARIANT OF IT) FOR THE AKNS

As in the case of the KdV,[10] this theorem concerns the representation of an integrable system on a peculiar differential algebra. This is the commutative differential algebra of formal Laurent series in one indeterminate x and complex coefficients, i.e.,

$$\mathcal{Q} := \left\{ q = \sum_{k=k_{\min}}^{+\infty} q_k x^k \,|\, q_k \in \mathbb{C} \ \ \forall\, k, k_{\min} = k_{\min}(q) \in \mathbb{Z} \right\}; \tag{2.1}$$

the product is the usual Cauchy product of series, and the derivation is

$$\partial_x \colon \mathcal{Q} \to \mathcal{Q}_x, \quad q \mapsto q_x := \sum_{k=k_{\min}}^{+\infty} k q_k x^{k-1}. \tag{2.2}$$

Clearly, we have

$$\mathcal{Q}_x = \{q \in \mathcal{Q} \,|\, q_{-1} = 0\} \tag{2.3}$$

and the map $\int \mathcal{Q} \to \mathbb{C}$, $\int q \mapsto q_{-1}$ is a linear isomorphism. For this reason, from now on we make the identifications

$$\int \mathcal{Q} \simeq \mathbb{C}, \quad \int q \simeq q_{-1} \quad \forall\, q \in \mathcal{Q} \tag{2.4}$$

(in Ref. 7, this was presented for simplicity as the very *definition* of $\int$). Of course, the above description of $\int q$ as the "residue" q_{-1} suggests to interpret it as a loop integral in $\mathbb{C}$ around zero.

We come to the Treves theorem for $\mathfrak{Z}_{\mathrm{AKNS}} \equiv \mathfrak{Z}$ and for the differential algebra (2.1) and (2.2). In our notations, this reads as follows.

Proposition 2.1 (Ref. 11): Let $h \in \mathfrak{Z} \subset \int\mathfrak{F}$, and consider its representation $h(\,)\colon \mathcal{Q}^2 \to \mathbb{C}$. Then

$$h(\tilde{q},\tilde{r}) = 0 \quad \forall\, \tilde{q} = e^{\varphi}\left(\frac{1}{x} + \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\chi}_k x^k\right), \ \tilde{r} = e^{-\varphi}\left(\frac{1}{x} - \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\rho}_k x^k\right) \tag{2.5}$$

$(\varphi, \alpha, \beta, \tilde{\chi}_k, \tilde{\rho}_k \in \mathbb{C})$.

As anticipated, our aim in this paper is to give a new proof of this result, based on the Bäcklund transformations. This technique will allow us to prove the following variant of the previous result.

Proposition 2.2: Let $h \in \mathfrak{Z}$; *then*

$$h(\tilde{q},\tilde{r}) = 0 \quad \forall\, \tilde{q} = e^{\varphi}\left(\frac{2}{x^2} + \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\chi}_k x^k\right),\ \tilde{r} = e^{-\varphi}\left(1 + \beta x^3 + \sum_{k=4}^{+\infty} \tilde{\rho}_k x^k\right) \tag{2.6}$$

$(\varphi, \alpha, \beta, \tilde{\chi}_k, \tilde{\rho}_k \in \mathbb{C})$.

Both Propositions 2.1 and 2.2 are proved in Sec. IV. Hereafter, as a preliminary step we discuss the AKNS Bäcklund transformation, in a formulation suitable for our purposes.

III. BÄCKLUND TRANSFORMATION FOR THE AKNS THEORY

Essentially, this is a transformation leaving invariant the AKNS conserved functionals. However, its description in the language of formal variational calculus requires some technical subtleties introduced hereafter. To this purpose, we consider besides $\mathfrak{F} := \mathbb{C}[\xi, \eta, \xi_x, \eta_x, \dots]_0$ a "copy" of it, say

$$\tilde{\mathfrak{F}} := \mathbb{C}[\tilde{\xi}, \tilde{\eta}, \tilde{\xi}_x, \tilde{\eta}_x, \dots]_0, \tag{3.1}$$

with the derivation such that $(\tilde{\xi})_x = \tilde{\xi}_x$, etc. Of course, there is a unique differential-algebraic isomorphism $\tilde{\cdot}: \mathfrak{F} \to \tilde{\mathfrak{F}}$, $F \mapsto \tilde{F}$ sending ξ, η into $\tilde{\xi}, \tilde{\eta}$. This also induces a linear isomorphism

$$\tilde{}: \int \mathfrak{F} \to \int \tilde{\mathfrak{F}},\ f = \int F \mapsto \tilde{f} := \int \tilde{F}. \tag{3.2}$$

We interpret $\mathfrak{F}$, $\tilde{\mathfrak{F}}$ as describing the "initial" and "final variables" for the "transformation" to be introduced. The latter is in fact defined implicitly in terms of an "auxiliary variable" ν; its description mixes together the initial auxiliary and final variables, so we introduce a third differential algebra

$$\mathfrak{M} := \mathbb{C}[\xi, \eta, \nu, \tilde{\xi}, \tilde{\eta}, \xi_x, \eta_x, \nu_x, \tilde{\xi}_x, \tilde{\eta}_x \dots]_0, \tag{3.3}$$

writing again ∂_x for its derivation. Up to trivial identifications, we have

$$\mathfrak{F}, \tilde{\mathfrak{F}} \subset \mathfrak{M}; \tag{3.4}$$

both $\mathfrak{F}$ and $\tilde{\mathfrak{F}}$ are strict differential subalgebras of $\mathfrak{M}$ [in the sense of (1.8)], so

$$\int \mathfrak{F} \simeq \int^{\mathfrak{M}} \mathfrak{F},\quad \int \tilde{\mathfrak{F}} \simeq \int^{\mathfrak{M}} \tilde{\mathfrak{F}} \subset \int \mathfrak{M}. \tag{3.5}$$

Definition 3.1: The AKNS Bäcklund ideal $\mathcal{I}_{\mathrm{AKNS}} \equiv \mathcal{I} \subset \mathfrak{M}$ *is the ideal of* $\mathfrak{M}$ *generated by the elements*

$$I_1 := \xi_x - \tilde{\xi}_x + \nu(\xi + \tilde{\xi}),\ I_2 := \eta_x - \tilde{\eta}_x + \nu(\eta + \tilde{\eta}),\ I_3 := \nu_x + \xi\eta - \tilde{\xi}\tilde{\eta}. \tag{3.6}$$

From standard commutative algebra,

$$\mathcal{I} = \left\{ \sum_{j=1}^{3} F_j I_j \,\middle|\, F_j \in \mathfrak{M}\ \forall\, j \right\}. \tag{3.7}$$

In the language of formal variational calculus, the Bäcklund invariance of the AKNS conserved functionals can be expressed as follows.

Proposition 3.2: Let $h \in \mathfrak{Z}_{\mathrm{AKNS}} \equiv \mathfrak{Z} \subset \mathfrak{F}$, *and define* $\tilde{h}$ *following* (3.2). *Then*

$$\tilde{h} - h \in \int \mathcal{I} \quad \left(\int \equiv \int^{\mathfrak{M}} \right). \tag{3.8}$$

The above proposition is essentially known in the literature, even though it is not usually formulated in the language of formal variational calculus. In any case, to make the paper self-contained we propose a proof in Appendix B.

In order to exemplify Eq. (3.8), let us consider the functionals h_i in Eq. (1.23) $(i=1,2,3,4)$ and their tilded images $\tilde{h}_1 = \int \tilde{\xi}\tilde{\eta}, \ldots$; it turns out that

$$\tilde{h}_1 - h_1 = -\frac{1}{2}\int I_3, \quad \tilde{h}_2 - h_2 = \frac{1}{4}\int (-\eta I_1 + \tilde{\xi} I_2 + \nu I_3),$$

$$\tilde{h}_3 - h_3 = \frac{1}{8}\int ((-\tilde{\eta}\nu + \tilde{\eta}_x) I_1 + (\xi\nu + \xi_x) I_2 + (\xi\eta + \tilde{\xi}\tilde{\eta} - \nu^2) I_3), \tag{3.9}$$

$$\tilde{h}_4 - h_4 = \frac{1}{16}\int ((\xi\eta^2 - \tilde{\xi}\eta^2 - \xi\eta\tilde{\eta} + 2\tilde{\xi}\eta\tilde{\eta} + \tilde{\xi}\tilde{\eta}^2 - \eta\nu^2 + \nu\tilde{\eta}_x - \tilde{\eta}_{xx}) I_1 + (-\xi\tilde{\xi}\eta + \tilde{\xi}^2\eta - 2\tilde{\xi}^2\tilde{\eta} + \tilde{\xi}\nu^2$$
$$+ \nu\xi_x + \xi\nu_x + \tilde{\xi}\nu_x + \xi_{xx}) I_2 + (-\xi\eta\nu + \tilde{\xi}\eta\nu + \xi\tilde{\eta}\nu - \tilde{\xi}\tilde{\eta}\nu + \nu^3 + \eta\xi_x + \tilde{\eta}\xi_x - \xi\eta_x - \tilde{\xi}\eta_x) I_3),$$

We now present the consequences of the previous statements in terms of concrete differential algebras. From now on $(\mathcal{Q}, \partial_x)$ is a commutative differential algebra; so, the generators I_j in Eq. (3.6) induce maps

$$I_j(\,)\colon \mathcal{Q}^5 \to \mathcal{Q}, \quad (q,r,v,\tilde{q},\tilde{r}) \mapsto I_j(q,r,v,\tilde{q},\tilde{r}),$$
$$I_1(q,\ldots,\tilde{r}) := q_x - \tilde{q}_x + v(q+\tilde{q}), \quad I_2(q,\ldots,\tilde{r}) := r_x - \tilde{r}_x + v(r+\tilde{r}), \quad I_3(q,\ldots,\tilde{r}) := v_x + qr - \tilde{q}\tilde{r} \tag{3.10}$$

(here and in the sequel $\tilde{q}$, $\tilde{r}$ are simply names for certain elements of $\mathcal{Q}$, employed for obvious reasons).

Definition 3.3: Let $\mathcal{Q}^2 := \mathcal{Q} \times \mathcal{Q}$ *and consider the set* $2^{\mathcal{Q}^2}$ *of all subsets of* $\mathcal{Q}^2$. *The AKNS Bäcklund transformation for* $\mathcal{Q}$ *is the map*

$$B_{\mathrm{AKNS}}(\,) \equiv B(\,)\colon \mathcal{Q}^2 \to 2^{\mathcal{Q}^2}, \quad (q,r) \mapsto B(q,r),$$
$$B(q,r) := \{(\tilde{q},\tilde{r}) \in \mathcal{Q}^2 \mid \exists\, v \in \mathcal{Q} \text{ s.t. } I_j(q,r,v,\tilde{q},\tilde{r}) = 0 \text{ for } j = 1,2,3\}. \tag{3.11}$$

Proposition 3.4: Let $h \in \mathfrak{Z}$ *and consider its representation* $h(\,)\colon \mathcal{Q}^2 \to \mathbb{C}$. *For all* $(q,r) \in \mathcal{Q}^2$ *and* $(\tilde{q},\tilde{r}) \in B(q,r)$, *it is*

$$h(\tilde{q},\tilde{r}) = h(q,r). \tag{3.12}$$

Proof: From Proposition 3.2 we know that $\tilde{h} - h = \int I$ for some I in the Bäcklund ideal $\mathcal{I}$. So, using the representation $I(\,)\colon \mathcal{Q}^5 \to \mathcal{Q}$ we find

$$h(\tilde{q},\tilde{r}) - h(q,r) = \int I(q,r,v,\tilde{q},\tilde{r}) \quad \forall\, (q,r,v,\tilde{q},\tilde{r}) \in \mathcal{Q}^5. \tag{3.13}$$

On the other hand, by comparison with (3.7) we have

$$I(\,) = \sum_{j=1}^{3} F_j(\,) I_j(\,), \tag{3.14}$$

where $F_j(\,)\colon \mathcal{Q}^5 \to \mathcal{Q}$ are certain polynomial maps. In particular, let $\tilde{q},\tilde{r} \in B(q,r)$; if v is as in (3.11), we have $I_j(q,r,v,\tilde{q},\tilde{r}) = 0$ implying $I(q,r,v,\tilde{q},\tilde{r}) = 0$, and Eq. (3.13) gives $h(\tilde{q},\tilde{r}) - h(q,r) = 0$. ■

IV. PROOFS OF PROPOSITIONS 2.1 AND 2.2

From now on, $(\mathcal{Q}, \cdot_x, \int)$ is the differential algebra of formal Laurent series described in Sec. II. For convenience, we consider therein the differential subalgebra of "holomorphic series,"

$$\mathcal{Z} := \left\{ q \in \mathcal{Q} | q = \sum_{k=0}^{+\infty} q_k x^k \right\}. \tag{4.1}$$

Trivially, we have

Lemma 4.1: Consider any $h \in \int\mathfrak{F}$ and its representation $h(\,)\colon \mathcal{Q}^2 \to \mathbb{C}$; then

$$h(\,) \restriction \mathcal{Z}^2 = 0. \tag{4.2}$$

Proof: Write $h = \int H$. If $q,r \in \mathcal{Z}$, it is also $H(q,r) \in \mathcal{Z}^2$, because this is a polynomial in q,r and their derivatives. Thus, the residue $h(q,r) = \int H(q,r)$ is zero. ■

We consider the AKNS Bäcklund transformation $B(\,)\colon \mathcal{Q}^2 \to 2^{\mathcal{Q}^2}$ (see Definition 3.3); then, combining the previous lemma with the Bäcklund invariance of all the AKNS conserved functionals (Proposition 3.4) we obtain the following.

Proposition 4.2: Let $h \in \mathfrak{Z}_{\mathrm{AKNS}} \equiv \mathfrak{Z}$; then

$$h(\,) \restriction B(\mathcal{Z}^2) = 0, \quad B(\mathcal{Z}^2) := \bigcup_{(q,r)\in\mathcal{Z}^2} B(q,r). \tag{4.3}$$

We now fix the attention on the set of Laurent series appearing in the Treves theorem 2.1, i.e.,

$$\mathcal{T} := \left\{ \tilde{q},\tilde{r} \in \mathcal{Q}^2 | \tilde{q} = e^{\varphi}\left(\frac{1}{x} + \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\chi}_k x^k\right), \right.$$

$$\left. \tilde{r} = e^{-\varphi} \left(\frac{1}{x} - \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\rho}_k x^k\right) \ (\varphi,\alpha,\beta,\tilde{\chi}_k,\tilde{\rho}_k \in \mathbb{C}) \right\}. \tag{4.4}$$

Lemma 4.3: (i) Let $\tilde{q},\tilde{r}$ be as in Eq. (4.4). Then, there are uniquely determined series of the form

$$q = e^{\varphi}\left(-\alpha + \sum_{k=2}^{+\infty} \chi_k x^k\right), \quad r = e^{-\varphi}\left(\alpha + \sum_{k=2}^{+\infty} \rho_k x^k\right), \quad v = -\frac{1}{x} + 2\beta x + \sum_{k=2}^{+\infty} v_k x^k, \tag{4.5}$$

such that

$$I_j(q,r,v,\tilde{q},\tilde{r}) = 0 \quad (j = 1,2,3). \tag{4.6}$$

(ii) Statement (i) implies

$$\mathcal{T} \subset B(\mathcal{Z}^2). \tag{4.7}$$

Proof: (i) Let $q,\ldots,\tilde{r}$ be as in Eqs. (4.4) and (4.5), and set for brevity $I_j \equiv I_j(q,r,v,\tilde{q},\tilde{r})$. Direct computation gives

$$I_1 = e^{\varphi}\sum_{k=1}^{+\infty} J_{1k}x^k,\ \ I_2 = e^{-\varphi}\sum_{k=1}^{+\infty} J_{2k}x^k,\ \ I_3 = \sum_{k=1}^{+\infty} I_{3k}x^k, \tag{4.8}$$

$$J_{11} := \chi_2 - 3\tilde{\chi}_2 + v_2,\ \ J_{12} := 2\chi_3 - 4\tilde{\chi}_3 + 2\beta^2 + v_3,\ \ J_{13} := 3\chi_4 - 5\tilde{\chi}_4 + \beta(2\chi_2 + 2\tilde{\chi}_2 + v_2) + v_4,$$
$$J_{1k} := k\chi_{k+1} - (k+2)\tilde{\chi}_{k+1} + \beta(2\chi_{k-1} + 2\tilde{\chi}_{k-1} + v_{k-1}) + v_{k+1} + \sum_{\ell=2}^{k-2} v_{k-\ell}(\chi_\ell + \tilde{\chi}_\ell)\ \ (k \geqslant 4), \tag{4.9}$$

$$J_{21} := \rho_2 - 3\tilde{\rho}_2 + v_2,\ \ J_{22} := 2\rho_3 - 4\tilde{\rho}_3 + 2\beta^2 + v_3,\ \ J_{23} := 3\rho_4 - 5\tilde{\rho}_4 + \beta(2\rho_2 + 2\tilde{\rho}_2 + v_2) + v_4,$$
$$J_{2k} := k\rho_{k+1} - (k+2)\tilde{\rho}_{k+1} + \beta(2\rho_{k-1} + 2\tilde{\rho}_{k-1} + v_{k-1}) + v_{k+1} + \sum_{\ell=2}^{k-2} v_{k-\ell}(\rho_\ell + \tilde{\rho}_\ell)\ \ (k \geqslant 4), \tag{4.10}$$

$$I_{31} := 2v_2 - \tilde{\rho}_2 - \tilde{\chi}_2,\ I_{32} := 3v_3 - \alpha(\rho_2 - \chi_2 + \tilde{\rho}_2 - \tilde{\chi}_2) - \tilde{\rho}_3 - \tilde{\chi}_3 - \beta^2,$$
$$I_{33} := 4v_4 - \alpha(\rho_3 - \chi_3 + \tilde{\rho}_3 - \tilde{\chi}_3) - \tilde{\rho}_4 - \tilde{\chi}_4 - \beta(\tilde{\rho}_2 + \tilde{\chi}_2), \tag{4.11}$$

$$I_{3k} := (k+1)v_{k+1} - \alpha(\rho_k - \chi_k + \tilde{\rho}_k - \tilde{\chi}_k) - \tilde{\rho}_{k+1} - \tilde{\chi}_{k+1} - \beta(\tilde{\rho}_{k-1} + \tilde{\chi}_{k-1})$$
$$+ \sum_{\ell=2}^{k-2} (\chi_{k-\ell}\rho_\ell - \tilde{\chi}_{k-\ell}\tilde{\rho}_\ell)(k \geqslant 4).$$

We must show that the equations $J_{1k}=0$, $J_{2k}=0$, $I_{3k}=0$ for all $k\geqslant 1$ have uniquely determined solutions for the coefficients χ_k, ρ_k, v_k $(k\geqslant 2)$.

The proof is recursive; for $k=1,2,3,\ldots$, the equation $I_{3k}=0$ determines v_{k+1}, and inserting the result into $J_{2k}=0$, $J_{1k}=0$ one determines, respectively, ρ_{k+1} and χ_{k+1}.

(ii) Let $(\tilde{q},\tilde{r}) \in \mathcal{T}$, and q,r,v as in (i). It is clear that $(q,r) \in \mathcal{Z}^2$; Eq. (4.6) means $(\tilde{q},\tilde{r}) \in B(q,r)$. ■

Proof of the Treves theorem (Proposition 2.1): Set together Eqs. (4.3) and (4.7). ■

In a similar way we now prove Proposition 2.2, that concerns the set

$$\mathcal{S} := \left\{ \tilde{q},\tilde{r} \in \mathcal{Q}^2 | \tilde{q} = e^{\varphi}\left(\frac{2}{x^2} + \alpha + \beta x + \sum_{k=2}^{+\infty} \tilde{\chi}_k x^k\right), \right.$$
$$\left. \tilde{r} = e^{-\varphi}\ \left(1 + \beta x^3 + \sum_{k=4}^{+\infty} \tilde{\rho}_k x^k\right),\ (\varphi,\alpha,\beta,\tilde{\chi}_k,\tilde{\rho}_k \in \mathbb{C})\right\}; \tag{4.12}$$

everything relies on the following.

Lemma 4.4: (i) Let $\tilde{q},\tilde{r}$ be as in Eq. (4.12). Then, there are uniquely determined series of the form

$$q = e^{\varphi}\sum_{k=2}^{+\infty} \chi_k x^k,\ \ r = e^{-\varphi}\left(-1 + \sum_{k=3}^{+\infty} \rho_k x^k\right),\ \ v = -\frac{2}{x} + \alpha x + \sum_{k=2}^{+\infty} v_k x^k \tag{4.13}$$

such that $I_j(q,r,v,\tilde{q},\tilde{r})=0$ for $j=1,2,3$.

(ii) Statement (i) implies

$$\mathcal{S} \subset B(\mathcal{Z}^2). \tag{4.14}$$

Proof: (i) Let $q,\dots,\tilde{r}$ be as in Eqs. (4.12) and (4.13), and $I_j \equiv I_j(q,r,v,\tilde{q},\tilde{r})$. Then

$$I_1 = e^{\varphi}\sum_{k=0}^{+\infty} J_{1k}x^k,\ \ I_2 = e^{-\varphi}\sum_{k=2}^{+\infty} J_{2k}x^k,\ \ I_3 = x\sum_{k=0}^{+\infty} J_{3k}x^k, \tag{4.15}$$

$$J_{10} := 2v_2 - 3\beta,\ \ J_{11} := 2v_3 - 4\tilde{\chi}_2 + \alpha^2,\ \ J_{12} := \chi_3 + 2v_4 + \alpha v_2 - 5\tilde{\chi}_3 + \alpha\beta,$$

$$J_{13} := 2\chi_4 + 2v_5 + \alpha v_3 + \beta v_2 - 6\tilde{\chi}_4 + \alpha(\chi_2 + \tilde{\chi}_2), \tag{4.16}$$

$$J_{1k} := (k-1)\chi_{k+1} + 2v_{k+2} - (k+3)\tilde{\chi}_{k+1} + \alpha v_k + \beta v_{k-1} + \alpha(\chi_{k-1} + \tilde{\chi}_{k-1}) + \sum_{\ell=2}^{k-2} v_{k-\ell}(\chi_\ell + \tilde{\chi}_\ell)\ \ (k \geqslant 4),$$

$$J_{22} := \rho_3 - 5\beta,\ \ J_{23} := 2\rho_4 - 6\tilde{\rho}_4,\ \ J_{24} := 3\rho_5 + \alpha(\rho_3 + \beta) - 7\tilde{\rho}_5,$$

$$J_{25} := 4\rho_6 + v_2\rho_3 + \beta v_2 - 8\tilde{\rho}_6 + \alpha(\rho_4 + \tilde{\rho}_4), \tag{4.17}$$

$$J_{2k} := (k-1)\rho_{k+1} - (k+3)\tilde{\rho}_{k+1} + \beta v_{k-3} + \alpha(\rho_{k-1} + \tilde{\rho}_{k-1}) + \sum_{\ell=3}^{k-2} v_{k-\ell}\rho_\ell + \sum_{\ell=4}^{k-2} v_{k-\ell}\tilde{\rho}_\ell\ \ (k \geqslant 6),$$

$$J_{30} := 2v_2 - 3\beta,\ \ J_{31} := 3v_3 - \chi_2 - \tilde{\chi}_2 - 2\tilde{\rho}_4,\ \ J_{32} := 4v_4 - \chi_3 - \tilde{\chi}_3 - 2\tilde{\rho}_5 - \alpha\beta,$$

$$J_{33} := 5v_5 - \chi_4 - \tilde{\chi}_4 - 2\tilde{\rho}_6 - \alpha\tilde{\rho}_4 - \beta^2,\ \ J_{34} := 6v_6 - \chi_5 - \tilde{\chi}_5 - 2\tilde{\rho}_7 - \alpha\tilde{\rho}_5 - \beta\tilde{\rho}_4 + \chi_2\rho_3 - \tilde{\chi}_2\beta, \tag{4.18}$$

$$J_{3k} := (k+2)v_{k+2} - \chi_{k+1} - \tilde{\chi}_{k+1} - 2\tilde{\rho}_{k+3} - \alpha\tilde{\rho}_{k+1} - \beta\tilde{\chi}_{k-2} - \beta\tilde{\rho}_k + \sum_{\ell=3}^{k-1} \chi_{k+1-\ell}\rho_\ell - \sum_{\ell=4}^{k-1} \tilde{\chi}_{k+1-\ell}\tilde{\rho}_\ell\ \ (k \geqslant 5).$$

Again, we must show that the equations $J_{1k}=0$, $J_{2k}=0$, $J_{3k}=0$ for all k have uniquely determined solutions for the coefficients χ_k,ρ_k,v_k.

In fact, from $J_{10}=0$ and $J_{11}=0$ one uniquely determines v_2, v_3; now, the equation $J_{30}=0$ is automatically fulfilled, and $J_{31}=0$ gives χ_2. At this point, we must determine v_{k+2}, ρ_{k+1}, and χ_{k+1} for $k \geqslant 2$, which is performed recursively in the following way. From $J_{1k}=0$ and $J_{3k}=0$ one computes v_{k+2} and χ_{k+1}; to find them, one must solve a linear system whose matrix $\left(\begin{smallmatrix} 2 & k-1 \\ k+2 & -1 \end{smallmatrix}\right)$ has determinant $-k(k+1) \neq 0$. Finally, from $J_{2k}=0$ one gets ρ_{k+1}.

(ii) Let $(\tilde{q},\tilde{r}) \in \mathcal{S}$, and q,r,v as in (i). Then $(q,r) \in \mathcal{Z}^2$, and statement (i) means $(\tilde{q},\tilde{r}) \in B(q,r)$. ■

Proof of Proposition 2.2: Set together Eqs. (4.3) and (4.14). ■

Remark: In any case, the following holds:

$$(\tilde{q},\tilde{r}) \in B(\mathcal{Z}^2),\ \ \tilde{q} = \sum_{k=a}^{+\infty} \tilde{q}_k x^k,\ \tilde{q}_a \neq 0,\ \ \tilde{r} = \sum_{k=b}^{+\infty} \tilde{r}_k x^k,\ \tilde{r}_b \neq 0,\ \ \min(a,b) < 0 \Rightarrow a + b = -2,$$

$$\tilde{q}_a\tilde{r}_b = -\min(a,b). \tag{4.19}$$

In fact, we are assuming $I_j \equiv I_j(q,r,v,\tilde{q},\tilde{r}) = 0$ for some holomorphic $q,r \in \mathcal{Z}$ and $v \in \mathcal{Q}$. To fix the ideas, let us assume $\min(a,b)=a$; then, from $I_1=0$ we easily infer $v = \sum_{k=-1}^{+\infty} v_k x^k$ with $v_{-1}=a$.

Inserting these facts into $I_3=0$, we obtain $a+b=-2$ and $\tilde{q}_a\tilde{r}_b=-a$. If $\min(a,b)=b$ we proceed similarly, using the equations $I_2=0$ and $I_3=0$.

Of course, if $(\tilde{q},\tilde{r})$ are in the subsets $\mathcal{T}$ or $\mathcal{S}$ we have, respectively, $a=b=-1$ or $a=-2$, $b=0$.

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APPENDIX A: MATRIX LAX OPERATORS: THE DRINFELD–SOKOLOV FORMULATION

Some more algebra: Consider any differential algebra $(\mathcal{U},\partial_x\equiv\cdot_x)$, possibly noncommutative. Then, the algebra of *differential operators with coefficients* in $\mathcal{U}$ is the associative (and noncommutative) algebra $\mathrm{Diff}(\mathcal{U})$ with generators

$$\partial_x,\ U\ (U\in\mathcal{U}) \tag{A1}$$

and defining relations

$$\underbrace{UV}_{\text{product in Diff}(\mathcal{U})} = \underbrace{UV}_{\text{product in }\mathcal{U}}\ ,\qquad \underbrace{\partial_x U}_{\text{product in Diff}(\mathcal{U})} = U\partial_x + U_x \qquad (U,V\in\mathcal{U}). \tag{A2}$$

Any $D\in\mathrm{Diff}(\mathcal{U})$ has a representation

$$D=\sum_{k=0}^{d} D_k\partial_x^k\ (d\in\mathbb{N},D_k\in\mathcal{U}\ \forall\, k), \tag{A3}$$

which is unique under the condition $D_d\neq 0$ if $d\neq 0$; the unique integer d determined in this way is called the *order* of the differential operator D. $\mathcal{U}$ can be identified with the subalgebra of $\mathrm{Diff}(\mathcal{U})$ made of zero order operators; if $\mathcal{U}$ has unity 1, this is also the unity of $\mathrm{Diff}(\mathcal{U})$ (so, the invertible zero order operators are just the invertible elements of $\mathcal{U}$).

For any vector space $\mathcal{V}$, we introduce the vector space of $n\times n$ matrices

$$\mathrm{Mat}_n(\mathcal{V})=\{\mathsf{V}=(V_{ab})_{a,b=1,\ldots,n}|V_{ab}\in\mathcal{V}\ \forall\, a,b\}; \tag{A4}$$

we often consider therein the supplementary subspaces $\mathrm{Diag}_n(\mathcal{V})$, $\mathrm{Off}_n(\mathcal{V})$ made, respectively, by the diagonal and off-diagonal matrices.

If $(\mathcal{V},\partial_x)$ is a differential algebra, $\mathrm{Mat}_n(\mathcal{V})$ is a differential algebra when equipped with the usual "row by column" product and with the "term by term" derivation $\mathsf{V}\mapsto\mathsf{V}_x:=(V_{ab,x})$. Up to trivial identifications, we have $\int\mathrm{Mat}_n(\mathcal{V})=\mathrm{Mat}_n(\int\mathcal{V})$ and $\int\mathsf{V}=(\int V_{ab})$. Of course, $\mathrm{Diag}_n(\mathcal{V})$ is a differential subalgebra of $\mathrm{Mat}_n(\mathcal{V})$. If $\mathcal{I}$ is an ideal, or a differential (∂_x-closed) ideal in $\mathcal{V}$, the same occurs for $\mathrm{Mat}_n(\mathcal{I})$ in $\mathrm{Mat}_n(\mathcal{V})$.

Consider again a vector space, now denoted for convenience with $\mathcal{W}$. We can build from it the vector space of formal series in one indeterminate λ,

$$\mathcal{W}(\lambda):=\left\{W=\sum_{i=i_{min}}^{+\infty} W_i\lambda^{-i}|i_{\min}=i_{\min}(W)\in\mathbb{Z},W_i\in\mathcal{W}\,\forall\, i\right\}; \tag{A5}$$

we will often fix the attention on the subspaces,

$$\mathcal{W}(\lambda)_{\leqslant}:=\left\{\sum_{i=0}^{+\infty} W_i\lambda^{-i}\right\},\quad \mathcal{W}(\lambda)_{<}:=\left\{\sum_{i=1}^{+\infty} W_i\lambda^{-i}\right\}. \tag{A6}$$

If $\mathcal{W}$ is a differential algebra with derivation $\partial_x\equiv\cdot_x$, then $\mathcal{W}(\lambda)$ is a differential algebra, with the usual Cauchy product of series and the derivation $\partial_x\colon\ W\mapsto W_x:=\Sigma_i W_{i,x}\lambda^{-i}$. Of course, $\mathcal{W}$ can be identified with the differential subalgebra of $\mathcal{W}(\lambda)$ made of series W with $W_i=0$ for $i\neq 0$; $\mathcal{W}(\lambda)_{\leqslant}$, $\mathcal{W}(\lambda)_{<}$ are also differential subalgebras. If $\mathcal{W}$ has unity 1, this is also the unity of $\mathcal{W}(\lambda)$; the subset

$$1 + \mathcal{W}(\lambda)_< = \left\{ 1 + \sum_{i=1}^{+\infty} W_i \lambda^{-i} \right\} \tag{A7}$$

is a group with respect to the Cauchy product.

To conclude these preliminaries we point out that the notation [,], employed in the sequel for matrices or differential operators, stands for the usual commutator.

Drinfeld–Sokolov theory: Let us consider a commutative differential algebra $(\mathcal{F}, \partial_x)$; to fix the ideas, one can think $\mathcal{F}$ to be the algebra (1.9) with generators ξ_s $(s=1, \ldots, \gamma)$, but for the moment this is not necessary. For a given n, we construct from it the matrix differential algebra $\mathrm{Mat}_n(\mathcal{F})$. In the sequel, elements of $\int\mathcal{F}$ and $\mathrm{Mat}_n(\int\mathcal{F})$ will be called, respectively, the *scalar* and the $n \times n$ *matrix integrals, or functionals* of $\mathcal{F}$.

For technical reasons appearing in the sequel, we need the direct sum of this algebra and the $n \times n$ matrices with complex entries, i.e.,

$$\mathrm{Mat}_n(\mathcal{F}) \oplus \mathrm{Mat}_n(\mathbb{C}), \tag{A8}$$

which is in an obvious way an associative algebra [the product beween elements of $\mathrm{Mat}_n(\mathcal{F})$ and $\mathrm{Mat}_n(\mathbb{C})$ is defined again row by column]; this algebra contains $\mathrm{Mat}_n(\mathcal{F})$ as an ideal. The derivation ∂_x of $\mathrm{Mat}_n(\mathcal{F})$ is extended to the previous direct sum, prescribing that it annihilates $\mathrm{Mat}_n(\mathbb{C})$; in this way, (A8) is a differential algebra and $\mathrm{Mat}_n(\mathcal{F})$ a differential ideal of it. Of course the unity of (A8) is $\mathsf{1} := \mathrm{diag}_n(1, \ldots, 1)$.

The next step is to form the differential algebra of formal series

$$(\mathrm{Mat}_n(\mathcal{F}) \oplus \mathrm{Mat}_n(\mathbb{C}))(\lambda) := \left\{ \mathsf{N} = \sum_{i=i_{\min}}^{+\infty} \mathsf{N}_i \lambda^{-i} \,|\, i_{\min} \in \mathbb{Z}, \mathsf{N}_i \in \mathrm{Mat}_n(\mathcal{F}) \oplus \mathrm{Mat}_n(\mathbb{C}) \ \forall\, i \right\} \tag{A9}$$

[which of course contains the differential ideal $\mathrm{Mat}_n(\mathcal{F})(\lambda)$, made of series as above with coefficients $\mathsf{N}_i \in \mathrm{Mat}_n(\mathcal{F})$]. The ultimate step is the algebra

$$\mathfrak{D}_n(\mathcal{F}) := \mathrm{Diff}((\mathrm{Mat}_n(\mathcal{F}) \oplus \mathrm{Mat}_n(\mathbb{C}))(\lambda)), \tag{A10}$$

made of differential operators with coefficients in the algebra (A9).

Definition A.1: A first order, $n \times n$ Lax operator is a differential operator of the form

$$\mathsf{L} \equiv \mathsf{L}_{\mathsf{A},\mathsf{S}} := \partial_x - \lambda \mathsf{A} - \mathsf{S} \in \mathfrak{D}_n(\mathcal{F}),$$
$$\mathsf{S} \in \mathrm{Mat}_n(\mathcal{F}), \ \mathsf{A} = \mathrm{diag}(a_1, \ldots, a_n) \in \mathrm{Diag}_n(\mathbb{C}), \ a_i \neq 0 \text{ for all } i, a_i \neq a_j \text{ for } i \neq j. \tag{A.11}$$

We will write $\mathfrak{L}_n(\mathcal{F})$ for the set of these operators.

The first result in the Drinfeld–Sokolov theory is a diagonalization theorem for these operators.

Proposition A.2: Consider an operator $\mathsf{L} = \mathsf{L}_{\mathsf{A},\mathsf{S}} \in \mathfrak{L}_n(\mathcal{F})$. Then, there is a pair of objects

$$\mathsf{U} = 1 + \sum_{i=1}^{+\infty} \mathsf{U}_i \lambda^{-i} \in 1 + \mathrm{Mat}_n(\mathcal{F})(\lambda)_<, \tag{A12}$$

$$\mathsf{H} = \sum_{i=0}^{+\infty} \mathsf{H}_i \lambda^{-i} \in \mathrm{Diag}_n(\mathcal{F})(\lambda)_\leqslant, \tag{A13}$$

such that

$$\mathsf{L} = \mathsf{U}(\partial_x - \lambda \mathsf{A} - \mathsf{H})\mathsf{U}^{-1}; \tag{A14}$$

moreover, the matrix functionals

$$\mathsf{h}_{\mathsf{L},i} \equiv \mathsf{h}_i := \int \mathsf{H}_i \quad (i = 0,1,2,\dots) \tag{A15}$$

are uniquely determined by L.

Proof: See Sec. I of Ref. 5. The main point is that Eq. (A14) is equivalent to $\mathsf{LU}=\mathsf{U}(\partial_x - \lambda\mathsf{A}-\mathsf{H})$, and that the expansion in powers of λ of both sides in this equality gives rise to recursion equations for the sequences (H_i), (U_i). ■

Definition A.3: Any pair (U,H) *as in Proposition A.2 will be called a diagonalizing pair for* L. *The matrix functionals* $\mathsf{h}_{\mathsf{L},i}$ *will be called the fundamental invariants of* L.

Remark: Suppose $(\mathcal{F},\partial_x)$ is a strict differential subalgebra of a commutative differential algebra $(\mathcal{M},\partial_x)$ [Eq. (1.8); recall that $\int\mathcal{F}\simeq\int^{\mathcal{M}}\mathcal{F}\subset\int\mathcal{M}$]. Then, by the uniqueness statement of the previous proposition, the diagonalizations of L as an element of $\mathfrak{L}_n(\mathcal{F})$, or as an element of $\mathfrak{L}_n(\mathcal{M})$, give rise to the same fundamental invariants which belong in any case to $\mathrm{Diag}_n(\int\mathcal{F})$.

The forthcoming proposition considers a situation of this kind; the result stated therein clarifies the origin of the term "invariant" for the functionals h_i.

Proposition A.4: Let $(\mathcal{M},\partial_x)$ *be a commutative differential algebra containing* $\mathcal{F}$ *as a strict differential subalgebra; further, let* $\widetilde{\mathcal{F}}$ *denote another strict differential subalgebra of* $\mathcal{M}$.

Consider two operators

$$\mathsf{L} = \mathsf{L}_{\mathsf{A},\mathsf{S}} \in \mathfrak{L}_n(\mathcal{F}),\ \widetilde{\mathsf{L}} = \mathsf{L}_{\mathsf{A},\widetilde{\mathsf{S}}} \in \mathfrak{L}_n(\widetilde{\mathcal{F}}) \tag{A16}$$

(*with the same* A) *and their fundamental invariants* $\mathsf{h}_{\mathsf{L},i}\equiv\mathsf{h}_i \in \mathrm{Diag}_n(\int\mathcal{F})$, $\mathsf{h}_{\widetilde{\mathsf{L}},i}\equiv\widetilde{\mathsf{h}}_i \in \mathrm{Diag}_n(\int\widetilde{\mathcal{F}})$.

Let $\mathcal{I}$ *denote an ideal of* $\mathcal{M}$, *and assume there is*

$$\mathsf{V} = 1 + \sum_{i=1}^{+\infty} \mathsf{V}_i\lambda^{-i} \in 1 + \mathrm{Mat}_n(\mathcal{M})(\lambda)_< \tag{A17}$$

such that

$$\widetilde{\mathsf{L}} - \mathsf{VLV}^{-1} \in \mathrm{Mat}_n(\mathcal{I})(\lambda)_{\leqslant}. \tag{A18}$$

Then

$$\widetilde{\mathsf{h}}_i - \mathsf{h}_i \in \mathrm{Diag}_n\left(\int\mathcal{I}\right) \quad (i = 0,1,2,\dots) \tag{A19}$$

(*where, in the last equation,* $\int\equiv\int^{\mathcal{M}}$).

In a few words, if $\mathsf{L},\widetilde{\mathsf{L}}$ are similar up to a series with coefficients in the ideal $\mathrm{Mat}_n(\mathcal{I})$, their fundamental invariants coincide up to elements of $\mathrm{Diag}_n(\int\mathcal{I})$. This result is essential for our purposes; since our language is slightly different from the one of Ref. 5, it is convenient to report the following.

Proof of Proposition A.4: We choose a diagonalizing pair (U,H) for L, so as to fulfill Eqs. (A12)–(A14), and proceed in three steps.

Step 1: There are

$$\mathsf{W} \in 1 + \mathrm{Mat}_n(\mathcal{M})(\lambda)_<,\ \mathsf{J} \in \mathrm{Mat}_n(\mathcal{I})(\lambda)_{\leqslant}\ \textit{such that}\ \widetilde{\mathsf{L}} = \mathsf{W}(\partial_x - \lambda\mathsf{A} - \mathsf{H} - \mathsf{J})\mathsf{W}^{-1}. \tag{A20}$$

In fact, assumption (A18) means $\widetilde{\mathsf{L}}=\mathsf{VLV}^{-1}+\mathsf{F}$, where $\mathsf{F}\in\mathrm{Mat}_n(\mathcal{I})(\lambda)_{\leqslant}$; from here and (A14) we get

$$\widetilde{\mathsf{L}} = \mathsf{VU}(\partial_x - \lambda\mathsf{A} - \mathsf{H})\mathsf{U}^{-1}\mathsf{V}^{-1} + \mathsf{F} = \mathsf{VU}(\partial_x - \lambda\mathsf{A} - \mathsf{H} + \mathsf{U}^{-1}\mathsf{V}^{-1}\mathsf{FVU})\mathsf{U}^{-1}\mathsf{V}^{-1}; \tag{A21}$$

this gives the thesis (A20), with $\mathsf{W}:=\mathsf{VU}$ and $\mathsf{J}:=-\mathsf{U}^{-1}\mathsf{FVU}$ [the relations $\mathsf{W}\in 1+\mathrm{Mat}_n(\mathcal{M})\times(\lambda)_<$, $\mathsf{J}\in\mathrm{Mat}_n(\mathcal{I})(\lambda)_{\leqslant}$ are easily checked from the previous definitions recalling that 1

$+\mathrm{Mat}_n(\mathcal{M})(\lambda)_<$ is a group, $\mathrm{Mat}_n(\mathcal{M})(\lambda)_\leqslant$ a subalgebra and $\mathrm{Mat}_n(\mathcal{I})$ an ideal].

Step 2: Consider the differential ideal $\mathcal{G}$ of $\mathcal{M}$ generated by $\mathcal{I}$ (i.e., the smallest differential ideal containing $\mathcal{I}$). Then $\tilde{\mathsf{L}}$, as an element of $\mathfrak{L}_n(\mathcal{M})$, admits a diagonalizing pair $(\tilde{\mathsf{U}},\tilde{\mathsf{H}})$ with $\tilde{\mathsf{H}}$ of the form

$$\tilde{\mathsf{H}} = \mathsf{H} + \mathsf{G},\ \ \mathsf{G} \in \mathrm{Diag}_n(\mathcal{G})(\lambda)_\leqslant. \tag{A22}$$

To prove this, we write

$$\tilde{\mathsf{U}} = \mathsf{W}\mathsf{Z},\ \ \mathsf{W} \text{ as in step 1, } \mathsf{Z} = 1 + \sum_{i=1}^{+\infty} \mathsf{Z}_i \lambda^{-i} \in 1 + \mathrm{Off}_n(\mathcal{G})(\lambda)_< \text{ to be found,} \tag{A23}$$

$$\tilde{\mathsf{H}} = \mathsf{H} + \mathsf{G} = \sum_{i=0}^{+\infty} (\mathsf{H}_i + \mathsf{G}_i)\lambda^{-i},\ \ \mathsf{G}_i \in \mathrm{Diag}_n(\mathcal{G}) \text{ to be found} \tag{A24}$$

(recall that Off_n stands for the the off-diagonal $n\times n$ matrices). Due to these representations and to Eq. (A20) for $\tilde{\mathsf{L}}$, the diagonalizing condition $\tilde{\mathsf{L}} = \tilde{\mathsf{U}}(\partial_x - \lambda\mathsf{A} - \tilde{\mathsf{H}})\tilde{\mathsf{U}}^{-1}$ is fulfilled if

$$(\partial_x - \lambda\mathsf{A} - \mathsf{H} - \mathsf{J})\mathsf{Z} = \mathsf{Z}(\partial_x - \lambda\mathsf{A} - \mathsf{H} - \mathsf{G}). \tag{A25}$$

Recalling that $\partial_x \mathsf{Z} = \mathsf{Z}\partial_x + \mathsf{Z}_x$ and expanding the last equation in powers of λ, we see that (A25) is fulfilled if

$$-\mathsf{G}_i + [\mathsf{A},\mathsf{Z}_{i+1}] = \mathsf{Z}_{i,x} - \mathsf{J}_i + \sum_{k=1}^{i} ([\mathsf{Z}_k,\mathsf{H}_{i-k}] + \mathsf{Z}_k\mathsf{G}_{i-k} - \mathsf{J}_{i-k}\mathsf{Z}_k)\ \ (i = 0,1,2,\dots) \tag{A26}$$

[intending $\mathsf{Z}_{0,x} := (1)_x = 0$ and $\Sigma_{k=1}^{0} := 0$]. We will show that the system (A26) can be solved recursively. To this purpose, we introduce the projections $\mathcal{D}_n, \mathcal{O}_n$ of $\mathrm{Mat}_n(\mathcal{M})$ onto the supplementary subspaces $\mathrm{Diag}_n(\mathcal{M})$, $\mathrm{Off}_n(\mathcal{M})$; furthermore, recalling that A is diagonal with nonzero and all different eigenvalues, we infer that $\mathrm{ad}_\mathsf{A} := [\mathsf{A},\cdot]$: $\mathrm{Off}_n(\mathcal{M}) \to \mathrm{Off}_n(\mathcal{M})$ is a linear isomorphism. These remarks yield for (A26) the solution

$$\mathsf{G}_i = \mathcal{D}_n\left(\mathsf{J}_i - \sum_{k=1}^{i} (\mathsf{Z}_k\mathsf{G}_{i-k} - \mathsf{J}_{i-k}\mathsf{Z}_k)\right), \tag{A27}$$

$$\mathsf{Z}_{i+1} = ad_\mathsf{A}^{-1}\left(\mathsf{Z}_{ix} - \mathcal{O}_n(\mathsf{J}_i) + \sum_{k=1}^{i} [\mathsf{Z}_k,\mathsf{H}_{i-k}] + \sum_{k=1}^{i} \mathcal{O}_n(\mathsf{Z}_k\mathsf{G}_{i-k} - \mathsf{J}_{i-k}\mathsf{Z}_k)\right)\ (i = 0,1,2,\dots)$$

(note that $[\mathsf{Z}_k,\mathsf{H}_{i-k}]$ is purely off-diagonal). From these equations, with $i=0$, one gets $\mathsf{G}_0 = \mathcal{D}_n(\mathsf{J}_0)$, $\mathsf{Z}_1 = -\mathrm{ad}_\mathsf{A}^{-1}\mathcal{O}_n(\mathsf{J}_0)$; subsequently, one uses recursively Eqs. (A27) to determine at each step $\mathsf{G}_i, \mathsf{Z}_{i+1}$. The fact that $\mathrm{Mat}_n(\mathcal{G})$ is a differential ideal and the structure of the above equations also make evident that $\mathsf{G}_i, \mathsf{Z}_{i+1}$ belong to $\mathrm{Mat}_n(\mathcal{G})$ for all i; by construction these matrices are, respectively, diagonal and off-diagonal as required.

Step 3: Conclusion of the proof. Let us intend $\int \equiv \int^{\mathcal{M}}$ (recalling the remark on $\int\mathcal{F}$ just before the statement of this proposition, and the analogous one for $\int\tilde{\mathcal{F}}$). Equation (A22) implies

$$\tilde{\mathsf{h}}_i - \mathsf{h}_i = \int \tilde{\mathsf{H}}_i - \int \mathsf{H}_i = \int \mathsf{G}_i \in \mathrm{Diag}_n\left(\int \mathcal{G}\right); \tag{A28}$$

the thesis (A19) follows from here, and from the remark that

$$\int \mathcal{G} = \int \mathcal{I}. \tag{A29}$$

To prove Eq. (A29), we note that any element of the differential ideal $\mathcal{G}$ has the form

$$G = \sum_{\ell \in \Lambda} F_\ell I_\ell^{(\sigma_\ell)} \ (\Lambda \text{ a finite set}, \ F_\ell \in \mathcal{M}, I_\ell \in \mathcal{I}, \sigma_\ell \in \mathbb{N} \ \ \forall\, \ell \in \Lambda), \tag{A30}$$

where $\cdot^{(\sigma_\ell)}$ indicates the σ_ℓth power of the derivation $\cdot_x$. Now, standard integration by parts gives

$$\int G = \int I, \ \ I := \sum_{\ell \in \Lambda} (-1)^{\sigma_\ell} F_\ell^{(\sigma_\ell)} I_\ell \in \mathcal{I}. \tag{A31}$$

■

We now review some known relations between Lax operators, their diagonalization and evolutionary problems. From now on, we work with the Gelfand–Dickey differential algebra,

$$\mathfrak{F} = \mathbb{C}[\xi_1, \dots, \xi_\gamma, \xi_{1,x}, \dots, \xi_{\gamma,x}, \dots]_0 \tag{A32}$$

[see Eq. (1.9)]. Also, we are given a vector field $X = (X_1, \dots, X_\gamma) \in \mathfrak{F}^\gamma$; as explained in Sec. I, there are Lie derivative operators $\mathcal{L}_X: \mathfrak{F} \to \mathfrak{F}$ and $\mathcal{L}_X: \int\mathfrak{F} \to \int\mathfrak{F}$ [see Eqs. (1.17) and (1.18)]; these induce "componentwisely" maps $\mathcal{L}_X$ of $\mathrm{Mat}_n(\mathfrak{F})$ or $\mathrm{Mat}_n(\int\mathfrak{F})$ into itself. Trivially, $\mathcal{L}_X$ can be extended to a map of $\mathrm{Mat}_n(\mathfrak{F}) \oplus \mathrm{Mat}_n(\mathbb{C})$ into itself, defining it to be zero on $\mathrm{Mat}_n(\mathbb{C})$.

Again trivially, we extend the Lie derivative to a map $\mathcal{L}_X$ of $[\mathrm{Mat}_n(\mathfrak{F}) \oplus \mathrm{Mat}_n(\mathbb{C})](\lambda)$ into itself, setting $\mathcal{L}_X(\Sigma_i \mathsf{N}_i \lambda^{-i}) := \Sigma_i (\mathcal{L}_X \mathsf{N}_i)\lambda^{-i}$; we finally define $\mathcal{L}_X: \mathfrak{D}_n(\mathfrak{F}) \to \mathsf{D}_n(F)$ by $\mathcal{L}_X(\Sigma_k \mathsf{D}_k \partial_x^k) := \Sigma_k (\mathcal{L}_X \mathsf{D}_k)\partial_x^k$.

Definition A.5: X is said to admit an $n \times n$ Lax formulation if there are an operator $\mathsf{L} = \mathsf{L}_{\mathsf{A},\mathsf{S}} \in \mathfrak{L}_n(\mathfrak{F}) \subset \mathfrak{D}_n(\mathfrak{F})$ and a zero-order operator $\mathsf{C} \in \mathrm{Mat}_n(\mathfrak{F})(\lambda) \subset \mathfrak{D}_n(\mathfrak{F})$ such that

$$\mathcal{L}_X \mathsf{L} = [\mathsf{L}, \mathsf{C}]. \tag{A33}$$

Proposition A.6: If X is admits a Lax formulation as above, the fundamental invariants $\mathsf{h}_{\mathsf{L},i} \equiv \mathsf{h}_i$ $(i = 0, 1, 2, \dots)$ are conserved matrix functionals for X,

$$\mathcal{L}_X \mathsf{h}_i = 0. \tag{A34}$$

Proof: Reference 5, Sec. I. ■

Of course, from here we get conserved scalar functionals taking all matrix elements $h_{i,ab} \in \int\mathfrak{F}$.

APPENDIX B: LAX FORMALISM AND BÄCKLUND TRANSFORMATIONS FOR THE AKNS THEORY

As in Sec. III, we consider the differential algebra,

$$\mathfrak{F} = \mathbb{C}[\xi, \eta, \xi_x, \eta_x, \dots], \tag{B1}$$

with two generators ξ, η, and the vector field $X_{\mathrm{AKNS}} \equiv X$. This is known to admit a Lax formulation of the type (A33), with $n = 2$; the matrices S, A of L, and the matrix C are given by

$$\mathsf{S} := \begin{pmatrix} 0 & \xi \\ \eta & 0 \end{pmatrix}, \ \ \mathsf{A} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ \ \mathsf{C} := \frac{1}{2}\begin{pmatrix} -\xi\eta & \xi_x \\ -\eta_x & \xi\eta \end{pmatrix} + \lambda \mathsf{S} + \lambda^2 \mathsf{A}. \tag{B2}$$

This operator has a diagonalizing pair $\mathsf{U} = 1 + \mathsf{U}_1/\lambda + \mathsf{U}_2/\lambda^2 + \mathsf{U}_3/\lambda^3 + \cdots$, $\mathsf{H} = \mathsf{H}_0 + \mathsf{H}_1/\lambda + \mathsf{H}_2/\lambda^2 + \mathsf{H}_3/\lambda^3 + \cdots$, where

$$\mathsf{U}_1 = \frac{1}{2}\begin{pmatrix} 0 & -\xi \\ \eta & 0 \end{pmatrix}, \ \ \mathsf{U}_2 = \frac{1}{4}\begin{pmatrix} 0 & -\xi_x \\ -\eta_x & 0 \end{pmatrix}, \tag{B3}$$

$$\mathsf{U}_3 = \frac{1}{8}\begin{pmatrix} 0 & -\xi_{xx} + \xi^2\eta \\ \eta_{xx} - \xi\eta^2 & 0 \end{pmatrix} \cdots,$$

$$\mathsf{H}_0 = 0,\ \mathsf{H}_1 = \frac{1}{2}\begin{pmatrix} \xi\eta & 0 \\ 0 & -\xi\eta \end{pmatrix},\ \mathsf{H}_2 = -\frac{1}{4}\begin{pmatrix} \xi\eta_x & 0 \\ 0 & \eta\xi_x \end{pmatrix},\ \mathsf{H}_3 = \frac{1}{8}\begin{pmatrix} \xi\eta_{xx} - \xi^2\eta^2 & 0 \\ 0 & -\eta\xi_{xx} + \xi^2\eta^2 \end{pmatrix},$$

$$\mathsf{H}_4 := \frac{1}{16}\begin{pmatrix} -\xi\eta_{xxx} + \xi\xi_x\eta^2 + 4\xi^2\eta\eta_x & 0 \\ 0 & -\eta\xi_{xxx} + \eta\eta_x\xi^2 + 4\eta^2\xi\xi_x \end{pmatrix}, \ldots. \tag{B4}$$

The fundamental invariants $\mathsf{h}_i := \int \mathsf{H}_i$ are conserved functionals for X; for all i, the diagonal elements of H_i are opposite up to total derivatives, so that

$$\mathsf{h}_i \equiv \mathsf{h}_{\mathrm{L},i} = \begin{pmatrix} h_i & 0 \\ 0 & -h_i \end{pmatrix}. \tag{B5}$$

For $i=1,2,3,4$, the conserved scalar functionals $h_i \in \int\mathfrak{F}$ are the ones appearing in Eq. (1.23).

Up to a rescaling of each element by a suitable constant, the sequence $(h_i)_{i=1,2,\ldots}$ can be identified with the basis of $\mathfrak{Z}_{\mathrm{AKNS}} \equiv \mathfrak{Z}$ considered in Ref. 11. [The basis in Ref. 11 is not defined via the Lax formalism but, rather, by a precise formulation of the known bi-Hamiltonian recursion scheme for the AKNS;[6] the fact that the functionals (h_i) fulfill this recursion scheme reflect a general feature of the Drinfeld–Sokolov approach: see again Ref. 5, Sec. I where a general construction is given for the bi-Hamiltonian structure of the evolution equations arising from matrix first order Lax operators.]

We come to the Bäcklund transformation. Let us recall the formalism of Sec. III; this involves the "initial variables" ξ,η generating $\mathfrak{F}$, the "final variables" $\tilde{\xi},\tilde{\eta}$ generating $\tilde{\mathfrak{F}}$, and the "auxiliary variable" ν generating with all of the previous ones in differential algebra $\mathfrak{M}$ [see Eq. (3.3)]. Of course, the "tilde" map $\tilde{}: \mathfrak{F} \to \tilde{\mathfrak{F}}$ induces componentwise a tilde map $\tilde{}: \mathrm{Mat}_n(\mathfrak{F}) \to \mathrm{Mat}_n(\tilde{\mathfrak{F}})$; the inclusions $\mathfrak{F}, \tilde{\mathfrak{F}} \subset \mathfrak{M}$ induce inclusions of the corresponding spaces of matrices, formal series in λ and differential operators. In particular, we fix the attention on the Lax operators,

$$\mathsf{L}_{\mathsf{A},\mathsf{S}} \equiv \mathsf{L} \in \mathfrak{D}_2(\mathfrak{F}) \subset \mathfrak{D}_2(\mathfrak{M}),\ \mathsf{L}_{\mathsf{A},\tilde{\mathsf{S}}} \equiv \tilde{\mathsf{L}} \in \mathfrak{D}_2(\tilde{\mathfrak{F}}) \subset \mathfrak{D}_2(\mathfrak{M}) \tag{B6}$$

[A,S as in Eq. (B2); as stipulated before, $\tilde{\mathsf{S}}$ means $\left(\begin{smallmatrix} 0 & \tilde{\xi} \\ \tilde{\eta} & 0 \end{smallmatrix}\right)$].

Lemma B.1: Let

$$\mathsf{V} := 1 + \frac{1}{2\lambda}\begin{pmatrix} \nu & \xi - \tilde{\xi} \\ \tilde{\eta} - \eta & -\nu \end{pmatrix}. \tag{B7}$$

Then

$$\tilde{\mathsf{L}} - \mathsf{V}\mathsf{L}\mathsf{V}^{-1} \in \mathrm{Mat}_2(\mathcal{I})(\lambda)_<, \tag{B8}$$

where $\mathcal{I}$ is the Bäcklund ideal of Definition 3.1.

Proof: One finds by direct computation that

$$\tilde{\mathsf{L}}\mathsf{V} - \mathsf{V}\mathsf{L} = \mathsf{V}_x - \tilde{\mathsf{S}}\mathsf{V} + \mathsf{V}\mathsf{S} - \lambda[\mathsf{A},\mathsf{V}] = \mathsf{I},\ \mathsf{I} := \frac{1}{2\lambda}\begin{pmatrix} I_3 & I_1 \\ -I_2 & -I_3 \end{pmatrix}, \tag{B9}$$

where I_j $(j=1,2,3)$ are the generators (3.6) of the Bäcklund ideal. This implies $\tilde{\mathsf{L}} - \mathsf{V}\mathsf{L}\mathsf{V}^{-1} = \mathsf{F}$, where $\mathsf{F} := \mathsf{I}\mathsf{V}^{-1} \in \mathrm{Mat}_2(\mathcal{I})(\lambda)_<$. ■

The previous lemma allows to give the following.

Proof of Proposition 3.2: The vector space $\mathfrak{Z}$ is generated by the sequence (h_i), so it suffices to prove that

$$\tilde{h}_i - h_i \in \int \mathcal{I} \quad (i = 1,2,3, \ldots). \tag{B10}$$

From Eq. (B5) and its tilded analogue, we know that

$$\begin{pmatrix} h_i & 0 \\ 0 & -h_i \end{pmatrix}, \quad \begin{pmatrix} \tilde{h}_i & 0 \\ 0 & -\tilde{h}_i \end{pmatrix} \tag{B11}$$

are the invariant matrix functionals of L and $\tilde{\mathsf{L}}$, respectively; by Proposition A.4 and Lemma B.1, these differ by elements of $\mathrm{Diag}_2(\int \mathcal{I})$, yielding the thesis. ■

As an example, in Eq. (3.9) we have given explicit representations of $\tilde{h}_i - h_i$ as integrals of elements of $\mathcal{I}$, for $i=1,2,3,4$; these representations have been computed specializing to this case the general argument employed to prove Proposition (A4). In particular, this has required the application of the recursion relations (A27) up to $i=4$.

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Angular intricacies in hot gauge field theories

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It is argued that in hot quantum field theories, "hard thermal loops" leading order calculations call for a definite sequence of angular averages and discontinuity (or imaginary part prescription) operations, and run otherwise into incorrect results. The 10 years old collinear singularity problem of hot QCD provides a dramatic illustration of that fate. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The intrinsic nonperturbative nature of nonzero temperature quantum field theories has long been recognized.[1] Naive thermal perturbation theory can nevertheless be devised, both in imaginary and real time formalisms,[2] but then, it promptly appears that, under certain circumstances, the original perturbative series must be reorganized. Such an example of reorganization is provided by the so-called *resummation program*.[3] This program, RP for short, is a resummation scheme of the leading order thermal fluctuations which, in the literature, are known under the spell of hard thermal loops. Whenever one is calculating a physical process related to thermal Green's functions whose external/internal legs are *soft*, it is mandatory to trade the naive thermal perturbation theory for the RP. The softness alluded to above, refers to momenta on the order of the soft scale gT, where T, the temperature, stands for the hard scale and g for any relevant (bare/renormalized) and small enough coupling constant.

The RP which has been set up in order to remedy an obvious lack of completeness of the naive thermal perturbation theory, has produced interesting results, but has also met serious obstructions in the infrared regime of the theories.[4,5] Within the resummation program itself, the solutions proposed so far,[5–7] however interesting in their own respect, can hardly be organized in a systematic way and display too much dependences on the process under consideration.

In this paper, we point out some overlooked aspects concerning "the historical derivations" of the famous RP *collinear singularity problem of hot* QCD.[5] The matter of the present paper has to do with the proper sequence of two operations that are of the utmost importance in the calculational context of hot quantum field theories. These operations are an angular average, on the one hand, and a discontinuity or imaginary part prescription, on the other hand. Though illustrated on the famous problem alluded to above, the point made here is relevant of a most universal property of hot quantum fields, because at $n \geqslant 3$, the hot gauge fields effective vertices are all defined by angular averages. As several of our previous and ongoing calculations have displayed, in effect, the pertinence of the advocated "proper sequence" extends far beyond the historical derivations to be recalled shortly.

The paper is organized as follows. Section II is a short reminder of the collinear singularity problem met in hot QCD, a more detailed introduction to the matter being given in Sec. II of Ref. 8. In Sec. III, we demonstrate that illicit mathematical steps have been taken, plaguing either of the

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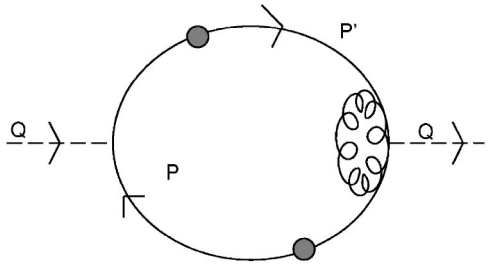

FIG. 1. A graph denoted by ($\star$, $\star$; 1) in the text, with two internal effective propagators ${}^{\star}S_{\alpha}(P(P'))$, of Eq. (2.2), depicted with a blob, and one HTL vertex correction $\Gamma_{\mu}^{\mathrm{HTL}}$ of Eq. (2.5), the other bare, γ_{μ}.

two distinct collinear problem historical derivations. Our conclusions are summarized in Sec. IV, whereas an appendix gathers the important calculational details of Sec. III.

Throughout the paper, we will be using the convention of upper case letters for quadrimomenta and lower case ones for their components, writing, for example, $P=(p_0,\vec{p})$. Our conventions for labelling internal and external momenta can be read off Fig. 1.

II. THE COLLINEAR SINGULARITY PROBLEM OF HOT QCD

This 10 years old issue is the following. The soft real photon emission rate out of a quark-gluon plasma in thermal equilibrium involves, in particular, the calculation of the quantity

$$\Pi_R(Q) = i\int \frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\mathrm{disc}_P\mathrm{Tr}\left\{{}^{\star}S_R(P){}^{\star}\Gamma_{\mu}(P_R,Q_R,-P'_A){}^{\star}S_R(P'){}^{\star}\Gamma^{\mu}(P_R,Q_R,-P'_A)\right\}. \tag{2.1}$$

The discontinuity is to be taken in the energy variable p_0, by forming the difference of R and A-indiced P-dependent quantities, and within standard notations, fermionic high-temperature limit (HTL) self-energies, effective propagators, and vertices are, respectively, given by

$${}^{\star}S_{\alpha}(P) = \frac{i}{\not{P} - \Sigma_{\alpha}(P) + i\epsilon_{\alpha}p_0}, \quad \alpha = R,A, \quad \epsilon_R = -\epsilon_A = \epsilon, \tag{2.2}$$

$$\Sigma_{\alpha}(P) = m^2\int \frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{\not{K}}}{\hat{K}\cdot P + i\epsilon_{\alpha}}, \quad m^2 = C_F\frac{g^2T^2}{8}, \tag{2.3}$$

$${}^{\star}\Gamma_{\mu}(P_{\alpha},Q_{\beta},P'_{\delta}) = -ie(\gamma_{\mu} + \Gamma_{\mu}^{\mathrm{HTL}}(P_{\alpha},Q_{\beta},P'_{\delta})), \tag{2.4}$$

$$\Gamma_{\mu}^{\mathrm{HTL}}(P_{\alpha},Q_{\beta},P'_{\delta}) = m^2\int \frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{k}_{\mu}\hat{\not{K}}}{(\hat{K}\cdot P + i\epsilon_{\alpha})(\hat{K}\cdot P' + i\epsilon_{\delta})}, \tag{2.5}$$

where $\hat{K}$ is the lightlike four vector $(1,\hat{k})$. As (2.4) is plugged into (2.1), four terms come about, three of them proportional to a collinear singularity. These singular terms are the two terms with one bare vertex γ_{μ}, the other $\Gamma_{\mu}^{\mathrm{HTL}}$, plus the term including two HTL vertices, $\Gamma_{\mu}^{\mathrm{HTL}}$. Thanks to an Abelian Ward identity peculiar to the high temperature limit, a partial cancellation of these collinear singularities occurs, but out of the term including two $\Gamma_{\mu}^{\mathrm{HTL}}$ vertices, a collinear singularity remains,

$$-2i\frac{e^2m^2}{q^2}\left(\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{1}{\hat{Q}\cdot\hat{K}+i\epsilon}\right)\int\frac{\mathrm{d}^4P}{(2\pi)^3}\delta(P\cdot\hat{Q})(1-2n_F(p_0))[\mathrm{Tr}(^\star S_A(P)\hat{\not{Q}})-\mathrm{Tr}(^\star S_R(P')\hat{\not{Q}})], \tag{2.6}$$

where, the soft photon being real, Q is the lightlike 4-vector $Q=q\hat{Q}=q(1,\hat{q})$, with q a real and positive number. In the literature, this result is ordinarily written in the form

$$\frac{C^{st}}{\varepsilon}\int\frac{d^4P}{(2\pi)^4}\delta(\hat{Q}\cdot P)(1-2n_F(p_0))\sum_{s=\pm1,V=P,P'}\pi\left(1-s\frac{v_0}{v}\right)\beta_s(V), \tag{2.7}$$

where the overall $1/\varepsilon$ comes from a dimensionally regularized evaluation of the factored out angular integration appearing in (2.6), and where $\beta_s(V)$ is related to the effective fermionic propagator usual parametrization,[2]

$$^\star S_\alpha(P)=\frac{i}{2}\sum_{s=\pm1}\hat{\not{P}}_s{}^\star\Delta^s(p_0+i\epsilon_\alpha,p) \tag{2.8}$$

with $\hat{P}_s=(1,s\hat{p})$, the label s referring to the two dressed fermion propagating modes. One has then

$$^\star\Delta^s(p_0+i\epsilon_\alpha,p)\equiv{}^\star\Delta^s_\alpha(p_0,p)=\alpha_s(p_0,p)-i\pi\epsilon(\epsilon_\alpha)\beta_s(p_0,p), \tag{2.9}$$

where $\epsilon(x)$ is the distribution "sign of x."

III. IMPROPER TRADITIONAL DERIVATIONS

The historical derivation just reminded above, however, is plagued with erroneous manipulations, which, following Ref. 5, are most easily described on the two simpler diagrams including one bare vertex γ_μ, the other $\Gamma^{\mathrm{HTL}}_\mu$. The R/A real time formalism conveys us to the expression

$$\Pi^{(\star,\star;1)}_R(Q)=-ie^2m^2\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\times\mathrm{disc}_{p_0}\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\mathrm{Tr}(^\star S_R(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}})}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}, \tag{3.1}$$

where the superscript $(\star,\star;1)$ on the left-hand side refers to a self-energy diagram involving two effective propagators and one vertex HTL correction, as depicted in Fig. 1. The steps leading to the collinear singularity of (3.1) are as follows. In consistency with the R/A formalism, and the standard mathematical definition of a discontinuity (ϵ is an infinitesimal parameter to be taken to zero in the end[9]), the discontinuity in the energy variable p_0 is taken by writing

$$\mathrm{disc}_{p_0}\frac{\mathrm{Tr}(^\star S_R(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}})}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}=\frac{\mathrm{Tr}(^\star S_R(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}})}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}-\frac{\mathrm{Tr}(^\star S_A(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}})}{(\hat{K}\cdot P-i\epsilon)(\hat{K}\cdot P'+i\epsilon)}. \tag{3.2}$$

Closing the p_0 integration contour in the upper half complex p_0 plane, one selects a pole term contribution to $\Pi^{(\star,\star;1)}_R(Q)$, which comes from the vertex $\Gamma^{\mathrm{HTL}}_\mu$ and reads

$$-ie^2m^2\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\times\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot P'+i\epsilon}\mathrm{Tr}(^\star S_A(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}}). \tag{3.3}$$

Since $P'=P+Q$, we have indeed, as a building block of (3.3), the expression

$$\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q+i\epsilon}\mathrm{Tr}(^\star S_A(P)\hat{\not{K}}{}^\star S_R(P')\hat{\not{K}}). \tag{3.4}$$

Here, it is traditionally claimed that the angular average develops a collinear singularity in a

neighborhood of $\hat{K}=\hat{Q}$, not balanced by the numerator, and whose "*residue*" is obtained by replacing everywhere $\hat{K}$ by $\hat{Q}$, except for the denominator. The result is then,

$$\frac{C^{st}}{\varepsilon}\frac{\delta(\hat{Q}\cdot P)}{q}\,\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{Q}}\overset{\star}{S}_R(P')\hat{\not{Q}}), \tag{3.5}$$

where the first factor, singular at $\varepsilon=0$, is obtained by using a dimensional regularization of the angular integral, and where the constant, C^{st}, is independent of P. Up to regular contributions that we do not consider here, this singular piece of (3.4) translates, for $\Pi_R^{(\star,\star;1)}(Q)$, into a singular result of

$$-\frac{C^{(st)}}{\varepsilon}\frac{e^2m^2}{q}\int\frac{\mathrm{d}^4P}{(2\pi)^3}(1-2n_F(p_0))\times\delta(\hat{Q}\cdot P)\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{Q}}\overset{\star}{S}_R(P')\hat{\not{Q}}). \tag{3.6}$$

The contribution of (3.6) to the soft photon emission rate being proportional to its imaginary part, the emission rate is plagued with a collinear singularity [as recalled in Sec. II, this very contribution cancels against a similar one in $\Pi_R^{(\star,\star;2)}(Q)$; but an uncancelled singular piece remains which, *mutatis mutandis*, is derived along the very same steps as taken here, in the simpler and more illustrative case of $\Pi_R^{(\star,\star;1)}(Q)$].

The RP is known to be ill defined in the infrared sector of hot gauge theories, and the above famous divergent result is one of the most compelling arguments in favor of this widespread opinion. Several solutions have been proposed ever since, which, however, do not meet with a general consensus. They display, in effect, too much dependences on the physical process under consideration, so that it seems reasonable to think of this, as an indication that things have not reached a satisfying enough state. Some decades ago, one may have written "*Our task as mathematicians (…) is to assist physicists in their work by throwing mathematical light if things grow too unsystematic or too complicated.*"[10] This is why it matters to stress that this 10 years old divergent and important result is incorrect, being derived on the basis of illicit mathematical steps. This can be seen as follows:

(i) Getting back to the building block expression (3.4), one can rewrite the trace as

$$\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{K}}\overset{\star}{S}_R(P')\hat{\not{K}})=\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{K}}\overset{\star}{S}_R(P')\hat{\not{K}})-\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{Q}}\overset{\star}{S}_R(P')\hat{\not{Q}})+\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{Q}}\overset{\star}{S}_R(P')\hat{\not{Q}}). \tag{3.7}$$

On the right-hand side of (3.7), the difference of the first two terms can be expressed as

$$\sum_{s,s'=\pm1}\overset{\star}{\Delta}{}_A^{s'}(P')\overset{\star}{\Delta}{}_R^{s}(P)\;(\hat{K}\cdot\hat{P}'_{s'}[\hat{P}_s\cdot(\hat{K}-\hat{Q})]+\hat{Q}\cdot\hat{P}_s[\hat{P}'_{s'}\cdot(\hat{K}-\hat{Q})]), \tag{3.8}$$

where the effective propagators representations (2.8) have been used. In this form, it is clear that these two terms pose no problem under the remaining angular integration of (3.4), and that the only potential trouble could come from the third term of (3.7), that is, from

$$\mathrm{Tr}(\overset{\star}{S}_A(P)\hat{\not{Q}}\overset{\star}{S}_R(P')\hat{\not{Q}})\times\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q+i\epsilon}. \tag{3.9}$$

As advertised after (3.4), a potentially singular behavior develops at $\hat{K}=\hat{Q}$. It has been taken care of by performing the angular integration at $D=3+2\varepsilon$ spatial dimensions,[5] and the so far admitted singular counterpart of (3.4) is then obtained under the form (3.5).

As shown in the Appendix, though, a direct evaluation of (3.9) is doable, and makes it clear that the traditional result (3.5) is incorrect. In view of (A4), we have in effect

$$\int \frac{d\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q+i\epsilon}=\frac{-i\Theta(-P^2)}{2qp}\int_0^{2\pi}\frac{d\varphi}{a+b\sin\varphi}=\frac{-i\Theta(-P^2)}{2qp}\times 4a\int_0^{\pi/2}\frac{d\varphi}{a^2-b^2\sin^2\varphi} \tag{3.10}$$

and the integral appearing on the right-hand side of (3.10) is dependent on the relative magnitude of coefficients a^2 and b^2. Corresponding to the condition $a^2=b^2$, that is to $\hat{Q}\cdot P=0$, a singularity is obtained, with, for (3.9), the resulting expression [see (A12)],

$$\mathrm{Tr}(^\star S_A(P)\hat{\not{Q}}^\star S_R(P')\hat{\not{Q}})\times\frac{-i\delta(\hat{Q}\cdot P)}{2q}\frac{-4p^2}{P^2-i\epsilon}\times\cot\eta_{|_{\eta=0^+}}, \tag{3.11}$$

where $\Theta(x)$ stands for the usual Heaviside step function.

Compared to the standard historical result (3.5), (3.11) presents a most interesting similarity, since, like the ε^{-1} logarithmic singularity of (3.5), a singular piece of $\cot\eta$, as $\eta\to 0$, factors out, in total independence of the remaining integrations to be performed on p_0 and $\vec{p}$.

However, as emphasized in the appendix, it appears that the terms which accompany these singularities are not the same, and, most importantly, that the singularities themselves are not the same since, in particular, the logarithmic nature of (3.5) is not recovered.

(ii) The traditional result (3.5) is also relevant of another, more important error, as being a systematic one, rather peculiar to the context of hot gauge field theories. Passing from (3.1) to (3.2) in effect, the prescription of discontinuity in p_0 is permuted with the angular integration on $\hat{K}$. Now, this permutation is an illicit mathematical step because, whatever the formalism in use, real or imaginary time, the discontinuity of the integral is in order, and not the integral of the discontinuity. Since a discontinuity is defined through a limiting procedure, it is long known that its permutability with an integration cannot be supposed to hold in general.

For the sake of a simpler and clear-cut illustration of our claim, we will focus on the "efficient" piece of (3.1), the expression

$$\mathrm{disc}_{p_0}\int\frac{d\hat{K}}{4\pi}\frac{1}{\hat{K}\cdot P+i\epsilon}\frac{1}{\hat{K}\cdot P'+i\epsilon}. \tag{3.12}$$

That this "efficient" piece be relevant to the problem under consideration, and in particular the one to be compared to the improper sequence expression (3.4), is shown in the Appendix. Let us begin with recalling that the improper sequence of discontinuity and integral operations has produced the corrected, still singular result,

$$\int\frac{d\hat{K}}{4\pi}\mathrm{disc}_{p_0}\frac{1}{\hat{K}\cdot P+i\epsilon}\frac{1}{\hat{K}\cdot P'+i\epsilon}=\frac{2i\delta(\hat{Q}\cdot P)}{q}\frac{p^2}{P^2-i\epsilon}\cot\eta_{|_{\eta=0^+}}. \tag{3.13}$$

On the other hand, we have[8]

$$\int\frac{d\hat{K}}{4\pi}\frac{1}{\hat{K}\cdot P+i\epsilon}\frac{1}{\hat{K}\cdot P'+i\epsilon}=\frac{1}{2Q\cdot P+i\epsilon q}\ln\frac{P'^2+i\epsilon p_0'}{P^2+i\epsilon p_0}. \tag{3.14}$$

Since $2Q\cdot P=P'^2-P^2$, this result is symmetric under the exchange $P\leftrightarrow P'$, as it should, and allows to calculate the proper sequence of the discontinuity and integration operations. One finds,

$$\mathrm{disc}_{p_0}\int\frac{d\hat{K}}{4\pi}\frac{1}{\hat{K}\cdot P+i\epsilon}\frac{1}{\hat{K}\cdot P'+i\epsilon}=\frac{i\pi\epsilon(p_0)\Theta(-P^2)}{Q\cdot P+i\epsilon q}. \tag{3.15}$$

The differences between the (corrected) improper sequence result (3.13) and the above proper sequence one, (3.15), are of utmost importance in the calculational context of hot quantum field

theories, because salient features emerge which reveal to be sound and general features, extending, beyond the present illustration, to any of the higher number of points HTL- vertices and related calculations.

(1) Staring at (3.14), one can observe how the angular average is able to reproduce all of the correct internal/external legs R/A specifications, the $i\epsilon q$, $i\epsilon p_0$, and $i\epsilon p_0'$, which are not manifest on the left-hand side. The same property can be observed on the angular identites (4.9)–(4.11) derived elsewhere.[8] A first important difference is therefore that the relevant $i\epsilon$ prescriptions of internal/external lines are preserved within the proper sequence, not along the reversed improper one. In calculations, it has been stressed that this drawback can only result into violent, structural inconsistencies.[11]

(2) A second essential difference is the sign distribution $\epsilon(p_0)$. In all of the real or imaginary time formalisms, and any possible resummation scheme,[8] sign distributions have long been noticed to be of paramount importance so as to preserve *integrable* and *nonintegrable* infrared singularity compensations.[12] As observed here again, correct sign distributions are a natural outcome of the calculational operations proper sequence (3.15), not of the improper one, (3.13), (A7), and (A8). That is, the proper sequence of angular average and discontinuity operations complies with the required, exact sign distributions and internal/external line prescriptions which, otherwise, are violated.

(3) The above two properties are not restricted to the soft photon emission rate problem, however important it is. Now, focusing on that problem again, the following summary may be in order. As displayed through Eqs. (A7)–(A9), the improper sequence result is not a systematically singular result. When the result comes out regular, at $a^2>b^2$ that is at $(\hat{Q}\cdot P)^2>0$, it still differs the proper sequence one, the shortcomings described above. At $\hat{Q}\cdot P=0$, the improper sequence result comes out effectively plagued with a divergence which factors out any possible calculation it is involved in, in total independence of the remaining integrations to be performed on p_0, $\vec{p}$. At variance with its original version, though, this divergence does not come out logarithmic, at least in a canonically devised dimensional regularization scheme, set up at $D=3+2\varepsilon$ spatial dimensions.

At this stage, it is worth noticing that when the proper sequence result (3.15) is plugged into the $\Pi_R^{(\star,\star;1)}(Q)$ calculation, then, the resulting contribution to the soft photon emission rate comes out regular (Ref. 14). In the same vein, it is interesting to stress also that the same property of regularity has been derived in Ref. 8, concerning any $\Pi_R^{(N,N';1)}(Q)$ and $\Pi_R^{(N,N';2)}(Q)$ contribution, where $N(N')$ are the numbers of HTL self-energy insertions (2.3) along the $P(P')$ internal lines. The proper sequence of discontinuity and angular average was followed throughout, whereas, again, the same overall factoring out mass singularity as (3.11), could be shown to appear along the improper, inverted sequence.

That makes the singularity so derived, definitely appear a fate of the improper sequence of discontinuity and angular average operations.

IV. CONCLUSION

Mathematically, the fact that the proper sequence of angular average and discontinuity operations are inverted by the so far conventional use, accounts for a substantial difference because a discontinuity is defined by a limiting procedure. The possibility of its permutation with an integration, should accordingly never be taken for granted *a priori*. In this respect, it is worth noticing that the authors of Ref. 5 (published version), while inverting the proper sequence of operations, were conscious of the risks this manipulation possibly entailed.

Though technically more involved of a step, we conclude that the angular averages inherent to the context of hot gauge field theories must definitely be performed in the first place, and in particular, before that any discontinuity and/or imaginary part prescriptions be actually taken. This sets in, we think, the general character and related importance of the point made in the present paper.

It is true that in the hot quantum field theories context, this is more of a trap as the formalisms in use are rather fuzzy about the distinction between discontinuity and imaginary part prescriptions which, then, can usually be permuted with integrations. Up to a trivial factor of 2, in effect, the one is generally mistaken for the other, whereas their difference, and in particular the prevalence of the discontinuity aspect over the imaginary part one, had been advocated in Ref. 13.

Ignoring that proper sequence may lead (and has led) to incorrect derivations and/or results. Not only have the infrared singularity cancellation patterns long revealed to be particularly sensitive to the angular averages and discontinuity operations proper sequence, but, as noticed in the Appendix, regular terms also, are the more endangered by an improper sequence calculation as the latter develops singularities.

Our point has been illustrated on the basis of the hot QCD collinear singularity problem, and it seems reasonable to think that this 10 years old and important issue should now be totally revisited within the proper sequence. Because of the complexity of the angular integrations inherent to the contribution of $\Pi_R^{(\star,\star;2)}(Q)$ (Ref. 8) it is a somewhat complicated task which could be deferred to a further publication.

However, it is certainly worth mentioning here, that we have been able to prove that the so far reputed singular contributions of type $\Pi_R^{(\star,\star;1)}(Q)$, come out regular, when taken within the correct, proper sequence of angular integration and discontinuity operations.[14]

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APPENDIX

On Eq. (3.10)

We proceed here to the direct calculation of (3.9), as alluded to in the main text, that is

$$\int \frac{\mathrm{d}\hat{K}}{4\pi}\mathrm{disc}_{p_0}\frac{1}{\hat{K}\cdot P+i\epsilon}\,\frac{1}{\hat{K}\cdot P'+i\epsilon}=\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q+i\epsilon}. \tag{A1}$$

If $\hat{p}\neq\hat{q}$, the calculation is most easily carried out in the orthonormal basis of vectors

$$\left\{\frac{\hat{p}\wedge\hat{q}}{\sin\alpha},\frac{\hat{p}\cos\alpha-\hat{q}}{\sin\alpha},\hat{p}\right\},\quad \cos\alpha=\hat{p}\cdot\hat{q}. \tag{A2}$$

We have then for (A1),

$$\begin{aligned}&\frac{-i}{2qp}\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{+1}\mathrm{d}\cos\theta\,\frac{\delta(p_0/p-\cos\theta)}{1-\cos\theta\cos\alpha+\sin\theta\sin\alpha\sin\varphi+i\epsilon}\\&\quad=\frac{-i\Theta(-P^2)}{2qp}\int_0^{2\pi}\frac{\mathrm{d}\varphi}{1-\dfrac{p_0}{p}\cos\alpha+\sin\left[\arccos\left(\dfrac{p_0}{p}\right)\right]\sin\alpha\sin\varphi+i\epsilon}.\end{aligned} \tag{A3}$$

This integral reads

$$\frac{-i\Theta(-P^2)}{2qp}\int_0^{2\pi}\frac{\mathrm{d}\varphi}{a+b\sin\varphi} \tag{A4}$$

at

$$a = 1 - \left(\frac{p_0}{p}\right)\hat{p}\cdot\hat{q} + i\epsilon,\ \ b = \eta\sqrt{-\frac{P^2}{p^2}}\,\eta'\sqrt{1-(\hat{p}\cdot\hat{q})^2},\ \ \eta,\eta' = \pm 1. \tag{A5}$$

Note that because of the constraint $\Theta(-P^2)$, we have $\mathrm{Re}(a)\geqslant 0$.

Three cases are now to be considered.

(i) $a^2 > b^2$. The result is then

$$\int_0^{2\pi}\frac{\mathrm{d}\varphi}{a+b\sin\varphi} = \frac{2\pi\epsilon(a)}{\sqrt{a^2-b^2}} \tag{A6}$$

as given[15] by formula 3.6151, and (A1) reads in this case as

$$(\mathrm{A1}) = \frac{-i\pi\Theta(-P^2)}{\sqrt{(Q\cdot P)^2 + i\epsilon}}. \tag{A7}$$

Note that, relevant of this case, is also the situation where no such basis as (A2) can be devised because $\hat{p}=\hat{q}$. Now, a direct evaluation of (A1) is then straightforward,

$$\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{-2i\pi\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q + i\epsilon} = \frac{i\pi\Theta(-P^2)}{q(p_0-p-i\epsilon)} = \frac{i\pi\Theta(-P^2)}{Q\cdot P - i\epsilon|_{\hat{p}=\hat{q}}} \tag{A8}$$

which results also from (A7) in the limit $\hat{p}=\hat{q}$.

(ii) $a^2 < b^2$. The integral would be undefined at $\sin^2\varphi = a^2/b^2$, and would be given the meaning of

$$4a\lim_{\eta=0}\left\{\int_0^{\arcsin(a/|b|)-\eta} + \int_{\arcsin(a/|b|)+\eta}^{\pi/2}\right\}\frac{\mathrm{d}\varphi}{a^2-b^2\sin\varphi}.$$

The result would then read

$$4a\lim_{\eta=0}\frac{\epsilon(a^2)}{\sqrt{a^2(b^2-a^2)}}\left\{\mathrm{Arth}\left(1-\frac{b^2}{\sqrt{a^2(b^2-a^2)}}\eta+\mathcal{O}(\eta^2)\right)\right.$$
$$\left.-\mathrm{Arcth}\left(1+\frac{b^2}{\sqrt{a^2(b^2-a^2)}}\eta+\mathcal{O}(\eta^2)\right)\right\} = 0 \tag{A9}$$

as given[15] by formula 2.5621. This case however, is not really to be considered in the present situation where we have $a^2-b^2=(\hat{Q}\cdot P)^2/p^2+i\epsilon$, that is, $\mathcal{R}e(a^2-b^2)\geqslant 0$.

(iii) $a^2=b^2$. This condition corresponds to $\hat{Q}\cdot P=0$, and we have

$$\int_0^{2\pi}\frac{\mathrm{d}\varphi}{a+b\sin\varphi} = \frac{4}{a}\int_0^{\pi/2}\frac{\mathrm{d}\varphi}{1-\sin^2\varphi} = -4\frac{p^2}{P^2-i\epsilon}\int_0^{\pi/2}\frac{\mathrm{d}\varphi}{1-\sin^2\varphi}. \tag{A10}$$

The integral does not exist, and it is noteworthy that, had we introduced a dimensional regularization at $D=3+2\varepsilon$ spatial dimensions,[5] then (A4) was multiplied by an overall factor of $(-P^2/p^2)^{\varepsilon}$, and the measure $\mathrm{d}\varphi$, by a factor of $\sin^{2\varepsilon}\varphi$.[16] The integral was then turned into

$$\int_0^{\pi/2}\mathrm{d}\varphi\frac{\sin^{2\epsilon}}{1-\sin^2\varphi} \tag{A11}$$

making it clear that, contrarily to the results obtained,[5] the dimensional regularization so introduced is not able to take care of the divergence developing in a neighbourhood of $\varphi=\pi/2$. A cutoff, $\eta=0^+$, may be introduced so as to supply the above integral with enough regularization, and one gets for (A10) the result

$$\frac{-4p^2}{P^2-i\epsilon}\lim_{\eta=0^+}\int_0^{\pi/2-\eta}\frac{\mathrm{d}\varphi}{1-\sin^2\varphi}=\frac{-4p^2}{P^2-i\epsilon}\lim_{\eta=0^+}\cot\eta. \tag{A12}$$

Clearly, a canonically devised dimensional scheme, is not able to reproduce the historical logarithmic divergence.

On expression (3.12)

The expression (3.12) is "efficient" in the sense of relevance for the problem under consideration, but this is obscured by the fact that an improper sequence of operations has been followed throughout the two historical derivations of the hot QCD collinear problem. Still, it is rather straightforward to see that (3.12) is the pertinent counterpart of the required comparison.

Relying again on the representations (2.8), we have

$$\mathrm{disc}_{p_0}\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\mathrm{Tr}\left({}^\star S_A(P)\hat{K}\,{}^\star S_R(P')\hat{K}\right)}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}=8\sum_{s,s'}{}^\star\Delta_R^{s'}(P')\left\{{}^\star\rho_R^s(P)\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}\cdot\hat{P}_s}{\hat{K}\cdot\hat{P}+i\epsilon}\frac{\hat{K}\cdot\hat{P}'_{s'}}{\hat{K}\cdot\hat{P}'+i\epsilon}\right.$$
$$\left.+{}^\star\Delta_R^s(P)\mathrm{disc}_{p_0}\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}\cdot\hat{P}_s}{\hat{K}\cdot\hat{P}+i\epsilon}\frac{\hat{K}\cdot\hat{P}'_{s'}}{\hat{K}\cdot\hat{P}'+i\epsilon}\right\}, \tag{A13}$$

where, within standard notations,[2]

$${}^\star\rho_R^s(P)=\mathrm{disc}_{p_0}{}^\star\Delta_R^s(P).$$

On the right-hand side of (A13), it appears clearly that it is the second term, entailing the proper sequence of discontinuity and integration, which compares with the improper sequence derivation (3.2) to (3.6). This second term can further be developed as

$$8\sum_{s,s'}{}^\star\Delta_R^{s'}(P'){}^\star\Delta_R^s(P)\mathrm{disc}_{p_0}\int\frac{\mathrm{d}\hat{K}}{4\pi}\left\{\frac{ss'}{pp'}+\frac{s'}{p'}\left(1-s\frac{p_0}{p}\right)\frac{1}{\hat{K}\cdot\hat{P}+i\epsilon}+\frac{s}{p}\left(1-s'\frac{p'_0}{p'}\right)\frac{1}{\hat{K}\cdot\hat{P}'+i\epsilon}\right.$$
$$\left.+\left(1-s\frac{p_0}{p}\right)\left(1-s'\frac{p'_0}{p'}\right)\frac{1}{(\hat{K}\cdot\hat{P}+i\epsilon)(\hat{K}\cdot\hat{P}'+i\epsilon)}\right\} \tag{A14}$$

whence the focus put on (3.12) as the "efficient" and simpler piece of the needed comparison with expression (3.13), since, starting from it and permuting the discontinuity with the integration, it is elementary to recover a result equivalent (not equal) to (3.5).

Equivalent but nonequal, because of the incorrect steps plaguing the traditional derivations, as in particular the factorization of a factor like $\mathrm{Tr}({}^\star S_A(P)\hat{Q}\,{}^\star S_R(P')\hat{Q})$. This simple, byproduct remark is enough of an argument to pin up the fact that not only the singular, but also the regular structure of the calculation is endangered by the improper sequence (this is of course so, because the improper sequence calculation generates an undefined integration).

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Conformal Killing horizons

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For time dependent black hole space–times the event horizon cannot be described by a Killing horizon. In the case when the space–time admits a timelike conformal Killing field, which becomes null on a boundary called the conformal stationary limit surface, one can locally describe the expanding event horizon by using this boundary, provided that it is a null geodesic hypersurface. In this case the boundary is called a conformal Killing horizon and is shown to be null and geodesic if and only if the twist of the conformal Killing trajectories on the hypersurface vanishes. Moreover if the space–time is conformally related to a stationary asymptotically flat black hole space–time, it is shown that this hypersurface is globally equivalent to the event horizon, provided that the conformal factor goes to a constant at null infinity. When the conformal stationary limit surface does not coincide with the conformal Killing horizon, a generalization of the weak rigidity theorem which establishes the conformal Killing property of the event horizon and the rigidity of its rotation is obtained. A physical definition of surface gravity for conformal Killing horizons is given, which is then used to formulate a generalized zeroth law of black hole physics. © *2004 American Institute of Physics.*
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I. INTRODUCTION

For more than 30 years, black hole physics has been one of the most active areas of research in both classical and quantum gravity. However almost all the research has been limited to isolated black holes, represented in general by the Kerr–Newman solution,[1] of which the Schwarzschild, Reissner-Nordström, and Kerr solutions are special cases. All these exact solutions share two basic characteristics: namely asymptotic flatness, and time independence which implies the existence of a global timelike Killing vector field, K, satisfying

$$\mathcal{L}_K \mathbf{g} = 0, \tag{1}$$

where $\mathcal{L}$ denotes the Lie derivative in the direction K and g is the metric of the space–time. While these black holes have been very useful for studying the physical effects like the classical tests and the quantum effects like black hole evaporation, they do not represent a realistic model.

In a realistic situation, the black hole is embedded in a cosmological background or surrounded by a local mass distribution and so it may cease to be time independent. Moreover the space–time becomes cosmological and nonflat at large distances from the black hole. One expects

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significant differences in the structure and properties of these black holes from the well-known isolated black holes, where even the passage from the Schwarzschild black hole to the Kerr black hole brings profound changes. In accordance with the strong rigidity theorem[2] the event horizon of a static or stationary asymptotically flat black hole is represented by the Killing horizon,[3] provided that the space–time is analytic, the fundamental matter fields obey well behaved hyperbolic equations and the stress-energy tensor satisfies the weak energy condition. The Killing horizon is defined as the union $H[K]=\cup H_i[K]$, where $H_i[K]$ is a connected component of the set of points forming a null hypersurface on which a Killing field K is null and not identically vanishing. The horizon Killing field K either coincides with the stationary Killing field, in which case the Killing horizon coincides with the static limit surface $(K|K)=0$, or the space–time admits at least one axial Killing field M such that[4] $[K,M]=0$. The latter case corresponds to a rotating asymptotically flat black hole in which the Killing horizon $H[\tilde{K}]$ is generated by

$$\tilde{K}=K+\Omega_H M, \tag{2}$$

where Ω_H is the angular velocity of the Killing horizon which is constant on $H[\tilde{K}]$. Moreover,[5] the Killing trajectories associated with the Killing field $\tilde{K}$ are null geodesics on $H[\tilde{K}]$ and coincide with the generators of the horizon.

According to the strong rigidity theorem in the case of a time dependent black hole space–time the event horizon cannot be defined as a Killing horizon and hence an alternative definition of a black hole must be found. Once a definition of an event horizon is found, one can then try to obtain exact solutions that describe dynamical black hole space–times. In the next section we address this problem by using the concepts of conformally stationary limit surfaces and conformal Killing horizons.[6]

If a space–time $(M,\mathbf{g})$ admits a conformal Killing vector field K satisfying

$$\mathcal{L}_K\mathbf{g}=2\phi\,\mathbf{g}, \tag{3}$$

where ϕ is related to the divergence of K by, $4\phi=-\mathrm{d}^\dagger K$, one can define a *conformal stationary limit surface* as the hypersurface Σ_0 on which K is null, i.e., the norm $N\equiv(K|K)=0$. To see the physical significance of this hypersurface it is first necessary to define a *conformal Killing observer* in the regions where K is timelike. This observer travels along a conformal Killing trajectory with a four velocity $u=e^{-\psi}K$, where $e^{2\psi}=N$, such that $(u|u)=1$ in a signature of -2. The function ϕ appearing in (3) is then equal to $(K|\mathrm{d}\psi)$, and hence is a measure of the rate of change of the scale along the conformal Killing trajectory. In the case of a Killing trajectory this function is zero implying that N remains constant along the trajectory. As the conformal Killing observer moves along the conformal Killing trajectory, he experiences a pure conformal change in the metric $\mathbf{g}$, in the sense that the metric can be written as $\mathbf{g}=f\mathbf{h}$, where f is related to ϕ, and is a function of space–time position and $\mathbf{h}$ is a function of position which is constant on any conformal Killing trajectory.[7] When the conformal Killing congruence of timelike curves is irrotational, i.e., the rotation or twist $\omega=\frac{1}{2}*(K\wedge\mathrm{d}K)$ vanishes, the observer concludes that the space–time is *conformally static*. Otherwise in the case of a nonzero ω, the space–time is seen as *conformally stationary*. In the regions where the conformal Killing field turns from timelike to spacelike such an observer cannot be defined. This leads to the boundary Σ_0 for the existence of such observers, where the conformal Killing field is null. Thus the name "conformal stationary limit surface."

For conformal Killing observers and sources the hypersurface Σ_0 is an infinite frequency shift surface. This can be seen by considering a conformal Killing source at S say, emitting photons at frequency μ_s, and a conformal Killing observer O receiving the photons at a frequency μ_0. If the photons from S to O travel along the null geodesic Γ with tangent vector k, then the frequency measured at O is proportional to $(u|k)$, where u is the four velocity of the observer. Also since Γ is a null geodesic, $(K|k)$ is constant along Γ, and hence it follows that the frequency shift obeys

$$\frac{\mu_s}{\mu_0} = \sqrt{\frac{N_0}{N_s}}. \tag{4}$$

So it is clear from (4) that when S lies on Σ_0 the observed frequency is zero, while when O lies on Σ_0 the observed frequency is infinite for finite emitted frequency μ_s. This explains why $N=0$ is a surface of infinite frequency shift for the conformal Killing observers and sources.

If the conformal stationary limit surface Σ_0 is itself a null surface then it is called a *conformal Killing horizon*. Dyer and Honig[6] proved that the hypersurface $N=0$ is a null surface, if and only if the rotation of the conformal Killing congruence has vanishing norm on the hypersurface, i.e., $(\omega|\omega)=0$. Moreover it was also shown that the conformal Killing trajectories are null pregeodesics on Σ_0 and therefore coincide with its null generators. Being a null geodesic hypersurface the conformal Killing horizon acts as a one-way membrane, i.e., the future null cone lies entirely on one side of the null surface such that future directed timelike directions cross the null surface in the same sense. In this way Σ_0 satisfies the local conditions for it to constitute the event horizon of a dynamical black hole space–time.

Time-dependent space–times admitting conformal Killing horizons can be obtained by applying a conformal transformation, $\tilde{\mathbf{g}}=\Omega^2\mathbf{g}$, to a stationary, asymptotically flat black hole space–time $(M,\mathbf{g})$ which admits a Killing horizon, Σ_0, generated by the Killing field K. Under a conformal transformation the Killing field K is mapped to a conformal Killing field, provided that $(K|\mathrm{d}\Omega)\neq 0$. Also since conformal transformations preserve causal structure as well as null geodesics, the hypersurface Σ_0 in the manifold $(M,\tilde{\mathbf{g}})$, is still a null surface whose null geodesic generators now coincide with the conformal Killing trajectories of K, i.e., it is a null geodesic hypersurface and therefore a conformal Killing horizon. In this way the conformal stationary limit surface and conformal Killing horizon in $(M,\tilde{\mathbf{g}})$, are the images of the corresponding stationary limit surface and Killing horizon in the space–time $(M,\mathbf{g})$. Such space–times are asymptotically conformally flat. However in general, there can be other space–times which are not asymptotically conformally flat, and which admit a timelike conformal field that generates a conformal Killing horizon.

In the next section we prove that the nullity of the conformal stationary limit surface requires a stronger necessary and sufficient condition than the one obtained earlier by Dyer and Honig[6] Moreover, in the case when the time dependent black hole space–time arises as a result of a conformal transformation on a stationary asymptotically flat space–time containing a Killing horizon, we prove that the conformal Killing horizon is globally equivalent to the event horizon, provided that the conformal factor goes to a constant at null infinity. This is an extension of the strong rigidity theorem[2] which establishes the conformal Killing property of the event horizon for such dynamic black hole space–times.

As discussed previously there are cases when the conformal stationary limit surface is a null surface and hence coincides with the conformal Killing horizon. These kind of space–times are conformally static. However there may be other cases where the conformal stationary limit surface is not a null surface. In this case one must assume the existence of another conformal Killing field which can be used with the above conformal Killing field K to construct a "mixed" conformal Killing field $\tilde{K}$ which has vanishing twist on the hypersurface $\tilde{\Sigma}_0, (\tilde{K}|\tilde{K})=0$. In this case the conformal stationary limit surface Σ_0 and the conformal Killing horizon $\tilde{\Sigma}_0$ do not coincide. This situation is analogous to the "mixed" Killing vector introduced in the Kerr space–time by Vishveshwara[8] and Carter,[3] where the stationary limit surface and the Killing horizon are separated by the ergosphere. This suggests that the so-called "weak rigidity theorem"[9] which establishes the Killing property of the horizon and the rigidity of its rotation for circular space–times, could be extended to conformal Killing horizons. This is done in Sec. III.

In the last section a physical definition of surface gravity for conformal Killing horizons similar to that for Killing horizons is given. This is then used to formulate a generalized zeroth law of black hole physics.

II. CONFORMAL KILLING TRAJECTORIES

The necessary and sufficient condition for a conformal stationary limit surface to be a null surface is given by the following theorem. Its proof is obtained in the framework of exterior calculus in order to make it easier and shorter. A concise introduction to the subject of exterior differential forms is given in Willmore.[10] We use the same symbol K to denote the conformal Killing field and its associated one form $\mathbf{g}(K)$.

Before proving the theorem we prove the following lemma.

Lemma 1: Let K be an arbitrary conformal Killing field with associated norm N and twist ω. Then

$$-\mathrm{d}K = \frac{1}{N}[2*(K\wedge\omega)+K\wedge\mathrm{d}N], \tag{5}$$

and

$$N(\mathrm{d}K|\mathrm{d}K) = (\mathrm{d}N|\mathrm{d}N) - 4(\omega|\omega) - 4\phi^2 N, \tag{6}$$

where $\phi=-\frac{1}{4}\mathrm{d}^{\dagger}K$.

Proof: Using the definition of the twist ω of the conformal Killing field K we have

$$-2*(K\wedge\omega) = 2i_K*\omega = i_K(K\wedge\mathrm{d}K).$$

Now

$$i_K(K\wedge\mathrm{d}K) = i_K K\wedge\mathrm{d}K - K\wedge i_K\,\mathrm{d}K = N\,\mathrm{d}K - K\wedge i_K\,\mathrm{d}K,$$

where

$$i_K\,\mathrm{d}K = -\mathrm{d}i_K\,K + \mathcal{L}_K K = -\mathrm{d}N + 2\phi K.$$

Hence

$$-2*(K\wedge\omega) = N\,\mathrm{d}K + K\wedge\mathrm{d}N,$$

which then gives the first identity

$$-\mathrm{d}K = \frac{1}{N}[2*(K\wedge\omega)+K\wedge\mathrm{d}N].$$

Then using the above identity we can write

$$N(\mathrm{d}K|\mathrm{d}K) = \frac{1}{N}[4(*(K\wedge\omega)|*(K\wedge\omega)) + 4(K\wedge\mathrm{d}N|*(K\wedge\omega)) + (K\wedge\mathrm{d}N|K\wedge\mathrm{d}N)].$$

Now

$$(*(K\wedge\omega)|*(K\wedge\omega)) = -(K\wedge\omega|K\wedge\omega) = -N(\omega|\omega),$$

because $(K|\omega)=0$. Moreover the cross term $(K\wedge\mathrm{d}N|*(K\wedge\omega))=0$ since it is proportional to $K\wedge K$. Finally

$$(K\wedge\mathrm{d}N|K\wedge\mathrm{d}N) = (K|K)(\mathrm{d}N|\mathrm{d}N) - (K|\mathrm{d}N)(K|\mathrm{d}N) = N(\mathrm{d}N|\mathrm{d}N) - 4\phi^2N^2,$$

since for a conformal Killing field $(K|\mathrm{d}N)=\mathcal{L}_K N=2\phi N$. Hence this gives

$$N(\mathrm{d}K|\mathrm{d}K) = \frac{1}{N}[-4N(\omega|\omega) + N(\mathrm{d}N|\mathrm{d}N) - 4\phi^2N^2],$$

from which we get the second identity

$$N(\mathrm{d}K|\mathrm{d}K) = (\mathrm{d}N|\mathrm{d}N) - 4(\omega|\omega) - 4\phi^2 N.$$

Theorem 1 (condition for CSLS to be a CKH): *If a space–time* $(M,\mathbf{g})$ *admits a timelike conformal Killing field* K *and* Σ_0 *denotes the surface* $\{N\equiv(K|K)=0\}$, *then the surface* Σ_0 *is a null surface (i.e., a conformal Killing horizon) if and only if*[11]

$$\omega = 0, \quad i_K\, \mathrm{d}K - 2\phi K \neq 0 \quad \textit{on } \Sigma_0, \tag{7}$$

where ω *denotes the rotation (twist) associated with the conformal Killing trajectories, and* ϕ *is the scalar function defined in (3).*

Proof: Let Σ_0 be a null surface such that $\mathrm{d}N$ is null on Σ_0. Then the orthogonality of $\mathrm{d}N$ and K on Σ_0 is evident from

$$(K|\mathrm{d}N) = \mathcal{L}_K N = (\mathcal{L}_K \mathbf{g})(K,K) + 2(K|[K,K]) = 0,$$

where the Leibnitz rule for the Lie derivative has been used together with the fact that the Lie bracket $[K,K]=\mathcal{L}_K K=0$, and $\mathcal{L}_K \mathbf{g}=2\phi\,\mathbf{g}$ for the CKV K. Since two orthogonal null vectors are proportional one must also have $K\wedge \mathrm{d}N=0$. Therefore from (5) which can be written in the form

$$2\,{}^*(K\wedge\omega) = -(N\,\mathrm{d}K + K\wedge \mathrm{d}N),$$

where $N=0$, it follows that $\omega=0$ on Σ_0. In addition

$$i_K\,\mathrm{d}K = \mathcal{L}_K K - \mathrm{d}i_K K = 2\phi K - \mathrm{d}N,$$

and so $\mathrm{d}N\neq 0$ implies $i_K\,\mathrm{d}K - 2\phi K \neq 0$.

Conversely let $\omega=0$, $i_K\,\mathrm{d}K - 2\phi K\neq 0$ on Σ_0. Then using (6), it follows that

$$(\mathrm{d}N|\mathrm{d}N) = N(\mathrm{d}K|\mathrm{d}K) - 4\phi^2 N = 0 \quad \text{on } \Sigma_0.$$

Then the assumption $i_K\,\mathrm{d}K - 2\phi K = -\mathrm{d}N \neq 0$ on Σ_0, implies that $\mathrm{d}N$ is null on Σ_0, which is therefore a null surface.

Having obtained the condition for the conformal stationary limit surface to be a conformal Killing horizon, one can easily show that the conformal Killing trajectories are null pregeodesics on the conformal Killing horizon. This property can be proved if one takes into account that the conformal Killing horizon by definition is a null surface, and hence its generators are null geodesics. As mentioned in the above proof the conformal Killing field K is tangent on Σ_0 to the generators, and so it follows that the conformal Killing trajectories on the conformal Killing horizon coincide with its generators and are therefore nonaffinely parametrized null geodesics. For this reason the conformal Killing horizon is sometimes referred to as a geodesic null hypersurface.

In the case when the time dependent black hole space–time admitting a conformal Killing horizon is conformally related to a static or stationary asymptotically flat black hole space–time, as described in the introduction, then one can say more about the role played by conformal Killing horizons. We will show in the next theorem that in this case the conformal Killing horizon, besides satisfying the local conditions for it to constitute an event horizon, is also globally equivalent to an event horizon $\mathcal{H}^+=\partial J^-(\mathcal{J}^+)\cap M$ of the black hole $\mathcal{B}=M-J^-(\mathcal{J}^+)$, provided that the conformal factor tends to a constant at null infinity.

Theorem 2 (extension of the strong rigidity theorem): *Consider a space–time* $(M,\tilde{\mathbf{g}})$ *which is conformally related to an analytic black hole space–time* $(M,\mathbf{g})$ *admitting a Killing horizon* Σ_0, *such that the conformal factor in* $\tilde{\mathbf{g}}=\Omega^2\mathbf{g}$ *goes to a constant at null infinity. Then the conformal Killing horizon* Σ_0 *in* $(M,\tilde{\mathbf{g}})$ *is globally equivalent to the event horizon, provided that the stress-energy tensor satisfies the weak energy condition.*

Proof: The proof of this theorem follows easily from the global definition of the event horizon and the properties of conformal transformations. The event horizon by definition is the boundary of the set $J^-(\mathcal{J}^+)$, which in turn is a union of terminal indecomposable past sets (TIPs). A TIP[12] is defined as the chronological past, $I^-(\gamma)$, of a future endless (or future inextendible, i.e., having no future end point[13]) causal curve γ. The TIPs are represented by the points on $\mathcal{J}^+$.[12] Each TIP being

a past-set[14] is unchanged if the metric is altered by the introduction of a finite conformal factor, and hence the global definition of an event horizon is conformally invariant, provided that the conformal factor tends to a constant such that the structure of conformal infinity in $(M,\tilde{\mathbf{g}})$ is preserved. This implies that in the manifold $(M,\mathbf{g})$, the event horizon $\partial J^-(\mathcal{J}^+)$ is a Killing horizon, while in the conformal manifold $(M,\tilde{\mathbf{g}})$ it is a conformal Killing horizon.

The case when the conformal factor goes to infinity on some surface S outside the Killing horizon Σ_0, needs special attention. At first it seems that since in this case the surface S is blown up to infinity in the conformal manifold $(M,\tilde{\mathbf{g}})$, the global definition $\partial J^-(\mathcal{J}^+)$ of the event horizon cannot be used. However one can show that in this situation the usual definition of event horizon is still applicable and hence the event horizon is a conformal Killing horizon as in the case of a finite conformal transformation. This can be shown by considering one of the TIPS, $I^-[\gamma]$ represented by the point p on $\mathcal{J}^+$, and generated by the null geodesic γ which intersects the surface S at a finite affine parameter λ_S in the manifold $(M,\mathbf{g})$. By the properties of conformal transformations, γ is still a null geodesic in $(M,\tilde{\mathbf{g}})$ with an affine parameter $\tilde{\lambda}$ related to λ by

$$\frac{d\tilde{\lambda}}{d\lambda} = c\Omega^2,$$

where c is a constant. From this it can be seen that the parameter λ_S in $(M,\mathbf{g})$ corresponds to $\tilde{\lambda}_S=\infty$ in $(M,\tilde{\mathbf{g}})$. This solves the problem for the case when Ω goes to infinity on some surface outside the Killing horizon.

III. ROTATING CONFORMAL KILLING HORIZONS

As discussed in the Introduction, there may be space–times where the conformal stationary limit surface $\{N\equiv(K|K)=0\}$ is not a null surface and hence does not coincide with the conformal Killing horizon. In this case besides the timelike conformal Killing field K, we consider another spacelike conformal Killing field M which commutes with K and which can be used in combination with it to construct a conformal Killing field $\tilde{K}$ that generates the conformal Killing horizon. This leads to a generalization of the weak rigidity theorem[9] which establishes the conformal Killing property of the event horizon for rotating black hole space–times, and the rigidity of its rotation. This is stated and proved after the following proposition.

Proposition 1: If K and M are two commuting conformal Killing fields with twist ω_K and ω_M, respectively, and $\tilde{K}$ and Ω are defined as

$$\tilde{K} = K + \Omega M, \quad \Omega = -\frac{W}{X},$$

where $X=(M|M)$ and $W=(K|M)$, then the twist of the vector field $\tilde{K}$ is given by

$$\omega_{\tilde{K}} = [(M|\omega_K) - \Omega(K|\omega_M)]\frac{M}{X}. \tag{8}$$

Proof: From the definition of $\tilde{K}$ it follows that

$$\tilde{K}\wedge d\tilde{K} = K\wedge dK + \Omega^2(M\wedge dM) + \Omega(K\wedge dM + M\wedge dK) - K\wedge M\wedge d\Omega.$$

Now since the two conformal Killing fields commute, $[M,K]=\mathcal{L}_M K=0$, one gets

$$dW = di_M K = -i_M\, dK + \mathcal{L}_M K = 2\phi_M K - i_M\, dK,$$

and

$$\mathrm{d}X = \mathrm{d}i_M\, M = -\, i_M\, \mathrm{d}M + \mathcal{L}_M M = 2\phi_M M - i_M\, \mathrm{d}M,$$

where ϕ_M is the scalar function associated with the conformal Killing field M and defined in (3). Therefore

$$\mathrm{d}\Omega = -\frac{1}{X}\left(\mathrm{d}W - \frac{W}{X}\mathrm{d}X\right) = \frac{1}{X}\left[i_M\left(\mathrm{d}K - \frac{W}{X}\mathrm{d}M\right) - 2\phi_M\left(K - \frac{W}{X}M\right)\right]. \tag{9}$$

Substituting for $\mathrm{d}\Omega$ in the expression for $\tilde{K}\wedge\mathrm{d}\tilde{K}$, gives

$$\begin{aligned}\tilde{K}\wedge\mathrm{d}\tilde{K} &= \frac{1}{X}[X(K\wedge\mathrm{d}K) - W(M\wedge\mathrm{d}K) - K\wedge M\wedge i_M\,\mathrm{d}K] + \frac{W}{X^2}[W(M\wedge\mathrm{d}M) - X(K\wedge\mathrm{d}M)\\ &\quad + K\wedge M\wedge i_M\,\mathrm{d}M]\\ &= \frac{1}{X} i_M\left[(M\wedge K\wedge\mathrm{d}K) + \frac{W}{X}(K\wedge M\wedge\mathrm{d}M)\right].\end{aligned} \tag{10}$$

Using the definitions of ω_M and ω_K, which represent the twist associated with M and K, respectively, and the fact that $*1=\eta$, where η is the volume form, we get

$$M\wedge K\wedge\mathrm{d}K = 2(M|\omega_K) * 1, \quad K\wedge M\wedge\mathrm{d}M = 2(K|\omega_M) * 1.$$

After substituting these in (10) and using $i_M * 1 = *M$, the identity in (8) is obtained by taking the dual of both sides of (10).

As in the case of the weak rigidity theorem[9] it is assumed that our space–time is circular or in other words orthogonally transitive. This means that the surfaces of transitivity are orthogonal to a family of surfaces of conjugate dimension. By Frobenius theorem[15] this requires that

$$\mathrm{d}K = \alpha_1\wedge K + \alpha_2\wedge M \tag{11}$$

and

$$\mathrm{d}M = \alpha_3\wedge K + \alpha_4\wedge M, \tag{12}$$

where α_i $(i=1,2,3,4)$, are arbitrary one-forms in $\Lambda^1 T^*$. Then the above two equations imply that

$$\mathrm{d}K\wedge K\wedge M = \mathrm{d}M\wedge M\wedge K = 0.$$

But $M\wedge K\wedge\mathrm{d}K = 2(M|\omega_K)\,\eta$ and similarly $K\wedge M\wedge\mathrm{d}M = 2(K|\omega_M)\,\eta$. This gives

$$(M|\omega_K) = (K|\omega_M) = 0.$$

Therefore as a corollary to the above proposition we can say that for a circular space–time admitting commuting, timelike, and spacelike conformal Killing fields K and M, respectively, the vector field $\tilde{K}$ defined by

$$\tilde{K} = K - \frac{(K|M)}{(M|M)}M,$$

is hypersurface orthogonal, i.e., $\omega_{\tilde{K}}=0$.

Theorem 3 (generalized weak rigidity theorem): *Consider a circular space–time admitting commuting timelike and spacelike conformal Killing fields K and M respectively, and let* $\tilde{\Sigma}_0$ *be the surface* $\{(\tilde{K}|\tilde{K})=0\}$, *where* $\tilde{K}=K+\Omega M$ *with* $\Omega=-W/X=-(K|M)/(M|M)$. *Then* Ω *is constant on* $\tilde{\Sigma}_0$, $\tilde{K}$ *is a conformal Killing field on* $\tilde{\Sigma}_0$, *and* $\tilde{\Sigma}_0$ *is a geodesic null hypersurface provided that the surface* $\tilde{\Sigma}_0$ *is regular.*

Proof: Using the commutativity of the conformal Killing fields, $\mathcal{L}_K M=[K,M]=0$, we can write

$$dW = di_K M = -i_K\, dM + \mathcal{L}_K M = *(K \wedge *\, dM) + 2\phi_K M,$$

$$dX = di_M M = -i_M\, dM + \mathcal{L}_M M = *(M \wedge *\, dM) + 2\phi_M M,$$

where now ϕ_K is the scalar field associated with K and defined by (3). Substituting this expression in (9) gives

$$d\Omega = -\frac{1}{X}[*(K \wedge *\, dM) + \Omega * (M \wedge *\, dM)] - \frac{2}{X}(\phi_K + \Omega\phi_M)M.$$

Taking the Hodge dual of both sides gives

$$*d\Omega = -\frac{1}{X}[\tilde{K} \wedge *\, dM] - \frac{2}{X}(\phi_K + \Omega\phi_M) * M. \tag{13}$$

From the above definition of $\tilde{K}$ it is easy to see that $(\tilde{K}|M)=0$ and $(\tilde{K}|\tilde{K})=(\tilde{K}|K)$. Applying i_M to (13) we have

$$i_M * d\Omega = \frac{1}{X}[\tilde{K} \wedge 2\omega_M] - \frac{2}{X}(\phi_K + \Omega\phi_M) i_M * M = \frac{1}{X}[\tilde{K} \wedge 2\omega_M],$$

since $i_M * M = 0$. Applying now i_K to the above expression, we get

$$i_K i_M * d\Omega = \frac{1}{X}[i_K\tilde{K} \wedge 2\omega_M - \tilde{K} \wedge 2i_K\omega_M] = \frac{2}{X}[(\tilde{K}|\tilde{K})\omega_M - (K|\omega_M)\tilde{K}].$$

But $(\tilde{K}|\tilde{K})=0$ on $\tilde{\Sigma}_0$ and by the circularity condition $(K|\omega_M)=0$. Therefore it follows that $i_K i_M * d\Omega = 0$ on $\tilde{\Sigma}_0$, and hence it is clear that $d\Omega$ can be expressed as a combination of the conformal Killing fields K and M on $\tilde{\Sigma}_0$, i.e., $d\Omega = aK + bM$, where a and b are two scalar fields. So for any vector field Y orthogonal to the conformal Killing fields one has $\mathcal{L}_Y\Omega = i_Y\, d\Omega = a(Y|K) + b(Y|M) = 0$ on $\tilde{\Sigma}_0$.

Moreover we can show using the definition of Ω that $\mathcal{L}_K\Omega = \mathcal{L}_M\Omega = 0$. For example,

$$\mathcal{L}_K\Omega = -\frac{\mathcal{L}_K W}{X} + \frac{W}{X^2}\mathcal{L}_K X. \tag{14}$$

But

$$\mathcal{L}_K W = \mathcal{L}_K(K|M) = (\mathcal{L}_K\mathbf{g})(K,M) + (K|[K,M]) = 2\phi_K(K|M),$$

and

$$\mathcal{L}_K X = \mathcal{L}_K(M|M) = (\mathcal{L}_K\mathbf{g})(M,M) + 2(M|[M,M]) = 2\phi_K(M|M).$$

Substituting these in (14) gives $\mathcal{L}_K\Omega = 0$. Similarly one can show that $\mathcal{L}_M\Omega = 0$. From this we conclude that Ω is constant on $\tilde{\Sigma}_0$, and thus the vector field $\tilde{K}$ is a conformal Killing field on $\tilde{\Sigma}_0$. As was shown above this field has vanishing twist on $\tilde{\Sigma}_0$, and hence since we assume that the surface $\tilde{\Sigma}_0$ is regular, i.e., $d(\tilde{K}|\tilde{K}) \neq 0$, theorem 1 implies that $\tilde{\Sigma}_0$ is a null geodesic hypersurface.

The space between the conformal stationary limit surface and the conformal Killing horizon provides a generalization of Penrose's ergosphere.

IV. SURFACE GRAVITY

We define the surface gravity, κ, for a space–time that admits a conformal Killing horizon Σ_0 generated by a conformal Killing field K, by the equation

$$\nabla_K K = \kappa K, \tag{15}$$

where the equality in the above equation applies only on Σ_0. In this way the surface gravity measures the extent to which the parametrization of the null geodesic congruence, represented by the conformal Killing trajectories on Σ_0, is not affine. This is regarded as the proper definition of surface gravity, because besides being a natural generalization of the surface gravity on Killing horizons, it also gives a physical interpretation to κ. Using the conformal Killing equations (3) which can be written in the form

$$\mathrm{d}N = -2\nabla_K K + 4\phi K, \tag{16}$$

we can write an alternative expression for the surface gravity by substituting (15) in the above equation, such that

$$\mathrm{d}N = -2\kappa K + 4\phi K = -2(\kappa - 2\phi)K. \tag{17}$$

When $\phi=0$ the above expression reduces to the well-known expression for surface gravity on Killing horizons which relates the one-form $\mathrm{d}N$ with the Killing field K, both of which are perpendicular to the Killing horizon.

An important difference between the properties of surface gravity on Killing horizons and the surface gravity on conformal Killing horizons, is that in the former case, the surface gravity along each Killing trajectory on the Killing horizon is constant, while in the latter case it scales up or down with ϕ along the conformal Killing trajectories generating the conformal Killing horizon. This can be shown by applying the Lie operator to both sides of (17), such that

$$\mathcal{L}_K \mathrm{d}N = -2\mathcal{L}_K[(\kappa - 2\phi)K]. \tag{18}$$

The left-hand side (LHS) of the above equation can be written as

$$\mathcal{L}_K\, \mathrm{d}N = \mathrm{d}\mathcal{L}_K N = 2\mathrm{d}(\phi N) = 2N\, \mathrm{d}\phi + 2\phi\, \mathrm{d}N,$$

where we have used the commutativity of the Lie derivative and exterior derivative when applied on scalars, together with the fact that $\mathcal{L}_K N = 2\phi N$ for a conformal Killing field K. Considering the right-hand side (RHS) and using $\mathcal{L}_K K = 2\phi K$, we have

$$\mathcal{L}_K[(\kappa - 2\phi)K] = 2\phi(\kappa - 2\phi)K + K\mathcal{L}_K[(\kappa - 2\phi)].$$

Therefore (18) becomes

$$2N\, \mathrm{d}\phi + 2\phi\, \mathrm{d}N = -4\phi(\kappa - 2\phi)K - 2K\mathcal{L}_K[(\kappa - 2\phi)].$$

On the conformal Killing horizon Σ_0, $N=0$ and from (17) $\mathrm{d}N = -2(\kappa - 2\phi)K$. So

$$\mathcal{L}_K(\kappa - 2\phi) = 0. \tag{19}$$

From this we conclude that in the conformal Killing case it is the combination, $\kappa - 2\phi$, which is constant along the null geodesic generators of the conformal Killing horizon Σ_0. In the case when K is a homothetic Killing field, i.e., ϕ is a constant, the situation is the same as in the Killing case, i.e., the surface gravity is constant along the homothetic Killing trajectories on the horizon. One would also like to consider the variation of $\kappa - 2\phi$ from one generator of Σ_0 to another in analogy to the generalized Hawking–Lichnerowicz theorem in the case of Killing horizons, which is also known as the zeroth law of black hole physics,[16] and which states that the surface gravity κ is constant over any connected component of the Killing horizon. This is discussed later on after we obtain an explicit expression for the surface gravity on conformal Killing horizons.

At this point we should remark that our definition of surface gravity on conformal Killing horizons is different than the one proposed earlier by Jacobson and Kang.[17] They suggested a conformally invariant definition of surface gravity κ_1 defined by

$$\mathrm{d}N = -2\kappa_1 K. \tag{20}$$

Unlike our definition this conformally invariant definition of surface gravity has no physical meaning attached to it. In our case the surface gravity as defined in (15) is not conformally invariant. To see this let us consider a conformal transformation $\tilde{\mathbf{g}}=\Omega^2\mathbf{g}$. Then in the conformal manifold $(M,\tilde{\mathbf{g}})$, (17) is written as

$$\mathrm{d}\tilde{N} = -2(\tilde{\kappa} - 2\tilde{\phi})\tilde{K}. \tag{21}$$

But $\tilde{N}=\Omega^2 N$ and hence on Σ_0

$$\mathrm{d}\tilde{N} = \Omega^2\ \mathrm{d}N + N\ \mathrm{d}\Omega^2 = \Omega^2\ \mathrm{d}N.$$

Also $\tilde{K}=\Omega^2 K$ and from the definition of the scalar function $\phi\left(\phi=\frac{1}{4}\nabla_c K^c\right)$, it follows that

$$\tilde{\phi} = \phi + \Omega^{-1}(K|\mathrm{d}\Omega).$$

Hence (21) gives

$$\mathrm{d}N = -2[\tilde{\kappa} - 2\phi - 2\Omega^{-1}(K|\mathrm{d}\Omega)]K.$$

Comparing this with the definition (17) we have

$$\tilde{\kappa} = \kappa + 2\Omega^{-1}(K|\mathrm{d}\Omega), \tag{22}$$

and hence unless Ω is a constant, the two surface gravities are different.

We now obtain an explicit expression for surface gravity on the conformal Killing horizon Σ_0 by using the fact that the twist ω associated with the conformal Killing field K vanishes on Σ_0. For this we use the identity,

$$(\mathrm{d}K|\mathrm{d}K) * K = i_K(\mathrm{d}K \wedge * \mathrm{d}K) = i_K\ \mathrm{d}K \wedge * \mathrm{d}K + \mathrm{d}K \wedge i_K * \mathrm{d}K. \tag{23}$$

The first part of this identity follows from the fact that

$$(\mathrm{d}K|\mathrm{d}K) = -\ *(\mathrm{d}K \wedge * \mathrm{d}K),$$

which implies that

$$(\mathrm{d}K|\mathrm{d}K)K = -K \wedge *(\mathrm{d}K \wedge * \mathrm{d}K),$$

such that

$$(\mathrm{d}K|\mathrm{d}K) * K = -\ *(K \wedge *(\mathrm{d}K \wedge * \mathrm{d}K)) = i_K(\mathrm{d}K \wedge * \mathrm{d}K).$$

Now using the definitions of N and ω, we have

$$i_K\ \mathrm{d}K = \mathcal{L}_K K - \mathrm{d}i_K\ K = 2\phi K - \mathrm{d}N \tag{24}$$

and

$$i_K * \mathrm{d}K = *(\mathrm{d}K \wedge K) = 2\omega, \tag{25}$$

such that (23) becomes

$$(\mathrm{d}K|\mathrm{d}K) * K = 2\phi K \wedge * \mathrm{d}K - \mathrm{d}N \wedge * \mathrm{d}K + 2\ \mathrm{d}K \wedge \omega.$$

Then using (17) and the fact that $\omega=0$ on Σ_0, this leads to

$$(\mathrm{d}K|\mathrm{d}K) * K = 2(\kappa - \phi)K \wedge * \mathrm{d}K,$$

which by (24) can also be written as

$$(\mathrm{d}K|\mathrm{d}K) * K = -2(\kappa-\phi) * i_K\, \mathrm{d}K = -2(\kappa-\phi)(2\phi * K - * \mathrm{d}N).$$

Finally using (17) we can write

$$(\mathrm{d}K|\mathrm{d}K) * K = -4(\kappa-\phi)^2 * K,$$

i.e.,

$$(\kappa-\phi)^2 = [-\tfrac{1}{4}(\mathrm{d}K|\mathrm{d}K)]_{\Sigma_0}. \tag{26}$$

After having shown that the combination $(\kappa-2\phi)$ is constant along the null generators of the conformal Killing horizon Σ_0, we now show that under certain assumptions this function is constant everywhere on Σ_0. In order to do this we first show that the quantity $(\kappa-2\phi)$ is conformally invariant under a general conformal transformation $\tilde{\mathbf{g}}=\Omega^2\mathbf{g}$, which maps the conformal Killing horizon Σ_0 in $(M,\mathbf{g})$, to another conformal Killing horizon in $(M,\tilde{\mathbf{g}})$. Thus letting $h=\kappa-2\phi$, Eq. (17) gives

$$-2\tilde{h}\tilde{K} = \mathrm{d}\tilde{N} = N\,\mathrm{d}\Omega^2 + \Omega^2\,\mathrm{d}N.$$

But $N=0$ on Σ_0 and hence

$$-2\tilde{h}\tilde{K} = \Omega^2\,\mathrm{d}N = -2h\Omega^2 K = -2h\tilde{K}.$$

Hence $h=\tilde{h}$.

The conformal invariance of h implies that if we start with a space–time $(M,\mathbf{g})$, admitting a Killing horizon on which h reduces to the surface gravity κ, then by the zeroth law of black hole physics together with the conformal invariance of h, we conclude that $\kappa-2\phi$ is constant on the conformal Killing horizon Σ_0 in the space–time $(M,\tilde{\mathbf{g}})$, provided that Einstein's equations hold with matter satisfying the dominant energy condition. Therefore in analogy to the Killing case, $\kappa-2\phi$ is not only constant along the null generators of Σ_0, but is constant over any connected component of Σ_0. Moreover by introducing another assumption, we now show that the constancy of $\kappa-2\phi$ on conformal Killing horizons is not only restricted to those cases in which the space–time admitting the conformal Killing horizon is obtained via a conformal transformation of a space–time with a Killing horizon.

So considering a space–time $(V,\mathbf{g})$ admitting a conformal Killing field K that generates a conformal Killing horizon H, we attempt to answer the following question: when does there exist at least locally on H, a conformally related metric $\tilde{\mathbf{g}}=\Omega^2\mathbf{g}$ such that K is a Killing field with respect to $\tilde{\mathbf{g}}$. It is not difficult to show that this requires finding a function Ω satisfying

$$(K|\mathrm{d}(\ln\Omega)) + \phi = 0, \tag{27}$$

or in coordinate form

$$K^c(\ln\Omega)_{,c} + \phi = 0,$$

where ϕ is the scalar function defined in (3) and a comma denotes partial differentiation. Clearly this is always possible at points $p\in H$ where the conformal Killing field K does not vanish. The problems in solving (27) occur at homothetic fixed points[18] of K on H, i.e., points $p\in H$ where $K=0$, but $\phi\neq 0$. A similar but more general question involving the algebra of conformal Killing fields $\mathcal{C}(\mathbf{g})$ on the entire space–time $(M,\mathbf{g})$ rather than a single conformal Killing field on a submanifold H of M, was considered first by Bilyalov[19] and Defrise-Carter[20] and recently by Hall and Steele.[21] Later Capocci[22] considered the case of a single conformal Killing field K in $(M,\mathbf{g})$ with a zero at $p\in M$ and gave sufficient conditions, for the existence of a conformally related metric defined on a neighborhood of p, with respect to which K is a Killing field. Hence returning to our case, in order to achieve the Killing property of K on H we can either apply the conditions stated by Capocci on H or, maybe easier, assume that there are no fixed points on H. In each case

the conformal Killing horizon H is mapped to a Killing horizon in $(V,\tilde{\mathbf{g}})$ on which the surface gravity is constant. Then the conformal invariance of h guarantees again that the quantity $\kappa-2\phi$ is constant on the conformal Killing horizon H in $(V,\mathbf{g})$. We have thus proved the following generalized version of the zeroth law of black hole physics.

Theorem 4 (generalized zeroth law): *If a space–time admits a conformal Killing horizon Σ_0 generated by a conformal vector field with no homothetic fixed points on Σ_0, then the quantity $\kappa-2\phi$ is constant everywhere on Σ_0, provided that Einstein's equations hold with matter satisfying the dominant energy condition.*

When $\phi=0$ it is clear that this theorem reduces to the well known zeroth law for Killing horizons.

V. CONCLUSION

In this work we have shown that conformal Killing horizons in time dependent black hole space–times can be used in general to describe locally the event horizon, both in the nonrotating case and in the rotating case. In the former case the conformally static limit surface coincides with the conformal Killing horizon, thus satisfying the necessary and sufficient conditions presented in theorem 1. In the latter case we have shown by generalizing the weak rigidity theorem, that the conformal stationary limit surface and the conformal Killing horizon are two distinct surfaces, with the space between them providing a generalization of Penrose's ergosphere. In the particular case when the black hole space–time admitting a conformal Killing horizon is the image of a conformal transformation applied to a stationary isolated black hole space–time, we have shown that the conformal Killing horizon is globally equivalent to the event horizon, provided that the conformal factor goes to a constant at null infinity. This is an extension of the strong rigidity theorem.

A physical definition of surface gravity, κ, on conformal Killing horizons was also given and later used to obtain a generalization of the zeroth law. The constancy of $\kappa-2\phi$ on the conformal Killing horizon, suggests that in general it is $\kappa-2\phi$, and not κ, to which the Hawking temperature is proportional, i.e., $T=(\kappa-2\phi)/2\pi$. This relation reduces to the usual one, $T=\kappa/2\pi$, for stationary asymptotically flat black holes, where the event horizon is a Killing horizon.

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The Poincaré equation: A new polynomial and its unusual properties

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The Poincaré equation, a second-order partial differential equation describing wave motions in a rotating spheroid of arbitrary eccentricity satisfying a certain set of the boundary condition, is studied. A new polynomial as the general solution of the Poincaré equation in spheroidal geometry is found for the first time. The paper focuses on some unusual and intriguing mathematical properties of the new Poincaré polynomial. The possible completeness of the set of eigenfunctions of the Poincaré equation in the form of the new polynomial is also discussed. The new Poincaré polynomial would provide a powerful basis for the mathematical analysis in many important geophysical and astrophysical problems. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1811786]

I. INTRODUCTION

Many geophysical and astrophysical problems are concerned with the following classical mechanic problem: Wave motions in an incompressible and inviscid fluid contained in an oblate spheroidal cavity rotating with constant angular velocity Ω (for example, Poincaré, 1885; Chandrasekhar, 1961; Greenspan, 1968; Zhang and Schubert, 2000). The spheroidal geometry of a planet or a star is mainly caused by its rapid rotation. The envelope of the spheroidal cavity, shown in Fig. 1, is usually described by the equation

$$s^2 + \frac{z^2}{1-\epsilon^2} = 1, \tag{1.1}$$

where (s,ϕ,z) are cylindrical polar coordinates with the unit vectors $(\mathbf{e}_s,\mathbf{e}_\phi,\mathbf{e}_z)$, $s=0$ represents the axis of rotation and ϵ is the eccentricity of the oblate spheroid, $0<\epsilon<1$. The limit $\epsilon\to 0$ corresponds to a special case for a sphere and the limit $\epsilon\to 1$ gives a flatted spheroidal disk.

The effect of rapid rotation results in fluid motions in the form of azimuthally traveling waves or oscillations in an oblate spheroidal cavity. The pressure of the wave motion and oscillations is governed by the well-known Poincaré equation (Lyttleton, 1953; Greenspan, 1968; Zhang *et al.*, 2001) which was derived more than a century ago by Poincaré (1885). Bryan (1889) discussed an implicit solution of the Poincaré equation using modified oblate spheroidal coordinates. It was first

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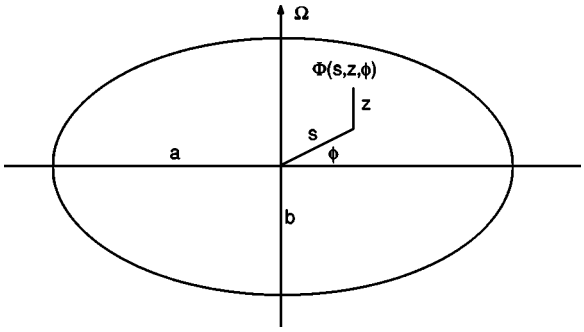

FIG. 1. Geometry of an oblate spheroid and cylindrical polar coordinates (s,z,ϕ). The major and minor axes of the oblate spheroid are $a=1$ and $b=\sqrt{1-\epsilon^2}$, respectively, with $0<\epsilon<1$. The pressure of wave motions is denoted by Φ.

recognized by Greenspan (1968) that the general solution for the Poincaré equation in spherical or spheroidal geometry is a double polynomial in terms of s and z. However, the explicit analytical expression for the double polynomial has not been found.

This paper presents the first explicit expression for the double polynomial as the general solution of the Poincaré equation in a spheroid of arbitrary eccentricity. The paper focuses on some unusual and intriguing mathematical properties of the new Poincaré polynomial, and the possible completeness of the set of eigenfunctions of the Poincaré equation in the form of the Poincaré polynomial.

II. THE NEW POINCARÉ POLYNOMIAL

In the following analysis, we shall use both cylindrical polar coordinates (s,ϕ,z) and spheroidal polar coordinates (η,ϕ,τ) which are related by

$$s^2=(\epsilon^2+\eta^2)(1-\tau^2),\quad z^2=\eta^2\tau^2. \tag{2.1}$$

The envelope of a spheroidal cavity in spheroidal polar coordinates is simply given by

$$\eta=\sqrt{1-\epsilon^2}. \tag{2.2}$$

Either the pressure Φ or the flow velocity $\mathbf{V}$ can be employed to describe the Poincaré problem in an oblate spheroid (Greenspan, 1968). The relationship between $\mathbf{V}$ and Φ is given by

$$\mathbf{V}=\frac{1}{2(1-\sigma^2)}\mathbf{e}_z\times\nabla\Phi-\frac{\hat{i}\sigma}{2(1-\sigma^2)}\nabla\Phi+\frac{\hat{i}}{2\sigma(1-\sigma^2)}(\mathbf{e}_z\cdot\nabla\Phi)\mathbf{e}_z, \tag{2.3}$$

where $\hat{i}=\sqrt{-1}$ and σ is the half frequency of a wave or an oscillation mode in a spheroid. Both the pressure Φ and the velocity $\mathbf{V}$ can be expressed as

$$\Phi=\Phi(\eta,\tau)e^{\hat{i}(2\sigma t+m\phi)},\quad \text{or}\quad \Phi=\Phi(s,z)e^{\hat{i}(2\sigma t+m\phi)}, \tag{2.4}$$

$$\mathbf{V}=\mathbf{V}(\eta,\tau)e^{\hat{i}(2\sigma t+m\phi)},\quad \text{or}\quad \mathbf{V}=\mathbf{V}(s,z)e^{\hat{i}(2\sigma t+m\phi)}, \tag{2.5}$$

where m is the azimuthal wave number of a wave. In cylindrical polar coordinates (s,ϕ,z), the pressure Φ is governed by the Poincaré equation in the form (Greenspan, 1968)

$$\left(\frac{1}{s}\frac{\partial\Phi}{\partial s}+\frac{\partial^2\Phi}{\partial s^2}-\frac{m^2}{s^2}\Phi\right)+\frac{(\sigma^2-1)}{\sigma^2}\frac{\partial^2\Phi}{\partial z^2}=0 \tag{2.6}$$

subject to the boundary condition

$$(1-\sigma^2)z\frac{\partial\Phi}{\partial z}-\sigma^2\left(\sqrt{1-\frac{z^2}{1-\epsilon^2}}\right)(1-\epsilon^2)\frac{\partial^2\Phi}{\partial s^2}-(1-\epsilon^2)m\sigma\Phi=0 \tag{2.7}$$

on the envelope of the spheroidal cavity give by (1.1). In spheroidal polar coordinates (η,ϕ,τ), the Poincaré equation has the more complicated form

$$C_{\tau\tau}\frac{\partial^2\Phi}{\partial\tau^2}+C_{\eta\eta}\frac{\partial^2\Phi}{\partial\eta^2}+C_\tau\frac{\partial\Phi}{\partial\tau}+C_\eta\frac{\partial\Phi}{\partial\eta}+C_{\tau\eta}\frac{\partial^2\Phi}{\partial\tau\,\partial\eta}+C_0\Phi=0, \tag{2.8}$$

where

$$C_{\tau\tau}=\frac{v^2}{w^4}\left(\tau^2u^2+\frac{(\sigma^2-1)}{\sigma^2}\eta^2v^2\right),$$

$$C_{\eta\eta}=\frac{u^2}{w^4}\left(\eta^2v^2+\frac{(\sigma^2-1)}{\sigma^2}\tau^2u^2\right),$$

$$C_\tau=\frac{\tau}{w^6}[-2w^4+u^2v^2(3\eta^2-\tau^2\epsilon^2)]+\frac{(\sigma^2-1)}{\sigma^2}\left(\frac{v^2}{\tau w^6}\right)[w^4-\eta^2w^2(1+\tau^2)-2\eta^2\tau^2(u^2+\epsilon^2v^2)],$$

$$C_\eta=\frac{\eta}{w^6}[2w^4+u^2v^2(3\tau^2\epsilon^2-\eta^2)]+\frac{(\sigma^2-1)}{\sigma^2}\left(\frac{u^2}{\eta w^6}\right)[w^4-\tau^2w^2(\epsilon^2-\eta^2)-2\eta^2\tau^2(u^2+\epsilon^2v^2)],$$

$$C_{\tau\eta}=-\frac{2\tau\eta u^2v^2}{\sigma^2w^4},$$

$$C_0=-\frac{m^2}{u^2v^2},$$

where

$$u=\sqrt{\eta^2+\epsilon^2},\quad v=\sqrt{1-\tau^2},\quad w=\sqrt{\eta^2+\epsilon^2\tau^2}.$$

The above equation is subject to the boundary condition

$$e_\eta\cdot\mathbf{V}=0\quad\text{at}\quad\eta=\sqrt{1-\epsilon^2}, \tag{2.9}$$

where $(\mathbf{e}_\eta,\mathbf{e}_\phi,\mathbf{e}_\tau)$ are the unit vectors for spheroidal polar coordinates. After solving the Poincaré equation for the pressure Φ, the flow velocity $\mathbf{V}$ can be readily obtained from (2.4).

There exist two different parities of solutions with respect to the equatorial plane, $\tau=0$ (or $z=0$), in a rotating spheroid. An equatorially symmetric solution (an even polynomial) is characterized by the symmetry property

$$(V_\tau,V_\phi,V_\eta,\Phi)(\tau,\phi,\eta)=(-V_\tau,V_\phi,V_\eta,\Phi)(-\tau,\phi,\eta), \tag{2.10}$$

or

$$(V_z,V_\phi,V_s,\Phi)(z,\phi,s)=(-V_z,V_\phi,V_s,\Phi)(-z,\phi,s), \tag{2.11}$$

while an equatorially antisymmetric solution (an odd polynomial) satisfies

$$(V_\tau,V_\phi,V_\eta,\Phi)(\tau,\phi,\eta)=(V_\tau,-V_\phi,-V_\eta,-\Phi)(-\tau,\phi,\eta), \tag{2.12}$$

or

$$(V_z, V_\phi, V_s, \Phi)(z, \phi, s) = (V_z, -V_\phi, -V_s, -\Phi)(-z, \phi, s). \tag{2.13}$$

Since the mathematical analyses for both the parities are nearly identical, we shall focus on the equatorially symmetric (even) polynomial.

The Poincaré equation (2.6) [or (2.8)] together with the boundary condition (2.7) [or (2.9)] defines an eigenvalue problem in spheroidal geometry. We find that the general explicit solution for (2.6) in cylindrical coordinates can be written as

$$\Phi(s,z) = \sum_{i=0}^{N} \sum_{j=0}^{N-i} C_{ijmN} \sigma^{2i} (1-\sigma^2)^j s^{m+2j} z^{2i+\delta}; \tag{2.14}$$

while in spheroidal polar coordinates the general solution is given by

$$\Phi(\eta, \tau) = \sum_{i=0}^{N} \sum_{j=0}^{N-i} C_{ijmN} \sigma^{2i} (1-\sigma^2)^j (uv)^{m+2j} (\eta\tau)^{2i+\delta}, \tag{2.15}$$

where C_{ijmN} is defined by

$$C_{ijmN} = \left[\frac{-1}{(1-\sigma^2\epsilon^2)}\right]^{i+j} \frac{[2(m+N+i+j+\delta)-1]!!}{2^{j+1}[2(i+\delta)-1]!!\,(N-i-j)!\,i!\,j!\,(m+j)!},$$

where the even polynomials are given by $\delta=0$, the odd polynomials correspond to $\delta=1$, and N is zero or a positive integer taking

$$N = (1-\delta), (2-\delta), (3-\delta), \ldots,$$

which characterizes the spatial complexity of a polynomial. The polynomial given by (2.14) or (2.15) represents the first explicit general solution for the Poincaré equation in a spheroid of arbitrary eccentricity.

The validity of polynomial (2.14) as solutions for the Poincaré equation can be verified by a direct substitution of (2.14) into (2.6). For example, in the case of the even polynomials, we obtain after shifting indices i and j by 1 in the resulting expression,

$$\begin{aligned}\left(\frac{1}{s}\frac{\partial\Phi}{\partial s} + \frac{\partial^2\Phi}{\partial s^2} - \frac{m^2}{s^2}\Phi\right) + \frac{(\sigma^2-1)}{\sigma^2}\frac{\partial^2\Phi}{\partial z^2} &= \sum_{i=0}^{N-1}\sum_{j=0}^{N-i-1} [4(j+1)(j+m+1)C_{i(j+1)mN} \\ &\quad - C_{(i+1)jmN}(2i+1)(2i+2)]F_{ij} \\ &= \sum_{i=0}^{N-1}\sum_{j=0}^{N-i-1}\left[\frac{(-1)^{i+j+1}[2(m+N+i+j)+1]!!}{2^j(N-i-j-1)!\,(1-\sigma^2\epsilon^2)^{(i+j)}}\right] \\ &\quad \times F_{ij}\left[\frac{(j+1)(j+m+1)}{(2i-1)!!\,i!\,(j+1)!\,(m+j+1)!}\right. \\ &\quad \left. - \frac{(2i+1)(i+1)}{(2i+1)!!\,(i+1)!\,j!\,(m+j)!}\right] \equiv 0\end{aligned} \tag{2.16}$$

for all values of N, m and σ, where F_{ij} is a function of m, σ, s and z.

Three components of the velocity $\mathbf{V}$ can be readily derived from (2.3). In cylindrical coordinates with $\mathbf{V}=(V_s, V_\phi, V_z)$, we obtain

$$V_s = \frac{-\hat{i}}{2}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i}(1-\sigma^2)^{j-1}(2j\sigma + m\sigma + m)s^{m+2j-1}z^{2i+\delta}, \tag{2.17}$$

$$V_\phi = \frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i}(1-\sigma^2)^{j-1}(2j+m+m\sigma)s^{m+2j-1}z^{2i+\delta}, \tag{2.18}$$

$$V_z = \frac{\hat{i}}{2}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i-1}(1-\sigma^2)^{j}(2i+\delta)s^{m+2j}z^{2i-1+\delta}. \tag{2.19}$$

In spheroidal polar coordinates with $\mathbf{V}=(V_\eta, V_\phi, V_\tau)$, we obtain

$$V_\eta = \frac{\hat{i}}{2w}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i-1}(1-\sigma^2)^{j-1}u^{m+2j-1}v^{m+2j}\eta^{2i-1}\tau^{2i+\delta} \times[-\eta^2\sigma(2j\sigma+m\sigma+m)+(2i+\delta)u^2(1-\sigma^2)], \tag{2.20}$$

$$V_\phi = \frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i}(1-\sigma^2)^{j-1}(2j+m+m\sigma)(uv)^{m+2j-1}(\eta\tau)^{2i+\delta}, \tag{2.21}$$

$$V_\tau = \frac{\hat{i}}{2w}\sum_{i=0}^{N}\sum_{j=0}^{N-i} C_{ijmN}\sigma^{2i-1}(1-\sigma^2)^{j-1}u^{m+2j}v^{m+2j-1}\eta^{2i}\tau^{2i-1+\delta} \times[\tau^2\sigma(2j\sigma+m\sigma+m)+(2i+\delta)v^2(1-\sigma^2)]. \tag{2.22}$$

We shall refer to polynomials given by (2.17)–(2.19) or (2.20)–(2.22) as the Poincaré polynomial, which represents the first general explicit solution for the flow velocity in a rotating spheroid of arbitrary eccentricity.

The eigenvalue σ (the half-frequency of a wave or an oscillation mode) can be determined by substituting (2.14) into (2.7), which yields

$$\sum_{n=0} F_N(\sigma)\mathcal{C}_n z^{2n+\delta} = 0, \tag{2.23}$$

where $\mathcal{C}_n$ are nonzero coefficients and $F_N(\sigma)$ is a polynomial of σ. Equation (2.23) implies that $F_N(\sigma)=0$, i.e.,

$$F_N(\sigma) = \left\{\frac{(-1)^N[2(N+m)]!\,(1-\delta)\sigma(1-\epsilon^2)(1-\sigma^2\epsilon^2)^N}{N!\,(N+m)!}\right\} - \sum_{j=0}^{N-1+\delta}(-1)^j\frac{[2(2N+m-j+\delta)]!}{[2(N-j)+\delta]!\,j!\,(2N+m-j+\delta)!}[(1-\epsilon^2)\sigma^2]^{N-j}(1-\sigma^2\epsilon^2)^j \times\{(1-\sigma)[2(N-j)+\delta]-m\sigma(1-\epsilon^2)\}=0. \tag{2.24}$$

For a given ϵ, m and N, there exist $(2N+\delta)$ different eigenvalues or $(2N+\delta)$ different polynomials. At this stage, it is convenient to introduce a triple index notation for the polynomial (eigenfunction) and the eigenvalue by denoting

$$\Phi \to \Phi_{Nnm}, \quad \mathbf{V} \to \mathbf{V}_{Nnm}, \quad \sigma \to \sigma_{Nnm}.$$

While $0 \leqslant N < \infty$ and $0 \leqslant m < \infty$, n has a finite range $n=1,2,3,\ldots,(2N+\delta)$ (which is the number of the roots in (2.24) for a given N). For example, when $N=1$ and $\delta=0$ (even polynomials), (2.24) gives

$$[(2m+3)(m+2)-2m(m+1)\epsilon^2]\sigma_{1nm}^2 - 2(2m+3)\sigma_{1nm} - m = 0. \tag{2.25}$$

For each nonzero wave number m and ϵ, there exist two different eigenvalues

TABLE I. Several examples of σ_{Nmn} for the odd polynomials with $m=2$ at two different eccentricities.

m,N,n	$(\sigma_{Nmn}, \epsilon=0)$	$(\sigma_{Nmn}, \epsilon=0.75)$
2, 0, 1	0.333 333 33	0.533 333 33
2, 1, 1	−0.381 668 34	−0.506 141 15
2, 1, 2	0.233 450 30	0.370 462 75
2, 1, 3	0.748 218 04	0.868 502 82
2, 2, 1	−0.653 999 82	−0.789 050 75
2, 2, 2	−0.254 996 76	−0.354 918 00
2, 2, 3	0.179 767 83	0.283 014 87
2, 2, 4	0.576 528 78	0.736 212 98
2, 2, 5	0.866 985 68	0.936 143 79
2, 3, 1	−0.780 643 60	−0.882 050 97
2, 3, 2	−0.512 288 56	−0.664 478 25
2, 3, 3	−0.192 054 27	−0.273 384 47
2, 3, 4	0.146 202 35	0.228 782 61
2, 3, 5	0.466 027 26	0.628 798 73
2, 3, 6	0.732 830 05	0.854 275 81
2, 3, 7	0.917 704 55	0.961 875 25
2, 4, 1	−0.848 974 15	−0.923 983 68
2, 4, 2	−0.658 613 53	−0.795 715 81
2, 4, 3	−0.421 330 28	−0.570 199 49
2, 4, 4	−0.154 159 53	−0.222 301 93
2, 4, 5	0.123 216 42	0.191 931 53
2, 4, 6	0.390 272 35	0.544 420 44
2, 4, 7	0.627 221 51	0.775 098 89
2, 4, 8	0.816 497 57	0.906 714 47
2, 4, 9	0.944 051 44	0.974 553 57

$$\sigma_{11m} = \frac{(2m+3)}{(m+2)(2m+3) - 2m(m+1)\epsilon^2}\left\{1 - \left[\frac{(m+2)^2-1}{(2m+3)} - \frac{2m^2(m+1)\epsilon^2}{(2m+3)^2}\right]^{1/2}\right\}, \quad (2.26)$$

$$\sigma_{12m} = \frac{(2m+3)}{(m+2)(2m+3) - 2m(m+1)\epsilon^2}\left\{1 + \left[\frac{(m+2)^2-1}{(2m+3)} - \frac{2m^2(m+1)\epsilon^2}{(2m+3)^2}\right]^{1/2}\right\}. \quad (2.27)$$

The corresponding eigenvectors are given by (2.17)–(2.19) or (2.20)–(2.22). Several more examples for σ_{Nnm} with $m=2$ are presented in Tables I and II.

III. UNUSUAL PROPERTIES OF THE POINCARÉ POLYNOMIAL

There are a number of well-known general properties of the the Poincaré equation which were discussed in detail by Greenspan (1968). The most important are that (i) the eigenvalue σ_{Nmn} is real and satisfies

$$-1 < \sigma_{Nmn} < 1, \quad (3.1)$$

and (ii) any eigenvector-eigenvalue pairs, $(\sigma_{Nmn}, \mathbf{V}_{Nmn})$ and $(\sigma_{N'm'n'}, \mathbf{V}_{N'm'n'})$, are orthogonal, i.e.,

$$\int_V \mathbf{V}^+_{Nmn} \cdot \mathbf{V}_{N'm'n'} dV = 0, \quad \text{if} \quad \sigma_{Nmn} \neq \sigma_{N'm'n'}, \quad (3.2)$$

where $\int_V$ denotes the integral over the volume of the solution domain and $\mathbf{V}^+_{Nmn}$ is the complex conjugate of $\mathbf{V}_{Nmn}$. It is of primary importance to note that the properties (3.1) and (3.2) are

TABLE II. Several examples of σ_{Nmn} for the even polynomials with $m=2$ at two different eccentricities.

m,N,n	$(\sigma_{Nmn}, \epsilon=0)$	$(\sigma_{Nmn}, \epsilon=0.75)$
2, 1, 1	−0.115 962 53	−0.120 732 39
2, 1, 2	0.615 962 53	0.779 555 92
2, 2, 1	−0.546 284 20	−0.691 729 37
2, 2, 2	−0.050 895 21	−0.051 845 64
2, 2, 3	0.442 124 48	0.610 969 67
2, 2, 4	0.821 721 59	0.911 631 56
2, 3, 1	−0.727 904 26	−0.845 899 01
2, 3, 2	−0.402 916 92	−0.545 179 59
2, 3, 3	−0.028 854 79	−0.029 163 32
2, 3, 4	0.344 837 69	0.495 420 97
2, 3, 5	0.667 945 80	0.808 631 90
2, 3, 6	0.896 892 48	0.951 531 70
2, 4, 1	−0.819 523 39	−0.906 553 47
2, 4, 2	−0.594 913 81	−0.742 402 07
2, 4, 3	−0.320 037 53	−0.447 935 81
2, 4, 4	−0.018 635 86	−0.018 765 14
2, 4, 5	0.282 672 06	0.414 244 83
2, 4, 6	0.557 170 13	0.715 761 49
2, 4, 7	0.780 489 42	0.884 989 71
2, 4, 8	0.932 778 97	0.969 185 23

derived directly from the basic equations without reference to particular geometry of the problem or the detailed structure of an eigenfunction.

In the nonlinear theory of the wave problem, the following integral

$$\int_V \mathbf{V}^+_{Nmn} \cdot \nabla^2 \mathbf{V}_{Nmn} dV \tag{3.3}$$

plays a key role in the higher-order problem. It can be readily shown that the integral (3.3) is always nonzero and negative in the geometries of an infinitely extended plane layer or a box or a cylinder or an annulus for which the eigenfunctions are not in the form of a polynomial. In spheroidal geometry, however, we have discovered an intriguing, unusual property of the Poincaré polynomial that

$$\int_V \mathbf{V}^+_{Nmn} \cdot \nabla^2 \mathbf{V}_{Nmn} dV \equiv 0, \tag{3.4}$$

for all values of ϵ, m, N, and σ. It should be emphasized that (3.4) holds only for spheroidal geometry in which its eigenfunction is in the form of a polynomial. The mathematical proof for (3.4) is rather complicated and lengthy, requiring the detailed structure of the Poincaré polynomial. Hence we focus on the case of the even (equatorially symmetric) polynomials since the proof for the odd polynomials is similar.

On the basis of explicit expressions (2.17)–(2.19) for the even polynomial ($\delta=0$), it is straightforward to carry out the relevant integration over the volume of the spheroid, which yields

$$\int_V \mathbf{V}^+_{Nmn} \cdot \nabla^2 \mathbf{V}_{Nmn} dV = D_1(\sigma)\mathcal{S}_1 + D_2(\sigma)\mathcal{S}_2 + D_3(\sigma)\mathcal{S}_3, \tag{3.5}$$

where $D_j(\sigma)$, $j=1,2,3$ are a nonzero function of σ and

$$\mathcal{S}_1 = \sum_{i=0}^{N}\sum_{k=1}^{N}\sum_{j=0}^{N-i}\sum_{l=0}^{N-k}(-1)^{i+j+k+l}\Delta^{2(i+k)}(1-\Delta^2)^{j+l} \times\frac{[2(m+N+i+j)-1]!!}{[2(l+k+i+j+m)-1]!!} \times\frac{[2(m+N+k+l)-1]!![2m(m+l+j)+4jl]}{(2i-1)!!\,(N-i-j)!\,i!\,j!\,(m+j)!} \times\frac{(2i+2k-3)!!\,(l+j+m-1)!}{(k-1)!\,l!\,(2k-3)!!\,(l+m)!\,(N-k-l)!}, \tag{3.6}$$

$$\mathcal{S}_2 = \sum_{i=0}^{N}\sum_{k=1}^{N}\sum_{j=0}^{N-i}\sum_{l=0}^{N-k}(-1)^{i+j+k+l}\Delta^{2(i+k)}(1-\Delta^2)^{j+l} \times\frac{[2(m+N+i+j)-1]!!}{[2(l+k+i+j+m)-1]!!} \times\frac{[2(m+N+k+l)-1]!!}{(2i-1)!!\,(N-i-j)!\,i!\,j!\,(m+j)!} \times\frac{(2i+2k-3)!!\,(l+j+m)!}{(k-1)!\,l!\,(2k-3)!!\,(l+m)!\,(N-k-l)!}, \tag{3.7}$$

$$\mathcal{S}_3 = \sum_{i=1}^{N}\sum_{k=2}^{N}\sum_{j=0}^{N-i}\sum_{l=0}^{N-k}(-1)^{i+j+k+l}\Delta^{2(i+k)}(1-\Delta^2)^{j+l} \times\frac{[2(m+N+i+j)-1]!!}{[2(l+k+i+j+m)-1]!!} \times\frac{[2(m+N+k+l)-1]!!}{(2i-1)!!\,(N-i-j)!\,(i-1)!\,j!\,(m+j)!} \times\frac{(2i+2k-5)!!\,(l+j+m)!}{(k-2)!\,l!\,(2k-3)!!\,(l+m)!\,(N-k-l)!}, \tag{3.8}$$

where

$$\Delta^2 = \frac{\sigma^2(1-\epsilon^2)}{(1-\sigma^2\epsilon^2)}.$$

We need to prove that

$$\mathcal{S}_1 = \mathcal{S}_2 = \mathcal{S}_3 \equiv 0$$

for all possible values of ϵ, m, σ and $N>1$. For $N=0$ and $N=1$, we can easily carry out the direct calculation. We shall only present the general proof for $\mathcal{S}_3\equiv 0$ because the proofs for $\mathcal{S}_1\equiv 0$ and $\mathcal{S}_2\equiv 0$ are rather similar.

First, we note that four indices (i,j,k,l) in (3.8) are intimately entangled. In consequence, a direct summation of (3.8) is generally impossible. An essential step in establishing $\mathcal{S}_3\equiv 0$ for all N is to introduce two additional indices, say α and β, by considering a new summation with six indices

$$\mathcal{P}_N^M = \sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha} Z_{\alpha,\beta}^M \sum_{i=1}^{N-M}\sum_{k=2}^{N-M}\sum_{j=0}^{N-i-M}\sum_{l=0}^{N-k-M} (-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta}$$
$$\times\frac{[2(m+N+i+j+\alpha+\beta)-1]!!}{[2(i+\alpha)-1)!!\,(N-i-j-M)!\,(i-1)!\,j!\,(m+j+\beta)!}$$
$$\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)!!\,(N-k-l-M)!\,(k-2)!\,l!\,(m+l+\beta)!}$$
$$\times\frac{(m+j+l+\beta)!\,[2(i+k+\alpha)-5)!!}{[2(m+i+j+k+l+\alpha+\beta+M)-1]!!}, \tag{3.9}$$

where coefficients $Z_{i,j}$ are generally nonzero and defined as

$$Z_{0,0}^0 = 1;$$

$$Z_{i,0}^{M+1} = (-1)^{M+1-i}\frac{(M+1)!}{(M+1-i)!\,i!}2^{M+1};$$

$$Z_{0,i}^{M+1} = (-2)^{M+1-i}\frac{(M+1)!}{(M+1-i)!\,i!}; \tag{3.10}$$

$$Z_{i,M+1-i}^{M+1} = 2^i\frac{(M+1)!}{(M+1-i)!\,i!};$$

$$Z_{i,j}^{M+1} = -2Z_{i,j}^M + 2Z_{i-1,j}^M + Z_{i,j-1}^M; \quad 1\leqslant i\leqslant(M-1), \quad 1\leqslant j\leqslant(M-i).$$

The precise values for the coefficients $Z_{i,j}^M$ are in fact not required in the mathematical proof. Clearly $\mathcal{S}_3$ and $\mathcal{P}_N^M$ are related by

$$\mathcal{S}_3 = \mathcal{P}_N^0.$$

In order to decouple the entangled indices, we first establish an important recurrence relation in the form

$$\mathcal{P}_N^0 = \frac{1}{(N-1)}\mathcal{P}_N^1 = \frac{1}{(N-1)(N-2)}\mathcal{P}_N^2 = \cdots. \tag{3.11}$$

Note that the expression (3.9) can be decomposed into the three different summations

$$\mathcal{P}_N^M = \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3, \tag{3.12}$$

where

$$\mathcal{Q}_1 = \frac{-1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha} Z_{\alpha,\beta}^M \sum_{i=1}^{N-M-1}\sum_{j=0}^{N-i-M-1}\sum_{k=2}^{N-M}\sum_{l=0}^{N-k-M} (-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha+1)}(1-\Delta^2)^{j+l+2\beta}$$
$$\times\frac{[2(m+N+i+j+\alpha+\beta)+1]!!}{[2(i+\alpha)+1)!!\,(N-i-j-M-1)!\,(i-1)!\,j!\,(m+j+\beta)!}$$
$$\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)!!\,(N-k-l-M)!\,(k-2)!\,l!\,(m+l+\beta)!}$$

$$\times\frac{(m+j+l+\beta)\,![2(i+k+\alpha)-3]!!}{[2(m+i+j+k+l+\alpha+\beta+M)+1]!!}, \tag{3.13}$$

$$\begin{aligned}\mathcal{Q}_2=&\frac{1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha}Z_{\alpha,\beta}^{M}\sum_{i=1}^{N-M-1}\sum_{j=0}^{N-i-M-1}\sum_{k=2}^{N-M}\sum_{l=0}^{N-k-M}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta}\\&\times\frac{[2(m+N+i+j+\alpha+\beta)-1]!!}{[2(i+\alpha)-1)\,!!\,(N-i-j-M-1)\,!\,(i-1)\,!\,j\,!\,(m+j+\beta)!}\\&\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)\,!!\,(N-k-l-M)\,!\,(k-2)\,!\,l\,!\,(m+l+\beta)!}\\&\times\frac{(m+j+l+\beta)\,![2(i+k+\alpha)-5]!!}{[2(m+i+j+k+l+\alpha+\beta+M)-1]!!},\end{aligned} \tag{3.14}$$

$$\begin{aligned}\mathcal{Q}_3=&\frac{-1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha}Z_{\alpha,\beta}^{M}\sum_{i=1}^{N-M-1}\sum_{j=0}^{N-i-M-1}\sum_{k=2}^{N-M}\sum_{l=0}^{N-k-M}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta+1}\\&\times\frac{[2(m+N+i+j+\alpha+\beta)+1]!!}{[2(i+\alpha)-1)\,!!\,(N-i-j-M-1)\,!\,(i-1)\,!\,j\,!\,(m+j+\beta+1)!}\\&\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)\,!!\,(N-k-l-M)\,!\,(k-2)\,!\,l\,!\,(m+l+\beta)!}\\&\times\frac{(m+j+l+\beta+1)\,![2(i+k+\alpha)-5]!!}{[2(m+i+j+k+l+\alpha+\beta+M)+1]!!}.\end{aligned} \tag{3.15}$$

For the recurrence relation, we require the further rearrangement of the summation so that the index $(M+1)$ appears in each term. After splitting $\mathcal{Q}_3$ into two parts and combining them with various terms in (3.13)–(3.15), $\mathcal{P}_N^M$ can be expressed in terms of the following three sums

$$\mathcal{P}_N^M=\mathcal{R}_1+\mathcal{R}_2+\mathcal{R}_3, \tag{3.16}$$

where

$$\begin{aligned}\mathcal{R}_1=&\frac{1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha}Z_{\alpha,\beta}^{M}\sum_{i=1}^{N-(M+1)}\sum_{j=0}^{N-i-(M+1)}\sum_{k=2}^{N-(M+1)}\sum_{l=0}^{N-k-(M+1)}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta}\Delta^4\\&\times\frac{2[2(m+N+i+j+\alpha+\beta)+1]!!}{[2(i+\alpha)+1)\,!!\,[N-i-j-(M+1)]\,!\,(i-1)\,!\,j\,!\,(m+j+\beta)!}\\&\times\frac{[2(m+N+k+l+\alpha+\beta)+1]!!}{[2(k+\alpha)-1)\,!!\,[N-k-l-(M+1)]\,!\,(k-2)\,!\,l\,!\,(m+l+\beta)!}\\&\times\frac{(m+j+l+\beta)\,![2(i+k+\alpha)-3]!!}{[2(m+i+j+k+l+\alpha+\beta+M+1)+1]!!},\end{aligned} \tag{3.17}$$

$$\mathcal{R}_2=\frac{1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha}Z_{\alpha,\beta}^{M}\sum_{i=1}^{N-(M+1)}\sum_{j=0}^{N-i-(M+1)}\sum_{k=2}^{N-(M+1)}\sum_{l=0}^{N-k-(M+1)}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2(\beta+1)}$$
$$\times\frac{[2(m+N+i+j+\alpha+\beta)+1]!!}{[2(i+\alpha)-1)!!\,[N-i-j-(M+1)]!\,(i-1)!\,j!\,(m+j+\beta)!}$$
$$\times\frac{[2(m+N+k+l+\alpha+\beta)+1]!!}{[2(k+\alpha)-3)!!\,[N-k-l-(M+1)]!\,(k-2)!\,l!\,(m+l+\beta+1)!}$$
$$\times\frac{(m+j+l+\beta+1)!\,[2(i+k+\alpha)-5]!!}{[2(m+i+j+k+l+\alpha+\beta+M+1)+1]!!},\tag{3.18}$$

$$\mathcal{R}_3=\frac{-1}{N-1-M}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M-\alpha}Z_{\alpha,\beta}^{M}\sum_{i=1}^{N-(M+1)}\sum_{j=0}^{N-i-(M+1)}\sum_{k=2}^{N-(M+1)}\sum_{l=0}^{N-k-(M+1)}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta}$$
$$\times\frac{2[2(m+N+i+j+\alpha+\beta)-1]!!}{[2(i+\alpha)-1)!!\,[N-i-j-(M+1)]!\,(i-1)!\,j!\,(m+j+\beta)!}$$
$$\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)!!\,[N-k-l-(M+1)]!\,(k-2)!\,l!\,(m+l+\beta)!}$$
$$\times\frac{(m+j+l+\beta)!\,[2(i+k+\alpha)-5]!!}{[2(m+i+j+k+l+\alpha+\beta+M+1)-1]!!}.\tag{3.19}$$

Evidently, by shifting α in $\mathcal{R}_1$ by 1, and shifting β in $\mathcal{R}_2$ by 1, combining the resulting three summations with the definition of (3.10), we obtain

$$\mathcal{P}_N^M=\frac{1}{N-(M+1)}\sum_{\alpha=0}^{M+1}\sum_{\beta=0}^{M+1-\alpha}Z_{\alpha,\beta}^{M+1}$$
$$\times\sum_{i=1}^{N-(M+1)}\sum_{k=2}^{N-(M+1)}\sum_{j=0}^{N-i-(M+1)}\sum_{l=0}^{N-k-(M+1)}(-1)^{i+j+k+l}\Delta^{2(i+k+2\alpha)}(1-\Delta^2)^{j+l+2\beta}$$
$$\times\frac{[2(m+N+i+j+\alpha+\beta)-1]!!}{[2(i+\alpha)-1)!!\,[N-i-j-(M+1)]!\,(i-1)!\,j!\,(m+j+\beta)!}$$
$$\times\frac{[2(m+N+k+l+\alpha+\beta)-1]!!}{[2(k+\alpha)-3)!!\,[N-k-l-(M+1)]!\,(k-2)!\,l!\,(m+l+\beta)!}$$
$$\times\frac{(m+j+l+\beta)!\,[2(i+k+\alpha)-5)!!}{[2(m+i+j+k+l+\alpha+\beta+M+1)-1]!!}.\tag{3.20}$$

Comparing (3.20) to (3.9), we have found the relationship between $\mathcal{P}_N^M$ and $\mathcal{P}_N^{M+1}$

$$\mathcal{P}_N^{M+1}=[N-(M+1)]\mathcal{P}_N^M.\tag{3.21}$$

In other words, we have proved that

$$\mathcal{S}_3=\mathcal{P}_N^0=\frac{1}{(N-1)}\mathcal{P}_N^1=\frac{1}{(N-1)(N-2)}\mathcal{P}_N^2=\ldots=\frac{1}{(N-1)!}\mathcal{P}_N^{N-2}.\tag{3.22}$$

A remarkable property of the summation (3.20) is that, when $M=N-2$, the indices (i,j) and the indices (α,β) become decoupled and, more significantly, the indices (k,l) are eliminated in the summation. It follows that the summation (3.20) at $M=N-2$ can be carried out explicitly

$$\mathcal{P}_N^{N-2} = \left\{ \sum_{\alpha=0}^{N-2} \sum_{\beta=0}^{N-2-\alpha} Z_{\alpha,\beta}^{N-2} \Delta^{4(\alpha+1)} (1-\Delta^2)^{2\beta} \frac{[2(m+N+\alpha+\beta)+3]!!}{(2\alpha+1)!!\,(m+\beta)!} \right\} \times \left\{ \sum_{i=1}^{2} \sum_{j=0}^{2-i} \Delta^{2i} (1-\Delta^2)^j \left[\frac{(-1)^{i+j}}{(i-1)!\,j!\,(2-i-j)!} \right] \right\}.$$

For any given parameters, $\mathcal{P}_N^{N-2}$ is identically zero because

$$\sum_{i=1}^{2} \sum_{j=0}^{2-i} \left[\frac{\sigma^{2i}(1-\sigma^2)^j (1-\epsilon^2)^i}{(1-\sigma^2\epsilon^2)^{i+j}} \right] \left[\frac{(-1)^{i+j}}{(i-1)!\,j!\,(2-i-j)!} \right] \equiv 0.$$

This implies, by the recurrence relation (3.22), that $\mathcal{S}_3 \equiv 0$.

IV. COMPLETENESS OF THE POINCARÉ EIGENFUNCTION

A fundamental mathematical question is completeness of the set of eigenfunctions of the Poincaré equation given by the new Poincaré polynomials (2.17)–(2.19). If the Poincaré eigenfunction is complete, it would revolutionize the mathematical analysis in many geophysical and astrophysical problems in which the effect of rotation is critically important and the relevant geometry is spheroidal.

Nearly all the existing analyses for geophysical and astrophysical fluid dynamical problems in rotating spherical or spheroidal systems employ the Legendre polynomial (for example, Chandrasekhar, 1961; Zhang, 1992). A major disadvantage in using the Legendre polynomial is that the rotational effect couples all the orders of the Legendre polynomial together. This makes the mathematical analysis using the Legendre polynomial in rotating systems rather complicated. The undesirable coupling comes from the fact that the Legendre polynomial is not associated with the differential operator in rotating systems. The Poincaré polynomials such as (2.17)–(2.19) would replace the Legendre polynomial to provide an extremely powerful basis for the mathematical analysis in rotating spherical or spheroidal systems.

It is unfortunate, however, that we find the mathematical proof for the completeness of the set of eigenfunctions of the Poincaré equation given by the new Poincaré polynomial (2.17)–(2.19) is too complicated to be tractable. We, therefore, look for numerical evidence indicating that the new Poincaré eigenfunction given by (2.17)–(2.19) is complete and can be used to expand an arbitrary velocity distribution in rotating spheroidal systems. We consider the problem of fluid motions in a rotating spheroid driven by an external force **F**, which is governed by the following two equations (Greenspan, 1968)

$$\frac{\partial \mathbf{V}}{\partial t} + 2\mathbf{e}_z \times \mathbf{V} + \nabla \Phi = \mathbf{F}, \tag{4.1}$$

$$\nabla \cdot \mathbf{V} = 0, \tag{4.2}$$

subject to the boundary condition

$$\mathbf{e}_\eta \cdot \mathbf{V} = 0 \quad \text{at } \eta = \sqrt{1-\epsilon^2}. \tag{4.3}$$

Generally speaking, it is a difficult task to solve (4.1)–(4.3) because of spheroidal geometry. However, assuming that the Poincaré eigenfunction given by (2.17)–(2.19) is complete, we can express solutions for (4.1) and (4.2) in the form

$$\mathbf{V} = \sum_{m,N,n} Z_{Nmn} \mathbf{V}_{Nmn} e^{\hat{i}m\phi}, \tag{4.4}$$

where the eigenvector $\mathbf{V}_{Nmn}$ are normalized such that

TABLE III. Numerical evidence for the completeness of the Poincaré polynomial. N_m denotes the largest N used in expansion (4.4), $l=3$ ($l=4$) uses the odd (even) Poincaré polynomial in the expansion.

N_m	$E(l=3)$	$E(l=4)$
5	0.0859	0.1594
6	0.0334	0.0572
7	0.0133	0.0192
8	0.0075	0.0105
9	0.0027	0.0031

$$\int_V |\mathbf{V}_{Nmn}|^2 dV = 1. \tag{4.5}$$

It follows that solutions of the problem defined by (4.1)–(4.3) in a spheroid is simply

$$\mathbf{V} = \sum_{m,N,n} \frac{\hat{i}}{2\sigma_{Nmn}} \left(\int_V \mathbf{F} \cdot \mathbf{V}^+_{Nmn} dV \right) \mathbf{V}_{Nmn} e^{\hat{i} m \phi}. \tag{4.6}$$

There are no difficulties to carry out the integral in (4.6) by using the explicit Poincaré polynomial found in this paper. The discovery of the explicit Poincaré polynomial thus offers a highly effective and efficient way to solve this rather difficult problem in a rotating spheroid of arbitrary eccentricity.

To test the completeness and the convergence of expansion (4.5), we consider a special case for a rotating fluid sphere ($\epsilon=0$) in which the flow motion is driven by

$$\mathbf{F} = \mathbf{e}_z \times \left[\nabla \frac{\partial (r\Psi)}{\partial r} - \mathbf{r} \nabla^2 \Psi \right], \tag{4.7}$$

where $\mathbf{r}$ is the position vector and

$$\Psi = r^l \sin(n\pi r) P_l^m(\cos\theta) e^{im\phi},$$

where $P_l^m(\cos\theta)$ is the standard Legendre polynomial. In this case, the exact solution for (4.1)–(4.3) with $\mathbf{F}$ given by (4.7) can be easily found and can be used to check the convergence of expansion (4.4). Our extensive calculations for various different cases strongly indicate that expansion (4.4) always converges to the exact solution. Two typical examples with $m=2$ and $n=2$ using the even and odd Poincaré polynomials are shown in Table III, in which the error E is defined by

$$E = \frac{1}{V} \int_V |\mathbf{V} - \mathbf{V}_{\text{exact}}| dV, \tag{4.8}$$

where $\mathbf{V}$ is given by the truncated expansion (4.4). There is clear numerical evidence suggesting the set of eigenfunctions given by the explicit Poincaré polynomial reported in this paper is complete.

V. SUMMARY

We have presented three significant new results on the classical Poincaré problem in this paper. First, an explicit polynomial as the general solution for the classical Poincaré problem in a spheroid of arbitrary eccentricity is found for the first time. Second, we have uncovered an intriguing integral property (3.4) that has important implications for the nonlinear wave theory in a rotating spheroid. It may also have important mathematical significance in connection with why an extremely complicated summation such as (3.20) vanishes identically and whether there exists

a simpler mathematical proof for (3.4). Thirdly, the possible completeness of the set of eigenfunctions given by the Poincaré polynomial opens an exciting new line in the research of many astrophysical fluid dynamical problems in a rotating spheroid. We are able to provide numerical evidence indicating that the Poincaré eigenfunction given by the Poincaré polynomials (2.17)–(2.19) is complete and can be used to expand an arbitrary velocity distribution in rotating spheroidal systems. However, a mathematical proof for the completeness of the Poincaré eigenfunction remains to be a challenging task.

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An approach to nonstandard quantum mechanics

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We use nonstandard analysis to formulate quantum mechanics in hyperfinite-dimensional spaces. Self-adjoint operators on hyperfinite-dimensional spaces have complete eigensets, and bound states and continuum states of a Hamiltonian can thus be treated on an equal footing. We show that the formalism extends the standard formulation of quantum mechanics. To this end we develop the Loeb-function calculus in nonstandard hulls. The idea is to perform calculations in a hyperfinite-dimensional space, but to interpret expectation values in the corresponding nonstandard hull. We further apply the framework to nonrelativistic quantum scattering theory. For time-dependent scattering theory, we identify the starting time and the finishing time of a scattering experiment, and we obtain a natural separation of time scales on which the preparation process, the interaction process, and the detection process take place. For time-independent scattering theory, we derive rigorously explicit formulas for the Møller wave operators and the S-matrix. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1812358]

I. INTRODUCTION

Quantum mechanics is conventionally formulated in a complex Hilbert space, $\mathcal{H}$. The possible states of a quantum system are associated with unit vectors in $\mathcal{H}$, and the observables are associated with self-adjoint linear operators on $\mathcal{H}$. A central role plays the Hamiltonian of the quantum system. The eigenvalues of the Hamiltonian are commonly interpreted as the energies of bound states of the system. Moreover, the values of the continuous part of the Hamiltonians spectrum are interpreted as the energies of "continuum" or scattering states. The interpretation is physically motivated, and we use the term "continuum state" in a physical sense in the following. While bound states can be identified with eigenvectors of the Hamiltonian, appropriate vectors do not exist in $\mathcal{H}$ for continuum states. Continuum states can be treated in the conventional Hilbert-space framework only approximately.[1]

The probably most prominent approach to solve this problem is the rigged-Hilbert-space formalism.[2–4] Within the rigged Hilbert-space formalism, continuum states are associated with linear functionals on a dense subspace $\mathcal{M}$ of $\mathcal{H}$. The linear functionals belong to the dual space $\mathcal{M}'$ of $\mathcal{M}$, which is a locally convex space and not a Hilbert space. In particular, we do not have a scalar product at hand. The rigged-Hilbert-space formalism is thus more complicated than the Hilbert-space formalism, and more efforts are required in mathematically rigorous applications. There exist further similar approaches to model continuum states, e.g., approaches that introduce lattices of Hilbert spaces or partial-inner-product spaces. These two approaches together with the rigged-Hilbert-space approach can be classified as "super-Hilbert-space" formalisms.[2] The main idea in common is to use linear functionals on (dense) subspaces of $\mathcal{H}$, and the mathematical complications are consequently of the same nature. If we look for an appropriate formalism, which includes a scalar product, we still face a mathematical-modelling problem.

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This paper suggests an approach to nonstandard quantum mechanics. This means that we use nonstandard analysis (NSA) to construct a framework where quantum mechanics can be formulated without the drawbacks mentioned above. Work in this direction is done in Ref. 5. However, this paper presents another approach that focuses more on eigenvector expansions. Eigenvector expansions are of great importance in practical applications since they simplify calculations. Within the approach, we are able to treat bound and continuum states on the same footing without losing the scalar product. However, we require a basic knowledge of NSA for the construction as it is presented in Ref. 6 (Ref. 7), for example. Nevertheless, a few remarks on NSA are made in the following.

NSA has its origin in logics and provides an astonishing rich formalism. The author of this paper believes that we should rather speak of nonstandard methods than of NSA since NSA suggests an application of nonstandard methods to analysis, but the term NSA is commonly used in the literature in a general sense. In this sense, NSA can be applied to a wide range of mathematical areas, e.g., real analysis, topology, measure theory, functional analysis, etc. NSA introduces rigorously many interesting objects like infinitesimals, infinitely large numbers, and functions that behave like Dirac's delta distribution. The author of this paper believes that these objects — which are not available in standard mathematics — make NSA rather attractive for physical applications.

The basic tool of NSA is the transfer principle. The transfer principle enables us to transfer sets and formulas from standard to nonstandard frameworks. Roughly speaking, every formula in a standard framework is true if, and only if, the corresponding transferred formula is true in the nonstandard framework. For the application of the transfer principle we however have to formulate formulas in a rather formal way marked by logics. The formal language appears laborious from the viewpoint of the concrete application, but we need the language to ensure rigorous results.

The paper is organized as follows. In Sec. II, the basic framework is introduced, and we start discussing its relationship to the standard framework used in quantum mechanics. We continue the discussion in Sec. III where we derive the required nonstandard function calculus. We establish then the final form of the approach to nonstandard quantum mechanics in Sec. IV. In Sec. V, we apply the framework to nonrelativistic scattering theory. We discuss first the impact of the approach on time-dependent scattering theory, and derive then explicit formulas within time-independent scattering theory. Finally, we summarize the results and conclude in Sec. VI.

II. NONSTANDARD EXTENSIONS

A. Spatial and operational extensions

NSA basically introduces extensions of superstructures that contain for a given context all mathematical objects of interest. Superstructures usually contain real numbers, complex numbers, functions, etc. The extension of a superstructure $\mathcal{V}$ is actually an injective mapping of $\mathcal{V}$ onto another superstructure $\mathcal{W}$. We note that there exist different types of extensions, but for applications of NSA polysaturated extensions are probably most convenient. For this reason, we assume a polysaturated extension ${}^\star:\mathcal{V}\to\mathcal{W}$ of a superstructure $\mathcal{V}$ that contains every standard mathematical object we will consider in this paper. Roughly speaking, the extension allows us to switch from the "standard world" $\mathcal{V}$ to the "nonstandard world" $\mathcal{W}$, in which we can use our standard mathematical objects of interest more conveniently, as we will see. In particular, $\mathcal{V}$ contains a complex Hilbert space $\mathcal{H}$ and linear operators on $\mathcal{H}$, which implies that appropriate counterparts are available in the "nonstandard world" $\mathcal{W}$. Moreover, for the sake of convenience we follow the common practice and drop the prefix * from many nonstandard objects when there is no ambiguity. For example, we write $r+s$ instead of $r^\star+s$ for $r,s\in{}^\star\mathbb{R}$. We obtain for our example a sensible simplification of notation since two hyper-real numbers can be added in the same manner as two real numbers.

As a consequence of polysaturation, there exists a hyperfinite-dimensional space H which externally contains $\mathcal{H}$,[8] i.e., $\{{}^\star x:x\in\mathcal{H}\}\subset H$. For the sake of convenience we simply write

$\mathcal{H} \subset H \subset {}^\star\mathcal{H}$. We use this result as an avenue to a nonstandard framework for quantum mechanics. Beside the well-known advantages of NSA, which are sketched in Sec. I, this approach has another important advantage: The transfer principle allows us to apply the results of linear algebra in finite-dimensional spaces to the hyperfinite-dimensional space H. We note that this idea is already known in the literature for a long time.[9,10]

The main goal in the following is to show that the formulation of quantum mechanics in an appropriate hyperfinite-dimensional space yields an extension of the standard formulation of quantum mechanics. We choose however a more general setting than outlined above, and assume only a dense subspace $\mathcal{M}$ of $\mathcal{H}$. We will see in Sec. IV B that this approach is quite convenient when we construct the hyperfinite dimensional space H in an example. However, by polysaturation there exists a hyperfinite-dimensional space H which externally contains $\mathcal{M}$, i.e., $\mathcal{M} \subset H \subset {}^\star\mathcal{M} \subset {}^\star\mathcal{H}$.

Proposition 1: Let $H \subset {}^\star\mathcal{H}$ be an internal Hilbert space that externally contains a dense subspace $\mathcal{M}$ of $\mathcal{H}$, and let O denote the projection of ${}^\star\mathcal{H}$ onto H, then ${}^\star x \approx O^\star x$ for all $x \in \mathcal{H}$.

Proof: Assume $x \in \mathcal{H}$. Since $\mathcal{M}$ is dense in $\mathcal{H}$ the internal statement $(\exists y \in H)\|{}^\star x - y\| < 1/n$ is true for all $n \in \mathbb{N}$. By the overflow principle there exists an infinite $m \in {}^\star\mathbb{N}$ for which $(\exists y \in H)\|{}^\star x - y\| < 1/m$ holds. Moreover, the (transferred) projection theorem states that $\|{}^\star x - O^\star x\| \leqslant \|{}^\star x - y\| < 1/m$.[1] □

Let us proceed with our discussion. As in proposition 1, let O denote the projection of ${}^\star\mathcal{H}$ onto H. O can be defined (as usual) by an orthonormal basis of H, as we show in the appendix. Moreover, let A be a self-adjoint operator with domain $\mathcal{D}(A)$, for which $\mathcal{M} \subset \mathcal{D}(A) \subset \mathcal{H}$ holds. Using the transfer principle we define the restriction of ${}^\star A$ to H by $B = O^\star A O$, and $B^\star x = O^\star(Ax) \approx {}^\star(Ax)$ for all $x \in \mathcal{M}$. B can thus be seen as a nonstandard extension of the restriction of A to $\mathcal{M}$. As shown in the Appendix, B is an internal hyperfinite-rank operator, and there exists an eigensystem $\{(\lambda_i, x_i)\}_{i=1}^h$ for B, which yields the representation

$$(\forall x, y \in H) \quad \langle x, By \rangle = \sum_{i=1}^{h} \lambda_i \langle x, x_i \rangle \langle x_i, y \rangle.$$

We note that h is the (nonstandard) dimension of H.

Our construction shows that there exist self-adjoint hyperfinite-rank operators, which yield extensions of standard self-adjoint operators in a certain sense. The relation is however rather weak at the moment since we do not know how the spectra and the function calculus of these operators are related. In particular, we may ask if nonstandard eigenvalues and nonstandard eigenvectors can be interpreted in a sensible way. To discuss these questions more thoroughly we introduce nonstandard hulls, which are important tools in NSA.[8] From a physical point of view, the introduction of nonstandard hulls is motivated by the assumption that infinitesimally different states cannot be distinguished in a measurement.

The definition of the nonstandard hull ${}^oH$ of the hyperfinite-dimensional space H introduces an equivalence relation on the set of finite nonstandard vectors, $\mathrm{fin}(H) = \{x \in H : \|x\| \in \mathrm{fin}({}^\star\mathbb{R})\}$. We note that $\mathrm{fin}({}^\star\mathbb{R})$ is the set of finite hyper-reals. Two vectors are equivalent if their difference has infinitesimal norm. The nonstandard hull ${}^oH$ of the space H is given as the quotient

$${}^oH = \mathrm{fin}(H)/H_0, \quad H_0 = \{x \in H : \|x\| \approx 0\},$$

$$\|{}^o x\| = \mathrm{st}(\|x\|), \quad \langle {}^o x, {}^o y \rangle = \mathrm{st}(\langle x, y \rangle). \tag{1}$$

${}^oH$ is a Hilbert space, and $\mathcal{H}$ is a closed subspace of ${}^oH$ by proposition 1. Especially, reconsidering our example above the equation $B^\star x = O^\star(Ax) \approx {}^\star(Ax)$ yields $Ax = {}^o(Bx)$ for all $x \in \mathcal{M}$. We note that we adopt the notation ${}^oH$ for the nonstandard hull of H as it is used in Refs. 9 and 10, instead of the notation $\hat{H}$ that seems to be more common.[6] The author of this paper believes that we gain a more uniform notation since, for example, for the standard part ${}^o r = \mathrm{st}(r)$ of $r \in \mathrm{fin}({}^\star\mathbb{R})$ we could also write $\hat{r}$, meaning an element of the nonstandard hull of ${}^\star\mathbb{R}$.

Furthermore, nonstandard hulls are defined also for finitely bounded nonstandard linear operators. If A is a bounded operator on $\mathcal{H}$, then $B=O^{\star}AO$ is finitely bounded and its nonstandard hull is defined as

$$
\begin{aligned}
{}^{o}B\,{}^{o}x &= {}^{o}(Bx) \quad \forall\, x \in \mathrm{fin}(H), \\
\|{}^{o}B\| &= \mathrm{st}(\|B\|).
\end{aligned}
\tag{2}
$$

Since A is bounded we obtain ${}^{\star}(Ax)\approx O^{\star}AO^{\star}x$ for $x\in\mathcal{H}$. Thus, ${}^{o}B$ is a self-adjoint bounded operator on ${}^{o}H$, which extends A, i.e., ${}^{o}Bx={}^{o}(B^{\star}x)=Ax$ for all $x\in\mathcal{H}$. We note that operational nonstandard extensions of this type are already discussed in Ref. 10. In particular, the relationship between the spectral resolution of bounded self-adjoint operators and their nonstandard extension is investigated. However, we come back to these results in Sec. II B.

B. Spectral properties of operator extensions

Hyperfinite-rank operators have convenient spectral properties, which are determined by linear algebra. If we consider a nonstandard extension B of a self-adjoint operator A as constructed in Sec. II A then we may naturally ask how the eigenvalues and eigenvectors of the hyperfinite-rank operator B are related to the spectral resolution of A. Let us focus first on the eigenvalues.

Lemma 1: Let B be a normal hyperfinite-rank operator, and let $\lambda\in\mathbb{C}$. Assume that for each $n\in\mathbb{N}$ there exists an $x_n\in H$ for which $\|x_n\|\approx 1$ and $\|\lambda x_n - Bx_n\|<1/n$ holds, then there exists a $\lambda'\in\sigma(B)$, and $\lambda\approx\lambda'$.

Proof: As shown in the Appendix, B has an eigensystem $\{(\lambda_i,x_i)\}_{i=1}^{h}$. Fix $\epsilon\in\mathbb{R}_+$, $\epsilon<1$, then

$$
(\forall\, n\in\mathbb{N})(\exists x\in H)\left(\|x\|>(1-\epsilon)\wedge\|\lambda x - Bx\|\leqslant\frac{1}{n}\right).
$$

By the overspill principle there exists an infinite $m\in{}^{\star}\mathbb{N}$ for which

$$
(\exists x_0\in H)\left(\|x_0\|>(1-\epsilon)\wedge\|\lambda x_0 - Bx_0\|\leqslant\frac{1}{m}\right)
$$

is true. Assume that there exists an $\epsilon'\in\mathbb{R}_+$ for which $|\lambda-\lambda'|\geqslant\epsilon'$ holds for all $\lambda'\in\sigma(B)$. Then,

$$
\|Bx_0-\lambda x_0\|^2=\sum_{i=1}^{h}|\lambda-\lambda_i|^2|\langle x_i,x_0\rangle|^2\geqslant(\epsilon')^2\sum_{i=1}^{h}|\langle x_i,x_0\rangle|^2=(\epsilon')^2\,\|x_0\|^2>(\epsilon')^2(1-\epsilon)^2
$$

and we obtain the contradiction $\|Bx_0-\lambda x_0\|>\epsilon'(1-\epsilon)>1/m$. There thus exists a $\lambda'\in\sigma(B)$ for which $\lambda\approx\lambda'$ holds. □

Proposition 2:

(1) Let B be a nonstandard extension of a self-adjoint operator A as constructed in Sec. II A, then for each $\lambda\in\sigma(A)$ there exists a $\lambda'\in\sigma(B)$ for which $\lambda\approx\lambda'$ holds, i.e., $\sigma(A)\subset{}^{o}NS(\sigma(B))$.
(2) Let B be a finitely bounded normal hyperfinite-rank operator, then $\sigma({}^{o}B)={}^{o}\sigma(B)$.

Proof:

(1) Let $\lambda\in\sigma(A)$, then for each $n\in\mathbb{N}$ there exists an $x_n\in\mathcal{M}$ for which $\|x_n\|=1$ and $\|(\lambda-A)x_n\|<1/n$ holds. Since $\mathcal{M}$ is externally contained in H, we obtain $\|(\lambda-B)^{\star}x_n\|\leqslant 1/n$ for each $n\in\mathbb{N}$, and by lemma 1 there exists a $\lambda'\in\sigma(B)$ with $\lambda\approx\lambda'$.
(2) We note that this statement can be proved also with the help of lemma 1. However, the statement is proved in a more general form in Ref. 8, and therefore we omit the proof. □

The first part of proposition 2 shows that the spectrum of A is approximated well by the eigenvalues of its nonstandard extension B. We can draw from this result a remarkable conclusion.

Let $\lambda \in \sigma(A)$, then there exists an eigenvalue $\lambda' \approx \lambda$ of B. Since B has a complete set of (normed) eigenvectors, there exists an $x \in H$ for which $Bx = \lambda' x$ holds. For each $y \in \mathcal{M}$ we obtain thus

$$\langle {}^o x, Ay \rangle = {}^o\langle x, B^\star y \rangle = st(\lambda')\,{}^o\langle x, {}^\star y \rangle = \lambda \langle {}^o x, y \rangle. \tag{3}$$

Equations of this type can usually be formulated only as eigenfunctional equations in super-Hilbert-space formalisms. The treatment of continuum states is therefore more complicated than the treatment of bound states in these frameworks. In a hyperfinite-dimensional space we can however treat both types of states on an equal footing. We note that work in this direction is also presented in Ref. 5 where the concept of ultraeigenvectors is introduced. The concept leads to similar equations, but ultraeigenvectors are not necessarily eigenvectors of a nonstandard extension. In particular, we generally do not obtain an eigenvector basis, which is simpler to use in applications as compared to projection-valued measures.

Moreover, if the operator A is bounded in proposition 2 then the nonstandard hull ${}^oB$ of B is a bounded self-adjoint operator on ${}^oH$. This case is extensively studied in Refs. 9 and 10. In particular, the operator A is then the restriction of ${}^oB$ to $\mathcal{H}$, and the projection-valued measure associated with A can be retrieved with the help of the eigenvectors of B. Unfortunately, most of the self-adjoint operators occurring in applications are unbounded. Also, we do not know how the function calculus of A is related to the function calculus of B, especially when we consider noncontinuous functions. We therefore use a more general approach that is related to nonstandard integration theory.

III. LOEB-FUNCTION CALCULUS

In our approach to nonstandard function calculus we introduce first projection-valued Loeb measures that are closely related to Loeb measures. The relationship is analogous to the relationship of standard projection-valued measures to finite Borel measures. We use projection-valued Loeb measures to prove a nonstandard spectral theorem and to establish the Loeb-function calculus. Finally, we use the results to introduce generalized nonstandard hulls, which we use in Sec. IV for the further discussion.

A. Projection-valued Loeb measures

Let $\mathcal{B}$ denote the set of Borel subsets of $\mathbb{R}$, and let P be a finite probability measure on $\mathcal{B}$. The associated probability space $(\mathbb{R}, \mathcal{B}, P)$ transfers to a finitely additive internal probability space, $({}^\star\mathbb{R}, {}^\star\mathcal{B}, {}^\star P)$. To be more general, we replace ${}^\star P$ by a finitely additive internal probability function μ, and consider the probability space $({}^\star\mathbb{R}, {}^\star\mathcal{B}, \mu)$. An important result of nonstandard measure theory is the construction of a Loeb (probability) space out of $({}^\star\mathbb{R}, {}^\star\mathcal{B}, \mu)$,[11] i.e., there exists a standard (σ-additive) probability space $({}^\star\mathbb{R}, {}^\star\mathcal{B}_L, \mu_L)$ such that

(1) ${}^\star\mathcal{B}_L$ is a σ-algebra with ${}^\star\mathcal{B} \subset {}^\star\mathcal{B}_L \subset \mathcal{P}({}^\star\mathbb{R})$,
(2) ${}^o\mu = \mu_L$ on ${}^\star\mathcal{B}$.

The sets $\Omega \in {}^\star\mathcal{B}_L$ are called Loeb measurable, and μ_L is called a Loeb measure. The σ-algebra ${}^\star\mathcal{B}_L$ is however related to the finitely additive internal probability function μ, i.e., we should rather write ${}^\star\mathcal{B}_L(\mu)$. To obtain a more general setting we introduce a smaller σ-algebra. Let Λ denote the set of finitely additive internal probability functions on ${}^\star\mathcal{B}$. The intersection $\mathcal{A} = \cap_{\mu \in \Lambda} {}^\star\mathcal{B}_L(\mu)$ is a σ-algebra, and contains the universally Loeb-measurable sets. For each $\mu \in \Lambda$ the space $({}^\star\mathbb{R}, \mathcal{A}, \mu_L)$ is a standard probability space. Moreover, ${}^\star\mathcal{B} \subset \mathcal{A}$ and ${}^o\mu = \mu_L$ on ${}^\star\mathcal{B}$.

Let χ_Ω denote the characteristic function of a set $\Omega \in {}^\star\mathcal{B}$. We may, for example, use the eigensystem of a normal hyperfinite-rank operator B to define a finitely additive internal projection-valued probability function:

$$E_\Omega = \chi_\Omega(B) = \sum_{\lambda_i \in \Omega} |x_i\rangle\langle x_i| = \sum_{i=1}^{h} \chi_\Omega(\lambda_i)|x_i\rangle\langle x_i| \quad (\Omega \in {}^\star\mathcal{B}). \tag{4}$$

We note that $\{E_\Omega\}$ is the projection-valued * measure of B. Generally, if we assume a finitely additive internal projection-valued probability function $\{E_\Omega\}_{\Omega \in {}^\star\mathcal{B}}$, e.g., a projection-valued * measure that is associated with an internal normal operator, then we can define for each normed vector $x \in H$, $\|x\|=1$, a probability function $\mu^{(x)}$ on ${}^\star\mathcal{B}$:

$$\mu^{(x)}(\Omega) = \|E_\Omega x\|^2 = \langle x, E_\Omega x\rangle \quad (\Omega \in {}^\star\mathcal{B}). \tag{5}$$

We denote the associated Loeb measure by $\mu_L^{(x)}$. Moreover, we introduce complex-valued Loeb measures. For $x,y \in \mathrm{fin}(H)$ let

$$\mu^{(x,y)}(\Omega) = \langle x, E_\Omega y\rangle \quad (\Omega \in {}^\star\mathcal{B}). \tag{6}$$

Since E_Ω is a projection, $\mu^{(x,y)}$ can be decomposed into four finitely additive positive internal functions on ${}^\star\mathcal{B}$ by polarization,[1]

$$\mu^{(x,y)} = \sum_{k=1}^{4} a_k \nu^{(k)}, \quad a_k \in {}^\star\mathbb{C}.$$

If $\nu^{(k)} \neq 0$ we can use the normalization $\nu^{(k)}({}^\star\mathbb{R})=1$ without any restriction. Each nonzero $\nu^{(k)}$ can be extended to an ordinary Loeb measure $\nu_L^{(k)}$. If $\mu^{(x,y)} \neq 0$ we can thus construct a finite complex-valued Loeb measure, $\mu_L^{(x,y)}$, that is the sum of up to four ordinary Loeb measures multiplied by appropriate complex factors. For the sake of completeness we define further $\mu_L^{(x,y)}=0$ if $\mu^{(x,y)}=0$.

The family of nonstandard hulls $\{{}^oE_\Omega\}_{\Omega \in {}^\star\mathcal{B}}$ is a family of projections on ${}^oH$, and $\mu_L^{(x,y)}(\Omega) = \langle {}^ox, {}^oE_\Omega {}^oy\rangle$ for all $x,y \in \mathrm{fin}(H)$, $\Omega \in {}^\star\mathcal{B}$. This result motivates us to extend the definition of ${}^oE_\Omega$ to all sets $\Omega \in \mathcal{A}$. For $\Omega \in {}^\star\mathcal{B}$ we denote the range of ${}^oE_\Omega$ by $R(\Omega)$, which is a closed subspace. For $\Omega \in \mathcal{A}$ let ${}^\star\mathcal{B}_\Omega = \{\Omega' \in {}^\star\mathcal{B} : \Omega' \subset \Omega\}$. We extend $R(\Omega)$ to $\mathcal{A}$ by

$$R(\Omega) = \mathrm{cl}\left(\bigcup_{\Omega' \in {}^\star\mathcal{B}_\Omega} R(\Omega') \right), \tag{7}$$

and define ${}^oE_\Omega$ as the projection of ${}^oH$ onto $R(\Omega)$. Using a statement in Ref. 12 on families of projections we conclude for $x \in H$, $\|x\|=1$,

$$\langle {}^ox, {}^oE_\Omega {}^ox\rangle = \sup_{\Omega' \in {}^\star\mathcal{B}_\Omega} \langle {}^ox, {}^oE_{\Omega'} {}^ox\rangle = \sup_{\Omega' \in {}^\star\mathcal{B}_\Omega} \mu_L^{(x)}(\Omega') = \mu_L^{(x)}(\Omega). \tag{8}$$

Theorem 2: Let $\{E_\Omega\}_{\Omega \in {}^\star\mathcal{B}}$ be a finitely additive internal projection-valued probability function, then $\{{}^oE_\Omega\}_{\Omega \in \mathcal{A}}$ defines a projection-valued Loeb measure.

Proof: We show that the family $\{{}^oE_\Omega\}_{\Omega \in \mathcal{A}}$ has the properties of a projection-valued measure.

(a) Assume $\Omega_1, \Omega_2 \in \mathcal{A}$, and $\Omega_1 \cap \Omega_2 = \emptyset$, then $\Omega_1' \cap \Omega_2' = \emptyset$ and $R(\Omega_1') \perp R(\Omega_2')$ for all $\Omega_1' \in {}^\star\mathcal{B}_{\Omega_1}$, $\Omega_2' \in {}^\star\mathcal{B}_{\Omega_2}$. Thus, $R(\Omega_1') \perp R(\Omega_2)$ for all $\Omega_1' \in {}^\star\mathcal{B}_{\Omega_1}$, $R(\Omega_1) \perp R(\Omega_2)$, and ${}^oE_{\Omega_1} {}^oE_{\Omega_2} = {}^oE_{\Omega_2} {}^oE_{\Omega_1} = 0$.

(b) Assume $\Omega_1, \Omega_2 \in \mathcal{A}$, and $\Omega_1 \subset \Omega_2$, then $R(\Omega_1) \subset R(\Omega_2)$, and ${}^oE_{\Omega_1} {}^oE_{\Omega_2} = {}^oE_{\Omega_2} {}^oE_{\Omega_1} = {}^oE_{\Omega_1}$.[12]

(c) Assume $\Omega_n \in \mathcal{A}$, $n \in \mathbb{N}$, and $\Omega_n \cap \Omega_m = \emptyset$ if $n \neq m$. Let $\Omega = \cup_n \Omega_n$, and let $P_N = \Sigma_{n=1}^N {}^oE_{\Omega_n}$. P_N is a projection since P_N is self-adjoint and $P_N^2 = P_N$ by (a).[1] For $x \in H$, $\|x\|=1$, we obtain by (b),

$$\|({}^oE_\Omega - P_N){}^ox\|^2 = \langle {}^ox, ({}^oE_\Omega - P_N){}^ox\rangle = \mu_L^{(x)}(\Omega) - \sum_{n=1}^{N} \mu_L^{(x)}(\Omega_n),$$

$$\lim_{N\to\infty}\|({}^oE_\Omega - P_N)^o x\|^2 = 0.$$

(d) Assume $\Omega_1,\Omega_2 \in \mathcal{A}$. Using (c) we obtain ${}^oE_{\Omega_1\cap\Omega_2} + {}^oE_{\Omega_1\setminus\Omega_2} = {}^oE_{\Omega_1}$, and using (a), (b) we obtain ${}^oE_{\Omega_1}{}^oE_{\Omega_2} = ({}^oE_{\Omega_1\cap\Omega_2} + {}^oE_{\Omega_1\setminus\Omega_2}){}^oE_{\Omega_2} = {}^oE_{\Omega_1\cap\Omega_2} = {}^oE_{\Omega_2}({}^oE_{\Omega_1\cap\Omega_2} + {}^oE_{\Omega_1\setminus\Omega_2}) = {}^oE_{\Omega_2}{}^oE_{\Omega_1}$.

B. Spectral theorem

We have seen in Sec. III A that a projection-valued ★ measure extends to a projection-valued Loeb measure $\{{}^oE_\Omega\}_{\Omega\in\mathcal{A}}$ on ${}^oH$. We now use this result to formulate a nonstandard spectral theorem. We note that the theorem is obtained not by transfer of a standard spectral theorem. It is rather an analog associated with Loeb integration theory.

We call a complex-valued function $f: {}^\star\mathbb{R}\to\mathbb{C}$ $\mathcal{A}$-measurable or Loeb measurable if $f^{-1}(\Omega) \in \mathcal{A}$ for each Borel set $\Omega\subset\mathbb{C}$. We note that st$(\cdot)$ is $\mathcal{A}$-measurable.[11]

Theorem 3: Let B be an internal self-adjoint operator on an internal Hilbert space H, let $\{{}^oE_\Omega\}_{\Omega\in\mathcal{A}}$ be the projection-valued Loeb measure associated with the projection-valued ★ measure of B, and let f be a complex-valued $\mathcal{A}$-measurable function, then $f(B)=\int f\ \mathrm{d}\,{}^oE$ is a normal operator on ${}^oH$, and $\sigma(f(B))\subset \mathrm{cl}(f(\sigma(B)))$.

Proof: First we note that if two vectors $x,y\in \mathrm{fin}(H)$ are approximately equal, $x\approx y$, then the associated Loeb measures are equal, $\mu_L^{(x)}=\mu_L^{(y)}$. Consequently, for $x,y\in{}^oH$ the Loeb measure $\langle x,{}^oE_\Omega y\rangle$ $(\Omega\in\mathcal{A})$ is well defined, and we use the notation $\mu_L^{(x,y)}=\langle x,{}^oE_\Omega y\rangle$ in this proof. The domain of f is given by

$$D(f(B)) = \left\{ x\in {}^oH: \int |f|^2\ \mathrm{d}\mu_L^{(x)} < \infty \right\}. \tag{9}$$

For $n\in\mathbb{N}$ let $\Omega_n=\{r\in{}^\star\mathbb{R}: |f(r)|\leqslant n\}$. Each Ω_n is measurable, $\Omega_n\in\mathcal{A}$. Let $x\in{}^oH$, and let $x_n = {}^oE_{\Omega_n}x$, then $x_n\in D(f(B))$ for all $n\in\mathbb{N}$, and $x=\lim_n x_n$. Hence, $\mathrm{cl}(D(f(B))={}^oH$. Let $f(B)^\dagger$ denote the adjoint of $f(B)$, and let z^* denote the complex conjugate of $z\in\mathbb{C}$. For $x\in D(f(B))$, $y\in D(f(B)^\dagger)$ we obtain

$$\langle x, f(B)^\dagger y\rangle = \langle f(B)x, y\rangle = \langle y, f(B)x\rangle^* = \left(\int f\ \mathrm{d}\mu_L^{(y,x)}\right)^* = \int f^*\ \mathrm{d}\mu_L^{(x,y)} = \langle x, f^*(B)y\rangle, \tag{10}$$

i.e., $f(B)^\dagger = f^*(B)$, $D(f(B)^\dagger)=D(f(B))$, and $f(B)$ is normal.

Let $\lambda\in\sigma(f(B))$, and let $\epsilon > o$. Since $f(B)$ is normal there exists an $x\in{}^oH$ for which $\|x\|=1$ and

$$\|(f(B)-\lambda)x\|^2 = \int |f-\lambda|^2\ \mathrm{d}\mu_L^{(x)} < \epsilon^2$$

holds. Let $\Omega_\epsilon=\{r\in{}^\star\mathbb{R}: |f(r)-\lambda|<\epsilon\} = f^{-1}(\{r\in\mathbb{R}: |r-\lambda|<\epsilon\})$, then $\mu_L^{(x)}(\Omega_\epsilon)>0$, and thus ${}^oE_{\Omega_\epsilon}\neq 0$. Moreover, there exists an $\Omega'_\epsilon\in{}^\star\mathcal{B}_{\Omega_\epsilon}$ for which $\mu_L^{(x)}(\Omega'_\epsilon)>0$ holds. Thus, $E_{\Omega'_\epsilon}\neq 0$ and $\Omega'_\epsilon\cap\sigma(B)\neq\emptyset$. Choose $\omega_\epsilon\in\Omega'_\epsilon\cap\sigma(B)$, then $|f(\omega_\epsilon)-\lambda|<\epsilon$, and thus $\lambda\in\mathrm{cl}(f(\sigma(B)))$. □

Corollary 1: Assume the conditions of theorem 3. If B is additionally a hyperfinite-rank operator, then

(1) $\sigma(f(B))=\mathrm{cl}(f(\sigma(B)))$,
(2) $\sigma({}^og(B))={}^og(\sigma(B))$ for finitely bounded $g\in{}^\star\mathcal{B}(\mathbb{R})$.

Proof:

(1) Let $\lambda\in\sigma(B)$, and let x be a corresponding eigenvector, then ${}^oE_{\{\lambda\}}{}^ox = {}^ox$, $f(B)^ox = f(\lambda)^ox$, and $f(\lambda)\in\sigma(f(B))$. Since $\sigma(f(B))$ is closed we obtain $\mathrm{cl}(f(\sigma(B)))\subset\sigma(f(B))$. The assertion follows now from theorem 3.

(2) Let $g \in {}^\star\mathcal{B}(\mathbb{R})$ be finitely bounded. Since B is a hyperfinite-rank operator we obtain $\sigma(g(B))=g(\sigma(B))$. Thus, $\sigma({}^o g(B))={}^o\sigma(g(B))={}^o g(\sigma(B))$ by proposition 2. □

If we consider in theorem 3 a real-valued function f, then we obtain a self-adjoint operator $f(B)$. For this operator, the standard spectral theorem yields the standard spectral representation. Since theorem 3 states an alternative nonstandard representation of $f(B)$ we clarify now the relationship between both representations.

Theorem 4: Let B be an internal self-adjoint operator on an internal Hilbert space H, let f be a real-valued $\mathcal{A}$-measurable function, and let g be a Borel function, then $g(f(B))=(g\circ f)(B)$.

Proof: For a Borel set $\Omega \in \mathcal{B}$ let $F_\Omega = {}^oE_{f^{-1}(\Omega)}$. F_Ω defines a projection-valued measure, and for $x \in \mathrm{fin}(H)$ we obtain

$$\mu_{f,L}^{(x)}(\Omega) = \mu_L^{(x)}(f^{-1}(\Omega)) = \langle {}^o x, {}^oE_{f^{-1}(\Omega)}\, {}^o x\rangle = \langle {}^o x, F_\Omega\, {}^o x\rangle.$$

Let us assume first that g is bounded, then we obtain for $\Omega \in \mathcal{B}$,

$$\int_\Omega g \, \mathrm{d}\mu_{f,L}^{(x)} = \int_{f^{-1}(\Omega)} g\circ f \, \mathrm{d}\mu_L^{(x)}.$$

We conclude that $\int g\, \mathrm{d}F = \int g\circ f \, \mathrm{d}\, {}^oE$. If we apply pointwise-convergence arguments the latter equation is valid for any Borel function g. In particular, for $g=i\mathrm{d}$ we obtain $f(B)=\int \omega \, \mathrm{d}F_\omega$, which is just the standard spectral representation. Since $\int g\, \mathrm{d}F = g(\int \omega \, \mathrm{d}F_\omega) = g(f(B))$ we obtain the statement of the theorem. □

We note that theorem 4 reveals the relationship between the standard and the nonstandard spectral representation of the self-adjoint operator $f(B)$: For each Borel set Ω we obtain $F_\Omega := \chi_\Omega(f(B)) = \int \chi_\Omega \circ f \, \mathrm{d}\, {}^oE = {}^oE_{f^{-1}(\Omega)}$, and $f(B)=\int \omega \, \mathrm{d}F_\omega$.

C. Nonstandard hulls

As pointed out in Sec. II operational nonstandard hulls are well known for finitely bounded internal operators. For infinite internal operators, however, ambiguities occur if we consider standard parts: Let B be a hyperfinite-rank operator that has an infinite eigenvalue λ, let x be the corresponding normed eigenvector, and let $y=x/\lambda$, then ${}^o y = 0$ but ${}^o(By) = {}^o x \neq 0$. We see by this example that for infinite internal operators an equation like ${}^oB\, {}^o x = {}^o(Bx)$ can generally not be true. The definition of nonstandard hulls for infinite internal operators is thus not straightforward. Nevertheless, if we consider self-adjoint internal operators then we can use the Loeb-function calculus for a sensible definition. The principal idea is to project those vectors out that cause the ambiguities. To arrive at a sensible definition we consider first finitely bounded internal operators. Moreover, let $\mathcal{B}(\mathbb{R})$ be the set of complex-valued Borel functions on $\mathbb{R}$.

Proposition 3: Let B be an internal self-adjoint operator on an internal Hilbert space H, let $\{{}^oE_\Omega\}_{\Omega\in A}$ be the projection-valued Loeb measure associated with the projection-valued * measure of B, and let $f \in {}^\star\mathcal{B}(\mathbb{R})$ be finitely bounded, then

$$\langle {}^o x, {}^o f(B)\, {}^o y\rangle = \mathrm{st}\left(\int f(\omega)\mathrm{d}\langle x, E_\omega y\rangle\right) = \int {}^o f \mathrm{d}\mu_L^{(x,y)} \quad (x,y \in \mathrm{fin}(H)). \tag{11}$$

Proof: We assume first that f is real valued. The generalization to complex-valued functions f is straightforward.

For $n \in {}^\star\mathbb{N}$, $k \in {}^\star\mathbb{Z}$ let $S_{k,n}=\{r \in {}^\star\mathbb{R} : k/n \leqslant f(r) < (k+1)/n\}$, and let $I_n=\{k \in {}^\star\mathbb{Z} : S_{k,n} \neq \emptyset\}$. Since f is finitely bounded I_n is hyperfinite. Moreover, ${}^\star\mathbb{R} = \cup_{k\in I_n} S_{k,n}$. Define $f_n = \Sigma_{k\in I_n} (k/n)\, \chi_{S_{k,n}}$, then $f_n \uparrow f$, and $|f_n(r)-f(r)| < 1/n$ for all $r \in {}^\star\mathbb{R}$. Moreover, ${}^o f_n \uparrow {}^o f (n \in \mathbb{N}))$, and

$$\int {}^o f d\mu_L^{(x,y)} = \lim_{n\in\mathbb{N}} \int {}^o f_n \mathrm{d}\mu_L^{(x,y)} \quad (x,y \in \mathrm{fin}(H))$$

$$= \lim_{n\in\mathbb{N}} \sum_{k\in I_n} \frac{k}{n} \mu_L^{(x,y)}(S_{k,n})$$

$$= \lim_{n\in\mathbb{N}}{}^{o}\sum_{k\in I_n} \int \frac{k}{n} \chi S_{k,n}(\omega) \mathrm{d}\langle x, E_\omega y\rangle$$

$$= {}^{o}\int f_n(\omega) \mathrm{d}\langle x, E_\omega y\rangle \quad (n \in {}^{\star}\mathbb{N}\setminus\mathbb{N})$$

$$= {}^{o}\int f(\omega) \mathrm{d}\langle x, E_\omega y\rangle$$

$$= {}^{o}\langle x, f(B) y\rangle = \left\langle {}^{o}x, {}^{o}f(B)\, {}^{o}y\right\rangle.$$

We note that we use $f_n(r) \approx f(r)$ for $n \in {}^{\star}\mathbb{N}\setminus\mathbb{N}$in the calculation. □

We note that if the operator B is finitely bounded in proposition 3 then the spectrum of B consists only of near-standard points, $\sigma(B) \subset \mathrm{fin}({}^{\star}\mathbb{R})$, and thus ${}^{o}B = \int_{\mathrm{fin}({}^{\star}\mathbb{R})} \mathrm{st}\ \mathrm{d}\,{}^{o}E$. Moreover, the last equation provides a correct approach for an extended definition of nonstandard hulls.

Definition 1: Let B be an internal self-adjoint operator on an internal Hilbert space H, and let $\{{}^{o}E_\Omega\}_{\Omega\in\mathcal{A}}$ be the projection-valued Loeb measure associated with the projection-valued * measure of B. The nonstandard hull of B is given by

$${}^{o}B = \int_{\mathrm{fin}\left({}^{\star}\mathbb{R}\right)} \mathrm{st}\ \mathrm{d}\,{}^{o}E.$$

This definition avoids the ambiguities mentioned above since the critical vectors, i.e., the vectors belonging to the range of ${}^{o}E_{\mathrm{fin}({}^{\star}\mathbb{N}\setminus{}^{\star}\mathbb{N})}$, are projected out. In particular, if x is an eigenvector of B in definition 1, then ${}^{0}B^{0}x = 0$ if x belongs to an infinite eigenvalue. We note that the statement $(\forall x \in \mathrm{fin}(H))\ {}^{0}B^{0}x = {}^{0}(Bx)$ holds for finitely bounded operators but not for infinite operators in definition 1. Generally, we obtain for $x, Bx \in \mathrm{fin}(H)$ rather

$${}^{0}B\,{}^{o}x = {}^{o}E_{\mathrm{fin}\left({}^{\star}\mathbb{R}\right)}\,{}^{o}(Bx). \tag{12}$$

IV. NONSTANDARD QUANTUM MECHANICS

A. Operational extensions

We continue now our discussion started in Sec. II. In particular, we consider a dense subset $\mathcal{M}$ of a Hilbert space $\mathcal{H}$, which is externally contained in a hyperfinite dimensional space H, and for which $\mathcal{M} \subset H \subset {}^{\star}\mathcal{M} \subset {}^{\star}\mathcal{H}$ holds. We note that $\mathcal{H} \subset {}^{o}H$ by proposition 1. We have seen in Sec. II that each bounded linear operator on $\mathcal{H}$ can be extended by a finitely bounded hyperfinite-rank operator on H, and that the extension is based on nonstandard hulls. In Sec. III we have worked out the connection of nonstandard hulls to the Loeb-function calculus. In particular, we have introduced nonstandard hulls for infinite self-adjoint internal operators. Now we use these results to generally establish the extension of standard self-adjoint operators to self-adjoint hyperfinite-rank operators.

Let A be a self-adjoint operator on $\mathcal{H}$, then $A' = \tan^{-1}(A)$ is a bounded self-adjoint operator on H. The hyperfinite-rank operator $B' = O\ {}^{\star}A' O$ is a nonstandard extension of A', i.e., ${}^{o}B'|_{\mathcal{H}} = A'$. We note that O denotes the projection of ${}^{\star}\mathcal{H}$ onto H. Moreover, we note that $\chi_{(-\pi/2,\pi/2)}(A')$

$=\chi_{\mathbb{R}}(A)=1$ and that $A=\tan(A')$. For $r\in\mathbb{R}$ let $\mathrm{tg}(r)=\tan(r\cdot\chi_{(-\pi/2,\pi/2)}(r))$. Since ${}^oB'|_{\mathcal{H}}=A'$ we obtain $\mathrm{tg}(A')=\mathrm{tg}({}^oB')|_{\mathcal{D}(\mathrm{tg}(A'))}$. Since $\mathrm{st}\circ\mathrm{tg}=\mathrm{tg}\circ\mathrm{st}$ on $\mathrm{fin}({}^\star\mathbb{R})$ we get further $\mathrm{tg}({}^oB')={}^o\mathrm{tg}(B')$ by proposition 3 and theorem 4, and thus $A=\mathrm{tg}(A')={}^o(\mathrm{tg}(B'))|_{\mathcal{D}(A)}$.

Our construction shows that for any standard self-adjoint operator A there exists a self-adjoint hyperfinite-rank operator B whose nonstandard hull extends A, i.e., $A={}^oB|_{\mathcal{D}(A)}$. In particular, we obtain $\sigma(A)\subset\sigma({}^oB)=\mathrm{cl}({}^o\mathrm{NS}(\sigma(B))$ by corollary 1. For each $\lambda\in\sigma(A)$ there exists thus a $\lambda'\in\sigma(B)$ for which $\lambda\approx\lambda'$ holds (cf. Sec. II B).

Definition 2: Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let H be an internal Hilbert space for which $\mathcal{H}\subset{}^oH$ holds and let B be an internal self-adjoint operator on H. B is called a nonstandard extension of A if $A={}^oB|_{\mathcal{D}(A)}$.

We note that the nonstandard extension of A is not unique. We discuss now how the function calculus of A is related to the function calculus of its nonstandard extensions.

Proposition 4: Let A be a standard self-adjoint operator and let B be a nonstandard extension of A. Then, for each real-valued Borel function g there exists an internal function f for which $g(A)x={}^o(f(B)^\star x)={}^of(B)x$ holds for all $x\in\mathcal{D}(g(A))$. In particular, $f(B)$ is a nonstandard extension of $g(A)$.

Proof: Let g be a real-valued Borel function and let $\{{}^oE_\Omega\}_{\Omega\in A}$ be the projection-valued Loeb measure associated with the projection-valued * measure of B. Since $g(A)=g({}^oB)|_{\mathcal{D}(g(A))}$ we conclude from theorem 4 that $g(A)x=\int_{\mathrm{fin}({}^\star\mathbb{R})}(g\circ\mathrm{st})\mathrm{d}{}^oEx$ $(x\in\mathcal{D}(g(A)))$. Moreover, for $x\in\mathcal{D}(g(A))$ let $\mu_L^{(x)}$ be the Loeb measure for which $\langle x,{}^oE_\Omega x\rangle=\mu_L^{(x)}(\Omega)$ $(\Omega\in\mathcal{A})$ holds. For each Loeb measure $\mu_L^{(x)}$ there exists an internal function f_x for which ${}^of_x=g\circ\mathrm{st}$ holds $\mu_L^{(x)}$ almost everywhere,[11] i.e., $\int_{\mathrm{fin}({}^\star\mathbb{R})}({}^of_x-g\circ\mathrm{st}^o)^2\mathrm{d}\|{}^oEx\|^2=0$. For $n\in\mathbb{N}$ let

$$f_{x,n}(\lambda):=\begin{cases}f_x(\lambda), & |f_x(\lambda)|\leqslant n,\\ 0, & \text{else},\end{cases}$$

then each $f_{x,n}$ is a finite internal function and $g(A)x=g({}^oB)x=\lim_n{}^of_{x,n}(B)x=\lim_n{}^o(f_{x,n}(B)^\star x)$. Hence, the internal sets

$$\Omega_{x,n}=\left\{f\in{}^\star(\mathbb{C}^{\mathbb{R}}):\left\|{}^\star(g(A)x)-f(B)^\star x\right\|<1/n\right\}$$

are nonempty for each $x\in\mathcal{D}(g(A))$, $n\in\mathbb{N}$. We note that $\Omega_{x,n}\subset\Omega_{x,m}$ for $n>m$. Moreover, for $x_1,\ldots,x_m\in\mathcal{D}(g(A))$ we consider the Loeb measure $\nu_L=\mu_L^{(x_1)}+\cdots+\mu_L^{(x_m)}$. For ν_L there exists also an internal function f for which ${}^of=g\circ\mathrm{st}$ holds ν_L almost everywhere.[11] In particular, ${}^of=g\circ\mathrm{st}$ holds $\mu_L^{(x_k)}$ almost everywhere for each $1\leqslant k\leqslant m$. If we define f_n with the help of f analogously as we have defined $f_{x,n}$ with the help of f_x then $g(A)x=g({}^oB)x_k=\lim_n{}^of_n(B)x_k=\lim_n{}^o(f_n(B)^\star x_k)$ for each $1\leqslant k\leqslant m$, and thus $\Omega_{x_1,n}\cap\cdots\cap\Omega_{x_m,n}\neq\emptyset$. The collection of internal sets $(\Omega_{x,n})_{x\in\mathcal{D}(g(A)),n\in\mathbb{N}}$ has thus the finite-intersection property, and by polysaturation there exists an internal $f\in\cap_{x\in\mathcal{D}(g(A)),n\in\mathbb{N}}\Omega_{x,n}$. In particular, we obtain $g(A)x={}^o(f(B)^\star x)$ for all $x\in\mathcal{D}(g(A))$.

Assume $x\in\mathcal{D}(g^2(A))$ and let $y=g(A)x$, then ${}^\star y\approx f(B)^\star x$ and ${}^\star(g^2(A)x)={}^\star(g(A)y)\approx f(B)^\star y$. Since $f(B)^\star y$ is finite we obtain $y=Py$ for the projection $P={}^o\chi_{\mathrm{fin}({}^\star\mathbb{R})}(f(B))$. Thus, $y={}^o(f(B)^\star x)=P{}^o(f(B)^\star x)={}^of(B)x$. Since $g(A)$ is essentially self-adjoint on $\mathcal{D}(g^2(A))$ we obtain $g(A)={}^of(B)|_{\mathcal{D}(g(A))}$. □

We note that the internal function in proposition 4 is not uniquely determined. In fact, if B is of hyperfinite rank we can even choose a * polynomial p for which $p(\lambda)=f(\lambda)$ holds for all eigenvalues λ of B, i.e., $f(B)=p(B)$. We can also restrict f to be a * continuous function or a * Borel function in proposition 4. We note also that if in proposition 4 the function g is bounded and continuous ($\mu_L^{(x)}$ almost everywhere for all $x\in\mathcal{H}$) then we may simply choose $f={}^\star g$.

Proposition 5: Let A be a standard self-adjoint operator and let B be a nonstandard extension of A. Let $(F_\Omega)_{\Omega\in\mathcal{B}}$ be the projection-valued measure associated with A and let $(E_\Omega)_{\Omega\in{}^\star\mathcal{B}}$ be the projection-valued * measure associated with B, then for each $\Omega\in\mathcal{B}$ there exists an $\Omega'\in{}^\star\mathcal{B}$ for which $F_\Omega x={}^oE_{\Omega'}x$ holds for all $x\in\mathcal{H}$.

Proof: Let $x\in\mathcal{D}(A)$, then $F_\Omega x=\chi_\Omega(A)x=\chi_\Omega({}^oB)x={}^oE_{\mathrm{st}^{-1}(\Omega)}x$ by theorem 4. Let $\mu_L^{(x)}$ be the

Loeb measure associated with $\langle x, {}^oE'_\Omega x\rangle$ ($\Omega' \in {}^\star\mathcal{B}$). There exists an $\Omega'_x \in {}^\star\mathcal{B}$ for which $\mu_L^{(x)}(\mathrm{st}^{-1}(\Omega)\Delta\Omega'_x)=0$ holds[11] ($\Omega\Delta\Omega' = (\Omega\setminus\Omega')\cup(\Omega'\setminus\Omega)$). We get in particular ${}^oE_{\Omega'_x}x = {}^oE_{\mathrm{st}^{-1}(\Omega)}x$. Let

$$\Gamma_{x,n} = \{\Omega' \in {}^\star\mathcal{B} : \|(E_{\Omega'} - E_{\Omega'_x})^\star x\| < 1/n\}.$$

The sets $\Gamma_{x,n}$ are internal and $\Gamma_{x,n} \subset \Gamma_{x,m}$ if $n > m$. Moreover, for $x_1, \ldots, x_m \in \mathcal{D}(A)$ we consider the Loeb measure $\nu_L = \mu_L^{(x_1)} + \cdots + \mu_L^{(x_m)}$. For ν_L there exists also an $\Omega' \in {}^\star\mathcal{B}$ for which $\nu_L(\mathrm{st}^{-1}(\Omega)\Delta\Omega')=0$ holds, i.e., ${}^oE_{\Omega'}x_k = {}^oE_{\mathrm{st}^{-1}(\Omega)}x_k$ for $1 \leqslant k \leqslant m$. The collection of internal sets $(\Gamma_{x,n})_{x\in\mathcal{D}(A),n\in\mathbb{N}}$ has thus the finite-intersection property, and by polysaturation there exists an $\Omega' \in \cap_{x\in\mathcal{D}(A),n\in\mathbb{N}}\Gamma_{x,n}$. In particular, ${}^oE_{\Omega'}x = {}^oE_{\mathrm{st}^{-1}(\Omega)}x$ for all $x \in \mathcal{D}(A)$, which proves the assertion. □

Let us come back to the discussion at the beginning of this section. We have seen that for any self-adjoint operator A on $\mathcal{H}$ there exist self-adjoint hyperfinite-rank operators on H that extend A in the sense of definition 2. Proposition 4 and proposition 5 provide further results that we discuss now from a physical point of view.

(1) If we want to model a standard measurement process we usually use a probability space $(\mathbb{R}, \mathcal{B}, \mu)$. The measure μ is related to a projection-valued measure of a self-adjoint operator A and a normalized state vector $x \in \mathcal{H}$. Proposition 5 suggests that we could also use a * probability space $(\mathbb{R}, {}^\star\mathcal{B}, \mu)$ to model the measurement process. The * measure μ is then related to the projection-valued * measure of a self-adjoint hyperfinite-rank extension B of A and the normalized vector $y = O^\star x/\|O^\star x\|$. We note that O denotes the projection of ${}^\star\mathcal{H}$ onto H and that $O^\star x \approx {}^\star x$.

(2) Proposition 4 tells us that the set of * Borel functions contains all functions that we need to retrieve standard results. We note that we may restrict ourselves to any set that contains the * polynomials, i.e., the * continuous functions, for example. In particular, for the time evolution we simply obtain $\exp(-iAt)x = {}^o(\exp(-iBt)y) = {}^o\exp(-iBt)x$ ($t \in \mathbb{R}$). We note that we use A, B, x, and y as in 1.

Following these two arguments we may formulate quantum mechanics in a hyperfinite-dimensional Hilbert space H, which extends the standard formulation in a Hilbert space $\mathcal{H}$. However, our results have a rather general nature so far. To demonstrate how a concrete formulation can be achieved we discuss Schrödinger representations as an example in Sec. IV B.

B. Schrödinger operators

The conventional Schrödinger representation of one-particle quantum mechanics is formulated in $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$. The momentum operator p and the position operator q are the closures of $i^{-1}\mathrm{d}/\mathrm{d}x$ and multiplication by x on $S(\mathbb{R})$. $S(\mathbb{R})$ is the space of functions of rapid decrease on $\mathbb{R}$, which is a domain of essential self-adjointness for p and q. Moreover, Schrödinger Hamiltonians are given by $A = p^2 + V(q)$, for which $V(\cdot)$ denotes a Borel function. We note that we restrict ourselves to the one-dimensional case and that the generalization to multidimensions is straightforward, as we will see.

Let $\{u_n\}_{n=o}^\infty$ be the basis of Hermite functions, let $h \in {}^\star\mathbb{N}\setminus\mathbb{N}$ be a fixed hypernatural number, and let H be the hyperfinite-dimensional space that has the basis $\{{}^\star u_n\}_{n=o}^h$. H externally contains the space $\mathcal{M}$ of finite linear combinations of $\{u_n\}_{n=0}^\infty$, which is dense in $\mathcal{H}$, and $H \subset {}^\star\mathcal{M}$. The triple $(\mathcal{M}, \mathcal{H}, H)$ thus realizes the setting described in Sec. II A.

We derive now explicit nonstandard extensions of several self-adjoint operators on $\mathcal{H}$. For example, let $O = \Sigma_{n=0}^h |{}^\star u_n\rangle\langle {}^\star u_n|$ be the projection from ${}^\star\mathcal{H}$ onto H associated with the Hermite-function basis $\{{}^\star u_n\}_{n=0}^h$, then the hyperfinite-rank operator $P = O^\star pO$ has a well-known simple representation, and for $x \in \mathcal{M}$ we obtain ${}^\star(px) = P^\star x$. Let $(E_\Omega)_{\Omega\in{}^\star\mathcal{B}}$ be the projection-valued

* measure associated with P. Since $P^{2\star}x$ is finite we obtain $px={}^o(P^\star x)={}^oE_{\mathrm{fin}(\mathbb{R})}{}^o(P^\star x)={}^oPx$ for $x\in\mathcal{M}$. In order to show that P is a nonstandard extension of p we prove that $p|_{\mathcal{M}}$ is essentially self-adjoint.

Let $x\in\mathcal{S}$ then there exists a sequence (x_n) in $\mathcal{M}$ that converges to x with respect to the topology of $\mathcal{S}$.[1] In particular, $\lim_n\|x-x_n\|=0$ and $\lim_n\|p(x-x_n)\|=0$. Let $\Gamma(p|_{\mathcal{M}})$ denote the graph of p restricted to $\mathcal{M}$. (px,x) is thus contained in the closure of $\Gamma(p|_{\mathcal{M}})$, i.e., $\Gamma(p|_S)\subset\mathrm{cl}(\Gamma(p|_{\mathcal{M}}))=\mathrm{cl}(\Gamma(p|_S))$. Since $p|_S$ is essentially self-adjoint we conclude that $p|_{\mathcal{M}}$ is also essentially self-adjoint and that $p={}^oP|_{\mathcal{D}(p)}$. P is thus a nonstandard extension of p. The following lemma generalizes our result.

Lemma 2: Let H be an internal Hilbert space and let $\mathcal{M}$ be a dense subset of a standard Hilbert space $\mathcal{H}$ for which $\mathcal{M}\subset H\subset{}^\star\mathcal{M}\subset{}^\star\mathcal{H}$ holds. Let A be a self-adjoint operator on $\mathcal{H}$, which is essentially self-adjoint on $\mathcal{M}$, and let O be the projection of ${}^\star\mathcal{H}$ onto H. Then, $B=O^\star AO$ is a nonstandard extension of A.

Proof: Let $(F_\Omega)_{\Omega\in{}^\star\mathcal{B}}$ be the projection-valued * measure associated with B. Since

$$\|B^\star x\|^2=\int_{{}^\star\mathbb{R}}\omega^2\mathrm{d}\langle{}^\star x,F_\omega{}^\star x\rangle$$

is finite for $x\in\mathcal{M}$ we conclude that

$$\int_{|\omega|>n}|\omega|\mathrm{d}\langle{}^\star x,F_\omega{}^\star x\rangle<\epsilon$$

for any standard $\epsilon>o$ and any $n\in{}^\star\mathbb{N}\backslash\mathbb{N}$. For a fixed standard $\epsilon>o$ there exists by the underflow principle an $n\in\mathbb{N}$ for which

$$\int_{|\omega|>n}|\omega|\mathrm{d}\langle{}^\star x,F_\omega{}^\star x\rangle<\epsilon$$

holds, and thus

$$\langle x,{}^o(B^\star x)\rangle=\mathrm{st}\left(\int_{{}^\star\mathbb{R}}\omega\mathrm{d}\langle{}^\star x,F_\omega{}^\star x\rangle\right)=\lim_{n\to\infty}\mathrm{st}\left(\int_{|\omega|\leqslant n}\omega\mathrm{d}\langle{}^\star x,F_\omega{}^\star x\rangle\right)=\langle x,{}^oBx\rangle\quad(x\in\mathcal{M}).$$

Moreover, by polarization we obtain $\langle y,{}^o(B^\star x)\rangle=\langle y,{}^oBx\rangle$ for $x,y\in\mathcal{M}$. Since ${}^o(B^\star x)=Ax\in\mathcal{H}$ we get

$$\left\|{}^o(B^\star x)\right\|=\sup_{y\in\mathcal{M}_1}|\langle y,{}^o(B^\star x)\rangle|=\sup_{y\in\mathcal{M}_1}|\langle y,{}^oBx\rangle|\leqslant\left\|{}^oBx\right\|,$$

using $\mathcal{M}_1=\{y\in\mathcal{M}:\|y\|=1\}$. Since

$$\|{}^o(B^\star x)\|=\|{}^oBx\|+\|{}^oF_{{}^\star\mathbb{R}\backslash\mathrm{fin}({}^\star\mathbb{R})}(B^\star x)\|$$

we obtain ${}^oF_{{}^\star\mathbb{R}\backslash\mathrm{fin}({}^\star\mathbb{R})}(B^\star x)=0$ and $Ax={}^o(B^\star x)={}^oBx$ for $x\in\mathcal{M}$. Since $A|_{\mathcal{M}}$ is essentially self-adjoint we obtain $A={}^oB|_{\mathcal{D}(A)}$. □

With the help of lemma 2 we gain explicit nonstandard extensions of many self-adjoint operators on $\mathcal{H}$. For example, since $q^n|_S$ and $p^n|_S(n\in\mathbb{N})$ are essentially self-adjoint we conclude in the same manner as for p that $Q^{(n)}=O^\star q^nO$ and $P^{(n)}=O^\star p^nO$ are nonstandard extensions, respectively. Also, if for a real Borel function V the operator $V(q)|_{\mathcal{M}}$ is essentially self-adjoint, which is for example true if V is bounded, then $W=O^\star V(q)O$ is a nonstandard extension of $V(q)$. We note that the matrix elements of W are given by explicit analytic expressions. Moreover, let us assume that the Schrödinger operator $A=p^2+V(q)$ is essentially self-adjoint on $\mathcal{M}$ and that $\mathcal{M}\subset\mathcal{D}(V(q))$. This requirement is fulfilled, for example, if V is a bounded Borel function (cf. Wüst's theorem[13]). Using lemma 2 we conclude that $B=O({}^\star p^2+{}^\star V(q))O=P^{(2)}+W$ is a nonstandard extension of A.

Without giving an explicit proof we note that we may even choose $V \in \mathcal{L}^2 + \mathcal{L}^\infty$ as in theorem X.15 of Ref. 13. Moreover, we note that in this example we simply may add the nonstandard extensions of p^2 and $V(q)$ to obtain a nonstandard extension of A. However, this is generally not valid since for two internal self-adjoint operators B_1 and B_2 the sum ${}^oB_1 + {}^oB_2$ is not necessarily defined although ${}^o(B_1 + B_2)$ is always defined.

V. APPLICATION IN SCATTERING THEORY

We apply in this section our nonstandard framework to nonrelativistic quantum scattering theory. First, we shortly review the concepts of conventional time-dependent scattering theory as it is presented in Ref. 14. We show then how the concepts fit into the framework, and discuss the physical impact. We finally derive explicit expressions for the Møller wave operators and the S-matrix.

A. Time-dependent scattering theory

In quantum scattering theory the Hamiltonian of the quantum system is the sum of a "free" Hamiltonian and an interaction potential, $A = A_0 + V$. If we consider a state x that was prepared in the remote past then the corresponding free state x_+ is given by $x = W^+ x_+ = \lim_{t \to -\infty} e^{iAt} e^{-iA_0 t} x_+$. W^+ is a Møller wave operator. Prerequisite is however that $\lim_{t \to -\infty} e^{iAt} e^{-iA_0 t} x_+$ exists. Analogously, the free state x_- that looks like x when it is detected in the far future is given by $x = W^- x_- = \lim_{t \to \infty} e^{iAt} e^{-iA_0 t} x_-$. We note that we use the convention of time-independent scattering theory that $t \to \mp\infty$ refers to $W^\pm$ (cf. Sec. 5.2, Ref. 14). The quantum system is complete if $W^+(\mathcal{H}) = W^-(\mathcal{H}) = \mathcal{H}_{ac}$. $\mathcal{H}_{ac}$ is the subspace of $\mathcal{H}$ that is connected to the absolutely continuous part of the spectrum of A.

Let us assume now an internal Hilbert space H, and self-adjoint hyperfinite-rank operators B and B_0 on H. We associate B_0 with the free Hamiltonian of the quantum system. Analogous to the conventional theory we are interested in the limits $W^\pm x = \lim_{t \to \pm\infty} ({}^o e^{iBt})({}^o e^{-iB_0 t}) x$ $(x \in {}^o H)$. Since we use NSA we can however give the terms "remote past" and "far future" a quantitative meaning. Let $Y_t = e^{iBt} e^{-iB_0 t}$ and let $L^\pm = \{x \in \mathrm{fin}(H) : \lim_{t \to \mp\infty} {}^o(Y_t x) \text{exists}\}$. We note that the spaces ${}^oL^\pm$ are closed subspaces of ${}^oH$ on which the Møller operators $W^\pm$ are defined. We assume in the following that the system is "reasonably" complete, i.e., that $W^+(L^+) \cap W^-(L^-)$ is a sensible set of physical states. This assumption is justified if we consider the nonstandard extension of a complete standard quantum system.

Lemma 3: $x \in L^\pm$ iff there exist infinite hyper-reals $T_{\pm,x}$ for which $W^{\pm o} x = {}^o(Y_t x)$ holds if t is infinite and $0 < (\mp t) \leqslant T_{\pm,x}$.

Proof: We carry out only the proof for L^-, since the proof for L^+ is analogous. Let $x \in \mathrm{fin}(H)$ and assume that there exists an infinite $T_{-,x}$ for which $W^{-o} x = {}^o(Y_t x)$ holds if t is infinite and $0 < t \leqslant T_{-,x}$. Since ${}^o(Y_t x) \in {}^oH$ there exists a $y \in \mathrm{fin}(H)$ for which ${}^o y = {}^o(Y_t x)$ holds. For a (standard) $\epsilon > 0$ let

$$\Gamma_\epsilon = \{T \in [0, T_{-,x}] : (\forall\, t \in [T, T_{-,x}]) \| y - Y_t x \| < \epsilon\}.$$

Since $T \in \Gamma_\epsilon$ if T is infinite and $T_{-,x} \geqslant T > 0$, and since Γ_ϵ is internal and nonempty there exists a finite $T_\epsilon \in \Gamma_\epsilon$. Hence, $(\forall\, t > {}^o T_\epsilon) \| W^{-o} x - {}^o(Y_t x) \| \leqslant \epsilon$, and thus $W^{-o} x = \lim_{t \to \infty} {}^o(Y_t x)$.

Now assume $W^{-o} x = \lim_{t \to \infty} {}^o(Y_t x)$. Since $W^{-o} x \in {}^oH$ there exists a $y \in \mathrm{fin}(H)$ for which ${}^o y = W^{-o} x$ holds. For each (standard) $\epsilon > 0$ there exists a T_ϵ for which $(\forall\, t > T_\epsilon) \| W^{-o} x - {}^o(Y_t x) \| < \epsilon$ holds. Let $T'_\epsilon = \max\{T_\epsilon, 1/\epsilon\}$, and let $F_t = \{s \in {}^\star\mathbb{R} : s \geqslant t\}$ for $t \in {}^\star\mathbb{R}$. The set

$$G_{\epsilon,x} = \{T \in F_{T'_\epsilon} : (\forall\, t \in [T'_\epsilon, T]) \| y - Y_t x \| < \epsilon\}$$

is nonempty and internal. By the overflow principle $G_{\epsilon,x}$ contains an infinite $T_{\epsilon,x}$, and by polysaturation the set

$$G_x = \bigcap_{\epsilon>0} [T'_\epsilon, T_{\epsilon,x}]$$

is nonempty, i.e., we can choose a $T_{-,x} \in G_x$. $T_{-,x}$ is infinite since $T_{-,x} > T'_\epsilon \geqslant 1/\epsilon$ for all $\epsilon > 0$. Moreover, if t is infinite and $t \leqslant T_{-,x}$ we obtain $(\forall \epsilon > 0) t \in [T'_\epsilon, T_{\epsilon,x}]$, and thus ${}^o y = W^- {}^o x = {}^o(Y_t x)$.□

Theorem 5: Assume that ${}^oH$ contains a standard Hilbert space $\mathcal{H}$, then there exist infinite hyper-reals $T_\pm$ for which $W^\pm {}^o x = {}^o(Y_t x)$ holds if t is infinite, $0 < (\mp t) \leqslant T_\pm$, $x \in L^\pm$, and ${}^o x \in \mathcal{H}$.

Proof: Again, we carry out only the proof for L^-, since the proof for L^+ is analogous. Let $x \in L^-$ and let $T_{-,x}$ be the infinite hyper-real determined by lemma 3. Since Y_t is finitely bounded for each $t \in {}^\star\mathbb{R}$ we obtain ${}^o(Y_t x) = {}^o(Y_t y)$ for all $y \approx x$. Thus, if t is infinite and $0 < t < T_{-,x}$ then $W^- {}^o y = {}^o(Y_t y)$ for all $y \approx x$. For $z \in \mathcal{H} \cap {}^o L^-$ we choose a representative $x \in L^-$ for which ${}^o x = z$ holds, and set $T'_{-,z} = T_{-,x}$. For $y \in L^-$ we obtain then $W^- z = {}^o(Y_t y)$ if t is infinite, $0 < t < T'_{-,z}$, and ${}^o y = z$. Let $G_{n,z} = [n, T'_{-,z}]$, then there exists an infinite $T_- \in \cap_{n \in \mathbb{N}, z \in \mathcal{H}} G_{n,z}$ by polysaturation. Since $T_- \leqslant T'_{-,z}$ for all $z \in \mathcal{H}$ we obtain the assertion. □

We note that theorem 5 is valid also if we replace $\mathcal{H}$ by any set of standard elements. The crucial point is that we use the properties of polysaturation in our proof, which limits the size of subsets of $L^\pm$ for which common hyper-reals $T_\pm$ can be determined. However, if we accept that we observe only a standard set of states in a scattering experiment, then theorem 5 yields an interesting result. Motivated by theorem 5, we may identify three phases of a scattering experiment: The preparation of the system is done in the remote past at infinite times t for which $-T_+ \leqslant t < 0$ holds. The scattering happens at finite times t, and the detection takes place in the far future at times t for which $0 < t \leqslant T_-$ holds. $-T_+$ and T_- may be interpreted as starting time and as finishing time of the experiment, respectively.

Moreover, we naturally obtain a separation of time scales within our nonstandard model: We observe the interacting system on a large time scale that is defined by the infinite time interval $[-T_+, T_-]$, whereas the interaction takes place on a small time scale that is defined by finite times, $t \in \mathrm{fin}({}^\star\mathbb{R})$. The separation of time scales, which cannot be done in standard models in the same manner, is a nice example of the strength of NSA. We note however that our result does not state that the preparation and the detection take place on the same time scale since the fraction T_-/T_+ is not necessarily finite.

B. Time-independent scattering theory

We discuss time-independent scattering theory in the following on the basis of our results for time-dependent scattering theory. In particular, we assume in this section the setting of theorem 5 and that H is hyperfinite-dimensional. As outlined in the discussion of theorem 5, we may assume especially two infinite hyper-reals $T_\pm$ that mark the starting and the finishing times of a scattering experiment. We introduce first a set of infinitesimals that is closely related to $T_\pm$. Let $T = \min\{T_-, T_+\}$, and let $\Gamma = \{t \approx 0 : t > 0 \text{ and } tT \text{ infinite}\}$. Γ is nonempty since, for example, $\{t/\sqrt{T} : {}^o t > 0 \text{ and } t \in \mathrm{fin}({}^\star\mathbb{R}_+)\} \subset \Gamma$. We note that Γ is a set of infinitesimals that depends only on $T_\pm$, and that is thus fundamentally related to the scattering system. We assume for the rest of the section that $\epsilon \in \Gamma$, i.e., $\epsilon \approx 0$, $\epsilon > 0$, and ϵt is infinite for $t \geqslant \min\{T_-, T_+\}$. Moreover, we use in the following transferred integration theory.

Lemma 4: Let $Y^\pm = Y_{\mp T_\pm/2}$, then

$$Y^\pm u \approx \int_0^{{}^\star\infty} \mathrm{d}s \; \epsilon e^{-\epsilon s} Y_{\mp s} u \tag{13}$$

if $u \in L^\pm$ and ${}^o u \in \mathcal{H}$.

Proof: Let $0 < {}^o\alpha < 1$, let $T_1 = 1/\sqrt{\epsilon}$, and let $T_2 = \alpha \min\{T_+, T_-\}$. Since $\|Y_s\| = 1$ for all $s \in {}^\star\mathbb{R}$ we obtain

$$\left\| \int_0^{{}^\star T_1} \mathrm{d}s \; \epsilon e^{-\epsilon s} Y_{\mp s} \right\| \leqslant \int_0^{{}^\star\sqrt{\epsilon}} \mathrm{d}s \; e^{-s} = 1 - e^{-\sqrt{\epsilon}} \approx 0,$$

$$\left\| \int_{T_2}^{\star\infty} \mathrm{d}s\ \epsilon e^{-\epsilon s} Y_{\mp s} \right\| \leqslant e^{-\epsilon T_2} \approx 0,$$

$$\int_{T_1}^{\star T_2} \mathrm{d}s\ \epsilon e^{-\epsilon s} Y_{\mp s} \approx \int_0^{\star\infty} \mathrm{d}s\ \epsilon e^{-\epsilon s} Y_{\mp s}.$$

Assume $u \in L^{\pm}$ and ${}^o u \in \mathcal{H}$. By theorem 5, $Y_{\mp s}\, u \approx Y^{\pm} u$ for $s \in [T_1, T_2]$, and thus

$$\int_{T_1}^{\star T_2} \mathrm{d}s\ \epsilon e^{-\epsilon s} Y_{\mp s} u \approx (e^{-\sqrt{\epsilon}} - e^{-\epsilon T_2}) Y^{\pm} u \approx Y^{\pm} u.$$

□

Lemma 4 enables us to deduce an explicit formula for the operators $W^{\pm} = {}^o Y^{\pm}$. Let $\{\lambda_j, x_j\}_{j=1}^h$ be an eigensystem of the free Hamiltonian B_0. If $u \in L^{\pm}$ and ${}^o u \in \mathcal{H}$ we obtain

$$\begin{aligned} Y^{\pm} u &\approx \int_0^{\star\infty} \mathrm{d}t\ \epsilon e^{-\epsilon t} Y_{\mp t} u = u \mp i \int_0^{\star\infty} \mathrm{d}t\ e^{-\epsilon t} e^{\mp iBt} V e^{\pm iB_0 t} u \quad (V = B - B_0) \\ &= u \mp i \sum_{j=1}^{h} u_j \int_0^{\star\infty} \mathrm{d}t\ e^{-\epsilon t} e^{\mp i(B-\lambda_j)t} V x_j \quad (u_j = \langle x_j, u \rangle) \\ &= u \pm i \sum_{j=1}^{h} u_j \frac{1}{\mp i(B - \lambda_j) - \epsilon} V x_j = \sum_{j=1}^{h} u_j \left(1 + \frac{1}{\lambda_j - B \pm i\epsilon} V \right) x_j. \end{aligned}$$

Theorem 6:

$$W^{\pm o} u = {}^o(Y^{\pm} u) = {}^o \sum_{j=1}^{h} u_j \left(1 + \frac{1}{\lambda_j - B \pm i\epsilon} V \right) x_j \tag{14}$$

if $u \in L^{\pm}$ and ${}^o u \in \mathcal{H}$.

Let $[Y^+, B_0] = Y^+ B_0 - B_0 Y^+$, and let $T_t = e^{iB_0 t}[Y^+, B_0] e^{-iB_0 t}$. We consider now the S-matrix, $S = (Y^-)^{\dagger} Y^+$, for which $\langle W^{-o} u, W^{+\ o} v \rangle = {}^o\langle u, Sv \rangle$ holds if $u \in L^-$, $v \in L^+$, and ${}^o u, {}^o v \in \mathcal{H}$.

Lemma 5:

$$\langle u, (S-1)v \rangle \approx -i \int_{-\star\infty}^{\star\infty} \mathrm{d}t\ e^{-\epsilon|t} \langle u, T_t v \rangle \tag{15}$$

if $u \in L^- \cap L^+$, $v \in L^+$, and ${}^o u, {}^o v \in \mathcal{H}$.

Proof: If $u \in L^- \cap L^+$, $v \in L^+$, and ${}^o u, {}^o v \in \mathcal{H}$ we obtain by lemma 4,

$$\langle u, (S-1)v \rangle = \langle u, (Y^- - Y^+)^{\dagger} Y^+ v \rangle \approx \int_0^{\star\infty} \epsilon e^{-\epsilon s} \langle u, (Y_t - Y_{-t})^{\dagger} Y^+ v \rangle.$$

Let $0 < {}^o\alpha < 1/2$, let $T_1 = 1/\sqrt{\epsilon}$, and let $T_2 = \alpha \min\{T_+, T_-\}$, then

$$\int_0^{\star\infty} \mathrm{d}t\ \epsilon e^{-\epsilon t} \langle u, (Y_t - Y_{-t})^{\dagger} Y^+ v \rangle \approx \int_{T_1}^{\star T_2} \mathrm{d}t\ \epsilon e^{-\epsilon t} \langle u, (Y_t - Y_{-t})^{\dagger} Y^+ v \rangle.$$

By theorem 5, we obtain for $t \in [T_1, T_2]$,

$$(Y_t)^{\dagger} Y^+ v \approx e^{iB_0 t} e^{-iBt} e^{-iB(T_+/2 - t)} e^{iB_0 (T_+/2 - t)} v = e^{iB_0 t} e^{-iBT_+/2} e^{iB_0 T_+/2} e^{-iB_0 t} v = e^{iB_0 t} Y^+ e^{-iB_0 t} v.$$

Analogously,

$$(Y_{-t})^{\dagger}Y^{+}v \approx e^{-iB_0t}e^{iBt}e^{-iB(T_+/2+t)}e^{iB_0(T_+/2+t)}v = e^{-iB_0t}e^{-iBT_+/2}e^{iB_0T_+/2}e^{iB_0t}v = e^{-iB_0t}Y^{+}e^{iB_0t}v.$$

Let $Z_t = e^{iB_0t}Y^{+}e^{-iB_0t}$, then

$$\int_{T_1}^{\star T_2} \mathrm{d}t\ \epsilon e^{-\epsilon t}\langle u,(Y_t - Y_{-t})^{\dagger}Y^{+}v\rangle \approx \int_{T_1}^{\star T_2} \mathrm{d}t\ \epsilon e^{-\epsilon t}\langle u,(Z_t - Z_{-t})v\rangle \approx \int_{0}^{\star \infty} \mathrm{d}t\ \epsilon e^{-\epsilon t}\langle u,(Z_t - Z_{-t})v\rangle.$$

We recognize that $^{\star}(\mathrm{d}/\mathrm{d}t)Z_t = -iT_t$, and obtain by partial integration

$$\int_{0}^{\star \infty} \mathrm{d}t\ \epsilon e^{-\epsilon t}\langle u,(Z_t - Z_{-t})v\rangle = -i\int_{0}^{\star \infty} \mathrm{d}t\ e^{-\epsilon t}\langle u,(T_t + T_{-t})v\rangle = -i\int_{-\star \infty}^{\star \infty} \mathrm{d}t\ e^{-\epsilon|t}\langle u,T_t v\rangle.$$

□

Let $T_{j,k} = \langle x_j,[Y^{+},B_0]x_k\rangle$ (the T-matrix). For $u \in L^{-} \cap L^{+}$, $v \in L^{+}$, and ${}^{o}u, {}^{o}v \in \mathcal{H}$ we obtain

$$\begin{aligned}
\langle u,(S-1)v\rangle &\approx -i\int_{-\star \infty}^{\star \infty} \mathrm{d}t\ e^{-\epsilon|t}\langle u,T_t v\rangle \\
&= -i\sum_{j,k=1}^{h} u_j^{*}v_k T_{j,k}\int_{-\star \infty}^{\star \infty} \mathrm{d}t\ e^{-\epsilon|t}e^{i(\lambda_j-\lambda_k)} \quad (u_j^{*} = \langle u,x_j\rangle, \quad v_k = \langle x_k,v\rangle) \\
&= -i\sum_{j,k=1}^{h} u_j^{*}v_k T_{j,k}\left(\frac{1}{i(\lambda_j-\lambda_k)+\epsilon} - \frac{1}{i(\lambda_j-\lambda_k)-\epsilon}\right) \\
&= -i\sum_{j,k=1}^{h} u_j^{*}v_k T_{j,k}\frac{-2\epsilon}{-(\lambda_j-\lambda_k)^2-\epsilon^2} = -2\pi i\sum_{j,k=1}^{h} u_j^{*}v_k\delta_{\epsilon}(\lambda_j-\lambda_k)T_{j,k}.
\end{aligned}$$

We note that since ϵ is a positive infinitesimal the function

$$\delta_{\epsilon}(x) = \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} \tag{16}$$

behaves like Dirac's delta distribution. [5]

Theorem 7:

$$\left\langle {}^{o}u, {}^{o}S^{o}v\right\rangle = {}^{o}\sum_{j,k=1}^{h} (\delta_{j,k} - 2\pi i\,\delta_{\epsilon}(\lambda_j-\lambda_k)T_{j,k})u_j^{*}v_k \tag{17}$$

if $u \in L^{-} \cap L^{+}$, $v \in L^{+}$, and ${}^{o}u, {}^{o}v \in \mathcal{H}$.

VI. SUMMARY AND CONCLUSIONS

We have formulated in this paper an approach to nonstandard quantum mechanics, i.e., we have introduced a mathematical framework that is based on NSA, and that can be appropriately applied to quantum mechanics. The principal step is the embedding of a dense subset of a standard complex Hilbert space $\mathcal{H}$ into a hyperfinite-dimensional space H. We have focused then on self-adjoint operators on $\mathcal{H}$, and have constructed appropriate extensions to self-adjoint hyperfinite-rank operators on H. To obtain a sensible interpretation of expectation values we have introduced further nonstandard hulls. We have defined the nonstandard hull ${}^{o}H$ of the hyperfinite-dimensional space H, which is a complex Hilbert space, and the nonstandard hulls of hyperfinite-rank operators on H. The idea is to perform calculations in H, and to interpret expectation values in the nonstandard hull ${}^{o}H$. To this end, we have developed the function calculus with respect to Loeb-measurable functions by introducing projection-valued Loeb measures. Using projection-valued Loeb measures we have proved then a nonstandard spectral theorem. With the help of the

spectral theorem we have shown how our nonstandard framework extends the standard framework used for quantum mechanics. As an example, we have applied our general results to Schrödinger representations of quantum mechanics.

Beside the mathematical results, which are rather interesting for their own, two important advantages are obtained by this approach. First, we can use nonstandard objects like infinitesimals, infinite numbers, or functions that behave like delta distributions in our framework. The availability of these objects is a general advantage of NSA as compared to standard mathematics. Second, since we perform calculations in a hyperfinite-dimensional space we can apply the transferred rules of linear algebra. In particular, self-adjoint hyperfinite-rank operators have complete sets of eigenvalues and eigenvectors. If we use this result to model the Hamiltonian of a quantum system we treat bound states and continuum states on the same footing. We note that this is also a feature of super-Hilbert space formalisms,[2,3] but the present approach seems to be more convenient for physical applications.

Moreover, we have applied the approach to nonrelativistic scattering theory. First we have extended standard time-dependent scattering theory to our framework. If we observe a standard set of states in a scattering experiment, as stated in theorem 5, then the extension yields two fundamental times of a scattering experiment that can be interpreted as the starting time, $-T_+$, and the finishing time, T_-, of the experiment. These times occur as infinite hyper-reals, and are not available in standard theories. Moreover, this result yields a natural separation of time scales: We observe the interacting system on a large time scale that is defined by the infinite time interval $[-T_+, T_-]$, whereas the interaction takes place on a small time scale that is defined by finite times, $t \in \mathrm{fin}({}^\star\mathbb{R})$. In particular, the preparation of the system is done in the remote past at infinite times t for which $-T_+ \leqslant t < 0$ holds, and the detection takes place in the far future at infinite times t for which $0 < t \leqslant T_-$ holds. We note however that this result does not state that the preparation and the detection processes take place on the same time scale since the fraction T_-/T_+ is not necessarily finite. Furthermore, we have applied our results to time-independent scattering theory. For time-independent scattering theory we have shown how concrete calculations work in the framework, and we have derived explicit formulas for the Møller wave operators and for the S-matrix. These formulas, which are well-known from standard physical text books, are proved rigorously.

From the author's point of view, the application of nonstandard methods to nonrelativistic scattering theory is rather fruitful. In particular, this example demonstrates the main advantages of the formalism mentioned above.

APPENDIX

The linear algebra in finite-dimensional subspaces of $\mathcal{H}$ is well known from standard textbooks. We need the results however to obtain the linear algebra in hyperfinite-dimensional subspaces of ${}^\star\mathcal{H}$ in the following. For this purpose, we formulate the standard results in a way that enables us to easily apply the transfer principle. However, although a presentation of nonstandard linear algebra should be available elsewhere, the author was not able to find an appropriate reference in the literature.

1. Linear algebra in finite-dimensional subspaces

Let $\mathcal{F}$ be the set of finite-dimensional subspaces of $\mathcal{H}$. For $F \in \mathcal{F}$ let $\mathrm{ONB}(F)$ be the set of orthonormal bases in F. The dimension d of F is the unique number of elements of each $B \in \mathrm{ONB}(F)$, i.e.,

$$(\exists d \in \mathbb{N})(\forall B \in \mathrm{ONB}(F)), \quad |B| = \mathrm{d}. \tag{A1}$$

We use here ONB as a function on $\mathcal{F}$. Let $\delta: \mathcal{H} \times \mathcal{H} \to \{0,1\}$ be the function defined by

$$\delta(x,y) = \begin{cases} 1, & x = y, \\ 0, & \text{else.} \end{cases}$$

The orthonormality of the bases can be expressed then as

$$(\forall B \in \mathrm{ONB}(F))(\forall x,y \in B), \quad \langle x,y\rangle = \delta(x,y),$$

and basis-set expansions are given by

$$(\forall B \in \mathrm{ONB}(F))(\forall x \in F), \quad x = \sum_{y\in B} \langle y,x\rangle y.$$

We denote the set of finite-rank operators on $\mathcal{H}$ by

$$\mathrm{LF} = \{f \in \mathcal{H}^{\mathcal{H}} : f \text{ is linear and } R(f) \in \mathcal{F}\}. \tag{A2}$$

$R(f)$ denotes the range of the function f. A finite-rank operator A on $\mathcal{H}$ is called normal if $A^\dagger A = AA^\dagger$, and we denote the set of normal finite-rank operators on $\mathcal{H}$ by

$$\mathrm{LFN} = \{A \in \mathrm{LF} : A^\dagger A = AA^\dagger\}. \tag{A3}$$

For $A \in \mathrm{LF}$ and $B \in \mathrm{ONB}(R(A))$ we can express the action of A on $R(A)$ as follows:

$$(\forall x \in R(A)), \quad Ax = \sum_{y\in B} \langle y,Ax\rangle y = \sum_{y,y'\in B} \langle y,Ay'\rangle\langle y',x\rangle y.$$

If A is normal, then $(\langle y,Ay'\rangle)_{y,y'\in B}$ is a normal matrix. Hence, there exists an eigensystem that can be used to express the action of A on $R(A)$, and we obtain

$$(\forall A \in \mathrm{LFN})(\exists B \in \mathrm{ONB}(R(A)))(\exists f \in \mathbb{C}^{\mathcal{H}})(\forall x \in R(A)),$$

$$Ax = \sum_{y\in B} f(y)\langle y,x\rangle y. \tag{A4}$$

The set $\{f(y)\}_{y\in B}$ is the set of eigenvalues of the restriction of A to $R(A)$.

2. Linear algebra in hyperfinite-dimensional subspaces

We assume in the sequel a polysaturated extension of the basic superstructure. Then, ${}^\star\mathcal{F}$ is the set of hyperfinite-dimensional subspaces of ${}^\star\mathcal{H}$. The transferred relation ${}^\star\mathrm{ONB}$ acts on ${}^\star\mathcal{F}$, and by the transfer principle we obtain for $F \in {}^\star\mathcal{F}$,

$$(\exists d \in {}^\star\mathbb{N})(\forall B \in {}^\star\mathrm{ONB}(F)), \quad |B| = d. \tag{A5}$$

We note that the dimension d of F is now a hypernatural number, which may be infinite. The orthonormality of the nonstandard bases is expressed by

$$(\forall B \in {}^\star\mathrm{ONB}(F))(\forall x,y \in B), \quad {}^\star\langle x,y\rangle = {}^\star\delta(x,y),$$

and the nonstandard basis-set expansions are given by

$$(\forall B \in {}^\star\mathrm{ONB}(F))(\forall x \in F), \quad x = \sum_{y\in B} {}^\star\langle y,x\rangle y.$$

Note that ${}^\star\langle\cdot,\cdot\rangle$ is the transferred scalar product, and that $\Sigma_{y\in B}$ may be a hyperfinite sum. The internal hyperfinite-rank operators on ${}^\star\mathcal{H}$ are given by the set

$$^{\star}\mathrm{LF} = \{f \in {}^{\star}(\mathcal{H}^{\mathcal{H}}) : f \text{ is linear and } R(f) \in {}^{\star}\mathcal{F}\}. \tag{A6}$$

A normal linear operator A on $^{\star}\mathcal{H}$ fulfills the condition $A^{\dagger}A = AA^{\dagger}$, and the set of normal hyperfinite-rank operators on $^{\star}\mathcal{H}$ is

$$^{\star}\mathrm{LFN} = \{A \in {}^{\star}\mathrm{LF} : A^{\dagger}A = AA^{\dagger}\}. \tag{A7}$$

For each $A \in {}^{\star}\mathrm{LFN}$ there exists an eigensystem, and we obtain

$$(\forall A \in {}^{\star}\mathrm{LFN})(\exists B \in {}^{\star}\mathrm{ONB}(R(A)))(\exists f \in {}^{\star}(\mathbb{C}^{\mathcal{H}}))(\forall x \in R(A)),$$

$$Ax = \sum_{y \in B} f(y)\,{}^{\star}\langle y, x\rangle y. \tag{A8}$$

Since each $A \in {}^{\star}\mathrm{LFN}$ is internal, the range of A, $R(A)$, is internal, $^{\star}\mathrm{ONB}(R(A))$ is internal, and each $B \in {}^{\star}\mathrm{ONB}(R(A))$ is internal. Moreover, $f \in {}^{\star}(\mathbb{C}^{\mathcal{H}})$ is internal, and the set of eigenvalues, $f(B)$, is thus internal too.

If we consider a standard eigensystem E then it is convenient to enumerate the elements, $E = \{(\lambda_1, x_1), \ldots, (\lambda_d, x_d)\}$, and $\mathrm{d} \in \mathbb{N}$ is the dimension. In the same manner we can denote a nonstandard eigensystem, assuming $\mathrm{d} \in {}^{\star}\mathbb{N}$.

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Stable quantum systems in anti–de Sitter space: Causality, independence, and spectral properties[a)]

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If a state is passive for uniformly accelerated observers in n-dimensional ($n \geqslant 2$) anti–de Sitter (Ads) space–time (i.e., cannot be used by them to operate a *perpetuum mobile*), they will (a) register a universal value of the Unruh temperature, (b) discover a PCT symmetry, and (c) find that observables in complementary wedge-shaped regions necessarily commute with each other in this state. The stability properties of such a passive state induce a "geodesic causal structure" on AdS and concommitant locality relations. It is shown that observables in these complementary wedge-shaped regions fulfill strong additional independence conditions. In two-dimensional AdS these even suffice to enable the derivation of a nontrivial, local, covariant net indexed by bounded space–time regions. All these results are model-independent and hold in any theory which is compatible with a weak notion of space–time localization. Examples are provided of models satisfying the hypotheses of these theorems. © *2004 American Institute of Physics.*
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I. INTRODUCTION AND BASIC ASSUMPTIONS

Quantum field theory in anti–de Sitter space–time (AdS) has been studied for almost 40 years (see, e.g., Refs. 1 and 20), primarily because it was found that AdS occurs as the ground state geometry in certain supergravity theories with gauged internal symmetry.[6,35] But it has become the object of an extraordinary amount of attention since the AdS–CFT correspondence has emerged. (We refer the interested reader to the SPIRES database, where a comprehensive list of articles on this topic can be retrieved.) There is therefore motivation to clarify in a model-independent setting and in a mathematically rigorous manner the universal properties of such theories, as implied by generally accepted and physically meaningful assumptions. This investigation has lead us to results which apparently have not been remarked in any form in the literature before.

AdS is a maximally symmetric and globally static solution of the vacuum Einstein equations. We consider here AdS of any dimension $n \geqslant 2$, except when explicitly stated otherwise. It can conveniently be described in terms of Cartesian coordinates in the ambient space $\mathbb{R}^{n+1}$ as the quadric surface

$$\mathrm{AdS}^n = \{ x \in \mathbb{R}^{n+1} | x^2 \doteq x_0^2 - x_1^2 - \cdots - x_{n-1}^2 + x_n^2 = R^2 \} \tag{1.1}$$

with metric $g = \mathrm{diag}(1,-1,\ldots,-1,1)$ in diagonal form. As the value of the radius R is not relevant for the results of this paper, we shall set it equal to 1 for convenience. The AdS^n isometry group is $\mathrm{O}(2,n-1)$ whose identity component will be denoted by $\mathrm{SO}_0(2,n-1)$. AdS^n is a homogeneous space of the group $\mathrm{SO}(2,n-1)$. It is not globally hyperbolic; indeed, it has closed timelike curves

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and has a timelike boundary at spatial infinity through which physical data can propagate. Although the covering space of AdS^n eliminates the closed timelike curves, it still has a timelike boundary at spatial infinity. We shall find some notable differences between the properties of quantum field theories on AdS^n and those of theories on the covering space.

As some of our basic assumptions are motivated by physical considerations concerning certain families of observables, we must collect some basic facts about observers in AdS. Let $x_O \in \mathrm{AdS}^n$ be any point and let $\lambda(t)$, $t \in \mathbb{R}$, be any one-parameter subgroup of $\mathrm{SO}_0(2,n-1)$ such that $t \mapsto \lambda(t)x_O$ is an orthochronous curve. (Note that AdS is time orientable.) We interpret this curve as the worldline of some observer. Among these observers will be those moving along a geodesic (henceforth, geodesic observers) and those experiencing a constant acceleration (uniformly accelerated observers). Points in a neighborhood of x_O will, in general, also give rise to orthochronous curves under the action of the chosen subgroup of $\mathrm{SO}_0(2,n-1)$, and we denote by W the connected neighborhood of x_O in AdS^n consisting of all such curves. Typically, W is the causal completion of the originally specified worldline. We view the region W as the maximal possible localization for any laboratory within the purview of the given observer. The associated dynamics are given by $e^{itM} \doteq U(\lambda(t))$ with suitable generator M. Since we are choosing a fixed parametrization of the pertinent subgroups of $\mathrm{SO}_0(2,n-1)$, the proper time of the observer is obtained by rescaling t with $((\dot{\lambda}(0)x_O)^2)^{1/2}$.

To become more precise, the geodesics of AdS^n are conic sections by two-planes containing the origin of the ambient space $\mathbb{R}^{n+1}$. So, one-parameter subgroups [see Appendix A for our notation concerning $\mathrm{SO}_0(2,n-1)$] $\lambda(t)$, $t \in \mathbb{R}$, of $\mathrm{SO}_0(2,n-1)$ of the form $\lambda\lambda_{0n}(t)\lambda^{-1}$, $t \in \mathbb{R}$, for some $\lambda \in \mathrm{SO}_0(2,n-1)$ generate admissible geodesic worldlines in the sense just indicated. These worldlines are closed, timelike curves, whose causal completion is the entire space AdS^n. Hence, the maximal laboratory localization region W for such geodesic observers must be the entire space–time, AdS^n. For uniformly accelerated observers, the corresponding one-parameter subgroups are of the form $\lambda\lambda_{01}(t)\lambda^{-1}$, $t \in \mathbb{R}$, for some $\lambda \in \mathrm{SO}_0(2,n-1)$. Their laboratory regions, called AdS wedges, are described immediately below. The algebras $\mathcal{A}(W)$ corresponding to any such wedge region as well as to $W = \mathrm{AdS}^n$ are taken to be weakly closed.

We define a "wedge" in AdS^n to be the causal completion of the worldline of a uniformly accelerated observer in AdS^n. To be concrete and in order to simplify the necessary computations, we consider the particular choice of region

$$W_R = \{ x \in \mathrm{AdS}^n | x_1 > |x_0|, x_n > 0 \}, \tag{1.2}$$

on which the one-parameter subgroup of boosts $\lambda_{01}(t)$, $t \in \mathbb{R}$, in the $0-1$ plane acts in an orthochronous manner. For any $x_O \in W_R$, the curve $t \mapsto \lambda_{01}(t)x_O$ is the worldline of a uniformly accelerated observer for which the causal completion is precisely W_R. By the assumed $\mathrm{SO}_0(2,n-1)$ covariance, all results concerning this wedge have natural extensions to all images of W_R under $\mathrm{SO}_0(2,n-1)$. We therefore define the set of AdS^n wedges to be

$$\mathcal{W} \doteq \{ \lambda W_R | \lambda \in \mathrm{SO}_0(2,n-1) \}. \tag{1.3}$$

These are maximal laboratory localizations for the uniformly accelerated observers.

We can now describe the four standing assumptions of this paper. A discussion of their physical motivation is given in Ref. 12, so we shall only expand upon the less familiar ones.

(i) There exists a strongly continuous, unitary, nontrivial representation U of the symmetry group $\mathrm{SO}_0(2,n-1)$ acting on a separable Hilbert space $\mathcal{H}$. (It is sufficient here to consider the subspace of "bosonic" states, so we shall not need to proceed to the covering group of the space–time symmetry group.)

(ii) On $\mathcal{H}$ act the global von Neumann algebra of observables $\mathcal{A} = \mathcal{A}(\mathrm{AdS}^n)$, which contains any observable measurable in AdS^n, and an isotonous family of von Neumann algebras $\{\mathcal{A}(W)\}_{W \in \mathcal{W}}$ associated with the wedges $\mathcal{W}$. Furthermore, one has

$$\bigvee_{W\in\mathcal{W}} \mathcal{A}(W) = \mathcal{A}. \tag{1.4}$$

(iii) For each wedge $W \in \mathcal{W}$ and $\lambda \in \mathrm{SO}_0(2,n-1)$, one has the equality

$$U(\lambda)\mathcal{A}(W)U(\lambda)^{-1} = \mathcal{A}(\lambda W). \tag{1.5}$$

The weak additivity condition (1.4) is a generalization of the natural idea that all observables are constructed out of local ones. But in contrast to Ref. 12, we do not assume that all observables can be constructed out of observables with arbitrarily small localization region. This is because there are nets of physical interest on curved space–times for which the condition (v) specified below holds but the algebras $\mathcal{A}(\mathcal{O})$ associated with all bounded open regions $\mathcal{O}$ are trivial.[13,31] Also, there exist examples in which the algebra $\mathcal{A}(\mathcal{O})$ is nontrivial only for sufficiently large bounded regions $\mathcal{O}$.[13] In both of these cases the assumption made in Ref. 12 is violated. We have therefore eliminated all assumptions referring to bounded regions.

We emphasize that we do not postulate from the outset any local commutation relations of the observables. For, in contrast to the case of globally hyperbolic space–times, the principle of Einstein causality does not provide any clues as to which observables in AdS should commute with each other. Instead, we shall *derive* such commutation relations from stability properties of the vacuum, which we now specify.

We shall assume that the state ω determined by Ω is passive (cf. Ref. 29 and Sec. 5.4.4 in Ref. 5) for the dynamical system $(\mathcal{A}(W), \mathrm{ad}U(\lambda(t)))$, for all geodesic and all uniformly accelerated observers described earlier. We recall that passivity is an expression of the Second Law of Thermodynamics. Since the vacuum is the most elementary system, all order parameters should have sharp values in this state. This is expressed by the weak mixing property

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left(\omega(A(t)B) - \omega(A(t))\omega(B)\right)\, dt = 0, \tag{1.6}$$

for all $A, B \in \mathcal{A}$, where $A(t) \doteq e^{itM}Ae^{-itM}$. The restriction of the state ω to $\mathcal{A}(W)$ is said to be central if $\omega(AB) = \omega(BA)$, for all $A, B \in \mathcal{A}(W)$. If this holds, then either Ω is annihilated by most of the observables in $\mathcal{A}(W)$ or $\mathcal{A}(W)$ is a finite algebra (cf. Sec. 8.1 in Ref. 26). In quantum field theory this is a physically pathological circumstance, which we shall exclude from consideration.

These basic features of the vacuum can be summarized as follows.

(iv) The vacuum vector Ω is cyclic for $\mathcal{A}$ and determines a passive, weakly mixing and noncentral state ω for all geodesic and all uniformly accelerated observers.

The standing assumptions (i)–(iv) are model-independent and physically natural. In this paper we shall show that these assumptions entail that for geodesic observers the vacuum ω is a ground state; uniformly accelerated observers in AdS will register a universal value of the Unruh temperature; they will discover a PCT symmetry; and they will find that observables localized in complementary wedge-shaped regions must commute in the vacuum state. Not only do such observables commute in this sense, but the corresponding algebras manifest strong properties of statistical independence, the nature of which will be studied in detail. We shall also see that these assumptions imply that quantum theories on AdS obey a geodesic causal structure.

Related results appeared in Ref. 12, and we revisit some of those arguments here in more detail than in that announcement. But our research in the intervening time has led not only to further results and a weakening of the assumptions, but also to a shift in our point of view, which now places emphasis on the locality and independence properties which can be derived from our assumptions. We establish independence properties going far beyond those announced in Ref. 12, and we prove an additional locality property of such theories on proper AdS^n which was not observed in Ref. 12. Moreover, we show that in two dimensions these suffice to construct a nontrivial, local, covariant net indexed by bounded space–time regions. We also explain how known examples of quantum fields on AdS fit into our scheme.

The primary lesson to be drawn from this paper is the observation that covariance and passivity properties of states induce strong algebraic relations between the observables, which may be interpreted as manifestations of Einstein causality. In our research program, the theories on AdS treated here serve as a theoretical laboratory to test this striking feature. But the insight gained in this analysis goes beyond this class of field theoretical models to quantum fields on other space–times. Further, it seems to be of relevance in the discussion of causality problems appearing in nonlocal theories, such as string theory and quantum field theory on noncommutative space–times.

II. UNRUH EFFECT, PCT SYMMETRY, AND WEAK LOCALITY

We now enter into the analysis of the implications of our standing assumptions (i)–(iv) by appealing to a deep result of Pusz and Woronowicz for general quantum dynamical systems.[29] In the present context this result says that the vacuum vector Ω is, as a consequence of its passivity and mixing properties, invariant under the dynamics of any of the observers discussed earlier (Ref. 29, Theorem 1.1). In particular, this entails that $M_{01}\Omega=0$ (and hence, by Lemma A.3, Ω is invariant under the entire group $U(\mathrm{SO}_0(2,n-1))$), and ω is either (Ref. 29, Theorem 1.3) a ground state for M_{01} (which is excluded by Lemma A.1), or satisfies, for some *a priori* unknown $\beta\geqslant 0$, the Kubo–Martin–Schwinger (KMS) condition. In fact, our assumptions exclude the possibility of $\beta=0$. In the proof of Lemma 4.1 in Ref. 29 it is shown that if $\beta=0$, then either ω is a trace state on $\mathcal{A}(W_R)$ or $M_{01}=0$. In the second case, one would have the triviality of the representation of the boost group and thus the triviality of $U(\mathrm{SO}_0(2,n-1))$, which is excluded by (i). The first case is excluded by assumption (iv). Therefore, for any pair of operators $A,B\in\mathcal{A}(W_R)$ there exists an analytic function F in the strip $\{z\in\mathbb{C}|0<\mathrm{Im}(z)<\beta\}$ with continuous boundary values at $\mathrm{Im}(z)=0$ and $\mathrm{Im}(z)=\beta$, which are given by

$$F(t)=\omega(AB(t)),\quad F(t+i\beta)=\omega(B(t)A), \tag{2.1}$$

respectively, for all $t\in\mathbb{R}$ and with $B(t)\doteq e^{itM_{01}}Be^{-itM_{01}}$. By the $\mathrm{SO}_0(2,n-1)$-covariance the same assertions are valid for the action of the groups $e^{itM_{0j}}$, $j=2,\ldots,n-1$, on the suitable wedge algebras.

In Appendix C it is proven that this analyticity entails that the theories we are considering here satisfy the Reeh–Schlieder property (cf. Lemma C.1). So the vacuum vector Ω is cyclic for the algebra $\mathcal{A}(W)$, given any $W\in\mathcal{W}$, and, by the KMS property, it is also separating for $\mathcal{A}(W)$ (Ref. 5, Corollary 5.3.9). Hence, the Tomita–Takesaki modular theory is applicable to $(\mathcal{A}(W),\Omega)$, for every $W\in\mathcal{W}$ (cf. Refs. 4 and 26). Let J_{W_R} denote the modular conjugation and $\Delta_{W_R}^{it}$ the modular unitaries associated to the pair $(\mathcal{A}(W_R),\Omega)$. Since the adjoint action of the strongly continuous unitary group $e^{itM_{01}}$, $t\in\mathbb{R}$, leaves the algebra $\mathcal{A}(W_R)$ invariant and satisfies the KMS condition, we must have $\Delta_{W_R}^{it}=e^{-\beta tM_{01}}$, for all $t\in\mathbb{R}$ (Ref. 26, Theorem 9.2.16). Hence, J_{W_R} is determined by the equation

$$J_{W_R}A\Omega=e^{-(\beta/2)M_{01}}A^*\Omega,\quad A\in\mathcal{A}(W_R). \tag{2.2}$$

A. Unruh temperature

The main task of this subsection is to determine the Unruh temperature β^{-1} and specific properties of the operator J_{W_R}. To this end we shall adapt methods employed in Ref. 3.

We show in Lemma B.1 that there exists a wedge $W_0\in\mathcal{W}$ such that $\lambda W_0\subset W_R$ for all λ in a neighborhood of the identity in $\mathrm{SO}_0(2,n-1)$. Therefore, for any $j=2,\ldots,n-1$ one has $\lambda_{0j}(s)W_0\subset W_R$ for the boosts $\lambda_{0j}(s)$ in the $0-j$ plane for all sufficiently small parameters s. From Eq. (A10) in Appendix A we have

$$e^{itM_{01}}e^{isM_{0j}}=e^{is(\cosh(t)M_{0j}+\sinh(t)M_{1j})}e^{itM_{01}}. \tag{2.3}$$

Thus we get for any vector $\Phi\in\mathcal{H}$ and operator $A^*\in\mathcal{A}(W_0)$:

$$\langle \Phi, e^{itM_{01}} e^{isM_{0j}} A^* e^{-isM_{0j}} \Omega \rangle = \langle \Phi, e^{is(\cosh(t)M_{0j} + \sinh(t)M_{1j})} e^{itM_{01}} A^* \Omega \rangle. \tag{2.4}$$

We are now in the position of employing the argument given in Ref. 12 to yield the equalities

$$J_{W_R} e^{isM_{0j}} = e^{is(\cos(\beta/2)M_{0j} + i \sin(\beta/2)M_{1j})} J_{W_R}. \tag{2.5}$$

As pointed out in Ref. 12, the operator on the left-hand side of this equation is antiunitary, which entails that β is an *integer* multiple of 2π, for otherwise the operator appearing in the exponential function on the right-hand side would not be skew-adjoint. By using the proof of Theorem 6.2 in Ref. 3 with $\mathcal{A}(\mathcal{O})$ replaced by $\mathcal{A}(W_0)$, one sees that its only possible value is $\beta = 2\pi$. Proceeding to the proper time scale of the observer, we conclude that he is exposed to the Unruh temperature $(1/2\pi)((\dot{\lambda}_{01}(0)x_O)^2)^{-1/2}$, in accordance with the value found in computations for some particular models[17,25] and also by more general considerations.[7]

For geodesic observers, Lemma A.1 is not applicable. In fact, ω cannot be a KMS state for $e^{itM_{0n}}$ on $\mathcal{A}$, the laboratory observable algebra for geodesic observers. Indeed, since the covariance assumption (iii) implies $U(\lambda)\mathcal{A}U(\lambda)^{-1} = \mathcal{A}$, for all $\lambda \in \mathrm{SO}_0(2, n-1)$, if $e^{itM_{0n}}$ were the modular group for Ω on $\mathcal{A}$, then modular theory would necessitate $U(\lambda)e^{itM_{0n}} = e^{itM_{0n}}U(\lambda)$, for all $\lambda \in \mathrm{SO}_0(2, n-1)$ (cf. Theorem 3.2.18 in Ref. 4). But this would only be possible if the representation $U(\mathrm{SO}_0(2, n-1))$ were trivial, which is excluded by assumption (i). So ω must be a ground state for $e^{itM_{0n}}$.

We have therefore established the following general facts:

Theorem 2.1: *Let standing assumptions (i)–(iv) hold. Then Ω is invariant under the action of $U(\mathrm{SO}_0(2, n-1))$ and each uniformly accelerated observer testing Ω in AdS^n finds a universal value $(1/2\pi)((\dot{\lambda}_{01}(0)x_O)^2)^{-1/2}$ of the Unruh temperature which depends only on his particular orbit. For geodesic observers ω is a ground state; in particular, M_{0n} is a positive operator.*

This result is a consequence of the passivity of ω, and this vacuum state is the only normal state on $\mathcal{A}$ which is passive for all observers. In light of Theorem 2.1, it is physically justified to identify the operator M_{0n} with the global energy operator.

The result $\beta = 2\pi$ and (Ref. 26, Theorem 9.2.16) permit us to completely determine the modular unitaries corresponding to the pair $(\mathcal{A}(W), \Omega)$, for all $W \in \mathcal{W}$.

Corollary 2.2: Given the standing assumptions (i)–(iv), the modular unitaries for the pair $(\mathcal{A}(W_R), \Omega)$ are given by

$$\Delta_{W_R}^{it} = e^{-i2\pi t M_{01}}, \quad t \in \mathbb{R}. \tag{2.6}$$

Covariance and the uniqueness of the modular objects yield similar results for Δ_W^{it}, for all $W \in \mathcal{W}$.

B. PCT symmetry

Having computed the modular unitaries and the value of the inverse temperature β seen by the uniformly accelerated observers, let us return now to the analysis of J_{W_R} and clarify its relation to space–time reflections. Plugging $\beta = 2\pi$ into Eq. (2.5), we see that for small s:

$$J_{W_R} e^{isM_{0j}} = e^{-isM_{0j}} J_{W_R}, \quad j = 2, \ldots, n-1. \tag{2.7}$$

This relation can be extended to arbitrary s by iteration, if one decomposes $e^{isM_{0j}}$ into an m-fold product $(e^{i(s/m)M_{0j}})^m$ for sufficiently large m. A similar argument with λ_{0j} replaced by λ_{0n} and Eq. (A10) replaced by Eq. (A8) yields

$$J_{W_R} e^{isM_{0n}} = e^{-isM_{0n}} J_{W_R}. \tag{2.8}$$

On the other hand, modular theory yields

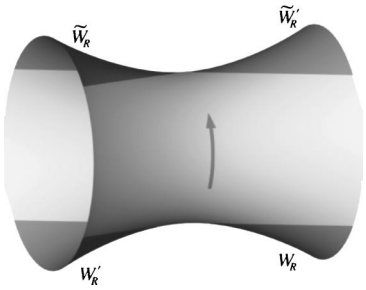

FIG. 1. Conjugate wedges in anti–de Sitter space and arrow of time.

$$J_{W_R} e^{isM_{01}} = e^{isM_{01}} J_{W_R}. \tag{2.9}$$

Since these one-parameter subgroups generate $\mathrm{SO}_0(2,n-1)$, the intertwining properties of J_{W_R} with all unitaries $U(\lambda) \in U(\mathrm{SO}_0(2,n-1))$ are determined.

Lemma 2.3: Given standing assumptions (i)–(iv), one has

$$J_{W_R} U(\lambda) = U(\theta_{01}\lambda\theta_{01}) J_{W_R}, \tag{2.10}$$

for all $\lambda \in \mathrm{SO}_0(2,n-1)$, *where* $\theta_{01} = \mathrm{diag}(-1,-1,1,\ldots,1)$ *is the reflection which changes the sign of the* $0-1$*-coordinates of the points in* AdS^n *(the reflection about the edge of the wedge* W_R*).*

Hence, if we define $U(\theta_{01}\lambda) \doteq J_{W_R} U(\lambda)$, for any $\lambda \in \mathrm{SO}_0(2,n-1)$, the following partial analog of the PCT-theorem can be proven.

Theorem 2.4: *If standing assumptions (i)–(iv) hold, then the unitary representation* U *of* $\mathrm{SO}_0(2,n-1)$ *extends to a representation of* $\mathrm{SO}(2,n-1)$ *in which the reflection* θ_{01} *is implemented by the antiunitary involution* J_{W_R}.

Proof: Note that $\mathrm{SO}(2,n-1)$ is the disjoint union of $\theta_{01}\mathrm{SO}_0(2,n-1)$ and $\mathrm{SO}_0(2,n-1)$. Since

$$U(\theta_{01}\lambda_1 \cdot \lambda_2) = J_{W_R} U(\lambda_1\lambda_2) = J_{W_R} U(\lambda_1) U(\lambda_2) = U(\theta_{01}\lambda_1) U(\lambda_2) \tag{2.11}$$

and

$$U(\theta_{01}\lambda_1 \cdot \theta_{01}\lambda_2) = U(\theta_{01}\lambda_1\theta_{01}) U(\lambda_2) = J_{W_R} U(\lambda_1) J_{W_R} U(\lambda_2) = U(\theta_{01}\lambda_1) U(\theta_{01}\lambda_2), \tag{2.12}$$

for all $\lambda_1, \lambda_2 \in \mathrm{SO}_0(2,n-1)$, the assertion follows.

Theorem 2.4 is a purely group-theoretic statement which does not yet say anything about the adjoint action of J_{W_R} on the observables. Results of that type require an additional assumption and will appear in a later publication.

C. Weak locality

In order to gain insight into the locality properties of the net, we consider the observables which are localized in the region

$$W_R' \doteq \{x \in \mathrm{AdS}^n \,|\, -x_1 > |x_0|, x_n > 0\}. \tag{2.13}$$

Throughout this subsection we shall only consider AdS^n of dimension $n \geq 3$. Since the regions W_R and W_R' are each one-half (on the same "side" of AdS^n—see Fig. 1 above) of the regions obtained by intersecting opposite wedge-shaped regions in the ambient space $\mathbb{R}^{n+1}$ with AdS^n, we call them opposite wedges. In general, if $W = \lambda W_R$, for some $\lambda \in \mathrm{SO}_0(2,n-1)$, then $W' = \lambda W_R'$.

In Ref. 12 it was shown that for $n \geq 3$ the earlier results entail that observables which are localized in complementary wedges are weakly local in the vacuum state. So we can state:

Theorem 2.5: *Under the assumptions (i)–(iv) and for* $n \geq 3$, *observables which are localized in opposite wedges of* AdS^n *are weakly local with respect to each other. Explicitly, for any* λ

$\in \mathrm{SO}_0(2,n-1)$ *and any* $A' \in \mathcal{A}(\lambda W_R')$, $B \in \mathcal{A}(\lambda W_R)$, *one has* $\langle \Omega, A'B\Omega\rangle = \langle \Omega, BA'\Omega\rangle$.

This result is also valid for theories in the covering space of AdS^n which satisfy (i)–(iv). A similar result was proven in Ref. 7 for two-point functions of quantum fields on the covering space of AdS^n satisfying a different set of assumptions in the Wightman framework.

The uniqueness of the modular objects and the covariance assumption (iii) give us a relation we shall use repeatedly in the following:

$$U(\lambda) J_W U(\lambda)^{-1} = J_{\lambda W}, \tag{2.14}$$

for all $W \in \mathcal{W}$ and all $\lambda \in \mathrm{SO}_0(2,n-1)$. Hence, since $\mathcal{A}(W_R') = e^{i\pi M_{12}} \mathcal{A}(W_R) e^{-i\pi M_{12}}$, Eq. (2.14) and the observations made above imply

$$J_{W_R'} = e^{i\pi M_{12}} J_{W_R} e^{-i\pi M_{12}} = J_{W_R} e^{-i2\pi M_{12}} = J_{W_R}. \tag{2.15}$$

Thus, the $\mathrm{SO}_0(2,n-1)$-covariance of the net entails

$$J_{W'} = J_W, \quad \text{for every } W \in \mathcal{W}. \tag{2.16}$$

If the algebras $\mathcal{A}(W)$ and $\mathcal{A}(W')$ commuted strongly with each other, it can be shown that (2.16) follows from modular theory. It is therefore of interest that (2.16) obtains when the algebras only weakly commute.

We continue with some further locality results, which distinguish theories on proper AdS from those on the covering space. We have chosen our wedge regions $W \in \mathcal{W}$ to be connected for physical reasons, as previously explained. But the intersection of the (connected) wedge $\mathbf{W}$ in the ambient space

$$\mathbf{W} = \{ x \in \mathbb{R}^{n+1} | x_1 > |x_0| \} \tag{2.17}$$

with AdS^n has two connected components, one of which is W_R and the other is the conjugate wedge

$$\widetilde{W}_R' = \{ x \in \mathrm{AdS}^n | x_1 > |x_0|, -x_n > 0 \}. \tag{2.18}$$

One has the geometric relations

$$\widetilde{W}_R = \theta_{01} \widetilde{W}_R' = -W_R \quad \text{and} \quad W_R' = -\widetilde{W}_R'. \tag{2.19}$$

Moreover, it is easy to see that

$$e^{i\pi M_{0n}} \mathcal{A}(W_R) e^{-i\pi M_{0n}} = \mathcal{A}(\widetilde{W}_R') \quad \text{and} \quad e^{i\pi M_{0n}} \mathcal{A}(W_R') e^{-i\pi M_{0n}} = \mathcal{A}(\widetilde{W}_R). \tag{2.20}$$

The rotation in the 0-n plane by π also reverses the orientation of the world lines $\lambda_{01}(t) x_O$ (cf. Eq. (A5)), so that the world lines in $\widetilde{W}_R'$ run in the same direction as those of W_R', while those in $\widetilde{W}_R$ have the same orientation as those in W_R. Explicitly, Corollary 2.2 implies that the modular unitaries for the pair $(\mathcal{A}(W_R'), \Omega)$ are given by

$$\Delta_{W_R'}^{it} = e^{i2\pi t M_{01}}, \quad t \in \mathbb{R}. \tag{2.21}$$

Hence, for all $t \in \mathbb{R}$, one has

$$\Delta_{\widetilde{W}_R}^{it} = e^{i\pi M_{0n}} \Delta_{W_R'}^{it} e^{-i\pi M_{0n}} = e^{i\pi M_{0n}} e^{i2\pi t M_{01}} e^{-i\pi M_{0n}} = e^{-i2\pi t M_{01}} = \Delta_{W_R}^{it}, \tag{2.22}$$

by (A5). So, $\{e^{-i2\pi t M_{01}}\}_{t \in \mathbb{R}}$ is the group of modular unitaries for $(\mathcal{A}(\widetilde{W}_R), \Omega)$, and we have the relation

$$J_{\tilde{W}_R} A\Omega = e^{-\pi M_{01}} A^* \Omega, \quad \text{for} \quad A \in \mathcal{A}(\tilde{W}_R). \tag{2.23}$$

Moreover, we may appeal to (2.16) and the modular theory to find

$$J_{\tilde{W}_R} A'\Omega = e^{\pi M_{01}} A'^* \Omega, \quad \text{for} \quad A' \in \mathcal{A}(\tilde{W}'_R). \tag{2.24}$$

From Eqs. (2.14) and (2.8) follow the equalities:

$$J_{\tilde{W}'_R} = e^{i\pi M_{0n}} J_{W_R} e^{-i\pi M_{0n}} = e^{i2\pi M_{0n}} J_{W_R} = J_{W_R}, \tag{2.25}$$

where we have used $e^{i2\pi M_{0n}} = 1$, valid in proper AdS but not in its covering space. Thus, by (2.16) we have for $n \geqslant 3$:

$$J_{W'_R} = J_{W_R} = J_{\tilde{W}_R} = J_{\tilde{W}'_R}. \tag{2.26}$$

We can now prove that $\mathcal{A}(\tilde{W}'_R)$ and $\mathcal{A}(W_R)$ are weakly local with respect to each other.

Theorem 2.6: *Under the assumptions (i)–(iv) and for $n \geqslant 3$, observables which are localized in W_R are weakly local with respect to observables localized in $\tilde{W}'_R$. Explicitly, for any $\lambda \in \mathrm{SO}_0(2, n-1)$ and any $A' \in \mathcal{A}(\lambda \tilde{W}'_R)$, $B \in \mathcal{A}(\lambda W_R)$, one has $\langle \Omega, A'B\Omega \rangle = \langle \Omega, BA'\Omega \rangle$.*

Proof: With the earlier preparations, one sees that for any $A' \in \mathcal{A}(\tilde{W}'_R)$ and $B \in \mathcal{A}(W_R)$, one has

$$\langle \Omega, A'^* B\Omega \rangle = \overline{\langle \Omega, B^* A'\Omega \rangle} = \overline{\langle \Omega, B^* J_{W_R} J_{W_R} A'\Omega \rangle} = \langle \Omega, Be^{-\pi M_{01}} e^{\pi M_{01}} A'^* \Omega \rangle = \langle \Omega, BA'^* \Omega \rangle. \tag{2.27}$$

Theorem 2.6 does not hold in the covering space of AdS^n, since, in general, $e^{i\pi M_{0n}}$ and J_{W_R} will not commute in such theories. Indeed, in Refs. 7 and 21 can be found examples of a free field theory on the covering space of AdS^n for which it can be shown that assumptions (i)–(iv) are satisfied, but the elements of $\mathcal{A}(W_R)$ and $\mathcal{A}(\tilde{W}'_R)$ do not commute in the vacuum state—see Appendix E for further discussion. However, for theories on proper AdS, Theorem 2.6 is consistent with a property of two-point functions observed in Ref. 7 and arrived at there by very different means and assumptions.

In Theorems 2.5 and 2.6 we see that the passivity of the vacuum state and the group relations in $\mathrm{SO}_0(2, n-1)$ have determined which regions in AdS^n are to have (weakly) commensurable observables. In theories on AdS where the basic fields satisfy standard *c*-number commutation relations, it follows from this result that such observables actually commute in the usual (operator) sense.[33] Indeed, it follows then that

$$\mathcal{A}(W'_R) \subset \mathcal{A}(W_R)' \quad \text{and} \quad \mathcal{A}(W_R) \subset \mathcal{A}(\tilde{W}'_R)'. \tag{2.28}$$

But assumptions (i)–(iv) do not imply the strong locality relations (2.28) in general. Indeed, consider a tempered Hermitian Fermi-type field ϕ with anticommutator

$$\phi(x)\phi(y) + \phi(y)\phi(x) = (W(x,y) + W(y,x)) \cdot 1, \tag{2.29}$$

where $W(x,y)$ is taken to be any $\mathrm{SO}_0(2, n-1)$-invariant two-point function satisfying the spectrum condition. [Specific examples are provided by two-point functions given in Ref. 21, Eq. (4.9).] This anticommutator does not vanish when x and y are in complementary wedges. The field ϕ generates a CAR-algebra with a quasifree state fixed by the two-point function

$$\omega(\phi(x)\phi(y)) = W(x,y). \tag{2.30}$$

Proceeding to the GNS representation with cyclic vector Ω, we conclude from Refs. 7 and 21 that this example satisfies all of our standing assumptions. Since $W(x,y)$ is symmetric when x, y are in complementary wedges, the weak locality is explicit.

As explained in Ref. 12, if (2.28) holds there are grounds to expect that the theory generically cannot have interaction. Theories which are weakly local but not strongly local escape that argument. In the following sections we shall therefore continue to explore consequences of standing assumptions (i)–(iv) when (2.28) does not hold, beginning with the nature of the independence of the algebras $\mathcal{A}(W_1)$, $\mathcal{A}(W_2)$ associated with suitable spacelike separated wedges. But, first, we make some further observations.

Assumptions (i)–(iv) entail that each wedge algebra $\mathcal{A}(W)$ is a factor (cf. the proof of Theorem 4.3). If wedge locality (2.28) held, then it would follow that $\mathcal{A}(W)\cap\mathcal{A}(W')=\mathbb{C}1$, i.e., no nontrivial observable can be localized in both W and W'. It is therefore of physical interest that this fact also follows directly from (i)–(iv) in the absence of (2.28).

Proposition 2.7: Let standing assumptions (i)–(iv) hold and let $n\geqslant 3$. *Then for any* $W\in\mathcal{W}$, *one has* $\mathcal{A}(W)\cap\mathcal{A}(W')=\mathbb{C}1$ *and* $\mathcal{A}(W)\vee\mathcal{A}(W')=B(\mathcal{H})$.

Proof: By covariance, it suffices to prove the assertion for $W=W_R$. Let $A\in\mathcal{A}(W_R)\cap\mathcal{A}(W_R')$ and $\mathcal{H}_0$ be the closure in $\mathcal{H}$ of $(\mathcal{A}(W_R)\cap\mathcal{A}(W_R'))\Omega$. Since $e^{i2t\pi M_{01}}$, respectively, $e^{-i2t\pi M_{01}}$, are the modular unitaries corresponding to $(\mathcal{A}(W_R),\Omega)$, respectively, $(\mathcal{A}(W_R'),\Omega)$, then with $\Delta=e^{2\pi M_{01}}$ one has

$$J_{W_R}\Delta^{1/2}A\Omega=A^*\Omega,\quad J_{W_R'}\Delta^{-1/2}A\Omega=A^*\Omega. \tag{2.31}$$

Hence, Eq. (2.26) entails that $\Delta^{1/2}=\Delta^{-1/2}$ on $\mathcal{H}_0$. Therefore, $\Delta A\Omega=A\Omega$, which yields $A\Omega=\Delta^{it}A\Omega=e^{i2t\pi M_{01}}A\Omega$, for all $t\in\mathbb{R}$. Hence, the mean ergodic theorem (see, e.g., Ref. 27) entails that $A\Omega=F_0A\Omega$, where F_0 is the projection onto the subspace of vectors in $\mathcal{H}$ each left invariant under $U(\mathrm{SO}_0(2,n-1))$, using Lemma A.3. Since the mixing property in condition (iii) entails that the rank of F_0 is 1 and since Ω is separating for $\mathcal{A}(W_R)$, it follows that A is a multiple of the identity. But this entails

$$\mathbb{C}1=J_W(\mathcal{A}(W)\cap\mathcal{A}(W'))J_W=J_W\mathcal{A}(W)J_W\cap J_W\mathcal{A}(W')J_W=\mathcal{A}(W)'\cap\mathcal{A}(W')', \tag{2.32}$$

using (2.26), so that $\mathcal{A}(W)\vee\mathcal{A}(W')=\mathcal{B}(\mathcal{H})$, for every $W\in\mathcal{W}$. □

Before we close this section, we have a final proposition to prove.

Proposition 2.8: Let standing assumptions (i)–(iv) hold, $n\geqslant 3$ *and* $W_1,W_2\in\mathcal{W}$. *If* $W_2\neq\pm W_1$, *then* $\mathcal{A}(W_1)\neq\mathcal{A}(W_2)$.

Proof: Since two unequal wedges $W_1,W_2\in\mathcal{W}$ have unequal reflections about their edges, unless W_2 coincides with W_1', $\widetilde{W}_1$ or $\widetilde{W}_1'$, Lemma 2.3 entails $J_{W_1}\neq J_{W_2}$ and, thus, $\mathcal{A}(W_1)\neq\mathcal{A}(W_2)$.

If $\mathcal{A}(W_1)\subset\mathcal{A}(W_1')$, then Theorem 2.5 entails that the restriction of ω to $\mathcal{R}(W_1)$ is a trace, which is excluded by assumptions (i) and (iii). Similarly Theorem 2.6 yields $\mathcal{A}(W_1)\neq\mathcal{A}(\widetilde{W}_1')$. □

III. THE SCHLIEDER PROPERTY

Many versions of the notion of independence of algebras of observables in spacelike separated regions have emerged in algebraic quantum theory (see Ref. 34 for a review), and most are logically independent of the usual notion of commensurability, which is that the algebras commute with each other elementwise. In this section we shall prove that algebras associated with properly spacelike separated wedges W_1,W_2 satisfy an extended form of the algebraic independence condition known as the Schlieder property, namely that $A_1\in\mathcal{A}(W_1),A_2\in\mathcal{A}(W_2)$ and $A_1A_2=0$ imply either $A_1=0$ or $A_2=0$. We shall say that two wedges W_1,W_2 are properly spacelike separated if $\lambda W_1\subset W_2'$ for all λ in some neighborhood of the identity in $\mathrm{SO}(2,n-1)$. Note that W and W' are not properly spacelike separated. Although in de Sitter and Minkowski spaces of dimension $n\geqslant 3$ such properly spacelike separated wedges do not exist, we show in Appendix B that they are plentiful in AdS.

The proof of an extended Schlieder property in AdS^n, $n\geqslant 3$, will be carried out in a series of steps.

Lemma 3.1: Let $W_1,W_2\in\mathcal{W}$ *be properly spacelike separated and let* $A_{1,k}\in\mathcal{A}(W_1)$, $A_{2,k}$

$\in \mathcal{A}(W_2), k=1,\ldots,n$. *If* $B \in \mathcal{B}(\mathcal{H})$ *is such that*

$$\sum_{k=1}^{n} A_{1,k} U(\lambda) B U(\lambda)^{-1} A_{2,k} = 0, \tag{3.1}$$

for all λ *in some neighborhood* $\mathcal{N} \subset \mathrm{SO}_0(2,n-1)$ *of the identity, then this equality holds for all* $\lambda \in \mathrm{SO}_0(2,n-1)$.

Proof: Choosing a smaller neighborhood $\mathcal{N}$, if necessary, it may be assumed that there exists a $W \in \mathcal{W}$ such that $W_1 \subset \lambda_0\lambda_1 W$ and $W_2 \subset \lambda_0\lambda_1 W'$ for $\lambda_0, \lambda_1 \in \mathcal{N}$. Let $s \mapsto \lambda_W(s)$ be the group of boosts inducing a positive timelike flow on the wedge W (and hence a negative timelike flow on W'). Setting $\lambda_1(s) \doteq \lambda_1 \lambda_W(s) \lambda_1^{-1}$ for $\lambda_1 \in \mathcal{N}$, it will first be shown that $B_s \doteq U(\lambda_1(s)) B U(\lambda_1(s))^{-1}$, $s \in \mathbb{R}$, satisfies the hypothesis of the lemma as well. Putting $\lambda(s) \doteq \lambda_0 \lambda_1 \lambda_W(s) \lambda_1^{-1} \lambda_0^{-1}$, $\lambda_0 \in N$, and picking arbitrary elements X_1, X_2 in $\mathcal{A}(W_1)$, $\mathcal{A}(W_2)$, respectively, one has

$$\begin{aligned} &\sum_{k=1}^{n} \langle \Omega, X_1 A_{1,k} U(\lambda_0) B_s U(\lambda_0)^{-1} A_{2,k} X_2 \Omega \rangle \\ &\quad = \sum_{k=1}^{n} \langle \Omega, X_1 A_{1,k} U(\lambda(s)) U(\lambda_0) B U(\lambda_0)^{-1} U(\lambda(s))^{-1} A_{2,k} X_2 \Omega \rangle = 0 \end{aligned} \tag{3.2}$$

for sufficiently small $|s|$. Now $s \mapsto U(\lambda(s))$ is, after rescaling s, the modular group corresponding to $(\mathcal{A}(\lambda_0\lambda_1 W), \Omega)$ and, similarly, $s \mapsto U(\lambda(s))^{-1}$ is the modular group corresponding to $(\mathcal{A}(\lambda_0\lambda_1 W'), \Omega)$. Since $\mathcal{A}(W_1) \subset \mathcal{A}(\lambda_0\lambda_1 W)$ and $\mathcal{A}(W_2) \subset \mathcal{A}(\lambda_0\lambda_1 W')$, it follows that

$$s \mapsto \langle \Omega, X_1 A_{1,k} U(\lambda(s)) U(\lambda_0) B U(\lambda_0)^{-1} U(\lambda(s))^{-1} A_{2,k} X_2 \Omega \rangle \tag{3.3}$$

extends to an analytic function on a strip of the upper complex half plane for each $k=1,\ldots,n$. By the preceding result, the corresponding sum of functions thus has to vanish for all $s \in \mathbb{R}$. As X_1, X_2 were arbitrary within the above limitations and Ω is cyclic for $\mathcal{A}(W_1)$ and $\mathcal{A}(W_2)$, respectively, one concludes that $\Sigma_{k=1}^{n} A_{1,k} U(\lambda_0) B_s U(\lambda_0)^{-1} A_{2,k} = 0$, $s \in \mathbb{R}$ and $\lambda_0 \in \mathcal{N}$.

Next, let $\lambda_1, \ldots, \lambda_m \in \mathcal{N}$. Setting $\lambda_i(s) \doteq \lambda_i \lambda_W(s) \lambda_i^{-1}$, $i=1,\ldots,m$, one deduces by induction on m that also

$$B_{s_1,\ldots,s_m} \doteq U(\lambda_m(s_m)) \cdots U(\lambda_1(s_1)) B U(\lambda_1(s_1))^{-1} \cdots U(\lambda_m(s_m))^{-1} \tag{3.4}$$

satisfies the hypothesis of the lemma for $s_1, \ldots, s_m \in \mathbb{R}$. Indeed, the case $m=1$ has just been proven. By the induction hypothesis and the group property of U, the assertion follows for $s_1, \ldots, s_{m-1} \in \mathbb{R}$ and small $|s_m|$. The argument presented in the preceding paragraph then entails that the assertion holds for all $s_m \in \mathbb{R}$.

But, according to Lemma A.2, the closure of the group generated by $\lambda_0 \lambda_W(s) \lambda_0^{-1}$, $\lambda_0 \in \mathcal{N}$, $s \in \mathbb{R}$, is $\mathrm{SO}_0(2,n-1)$. Hence, taking into account that U is a continuous representation, it follows by (weak operator) continuity of $\lambda \mapsto U(\lambda) B U(\lambda)^{-1}$ that these operators satisfy the hypothesis of the lemma as well, thereby completing its proof.

In the following, we shall say that the wedge W_1 is properly contained in the wedge W_2 and shall write $W_1 \Subset W_2$ if there exists a neighborhood $\mathcal{N}$ of the origin in $\mathrm{SO}_0(2,n-1)$ such that $\lambda W_1 \subset W_2$, for all $\lambda \in \mathcal{N}$. Again, note that in de Sitter space and Minkowski space of dimension $n \geqslant 3$ such pairs of wedges do not exist, but in AdS they are abundant (see Appendix B).

Lemma 3.2: Let W_1, W_2 *be properly spacelike separated, let* W *be any wedge such that* W_1, W_2 *are properly contained in* W *and* W', *respectively. If* $A_{1,k}$, $A_{2,k}, k=1,\ldots,n$, *are elements of* $\mathcal{A}(W_1)$ *and* $\mathcal{A}(W_2)$, *respectively, such that* $\Sigma_{k=1}^{n} A_{1,k} A_{2,k} = 0$, *one has*

$$\sum_{k=1}^{n} A_{1,k} U(\lambda_1) B_1 U(\lambda_1)^{-1} \cdots U(\lambda_m) B_m U(\lambda_m)^{-1} A_{2,k} = 0, \tag{3.5}$$

for $m \in \mathbb{N}$ *and* $B_i \in \mathcal{A}(W)'$, $\lambda_i \in \mathrm{SO}_0(2,n-1), i=1,\ldots,m$.

Proof: The proof of the lemma proceeds by induction on m. Let $\mathcal{N}$ be a neighborhood of the identity in $\mathrm{SO}_0(2,n-1)$ such that $\lambda_0^{-1}W_1 \subset W$ for $\lambda_0 \in \mathcal{N}$. Then

$$U(\lambda_0)^{-1}A_{1,k}U(\lambda_0) \in \mathcal{A}(\lambda_0^{-1}W_1) \subset \mathcal{A}(W) = (J_W\mathcal{A}(W)J_W)'. \tag{3.6}$$

So $A_{1,k}$ and $U(\lambda_0)B_0U(\lambda_0)^{-1}$ commute for any $B_0 \in J_W\mathcal{A}(W)J_W$ and consequently

$$0 = U(\lambda_0)B_0U(\lambda_0)^{-1}\sum_{k=1}^{n} A_{1,k}A_{2,k} = \sum_{k=1}^{n} A_{1,k}U(\lambda_0)B_0U(\lambda_0)^{-1}A_{2,k}. \tag{3.7}$$

By the preceding lemma, this equality extends to all $\lambda_0 \in \mathrm{SO}_0(2,n-1)$. Assuming now that the statement holds for m, one has with the same choices of B_0 and λ_0 as in the preceding step

$$\begin{aligned} 0 &= \sum_{k=1}^{n} U(\lambda_0)B_0U(\lambda_0)^{-1}A_{1,k}U(\lambda_1)B_1U(\lambda_1)^{-1}\cdots U(\lambda_m)B_mU(\lambda_m)^{-1}A_{2,k} \\ &= \sum_{k=1}^{n} A_{1,k}U(\lambda_0)B_0U(\lambda_0)^{-1}U(\lambda_1)B_1U(\lambda_1)^{-1}\cdots U(\lambda_m)B_mU(\lambda_m)^{-1}A_{2,k}, \end{aligned} \tag{3.8}$$

for $B_i \in J_W\mathcal{A}(W)J_W$, $\lambda_i \in \mathrm{SO}_0(2,n-1), i=1,\ldots,m$. Taking into account that U is a representation of $\mathrm{SO}_0(2,n-1)$, this implies (after an obvious redefinition of $\lambda_1,\ldots,\lambda_m$):

$$\sum_{k=1}^{n} A_{1,k}U(\lambda_0)(B_0U(\lambda_1)B_1U(\lambda_1)^{-1}\cdots U(\lambda_m)B_mU(\lambda_m)^{-1})U(\lambda_0)^{-1}A_{2,k} = 0. \tag{3.9}$$

Applying once more the preceding lemma, one concludes that

$$\sum_{k=1}^{n} A_{1,k}U(\lambda_0)B_0U(\lambda_0)^{-1}U(\lambda_1)B_1U(\lambda_1)^{-1}\cdots U(\lambda_m)B_mU(\lambda_m)^{-1}A_{2,k} = 0, \tag{3.10}$$

for $B_i \in J\mathcal{A}(W)J$, $\lambda_i \in \mathrm{SO}_0(2,n-1), i=0,1,\ldots,m$, completing the proof.

In the next step of our argument we make use of the relation $J_WU(\lambda)J_W = U(\theta\lambda\theta)$, where θ is the reflection about the edge of W (cf. Lemma 2.3). Because of weak additivity, Proposition 2.7 and the preceding relation we have

$$\bigvee_{\lambda} U(\lambda)J_W\mathcal{A}(W)J_WU(\lambda)^{-1} = J_W\Big(\bigvee_{\lambda} U(\lambda)\mathcal{A}(W)U(\lambda)^{-1}\Big)J_W = J_W\mathcal{B}(\mathcal{H})J_W = \mathcal{B}(\mathcal{H}), \tag{3.11}$$

showing that $\mathcal{B}(\mathcal{H})$ is the weak operator closure of the algebra generated by the operators $U(\lambda)J_WBJ_WU(\lambda)^{-1}$, $B \in \mathcal{A}(W)$, $\lambda \in \mathrm{SO}_0(2,n-1)$. It therefore follows that for any collection of operators $A_{1,k}$, $A_{2,k}$ as in the preceding lemma one has

$$\sum_{k=1}^{n} A_{1,k}BA_{2,k} = 0, \quad B \in \mathcal{B}(\mathcal{H}). \tag{3.12}$$

Taking into account that $\mathcal{B}(\mathcal{H})$ contains in particular all operators of rank 1, we conclude that for any normal state $\tilde{\omega}$ on $\mathcal{B}(\mathcal{H})$ we have

$$\sum_{k=1}^{n} \tilde{\omega}(A_{1,k})A_{2,k} = 0 = \sum_{k=1}^{n} A_{1,k}\tilde{\omega}(A_{2,k}). \tag{3.13}$$

So we have established that properly spacelike separated wedge algebras manifest a strong form of algebraic independence which implies the Schlieder property.

Proposition 3.3: Let standing assumptions (i)–(iv) hold and let W_1 *and* W_2 *be properly space-*

like separated wedges. For any $A_{1,k} \in \mathcal{A}(W_1)$ *and* $A_{2,k} \in \mathcal{A}(W_2), k=1,\ldots,n$, *such that* $\Sigma_{k=1}^{n} A_{1,k}A_{2,k}=0$, *relation (3.13) must hold for all normal states* $\tilde{\omega}$ *on* $\mathcal{B}(\mathcal{H})$. *In particular, if* $A_1A_2=0$, *then either* $A_1=0$ *or* $A_2=0$.

If the algebras $\mathcal{A}(W_1)$ and $\mathcal{A}(W_2)$ were mutually commuting, then the Schlieder property is equivalent to C^*-independence.[32] However, in the noncommuting case, the Schlieder condition is strictly weaker than C^*-independence,[24] and it is an open question in our setting whether C^*-independence holds if $\mathcal{A}(W_1)$ and $\mathcal{A}(W_2)$ do not commute.

IV. THE SPLIT PROPERTY

We shall next show that if W_1 is properly contained in W_2, then there exists a type I factor $\mathcal{M}$ such that $\mathcal{A}(W_1) \subset \mathcal{M} \subset \mathcal{A}(W_2)$, as long as the multiplicity of the eigenvalues of M_{0n} does not grow too fast. Hence, with this additional assumption, the algebras $\mathcal{A}(W_1)$ and $\mathcal{A}(W_2)'$ manifest a particularly strong form of statistical independence.

Since AdS^n is periodic in the time variable and M_{0n} is a positive operator, the spectrum of M_{0n} is a subset of $\mathbb{N}_0=\{0\}\cup\mathbb{N}$. If the multiplicities of the eigenvalues of M_{0n} do not increase too rapidly, then $e^{-\gamma M_{0n}}$ is a trace class operator for any $\gamma>0$. In Appendix D we exhibit simple examples, constructed from irreducible unitary positive energy representations of $\mathrm{SO}_0(2,n-1)$, where this situation obtains. We formulate this assumption explicitly as condition (NC).

(NC). There exist constants $c_0>0$ and $0<k_0<1$ such that the spectral multiplicities $\boldsymbol{\mu}_m$ of the eigenvalues m of M_{0n} are bounded by $\boldsymbol{\mu}_m \leqslant e^{c_0 m^{k_0}}$, $m \in \mathbb{N}_0$.

It is particularly straightforward to establish the "split property" in the presence of condition (NC). In fact, in Ref. 16, Theorem 3.2 it was shown that in conformally invariant theories a trace-class condition on the exponentiated conformal Hamiltonian entails that suitable inclusions are split. We indicate here a somewhat different and more explicit argument. To this end, we recall the following lemma (Ref. 10, Lemma 2.3).

Lemma 4.1: Let $U(t)=e^{itH}$, $t \in \mathbb{R}$, *determine a strongly continuous one-parameter group of unitary operators with positive generator H and invariant unit vector* $\Omega \in \mathcal{H}$. *Moreover, let* $\mathcal{A}$ *and* $\mathcal{B}$ *be von Neumann algebras satisfying*

$$U(t)\mathcal{A}U(t)^{-1} \subset \mathcal{B}, \tag{4.1}$$

for all $|t|<\delta$ *and some* $\delta>0$. *Then there exists a continuous function* $f:\mathbb{R}\to\mathbb{R}$ *which decreases almost exponentially, i.e.,* $\sup_\omega |f(\omega)|e^{|\omega|^k}<\infty$, *for any* $0<k<1$, *such that*

$$\langle \Omega, AB'\Omega\rangle = \langle \Omega, Af(H)B'\Omega\rangle + \langle \Omega, B'f(H)\Omega\rangle, \tag{4.2}$$

for all $A \in \mathcal{A}$ *and* $B' \in \mathcal{B}'$.

We use this to establish the following general result.

Proposition 4.2: Let $U(t)=e^{itH}$, $t \in \mathbb{R}$, *be a strongly continuous one-parameter group of unitary operators with an (up to a phase) unique invariant unit vector* $\Omega \in \mathcal{H}$ *and with a generator H having spectrum in* $\mathbb{N}_0$ *and spectral multiplicities bounded by* $\boldsymbol{\mu}_m \leqslant e^{c_0 m^{k_0}}$, $m \in \mathbb{N}_0$, *for fixed* $c_0>0$ *and* $0<k_0<1$. *Moreover, let* $\mathcal{A}$ *and* $\mathcal{B}$ *be type III factors with* Ω *cyclic and separating for both and satisfying*

$$U(t)\mathcal{A}U(t)^{-1} \subset \mathcal{B}, \tag{4.3}$$

for all $|t|<\delta$ *and some* $\delta>0$. *Then there exists a type I factor* $\mathcal{M}$ *such that* $\mathcal{A} \subset \mathcal{M} \subset \mathcal{B}$.

Proof: Consider the algebraic tensor product $\mathcal{A}\odot\mathcal{B}'$ and two of its representations

(a) $(\pi, \mathcal{H}, \Omega)$ with $\pi(A\odot B') \doteq AB'$,
(b) $(\pi_p, \mathcal{H}\otimes\mathcal{H}, \Omega\otimes\Omega)$ with $\pi_p(A\odot B') \doteq A\otimes B'$

in an obvious notation. By the preceding lemma, one has

$$\langle \Omega, \pi(A \odot B')\Omega \rangle = \langle \Omega, AB'\Omega \rangle = \langle \Omega, Af(H)B'\Omega \rangle + \langle \Omega, B'f(H)\Omega \rangle. \tag{4.4}$$

Let P_Ω be the projection onto $\mathbb{C}\Omega \subset \mathcal{H}$ and let V be the unitary flip on $\mathcal{H} \otimes \mathcal{H}$:

$$V\Phi \otimes \Psi \doteq \Psi \otimes \Phi, \quad \Phi, \Psi \in \mathcal{H}. \tag{4.5}$$

Taking into account that $f(H)$ is a trace class operator on $\mathcal{H}$, because of the assumptions on the spectrum of H and the rapid decay of f, one may conclude from (4.4) that

$$\langle \Omega, \pi(A \odot B')\Omega \rangle = tr_{\mathcal{H}\otimes\mathcal{H}}([V(f(H) \otimes P_\Omega) + (P_\Omega \otimes f(H))V]A \otimes B'), \tag{4.6}$$

where the operator in square brackets is of trace class on $\mathcal{H} \otimes \mathcal{H}$. Thus

$$\langle \Omega, \pi(A \odot B')\Omega \rangle = \omega_p(\pi_p(A \odot B')), \tag{4.7}$$

where ω_p is some normal functional with respect to the representation π_p. Since the left-hand side defines a state on $A \odot \mathcal{B}'$, so does the right-hand side; hence, ω_p is, in fact, a state on $\pi_p(\mathcal{A} \odot \mathcal{B}')^- = \mathcal{A} \overline{\otimes} \mathcal{B}'$. Since $\mathcal{A}, \mathcal{B}'$ are type III factors, so is their tensor product. Moreover, $\Omega \otimes \Omega$ is a cyclic and separating vector for $\mathcal{A} \overline{\otimes} \mathcal{B}'$, since Ω is cyclic and separating for $\mathcal{A}$ and $\mathcal{B}'$. Hence ω_p is represented by a vector $\Omega_p \in \mathcal{H} \otimes \mathcal{H}$, and one has

$$\langle \Omega, \pi(A \odot B')\Omega \rangle = \langle \Omega_p, \pi_p(A \odot B')\Omega_p \rangle, \quad A \in \mathcal{A}, B' \in \mathcal{B}'. \tag{4.8}$$

Since Ω is cyclic for $\pi(\mathcal{A} \otimes \mathcal{B}')$, one concludes that π is unitarily equivalent to some subrepresentation of π_p. But, due to the fact that $\pi_p(\mathcal{A} \otimes \mathcal{B}')$ is a factor of type III, any subrepresentation of π_p is equivalent to π_p; hence, π and π_p are unitarily equivalent.

So let $W: \mathcal{H} \otimes \mathcal{H} \to \mathcal{H}$ be a unitary such that

$$AB' = \pi(A \odot B') = W\pi_p(A \odot B')W^{-1} = WA \otimes B'W^{-1}. \tag{4.9}$$

Since $\mathcal{A} \otimes 1 \subset \mathcal{B}(\mathcal{H}) \otimes 1 \subset (1 \otimes \mathcal{B}')'$, one concludes, after applying the adjoint action of W to this chain of inclusions,

$$\mathcal{A} \subset W(\mathcal{B}(\mathcal{H}) \otimes 1)W^{-1} \subset \mathcal{B}'' = \mathcal{B}, \tag{4.10}$$

where $\mathcal{M} \doteq W(\mathcal{B}(\mathcal{H}) \otimes 1)W^{-1}$ is a type I factor. □

We can now prove the following theorem for our immediate purposes.

Theorem 4.3: *Let the assumptions (i)–(iv) and (NC) hold. Then for any wedges W_1 and W_2 such that*

$$e^{itM_{0n}}\mathcal{A}(W_1)e^{-itM_{0n}} \subset \mathcal{A}(W_2), \tag{4.11}$$

for all sufficiently small $t \in \mathbb{R}$, there exists a type I_∞ factor $\mathcal{M}$ such that $\mathcal{A}(W_1) \subset \mathcal{M} \subset \mathcal{A}(W_2)$.

Remark: Of course, if $W_1 \Subset W_2$, then (4.11) holds.

Proof: Our passivity and mixing assumptions entail that $\mathcal{A}(W)$ is a type III_1 factor, for all $W \in \mathcal{W}$ (Ref. 29, Theorem 4.3). The theorem then follows at once from Proposition 4.2.

Note that in de Sitter space and Minkowski space of dimension $n \geqslant 3$ no inclusions of wedge algebras can be split. For Minkowski space this was observed in Ref. 8; in de Sitter space $W_1 \subset W_2$ entails $W_1 = W_2$.

The earlier results hold only for theories on proper AdS. If the covering space of AdS is considered, then condition (NC) must be replaced by the condition that the map

$$\mathcal{A}(W) \ni A \mapsto e^{-\gamma M_{0n}}A\Omega, \tag{4.12}$$

is nuclear, for all $\gamma > 0$.[9] The proof presented in Ref. 9 is formulated in terms of double cone algebras in Minkowski space but carries over to the present situation without difficulty.

V. LOCAL NETS ON TWO-DIMENSIONAL AdS

In this section we prove that standing assumptions (i)–(iv) and the spectral condition (NC) entail the existence of a nontrivial, covariant and local subnet in two-dimensional AdS. It is noteworthy that locality properties can be derived in these circumstances, and it would be of interest to see whether the same is also true in higher-dimensional AdS.

In two-dimensional AdS, the set of all wedge-shaped regions consists of two disconnected pieces $\{\lambda W_R|\lambda \in \mathrm{SO}_0(2,n-1)\}$ and $\{\lambda W_L|\lambda \in \mathrm{SO}_0(2,n-1)\}$, where $W_L = W_R'$. The former (respectively, latter) will be denoted by $\mathcal{W}_R(\mathcal{W}_L)$ and called the class of right wedges (left wedges). Note that $W \in \mathcal{W}_R$ if and only if $W' \in \mathcal{W}_L$. We assume as before that

$$\mathcal{A} = \bigvee_{W \in \mathcal{W}_R} \mathcal{A}(W), \tag{5.1}$$

and that Ω is cyclic for $\mathcal{A}$. Hence, once again, Proposition C.1 yields the cyclicity of Ω for every $\mathcal{A}(W)$, $W \in \mathcal{W}_R$.

In AdS^2 the edge of a wedge is a single point. For each point $a \in \mathrm{AdS}^2$ we shall denote by W_a the unique element of $\mathcal{W}_R$ whose edge is a. Then W_a' is the unique element of $\mathcal{W}_L$ whose edge is a. For $a,b \in \mathrm{AdS}^2$ such that $W_b \Subset W_a$ we define the open sets (double cones) $\mathcal{O}_{a,b} = W_a \cap W_b'$. Corresponding to $\mathcal{O}_{a,b}$ we define the von Neumann algebra

$$\mathcal{B}(\mathcal{O}_{a,b}) = \mathcal{A}(W_a) \cap \mathcal{A}(W_b)'. \tag{5.2}$$

Note that $\mathcal{O}_{a,b} \subset \mathcal{O}_{c,d}$ if and only if $W_a \subset W_c$ and $W_d \subset W_b$. The isotony of the original net of wedge algebras then implies

$$\mathcal{B}(\mathcal{O}_{a,b}) \subset \mathcal{B}(\mathcal{O}_{c,d}), \tag{5.3}$$

i.e., the isotony of the net $\{\mathcal{B}(\mathcal{O}_{a,b})|a,b \in \mathrm{AdS}^2\}$. The covariance of the original net of wedge algebras entails

$$U(\lambda)\mathcal{B}(\mathcal{O}_{a,b})U(\lambda)^{-1} = U(\lambda)(\mathcal{A}(W_a) \cap \mathcal{A}(W_b)')U(\lambda)^{-1} = \mathcal{A}(\lambda W_a) \cap \mathcal{A}(\lambda W_b)' = \mathcal{B}(\lambda \mathcal{O}_{a,b}) \tag{5.4}$$

for all $\lambda \in \mathrm{SO}(2,n-1)$.

In general, there is no reason for such relative commutants of wedge algebras to be nontrivial. But in our setting they turn out to be very large algebras, having a dense G_δ set of cyclic vectors.

Proposition 5.1: If conditions (i)–(iv) and (NC) hold in a theory on two-dimensional AdS and $W_b \Subset W_a$, *then* $\mathcal{B}(\mathcal{O}_{a,b})$ *is a type* III_1 *factor*.

Proof: If W_b is properly contained in W_a, then from Theorem 4.3 one has the existence of a type I factor $\mathcal{M}$ such that $\mathcal{A}(W_b) \subset \mathcal{M} \subset \mathcal{A}(W_a)$. From the proof of Theorem 2.1 in Ref. 18 there exists a unitary mapping $\mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ such that $U\mathcal{A}(W_b)U^{-1} = \mathcal{A}(W_b) \otimes 1$ and $U\mathcal{A}(W_a)U^{-1} = \mathcal{B}(\mathcal{H}) \otimes \mathcal{A}(W_a)$. Using Takesaki's commutant theorem for tensor products (cf. Ref. 26, Theorem 11.2.16) one therefore sees that

$$\mathcal{B}(\mathcal{O}_{a,b}) = \mathcal{A}(W_a) \cap \mathcal{A}(W_b)' = U^{-1}((\mathcal{B}(\mathcal{H}) \otimes \mathcal{A}(W_a)) \cap (\mathcal{A}(W_b)' \otimes \mathcal{B}(\mathcal{H})))U = U^{-1}\mathcal{A}(W_b)' \otimes \mathcal{A}(W_a)U. \tag{5.5}$$

Since $\mathcal{A}(W_a)$ and $\mathcal{A}(W_b)$ are type III_1 factors (cf. proof of Theorem 4.3), the algebra $\mathcal{A}(W_b)' \otimes \mathcal{A}(W_a)$ and, thus, also $\mathcal{B}(\mathcal{O}_{a,b})$ is a type III_1 factor (cf. Ref. 26, Corollary 11.2.17 and Ref. 15, Theorems 1.3.4 and 3.4.1).

We have seen previously that assumptions (i)–(iv) prescribe the sense in which "spacelike separated" is to be understood in AdS^n. Hence, the region $\mathcal{O}_{a,b}$ is spacelike separated from $\mathcal{O}_{c,d}$ if there exists a wedge W such that $\mathcal{O}_{a,b} \subset W$ and $\mathcal{O}_{c,d} \subset W'$. Without loss of generality, we may assume for concreteness that $W \in \mathcal{W}_R$, so that $W_a \subset W \subset W_d$. Then one finds that the local algebras satisfy locality

$$\mathcal{B}(\mathcal{O}_{a,b}) = \mathcal{A}(W_a) \cap \mathcal{A}(W_b)' \subset \mathcal{A}(W) \subset \mathcal{A}(W_c)' \vee \mathcal{A}(W_d) = \mathcal{B}(\mathcal{O}_{c,d})'. \tag{5.6}$$

We summarize these findings in the following theorem.

Theorem 5.2: If conditions (i)–(iv), (NC) and (5.1) hold in a theory on two-dimensional AdS, then the above construction yields a nontrivial, covariant and local net $\mathcal{O} \mapsto \mathcal{B}(\mathcal{O})$ *based on double cones* $\mathcal{O} \subset AdS^2$, *in which each algebra* $\mathcal{B}(\mathcal{O})$ *is a factor of type* III_1.

One can similarly define a second nontrivial, covariant, and local net from a given net of wedge algebras based upon the wedges in $\mathcal{W}_L$. These two local nets coincide if the initial nets of wedge algebras are local with respect to each other, $\mathcal{A}(W') \subset \mathcal{A}(W)'$.

We wish to sketch some consequences of this construction. The weakly local, but quite nonlocal net fixed by the field ϕ given in Eq. (2.29) is also well-defined in two-dimensional AdS, as long as the two-point function $W(x,y)$ is suitably chosen. The preceding construction yields many nontrivial observables localized in precompact subsets of AdS^2 and associated with this field. In terms of the original, simply expressed field, these local observables are quite complicated objects. This suggests the possibility of constructing complex local objects from relatively simple nonlocal fields.

In Ref. 14 the existence of split inclusions of wedge algebras was replaced by a modular nuclearity condition to employ the above construction in theories on two-dimensional Minkowski space. This modular nuclearity condition has been verified[28] in a factorizing S-matrix model with S-matrix not equal to the identity. The basic field in that model has algebraic relations similar to those of our field ϕ. Since in some suitable sense quantum theories on AdS become close to theories on Minkowski space as the AdS radius becomes sufficiently large, one may expect that the model on AdS^2 determined by ϕ also describes physics which goes beyond that of generalized free fields. These matters shall be further investigated elsewhere.

VI. CONCLUSIONS AND FURTHER REMARKS

We have thus shown that stability properties of a state carrying the interpretation of a "vacuum" imply a PCT theorem, the uniqueness of the Unruh temperature, as well as commensurability and independence properties of the observables in any quantum field theory on AdS. Such implications exist also in other space–times, but they are of particular interest in the case of AdS, where the causal structure is such that it is not clear *a priori* how to define "mutually spacelike regions," and therefore it is not clear which locality relations are physically meaningful. Nor is it sufficient to sidestep the issue by appealing to theories on the covering space of AdS^n. In fact, we have seen that observables in opposite wedges W and W' or in conjugate wedges W and $\widetilde{W}'$ necessarily commute with each other, either weakly or strongly. The former fact can seem natural from the point of view of the covering space of AdS^n, but the latter can certainly not be observed in theories on the covering space. It is remarkable that locality properties can be determined by stability assumptions. Indeed, we showed that in two-dimensional AdS these stability assumptions and a weak growth condition on the eigenvalues of M_{02} entail the existence of a nontrivial, covariant, local net indexed by bounded regions in AdS. It would be of interest to determine if the same is true of theories on higher dimensional AdS.

It was conjectured by Bros, Epstein, and Moschella in Ref. 7 that the assumptions made in that paper should follow from our standing assumptions. This would be an interesting matter to settle, since it would allow one to derive more detailed information about the analyticity properties of the two-point function of quantum fields on AdS.

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APPENDIX A: UNITARY REPRESENTATIONS OF THE AdS GROUP

The algebraic properties of the strongly continuous unitary representation of $\mathrm{SO}_0(2,n-1)$ assumed to exist in (i) are of crucial importance to us. As a convenience to the reader, we collect the relevant properties here. Many of the arguments in this section are adapted from Ref. 3. Given any such representation U and a coordinate system on AdS^n, we denote by $M_{\mu\nu}, \mu,\nu = 0,1,\ldots,n$, the corresponding self-adjoint generators. On a dense, invariant domain of analytic vectors in $\mathcal{H}$, they fulfill the following Lie-algebraic relations:

$$[M_{\mu\nu},M_{\rho\sigma}] = -ig_{\mu\rho}M_{\nu\sigma} + ig_{\mu\sigma}M_{\nu\rho} - ig_{\nu\sigma}M_{\mu\rho} + ig_{\nu\rho}M_{\mu\sigma}, \tag{A1}$$

where $g=\mathrm{diag}(1,-1,\ldots,-1,1)$, $\mu,\nu=0,1,\ldots,n$. In particular, the operator M_{01} generates the action of the boosts λ_{01}:

$$U(\lambda_{01}(t)) = e^{itM_{01}}, \quad t \in \mathbb{R}, \tag{A2}$$

and similarly for the operators $M_{0j}, j=2,\ldots,n-1$. M_{0n} is the generator of the time translations. Any of the operators $M_{0j}, j=1,\ldots,n$, may be taken to be the operator M discussed in the Introduction (see Sec. I). If $n\geqslant 3$, the operators $M_{jk}, j,k=1,\ldots,n-1$, are the generators of spatial rotations, whereas $M_{jn}, j=2,\ldots,n-1$ generate other subgroups of boosts obtained from the first-mentioned by temporal rotation. If $n=2$, then M_{01} and M_{12} are generators of boosts and there are no spatial rotations.

The Lie-algebraic relations (A1) yield the equality

$$e^{isM_{0n}}M_{01}e^{-isM_{0n}} = \cos(s)M_{01} - \sin(s)M_{1n}, \tag{A3}$$

which implies

$$e^{i\pi M_{0n}}M_{01}e^{-i\pi M_{0n}} = -M_{01}. \tag{A4}$$

Hence, M_{01} cannot be a positive operator on $\mathcal{H}$. Since the representation $U(\mathrm{SO}_0(2,n-1))$ is nontrivial, we may conclude the following lemma from the assumed $\mathrm{SO}_0(2,n-1)$-covariance.

Lemma A.1: The operators $M_{0j}, j=1,\ldots,n-1$, cannot be positive on $\mathcal{H}$ and thus Ω cannot be a ground state for the group $e^{itM_{0j}}$.

The Lie-algebraic relations (A1) also imply the following group relations:

$$e^{isM_{0n}}e^{itM_{01}}e^{-isM_{0n}} = e^{it(\cos(s)M_{01}-\sin(s)M_{1n})}; \tag{A5}$$

$$e^{isM_{0j}}e^{itM_{01}}e^{-isM_{0j}} = e^{it(\cosh(s)M_{01}-\sinh(s)M_{1j})}, \quad j=2,\ldots,n-1; \tag{A6}$$

$$e^{isM_{j1}}e^{itM_{01}}e^{-isM_{j1}} = e^{it(\cos(s)M_{01}-\sin(s)M_{j0})}, \quad j=2,\ldots,n-1; \tag{A7}$$

$$e^{isM_{01}}e^{itM_{0n}}e^{-isM_{01}} = e^{it(\cosh(s)M_{0n}-\sinh(s)M_{1n})}. \tag{A8}$$

Of course, Eqs. (A6) and (A7) are vacuous if $n=2$. We shall establish a few necessary tools.

Lemma A.2: Let $\mathcal{N}\subset \mathrm{SO}_0(2,n-1)$ be any neighborhood of the identity in $\mathrm{SO}_0(2,n-1)$. Then the closure $\mathcal{U}_\mathcal{N}$ in the strong operator topology of the group generated by the unitaries $U(\lambda\lambda_{01}(t)\lambda^{-1})$, $t\in\mathbb{R}$, $\lambda\in\mathcal{N}$, contains $U(\mathrm{SO}_0(2,n-1))$.

Proof: Consider first $n\geqslant 3$. From (A6) it follows that for all sufficiently small $|s|$ and for all $t\in\mathbb{R}$, $\mathcal{U}_\mathcal{N}$ contains the operator $e^{it(\cosh(s)M_{01}-\sinh(s)M_{1j})}$ for $j=2,\ldots,n-1$. With fixed s, the Trotter product formula[30] applied to the product of the one–parameter groups $e^{it(\cosh(s)M_{01}-\sinh(s)M_{1j})}$ and $e^{it\,\cosh(s)M_{01}}\in\mathcal{U}_\mathcal{N}$ implies that the rotations $e^{-it\,\sinh(s)M_{1j}}$, $j=2,\ldots,n-1$, are also contained in $\mathcal{U}_\mathcal{N}$.

Similarly, Eqs. (A5) and (A7) entail that the operators $e^{itM_{1n}}$ and $e^{itM_{j0}}$, $j=2,\ldots,n-1$, $t\in\mathbb{R}$, are contained in $\mathcal{U}_{\mathcal{N}}$. Since the group $U(\mathrm{SO}_0(2,n-1))$ is generated by these subgroups, the proof is complete for $n\geqslant 3$.

If $n=2$, then the same argument applied to (A5) entails that the group $e^{itM_{12}}$, $t\in\mathbb{R}$, is contained in $\mathcal{U}_{\mathcal{N}}$. One may then apply the same reasoning to the equality

$$e^{isM_{12}}e^{itM_{01}}e^{-isM_{12}}=e^{it(\cosh(s)M_{01}-\sinh(s)M_{02})} \tag{A9}$$

to conclude that also the group $e^{itM_{02}}$, $t\in\mathbb{R}$, is contained in $\mathcal{U}_{\mathcal{N}}$. The assertion now follows for $n=2$.

Lemma A.3: Let $\Psi\in\mathcal{H}$ satisfy $U(\lambda_{01}(t))\Psi=\Psi$, for all $t\in\mathbb{R}$. Then $U(\lambda)\Psi=\Psi$, for all $\lambda\in\mathrm{SO}_0(2,n-1)$.

Proof: Consider first $n\geqslant 3$. Using the equation

$$e^{isM_{01}}e^{itM_{0j}}e^{-isM_{01}}=e^{it(\cosh(s)M_{0j}+\sinh(s)M_{1j})},\quad j=2,\ldots,n-1, \tag{A10}$$

and setting $t=2re^{-|s|}$, the continuity of the representation $U(\mathrm{SO}_0(2,n-1))$ implies that

$$\lim_{s\to\pm\infty}e^{isM_{01}}e^{i2re^{-|s|}M_{0j}}e^{-isM_{01}}=e^{ir(M_{0j}\pm M_{1j})}, \tag{A11}$$

for $j=2,\ldots,n-1$, where the limit is the strong operator limit on $\mathcal{H}$. But then, by hypothesis, one has

$$\lim_{s\to\pm\infty}\left\|e^{isM_{01}}e^{i2re^{-|s|}M_{0j}}e^{-isM_{01}}\Psi-\Psi\right\|=\lim_{s\to\pm\infty}\left\|e^{i2re^{-|s|}M_{0j}}\Psi-\Psi\right\|=0, \tag{A12}$$

since $e^{i2re^{-|s|}M_{0j}}$ converges strongly to the identity 1 on $\mathcal{H}$ as $s\to\pm\infty$. These two equations then imply

$$e^{ir(M_{0j}\pm M_{1j})}\Psi=\Psi, \tag{A13}$$

for all $r\in\mathbb{R}$ and $j=2,\ldots,n-1$. Similarly, the equation

$$e^{isM_{01}}e^{itM_{1n}}e^{-isM_{01}}=e^{it(\cosh(s)M_{1n}+\sinh(s)M_{0n})} \tag{A14}$$

yields

$$e^{ir(M_{1n}\pm M_{0n})}\Psi=\Psi, \tag{A15}$$

for all $r\in\mathbb{R}$. By using the Trotter product formula again and taking suitable limits, it is clear that $M_{0j}\Psi=0=M_{1j}\Psi$, for all $j=0,\ldots,n$. Equation (A1) then implies that Ψ is annihilated by all of the generators $M_{\mu\nu}$, which yields the assertion for $n\geqslant 3$.

If $n=2$, Eq. (A14) yields

$$e^{ir(M_{12}\pm M_{02})}\Psi=\Psi, \tag{A16}$$

for all $r\in\mathbb{R}$, and thus $M_{12}\Psi=0=M_{02}\Psi$. The assertion then follows for $n=2$.

We mention that Lemma A.3 is also stated (without explicit proof) as Lemma 5.4 in Ref. 7.

APPENDIX B: WEDGE INCLUSIONS IN AdS

Here we give the proof of some useful geometric properties of the subregions of AdS^n which we have identified as the correct choice of wedges in AdS^n. Indeed, we wish to show that for any wedge $W\in\mathcal{W}$ there exist wedges $W_0\in\mathcal{W}$ which are properly contained in W, $W_0\Subset W$, respectively, such that W_0' is properly spacelike separated from W, $W\Subset W_0$. In fact, such wedges are quite abundant. These results are to be contrasted with the situation in de Sitter space, where de Sitter

wedges satisfy $W_1 \subset W_2$ if and only if $W_1 = W_2$.[11] In Minkowski space of dimension $n \geq 3$, two wedges form an inclusion $W_1 \subset W_2$ only if W_1 is a suitable translation of W_2. Hence, also in the latter case there do not exist properly spacelike separated wedges.

It is convenient to use the following description of W_R:

$$W_R = \{x \in \mathrm{AdS}^n | e_\pm \cdot x < 0, x \cdot e_4 > 0\}, \tag{B1}$$

where $e_\pm = (\pm 1, 1, 0, \ldots, 0)$ and $e_4 = (0, \ldots, 0, 1)$. Consider the lightlike vectors $f_\pm = (\pm 1, c, 0, \ldots, 0, s)$, where $s > 0$ and $c^2 = 1 + s^2$, and the wedge they determine

$$W_0 \doteq \{x \in \mathrm{AdS}^n | x \cdot f_\pm < 0, x \cdot e_4 > 0\}. \tag{B2}$$

The edge of this wedge is the spacelike submanifold

$$\mathcal{E}_1 \doteq \{(0, s(1+\boldsymbol{\sigma}^2)^{1/2}, \boldsymbol{\sigma}, c(1+\boldsymbol{\sigma}^2)^{1/2}) | \boldsymbol{\sigma} \in \mathbb{R}^{n-2}\}, \tag{B3}$$

which is contained in W_R.

Lemma B.1: With the earlier definitions, for any $t \in \mathbb{R}$ there exists a neighborhood $\mathcal{N}$ of the identity in $\mathrm{SO}_0(2, n-1)$ such that $\lambda \lambda_{01}(t) W_0 \subset W_R$ for all $\lambda \in \mathcal{N}$. Hence, for any wedge $W_2 \in \mathcal{W}$ there exist wedges $W_1, W_3 \in \mathcal{W}$ such that $W_1 \Subset W_2$ and W_2 and W_3 are properly spacelike separated.

Proof: In order to show that $\lambda \lambda_{01}(t) \overline{W_0} \subset W_R$ for λ in a neighborhood of the identity, it suffices to show that the characteristic boundary of $\lambda \lambda_{01}(t) \overline{W_0}$ is contained in W_R: $\lambda \lambda_{01}(t)(\mathcal{E}_1 + \mathbb{R}_+ f_\pm) \subset W_R$, i.e., $\lambda \lambda_{01}(t)(x + l f_\pm) \in W_R$, for all $l \geq 0$, $x \in \mathcal{E}_1$. Since λ is to be in a neighborhood of the identity 1, consider $\lambda = 1 + M$, where $\|M\| < \varepsilon$ and $\|\cdot\|$ is the norm on the $(n+1) \times (n+1)$ matrices with real entries. Then one has

$$\begin{aligned} \lambda \lambda_{01}(t)(x + l f_+) \cdot e_\pm &= (\pm \sinh(t) - \cosh(t)) s (1+\boldsymbol{\sigma}^2)^{1/2} + l(\pm \cosh(t) \pm c \sinh(t) - \sinh(t) - c \cosh(t)) \\ &\quad + M \lambda_{01}(t) x \cdot e_\pm + l M \lambda_{01}(t) f_+ \cdot e_\pm \leq (\pm \sinh(t) - \cosh(t)) s (1+\boldsymbol{\sigma}^2)^{1/2} + \|M\| \|e_\pm\| \\ &\quad \times \{\|\lambda_{01}(t) x\| + l \|\lambda_{01}(t) f_+\|\}, \end{aligned} \tag{B4}$$

where use was made of the fact that

$$\pm \cosh(t) \pm c \sinh(t) - \sinh(t) - c \cosh(t) = (\mp 1 + c)(\pm \sinh(t) - \cosh(t)) < 0. \tag{B5}$$

But $\|\lambda_{01}(t) f_\pm\| \leq 2 \cosh(t)$, $\|\lambda_{01}(t) x\| \leq \cosh(t)(1 + c^2 + 2s^2)^{1/2}(1 + \boldsymbol{\sigma}^2)^{1/2}$ and $\|e_\pm\| = \sqrt{2}$. In addition, $\pm \sinh(t) - \cosh(t) < 0$, for all $t \in \mathbb{R}_+$. Hence, if ε is sufficiently small, there exists a $\delta < 0$ (depending on t) such that

$$\lambda \lambda_{01}(t)(x + l f_+) \cdot e_\pm \leq \delta < 0, \quad x \in \mathcal{E}_1, l \geq 0. \tag{B6}$$

Similarly, one shows that

$$\lambda \lambda_{01}(t)(x + l f_-) \cdot e_\pm \leq \delta < 0, \quad x \in \mathcal{E}_1, l \geq 0, \tag{B7}$$

for suitably small ε.

Since $(\lambda W)' = \lambda W'$, for all $\lambda \in \mathrm{SO}_0(2, n-1)$ and $W \in \mathcal{W}$, it is clear that W_2 and W_3' are properly spacelike separated if and only if $W_2 \Subset W_3$. Thus, since $\mathcal{W} = \{\lambda W_R | \lambda \in \mathrm{SO}_0(2, n-1)\}$, the remaining assertions follow at once. □

It is of interest to note that in AdS^n, $n \geq 3$, there exists a wedge $W_2 \in \mathcal{W}$ such that $\overline{W_2} \subset W_R$, but in any neighborhood of the identity of $\mathrm{SO}_0(2, n-1)$ there exists some λ such that $\lambda W_2 \not\subset W_R$.

APPENDIX C: THE REEH–SCHLIEDER PROPERTY

We prove that the theories we are considering here must satisfy the Reeh–Schlieder property for the wedge algebras. Let $W \in \mathcal{W}$ be a wedge, and let $\mathcal{B}(W)$ denote the *–algebra consisting of

all $B \in \mathcal{A}(W)$ for which there exists a neighborhood $\mathcal{N}(B)$ of the identity in $\mathrm{SO}_0(2,n-1)$ such that $B(\lambda) \doteq U(\lambda)BU(\lambda)^{-1} \in \mathcal{A}(W)$, for all $\lambda \in \mathcal{N}(B)$. Note that Lemma B.1 entails that there exists a wedge $W_0 \in \mathcal{W}$ such that $\mathcal{A}(W_0) \subset \mathcal{B}(W)$.

Proposition C.1: Let assumptions (i)–(iv) obtain. Then Ω *is cyclic for* $\mathcal{A}(W)$*, given any* $W \in \mathcal{W}$.

Proof: (This proof is a straightforward adaptation of an argument given in Ref. 3.) Let $W, W_0 \in \mathcal{W}$ and $\mathcal{B}(W)$ be as described earlier and let $\mathcal{N}$ be a neighborhood of the identity in $\mathrm{SO}_0(2,n-1)$ such that $\lambda^{-1}W_0 \subset W$, for all $\lambda \in \mathcal{N}$. By the covariance assumption (iii), it suffices to consider $W = W_R$. Further, let $\Psi \in \mathcal{H}$ be orthogonal to the set of vectors $\mathcal{A}(W)\Omega$.

Since $\mathcal{B}(W) \subset \mathcal{A}(W)$, Ψ is also orthogonal to $\mathcal{B}(W)\Omega$. From the definition of $\mathcal{B}(W)$ and the continuity of the representation U, it is clear that for any $B \in \mathcal{B}(W)$ and $\lambda \in \mathcal{N}$ as described above there exists an $\varepsilon > 0$ such that $B(\lambda\lambda_{01}(t)\lambda^{-1}) \in \mathcal{B}(W)$, for all $|t| < \varepsilon$. Therefore, one has

$$\langle \Psi, B(\lambda\lambda_{01}(t)\lambda^{-1})\Omega \rangle = 0, \tag{C1}$$

for $|t| < \varepsilon$. Since $\lambda\lambda_{01}(t)\lambda^{-1}W_0 \subset \lambda W$, one also has $B(\lambda\lambda_{01}(t)\lambda^{-1}) \in \mathcal{A}(\lambda W)$, for all $t \in \mathbb{R}$. Hence, by the KMS property of the restriction of ω to $\mathcal{A}(\lambda W)$, the function

$$t \mapsto B(\lambda\lambda_{01}(t)\lambda^{-1})\Omega, \quad t \in \mathbb{R}, \tag{C2}$$

extends analytically to a vector-valued function in the strip $\{z \in \mathbb{C} | 0 < \mathrm{Im}(z) < \beta/2\}$ with continuous boundary values. Therefore, one must have

$$\langle U(\lambda\lambda_{01}(t)\lambda^{-1})^{-1}\Psi, B\Omega \rangle = \langle \Psi, B(\lambda\lambda_{01}(t)\lambda^{-1})\Omega \rangle = 0, \tag{C3}$$

for all $t \in \mathbb{R}$ and $B \in \mathcal{B}(W)$. By iterating this argument, it follows that for $\lambda_1, \ldots, \lambda_k \in \mathcal{N}$ and $t_1, \ldots, t_k \in \mathbb{R}$,

$$\langle U(\lambda_1\lambda_{01}(t_1)\lambda_1^{-1})^{-1} \cdots U(\lambda_k\lambda_{01}(t_k)\lambda_k^{-1})^{-1}\Psi, B\Omega \rangle = 0. \tag{C4}$$

Lemma A.2 then implies that $U(\lambda)\Psi$ is orthogonal to $\mathcal{B}(W)\Omega$, for any $\lambda \in \mathrm{SO}_0(2,n-1)$, and hence Ψ is orthogonal to $U(\lambda)^{-1}\mathcal{B}(W)\Omega = \mathcal{B}(\lambda^{-1}W)\Omega$.

Moreover, since $\mathcal{B}(W)$ is a *-algebra, $B^*U(\lambda)\Psi$ is orthogonal to $\mathcal{B}(W)\Omega$, for any $B \in \mathcal{B}(W)$ and $\lambda \in \mathrm{SO}_0(2,n-1)$. Hence, by induction, for any $\lambda_1, \ldots, \lambda_k \in \mathrm{SO}_0(2,n-1)$ and $B_1, \ldots, B_k \in \mathcal{B}(W)$ one has

$$\langle \Psi, B_1(\lambda_1) \cdots B_k(\lambda_k)\Omega \rangle = 0. \tag{C5}$$

Putting these results together, it now follows that Ψ is orthogonal to $(\cup_{\lambda \in \mathrm{SO}_0(2,n-1)} U(\lambda)\mathcal{B}(W)U(\lambda)^{-1})\Omega$. And since $\mathcal{A}(W_0) \subset \mathcal{B}(W)$, one observes

$$\Big(\bigvee_{\lambda \in \mathrm{SO}_0(2,n-1)} \mathcal{B}(\lambda W) \Big)\Omega \supset \Big(\bigvee_{\lambda \in \mathrm{SO}_0(2,n-1)} \mathcal{A}(\lambda W_0) \Big)\Omega = \mathcal{A}\Omega, \tag{C6}$$

by the assumption of weak additivity (1.4). Thus, Ψ is orthogonal to $\mathcal{A}\Omega$. As Ω is cyclic for $\mathcal{A}$, the assertion is proven.

APPENDIX D: MULTIPLICITY OF ENERGY LEVELS AND NUCLEARITY

In this appendix we wish to prove that given any irreducible unitary positive energy representation U_1 of the anti–de Sitter group $\mathrm{SO}_0(2,n-1)$ on a Hilbert space $\mathcal{H}_1$, then the corresponding unitary representation U obtained by "second quantization" on the bosonic or fermionic Fock space $\mathcal{H}$ based upon $\mathcal{H}_1$ satisfies condition (NC). Hence the free field examples discussed in the main text and Appendix E satisfy (NC). To verify this, we shall have need of some basic results about unitary representations of $\mathrm{SO}_0(2,n-1)$. We merely recall these and refer the reader to Refs. 19–21 for details and proofs. We shall present the case $n=4$; the situation is similar for the other cases.

Let $SO(2)\otimes SO(3)\subset \mathrm{SO}_0(2,3)$ be the maximal compact subgroup consisting of the "time rotations" around AdS^4 and the spatial rotations. Restricting U_1 to this compact group, the Hilbert space $\mathcal{H}_1$ decomposes into a direct sum of corresponding irreducible subspaces which are labeled by the energy $n\in\mathbb{N}$ and angular momentum $l\in\mathbb{N}_0$. It has been shown in Ref. 19 that in this decomposition there appear only representations where $l<n$. Moreover, for given (n,l), the number of these representations is bounded by $l+1$. Taking these facts into account, the multiplicity μ_n of the eigenvalue n of the generator of the time rotations on $\mathcal{H}_1$ can be estimated by $\mu_n \leqslant \Sigma_{l=0}^{n-1}(2l+1)(l+1)\leqslant 2n^3$, $n\in\mathbb{N}$.

Next, let M_{04} be the generator of the time rotations on the Fock space $\mathcal{H}$. The bound given earlier entails by standard arguments in statistical mechanics that in the bosonic case the corresponding partition function satisfies, for any $\gamma>0$:

$$\begin{aligned}\ln \operatorname{tr} e^{-\gamma M_{04}} &= -\sum_n \mu_n \ln(1-e^{-\gamma n})\\ &\leqslant \sum_n 2n^3 \frac{e^{-\gamma n}}{1-e^{-\gamma}} = \frac{2}{1-e^{-\gamma}}(-\partial_\gamma)^3 \frac{1}{1-e^{-\gamma}}\\ &\leqslant \frac{12e^{-\gamma}}{(1-e^{-\gamma})^5} \leqslant \frac{12\cdot 5^5}{\gamma^5}. \end{aligned} \tag{D1}$$

Denoting by $\boldsymbol{\mu}_n$ the multiplicity of the eigenvalue n of M_{04}, $n\in\mathbb{N}_0$, we obtain the estimate

$$\operatorname{tr} e^{-\gamma M_{04}} = \sum_n \boldsymbol{\mu}_n e^{-\gamma n} \leqslant e^{12\cdot 5^5/\gamma^5}, \tag{D2}$$

which implies

$$\boldsymbol{\mu}_n \leqslant e^{\gamma n + 12\cdot 5^5/\gamma^5}, \tag{D3}$$

for all $n\in\mathbb{N}_0$ and $\gamma>0$. With the choice $\gamma=5n^{-1/6}$, we conclude that

$$\boldsymbol{\mu}_n \leqslant e^{17n^{5/6}}, \quad n\in\mathbb{N}_0. \tag{D4}$$

A similar argument applies also to the fermionic case and in any number of space–time dimensions. Hence we have the following result.

Proposition D.1: In any free boson or fermion model based upon an irreducible positive energy representation of the anti–de Sitter group, condition (NC) holds.

APPENDIX E: EXAMPLES

In this appendix we shall discuss some examples of nets and states which fulfill standing assumptions (i)–(iv), as well as the condition (NC). Because AdS is not globally hyperbolic, the standard means of obtaining examples do not suffice. Free field models on AdS have been discussed in a series of papers by Fronsdal[20–23] and by Avis, Isham, and Storey.[1] More recently, the Wightman functions of quantum field models on AdS satisfying certain general conditions have been treated rigorously in Ref. 7. In addition, models of quantum field theories on AdS can also be obtained *via* holography[31] (see also Ref. 2). We begin our discussion with the latter.

In an elegant paper[31] Rehren has given rigorous mathematical meaning to the notion of holography, namely the correspondence between theories on AdS^n and conformally invariant theories on the boundary CM_{n-1} of AdS^n, compactified $(n-1)$-dimensional Minkowski space. He shows that between the set of wedges W in AdS and the set of (conformal images of) double cones C in the boundary there exists a canonical bijection α which preserves inclusions and causal complements, and intertwines the actions of the anti–de Sitter group and of the conformal group (which are isomorphic groups):

$$\alpha(\lambda(W)) = \tilde{\lambda}(\alpha(W)), \quad \alpha^{-1}(\tilde{\lambda}(C)) = \lambda(\alpha^{-1}(C)), \tag{E1}$$

where $\tilde{\lambda}$ is the restriction of the action of $\lambda \in \mathrm{SO}_0(2,n-1)$ to the boundary. The double cone $C = \alpha(W)$ is defined to be the intersection of W with the boundary. Hence, given a net $\{\tilde{\mathcal{A}}(\alpha(W))\}$ associated with a (for example) free quantum field on CM_{n-1} and a vacuum state $\tilde{\omega}$ on this net, one can define a net $\{\mathcal{A}(W)\}$ and state ω on AdS^n by

$$\mathcal{A}(W) \doteq \tilde{\mathcal{A}}(\alpha(W)), \quad \omega(A) \doteq \tilde{\omega}(A), \tag{E2}$$

for every $A \in \mathcal{A}(W) = \tilde{\mathcal{A}}(\alpha(W))$. From the results in Ref. 31 it is easy to show that the resulting theory on AdS^n fulfills our assumptions (i)–(iv), provided the underlying net on CM_{n-1} complies with the standard assumptions of conformal Minkowski space theories. In such theories one also has the equality $\mathcal{A}(W) = \mathcal{A}(-W)$, for every $W \in \mathcal{W}$. The CGMA and the modular stability condition, formulated in Ref. 11, both obtain in these models.

Using an irreducible representation of $\mathrm{SO}_0(2,3)$, Fronsdal[21] defines Hermitian free fields on the covering space of AdS^4; only if the energy spectrum of the theory is contained in $\mathbb{N}_0$ does his field restrict to AdS proper. In this latter case, Fronsdal's model satisfies assumptions (i)–(iv), as well as (NC)—see later and Appendix D. Moreover, the elements of $\mathcal{A}(W)$ commute weakly with those of $\mathcal{A}(\tilde{W}')$. Yet if the energy spectrum is not a subset of $\mathbb{N}_0$, this feature is no longer present, confirming our expectation that Theorem 2.6 cannot hold in general for fields not manifesting the periodicity in time required to enable them to be defined on AdS. We note that since in his examples the fields are invariant under the map $x \mapsto -x$, one has $\mathcal{A}(\tilde{W}') = \mathcal{A}(W') = \mathcal{A}(W)'$.

In Ref. 1 Avis, Isham, and Storey use an embedding of (the covering space of) AdS into the static Einstein universe to construct a free quantum field on AdS. Since the static Einstein universe is globally hyperbolic, one can rigorously construct free fields and the associated nets of local algebras in (subsets of) that space–time. And since the covering space of AdS can be conformally embedded into the Einstein universe, one can define free massless, i.e., conformally invariant, fields on AdS. However, the matter is complicated by the fact that one must find suitable boundary conditions at spacelike infinity in AdS—we must refer the reader to Ref. 1 for details. Since the resultant fields manifest the necessary periodicity in the time variable, they may be understood to be defined on AdS. Inspection of the resulting representations then led them to construct analogous representations of "conformally coupled massive" free fields on AdS. From the construction of their examples and the results in Ref. 7 it follows that standing assumptions (i)–(iv) hold. All of their examples are consistent with Theorem 2.6.

In Ref. 7 an axiomatic study is made of quantum fields on the covering space of AdS from the point of view of a suitable modification of the Wightman function approach to quantum field theory on Minkowski space. Explicit examples of two-point functions satisfying their assumptions are given there, which include Fronsdal's examples. A subclass of those two-point functions restrict to AdS; it is of interest to note that such two-point functions are characterized by a certain uniformity property—cf. Sec.6 in Ref. 7. Using the results of Refs. 7 and 29 it is easy to show that free fields built upon those two-point functions satisfy our assumptions (i)–(iv); the elements of a subclass also satisfy assumption (NC). The authors of Ref. 7 also observe that the locality property proven in Theorem 2.6 obtains only in those free field models which restrict to AdS proper (Ref. 7, p. 509).

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Marginal distributions in $(2N)$-dimensional phase space and the quantum $(N+1)$ marginal theorem

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We study the problem of constructing a probability density in $2N$-dimensional phase space which reproduces a given collection of n joint probability distributions as marginals. Only distributions authorized by quantum mechanics, i.e., depending on a (complete) commuting set of N variables, are considered. A diagrammatic or graph theoretic formulation of the problem is developed. We then exactly determine the set of "admissible" data, i.e., those types of data for which the problem always admits solutions. This is done in the case where the joint distributions originate from quantum mechanics as well as in the case where this constraint is not imposed. In particular, it is shown that a necessary (but not sufficient) condition for the existence of solutions is $n \leqslant N+1$. When the data are admissible and the quantum constraint is not imposed, the general solution for the phase space density is determined explicitly. For admissible data of a quantum origin, the general solution is given in certain (but not all) cases. In the remaining cases, only a subset of solutions is obtained. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In quantum theory, we usually assume that probability densities for eigenvalues of two noncommuting observables cannot be measured by the same experimental setup. A related theoretical question is: Does there exist a joint probability distribution of the eigenvalues of two such observables A and B which correctly reproduces the individual probabilities for A and for B as marginals (i.e., on integration over the eigenvalues of the other observable). Perhaps surprisingly, the answer to this question is yes. More generally, for a system with N configuration space variables $q_1, q_2, \ldots, q_N$, consider complete commuting sets (CCS) $S_1, S_2, \ldots, S_n$ of observables, each S_i consisting of some coordinate and some momentum variables (where S_i and S_j must contain some mutually noncommuting observables to be considered distinct CCS). Is there a joint probability density $\rho(q_1, \ldots, q_N, p_1, \ldots, p_N)$ whose marginals reproduce the quantum probability

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densities of the different CCS, $S_1, S_2, \ldots, S_n$? We shall prove that a necessary condition for this to be possible for arbitrary quantum states is $n \leqslant N+1$; this result is a precise no go theorem for simultaneous realization of more than $(N+1)$ quantum marginals.

Actually, this no go theorem also has applications to the classical arena of joint time-frequency distributions in signal processing and joint position-wave number distributions in image processing. It is therefore useful to state the problem in a general setting encompassing both classical and quantum mechanics.

Consider the general problem of reconstructing a probability density over $\mathbb{R}^M$, given a set of n associated joint probability distributions over subspaces of $\mathbb{R}^M$. In this general setting the problem can be stated as follows. Suppose first that a probability density $\rho(y_1, \ldots, y_M)$ is given and define the marginal distributions

$$\sigma_\alpha(Y_\alpha) = \int dY'_\alpha \rho(y_1, \ldots, y_M) \quad (\alpha = 1, \ldots, n), \tag{1.1}$$

where $Y_\alpha \cup Y'_\alpha$ is, for each α, a partition of $\{y_1, \ldots, y_M\}$. These joint distributions obey a set of compatibility conditions. Indeed, let $Y_{\alpha\beta}$ be the set of variables that $\sigma_\alpha(Y_\alpha)$ and $\sigma_\beta(Y_\beta)$ have in common and introduce the partitions $Y_\alpha = Y_{\alpha\beta} \cup Y'_{\alpha\beta}$ and $Y_\beta = Y_{\alpha\beta} \cup Y''_{\alpha\beta}$. Then Eq. (1.1) implies

$$\int dY'_{\alpha\beta} \sigma_\alpha(Y_{\alpha\beta}, Y'_{\alpha\beta}) = \int dY''_{\alpha\beta} \sigma_\beta(Y_{\alpha\beta}, Y''_{\alpha\beta}). \tag{1.2}$$

Conversely, suppose that a set $\{\sigma_1, \ldots, \sigma_n\}$ of joint probability distributions is given, which satisfies the compatibility conditions (1.2). Is it always possible to find some probability density ρ which reproduces them as marginals, in accordance with Eq. (1.1)? In the affirmative, how can we "reconstruct" such ρ's? It turns out that Eq. (1.2) is in general only necessary conditions for the existence of a positive density ρ, and our problem is precisely to solve the questions of existence, multiplicity, and explicit determination of the ρ's (if any).

Actually, we address these questions not in such a general setting, but in the case where $\mathbb{R}^M = \mathbb{R}^{2N}$ is the phase space of some physical system with coordinates y_j identified with conjugate canonical variables $\{q_j, p_j\}_{j=1}^N$ and where all distributions σ_α depend on exactly N variables $x_1, \ldots, x_N$ restricted by the condition $x_i = q_i$ or p_i $(i = 1, \ldots, N)$. The reason for this choice lies in the motivation of the problem within the context of quantum mechanics. Indeed, the functions σ_α just introduced can then be understood as quantum probability distributions associated with n complete commuting sets of observables (CCS), selected among 2^N possible choices (the 2^N possible assignments of the variables x_i). By "*quantum* probability distributions" is meant here a set of functions $\sigma_\alpha(x_1, \ldots, x_N)$ derived from a common wave function $\langle q_1, \ldots, q_N | \psi \rangle$ (in the Schrödinger representation), in accordance with the formula

$$\sigma_\alpha(x_1, \ldots, x_N) = |\langle x_1, \ldots, x_N \rangle \psi|^2 \quad (\alpha = 1, \ldots, n), \tag{1.3}$$

or more generally, for a mixed quantum state described by the density operator $\hat{\rho}$,

$$\sigma_\alpha(x_1, \ldots, x_N) = \langle x_1, \ldots, x_N | \hat{\rho} | x_1, \ldots, x_N \rangle \quad (\alpha = 1, \ldots, n). \tag{1.4}$$

The problem in this physical framework is directly related to the construction of "maximally realistic quantum mechanics," a program initiated by Roy and Singh in 1995 (Ref. 1) and intensively pursued since then.[2–4] Without entering a detailed discussion of this relationship from the viewpoint of quantum physics (for which we refer the reader to Refs. 1–4), let us recall the main results gained so far. In Ref. 2 it was shown that for any $N \geqslant 2$, a set of $n = N+1$ quantum probability distributions of the special form

$$\{\sigma_1(q_1, q_2, \ldots, q_N), \sigma_2(p_1, q_2, \ldots, q_N), \sigma_3(p_1, p_2, q_3, \ldots, q_N), \ldots, \sigma_{N+1}(p_1, p_2, \ldots, p_N)\} \tag{1.5}$$

can be realized as a set of marginals of a common phase space probability density $\rho(q_1, \ldots, q_N, p_1, \ldots, p_N)$. Further the "no go" conjecture was made that for $n \geqslant N+2$ (and for any

choice of n distinct CCS), there exist sets $\{\sigma_1,\ldots,\sigma_n\}$ of quantum probability distributions which cannot be recovered as marginals of some ρ. The determination of the most general density ρ reproducing the set (1.5), as well as the status of sets of CCS-distributions different from (1.5) and not necessarily of a quantum origin (i.e., mutually compatible but not necessarily construed according to Eq. (1.4)), were left as open questions. In Ref. 4, hereafter denoted by (I), complete answers to these questions were given in the special case $N=2$ (see also Ref. 3 for a brief summary). In particular, the general positive solution ρ of the equations

$$\begin{cases} \int dp_1 dp_2 \rho(q_1,q_2,p_1,p_2) = \sigma_1(q_1,q_2), \\ \int dq_1 dp_2 \rho(q_1,q_2,p_1,p_2) = \sigma_2(p_1,q_2), \\ \int dq_1 dq_2 \rho(q_1,q_2,p_1,p_2) = \sigma_3(p_1,p_2), \end{cases} \tag{1.6}$$

was worked out for an arbitrary set $\{\sigma_1,\sigma_2,\sigma_3\}$ (quantum or not) and the "no go" conjecture stated above was proved for $N=2$. In fact, it was shown that a necessary and sufficient condition for $n(\leqslant 4)$ arbitrarily given compatible σ_α's to be marginals of a probability density in four-dimensional phase space is $n\leqslant 3$ ("Three marginal theorem"). These results were obtained by first deriving certain correlation inequalities between the σ_α's from the mere existence of a positive and normalized ρ. Such inequalities, which are the analogs in phase space of the standard Bell inequalities for spin variables,[5] turn out to have an interest of their own in the context of quantum physics, as discussed in Refs. 3 and 4.

The generalization of the study performed in (I) to the case of an arbitrary number n of CCS-distributions of any species in a phase space of arbitrary dimension $2N$, which is precisely the aim of the present work, is not a straightforward task. It will be accomplished by means of two main tools: the Bell-type inequalities just mentioned (it turns out that no new correlation inequalities, proper to the $2N$-dimensional case, are needed for the present purpose) and a specific diagrammatic formulation of the problem which appears essential both for a concise exposition of our final statements and for their proof. In this way, we shall be able to treat the problem exhaustively and to give, in the general case, definite answers to the questions previously posed, in the form of a clear-cut theorem. This theorem will be stated at once in Sec. II (Theorem 1), after having introduced a set of appropriate definitions. As a by-product, the theorem affords a proof of the "no go" conjecture for any N (Theorem 2). On the positive side, it considerably extends early results of Cohen and Zaparovanny[6] for two marginals with non intersecting sets of variables by simultaneous realizability of $N+1$ marginals which have intersecting sets of variables as well. The rest of the paper (Secs. III–V) is almost entirely devoted to the (quite long!) proof of Theorem 1, and is therefore mainly technical. Our concluding comments are presented in Sec. VI.

II. DEFINITIONS AND RESULTS

In order to give our results a precise and unambiguous form, we introduce the following definitions:

(1) A CCS-distribution (CCS for Complete Commuting Set) in N dimensions is a probability distribution [Here and in the following, probability distributions are understood as positive normalized measures, with an absolutely continuous part and (possibly) Dirac measures.] $\sigma(x_1,\ldots,x_N)$, with $x_j=q_j$ or p_j for each index j.

The CCS-distributions can occur in 2^N different types, each type corresponding to one choice of the N-tuple of arguments.

(2) An n-chain is a set $\{\sigma_1,\ldots,\sigma_n\}$ of *mutually compatible* CCS-distributions of distinct types. Here, the mutual compatibility conditions (1.2) read, for any pair $\{\sigma_\alpha(Y_\alpha),\sigma_\beta(Y_\beta)\}$, where

$Y_\alpha=\{y_1,\ldots,y_r,Y\}$, $Y_\beta=\{y'_1,\ldots,y'_r,Y\}$ and y'_j is the conjugate of y_j ($y'_j=q_j$ or p_j according as $y_j=p_j$ or q_j),

$$\int dy_1\cdots dy_r\sigma_\alpha(y_1,\ldots,y_r,Y)=\int dy'_1\cdots dy'_r\sigma_\beta(y'_1,\ldots,y'_r,Y). \tag{2.1}$$

Thus, an n-chain is a possible candidate for a set of n marginals, i.e., joint probability distributions obtained from some phase space probability distribution [we shall use sometimes the notation $\rho(\mathbf{q},\mathbf{p})$] $\rho(q_1,\ldots,q_N,p_1,\ldots,p_N)$ by integrating over some of the arguments.

The type of an n-chain is defined by the types of its elements.

(3) An n-chain is admissible if there exists at least one phase space probability distribution ρ reproducing all the CCS distributions of the n-chain, namely such that

$$\sigma_\alpha(x_1,\ldots,x_N)=\int dx'_1\cdots dx'_N\rho(q_1,\ldots,q_N,p_1,\ldots,p_N)\ \ (\alpha=1,\ldots,n), \tag{2.2}$$

where x'_i is the conjugate of x_i. Equation (2.2) imply (2.1). Using the notation $Z_\alpha=\{x_1,\ldots,x_N\}$, $Z'_\alpha=\{x'_1,\ldots,x'_N\}$, and $d^NZ'_\alpha=dx'_1\cdots dx'_N$, (2.2) can be rewritten as

$$\sigma_\alpha(Z_\alpha)=\int d^NZ'_\alpha\rho(\mathbf{q},\mathbf{p})\ \ (\alpha=1,\ldots,n).$$

(4) An n-chain is a quantum n-chain if there exists at least one quantum state described by the density operator $\hat{\rho}$ such that Eq. (1.4) holds.

Note that in that case the compatibility conditions (2.1) are automatically satisfied.

(5) Two CCS-distributions σ_α and σ_β are contiguous if they differ by the assignment of only one variable x_i (to q_i and p_i), namely

$$\sigma_\alpha(x_1,\ldots,x_{i-1},q_i,x_{i+1},\ldots,x_N)\text{ and }\sigma_\beta(x_1,\ldots,x_{i-1},p_i,x_{i+1},\ldots,x_N).$$

We call i the index of the pair $\{\sigma_\alpha,\sigma_\beta\}$.

(6) To each n-chain we associate a graph which is constructed as follows:

(a) To every CCS-distribution of the chain, associate a vertex characterized by the collection of the variables of this distribution;

(b) Connect two vertices by a link if they correspond to contiguous CCS-distributions. We call index of the link the index of the pair of contiguous CCS-distributions, and we say that the two vertices are contiguous.

As usual, there are connected and disconnected graphs, tree graphs and graphs with loops. A graph G completely determines the type of the associated n-chain, so that we can speak of a chain of type G.

(7) An n-chain and its associated graph are said to be proper if no two links have the same index.

Since there are at most N possible indices, a proper graph has at most N links, and thus, if it is connected, at most $(N+1)$ vertices. Furthermore, a graph with a loop cannot be proper. Therefore, a connected proper graph is necessarily a tree graph with at most $(N+1)$ vertices.

(8) A graph G is fully admissible if all n-chains of type G are admissible.

A graph G is quantum admissible if all quantum n-chains of type G are admissible.
Full admissibility entails quantum admissibility.
A graph G is nonadmissible if it is not quantum (and *a fortiori* not fully) admissible.

(9) Let a nonconnected graph G be subgraph of a connected graph G_c. We call insertions the vertices of G_c which are not vertices of G. G_c is called G-simple if all its insertions have only two legs.

In the following, in order to shorten the writing, particularly when drawing graphs, we often replace the variables q_j and p_j by the indices j and j', respectively. For example, to a CCS-distribution $\sigma(q_1,p_2,q_3)$ we associate the vertex $\boxed{12'3}$ in a rectangle box. As for the inserted vertices, we use instead round boxes, e.g., (12′3).

We are now in a position to give a complete characterization of the graphs, or equivalently of the types of n-chains, according to their (full, quantum or non) admissibility.

Theorem 1:

(1) If a graph G is proper and connected, then it is fully admissible.
(2) If G is proper but nonconnected, then

(a) if G is subgraph of a proper connected graph G_c, then

(i) if G_c is G-simple, G is fully admissible,
(ii) if G_c is not G-simple, G is quantum, but not fully, admissible,

(b) *if G is not subgraph of a proper connected graph G_c, then it is nonadmissible.*

(3) *If G is nonproper, then it is nonadmissible.*

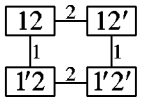
This theorem is complemented by the explicit construction of all the phase space distributions ρ reproducing a given chain of type G, a construction which is completed only in the case of full admissibility, that is to say when G is either connected and proper, or subgraph of a connected, proper and G-simple graph G_c (see Sec. IV B). In the case of quantum admissibility, when the connected graph G_c is proper but not G-simple, the situation is not as favorable and the general expression of ρ is not known (see Sec. V B 2).

Remarks:

(1) Given a graph G, a proper G_c, when there is one (case 2a), is in general not unique. It is a consequence of the theorem that either all the proper G_c's are G-simple, or none of them is.

Notice that this is a pure graph theoretic statement.

(2) For $N=2$, the main result of Sec. IV of (I), which was derived from Bell-type correlation inequalities, is the following: both in the classical and quantum cases, there exist 4-chains $\sigma_1(q_1,q_2)$, $\sigma_2(p_1,q_2)$, $\sigma_3(q_1,p_2)$, and $\sigma_4(p_1,p_2)$ which cannot be reproduced as marginals of any probability distribution $\rho(\mathbf{q},\mathbf{p})$. In the language of the present paper, this can be rephrased as:

The nonproper graph  *is non admissible.*

This is the simplest case of part 3 of the above theorem, and actually it is the clue of its proof.

An immediate corollary of Theorem 1 is

Theorem 2 ($N+1$ Marginal Theorem):

A necessary condition for all quantum n-chains of a given type to be admissible is $n \leqslant N+1$.

It suffices to use parts 2b and 3 of Theorem 1 and to note that G cannot have more vertices than G_c, and that a proper G_c has at most $N+1$ vertices (see the remark after the above definition 7 of *proper* n-chains and graphs).

Notice that, in contradistinction with the *three* marginal theorem of (I), the above theorem gives only a necessary condition. This is because only proper connected graphs G_c are involved when $N=2$ and $n \leqslant N+1$, whereas nonproper connected G_c's do appear as soon as $N \geqslant 3$. Of course, for proper connected graphs G for which n must be $\leqslant N+1$, part 1 of Theorem 1 guarantees admissibility for $N \geqslant 3$ also.

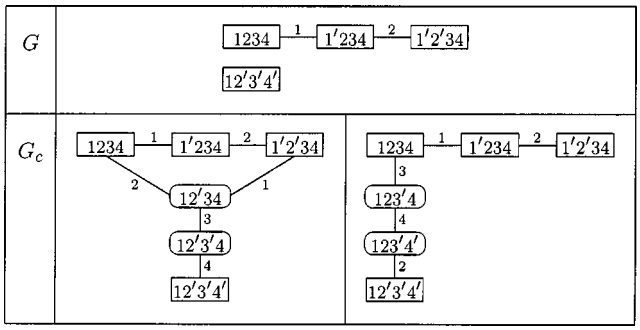


FIG. 1. A nonconnected proper graph G which is not subgraph of any proper connected graph G_c: G is nonadmissible. Two possible (nonproper) G_c's are shown: one with a loop, the other one a tree graph.

Theorem 1 will be proved in Secs. III–V. In order to help understanding its content, we give in Figs. 1 and 2 examples of the various cases encountered.

III. NONPROPER GRAPHS

Consider a nonproper graph G. By definition, there exist at least two links with the same index (say 1) connecting a first pair of vertices (V, V') and a second pair (W, W'). Then there necessarily exists a second index (say 2) such that the variables x_1 and x_2 have in the four vertices V, V', W, and W' the assignments as shown in Fig. 3.

Quite generally, in a graph G (proper or not), a set of four vertices where a pair of variables takes the four possible assignments will be called a *critical quartet*.

We now prove

Lemma 1: A graph G containing a critical quartet is nonadmissible.

Given an n-chain $\{\sigma_\alpha\}_{\alpha=1,\ldots,n}$ of type G in N dimensions and a partition of the set of indices $\{1,\ldots,N\}=J\cup K$, let us introduce the distributions

$$\tilde{\sigma}_\alpha(X_J)=\int \prod_{k\in K} dx_k \sigma_\alpha(X_J,X_K).$$

Some of these $\tilde{\sigma}_\alpha$'s may coincide. We call *J-reduced n′-chain* the maximal set of n' distinct $\tilde{\sigma}_\alpha$'s $(n'\leqslant n)$. Obviously, a necessary condition for the n-chain to be admissible is that the associated J-reduced n'-chain be admissible. Now, consider a quantum n-chain constructed with a factorized wave function of the form

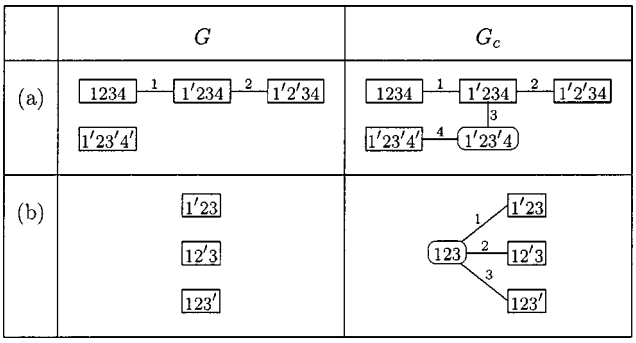


FIG. 2. (a) A nonconnected proper graph G which is subgraph of a proper connected G-simple graph G_c: G is fully admissible. (b) A nonconnected proper graph G which is subgraph of a proper connected non G-simple graph G_c: G is quantum but not fully admissible.

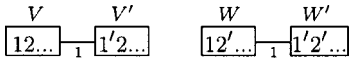


FIG. 3. Critical quartet in a nonproper graph.

$$\Psi(q_1, \ldots, q_N) = \Psi_1(Q_J)\Psi_2(Q_K). \tag{3.1}$$

Choosing then $J=\{1,2\}$, to be the indices of a critical quartet, our results in (I) (see Remark 2 after Theorem 1) immediately imply the nonadmissibility of the J-reduced 4-chain. Hence, the nonadmissibility of the n-chain σ_α itself, and Lemma 1 follows.

This establishes part 3 of Theorem 1, namely that a nonproper graph G is nonadmissible.

IV. CONNECTED PROPER GRAPHS

Let G be a connected proper graph. We establish part 1 of Theorem 1 by associating to any chain of type G a particular phase space distribution ρ_0 reproducing this chain. The explicit construction of such a ρ_0 is described in Sec. IV A. In Sec. IV B, we derive the expression of the most general phase space distribution reproducing the given chain.

A. Particular solution

Let $\mathcal{C}_n=\{\sigma_1, \ldots, \sigma_n\}$ be an n-chain of type G. Since G is a proper tree graph with $(n-1)$ links, there are exactly $(N-n+1)$ variables which have the same assignments in all the distributions σ_α. After a possible renumbering of the indices of the x_i's, we can therefore assume that in $\sigma_\alpha(x_1, \ldots, x_{n-1}, x_n, \ldots, x_N)$ the assignment of each of the variables $x_n, \ldots, x_N$ is independent of α. These variables, which will play a purely passive role, are henceforth denoted collectively by T, whereas T' will stand for the set of conjugate variables $\{x'_n, \ldots, x'_N\}$.

The solution $\rho_0(q_1, \ldots, q_N, p_1, \ldots, p_N)$ of Eq. (2.2) is constructed as the product of "vertex functions," "propagators" and an arbitrary positive function of T'. The former elements are defined by the following "Feynman rules:"

1) to each vertex $\boxed{x_1, \ldots, x_N}$ of G, we associate the vertex function $\sigma_\alpha(x_1, \ldots, x_N)$ of the chain $\mathcal{C}_n$,

2) for each link l_i of G carrying the index i, by using the compatibility condition (2.1) for the pair $\{\sigma_{\alpha i}, \sigma_{\beta i}\}$ of contiguous CCS-distributions attached to this link, we define the integrated distribution

$$\sigma_{\alpha_i\beta_i}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N) = \int dq_i \sigma_{\alpha_i}(x_1, \ldots, x_{i-1}, q_i, x_{i+1}, \ldots, x_N)$$
$$= \int dp_i \sigma_{\beta_i}(x_1, \ldots, x_{i-1}, p_i, x_{i+1}, \ldots, x_N). \tag{4.1}$$

Then, to the link l_i we associate the propagator

$$\varpi_i(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N) \equiv \begin{cases} \dfrac{1}{\sigma_{\alpha_i\beta_i}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N)} & \text{if } (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N) \in S_{\alpha_i\beta_i}, \\ 0 \quad \text{otherwise}, \end{cases} \tag{4.2}$$

where $\mathcal{S}_{\alpha_i\beta_i}$ is the (essential) support of $\sigma_{\alpha_i\beta_i}$.

The support properties of the σ_α's, $\sigma_{\alpha\beta}$'s, and ρ_0, and the relations between them (due to compatibility and positivity) are not innocent in the forthcoming considerations, and we should pay attention to them. However, doing so leads to cumbersome technicalities which are in fact

straightforward generalizations of those developed in the rigorous proof of Theorem 1 in (I) for the case $N=2$. Thus, in this Sec. IV, we shall ignore such inessential complications.

The function ρ_0 is then written as

$$\rho_0 = \left(\prod_{\alpha=1}^{n} \sigma_\alpha \prod_{i=1}^{n-1} \varpi_i \right) \zeta, \tag{4.3}$$

where $\zeta(T')$ is an arbitrary non-negative function in $L^1(\mathbb{R}^{N-n+1}, d^{N-n+1}T')$ with normalization

$$\int d^{N-n+1}T'\, \zeta(T') = 1. \tag{4.4}$$

That the expression (4.3) for ρ_0 solves Eq. (2.2) results from the following property:

Let $\hat{V}=\boxed{x_1,\ldots,x_N}$ be a one-leg vertex of the proper tree graph G and i be the index of the link $\hat{l}$ attached to it. Let $\hat{\sigma}(x_1,\ldots,x_N)$ be the corresponding element of the chain $\mathcal{C}_n$. Then

$$\int dq_i \rho_0^{(n)}(\mathbf{q},\mathbf{p}) = \rho_0^{(n-1)}(q_1,\ldots,q_{i-1},q_{i+1},\ldots,q_N,p_1,\ldots,p_N) \text{ if } x_i = q_i,$$

$$\int dq_i \rho_0^{(n)}(\mathbf{q},\mathbf{p}) = \rho_0^{(n-1)}(q_1,\ldots,q_N,p_1,\ldots,p_{i-1},p_{i+1},\ldots,p_N) \text{ if } x_i = p_i, \tag{4.5}$$

where $\rho_0^{(n)}$ is the above defined ρ_0 associated with the n-chain $\mathcal{C}_n$, and $\rho_0^{(n-1)}$ is the ρ_0 similarly associated with the $(n-1)$-chain $\mathcal{C}_{n-1}$ obtained from $\mathcal{C}_n$ by removing the CCS-distribution $\hat{\sigma}$. Notice that the reduced chain $\mathcal{C}_{n-1}$ corresponds to the reduced graph $G^{(n-1)}$ obtained from G by removing the one-leg vertex $\hat{V}$ and the link $\hat{l}$. Hence $\rho_0^{(n-1)}=\rho_0/(\hat{\sigma}\overline{\omega_i})$.

Equation (5.5) holds because: (*i*) in $\rho_0^{(n)}$ the variable x_i appears only in the factor $\hat{\sigma}$, (*ii*) the propagator of the link $\hat{l}$ is precisely the inverse of the integral of $\hat{\sigma}$ over x_i.

Now, given any σ_α in the chain $\mathcal{C}_n$, corresponding to the vertex V_α of G, one can start the reduction $G^{(n)} \to G^{(n-1)}$ of the tree graph $G^{(n)} \equiv G$ at some arbitrarily chosen one-leg vertex $\hat{V} \neq V_\alpha$, and repeat it $(n-1)$ times in such a way that one is left with the graph $G^{(1)}$ consisting solely of the vertex V_α. To this "peeling process" $G^{(n)} \to G^{(n-1)} \to \cdots \to G^{(1)}$ of tree graphs is naturally associated, via Eqs. (4.5), a reduction $\rho_0 \equiv \rho_0^{(n)} \to \rho_0^{(n-1)} \to \cdots \to \rho_0^{(1)}$ of functions $\rho_0^{(m)}$, which eventually produces

$$\rho_0^{(1)}(x_1,\ldots,x_{n-1},T,T') = \int dx_1' \cdots dx_{n-1}' \rho_0 = \sigma_\alpha(x_1,\ldots,x_{n-1},T)\zeta(T'), \tag{4.6}$$

and hence, by integrating over T':

$$\int dx_1' \cdots dx_N' \rho_0 = \sigma_\alpha(x_1,\ldots,x_N). \tag{4.7}$$

Notice that, although the order of the repeated integrations over the x_i''s is imposed by the steps of the peeling process, this order becomes obviously irrelevant in the above equation: Eq. (2.2) is valid for $\rho=\rho_0$ indeed.

Finally, to illustrate our Feynman rules, let us take as an example the graph $G^{(5)}$ of Fig. 4. The distribution ρ_0 associated with any 5-chain of type $G^{(5)}$ is

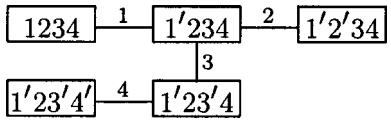


FIG. 4. A proper connected graph with $N=4$ and $N=5$.

$$\rho_0(\mathbf{q},\mathbf{p}) = \sigma_1(q_1q_2q_3q_4)\frac{1}{\sigma_{12}(q_2q_3q_4)}\sigma_2(p_1q_2q_3q_4)\frac{1}{\sigma_{23}(p_1q_3q_4)}\sigma_3(p_1p_2q_3q_4)\frac{1}{\sigma_{24}(p_1q_2q_4)}$$
$$\times\sigma_4(p_1q_2p_3q_4)\frac{1}{\sigma_{45}(p_1q_2p_3)}\sigma_5(p_1q_2p_3p_4).$$

Here and in the sequel, we keep writing the propagators as $1/\sigma_{\alpha\beta}$, although they are strictly given by Eq. (4.2).

B. General solution

Let us define the n following positive measures, each one associated to a particular component σ_α of the n-chain $\mathcal{C}_n$:

$$d\mu_\alpha = \begin{cases} \dfrac{\rho_0(\mathbf{q},\mathbf{p})}{\sigma_\alpha(Z_\alpha)}d^NZ'_\alpha & \text{if } Z_\alpha=(x_1,\ldots,x_N)\in\mathcal{S}_\alpha, \\ 0 \quad \text{otherwise}, \end{cases} \tag{4.8}$$

where $\mathcal{S}_\alpha$ denotes the (essential) support of σ_α. Due to Eq. (4.7) these $(x_1,\ldots,x_N)$-dependent measures [notice also that the $d\mu_\alpha$'s are continuous linear mappings of $L^1(\mathbb{R}^{2N},\rho_0d^Nqd^Np)$ into itself] are normalized for all $(x_1,\ldots,x_N)\in\mathcal{S}_\alpha$.

It is convenient to write the general solution ρ we are looking for in the form

$$\rho=\rho_0(1+\lambda h). \tag{4.9}$$

Here, the function $h(\mathbf{q},\mathbf{p})$ will be chosen as to ensure Eq. (2.2), which results in the linear equations

$$\int d^NZ'_\alpha\rho_0(\mathbf{q},\mathbf{p})h(\mathbf{q},\mathbf{p})=0 \quad (\alpha=1,\ldots,n), \tag{4.10}$$

whereas the real constant λ is a normalization factor which will be useful to control the positivity of ρ. Thanks to definitions (4.8), Eq. (4.10) is equivalent to

$$\int d\mu_\alpha h=0 \quad (\alpha=1,\ldots,n). \tag{4.11}$$

We then observe that, for any α and any function g in $L^1(\mathbb{R}^{2N},\rho_0d^Nqd^Np)$

$$\int d\mu_\alpha\left(\int d\mu_\alpha g\right)=\int d\mu_\alpha g, \tag{4.12}$$

since $\int d\mu_\alpha g$ does not depend any longer on the integration variables $(x'_1,\ldots,x'_N)$ and $d\mu_\alpha$ is normalized. That is, the linear operators $P_\alpha: L^1(\mathbb{R}^{2N},\rho_0d^Nqd^Np)\to L^1(\mathbb{R}^{2N},\rho_0d^Nqd^Np)$ defined by $P_\alpha g=\int d\mu_\alpha g$ are projectors,

$$P_\alpha^2=P_\alpha \quad (\alpha=1,\ldots,n). \tag{4.13}$$

The set $\{P_\alpha\}$ enjoys certain algebraic properties which are crucial for the construction of the general solution h of Eq. (4.11).

Lemma 2:

(a) The projectors P_α and P_β associated with any pair $\{V_\alpha, V_\beta\}$ of contiguous vertices commute

$$[P_\alpha, P_\beta] = 0. \tag{4.14}$$

(b) If V_α, V_β, and V_γ, are three vertices of the connected proper (tree) graph G such that V_α belongs to the (unique) path connecting V_β to V_γ, and is contiguous to at least one of these two vertices, then

$$P_\gamma P_\alpha P_\beta = P_\gamma P_\beta. \tag{4.15}$$

The proof is given in Appendix A. We stress that the contiguity of V_α with V_β or V_γ is essential for the validity of Eq. (4.15).

Let us now introduce the central object of our construction, namely the operator

$$\Pi = 1 - \sum_{\alpha=1}^{n} P_\alpha + \sum_{i=1}^{n-1} P_{\alpha_i} P_{\beta_i}, \tag{4.16}$$

where P_{α_i} and P_{β_i} denote the operators P associated with the two (contiguous) vertices V_{α_i} and V_{β_i} attached to the link with index i. Thanks to Lemma 2, it is readily shown that Π is annihilated by all the projectors P_α:

$$P_\gamma \Pi = 0 \quad (\gamma = 1, \ldots, n). \tag{4.17}$$

Indeed

$$P_\gamma \Pi = P_\gamma - \sum_{\alpha=1}^{n} P_\gamma P_\alpha + \sum_{i=1}^{n-1} P_\gamma P_{\alpha_i} P_{\beta_i} = - P_\gamma \sum_{\substack{\alpha=1 \\ \alpha \neq \gamma}}^{n} P_\alpha + \sum_{i=1}^{n-1} P_\gamma P_{\alpha_i} P_{\beta_i}. \tag{4.18}$$

But, according to Eq. (4.15):

$$P_\gamma P_{\alpha_i} P_{\beta_i} = P_\gamma P_{\delta_i}, \tag{4.19}$$

where $\delta_i = \beta_i$ (resp. α_i) if V_{α_i} (resp. V_{β_i}) belongs to the path connecting V_γ to V_{β_i} (resp. V_{α_i}). Hence

$$\sum_{i=1}^{n-1} P_\gamma P_{\alpha_i} P_{\beta_i} = P_\gamma \sum_{\substack{\alpha=1 \\ \alpha \neq \gamma}}^{n} P_\alpha, \tag{4.20}$$

which entails Eq. (4.17) (the property $\Pi P_\gamma = 0$ $(\gamma = 1, \ldots, n)$, which also holds as a consequence of Eq. (4.15), will not be used here). Note that Eq. (4.20) would not be valid if the graph G were not connected.

Furthermore, Π is itself a projector:

$$\Pi^2 = \Pi, \tag{4.21}$$

as immediately deduced from

$$\Pi^2 = \left(1 - \sum_{\alpha=1}^{n} P_\alpha + \sum_{i=1}^{n-1} P_{\alpha_i} P_{\beta_i} \right) \Pi$$

and Eq. (4.17). This operator allows us to write down at once the general solution of Eq. (4.11), i.e.,

$$P_\alpha h = 0 \quad (\alpha = 1, \ldots, n), \tag{4.22}$$

as

$$h = \Pi f, \tag{4.23}$$

where f is an arbitrary function in $L^1(\mathbb{R}^{2N}, d^N q d^N p)$. That Eq. (4.23) implies Eq. (4.22) is trivial due to Eq. (4.17). Conversely, any function h satisfying Eq. (4.22) assumes the form (4.23): since then $h = \Pi h$, it suffices to take $f = h$.

We now have to give the representation formula for h resulting from Eqs. (4.23) and (4.16) an explicit form in terms of the data of the problem, namely, the elements of the chain $\mathcal{C}_n$. For this purpose, it is necessary to use appropriate notations. First, we denote by Z_α the collection of arguments of the vertex function σ_α, and Z'_α the collection of the conjugate arguments (a notation already used in the definition (4.8)). Then

$$(P_\alpha f)(Z_\alpha) = \frac{1}{\sigma_\alpha(Z_\alpha)} \int d^N Z'_\alpha \rho_0(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p}). \tag{4.24}$$

Second, we denote by $\sigma_{\alpha_i}(X_i, x_i)$ and $\sigma_{\beta_i}(X_i, x'_i)$ the vertex functions of the vertices V_{α_i} and V_{β_i}, where $X_i = \{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N\}$. Accordingly, we write $\rho_0(X_i, X'_i, x_i, x'_i)$ for $\rho_0(\mathbf{q},\mathbf{p})$, where $X'_i = \{x'_1, \ldots, x'_{i-1}, x'_{i+1}, \ldots, x'_N\}$, and so on. With these notations

$$(P_{\alpha_i} P_{\beta_i} f)(X_i) = \int d^{N-1} X'_i dx'_i \frac{\rho_0(X_i, X'_i, x_i, x'_i)}{\sigma_{\alpha_i}(X_i, x_i)} (P_{\beta_i} f)(X_i, x'_i), \tag{4.25}$$

and

$$(P_{\beta_i} f)(X_i, x'_i) = \int d^{N-1} X'_i dx_i \frac{\rho_0(X_i, X'_i, x_i, x'_i)}{\sigma_{\beta_i}(X_i, x'_i)} f(X_i, X'_i, x_i, x'_i). \tag{4.26}$$

In the r.h.s. of Eq. (4.25), one observes that the integral $\int d^{N-1} X'_i \rho_0$ can be performed explicitly by means of the "peeling process" described in Sec. IV A,

$$\int d^{N-1} X'_i \rho_0(X_i, X'_i, x_i, x'_i) = \frac{\sigma_{\alpha_i}(X_i, x_i) \sigma_{\beta_i}(X_i, x'_i)}{\sigma_{\alpha_i \alpha_i}(X_i)}. \tag{4.27}$$

This equation obtains by stopping the peeling process at the reduced graph made of the two vertices V_{α_i}, V_{β_i} and the link between them. Here appears the propagator $1/\sigma_{\alpha_i \beta_i}$ with

$$\sigma_{\alpha_i \beta_i}(X_i) = \int dx_i \sigma_{\alpha_i}(X_i, x_i) = \int dx'_i \sigma_{\beta_i}(X_i, x'_i). \tag{4.28}$$

Then, inserting Eqs. (4.26) and (4.27) in Eq. (4.25), one gets, after simplifications,

$$(P_{\alpha_i} P_{\beta_i} f)(X_i) = \int d^{N-1} X'_i dx_i dx'_i \frac{\rho_0(X_i, X'_i, x_i, x'_i)}{\sigma_{\alpha_i \beta_i}(X_i)} f(X_i, X'_i, x_i, x'_i). \tag{4.29}$$

Finally, collecting Eqs. (4.23), (4.16), (4.24), and (4.29), we obtain the expression of the function h we were looking for

$$h(\mathbf{q},\mathbf{p}) = f(\mathbf{q},\mathbf{p}) - \sum_{\alpha=1}^{n} \frac{1}{\sigma_\alpha(Z_\alpha)} \int d^N Z'_\alpha \rho_0(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p}) + \sum_{i=1}^{n-1} \frac{1}{\sigma_{\alpha_i \beta_i}(X_i)} \int d^{N-1} X'_i dx_i dx'_i \rho_0(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p}). \tag{4.30}$$

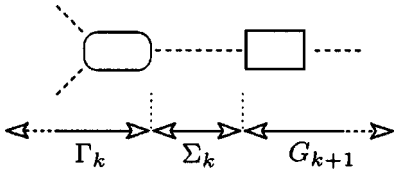


FIG. 5. The diagram Γ_{k+1}.

Equations (4.9) and (4.30) provide us with the general solution ρ of the linear system (2.2). It remains to enforce the positivity of this solution. Let us denote by m_+ (resp. $-m_-$) the (essential) supremum (resp. infimum) of h. Because of Eq. (4.10), m_+ and m_- are strictly positive when h does not vanish identically. Then, from Eq. (4.9), the condition $\rho \geqslant 0$ is equivalent to the condition on the parameter λ

$$-\frac{1}{m_+} \leqslant \lambda \leqslant \frac{1}{m_-}. \tag{4.31}$$

We stress that the allowed interval $[-(1/m_+),(1/m_-)]$ is not zero as soon as the range of the arbitrary function f is (essentially) bounded. Indeed, assuming that $A \leqslant f \leqslant B$ (almost) everywhere, one finds from Eq. (4.30) that $m_\pm \leqslant n(B-A)$.

Equations (4.9), (4.30), and (4.31) for ρ constitute the generalization of the results in Sec. V of (I) (see Eqs. (5.8)–(5.10) there) to phase spaces of arbitrary dimension, in one case of full admissibility (connected proper graphs).

V. NONCONNECTED PROPER GRAPHS

Throughout this section, devoted to the proof of part 2 of Theorem 1, a vertex (or insertion) with only two legs will be called *simple vertex*.

A. Nonproper G_c

Our purpose here is to establish part 2b of Theorem 1. To this end we first construct a particular connected graph G_c such that the proper graph G is subgraph of G_c. By hypothesis G_c is not proper. We then show that this implies the existence of at least one critical quartet in the graph G. According to Lemma 1, the statement 2b immediately follows.

Let $G=\cup_k G_k$ be the decomposition of a proper graph G into connected components G_k's. Each G_k is a proper graph, hence a tree. We connectify G recursively according to the following scheme. Assume we have already connectified the components $G_1,\ldots,G_k$ into a connected *diagram* Γ_k. We define Γ_{k+1} as follows. Let us call segment a linear chain of inserted simple vertices and links, and define its length by the number of its links. We choose one of the shortest segments which connect Γ_k to the component G_r $(r=k+1,\ldots)$. Among the G_r's we select one, say G_{k+1}, which minimizes the length of the attached segment. We call Σ_k this segment. The diagram Γ_{k+1} is defined by $\Gamma_{k+1}=\Gamma_k \cup G_{k+1} \cup \Sigma_k$.

Note that:

(1) In the above construction, two contiguous vertices of a Γ are not necessarily linked, so that the *diagrams* Γ are not always *graphs* as defined in Sec. II. The advantage of this construction is that the Γ_k's are trees.
(2) The segment Σ_k is attached to G_{k+1} through a vertex of G and attached to Γ_k through either a vertex of G or an inserted vertex of Γ_k (as represented in Fig. 5). In the latter case, this inserted vertex becomes nonsimple (if it was simple before).
(3) There is in general some arbitrariness in the construction of the Γ_k's. First, the recursive process has to be initialized by the choice of one component as Γ_1. Next, in the subsequent steps of the process, there is a possible arbitrariness in the choice of G_{k+1} and its attached segment.

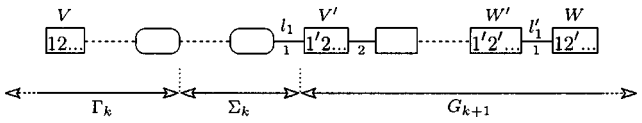


FIG. 6. Case a.

Once this connectification process is completed, we end up with a connected tree diagram Γ_c which contains all the components of G. If Γ_c is not a graph, we obtain a graph G_c by adding links between all pairs of contiguous vertices which are still not linked in Γ_c.

G_c and Γ_c may coincide or not. In the latter case, it is important to notice that G_c and Γ_c are still either both proper or both nonproper. This follows from the fact that (i) when going from Γ_c to G_c, a loop of G_c is created each time one adds a link, (ii) a loop contains at least two pairs of links carrying the same index.

Let us define the diagrams Ω_k by

$$\Omega_k = \Gamma_k \cup G_{k+1} \cup G_{k+2} \cup \cdots$$

which satisfy the inclusion relations

$$\Omega_1 \equiv G \subset \Omega_2 \subset \cdots \subset \Omega_c \equiv \Gamma_c \subset G_c.$$

Now, by hypothesis G_c, and thus also $\Omega_c = \Gamma_c$, are nonproper, whereas $\Omega_1 = G$ is proper. This implies the existence of an integer k such that $\Omega_k \subset \Omega_{k+1}$ with Ω_k proper and Ω_{k+1} nonproper. From the observation that

$$\Omega_{k+1} = \Omega_k \cup \Sigma_k,$$

we deduce that there exists at least one index, say 1, which is carried by just two links, one l_1 in Σ_k and a second one l_1' in Ω_k. The link l_1' may appear either in Γ_k or in the components $G_{k+1}, \ldots$ of G, which leads us to distinguish three cases:

(a) $l_1' \subset G_{k+1}$,
(b) $l_1' \subset \Gamma_k$,
(c) $l_1' \subset G_{k+2}$ or G_{k+3} or ….

We now proceed with a few remarks which will be useful in the forthcoming argument, although not always explicitly refered to thereby:

(1) All the end points (one leg vertices) of the Γ_k's belong to G.
(2) Any link of a Γ_k belongs to at least one linear chain with end vertices belonging to G.
(3) On a segment, the indices of the links can be reordered at our convenience. This should be kept in mind when constructing the Γ_k's.
(4) Two links carrying the same index cannot be attached to a common vertex.

As a consequence of these last two remarks, since all the Σ_k's are shortest connecting chains.
(5) All segments Σ_k are proper.
(6) On a connected tree Γ_k, the (unique) path joining two links carrying the same index contains either two vertices of G, or one vertex of G and one inserted nonsimple vertex, or two inserted nonsimple vertices.

Case a:

Let V be any vertex of Γ_k belonging to G, and V' be the vertex of G_{k+1} where the segment Σ_k attaches. Figure 6 exhibits the relevant part of Ω_{k+1}, namely the linear chain joining the vertices V and V', and the linear chain from V' to the link l_1' in G_{k+1}. Moreover, in accordance with Remark 3, we have attached the link l_1 to V'. We have also called 2 the index of the other link attached to V'.

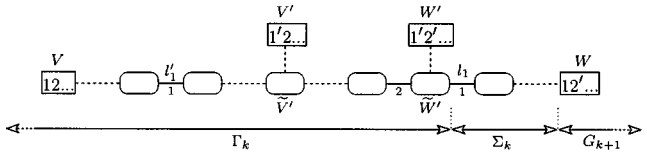


FIG. 7. Case b.

According to Remarks 3 and 4, there is no link with index 2 in Σ_k. Furthermore, since $\Gamma_k \cup G_{k+1}$ is proper, no new link of index 1 or 2 can appear in the linear chain connecting V to W. As a consequence, the vertices V, V', W, and W' constitute a critical quartet.

Case b:

The relevant part of Ω_{k+1} is displayed in Fig. 7. Here, V is a vertex of Γ_k belonging to G, such that the (unique) path joining it to Σ_k contains the link l_1'.

The existence of the nonsimple vertices $\widetilde{V}'$ and $\widetilde{W}'$ results from Remark 6. They may possibly coincide with respectively the vertices V' and W' of G. As previously, no new index 1 or 2 can appear in the chain displayed in Fig. 7, which implies that the vertices V, V', W, and W' constitute a critical quartet.

Case c:

In that case, the relevant part of Ω_{k+1} is made of two disconnected parts, as displayed in Fig. 8. As previously, the nonsimple inserted vertex $\widetilde{V}$ may possibly coincide with V.

Let us denote by I the set of indices appearing (each only once) in the links between V and $\widetilde{V}$, by J the set of indices appearing in the segment Σ_k but the index 1, and by K all the remaining indices. We can assume $I \cap J = \emptyset$ (otherwise the configuration would also enter the case b). We further split the sets I, J, and K as $I = I_1 \cup I_2$, $J = J_1 \cup J_2$, $K = K_1 \cup K_2$. Here, I_1 and I_2 are introduced to separate the variables which have the same or different assignments in the vertices V on the one hand and in the vertices W and W' on the other hand, and similarly for the splitting of J and K. Then $\{1, I_1, I_2, J_1, J_2, K_1, K_2\}$ is a partition of $\{1, 2, \ldots, N\}$, and the assignments of the variables in the vertices V, V', W, and W' of G, and $\widetilde{V}$ take the form

$$\begin{cases} V = \{1\mathcal{I}_1\mathcal{I}_2\mathcal{J}_1\mathcal{J}_2\mathcal{K}_1\mathcal{K}_2\}, \\ \widetilde{V} = \{1\mathcal{I}_1'\mathcal{I}_2'\mathcal{J}_1\mathcal{J}_2\mathcal{K}_1\mathcal{K}_2\}, \\ V' = \{1'\mathcal{I}_1'\mathcal{I}_2'\mathcal{J}_1'\mathcal{J}_2'\mathcal{K}_1\mathcal{K}_2\}, \\ W = \{1\mathcal{I}_1\mathcal{I}_2'\mathcal{J}_1\mathcal{J}_2'\mathcal{K}_1\mathcal{K}_2'\}, \\ W' = \{1'\mathcal{I}_1\mathcal{I}_2'\mathcal{J}_1\mathcal{J}_2'\mathcal{K}_1\mathcal{K}_2'\}. \end{cases} \tag{5.1}$$

In these formulas, $\mathcal{I}_1, \mathcal{I}_2, \ldots$ represent collections of variables q and p. In accordance with our convention (see Sec. II), $\mathcal{I}_1$ is written as a set of indices, namely those of I_1 but each one being primed or not. As for $\mathcal{I}_1'$, it is written as a set of the same indices, nonprimed (resp. primed) if primed (resp. nonprimed) in $\mathcal{I}_1$. Similarly for the other sets $\mathcal{I}_2, \mathcal{I}_2', \ldots$.

Let us define the distance $d(U, U')$ between two vertices U and U' as the number of variables with different assignments in U and U'. Inspecting Eq. (5.1), one readily obtains

$$\begin{cases} d(\widetilde{V}, V') = 1 + j_1 + j_2, \\ d(\widetilde{V}, W) = i_1 + j_2 + k_2, \end{cases} \tag{5.2}$$

where $j_1 = \text{card } J_1$, and so on. Since Σ_k is one of the shortest segments connecting Γ_k to one of the components $G_{k+1}, G_{k+2}, \ldots$, one must have $d(\widetilde{V}, V') \leqslant d(\widetilde{V}, W)$, which entails

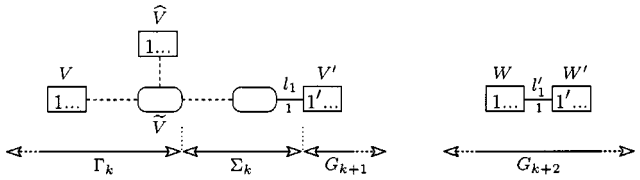


FIG. 8. Case c.

$$i_1 + k_2 \geqslant 1.$$

This means that the sets I_1 and K_2 cannot be both empty. If $K_2 \neq \emptyset$, we choose the index 2 in K_2, so that the vertices V, V', W, and W' constitute a critical quartet. If $K_2 = \emptyset$, I_1 is not empty, $\tilde{V}$ does not coincide with V, and thus $\tilde{V}$ is a nonsimple inserted vertex, necessarily linked in Γ_k to a vertex $\hat{V}$ of G as displayed in Fig. 8. Choosing now the index 2 in I_1, one finds that the vertices $\hat{V}$, V', W, and W' constitute a critical quartet.

B. Proper G_c

When G is subgraph of a *proper* connected graph G_c, the latter is a tree graph which can be decomposed into the connected components G_i of G and connecting segments Σ_k, even when G_c does not coincide with the specific graph G_c constructed in the previous Sec. V A. One needs to distinguish two cases:

(a) All the segments Σ_k's are disjoint. Then all insertions are simple and G_c is G-simple.
(b) At least two segments have one common vertex. This vertex is not a simple insertion and thus G_c is not G-simple.

1. G-simple G_c

Here, as in Sec. IV, we establish part 2.a.i of Theorem 1 by associating to any chain $\mathcal{C}$ of type G a particular phase space distribution ρ_0 reproducing this chain. We also give the general form of the ρ's reproducing the chain.

The construction of ρ_0 proceeds through the "Feynman rules" of Sec. IV A, complemented with propagators associated with the segments of G_c. Let Σ be such a segment connecting the vertices V_α and V_β of G, and let r be its length. Let $\sigma_\alpha(X,Y)$ and $\sigma_\beta(X,Y')$ be the corresponding vertex functions of $\mathcal{C}$, where X (resp. Y) denote the set of variables which have the same (resp. a different) assignment in σ_α and σ_β. The compatibility of σ_α and σ_β allows us to define

$$\sigma_{\alpha\beta}(X) \equiv \int d^r Y \sigma_\alpha(X,Y) = \int d^r Y' \sigma_\beta(X,Y'). \tag{5.3}$$

For different segments Σ_l labelled by the index l, we use the notation $\sigma_{\alpha_l\beta_l}(X_l)$.

To the segment Σ_l we now associate the propagator

$$\varpi_l(X_l) = \begin{cases} \dfrac{1}{\sigma_{\alpha_l\beta_l}(X_l)} & \text{if } X_l \in \mathcal{S}_{\alpha_l\beta_l}, \\ 0 \quad \text{otherwise}, \end{cases} \tag{5.4}$$

where $\mathcal{S}_{\alpha_l\beta_l}$ is the support of $\sigma_{\alpha_l\beta_l}$. This amounts to consider Σ_l as a new kind of link (in the graph G_c) which we call *composite link*. Then the function ρ_0 reads

$$\rho_0(\mathbf{q},\mathbf{p}) = \left(\prod_{\alpha=1}^{n} \sigma_\alpha(Z_\alpha)\right)\left(\prod_{l=1}^{n-1} \varpi_l(X_l)\right)\zeta(T'), \tag{5.5}$$

where the second product in the r.h.s. is performed on all links, namely the links of G and the composite links of G_c. Note that, since G_c is a connected tree, the total number of links is $(n-1)$. As for the function $\zeta(T')$, which is arbitrary but non-negative and normalized, it takes care of the "passive" variables $T=\{x_n, x_{n+1}, \ldots, x_N\}$ and their conjugate T', as in Eq. (4.3).

The proof that the ρ_0 of Eq. (5.5) solves Eq. (2.2) relies on the "peeling process" described in Sec. IV A. Here, this process has to be extended to the case where the one-leg vertex $\hat{V}$ introduced there is attached to a composite link. Let $\hat{\sigma}(X,Y)$ be the vertex function of $\mathcal{C}$ associated to $\hat{V}$, where X (resp. Y) is the set of variables whose assignment does not change (resp. changes) through the composite link. Then Eqs. (4.5) become

$$\int d^r Y \rho_0^{(m)}(\mathbf{q},\mathbf{p}) = \rho_0^{(m-1)}(X,X',Y'), \tag{5.6}$$

and the rest of the proof is completely similar to that given in Sec. IV A.

The determination of the general solution ρ of Eq. (2.2) is also carried out along the lines followed in Sec. IV B, by using this time the extended peeling process. The definitions of the measures $d\mu_\alpha$ and of the projectors P_α (which now involve the function ρ_0 of Eq. (5.5)) are unchanged. The Lemma 2 still holds, though with an extended acceptation of "contiguity": two vertices V_{α_l} and V_{β_l} of G connected by a composite link Σ_l of G_c are declared contiguous. Actually, only minor changes are needed to generalize the proof given in Appendix A (essentially the substitution $x_i \to Y$). The operator Π is now defined as

$$\Pi = 1 - \sum_{\alpha=1}^{n} P_\alpha + \sum_{l=1}^{n-1} P_{\alpha_l} P_{\beta_l}, \tag{5.7}$$

where the last sum in the r.h.s. is a sum over all links of G_c, composite or not. Its properties (4.17) and (4.21) remain true and, with ρ written as in Eq. (4.9), one finds that the general solution for h is given again by Eq. (4.23). A change then occurs in Eq. (4.27) when the two vertices V_{α_i} and V_{β_i} there become two vertices V_{α_l} and V_{β_l} connected by a composite link. In this case Eq. (4.27) becomes

$$\int d^{N-r_l} X_l' \rho_0(X_l, X_l', Y_l, Y_l') = \frac{\sigma_{\alpha_l}(X_l, Y_l)\sigma_{\beta_l}(X_l, Y_l')}{\sigma_{\alpha_l\beta_l}(X_l)}. \tag{5.8}$$

One ends up with the following expression of h, generalizing the representation formula (4.30)

$$h(\mathbf{q},\mathbf{p}) = f(\mathbf{q},\mathbf{p}) - \sum_{\alpha=1}^{n} \frac{1}{\sigma_\alpha(Z_\alpha)} \int d^N Z_\alpha' \rho_0(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p}) + \sum_{l=1}^{n-1} \frac{1}{\sigma_{\alpha_l\beta_l}(X_l)} \int d^{N-r_l} X_l' d^{r_l} Y_l d^{r_l} Y_l' \rho_0(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p}). \tag{5.9}$$

We remind the reader that, in this formula:

(i) f is an arbitrary function in $L^1(\mathbb{R}^{2N}, \rho_0 d^N q d^N p)$;
(ii) the first sum in the r.h.s. is over all vertices V_α of G; Z_α denotes the collection of arguments of the vertex function σ_α and Z_α' the collection of conjugate arguments;

(iii) the second sum is over all links (of length r_l), that is the simple links of G and the composite links of G_c; the definition of the functions $\sigma_{\alpha_l\beta_l}$ occurring in the sum, as well as the meaning of the collections of variables X_l, X'_l, Y_l, and Y'_l, are provided by Eq. (5.3), which reduces to Eq. (4.28) in the case of a simple link of index i.

2. Non G-simple G_c

Part 2.a.ii of Theorem 1 remains to be proven.

Consider first an arbitrary *quantum* chain $\mathcal{C}$ of type G. The CCS-distributions of $\mathcal{C}$ are then expressed in terms of some density operator $\hat{\rho}$, in accordance with Eq. (1.4). But, in this case, a set of CCS-distributions associated with the insertions of G_c can also be computed through these equations. One thus obtains an extended chain $\mathcal{C}_c$ of compatible CCS-distributions associated with all the vertices of G_c. Since G_c is proper, the chain $\mathcal{C}_c$ admissible (irrespective of the fact that G_c is not G-simple), which implies the admissibility of $\mathcal{C}$. Hence the quantum admissibility of the graph G.

To prove that G is not fully admissible, we show that there are (nonquantum) chains of type G which are not admissible.

By assumption G_c contains at least one insertion V with $k \geqslant 3$ legs, say the vertex $\boxed{12\ldots N}$ with legs carrying the indices $j=1,2,\ldots,k$. These legs connect V to k subgraphs $G_c^{(j)}$ of G_c which are proper connected trees, but mutually disconnected (otherwise G_c would contain loops). By removing all the insertions, together with their legs, from each of the $G_c^{(j)}$'s, we obtain k subgraphs $G^{(j)}$ of G which are proper (not necessarily connected) trees. The vertices $V_l^{(j)}$ of each $G^{(j)}$ are of the form $\boxed{1,2,\ldots,j-1,j',j+1,\ldots,k,\mathcal{J}_l^{(j)}}$, where $\mathcal{J}_l^{(j)}$ represents a set $\{k+1,k+2,\ldots,N\}$ of indices, each one being primed or not.

We now use the following lemma, the proof of which is given in Appendix B.

Lemma 3:

In a $2k$*-dimensional phase space with* $k \geqslant 3$, *there exist k-chains of compatible distributions* $\{\tau_1(p_1,q_2,q_3,\ldots,q_k),\ \tau_2(q_1,p_2,q_3,\ldots,q_k),\ \ldots,\ \tau_k(q_1,q_2,\ldots,q_{k-1},p_k)\}$ *which are not admissible.*

Let us construct a chain $\mathcal{C}$ of type G by assigning to each vertex $V_l^{(j)}$ of $G^{(j)}$ $(j=1,\ldots,k)$ the CCS-distributions

$$\sigma_l^{(j)}(q_1,\ldots,q_{j-1},p_j,q_{j+1},\ldots,q_k,X_l^{(j)}) = \tau_j(q_1,\ldots,q_{j-1},p_j,q_{j+1},\ldots,q_k)\tilde{\sigma}_l^{(j)}(X_l^{(j)}), \tag{5.10}$$

where $X_l^{(j)}$ denotes the set of variables x_i corresponding to $\mathcal{J}_l^{(j)}$ and the $\tilde{\sigma}_l^{(j)}$'s are arbitrary probability distributions depending on these variables, only subjected to the opposite compatibility conditions. (That such $\tilde{\sigma}_l^{(j)}$'s always exist is easy to see, e.g., by choosing completely factorized forms for them.) The elements of the chain $\mathcal{C}=\{\sigma_l^{(j)}\}_{j=1,\ldots,k;l}$ are evidently compatible CCS-distributions. Let us pretend that these distributions are marginals of some phase space density ρ. Then, by defining the reduced density

$$\tilde{\rho}(q_1,\ldots,q_k,p_1,\ldots,p_k) = \int dq_{k+1}dp_{k+1}\cdots dq_N dp_N \rho(\mathbf{q},\mathbf{p}) \tag{5.11}$$

in a $2k$-dimensional phase space, one finds that

$$\tau_j = \int d^{N-k}X_l^{(j)}\sigma_l^{(j)} \text{ (any } l),$$

$$= \int dp_1\cdots dp_{j-1}dq_j dp_{j+1}\cdots dp_k\tilde{\rho} \ (j=1,\ldots,k). \tag{5.12}$$

This would mean that the reduced k-chain $\tilde{\mathcal{C}}=\{\tau_j\}_{j=1,\ldots,k}$ is always admissible, in contradistinction with Lemma 3. We conclude that there exist chains of type G which are not admissible.

The two statements in part 2.a.ii of Theorem 1 are now established and the proof of this theorem is complete.

Finally, we would like to obtain an explicit expression of all the phase space densities ρ solving Eq. (2.2) for a given quantum chain $\mathcal{C}$ of type G, by following again the method of Sec. IV. However, serious complications crop up in the final step of the procedure.

First, a particular solution ρ_0 is obtained by applying formula (4.3) *to the extended chain* $\mathcal{C}_c$. Alternatively, one can determine other particular solutions ρ_0' by using, instead of $\mathcal{C}_c$, the chains $\mathcal{C}_c'$ obtained from $\mathcal{C}_c$ by removing all or some of the *simple* insertions of G_c and applying the procedure of Sec. V B 1 involving composite links and their associated propagators. Whatever ρ_0 is chosen, we keep writing the general solution in the form $\rho=\rho_0(1+\lambda h)$, as in Eq. (4.9).

Then a change appears in the determination of the function h, because one does not have to require the density ρ to reproduce all the CCS-distributions of the chain $\mathcal{C}_c$ (or $\mathcal{C}_c'$), but only those of the given chain $\mathcal{C}$. This means that h should satisfy Eq. (4.22), where the index α now refers to the only elements of the *initial chain* $\mathcal{C}$. As a consequence, the form (4.16) of the appropriate operator Π (to be used in Eq. (4.23)) is no longer valid, since the properties (4.17) and (4.21) hold only if the underlying graph is *connected*. Notice that a similar difficulty already appeared when dealing with G-simple graphs G_c in the previous subsection. There, it was overcome by introducing composite links which eventually allowed us to remove the insertions of G_c. Unfortunately, no such device presents itself for non G-simple G_c's, and constructing the "good" projector Π in this case seems to be quite a difficult problem, which we leave unsolved here.

Of course, the projector Π_c associated with the chain $\mathcal{C}_c$ already provides us with a large class of solutions, but certainly not all the solutions.

VI. CONCLUSIONS

We have investigated the extent to which it is possible to reproduce a given set of joint probability distributions $\sigma_\alpha(x_1,x_2,\ldots,x_N)$ with $x_i=q_i$ or p_i, in arbitrary number n and with arbitrary position-momentum assignments of the x_i's, as marginals of some probability density $\rho(\mathbf{q},\mathbf{p})$ in $2N$-dimensional phase space. We have been able to give a complete characterization of those sets which can always be reproduced by a $\rho(\mathbf{q},\mathbf{p})$ (admissible sets), irrespective of the functional form of the σ_α's provided they are compatible, and both for quantum probability distributions σ_α and for more general (classical) ones. This has been achieved by introducing a specific, powerful diagrammatic method and by relying on previous results[3,4] obtained in the case $N=2$ by means of Bell-type inequalities in phase space.

When both classical and quantum sets $\{\sigma_\alpha\}_{\alpha=1,\ldots,n}$ are admissible, we have constructed the general solution $\rho(\mathbf{q},\mathbf{p})$ of the problem. When only quantum sets are admissible, we have the explicit expression of a large class of solutions, which however is not exhaustive. Concerning the dynamical aspect which is completely ignored in this paper, our results in the quantum case motivate the construction of realistic quantum mechanics reproducing $(N+1)$ marginals at all times t and thus considerably improving on the de Broglie–Bohm mechanics,[7] which reproduces only one σ_α (the position probability distribution $\sigma(\mathbf{q},t)$).

On the other hand, all cases of nonadmissibility have been identified. For quantum σ_α's again, this may be viewed as a general contextuality theorem of the Gleason–Kochen–Specker-type,[8] which also extends a previous result of this type due to Martin and Roy.[9] At the same time, this provides a proof of a long-standing conjecture, the "$(N+1)$ marginal theorem."

From the mathematical standpoint, the parts of our main theorem (Theorem 1), pertaining to the quantum case are essentially new statements concerning multidimensional Fourier transforms in $L^2(\mathbb{R}^{2N},d^Nqd^Np)$. These statements vastly extend the results of Cohen and Zaparovanny[6] for two nonintersecting marginals to the case of $N+1$ marginals containing overlapping variables.

In classical image processing previous constructions of joint probability densities for position and wave number vectors which reproduce just two marginals (the position vector probability density and the wave number vector probability density) can now be extended to reproduce $N+1$ marginals whenever the admissibility conditions are obeyed. This has potential for new applications in classical signal and image processing.[10]

In the quantum arena the $N+1$ marginal theorem proved here makes precise the extent to which noncommuting CCS can be simultaneously realized extending the $N=2$ results of (I). Our results completely settle, at a formal level, the question of "maximal reality" raised and already investigated in special cases.[1–4] Their possible relevance for related fundamental problems of quantum theory (in particular for helping towards a clarification of the still controversial problem of measurement) remains to be explored.

At a practical level, the theorem is intimately related to quantum entanglement. The impossibility of reproducing more than $N+1$ marginals stems from allowing the most general entangled states. This indicates a direction in which the present work can be extended and applied to quantum information theory. For example, for partially separable quantum states, one may obtain theorems allowing positive phase space densities with more than $N+1$ marginals agreeing with quantum probabilities. To make this point forcefully suppose that $q_1, q_2, \ldots, q_N$ are coordinates of N particles and the quantum state $\hat{\rho}$ is separable (i.e., completely separable),

$$\hat{\rho} = \sum_r \mu_r \bigotimes_{i=1}^{N} \hat{\rho}_r^{(i)}, \tag{6.1}$$

where $\mu_r > 0$, $\Sigma_r \mu_r = 1$, and $\hat{\rho}_r^{(i)}$ is a density operator for the ith particle. We demonstrate now that the 2^N quantum probability densities

$$\sigma(x_1, x_2, \ldots, x_N) = \langle x_1, \ldots, x_N | \hat{\rho} | x_1, \ldots, x_N \rangle = \sum_r \mu_r \prod_{i=1}^{N} \langle x_i | \hat{\rho}_r^{(i)} | x_i \rangle \tag{6.2}$$

obtained by choosing $x_i = q_i$ or p_i, can all be reproduced as marginals of a single positive phase space density,

$$\rho(\mathbf{q}, \mathbf{p}) = \sum_r \mu_r \prod_{i=1}^{N} \langle q_i | \hat{\rho}_r^{(i)} | q_i \rangle \langle p_i | \hat{\rho}_r^{(i)} | p_i \rangle. \tag{6.3}$$

As before, denoting by x_i' the variable conjugate to x_i we obtain the 2^N equations

$$\int dx_1' \cdots dx_N' \rho(\mathbf{q}, \mathbf{p}) = \sum_r \mu_r \prod_{i=1}^{N} \langle x_i | \hat{\rho}_r^{(i)} | x_i \rangle = \sigma(x_1, x_2, \ldots, x_N), \tag{6.4}$$

which are the desired marginal conditions. We have used the normalization conditions

$$\int dx_i' \langle x_i' | \hat{\rho}_r^{(i)} | x_i' \rangle = 1. \tag{6.5}$$

We therefore expect that partial separability will allow a number of marginals intermediate between $N+1$ and 2^N to agree with quantum probabilities. We also expect that future work will demonstrate and exploit phase space Bell inequalities for general N following from hypotheses of marginal conditions or of quantum separability.

ACKNOWLEDGMENT

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APPENDIX A: PROOF OF LEMMA 2

1. Commutation relation (4.14)

Consider two contiguous vertices V_α and V_β of G connected by a link l_i with index i, and denote by $\sigma_\alpha(x_i, X, T)$ and $\sigma_\beta(x_i', X, T)$ the corresponding distributions of the chain $\mathcal{C}_n$, where $X = \{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_{n-1}\}$. By removing the link l_i, the proper tree graph G is broken in two

connected components G_α and G_β: $G=G_\alpha \cup l_i \cup G_\beta$. To this splitting clearly corresponds a partition $\{X_\alpha, X_\beta\}$ of the variables X such that, among X and their conjugate X', all the variables $\{X_\alpha, X'_\alpha, X_\beta\}$ and only them appear in the vertices of G_α, whereas all the variables $\{X_\alpha, X_\beta, X'_\beta\}$ and only them appear in the vertices of G_β. In parallel, the particular solution ρ_0 given in Eq. (4.3) factorizes as

$$\rho_0 = \frac{\rho_\alpha \rho_\beta}{\sigma_{\alpha\beta}} \zeta, \tag{A1}$$

where the function ρ_α (the "ρ_0/ζ" of the subchain of $\mathcal{C}_n$ of type G_α) depends only on $(x_i, X_\alpha, X'_\alpha, X_\beta)$, the function ρ_β depends only on $(x'_i, X_\alpha, X_\beta, X'_\beta)$, and

$$\sigma_{\alpha\beta}(X,T) = \int dx_i \sigma_\alpha(x_i, X, T) = \int dx'_i \sigma_\beta(x'_i, X, T).$$

The measures $d\mu_\alpha$ and $d\mu_\beta$ as defined by Eq. (4.8) now take the form

$$\begin{cases} d\mu_\alpha = \dfrac{\rho_\alpha}{\sigma_\alpha} dX'_\alpha \dfrac{1}{\sigma_{\alpha\beta}} \rho_\beta dX'_\beta dx'_i \zeta dT', \\ d\mu_\beta = \rho_\alpha dX'_\alpha \dfrac{1}{\sigma_{\alpha\beta}} \dfrac{\rho_\beta}{\sigma_\beta} dX'_\beta dx_i \zeta dT'. \end{cases} \tag{A2}$$

Hence, for any $g(\mathbf{q},\mathbf{p}) \in L^1(\mathbb{R}^{2N}, \rho_0 d^N q d^N p)$:

$$P_\alpha P_\beta g = \frac{1}{\sigma_{\alpha\beta}} \int dx'_i \int dX'_\alpha \frac{\rho_\alpha}{\sigma_\alpha} \int dX'_\beta \rho_\beta \int dT' \zeta (P_\beta g).$$

The integrations over X'_α, X'_β, and T' can be performed explicitly since $P_\beta g$ does not depend on these variables. Noticing that

$$\int dX'_\alpha \rho_\alpha = \sigma_\alpha, \quad \int dX'_\beta \rho_\beta = \sigma_\beta, \tag{A3}$$

and taking account of Eq. (4.4), we get

$$P_\alpha P_\beta g = \frac{1}{\sigma_{\alpha\beta}} \int dx'_i \sigma_\beta (P_\beta g), \tag{A4}$$

$$= \frac{1}{\sigma_{\alpha\beta}} \int dx'_i \sigma_\beta \frac{1}{\sigma_{\alpha\beta}} \int dx_i dX'_\alpha dX'_\beta dT' \rho_\alpha \frac{\rho_\beta}{\sigma_\beta} \zeta g. \tag{A5}$$

Since σ_β does not depend on x_i, X'_α, and X'_β, the factors σ_β and $1/\sigma_\beta$ in Eq. (A5) cancel each other. This gives

$$P_\alpha P_\beta g = \frac{1}{(\sigma_{\alpha\beta})^2} \int dx_i dx'_i dX'_\alpha dX'_\beta dT' \rho_\alpha \rho_\beta \zeta g. \tag{A6}$$

The r.h.s. of this equation is symmetric in $\alpha \leftrightarrow \beta$, which establishes Eq. (4.14).

2. Relation (4.15)

Let V_α, V_β, and V_γ be now three vertices of G such that V_α belongs to the path connecting V_γ to V_β and is contiguous to V_β. Consider again the connected subgraphs G_α and G_β defined in Appendix A1 above, together with the partition $\{X_\alpha, X_\beta\}$ of the variables X, and distinguish in G_α the linear subgraph $G_{\alpha\gamma}$ made of the vertices V_α, V_γ and the path connecting them. Denote by I_{α_1}

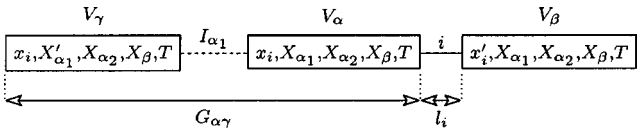

FIG. 9. The path between V_γ and V_β in G.

the set of indices of the links of $G_{\alpha\gamma}$ and by I_{α_2} the set of indices of the remaining links in G_α. To this splitting corresponds a further partition $\{X_{\alpha_1}, X_{\alpha_2}\}$ of the variables X_α, as indicated in Fig. 9.

With a factorization of the measure $d\mu_\gamma$ analogous to those of Eq. (A2), we can write

$$P_\gamma P_\alpha P_\beta g = \int dX_{\alpha_1} dX'_{\alpha_2} dX'_\beta dx'_i dT' \frac{\rho_\alpha}{\sigma_\gamma} \frac{1}{\sigma_{\alpha\beta}} \rho_\beta \zeta (P_\alpha P_\beta g). \tag{A7}$$

Here, we can perform explicitly the integrations over x'_i, X'_β, X'_{α_2}, and T', for $P_\alpha P_\beta g$ does not depend on these variables. First

$$\int dx'_i dX'_\beta \rho_\beta = \int dx'_i \sigma_\beta = \sigma_{\alpha\beta}. \tag{A8}$$

The left equality in Eq. (A8) results, as in Eq. (A3), from the "peeling process" (described in Sec. IV A) corresponding to the reduction of the graph G_β to the vertex V_β. Similarly, the (partial) peeling process corresponding to the reduction $G_\alpha \to G_{\alpha\gamma}$ yields

$$\int dX'_{\alpha_2} \rho_\alpha = \rho_{\alpha\gamma}, \tag{A9}$$

where $\rho_{\alpha\gamma}$ is the "ρ_0/ζ" of the subchain of type $G_{\alpha\gamma}$. Thanks to Eqs. (A8), (A9), and (4.7), Eq. (A7) boils down to

$$P_\gamma P_\alpha P_\beta g = \int dX_{\alpha_1} \frac{\rho_{\alpha\gamma}}{\sigma_\gamma} (P_\alpha P_\beta g)$$

or, by inserting the expression (A4) of $P_\alpha P_\beta g$:

$$P_\gamma P_\alpha P_\beta g = \int dX_{\alpha_1} \frac{\rho_{\alpha\gamma}}{\sigma_\gamma} \int dx'_i \frac{\sigma_\beta}{\sigma_{\alpha\beta}} (P_\beta g). \tag{A10}$$

On the other hand,

$$P_\gamma P_\beta g = \int dX_{\alpha_1} dX'_{\alpha_2} dX'_\beta dx'_i dT' \frac{\rho_0}{\sigma_\gamma} \zeta (P_\beta g), \tag{A11}$$

where the integrations over X'_β, X'_{α_2}, and T' can be performed explicitly since $P_\beta g$ does not depend on these variables. The integration over X'_β first produces, through the partial peeling process corresponding to $G \to (G_\alpha \cup l_i \cup V_\beta)$:

$$\int dX'_\beta \rho_0 = \rho_\alpha \frac{1}{\sigma_{\alpha\beta}} \sigma_\beta. \tag{A12}$$

Then Eqs. (A9) and (4.4) are used again for the integrations over X'_{α_2} and T', respectively. Altogether, this reduces the expression (A11) to the r.h.s. of Eq. (A10). Therefore $P_\gamma P_\alpha P_\beta g = P_\gamma P_\beta g$, which establishes Eq. (4.15) in the case where V_α is contiguous to V_β.

The proof of Eq. (4.15) in the case where V_α is contiguous to V_γ is completely similar.

Q.E.D.

APPENDIX B: PROOF OF LEMMA 3

We construct a particular k-chain of compatible distributions τ_j and we prove that there is no positive phase space density ρ reproducing these distributions as marginals. We take τ_j of the form:

$$\tau_j(q_1,\ldots,q_{j-1},p_j,q_{j+1},\ldots,q_k)=\gamma_j(p_j)\overline{\tau_j}(q_1,\ldots,q_{j-1},q_{j+1},\ldots,q_k)\ (j=1,\ldots,k),$$

where $\{\overline{\tau_1},\ldots,\overline{\tau_k}\}$ is a k-chain of compatible, reduced distributions and the $\gamma_j(p_j)$'s are arbitrary, normalized one variable distributions.

Let us look for a phase space density ρ reproducing the τ_j's. The $\overline{\tau_j}$'s are given in terms of the configuration space density

$$\overline{\rho}(q_1,\ldots,q_k)\equiv\int d^k p\rho(q_1,\ldots,q_k,p_1,\ldots,p_k) \tag{B1}$$

as

$$\overline{\tau_j}(q_1,\ldots,q_{j-1},q_{j+1},\ldots,q_k)=\int dq_j\overline{\rho}(q_1,\ldots,q_k). \tag{B2}$$

We now choose the $\overline{\tau_j}$'s as follows:

$$\begin{cases}\overline{\tau_1}(q_2,\ldots,q_k)=\displaystyle\prod_{r=2}^{k}T_r-\prod_{r=2}^{k}U_r,\\ \overline{\tau_j}(q_1,\ldots,q_{j-1},q_{j+1},\ldots,q_k)=\displaystyle\prod_{\substack{r=1\\ r\neq j}}^{k}T_r+\prod_{\substack{r=1\\ r\neq j}}^{k}U_r,\quad (j=2,\ldots,k),\end{cases} \tag{B3}$$

where

$$\begin{cases}T_r=\frac{1}{2}[\delta(q_r-1)+\delta(q_r+1)],\\ U_r=\frac{1}{2}[\delta(q_r-1)-\delta(q_r+1)],\end{cases}\quad (r=1,\ldots,k).$$

The $\overline{\tau_j}$'s, which appear as sums of 2^{k-2} monomials of the form

$$\frac{1}{2^{k-2}}\prod_{\substack{r=1\\ r\neq j}}^{k}\delta(q_r-\varepsilon_r)\quad \varepsilon_r=\pm 1,$$

are obviously positive and normalized. Furthermore,

$$\int dq_i\overline{\tau_j}(q_1,\ldots,q_{j-1},q_{j+1},\ldots,q_k)=\prod_{\substack{r=1\\ r\neq i,j}}^{k}T_r\quad (i\neq j).$$

The r.h.s. of this equation is symmetric in $i\leftrightarrow j$, which entails the compatibility of the $\overline{\tau_j}$'s.

Clearly, the most general *positive* $\overline{\rho}$ obeying Eqs. (B2) is the sum of 2^k terms proportional to $\Pi_{r=1}^{k}\delta(q_r-\varepsilon_r)$. Equivalently, $\overline{\rho}$ can be written as a homogeneous polynomial $P(\{T_r\},\{U_r\})$ of degree k which, for each index r, is linear in T_r and U_r. Then, since $\int dq_jT_j=1$ and $\int dq_jU_j=0$, we can express $\int dq_j\overline{\rho}$ as $\partial P/\partial T_j$, so that Eqs. (B2) and (B3) yield

$$\begin{cases} \dfrac{\partial P}{\partial T_1} = \displaystyle\prod_{r=2}^{k} T_r - \prod_{r=2}^{k} U_r, \\ \dfrac{\partial P}{\partial T_j} = \displaystyle\prod_{\substack{r=1 \\ r\neq j}}^{k} T_r + \prod_{\substack{r=1 \\ r\neq j}}^{k} U_r \ (j = 2, \ldots, k). \end{cases}$$

The general solution of these equations is

$$P = \prod_{r=1}^{k} T_r - T_1 \prod_{r=2}^{k} U_r + \sum_{j=2}^{k} T_j \prod_{\substack{r=1 \\ r\neq j}}^{k} U_r + \lambda \prod_{r=1}^{k} U_r, \tag{B4}$$

where λ is an arbitrary real parameter.

Now, whatever the value of λ is, P, and thus ρ, are not positive. To show this, it is sufficient to look at the coefficients of the two monomials

$$\delta(q_1 + 1) \prod_{r=2}^{k} \delta(q_r - 1) \text{ and } \delta(q_1 - 1)\delta(q_2 + 1)\delta(q_3 + 1) \prod_{r=4}^{k} \delta(q_r - 1)$$

which appear in Eq. (B4) if $k \geqslant 3$. One finds $-(k-1+\lambda)/2^k$ and $(k-5+\lambda)/2^k$, respectively, the sum of which is independent of λ and negative. Q.E.D.

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The moduli space of three-qutrit states

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We study the invariant theory of trilinear forms over a three-dimensional complex vector space, and apply it to investigate the behavior of pure entangled three-partite qutrit states and their normal forms under local filtering operations (SLOCC). We describe the orbit space of the SLOCC group $\mathrm{SL}(3,\mathbb{C})^{\times 3}$ both in its affine and projective versions in terms of a very symmetric normal form parametrized by three complex numbers. The parameters of the possible normal forms of a given state are roots of an algebraic equation, which is proved to be solvable by radicals. The structure of the sets of equivalent normal forms is related to the geometry of certain regular complex polytopes. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The invariant theory of trilinear forms over a three-dimensional complex vector space is an old subject with a long history, which, as we shall see, appears even longer if we take into account certain indirect but highly relevant contributions.[1–4] This question has been recently revived in the field of Quantum Information Theory as the problem of classifying entanglement patterns of three-qutrit states.

Indeed, since the advent of quantum computation and quantum cryptography, entanglement has been promoted to a resource that allows quantum physics to perform tasks that are classically impossible. Quantum cryptography[5,6] proved that this gap even exists with small systems of two entangled qubits. Furthermore, it is expected that the study of higher dimensional systems and of multipartite (e.g., 3-partite) states would lead to more applications. A seminal example is the so-called 3-qutrit Aharonov-state, which "*is so elegant it had to be useful*":[7] Fitzi, Gisin, and Maurer[7] found out that the classically impossible Byzantine agreement problem[8] can be solved using 3-partite qutrit states. From a more fundamental point a view, the Aharonov state led to nontrivial counterexamples of the conjectures on additivity of the relative entropy of entanglement[9] and of the output purity of quantum channels.[10] Obviously, these results provide a strong motivation for studying 3-partite qutrit states. Furthermore, interesting families of higher-dimensional states are perfectly suited to address questions concerning local realism and Bell inequalities (see, e.g., Ref. 11 for a study of three-qutrit correlations).

It is therefore of interest to find some classification scheme for three-qutrit states. A possible direction is to look for classes of equivalent states, in the sense that they are equivalent up to local unitary transformations[12–14] or local filtering operations (also called SLOCC operations).[14–19] In the case of three qubits, especially the last classification proved to yield a lot of insights (the

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classification up to local unitaries has too many parameters left); the reason for that is that in the closure of each generic orbit induced by SLOCC operations, there is a unique state (up to local unitary transformations) with maximal entanglement.[14,17]

In Ref. 19, a numerical method converging to such a maximally entangled state has been described. It has been experimentally observed that, when applied to a three-qutrit state, this method converged to a very special normal form. We shall provide a formal proof of this property, and then study in some detail the geometry of those normal forms. Precise statements of the results are summarized in the forthcoming section.

II. RESULTS

Let $V=\mathbb{C}^3$ and $\mathcal{H}=V\otimes V\otimes V$ regarded as a representation of the group $G=\mathrm{SL}(3,\mathbb{C})^{\times 3}$. The elements of $\mathcal{H}$ will be interpreted either as three-qutrit states

$$|\psi\rangle = \sum_{i,j,k=0}^{2} A_{ijk}|i,j,k\rangle \tag{1}$$

or as trilinear forms

$$f = f(\mathbf{x},\mathbf{y},\mathbf{z}) = \sum_{i,j,k=0}^{2} A_{ijk}x_i y_j z_k, \tag{2}$$

that is, we identify the basis state $|ijk\rangle$ with the monomial $x_i y_j z_k$. If $g=(g^{(1)},g^{(2)},g^{(3)})\in G$ is a triple of matrices, we define $x'_i=\Sigma_p g^{(1)}_{ip}x_p$, $y'_j=\Sigma_q\, g^{(2)}_{jq}y_q$, $z'_k=\Sigma_r\, g^{(3)}_{kr}z_r$, and the coefficients A'_{ijk} by the condition

$$\sum A'_{ijk}x'_i y'_j z'_k = \sum A_{ijk}x_i y_j z_k, \tag{3}$$

the action of G on $\mathcal{H}$ being defined by

$$g\cdot A = \sum A'_{ijk}x_i y_j z_k, \tag{4}$$

It has been shown by Vinberg[20] that a generic state can be reduced to the normal form

$$A'_{ijk} = u\,\delta_{ijk} + \frac{w-v}{2}\epsilon_{ijk} + \frac{w+v}{2}|\epsilon_{ijk}| \tag{5}$$

(where δ_{ijk} is the Kronecker symbol and ϵ_{ijk} the completely antisymmetric tensor) by an appropriate choice of $g\in G$.

Our first result is as follows.

Theorem II.1: *When applied to a generic 3-qutrit state (1) the numerical algorithm of Ref. 19 converges to a state which is a Vinberg normal form, generically in the same G-orbit as* $|\psi\rangle$.

As proved in Refs. 14 and 19, the normal form $|\psi'\rangle$ is unique up to local unitary transformations. More precisely, we have the following.

Theorem II.2: *A generic state has exactly* 648 *different normal forms. For special states, this number can be reduced to* 216, 72, 27 *or* 1. *Moreover, the coefficients u, v, w of the normal form can be computed algebraically.*

Theorem II.3: *The coefficients of the normal forms are determined, up to a sign, by an algebraic equation of degree* 1296, *which is explicitly solvable by radicals.*

To form this equation, we need some notions of invariant theory.

A polynomial $P(A)$ in the coefficients A_{ijk} is an *invariant* of the action of G on $\mathcal{H}$ if $P(A')=P(A)$ for all $g\in G$. These invariants form a graded algebra R (any invariant P is a sum of homogeneous invariants) and the first issue is to determine the dimension of the space R_d of homogeneous invariants of degree d. The Hilbert series

$$h(t) = \sum_{d \geqslant 0} \dim R_d t^d \tag{6}$$

is known[20]

$$h(t) = \frac{1}{(1-t^6)(1-t^9)(1-t^{12})} \tag{7}$$

and in fact, one can prove that R is a polynomial algebra generated by three algebraically independent invariants of respective degree 6, 9, and 12.

The modern way to prove this result is due to Vinberg, who obtained it from his notion of Weyl group of a graded Lie algebra, applied to a Z_3-grading of the exceptional Lie algebra E_6.[21]

In Sec. III, we shall explain how it can be deduced from the work of Chanler.[22] We prove that certain invariants I_6, I_9, and I_{12} introduced in Ref. 22 are indeed algebraic generators of R and explain how to compute them from the numerical values of the coefficients A_{ijk}, by expressing them in terms of *transvectants*, that is, by means of certain differential polynomials in the form f, rather than in terms of the classical symbolic notation. Given the values of the invariants for a particular state, we show how to form and solve the system of algebraic equations determining the coefficients, u, v, w of the normal form.

Let $a=I_6$, $b=I_{12}$, and $c=I_{18}$ (a certain polynomial in the fundamental invariants). Then, the symmetric functions of u^3, v^3, and w^3

$$\psi = u^3 + v^3 + w^3, \quad \chi = u^3v^3 + u^3w^3 + v^3w^3, \quad \lambda = 216u^3v^3w^3 \tag{8}$$

satisfy

$$\psi^2 - 12\chi - a = 0,$$

$$\psi^4 + \lambda\psi - b = 0,$$

$$\psi^6 - \tfrac{5}{2}\lambda\psi^3 - \tfrac{1}{8}\lambda^2 - c = 0. \tag{9}$$

Theorem II.4: *The system (9) has generically* 1296 *solutions* (u,v,w)*, which can be obtained by solving a chain of algebraic equations of degree at most* 4*. Only* 648 *of them give the correct sign for* I_9*. The number of solutions (with the correct sign for* I_9*) can be reduced only to* 216, 72, 27 *or* 1*. Moreover, the isotropy groups of these degenerate orbits can be determined, and the configuration of the points* (u,v,w) *in* $\mathbb{C}^3$ *can be interpreted in terms of the geometry of regular complex polyhedra.*

The details are given in Sec. VII.

III. THE FUNDAMENTAL INVARIANTS

In this section, we describe the fundamental invariants, as well as the other concomitants obtained by Chanler,[22] in a form suitable for calculations, in particular for their numerical evaluation (see also Refs. 23 and 24).

As already mentioned, we shall identify a three-qutrit state $|\psi\rangle \in \mathcal{H}$ with a trilinear form

$$f(\mathbf{x},\mathbf{y},\mathbf{z}) = \sum_{1 \leqslant i,j,k \leqslant 3} A_{ijk} x_i y_j z_k \tag{10}$$

in three ternary variables. To construct its fundamental invariants, we shall need the notion of a transvectant, which is defined by means of Cayley's omega process (see, e.g., Ref. 25).

Let f_1, f_2, and f_3 be three forms in a ternary variable $\mathbf{x}=(x_1,x_2,x_3)$. Their tensor product $f_1 \otimes f_2 \otimes f_3$ is identified with the polynomial $f_1(\mathbf{x}^{(1)})f_2(\mathbf{x}^{(2)})f_3(\mathbf{x}^{(3)})$ in the three independent ternary variables $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$ and $\mathbf{x}^{(3)}$. We use the "trace" notation of Olver[26] to denote the multiplication map $f_1 \otimes f_2 \otimes f_3 \to f_1 f_2 f_3$, that is,

$$\operatorname{tr} f_1(\mathbf{x}^{(1)})f_2(\mathbf{x}^{(2)})f_3(\mathbf{x}^{(3)}) = f_1(\mathbf{x})f_2(\mathbf{x})f_3(\mathbf{x}). \tag{11}$$

Cayley's operator $\Omega_{\mathbf{x}}$ is the differential operator

$$\Omega_{\mathbf{x}} = \begin{vmatrix} \frac{\partial}{\partial x_1^{(1)}} & \frac{\partial}{\partial x_1^{(2)}} & \frac{\partial}{\partial x_1^{(3)}} \\ \frac{\partial}{\partial x_2^{(1)}} & \frac{\partial}{\partial x_2^{(2)}} & \frac{\partial}{\partial x_2^{(3)}} \\ \frac{\partial}{\partial x_3^{(1)}} & \frac{\partial}{\partial x_3^{(2)}} & \frac{\partial}{\partial x_3^{(3)}} \end{vmatrix}. \tag{12}$$

Now, we consider three independent ternary variables $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ together with the associated dual (contravariant) variables $\xi=(\xi_1,\xi_2,\xi_3)$, $\eta=(\eta_1,\eta_2,\eta_3)$, $\zeta=(\zeta_1,\zeta_2,\zeta_3)$ [that is, ξ_i is the linear form on the $\mathbf{x}$ space such that $\xi_i(x_j)=\delta_{ij}$].

A *concomitant* of f is, by definition, a polynomial F in the A_{ijk}, $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$, ξ, η, ζ, such that if $g=(g_1,g_2,g_3)\in \mathrm{SL}(3,\mathbb{C})^3$, then, with A', $\mathbf{x}'$, etc., as above,

$$F(A';\mathbf{x}',\mathbf{y}',\mathbf{z}';\xi',\eta',\zeta') = F(A;\mathbf{x},\mathbf{y},\mathbf{z};\xi,\eta,\zeta). \tag{13}$$

The algebra of concomitants admits only one generator of degree 1 in the A_{ijk}, which is the form f itself. Other concomitants can be deduced from f and the three absolute invariants $P_\alpha=\Sigma\xi_i x_i$, $P_\beta=\Sigma\eta_j y_j$, and $P_\gamma=\Sigma\zeta_k z_k$, using transvectants. If F_1, F_2, and F_3 are three 6-tuple forms in the independent ternary variables $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$, ξ, η, and ζ, one defines for any $(n_1,n_2,n_3)\times(m_1,m_2,m_3)\in\mathbb{N}^3\times\mathbb{N}^3$ the multiple transvectant of F_1, F_2, and F_3 by

$$(F_1,F_2,F_3)^{n_1n_2n_3}_{m_1m_2m_3} = \operatorname{tr}\quad \Omega_{\mathbf{x}}^{n_1}\Omega_{\mathbf{y}}^{n_2}\Omega_{\mathbf{z}}^{n_3}\Omega_{\xi}^{m_1}\Omega_{\eta}^{m_2}\Omega_{\zeta}^{m_3}\prod_{i=1}^{3} F_i(\mathbf{x}^{(i)},\mathbf{y}^{(i)},\mathbf{z}^{(i)};\xi^{(i)},\eta^{(i)},\zeta^{(i)}). \tag{14}$$

For convenience, we will set $(F_1,F_2,F_3)^{n_1n_2n_3}=(F_1,F_2,F_3)^{n_1n_2n_3}_{000}$. The concomitants of degree 2 given by Chanler[22] can be obtained using these operations,

$$Q_\alpha = (f,f,P_\beta P_\gamma)^{011}, \tag{15}$$

$$Q_\beta = (f,f,P_\alpha P_\gamma)^{101}, \tag{16}$$

$$Q_\gamma = (f,f,P_\alpha P_\beta)^{110}. \tag{17}$$

The invariant I_6 is then

$$I_6 = \tfrac{1}{96}(Q_\alpha,Q_\alpha,Q_\alpha)^{200}_{011} = \tfrac{1}{96}(Q_\beta,Q_\beta,Q_\beta)^{020}_{101} = \tfrac{1}{96}(Q_\gamma,Q_\gamma,Q_\gamma)^{002}_{110}. \tag{18}$$

There is an alternative expression using only the ground form f,

$$I_6 = \frac{1}{1152}(f^2,f^2,f^2)^{222}. \tag{19}$$

Now, in degree 3 the covariants B_α, B_β, and B_γ of Ref. 22 are

$$B_\alpha = (f,f,f)^{011}, \tag{20}$$

$$B_\beta = (f,f,f)^{101}, \tag{21}$$

$$B_\gamma = (f,f,f)^{110}. \tag{22}$$

The other concomitants found by Chanler can be written in a similar way,

$$C_{\alpha\beta} = \tfrac{1}{4}(f, f, fP_\beta)^{110}, \tag{23}$$

$$C_{\beta\alpha} = \tfrac{1}{4}(f, f, fP_\alpha)^{110}, \tag{24}$$

$$C_{\alpha\gamma} = \tfrac{1}{4}(f, f, fP_\gamma)^{101}, \tag{25}$$

$$C_{\gamma\alpha} = \tfrac{1}{4}(f, f, fP_\alpha)^{101}, \tag{26}$$

$$C_{\beta\gamma} = \tfrac{1}{4}(f, f, fP_\gamma)^{011}, \tag{27}$$

$$C_{\gamma\beta} = \tfrac{1}{4}(f, f, fP_\beta)^{011}, \tag{28}$$

$$D_\alpha = -2(fP_\beta, fP_\gamma, f)^{111}, \tag{29}$$

$$D_\beta = 2(fP_\alpha, fP_\gamma, f)^{111}, \tag{30}$$

$$D_\gamma = -2(fP_\alpha, fP_\beta, f)^{111}, \tag{31}$$

$$E_\alpha = (Q_\alpha, f, P_\alpha)^{100}, \tag{32}$$

$$E_\beta = (Q_\beta, f, P_\beta)^{010}, \tag{33}$$

$$E_\gamma = (Q_\gamma, f, P_\gamma)^{001}, \tag{34}$$

$$G_\alpha = -\tfrac{3}{8}(fP_\beta, fP_\gamma, f)^{011} + \tfrac{5}{16}(fP_\beta P_\gamma, f, f)^{011}, \tag{35}$$

$$G_\beta = -\tfrac{3}{8}(fP_\alpha, fP_\gamma, f)^{101} + \tfrac{5}{16}(fP_\alpha P_\gamma, f, f)^{101}, \tag{36}$$

$$G_\gamma = -\tfrac{3}{8}(fP_\alpha, fP_\beta, f)^{110} + \tfrac{5}{16}(fP_\alpha P_\beta, f, f)^{110}, \tag{37}$$

$$H = \tfrac{1}{2}(fP_\alpha, fP_\beta, fP_\gamma)^{111}. \tag{38}$$

Here, we have combined the concomitants of degrees 0, 1, and 2 into independent concomitants of degree 3. Next, we have chosen the scalar factors so that the syzygies given by Chanler[22] hold in the form

$$H + E_\alpha - E_\gamma + D_\beta P_\beta = 0, \tag{39}$$

$$H + E_\beta - E_\alpha + D_\gamma P_\gamma = 0, \tag{40}$$

$$H + E_\gamma - E_\beta + D_\alpha P_\alpha = 0, \tag{41}$$

$$3C_{\alpha\beta} - B_\gamma P_\beta = 0, \tag{42}$$

$$3C_{\beta\alpha} - B_\gamma P_\alpha = 0, \tag{43}$$

$$3C_{\alpha\gamma} - B_\beta P_\gamma = 0, \tag{44}$$

$$3C_{\gamma\alpha} - B_\beta P_\alpha = 0, \tag{45}$$

$$3C_{\beta\gamma} - B_\alpha P_\gamma = 0, \tag{46}$$

$$3C_{\gamma\beta} - B_\alpha P_\beta = 0, \tag{47}$$

$$6G_\alpha - 3Q_\alpha f + B_\alpha P_\beta P_\gamma = 0, \tag{48}$$

$$6G_\beta - 3Q_\beta f + B_\beta P_\alpha P_\gamma = 0, \tag{49}$$

$$6G_\gamma - 3Q_\gamma f + B_\gamma P_\alpha P_\beta = 0. \tag{50}$$

One can remark that a basis of the space of the concomitants of degree 3 found by Chanler can be constructed using only transvections and products from smaller degrees,

$$f^3, Q_\alpha f, Q_\beta f, Q_\gamma f, B_\alpha, B_\beta, B_\gamma, D_\alpha, D_\beta, D_\gamma, E_\alpha. \tag{51}$$

The knowledge of these concomitants allows one to construct the invariants I_9 and I_{12},

$$I_9 = \tfrac{1}{576}(E_\alpha, E_\beta, E_\beta)^{111}_{111}, \tag{52}$$

$$I_{12} = \frac{1}{124\,416}(B_\alpha f, B_\alpha f, B_\alpha f)^{411}. \tag{53}$$

These expressions, which can be easily implemented in any computer algebra system, will prove convenient to compute the specializations discussed in the sequel.

IV. NORMAL FORM AND INVARIANTS

It will now be shown that a generic state can be reduced to the normal form

$$A_{ijk} = u\,\delta_{ijk} + \frac{w-v}{2}\epsilon_{ijk} + \frac{w+v}{2}|\epsilon_{ijk}|, \tag{54}$$

where ϵ_{ijk} is the alternating tensor, or, otherwise said, that the generic trilinear form $f(\mathbf{x},\mathbf{y},\mathbf{z})$ is equivalent to some

$$\begin{aligned} N_{uvw}(\mathbf{x},\mathbf{y},\mathbf{z}) = {} & u(x_1y_1z_1 + x_2y_2z_2 + x_3y_3z_3) + v(x_1y_3z_2 + x_2y_1z_3 + x_3y_2z_1) \\ & + w(x_1y_2z_3 + x_2y_3z_1 + x_3y_1z_2). \end{aligned} \tag{55}$$

For such a state, the local density operators are all proportional to the identity. This property is automatically satistfied by the limiting state obtained from the numerical method of Ref. 19, and implies maximal entanglement as well. Since this algorithm amounts to an infinite sequence of invertible local filtering operations, the genericity of Vinberg's normal form, together with the previously mentioned properties, implies convergence to a Vinberg normal form for a generic input state, that is, our Theorem II.1 (see also Refs. 27 and 28).

This normal form is in general not unique, and the relations between the various N_{uvw} in a given orbit is an interesting question, which will be addressed in the sequel.

Although, the validity of this normal form follows from Vinberg's theory,[21] it can also be proved in other ways, some of them being particularly instructive. We shall detail one of these possibilities, which will give us the opportunity to introduce some important polynomials, playing a role in the algebraic calculation of the normal form and in the geometric discussion of the orbits.

The shortest possibility, although not the most elementary, relies on the results of Ref. 22, and starts with computing the invariants of N_{uvw}. We then use a few results of algebraic geometry, which can be found in Ref. 29. Let us denote by $C_k \equiv C_k(u,v,w)$ $(k=6,9,12)$ the values of the I_k on N_{uvw}. Direct calculation gives, denoting by m_{pqr} the monomial symmetric functions of u,v,w (sum of all distinct permutations of the monomial $u^p v^q w^r$),

$$C_6 = m_{(6)} - 10m_{(3,3)}, \tag{56}$$

$$C_9 = (u^3 - v^3)(u^3 - w^3)(v^3 - w^3), \tag{57}$$

$$C_{12} = m_{(12)} + 4m_{(9,3)} + 6m_{(6,6)} + 228m_{(6,3,3)}. \tag{58}$$

It is easily checked by direct calculation that the Jacobian of these three functions is nonzero for generic values of (u,v,w). Actually, its zero set consists of 12 planes, whose geometric significance will be discussed below.

Let us denote by $\varphi: \mathcal{H} \xrightarrow{(I_6,I_9,I_{12})} \mathbb{C}^3$, the map sending a trilinear form to its three invariants, so that $(C_6,C_9,C_{12}) = \varphi(N_{uvw})$. Let $S = \{N_{uvw} | (u,v,w) \in \mathbb{C}^3\}$ be the three-dimensional space of normal forms. The nonvanishing of the Jacobian proves that φ induces a dominant mapping from S to $\mathbb{C}^3$ (that is, the direct image of any nonempty open subset of S contains a nonempty open subset of $\mathbb{C}^3$). Note that the independence of C_6,C_9,C_{12} implies the independence of I_6,I_9,I_{12}. Now, Chanler[22] has shown that I_6,I_9,I_{12} separate the orbits in general position. This proves that the field of rational invariants of G is freely generated by I_6,I_9,I_{12} (Ref. 29, Lemma 2.1). As a consequence, φ is a *rational quotient* (Ref. 29, Sec. 2.4) for the action of G on $\mathcal{H}$ (actually, this also implies that φ is a categorical quotient, by Ref. 29, Proposition 2.5 and Theorem 4.12, using that $\varphi_{|S}$ is surjective, whence also φ).

There exists a nonempty open subset Y_0 of $\mathbb{C}^3$ such that the fiber of φ over each of its points is the closure of an orbit (Ref. 29, Proposition 2.5). Let then $U_0 = \varphi^{-1}(Y_0)$. This set cuts S since $\varphi_{|S}$ is dominant. Let U_1 be the union of all orbits having maximal dimension (a nonempty open set, the function *dimension of the orbit* being lower semicontinuous). It is easy to see that U_1 intersects S (for instance at $u=1$, $v=1$, $w=-1$, whose orbit has dimension $24 = \dim G$, as may be checked by direct calculation). Let $S_0 = U_1 \cap S$, a dense open subset of S. The set $\varphi^{-1}\varphi(S_0)$ thus contains a dense open subset U_2 of $\mathcal{H}$. One then checks that $U_0 \cap U_1 \cap U_2$ (a dense open subset, as an intersection of dense open subsets of an irreducible space) is contained in GS. This proves $\overline{GS} = \mathcal{H}$, that is, the normal form N_{uvw} is generic.

Let us remark that the above discussion also proves, thanks to Igusa's theorem (Ref. 29, Theorem 4.12) that $\mathbb{C}[\mathcal{H}]^G = \mathbb{C}[I_6,I_9,I_{12}]$, that is, the algebra of invariants is freely generated by Chanler's invariants.

Is is also possible to give a direct proof of the normal form by using the same technique as in Ref. 22. Chanler's method relies on the geometry of plane cubics, which will play a prominent role in the sequel.

V. THE FUNDAMENTAL CUBICS

The trilinear form $f(\mathbf{x},\mathbf{y},\mathbf{z})$ can be encoded in three ways by a 3×3 matrix of linear forms $M_x(\mathbf{x})$, $M_y(\mathbf{y})$, and $M_z(\mathbf{z})$, defined by

$$f(\mathbf{x},\mathbf{y},\mathbf{z}) = {}^t\mathbf{y} M_x(\mathbf{x})\mathbf{z} = {}^t\mathbf{x} M_y(\mathbf{y})\mathbf{z} = {}^t\mathbf{x} M_z(\mathbf{z})\mathbf{y} \tag{59}$$

and the classification of trilinear forms amounts to the classification of one of these matrices, say $M_x(\mathbf{x})$ up to left and right multiplication by elements of $\mathrm{SL}(3,\mathbb{C})$ and action of $\mathrm{SL}(3,\mathbb{C})$ on the variable $\mathbf{x}$.

The most immediate covariants of f are the determinants of these matrices

$$X(\mathbf{x}) = \det M_x(\mathbf{x}) = \tfrac{1}{6}B_\alpha, \tag{60}$$

$$Y(\mathbf{y}) = \det M_y(\mathbf{y}) = \tfrac{1}{6}B_\beta, \tag{61}$$

$$Z(\mathbf{z}) = \det M_z(\mathbf{z}) = \tfrac{1}{6}B_\gamma. \tag{62}$$

These are ternary cubic forms, and for generic f the equations $X(\mathbf{x})=0$, etc., will define nonsingular cubics (elliptic curves) in $\mathbb{P}^2$. It is shown in Ref. 24 that whenever one of these curves is elliptic, so are the other two ones, and moreover, all three are projectively equivalent. Actually, one can check by direct calculation that they have the same invariants. When $f=N_{uvw}$, these three cubics have even the same equation and are in the Hesse canonical form[30]

$$X(\mathbf{x}) = -\phi(x_1^3 + x_2^3 + x_3^3) + \psi x_1 x_2 x_3 = Y(\mathbf{x}) = Z(\mathbf{x}), \tag{63}$$

where we introduced, following the notation of Ref. 2,

$$\phi = uvw, \quad \psi = u^3 + v^3 + w^3. \tag{64}$$

The Aronhold invariants of the cubics (63) are given by

$$6^4 S = -\phi(\psi^3 + (6\phi)^3), \tag{65}$$

$$6^6 T = (6\phi)^6 + 20(6\phi^3)\psi^3 - 8\psi^6. \tag{66}$$

These are of course invariants of f. We recognize that $6^4S=-C_{12}$, and we introduce an invariant I_{18} such that $C_{18}=I_{18}(N_{uvw})=6^6T$. The three cubics have the same discriminant $64S^3+T^2$, known to be proportional to the hyperdeterminant of f (see Refs. 31 and 32), which we normalize as

$$\Delta = 27(64S^3 + T^2). \tag{67}$$

Then $\Delta = C'^3_{12}$, where C'_{12} is the product of 12 linear forms

$$\begin{aligned} C'_{12} = {} & uvw(u+v+w)(\varepsilon u+v+w)(u+\varepsilon v+w)(\varepsilon^2 u+\varepsilon v+w)(u+\varepsilon^2 v+w) \\ & \times (\varepsilon u+\varepsilon v+w)(\varepsilon^2 u+v+w)(\varepsilon u+\varepsilon^2 v+w)(\varepsilon^2 u+\varepsilon^2 v+w), \end{aligned} \tag{68}$$

where $\varepsilon = e^{2i\pi/3}$, so that $C'_{12}=0$ is the equation in $\mathbb{P}^2$ of the twelve lines containing 3×3 the nine inflection points of the pencil of cubics,

$$u^3 + v^3 + w^3 + 6m\, uvw = 0, \tag{69}$$

obtained from X, Y, Z by treating the original variables as parameters. We note also that the Jacobian of C_6, C_9, C_{12} is proportional to C'^2_{12}.

VI. SYMMETRIES OF THE NORMAL FORMS

In this section, we will prove Theorem II.2. That is, a generic f has 648 different normal forms [the points (u,v,w) for which this number is reduced will be studied in Sec. VII].

To prove the theorem, we remark that the Hilbert series (7) is also the one of the ring of invariants of G_{25}, the group number 25 in the classification of irreducible complex reflection groups of Shephard and Todd.[4] This group, which we will denote for short by K, has order 648. It is one of the groups considered by Maschke[2] in his determination of the invariants of the symmetry group of the 27 lines of a general cubic surface in $\mathbb{P}^3$ (a group with 51 840 elements, which is related to the exceptional root system E_6). To define K, we first have to introduce Maschke's group H, a group of order 1296, which is generated by the matrices of the linear transformations on $\mathbb{C}^3$ given in Table I.

TABLE I. The generators of H.

	A	B	C	D	E
u'	v	u	u	u	$1/i\sqrt{3}(u+v+w)$
v'	w	w	εv	εv	$1/i\sqrt{3}(u+\varepsilon v+\varepsilon^2 w)$
w'	u	v	$\varepsilon^2 w$	εw	$1/i\sqrt{3}(u+\varepsilon^2 v+\varepsilon w)$

This group contains in particular the permutation matrices, and simultaneous multiplication by $\pm\varepsilon^k$, since $E^2=-B$. The subgroup K is the one in which odd permutations can appear only with a minus sign. It is generated by A,C,D,E.

Then, as proved by Maschke, the algebra of invariants of K in $\mathbb{C}[u,v,w]$ is precisely $\mathbb{C}[C_6,C_9,C_{12}]$.

Hence, we can conclude that K is the symmetry group of the normal forms N_{uvw}. There was another, equally natural possibility leading to the same Hilbert series. The symmetry group L of the equianharmonic cubic surface $\Sigma: z_0^3+z_1^3+z_2^3+z_3^3=0$ acting on the homogeneous coordinate ring $\mathbb{C}[\Sigma]$ has as fundamental invariants the elementary symmetric functions of the z_i^3, the first one being 0 by definition, so that the Hilbert series of $\mathbb{C}[\Sigma]^L$ coincides with (7). Moreover, L is also of order 648, but it is known that it is not isomorphic to K.

Taking into account the results of Sec. IV, we see that

$$S=\{N_{uvw}|(u,v,w)\in\mathbb{C}^3\} \tag{70}$$

is what is usually called a Chevalley section of the action of G on $\mathcal{H}$, with Weyl group K (see Ref. 29, p. 174).

VII. THE FORM PROBLEM

This section contains the proofs of Theorems II.3 and II.4. Klein (see Ref. 33) has introduced and investigated the notion of "Formenproblem" associated to a finite group action. This is the following: given the numerical values of the invariants, compute the coordinates of a point of the corresponding orbit.

In our case, we shall see that the problem of finding the parameters (u,v,w) of the normal form of a given generic f, given the values of the invariants, can be reduced to a chain of algebraic equations of degree at most 4, hence sovable by radicals.

Let $a=I_6$, $b=I_{12}$ and $c=I_{18}$ (we start with I_{18}, because C_{18} is a symmetric function of u^3,v^3,w^3, and at the end of the calculation, select the solutions which give the correct sign for C_9, which is alternating).

What we have to do is to determine the elementary symmetric functions $e_1=\psi, e_2=\chi, e_3=\phi^3$ of u^3,v^3,w^3. Let $\lambda=216\phi^3$. Then,

$$\psi^4+\lambda\psi-b=0, \tag{71}$$

$$\psi^6-\tfrac{5}{2}\lambda\psi^3-\tfrac{1}{8}\lambda^2-c=0. \tag{72}$$

Eliminating λ from these equations, we get a quartic equation for ψ^2,

$$27\psi^8-18b\psi^4-8c\psi^2-b^2=0. \tag{73}$$

The discriminant (with respect to ψ) of this polynomial is proportional to $D=b^2(b^3-c^2)^4$. When it is nonzero, we get eight values for e_1, each of which determines univocally e_2 and e_3. Hence, we obtain eight cubic equations whose roots are the possible values of u^3,v^3,w^3. This gives eight sets, whence $8\times6=48$ triples, each of which providing generically 27 values of (u,v,w), in all $48\times27=1296$ triples corresponding to the given values of a,b,c, among which exactly $1296/2=648$ give the correct sign for I_9. The common discriminant of the eight cubics is $\delta=a^3-3ab$

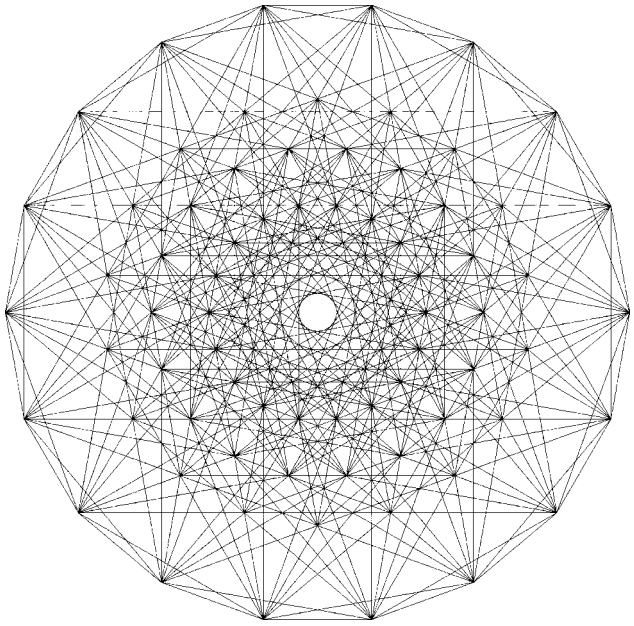

FIG. 1. The polyhedron 2{4}3{3}3.

$+2c$. Clearly, when $\delta \neq 0$, we will have 648 triples. If $\delta = 0$, one can check that the cubics cannot have a triple root, and that no root is zero. Hence, in this case, we obtain again 648 triples.

If $D=0$, we can have $b^3=c^2$ or $b=0$. In the first case, setting $b=q^2, c=q^3$, the equation becomes

$$(\psi^2 - q)^3(\psi^2 + 2q)^3 = 0. \tag{74}$$

In this case, we get only four quartics for ψ^2. If $C_9 \neq 0$, we obtain 216 triples. If $C_9=0$ and $b=a^2/4$, $c=-a^3/8$ we obtain again 216 triples which form the centers of the edges of a complex polyhedron of type 2{4}3{3}3 in $\mathbb{C}^3$ (see Fig. 1), in the notation of Ref. 34. The vertices of this polyhedron are the vertices of two reciprocal Hessian polyhedra (see Fig. 2) and its edges join each vertex of one Hessian polyhedron to the eight closest vertices of the other one. In Fig. 2, the edges of the Hessian polyhedron, which are complex lines, are represented by real equilateral triangles, so that the figure can as well be interpreted as a two-dimensional projection of a six-dimensional Gosset polytope 2_{21}. If $C_9=0$ and $b=a^2$, $c=a^3$, we obtain only 72 triples which

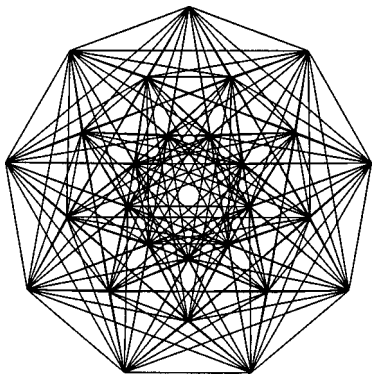

FIG. 2. The Hessian polyhedron.

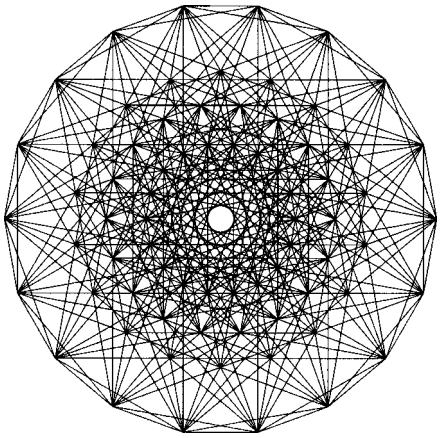

FIG. 3. The polyhedron 3{3}3{4}2.

are the centers of the edges of a Hessian polyhedron and the vertices of a complex polytope of type 3{3}3{4}2 (see Fig. 3).

In the case where $b=0$, we have to distinguish between the cases $c\neq 0$ and $c=0$. If $c\neq 0$, we find 648 triples, whatever the value of a. If $c=0$, we obtain 27 triples if $a\neq 0$, and only one if $a=0$.

Indeed, for $b=c=0$, the ψ-equation reduces to $\psi^8=0$, and all the cubics collapse to $12U^3-aU=0$. For $a\neq 0$ we obtain precisely 27 triples (u,v,w) which form the vertices of a Hessian polyhedron in $\mathbb{C}^3$ (see Ref. 1).

From the results of Ref. 3 about the arrangement of 12 planes formed by the mirrors of the pseudoreflections of $K=G_{25}$, we can determine the structure of the stabilizers of the normal forms. The only nontrivial cases are as follows:

(i) the orbits with 216 elements, for which the stabilizer is the cyclic group C_3;
(ii) the orbits with 72 elements, for which it is $C_3\times C_3$;
(iii) the Hessian orbits with 27 elements, for which it is the group G_4 of the Shephard–Todd classification.

These results can be regarded as a complete description of the moduli space of three-qutrit states. To see what this means, let us recall some definitions from geometric invariant theory.

It is well known that it in general, the orbits of a group action on an algebraic variety cannot be regarded as the points of an algebraic variety. To remedy this situation, one has to discard certain degenerate orbits. It is then possible to construct a *categorical quotient* and a *moduli space*, which describe the geometry of sufficiently generic orbits, respectively, in the affine and projective situation.

The *categorical quotient* $Y=\mathcal{H}//G$ is defined as the affine variety whose affine coordinate ring is the ring of polynomial invariants $R=\mathbb{C}[\mathcal{H}]^G$. The moduli space is the projective variety $\mathcal{M}=\mathrm{Proj}(R)$ of which R is the homogeneous coordinate ring. It is the quotient of the set $\mathbb{P}(\mathcal{H})^{\mathrm{ss}}$ of *semistable* points by the action of G (by definition, a point is semistable iff at least one of its algebraic invariants is nonzero, see Ref. 29).

Now, since in our case the algebra of invariants is a polynomial algebra, we see that the categorical quotient is just the affine space $\mathbb{C}^3$.

The moduli space is more interesting. The projective variety whose homogeneous coordinate ring is a polynomial algebra over generators of respective degrees $d_1,\ldots,d_m$ is called a *weighted projective space* $\mathbb{P}(d_1,\ldots,d_m)$. Hence, by definition, our moduli space $\mathcal{M}$ is the weighted projective space $\mathbb{P}(6,9,12)\simeq\mathbb{P}(2,3,4)$. It is known that this space is isomorphic to $\mathbb{P}(1,2,3)$,[35] which in turn can be embedded as a sextic surface in $\mathbb{P}^6$, the so-called *del Pezzo surface* F^6 (see Ref. 36). The del Pezzo surfaces are very interesting objects, known to be related to the exceptional root systems (see, e.g., Ref. 37).

The above results can then be interpreted as a description of the singularities of $\mathcal{M}$, since one can view it as the quotient of the projective plane $\mathbb{P}^2$ of the parameters $(u:v:w)$ under the projective action of G_{25}. We have described this quotient as a 648-fold ramified covering $\mathbb{P}^2 \to \mathcal{M}$, and analyzed its ramification locus.

VIII. CONCLUSION

A problem of current interest in Quantum Information Theory has been connected to various important mathematical works, scattered on a period of more than one century from Ref. 2 in 1889 to Ref. 27 in 2000, in general independent of each other and apparently discussing different subjects. Relying on all these works, we have described the geometry of the normal forms of semistable orbits of three-qutrit states under the action of $\mathrm{SL}(3,\mathbb{C})^{\times 3}$, the group of local filtering (SLOCC) operations. From a physical point of view, our results can be expected to provide a good starting point for studying the richness of the entanglement of three qutrits and its differences with that of the simpler qubit systems. From a mathematical point of view, we have worked out an interesting example of a problem in invariant theory, using both classical algebraic and modern geometric methods, found a surprising connection with the geometry of complex polytopes, and applied Klein's vision of Galois theory to the explicit solution of an algebraic equation of degree 648.

Also, this example provides a good illustration of the ideas presented in Refs. 14 and 17.

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Fundamental properties of Tsallis relative entropy

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Fundamental properties for the Tsallis relative entropy in both classical and quantum systems are studied. As one of our main results, we give the parametric extension of the trace inequality between the quantum relative entropy and the minus of the trace of the relative operator entropy given by Hiai and Petz. The monotonicity of the quantum Tsallis relative entropy for the trace preserving completely positive linear map is also shown without the assumption that the density operators are invertible. The generalized Tsallis relative entropy is defined and its subadditivity is shown by its joint convexity. Moreover, the generalized Peierls–Bogoliubov inequality is also proven. © *2004 American Institute of Physics.*
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I. INTRODUCTION

In the field of the statistical physics, Tsallis entropy was defined in Ref. 28 by $S_q(X)=-\Sigma_x p(x)^q \ln_q p(x)$ with one parameter q as an extension of Shannon entropy, where q-logarithm is defined by $\ln_q(x)\equiv(x^{1-q}-1)/(1-q)$ for any non-negative real number q and x, and $p(x)\equiv p(X=x)$ is the probability distribution of the given random variable X. We easily find that the Tsallis entropy $S_q(X)$ converges to the Shannon entropy $-\Sigma_x p(x)\log p(x)$ as $q\to 1$, since q-logarithm uniformly converges to natural logarithm as $q\to 1$. Tsallis entropy plays an essential role in nonextensive statistics, which is often called Tsallis statistics, so that many important results have been published from the various points of view.[29] As a matter of course, the Tsallis entropy and its related topics are mainly studied in the field of statisitical physics. However the concept of entropy is important not only in thermodynamical physics and statistical physics but also in information theory and analytical mathematics such as operator theory and probability theory. Recently, information theory has been in progress as quantum information theory[19] with the help of the operator theory[5,12] and the quantum entropy theory.[20] To study a certain entropic quantity is important for the development of information theory and the mathematical interest itself. In particular, the relative entropy is fundamental in the sense that it produces the entropy and the mutual information as special cases. Therefore in the present paper, we study properties of the Tsallis relative entropy in both the classical and quantum systems.

In the rest of this section, we will review several fundamental properties of the Tsallis relative entropy, as giving short proofs for the convenience of the readers. See Refs. 7, 27, and 26, for the pioneering works of the Tsallis relative entropy and their applications in the classical system.

Definition 1.1: We suppose a_j and b_j are probability distributions satisfying $a_j\geqslant 0$, $b_j\geqslant 0$, and

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$\Sigma_{j=1}^{n} a_j = \Sigma_{j=1}^{n} b_j = 1$. Then we define the Tsallis relative entropy between $A=\{a_j\}$ and $B=\{b_j\}$, for any $q \geqslant 0$ as

$$D_q(A|B) \equiv -\sum_{j=1}^{n} a_j \ln_q \frac{b_j}{a_j}, \tag{1}$$

where q-logarithm function is defined by $\ln_q(x) \equiv (x^{1-q}-1)/(1-q)$ for non-negative real number x and q, and we make a convention $0 \ln_q \infty \equiv 0$.

Note that $\lim_{q\to 1} D_q(A|B) = D_1(A|B) \equiv \Sigma_{j=1} a_j \log(a_j/b_j)$, which is known as relative entropy (which is often called Kullback–Leibler information, divergence or cross entropy). For the Tsallis relative entropy, the following proposition is known.

Proposition 1.2:

(1) (Non-negativity) $D_q(A|B) \geqslant 0$.
(2) (Symmetry) $D_q(a_{\pi(1)}, \ldots, a_{\pi(n)} | b_{\pi(1)}, \ldots, b_{\pi(n)}) = D_q(a_1, \ldots, a_n | b_1, \ldots, b_n)$.
(3) (Possibility of extention) $D_q(a_1, \ldots, a_n, 0 | b_1, \ldots, b_n, 0) = D_q(a_1, \ldots, a_n | b_1, \ldots, b_n)$.
(4) (Pseudoadditivity)

$$D_q(A^{(1)} \times A^{(2)} | B^{(1)} \times B^{(2)}) = D_q(A^{(1)}|B^{(1)}) + D_q(A^{(2)}|B^{(2)}) + (q-1) D_q(A^{(1)}|B^{(1)}) D_q(A^{(2)}|B^{(2)}),$$

where

$$A^{(1)} \times A^{(2)} = \{a_j^{(1)} a_j^{(2)} | a_j^{(1)} \in A^{(1)}, a_j^{(2)} \in A^{(2)}\},$$

$$B^{(1)} \times B^{(2)} = \{b_j^{(1)} b_j^{(2)} | b_j^{(1)} \in B^{(1)}, b_j^{(2)} \in B^{(2)}\}.$$

(5) (Joint convexity) For $0 \leqslant \lambda \leqslant 1$, any $q \geqslant 0$ and the probability distributions $A^{(i)} = \{a_j^{(i)}\}$, $B^{(i)} = \{b_j^{(i)}\}$ $(i=1,2)$, we have

$$D_q(\lambda A^{(1)} + (1-\lambda) A^{(2)} | \lambda B^{(1)} + (1-\lambda) B^{(2)}) \leqslant \lambda D_q(A^{(1)}|B^{(1)}) + (1-\lambda) D_q(A^{(2)}|B^{(2)}).$$

(6) (Strong additivity)

$$\begin{aligned} &D_q(a_1, \ldots, a_{i-1}, a_{i_1}, a_{i_2}, a_{i+1}, \ldots, a_n | b_1, \ldots, b_{i-1}, b_{i_1}, b_{i_2}, b_{i+1}, \ldots, b_n) \\ &= D_q(a_1, \ldots, a_n | b_1, \ldots, b_n) + b_i^{1-q} a_i^q D_q\left(\frac{a_{i_1}}{a_i}, \frac{a_{i_2}}{a_i} \middle| \frac{b_{i_1}}{b_i}, \frac{b_{i_2}}{b_i} \right), \end{aligned}$$

where $a_i = a_{i_1} + a_{i_2}$, $b_i = b_{i_1} + b_{i_2}$.

Proof: (1) follows from the convexity of the function $-\ln_q(x)$:

$$D_q(A|B) \equiv -\sum_{j=1}^{n} a_j \ln_q \frac{b_j}{a_j} \geqslant -\ln_q\left(\sum_{j=1}^{n} a_j \frac{b_j}{a_j} \right) = 0.$$

(2) and (3) are trivial. (4) follows by the direct calculation. (5) follows from the generalized log-sum inequality:[7]

$$\sum_{i=1}^{n} \alpha_i \ln_q\left(\frac{\beta_i}{\alpha_i} \right) \leqslant \left(\sum_{i=1}^{n} \alpha_i \right) \ln_q\left(\frac{\sum_{i=1}^{n} \beta_i}{\sum_{i=1}^{n} \alpha_i} \right), \tag{2}$$

for non-negative numbers α_i, β_i $(i=1,2,\ldots,n)$ and any $q \geqslant 0$. We define the function L_q for $q \geqslant 0$ to prove (6) as

$$L_q(x,y) \equiv -x \ln_q \frac{y}{x}$$

and

$$a_{i_1} = a_i(1-s), \quad b_{i_1} = b_i(1-t),$$

$$a_{i_2} = a_i s, \quad b_{i_2} = b_i t.$$

Then we have

$$L_q(x_1x_2,y_1y_2) = x_2L_q(x_1,y_1) + x_1L_q(x_2,y_2) + (q-1)L_q(x_1,y_1)L_q(x_2,y_2),$$

which implies the claim with easy calculations. ■

Remark 1.3: 1. (1) of Proposition 1.2 implies

$$S_q(A) \leqslant \ln_q n,$$

since we have

$$D_q(A|U) = -n^{q-1}(S_q(A) - \ln_q n),$$

for any $q \geqslant 0$ and two probability distributions $A=\{a_j\}$ and $U=\{u_j\}$, where $u_j = 1/n$, $(^\forall j)$, where the Tsallis entropy is represented by

$$S_q(A) \equiv -\sum_{j=1}^{n} a_j^q \ln_q a_j.$$

2. (4) of Proposition 1.2 is reduced to the pseudoadditivity for the Tsallis entropy:

$$S_q(A^{(1)} \times A^{(2)}) = S_q(A^{(1)}) + S_q(A^{(2)}) + (1-q)S_q(A^{(1)})S_q(A^{(2)}). \tag{3}$$

3. (5) of Proposition 1.2 recover the concavity for the Tsallis entropy, by setting $B^{(1)} = \{1,0,\ldots,0\}$, $B^{(2)} = \{1,0,\ldots,0\}$.

4. (6) of Proposition 1.2 is reduced to the strong additivity for the Tsallis entropy:

$$S_q(a_1,\ldots,a_{i-1},a_{i_1},a_{i_2},a_{i+1},\ldots,a_n) = S_q(a_1,\ldots,a_{i-1},a_i,a_{i+1},\ldots,a_n) + a_i^q S_q\left(\frac{a_{i1}}{a_i},\frac{a_{i2}}{a_i}\right).$$

We finally show the monotonicity for the Tsallis relative entropy. To this end, we introduce some notations. We consider the transition probability matrix W: $\mathcal{A} \to \mathcal{B}$, which can be identified to the matrix having the conditional probability W_{ji} as elements, where $\mathcal{A}$ and $\mathcal{B}$ are alphabet sets (finite sets) and $\Sigma_{j=1}^m W_{ji} = 1$ for all $i=1,\ldots,n$. By $A=\{a_i^{(\mathrm{in})}\}$ and $B=\{b_i^{(\mathrm{in})}\}$, two distinct probability distributions in the input system $\mathcal{A}$ are denoted. Then the probability distributions in the output system $\mathcal{B}$ are represented by $WA=\{a_j^{(\mathrm{out})}\}$, $WB=\{b_j^{(\mathrm{out})}\}$, where $a_j^{(\mathrm{out})} = \Sigma_{i=1}^n a_i^{(\mathrm{in})} W_{ji}$, $b_j^{(\mathrm{out})} = \Sigma_{i=1}^n b_i^{(\mathrm{in})} W_{ji}$, in terms of $W=\{W_{ji}\}$ $(i=1,\ldots,n; j=1,\ldots,m)$. Then we have the following.

Proposition 1.4: In the above notation, for any $q \geqslant 0$, we have

$$D_q(WA|WB) \leqslant D_q(A|B).$$

Proof: Applying the generalized log-sum inequality Eq. (2), we have

$$D_q(WA|WB) = -\sum_{j=1}^{m} a_j^{(\mathrm{out})} \ln_q \frac{b_j^{(\mathrm{out})}}{a_j^{(\mathrm{out})}} = -\sum_{j=1}^{m}\sum_{i=1}^{n} a_i^{(\mathrm{in})} W_{ji} \ln_q \frac{\sum_{i=1}^{n} b_i^{(\mathrm{in})} W_{ji}}{\sum_{i=1}^{n} a_i^{(\mathrm{in})} W_{ji}} \leqslant$$

$$-\sum_{j=1}^{m}\sum_{i=1}^{n} a_i^{(\mathrm{in})} W_{ji} \ln_q \frac{b_i^{(\mathrm{in})} W_{ji}}{a_i^{(\mathrm{in})} W_{ji}} = -\sum_{i=1}^{n} a_i^{(\mathrm{in})} \ln_q \frac{b_i^{(\mathrm{in})}}{a_i^{(\mathrm{in})}} = D_q(A|B).$$

■

We note that the above proposition is a special case of the monotonicity of f divergence[9] for the convex function f. Closing the introduction, we should also note here that the Tsallis entropy can be derived by a simple transformation from Rényi entropy which was used before the Tsallis one in the mathematical literature. See Ref. 4 on the details of Rényi entropy, in particular see pp. 184–191 of Ref. 4 for the relation to the structural a-entropy[14] [or called the entropy of type β (Ref. 10)], which is one of the nonextensive entropies including the Tsallis entropy.

II. QUANTUM TSALLIS RELATIVE ENTROPY AND ITS PROPERTIES

In Refs. 1 and 2, the quantum Tsallis relative entropy was defined by

$$D_q(\rho|\sigma) \equiv \frac{1 - \mathrm{Tr}[\rho^q \sigma^{1-q}]}{1-q} \tag{4}$$

for two density operators ρ and σ and $0 \leqslant q < 1$, as one parameter extension of the definition of the quantum relative entropy by Umegaki[30]

$$U(\rho|\sigma) \equiv \mathrm{Tr}[\rho(\log \rho - \log \sigma)]. \tag{5}$$

See Chap. II written by Rajagopal in Ref. 29, for the quantum version of Tsallis entropies and their applications.

For the quantum Tsallis relative entropy $D_q(\rho|\sigma)$ and the quantum relative entropy $U(\rho|\sigma)$, the following relations are known.

Proposition 2.1 [Ruskai–Stillinger[24] (see also Ref. 21)]: For the strictly positive operators with a unit trace ρ and σ, we have

(1) $D_q(\rho|\sigma) \leqslant U(\rho|\sigma) \leqslant D_{2-q}(\rho|\sigma)$ for $0 \leqslant q < 1$.
(2) $D_{2-q}(\rho|\sigma) \leqslant U(\rho|\sigma) \leqslant D_q(\rho|\sigma)$ for $1 < q \leqslant 2$.

Note that both sides in both inequalities converge to $U(\rho|\sigma)$ as $q \to 1$. We must extend this definition of the Tsallis relative entropy Eq. (4) for $0 \leqslant q \leqslant 2$ and impose the invertibility on the density operators of $D_{2-q}(\rho|\sigma)$ for $0 \leqslant q < 1$ and of $D_q(\rho|\sigma)$ for $1 < q \leqslant 2$.

Proof: Since we have for any $x > 0$ and $t > 0$,

$$\frac{1 - x^{-t}}{t} \leqslant \log x \leqslant \frac{x^t - 1}{t},$$

the following inequalities hold for any $a, b, t > 0$:

$$a\left(\frac{1 - a^{-t} b^t}{t}\right) \leqslant a \log \frac{a}{b} \leqslant a\left(\frac{a^t b^{-t} - 1}{t}\right). \tag{6}$$

Let $\rho = \Sigma_i \lambda_i P_i$ and $\sigma = \Sigma_j \mu_j Q_j$ be the spectral decompositions. Since $\Sigma_i P_i = \Sigma_j Q_j = I$, then we have

$$\mathrm{Tr}\left[\frac{\rho^{1+t}\sigma^{-t}-\rho}{t}-\rho(\log\rho-\log\sigma)\right]=\sum_{i,j}\mathrm{Tr}\left[P_i\left\{\frac{\rho^{1+t}\sigma^{-t}-\rho}{t}-\rho(\log\rho-\log\sigma)\right\}Q_j\right]$$
$$=\sum_{i,j}\mathrm{Tr}\left[P_i\left(\frac{1}{t}\lambda_i^{1+t}\mu_j^{-t}-\frac{1}{t}\lambda_i-\lambda_i\log\lambda_i+\lambda_i\log\mu_j\right)Q_j\right]$$
$$=\sum_{i,j}\left(\frac{1}{t}\lambda_i^{1+t}\mu_j^{-t}-\frac{1}{t}\lambda_i-\lambda_i\log\lambda_i+\lambda_i\log\mu_j\right)\mathrm{Tr}[P_iQ_j]\geqslant 0.$$

The last inequality in the above is due to the inequality of the right-hand side of Eq. (6). Thus we have

$$\mathrm{Tr}[\rho(\log\rho-\log\sigma)]\leqslant\frac{1}{t}\mathrm{Tr}[\rho^{1+t}\sigma^{-t}-\rho].$$

The left-hand side inequality is proven by a similar way. Thus setting $1-q=t(>0)$ in the above, we have (1) in Proposition 2.1. Also we have (2) in Proposition 2.1, by setting $q-1=t(>0)$. ■

We next consider another relation on the quantum Tsallis relative entropy. In Ref. 11, the relative operator entropy was defined by

$$S(\rho|\sigma)\equiv\rho^{1/2}\log(\rho^{-1/2}\sigma\rho^{-1/2})\rho^{1/2},$$

for two strictly positive operators ρ and σ. If ρ and σ are commutative, then we have $U(\rho|\sigma)=-\mathrm{Tr}[S(\rho|\sigma)]$. For this relative operator entropy and the quantum relative entropy $U(\rho|\sigma)$, Hiai and Petz proved the following relation:

$$U(\rho|\sigma)\leqslant-\mathrm{Tr}[S(\rho|\sigma)],\tag{7}$$

in Ref. 15 (see also Ref. 16).

In our previous papers,[32] we introduced the Tsallis relative operator entropy $T_q(\rho|\sigma)$ as a parametric extension of the relative operator entropy $S(\rho|\sigma)$ such as

$$T_q(\rho|\sigma)\equiv\frac{\rho^{1/2}(\rho^{-1/2}\sigma\rho^{-1/2})^{1-q}\rho^{1/2}-\rho}{1-q},$$

for $0\leqslant q<1$ and strictly positive operators ρ and σ, in the sense that

$$\lim_{q\to1}T_q(\rho|\sigma)=S(\rho|\sigma).\tag{8}$$

Actually we should note that there is a slight difference between the two parameters q in the present paper and λ in the previous paper,[32] which is an extension of Ref. 13. If ρ and σ are commutative, then we have $D_q(\rho|\sigma)=-\mathrm{Tr}[T_q(\rho|\sigma)]$. Also we now have that

$$\lim_{q\to1}D_q(\rho|\sigma)=U(\rho|\sigma).\tag{9}$$

These relations, Eq. (7), Eq. (8), and Eq. (9) naturally lead us to show the following theorem as a parametric extension of Eq. (7).

Theorem 2.2: For $0\leqslant q<1$ and any strictly positive operators with unit trace ρ and σ, we have

$$D_q(\rho|\sigma)\leqslant-\mathrm{Tr}[T_q(\rho|\sigma)].\tag{10}$$

Proof: We denote the α-power mean $\sharp_\alpha$ by $A\sharp_\alpha B\equiv A^{1/2}(A^{-1/2}BA^{-1/2})^\alpha A^{1/2}$. From Theorem 3.4 of Ref. 16, we have

$$\mathrm{Tr}[e^A \sharp_\alpha e^B] \leqslant \mathrm{Tr}[e^{(1-\alpha)A+\alpha B}]$$

for any $\alpha \in [0,1]$. Setting $A=\log \rho$ and $B=\log \sigma$, we have

$$\mathrm{Tr}[\rho \sharp_\alpha \sigma] \leqslant \mathrm{Tr}[e^{\log \rho^{1-\alpha}+\log \sigma^\alpha}].$$

Since the Golden–Thompson inequality $\mathrm{Tr}[e^{A+B}] \leqslant \mathrm{Tr}[e^A e^B]$ holds for any Hermitian operators A and B, we have

$$\mathrm{Tr}[e^{\log \rho^{1-\alpha}+\log \sigma^\alpha}] \leqslant \mathrm{Tr}[e^{\log \rho^{1-\alpha}} e^{\log \sigma^\alpha}] = \mathrm{Tr}[\rho^{1-\alpha}\sigma^\alpha].$$

Therefore

$$\mathrm{Tr}[\rho^{1/2}(\rho^{-1/2}\sigma\rho^{-1/2})^\alpha \rho^{1/2}] \leqslant \mathrm{Tr}[\rho^{1-\alpha}\sigma^\alpha]$$

which implies the theorem by taking $\alpha=1-q$. ■

Corollary 2.3 (Hiai–Petz[15,16]): For any strictly positive operators with unit trace ρ and σ, we have

$$\mathrm{Tr}[\rho(\log \rho - \log \sigma)] \leqslant \mathrm{Tr}[\rho \log(\rho^{1/2}\sigma^{-1}\rho^{1/2})]. \tag{11}$$

Proof: It follows by taking the limit as $q \to 1$ in both sides of Eq. (10). ■

Thus the result proved by Hiai and Petz in Refs. 15 and 16 is recovered as a special case of Theorem 2.2.

For the quantum Tsallis relative entropy $D_q(\rho|\sigma)$, (i) pseudoadditivity and (ii) non-negativity are shown in Ref. 1, moreover (iii) joint convexity and (iv) monotonicity for projective mesurements, are shown in Ref. 2 Here we show the unitary invariance of $D_q(\rho|\sigma)$ and the monotonicity of that for the trace-preserving completely positive linear map.

Proposition 2.4: For $0 \leqslant q < 1$ and any density operators ρ and σ, the quantum relative entropy $D_q(\rho|\sigma)$ has the following properties.

(1) (Non-negativity) $D_q(\rho|\sigma) \geqslant 0$.
(2) (Pseudoadditivity) $D_q(\rho_1 \otimes \rho_2|\sigma_1 \otimes \sigma_2) = D_q(\rho_1|\sigma_1) + D_q(\rho_2|\sigma_2) + (q-1)D_q(\rho_1|\sigma_1)D_q(\rho_2|\sigma_2)$.
(3) (Joint convexity) $D_q(\Sigma_j \lambda_j \rho_j | \Sigma_j \lambda_j \sigma_j) \leqslant \Sigma_j \lambda_j D_q(\rho_j|\sigma_j)$.
(4) The quantum Tsallis relative entropy is invariant under the unitary transformation U:

$$D_q(U\rho U^* | U\sigma U^*) = D_q(\rho|\sigma).$$

Proof: Since it holds that $f(q,x,y) \equiv (x - x^q y^{1-q})/(1-q) - (x-y) \geqslant 0$ for $x \geqslant 0$, $y \geqslant 0$, and $0 \leqslant q < 1$, we have $D_q(\rho|\sigma) \geqslant \mathrm{Tr}[\rho - \sigma]$, which implies (1), since ρ and σ are density operators. (See Proposition 3.16 of Ref. 21 on the so-called Klein inequality.)

(2) follows by the direct calculation.

(3) follows from the Lieb's theorem that for any operator Z and and $0 \leqslant t \leqslant 1$, the functional $f(A,B) \equiv \mathrm{Tr}[Z^* A^t Z B^{1-t}]$ is joint concave with respect to two positive operators A and B.

(4) is obvious by the use of Stone–Weierstrass approximation theorem. (It also can be shown by the application of Theorem 2.5.) ■

(1) of the above proposition follows from the generalized Peierls–Bogoliubov inequality which will be shown in the next section.

In Ref. 22, the monotonicity for more generalized relative entropy was shown under the assumption of the invertibility of the density operators. Here we show the monotonicity for the quantum Tsallis relative entropy in the case of $0 \leqslant q < 1$ without the assumption of the invertibility of the density operators.

Theorem 2.5: For any trace-preserving completely positive linear map Φ, any density operators ρ and σ and $0 \leqslant q < 1$, we have

$$D_q(\Phi(\rho)|\Phi(\sigma)) \leqslant D_q(\rho|\sigma).$$

Proof: We prove this theorem in a similar way as Ref. 18. To this end, we first prove the monotonicity of $D_q(\rho|\sigma)$ for the partial trace Tr_B in the composite sysytem AB. Let ρ^{AB} and σ^{AB} be density operators in the composite system AB. From Refs. 20 and 31, there exists unitary operators U_j and the probability p_j such that

$$\rho^A \otimes \frac{I}{n} = \sum_j p_j (I \otimes U_j)\rho^{AB}(I \otimes U_j)^* ,$$

where n and I present the dimension and identity operator of the system B, $\rho^A = \mathrm{Tr}_B[\rho^{AB}]$ and $\sigma^A = \mathrm{Tr}_B[\sigma^{AB}]$. By the help of the joint concavity and the unitary invariance of the Tsallis relative entropy, we thus have

$$\begin{aligned} D_q\left(\rho^A \otimes \frac{I}{n} \middle| \sigma^A \otimes \frac{I}{n}\right) &\leqslant \sum_j p_j D_q((I \otimes U_j)\rho^{AB}(I \otimes U_j)^* | (I \otimes U_j)\sigma^{AB}(I \otimes U_j)^*) \\ &= \sum_j p_j D_q(\rho^{AB}|\sigma^{AB}) = D_q(\rho^{AB}|\sigma^{AB}). \end{aligned}$$

Since

$$D_q\left(\rho^A \otimes \frac{I}{n} \middle| \sigma^A \otimes \frac{I}{n}\right) = D_q(\rho^A|\sigma^A),$$

we thus have

$$D_q(\mathrm{Tr}_B(\rho^{AB})|\mathrm{Tr}_B(\sigma^{AB})) \leqslant D_q(\rho^{AB}|\sigma^{AB}). \tag{12}$$

It is known[25] (see also Refs. 8, 18, and 19) that every trace-preserving completely positive linear map Φ has the following representation with some unitary operator U^{AB} on the total system AB and the projection (pure state) P^B on the subsystem B,

$$\Phi(\rho^A) = \mathrm{Tr}_B\, U^{AB}(\rho^A \otimes P^B)U^{AB*}.$$

Therefore we have the following result, by the result of Eq. (12) and the unitary invariance of $D_q(\rho|\sigma)$ again,

$$D_q(\Phi(\rho^A)|\Phi(\sigma^A)) \leqslant D_q(U^{AB}(\rho^A \otimes P^B)U^{AB*}|U^{AB}(\sigma^A \otimes P^B)U^{AB*}) = D_q(\rho^A \otimes P^B|\sigma^A \otimes P^B)$$

which implies our claim, since $D_q(\rho^A \otimes P^B|\sigma^A \otimes P^B) = D_q(\rho^A|\sigma^A)$. ■

Setting $\sigma = (1/n)I$ in Theorem 2.5, we have the following corollary.

Corollary 2.6: For any trace-preserving completely positive linear unital map Φ, any density operator ρ and $0 \leqslant q < 1$, we have

$$H_q(\Phi(\rho)) \geqslant H_q(\rho),$$

where $H_q(X) = (\mathrm{Tr}[X^q] - 1)/(1-q)$ represents the Tsallis entropy for density operator X, which is often called the quantum Tsallis entropy.

We note that Theorem 2.5 for the fixed σ, namely the monotonicity of the quantum Tsallis relative entropy in the case of $\Phi(\sigma) = \sigma$, was proved in Ref. 3 to establish Clausius' inequality.

Remark 2.7: It is known[19] (see also Ref. 23) that there is an equivalent relation between the monotonicity for the quantum relative entropy and the strong subadditivity for the quantum entropy. However in our case, we have not yet found such a relation. Because the pseudoadditivity of the q-logarithm function,

$$\ln_q xy = \ln_q x + \ln_q y + (1-q)\ln_q x \ln_q y,$$

disturbs us to derive the beautiful relation such as

$$D_q(p(x,y)|p(x)p(y)) = S_q(p(x)) + S_q(p(y)) - S_q(p(x,y))$$

for the Tsallis relative entropy $D_q(p(x,y)|p(x)p(y))$, the Tsallis entropy $S_q(p(x))$, $S_q(p(y))$, and the Tsallis joint entropy $S_q(p(x,y))$, even if our stage is in the classical system.

III. GENERALIZED TSALLIS RELATIVE ENTROPY

For any two positive operators A, B and any real number $q \in [0,1)$, we can define the generalized Tsallis relative entropy.

Definition 3.1:

$$D_q(A\|B) \equiv \frac{\mathrm{Tr}[A] - \mathrm{Tr}[A^q B^{1-q}]}{1-q}.$$

To avoid the confusions of readers, we use the different symbol $D_q(\cdot\|\cdot)$ for the generalized Tsallis relative entropy.

Since Lieb's concavity theorem is available for any positive operators A and B, the generalized Tsallis relative entropy has a joint convexity,

$$D_q\left(\sum_j \lambda_j A_j \middle\| \sum_j \lambda_j B\right) \leqslant \sum_j \lambda_j D_q(A_j\|B_j), \tag{13}$$

for the positive number λ_j satisfying $\Sigma_j \lambda_j = 1$ and any positive operators A_j and B_j. Then we have the subadditivity of the generalized Tsallis relative entropy between A_1+A_2 and B_1+B_2.

Theorem 3.2: For any positive operators A_1, A_2, B_1, and B_2, and $0 \leqslant q < 1$, we have the subadditivity

$$D_q(A_1 + A_2\|B_1 + B_2) \leqslant D_q(A_1\|B_1) + D_q(A_2\|B_2). \tag{14}$$

Proof: First we note that we have the following relation for any numbers α and β, and two positive operators A and B,

$$D_q(\alpha A\|\beta B) = \alpha D_q(A\|B) - \alpha \ln_q \frac{\beta}{\alpha} \mathrm{Tr}[A^q B^{1-q}]. \tag{15}$$

Now from Eq. (13), we have

$$D_q(\lambda_1 X_1 + \lambda_2 X_2\|\lambda_1 Y_1 + \lambda_2 Y_2) \leqslant \lambda_1 D_q(X_1\|Y_1) + \lambda_2 D_q(X_2\|Y_2)$$

for any positive operators X_1, X_2, Y_1, and Y_2, and λ_1, λ_2 ($\lambda_1+\lambda_2=1$). Setting $A_i = \lambda_i X_i$ and $B_i = \lambda_i Y_i$ for $i=1,2$ in the above inequality, we have

$$D_q(A_1 + A_2\|B_1 + B_2) \leqslant \lambda_1 D_q\left(\frac{A_1}{\lambda_1}\middle\|\frac{B_1}{\lambda_1}\right) + \lambda_2 D_q\left(\frac{A_2}{\lambda_2}\middle\|\frac{B_2}{\lambda_2}\right).$$

Thus we have our claim due to Eq. (15). ■

As a famous inequality in statistical physics, the Peierls–Bogoliubov inequality[17,6] is known. Finally, we prove the generalized Peierls–Bogoliubov inequality for the generalized Tsallis relative entropy in the following.

Theorem 3.3: For any positive operators A and B, $0 \leqslant q < 1$,

$$D_q(A\|B) \geqslant \frac{\mathrm{Tr}[A] - (\mathrm{Tr}[A])^q (\mathrm{Tr}[B])^{1-q}}{1-q}.$$

Proof: In general, we have the following Hölder's inequality:

$$|\mathrm{Tr}[XY]| \leqslant \mathrm{Tr}[|X|^s]^{1/s}\,\mathrm{Tr}[|Y|^t]^{1/t}, \tag{16}$$

for any bounded linear operators X and Y satisfying $\mathrm{Tr}[|X|^s]<\infty$ and $\mathrm{Tr}[|Y|^t]<\infty$ and for any $1<s<\infty$ and $1<t<\infty$ satisfying $(1/s)+(1/t)=1$. By setting $X=A^q$, $Y=B^{1-q}$, and $s=1/q$, $t=1/(1-q)$ in Eq. (16), we have

$$\mathrm{Tr}[A^qB^{1-q}] \leqslant (\mathrm{Tr}[A])^q(\mathrm{Tr}[B])^{1-q},$$

which implies our claim. ■

Note that Theorem 3.3 can be considered a noncommutative version of Eq. (2). If A and B are density operators, then the non-negativity of the quantum Tsallis relative entropy follows from Theorem 3.3.

IV. CONCLUSION

As we have seen, the monotonicity of the quantum Tsallis relative entropy for the trace-preserving completely positive map was shown. Also the trace inequality between the Tsallis quantum relative entropy and the Tsallis relative operator entropy was shown. It is remarkable that our inequality recovers the famous inequality shown by Hiai–Petz as $q\to 1$.

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Crystal bases and generalized Lascoux–Leclerc–Thibon (LLT) algorithm for the quantum affine algebra $U_q(C_n^{(1)})$

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In this paper, we give a realization of crystal bases of the fundamental representations over $U_q(C_n^{(1)})$ in terms of Young diagrams k introduced by Premat. Further, we give a generalized Lascoux–Leclerc–Thibon algorithm for computing the global bases. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1811791]

I. INTRODUCTION

In Refs. 11, 12, and 17, the *crystal basis* theory or *canonical basis* theory for the integrable modules over quantum groups $U_q(\mathfrak{g})$ was developed by Kashiwara and Lusztig, independently. Roughly speaking, crystal bases are the bases of representations of $U_q(\mathfrak{g})$ as the parameter q tends to zero, and they give a structure of colored oriented graphs, called the *crystal graphs*, which reflect the combinatorial structure of integrable modules. Hence one of the important problems in the crystal basis theory is to give explicit realization of crystals.

The Fock space representations of affine Lie algebras play an important role in the soliton theory. In Ref. 5, Hayashi gave the Fock space representation of $U_q(A_n^{(1)})$ and realized the fundamental representations. From Hayashi's results, Misra and Miwa gave an explicit characterization of the crystal basis for the basic representations of $U_q(A_n^{(1)})$ using colored Young diagrams.[18] In Ref. 4, this construction was generalized to all irreducible hight weight representations $V(\lambda)$ with a dominant integral weight λ of $U_q(A_n^{(1)})$. In Ref. 10, Kang, Misra, and Miwa gave the Fock space representation of $U_q(C_n^{(1)})$, $U_q(A_{2n}^{(2)})$, and $U_q(D_{n+1}^{(2)})$. Moreover, they realized all level one representations $V(\Lambda_k)$ for $U_q(C_n^{(1)})$, and they realized the level two representations $V(2\Lambda_0)$, $V(\Lambda_1), \ldots, V(\Lambda_n)$ [resp., $V(\Lambda_n)$] for $U_q(A_{2n}^{(2)})$ [resp., $U_q(D_{n+1}^{(2)})$].

In Ref. 6, Kang constructed the crystal graphs $B(\lambda)$ of the basic representations using *reduced proper Young walls* for the classical quantum affine algebras except $U_q(C_n^{(1)})$. The $C_n^{(1)}$ case was more difficult to deal with because the level 1 perfect crystal for this type is intrinsically of level 2. In Ref. 3, using the notion of *splitting block*, Hong, Kang and Lee overcame this difficulty. But, this realization is so complex and so difficult to deal with. In Ref. 19, Premat constructed the Fock space representation $\mathcal{F}(\Lambda_k)$ over $U_q(C_n^{(1)})$ using, two-dimensional object, colored Young diagrams and she showed that the connected component $\mathcal{Y}(\Lambda_k)$ in $\mathcal{F}(\Lambda_k)$ containing the maximal vector ϕ_k of weight Λ_k is isomorphic to $B(\Lambda_k)$. One of the main results in this paper is to give a characterization of $\mathcal{Y}(\Lambda_k)$.

On the other hand, from crystal graphs, Kashiwara recovered the true bases of $U_q(\mathfrak{g})$-modules which are called *global bases* in a canonical way.[12] But, in general, it is difficult to find global bases. In Ref. 13, Lascoux, Leclerc, and Thibon gave an algorithm, called LLT algorithm, for computing the global bases of the basic representations over $U_q(A_n^{(1)})$. Moreover, they gave a conjecture that there is a connection between the representation theory of the quantum affine

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algebras and the Hecke algebras. This conjecture was proved by Ariki.[1] There are several variants of LLT algorithm using Young diagrams for the classical Lie algebras and Young walls for affine types $A^{(2)}_{2n-1}$, $B^{(1)}_n$, $D^{(1)}_n$, $D^{(2)}_{n+1}$, and $C^{(1)}_2$.[7–9,14–16] In this paper, we give a generalized LLT algorithm using colored Young diagrams introduced by Kang, Misra, Miwa,[10] and Premat.[19]

II. THE FOCK SPACE REPRESENTATION FOR $U_q(C^{(1)}_n)$

The basic concepts on quantum groups and crystal bases may be found in many articles and books (for example Refs. 2, 11, and 12). We refer the readers to these references. In this section, we mostly explain the Fock space representation for $U_q(C^{(1)}_n)$ constructed by Premat.[19]

Let $U_q(\mathfrak{g})=U_q(C^{(1)}_n)$ be the quantum affine algebra of type $C^{(1)}_n$ and $I=\{0,1,\ldots,n\}$ be the index set for simple roots of $U_q(\mathfrak{g})$. Let $P^\vee=(\oplus_{i\in I}\mathbb{Z}h_i)\oplus\mathbb{Z}d$ and $P=(\oplus_{i\in I}\mathbb{Z}\Lambda_i)\oplus\mathbb{Z}\delta$ be the dual weight lattice and the weight lattice, respectively. Moreover, α_i $(i\in I)$, δ, Λ_i $(i\in I)$ are the simple roots, null root, fundamental weights, respectively, and e_i, f_i, K_i, q^d are the generators of $U_q(C^{(1)}_n)$. Further, $P^+=(\oplus_{i\in I}\mathbb{Z}_{\geqslant 0}\Lambda_i)\oplus\mathbb{Z}\delta$ is the set of dominant weights, and $\tilde{e}_i$, $\tilde{f}_i$ are the Kashiwara operators.

A *Young diagram* Y $k\in I$ is a sequence $\{y_l\}_{l\in\mathbb{N}}$ of integers such that

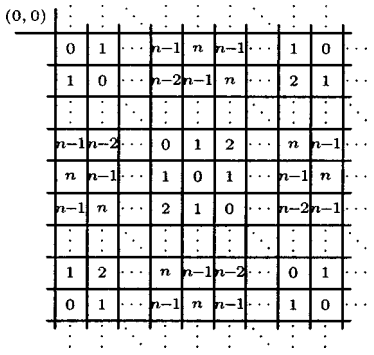
$$\text{(i) } y_l\leqslant y_{l+1} \text{ for all } l\in\mathbb{N},\quad \text{(ii) } y_l=k \text{ for all } l\gg 0,$$

where $\mathbb{N}$ is the set of positive integers. The empty Young diagram $\{k,k,\ldots\}$ k will be denoted by ϕ_k and we denote by $\mathcal{Z}(\Lambda_k)$ the set of all Young diagrams k. Define the *Fock space* of weight Λ_k by

$$\mathcal{F}(\Lambda_k)=\bigoplus_{Y\in\mathcal{Z}(\Lambda_k)}\mathbb{Q}(q)Y,$$

where $\mathbb{Q}$ is the set of rational numbers.

The Young diagram $Y=\{y_l\}_{l\in\mathbb{N}}$ k is represented by the region $\{(x,y)\,|\,x\in\mathbb{N},y\geqslant y_x\}$ in the following colored xy-plane

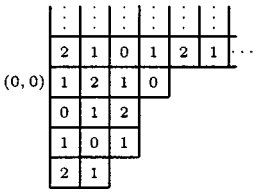
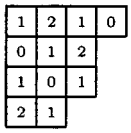


All Young diagrams of charge k contain the region $\{(x,y)\,|\,x\in\mathbb{N},y\geqslant k\}$ corresponding to ϕ_k. Hence for simplicity, when we represent a Young diagram, we remove this region ϕ_k, and so the empty Young diagram ϕ_k is meaningful. We also define the map wt: $\mathcal{F}(\Lambda_k)\to P$ by

$$\mathrm{wt}(Y)=\Lambda_k-\sum_{i\in I}k_i\alpha_i,$$

where k_i is the number of i-colored boxes in Y that have been added to the ϕ_k.

Example 1.1: For $n=2$, a Young diagram $Y=\{-3,-3,-2,0,1,1,\ldots\}$ 1 is represented as follows:

$Y =$  $=$  .

Further, we have

$$\mathrm{wt}(Y) = \Lambda_1 - (3\alpha_0 + 6\alpha_1 + 3\alpha_2).$$

Let $Y=\{y_l\}_{l\in\mathbb{N}} \in \mathcal{Z}(\Lambda_k)$. If $y_l \neq y_{l+1}$ for some $l \in \mathbb{N}$, the site (l, y_{l+1}) [resp., $(l+1, y_{l+1}-1)$] is called a *concave* (resp., *addable*) *corner* of Y, and the site (l, y_l) is called a *convex* or *removable corner* of Y. Moreover, the site $(0, y_1)$ [resp., $(1, y_1-1)$] is also called a *concave* (resp., *addable*) *corner*. Moreover, the site (l, y) with coloring i is called an *i-colored corner*. Note that the definition of addable (resp., convex) corner of Young diagram Y k is similar to that of admissible slot (resp., removable block) in Young walls.[6]

Example 1.2: The Young diagram Y in Example 1.1 has a 0-colored addable corner $(3,-3)$, and 1-colored addable corners $(1,-4)$, $(4,-1)$, and (5, 0). Moreover, it has a 0-colored convex (removable) corner (4, 0), 1-colored convex (removable) corners $(2,-3)$ and $(3,-2)$.

Now, following Refs. 10 and 19, we define an action of $U_q(\mathfrak{g})$ on $\mathcal{F}(\Lambda_k)$. For $(x,y) \in \mathbb{N}\times\mathbb{Z}$, we define $E_{(x,y)}$, $F_{(x,y)}$, $T^{\pm}_{(x,y)}: \mathcal{F}(\Lambda_k) \to \mathcal{F}(\Lambda_k)$ as follows:

$$E_{(x,y)}(Y) = \begin{cases} Y \nearrow (x,y) & \text{if } (x,y) \text{ is a convex corner,} \\ 0 & \text{otherwise,} \end{cases}$$

$$F_{(x,y)}(Y) = \begin{cases} Y \swarrow (x,y) & \text{if } (x,y) \text{ is an addable corner,} \\ 0 & \text{otherwise,} \end{cases}$$

$$T^{\pm}_{(x,y)}(Y) = \begin{cases} q_i^{\pm} Y & \text{if } (x,y) \text{ is a } i\text{-colored concave corner,} \\ q_i^{\mp} Y & \text{if } (x,y) \text{ is a } i\text{-colored convex corner,} \\ Y & \text{otherwise.} \end{cases}$$

Here, $Y \nearrow (x,y)$ (resp., $Y \swarrow (x,y)$) is the Young diagram k obtained by removing (resp., adding) the site (x,y) from Y (resp., to Y).

Define the order $>$ on $\mathbb{N}\times\mathbb{Z}$ as follows: $(x,y) > (x',y')$ if and only if $x+y > x'+y'$. We define linear operators E_i, F_i, $T_i^{\pm}$ $(i \in I)$ and $T_d: \mathcal{F}(\Lambda_k) \to \mathcal{F}(\Lambda_k)$ as follows:

$$E_i = \sum_{(x,y)\in\mathbb{N}\times\mathbb{Z}} \left(\prod_{(x',y')<(x,y)} T^{-}_{(x',y')} \right) E_{(x,y)},$$

$$F_i = \sum_{(x,y)\in\mathbb{N}\times\mathbb{Z}} \left(\prod_{(x',y')>(x,y)} T^{+}_{(x',y')} \right) F_{(x,y)},$$

$$T_i^{\pm} = \prod_{(x,y)\in\mathbb{N}\times\mathbb{Z}} T^{\pm}_{(x,y)},$$

and for $Y \in \mathcal{Z}(\Lambda_k)$, $T_d(Y) = q^{-(\text{the number of 0-colored corners in } Y)}$. Here, the sites (x,y) and (x',y') are i-colored corners.

Then we have

Theorem 1.3 (Refs. 10 and 19): (a) *The Fock space* $\mathcal{F}(\Lambda_k)$ $(k \in I)$ *is a* $U_q(\mathfrak{g})$*-module under the action of* e_i, f_i, q^{h_i} *and* q^d *is given by that of* E_i, F_i, T_i *and* T_d, *respectively*.

(b) *The* $U_q(\mathfrak{g})$*-module* $\mathcal{F}(\Lambda_k)$ *lies in the category* $\mathcal{O}_{\text{int}}$, *where* $\mathcal{O}_{\text{int}}$ *is the category of integrable modules in* Refs. 2, 11, and 12.

Corollary 1.4 (Refs. 10 and 19): There is a $U_q(\mathfrak{g})$*-module isomorphism from* $U_q(\mathfrak{g})\phi_k$ *to the irreducible highest weight module* $V(\Lambda_k)$ *with the highest weight* Λ_k.

Let $\mathbf{A}_0=\{f/g \in \mathbb{Q}(q) \mid f,g \in \mathbb{Q}[q], g(0) \neq 0\}$ be the localization of $\mathbb{Q}[q]$ at $q=0$.

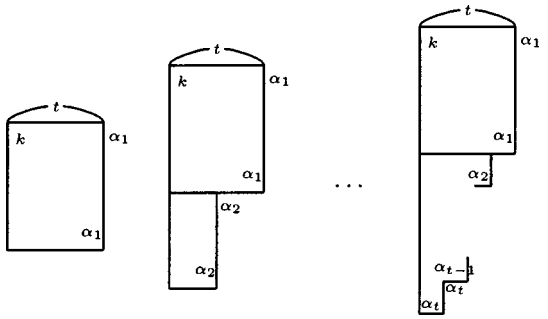
Theorem 1.5 (Refs. 10 and 19): *Let* $L(\mathcal{F}(\Lambda_k))=\Sigma_{Y \in \mathcal{F}(\Lambda_k)}\mathbf{A}_0 Y$ *and* $B(\mathcal{F}(\Lambda_k))=\{Y+qL(\mathcal{F}(\Lambda_k)) \mid Y \in \mathcal{Z}(\Lambda_k)\}$. *Then* $(L(\mathcal{F}(\Lambda_k)), B(\mathcal{F}(\Lambda_k)))$ *is a crystal base for the integrable* $U_q(\mathfrak{g})$*-module* $\mathcal{F}(\Lambda_k)$.

Now, we give a crystal structure on $\mathcal{Z}(\Lambda_k)$. Let $Y \in \mathcal{Z}(\Lambda_k)$ and $(x_1,y_1)>(x_2,y_2)>\cdots>(x_i,y_i)$ be the i-colored convex or addable corners of Y. At first, to each i-colored convex or addable corner (x_j,y_j) $(j=1,\ldots,l)$, we assign its i-signature $sgn(x_j,y_j)$ as $-$ (resp., $+$) if it is a convex (resp., addable) corner. From the sequence $(sgn(x_1,y_1),\ldots,sgn(x_l,y_l))$ of $+$'s and $-$'s, cancel out every $(+,-)$-pair to obtain a sequence of $-$'s followed by $+$'s, reading from left to right. This sequence is called the *i-signature* of Y.

We define $\tilde{f}_i Y$ to be the Young diagram k obtained from Y by adding the i-colored box to the i-colored addible corner corresponding to the left-most $+$ in the i-signature of Y. We define $\tilde{f}_i Y=0$ if there is no $+$ in the i-signature of Y. We define $\tilde{e}_i Y$ to be the Young diagram k obtained from Y by removing the i-colored convex corner corresponding to the right-most $-$ in the i-signature of Y. We define $\tilde{e}_i Y=0$ if there is no $-$ in the i-signature of Y.

Theorem 1.6 (Ref. 19): *The operators* $\tilde{e}_i$ *and* $\tilde{f}_i$ *defined above coincide with the Kashiwara operators*.

Using Theorem 1.3 and Theorem 1.6, it is easy to find all maximal vectors in $\mathcal{Z}(\Lambda_k)$. That is, if the rightmost convex corner C_v of a maximal vector Y is a α-colored corner, by the definition of Kashiwara operators, there should exist a α-colored addable corner in the right hand side of C_v which must be the rightmost addable corner. Applying this argument to other convex corners, we can obtain a maximal vector. The following are maximal vectors consisting of t columns $(t \geqslant 1)$:



(1.1)

In particular, consider the case $\mathfrak{g}=C_2^{(1)}$. Let $a(m)$ be the number of partitions of m on the set $\frac{1}{2}\mathbb{Z}_{>0}=\{\frac{1}{2},1,\frac{3}{2},\ldots,\}$, and $b(m)$ be the number of partitions of $m+\frac{1}{2}$ on the set $\frac{1}{2}\mathbb{Z}_{>0}$. Let $c(m)$ be the number of partitions of m on the set $\{1,3,5,\ldots\}\cup\{1',2',3',\ldots\}$ such that $2k-1=(2k-1)'$ $(k \geqslant 1)$. For instance, since

$$3'=3=2'+1'=2'+1=1'+1'+1'=1'+1'+1=1'+1+1=1+1+1,$$

we have $c(3)=8$.

Proposition 1.7: Let $\mathfrak{g}=C_2^{(1)}$ *and let* Λ_k $(k=0,1,2)$ *be a dominant integral weight. Then we have*

$$\mathcal{F}(\Lambda_k)=\begin{cases}(\oplus_{m\geqslant 0}V(\Lambda_k-m\delta)^{\oplus a(m)})\oplus(\oplus_{m\geqslant 0}V(\Lambda_k-m\delta-\alpha_k-\alpha_1)^{\oplus b(m)}) & \text{if } k=0,2,\\ \oplus_{m\geqslant 0}V(\Lambda_k-m\delta)^{\oplus c(m)} & \text{if } k=1.\end{cases}$$

Proof: Since the proof is similar, we only check the $\mathcal{F}(\Lambda_1)$-case. By (1.1), the maximal vectors M_t $(t\geqslant 1)$ with the least number of boxes among the maximal vectors consisting of t columns are as follows:

$$M_1=\begin{array}{|c|}\hline 1\\\hline 2\\\hline 1\\\hline 0\\\hline\end{array},\qquad M_2=\begin{array}{|c|c|}\hline 1&0\\\hline 2&1\\\hline\end{array},\qquad M_3=\begin{array}{|c|c|c|}\hline 1&0&1\\\hline 2&1&0\\\hline 1&2&1\\\hline 0&1&2\\\hline\end{array},\qquad M_4=\begin{array}{|c|c|c|c|}\hline 1&0&1&2\\\hline 2&1&0&1\\\hline\end{array},\qquad \cdots$$

Let Y be a maximal vector which is not the empty diagram ϕ_1. Then Y is obtained by attaching some maximal vectors $M_{t_1},\ldots,M_{t_2}$. For instance, the maximal vector

$$M=\begin{array}{|c|c|c|c|}\hline 1&0&1&2\\\hline 2&1&0&1\\\hline\end{array}\\\begin{array}{|c|c|}\hline 1&2\\\hline 0&1\\\hline\end{array}\\\begin{array}{|c|}\hline 1\\\hline 2\\\hline 1\\\hline 0\\\hline\end{array}$$

is obtained by attaching M_1, M_2, and M_4. We associate p_j's for M_{t_j} as follows:

$$p_j=\begin{cases}t_j & \text{if } t_j \text{ is odd},\\ \left(\dfrac{t_j}{2}\right)' & \text{if } t_j \text{ is even}.\end{cases}$$

Then $(p_j)_{j=1}^s$ forms a partition on $\{1,3,5,\ldots\}\cup\{1',2',3',\ldots\}$ and $\mathrm{wt}(Y)=\Lambda_1-(\Sigma_{j=1}^s p_j)\delta$. Therefore, it is easy to see that the number of maximal vectors with weight $\Lambda_1-m\delta$ is $c(m)$. Conversely, for a given partition $(p_j)_{j=1}^s$ of m on $\{1,3,5,\ldots\}\cup\{1',2',3',\ldots\}$, we can find a unique Young diagram $Y\in\mathcal{Z}(\Lambda_1)$ 1 with $\mathrm{wt}(Y)=\Lambda_1-m\delta$, which is obtained by attaching maximal vectors M_{t_j}'s, where

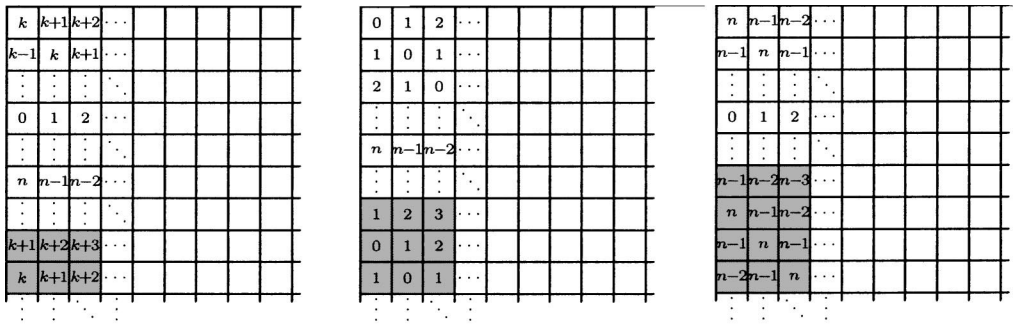
$$t_j=\begin{cases}p_j & \text{if } p_j\in\{1,3,5,\ldots\},\\ 2q_j & \text{if } p_j\in\{1',2',3'\ldots\} \text{ and } p_j=q_j'.\end{cases}$$

□

Until now, we described the Fock space representation $\mathcal{F}(\Lambda_k)$ and the crystal structure on $\mathcal{Z}(\Lambda_k)$ given by Premat. But, she did not give explicit description of the crystal basis $\mathcal{Y}(\Lambda_k)$ of the fundamental representation $U_q(\mathfrak{g})\phi_k=V(\Lambda_k)$. In next section, we deal with it.

III. CHARACTERIZATION OF THE CRYSTAL BASIS $\mathcal{Y}(\Lambda_k)$

Let Y be a Young diagram k. It is represented by some region in the following xy-planes with coloring.



$(k \neq 0, n)$ $(k = 0)$ $(k = n)$

In the above xy-planes, we denote by C_i^+ the ith column of xy-plane and we can find regions in C_{i-1}^+ with the same coloring as C_i^+. Among these, we denote by C_{i-1}^- the largest region. The shaded parts in above xy-planes represent C_1^-, C_2^-, and C_3^-.

Now, consider 0-colored or n-colored corners in the first row. We write these sites $(x_i, k-1)$ with $i \geqslant 1$ from left to right. Then $(x_i+1, k-1)$ and $(x_i, k-2)$ are the sites of the same coloring. For example, in Figs. 1 and 2, the third site and the seventh site in the first row are n-colored and 0-colored corners, respectively. That is, $x_1=3$ and $x_2=7$. Also, both the fourth site in the first row and the third site in the second row are 3-colored corners, and both the eighth site in the first row and the seventh site in the second row are 1-colored corners, and so on. Let U_i $(i \geqslant 1)$ be the area consisting of sites (x,y) such that $x+y \geqslant x_i+k$. Then it is easy to see that there is an area which is symmetric to U_i with respect to the line $l_i=\{(x,y)|x+y=x_i+k-1\}$. That is, $\{(x,y)|x \geqslant x_i, x+y<x_i+k-1\}$. We denote by L_i this region. For $k \neq 0$, n, we denote by U_0 (resp., L_0) the area consisting of corners (x,y) such that $x+y>k$ (resp., $x+y<-k$). For $k=0$, n, we also denote by U_0 (resp., L_0) the area consisting of corners (x,y) such that $x+y>k$ (resp., $x+y<k$). Notice that if we set

$$l_0 = \begin{cases} \{(x,y)|x+y=0\} & \text{if } k \neq n, \\ \{(x,y)|x+y=n\} & \text{if } k=n, \end{cases}$$

then U_0 and L_0 are symmetric to each other with respect to the line l_0. Note that for $k=0$, n, U_1 (resp., L_1) is equal to U_0 (resp., L_0). For instance, the shaded parts in Fig. 1 represent U_0, L_0, and in Fig. 2, the shaded parts represent U_1 and L_1 for the Young diagram 2 of $C_4^{(1)}$.

Now, for each $Y \in \mathcal{Z}(\lambda)$, we denote by $Y \cap U_i$ (resp., $Y \cap L_i$) for $i=0,1,\ldots,n$ the set of all common sites in Y and U_i (resp., L_i) and denote by $|Y \cap L_i|$ the diagram obtained by reflecting $Y \cap L_i$ with respect to the line l_i. Finally, for the sites $(x,y) \in U_i$ and $(x',y') \in L_i$, we say that (x,y) corresponds to (x',y') if (x,y) is symmetric to (x',y') with respect to l_i.

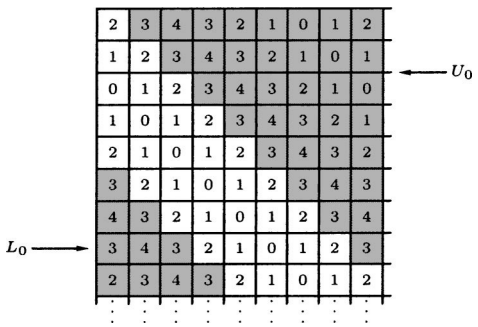


FIG. 1. U_0 and L_0.

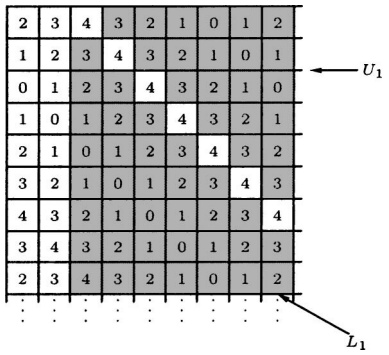


FIG. 2. U_1 and L_1.

Example 2.1: Let $\mathfrak{g}=C_4^{(1)}$ and let

$$Y = \begin{array}{|c|c|c|c|}\hline 0&1&2&3\\\hline 1&0\\\cline{1-2} 2&1\\\cline{1-2} 3\\\cline{1-1}\end{array}$$

be a Young diagram 0. Then

$$Y\cap U_1=\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array},\quad Y\cap L_1=\begin{array}{|c|c|}\hline 1\\\hline 2&1\\\hline 3\\\cline{1-1}\end{array},\quad \text{and}\quad |Y\cap L_1|=\begin{array}{|c|c|c|}\hline 1&2&3\\\hline 1\\\cline{1-1}\end{array}.$$

Now, we introduce some configuration conditions.

Definition 2.2: (a) Assume that $Y\in\mathcal{Z}(\Lambda_k)$ has i-convex corners $(x_1,y_1)\in U_j$ and $(x_2,y_2)\in L_j$ corresponding to each other for some $j=0,1,2,\ldots$. If there is no i-concave corner between (x_1,y_1) and (x_2,y_2), we say that Y satisfies the *configuration condition* (**C1**).

(b) Assume that $Y\in\mathcal{Z}(\Lambda_k)$ has an i-convex corner $(x_1,y_1)\in U_j$ and an i-addable corner $(x_2,y_2)\in L_j$ corresponding to each other for some $j=0,1,2,\ldots$. We say that Y satisfies the *configuration condition* (**C2**) unless there is another i-addable corner between (x_1,y_1) and (x_2,y_2), and the i-signature of the diagram $\{(x,y)\in Y\,|\,x_2+y_2<x+y<x_1+y_1\}$ does not have $+$'s, i.e., $\emptyset=(\cdot)$ or $(-,-,-,\ldots)$.

(c) Assume that $Y\in\mathcal{Z}(\Lambda_k)$ has i-addable corners $(x_1,y_1)\in U_j$ and $(x_2,y_2)\in L_j$ corresponding to each other for some $j=0,1,2,\ldots$. We say that Y satisfies the *configuration condition* (**C3**) unless there is another i-addable corner between (x_1,y_1) and (x_2,y_2), and the i-signature of the diagram $\{(x,y)\in Y\,|\,x_2+y_2<x+y<x_1+y_1\}$ is $\emptyset=(\cdot)$.

From now on, for simplicity, we call the i-signature of the diagram $\{(x,y)\in Y\,|\,x_2+y_2<x+y<x_1+y_1\}$ the i-signature between (x_1,y_1) and (x_2,y_2).

Example 2.3: Let $\mathfrak{g}=C_3^{(1)}$ and let

$$Y = \begin{array}{|c|c|c|c|c|}\hline 0&1&2&3&2\\\hline 1&0&1&2\\\cline{1-4} 2\\\cline{1-1} 3\\\cline{1-1} 2\\\cline{1-1}\end{array}\quad.$$

be a Young diagram 0. The shaded parts $(1,-5)$ and $(5,-1)$ represent the 2-colored convex corners corresponding to each other. Since there is a 2-colored addable corner $(4,-2)$ between these convex corners, Y does not satisfy the configuration condition (**C1**).

Let $Y \in \mathcal{Z}(\Lambda_k)$ be a Young diagram k. Let C_v be the maximal convex corner in Y with respect to the order $>$ on $\mathbb{N}\times\mathbb{Z}$ and assume that C_v is a α-colored corner. Then we denote by C_a the maximal α-addable corner. Now, we define $\hat{Y}$ to be the Young diagram k obtained from Y by removing all α-colored convex corners between C_v and C_a in Y.

Example 2.4: (a) For $\mathfrak{g}=C_3^{(1)}$ and $\lambda=\Lambda_0$, let

$$Y = \begin{array}{|c|c|c|c|c|}\hline 0&1&2&3&2\\\hline 1\\\cline{1-1} 2\\\cline{1-1}\end{array} \in \mathcal{Z}(\lambda),$$

where the shaded corner represents the maximal convex corner C_v. In this case, there is no 2-addable corner and so $\hat{Y}$ is the Young diagram 0 obtained by removing all 2-colored convex corners. That is,

$$\hat{Y} = \begin{array}{|c|c|c|c|}\hline 0&1&2&3\\\hline 1\\\cline{1-1}\end{array}$$

(b) For $\mathfrak{g}=C_3^{(1)}$ and $\lambda=\Lambda_1$, let

$$Y = \begin{array}{|c|c|c|c|c|}\hline 1&2&3&2&1\\\hline 0&1&2&3&2\\\hline 1&0&1\\\cline{1-3} 2\\\cline{1-1}\end{array} \in \mathcal{Z}(\lambda),$$

where the shaded corner represents the maximal convex corner C_v. Since there exists C_a in Y, $\hat{Y}$ is the Young diagram 1 obtained by removing the 2-colored convex corner C_v. That is,

$$\hat{Y} = \begin{array}{|c|c|c|c|c|}\hline 1&2&3&2&1\\\hline 0&1&2&3\\\cline{1-4} 1&0&1\\\cline{1-3} 2\\\cline{1-1}\end{array}$$

Now, we are ready to give an explicit description of the crystal graph $\mathcal{Y}(\Lambda_k)$.

Theorem 5: *The crystal basis $\mathcal{Y}(\Lambda_k)$ of $V(\Lambda_k)=U_q(\mathfrak{g})\phi_k$ is realized as the set of Young diagrams $Y \in \mathcal{Z}(\Lambda_k)$ k satisfying the following conditions*:

(I) *for each* $i=2,3,\ldots$, $Y\cap C_{i-1}^{-}\subset Y\cap C_i^{+}$,
(II) *for each* $i=0,1,2,\ldots$, $|Y\cap L_i|\subset Y\cap U_i$,
(III) *if we set* $Y_0=Y$, $Y_1=\hat{Y}$ *and* $Y_k=\widehat{Y_{k-1}}$, *every* Y_k *satisfies configuration conditions* (**C1**), (**C2**), *and* (**C3**).

Remark 2.6: (a) In Theorem 2.5 (I), we regard $Y\cap C_{i-1}^{-}$ and $Y\cap C_i^{+}$ as only diagrams without coordinates, that is, (I) means that if we put $Y\cap C_{i-1}^{-}$ and $Y\cap C_i^{+}$ on the xy-plane left-top adjusted, then $Y\cap C_{i-1}^{-}$ is a subdiagram of $Y\cap C_i^{+}$.

(b) If $Y \in \mathcal{Y}(\Lambda_k)$ is a Young diagram k, then $\hat{Y}$ also belongs to $\mathcal{Y}(\Lambda_k)$.

Example 2.7: (a) Let $\mathfrak{g}=C_2^{(1)}$ and let

$$Y = \begin{array}{|c|c|c|c|}\hline 1&2&1&0\\\hline 0&1&2\\\cline{1-3} 1&0&1\\\cline{1-3} 2&1&0\\\cline{1-3} 1&2&1\\\cline{1-3} 0\\\cline{1-1}\end{array} .$$

Then we have

$$Y \cap C_2^+ = \begin{array}{|c|}\hline 2\\\hline 1\\\hline 0\\\hline 1\\\hline 2\\\hline\end{array}, \quad Y \cap C_3^+ = \begin{array}{|c|}\hline 1\\\hline 2\\\hline 1\\\hline 0\\\hline 1\\\hline\end{array}, \quad Y \cap C_4^+ = \begin{array}{|c|}\hline 0\\\hline\end{array},$$

$$Y \cap C_1^- = \begin{array}{|c|}\hline 2\\\hline 1\\\hline 0\\\hline\end{array}, \quad Y \cap C_2^- = \begin{array}{|c|}\hline 1\\\hline 2\\\hline\end{array}, \quad \text{and} \quad Y \cap C_3^- = \begin{array}{|c|}\hline 0\\\hline 1\\\hline\end{array}.$$

Therefore,

$$Y \cap U_1 = \subseteq Y \cap C_2^+,\ Y \cap C_2^- \subseteq Y \cap C_3^+, \text{ and } Y \cap C_3^- \nsubseteq Y \cap C_4^+.$$

(b) In Example 2.1, we have

$$Y \cap U_1 = \begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}, \quad Y \cap L_1 = \begin{array}{|c|c|}\hline 1&\multicolumn{1}{c}{}\\\hline 2&1\\\hline 3&\multicolumn{1}{c}{}\\\cline{1-1}\end{array}, \quad \text{and} \quad |Y \cap L_1| = \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 1&\multicolumn{2}{c}{}\\\cline{1-1}\end{array}.$$

Therefore, $Y \cap U_1 \ngeq |Y \cap L_1|$ and so Y does not belong to $\mathcal{Y}(\Lambda_0)$.

(c) Let $\mathfrak{g} = C_4^{(1)}$ and let

$$Y = \begin{array}{|c|c|c|c|c|c|c|}\hline 0&1&2&3&4&3&2\\\hline 1&0&1&2&3&\multicolumn{2}{c}{}\\\cline{1-5} 2&1&0&1&2&\multicolumn{2}{c}{}\\\cline{1-5} 3&2&\multicolumn{5}{c}{}\\\cline{1-2} 4&\multicolumn{6}{c}{}\\\cline{1-1} 3&\multicolumn{6}{c}{}\\\cline{1-1} 2&\multicolumn{6}{c}{}\\\cline{1-1}\end{array}.$$

be a Young diagram 0. Then Y does not satisfy the configuration condition (**C2**), which implies $Y \notin \mathcal{Y}(\Lambda_0)$.

IV. GENERALIZED LLT ALGORITHM

In this section, we give a generalized LLT algorithm, which is an algorithm for constructing the global basis $\mathcal{G}(\Lambda_k)$ of the irreducible highest weight module $V(\Lambda_k)$ of level 1 over $U_q(\mathfrak{g})$. More precisely, for a Young diagram Y k in $\mathcal{Y}(\Lambda_k)$, we give an algorithm of computing the corresponding global basis element $G(Y)$ as a linear combination of Young diagrams k in $\mathcal{Z}(\Lambda_k)$.

We recall the notion of global basis. Consider a $\mathbb{Q}$-algebra involution–of $U_q(\mathfrak{g})$ defined by

$$\overline{e_i} = e_i,\ \overline{f_i} = f_i,\ \overline{q^h} = q^{-h},\ \overline{q} = q^{-1} \text{ for } i \in I,\ h \in P^\vee.$$

Then we have a $\mathbb{Q}$-linear automorphism of $V(\lambda)$ given by

$$Pv_\lambda \mapsto \overline{P}v_\lambda \text{ for } P \in U_q(\mathfrak{g})$$

with the highest weight vector v_λ of $V(\lambda)$. Let $\mathbf{A} = \mathbb{Q}[q, q^{-1}]$. Let $U_{\mathbf{A}}^-$ be the $\mathbf{A}$-subalgebra of $U_q(\mathfrak{g})$ generated by $f_i^{(n)}$ $(i \in I, n \in \mathbb{Z}_{\geqslant 0})$ and set $V(\lambda)_{\mathbf{A}} = U_{\mathbf{A}}^- v_\lambda$. Let $(L(\lambda), B(\lambda))$ be a crystal basis of the irreducible highest weight $U_q(\mathfrak{g})$-module $V(\lambda)$ with a dominant integral weight λ. Then there is a unique $\mathbf{A}$-basis $\mathcal{G}(\lambda) = \{G(b) \in V(\lambda)_{\mathbf{A}} \cap L(\lambda) \,|\, b \in B(\lambda)\}$ of $V(\lambda)_{\mathbf{A}}$ such that

$$\overline{G(b)} = G(b),\ G(b) \equiv b \bmod qL(\lambda) \text{ for all } b \in B(\lambda).$$

The basis $\{G(b)\}$ is called the *global basis* of $V(\lambda)$ corresponding to the crystal basis $B(\lambda)$ (Ref. 12).

Now, we are ready to describe the generalized LLT algorithm. At first, we consider the action of divided powers $f_i^{(r)}$ on the Young diagrams k.

Lemma 3.1: Let Y be a Young diagram k, and write

$$f_i^{(r)}Y = \sum_{\substack{Z\in Z(\Lambda_k)\\ wt(Z)=wt(Y)-r\alpha_i}} Q_{Y,Z}(q)Z,$$

where $Q_{Y,Z}(q)\in\mathbb{Q}(q)$. Then we have $Q_{Y,Z}(q)\in\mathbb{Z}[q,q^{-1}]$.

Proof: If $Z\in\mathcal{Z}(\Lambda_k)$ satisfies $Q_{Y,Z}(q)\neq 0$, we can find a unique sequence of Young diagrams k, $Y=Y_0,Y_1,\ldots,Y_r=Z$ such that

(i) $Y_{k+1}=Y_k\swarrow(x_{k+1},y_{k+1})$ for an i-colored addable corner (x_{k+1},y_{k+1}),
(ii) the site (x_{k+1},y_{k+1}) is smaller than the site (x_k,y_k).

For each k, let $Q_{Y_k,Y_{k+1}}(q)$ be the coefficient of Y_{k+1} in f_iY_k and let

$$Q^{\circ}_{Y,Z}(q)=\prod_{k=0}^{r-1}Q_{Y_k,Y_{k+1}}(q)\in\mathbb{Z}[q,q^{-1}].$$

Then by induction on r, we can see that

$$Q_{Y,Z}(q)=Q^{\circ}_{Y,Z}(q)q_i^{r(r-1)/2}\in\mathbb{Z}[q,q^{-1}]. \tag{3.1}$$

□

For Y in $\mathcal{Z}(\Lambda_k)$, we associate a sequence $\|Y\|=(\ldots,y_{-1},y_0,y_1,\ldots)$, where y_i is the number of sites (x,y) in Y such that $x+y=i$. For Y and Z in $\mathcal{Z}(\Lambda_k)$, consider the associated sequences $\|Y\|=(\ldots,y_{-1},y_0,y_1,\ldots)$ and $\|Z\|=(\ldots,z_{-1},z_0,z_1,\ldots)$. We define $Y>Z$ if and only if there exists p such that $y_i=z_i$ for all $i>p$ and $y_p>z_p$. Then we have

Proposition 3.2: Let $Y\in\mathcal{Y}(\Lambda_k)$ be a Young diagram k. Suppose that $wt(\hat{Y})=wt(Y)+r\alpha_i$. Then

$$f_i^{(r)}\hat{Y}=Y+\sum_{\substack{wt(Z)=wt(Y)\\ Y>Z}}Q_{\hat{Y},Z}(q)Z,$$

where $Q_{\hat{Y},Z}(q)\in\mathbb{Z}[q,q^{-1}]$.

Proof: Recall that $\hat{Y}$ is obtained from Y by removing i-colored convex corners between maximal convex corner C_v and the maximal i-colored addable corner C_a. Then it is easy to see that $Q_{\hat{Y},Z}(q)=0$ unless $Y\geqslant Z$ and $wt(Y)=wt(Z)$. Further, there is a unique sequence of Young diagrams k, $\hat{Y}=Y_0,Y_1,\ldots,Y_r=Y$ such that

(i) $Y_{k+1}=Y_k\swarrow(x_{k+1},y_{k+1})$ for some i-colored addable corner (x_{k+1},y_{k+1}),
(ii) there is no addable corner located above the site (x_k,y_k) with respect to the ordering $>$ on $\mathbb{N}\times\mathbb{Z}$.

In this case, it is easy to see that $Q_{Y_k,Y_{k+1}}(q)=q_i^{-k}$ and so

$$Q^{\circ}_{\hat{Y},Y}(q)=\prod_{k=0}^{r-1}Q_{Y_k,Y_{k+1}}(q)=q_i^{-r(r-1)/2}.$$

Therefore, by (3.1) $Q_{\hat{Y},Y}(q)=1$. □

Definition 3.3: Let $Y \in \mathcal{Y}(\Lambda_k)$ be a Young diagram k. Then we have the unique sequence of Young diagrams k in $\mathcal{Y}(\Lambda_k)$ such that $Y=Y_0$, $Y_1=\hat{Y}_0, \ldots, Y_{k+1}=\hat{Y}_k, \ldots, Y_N=\hat{Y}_{N-1}=\phi_k$. Suppose that $Y_k=\hat{Y}_{k-1}$ is obtained by removing r_k-many i_k-colored convex corners from Y_{k-1}. We define

$$A(Y) = f_{i_1}^{(r_1)} \cdots f_{i_N}^{(r_N)} \phi_k \in V(\Lambda_k)_{\mathbf{A}}. \tag{3.2}$$

By definition, $\overline{A(Y)}=A(Y)$. We write

$$A(Y) = \sum_{Z \in Z(\Lambda_k)} A_{Y,Z}(q) Z,$$

where $A_{Y,Z}(q) \in \mathbb{Q}(q)$. Then we have

Proposition 3.4: Let $Y \in \mathcal{Y}(\Lambda_k)$ *be a Young diagram* k. *Then for a Young diagram* $Z \in \mathcal{Z}(\Lambda_k)$ k, *we have*

$$A(Y) = Y + \sum_{\substack{wt(Z)=wt(Y) \\ Y>Z}} A_{Y,Z}(q) Z,$$

where $A_{Y,Z}(q) \in \mathbb{Z}|q, q^{-1}|$.

Proof: By Lemma 3.1 and Proposition 3.2, it is clear that $A_{Y,Z}(q) \in \mathbb{Z}|q, q^{-1}|$ and $A_{Y,Y}(q)=1$. Therefore, it suffices to show that $A_{Y,Z}(q)=0$ unless $Y \geqslant Z$ and $wt(Y)=wt(Z)$. Now, we use the induction on N. If $N=1$, it is just the Proposition 3.2. Suppose that

$$f_{i_{j+1}}^{(r_{j+1})} \cdots f_{i_N}^{(r_N)} \phi_k = Y_{j+1} + \sum_{Y_{j+1}>Z} A_{Y_{j+1},Z}(q) Z.$$

Then

$$\begin{aligned} f_{i_j}^{(r_j)} f_{i_{j+1}}^{(r_{j+1})} \cdots f_{i_N}^{(r_N)} \phi_k &= f_{i_j}^{(r_j)} Y_{j+1} + \sum_{Y_{j+1}>Z} A_{Y_{j+1},Z}(q) f_{i_j}^{(r_{i_j})} Z \\ &= Y_j + \sum_{Y_j>W} Q_{Y_j,W}(q) W + \sum_{Y_{j+1}>Z} A_{Y_{j+1},Z}(q) \sum_W Q_{Z,W}(q) W. \end{aligned}$$

Let $\|Y_{j+1}\|=(\ldots, y_{-1}, y_0, y_1, \ldots)$ and $\|Z\|=(\ldots, z_{-1}, z_0, z_1, \ldots)$ and let p be the largest integer such that $y_p > z_p$ and $y_q=z_q$ $(q>p)$. Let α be the coloring of (x,y) such that $x+y=p$. If i_j is not α, it is easy to see that $Y_j > W$. If i_j is α, by definition of Y, we can see that Y_j and W are obtained by adding i_j-many α's to the addable corners (x,y) such that $x+y>p$. Hence $Y_j > W$. □

Let $\mathcal{G}(\Lambda_k)=\{G(Y) \mid Y \in \mathcal{Y}(\Lambda_k)\}$ be a global basis of $V(\Lambda_k)_A$. For $Y \in \mathcal{Y}(\Lambda_k)$, let us write

$$G(Y) = \sum_{Z \in \mathcal{Z}(\Lambda_k)} G_{Y,Z}(q) Z \in V(\Lambda_k)_{\mathbf{A}} \cap \mathcal{L}(\Lambda_k),$$

where $G_{Y,Z}(q) \in \mathbf{A}_0$. Since $\mathcal{G}(\Lambda_k)$ is a $\mathbf{A}$-basis of $V(\Lambda_k)_{\mathbf{A}}$, it is easy to see that $G_{Y,Z}(q) \in \mathbb{Q}[q, q^{-1}]$. Further, $G(Y) \equiv Y \bmod q\mathcal{L}(\mathcal{F}(\Lambda_k))$ implies (i) $G_{Y,Z}(q) \in \mathbb{Q}[q]$, (ii) $G_{Y,Z}(q) \in q\mathbb{Q}[q]$ unless $Y=Z$, (iii) $G_{Y,Y}(q)=1$.

On the other hand, since $\mathcal{G}(\Lambda_k)$ and $\mathcal{A}(\Lambda_k)$ are both $\mathbb{Q}(q)$-basis of $V(\Lambda_k)$, there is a matrix $H=(H_{Y,W}(q))_{Y,W \in \mathcal{Y}(\Lambda_k)}$ such that

$$G(Y) = \sum_{W \in \mathcal{Y}(\Lambda_k)} H_{Y,W}(q) A(W).$$

Since $\overline{G(Y)}=G(Y)$ and $\overline{A(W)}=A(W)$, $H_{Y,W}(q)=H_{Y,W}(q^{-1})$.

Proposition 3.5 (cf. Ref. 8):

(a) *$H_{Y,W}(q)$ satisfies the following properties*:

(i) $H_{Y,W}(q) \in \mathbb{Q}[q,q^{-1}]$,
(ii) $H_{Y,W}(q)=0$ *unless* $Y \geqslant W$ *and* $wt(Y)=wt(W)$,
(iii) $H_{Y,Y}(q)=1$.

(b) $A(\Lambda_k)=\{A(Y)\,|\,Y \in \mathcal{Y}(\Lambda_k)\}$ *is an* **A**-*basis of* $V(\Lambda_k)_A$.

Proof: The proof is the same as that of Proposition 7.12 in Ref. 17. □

By above proposition, for each $Y \in \mathcal{Y}(\Lambda_k)_\lambda$ $(\lambda \leqslant \Lambda_k)$, we have

$$A(Y) = G(Y) + \sum_{\substack{Z \in \mathcal{Y}(\Lambda_k)_\lambda \\ Y>Z}} \gamma_{Y,Z}(q)G(Z), \tag{3.3}$$

where $\gamma_{Y,Z}(q) \in \mathbb{Q}[q,q^{-1}]$ and $\gamma_{Y,Z}(q)=\gamma_{Y,Z}(q^{-1})$. If Y is the minimal element in $\mathcal{Y}(\Lambda_k)_\lambda$, then $G(Y)=A(Y)$. Suppose that Y is not minimal and $G(Y')$ are given for $Y' \in \mathcal{Y}(\Lambda_k)_\lambda$ such that $Y' < Y$. Then $\gamma_{Y,Y'}(q)$ are completely determined as follows:

(1) if Y' is the maximal one such that $Y > Y'$ and $A_{Y,Y'}(q)=\Sigma_{i=-r'}^{r} a_i q^i$, then $\gamma_{Y,Y'}(q)=\Sigma_{i=1}^{r'} a_i(q^i + q^{-i}) + a_0$;
(2) if the coefficient of Y' in $A(Y) - \Sigma_{Y>Z>Y'} \gamma_{Y,Z}(q)G(Z)$ is $\Sigma_{i=-r'}^{r} a_i q^{-i}$, then $\gamma_{Y,Y'}(q)=\Sigma_{i=1}^{r'} a_i(q^i + q^{-i}) + a_0$.

From the description of the algorithm, we have

Theorem 3.6: *For a Young diagram $Y \in \mathcal{Y}(\Lambda_k)_\lambda$ $(\lambda \leqslant \Lambda_k)$ k, the corresponding global basis element $G(Y)$ is of the following form*

$$G(Y) = Y + \sum_{\substack{Z \in \mathcal{Z}(\Lambda_k)_\lambda \\ Y>Z}} G_{Y,Z}(q)Z, \tag{3.4}$$

where $G_{Y,Z}(q) \in q\mathbb{Z}[q]$ for $Y \neq Z$.

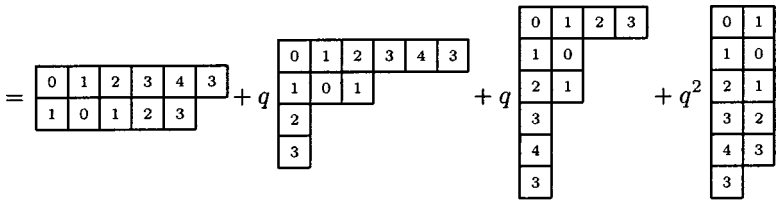
Example 3.7: Let $g=C_4^{(1)}$. In this case, $q_0=q_4=q^2$ and $q_1=q_2=q_3=q$. The following are the all Young diagrams 0 with the weight $\Lambda_0-(2\alpha_0+3\alpha_1+2\alpha_2+3\alpha_3+\alpha_4)$.

$$Y_1 = \begin{array}{|c|c|c|c|c|c|}\hline 0&1&2&3&4&3\\\hline 1&0&1&2&3\\\cline{1-5}\end{array} \quad \text{and} \quad Y_2 = \begin{array}{|c|c|c|c|c|c|}\hline 0&1&2&3&4&3\\\hline 1&0&1\\\cline{1-3} 2\\\cline{1-1} 3\\\cline{1-1}\end{array}\ .$$

Now, $Y_1 > Y_2$ and

$$= \begin{array}{|c|c|c|c|c|c|}\hline 0&1&2&3&4&3\\\hline 1&0&1\\\cline{1-3} 2\\\cline{1-1} 3\\\cline{1-1}\end{array} + q \begin{array}{|c|c|c|c|}\hline 0&1&2&3\\\hline 1&0&1\\\cline{1-3} 2\\\cline{1-1} 3\\\cline{1-1} 4\\\cline{1-1} 3\\\cline{1-1}\end{array} + q \begin{array}{|c|c|c|c|c|c|}\hline 0&1&2&3&4&3\\\hline 1&0\\\cline{1-2} 2&1\\\cline{1-2} 3\\\cline{1-1}\end{array} + q^2 \begin{array}{|c|c|c|c|}\hline 0&1&2&3\\\hline 1&0\\\cline{1-2} 2&1\\\cline{1-2} 3\\\cline{1-1} 4\\\cline{1-1} 3\\\cline{1-1}\end{array}\ .$$

Moreover,



and so $A(Y_1)=Y_1+q\mathcal{L}(\Lambda_0)$. Therefore, $G(Y_1)=A(Y_1)$.

Remark 3.8: Indeed, we have a Young diagram $Y\in\mathcal{Z}(\lambda)$ such that $A(Y)\neq G(Y)$. But, in general, it is composed of a lot of colored boxes.

V. THE PROOF OF THE MAIN THEOREM

In this section, we give a proof of our main theorem. Let $\mathcal{Y}(\Lambda_k)$ be the set of Young diagrams k satisfying the conditions of the Theorem 2.5.

By Corollary 1.4 and Theorem 1.5, it suffices to prove the following statements:

(1) For all $i\in I$ we have $\tilde{e}_i\mathcal{Y}(\Lambda_k)\subset\mathcal{Y}(\Lambda_k)\cup\{0\}$, $\tilde{f}_i\mathcal{Y}(\Lambda_k)\subset\mathcal{Y}(\Lambda_k)\cup\{0\}$.
(2) If $Y\in\mathcal{Y}(\Lambda_k)$ and $\tilde{e}_iY=0$ for all $i\in I$, then $Y=\phi_k$.

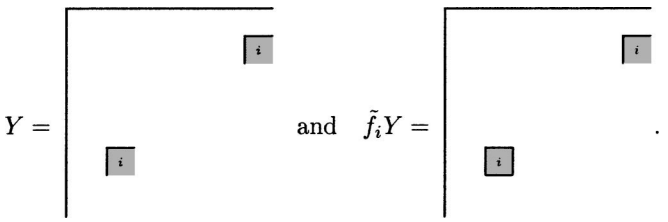
But, thanks to (1.1), it is easy to see that all maximal Young diagrams k except ϕ_k does not satisfy the condition (II). Hence (2) is proved. For (1), let $y\in\mathcal{Y}(\Lambda_k)$ be a Young diagram k. Suppose that $\tilde{f}_iY$ does not belong to $\mathcal{Y}(\Lambda_k)$. It means that $\tilde{f}_iY$ violates at least one of the conditions (I)–(III).

Case I. suppose that $\tilde{f}_iY$ does not satisfy the condition (I). Then there exists an i-colored convex corner in C_k^- for some k, where i-colored box can be added to get $\tilde{f}_iY$ such that

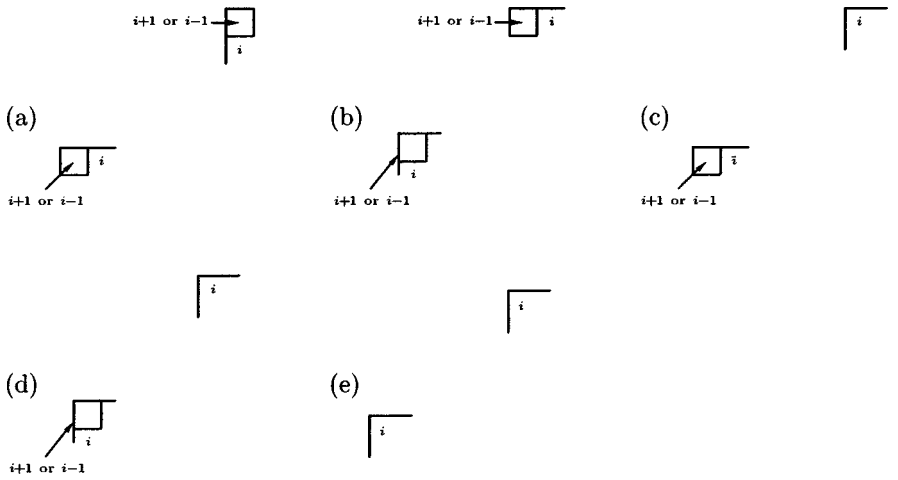
$$\tilde{f}_iY\cap C_k^-\not\subseteq\tilde{f}_iY\cap C_{k+1}^+.$$

Moreover, since Y satisfies the condition (I), there should exist the i-colored addable corner in C_{k+1}^+ of $\tilde{f}_iY$, which implies that Y has i-colored addable corners in both C_k^- and C_{k+1}^+. But, by the definition of Kashiwara operators, it is a contradiction.

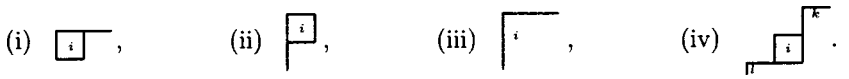
Case II. Suppose that $\tilde{f}_iY$ does not satisfy the condition (II). Then Y has i-colored addable corners (x,y) and (x',y') corresponding to each other, and Y and $\tilde{f}_iY$ have the following form:



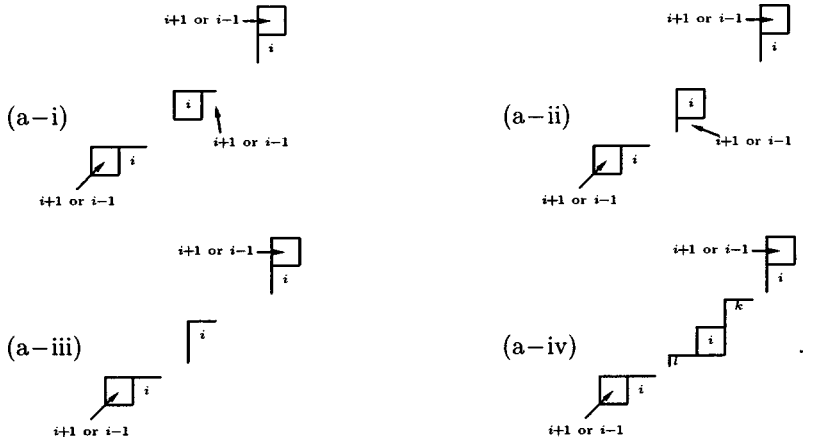
By the condition (II), we have the following possibilities for Y:



By the definition of Kashiwara operator $\tilde{f}_i$, there should be a convex i-colored corner between (x,y) and (x',y') in Y. Hence, one of the following diagrams appears between the corners (x,y) and (x',y').



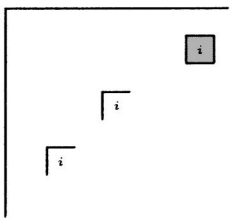
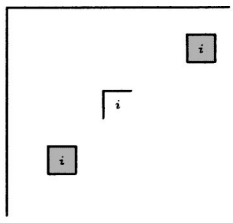
Consider the case (a). Then we have the following four cases:



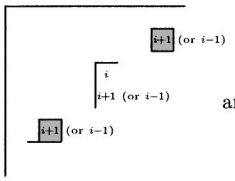
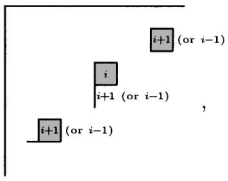
For the case (a-i) and (a-ii), if Y has $(i+1)$-colored [resp., $(i-1)$-colored] convex corner and $(i+1)$-colored [resp., $(i-1)$-colored] addable corner, it contradicts to the configuration condition (**C1**). If Y has $(i+1)$-colored [resp., $(i-1)$-colored] convex corner and $(i-1)$-colored [$(i+1)$-colored] addable corner, then we can check that Y_t for some $t \geqslant 0$ cannot satisfy the configuration condition (**C1**) for the $(i-1)$-color [$(i+1)$-color]. In case (a-iii), it is easy to see that Y does not satisfy the configuration condition (**C1**). In case (a-iv), thanks to the pattern of coloring in xy-plane, we can check that Y_t for some t cannot satisfy the configuration condition (**C1**). For the remaining cases, we can give a proof by the similar method.

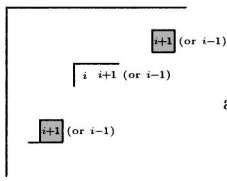
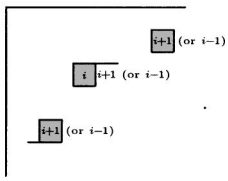
Case III. Suppose that $\tilde{f}_i Y$ does not satisfy the condition (III). Then there is a Young diagram $(\tilde{f}_i Y)_l$ which does not satisfy one of the configuration conditions (**C1**), (**C2**), (**C3**). At first, consider the case $l=0$. That is, suppose that $\tilde{f}_i Y$ does not satisfy one of the configuration conditions

(**C1**), (**C2**) and (**C3**). At first, suppose that $\tilde{f}_i Y$ violates the configuration condition (**C1**). If C_v of $\tilde{f}_i Y$ is a i-colored convex corner, then Y and $\tilde{f}_i Y$ have the following form:

$Y =$  and $\tilde{f}_i Y =$  .

By the definition of Kashiwara operator $\tilde{f}_i$, it is easy to see that the i-signature between i-colored convex corner C_v and i-colored addable corner corresponding to C_v in Y is $\emptyset=(\cdot)$ or $(-, -, -, \ldots)$. Since Y satisfies the configuration condition (**C2**), it is a contradiction. If C_v of $\tilde{f}_i Y$ is a $(i+1)$-colored or $(i-1)$-colored convex corner, then Y and $\tilde{f}_i Y$ have the following possibilities:

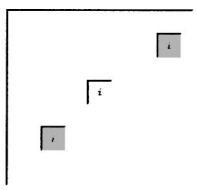
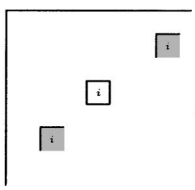
(a) $Y =$  and $\tilde{f}_i Y =$  ,

(b) $Y =$  and $\tilde{f}_i Y =$  .

Here, the left hand side or the upside of C_v is i-colored. In any case, by the pattern of coloring in xy-plane and the condition (II) which Y should satisfy, Y_t for some t can not satisfy the configuration condition (**C1**). It is a contradiction. Similarly, for the remaining cases, we can see that it contradicts to the fact that $Y \in \mathcal{Y}(\Lambda_k)$.

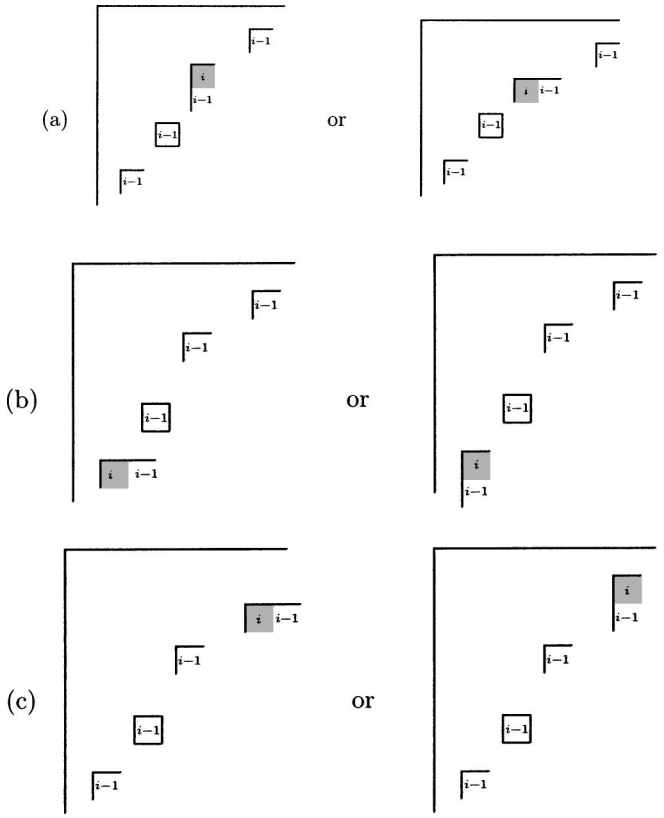
By the similar argument, if $\tilde{f}_i Y$ violates the configuration condition (**C2**), we can show that Y does not satisfy the configuration condition (**C2**) or (**C3**).

Finally, suppose that $\tilde{f}_i Y$ violates the configuration condition (**C3**). If the addable corners of $\tilde{f}_i Y$ which violate (**C3**) are i-colored corners, then Y and $\tilde{f}_i Y$ have the following form:

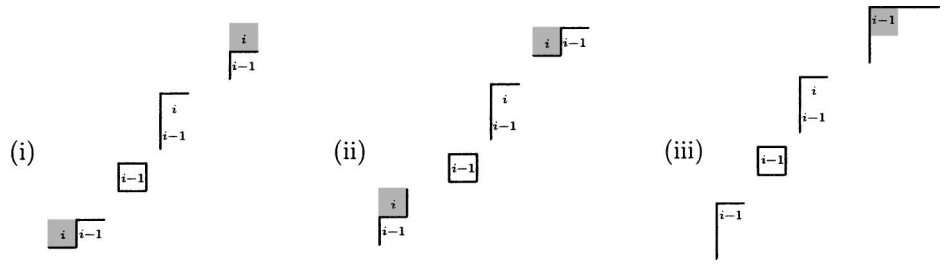
$Y =$  and $\tilde{f}_i Y =$  .

Note that i-signature of Y between above two i-addable corners is $(+)$. Hence, by the definition of Kashiwara operator $\tilde{f}_i$, it is impossible.

If the addable corners of $\tilde{f}_i Y$ which violate (**C3**) are $(i-1)$-colored corners, then Y should be one of the following forms:

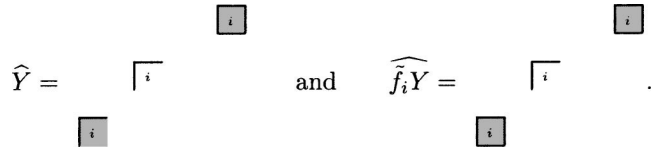


Here, the shaded parts represent the sites where i-colored box will be added in $\tilde{f}_i Y$. Consider the first case of (a). Then we have the following cases:

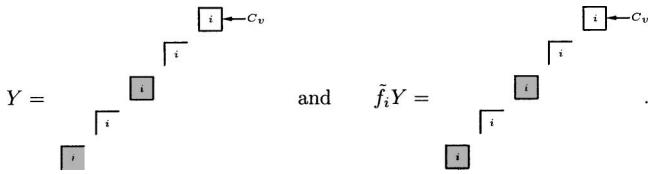


The cases (i) and (ii) violate the configuration condition (**C1**). Further, for the case (iii), we can see that Y_t for some t has the form of (i) and (ii). It is a contradiction. The case (b) is also proved by the similar argument. Moreover, the case (c) cannot appear by the condition (I).

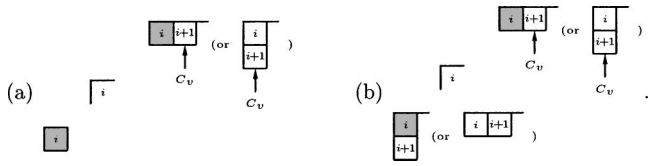
Now, suppose that $(\tilde{f}_i Y)_{l>0}$ does not satisfy one of the configuration conditions (**C1**), (**C2**), (**C3**). Consider the case (**C1**). Using Remark 2.6 (b) and induction argument, we may assume that $\widehat{\tilde{f}_i Y}$ violates the configuration condition (**C1**). If C_v is a α-colored $(\alpha \neq i, i \pm 1)$ corner, $\hat{Y}$ and $\widehat{\tilde{f}_i Y}$ have the following forms:



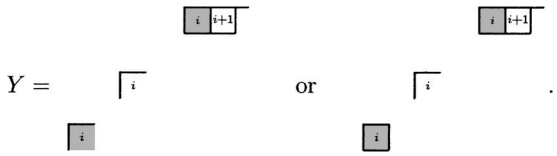
In this case, since $\alpha \neq i, i\pm 1$, it is straightforward to see $\tilde{f}_i\hat{Y} = \widehat{\tilde{f}_i Y}$. Moreover, it means that $\hat{Y}$ violates the configuration condition (**C1**), which is a contradiction. Secondly, if C_v is a i-colored corner, then Y and $\tilde{f}_i Y$ are the following forms:



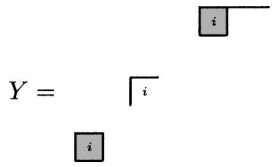
But, in this case, $\tilde{f}_i Y$ does not satisfy the configuration condition (**C1**), which is a contradiction. Finally, if C_v is a $(i+1)$ or $(i-1)$-colored corner, $\tilde{f}_i Y$ is one of the following forms:



In case (a), we have



Then $\hat{Y}$ violates the configuration condition (**C1**) or (**C2**), which is a contradiction. For the case (b), we have



Moreover, Y does not satisfy the configuration condition (**C1**), which is a contradiction.

By the similar argument, we can see that $(\tilde{f}_i Y)_l$ for all l satisfy the configuration conditions (**C2**) and (**C3**). Therefore, $\tilde{f}_i Y$ satisfies the condition (III).

Similarly, we can see that $\tilde{e}_i Y$ belongs to $\mathcal{Y}(\Lambda_k) \cup \{0\}$. □

ACKNOWLEDGMENTS

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Harmonic analysis of linear fields on the nilgeometric cosmological model

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To analyze linear field equations on a locally homogeneous space–time by means of separation of variables, it is necessary to set up appropriate harmonics according to its symmetry group. In this paper, the harmonics are presented for a spatially compactified Bianchi II cosmological model—the *nilgeometric model*. Based on the group structure of the Bianchi II group (also known as the Heisenberg group) and the compactified spatial topology, the irreducible differential regular representations and the multiplicity of each irreducible representation, as well as the explicit form of the harmonics are all completely determined. They are also extended to vector harmonics. It is demonstrated that the Klein–Gordon and Maxwell equations actually reduce to systems of ODEs, with an asymptotic solution for a special case. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1811373]

I. INTRODUCTION

A basic strategy to analyze linear field equations on a given space–time, like linear perturbation equations of Einstein's equation, is to separate the equations using appropriate harmonics. The harmonics for a given manifold are in general determined by the underlying symmetry group (isometry group) and the topology of the manifold. The simplest example is that of a commutative group acting on a flat manifold. If the manifold is compactified to, e.g., a torus, then functions on the manifold are expanded in the form of usual Fourier series. When the group is noncommutative, however, the harmonics become much more complicated. The most familiar example in homogeneous cosmology is the SU(2) (Bianchi IX) case,[2,6,8] where one needs to use the spherical harmonics (and their generalization to vector and tensor harmonics if necessary) to separate field variables. A notable nontrivial example is the $H^2\times\mathbf{R}$ (Bianchi III) case[17,13] with compactified three-dimensional manifold. Since such a manifold is a direct product of two submanifolds, a closed hyperbolic plane and a circle, the harmonics are simply given by making products of those for the two lower dimensional manifolds. Note that the Bianchi III belongs to Class B.[4] Separations of variables regarding locally rotationally symmetric (LRS) Class A Bianchi types (and gravitational perturbations) were discussed in Refs. 3 and 9 without compactification.

In this paper we consider the *generic* (i.e., non-LRS) Bianchi II model *with* compactification. The Bianchi II type is one of the class A types. The underlying symmetry group is the three-dimensional Heisenberg group H_1, which we refer to as the Bianchi II group G_{II}. The Bianchi II homogeneous manifolds correspond to Thurston's nilgeometry.[20] We will refer to spatially compactified Bianchi II space–times (i.e., ones obtained from Bianchi II spatially homogeneous space–times by compactifying the homogeneous spatial sections) as *nilgeometric cosmological models* (to distinguish from the conventional open models).

By considering a compactified (spatial) manifold we have the following merits: (1) a compact Cauchy surface makes it natural to view the field equations as an initial value problem in cosmo-

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logical context, (2) a finite spatial volume is physically reasonable, and (3) functional analysis on a compact manifold is much easier and tractable than one on an open manifold, since we can avoid many complexities involved in continuous spectra and those for the convergence of integrals (remember the contrast between Fourier series analysis on the "compactified space" $S^1=\mathbf{R}^1/\mathbf{Z}$ and Fourier analysis on the open space $\mathbf{R}$).

We also mention that a motivation of considering compactified manifolds also comes from recent evidence that the spatial topology and global dynamical properties of solutions of Einstein's equation are related in some ways. In particular, recent results[1,5] suggest a very general picture of how an appropriately conformally transformed spatial manifold evolves in time by the vacuum Einstein equation, depending upon its topology. This picture motivates us to study linear perturbation equations for locally homogeneous solutions which have various spatial topologies.

Fortunately, although it is not as trivial as the torus compactification of a flat manifold, the compactification of Bianchi II manifolds (or Bianchi II type space–times) is not very difficult. We will describe our compactification following Refs. 10, 15, and 16.

In this paper we explore detailed properties for the scalar and vector harmonics. We also demonstrate separation of variables for the Klein–Gordon scalar field equation and the source-free Maxwell equation. Although generalization to tensor harmonics is straightforward we leave their explicit presentation to a subsequent paper as well as a study of linear perturbations. This paper is intended to lay a solid basis for exploring those more complicated problems, or to be useful for many applications on the nilgeometric space–time model like quantum field analysis.

Some of the mathematical background assumed in this paper and some related results obtained are the following. As well known (e.g., Ref. 32), the harmonics on a manifold M on which a transformation group G acts are naturally obtained through irreducible decomposition of a representation T, called the *regular representation*, of G on $L^2(M)$. Let $g\in G$ and let $f(x)\in L^2(M)$. The (right) regular representation $(T,L^2(M))$ is given by the homomorphism $T:g\to T_g$, where T_g is the right translation map $T_g:f(x)\to f(xg)$.[22] In fact, letting $g,g'\in G$, we can see $T_gT_{g'}f(x)=(T_{g'}f)(xg)=f(xgg')=T_{gg'}f(x)$, showing T is a representation (homomorphism), $T_gT_{g'}=T_{gg'}$. This representation is however *not* irreducible in general. The appropriate harmonics on M are naturally obtained through an irreducible decomposition of $(T,L^2(M))$.

In our context, the transformation group G is the Bianchi II group G_{II}, which acts on $\tilde{M}=\mathbf{R}^3$ from the left simply transitively, i.e., for arbitrary $p,q\in\tilde{M}$ there exists a unique element $g\in G$ such that $gp=q$. Thanks to this property, choosing an arbitrary fixed point $o\in\tilde{M}$, e.g., the coordinate origin, one can identify the group G_{II} and the manifold $\tilde{M}$, $G_{\mathrm{II}}=\tilde{M}$, by associating go with g. With this identification, the manifold $\tilde{M}$ is also the group G_{II}, and therefore the right action of G_{II} on $\tilde{M}$ is also naturally defined. We make $\tilde{M}$ compact by identifying points by left action of a discrete subgroup $A\subset G_{\mathrm{II}}$, $M=A\backslash\tilde{M}$. The (right) regular representation $(T,L^2(A\backslash\tilde{M}))$ on this space is indeed well defined, since keeping in mind the fact that we can identify an arbitrary function on $A\backslash\tilde{M}$ with an "automorphic function" $f(x)$ on $\tilde{M}$ such that $f(x)=f(Ax)$, we can confirm the consistency $T_gf(Ax)=f(Axg)=f(xg)=T_gf(x)$. This shows the consistency of the fact that we choose the "right" regular representation, i.e., since we want to define the (Killing) symmetry of the manifold with respect to the left action, and make a quotient by the left one, the regular representation on the quotient should be the right one for commutativity. The universal covering manifold $(\tilde{M},\tilde{q}^{(0)})$ with a standard left invariant metric $\tilde{q}^{(0)}$ naturally defines a left invariant measure $\mathrm{d}\mu_0\equiv\mathrm{d}\mu_L$ on $\tilde{M}$, for which we can define the natural inner product on $L^2(\tilde{M})$. Since for the Bianchi II group this measure is also right invariant $\mathrm{d}\mu_L\propto\mathrm{d}\mu_R$, i.e., G_{II} is unimodular, the right regular representation $(T,L^2(A\backslash\tilde{M}))$ with the inner product is unitary; $\int_M|f(xg)|^2\,\mathrm{d}\mu_0=\int_M|f(x)|^2\mathrm{d}\mu_0$.

Our mode functions on M will be denoted as ϕ_{l,m,n_0} (or φ_{l,m,n_0} on the space–time $M\times\mathbf{R}$) for generic modes with $m\neq0$. The index m labels inequivalent irreducible representations, while the index n_0 labels ones in equivalent representations. For fixed m and n_0, the functions $\{\phi_l\}_{l=0}^{\infty}$ work

as a set of basis functions for the irreducible representation space specified by m and n_0. Each single ϕ_l spans the eigenspace of an operator denoted as L^2, which is like a total angular momentum operator.

For the purpose of separation of variables, the most important relations are those for the differential representation, which is a linear transformation acting on the representation space spanned by mode functions. Those relations are written in terms of group-invariant differential operators denoted as χ_I $(I=1-3)$. [See Eqs. (4.14) and (7.9).] Indeed, since group-invariant field equations like the Klein–Gordon equation can be written with no explicit coordinate dependences if it is written with the invariant operators, these relations are found to provide the key to separate the equations.

The formulas for the differential representation however do not provide complete information about the representation. For example, they do not tell whether the representation specified by m does exist in $(T,L^2(M))$, or how many equivalent copies of a representation exist in $(T,L^2(M))$. To see how the representation $(T,L^2(M))$ is decomposed to irreducible representations we need to find all the appropriate mode functions on M. In this paper, the universal covering manifold $\tilde{M}$ (with a group invariant standard metric) is compactified to a circle bundle over the torus. The regular representation $(T,L^2(M))$ is completely reducible, and as a result of finding of the mode functions on the given topology of M we find the following.

Theorem 1.1: *Let M be the circle bundle over the torus with Euler class $e=1$ [see Eq. (2.15) for its fundamental group], and let $(T,L^2(M))$ be the regular representation of the Bianchi II group G_{II}. Then, it holds that*

$$T=\Big(\bigoplus_{m\in\mathbf{Z}\setminus\{0\}}|m|T_m\Big)\oplus\Big(\bigoplus_{k_1,k_2\in\mathbf{Z}}\mathbf{1}_{k_1,k_2}\Big), \tag{1.1}$$

where T_m is an infinite dimensional irreducible representation, $\mathbf{1}_{k_1,k_2}$ is a one-dimensional irreducible representation, and the coefficient $|m|$ stands for the multiplicity in T_m. $\mathbf{Z}\setminus\{0\}$ represents nonzero integers.

(See Ref. 30, Secs. X and XI and references therein for some related mathematical works.) This decomposition expresses the completeness of the harmonics we construct. In particular, this decomposition does not depend on the Teichmüller (or moduli) parameters of M. From the Stone–von Neumann theorem,[19,30] T_m is equivalent to a corresponding Schrödinger representation.

Construction of vector (or tensor) harmonics is not difficult on the one hand. However the important point is to divide each irreducible space of vectors into subspaces such that each subspace is invariant under the action of the operator L^2. This feature is necessary to obtain decoupled systems of ODEs when the background space–time has an additional symmetry. We define three kinds of vector harmonics, two of which have this property.

The plan of the paper is as follows. In the next section we describe the background solution and also account for some basic facts. Section III sets up some basic eigenvalues used to label mode functions, based on the compactification of the spatial manifold. In Sec. IV we make algebraic discussions to derive the χ relations. Section V is devoted to construction of the mode functions on the spatial manifold. In Sec. VI the mode functions constructed on the spatial manifold are generalized to those on the space–time. While Secs. IV–VI deal with the generic modes, Sec. VII deals with the exceptional modes, the U(1)-symmetric modes, which complete all possible (scalar) modes. The results so far are applied to the Klein–Gordon equation and the reduced ODEs are explicitly given, with an asymptotic solution for a special case, in Sec. VIII. In Sec. IX we develop the vector harmonics. Section X is devoted to an application to Maxwell's equation. The final section is devoted to the conclusion.

This paper is a full account, with much generalizations and development, of the subject outlined in Sec. III of Ref. 13. Although most notations remain the same, one of the changes is that a quotient by the left action is now written $A\backslash\tilde{M}$ instead of $\tilde{M}/A$ to make clear which action is used. We employ the abstract index notation[21] and use leading italic letters $a,b,\ldots$ to denote abstract indices for vectors and tensors in Secs. VIII–X. In the other sections however we write them without abstract indices. We often drop the tensor product symbol and write, e.g., $(\sigma^1)^2$

instead of $\sigma^1 \otimes \sigma^1$. Beware that since vectors are also used as differential operators, products of them like $(\chi_1)^2$ can stand for second order derivatives like $\chi_1\chi_1$ or tensor products like $\chi_1 \otimes \chi_1$, depending upon the quantity considered.

II. THE BACKGROUND SOLUTION

Our background solution is specified by the following: (1) it is a solution of the vacuum Einstein equation, (2) it is spatially locally homogeneous of Bianchi II type, and (3) its spatial manifold is compact without boundary, in other words, *closed*. (An explicit topology will be chosen later.)

A Bianchi type II solution is characterized by the fact that the solution (or the universal cover of it) is invariant under the action of the *Bianchi II group* G_{II}, which is a three-dimensional nilpotent (e.g., Ref. 19) Lie group. The group multiplication is given by

$$(a,b,c)(a',b',c') = (a + a', b + b', c + c' + ab'), \tag{2.1}$$

for $(a,b,c),(a',b',c') \in G_{\mathrm{II}}$. (Note: To save space we try to express components of group elements in a row form as above, but a column form is also equally used when it is more convenient.)

Let $\tilde{M} = \mathbf{R}^3$ be the simply connected open manifold with coordinates (x,y,z). We can define the group action on this manifold identifying the group manifold G_{II} with $\tilde{M}$. The left action is therefore expressed as

$$(a,b,c)(x,y,z) = (a + x, b + y, c + z + ay), \tag{2.2}$$

where $\mathbf{a} = (a,b,c) \in G_{\mathrm{II}}$, and $\mathbf{x} = (x,y,z) \in \tilde{M} (\simeq G_{\mathrm{II}})$. Let ξ_I $(I = 1,2,3)$ be the generators of the one-parameter subgroups $(a,0,0)$, $(0,b,0)$, and $(0,0,c) \in G_{\mathrm{II}}$. It is easy to find that they are expressed

$$\xi_1 = \frac{\partial}{\partial x} + y\frac{\partial}{\partial z}, \quad \xi_2 = \frac{\partial}{\partial y}, \quad \xi_3 = \frac{\partial}{\partial z}. \tag{2.3}$$

Similarly, the generators of the right actions and their dual one-forms are given by

$$\chi_1 = \frac{\partial}{\partial x}, \quad \chi_2 = \frac{\partial}{\partial y} + x\frac{\partial}{\partial z}, \quad \chi_3 = \frac{\partial}{\partial z},$$

$$\sigma^1 = \mathrm{d}x, \quad \sigma^2 = \mathrm{d}y, \quad \sigma^3 = \mathrm{d}z - x\,\mathrm{d}y. \tag{2.4}$$

These vectors χ_I and one-forms σ^I $(I = 1-3)$ are called the *invariant vectors or one-forms* of G_{II}, since they are left invariant;

$$\mathcal{L}_{\xi_I}\chi_J = [\xi_I, \chi_J] = 0 = \mathcal{L}_{\xi_I}\sigma^J, \quad I,J = 1-3, \tag{2.5}$$

where $\mathcal{L}_{\xi_I}$ is the Lie derivative with respect to ξ_I. The invariant vectors satisfy the following commutation relations:

$$[\chi_1,\chi_2] = \chi_3, \quad [\chi_2,\chi_3] = 0, \quad [\chi_3,\chi_1] = 0. \tag{2.6}$$

The vectors ξ_I $(I = 1,2,3)$ are *Killing vectors* for the metric of the form $\tilde{q} = \tilde{q}_{IJ}\sigma^I \otimes \sigma^J$ with the components $\tilde{q}_{IJ}$ being constants. Riemannian manifold $(\tilde{M},\tilde{q})$ is called *homogeneous*, since G_{II} acts transitively on it as its isometry group.

A homogeneous metric is called *locally rotationally symmetric (LRS)* if it has a fourth independent Killing vector ξ_4. Bianchi type II LRS metrics are given by the metrics of the form $\tilde{q}^{(\mathrm{LRS})} = \tilde{q}_{11}((\sigma^1)^2 + (\sigma^2)^2) + \tilde{q}_{33}(\sigma^3)^2$, since such a metric has an additional Killing vector, given by

$$\xi_4 = -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} + \frac{1}{2}(x^2 - y^2)\frac{\partial}{\partial z}. \tag{2.7}$$

This Killing vector generates the following one-parameter isometries $s_\theta = e^{\theta\xi_4}$ for the metric $\tilde{q}^{(\mathrm{LRS})}$:

$$s_\theta : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} R_\theta \begin{pmatrix} x \\ y \end{pmatrix} \\ z + \zeta_\theta(x,y) \end{pmatrix}, \tag{2.8}$$

where $(x,y,z) \in \tilde{M}$, R_θ is the rotation matrix $R_\theta = \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right)$, and

$$\zeta_\theta(x,y) \equiv \tfrac{1}{2}((x^2 - y^2)\cos\theta - 2xy\sin\theta)\sin\theta. \tag{2.9}$$

An LRS manifold $X = (\tilde{M}, \tilde{q}^{(\mathrm{LRS})})$ has as a result a four-dimensional isometry group Isom X. Let $\mathrm{Isom}_0 X$ be its identity component, i.e., the component connected to the identity. An element $\alpha \in \mathrm{Isom}_0 X$ can be uniquely expressed as the composite $(\alpha_1, \alpha_2, \alpha_3) \circ s_\theta$ for a choice of $(\alpha_1, \alpha_2, \alpha_3) \in G_{\mathrm{II}}$ and s_θ.

The one-parameter diffeomorphism s_θ plays an important role even when the metric is not LRS. It forms a one-parameter subgroup of the automorphism group of G_{II}, which induces on the cotangent space a rotation of the invariant one-forms,

$$s_{\theta *} : \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix} \to \begin{pmatrix} R_\theta \begin{pmatrix} \sigma^1 \\ \sigma^2 \end{pmatrix} \\ \sigma^3 \end{pmatrix}. \tag{2.10}$$

The induced map s_θ^* on the tangent space acts on the invariant vectors χ_I the same way with replacement $R_\theta \to R_{-\theta}$ above. The significance of the automorphisms of Bianchi groups was first fully recognized by Jantzen.[7] Maps $s_{\theta *}$ or s_θ^* will be used in this paper in several contexts.

We can obtain the space–time metric for the conventional Bianchi cosmology assuming that all the components with respect to the invariant frame $(\mathrm{d}t, \sigma^I)$ formed by the invariant one-forms and the timelike basis dt are functions of time t only. The vacuum Bianchi II solution $\tilde{g}$ was first obtained by Taub.[18] We write that metric in the following form using our invariant one-forms (2.4):

$$\tilde{g} = -N^2(t)\mathrm{d}t^2 + q_1(t)(\sigma^1)^2 + q_2(t)(\sigma^2)^2 + q_3(t)(\sigma^3)^2, \tag{2.11}$$

where

$$N^2 = 1 + \beta^2 t^{4p_3}, \quad q_1 = t^{2p_1}N^2, \quad q_2 = t^{2p_2}N^2, \quad q_3 = 16p_3^2\beta^2 t^{2p_3}/N^2. \tag{2.12}$$

Parameters p_i $(i = 1,2,3)$ and β are constants such that $\beta > 0$, $p_3 \neq 0$, and

$$\Sigma p_i = \Sigma p_i^2 = 1. \tag{2.13}$$

When $p_1 = p_2$, the solution is LRS. Although there exist two possible such cases $(p_1, p_2, p_3) = (0,0,1)$ (case I LRS) and $(2/3, 2/3, -1/3)$ (case II LRS), these two solutions represent equivalent one-parameter solutions. In fact, we can check that the case I LRS solution with $\beta = \beta_{\mathrm{I}}$ is isometric to the case II LRS solution with $\beta = \beta_{\mathrm{II}} = 3^{-2/3}\beta_{\mathrm{I}}^{-1/3}$. When we are interested in an LRS solution, the case II LRS solution may be preferable, since the time coordinate t in this solution approaches the proper time τ at future infinity. This will make comparisons with other models like the Bianchi type III[17,13] more straightforward.

It is also worth pointing out that a solution $\tilde{g}$ with (p_1, p_2, p_3) is isometric to another solution $\tilde{g}'$ with p_1 and p_2 swapped. In fact, it is at once using Eq. (2.10) to see that $\tilde{g}'$ is the metric induced by $s_{\pi/2}$; $\tilde{g}' = s_{\pi/2 *}\tilde{g}$. We can therefore without loss of generality assume, e.g., $p_1 \leqslant p_2$.

We denote the conventional solution described so far as $(\tilde{M} \times \mathbf{R}, \tilde{g})$, and call it the *universal*

covering solution. On the other hand, our spatially closed solution, denoted $(M\times\mathbf{R},g)$, is obtained introducing a spatial compactification with it. We express the solution as

$$(M\times\mathbf{R},g)=\Gamma\backslash(\tilde{M}\times\mathbf{R},\tilde{g}), \tag{2.14}$$

using an appropriate discrete subgroup Γ of G_{II} which acts spatially from the left on the solution. The metric g here is the one induced from $\tilde{g}$. (g and $\tilde{g}$ are therefore locally isometric to each other.) While there are infinitely many possible compactifications (i.e., spatial topologies), we for definiteness specify the spatial manifold M to be "the circle bundle over the 2-torus with Euler class $e=1$." (See, e.g., Refs. 12 and 31. In general, a closed Bianchi II manifold is a *Seifert fiber space* over a Euclidean orbifold.) The fundamental group can be represented in the standard notation as

$$\pi_1(M)=\langle g_1,g_2,g_3;[g_1,g_2]=g_3,[g_1,g_3]=1,[g_2,g_3]=1\rangle, \tag{2.15}$$

where the brackets stand for group commutators, $[a,b]\equiv aba^{-1}b^{-1}$. The procedure for the actual compactification is described in the next section. The resulting spatially compactified generalization was first constructed and discussed in Ref. 15. Note that as a result of the compactification the spatial manifold specified by $t=$constant is now *locally homogeneous* (e.g., Ref. 12), and the space–time solution is said to be *spatially locally homogeneous*.

As shown in Ref. 15, Γ contains four free parameters [see Eq. (6.1)]. Our spatially closed solution (2.14) therefore forms a *six* parameter solution (since the universal cover has as we have seen *two* independent parameters, β and, e.g., p_3).

III. COMPACTIFICATION AND EIGENVALUES

To proceed, we need to describe the compactification of the spatial manifold and thereby define some eigenvalues.

Let us first describe a canonical way of expressing the Bianchi type II locally homogeneous manifold (M,q). Let $\tilde{q}^{(0)}$ be the standard metric given by

$$\tilde{q}^{(0)}=(\sigma^1)^2+(\sigma^2)^2+(\sigma^3)^2 \tag{3.1}$$

and let

$$\mathcal{N}\equiv(\tilde{M},e^{2\alpha}\tilde{q}^{(0)}) \tag{3.2}$$

be the *standard conformal manifold*, with $e^{2\alpha}$ being a constant conformal factor. Then,[10] the manifold (M,q_{ab}) can be expressed as a quotient of the standard conformal manifold (with an appropriate choice of the factor $e^{2\alpha}$),

$$(M,q)=A\backslash\mathcal{N}, \tag{3.3}$$

where A is an appropriate discrete subgroup of the isometry group of $\mathcal{N}$, $A\subset\mathrm{Isom}\,\mathcal{N}$.

The subgroup A must be isomorphic to the fundamental group $\pi_1(M)$ given by (2.15). (In fact, M is a Haken manifold.[31]) This means that A must be an embedding of $\pi_1(M)$ into the isometry group Isom $\mathcal{N}$. Let $\mathbf{a}_i\in\mathrm{Isom}\,\mathcal{N}$ $(i=1,2,3)$ be the image of π_1-generator g_i by such an embedding. Following the procedure shown in Ref. 10, we find that it is possible to parametrize them in the following way:[23]

$$\mathbf{a}_1=(u,\delta,0),\quad \mathbf{a}_2=(0,2\pi v,0),\quad \mathbf{a}_3=(0,0,2\pi uv). \tag{3.4}$$

Here, $\mathbf{a}_i\in G_{\mathrm{II}}\subset\mathrm{Isom}\,\mathcal{N}$.[24] We denote $A=\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}$. The three real parameters u, v, and δ are called the *Teichmüller parameters of geometric structure* for the locally homogeneous 3-manifold (M,q).

We construct the harmonics on (M,q) by two steps; first we do a construction on a covering manifold, denoted $(\overline{M},\overline{q})$, and then superpose appropriate subset of the harmonics to obtain those on (M,q). The *auxiliary manifold* $(\overline{M},\overline{q})$ is simply defined by removing $\mathbf{a}_1$ from A, i.e., $(\overline{M},\overline{q})$

$=\overline{A}\backslash\mathcal{N}$, where $\overline{A}=\{\mathbf{a}_2,\mathbf{a}_3\}$. $\overline{A}$ is a commutative subgroup of A, and therefore $\overline{M}$ is homeomorphic to the much tractable manifold $T^2\times\mathbf{R}$. In fact, we can easily see that it is each $x=$constant plane in $\mathcal{N}$ that is compactified to a 2-torus.

Now, let us introduce some important operators. We define the "total angular momentumlike" operator

$$\mathsf{L}^2 \equiv (\mathcal{L}_{\chi_1})^2 + (\mathcal{L}_{\chi_2})^2, \tag{3.5}$$

using the Lie derivatives $\mathcal{L}_{\chi_1}$ and $\mathcal{L}_{\chi_2}$. Note that when acting on a scalar, it becomes a simple form

$$\mathsf{L}^2 = (\chi_1)^2 + (\chi_2)^2, \tag{3.6}$$

which also coincides with the Laplacian Δ_0 with respect to the standard metric $\tilde{q}^{(0)}$, up to square of χ_3,

$$\Delta_0 = \mathsf{L}^2 + (\chi_3)^2, \tag{3.7}$$

when acting on a scalar. Here, χ_I $(I=1,2,3)$ are regarded as differential operators. It is quite important to recognize that operators χ_I are well defined not only on the universal cover $\tilde{M}$ but also on the compactified manifold $M=A\backslash\tilde{M}$. In other words, the induced vector fields $\pi^*\chi_I$ on M for the covering map $\pi:\tilde{M}\to M=A\backslash\tilde{M}$ is well defined because of the invariance of χ_I under the action of $A\subset G_{\mathrm{II}}$. (For simplicity we do not explicitly write π^*, and identify $\pi^*\chi_I$ and χ_I.) Since $\overline{A}$ is also a subgroup of G_{II}, χ_I are well defined on $\overline{M}$, also. The globally defined invariant operators χ_I work as the fundamental derivative operators, since any group-invariant field equations become independent of coordinates when they are written with χ_I. This coordinate-free property of the field equations is necessary to be able to reduce the field equation to ordinary differential equations.

The operator χ_3, called the *fiber generator*, has a special importance, since it commutes with all the invariant operators χ_I. In other words, χ_3 is the *center* of the Bianchi II algebra. As a direct consequence of Schur's lemma, such an operator must be diagonalized to obtain an irreducible representation of the regular representation mentioned in the Introduction.

The operator $\mathsf{L}^2=(\chi_1)^2+(\chi_2)^2$ commutes with χ_3, since χ_3 is the center. We may therefore be able to diagonalize our mode functions with respect to both χ_3 and L^2. Also, consider another operator $\xi_2=\partial/\partial y$, which we can find commutes with both L^2 and χ_3, so we may diagonalize the mode functions with respect to ξ_2, also. This operator however is *not* well defined on M, but on $\overline{M}$. This is the reason we consider the auxiliary manifold $\overline{M}$. The existence of ξ_2 is important to make it possible to perform separation of variables for the eigenvalue equation for L^2 (see below).

Let $i\mu$ and $i\nu$ be eigenvalues for the operators χ_3 and ξ_2,

$$\chi_3\overline{\phi}=i\mu\overline{\phi}, \quad \xi_2\overline{\phi}=i\nu\overline{\phi}. \tag{3.8}$$

The function $\overline{\phi}$ is supposed to be an appropriate mode function on $\overline{M}$. Also, we define λ by $\mathsf{L}^2\overline{\phi}=-\lambda^2\overline{\phi}$. The solution of these equations is given by

$$\overline{\phi}=X(x)e^{i\mu z}e^{i\nu y}, \tag{3.9}$$

where the function $X(x)$ is a solution of the following "harmonic oscillator Schrödinger equation":

$$\frac{\mathrm{d}^2X}{\mathrm{d}x^2}+(\lambda^2-(\mu x+\nu)^2)X=0. \tag{3.10}$$

For $\overline{\phi}$ to be well defined on $\overline{M}$, it must be an automorphic function such that $\overline{\phi}(\overline{A}\mathbf{x})=\overline{\phi}(\mathbf{x})$.[25] From this condition we find

$$\mu = \mu(m) = m/(uv), \quad m \in \mathbf{Z},$$

$$\nu = \nu(n) = n/v, \quad n \in \mathbf{Z}. \tag{3.11}$$

We call μ, m, ν, and n, respectively, the *fiber eigenvalue*, *fiber index*, *auxiliary eigenvalue*, and *auxiliary index*. We call λ^2 the *total eigenvalue*. The spectrum of λ^2 is determined in the next section.

IV. IRREDUCIBLE DIFFERENTIAL REPRESENTATIONS

It is not difficult to determine the irreducible representations of the regular representation in their differential form, i.e., the differential representations of the Bianchi II algebra. In fact, it will be found that this procedure is similar to the one in determining quantum states of the harmonic oscillator, since L^2 (or the scalar Laplacian Δ_0) has essentially the same algebraic structure as that of the Hamiltonian of the oscillator.

As mentioned in the preceding section since the fiber generator χ_3 must be a constant when acting on an irreducible subspace, the fiber index $m \in \mathbf{Z}$ is constant in this space. We therefore assume that m is fixed throughout this section. It may be helpful to bear in mind that as for the correspondence to quantum mechanics, the fiber eigenvalue $\mu = m/uv$ corresponds to the Planck constant h, while χ_1 and χ_2 correspond, respectively, to the position x and momentum p operators, as in $[x,p]=ih \Leftrightarrow [\chi_1,\chi_2]=\chi_3=i\mu$. Remember however that our representation space is $L^2(M)$ instead of $L^2(\mathbf{R})$.

In this section we deal with the generic $m \neq 0$ case. The exceptional $m=0$ case will be discussed in Sec. VII.

Let ϕ be an eigenfunction on M for the operators χ_3 and L^2, i.e., $\chi_3\phi = i\mu\phi$, and $\mathsf{L}^2\phi = -\lambda^2\phi$. It is helpful to introduce a symbol signifying the sign of the fiber eigenvalue, which allows us to discuss both $m \gtrless 0$ cases simultaneously; we define

$$\varsigma \equiv \mathrm{sign}(m) = \mathrm{sign}(\mu) \quad (m \neq 0). \tag{4.1}$$

Let us then define

$$\mathcal{A}_1 \equiv \frac{1}{\sqrt{2}}(\chi_1 + \varsigma i\chi_2), \quad \mathcal{A}_2 \equiv \frac{1}{\sqrt{2}}(\chi_1 - \varsigma i\chi_2), \quad \mathcal{A}_3 \equiv -\varsigma i\chi_3. \tag{4.2}$$

Then, we immediately find the following commutation relations:

$$[\mathsf{L}^2, \mathcal{A}_1] = \varsigma 2i\mathcal{A}_1\chi_3, \quad [\mathsf{L}^2, \mathcal{A}_2] = -\varsigma 2i\mathcal{A}_2\chi_3. \tag{4.3}$$

This means that $\mathcal{A}_1$ and $\mathcal{A}_2$ are, respectively, a *raising and lowering operator* for the total eigenvalue λ^2. In fact, since

$$\mathsf{L}^2\mathcal{A}_1\phi = ([\mathsf{L}^2, \mathcal{A}_1] + \mathcal{A}_1\mathsf{L}^2)\phi = (\varsigma 2i\mathcal{A}_1\chi_3 + \mathcal{A}_1\mathsf{L}^2)\phi = -(2|\mu| + \lambda^2)\mathcal{A}_1\phi, \tag{4.4}$$

$\mathcal{A}_1\phi$ is an eigenfunction for $\lambda'^2 = \lambda^2 + 2|\mu|$. Similarly, $\mathcal{A}_2\phi$ is an eigenfunction for $\lambda'^2 = \lambda^2 - 2|\mu|$.

Taking into account the fact that $\mathcal{A}_1$ and $\mathcal{A}_2$ change the eigenvalue λ^2 by $\pm 2|\mu(m)|$, we can without loss of generality assume the form of spectrum as

$$\lambda^2 = |\mu|(2l + c_m), \tag{4.5}$$

where

$$l = 0, 1, \ldots . \tag{4.6}$$

The value for $l=0$, $\lambda^2 = \lambda_0^2 \equiv |\mu| c_m$, corresponds to the smallest one for given m, which must exist because minus the Laplacian $-\Delta_0 = -\mathsf{L}^2 - (\chi_3)^2 = -(\mathsf{L}^2 + \mu^2)$ can have only non-negative eigenvalues. We call l the *spin index*.

At this point we know the eigenmode is specified by the pair of integers (l,m), so the corresponding eigenfunction can be expressed with these labels $\phi_{l,m}$. As we remarked since the value of m does not change in an irreducible space, we drop m and write ϕ_l for simplicity.

Let us write down the whole relations we have as

$$\begin{aligned} \mathsf{L}^2\phi_l &= -|\mu|(2l+c_m)\phi_l, \\ \mathcal{A}_3\phi_l &= |\mu|\phi_l, \\ \mathcal{A}_1\phi_l &= \alpha_l\phi_{l+1}, \\ \mathcal{A}_2\phi_l &= \beta_l\phi_{l-1}, \end{aligned} \tag{4.7}$$

where we have introduced unknown constants α_l and β_l, which possibly depend on l.

Note the following identity that can be easily checked by a direct computation:

$$\mathsf{L}^2 = 2\mathcal{A}_1\mathcal{A}_2 - \mathcal{A}_3. \tag{4.8}$$

Using Eqs. (4.7), this implies $-|\mu|(2l+c_m)=2\alpha_{l-1}\beta_l-|\mu|$, i.e.,

$$\alpha_{l-1}\beta_l = -|\mu|\left(l+\frac{c_m-1}{2}\right). \tag{4.9}$$

Because of the arbitrariness of constant multipliers for the eigenfunctions ϕ_l, we may set α_l or β_l arbitrarily, but once it is set, the other is constrained from this relation. We take[26]

$$\alpha_l = -\sqrt{|\mu|}, \quad \beta_l = \sqrt{|\mu|}\left(l+\frac{c_m-1}{2}\right). \tag{4.10}$$

These do satisfy Eq. (4.9). Then, since we defined l so that $l=0$ gives, for given $m\neq 0$, the smallest eigenvalue of $-\mathsf{L}^2$, we should have

$$\mathcal{A}_2\phi_0 = \beta_0\phi_{-1} = \sqrt{|\mu|}\left(\frac{c_m-1}{2}\right)\phi_{-1} = 0, \tag{4.11}$$

implying

$$c_m = 1. \tag{4.12}$$

So, now we have

$$\alpha_l = -\sqrt{|\mu|}, \quad \beta_l = \sqrt{|\mu|}\, l. \tag{4.13}$$

Gathering Eqs. (4.2), (4.7), and (4.13), we arrive at the following set of relations:

$$\begin{aligned} \chi_1\phi_l &= -\sqrt{\frac{|\mu|}{2}}(\phi_{l+1}-l\phi_{l-1}), \\ \chi_2\phi_l &= \varsigma i\sqrt{\frac{|\mu|}{2}}(\phi_{l+1}+l\phi_{l-1}), \\ \chi_3\phi_l &= i\mu\phi_l, \\ l &= 0,1,\ldots. \end{aligned} \tag{4.14}$$

In particular,

$$\mathsf{L}^2\phi_l = -\lambda_l^2\phi_l, \quad \lambda_l^2 \equiv |\mu|(2l+1). \tag{4.15}$$

Now, we have found the following. A "ground state" ϕ_0 is determined as a solution for the two equations

$$\mathcal{A}_3\phi_0 = |\mu|\phi_0, \quad \mathcal{A}_2\phi_0 = 0. \tag{4.16}$$

Note that the function ϕ_0 obtained this way is automatically an eigenfunction of L^2 as seen from the identity (4.8). The excited states ϕ_l are determined by successively multiplying the raising operator $(-1/\sqrt{|\mu|})\mathcal{A}_1$, i.e.,

$$\phi_l = \left(-\frac{\mathcal{A}_1}{\sqrt{|\mu|}}\right)^l \phi_0. \tag{4.17}$$

The space spanned by these functions, $L_m^2(M) \equiv \{\Sigma_{l=0}^{\infty} a_l\phi_l | a_l \in \mathbf{C}\} \cap L^2(M)$, gives an irreducible subspace of $L^2(M)$. In other words, the restriction of the regular representation T to $L_m^2(M)$, denoted as $(T_m, L_m^2(M))$, gives an irreducible representation. The differential representation $(\mathrm{d}T_m, L_m^2(M))$ is given by Eqs. (4.14), which will be repeatedly used to separate the field equations. For convenience, we call these relations the χ *relations*.

V. MODE FUNCTIONS ON THE COMPACTIFIED MANIFOLD

In this section we solve the eigenvalue equations for the mode functions ϕ_l under the appropriate automorphic conditions. As a result we find how many equivalent copies of the irreducible representation T_m are contained in T, in other words, the multiplicity of T_m is determined. The explicit form of ϕ_l itself is also of great interest. In this section we continue to assume $m \neq 0$.

One of the possible procedures to find the explicit form of ϕ_l is to solve the equations (4.16) to find ϕ_0 and compute successive differential operations in Eq. (4.17) to find general ϕ_l. Another procedure is to directly solve the eigenvalue equation $\mathsf{L}^2\phi_l = -\lambda^2\phi_l$ for general spin index l. While both ways are possible, we take the latter, which provides a quicker way of identifying the solutions with known functions.

As remarked in Sec. III, let us find the mode functions on $\overline{M}$ first. Note that Eq. (3.10) becomes (attaching index l to X)

$$\frac{\mathrm{d}^2X_l}{\mathrm{d}\zeta^2} + \left(l + \frac{1}{2} - \frac{\zeta^2}{4}\right)X_l = 0, \tag{5.1}$$

if we define

$$\zeta = \mathfrak{s}\sqrt{\frac{2}{|\mu|}}(\mu x + \nu). \tag{5.2}$$

Independent solutions to the above equation are given by $D_l(\zeta)$ and $D_{-l-1}(i\zeta)$, where $D_l(\zeta)$ is the Weber parabolic cylinder function. When l is zero or a positive integer, $D_l(\zeta)$ can be expressed using the Hermite polynomial $H_l(\zeta)$,

$$D_l(\zeta) = e^{-(1/4)\zeta^2}H_l(\zeta). \tag{5.3}$$

Our convention for the Hermite polynomial is $H_l(\zeta) = (-1)^l e^{(1/2)\zeta^2}(\mathrm{d}^l/\mathrm{d}\zeta^l)e^{-(1/2)\zeta^2}$.

Since ϕ_0 must be annihilated by $\mathcal{A}_2$ the appropriate choice is found to be $D_l(\zeta)$, i.e., we must take $X_l = \mathrm{const} \times D_l(\zeta)$. In fact, the equation $\mathcal{A}_2\overline{\phi_0} = 0$ together with the separation form $\overline{\phi_l} = X_l(x)e^{i\nu y}e^{i\mu z}$, implies $(\mathrm{d}/\mathrm{d}\zeta + (1/2)\zeta)X_0 = 0$, with the solution being $X_0 = \mathrm{const} \times e^{-(1/4)\zeta^2}$. This coincides with the one claimed for $l=0$. [Conversely, as we will see, functions ϕ_l constructed using these X_l can satisfy the desired relations (4.14) for all l, which justifies our choice.]

The mode functions on $\overline{M}$ are therefore, attaching indices m and n, given by

$$\overline{\phi}_{l,m,n}(\mathbf{x}) = C_l D_l\left(\pm\sqrt{\frac{2}{|\mu|}}(\mu x+\nu)\right)e^{i\mu z}e^{i\nu y}, \tag{5.4}$$

where C_l are constants and μ and ν are defined in Eqs. (3.11).

The constants C_l are determined by requiring that the functions $\overline{\phi}_{l,m,n}(\mathbf{x})$ obey the χ relations (4.14). Using the widely known formulas

$$D_l'(\zeta) = -\tfrac{1}{2}(D_{l+1}(\zeta) - lD_{l-1}(\zeta)),$$

$$\zeta D_l(\zeta) = D_{l+1}(\zeta) + lD_{l-1}(\zeta), \tag{5.5}$$

we can easily find $C_{l+1}=C_l$, i.e., they are constants that do not depend on l;

$$C_l = C. \tag{5.6}$$

[Actually, this is the reason we choose Eqs. (4.13).] The constant C may be determined by a normalization of the square integral on M. (See below.)

The mode functions on M are, as mentioned, expressed as an infinite sum of these eigenfunctions on $\overline{M}$. Remember that they must be invariant under the action of $A=\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}$, and the functions $\overline{\phi}_{l,m,n}$ are already invariant under $\overline{A}=\{\mathbf{a}_2,\mathbf{a}_3\}$. We therefore want to make a linear combination of $\overline{\phi}_{l,m,n}$ so that it is invariant under $\mathbf{a}_1$. Recalling the multiplication rule (2.2), we find the following transformation law [cf. Ref. 13, Eq. (3.15)]:

$$\overline{\phi}_{l,m,n}(\mathbf{a}_1\mathbf{x}) = e^{i(\delta/v)n}\overline{\phi}_{l,m,n+m}(\mathbf{x}). \tag{5.7}$$

From this we can see that the following function ϕ_{l,m,n_0}, defined as an infinite sum, is actually invariant under the action of $\mathbf{a}_1$ (cf. Ref. 13, Theorem 3.1), i.e., $\phi_{l,m,n_0}(\mathbf{a}_1\mathbf{x})=\phi_{l,m,n_0}(\mathbf{x})$ for

$$\phi_{l,m,n_0}(\mathbf{x}) = \sum_{k=-\infty}^{\infty} e^{i\delta\{n_0k+m[k(k-1)/2]\}}\overline{\phi}_{l,m,n_0+mk}(\mathbf{x}), \tag{5.8}$$

where $l=0,1,\ldots,\infty$, $|m|=1,2,\ldots,\infty$, $n_0=0,1,\ldots,|m|-1$. The sum is convergent at any point $\mathbf{x}$. It is easy to see that since the functions $\overline{\phi}_{l,m,n}(\mathbf{x})$ satisfy the relations (4.14), so do $\phi_{l,m,n_0}(\mathbf{x})$. These functions are therefore the right mode functions on $M=A\backslash\tilde{M}$.

As a result of the compactification, the index n_0 for the mode functions on M is now bounded by $|m|$. $|m|$ is the *multiplicity* of the modes specified by the same l and m. Since for each n_0 the functions $\phi_{l,m}$ span an irreducible subspace of $L^2(M)$, $|m|$ is also the multiplicity of the irreducible representation T_m contained in T.

We can summarize the results as follows.

Theorem 5.1: *There exist $|m|$ different sets of mode functions $\{\phi_l(\mathbf{x})\}_{l=0}^{\infty}$ that satisfy the relations (4.14) on the compactified manifold $(M,q_{ab})=A\backslash\mathcal{N}$ (with M being the S^1-bundle over the 2-torus with Euler class $e=1$).*

Let us discuss how the mode functions can be normalized. We define the inner product in $L^2(M)$ as

$$(f,g) \equiv \int_M fg^*\,\mathrm{d}\mu_0, \tag{5.9}$$

where g^* is the complex conjugate of g, $\mathrm{d}\mu_0=\sigma^1\wedge\sigma^2\wedge\sigma^3=\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ is the standard invariant measure. We want to determine the square norm

$$N_l \equiv (\phi_l,\phi_l). \tag{5.10}$$

We first observe the following.

Lemma 5.2: The invariant operators χ_I $(I=1-3)$ *in* $L^2(M)$ *are anti-self-adjoint,* $\chi_I^\dagger=-\chi_I$.
Proof: Since

$$(\chi_I f,g)=\int_M (\chi_I(fg^*)-f\chi_I g^*)\mathrm{d}\mu_0=\mathcal{I}_I-(f,\chi_I g), \tag{5.11}$$

we need to show $\mathcal{I}_I\equiv\int_M \chi_I(fg^*)\mathrm{d}\mu_0=0$. In fact, when, e.g., $I=1$, we can show $\mathcal{I}_1=\int_M \chi_1(fg^*)\sigma^1\wedge\sigma^2\wedge\sigma^3=\int_M \mathrm{d}(fg^*\sigma^2\wedge\sigma^3)$, which is from Stoke's theorem $\int_{\partial M} fg^*\sigma^2\wedge\sigma^3=0$. Here, we have used the identity

$$\mathrm{d}f=(\chi_1 f)\sigma^1+(\chi_2 f)\sigma^2+(\chi_3 f)\sigma^3, \tag{5.12}$$

which is valid for an arbitrary function f on M, and also used the relation $\mathrm{d}(\sigma^2\wedge\sigma^3)=0$, which is confirmed from the definition (2.4). The other cases $I=2,3$ are the same, since $\mathrm{d}(\sigma^1\wedge\sigma^3)=\mathrm{d}(\sigma^1\wedge\sigma^2)=0$. ■

Remark: Operators $(1/i)\chi_I$ $(I=1-3)$ are self-adjoint.

Corollary 5.3: In $L^2(M)$, $\mathcal{A}_1^\dagger=-\mathcal{A}_2$.

Proof: $\mathcal{A}_1^\dagger=2^{-1/2}(\chi_1+\mathfrak{s}i\chi_2)^\dagger=2^{-1/2}(\chi_1^\dagger-\mathfrak{s}i\chi_2^\dagger)=-2^{-1/2}(\chi_1-\mathfrak{s}i\chi_2)=-\mathcal{A}_2$. ■

Returning to the issue of N_l, consider $N_{l+1}=(\phi_{l+1},\phi_{l+1})$. When $m\neq 0$, from Eqs. (4.7) and Corollary 5.3 we have

$$\mathcal{N}_{l+1}=\frac{1}{\alpha_l\alpha_l^*}(\mathcal{A}_1\phi_l,\mathcal{A}_1\phi_l)=\frac{1}{\alpha_l\alpha_l^*}(\phi_l,\mathcal{A}_1^\dagger\mathcal{A}_1\phi_l)=\frac{-1}{\alpha_l\alpha_l^*}(\phi_l,\mathcal{A}_2\mathcal{A}_1\phi_l)=\frac{-1}{\alpha_l\alpha_l^*}(\phi_l,\beta_{l+1}\alpha_l\phi_l)=\frac{-\beta_{l+1}^*}{\alpha_l}N_l. \tag{5.13}$$

Substituting our choice (4.13) of α_l and β_l we have

$$N_{l+1}=(l+1)N_l. \tag{5.14}$$

Taking $N_0=1$ we conclude

$$N_l=l!\,. \tag{5.15}$$

Now, we have the following.

Theorem 5.4: *Suppose that* ϕ_l *are mode functions on* $(M,q_{ab})=A\backslash\mathcal{N}$ *such that they satisfy the relations (4.14). Multiplying the same constant normalization factor* C *to all* ϕ_l, $\phi_l\to C\phi_l$, *does not change those relations. By choosing* C *appropriately, we can make the normalization*

$$(\phi_{l,m,n_0},\phi_{l',m',n_0'})=l!\,\delta_{ll'}\delta_{mm'}\delta_{n_0n_0'} \tag{5.16}$$

hold.

Proof: The orthogonality for m and m' is apparent from the fact that $\mu(m)$ is the eigenvalue of the self-adjoint operator $(1/i)\underline{\chi}_3$. The orthogonality for n_0 and n_0' comes from the orthogonality among the mode functions on $\bar{M}$:

$$(\bar{\phi}_{l,m,n},\bar{\phi}_{l,m,n'})_{\bar{M}}\equiv\int_{\bar{M}}\bar{\phi}_{l,m,n}\bar{\phi}_{l,m,n'}^*\,\mathrm{d}\mu_0=0\quad(n\neq n'), \tag{5.17}$$

which is also apparent from the fact that the operator $(1/i)\xi_2$, of which eigenvalues are $\nu(n)$, is self-adjoint on $L^2(\bar{M})$. Observing that when $n_0\neq n_0'$, ϕ_{l,m,n_0}, and $\phi_{l,m,n_0'}$ are linear combinations in different sets $\{\bar{\phi}_{l,m,n}\}_{n\in\mathcal{N}_1}$ and $\{\bar{\phi}_{l,m,n}\}_{n\in\mathcal{N}_2}$, $\mathcal{N}_1\cap\mathcal{N}_2=\varnothing$, we can easily see

$$\int_{\bar{M}} \phi_{l,m,n_0} \phi^*_{l,m,n_0'} \, \mathrm{d}\mu_0 = 0 \quad (n_0 \neq n_0'), \tag{5.18}$$

which in turn implies the orthogonality for n_0 and n_0' in $L^2(M)$. The other part has already been proven. ■

Remark: The constant C does not depend on l, but can depend on m and n_0, so we may write $C = C_{m,n_0}$.

Apparently, if we define

$$\phi^{(\mathrm{n})}_{l,m,n_0} \equiv \frac{1}{\sqrt{l!}} \phi_{l,m,n_0}, \tag{5.19}$$

they become orthonormal to each other,

$$(\phi^{(\mathrm{n})}_{l,m,n_0}, \phi^{(\mathrm{n})}_{l',m',n_0'}) = \delta_{ll'} \delta_{mm'} \delta_{n_0 n_0'}. \tag{5.20}$$

As seen from Eqs. (5.13) and (4.9) this corresponds to choosing

$$\alpha^{(\mathrm{n})}_l = e^{i\Theta_l} \sqrt{|\mu|(l+1)}, \quad \beta^{(\mathrm{n})}_l = -e^{-i\Theta_l} \sqrt{|\mu| l}, \tag{5.21}$$

where Θ_l is an arbitrary phase factor, which we may want to take zero, $\Theta_l = 0$. Substituting $\alpha_l = \alpha^{(\mathrm{n})}_l$ and $\beta_l = \beta^{(\mathrm{n})}_l$ into Eqs. (4.7) we have another version of χ relations for $\phi^{(\mathrm{n})}_{l,m,n_0}$, which have the most direct correspondence to the usual relations between the quantum states of the harmonic oscillator. As mentioned however we employ the unnormalized ϕ_l in this paper for the convenience of computation.

VI. FURTHER TRANSFORMATION

The mode functions $\phi_{l,m,n_0}(\mathbf{x})$ shown in the preceding section are *not* well defined on the general space–time solution $(M \times \mathbf{R}, g) = \Gamma \backslash (\tilde{M} \times \mathbf{R}, \tilde{g})$, because of the fact $A \neq \Gamma$. Remember that $\Gamma \subset G_{\mathrm{II}}$ is a four-parameter embedding, while A is a three-parameter one. This incompatibility means that we cannot identify the coordinates $\mathbf{x}$ in $\mathcal{N}$ with the spatial coordinates $\mathbf{x}$ in $(\tilde{M} \times \mathbf{R}, \tilde{g})$.[27] Although it is expected that an appropriate diffeomorphism can make the mode functions well defined on the space–time, such a diffeomorphism can affect the χ relations. In the following, we show by explicit computations that this is the case but a further renormalization makes the mode functions retain the original χ relations.

As shown in Ref. 15, the covering group Γ can be parametrized as

$$\Gamma = \{\gamma_1, \gamma_2, \gamma_3\} = \left\{ \begin{pmatrix} R_{-\theta} \begin{pmatrix} u \\ \delta \end{pmatrix} \\ 0 \end{pmatrix}, \begin{pmatrix} R_{-\theta} \begin{pmatrix} 0 \\ 2\pi v \end{pmatrix} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 2\pi u v \end{pmatrix} \right\}, \tag{6.1}$$

where $\gamma_i \in G_{\mathrm{II}}$, and θ, u, δ, and v are real parameters.[28,29] Let $(M, q) = \Gamma \backslash (\tilde{M}, \tilde{q}_{ab})$ be the *spatial section* of the solution, where $\tilde{q}$ is the spatial part of $\tilde{g}$. For convenience of considering diffeomorphisms between the spatial universal cover $(\tilde{M}, \tilde{q}_{ab})$ and the standard conformal manifold $\mathcal{N} = (\tilde{M}, e^{2\alpha} \tilde{q}^{(0)})$, let us distinguish the latter manifold (without metric structure) by denoting $\tilde{M}'$. This distinction is meant to be helpful just to keep track of the direction of the diffeomorphisms we consider.

Let ψ be a diffeomorphism,

$$\psi : \tilde{M} \to \tilde{M}' \tag{6.2}$$

such that

$$\Gamma = \psi^{-1} \circ A \circ \psi. \tag{6.3}$$

Then, the induced function of $\phi_{l,m,n_0}(\mathbf{x})$ will be invariant under Γ, since so is $\phi_{l,m,n_0}(\mathbf{x})$ under A.

We can find ψ in Isom $\mathcal{N}$, which is explicitly given by

$$\psi = \mathbf{b} \circ s_\theta, \tag{6.4}$$

where $\mathbf{b} \in G_{\mathrm{II}}$ is

$$\mathbf{b} = (\pi v \cos\theta \sin\theta, u^{-1}(-\zeta_{-\theta}(u,\delta) + \pi\delta v \sin\theta \cos\theta), 0). \tag{6.5}$$

We have, for simplicity, chosen the third component of $\mathbf{b}$ as zero, though it can be an arbitrary constant. The induced vectors $\psi^* \chi_I$ on $\tilde{M}'$ becomes a linear transformation of χ_I, due to the property that elements in Isom $\mathcal{N}$ are automorphisms of G_{II}. Note that when acting on the vectors χ_I, the induced map $\psi^* = \mathbf{b}^* \circ s_\theta^*$ becomes the same as s_θ^*, since χ_I are by definition invariant under the induced map $\mathbf{b}^*$ for $\mathbf{b} \in G_{\mathrm{II}}$. Therefore from (the vector version of) Eq. (2.10), we have

$$\psi^* : \begin{pmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix} \to \begin{pmatrix} \psi^*\chi_1 \\ \psi^*\chi_2 \\ \psi^*\chi_3 \end{pmatrix} = \begin{pmatrix} R_{-\theta}\begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} \\ \chi_3 \end{pmatrix}. \tag{6.6}$$

Let $\phi_l^{(\mathrm{ss})}(\mathbf{x}) \equiv (\psi_* \phi_l)(\mathbf{x}) = \phi_l \circ \psi(\mathbf{x})$, where $\mathbf{x} \in \tilde{M}$. [Superscript (ss) stands for "spatial section."] Then,

$$\chi_1 \phi_l^{(\mathrm{ss})} = \chi_1(\psi_* \phi_l) = (\psi^* \chi_1)\phi_l \circ \psi = (\cos\theta \chi_1 + \sin\theta \chi_2)\phi_l \circ \psi = \sqrt{\frac{|\mu|}{2}}(-e^{-i\theta}\phi_{l+1} + e^{i\theta} l \phi_{l-1}) \circ \psi$$

$$= \sqrt{\frac{|\mu|}{2}}(-e^{-i\theta}\phi_{l+1}^{(\mathrm{ss})} + e^{i\theta} l \phi_{l-1}^{(\mathrm{ss})}), \tag{6.7}$$

where we have used the relations (4.14). Similarly, we obtain

$$\chi_2 \phi_l^{(\mathrm{ss})} = \mathrm{s}i \sqrt{\frac{|\mu|}{2}}(e^{-i\theta}\phi_{l+1}^{(\mathrm{ss})} + e^{i\theta} l \phi_{l-1}^{(\mathrm{ss})}), \tag{6.8}$$

and $\chi_3 \phi_l^{(\mathrm{ss})} = i\mu \phi_l^{(\mathrm{ss})}$. These relations are different from the original χ relations (4.14) unless θ is a multiple of 2π.

However, it is possible to renormalize $\phi_l^{(\mathrm{ss})}$ so that the original χ relations are recovered. It is straightforward to check that

$$\varphi_l = e^{i\theta l} \phi_l^{(\mathrm{ss})} \tag{6.9}$$

gives such a renormalized function. Thus, we have found that the functions $\varphi_l = e^{i\theta l}\phi_l \circ \psi$ with ϕ_l given by Eq. (5.8) and ψ being Eq. (6.4), are served as the right mode functions on the spatial section (and therefore on the space–time) that satisfy the relations (4.14). This provides a direct proof of the following.

Theorem 6.1: *There exist $|m|$ different sets of time-independent mode functions $\{\varphi_{l,m}(\mathbf{x})\}_{l=0}^{\infty}$ on the spatially closed Bianchi II solution $(M \times \mathbf{R}, g) = \Gamma \backslash (\tilde{M} \times \mathbf{R}, \tilde{g})$ such that they satisfy the relations (4.14).*

VII. U(1)-SYMMETRIC MODES

Let us, for completeness, consider the modes with the fiber index m being zero. We call these modes U(1)-*symmetric*, since they are constant along the U(1) ($\simeq S^1$) fibers.

Let ϕ be an eigenfunction for $m=0$, i.e., $\chi_3 \phi = (\partial\phi/\partial z) = 0$. This in turn implies that χ_1 and χ_2 are commutative when acting on ϕ,

$$[\chi_1,\chi_2]\phi=0, \tag{7.1}$$

since $[\chi_1,\chi_2]=\chi_3$. Due to this property, the harmonics describing the $m=0$ subspace of $L^2(M)$ become the usual Fourier expansion on a torus. (Thus, together with the results for the generic modes we obtain Theorem 1.1.) In the following we explicitly determine the spectrum of the eigenvalues for the operators χ_1 and χ_2 in terms of the space–time moduli parameters u, δ, v, and θ.

Let us first work on the 3-manifold $A\backslash\mathcal{N}$ (not on the space–time manifold) as we did for the generic $(m\neq 0)$ case. Taking the form of A into account, we label the mode functions with the following equations:

$$(u\chi_1+\delta\chi_2)\phi=2\pi i k_1\phi,$$

$$v\chi_2\phi=ik_2\phi, \tag{7.2}$$

where the eigenvalues k_1 and k_2 are to be used as labels. Let us therefore write the solution of these equations as $\phi=\phi^{(0)}_{k_1,k_2}(\mathbf{x})=\phi^{(0)}_{k_1,k_2}(x,y)$, which is given by

$$\phi^{(0)}_{k_1,k_2}=\text{const}\times e^{(i/u)[2\pi k_1 x+(k_2/v)(-\delta x+uy)]}. \tag{7.3}$$

Since, recalling the rule (2.2),

$$\phi^{(0)}_{k_1,k_2}(\mathbf{a}_1\mathbf{x})=\phi^{(0)}_{k_1,k_2}(x+u,y+\delta)=\phi^{(0)}_{k_1,k_2}(\mathbf{x})e^{2\pi i k_1},$$

$$\phi^{(0)}_{k_1,k_2}(\mathbf{a}_2\mathbf{x})=\phi^{(0)}_{k_1,k_2}(x,y+2\pi v)=\phi^{(0)}_{k_1,k_2}(\mathbf{x})e^{2\pi i k_2}, \tag{7.4}$$

we find

$$k_1\in\mathbf{Z},\quad k_2\in\mathbf{Z}, \tag{7.5}$$

for $\phi^{(0)}_{k_1,k_2}$ to be well defined on $M=A\backslash\tilde{M}$. The remaining condition $\phi^{(0)}_{k_1,k_2}(\mathbf{a}_3\mathbf{x})=\phi^{(0)}_{k_1,k_2}(\mathbf{x})$ is trivial.

Therefore from Eqs. (7.2) the χ relations for the U(1)-symmetric modes are

$$\chi_1\phi^{(0)}_{k_1,k_2}=iK_1(k_1,k_2)\phi^{(0)}_{k_1,k_2},$$

$$\chi_2\phi^{(0)}_{k_1,k_2}=iK_2(k_2)\phi^{(0)}_{k_1,k_2}, \tag{7.6}$$

$$\chi_3\phi^{(0)}_{k_1,k_2}=0,$$

where

$$K_1(k_1,k_2)\equiv\frac{1}{u}\left(2\pi k_1-\frac{\delta}{v}k_2\right),$$

$$K_2(k_2)\equiv\frac{k_2}{v}. \tag{7.7}$$

To extend the mode functions on the space–time manifold $\Gamma\backslash(\tilde{M}\times\mathbf{R},\tilde{g})$, we need to apply the diffeomorphism ψ defined in Eq. (6.4) again, and as a result the spectrum of the eigenvalues are altered. (Contrary to the generic case, any renormalizations of the resulting mode functions do not affect the χ relations.)

As in the preceding section, let us define $\varphi^{(0)}_{k_1,k_2}\equiv\phi^{(0)}_{k_1,k_2}\circ\psi$. Then, from Eq. (6.6), we have, e.g.,

$$\chi_1\varphi^{(0)}_{k_1,k_2} = (\psi^*\chi_1)\phi^{(0)}_{k_1,k_2}\circ\psi = (\cos\ \theta\chi_1 + \sin\ \theta\chi_2)\phi^{(0)}_{k_1,k_2}\circ\psi = i(\cos\ \theta K_1 + \sin\ \theta K_2)\varphi^{(0)}_{k_1,k_2}. \quad (7.8)$$

A similar result is also obtained for $\chi_2\varphi^{(0)}_{k_1,k_2}$. We write the final form of the relations as follows:

$$\chi_1\varphi^{(0)}_{k_1,k_2} = i\kappa_1(k_1,k_2)\varphi^{(0)}_{k_1,k_2},$$

$$\chi_2\varphi^{(0)}_{k_1,k_2} = i\kappa_2(k_1,k_2)\varphi^{(0)}_{k_1,k_2}, \quad (7.9)$$

$$\chi_3\varphi^{(0)}_{k_1,k_2} = 0, \quad k_1 \in \mathbf{Z}, \quad k_2 \in \mathbf{Z},$$

where

$$\kappa_1(k_1,k_2) \equiv \cos\ \theta K_1(k_1,k_2) + \sin\ \theta K_2(k_2),$$

$$\kappa_2(k_1,k_2) \equiv -\sin\ \theta K_1(k_1,k_2) + \cos\ \theta K_2(k_2). \quad (7.10)$$

Now, we have the following.

Theorem 7.1: *There exist time-independent mode functions* $\varphi^{(0)}_{k_1,k_2}(\mathbf{x})$, $k_1,k_2 \in \mathbf{Z}$, *on the spatially closed Bianchi II solution* $(M\times\mathbf{R},g)=\Gamma\backslash(\tilde{M}\times\mathbf{R},\tilde{g})$ *such that they satisfy the relations (7.9).*

VIII. APPLICATION TO THE KLEIN–GORDON EQUATION

As an example, let us consider the Klein–Gordon equation

$$(g^{ab}\nabla_a\nabla_b - m_\Phi^2)\Phi = 0, \quad (8.1)$$

where $m_\Phi \geqslant 0$ is the mass of the field Φ. ∇_a is the covariant derivative operator associated with the space–time metric g_{ab}. It is straightforward to see that this equation on our background can be expressed, using the invariant operators χ_I, as

$$\left(\frac{-1}{\sqrt{-g}}\frac{\partial}{\partial t}\left(\sqrt{-g}N^{-2}\frac{\partial}{\partial t}\right) + \Delta_q - m_\Phi^2\right)\Phi = 0, \quad (8.2)$$

where Δ_q is the Laplacian with respect to the spatial metric q_{ab},

$$\Delta_q = q_1^{-1}(\chi_1)^2 + q_2^{-1}(\chi_2)^2 + q_3^{-1}(\chi_3)^2, \quad (8.3)$$

and $\sqrt{-g} \equiv \sqrt{-\det\ g_{ab}} = 4|p_3|\beta t N^2$.

Let us consider a generic irreducible component of Φ, i.e., $\Phi = \Phi_{m,n_0}$, $m \neq 0$. We can expand this component as

$$\Phi(t,\mathbf{x}) = \sum_{l=0}^{\infty} a_l(t)\varphi_l(\mathbf{x}), \quad (8.4)$$

where $\varphi_l = \varphi_{l,m,n_0}$ are the mode functions mentioned in Theorem 6.1.

From the relations (4.14), we have

$$(\chi_1)^2\varphi_l = \frac{|\mu|}{2}(\varphi_{l+2} - (2l+1)\varphi_l + l(l-1)\varphi_{l-2}),$$

$$(\chi_2)^2\varphi_l = -\frac{|\mu|}{2}(\varphi_{l+2} + (2l+1)\varphi_l + l(l-1)\varphi_{l-2}), \quad (8.5)$$

$$(\chi_3)^2\varphi_l = -\mu^2\varphi_l,$$

from which we immediately obtain the following wave equations for $a_l(t)$:

$$\ddot{a}_l + \frac{1}{t}\dot{a}_l + Z(t)a_l = I(t;a_{l-2},a_{l+2}), \tag{8.6}$$

where

$$Z(t) \equiv \frac{\mu^2}{16(p_3)^2\beta^2}(1+\beta^2t^{4p_3})^2t^{-2p_3} + m_\Phi^2(1+\beta^2t^{4p_3}) + \frac{2l+1}{2}|\mu|(t^{-2p_1}+t^{-2p_2}), \tag{8.7}$$

with the inhomogeneous term I being

$$I(t;a_{l-2},a_{l+2}) \equiv \frac{|\mu|}{2}(t^{-2p_1}-t^{-2p_2})(a_{l-2}+(l+2)(l+1)a_{l+2}). \tag{8.8}$$

[In $I(t;a_{l-2},a_{l+2})$, a_{l-2} should be regarded zero when $l=0$ and 1.]

Note that the inhomogeneous term I introduces couplings with the next neighboring modes with $l\pm2$. The Eqs. (8.6) therefore comprise two systems of infinite number of equations, the one with $l=$even and the one with $l=$odd, unless the background is LRS. When on the other hand the background is LRS, each equation (8.6) for a given l becomes closed itself, due to the vanishing of the inhomogeneous term I.

When the background is LRS, we can find future ($t\to\infty$) asymptotic solutions.

Proposition 8.1: On the LRS Bianchi II vacuum solution with $p_1=p_2=2/3$ and $p_3=-1/3$, the scalar field equation (8.6) for a generic mode has the following fundamental solutions as $t\to\infty$:

$$y_l^{\pm}(t) = t^{-2/3}e^{\pm i\mu T_{\mathrm{KG}}(t)}(1+o(1)), \tag{8.9}$$

where

$$T_{\mathrm{KG}}(t) \equiv \frac{9}{16\beta}t^{4/3} + \frac{\beta m_\Phi^2}{\mu^2}t^{2/3} + \left(\frac{3\beta}{4} - \frac{8\beta^3m_\Phi^4}{27\mu^4}\right)\log t. \tag{8.10}$$

The symbol $o(1)$ stands for a function such that $\lim_{t\to\infty} o(1)=0$.

Proof: This result is a generalization of Theorem 3.4, Ref. 13, with finite mass m_Φ. As emphasized there, it is an appropriate choice of new time variable that is essential to obtain an asymptotic solution. In the present case an appropriate choice $T(t)$ is given by

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{3}{4\beta}t^{1/3} + \frac{2\beta m_\Phi^2}{3\mu^2}t^{-1/3} + \left(\frac{3\beta}{4} - \frac{8\beta^3m_\Phi^4}{27\mu^4}\right)\frac{1}{t}. \tag{8.11}$$

Following the procedure shown in the reference, one obtains the asymptotic solution (8.9). ■

It is worth noticing that the asymptotic solution only depends on the fiber index m and the other index l does not affect them. See the final section for more discussion.

IX. VECTOR HARMONICS

Let us discuss how we can construct the vector harmonics.

Fortunately, this is on the one hand a trivial issue as the invariant frame $\{\sigma^I,\chi_I\}$ is well defined on the compactified manifold M (and on the space–time manifold $M\times\mathbf{R}$). This means we can define the components $T_{I\cdots}{}^{J\cdots}$ of any type of tensor $T_{a\cdots}{}^{b\cdots}$ with respect to this invariant frame,

$$T_{I\cdots}{}^{J\cdots} = T_{a\cdots}{}^{b\cdots}\chi_I{}^a\cdots\sigma_b{}^J\cdots. \tag{9.1}$$

All we must do is expand these components with respect to the scalar harmonics ϕ_{l,m,n_0} and $\phi^{(0)}_{k_1,k_2}$. This procedure corresponds to using the set of one-forms $\{\phi_l\sigma_a{}^1,\phi_l\sigma_a{}^2,\phi_l\sigma_a{}^3\}_{l=0}^{\infty}$ as vector har-

monics for given $m\neq 0$ and n_0. (As for $m=0$, ϕ_l should of course be replaced by $\phi^{(0)}_{k_1,k_2}$.) On the space–time manifold, we also need the timelike mode vectors, as well as the replacement $\phi_{l,m,n_0} \to \varphi_{l,m,n_0}$. We therefore can define the following harmonics (basis mode vectors):

$$(V'^0_l)_a \equiv \varphi_l(\mathrm{d}t)_a, \quad (V'^1_l)_a \equiv \varphi_l\sigma^1_a, \quad (V'^2_l)_a \equiv \varphi_l\sigma^2_a, \quad (V'^3_l)_a \equiv \varphi_l\sigma^3_a \tag{9.2}$$

(or the one with $\varphi^{(0)}_{k_1,k_2}$ instead of φ_l for $m=0$). We call them the *simple vector harmonics*.

The advantage of considering these harmonics is that they are apparently complete (since the scalar harmonics used are complete). However, this choice of harmonics does not reflect very well the group structure regarding the rotational automorphisms (2.10). A more natural and convenient choice can be obtained by using the "spherical bases"[9] $\mathcal{A}_I$ ($I=1-3$) defined in Eqs. (4.2), or their duals such that $\mathcal{A}_I{}^a\varrho_a{}^J=\delta^J_I$;

$$\varrho^1 \equiv \frac{1}{\sqrt{2}}(\sigma^1 - \varsigma i\sigma^2), \quad \varrho^2 \equiv \frac{1}{\sqrt{2}}(\sigma^1 + \varsigma i\sigma^2), \quad \varrho^3 \equiv \varsigma i\sigma^3. \tag{9.3}$$

Using these we can set up new harmonics as

$$(V^0_l)_a \equiv \varphi_l(\mathrm{d}t)_a, \quad (V^1_l)_a \equiv \varphi_{l+1}\varrho_a{}^1, \quad (V^2_l)_a \equiv \varphi_{l-1}\varrho_a{}^2, \quad (V^3_l)_a \equiv \varphi_l\varrho_a{}^3. \tag{9.4}$$

(When $m=0$ we just use the same harmonics as the simple harmonics.) Beware that $\varphi_{l\pm1}$ are used to define $(V^1_l)_a$ and $(V^2_l)_a$. The reason will become clear below. Because of this index correspondence, we should think that the harmonics $\{(V^I_l)_a\}^3_{I=0}$ are defined for $l\geqslant -1$ (not for $l\geqslant 0$). The basis $(V^I_{-1})_a$ for $l=-1$ is nonzero only for $I=1$, and the others should simply be regarded as zero. We call these harmonics the *polarized vector harmonics* or the *standard vector harmonics*.

We can confirm that for given m, the simple harmonics and the polarized harmonics span the same space of vector fields. This ensures the completeness of the polarized vector harmonics.

Theorem 9.1: *For given fiber index $m\in\mathbf{Z}$ (and given auxiliary index n_0), the linear span of the simple harmonics*

$$\mathrm{Span}(V'^m) \equiv \left\{ \sum_{l=0}^{\infty}\sum_{I=0}^{3} c_{I,l}(V'^I_l)_a \,\middle|\, c_{I,l}\in\mathbf{C} \right\} \quad (m\neq 0) \tag{9.5}$$

(*the $m=0$ case is defined similarly) and that of the polarized harmonics*

$$\mathrm{Span}(V^m) \equiv \left\{ \sum_{l=-1}^{\infty}\sum_{I=0}^{3} c_{I,l}(V^I_l)_a \,\middle|\, c_{I,l}\in\mathbf{C} \right\} \quad (m\neq 0) \tag{9.6}$$

(*the $m=0$ case is defined similarly) are the same*,

$$\mathrm{Span}(V'^m) = \mathrm{Span}(V^m). \tag{9.7}$$

Proof: This is trivial for the $m=0$ case, since in this case the two kinds of harmonics are the same. So, we can assume $m\neq 0$. From the definition (9.4), it is apparent that each basis one-form V^I_l of the polarized harmonics for given m can be expressed as a linear combination of the simple harmonics belonging to the same m. Conversely, each basis one-form V'^I_l of the simple harmonics for given m can be expressed as a linear combination of the polarized harmonics with the same m as

$$V'^0_l = V^0_l,$$

$$V'^1_l = \frac{1}{\sqrt{2}}(V^1_{l-1} + V^2_{l+1}), \tag{9.8}$$

$$V_l'^2 = \frac{si}{\sqrt{2}}(V_{l-1}^1 - V_{l+1}^2),$$

$$V_l'^3 = V_l^3.$$

Therefore the two sets are related by a regular linear transformation, which proves the identity of the two spans. ■

The significance of the polarized harmonics is that for given l (and as usual, given m and n_0), the space spanned by them

$$\mathrm{Span}(V_l) \equiv \left\{ \sum_{I=0}^{3} c_I (V_l^I)_a \,\middle|\, c_I \in \mathbf{C} \right\} \tag{9.9}$$

is invariant under the operation of L^2. To show this, let us start with observing the commutation relations

$$[\mathcal{A}_1, \mathcal{A}_2] = \mathcal{A}_3, \quad [\mathcal{A}_1, \mathcal{A}_3] = 0, \quad [\mathcal{A}_2, \mathcal{A}_3] = 0, \tag{9.10}$$

from which one can immediately have

$$\mathcal{L}_{\mathcal{A}_I} \mathcal{A}_J = [\mathcal{A}_I, \mathcal{A}_J] = \epsilon_{IJ3} \mathcal{A}_3, \tag{9.11}$$

where ϵ_{IJK} is the unit skew symmetric symbol; $\epsilon_{123} = +1$, $\epsilon_{IJK} = \epsilon_{[IJK]}$. Then, noting the duality $A_J^{\ a} \varrho_a^{\ K} = \delta_J^K$, it is also easy to see

$$\mathcal{L}_{\mathcal{A}_I} \varrho^J = -\delta_3^J \epsilon_{IK3} \varrho^K. \tag{9.12}$$

From this equation and the χ relations, as well as the identity

$$\mathsf{L}^2 = \mathcal{L}_{\mathcal{A}_1} \mathcal{L}_{\mathcal{A}_2} + \mathcal{L}_{\mathcal{A}_2} \mathcal{L}_{\mathcal{A}_1}, \tag{9.13}$$

one obtains

$$\mathsf{L}^2(\varphi_l \varrho^I) = -\lambda_l^2 \varphi_l \varrho^I - 2\sqrt{|\mu|}\,\delta_3^I (\varphi_{l+1} \varrho^1 + l \varphi_{l-1} \varrho^2). \tag{9.14}$$

This equation happens to be valid when $I = 0$, as well. Converting to our bases (9.4), we obtain the following statement.

Lemma 9.2: Let V_l^I $(I = 0-3)$ *be the basis mode one-forms defined in Eqs. (9.4), and let* L^2 *be the second order Lie derivative operator defined in Eq. (3.5) . Then, it holds that*

$$\begin{aligned} \mathsf{L}^2 V_l^0 &= -\lambda_l^2 V_l^0, \\ \mathsf{L}^2 V_l^1 &= -\lambda_{l+1}^2 V_l^1, \\ \mathsf{L}^2 V_l^2 &= -\lambda_{l-1}^2 V_l^2, \\ \mathsf{L}^2 V_l^3 &= -\lambda_l^2 V_l^3 - 2\sqrt{|\mu|}(V_l^1 + IV_l^2), \end{aligned} \tag{9.15}$$

where $-\lambda_l^2$ *is the eigenvalue of* L^2 *with respect to the mode function* φ_l*, defined in Eq. (4.15).*

Note that the right-hand sides of Eqs. (9.15) are linear combinations of $\{V_l^I\}_{I=0}^3$ belonging to given l. This proves the invariance we claimed.

Theorem 9.3: *The linear span* $\mathrm{Span}(V_l)$*, defined in Eq. (9.9), of the harmonics* $\{V_l^I\}_{I=0}^3$ *is invariant under the operation of* L^2,

$$\mathsf{L}^2\ \mathrm{Span}(V_l) \subset \mathrm{Span}(V_l). \tag{9.16}$$

Thanks to this property, if the background space–time is LRS and the field equation is invariant under the LRS-action induced by s_θ as well as the usual group action, the ODEs reduced from the field equation become all independent from the others. In other words, "each l" decouples from the others in case of LRS. (This property does not occur for the simple harmonics, since the linear span of them for a given l is *not* L^2 invariant.)

Before ending this section let us mention the approach taken in Ref. 13, Sec. III, which was based on the analogy of the spherically symmetric case[11] or the Bianchi III hyperbolically symmetric case.[17] Let us denote the harmonics used in the reference with double primes like $(V_l''^I)_a$. $V_l''^0$ and $V_l''^3$ are defined in the same way (up to constant multiplication factor) as the polarized ones,

$$V_l''^0 = V_l^0, \quad V_l''^3 = \varsigma\mu V_l^3. \tag{9.17}$$

$V_l''^0$ is called the *timelike basis one-form*, while $V_l''^3$ is called the *fiber basis one-form*. Let us then consider the "plane field" spanned by χ_1 and χ_2, which is horizontal to the base manifold. This horizontal plane field is invariant under the natural actions of the fibers generated by χ_3. We define the "area two-form" ε of this field by $\varepsilon_{ab}=2\sigma^1{}_{[a}\sigma^2_{b]}$ (although the plane field is not integrable). We define the *horizontal gradient (HG) basis one-form* (corresponding to the "even" one-form[11,17]) by taking gradient of the scalar harmonics and subtracting the fiber part,

$$(V_l''^1)_a = \partial_a\varphi_l - (V_l''^3)_a = (\chi_1\varphi_l)\sigma_a{}^1 + (\chi_2\varphi_l)\sigma_a{}^2 = \sqrt{\frac{|\mu|}{2}}(-(\varphi_{l+1} - l\varphi_{l-1})\sigma_a{}^1 + \varsigma i(\varphi_{l+1} + l\varphi_{l-1})\sigma_a{}^2). \tag{9.18}$$

And, we define the *dual horizontal gradient (DHG) basis one-form* (corresponding to the "odd" one-form) by taking the dual gradient associated with ε,

$$(V_l''^2)_a = i\varepsilon_a{}^b\partial_b\varphi_l = i((\chi_2\varphi_l)\sigma_a{}^1 - (\chi_1\varphi_l)\sigma_a{}^2) = \sqrt{\frac{|\mu|}{2}}(-\varsigma(\varphi_{l+1} + l\varphi_{l-1})\sigma_a{}^1 + i(\varphi_{l+1} - l\varphi_{l-1})\sigma_a{}^2). \tag{9.19}$$

To raise an index for ε_{ab} we use the (inverse of the) standard Bianchi II metric $h^{(0)ab}=\chi_1{}^a\chi_1{}^b + \chi_2{}^a\chi_2{}^b + \chi_3{}^a\chi_3{}^b$. It is clear that the harmonics $V_l'' \equiv \{(V_l''^I)_a\}_{I=0}^3$ are equivalent (i.e., their span is the same) to the polarized harmonics $V_l \equiv \{(V_l^I)_a\}_{I=0}^3$ *for each* l, since they are merely related to each other by a regular linear transformation, as seen from the relations

$$V_l''^1 = -\sqrt{|\mu|}(V_l^1 - IV_l^2), \quad V_l''^2 = -\varsigma\sqrt{|\mu|}(V_l^1 + IV_l^2), \tag{9.20}$$

as well as (9.17). We call these harmonics the *mixed vector harmonics*. This choice is particularly convenient for Maxwell's equation, since the U(1)-gauge transformation, $A_a \to A_a + \partial_a f$, does not affect the component for the DHG basis one-form (9.19). (As a result, this component itself becomes gauge invariant. See the next section.)

X. APPLICATION TO MAXWELL'S EQUATION

As an application let us consider the source-free Maxwell equation $\nabla^a F_{ab} = 0$. Since the electromagnetic field F_{ab} is given by (twice) the exterior derivative of the vector potential A_a; $F_{ab} = \partial_a A_b - \partial_b A_a$, this equation can be dealt with by vector harmonics.

Let us consider the irreducible component belonging to given $m \neq 0$ and n_0. For this component we can expand the vector potential as follows:

$$A_a = \sum_{l=-1}^{\infty} \sum_{I=0}^{3} \gamma_I^{(l)}(t)(V_l''^I)_a, \tag{10.1}$$

where $(V_l''^I)_a$ are the mixed vector harmonics. The four kinds of functions of time $\gamma_I^{(l)}(t)$ ($I = 0-3$) serve as the field variables.

The quantities we are interested in are the U(1)-gauge invariant variables, which can be easily found by inspecting components of the field strength $F_{ab} = \partial_a A_b - \partial_b A_a$. We obtain the following four independent U(1)-invariant variables:

$$Q_1^{(l)} = \gamma_1^{(l)} - \gamma_3^{(l)}, \quad Q_2^{(l)} = \gamma_2^{(l)}, \quad P_1^{(l)} = \dot{\gamma}_1^{(l)} - \gamma_0^{(l)}, \quad P_2^{(l)} = \dot{\gamma}_2^{(l)}. \tag{10.2}$$

Although function $P_3 \equiv \dot{\gamma}_3 - \gamma_0$ is also invariant, it is found that it can be (consistently) solved with the others, due to the constraint part of Maxwell's equation $0 = (\partial_t)^a \nabla^b F_{ab}$, which can be written, using the invariant operator, as

$$0 = N^{-1}(q_1^{-1}\chi_1 \dot{A}_1 + q_2^{-1}\chi_2 \dot{A}_2 + q_3^{-1}\chi_3 \dot{A}_3) - \Delta_q A_0, \tag{10.3}$$

where $A_0 \equiv N^{-1}(\partial_t)^a A_a$ and $A_I \equiv \chi_I^a A_a$ ($I = 1-3$). Laplacian Δ_q is given in Eq. (8.3). The evolution equations $0 = \chi_I^a \nabla^b F_{ab}$ ($I = 1-3$) can similarly be written

$$\begin{aligned} 0 = &- N^{-1}\dot{F}_{0I} + q_1^{-1}\chi_1 F_{1I} + q_2^{-1}\chi_2 F_{2I} + q_3^{-1}\chi_3 F_{3I} + N^{-1}q_I^{-1}\dot{q}_I F_{0I} - (2N)^{-1}(q_1^{-1}\dot{q}_1 + q_2^{-1}\dot{q}_2 + q_3^{-1}\dot{q}_3)F_{0I} \\ &+ (q_1 q_2)^{-1} q_3 \delta_I^3 F_{12} \end{aligned} \tag{10.4}$$

(no sum for repeated indices), where $F_{0I} \equiv N^{-1}(\partial_t)^a \chi_I^{\ b} F_{ab}$ and $F_{IJ} \equiv \chi_I^{\ a}\chi_J^{\ b} F_{ab}$. After a rather lengthy computation they become the following:

$$\begin{aligned} \dot{Q}_1^{(l)} &= P_1^{(l)} + \frac{(q_1^{-1} + q_2^{-1})q_3}{2|\mu|}((2l+1)P_1^{(l)} + \varsigma P_2^{(l)}) + I_{Q_1}, \\ \dot{Q}_2^{(l)} &= P_2^{(l)}, \\ \dot{P}_1^{(l)} &= \left(\frac{\dot{N}}{N} - \frac{1}{2}\frac{\dot{q}_3}{q_3}\right)P_1^{(l)} - \mu^2 \frac{N^2}{q_3} Q_1^{(l)} + I_{P_1}, \\ \dot{P}_2^{(l)} &= \left(\frac{\dot{N}}{N} - \frac{1}{2}\frac{\dot{q}_3}{q_3}\right)P_2^{(l)} - \mu^2 \frac{N^2}{q_3} Q_2^{(l)} - \frac{\mu}{2} N^2 (q_1^{-1} + q_2^{-1})(Q_1^{(l)} + \varsigma(2l+1)Q_2^{(l)}) + I_{P_2}, \end{aligned} \tag{10.5}$$

where the inhomogeneous terms are

$$I_{Q_1} \equiv -\frac{(q_1^{-1}-q_2^{-1})q_3}{2|\mu|}\{(l+2)(l+1)(P_1^{(l+2)}-\varsigma P_2^{(l+2)})+(P_1^{(l-2)}+\varsigma P_2^{(l-2)})\},$$

$$I_{P_1} \equiv \frac{N^2}{4}(q_1^{-1}-q_2^{-1})|\mu|\{(l+2)(Q_1^{(l+2)}+\varsigma(2l+5)Q_2^{(l+2)})-l^{-1}(Q_1^{(l-2)}+\varsigma(2l-3)Q_2^{(l-2)})\}$$
$$-\frac{1}{4}\left(\frac{\dot q_1}{q_1}-\frac{\dot q_2}{q_2}\right)\{(l+2)(P_1^{(l+2)}-\varsigma P_2^{(l+2)})+l^{-1}(P_1^{(l-2)}+\varsigma P_2^{(l-2)})\}, \tag{10.6}$$

$$I_{P_2} \equiv \frac{N^2}{4}(q_1^{-1}-q_2^{-1})|\mu|\{(l+2)(\varsigma Q_1^{(l+2)}+(2l+5)Q_2^{(l+2)})+l^{-1}(\varsigma Q_1^{(l-2)}+(2l-3)Q_2^{(l-2)})\}$$
$$-\frac{1}{4}\left(\frac{\dot q_1}{q_1}-\frac{\dot q_2}{q_2}\right)\{(l+2)(\varsigma P_1^{(l+2)}-P_2^{(l+2)})-l^{-1}(\varsigma P_1^{(l-2)}+P_2^{(l-2)})\}.$$

Again, we can see the same qualitative features in the Klein–Gordon equations; we have two systems of infinite number of equations, the one with $l=$even and the one with $l=$odd, unless the background is LRS. When the background is LRS, the couplings between mode l and the next neighbors $l\pm2$ are cut off due to the vanishing of the inhomogeneous terms I_{Q_1}, I_{P_1} and I_{P_2} and this makes each system of four first-order equations (10.5) for given l closed itself. This is of course a result of the invariance described in Theorem 9.3.

XI. CONCLUSION

There are three main results about basic properties for the nilgeometric harmonics obtained in this paper. They are (i) the irreducible decomposition of the regular representation (Theorem 1.1), (ii) the explicit form of the mode functions, and (iii) the differential representation formula, the χ relations [see Eqs. (4.14) and (7.6)]. The decomposition (i) represents the completeness of our harmonics. As for the point (ii), remember that we have two kinds of formula, the one for the canonical manifold and the one for the space–time manifold. The former is given in Eqs. (5.8) and (7.3), while the latter is obtained by the transformations explicitly given in Secs. VI and VII. Remember also that the χ relations are the most important for the purpose of separation of variables. We also have generalized the (scalar) harmonics to vector harmonics, and demonstrated separation of variables for a scalar equation (the Klein–Gordon equation) and a vector equation (the Maxwell equation).

As we have seen, when the fiber index m is nonzero the ODEs reduced from a field equation, e.g., the ones from the KG equation, become systems of *infinite number of* simultaneous equations. In this sense, infinite number of different modes are coupled to each other. This is a result of the fact that the corresponding irreducible representation is infinite dimensional. When the background is LRS however, the couplings between the modes are cut off and as a result, each single reduced KG equation becomes closed itself. Although the Maxwell equations give rise to much more complicated reduced equations because of the multiple components of the field variable, it has the same feature that the couplings between modes disappear when the background is LRS. It is also apparent that the linear perturbation equations will have the same feature if we choose the tensor harmonics so as to possess the invariance under L^2 like the vector harmonics do (cf. Theorem 9.3).

An interesting fact is that as shown in Sec. VIII, the future asymptotic solution of the LRS KG wave equation depends only on the fiber index m and does not depend on the spin index l. This fact seems to indicate a clue for analyzing the generic non-LRS cases, since it suggests that the couplings between the modes asymptotically disappear even when the background is non-LRS, at least if the background is close enough to the LRS one. See Ref. 14 for the same ("fiber term

dominated") behavior of other models (Bianchi VIII and III). Detailed studies of the non-LRS cases, as well as linear perturbations of the nilgeometric model, will be reported elsewhere, on the basis of this work.

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[22] The "left" regular representation can also be defined similarly. We take the "right" one for the reason explained below.
[23] In Refs. 10, 15, and 16, the second component of $\mathbf{a}_1$ was taken zero instead of the first component of $\mathbf{a}_2$. It is however not difficult to see that those two choices are equivalent (*conjugate*) to each other following the procedure shown in the same references. The present parametrization will be proved more convenient for our purpose.
[24] While Isom $\mathcal{N}$ is four-dimensional, the extra isometries are not necessary for us to represent $\mathbf{a}_i$, resulting in $\mathbf{a}_i \in G_{\mathrm{II}}$ here. Remark however that to obtain this representation the fourth-dimensional isometries play an essential role, especially to delete the first component of $\mathbf{a}_2$.
[25] Like this, we consider any functions on M or $\overline{M}$ as functions on the universal cover $\tilde{M}=\mathbf{R}^3$. If $f(Ax)=f(x)$ holds we regard $f(x)$ as a function on $M=A\backslash\tilde{M}$. Similarly, If $f(\overline{A}x)=f(x)$ holds, $f(x)$ is a function on $\overline{M}=\overline{A}\backslash\tilde{M}$. Those functions are called *automorphic functions*.
[26] We could impose a unitary condition on $\mathcal{A}_i$ $(i=1,2)$ to make the choice of α_l and β_l unique, although there is no strong reason to do so for our purpose. On the other hand, our present choice (4.10) makes the final formula [see Eqs. (4.14)] to some extent simpler, with less square roots appearing in the formula than in the one obtained requiring the unitary condition. It is however easy to convert the resulting mode functions into those for unitary $\mathcal{A}_i$. See the last paragraph of Sec. V.
[27] We are assuming that the action of A on the space–time manifold $\tilde{M}\times\mathbf{R}$ is defined by $A\circ(\mathbf{x},t)=(A\circ\mathbf{x},t)$, $(\mathbf{x},t)\in\tilde{M}\times\mathbf{R}$. (Apparently, the same equality for Γ defines its action on $\tilde{M}$.)
[28] The parametrization among the free parameters has been rearranged from Ref. 15 so that it is convenient for our purpose.

[29] Although we use, for convenience, the same symbols θ, u, δ, and v as in A here, it is worth emphasizing that their meaning is distinctly different; those in Γ are moduli parameters of *space–time*, while those in A are the Teichmüller (or moduli) parameters of *space*, which are functions of time in space–time (Refs. 15 and 16). The space–time moduli parameters parametrize the admissible initial values and velocities of the Teichmüller parameters.

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Remote preparation of arbitrary ensembles and quantum bit commitment

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The Hughston–Jozsa–Wootters theorem shows that any finite ensemble of quantum states can be prepared "at a distance," and it has been used to demonstrate the insecurity of all bit commitment protocols based on finite quantum systems without superselection rules. In this paper, we prove a generalized HJW theorem for arbitrary ensembles of states on a C^*-algebra. We then use this result to demonstrate the insecurity of bit commitment protocols based on infinite quantum systems, and quantum systems with Abelian superselection rules. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1812827]

I. INTRODUCTION

Recent work in quantum cryptography has focused on questions of which sorts of information-transfer protocols are secure from attempts at cheating by an intruder or by one of the participants. As early as 1984, the question was raised whether quantum theory would permit a secure bit commitment protocol, i.e., a protocol in which a bit of information is committed by one party Alice to another party Bob, such that Alice cannot change her commitment, and such that Bob cannot determine Alice's commitment until given further information by Alice. An initial protocol using pairs of polarized photons was proposed by Bennett and Brassard;[2] however, Bennett and Brassard showed that this protocol can be cheated by exploiting the nonlocal correlations of the EPR-Bohm state.

A number of other quantum bit commitment protocols have been proposed in the intervening years (see Refs. 3, 4, and 6 for reviews). Most of these protocols rely on the fact that a non-pure-density operator corresponds to more than one ensemble of quantum states. In particular, two different ensembles on a composite system can induce the same density operator on a local system. Thus, if Alice encodes her bits into these two ensembles, then Bob cannot possibly determine Alice's commitment until she provides further information about the composite system.

However, Lo and Chau[15] and Mayers[16,17] show that, as a consequence of the Hughston–Jozsa–Wootters (HJW) theorem, if a bit commitment protocol is concealing against Bob, then it is not binding against Alice. (Kent's[12] relativistic bit commitment protocol does not rely on the existence of alternative decompositions of a density operator, and so its security is not challenged by the Mayers–Lo–Chau result.) That is, if the ensembles prepared in the protocol are indistinguishable to Bob (i.e., correspond to approximately the same local density operator), then Alice can "steer" between these ensembles after the Commit stage of the protocol.

HJW Theorem:[10] *Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be finite-dimensional Hilbert spaces, let $\{D_i\}_{i=1}^n$ be density operators on $\mathcal{H}_B$, and let x be a unit vector in $\mathcal{H}_A \otimes \mathcal{H}_B$ such that $\mathrm{Tr}_A(P_x) = \Sigma_{i=1}^n \lambda_i D_i$. Then there are positive operators $\{A_i\}_{i=1}^n$ in $\mathcal{B}(\mathcal{H}_A) \otimes I$ such that*

$$\langle A_i^{1/2} x | B A_i^{1/2} x \rangle = \lambda_i \mathrm{Tr}(D_i B), \tag{1}$$

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for all $B \in I \otimes \mathcal{B}(\mathcal{H}_B)$.

Thus, the HJW theorem shows that any *finite* decomposition of $\mathrm{Tr}_A(P_x)$ can be prepared from the state P_x by a measurement operation on $\mathcal{H}_A$. However, all nonpure density operators have countably infinite convex decompositions, as well as uncountably infinite integral decompositions. For the case of countably infinite decompositions, Cassinelli *et al.*[7] have proved a generalized HJW theorem, but their results do not cover the case of integral decompositions. What is more, the HJW theorem and its generalization by Cassinelli *et al.* apply only to a very narrow class of quantum systems—namely those whose observables are represented by type I von Neumann factors. Thus, these results do not directly establish the insecurity of bit commitment protocols that employ systems with nontrivial superselection rules (represented by direct sums of type I von Neumann factors), or bit commitment protocols that employ infinite quantum systems (represented by type II or type III von Neumann algebras).

In this paper, we prove a generalized HJW theorem for arbitrary ensembles of states on a C^*-algebra. We show first (in Sec. II) that each measure on the state space of a C^*-algebra $\mathcal{B}$ gives rise to a positive-operator-valued measure with range in the commutant $\mathcal{B}'$ of $\mathcal{B}$. (This first result is completely general, and does not impose any restrictions on the C^*-algebra $\mathcal{B}$.) We then show that when $\mathcal{B}'$ is a hyperfinite von Neumann algebra, there is a completely positive instrument that prepares the relevant ensemble of states on $\mathcal{B}$. In Sec. III we apply our results to the question of the security of bit commitment protocols.

II. GENERALIZED HJW THEOREM

Our first result (Theorem 1) shows that for any C^*-algebra $\mathcal{B}$ of operators acting on a Hilbert space $\mathcal{H}$, a measure on the state space of $\mathcal{B}$ gives rise to a corresponding POV measure with values in the commutant $\mathcal{B}' = \{A \in \mathcal{B}(\mathcal{H}) : [A,B] = 0 \text{ for all } B \in \mathcal{B}\}$. For the case that $\mathcal{B} = I \otimes \mathcal{M}_n$, where $\mathcal{M}_n$ is the C^*-algebra of $n \times n$ matrices over $\mathbb{C}$, our result yields an alternate proof of the original HJW theorem.

Let K denote the compact convex set of states of $\mathcal{B}$ with the weak* topology. [A net $\{\omega_a\}_{a \in \mathbb{A}}$ of states of $\mathcal{B}$ converges in the weak* topology to a state ω just in case, for each $B \in \mathcal{B}, \lim_a \omega_a(B) = \omega(B)$. If $\mathcal{B} = \mathcal{M}_n$, then the weak* topology on states is equivalent to the standard topology on density operators.] In this paper, we consider positive regular measures on (K, Σ), where Σ is the Borel σ-algebra of K. When we say that μ is a measure, it can be assumed that μ is positive and regular.

Definition (Ref. 1, p. 12): If μ is a measure on the state space K, then the state

$$\rho_\mu = \mu(K)^{-1} \int x \, d\mu(x), \tag{2}$$

is called the *barycenter* of μ. Measures μ and ν on K are said to be *equivalent* if they have the same barycenter.

Let K be the convex set of density operators on $\mathbb{C}^n$. If ρ is a density operator and μ is a finitely supported measure on K with barycenter ρ, then Hughston *et al.* call μ a *ρ-ensemble*. So, the set of ρ-ensembles consists of those measures on K that have barycenter ρ, and that are supported on a finite set. In this paper, we consider all measures with barycenter ρ, and not just those with finite support.

Notation: If x is a vector in $\mathcal{H}$, we let $\omega_x(A) = \langle x | Ax \rangle$, for all $A \in \mathcal{B}(\mathcal{H})$. If $\mathcal{B}$ is a set of operators on $\mathcal{H}$, we let $\mathcal{B}x = \{Bx : B \in \mathcal{B}\}$, and we let $[\mathcal{B}x]$ denote the closed linear span of $\mathcal{B}x$.

Lemma 1 (Ref. 11, Proposition. 7.3.5): If $\mathcal{B}$ is a C^*-algebra of operators acting on the Hilbert space $\mathcal{H}$ and ρ is a positive linear functional on $\mathcal{B}$ such that $\rho \leqslant \omega_x|_{\mathcal{B}}$ for some vector x in $\mathcal{H}$, then there is a positive operator H in the unit ball of $\mathcal{B}'$ such that $\rho(A) = \omega_x(HA) = \omega_{H^{1/2}x}(A)$, for all $A \in \mathcal{B}$.

Proof: Define a conjugate-bilinear functional φ on $\mathcal{B}x$ by setting $\varphi(Ax, Bx) = \rho(A^*B)$. Then,

$$|\varphi(Ax,Bx)|^2 = |\rho(A^*B)|^2 \leq \rho(A^*A)\rho(B^*B) \leq \|Ax\|^2\|Bx\|^2. \tag{3}$$

The first inequality follows from the Cauchy–Schwartz inequality for the inner product $\langle A|B\rangle_\rho = \rho(A^*B)$ on $\mathcal{B}$. Thus φ is positive and bounded by 1. It follows that φ has a unique extension to the subspace $[\mathcal{B}x]$. Moreover, the Riesz representation theorem entails that there is a positive operator H on $[\mathcal{B}x]$ such that $\|H\| \leq 1$ and $\varphi(Ax,Bx) = \langle Ax|HBx\rangle$. In particular, $\rho(A) = \langle x|HAx\rangle = \omega_x(HA)$ for all $A \in \mathcal{B}$. Extend H to the entire Hilbert space $\mathcal{H}$ by setting it to zero on $\mathcal{H} \ominus [\mathcal{B}x]$. Since

$$\langle Ax|HCBx\rangle = \rho(A^*CB) = \rho((C^*A)^*B) \tag{4}$$

$$= \langle C^*Ax|HBx\rangle = \langle Ax|CHBx\rangle \tag{5}$$

for all C in $\mathcal{B}$, it follows that $[H,C]=0$ on $[\mathcal{B}x]$. Since $[H,C]=0$ on $\mathcal{H} \ominus [\mathcal{B}x]$, it follows that $[H,C]=0$ on the entire Hilbert space. Therefore, $H \in \mathcal{B}'$. □

The following result is a special case of a theorem proved by Tomita[25] in 1956 (compare with Ref. 5, Lemma 4.1.21, Proposition 4.1.22).

Theorem 1: *Let $\mathcal{B}$ be a C^*-algebra acting on the Hilbert space $\mathcal{H}$, and let μ be a probability measure on the state space of $\mathcal{B}$. If there is a unit vector x in $\mathcal{H}$ such that $\omega_x|_{\mathcal{B}}$ is the barycenter of μ, then there is a POV measure* **A** *with range in $\mathcal{B}'$ such that*

$$\langle A(S)^{1/2}x|BA(S)^{1/2}x\rangle = \int_S \omega(B)d\mu(\omega), \tag{6}$$

for all $S \in \Sigma$ and $B \in \mathcal{B}$.

Proof: Let S be a Borel subset of the state space of $\mathcal{B}$, and let $\rho_S = \int_S \omega d\mu(\omega)$. Then ρ_S is a positive linear functional on $\mathcal{B}$ with $\rho_S \leq \omega_x|_{\mathcal{B}}$. By Lemma 1, there is a positive operator $A(S)$ in the unit ball of $\mathcal{B}'$ such that $\rho_S(B) = \omega_x(A(S)B)$ for all $B \in \mathcal{B}$, and $A(S)=0$ on $\mathcal{H} \ominus [\mathcal{B}x]$. In order to verify that $S \mapsto A(S)$ is countably additive, suppose that $\{S_i : i \in \mathbb{N}\}$ are disjoint Borel subsets, and let $S = \cup_{i=1}^{\infty} S_n$. Then for fixed $B \in \mathcal{B}$,

$$\sum_{i=1}^{\infty} \chi_{S_i}(\omega) \cdot \omega(B) = \chi_S(\omega) \cdot \omega(B), \tag{7}$$

and so the monotone convergence theorem entails that

$$\sum_{i=1}^{\infty} \left(\int_{S_i} \omega(B)d\mu(\omega) \right) = \int_S \omega(B)d\mu(\omega) = \langle x|A(S)Bx\rangle. \tag{8}$$

Furthermore, countable additivity of the map $Z \mapsto \langle x|ZBx\rangle$ entails that

$$\left\langle x \middle| \left(\sum_{i=1}^{\infty} A(S_i) \right) Bx \right\rangle = \sum_{i=1}^{\infty} \langle x|A(S_i)Bx\rangle. \tag{9}$$

Replacing B with B^*C, where $B,C \in \mathcal{B}$, we have

$$\left\langle Bx \middle| \sum_{i=1}^{\infty} A(S_i)Cx \right\rangle = \langle Bx|A(S)Cx\rangle, \tag{10}$$

and therefore $(\Sigma_{i=1}^{\infty} A(S_i))y = A(S)y$, for all $y \in [\mathcal{B}x]$. Since $A(S)=0$ on $\mathcal{H} \ominus [\mathcal{B}x]$, it follows that $\Sigma_{i=1}^{\infty} A(S_i) = A(S)$. □

Thus, if μ is a measure on the state space of Bob's algebra $\mathcal{B}$, Alice's algebra $\mathcal{A}=\mathcal{B}'$ contains the range of a POV measure $\mathbf{A}$ satisfying Eq. (6). But this does not yet yield the conclusion that Alice can prepare the ensemble μ on Bob's system—for that, we need to show that Alice has an "instrument" corresponding to the POV measure $\mathbf{A}$.

Definition:[9,19] Let (X,Σ) be a Borel space. A *completely positive (CP) instrument* on $\mathcal{B}(\mathcal{H})$ is a map $\mathcal{E}:\Sigma\times\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ such that

(1) for fixed $B\in\mathcal{B}(\mathcal{H})$, $\mathcal{E}[\cdot](B)$ is σ-additive in the weak-operator topology;
(2) for fixed $S\in\Sigma$, $\mathcal{E}[S](\cdot)$ is a completely positive linear map such that $\mathcal{E}[S](I)\leqslant I$.

Since the map $\mathcal{E}[S](\cdot),(S\in\Sigma)$, is positive, it is automatically norm-continuous. If, in addition, each such map is weak-operator continuous on bounded sets, then $\mathcal{E}$ is said to be *normal*. [A net $\{A_a\}_{a\in\mathbb{A}}$ of bounded operators on $\mathcal{H}$ converges in the weak-operator topology to an operator A just in case $\lim_a\langle x|A_a y\rangle=\langle x|Ay\rangle$ for all vectors x,y in $\mathcal{H}$.] However, we do not require instruments to be normal, because continuous PV measures give rise to non-normal instruments,[9,23] and a continuous ensemble of states on $\mathcal{B}$ will give rise to a continuous PV measure in $\mathcal{B}'$.

Each instrument $\mathcal{E}$ determines a unique POV measure $\mathbf{A}$ via the formula

$$A(S)\equiv\mathcal{E}[S](I)\quad(S\in\Sigma). \tag{11}$$

If Eq. (11) holds for an instrument $\mathcal{E}$ and a POV measure $\mathbf{A}$, then $\mathcal{E}$ and $\mathbf{A}$ are said to be *compatible*. For any given POV measure $\mathbf{A}$, there are many instruments that are compatible with $\mathbf{A}$. In fact, if Φ is a CP projection of $\mathcal{B}(\mathcal{H})$ with $\mathrm{ran}(\Phi)\subseteq\mathrm{ran}(\mathbf{A})'$, then

$$\mathcal{E}[S](B)=A(S)\Phi(B)\quad(S\in\Sigma,B\in\mathcal{B}(\mathcal{H})) \tag{12}$$

is compatible with $\mathbf{A}$. In particular, if ρ is a state on $\mathcal{B}(\mathcal{H})$, then

$$\mathcal{E}[S](B)=A(S)\rho(B)\quad(S\in\Sigma,B\in\mathcal{B}(\mathcal{H})) \tag{13}$$

is compatible with $\mathbf{A}$.

Thus, given a POV measure $\mathbf{A}$ with range in Alice's algebra $\mathcal{A}=\mathcal{B}'$, we can easily find an instrument $\mathcal{E}$ that is compatible with $\mathbf{A}$. However, it does not follow that Alice can in any sense measure $\mathbf{A}$ with the instrument $\mathcal{E}$, because $\mathcal{E}$ may not be "local" to Alice's system. In particular, an instrument that is local to Alice's system should not disturb the statistics of measurements of observables in Bob's algebra $\mathcal{B}=\mathcal{A}'$. In other words, for any state ρ on $\mathcal{B}$, the equation

$$\rho(\mathcal{E}[X](B))=\rho(B) \tag{14}$$

should hold for all $B\in\mathcal{B}$. But Eq. (14) holds for all states ρ on $\mathcal{B}$ iff the CP map $\mathcal{E}[X](\cdot)$ is the identity on $\mathcal{B}$. Thus, we capture the locality requirement with the following definition.

Definition: An instrument $\mathcal{E}$ is *local* to an algebra $\mathcal{A}$ just in case $\mathcal{E}[S](B)=\mathcal{E}[S](I)B$, for all $B\in\mathcal{A}'$ and $S\in\Sigma$.

Of course, if $\mathbf{A}$ is a POV measure on $\mathbb{N}$, there is a canonical instrument $\mathcal{E}^{\mathbf{A}}$ that is compatible with $\mathbf{A}$ and local to any algebra containing $\mathrm{ran}(\mathbf{A})$:

$$\mathcal{E}^{\mathbf{A}}[S](B)=\sum_{n\in S}A_n^{1/2}BA_n^{1/2}\quad(S\subseteq\mathbb{N},B\in\mathcal{B}(\mathcal{H})). \tag{15}$$

We wish to extend this result to show that for each POV measure $\mathbf{A}$ with range in a C^*-algebra $\mathcal{A}$, there is a CP instrument $\mathcal{E}^{\mathbf{A}}$ that is compatible with $\mathbf{A}$ and local to $\mathcal{A}$. In this paper, we prove this result for finite quantum systems (Theorem 2), and for infinite quantum systems that can be approximated, in an appropriate sense, by finite quantum systems (Theorem 3). While our proof for the finite case uses only elementary linear algebra, our proof for the infinite case is nonconstructive (i.e., invokes the axiom of choice in the form of the Tychonoff product theorem), and uses tools from the theory of operator algebras.

We first show that if Alice has a finite quantum system, then she can perform a "maximally disturbing" local operation—i.e., an operation that maps all her states to the maximally mixed state.

Lemma 2: If $\mathcal{A}$ is finite-dimensional C^*-algebra on the Hilbert space $\mathcal{H}$, then there is a completely positive projection Φ from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{A}'$. In particular, Φ maps $\mathcal{A}$ onto $\mathbb{C}I$.

Proof (Compare with Ref. 11, Proposition 8.3.11, and Ref. 22): Since $\mathcal{A}$ is finite-dimensional, $\mathcal{A}=\bigoplus_{i=1}^{m}\mathcal{M}_{n(i)}$ for some positive integers $n(1),\ldots,n(m)$. Consider the following statement:

(†) There is a projective unitary representation $g\mapsto W(g)$ of a finite group G in $\mathcal{A}$ such that $\{W(g):g\in G\}$ spans $\mathcal{A}$.

We first show that (†) holds when $\mathcal{A}=\mathcal{M}_n$. Let $\{|0\rangle,\ldots,|n-1\rangle\}$ be a basis for $\mathbb{C}^n$, and for each $g\in\mathbb{Z}_n\times\mathbb{Z}_n$ let $W(g)$ be the unitary operator on $\mathbb{C}^n$ defined by

$$W(g)|a\rangle = e^{ig_1a}|a+g_2\rangle \quad (a=1,\ldots,n). \tag{16}$$

Then $g\mapsto W(g)$ is a projective representation of $\mathbb{Z}_n\times\mathbb{Z}_n$ with bicharacter $\xi(g,h)=e^{ig_1h_2}$; i.e., $W(g)W(h)=e^{ig_1h_2}W(g+h)$. Furthermore, $\{W(g):g\in\mathbb{Z}_n\times\mathbb{Z}_n\}$ is an orthonormal basis for $\mathcal{M}_n$ relative to the inner product $\langle A|B\rangle_2=\mathrm{Tr}(A^*B)$. Thus, we have established (†) for the case that $\mathcal{A}=\mathcal{M}_n$. We now show that (†) holds when $\mathcal{A}=\bigoplus_{i=1}^{m}\mathcal{M}_{n(i)}$. Indeed, let

$$G=\bigoplus_{i=1}^{m}[\mathbb{Z}_{n(i)}\times\mathbb{Z}_{n(i)}], \tag{17}$$

and take the direct sum of the corresponding projective representations.

We now show that if (†) holds, then there is a CP projection from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{A}'$. For each $g\in G$, define an automorphism α_g of $\mathcal{B}(\mathcal{H})$ by

$$\alpha_g(A)=W(g)^*AW(g) \quad (B\in\mathcal{B}(\mathcal{H})). \tag{18}$$

Then $\mathcal{G}=\{\alpha_g:g\in G\}$ is a finite group of automorphisms of $\mathcal{B}(\mathcal{H})$. If $\alpha(A)=A$ for all $\alpha\in\mathcal{G}$, then $AW(g)=W(g)A$ for all $g\in G$, and $A\in\mathcal{A}'$. Thus,

$$\Phi(A)=|\mathcal{G}|^{-1}\sum_{\alpha\in\mathcal{G}}\alpha(A) \quad (A\in\mathcal{B}(\mathcal{H})) \tag{19}$$

is a CP projection from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{A}'$. □

We are now prepared to prove a generalized HJW theorem, valid for all finite quantum systems (i.e., systems whose algebra of observables is finite-dimensional). In particular, if the C^*-algebra $\mathcal{B}'$ is finite-dimensional, then the product $\Phi\otimes\mathbf{A}$ of the maximally disturbing operation Φ (from Lemma 2) and the POV measure $\mathbf{A}$ (from Theorem 1) yields an instrument that prepares the ensemble μ on system $\mathcal{B}$.

Theorem 2 (Generalized HJW Theorem): *Let $\mathcal{B}$ be a C^*-algebra acting on the Hilbert space $\mathcal{H}$, let x be a unit vector in $\mathcal{H}$, and let μ be a measure on the state space of $\mathcal{B}$ such that $\omega_x|_{\mathcal{B}}$ is the barycenter of μ. If $\mathcal{B}'$ is finite-dimensional, then there is a CP instrument $\mathcal{E}$ on $\mathcal{B}(\mathcal{H})$ that is local to $\mathcal{B}'$ and*

$$\langle x|\mathcal{E}[S](B)x\rangle=\int_S\omega(B)d\mu(\omega), \tag{20}$$

for all $S\in\Sigma$ and $B\in\mathcal{B}$.

Proof: By Lemma 2, there is a CP projection Φ from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{A}'$. Let $\mathcal{E}=\Phi\otimes\mathbf{A}$, where $\mathbf{A}$ is the POV measure defined in Theorem 1. That is,

$$\mathcal{E}[S](B)=\Phi(B)A(S), \tag{21}$$

for all $S\in\Sigma$ and $B\in\mathcal{B}(\mathcal{H})$. □

This generalized HJW theorem applies to bit commitment protocols that employ continuous ensembles on finite quantum systems (e.g., continuous measures on the Bloch sphere), and to finite quantum systems with Abelian superselection rules (direct sums of matrix algebras). However, this first result leaves open the possibility of secure bit commitment protocols that employ infinite quantum systems. So, in the following subsection, we prove a more general HJW theorem that also applies to infinite quantum systems.

A. HJW theorem for hyperfinite algebras

Definition: A von Neumann algebra $\mathcal{R}$ is said to be *hyperfinite* just in case there is an upward directed family $\{\mathcal{R}_a\}_{a\in\mathbb{A}}$ of finite-dimensional C^*-algebras such that $\mathcal{R}$ is the weak-operator closure of $\cup_{a\in\mathbb{A}}\mathcal{R}_a$.

As in the finite case, an observer with a hyperfinite von Neumann algebra can perform a maximally disturbing measurement operation.

Lemma 3: If $\mathcal{R}$ is a hyperfinite von Neumann algebra acting on the Hilbert space $\mathcal{H}$, then there is a completely positive projection Φ from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{R}'$. In particular, Φ maps $\mathcal{R}$ onto $\mathbb{C}I$.

Notation: For an arbitrary operator B in $\mathcal{B}(\mathcal{H})$ we write $\mathrm{co}_{\mathcal{R}}(B)^-$ for the weak-operator closed convex hull of $\{UBU^*: U\in\mathcal{R}, U \text{ unitary}\}$.

Proof (Compare with Ref. 11, Proposition. 8.3.11; Exercise 8.7.24, and Ref. 22): Let $\{\mathcal{R}_a: a\in\mathbb{A}\}$ be an increasing net of finite-dimensional C^*-algebras on $\mathcal{H}$ such that

$$\left(\cup_{a\in\mathbb{A}}\mathcal{R}_a\right)^- = \mathcal{R}, \tag{22}$$

where $\mathcal{X}^-$ denotes the weak-operator closure of $\mathcal{X}$. By Lemma 2, for each $a\in\mathbb{A}$ there is a CP projection Φ_a from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{R}_a'$. Let

$$X = \prod_{B\in\mathcal{B}(\mathcal{H})} \mathrm{co}_{\mathcal{R}}(B)^- \tag{23}$$

be the product topological space, where each factor is equipped with the weak-operator topology. For fixed $B\in\mathcal{B}(\mathcal{H})$, $\mathrm{co}_{\mathcal{R}}(B)^-$ is weak-operator closed and bounded, and is therefore weak-operator compact (Ref. 11, Theorem 5.1.3). Thus, the Tychonoff product theorem entails that X is compact. Let $\mathcal{M}$ be the subset of X consisting of mappings Φ that are positive, linear, normalized, and such that

$$\Phi(R_1'BR_2') = R_1'\Phi(B)R_2', \tag{24}$$

for all $R_1', R_2'\in\mathcal{R}'$ and for all $B\in\mathcal{B}(\mathcal{H})$. Since $\mathcal{M}$ is closed in X, $\mathcal{M}$ is compact, and $\{\Phi_a: a\in\mathbb{A}\}$ has a limit point $\Phi\in\mathcal{M}$. Note that $\lim_a\Phi_a=\Phi$ iff, for each fixed $B\in\mathcal{B}(\mathcal{H})$, $\text{w-lim}_a\Phi_a(B)=\Phi(B)$. We claim that $\Phi(B)\in\mathcal{R}'$ for each $B\in\mathcal{B}(\mathcal{H})$. Let $A\in\cup_{a\in\mathbb{A}}\mathcal{R}_a$; that is, there is an $m\in\mathbb{A}$ such that $A\in\mathcal{R}_m$. Then, $A\Phi_a(B)=\Phi_a(B)A$, for all $a\geqslant m$. Since the maps $Z\mapsto AZ$ and $Z\mapsto ZA$ are weak-operator continuous,

$$A\left[\text{w-}\lim_{a\geqslant m}\Phi_a(B)\right] = \text{w-}\lim_{a\geqslant m}[A\Phi_a(B)] = \text{w-}\lim_{a\geqslant m}[\Phi_a(B)A] \tag{25}$$

$$=\left[\text{w-}\lim_{a\geqslant m}\Phi_a(B)\right]A. \tag{26}$$

Since $\Phi(B)=\text{w-}\lim_a\Phi_a(B)=\text{w-}\lim_{a\geqslant m}\Phi_a(B)$, it follows that $A\Phi(B)=\Phi(B)A$. Since A was an arbitrary element of $\cup_{a\in\mathbb{A}}\mathcal{R}_a$, $\Phi(B)\in(\cup_{a\in\mathbb{A}}\mathcal{R}_a)'=\mathcal{R}'$. Therefore $\mathrm{ran}(\Phi)=\mathcal{R}'$. Finally, since Φ is an $\mathcal{R}'$-bimodule mapping [i.e., Eq. (24) holds], Φ is idempotent and completely positive (Ref. 24, Corollary 3.4). □

Again, a maximally disturbing operation Φ can be tensored with the POV measure **A** to yield an instrument that prepares the ensemble μ on Bob's system.

Theorem 3 (Generalized HJW Theorem): *Let $\mathcal{B}$ be a C^*-algebra acting on the Hilbert space $\mathcal{H}$, let x be a unit vector in $\mathcal{H}$, and let μ be a measure on the state space of $\mathcal{B}$ such that $\omega_x|_{\mathcal{B}}$*

is the barycenter of μ. If $\mathcal{B}'$ is hyperfinite, then there is a CP instrument $\mathcal{E}$ on $\mathcal{B}(\mathcal{H})$ that is local to $\mathcal{B}'$ and

$$\langle x|\mathcal{E}[S](B)x\rangle = \int_S \omega(B)d\mu(\omega), \tag{27}$$

for all $S \in \Sigma$ and $B \in \mathcal{B}$.

Proof: The proof is identical to the proof of Theorem 2, with Lemma 3 replacing Lemma 2.□

III. APPLICATION TO BIT COMMITMENT

The Mayers–Lo–Chau theorem shows that when $\mathcal{A}=\mathcal{M}_n\otimes I$ and $\mathcal{B}=\mathcal{A}'$, and when bits are encoded in finite ensembles, then $(\mathcal{A},\mathcal{B})$ cannot be used to implement a secure bit commitment protocol. The generalized HJW theorem allows us to extend this result to the case where $\mathcal{A}(=\mathcal{B}')$ is an arbitrary hyperfinite von Neumann algebra, and to encodings that employ arbitrary ensembles of states on $\mathcal{B}$. In particular, the generalized HJW theorem entails that there can be no secure bit commitment protocol using infinite (hyperfinite) quantum systems, or quantum systems with Abelian superselection rules.

A. Bit commitment with infinite quantum systems

The quantum bit commitment protocols that have been proposed to date employ finite quantum systems. In this subsection, we describe a bit commitment protocol that employs continuous ensembles of states on infinite qubit lattices. Since this protocol does not fall within the range of validity of the HJW theorem, it is immune to current no-go theorems against bit commitment. However, we show that this protocol can be cheated by exploiting the nonlocal correlations of an "infinitely entangled" EPR state (see Ref. 13).

Let $|0,0\rangle$ and $|0,1\rangle$ be orthogonal unit eigenvectors of σ_x, and let $|1,0\rangle$ and $|1,1\rangle$ be orthogonal unit eigenvectors of σ_y. Then, heuristically, the states of a one-dimensional infinite qubit lattice include vectors of the form

$$\|b,s\rangle\rangle =_{\text{def}} \otimes_{i=1}^{\infty}|b,s(i)\rangle \quad (s \in (\mathbb{Z}_2)^{\omega}), \tag{28}$$

with $b=0$ or $b=1$. (We provide a rigorous definition of these states below.)

During the Commit stage of the protocol, Alice performs operations on a composite $(\mathcal{A},\mathcal{B})$ consisting of two lattice systems $\mathcal{A}$ and $\mathcal{B}$, and she then sends system $\mathcal{B}$ to Bob. During the Unveil stage, Alice makes measurements on $\mathcal{A}$, and sends classical information to Bob, who then makes measurements on $\mathcal{B}$.

Commit: For $b=0,1$, Alice chooses a random sequence $s \in (\mathbb{Z}_2)^{\omega}$, and prepares the state

$$\|b,s\rangle\rangle_A \otimes \|b,s\rangle\rangle_B.$$

Alice holds part A, and sends part B to Bob. (So, the ensemble Bob receives is an equal mixture over $\|b,s\rangle\rangle$, for $s \in (\mathbb{Z}_2)^{\omega}$.)

Unveil: Alice measures the observable

$$A_b = \sum_{i=1}^{\infty} \frac{2}{3^i} P_b^{(i)},$$

on her systems, where $P_b=\frac{1}{2}(I+\sigma_b)$ and

$$P_b^{(i)} = I \otimes \cdots I \otimes P_b \otimes I \otimes \cdots.$$

(Each state $\|b,s\rangle\rangle$ is an eigenstate of A_b, and when $s_1 \neq s_2$, $\|b,s_1\rangle\rangle$ and $\|b,s_2\rangle\rangle$ assign different values to A_b.) Alice sends the results of her measurements (a list of numbers in the Cantor set) to Bob. Bob measures A_b on his systems and compares his numbers with Alice's. Bob accepts if the two lists agree, and rejects if the two lists disagree.

Let ρ_b be the state that Bob receives. It is intuitively clear that if Alice follows the protocol honestly, then $\rho_0=\rho_1$, and so Bob cannot cheat. (We prove this fact below.)

We now tighten up the mathematical description of the systems involved in the protocol. The observables of a one-dimensional qubit lattice are represented by the C^*-algebraic infinite direct product

$$\mathcal{A} = \bigotimes_{i\in\mathbb{N}} \mathcal{M}_{n(i)}, \tag{29}$$

where $n(i)=2$ for each $i\in\mathbb{N}$. For each $i\in\mathbb{N}$ and $A\in\mathcal{M}_2$, let

$$A^{(i)} = I\otimes\cdots\otimes I\otimes A\otimes I\cdots, \tag{30}$$

where A is in the ith position. If for each $i\in\mathbb{N}, \omega_i$ is a state of $\mathcal{M}_2$, then there is a unique state $\otimes_{i=1}^{\infty}\omega_i$ of $\mathcal{A}$ defined by

$$(\otimes_{i=1}^{\infty}\omega_i)(A^{(j)}) = \omega_j(A). \tag{31}$$

Furthermore, $\otimes_{i=1}^{\infty}\omega_i$ is pure iff each ω_i is pure, and is a trace iff each ω_i is a trace (Ref. 11, Proposition 11.4.7). Thus, if $\{|i\rangle : i\in\mathbb{N}\}$ are unit vectors in $\mathbb{C}^2$, then $\otimes_{i=1}^{\infty}|i\rangle$ can be used to denote the corresponding pure state of $\mathcal{A}$. In particular, for any $s\in(\mathbb{Z}_2)^{\omega}$, $\|b,\ s\rangle\rangle$ does in fact correspond to a pure state of $\mathcal{A}$.

Let $\mathcal{B}$ be an isomorphic copy of $\mathcal{A}$. Since $\mathcal{A}$ is a uniform limit of an increasing sequence of finite-dimensional algebras, it is nuclear; i.e., there is a unique norm on the algebraic tensor product $\mathcal{A}\odot\mathcal{B}$ whose completion is a C^*-algebra. We denote this C^*-algebra by $\mathcal{A}\otimes\mathcal{B}$. We now establish the existence of the ensembles described in the protocol, and we show that they give rise to the same quantum state (namely, the "maximally mixed" tracial state) on system $\mathcal{B}$.

Proposition 4: If μ is the normalized Haar measure on $(\mathbb{Z}_2)^{\omega}$, then there is a probability measure μ_b on the state space of $\mathcal{A}\otimes\mathcal{B}$ such that

$$\mu_b(\{\|b,s\rangle\rangle_A\otimes\|b,s\rangle\rangle_B : s\in S\}) = \mu(S), \tag{32}$$

for every Borel subset S of $(\mathbb{Z}_2)^{\omega}$. Furthermore, if ρ_b is the barycenter of μ_b, then $\rho_b|_{I\otimes\mathcal{B}}$ is the tracial state.

To establish the first part of Proposition 4, it will suffice to show that

$$s \overset{\varphi}{\mapsto} \|b,s\rangle\rangle_A\otimes\|b,s\rangle\rangle_B \tag{33}$$

is a continuous mapping of $(\mathbb{Z}_2)^{\omega}$ into the state space of $\mathcal{A}\otimes\mathcal{B}$ (with the weak* topology), for then the induced measure $\mu_b=\mu\circ\varphi^{-1}$ will satisfy Eq. (32).

Let $G=\Sigma_{i\in\mathbb{N}}(\mathbb{Z}_2\oplus\mathbb{Z}_2)_i$ be the direct sum of a countable number of copies of $\mathbb{Z}_2\oplus\mathbb{Z}_2$. Elements of G are sequences with values in $\mathbb{Z}_2\oplus\mathbb{Z}_2$ that differ from the identity (0, 0) in only finitely many positions. Let $V_{(0,0)}=I$, $V_{(0,1)}=\sigma_x, V_{(1,0)}=\sigma_y$, and $V_{(1,1)}=\sigma_z$, and, for any $s\in G$, let

$$U(s) =_{\text{def}} V_{s(1)}\otimes V_{s(2)}\otimes V_{s(3)}\otimes\cdots\in\mathcal{A}. \tag{34}$$

Then the set $\{U(s) : s\in G\}$ is linearly dense in $\mathcal{A}$. Let H_b denote the subgroup of G generated by those sequences s with the property that $s(i)=(0,0)$ or $s(i)=(b,b\oplus 1)$ for all $i\in\mathbb{N}$. Then, $\{U(s) : s\in H_b\}$ generates an Abelian subalgebra of $\mathcal{A}$, namely, the algebra generated by the spin operator $V_{(b,b\oplus 1)}$ at each lattice site.

Lemma 5: If $\mathcal{C}$ is the Abelian subalgebra of $\mathcal{A}$ generated by $\{U(s): s \in H_b\}$, then the pure state space of $\mathcal{C}$ is homeomorphic to $(\mathbb{Z}_2)^\omega$.

Proof: The Abelian C^*-algebra $\mathcal{C}$ is isomorphic to the C^*-algebra $C(X)$ of continuous complex-valued functions on X, where X is the pure state space of $\mathcal{C}$ equipped with the weak* topology. Furthermore, if $C(X)$ and $C(Y)$ are isomorphic, then X and Y are homeomorphic. Thus, if $\mathcal{C} \simeq C(Y)$, then the space of pure states of $\mathcal{C}$ is homeomorphic to Y. Now, $\mathcal{C} \simeq \bigotimes_{i=1}^{\infty} \mathcal{N}_i$, where $\mathcal{N}_i$ is the Abelian algebra generated by σ_b. Since $\mathcal{N}_i$ is isomorphic to $C(\mathbb{Z}_2)$,

$$\bigotimes_{i=1}^{\infty} \mathcal{N}_i \simeq \bigotimes_{i=1}^{\infty} C(\mathbb{Z}_2) \simeq C((\mathbb{Z}_2)^\omega), \tag{35}$$

where $(\mathbb{Z}_2)^\omega$ is equipped with the product topology (see Ref. 11, pp. 910–911; Proposition 11.4.3). Therefore the pure state space of $\mathcal{C}$ is homeomorphic to $(\mathbb{Z}_2)^\omega$. □

Since $\mathcal{C}$ is isomorphic to $C((\mathbb{Z}_2)^\omega)$, there is (by the Riesz representation theorem) a one-to-one correspondence between positive normalized measures on $(\mathbb{Z}_2)^\omega$ and states on $\mathcal{C}$.

Lemma 6: If μ is the Haar measure on $(\mathbb{Z}_2)^\omega$, then the barycenter of μ is $\tau|_{\mathcal{C}}$, where τ is the trace on $\mathcal{A}$.

Proof: Let $\sigma(\mathcal{C})$ denote the pure state space of $\mathcal{C}$, and let $\rho = \int_{\sigma(\mathcal{C})} \omega d\mu(\omega)$ be the barycenter of μ. To show that $\rho = \tau$, it will suffice to show that $\rho(U(s)) = 0$ whenever $s \in H_b - \{e\}$. Indeed, if $s \neq e$, then there is an $i \in \mathbb{N}$ such that $s(i) = (b, b \oplus 1)$. Let s' be the element of $\oplus_{i=1}^{\infty}(\mathbb{Z}_2 \oplus \mathbb{Z}_2)_i$ such that $s'(j) = s(j)$ when $j \neq i$, and $s'(i) = (b \oplus 1, b)$. Then $U(s')^* U(s) U(s') = -U(s)$. Since μ is translation-invariant, $\rho(U(s)) = -\rho(U(s))$. Therefore $\rho(U(s)) = 0$. □

Lemma 7: There is a completely positive projection Φ from $\mathcal{A}$ onto $\mathcal{C}$ such that $\tau(\Phi(A)) = \tau(A)$ for all A in $\mathcal{A}$.

Proof: For each $t \in \mathbb{R}$, define an automorphism α_t of $\mathcal{A}$ by

$$\alpha_t(B) = e^{-itA_b} B e^{itA_b} \quad (B \in \mathcal{A}). \tag{36}$$

Since A_b is bounded, the map $t \mapsto \alpha_t(B)$ is norm-continuous. If ν is an invariant mean on $\mathbb{R}$, then

$$\Phi(B) = \int_{\mathbb{R}} \alpha_t(B) d\nu(t) \quad (B \in \mathcal{A}) \tag{37}$$

is a positive linear map on $\mathcal{A}$ (Ref. 20, Lemma 7.4.4). (To show that Φ is completely positive, it will suffice to show that the range of Φ is Abelian.) Clearly $\Phi(C_1 B C_2) = C_1 \Phi(B) C_2$ for all $C_1, C_2 \in \mathcal{C}$, and $B \in \mathcal{A}$. In particular, $\Phi(C) = C$ for all $C \in \mathcal{C}$. To see that the image of Φ lies in $\mathcal{C}$, let s be an element of $G = \Sigma_{i \in \mathbb{N}}(\mathbb{Z}_2 \oplus \mathbb{Z}_2)_i$. If $s \in H_b$, then $U(s) \in \mathcal{C}$ and $\Phi(U(s)) = U(s)$. Suppose then that $s \notin H_b$; that is, there is an $i \in \mathbb{N}$ such that either $s(i) = (b \oplus 1, b)$ or $s(i) = (1, 1)$. (It will suffice to consider the first case; the second case follows by symmetry.) Then

$$U(s) = V_{s(1)} \otimes \cdots \otimes V_{s(i-1)} \otimes V_{s(i)} \otimes V_{s(i+1)} \otimes \cdots, \tag{38}$$

and

$$\Phi(U(s)) = V_{s(1)} \otimes \cdots \otimes V_{s(i-1)} \otimes B_i \otimes V_{s(i+1)} \otimes \cdots, \tag{39}$$

where

$$B_i = \int_{\mathbb{R}} e^{-itP_b} [V_{(b \oplus 1, b)}] e^{itP_b} d\nu(t) = 0. \tag{40}$$

Thus, $\Phi(U(s)) = 0$. Since $\{U(s): s \in G\}$ spans $\mathcal{A}$, it follows that $\mathrm{ran}(\Phi) = \mathcal{C}$. To see that $\tau = \tau \circ \Phi$, note that every nonidentity element of $\{U(s): s \in G\}$ is trace-free. If $s \in H_b$, then $\Phi(U(s)) = U(s)$ and therefore $\tau(\Phi(U(s))) = \tau(U(s))$. If $s \notin H_b$, then $\Phi(U(s)) = 0$ and $\tau(U(s)) = 0$. Since τ and $\tau \circ \Phi$ are continuous linear functionals, $\tau = \tau \circ \Phi$. □

The mapping $\Psi=\Phi\otimes\Phi$ is a CP projection from $\mathcal{A}\otimes\mathcal{B}$ onto $\mathcal{C}\otimes\mathcal{C}$, and its adjoint Ψ^* is a weak* continuous mapping from the state space of $\mathcal{C}\otimes\mathcal{C}$ into the state space of $\mathcal{A}\otimes\mathcal{B}$. Let $\sigma(\mathcal{C}\otimes\mathcal{C})$ denote the pure state space of $\mathcal{C}\otimes\mathcal{C}$, and let $\sigma(\mathcal{A}\otimes\mathcal{B})$ denote the pure state space of $\mathcal{A}\otimes\mathcal{B}$. Using Ψ^* again to denote the restriction of Ψ^* to $\sigma(\mathcal{C}\otimes\mathcal{C})$, and identifying $\sigma(\mathcal{C}\otimes\mathcal{C})$ with $(\mathbb{Z}_2)^\omega\times(\mathbb{Z}_2)^\omega$, it follows that Ψ^* is a continuous injection of $(\mathbb{Z}_2)^\omega\times(\mathbb{Z}_2)^\omega$ into $\sigma(\mathcal{A}\otimes\mathcal{B})$. Note that

$$\Psi^*[(s,s)] = \|b,s\rangle\rangle_A \otimes \|b,s\rangle\rangle_B \tag{41}$$

and so the mapping

$$s \overset{\varphi}{\mapsto} \|b,s\rangle\rangle_A \otimes \|b,s\rangle\rangle_B = (\Psi^* \circ \Delta)(s), \tag{42}$$

where $\Delta(s)=(s,s)$, is continuous, which establishes the first part of Proposition 4.

Now let ρ_b denote the barycenter of μ_b, and let $\nu_b =_{\text{def}} \mu\circ(\Phi^*)^{-1}$ denote the measure on $\sigma(\mathcal{B})$ induced by Φ^* from the measure μ on $\sigma(\mathcal{C})$. Then for any $B\in\mathcal{B}$,

$$\rho_b(I\otimes B) = \int_{\sigma(\mathcal{A}\otimes\mathcal{B})} \omega(I\otimes B)\,d\mu_b(\omega) = \int_{\sigma(\mathcal{B})} \omega(B)\,d\nu_b(\omega) \tag{43}$$

$$= \int_{\sigma(\mathcal{C})} \omega(\Phi(B))\,d\mu(\omega) = \tau(\Phi(B)) = \tau(B). \tag{44}$$

This establishes the second part of Proposition 4. Thus, μ_0 and μ_1 are the ensembles prepared by Alice if she follows the protocol honestly.

Finally, we show that Alice can cheat by preparing an entangled state during the Commit stage rather than μ_0 or μ_1. In particular, if for each $i\in\mathbb{N}$, $\psi_i=\psi$ is the Bohm-EPR state of $\mathcal{M}_2\otimes\mathcal{M}_2$, then $\omega=_{\text{def}}\otimes_{i=1}^{\infty}\psi_i$ is a pure state of $\bigotimes_{i=1}^{\infty}(\mathcal{M}_{n(i)}\otimes\mathcal{M}_{n(i)})=\mathcal{A}\otimes\mathcal{B}$.[13] It is not difficult to see, then, that if Alice performs a nonselective measurement of A_b [represented by the CP map in Eq. (36)] when $\mathcal{A}\otimes\mathcal{B}$ is in state ω, then the posterior state is the ensemble μ_b. Therefore, if Alice prepares ω during the Commit stage, then she can unveil either 0 or 1.

B. Bit commitment and superselection rules

It has recently been argued by Mayers, Kitaev, and Preskill,[14,18] in response to a question raised by Popescu,[21] that the no-go theorem for bit commitment extends to the case of quantum systems with superselection rules. The generalized HJW theorem provides another route to this result, at least for systems whose superselection rules are Abelian. In the case of Abelian superselection rules, $\mathcal{A}=\mathcal{B}'$; that is, Alice can perform any operation that commutes with Bob's measurement operations. And the generalized HJW theorem shows that an observer with algebra $\mathcal{B}'$ can steer system $\mathcal{B}$ into any ensemble consistent with $\omega_x|_{\mathcal{B}}$. Thus, a bit commitment protocol is perfectly concealing against Bob only if it is not binding against Alice. However, the generalized HJW theorem has nothing to say (directly) about Alice's ability to cheat when both systems are governed by non-Abelian superselection rules (in which case $\mathcal{A}\subset\mathcal{B}'$).

Mayers *et al.*[14] claim that—HJW theorem aside—Alice can always steer Bob's system into the state of her choice by adding, if necessary, an appropriate ancilla to her system. Their argument is based on a more general claim that restrictions imposed by superselection rules on a local system can always be effectively removed by embedding the local system in a larger system (in particular, by adding an ancilla).

The formalism of elementary quantum mechanics imposes no restriction on adding ancillae. However, in the setting of algebraic quantum field theory, an observer can measure only those observables that correspond to her space–time region. As a result, adding ancillae is not permitted—at least if "adding an ancilla" is interpreted to mean that Alice can measure observables that are not in her local observable algebra $\mathcal{R}(O_A)$. Thus, in this richer theoretical framework, Alice is subject to further constraints on her ability to simulate any operation that commutes

with Bob's measurement operations, and these constraints could—it seems theoretically possible—prevent Alice from cheating in a bit commitment protocol. (It would be interesting to explore connections between the formal condition $\mathcal{A}\subset\mathcal{B}'$ and relativistic constraints of the sort exploited by Kent's[12] bit commitment protocol.)

C. Limitations on the generalized HJW theorem

Let us say that a bit commitment protocol employs a *quantum encoding* just in case Alice encodes her choice of a bit 0 or 1 in two ensembles μ_0 or μ_1 of quantum states. Then, even in the case of bit commitment schemes that employ quantum encodings, there is one further assumption of the generalized HJW theorem that is not *prima facie* guaranteed to hold in any bit commitment protocol: the assumption that the barycenter of μ_b is a *vector* state. (Let us call this latter assumption the *vector state assumption*.)

First, it is not difficult to find pairs of C^*-algebras $(\mathcal{A},\mathcal{B})$, and measures μ_b on the state space of $\mathcal{B}$ such that the vector state assumption does not hold: e.g., let $\mathcal{B}=\mathcal{M}_2$, and let μ_b be the measure on the state space of $\mathcal{B}$ that assigns $\frac{1}{2}$ to each of $\frac{1}{2}(I+\sigma_b)$ and $\frac{1}{2}(I-\sigma_b)$. (Of course, this trivial example could not be used to construct a secure bit commitment protocol, since Alice could not perform any nontrivial measurements to verify her commitment to Bob.) However, the vector state assumption does hold when $\mathcal{B}$ has a separating vector in $\mathcal{H}$.

Definition: A vector x in the Hilbert space $\mathcal{H}$ is said to be *separating* for the C^*-algebra $\mathcal{B}$ just in case $Bx=0$ only if $B=0$ for all $B\in\mathcal{B}$.

Proposition 8 (Ref. 11, Theorem 7.3.8): If $\mathcal{B}$ is a C^*-algebra acting on the Hilbert space $\mathcal{H}$ and if $\mathcal{B}$ has a separating vector x in $\mathcal{H}$, then each state of $\mathcal{B}$ is implemented by some vector in $\mathcal{H}$.

Thus, if $\mathcal{B}$ has a separating vector in the Hilbert space $\mathcal{H}$ (and if $\mathcal{A}=\mathcal{B}'$), then any ensemble of states on $\mathcal{B}$ corresponds to a state $\omega_x|_{\mathcal{B}}$ induced by a vector x in $\mathcal{H}$, and the generalized HJW theorem entails that any two equivalent ensembles can be prepared at a distance (from a common state). For example, $\mathcal{B}=I_A\otimes\mathcal{B}(\mathcal{H}_B)$ has a separating vector in $\mathcal{H}_A\otimes\mathcal{H}_B$ if and only if $\dim(\mathcal{H}_B)\leqslant\dim(\mathcal{H}_A)$.[8] So, in the case of elementary quantum systems, by adding an ancilla, Alice can "make her Hilbert space as large as Bob's," which ensures that their joint Hilbert space $\mathcal{H}=(\mathcal{H}_{A'}\otimes\mathcal{H}_A)\otimes\mathcal{H}_B$ contains a vector representative of each of Bob's states.

Nonetheless, there are C^*-algebras that do not have—and could not have, in any faithful representation—a separating vector, e.g., C^*-algebras which contain an uncountable family of mutually orthogonal projection operators. But if $\mathcal{B}$ does not have a separating vector, then the HJW theorem does not show that an observer with algebra $\mathcal{B}'$ could perform operations that prepare any one of two equivalent measures on the state space of $\mathcal{B}$ (from a common ancestor state). Until the HJW theorem is generalized to cover such cases, there remains a small, but theoretically crucial, loophole in current proofs of the impossibility of secure bit commitment.

IV. CONCLUSION

We have shown, subject to a mild constraint (viz., that the systems involved are "hyperfinite"), that any two equivalent measures on the state space of a C^*-algebra can be prepared "at a distance." This result generalizes the Hughston–Jozsa–Wootters theorem, and so can be used to extend the Mayers–Lo–Chau argument against the security of quantum bit commitment protocols.

However, the results proved to date—including the results in this paper—are not yet sufficient to rule out the security of any conceivable quantum bit commitment protocol. First, it remains an open question whether an analog of the HJW theorem holds for any system whose observables can be represented by self-adjoint operators in some abstract (not necessarily nuclear) C^*-algebra. Second, in order to invoke the HJW theorem in an argument against bit commitment, one must make further physical assumptions—e.g., that the states on Bob's system correspond to vector states of some larger system S, and that Alice can perform any operation on S that commutes with Bob's measurement operations—that have yet to be justified in a fully general context.

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Chaos in the case of two fixed black holes

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We study the structure of chaos in the relativistic problem of particles moving in the field of two fixed black holes M_1 and M_2 by considering the asymptotic curves of some simple unstable periodic orbits on a surface of section. These curves consist of infinite arcs reaching the two black holes. Most orbits starting along these curves (asymptotic orbits) escape, i.e., they fall into the black holes M_1 (type I orbits) and M_2 (type II orbits). The number of the remaining orbits after n iterations (intersections with the surface of section) decreases exponentially with n. The asymptotic curves intersect at infinite homoclinic and heteroclinic points. We study in detail the forms of the asymptotic orbits with emphasis on the homoclinic and heteroclinic orbits. The homoclinic and heteroclinic intersections are confined in certain intervals along the asymptotic curves. Every homoclinic and heteroclinic orbit is the limit of infinite more homoclinic and heteroclinic orbits. Between an asymptotic orbit falling on the black hole M_1 and another orbit falling on the black hole M_2 there are infinite homoclinic and heteroclinic orbits and infinite transitions between type I and type II orbits. Therefore the orbits of type I and II form fractal sets. The nonasymptotic curves falling on the black holes M_1 and M_2 also form fractal sets. The black holes act as attractors and the areas on the surface of section are not conserved despite the fact that the system is conservative. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1782672]

I. INTRODUCTION

The relativistic system of two fixed black holes is important because it has a large degree of chaos, while the corresponding classical problem is completely ordered (integrable) and does not have any chaos at all.[1,2] In the case of orbits of photons (null geodesics) and of particles (timelike geodesics) with hyperbolic or parabolic energy almost all orbits either escape to infinity, or fall on a black hole, while in the case of particles with elliptic energy many orbits fall on one of the two black holes.

In the present paper we explore the structure of chaos by studying the forms of the asymptotic curves and of the corresponding asymptotic orbits. We study in detail a case with particular values of the energy and masses of the black holes, but this case is typical of most other cases.

The basic characteristic feature of chaos is the existence of asymptotic manifolds intersecting along homoclinic and heteroclinic orbits. On a surface of section $x=0$ (with $\dot{x}>0$) there are asymptotic curves intersecting along homoclinic and heteroclinic points. The asymptotic curves are composed of infinite disjoint arcs reaching the black holes. The structure of these arcs is discussed in Sec. II.

Section III describes the main simple periodic orbits (i.e., periodic orbits of period 1) and the main homoclinic intersections of their asymptotic curves. Then Sec. IV describes in detail the forms of the orbits starting on an asymptotic curve, i.e., the asymptotic orbits. Of special interest are the homoclinic and heteroclinic orbits connecting various periodic orbits to each other. There are infinite homoclinic and heteroclinic points along an asymptotic curve. However, the homoclinic and heteroclinic points are confined in certain domains of the phase space, leaving most of the phase space without any such points.

As a consequence of the existence of heteroclinic orbits connecting periodic orbits around M_1 and M_2 the sets of points along an asymptotic curve leading to one or the other black hole are fractal.

In Sec. V we find the basins of attraction of nonperiodic and nonasymptotic orbits, leading to the black holes M_1 and M_2. These basins consist of compact domains and of infinite filaments mixed in a fractal way.

In Sec. VI we consider briefly what happens for other values of the masses of the black holes and in Sec. VII we summarize our conclusions.

Finally, in an Appendix we consider theoretically the orbits very close to a black hole and explain the forms of the asymptotic curves when they reach the black holes.

II. ASYMPTOTIC CURVES AND ASYMPTOTIC ORBITS

Our study consists mainly of an exhaustive numerical exploration of orbits of particles (timelike geodesics) in a number of cases, with a representative value of the energy $E=\sqrt{0.5}$. We use standard numerical integration methods (fourth order Runge–Kutta), as in our previous papers (Refs. 1 and 2) and we checked the accuracy by requiring that any error in the energy conservation should be less than 10^{-10}. The energy we use is of the elliptic type ($0<E<1$), therefore there are no escapes to infinity. The mass of the black hole M_2 is always taken equal to $M_2=1$, while M_1 takes various values. In particular for $M_1=1.1$, there are two simple (almost circular) orbits around M_1 (orbits of types a, a'), two simple orbits around M_2 (orbits of types b, b') and an orbit like a hyperbolic arc [orbit of type h, intersecting the z axis and reaching the curve of zero velocity (CZV) at two symmetric points].[2]

These are the only simple periodic orbits, i.e., orbits intersecting the z axis at only one point perpendicularly (with $x=\dot{z}=0$ and $\dot{x}>0$).

In most cases all simple periodic orbits are unstable. However, there is a small interval of values of M_1 (around $M_1=1.324$), where the orbit a' is stable, and another small interval of values of M_1 (around $M_1=0.908$) where the orbit b' is stable.[2]

We study now in detail the asymptotic curves and the corresponding asymptotic orbits from the inner unstable periodic orbit of type a in the case $M_1=1.1$. This orbit (O) has $z_0=2.504\,568\,37$, $\dot{z}_0=0$.

The eigenvalue of the inner orbit a is $\lambda=32.330\,01$, the direction of the unstable eigenvector is $d\dot{z}/dz=0.0983$ and the direction of the stable eigenvector is -0.0983.

We have calculated 2×10^4 asymptotic orbits along the (upper) unstable eigenvector with a step $\Delta x=10^{-8}$. All these orbits approach asymptotically the periodic orbit O for negative time tending to $-\infty$, while for positive time they deviate further and further from O. The whole set of initial conditions has a length $\Delta x=2\times10^{-4}$. In this interval the deviations of the eigenvector from the corresponding asymptotic curve are very small, namely smaller than 2×10^{-7}. The deviations of the nth images of the 2×10^4 points from the asymptotic curves are even smaller, by a factor λ^n.

The first iterations of the original points reach a distance of order $2\times10^4\lambda\approx6.5\times10^{-3}$ and the second iterations reach a distance of order $2\times10^{-4}\lambda^2\approx0.2$. But the third iterations reach a large distance and are appreciably curved (Fig. 1). The numbers m along the asymptotic curve mark the third iterations of the initial points with distance $m\times10^{-8}$ from the periodic orbit, where m varies from 1 up to 20 000.

In Fig. 1 we see three arcs of the asymptotic curve. The first arc (1) starts at the periodic orbit (O) towards larger z with $\dot{z}$ small positive. This curve is continued with $\dot{z}<0$, and z reaches a maximum near $z=4$. Then it turns to smaller z until it reaches the black hole $z=1$, with $\dot{z}=-0.75$ (point M_1^-). The point marked 6722 is the third intersection of an orbit with initial distance $m\times10^{-8}$, along the unstable asymptotic curve from O, with $m=6722$. The orbits $m=6723-9051$ do not have a third image in Fig. 1, because these orbits fall into the black hole $z=1$ before their third intersection with the z axis with $\dot{x}>0$. The same points in Fig. 2 are the fourth iterations of the original points with $m=(6723/\lambda)-(9051/\lambda)\approx208-279$. The orbits with initial conditions $m=9052-11\,014$ in Fig. 1 ($m=280-340$ in Fig. 2) form the second arc (2). This

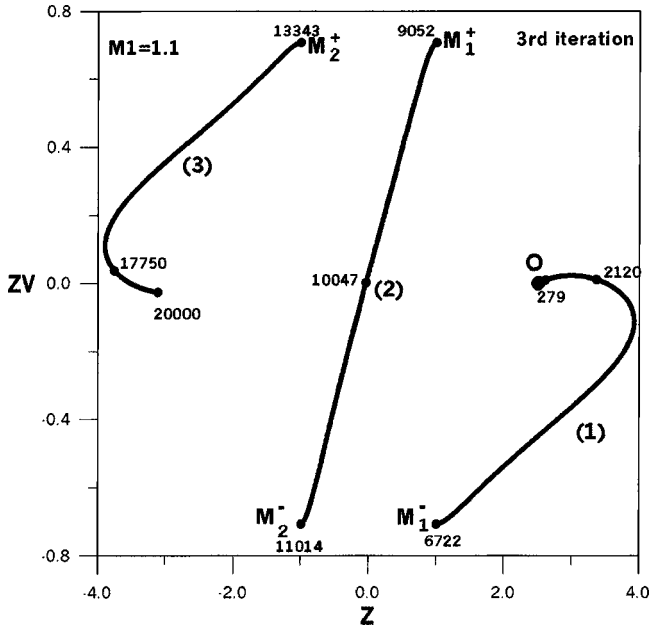

FIG. 1. An unstable asymptotic curve from the unstable periodic orbit O ($z_0=2.504\,568\,37$, $\dot{z}_0=0$) on a surface of section $(z,\dot{z})$ for $M_1=1.1$, $M_2=1$, $E=\sqrt{0.5}$. The numbers (m) indicate the third intersections of the z axis (with $\dot{x}>0$) by asymptotic orbits starting close to O (at distances $m\times10^{-8}$ along the asymptotic curve). The first part of this curve (1) starts at O and reaches the black hole $z=1$. The second part (2) starts at $z=1$ and reaches the second black hole $z=-1$. The third part (3) starts at $z=-1$ and continues beyond at $m=20\,000$.

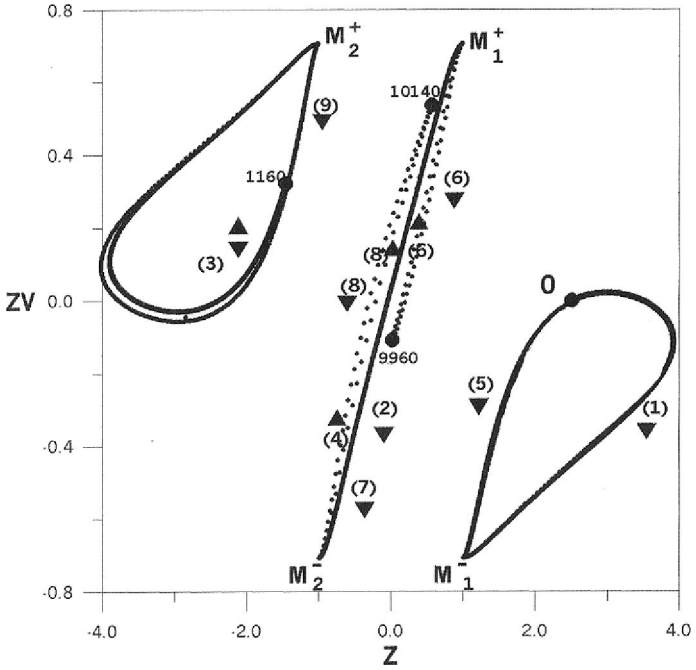

FIG. 2. The fourth iterations of orbits starting close to the unstable periodic orbit O along the unstable asymptotic curve at distances $m\times10^{-8}$. This curve consists of various arcs (1), (2),…,(9). The first arc starts at the periodic orbit O and ends at the black hole $z=1$. The other arcs start and end at a black hole. The numbers mark the turning points of the arcs (3), (6), and (8).

arc starts at the point M_1^+ ($z=1$, $\dot{z}=0.75$) and terminates at the point M_2^- ($z=-1$, $\dot{z}=-0.75$). The orbits of this arc have again a third intersection with the z axis ($\dot{x}>0$) before falling into a black hole. This third intersection is between the black holes M_1 and M_2.

The orbits with initial conditions $m=11\,015-13\,342$ in Fig. 1 (or $m=340-412$ in Fig. 2) do not have a third intersection; all these orbits fall into the black hole $z=-1$ before a third intersection with the z axis ($\dot{x}>0$). Finally, the orbits with initial conditions $m=13\,343-20\,000$ have third iterates with $z<-1$, i.e., below the black hole M_2 [third arc (3)].

The asymptotic curve continues beyond the third iteration of the point with $m=20\,000$ marked in Fig. 1. The third iteration of the initial point with $m=20\,000$ has the same position on the phase space with the fourth iteration of an initial point with $m=20\,000/\lambda\approx 615$. Thus, the points of Fig. 2 with $m<615$ belong to the arcs given in Fig. 1, and the points with $m>615$ belong to the continuation of the unstable asymptotic curve.

Figure 2 contains nine successive arcs of the asymptotic curve from the periodic orbit O, composed of the fourth iterations of the point m (with initial distance $m\times 10^{-8}$ along the asymptotic curve close to O). These arcs are separated by gaps in m, containing orbits that do not have fourth iterations. These arcs and gaps are as follows:

Arc (1) from $m=0$(O) to $m=207$ (point M_1^-),

Gap from $m=208$ to $m=279$,

Arc (2) from $m=280$ (point M_1^+) to $m=340$ (M_2^-),

Gap from $m=341$ to $m=412$,

Arc (3) from $m=413$ (point M_2^+) to $m=2054$ (M_2^+),

Gap from $m=2055$ to $m=2120$,

Arc (4) from $m=2121$ (point M_2^-) to $m=2175$ (M_1^+),

Gap from $m=2175$ to $m=2240$,

Arc (5) from $m=2241$ (point M_1^-) to $m=2748$ (M_1^-),

Gap from $m=2749$ to $m=9917$,

Arc (6) from $m=9918$ (point M_1^+) to $m=9986$ (M_1^+),

Gap from $m=9987$ to $m=10\,047$,

Arc (7) from $m=10\,048$ (point M_1^+) to $m=10\,052$ (M_2^-),

Gap from $m=10\,053$ to $m=10\,107$,

Arc (8) from $m=10\,108$ (point M_2^-) to $m=10\,185$ (M_2^-),

Gap from $m=10\,186$ to $m=17\,750$,

Arc (9) from $m=17\,751$ (point M_2^+) to $m=18\,276$ (M_2^+).

We give this detailed information in order to show the various types of arcs. After the arc (1) that starts at O and terminates at M_1 all other arcs start and terminate at M_1 or M_2.

There are three types of arcs: (a) arcs starting at M_1^- and terminating at the same point [arc (5)], (b) arcs starting at M_2^+ and terminating at the same point [arcs (3) and (9)], and (c) arcs close to the diagonal M_1^+, M_2^-. These orbits are of four subtypes: (c1) starting at M_1^+ and terminating at M_2^- [arcs (2) and (7)], (c2) starting at M_2^- and terminating at M_1^+ [arc (4)], (c3) starting at M_1^+ and terminating at the same point [arc (6)], or (c4) starting at M_2^- and terminating at the same point [arc (8)].

TABLE I. Intervals of escaping orbits.

m	Δm	Into
	(1) Escape-3 intervals (escaping before the third iteration)	
6723–9051	2328	M_1
11 015–13 342	2327	M_2
	(2) Escape-4 intervals (escaping before the fourth iteration)	
208–279	71	M_1
341–412	72	M_2
2055–2120	65	M_2
2176–2240	64	M_1
2749–9917	7168	M_1 (including the escape-3)
9987–10047	60	M_1
10 053–10 107	54	M_2
10 186–17 750	7564	M_2 (including the escape-3)
18 277–18 330	53	M_2
18 380–18 440	60	M_1
19 080–20 000+	920+	M_1

We notice also that certain intervals of m along arcs, or intervals in gaps (intervals of escape) are rather short while other intervals are quite long. The escape intervals up to $m=20\,000$ are given in Table I.

Before the third iteration a total interval $\Sigma\Delta m \approx 4660$ escape, and before the fourth iteration a total interval $\Sigma\Delta m = 16\,150$ escape up to $m=20\,000$. There remains 77% of the original set of points m after the third iteration and 19% after the fourth iteration.

After the fourth iteration only intervals summing up to less than $\Sigma\Delta m = 4000$ remain. Further intervals escape before the fifth, sixth, etc., iterations. After the fifth iteration there remains only a total interval $\Sigma\Delta m = 462$, i.e., 2.3% and after the sixth iteration a total interval $\Sigma\Delta m = 52$, i.e., 0.26%. As the order of iteration increases, the remaining intervals become very small.

The remaining total interval after the nth iteration follows approximately the relation

$$\ln(\Sigma\Delta m) = a - bn \tag{1}$$

with $a=16.2758$ and $b=2.080\,58$, i.e., $\Sigma\Delta m$ is reduced exponentially with n.

The splitting of the asymptotic curve into pieces separated by sets of orbits that fall into one of the two black holes is remarkable. It reminds us of the splitting of the asymptotic curves in a potential with escapes, by sets of orbits that escape to infinity.[3] In that case the separate arcs of the asymptotic curves do not terminate abruptly but after infinite rotations around an "escape domain." However, in the present case the arcs of the asymptotic curve terminate abruptly at the black holes ($z=\pm 1$, $\dot{z}=\pm 0.75$). A theoretical explanation of this effect is given in the Appendix.

Now the question arises whether there is a continuity between the orbits that fall into the black holes in Figs. 1 and 2 before and after a third or a fourth iteration.

This question is easy to answer. Consider two orbits marked $m=6722$ and $m=9052$ in Fig. 3. The orbit $m=6722$ has a third intersection with the z axis ($\dot{x}>0$) a little above $z=1$, while the orbit $m=6723$ does not have a third intersection. The two orbits are so close that they cannot be separated in Fig. 3. Both orbits make a small angle with the z axis above $z=1$ as they reach the black hole M_1 (small positive, i.e., clockwise from the upper z axis for $m=6722$ and small negative, i.e., counterclockwise for $m=6723$). The orbit $m=6723$ is slightly below the orbit $m=6722$ near the black hole $z=1$ and reaches the black hole from the left of the z axis without a third intersection with the z axis. Thus, the continuity between the orbits $m=6722$ and $m=6723$

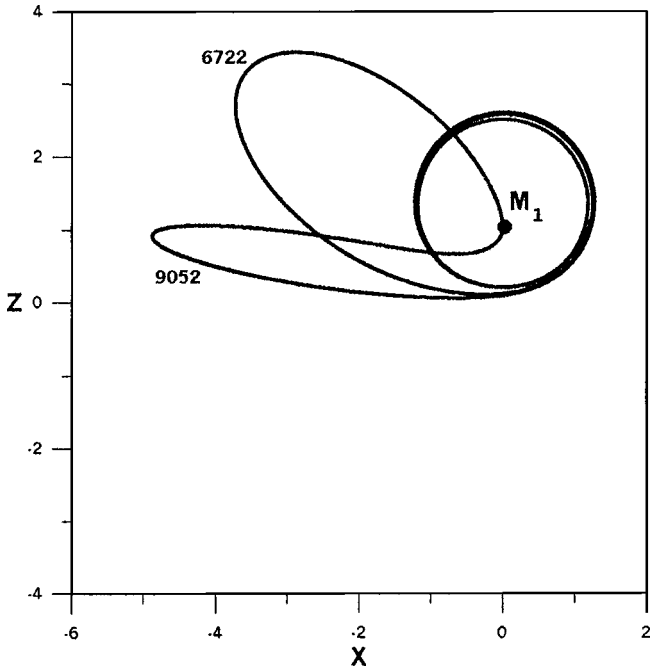

FIG. 3. The orbits with $m=6722$ and $m=9052$ reach the black hole M_1. The first orbit intersects the z axis ($\dot{x}=0$) for a third time above and very close to M_1, while the second orbit intersects this axis below and very close to M_1. The orbits with $6723<m<9051$ reach M_1 from the left, without intersecting for a third time the z axis.

close to the black hole is obvious. As m increases from $m=6722$ to $m=9052$ the orbits reach the black hole $z=1$ from the left of the z axis making larger and larger negative angles with the z axis until they reach an angle very close to $-180°$. The orbit $m=9051$ does not have a third intersection with the z axis, while the orbit $z=9052$ has a third intersection just below $z=1$. Again the continuity between these orbits is obvious.

Similar results refer to the fourth and higher order intersections. The orbits between $m=208$ and $m=279$ in Fig. 2 do not have a fourth intersection with the z axis ($\dot{x}>0$). These orbits correspond to the orbits $m=6723$ ($=208\lambda$) and $m=9051$ ($=279\lambda$) that do not have third intersections. In Fig. 4 the orbit $m=279$ does not have a fourth intersection with the z axis (with $\dot{x}>0$) but the orbit $m=280$ does have such a fourth intersection just below $z=1$, and there is an obvious continuity between the orbits $m=279$ and $m=280$.

The orbit $m=341$ of Fig. 4 corresponds to the orbit with $m=11\,015$ in Fig. 1. This orbit does not have a fourth intersection with the z axis ($\dot{x}>0$), but reaches the black hole $z=-1$ before the fourth intersection. But the orbit with $m=340$ does have a fourth intersection with the z axis just above the black hole $z=-1$. The continuity between the orbits $m=340$ and $m=341$ is again obvious.

III. PERIODIC ORBITS: HOMOCLINIC AND HETEROCLINIC INTERSECTIONS

The periodic orbits in a system of two fixed black holes have been studied by Contopoulos[1,2] and by Contopoulos and Papadaki.[4]

In the present case we consider the most simple periodic orbits in the case ($M_1=1.1$, $M_2=1$, $E=\sqrt{0.5}$). There are two periodic orbits of period 1 around M_1 [inner orbit (a) and outer orbit (a')], two periodic orbits around M_2 [inner orbit (b) and outer orbit (b')], and the orbit (h), which is like an arc of a hyperbola. The main periodic orbits starting at the points ($z, x=0, \dot{z}=0$) are given in Table II, together with their absolutely larger eigenvalues λ (Fig. 5). The orbits (a), (a') and (b), (b') can be described also in the opposite direction of rotation and then they are called ($\overline{a}, \overline{a'}, \overline{b}, \overline{b'}$).

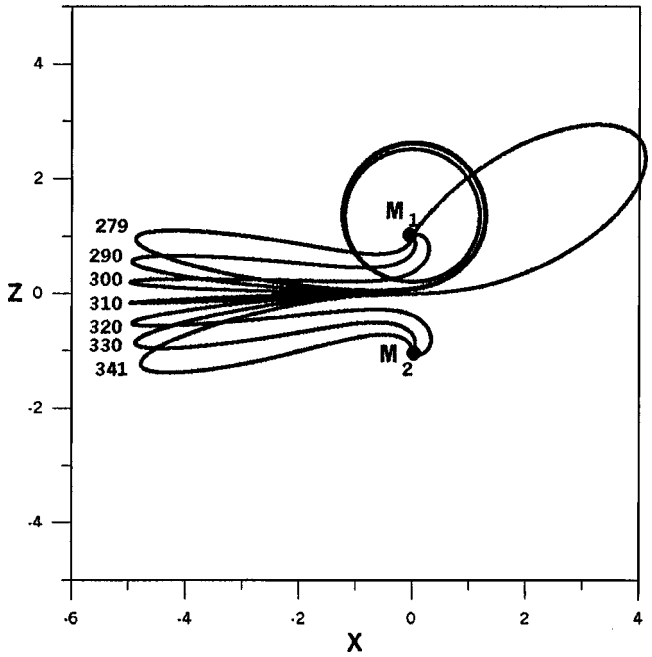

FIG. 4. The orbits with $m=279$, 290, 300 fall into M_1 after a loop to the left and have $\dot{z}>0$ at their minimum x. The orbits with $m=320$, 330, 341 fall into M_2 after a loop to the left and have $\dot{z}<0$ at their minimum x. The orbit $m=310$ has $\dot{z}<0$ at its minimum x, but reaches M_1.

The most important periodic orbits are the orbits (a), $(\overline{a})$ and (b), $(\overline{b})$ because all orbits crossing them inwards fall into the black holes M_1 and M_2, respectively.[1]

The above periodic orbits have multiplicity 1, i.e., they have only one intersection with the z axis and $\dot{x}>0$. The characteristic curve of the periodic orbit h is given in Fig. 6. This curve gives z as a function of M_1 for $M_2=1$ and $E=\sqrt{0.5}$. For $M_1<1$ the orbit h has $z>0$ and it is curved upwards, and for $M_1\to 0$ it tends to a straight line along the z axis above M_1. For $M_1>1$ the orbit h has $z<0$ and it is curved downwards. As $M_1\to\infty$ this orbit tends to a straight line along the z axis below M_2. The characteristics of the orbits (a,a',b,b') are given by Contopoulos.[2]

Besides the most simple periodic orbits above, there are several types of orbits of higher multiplicity. Such orbits are shown in Figs. 7(a)–7(c). The orbit of Fig. 7(a) makes a rotation around M_1 and reaches the curve of zero velocity (CZV) with $\dot{z}=0$ at two symmetric points with respect to the z axis.

The orbits of Fig. 7(b) are of type (8). The upper one makes a rotation around M_1 and then it is elongated symmetrically to the left and to the right, without reaching the CZV. Similarly the lower orbit makes a rotation around M_2 and has two symmetric extensions to the left and to the right above M_2 without reaching the CZV.

TABLE II. Positions and eigenvalues of simple periodic orbits.

	$z(\dot{x}>0)$	$z(\dot{x}<0)$	λ
(inner orbit a)	2.504 568 37	0.207 983 90	32.330 01
(outer orbit a')	3.445 740 37	0.147 178 12	−34.642 86
(inner orbit b)	−2.161 083 40	−0.306 298 55	47.561 40
(outer orbit b')	−3.762 971 63	−0.206 429 38	−60.913 58
(orbit h)	−0.044 139 73	−0.044 139 73	10 384.373

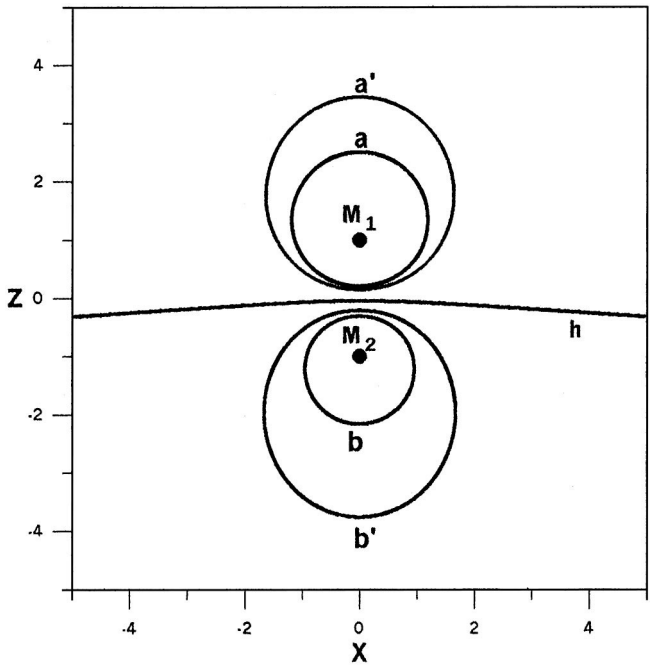

FIG. 5. The inner and outer periodic orbits (a), (a'), (b), and (b') and the hyperbolic type periodic orbit (h). In all cases $M_1=1.1$, $M_2=1$, $E=\sqrt{0.5}$.

Finally, the orbit of Fig. 7(c) makes two rotations, one around M_1 and one around M_2, and has two symmetric extensions to the left and to the right without reaching the CZV.

There are further periodic orbits that have more than one extension to the left and to the right, orbits that make two, or more, rotations around M_1, and/or M_2, and even more complicated periodic orbits.[1,2,4]

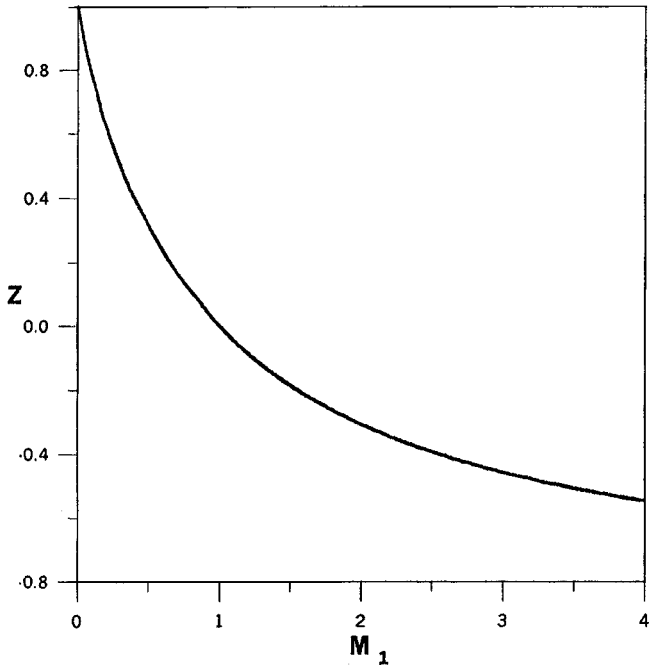

FIG. 6. The characteristic of the orbit h for $M_2=1$, $E=\sqrt{0.5}$, while M_1 varies for 0 to $M_1=4$.

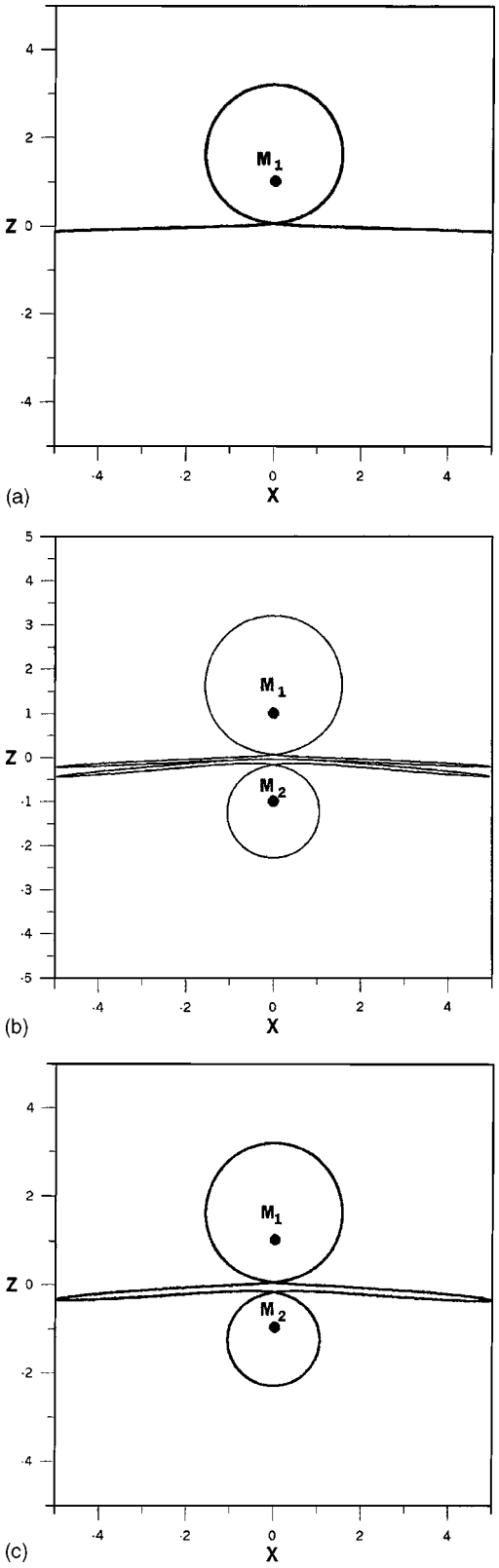

FIG. 7. (a), (b), (c). Various periodic orbits that make a rotation around M_1 and/or M_2.

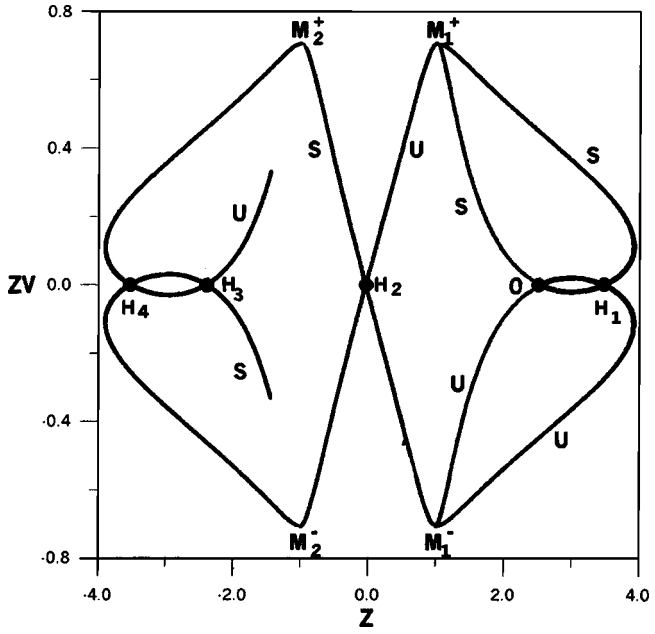

FIG. 8. The stable and unstable asymptotic curves of the orbit O [inner orbit (a) for $M_1=1.1$, $M_2=1$, $E=\sqrt{0.5}$] intersect at an infinity of homoclinic points like H_1, H_2, H_3, H_4.

We study now, the asymptotic curves of some of the main periodic orbits above and find their homoclinic and heteroclinic intersections.

In Fig. 8 we give the stable and unstable asymptotic curves of the (unstable) inner periodic orbit (a), marked O. We mark four main homoclinic points H_1, H_2, H_3, H_4, but there are infinitely more homoclinic points. The points H_1, H_2, H_3, H_4 are close to the periodic orbits a', h, b, and b', respectively. Namely they all have $\dot{z}=0$ and (m,z) given in Table III.

The points H_1, H_2, H_3, H_4 exist already in the arcs of the third iterations, given in Fig. 1, but their values m in Table III correspond to their fourth iterations.

In Fig. 9 we give one unstable asymptotic curve of the inner orbit (a) [the curve starting upwards and to the right from the point (a)] and the stable asymptotic curve of the orbit (h). The unstable asymptotic curves of the orbits (a) and (h) are close to each other, but they do not intersect themselves or each other. In the same way the stable asymptotic curves of the orbits (a) and (h) do not intersect themselves or each other. But the unstable asymptotic curve of (a) intersects the stable asymptotic curve of (h) at infinite heteroclinic points. Thus, we have an infinity of heteroclinic orbits near the point $m=311$. These heteroclinic points are confined in the interval between $m^*=307.643\,390$ and $m^{**}=314.384\,627$ (defined in the next section). In this interval we find infinite homoclinic orbits and heteroclinic orbits connecting (a) with other simple periodic orbits.

In a similar way we have infinite homoclinic and heteroclinic points between the asymptotic

TABLE III. Positions of homoclinic points and of nearby periodic orbits.

$m(H_1)=75$	$z(H_1)=3.500\,48$	$z(a')=3.445\,74$
$m(H_2)=311$	$z(H_2)=-0.041\,66$	$z(h)=-0.044\,14$
$m(H_3)=713$	$z(H_3)=-2.3947$	$z(b)=-2.161\,08$
$m(H_4)=576$	$z(H_4)=-3.5195$	$z(b')=-3.762\,97$

curves of the orbits (a), (a'), (b), (b') and so on. The homoclinic and heteroclinic points are confined in some regions in an extended neighborhoods of the points O, H_1, H_2, H_3, H_4 of Fig. 8. We will describe now the corresponding orbits in some detail.

IV. THE FORMS OF ORBITS STARTING ALONG AN ASYMPTOTIC CURVE

We consider now the changes of the forms of the orbits as we vary the initial point m along the unstable asymptotic curve of the periodic orbit (a). In Fig. 4 we see orbits that fall into M_1 (type I orbits) like $m=279$, and orbits that fall into M_2 (type II orbits), like $m=341$. All the orbits of Fig. 4 start very close to each other forming three almost circular rotations clockwise around M_1 and then an oscillation to the left. Only the last oscillation to the left is substantially different for different orbits. As m increases from $m=279$ this last oscillation becomes thinner. Similarly as m decreases from $m=341$ the last oscillation also becomes thinner. The orbits of type I in Fig. 4 up to $m=300$ have $\dot{z}>0$ at their minimum x along this last oscillation while the orbits $m=320-341$ in this figure are of type II and have $\dot{z}<0$ at their minimum x. On the other hand, the orbit $m=310$ is of type I but it has $\dot{z}<0$ at its minimum x and after this minimum it has an oscillation to the right before reaching M_1.

Between the orbits $m=300$ and $m=320$ there are many transitions between various types of orbits. As m increases beyond $m=300$ the oscillation to the left becomes very thin and for $m=m^*\approx 307.643\,390$ it becomes infinitely thin, i.e., the orbit is reflected along the same path, having $\dot{z}=0$ at its minimum z. This orbit reaches the inverse periodic orbit $(\overline{a})$ after infinite rotations counterclockwise around M_1 (Fig. 10). Therefore this critical orbit is heteroclinic between the orbit (a) and the inverse orbit $(\overline{a})$. We call it "first heteroclinic orbit." The orbits close to m^* with $m<m^*$ have $\dot{z}>0$ at their minimum x while the orbits with $m>m^*$ have $\dot{z}<0$ at this minimum. All the orbits with $74.94<m<m^*$ are of type I, i.e., they fall into the black hole M_1.

The critical value $m=m^*=307.643\,390$ is found as follows. All orbits having m in the interval $280<m<306.7$ fall into M_1 after a fourth intersection of the z axis with $\dot{x}>0$ but before a fifth intersection. The orbit $m=306.8$ makes first three clockwise rotations around M_1, then goes to the left reaching a minimum x near the CZV and then returns and makes a complete turn counterclockwise around M_1 and is the first orbit with this accuracy (i.e., with so many decimals) that has a fifth intersection with the z axis just below M_1.

The orbit with $m_0=307.613$ makes two counterclockwise rotations (six intersections in total), $m_1=307.642\,411\,0$ makes three counterclockwise rotations (seven intersections in total), $m_2=307.643\,360\,1$ makes four counterclockwise rotations (eight intersections in total), $m_3=307.643\,389\,5$ makes five counterclockwise rotations (nine intersections in total). The last orbit (Fig. 10) is very close to the "first" heteroclinic orbit.

The intervals between these successive orbits are equal to $\Delta m_1=0.029\,41$, $\Delta m_2=0.000\,949$, $\Delta m_3=0.000\,0294$. Each successive interval is smaller by a factor close to the eigenvalue $\lambda=32.33$ of the periodic orbit $(\overline{a})$.

The reason is the following. The successive intersections of the $(z,\dot{z})$ plane by the heteroclinic orbit m^* connecting the orbits (a) and $(\overline{a})$ approach the orbit $(\overline{a})$ by a factor λ at each iteration, where λ is the (larger) eigenvalue of the orbit $(\overline{a})$. An orbit starting at m close to m^* with $m<m^*$, has six, seven, etc., intersections with the $(z,\dot{z})$ plane close to the corresponding intersections of the heteroclinic orbit m^* at distances $d_6(m)$, $d_7(m)$, etc., increasing by a factor λ at each iteration. If now the initial differences $|m_i-m^*|$ decrease by factors λ ($|m_i-m^*|\approx|m_0-m^*|/\lambda^i$), the corresponding distances at the sixth intersection $d_6(m_i)$ decrease approximately by the same factors $[d_6(m_i)=d_6(m_0)/\lambda^i]$. Then as the distances $d_7(m_i)$, $d_8(m_i)$ increase by λ at each iteration we reach the initial distance $d_6(m_0)$ at the $(6+i)$ iteration $[d_{6+i}(m_i)\approx d_6(m_0)]$. If now the m_0 orbit escapes to the black hole after its sixth intersection, the orbit m_i escapes after its $(6+i)$ intersection.

As the successive intervals $|m_i-m^*|$ decrease by a factor λ, the intervals $|m_i-m_{i-1}|$ also decrease by the same factor. Thus we can calculate m^* as the limit of an infinite series beyond $m_2=307.643\,360\,1$ by adding to m_2 the sum

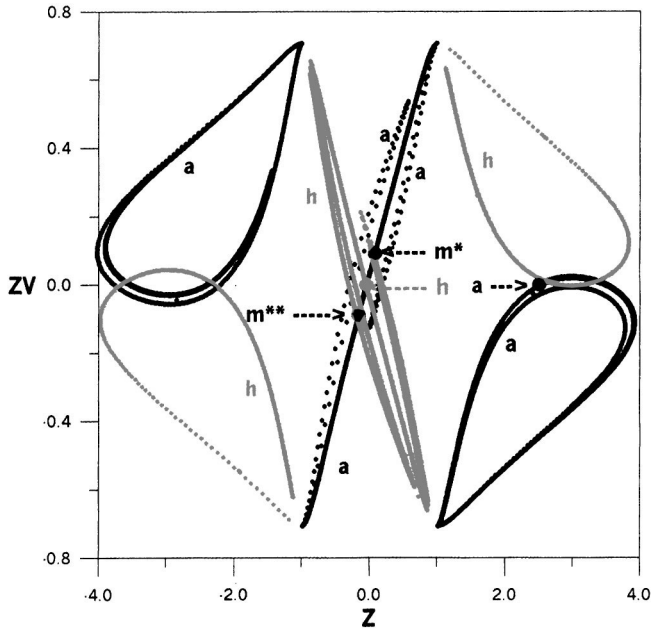

FIG. 9. The unstable asymptotic curve of the orbit (a) (black) and the stable asymptotic curve of the orbit (h) (gray) intersect at an infinity of heteroclinic points close to H_2 ($m=311$), but also close to O and some other points of this figure. The main homoclinic and heteroclinic points along the arc (2) of the unstable asymptotic curve of the orbit (a) are confined between the points $m*$ and $m**$.

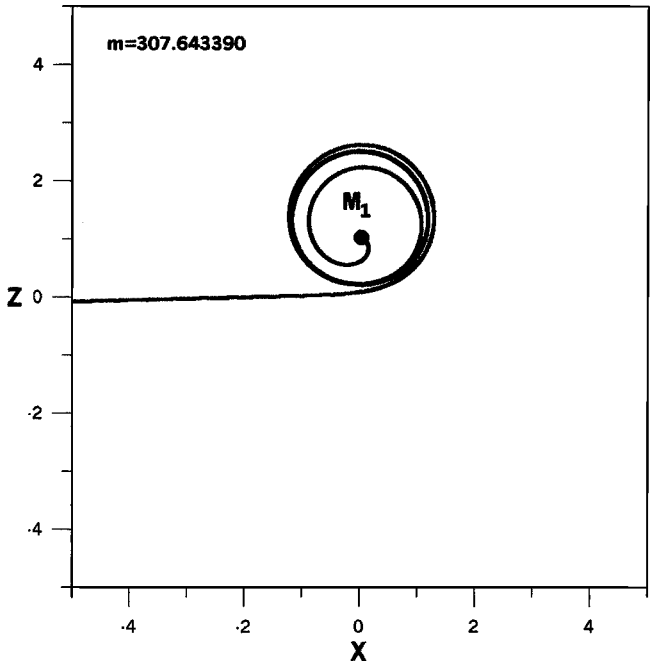

FIG. 10. The orbit $m=307.643\,390$ is very close to a heteroclinic orbit joining the periodic orbits (a) and ($\overline{a}$). The heteroclinic orbit is the limit of orbits starting above the periodic orbit (a) and intersecting the z axis n times with $\dot{x}>0$ where $n=5,6,7,8,9$, etc. This orbit has $\dot{z}=0$ at its minimum x.

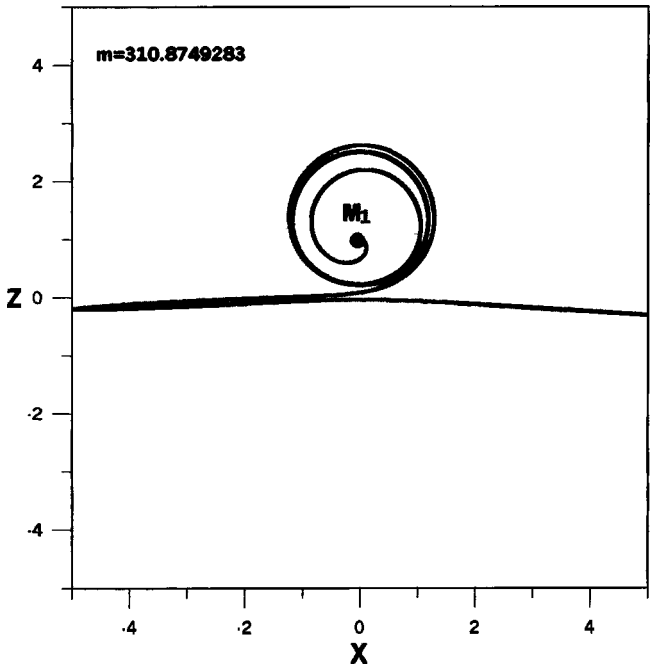

FIG. 11. The orbit $m=310.874\,928\,3$ is very close to a heteroclinic orbit joining (a) and $(\overline{a})$ that has $(\dot{z}=0)$ at its maximum x. This heteroclinic orbit is the limit of orbits having $n=6,7,8,\ldots$ intersections with the z axis with $\dot{x}>0$. These orbits have $\dot{z}<0$ at their minimum x.

$$\Sigma\Delta m=\frac{0.000\,029\,4}{1-\dfrac{1}{32.33}}=0.000\,030\,3, \tag{2}$$

hence the limiting value of m is $m^*=307.643\,360\,1+0.000\,030\,3=307.643\,390\,4$. All other homoclinic and heteroclinic orbits have been calculated in the same way.

If we proceed beyond $m=m^*$ we have orbits with $\dot{z}<0$ at their minimum x. The orbits a little beyond $m=310$ (Fig. 4) have also an oscillation to the right with $\dot{z}>0$ at the maximum x. As m increases beyond $m=310$ this oscillation becomes thinner and for m very close to $\overline{m}=310.874\,928\,3$ (Fig. 11) the orbit has $\dot{z}=0$ at its maximum x. The orbit returns along the same path and approaches the orbit $(\overline{a})$ after reaching a minimum x, following the maximum x with $\dot{z}=0$, and then making infinite counterclockwise rotations around M_1. This orbit is a second heteroclinic orbit $(a\rightarrow\overline{a})$ but of different form from the first heteroclinic orbit.

Between the first and the second heteroclinic orbits there are infinite heteroclinic orbits connecting the periodic orbit (a) with its opposite orbit $(\overline{a})$. In fact, close to the first heteroclinic orbit but with m larger than m^*, there are orbits that make one rotation counterclockwise around M_1 after their minimum x and then make an oscillation to the right. An orbit very close to $m=307.797\,852\,2$ after a counterclockwise rotation around M_1 reaches a maximum x with $\dot{z}=0$ and returns along the same path making infinite counterclockwise rotations around M_1. Therefore it is again a heteroclinic orbit connecting the orbits (a) and $(\overline{a})$.

Even closer to the first heteroclinic orbit there are orbits with two or more counterclockwise rotations around M_1 after their minimum x, that have also an oscillation to the right reaching a maximum x with $\dot{z}=0$. All these orbits are heteroclinic between (a) and $(\overline{a})$. The limit of these heteroclinic orbits is the original heteroclinic orbit m^*.

Close to the second heteroclinic orbit $\overline{m}$, but with smaller m, there are orbits that make some

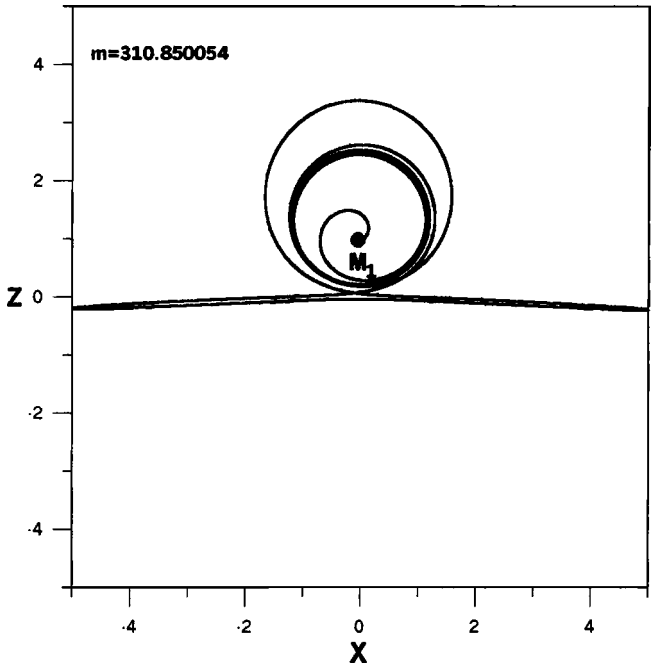

FIG. 12. The orbit $m=310.850\,054$ is very close to a homoclinic orbit for the periodic orbit (a). It is the limit of orbits having an oscillation to the left with $\dot{z}<0$ at their minimum x, then an oscillation to the right with $\dot{z}>0$ at their maximum x and then make $n=1,2,3,4\ldots$ rotations clockwise around M_1.

clockwise rotations around M_1 before reaching M_1. In particular an orbit close to $m_a=310.850\,054$ (Fig. 12) makes infinite clockwise rotations before reaching M_1. This orbit is homoclinic to the periodic orbit (a).

All the orbits between the homoclinic orbit near $m_a=310.850\,054$ (Fig. 12) and the heteroclinic orbit near $\overline{m}=310.874\,928\,3$ (Fig. 11) fall into M_1. The progression of such orbits is seen in Fig. 13. The number of clockwise rotations around M_1 is infinite for the homoclinic orbit m_a, but as m increases beyond m_a the number of rotations decreases. The orbits of Fig. 13 make first three clockwise rotations around M_1 and then they extend to the left and later to the right after a fourth intersection with the z axis. After reaching a maximum x the orbit $m=310.851$ makes one and one-half clockwise rotations around M_1 and then falls into M_1. The orbit $m=310.860$ after its maximum x makes about one clockwise rotation before falling into M_1. The orbits $m=310.868$, $m=310.873$ both have only one extension to the left, after their maximum x, but the latter starts to form a counterclockwise rotation around M_1, as it approaches M_1, and has one more intersection with the z axis. As m increases further and approaches $\overline{m}$ the number of counterclockwise rotations around M_1 increases and tends to infinity.

Close to the heteroclinic orbits joining (a) and $(\overline{a})$, with extra rotations around M_1 before the oscillation to the right with $\dot{z}=0$ at their maximum x, there are further homoclinic orbits from the orbit (a) to the same orbit (a) for slightly smaller m. For example, there is a homoclinic orbit making an oscillation to the left with $\dot{z}<0$ at its minimum x, then a counterclockwise rotation around M_1 and an oscillation to the right with $\dot{z}>0$ at its maximum x, and then infinite clockwise rotations around M_1. There is an infinity of homoclinic orbits with n counterclockwise rotations around M_1 after an oscillation to the left and before an oscillation to the right. The value of m for these homoclinic orbits decreases with increasing n, and as n tends to infinity $m\rightarrow m^*$. The calculation of these higher order orbits is difficult, because we reach the limit of double precision accuracy.

There are more heteroclinic orbits, connecting (a) with $(\overline{a})$, (a'), $(\overline{a'})$, (h), (b), (b'), $(\overline{b})$, and $(\overline{b'})$.

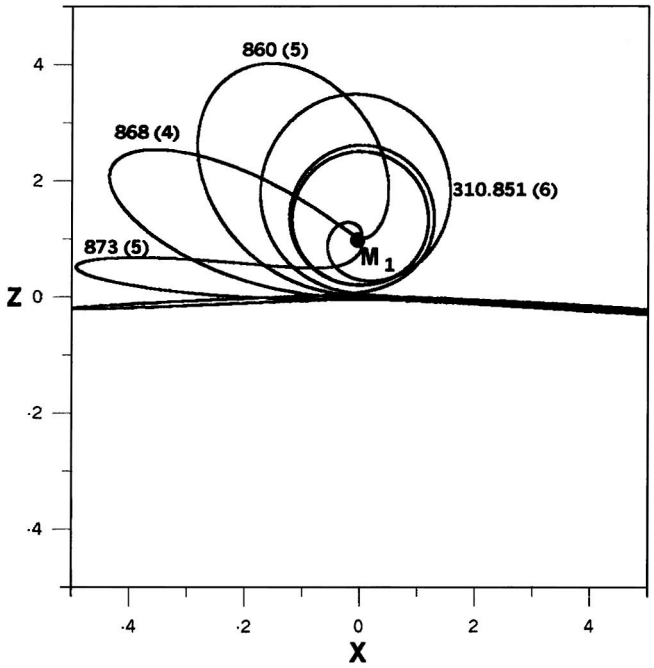

FIG. 13. All the orbits between the homoclinic orbit close to $m_1=310.850\,054$ and the heteroclinic orbit close to $m_2=310.874\,828\,3$ fall into M_1. Their total number of intersections with the z axis (with $\dot{x}>0$) is shown in parentheses.

The most important among these heteroclinic orbits is the orbit $m=m^{**}=314.384\,627$, that connects (a) with the inverse orbit $(\bar{b})$, around M_2 (Fig. 14). This is the last heteroclinic orbit in an interval of values of m around $m=311$, because all the orbits with $m>m^{**}$ up to $m=559$ reach the black hole M_2.

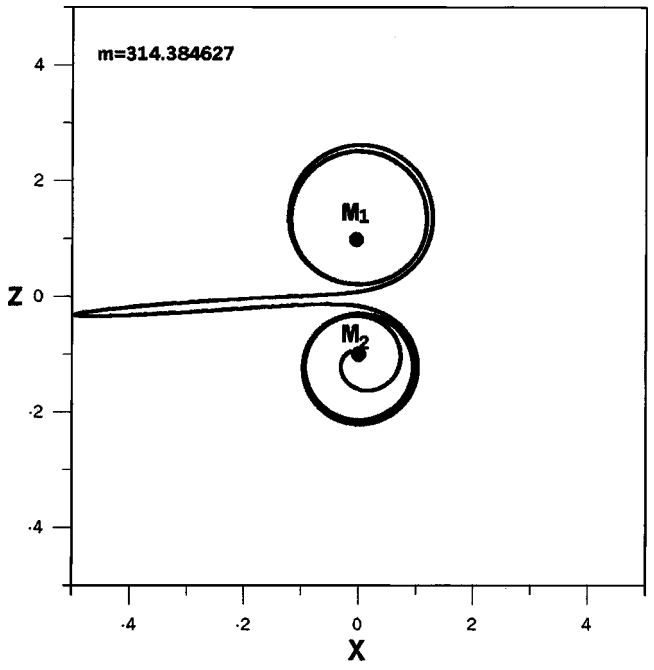

FIG. 14. The orbit $m=314.384\,627$ is very close to a heteroclinic orbit connecting (a) with (b).

In the inner neighborhood of m^{**}, i.e., for small negative $(m-m^{**})$, there are infinite heteroclinic and homoclinic orbits and transitions from orbits falling into M_1 (type I) and orbits falling into M_2 (type II). Such orbits make a number of clockwise rotations around M_2 close to the periodic orbit $(\overline{b})$ after reaching their minimum x, and then recede outwards from the orbit $(\overline{b})$ in various directions. If we try to find accurately the transitions between these orbits we have problems with accuracy, because we must go to decimal places beyond those secured by double precision.

However, if we calculate orbits with even smaller m then the main transitions are clearly defined.

As we have seen in Fig. 13 an interval $\Delta m=\overline{m}-m_a$ of orbits falling into M_1 is terminated on the one side by an homoclinic orbit and on the other side by an orbit heteroclinic with the inverse orbit $(\overline{a})$. All the orbits between them are of type I.

In general an interval Δm of orbits of type I is terminated by a homoclinic orbit $(a\rightarrow a)$ and a heteroclinic orbit $(a\rightarrow\overline{a})$, while an interval Δm of orbits of type II is terminated by two heteroclinic orbits $(a\rightarrow b)$ and $(a\rightarrow\overline{b})$. However there are also cases where the orbits at the ends of such an interval Δm are of the same type, e.g., $(a\rightarrow\overline{a})$ and $(a\rightarrow\overline{a})$. In this case the heteroclinic orbits $(a\rightarrow\overline{a})$ at the ends of the interval Δm are different in form, although they approach the same orbit $(\overline{a})$.

Transitions between orbits of type I and type II occur near every homoclinic and heteroclinic orbit. For example, while all the orbits close to $m^*=307.643\,390$ (Fig. 10) with $m<m^*$ fall into M_1 after a number of clockwise rotations around M_1, the orbits with $m>m^*$ may fall either into M_1, or M_2. Such orbits with $m>m^*$ have $\dot{z}<0$ at their minimum x, but then they form a number of rotations counterclockwise around M_1, close to the orbit $(\overline{a})$, and later they recede away from this orbit. Some of them make a number of rotations around M_2 and finally they fall into M_1, or M_2. Therefore the sets of orbits falling into M_1 and M_2 are fractal.

In Fig. 9 we see that along the diagonal part of the asymptotic curve [arc (2)], there is only a relatively small part, between m^* and m^{**}, that contains infinite heteroclinic and homoclinic orbits and correspondingly infinite intervals of orbits of types I and II. On the other hand, all orbits on the diagonal above m^* are of type I and all orbits below m^{**} are of type II.

In Fig. 8 we see the heteroclinic points H_1, H_2, H_3, H_4 which have initial conditions given in Table III. Up to now we have considered in detail the region close to H_2 $(m\approx 311)$. A characteristic feature of the orbits in this region is an oscillation to the left (Figs. 10–14) with $\dot{z}$ equal to zero or to a small negative near the minimum x.

If we come now to the orbits near $m=559$ we see that they do not have this oscillation to the left. In Fig. 15 we show two orbits close to the heteroclinic orbit from (a) to (b). These orbits start asymptotically at the orbit (a) for $t\rightarrow-\infty$. After the initial time $t=0$ they make three clockwise rotations around M_1, and four counterclockwise rotations around M_2. The first rotation around M_2 is close to the orbit (b') and the following three rotations are very close to the orbit (b). Then the orbit $m=559.1297$ makes one more rotation around M_2 and falls into M_2, while the orbit $m=559.1298$ makes one rotation clockwise around M_1 and falls into M_1. The orbit $m=m^{***}=559.1297$ is very close to the heteroclinic orbit that reaches the orbit (b) after infinite oscillations around M_2 as t tends to infinity.

All the orbits with m between $m^{**}=314.384\,627$ to $m^{***}=559.1297$ are of type II, i.e., they fall into M_2 (Fig. 16). It is remarkable that the orbits in this interval change fast only for m close to m^{**} or m^{***} while far from these limiting values they change slowly. Then there is an interval of values of m up to $m^{****}\approx 576$ with several transitions between orbits of type I and of type II, followed by a large interval of orbits of type I, up to about $m\approx 726$, and so on.

In general we find the following:

(1) Between an asymptotic orbit of type I (falling into M_1) and an orbit of type II (falling into M_2) there is always a homoclinic (or heteroclinic) orbit. The original point of this orbit on the phase space is at the intersection of the asymptotic curves of the original periodic orbit

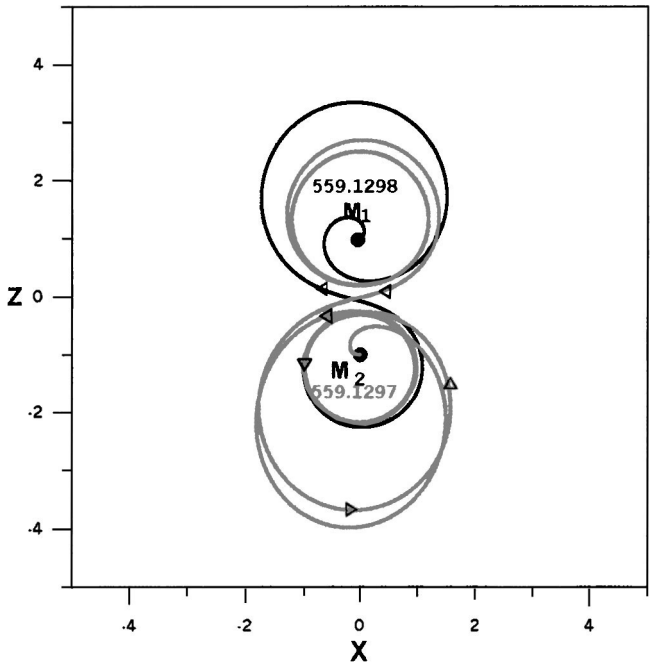

FIG. 15. The orbit $m=m^{***}=559.1297$ is close to a heteroclinic orbit connecting (a) and (b). All orbits in the large interval $m^{**}=314.3846\ldots<m<m^{***}$ are of type II. But orbits with $m>m^{***}$ are either of type I ($m=559.1298$) or of type II.

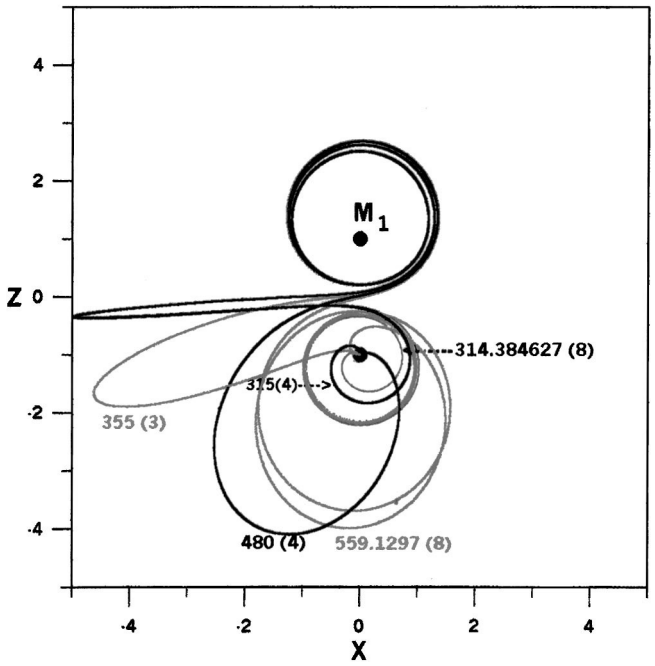

FIG. 16. All the orbits between $m^{**}=314.384\,628$ [heteroclinic to ($\bar{b}$)], and $m^{***}=559.1297$ [heteroclinic to (b)] are of type II. In parentheses we give the total numbers of intersections of the z axis (with $\dot{x}>0$) after the initial points.

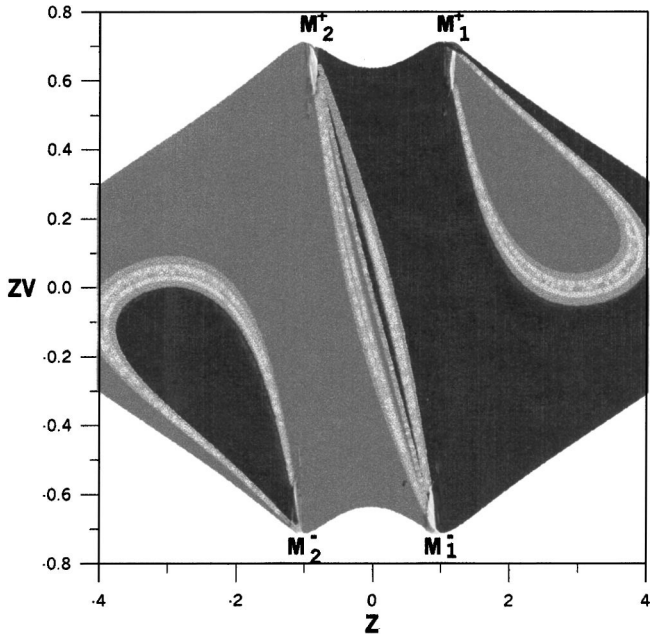

FIG. 17. Basins of attraction of the black holes M_1 and M_2. We distinguish the orbits that fall into M_1 (black), or M_2 (gray) before an intersection with the z axis, (with $\dot{x}>0$) or after only one intersection. The white regions represent orbits that fall into M_1, or M_2 after more than one intersection.

(a) and of the same, or another, periodic orbit. This orbit is homoclinic in the first case and heteroclinic in the second case.

(2) Near every homoclinic or heteroclinic orbit there are infinite intervals of orbits of types I and II. The intervals of type I are terminated by homoclinic orbit ($a\to a$) and heteroclinic orbits ($a\to\overline{a}$). The intervals of type II are terminated by two heteroclinic orbits of types ($a\to b$) and ($a\to\overline{b}$).

If we reduce m by a factor λ we find the same orbits as above after one more iteration (orbits of types I and II, and homoclinic and heteroclinic orbits). For example, the orbits close to $m=311$ considered above near their fourth intersection, are also represented by orbits near $m=311/\lambda\approx 9.5$ at their fifth intersection. Similar results appear for m equal to m/λ^2, m/λ^3, etc., after two, three, etc., more intersections with the z axis. Therefore very close to the periodic orbit O, along its unstable asymptotic curve, there are infinite transitions of types I and II orbits and infinite homoclinic and heteroclinic orbits connecting the orbit (a) with itself, or with the periodic orbits ($\overline{a}$), (a'), ($\overline{a'}$), (h), (b), (b'), ($\overline{b}$), ($\overline{b'}$).

V. BASINS OF ATTRACTION AND CHAOS

If we exclude the periodic orbits and the small islands of stability around stable periodic orbits, all other orbits fall into the black holes M_1 and M_2. The basins of attraction of the two black holes on the surface of section are shown in Fig. 17. The black regions fall into M_1 and the gray regions fall into M_2. Each basin consists of large compact regions of initial conditions falling into one black hole, and of thin filaments that have a fractal structure.

The largest regions are called 0-iterations, because they fall into M_1 or M_2, before any intersection with the z axis (with $\dot{x}>0$). These regions are surrounded by elongated regions that fall into M_1 or M_2, after one intersection with the z axis. Furthermore, there are thin filaments of 0, 1, 2 iterations, etc.

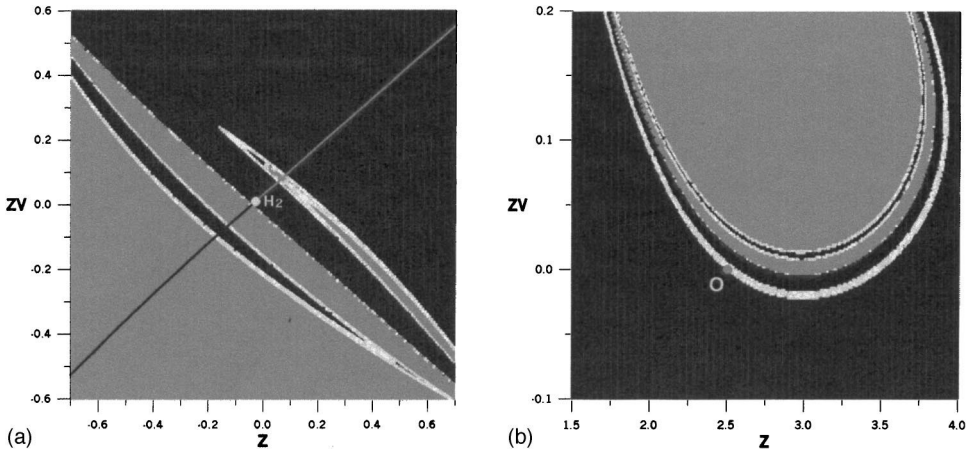

FIG. 18. (a), (b). Details of Fig. 17: Orbits that fall into M_1 (black), or M_2 (gray), before a second intersection. The orbits in the white regions fall into one of the black holes after the second iteration. The line in (a) is the arc (2) of the unstable asymptotic curve of the orbit O, marked in (b).

In Figs. 18(a) and 18(b) we see some of the regions of 0 iteration and 1 iteration, in greater detail. Near the homoclinic and heteroclinic, orbits pass thin filaments of arbitrarily high order. These filaments form fractal sets in the same way as the initial conditions of the asymptotic curves that lead to M_1 or M_2, close to the homoclinic and heteroclinic orbits.

The fact that many orbits fall into M_1 or M_2, produces a nonpreservation of areas on the surface of the section. In Fig. 19 we see the successive images of a small circle of radius $R=0.001$ around the periodic orbit O. The first iteration produces an elongated ribbon like an ellipse with the same area as the circle [Fig. 19(a)]. (This ribbon is so thin that its thickness is not apparent in this figure.) The second, third, and fourth iterations [Fig. 19(b)] produce thinner regions with the same area. However the fifth iteration produces a much longer ribbon that consists of three parts and reaches the black holes M_1 and M_2 [Fig. 19(c)]. This ribbon has an area smaller than the original circle. Therefore, the surface of section is not a "Poincaré surface of section," in which the areas are preserved.

The loss of areas and the very existence of basins of attraction characterizes dissipative systems. This seems strange because our problem is conservative. However, the existence of singularities along the orbits of most initial conditions relaxes the consequences of the conservative character of our system. The problem of two fixed black holes has many characteristics of a chaotic scattering system. But in general chaotic scattering systems lead to escapes to infinity, while here most motions are led to the points M_1 and M_2 at a finite distance.

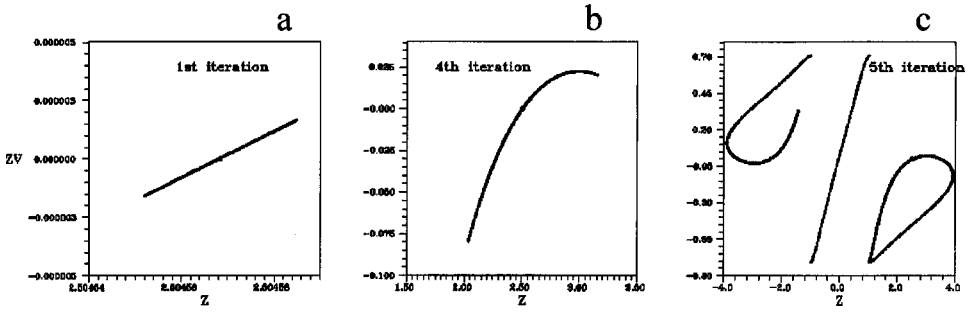

FIG. 19. (a), (b), (c). The images of a circle of radius $R=0.001$ around O on the surface of section $(z,\dot{z})$ at (*a*) the first iteration, (*b*) the fourth iteration, and (*c*) the fifth iteration.

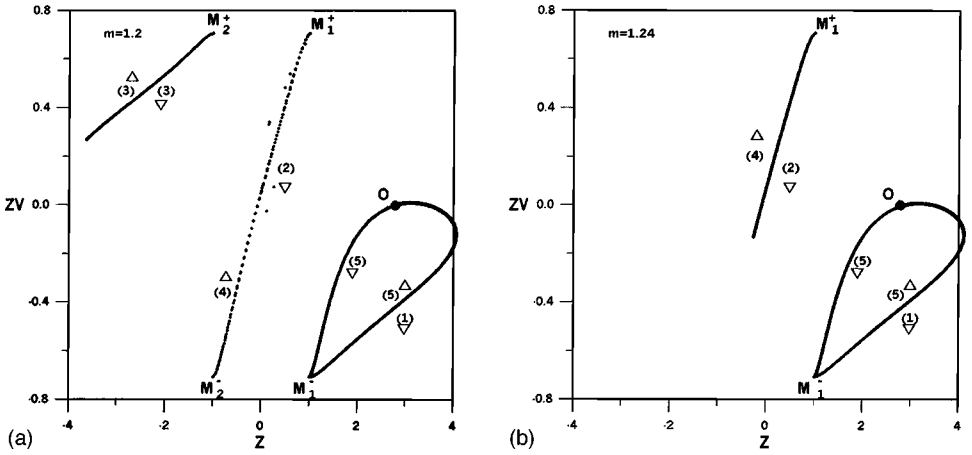

FIG. 20. The unstable asymptotic curve of the orbit O in the cases (a) $M_1=1.2$ and (b) $M_1=1.24$.

At this point we should emphasize a difference between the relativistic problem of two fixed black holes and the corresponding classical problem of two fixed centers. In the second case the phase space extends to infinity along the velocity axis ($\dot{z}$), Therefore although we do not have escapes in coordinate space, we do have escapes in velocity space. But in the relativistic problem with elliptic energy we do not have escapes to infinity, neither in the coordinates nor in the velocities.

We conclude that when the orbits in a conservative system are attracted to one or more singular points, the system does not have some of the usual properties of generic conservative systems, but has some (not all) of the properties of dissipative systems.

VI. OTHER CASES

If we vary the mass M_1 while keeping $M_2=1$ and the energy constant ($E=\sqrt{0.5}$) the positions of the periodic orbits and of the asymptotic curves change. As M_1 increases the orbits (a) and (a') approach each other and for $M_1=M_{1\,\max}=1.3257$ they join and disappear.

For M_1 close to the maximum $M_{1\,\max}$ the orbit (a') is stable.[2] The asymptotic curves of the orbit (a) starting at the point O surround the island of stability. The homoclinic point H_1, beyond the island, also approaches the orbit O.

As M_1 increases beyond $M_1=1.1$ the part (3) of the (upper) asymptotic curve of the orbit (a) (Fig. 2) becomes shorter [Fig. 20(a)] and disappears for some value of M_1 larger than $M_1=1.2$. For still larger M_1 the branches (2) and (4) join each other and they no longer reach the point M_2^- of Fig. 2 [Fig. 20(b)]. As M_1 increases further the branches (2)–(4) disappear, and for even larger M_1 the branches (1) and (5) join each other and they do not reach the point M_1^- [Fig. 21(a)].

The point H_1 is the first homoclinic point on the right of the orbit O with $\dot{z}=0$. At this point the curve U from O crosses the curve S outwards. The first image of H_1 is the homoclinic point H'_1, and between H_1 and H'_1 the curve U crosses the curve S inwards at the point H_1^-. The branches (1) and (5) in the case of Fig. 21(a) form an elongated lobe U on the right of O, reaching a point with maximum distance from O and terminating at the point H_1^-. Between O and H_1 there is the unstable periodic point a'.

For still larger M_1 [Fig. 21(b)] the lobe becomes smaller. In this case between the periodic orbit O and the homoclinic point H_1 there is an island of stability surrounding the periodic orbit a' which is stable in this case. This island consists of a set of closed invariant curves, surrounded by four small secondary islands. As M_1 increases further the points O and H_1 approach each other and the periodic orbits, the islands, and the asymptotic curves disappear for $M_1>1.3257$.

The evolution of the lobe from H_1 to H'_1 along the unstable asymptotic curve from the periodic orbit O can be described as follows. For relatively large M_1 [$M_1=1.325$; Fig. 21(b)] this

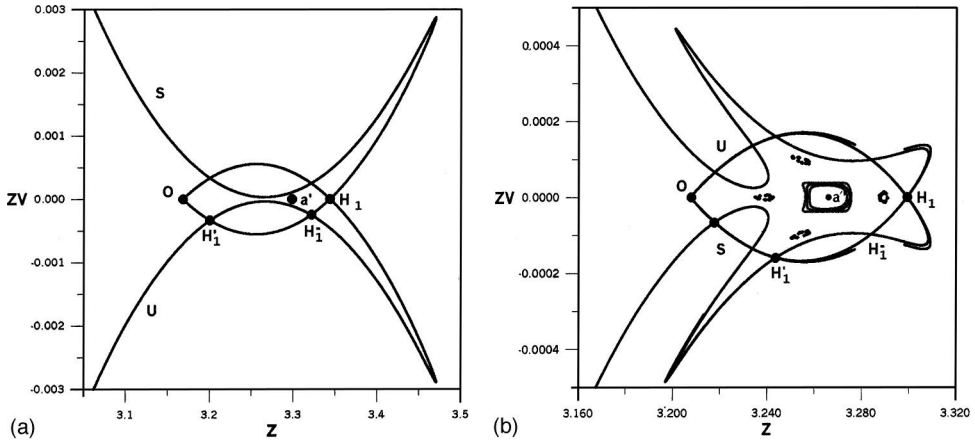

FIG. 21. The unstable and stable asymptotic curves close to the orbit O for (a) $M_1=1.322$ and (b) $M_1=1.325$. Some of the main homoclinic points are marked. In the second case some stable islands appear between O and H_1. The orbit (a') is unstable for $M_1=1.322$ and stable for $M_1=1.325$.

lobe is rather short, but it becomes longer as M_1 decreases [Fig. 21(a)]. For smaller M_1 this lobe is very long and reaches the black hole M_1 at the point M_1^-. For even smaller values of M_1 there is a second (separated) part of this lobe starting and ending at the point M_1^+ [Fig. 20(b)] and reaching a maximum distance from M_1 close to the diagonal $M_1^+ M_2^-$. For smaller M_1 this part of the lobe terminates at the point M_2^- and for still smaller M_1 there is a third (separated) part of the same lobe starting at the point M_2^+ and reaching a maximum distance from M_2^+ along the average asymptotic curve [average between the two arcs of the branch (3)] [Figs. 20(a) and 2].

When $M_1 > M_{1\,\max}$ there are no orbits (a) and (a'). In these cases the orbits (b) and (b') in some sense take the place of the orbits (a) and (a'). Namely when both orbits (a) and (b) are present the asymptotic curves of the orbit (b) (stable and unstable) are close to the asymptotic curves of the orbit (a) and when the asymptotic curves of the orbit (a) disappear they are replaced by the asymptotic curves of the orbit (b). An example is given in Fig. 22 for $M_1=1.326$. This value of M_1 is a little above the maximum value of M_1 ($M_{1\,\max}=1.3257$) beyond which the orbits (a) and (a') do not exist. This curve is qualitatively similar to the unstable asymptotic curve of the orbit (a) for $M_1=1.1$ (Fig. 2) although there are quantitative differences. Because of this similarity the overall structure of the phase space giving the basins of attraction does not change appreciably from Fig. 17.

VII. CONCLUSIONS

The main results of the present study are the following.

(1) The asymptotic curves of the main unstable periodic orbits in the case of two fixed black holes are composed of discontinuous arcs reaching one or two black holes. Some arcs join one black hole with the other, but there are also many arcs that start and terminate at the same black hole. The limiting forms of these arcs close to the black hole are explained theoretically in the Appendix.

(2) The orbits with initial conditions on the asymptotic curves are asymptotic orbits, i.e., they tend to the periodic orbit (a) as $t\to-\infty$. Most of these orbits fall into one or the other black hole. However, there are infinite doubly asymptotic orbits that tend to the same periodic orbit (homoclinic orbits) or to another periodic orbit (heteroclinic orbits) as $t\to\infty$.

(3) There is a continuity of the orbits falling into a black hole before and after n iterations (n intersections with a surface of section $x=0$ with $\dot{x}>0$).

(4) The asymptotic orbits are defined along an unstable asymptotic curve by their distances $m\times10^{-8}$ from the periodic orbit (in our calculations m varies from 1 to 20 000). At every itera-

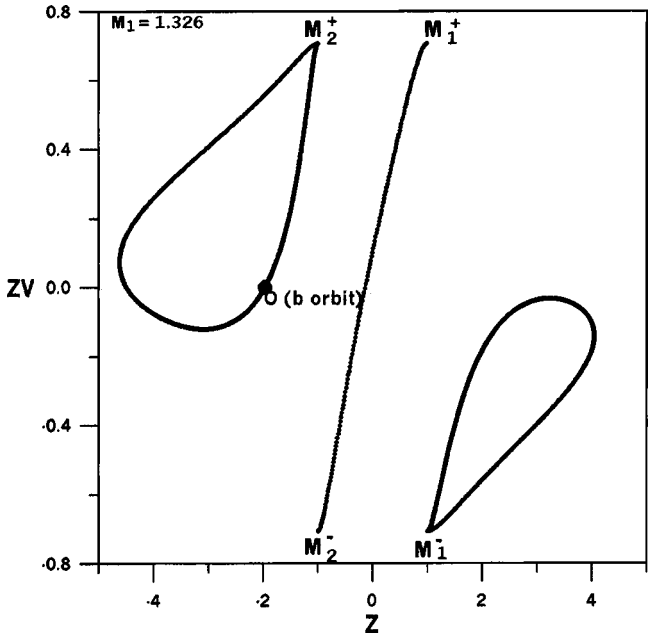

FIG. 22. Parts of the unstable asymptotic curve of the orbit (b) for $M_1=1.326$ ($M_2=1, E=\sqrt{0.5}$). This value of M_1 is just above the maximum $M_{1\,\max}$ for the existence of the orbits (a) and (a').

tion the distance $m\times 10^{-8}$ increases by a factor $\approx\lambda$, where λ is the larger (absolutely) eigenvalue of the periodic orbit. The measure $\Sigma\Delta m$ of orbits that have not reached a black hole after n iterations decreases exponentially with n.

(5) There are five types of simple periodic orbits (orbits of period 1). Two of them surround the black hole $M_1(a,a')$, two surround the black hole $M_2(b,b')$, and one (h) is like an arc of a hyperbola between the orbits (a), (a') and (b), (b'). The orbits (a,a',b,b') can be described also in the inverse direction $(\overline{a},\overline{a'},\overline{b},\overline{b'})$, while the orbit h is the same with its inverse. The sets of orbits falling into one black hole (M_1 or M_2) as $t\to\infty$, are limited by homoclinic or heteroclinic orbits asymptotic to the smaller periodic orbits around M_1 [orbits (a), $(\overline{a})$] and around M_2 [orbits (b), $(\overline{b})$].

(6) The distances Δm between asymptotic orbits falling into M_1 (or M_2 after $n=1,2$, etc., rotations around M_1 (or M_2) decrease by a factor $\approx\lambda$, where λ is the eigenvalue of the orbit (a) or (a') in the first case, and of the orbit (b) or (b') in the second case. The limit of such orbits is the homoclinic orbit connecting (a) with (a) or a heteroclinic orbit connecting (a) with (a'), (b), (b'), or the inverse orbits $(\overline{a})$, $(\overline{a'})$, $(\overline{b})$, $(\overline{b'})$.

(7) There are infinite intervals Δm of orbits of type I (falling into M_1) and of type II (falling into M_2) close to every homoclinic or heteroclinic orbit. These intervals are limited by homoclinic or heteroclinic orbits between the inner periodic orbits around M_1 and M_2. The limiting orbits are of types $a\to a$, $a\to\overline{a}$ for intervals of type I and of types $a\to b$, $a\to\overline{b}$ for intervals of type II. Therefore the sets of orbits of types I and II are fractal.

(8) The homoclinic and heteroclinic orbits are confined in relatively small intervals along an asymptotic curve. Such an interval containing infinite homoclinic and heteroclinic orbits in Fig. 10 [arc (2)] is confined between $m^*\approx 307.64$ and $m^{**}\approx 314.38$. On the other hand, all orbits in a large interval $74.94<m<m^*$ fall into M_1 and all orbits in the interval $m^{**}<m<559.12$ fall into M_2.

(9) Similar intervals containing infinite homoclinic and heteroclinic orbits appear in other arcs of the asymptotic curve. In particular if we take an interval $(m^*/\lambda, m^{**}/\lambda)$ close to the periodic

orbit O we have the same transitions after one more iteration. Similar orbits appear in the intervals $(m*/\lambda^2, m**/\lambda^2)$ and so on. Therefore close to O there are infinite sets of homoclinic and heteroclinic orbits.

(10) An exploration of the whole phase space gives the domains of escape into the black holes M_1 and M_2 after some iterations beyond the initial points. There are large domains of orbits that escape immediately into M_1 and M_2 and fractal regions with escapes into M_1 or M_2, after any number of iterations (0,1,2…). As most orbits fall into the black holes after a finite time one cannot calculate a Lyapunov characteristic number. Nevertheless the fractal mixing of the various domains of escape gives another way to establish the chaotic behavior of the system of two black holes.

(11) The areas on a surface of section are not preserved. Therefore the surface of section $x=0$ ($\dot{x}>0$) is not a "Poincaré surface of section." The black holes act as attractors despite the fact that the system is conservative. Therefore the system of two fixed black holes has certain properties of dissipative systems.

The last conclusion, together with the fact that the sets of orbits falling on the two black holes are fractal, are the main results of the present study.

ACKNOWLEDGMENT

This research was supported by the Academy of Athens (program 200/557).

APPENDIX: ORBITS VERY CLOSE TO A BLACK HOLE

The equations of motion in the case of two black holes are[5,1]

$$\frac{\mathrm{d}}{\mathrm{d}s}(U^2Q^2\dot{\psi}^2) = E^2\dot{\psi}\frac{\partial}{\partial\psi}\left[U^2Q\left(U^2-\frac{\delta_1}{E^2}\right)\right],$$
$$\frac{\mathrm{d}}{\mathrm{d}s}(U^2Q^2\dot{\theta}^2) = E^2\dot{\theta}\frac{\partial}{\partial\theta}\left[U^2Q\left(U^2-\frac{\delta_1}{E^2}\right)\right], \tag{A1}$$

where ψ and θ are prolate spheroidal coordinates in the case of particles moving on a meridian plane of a potential U with

$$U=\frac{1+[(\mathrm{M}_1+\mathrm{M}_2)\cosh\psi+(\mathrm{M}_1-\mathrm{M}_2)\cos\theta]}{Q} \tag{A2}$$

and

$$Q=\sinh^2\psi+\sin^2\theta>0, \tag{A3}$$

E is the value of the energy, which is assumed of the elliptic type, i.e., $0<E<1$, and s is the proper time, while the dot means a derivative with respect to s; $\delta_1=0$ for photons and $\delta_1=1$ for particles.

The coordinates x and z are

$$x=\sinh\psi\sin\theta,\quad z=\cosh\psi\cos\theta, \tag{A4}$$

and at the black hole M_1 we have $\psi=\theta=0$. Along the z axis, above M_1, we have $\theta=0$, and below M_1 we have $\psi=0$.

We consider now motions close to the black hole M_1. Then ψ and θ are small quantities, and to second order

$$x=\psi\theta,$$

$$z - 1 = \tfrac{1}{2}(\psi^2 - \theta^2). \tag{A5}$$

The largest term of U is

$$U = \frac{2M_1}{\psi^2 + \theta^2}. \tag{A6}$$

The largest terms of the equations of motion (A1) are

$$\begin{aligned} \frac{d}{ds}\left(\frac{\dot{\psi}}{\psi^2 + \theta^2}\right) &= -\frac{3E^2\psi}{(\psi^2 + \theta^2)^3}, \\ \frac{d}{ds}\left(\frac{\dot{\theta}}{\psi^2 + \theta^2}\right) &= -\frac{3E^2\theta}{(\psi^2 + \theta^2)^3}. \end{aligned} \tag{A7}$$

Multiplying the first equation by θ and the second equation by ψ and substracting we find

$$(\psi^2 + \theta^2)(\theta\ddot{\psi} - \psi\ddot{\theta}) - 2(\theta\dot{\psi} - \psi\dot{\theta})(\psi\dot{\psi} + \theta\dot{\theta}) = 0 \tag{A8}$$

and if we write

$$J = \theta\dot{\psi} - \psi\dot{\theta} \tag{A9}$$

we derive

$$Q\dot{J} - J\dot{Q} = 0. \tag{A10}$$

Therefore,

$$\frac{J}{Q} = c \ \text{(constant)}. \tag{A11}$$

This relation is written

$$\frac{\dfrac{d}{ds}\left(\dfrac{\psi}{\theta}\right)}{1 + \left(\dfrac{\psi}{\theta}\right)^2} = \frac{d}{ds}\tan^{-1}\left(\frac{\psi}{\theta}\right) = c \tag{A12}$$

and integrating we derive

$$\tan^{-1}(\psi/\theta) = cs + c' \tag{A13}$$

or

$$\psi = \theta\tan(cs + c') = \theta q, \tag{A14}$$

where s is zero when a particle hits the black hole.

In order to complete the integration close to the black hole we take the second equation (A7) and find

$$\ddot{\theta} - \frac{2\dot{\theta}^2}{\theta} - 2\dot{\theta}qc = -\frac{3E^2}{\theta^3(1 + q^2)^2}. \tag{A15}$$

The second member is large if θ is close to zero. Assuming

$$\theta = \alpha s^m \tag{A16}$$

we find that the second member is $-3E^2 s^{-3m}/a^3(1+q^2)^2$, while the most important terms of the first member are $as^{m-2}[m(m-1)-2m^2]$. The first and second members are of the same order iff $m=0.5$. Then we find

$$a^4 = \frac{4E^2}{(1+q^2)^2} \tag{A17}$$

and

$$z-1 = \frac{1}{2}\theta^2(q^2-1) = \frac{1}{2}a^2 s(q^2-1) = \pm E\left(\frac{q^2-1}{q^2+1}\right)s \tag{A18}$$

while

$$x = \theta^2 q. \tag{A19}$$

Thus the angle between the orbit and the z axis has a tangent equal to

$$\frac{x}{(z-1)} = \frac{2q}{q^2-1}. \tag{A20}$$

When the asymptotic curve reaches the black hole $z=1$ [e.g., at the third intersection in Fig. 1 for m near $m=6722$ (Fig. 3)], the tangent of the angle $x/(z-1)$ tends to zero, i.e., q tends to zero. Therefore, from Eq. (A18) we derive $\dot{z}=\pm E$ (and $\ddot{z}=0$). This is verified numerically for $E=\sqrt{0.5}$ in Fig. 1 where the value of $\dot{z}$ at $m=6722$ is $\ddot{z}=-0.71$ and very close to it the asymptotic curve is horizontal, i.e., $\ddot{z}=0$. The same happens near $m=9052$, where the tangent of the angle between the orbit and the z axis is close to 180°, i.e., $x/|z-1|$ again tends to zero, hence $q\to 0$ and $\dot{z}=\pm E$, $\ddot{z}=0$.

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On the form factor for the unitary group

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We study the combinatorics of the contributions to the form factor of the group $U(N)$ in the large N limit. This relates to questions about semiclassical contributions to the form factor of quantum systems described by the unitary ensemble.
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I. INTRODUCTION

The *form factor* associated to a self-adjoint operator H is a real-valued function describing statistical properties of its spectrum. For sake of simplicity we assume that H acts on finite-dimensional Hilbert space and thus has eigenvalues $E_1,\ldots,E_N\in\mathbb{R}$. Then we consider the Fourier transform of the measure

$$\mu:=\frac{1}{N}\sum_{j,k=1}^{N}\delta_{E_j-E_k}$$

and obtain the form factor

$$K(t):=\int_{\mathbb{R}}\exp(-itE)\mathrm{d}\mu(E)=\frac{1}{N}|\mathrm{tr}(U(t))|^2,$$

with the unitary time evolution $U(t):=\exp(-iHt)$ generated by H.

It is an empirical fact and a physical conjecture (see Bohigas, Giannoni, and Schmit[8] and also Ref. 15) that most form factors encountered in physical quantum systems resemble the form factor associated to a so-called random matrix ensemble (see Mehta[18]).

The simplest of these is the so-called *unitary ensemble* on which we shall concentrate below. This is given by the unitary group $U(N)$ equipped with Haar probability measure μ_N. Its form factor is defined as

$$K_N(t):=\frac{1}{N}\langle|\mathrm{tr}(U^t)|^2\rangle_N\quad(t\in\mathbb{Z}),\tag{1.1}$$

with the expectation $\langle f\rangle\equiv\langle f\rangle_N:=\int_{U(N)}f\mathrm{d}\mu_N$ of a continuous function $f:U(N)\to\mathbb{C}$.

As the map $U\mapsto\mathrm{tr}(U^t)$ is a class function on the unitary group, we can apply Weyl's integration formula

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$$\int_{\mathrm{U}(N)} f \mathrm{d}\mu_N = \frac{1}{N!} \int_{\mathbb{T}^N} f \Delta^2 \mathrm{d}\nu_N \tag{1.2}$$

to evaluate (1.1). In (1.2) $f: \mathrm{U}(N) \to \mathbb{C}$ is assumed to be a class function. $\mathbb{T}^N \subseteq \mathrm{U}(N)$ is a maximal torus and may be identified with the subgroup of diagonal matrices. $\mathrm{d}\nu_N$ denotes Haar measure on $\mathbb{T}^N$. Finally for $h := \mathrm{diag}(h_1, \ldots, h_N) \in \mathbb{T}^n \subseteq \mathrm{U}(N)$

$$\Delta(h) := \sum_{1 \leqslant j < k \leqslant N} |h_j - h_k|$$

is the modulus of Vandermonde's determinant for $h_1, \ldots, h_N$. The combinatorial factor $N!$ is the order of the symmetric group S_N making its appearance as the Weyl group, see, e.g., Fulton and Harris.[13]

With these data, the form factor is evaluated,

$$K_N(t) = \begin{cases} N, & t = 0, \\ |t|/N, & 0 < |t| \leqslant N \quad (t \in \mathbb{Z}), \\ 1, & N < |t|. \end{cases} \tag{1.3}$$

This calculation is based on the eigenvalues $h_1, \ldots, h_N$ of the unitary matrix. [As the N eigenvalues of $U \in \mathrm{U}(N)$ have mean distance $2\pi/N$, note that the natural argument of the form factor would be t/N instead of t. However, in order to simplify notation, we use the parameter $t \in \mathbb{Z}$.]

In Ref. 6, Berry proposed a semiclassical evaluation of the form factor for quantum systems, based on the periodic orbits of the principal symbol (Hamiltonian function) of the Hamiltonian operator. For the different random matrix ensembles he derived in the range $0 < t \ll N$ the leading order of $K_N(t)$, which is linear in t/N.

More precisely, semiclassical theory based on the Gutzwiller trace formula provides a link between spectral quantities of the quantum Hamiltonian and properties of the chaotic dynamics of the corresponding classical system. In this approach the spectral two-point correlation function and its Fourier transform, namely the form factor, are calculated by approximating the density of states using the trace formula. This formula expresses them by sums over contributions from pairs of classical periodic trajectories.

If one includes only pairs of equal or time-reversed orbits (the so-called "diagonal approximation") then the form factor agrees with random matrix theory, asymptotically close to the origin (long-range correlations).

A more systematic approach will require a complete control of all the other contributions. A first step towards an understanding of the "off-diagonal" contributions have been achieved in Ref. 7. But only recently, beginning with the article by Sieber and Richter,[23] contributions involving pairs of periodic orbits were systematically considered in order to explain higher order terms in t/N.

In particular, for the geodesic flow on constant negative curvature, a particular family of pairs of periodic orbits have been presented in Refs. 23 and 22, which turned out to be relevant for the first correction to the diagonal approximation for the spectral form factor. These orbits pairs are given by trajectories which exhibit self-intersection with small intersection angles. This result has been generalized recently to more general uniformly hyperbolic dynamical systems.[24]

The combinatorics, however, turned out to be highly nontrivial. These combinatorial difficulties in handling high order corrections to the semiclassical expression of the form factor persist also in the context of quantum graphs, Refs. 16 and 17, where these off-diagonal contributions have been explored up to the third order.[3–5]

In our opinion the complex combinatorics should first be studied in the simplest situation possible, that is, on the group level. Here the unitary ensemble is the simplest one, since the case of the orthogonal or symplectic ensemble involves additional elements like the Brauer algebra, see Ref. 12.

Now we collect the main points of the paper.

We want to compare the form factor $K_N(t)$ with the diagonal contribution

$$\frac{t}{N}\Delta_N^{\max}(t) \quad \text{with} \quad \Delta_N^{\max}(t) := \sum_{i_1,\ldots,i_k=1}^{N} \left\langle \prod_{k=1}^{t} |U_{i_k i_{k+1}}|^2 \right\rangle_N \tag{1.4}$$

(note that only sum over *one* t-tuple of indices in $\Delta_N^{\max}$, hence the name *diagonal contribution*).

The expectation values of products of matrix entries in (1.4) and (1.1) can be evaluated using the well-known formula (2.1), that is, by summing class functions on the symmetric group S_t.

So in Sec. II we introduce some notation concerning the symmetric group.

In Sec. III we discuss the relation between the class functions V and $\mathcal{N}$ on S_t used in (2.1). As stated in Proposition 3.3 they are mutual inverses in the group algebra of S_t.

As a simple by-product, this leads to a rederivation of Eq. (1.2) in the linear regime $|t| \leqslant N$ (Remarks 3.6).

In Sec. IV we study the relation between a natural metric on S_t and the joint operation on the associated partition lattice $\mathcal{P}_t$ (Proposition 4.1).

Section V starts by a (partial) justification of our above definition (1.4), and an estimate of its contributions in terms of formula (2.1). Here the interplay between the partition lattice and cyclic permutation becomes essential (Proposition 5.4). Although Proposition 5.4 is a statement about the $N \to \infty$ limit, we present evidence for our conjecture 5.8 which is a uniform in $N \geqslant t$ version of Proposition 5.4.

In Sec. VI we first prove that only derangements (that is, fixed point free permutations) are involved in the diagonal approximation (Proposition 6.2). Then we estimate the number of contributions to $\Delta_N^{\max}$ with a given power of N (Proposition 6.3).

This leads us to our main result in Sec. VII: Assuming Conjecture 5.8, there exists a subinterval $I := [\varepsilon, C-\varepsilon] \subset [0,1]$ such that the diagonal approximation converges uniformly to the form factor if $t/N \in I$ (Theorem 7.1).

II. GENERALITIES ON THE SYMMETRIC GROUP

As already mentioned in the Introduction, the symmetric group S_t of permutations of the set $[t] := \{1, \ldots, t\}$ plays an important role in the analysis of the unitary ensemble.

We begin by introducing some notation, see Ref. 20 for more information. For $\sigma \in S_t$ the *cycle length* of $i \in [t]$ is the smallest $n \in \mathbb{N}$ with $\sigma^n(i) = i$. i is a *fixed point* of σ if $n = 1$. The *cycle* of i is given by $(i, \sigma(i), \ldots, \sigma^{n-1}(i))$, and can be interpreted as the group element of S_t which permutes the $\sigma^k(i)$ in the prescribed order, leaving the other elements of $[t]$ fixed.

$e \in S_t$ denotes the identity element.

Writing a group element $\sigma \in S_t \backslash \{e\}$ as a product of disjoint cycles $\sigma = \sigma^{(1)}, \ldots, \sigma^{(k)}$, we sometimes omit the fixed points.

Two lattices are associated with the symmetric group S_t:

(i) The *partition lattice* $\mathcal{P}_t$ of *set partitions* $p = \{a_1, \ldots, a_k\}$, with *atoms* or *blocks* $a_l \subseteq [t]$ ($a_l \cap a_m = \emptyset$ for $l \neq m$, $a_l \neq \emptyset$ and $\cup_{l=1}^k a_l = [t]$). $p \in \mathcal{P}_t$ is called *finer* than $q \in \mathcal{P}_t$ (and q *coarser* than p, denoted by $p \leqslant q$) if every block of p is contained in a block of q. The meet $p \vee q$ of $p, q \in \mathcal{P}_t$ is the unique finest element coarser than p and q. We define the rank $|p|$ of the partition $p = \{a_1, \ldots, a_k\} \in \mathcal{P}_t$ by $|p| := k$ (note that this is called the corank in Ref. 1).

(ii) The *dominance order* $\mathcal{D}_t$ of *number partitions* $\lambda = (\lambda_1, \ldots, \lambda_k) \in \mathcal{D}_t$ of $t \in \mathbb{N}$ (with $\lambda_l \in \mathbb{N}, \lambda_{l+1} \leqslant \lambda_l$ and $\Sigma_{l=1}^k \lambda_l = t$). The map

$$\mathcal{P}_t \to \mathcal{D}_t, \quad \{a_1, \ldots, a_k\} \mapsto (|a_1|, \ldots, |a_k|)$$

induces an order relation and a rank function on $\mathcal{D}_t$.

See Ref. 1 for more information.

Each permutation $\sigma \in S_t$ partitions $[t]$ into atoms belonging to the same cycle of σ. Thus we have a map

$$S_t \to \mathcal{P}_t, \quad \sigma \mapsto \hat{\sigma}.$$

If the context is clear, we omit the hat. In particular $|\sigma| := k$ if $\sigma = \sigma^{(1)}, \ldots, \sigma^{(k)}$ is the disjoint cycle decomposition of σ (including fixed points).

Examples 2.1: (1) $\sigma = (124)(3) \in S_4$ and $\rho = (142)(3) \in S_4$ have the set partition $\hat{\sigma} = \hat{\rho} = \{\{1,2,4\},\{3\}\} \in \mathcal{P}_4$ and number partition $[\sigma] = [\rho] = (3,1) \in \mathcal{D}_4$ (here $[\sigma] := \{\alpha^{-1}\sigma\alpha \,|\, \alpha \in S_t\}$ denotes the conjugacy class of $\sigma \in S_t$).

(2) $\sigma = (12)(34) \in S_4$ and $\rho = (13)(24) \in S_4$ have rank $|\sigma| = |\rho| = 2$, whereas $|\sigma \vee \rho| = |\{\{1,2,3,4\}\}| = 1$.

The importance of the dominance order $\mathcal{D}_t$ for the symmetric group is obvious, as the elements of $\mathcal{D}_t$ naturally enumerate the conjugacy classes of S_t. Thus they also enumerate the irreducible representations and their characters,

$$\chi_\lambda : S_t \to \mathbb{R} \quad (\lambda \in \mathcal{D}_t).$$

In the present context the importance of the partition lattice $\mathcal{P}_t$ comes from the following identity.

Lemma 2.2: For all $t, N, k \in \mathbb{N}$ and $\pi_1, \ldots, \pi_k \in S_t$,

$$\sum_{(i_1,\ldots,i_t)\in[N]^t} \prod_{l=1}^{k} \left(\prod_{j=1}^{t} \delta_{i_j}^{i_{\pi_l(j)}} \right) = N^{|\pi_1 \vee \ldots \vee \pi_k|}.$$

From now on our standing assumption relating the groups S_t and $\mathrm{U}(N)$ is $t \leqslant N$. Then the following important formula can be found in Ref. 21, see also Ref. 10,

$$\langle U_{a_1 b_1} \cdots U_{a_s b_s} \overline{U}_{\alpha_1 \beta_1} \cdots \overline{U}_{\alpha_t \beta_t} \rangle_N = \delta_t^s \sum_{\sigma,\pi \in S_t} V_N(\sigma^{-1}\pi) \prod_{k=1}^{t} \delta_{a_k}^{\alpha_{\sigma(k)}} \delta_{b_k}^{\beta_{\pi(k)}}, \tag{2.1}$$

where for $N \geqslant t$ the class function $V \equiv V_N : S_t \to \mathbb{R}$ is given by

$$V_N := \sum_{\lambda \in \mathcal{D}_t} \frac{\chi_\lambda(e)}{t!\, f_\lambda(N)} \chi_\lambda. \tag{2.2}$$

f_λ is a polynomial in N of order t vanishing at certain integers,

$$f_\lambda(N) := \sum_{\sigma \in S_t} \frac{\chi_\lambda(\sigma) N^{|\sigma|}}{\chi_\lambda(e)} = \prod_{i=1}^{k} \frac{(N + \lambda_i - i)!}{(N-i)!} \quad (\lambda \in \mathcal{D}_t) \tag{2.3}$$

(see Appendix A of Ref. 21).

Recalling the correspondence between irreducible representations of S_t and conjugacy classes of S_t, i.e., ordered number partitions $\lambda = (\lambda_1, \ldots, \lambda_k) \in \mathcal{D}_t$, $\lambda_1 \geqslant \cdots \geqslant \lambda_k$, of t, by evaluating Frobenius' formula the dimension $\chi_\lambda(e)$ of the representation appearing in (2.2) equals

$$\chi_\lambda(e) = t! \, \frac{\prod_{i<j} (\lambda_i - \lambda_j + j - i)}{\prod_i (\lambda_i + k - i)!} \quad (\lambda \in \mathcal{D}_t),$$

see Ref. 13, Eq. (4.11).

III. THE LINEAR REGIME OF THE FORM FACTOR

Next we decompose the form factor $K_N(t)$ into a sum of products of the class functions V_N and $\mathcal{N} : \sigma \mapsto N^{|\sigma|}$ on S_t. This will allow us to compare it with the diagonal contribution to be introduced in Sec. V.

As a side effect, we will rederive its concrete form (1.3) for $|t| \leqslant N$. Since $K_N(0) = N^{-1}(\mathrm{tr}(\mathbb{1}_N))^2 = N$ and $K_N(-t) = K_N(t)$, we effectively only need to consider the regime $0 < t \leqslant N$ where K_N is linear.

Evaluating $\mathrm{tr}(U^t)$ as $\Sigma_{i\in[N]^t}\Pi_{k=1}^{t} U_{i_k i_{k+1}}$ in (1.1), we get a cyclic ordering of the subindices, given by the circular permutation

$$\tau := (1,2,\ldots,t) \in S_t.$$

Conjugation of $\sigma \in S_t$ by τ will be denoted by $\sigma_+ := \tau^{-1}\sigma\tau$.

Given $t \in \mathbb{N}$ and the permutation group S_t, we denote by

$$\mathcal{C}_t := \{\sigma \in S_t \,|\, |\sigma| = 1\}$$

the set of *circular permutations*. This subset is of cardinality

$$|\mathcal{C}_t| = (t-1)!\,,$$

and every $\sigma \in \mathcal{C}_t$ can be written in the form $\sigma = \pi^{-1}\tau\pi,\ \pi \in S_t$.

Lemma 3.1: The sets

$$M(\phi,\phi') := \{(\pi,\sigma) \in S_t \times S_t \,|\, \phi = \pi^{-1}\sigma_+, \phi' = \pi^{-1}\sigma\} \quad (\phi,\phi' \in S_t)$$

are of size

$$|M(\phi,\phi')| = \begin{cases} t, & \phi'\tau\phi^{-1} \in \mathcal{C}_t, \\ 0, & \text{otherwise}, \end{cases}$$

and form a partition of $S_t \times S_t$.

Proof:

(1) By definition of $M(\phi,\phi')$ any given pair $(\pi,\sigma) \in S_t \times S_t$ lies in exactly one subset $M(\phi,\phi') \subseteq S_t \times S_t$, namely in $M(\pi^{-1}\sigma_+, \pi^{-1}\sigma)$.

(2) If $(\pi,\sigma) \in M(\phi,\phi')$ then $\phi'\tau\phi^{-1} = \pi^{-1}\tau\pi \in \mathcal{C}_t$. Then the t different

$$(\tau^l\pi, \tau^l\sigma) \in S_t \times S_t \quad (l = 0,\ldots,t-1)$$

are in $M(\phi,\phi')$, too. As thus there are exactly $\mathcal{C}_t \times S_t = (t-1)! \times t!$ pairs $(\phi,\phi') \in S_t \times S_t$ with cardinality of the corresponding atoms $|M(\phi,\phi')| \geqslant t$, but $S_t \times S_t = t! \times t!$, their cardinality must be exactly t. □

Proposition 3.2: For all $t \leqslant N \in \mathbb{N}$, *the form factor* (1.1) *equals*

$$K_N(t) = \frac{t}{N} \cdot \sum_{\substack{\phi,\phi' \in S_t \\ \phi'\tau\phi^{-1} \in \mathcal{C}_t}} V_N(\phi') N^{|\phi|} \tag{3.1}$$

$$= \frac{t}{N} \cdot \sum_{\gamma \in \mathcal{C}_t} \sum_{\phi \in S_t} V_N(\gamma\phi\tau^{-1}) N^{|\phi|}. \tag{3.2}$$

Proof: Using subindices (mod t),

$$\langle|\mathrm{tr}(U^t)|^2\rangle_N = \sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \langle U_{i_1 i_2}\cdots U_{i_t i_1}\overline{U}_{j_1 j_2}\cdots\overline{U}_{j_t j_1}\rangle_N$$

$$= \sum_{\pi,\sigma\in S_t} V_N(\pi^{-1}\sigma)\cdot \sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \prod_{k=1}^{t} \delta^{j_{\pi(k)}}_{i_k}\cdot\delta^{j_{\sigma(k+1)}}_{i_{k+1}} = \sum_{\pi,\sigma\in S_t} V_N(\pi^{-1}\sigma)\cdot N^{|\pi^{-1}\sigma_+|}, \qquad (3.3)$$

since

$$\sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \prod_{k=1}^{t} \delta^{j_{\pi(k)}}_{i_k}\cdot\delta^{j_{\sigma(k+1)}}_{i_{k+1}} = \sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \prod_{k=1}^{t} \delta^{j_{\pi(k)}}_{i_k}\cdot\delta^{j_{\sigma\tau(k)}}_{i_{\tau(k)}}$$

$$= \sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \prod_{k=1}^{t} \delta^{j_{\pi(k)}}_{i_k}\cdot\delta^{j_{\sigma_+(k)}}_{i_k} = \sum_{\substack{i_1,\ldots,i_t\\ j_1,\ldots,j_t}} \prod_{k=1}^{t} \delta^{j_{\pi(k)}}_{i_k}\cdot\delta^{j_{\pi^{-1}\sigma_+(k)}}_{j_k} = \sum_{j_1,\ldots,j_t} \prod_{k=1}^{t} \delta^{j_{\pi^{-1}\sigma_+(k)}}_{j_k}.$$

In the last step of (3.3) we used Lemma 2.2. Equation (3.1) now follows from Lemma 3.1. In (3.1) we can write $\phi' = \phi\tau^{-1}\gamma$ for a unique $\gamma\in\mathcal{C}_t$, This implies the second equation. □

To further evaluate these expressions for the form factor, we remind the reader of some general group theoretical notions.

Let G be a finite group with normalized counting measure, that is, the inner product

$$\langle f_1, f_2\rangle := \frac{1}{|G|}\sum_{g\in G}\overline{f_1(g)}f_2(g) \quad (f_1, f_2\in L^2(G)). \qquad (3.4)$$

The characters of the irreducible representations are orthonormal with respect to this inner product and form a basis of the subspace of class functions.

On $L^2(G)$ we have the unitary operators of left and right translations, given by

$$R_h f(g) := f(gh), \quad L_h f(g) := f(hg) \quad (g,h\in G).$$

For irreducible characters $\chi_\mu, \chi_\lambda : G\to\mathbb{C}$ one has

$$\langle\chi_\lambda, L_g\chi_\mu\rangle = \langle\chi_\lambda, R_g\chi_\mu\rangle = \delta_{\lambda\mu}\frac{\chi_\lambda(g)}{\chi_\lambda(e)} \quad (g\in G), \qquad (3.5)$$

see Ref. 11, Eq. (31.16).

We now consider the group algebra $K[S_t]$ of the symmetric group, K denoting a field, i.e., the K-vector space $\{f: S_t\to K\}$, with multiplication of $f, g\in K[S_t]$ given by

$$f * g(\alpha) := \sum_{\sigma\in S_t} f(\sigma)g(\sigma^{-1}\alpha) = \sum_{\sigma\in S_t} f(\alpha\sigma^{-1})g(\sigma) \quad (\alpha\in S_t)$$

and neutral element $\mathbb{1}_e\in K[S_t]$.

More specifically we use the field $K := \mathbb{C}(N)$ of rational functions and denote by $\mathcal{N}\in K[S_t]$ the monomial-valued function

$$\mathcal{N}(\alpha) := N^{|\alpha|} \quad (\alpha\in S_t)$$

(which, like $\mathbb{1}_e$, is a class function).

Proposition 3.3: $V=\mathcal{N}^{-1}$.

Proof: We have, using Eq. (2.3),

$$V(\phi)=\sum_{\lambda\in\mathcal{D}_t}\frac{\chi_\lambda(\phi)\chi_\lambda(e)}{t!\,f_\lambda(N)}=\frac{1}{t!}\sum_{\lambda\in\mathcal{D}_t}\frac{\chi_\lambda(\phi)(\chi_\lambda(e))^2}{\sum_{\sigma\in S_t}\chi_\lambda(\sigma)N^{|\sigma|}}.$$

Thus (as $|\sigma^{-1}|=|\sigma|$) we must prove that

$$\sum_{\lambda\in\mathcal{D}_t}\frac{\sum_{\omega\in S_t}\chi_\lambda(\alpha\omega)N^{|\omega|}}{\sum_{\sigma\in S_t}\chi_\lambda(\sigma)N^{|\sigma|}}(\chi_\lambda(e))^2=t!\,\mathbb{1}_e(\alpha). \tag{3.6}$$

In order to show that the left-hand side (lhs) is in fact independent of N (if $N\geqslant t$ so that the denominator does not vanish), for $\sigma\in S_t$ we sum over the conjugacy class $[\sigma]\subseteq S_t$ of σ, using that $|\rho\sigma\rho^{-1}|=|\sigma|$.

More specifically we claim the existence of a constant $C_\lambda(\alpha)$ such that for all $\sigma\in S_t$,

$$\sum_{\tilde\sigma\in[\sigma]}\chi_\lambda(\alpha\tilde\sigma)=C_\lambda(\alpha)\sum_{\tilde\sigma\in[\sigma]}\chi_\lambda(\tilde\sigma). \tag{3.7}$$

Equivalently we show that

$$\mathcal{L}_\lambda(\sigma)\equiv\mathcal{L}_\lambda(\alpha,\sigma):=\sum_{\rho\in S_t}\chi_\lambda(\alpha\rho\sigma\rho^{-1})$$

equals $C_\lambda(\alpha)\cdot r_\lambda(\sigma)$ with $r_\lambda(\sigma):=\Sigma_{\rho\in S_t}\chi_\lambda(\rho\sigma\rho^{-1})=t!\,\chi_\lambda(\sigma)$.

Now for $\alpha\in S_t$,

$$\mathcal{L}_\lambda(\sigma)=\sum_{\rho\in S_t}\chi_\lambda((\rho^{-1}\alpha\rho)\sigma)=\frac{|S_t|}{|[\alpha]|}\sum_{\pi\in[\alpha]}\chi_\lambda(\pi\sigma)=\frac{t!}{|[\alpha]|}\sum_{\pi\in[\alpha]}L_\pi\chi_\lambda(\sigma).$$

$\mathcal{L}_\lambda$ being a class function, we write it in the form

$$\mathcal{L}_\lambda=\sum_{\mu\in\mathcal{D}_t}\mathrm{d}_\mu\chi_\mu \tag{3.8}$$

and determine the coefficients d_μ using the orthonormality relation $\langle\chi_\lambda,\chi_\mu\rangle=\delta_{\lambda\mu}$. By Eq. (3.5),

$$\langle L_\pi\chi_\lambda,\chi_\mu\rangle=\delta_{\lambda\mu}\frac{\chi_\lambda(\pi)}{\chi_\lambda(e)}$$

which leads to

$$\mathrm{d}_\mu=\delta_{\lambda\mu}\frac{t!}{|[\alpha]|\chi_\lambda(e)}\sum_{\pi\in[\alpha]}\chi_\lambda(\pi).$$

Inserting this into (3.8) we see that $C_\lambda(\alpha)$ in (3.7) equals

$$C_\lambda(\alpha)=\frac{1}{|[\alpha]|\chi_\lambda(e)}\sum_{\pi\in[\alpha]}\chi_\lambda(\pi).$$

Using

$$\sum_{\sigma\in S_t}\chi_\lambda(\alpha\sigma)N^{|\sigma|}=C_\lambda(\alpha)\sum_{\sigma\in S_t}\chi_\lambda(\sigma)N^{|\sigma|},$$

the lhs of (3.6) equals

$$\frac{1}{|[\alpha]|}\sum_{\lambda\in\mathcal{D}_t}\sum_{\pi\in[\alpha]}\chi_\lambda(\pi)\chi_\lambda(e)=\frac{1}{|[\alpha]|}\sum_{\pi\in[\alpha]}\sum_{\lambda\in\mathcal{D}_t}\chi_\lambda(\pi)\chi_\lambda(e)$$

$$=\frac{1}{|[\alpha]|}\sum_{\pi\in[\alpha]}\mathbb{1}_e(\pi)\sum_{\lambda\in\mathcal{D}_t}(\chi_\lambda(e))^2=\frac{1}{|[\alpha]|}\mathbb{1}_e(\alpha)t!=\mathbb{1}_e(\alpha)t!, \quad (3.9)$$

using the identity

$$\sum_{\lambda\in\mathcal{D}_t}\chi_\lambda(e)^2=t!$$

in (3.9), see Chap. 5.2 in Ref. 20 and 19. This proves (3.6). □

We redefine the inner product (3.4) on $\mathbb{C}[S_t]$ omitting the factor $1/|S_t|=1/t!$,

$$\langle f_1,f_2\rangle:=\sum_{\sigma\in S_t}\overline{f_1(\sigma)}f_2(\sigma)(f_1,f_2:S_t\to\mathbb{C}). \quad (3.10)$$

So the irreducible characters are now of norm $t!$. Anyhow we are now more interested in the following sets of functions.

Instead of considering the field $\mathbb{C}(N)$ of rational functions in the variable N we will now specialize the value $N\in\mathbb{N}$, $N\geqslant t$.

Define for $\sigma\in S_t$ the translates of $\mathcal{N}$,

$$\hat{q}_\sigma\in\mathbb{C}[S_t],\quad \hat{q}_\alpha(\sigma):=N^{|\sigma^{-1}\alpha|}\quad(\alpha\in S_t).$$

Similarly we define the translates

$$V_\sigma\in\mathbb{C}[S_t],\quad V_\alpha(\sigma):=V_N(\sigma^{-1}\alpha)\quad(\alpha\in S_t)$$

of V_N.

Lemma 3.4: For $N\geqslant t$ the $\hat{q}_\sigma$, $\sigma\in S_t$ form a basis of the vector space $\mathbb{C}[S_t]$, with dual basis V_σ, $\sigma\in S_t$.

Proof: Considered as rational functions, for $\alpha,\beta\in S_t$ the inner product equals

$$\langle V_\alpha,\hat{q}_\beta\rangle=\sum_{\sigma\in S_t}V_N(\sigma^{-1}\alpha)N^{|\sigma^{-1}\beta|}=\sum_{\sigma\in S_t}V_N(\alpha^{-1}\sigma)N^{|\sigma^{-1}\beta|}=\sum_{\rho\in S_t}V_N(\rho)N^{|\rho^{-1}(\alpha^{-1}\beta)|}=V*\mathcal{N}(\alpha^{-1}\beta)=\delta_\alpha^\beta.$$

Specializing the value of N, this duality relation is true as long as the rational functions are defined. By inspection of the definition (2.2) of V_N [in particular of the f_λ defined in (2.3)] this is the case as long as $N\geqslant t$. As the number of the V_α and of the $\hat{q}_\beta$ both equals $\dim(\mathbb{C}[S_t])=t!$, these are indeed bases. □

Corollary 5: For $t\leqslant N$

$$\sum_{\sigma\in S_t}V_N(\alpha\sigma^{-1})N^{|\sigma|}=\mathbb{1}_e(\alpha)\quad(\alpha\in S_t).$$

Remarks 3.6: (1) Corollary 3.5 allows us to regain formula (1.3), i.e.,

$$K_N(t)=\frac{t}{N}\quad\text{for}\quad 0<t\leqslant N.$$

Using Proposition 3.2 we have

$$K_N(t)=\frac{t}{N}\sum_{\gamma\in C_t}\sum_{\phi\in S_t}V_N(\gamma\phi\tau^{-1})N^{|\phi|}=\frac{t}{N}\sum_{\gamma\in C_t}\sum_{\sigma\in S_t}V_N(\sigma)N^{|\gamma^{-1}\sigma\tau|}=\frac{t}{N}\sum_{\gamma\in C_t}\mathbb{1}_\gamma(\tau)=\frac{t}{N}.$$

(2) As $V_N:S_t\to\mathbb{R}$ is a class function, we can also use the notation

$$V_N:\mathcal{D}_t \to \mathbb{R}, \quad V_N([\sigma]) := V_N(\sigma).$$

Then we can calculate V_N using Proposition 3.3. Some examples,

(i) for $t=1$ we have $V_N(1)=1/N$;
(ii) for $t=2$ and denominator $D_2 := N(N^2-1)$ we have

$$V_N(1,1) = \frac{N}{D_2}, \quad V_N(2) = -\frac{1}{D_2},$$

(iii) for $t=3$ and $D_3 := N^3(N^2-1)(N^2-4)$ we have

$$V_N(1,1,1) = \frac{N^4-2N^2}{D_3}, \quad V_N(2,1) = -\frac{N^3}{D_3} \quad \text{and} \quad V_N(3) = \frac{2N^2}{D_3}.$$

(3) The large N asymptotics of $V_N:\mathcal{D}_t \to \mathbb{R}$ for $\lambda=(\lambda_1,\ldots,\lambda_k)$ is given by

$$V_N(\lambda) \sim (-1)^{t-k} N^{k-2t} \prod_{l=1}^{k} C_{\lambda_l} \quad (N \to \infty) \tag{3.11}$$

with the Catalan number $C_l := \binom{2l-2}{l-1}/l$, see Ref. 21.

IV. THE RANK FUNCTION AND THE JOIN OF PARTITIONS

It is useful to give a geometric meaning to our estimates. For this purpose we equip the symmetric group S_t with the metric

$$d:S_t \times S_t \to \{0,1,\ldots,t\}, \quad d(\sigma,\gamma) = t - |\sigma\gamma^{-1}|.$$

The easiest way to visualize this metric is to consider the $\binom{t}{2}$-regular *Cayley graph* (S_t,E_t) having the symmetric group as its vertex set, and edge set

$$E_t := \{(\rho,\rho') \in S_t \times S_t | \rho^{-1}\rho' \text{ is a transposition}\}.$$

Proposition 4.1: (1) *$d(\sigma,\gamma)$ is the distance between the vertices σ and γ on the Cayley graph (S_t,E_t). So in particular the metric d is invariant under the left and right self-actions of S_t.*

(2) $|\pi\vee\sigma| = \min\{|\pi\mu^{-1}| \,|\, \mu \leqslant \sigma\} \quad (\pi,\sigma \in S_t)$.

So in particular

$$d(\pi,\sigma) \leqslant t - |\pi\vee\sigma|.$$

(3) $d(\rho,\rho') \geqslant ||\rho\vee\sigma| - |\rho'\vee\sigma|| \quad (\rho,\rho',\sigma \in S_t)$.

Proof:

(1) For $\rho := \sigma\gamma^{-1}$ with disjoint cycle decomposition $\rho=\rho_1,\ldots,\rho_k$ we have $d(\sigma,\gamma)=d(\rho,e)=t-k=\Sigma_{i=1}^{k}(l_i-1)$, l_i being the length of ρ_i. Exactly $l-1$ transpositions are needed to form a cycle of length l.
(2) Let $(c_1,\ldots,c_m)$, $c_k \subseteq \{1,\ldots,t\}$ be the partition corresponding to the cycles of π. We consider the graph (V,E) with vertex set $V := \{c_1,\ldots,c_m\}$ and edges $\{c_i,c_j\} \in E$ for which there are elements $e_i \in c_i$, $e_j \in c_j$ which belong to the same cycle of σ. Choose for each connected component of (V,E) a spanning tree and representatives $\{e_i,e_j\}$ of its edges. Then by construction the product μ_0 of the transpositions (e_i,e_j) meets $\mu_0 \leqslant \sigma$, and $|\pi\mu_0^{-1}| = |\pi\vee\sigma|$. Any $\mu \leqslant \sigma$ can be written in the form $\mu=\rho\mu_0$ with $\rho \leqslant \sigma$. As no cycles of $\pi\mu_0^{-1}$ can be joined by right multiplication with $\rho^{-1} \leqslant \sigma$, the statement follows.
(3) By symmetry of the metric d we assume $|\rho\vee\sigma| \geqslant |\rho'\vee\sigma|$ and choose $\mu_0 \leqslant \sigma$ so that $|\rho'\vee\sigma| = |\rho'\mu_0^{-1}|$. Then, again by part (2) of the proposition

$$0 \leqslant |\rho \vee \sigma| - |\rho' \vee \sigma| \leqslant |\rho\mu_0^{-1}| - |\rho'\mu_0^{-1}|.$$

By part (1) of the proposition

$$|\rho\mu_0^{-1}| - |\rho'\mu_0^{-1}| \leqslant d(\rho\mu_0^{-1}, \rho'\mu_0^{-1}) = d(\rho, \rho')$$

since multiplication by a transposition changes the number of cycles by one, and since d is invariant under right multiplication. □

Remark 4.2: As the elements $\rho = \sigma = (12)(34)$, $\rho' = (13)(24)$ of S_4 show, in general the inequality $||\rho \vee \sigma| - |\rho' \vee \sigma|| \leqslant ||\rho| - |\rho'||$ does **not** hold. The reverse inequality is wrong.

V. THE DIAGONAL CONTRIBUTION

We now define and study the *diagonal approximation* for the unitary ensemble.

Setting $[N] := \{1, \ldots, N\}$, the diagonal contribution is defined by

$$\Delta_N(t) := \sum_{i \in [N]^t} \mathrm{per}(i) \left\langle \prod_{k=0}^{t-1} |U_{i_k i_{k+1}}|^2 \right\rangle, \tag{5.1}$$

where $\mathrm{per}(i)$ denotes the period of i. In fact [see (2.1)], only those terms of the form factor

$$K_N(t) = \sum_{i,j \in [N]^t} \left\langle \prod_{k=0}^{t-1} U_{i_k i_{k+1}} \overline{U}_{j_k j_{k+1}} \right\rangle$$

can be nonzero for which the sets

$$m_i(r) := \{k \in [t] | i_k = r\}$$

have equal multiplicity $[|m_i(r)| = m_i(r)$ for all $r \in [N]]$.

In this case, if only multiplicities $|m_i(r)| \leqslant 1$ occur for i, there is a unique permutation σ with $j_{\sigma(k)} = i_k$ (and $\pi := \tau\sigma\tau^{-1}$ with $j_{\pi(k)+1} = i_{k+1}$), but in general we have

$$K_N(t) = \sum_{i,j \in [N]^t} \sum_{\kappa^{(1)}, \kappa^{(2)} \in S(m;(1)) \times \cdots \times S(m;(N))} V((\sigma\kappa^{(1)})^{-1} \pi \kappa^{(2)}).$$

As the dominant (in N) contributions are the ones with $V(e)$, i.e., $\sigma = \tau^l$ for some l, we call the sum

$$\Delta_N(t) = \sum_{i,j \in [N]^t \exists l \text{ with } j_{k+l} = i_k} \left\langle \prod_{k=0}^{t-1} U_{i_k i_{k+1}} \overline{U}_{j_k j_{k+1}} \right\rangle \tag{5.2}$$

$$= \sum_{i \in [N]^t} \mathrm{per}(i) \left\langle \prod_{k=0}^{t-1} |U_{i_k i_{k+1}}|^2 \right\rangle \tag{5.3}$$

the *diagonal contribution*.

If $|m_i(r)| \leqslant 1$, then only terms $V(e)$ occur in $\langle \Pi_{k=0}^{t-1} |U_{i_k i_{k+1}}|^2 \rangle$.

The number of all terms in $\Sigma_{i_1, \ldots, i_t}$ being N^t, for $k | t$,

$$I_k := \{(i_1, \ldots, i_t) | i_{l+k} = i_l\}$$

is the set of terms with $\mathrm{per}(i_1, \ldots, i_t) | k$. So the number of terms with $\mathrm{per}(i) < t$ equals

$$\sum_{r>1,r|t} |I_{t/r}|\mu(r),$$

with the Möbius μ function. As $|I_k|=N^k$, this is only of order $N^{t/2}\log(t)$ and thus negligible compared to $|I_t|=N^t$ as $N\to\infty$.

For these reasons, we just define and study a function similar to (5.1) but replacing the period by its maximal value t. In fact for simplicity of notation we use the constant one instead,

$$\Delta_N^{\max}(t) := \sum_{i_1,\ldots,i_t} \left\langle \prod_{k=0}^{t-1} |U_{i_k i_{k+1}}|^2 \right\rangle.$$

A basic manipulation yields the following.

Proposition 5.1:

$$\Delta_N^{\max}(t) = \sum_{\pi,\sigma\in S_t} V_N(\pi^{-1}\sigma) N^{|\pi\vee\sigma_+|}. \tag{5.4}$$

Proof: Using (2.1),

$$\Delta_N^{\max}(t) = \sum_{i\in[N]^t} \sum_{\pi,\sigma\in S_t} V_N(\pi^{-1}\sigma)\cdot \prod_{k=0}^{t-1} \delta_{i_k}^{i_{\pi(k)}}\cdot\delta_{i_{k+1}}^{i_{\sigma(k+1)}} = \sum_{i\in[N]^t} \sum_{\pi,\sigma\in S_t} V_N(\pi^{-1}\sigma)\cdot \prod_{k=0}^{t-1} \delta_{i_k}^{i_{\pi(k)}}\cdot\delta_{i_k}^{i_{\tau^{-1}\sigma\tau(k)}}. \tag{5.5}$$

Lemma (2.2) now gives the result. □

A first easy observation is that for *bounded* t,

$$\Delta_N^{\max}(t) = 1 + \mathcal{O}(1/N^2).$$

This follows by inserting (3.11) into (5.4).

Remark 5.2: In general for $0<t\leqslant N$ **neither** $K_N(t)=(1/N)\Delta_N(t)$ **nor** $K_N(t)=(t/N)\Delta_N^{\max}(t)$, although both equations hold for $N=1$ and $N=2$. Already for $t=3\leqslant N$,

$$\Delta_N(3) = \frac{3N^3}{D_3}(N^4-7N^2+4N+2) \neq 3 = NK_N(3)$$

and

$$\Delta_N^{\max}(3) = \frac{N^3}{D_3}(N^4-3N^2-6N+8) \neq 1 = N\frac{K_N(3)}{3},$$

with denominator $D_3=N^3(N^2-1)(N^2-4)$.

So the diagonal approximation is not exact.

Remark 5.3: Note that we can also write[25]

$$\Delta_N^{\max}(t) = \mathrm{tr}\langle M^t\rangle_N,$$

where M is the doubly stochastic matrix with elements $M_{i,j} := |U_{i,j}|^2$. In Ref. 2 it has been shown that if $\lambda_1=1,\lambda_2,\ldots,\lambda_N$ are the eigenvalues of M ($|\lambda_1|\geqslant|\lambda_2|\geqslant\cdots\geqslant|\lambda_N|$), then

$$\langle|\lambda_j|\rangle_N \to 0, \quad j=2,\ldots,N.$$

Moreover, the expectation of the second eigenvalue $\langle|\lambda_2|\rangle$ is of order $1/\sqrt{N}$. This upper bound is not helpful to show convergence of the trace to 1, namely this does not allow to bound expectations of positive powers $\langle|\lambda_j|^t\rangle$. [For a generic random variable X with values in [0,1], like $X := |\lambda_2|$ the lower, respectively, upper bounds

$$\mathbb{E}(X)^t \leqslant \mathbb{E}(X^t) \leqslant \mathbb{E}(X) \quad (t \in \mathbb{N}),$$

following from Jensen's inequality (applied to the convex function $x \mapsto x^t$), respectively, convolution inequality are optimal in general. This can be seen [for $c = \mathbb{E}(X) \in [0,1]$] by considering the cases of X distributions δ_c, respectively $(1-c)\delta_0 + c\delta_1$. Even for an ac distribution like in our case the falloff in t is not exponential.]

This last remark forces us to investigate more carefully each single contribution to the diagonal contribution. In particular, as we will see in the rest of the paper, the combinatorics become essential in order to bound uniformly the difference of the diagonal approximation to the form factor. This difference becomes large above the regime $t=N$. According to (3.11) the terms in the sum (5.4) have fluctuating sign,

$$\operatorname{sign}(V_N(\pi^{-1}\sigma)) = (-1)^{d(\pi,\sigma)}.$$

This makes it advisable to perform a partial summation before estimating terms in absolute value. We thus rewrite the sum over π in (5.4) in the form of an inner product,

$$\Delta_N^{\max}(t) = \sum_{\sigma \in S_t} \langle V_N, \hat{p}_\sigma \rangle \quad \text{with} \quad \hat{p}_\sigma(\alpha) := N^{|\sigma\alpha^{-1} \vee \sigma_+|}. \tag{5.6}$$

Proposition 5.4: There exists a function $C_t : S_t \to \{0,1\}$ such that

$$\langle V_N, \hat{p}_\sigma \rangle_N = N^{|\sigma \vee \sigma_+| - t}(C_t(\sigma) + \mathcal{O}(1/N)) \quad (\sigma \in S_t).$$

Proof: For $\sigma \in S_t$ the symmetric group is partitioned into the sets

$$B_n := \{\alpha \in S_t \,|\, |\alpha \vee \sigma_+| = |\sigma_+| - n \quad (n = 0, \ldots, |\sigma| - 1).$$

The metric d on S_t is then used to introduce for $\gamma \in B_n$,

$$B(\gamma) := \left\{ \alpha \in \bigcup_{k=0}^{n} B_k \,\middle|\, |\alpha \vee \sigma_+| - |\gamma \vee \sigma_+| = d(\alpha, \gamma) \right\}.$$

Observe that by part (3) of Lemma 4.1 we always have

$$0 \leqslant |\alpha \vee \sigma_+| - |\gamma \vee \sigma_+| \leqslant d(\alpha, \gamma). \tag{5.7}$$

In particular γ is the only element in $B(\gamma) \cap B(n)$. This enables us to define for $n = 0, \ldots, |\sigma| - 1$,

$$C_t(\gamma) := 1 - \sum_{\alpha \in B(\gamma) \setminus \{\gamma\}} C_t(\alpha) \quad (\gamma \in B_n), \tag{5.8}$$

and the approximants

$$\tilde{p}_\sigma : S_t \to \mathbb{R}, \quad \tilde{p}_\sigma := \sum_{\gamma \in S_t} C_t(\gamma) N^{|\gamma \vee \sigma_+| - t} \hat{q}_{\gamma^{-1}\sigma} \quad (\sigma \in S_t)$$

of the functions $\hat{p}_\sigma$.

(i) Next we prove that C_t only takes the values 0 and 1. This follows from the definition (5.8), if we can show that each γ has exactly one *predecessor* in

$$P := \{\alpha \in S_t \,|\, C_t(\alpha) = 1\},$$

that is, $|B(\gamma) \cap P| = 1$. This is done by induction in n, with

$$\gamma \in P \cap B_n \quad (n = 0, \ldots, |\sigma| - 1)$$

and noting that $P \cap B_0 = B_0$ [the $\gamma \in B_0$ are their own predecessors so that $C_t(\gamma) = 1$].

(ii) For the induction step we use the directed graph (S_t, E) with vertex set S_t and edges

$$(\alpha,\beta)\in E \Leftrightarrow d(\alpha,\beta)=1 \text{ and } \alpha\in B_n,\beta\in B_{n-1} \text{ for some } n\in\{1,\ldots,|\sigma|-1\}.$$

By the triangle inequality for $\gamma\in B(n)$ the set $B(\gamma)$ contains all $\alpha\in B_k, 0\leqslant k\leqslant n$ for which there exists a directed chain

$$\gamma=c_n,c_{n-1},\ldots,c_k=\alpha \text{ from } \gamma \text{ to } \alpha \text{ with } c_l\in B_l \text{ and } (c_l,c_{l-1})\in E \quad (l=k+1,\ldots,n).$$

Conversely all $\alpha\in B(\gamma)$ are of that form. Namely for $\alpha\in B(\gamma)\cap B_k$ we know that $d(\alpha,\gamma)=n-k$ so that there exist $c_n,\ldots,c_k\in S_t$ with $c_k=\gamma, c_k=\alpha$ and $d(c_{l-1},c_l)=1$. As $||c_{l-1}\vee\sigma_+|-|c_l\vee\sigma_+||\leqslant d(c_{l-1},c_l)=1$ and $|c_n\vee\sigma_+|=n, |c_k\vee\sigma_+|=k$, we conclude $|c_l\vee\sigma_+|=l$ so that $(c_l,c_{l-1})\in E$.

(iii) This shows that $\alpha\in P$ if there does not exist an edge $(\alpha,\beta)\in E$, and thus $|B(\gamma)\cap P|\geqslant 1$ (as every directed chain starting at γ ends somewhere). To prove that $|B(\gamma)\cap P|=1$, we need a more precise characterization of the predecessors $\alpha\in P$. As there does not exist an edge of the form (α,β) in E, for all neighbors $\beta\in S_+$ of α [i.e., $d(\alpha,\beta)=1$] we have $|\beta\vee\sigma_+|\leqslant|\alpha\vee\sigma_+|$. In other words if β differs from α by a transposition, and if two blocks of $\hat{\sigma}_+\in P_t$ belong to the same block of $\alpha\vee\sigma_+$, then they belong to the same block of $\beta\vee\sigma_+$.

(iv) We model this by considering for given $\sigma\in S_t$ the directed multigraph

$$G_\alpha=(V_\alpha,\mathcal{E}_\alpha)$$

associated to $\alpha\in S_t$. The vertex set of $G(\alpha)$ equals $V_\alpha:=\{\hat{\sigma}_{+,1},\ldots,\hat{\sigma}_{+,m}\}$, with $\hat{\sigma}_{+,1},\ldots,\hat{\sigma}_{+,m}\subseteq[N]$ the blocks of the set partition $\hat{\sigma}_+\in P_t$. The multiplicity of the directed edge $(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j})\in V_\alpha\times V_\alpha$ is given by

$$\mathcal{E}_\alpha: V_\alpha\times V_\alpha\setminus\Delta\to\mathbb{N}_0, \mathcal{E}_\alpha(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j}):=|\{(u,v)\in\hat{\sigma}_{+,i}\times\hat{\sigma}_{+,j}|\alpha(u)=v\}.$$

The in and out degrees of the blocks $\hat{\sigma}_{+,i}$ coincide, that is $\mathcal{E}^+_\alpha(\hat{\sigma}_{+,i})=\mathcal{E}^-_\alpha(\hat{\sigma}_{+,i})$ for

$$\mathcal{E}^+_\alpha(\hat{\sigma}_{+,i}):=\sum_{\hat{\sigma}_{+,j}}\mathcal{E}_\alpha(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j}), \quad \mathcal{E}^-_\alpha(\hat{\sigma}_{+,i}):=\sum_{\hat{\sigma}_{+,j}}\mathcal{E}_\alpha(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j}).$$

Henceforth we omit the superscripts $\pm$ and simply refer to the *degree* $\mathcal{E}_\alpha(\hat{\sigma}_{+,i})=\mathcal{E}^\pm_\alpha(\hat{\sigma}_{+,i})$ of the block.

(v) All ancestors $\alpha\in P$ have multigraphs G_α which have two-connected components, that is, the number of connected components cannot be increased by reducing a single degree $\mathcal{E}(\hat{\sigma}_{+,i})$ by one. This can be seen by noticing that for every $\alpha\in S_t$ the number of connected components of G_α equals $|\alpha\vee\sigma_+|$, and using that the $\alpha\in P$ do not have neighbors β with $|\beta\vee\sigma_+|=|\alpha\vee\sigma_+|+1$.

(vi) To prove $|B(\gamma)\cap P|=1$, we assume that $\alpha^{(1)},\alpha^{(2)}\in B(\gamma)\cap P$. So there exist directed chains $\gamma=c^{(i)}_n,c^{(i)}_{n-1},\ldots,c^{(i)}_{k^{(i)}}=\alpha^{(i)}$ [with $(c^{(i)}_l,c^{(i)}_{l-1})\in E$] from γ to $\alpha^{(i)}, i=1,2$, and we are to show that $\alpha^{(1)}=\alpha^{(2)}$. In each step the number $|c^{(1)}_l\vee\sigma_+|=|c^{(2)}_l\vee\sigma_+|=l$ of connected components of the multigraphs $G_{c^{(i)}_l}$ is reduced by one. That is, all connected components of the multigraph G_γ are broken into their two-connected subcomponents,

$$\mathcal{E}_{\alpha^{(i)}}\leqslant\mathcal{E}_\gamma \quad \text{and} \quad \mathcal{E}_{\alpha^{(i)}}(\hat{\sigma}_{+,j})\neq 1 \quad (i=1,2,\ j=1,\ldots,m).$$

In fact this shows that $\mathcal{E}_{\alpha^{(1)}}=\mathcal{E}_{\alpha^{(2)}}$ so that the multigraphs of $\alpha^{(1)}$ and $\alpha^{(2)}$ coincide.
The multiplicity $\mathcal{E}_\gamma(\hat{\sigma}_{+,i}\hat{\sigma}_{+,j})$ of a directed edge of G_α is reduced only if $\mathcal{E}_\gamma(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j})=1$. So not only $\mathcal{E}_{\alpha^{(1)}}(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j})=\mathcal{E}_{\alpha^{(2)}}(\hat{\sigma}_{+,i},\hat{\sigma}_{+,j})$ but the chains connecting γ with $\alpha^{(1)}=\alpha^{(2)}$.

(vii) We now know that $C_t(\alpha)$ only takes the values 0 and 1, and that $\tilde{p}_\sigma=\Sigma_{\gamma\in P}N^{|\gamma\vee\sigma_+|-t}\hat{q}_{\gamma^{-1}\sigma}$. This implies

$$\langle V_N,\tilde{p}_\sigma\rangle_N=\sum_{\gamma\in P}N^{|\gamma\vee\sigma_+|-t}\langle V_N,\hat{q}_{\gamma^{-1}\sigma}\rangle_N=C_t(\sigma)N^{|\sigma\vee\sigma_+|-t}.$$

It remains to show that

$$\langle V_N, \hat{p}_\sigma \rangle_N = \langle V_N, \tilde{p}_\sigma \rangle_N + \mathcal{O}(N^{|\sigma \vee \sigma_+| - t - 1}).$$

But, denoting the unique predecessor of $\beta \in S_t$ by $P(\beta)$ [that is $\{P(\beta)\} = B(\beta) \cap P$], we have

$$\tilde{p}_\sigma(\beta^{-1}\sigma) = \sum_{\gamma \in P} N^{|\gamma \vee \sigma_+| - d(\gamma,\beta)} = N^{|P(\beta) \vee \sigma_+| - d(P(\beta),\beta)} + \sum_{\substack{\gamma \in P \\ \gamma \neq P(\beta)}} N^{|\gamma \vee \sigma_+| - d(\gamma,\beta)}.$$

By definition of $B(\gamma)$ the exponent of the first term equals

$$|P(\beta) \vee \sigma_+| - d(P(\beta), \beta) = |\beta \vee \sigma_+|,$$

whereas the exponents of the second term are smaller:

$$|\gamma \vee \sigma_+| - d(\gamma, \beta) < |\beta \vee \sigma_+|$$

on the other hand,

$$\hat{p}_\sigma(\beta^{-1}\sigma) = N^{|\beta \vee \sigma_+|},$$

proving the claim. □

If $\sigma \in S_t$ consists of a single nontrivial cycle, the estimate of Proposition 5.4 can be replaced by an identity (Proposition. 5.6 below).

We prepare this by a sum rule for the class function $\mathcal{N}$.

Lemma 5.5: For all $k \in \mathbb{N}$,

$$\sum_{\sigma \in S_k} N^{|\sigma|} = \prod_{l=0}^{k-1} (N + l). \tag{5.9}$$

Proof: For $k=1$ both sides equal N. So assume the formula to hold for $k-1$, so that

$$\sum_{\tilde{\sigma} \in S_k, \tilde{\sigma}(k)=k} N^{|\tilde{\sigma}|} = N \prod_{l=0}^{k-2} (N + l). \tag{5.10}$$

The group elements $\sigma \in S_k$ either have k as a fixed point s or can uniquely be written in the form

$$\sigma = (l,k)\tilde{\sigma}$$

with $l \in \{1, \ldots, k-1\}$ and $\tilde{\sigma}(k) = k$. As in the second case $|\sigma| = |\tilde{\sigma}| - 1$,

$$\sum_{l=1}^{k-1} \sum_{\tilde{\sigma} \in S_k, \tilde{\sigma}(k)=k} N^{|\tilde{\sigma}|} = (k-1) \prod_{l=0}^{k-2} (N + l). \tag{5.11}$$

Adding the contributions (5.10) and (5.11) yields (5.9). □

We now decompose $\hat{p}_\sigma$ in the form

$$\hat{p}_\sigma = \sum_{\gamma \in S_t} c_\gamma \hat{q}_\gamma \quad \text{with} \quad c_\gamma := \langle V_\gamma, \hat{p}_\sigma \rangle.$$

Proposition 5.6: For a cycle $\sigma = (i_1 + 1, \ldots, i_k + 1) \in S_t$ [and $\sigma_+ = (i_1, \ldots, i_k)$]

$$\hat{p}_\sigma = \left(\prod_{l=1}^{k-1} (N + l) \right)^{-1} \sum_{\gamma' \preccurlyeq \sigma_+} \hat{q}_{\gamma' \sigma}. \tag{5.12}$$

Proof: (i) We evaluate both sides on $\tilde{\alpha} \in S_t$ and write $\tilde{\alpha}$ as $\tilde{\alpha} = \alpha\sigma$ to simplify expressions. Then

$$\hat{p}_\sigma(\alpha\sigma) = N^{|\alpha^{-1}\vee\sigma_+|} \quad \text{and} \quad \hat{q}_{\gamma'\sigma}(\alpha\sigma) = N^{|\alpha^{-1}\gamma'|}. \tag{5.13}$$

(ii) Next we write α as a product of disjoint cycles z_j and note that

$$|z_j\alpha^{-1}\vee\sigma_+| - |z_j\alpha^{-1}\gamma'| = |\alpha^{-1}\vee\sigma_+| - |\alpha^{-1}\gamma'|$$

if z_j and σ_+ are disjoint. We thus can reduce α to a product of cycles intersecting σ_+.

(iii) So we assume that all cycles z_j of α intersect $\sigma_+=(i_1,\ldots,i_k)$,

$$z_j = (i_{\pi(1)},\tilde{z}_1,\ldots,\tilde{z}_2,i_{\pi(2)},\tilde{z}_3,\ldots,\tilde{z}_{2s-2},i_{\pi(s)},\tilde{z}_{2s-1},\ldots,\tilde{z}_{2s})$$

with $\tilde{z}_n \in \{1,\ldots,t\}\backslash\{i_1,\ldots,i_k\}$. Then

$$(i_{\pi(s)},i_{\pi(s-1)},\ldots,i_{\pi(1)})z_j = (i_{\pi(1)},\tilde{z}_1,\ldots,\tilde{z}_2)(i_{\pi(2)},\tilde{z}_3,\ldots,\tilde{z}_4)\cdots(i_{\pi(s)},\tilde{z}_{2s-1},\ldots,\tilde{z}_{2s})$$

is a product of disjoint cycles intersecting the cycle σ_+ only at $i_{\pi(n)}$. Furthermore,

$$(i_{\pi(s)},i_{\pi(s-1)},\ldots,i_{\pi(1)}) \leqslant \sigma_+$$

so that the map

$$\gamma' \mapsto (i_{\pi(s)},i_{\pi(s-1)},\ldots,i_{\pi(1)})\gamma'$$

simply permutes the γ' in $\Sigma_{\gamma'\leqslant\sigma_+}\hat{q}_{\gamma'\sigma}$. This allows to reduce to the case of simple intersections.

(iv) We thus assume that the cycles z_j in the decomposition of α intersect σ_+ exactly in one point, say i_j. Under this assumption, by Lemma 5.5 and (5.13)

$$\left(\prod_{l=1}^{k-1}(N+l)\right)^{-1}\sum_{\gamma'\leqslant\sigma_+}\hat{q}_{\gamma'\sigma}(\alpha\sigma) = \left(\prod_{l=1}^{k-1}(N+l)\right)^{-1}N^{|\alpha^{-1}|-k}\sum_{\gamma\in S_k}N^{|\gamma|} = N^{|\alpha^{-1}|-k+1} = N^{|\alpha^{-1}\vee\sigma_+|} = \hat{p}_\sigma(\alpha\sigma),$$

proving the assertion. □

Corollary 5.7: For a cycle $\sigma=(i_1,\ldots,i_k)\in S_t$ of length k

$$\langle V_N,\hat{p}_\sigma\rangle = \begin{cases} 1, & k=1 \text{ that is } \sigma=e,\\ 0, & 1<k<t\\ \left(\prod_{l=1}^{t-1}(N+l)\right)^{-1}, & k=t. \end{cases} \tag{5.14}$$

Proof: This follows from Proposition 5.6 with $\langle V_N,\hat{q}_\sigma\rangle=\delta_{e,\sigma}$ (Lemma 3.4), remarking that only for $k=1$ or $k=t$ there is a $\gamma'\leqslant\sigma_+$ with $\gamma'\sigma=e$. □

This result and numerical experiments support the following conjecture (compare with Proposition 5.4).

Conjecture 5.8: There exists a constant $C_1\geqslant 1$ such that for all $t\leqslant N\in\mathbb{N}$,

$$|\langle V_N,\hat{p}_\sigma\rangle_N| \leqslant C_1N^{|\sigma\vee\sigma_+|-t} \quad (\sigma\in S_t).$$

VI. DERANGEMENTS AND CIRCULAR ORDER

We now show that, apart from the identity, only the *derangements*, that is the fixed-point free permutations

$$D_t := \{\sigma\in S_t | \sigma(k)\neq k \quad \text{for all} \quad k\in\{1,\ldots,t\}\}$$

contribute in the sum (5.6).

This will follow from a statement of independent interest.

Proposition 6.1: For $k=1,\ldots,t+1$ denote by $S_t^{(k)}$ the subgroup

$$S_t^{(k)} := \{\sigma \in S_{t+1} | \sigma(k) = k\},$$

and by $I_k : S_t \to S_t^{(k)}$ *the isomorphism induced by the injection*

$$\tilde{I}_k : \{1, \ldots, t\} \hookrightarrow \{1, \ldots, t+1\}, \quad \tilde{I}_k(i) = \begin{cases} i, & 1 \leqslant i < k, \\ i+1, & i \geqslant k. \end{cases}$$

Then for $\sigma = I_{k+1}(\tilde{\sigma})$ *and*

$$\hat{p}_{\tilde{\sigma}} = \sum_{\tilde{\gamma} \in S_t} c_{\tilde{\gamma}}\, \hat{q}_{\tilde{\gamma}\tilde{\sigma}},$$

we have

$$\hat{p}_\sigma = \sum_{\tilde{\gamma} \in S_t} c_{\tilde{\gamma}}\, \hat{q}_{I_k(\tilde{\gamma})\sigma}.$$

Proof: (i) For $\beta \in S_t^{(k)} \subset S_{t+1}$, that is $\beta = I_k(\tilde{\beta})$ with $\tilde{\beta} \in S_t$,

$$\hat{p}_\sigma(\beta\sigma) = N^{|I_k(\tilde{\beta}) \vee \sigma_+|} = N^{|I_k(\tilde{\beta}) \vee (I_{k+1}(\tilde{\sigma}))_+|} = N^{|I_k(\tilde{\beta}) \vee I_k(\tilde{\sigma}_+)|} = N^{|\tilde{\beta} \vee \tilde{\sigma}_+| + 1} = N \hat{p}_{\tilde{\sigma}}(\tilde{\beta}\tilde{\sigma})$$

and similarly

$$\hat{q}_{I_k(\tilde{\gamma})\sigma}(\beta\sigma) = N^{|I_k(\tilde{\gamma})(I_k(\tilde{\beta}))^{-1}|} = N^{|I_k(\tilde{\gamma}\tilde{\beta}^{-1})|} = N^{|\tilde{\gamma}\tilde{\beta}^{-1}| + 1} = N \hat{q}_{\tilde{\gamma}\tilde{\sigma}}(\tilde{\beta}\tilde{\sigma}).$$

(ii) The other elements of S_{t+1} can be uniquely written as a product of a transposition $(l,k) \in S_{t+1}$ and $\beta = I_k(\tilde{\beta}) \in S_t^{(k)}$. In that case a similar argument leads to

$$\hat{p}_\sigma(\beta\sigma) = \hat{p}_{\tilde{\sigma}}(\tilde{\beta}\tilde{\sigma}) \quad \text{and} \quad \hat{q}_{I_k(\tilde{\gamma})\sigma}(\beta\sigma) = \hat{q}_{\tilde{\gamma}\tilde{\sigma}}(\tilde{\beta}\tilde{\sigma}).$$

(iii) So in any case the proportionality factor does not depend on $\tilde{\gamma}$. □

Proposition 6.2: For all $t \leqslant N \in \mathbb{N}$,

$$\langle V_N, \hat{p}_\sigma \rangle = 0 \quad \textit{for } \sigma \in S_t \setminus D_t,\ \sigma \neq e. \tag{6.1}$$

Proof: Lemma 3.4 implies the formula

$$\langle V_N, \hat{q}_\sigma \rangle = \delta_e^\sigma.$$

So (6.1) is equivalent to show that for these σ in the base decomposition

$$\hat{p}_\sigma = \sum_{\gamma \in S_t} c_\gamma \hat{q}_{\gamma\sigma}$$

of $\hat{p}_\sigma$ the coefficient $c_{\sigma^{-1}}$ equals zero. These σ have a fixed point $k+1 \pmod t$ which has the additional property that $k \pmod t$ is *not* a fixed point. So $\sigma = I_{k+1}(\tilde{\sigma})$ with $\tilde{\sigma} \in S_{t-1}, \tilde{\sigma}(k) \neq k$. The base decomposition $\hat{p}_{\tilde{\sigma}} = \Sigma_{\tilde{\gamma} \in S_{t-1}}\, c_{\tilde{\gamma}} \hat{q}_{\tilde{\gamma}\tilde{\sigma}}$ leads to $\hat{p}_\sigma = \Sigma_{\tilde{\gamma} \in S_{t-1}}\, c_{\tilde{\gamma}} \hat{q}_{I_k(\tilde{\gamma})\sigma}$, see Propostion 6.1.

Thus if the $\tilde{\gamma} \in S_{t-1}$ term in (6.1) would be nonzero, it would be of the form $\langle V_N, \hat{p}_\sigma \rangle = c_{\tilde{\gamma}}$ for $\tilde{\gamma} \in S_{t-1}$ with $I_k(\tilde{\gamma}) = \sigma^{-1} = I_{k+1}(\tilde{\sigma}^{-1})$ or $I_{k+1}(\tilde{\sigma}) = I_k(\tilde{\gamma}^{-1})$. But this would imply $\tilde{\sigma}(k) = k$, contradicting the assumption. □

It is known that

$$|D_t| \sim \frac{|S_t|}{e} \quad \text{as} \quad t \to \infty.$$

So it could seem that we would only gain an unimportant factor $1/e$ by restricting the summation in (5.6) to the derangements (and the identity).

This is not so, since we can use the structure of the derangements under the τ action in our estimation.

For that purpose we now partition the derangements D_t by setting

$$D_t(k) := \{\sigma \in D_t \,|\, |\sigma \vee \sigma_+| = k \quad (k = 1, \ldots, t).$$

So $D_t(k) = \emptyset$ for $k > t/2$, and we estimate the cardinalities of these sets.

Proposition 6.3: There exists a $C_2 \geq 1$ such that for all $t \in \mathbb{N}$

$$|D_t(k)| \leq k C_2^k (t - k + 1)! \quad (k = 1, \ldots, \lfloor t/2 \rfloor).$$

Proof: Remark that the statement becomes trivial for $k = 1$ so that in the proof we assume $k \geq 2$.

(i) Each $\sigma \in D_t(k)$ induces a set partition

$$B(\sigma) \equiv B = (B_1, \ldots, B_k)$$

of $\{1, \ldots, t\}$ into the blocks of $\sigma \vee \sigma_+$ which is unique if you assume $|B_{l+1}| \geq |B_l|$ and $\min(B_l) \leq \min(B_{l+1})$ if $|B_{l+1}| = |B_l|$. As each B_l contains at least one cycle of σ (or rather the block corresponding to the cycle in the partition of σ), we have $|B_l| \geq 2$.

(ii) Next we consider the intersections

$$C_{l,m} := B_l \cap B_m^+ \quad (l, m \in \{1, \ldots, k\})$$

with the atoms $B_m^+ := \tau(B_m) = \{j + 1 \,|\, j \in B_m\}$ of the shifted set partition B^+. We thus get a set partition

$$C(\sigma) \equiv C = (C_{1,1}, \ldots, C_{k,k})$$

of $\{1, \ldots, t\}$ which is finer than B and B^+ but may contain empty atoms $C_{l,m}$. However, as σ is a derangement, we know that if $C_{l,m}(\sigma)$ is nonempty, it is a union of cycles of σ so that in any case $|C_{l,m}(\sigma)| \neq 1$.

(iii) We now estimate $|D_t(k)|$ by

$$|D_t(k)| \leq \sum_{b=(b_1,\ldots,b_k)} Y(b),$$

where $2 \leq b_1 \leq \cdots \leq b_k, \Sigma_{l=1}^k b_l = t$, and

$$Y(b) := |\{\sigma \in D_t \,|\, |B_l(\sigma)| = b_l, l = 1, \ldots, k\}.$$

(iv) This quantity, in turn is estimated by

$$Y(b) \leq \sum_{c=(c_{1,1},\ldots,c_{k,k})} X(c) \prod_{l,m=1}^{k} c_{l,m}!, \tag{6.2}$$

where now $c_{l,m} \in \{0, \ldots, b_l\} \setminus \{1\}$ with $\Sigma_{m=1}^k c_{l,m} = b_l$ and

$$X(c) = |\{B = (B_1, \ldots, B_k) \,||C_{l,m}| = c_{l,m}\}.$$

Here $\{B_1, \ldots, B_k\}$ is an arbitrary set partition of $\{1, \ldots, t\}$ with enumeration fixed by demanding $2 \leq |B_1| \leq \ldots \leq |B_k|$ and, again, $\min(B_l) \leq \min(B_{l+1})$ if $|B_l| = |B_{l+1}|$. Denoting as before by $C_{l,m}$ the intersection $B_l \cap B_m^+$ formula (6.2) follows by our above remark that all $\sigma \in D_t$ with $C_{l,m}(\sigma) = C_{l,m}$ have a cycle partition finer than $C = (C_{1,1}, \ldots, C_{k,k})$ and there are $c_{l,m}!$ ways to permute the set $C_{l,m}$.

We bound $X(c)$ by considering the directed multigraph $G = G(c)$ with vertex set $V := \{1, \ldots, k\}$ and $c_{l,m}$ unlabeled directed edges from vertex l to m. Then

$$X(c) \leqslant X_G(c), \tag{6.3}$$

where $X_G(c)$ is the number of closed Euler trails on G. This can be seen as follows:

(1) The length of any closed Euler trail equals $\Sigma_{l,m=1}^{k} c_{l,m} = t$.
(2) Any closed directed Euler trail on G (shortly called *trail* from now on) is uniquely characterized by the sequence $(v_1, \ldots, v_t)$ of vertices $v_j \in V$ it visits. This is due to our assumptions that the edges from l to m are unlabeled, and that the beginning of the closed trail is marked.
(3) A set partition $B = (B_1, \ldots, B_k)$ of $\{1, \ldots, t\}$ gives rise to a sequence $(v_1, \ldots, v_t)$ of vertices $v_i \in V$, where $v_i := j$ if $i \in B_j$. Using a t-periodic notation with $v_{t+1} = v_1$, we have

$$\left|\{i \in \{1, \ldots, t\} | (v_i, v_{i+1}) = (l,m)\}\right| = c_{l,m} \quad (l,m \in \{1, \ldots, k\}).$$

Thus B gives rise to a trail in $G(c)$ rooted at $v_1 \in V$.

It may be remarked that we have equality in (6.3) if the vertices of the directed multigraph $G(c)$ can be discerned by their outdegree, that is $b_1 < \cdots < b_k$. Then, given a Euler trail with sequence $(v_1, \ldots, v_t)$, we define the partition $(B_1, \ldots, B_k)$ by setting $B_j := \{i \in \{1, \ldots, t\} | v_i = j\}$.

(i) To get an upper bound on $X_G(c)$ we select a root vertex $j \in V$ and consider the Euler trails in $G(c)$ beginning at j. By the BEST formula their number equals

$$b_j^R T_j(c) \cdot \frac{\prod_{l=1}^{k} (b_l - 1)!}{\prod_{l,m=1}^{k} c_{l,m}!}, \tag{6.4}$$

where $T_j(c)$ is the number of directed spanning trees rooted at j. Equation (6.4) is derived from Theorem 13 in Chap. I of Ref. 9 by noting that, unlike here, Bollobas considers directed multigraphs with labeled edges. Here the *reduced out degree*

$$b_l^R := \sum_{m=1}^{k} c_{l,m}^R \text{ with } c_{l,m}^R := 1 \text{ if } c_{l,m} > 0 \text{ and } c_{l,m}^R := 0 \text{ otherwise}.$$

(ii) The number of directed spanning trees rooted at j equals the $(k-1) \times (k-1)$ minor of the $k \times k$ degree matrix,

$$\mathrm{diag}(b_1^R, \ldots, b_k^R) - (c_{l,m}^R)_{l,m=1}^{k}$$

obtained by deleting the jth row and the jth column. This number is known to be independent of j, and we call it $\Delta(c^R)$.
By this remark and (6.4),

$$X_G(c) \leqslant t\Delta(c^R) \frac{\prod_{l=1}^{k} (b_l - 1)!}{\prod_{l,m=1}^{k} c_{l,m}!}, \tag{6.5}$$

since $\Sigma_{j=1}^{k} b_j^R \leqslant \Sigma_{j=1}^{k} b_j = t$.
(iii) From (6.2) and (6.5) we obtain the estimate

$$Y(b) \leqslant t\prod_{l=1}^{k}(b_l-1)!\sum_{c=(c_{1,1},\ldots,c_{k,k})}\Delta(c^R). \tag{6.6}$$

A bound on $\Delta(c^R)$ only depending on the reduced out degrees $b_1^R,\ldots,b_k^R$ can be found in Ref. 14. We use it in the slightly weakened version,

$$\Delta(c^R) \leqslant \frac{1}{2}\prod_{l=1}^{k} b_l^R,$$

and thus get from (6.6)

$$Y(b) \leqslant \frac{t}{2}\prod_{l=1}^{k}[b_l^R(b_l-1)!]\cdot\sum_c 1. \tag{6.7}$$

(iv) The cardinality $\Sigma_c\,1$ of number partitions $c=(c_{1,1},\ldots,c_{k,k})$ compatible with the number partition $(b_1,\ldots,b_k)$ of t is calculated as follows:

$$\sum_c 1 = \prod_{l=1}^{k}\left|\left\{(c_{l,1},\ldots,c_{l,k})\,|\,c_{l,m}\neq 1 \text{ and}\sum_{m=1}^{k} c_{l,m}=b_l\right\}\right|.$$

But

$$\begin{aligned}
&\left|\left\{(c_{l,1},\ldots,c_{l,k})\,|\,c_{l,m}\neq 1 \text{ and}\sum_{m=1}^{k} c_{l,m}=b_l\right\}\right| \\
&\quad=\sum_{U\subseteq\{1,\ldots,k\}}\left|\left\{(c_{l,1},\ldots,c_{l,k})\,|\,c_{l,m}\geqslant 2 \text{ if } m\right.\right. \\
&\quad\left.\left.\in U \text{ and } c_{l,m}=0 \text{ otherwise}, \sum_{m\in U} c_{l,m}=b_l\right\}\right| \\
&\quad=\sum_{r=1}^{\min(k,\lfloor b_l/2\rfloor)}\sum_{|U|=r}\binom{b_l-r-1}{r-1} \\
&\quad=\sum_{r=1}^{\min(k,\lfloor b_l/2\rfloor)}\binom{b_l-r-1}{r-1}\binom{k}{r},
\end{aligned}$$

so that (6.7) reduces to

$$Y(b)\leqslant\frac{t}{2}\prod_{l=1}^{k}\left[b_l^R(b_l-1)!\sum_{r=1}^{\min(k,\lfloor b_l/2\rfloor)}\binom{b_l-r-1}{r-1}\binom{k}{r}\right]. \tag{6.8}$$

(v) We bound the sums appearing in (6.8), depending on the relative size of k and b_l. Remember our assumption $k\geqslant 2$.

We set $\hat{b}:=\lfloor b/2\rfloor$.

(1) For all $k,b\geqslant 2$ we have the estimate

$$\sum_{r=1}^{\min(k,\hat{b})}\binom{b-r-1}{r-1}\binom{k}{r}\leqslant\sum_{r=1}^{\min(k,b-1)}\binom{b-r-1}{r-1}\binom{k}{r}\leqslant\sum_{r=1}^{\min(k,b-1)}\binom{b-2}{r-1}\binom{k}{k-r}=\binom{k+b-2}{k-1}. \tag{6.9}$$

(2) For all $k\geqslant b\geqslant 2$ and $r\leqslant\hat{b}$ we use the inequality $\binom{k}{r}\leqslant\binom{k}{\hat{b}}\leqslant\binom{k}{\lfloor k/2\rfloor}$ to show

$$\sum_{r=1}^{\min(k,\hat{b})}\binom{b-r-1}{r-1}\binom{k}{r}\leqslant\left(\sum_{r=1}^{\hat{b}}\binom{b-r-1}{r-1}\right)\binom{k}{\hat{b}}=\frac{g^{b-1}-\left(\frac{-1}{g}\right)^{b-1}}{\sqrt{5}}\binom{k}{\hat{b}}\qquad(6.10)$$

with the golden mean $g:=(1+\sqrt{5})/2$, since the sum of the binomials equals the Fibonacci numbers.

(vi) The reduced out degree b_l^R is bounded by

$$b_l^R=\sum_{m=1}^{k}c_{l,m}^R\leqslant\min(k,\hat{b}_l)\leqslant\frac{2k\hat{b}_l}{k+\hat{b}_l}.\qquad(6.11)$$

Instead of summing (6.8) over the ensemble of $b=(b_1,\ldots,b_k)$ with $2\leqslant b_1\leqslant\cdots\leqslant b_k$ and $\Sigma_{l=1}^k b_l=t$, we shift the b_l by 2 and set for $\tilde{k}\leqslant k$,

$$Y_k(b_1,\ldots,b_{\tilde{k}};t):=\frac{t}{2}k^{k-\tilde{k}}\prod_{l=1}^{\tilde{k}}b_l^R(b_l+1)!\sum_{r=1}^{\min(k,\hat{b}_l)}\binom{b_l-r+1}{r-1}\binom{k}{r},$$

with $\hat{b}_l:=\lfloor b_l/2\rfloor+1$ and b_l^R is redefined as $\min(k,\hat{b}_l)$. Then for $b_l\geqslant 0$

$$Y_G(b_1+2,\ldots,b_k+2)\leqslant Y_k(b_1,\ldots,b_k;t)\qquad(6.12)$$

and our aim is to find a $C\geqslant 1$, independent of k and t, such that the recursion

$$\sum_{\substack{0\leqslant b_1\leqslant\cdots\leqslant b_{\tilde{k}+1}\\ \mathrm{P}_{l=1}^{\tilde{k}+1}b_l=t-2k}}(b_1,\ldots,b_{\tilde{k}+1};t)\leqslant C\sum_{\substack{0\leqslant b_1\leqslant\cdots\leqslant b_{\tilde{k}}\\ \mathrm{P}_{l=1}^{\tilde{k}}b_l=t-2k}}Y_k(b_1,\ldots,b_{\tilde{k}};t)\qquad(6.13)$$

in $\tilde{k}$ holds true. Assuming (6.13), we obtain from (6.12),

$$\sum_{\substack{2\leqslant b_1\leqslant\cdots\leqslant b_k\\ \mathrm{P}_{l=1}^{k}b_l=t}}Y_G(b_1,\ldots,b_k)\leqslant ke(ce)^{k-1}(t-k+1)!,$$

since

$$\begin{aligned}Y_k(t-2k;t)&\leqslant\frac{t}{2}k^{k-1}\min\left(k,\left\lfloor\frac{t}{2}-k\right\rfloor+1\right)(t-2k+1)!\binom{k+t-2k}{k-1}\\&=\frac{t}{2}\frac{k^k}{k!}\min\left(k\left\lfloor\frac{t}{2}-k\right\rfloor+1\right)(t-k)!\leqslant ke^k(t-k+1)!.\end{aligned}$$

Using (6.9) and (6.13) follows from the recursion

$$\begin{aligned}&\sum_{l=0}^{\hat{b}-1}\hat{l}(l+1)!\left(\sum_{r=1}^{\min(k,\hat{l})}\binom{l-r+1}{r-1}\binom{k}{r}\right)b\hat{}\,l(b-l+1)!\binom{k+b-l}{k-1}\\&\quad\leqslant C\cdot k(\hat{b})(b+1)!\binom{k+b}{k-1},\end{aligned}$$

with $\hat{l}=\lfloor l/2\rfloor+1$. This is equivalent to the claim

$$\sum_{l=0}^{\hat{b}-1} \hat{l}(l+1)! \left(\sum_{r=1}^{\min(k,\hat{l})} \binom{l-r+1}{r-1} \binom{k}{r} \right) b \hat{-} l \prod_{r=1}^{l} \frac{1}{k+b-r+1} \leqslant Ck\hat{b}. \tag{6.14}$$

Depending on the relative size of k and b, we estimate the lhs of (6.14) in two ways.

(i) Using (6.9), we get the uppper bound for the lhs of (6.14),

$$\sum_{l=0}^{\hat{b}-1} \hat{l}(l+1)! \binom{k+l}{k-1} b \hat{-} l \prod_{r=1}^{l} \frac{1}{k+b-r+1} = k \sum_{l=0}^{\hat{b}-1} \hat{l} b \hat{-} l \prod_{r=1}^{l} \frac{k+r}{k+b-r+1}. \tag{6.15}$$

We write the product in (6.15) in the form

$$\prod_{r=1}^{l} \frac{k+r}{k+b-r+1} = \exp\left(\sum_{r=1}^{l} g(r) \right) \quad \text{with} \quad g(r) := \ln\left(\frac{k+r}{k+b-r+1} \right).$$

For $r \leqslant l \leqslant b \hat{-} 1$ not only $g(r) \leqslant 0$ and $g(r) \geqslant g(r-1)$ but also (for all real such r)

$$g''(r) = \frac{1}{(k+b-r+1)^2} - \frac{1}{(k+r)^2} \leqslant 0.$$

So $\Sigma_{r=1}^{l} g(r) \leqslant lg[(1+l)/2] \leqslant lg(\hat{b}/2)$ or

$$\prod_{r=1}^{l} \frac{k+r}{k+b-r+1} \leqslant \lambda^l \quad \text{with} \quad \lambda := \frac{k+\frac{\hat{b}}{2}}{k+b-\frac{\hat{b}}{2}+1}. \tag{6.16}$$

For $k \leqslant b$ we have the uniform bound $\lambda \leqslant \frac{3}{4}$.
Inserting (6.16) in (6.15) and noting that $b \hat{-} l \leqslant \hat{b}$ and $\hat{l} \leqslant (l/2)+1$, we get (6.14) with

$$C := \sum_{l=0}^{\infty} \left(\frac{l}{2} + 1 \right) \left(\frac{3}{4} \right)^l = 10.$$

(ii) For $k \geqslant b$ we insert (6.10) in the lhs of (6.14) which is thus bounded by

$$\sum_{l=0}^{\hat{b}-1} \hat{l}(l+1)! \, g^l \binom{k}{\hat{l}-1} b \hat{-} l \prod_{r=1}^{l} \frac{1}{k+b-r+1} = \sum_{l=0}^{\hat{b}-1} \hat{l} b \hat{-} l g^l \binom{k}{\hat{l}-1} \prod_{r=1}^{l} \frac{r+1}{k+b-r+1}.$$

By an argument similar to the one leading to (6.16),

$$\begin{aligned}
\sum_{l=0}^{\hat{b}-1} \hat{l} b \hat{-} l g^l \binom{k}{\hat{l}-1} \prod_{r=1}^{l} \frac{r+1}{k+b-r+1} &= \sum_{l=0}^{\hat{b}-1} \hat{l}^2 b \hat{-} l \prod_{r=1}^{\lfloor l/2 \rfloor} \frac{g^2(r+\hat{l})}{(k+b-r+1)(k+b-r-\lfloor l/2 \rfloor+1)} \\
&\leqslant \sum_{l=0}^{\hat{b}-1} \hat{l}^2 b \hat{-} l \prod_{r=1}^{\lfloor l/2 \rfloor} \frac{g^2}{k+b-r+1} \leqslant \hat{b} \sum_{l=0}^{\hat{b}-1} \hat{l}^2 \left(\frac{g}{2} \right)^l \\
&\leqslant \hat{b} \sum_{l=0}^{\infty} \left(\frac{l^2}{4} + l + 1 \right) \left(\frac{g}{2} \right)^l \\
&= \frac{1}{4}(161 + 71\sqrt{5}) < 80,
\end{aligned}$$

assuming $k \geqslant 4$ and treating $k=2$ and $k=3$ separately. □

VII. THE ASYMPTOTIC ESTIMATE

Now we are ready to present our asymptotic result.

Theorem 7.1: *Under the assumption of Conjecture 5.8 the form factor K_N is approximated by the diagonal contribution in the following sense.*

For all $\varepsilon > 0$ uniformly in $t/N \in [\varepsilon, (e/C_2)(1-\varepsilon)]$

$$\left| K_N(t) - \frac{t}{N}\Delta_N^{\max}(t) \right| \to 0 \quad (N \to \infty).$$

Proof: As $K_N(t) = t/N$ for the t-values under consideration,

$$\Delta_N^{\max}(t) = \sum_{\sigma \in S_t} \langle V_N, \hat{p}_\sigma \rangle$$

[Eq. (5.6)], and $\langle V_N, \hat{p}_e \rangle = 1$ (Corollary 5.7), we need to show that

$$\sum_{\sigma \in S_t \setminus \{e\}} \langle V_N, \hat{p}_\sigma \rangle \to 0 \quad (N \to \infty).$$

Using Proposition 6.2 this amounts to show

$$\sum_{\sigma \in D_t} \langle V_N, \hat{p}_\sigma \rangle \to 0 \quad (N \to \infty),$$

which is implied by the asymptotic vanishing of

$$\sum_{k=1}^{\lfloor t/2 \rfloor} \sum_{\sigma \in D_t(k)} |\langle V_N, \hat{p}_\sigma \rangle| \leqslant C_1 \sum_{k=1}^{\lfloor t/2 \rfloor} k C_2^k (t-k+1)!\, N^{k-t},$$

using Conjecture 5.8 and Proposition 6.3. Under our assumptions for t/N,

$$\sum_{k=1}^{\lfloor t/2 \rfloor} k C_2^k (t-k+1)!\, N^{k-t} \leqslant tN \sum_{k=1}^{\lfloor t/2 \rfloor} C_2^k \left(\frac{t-k+1}{N^e} \right)^{t-k+1} \leqslant N^2 \sum_{k=1}^{\lfloor t/2 \rfloor} C_2^k \left(\frac{1-\varepsilon}{C_2} \right)^{t-k+1} \leqslant N^2 C_2^{-1} \sum_{k=1}^{\lfloor t/2 \rfloor} (1-\varepsilon)^{t-k+1}$$

$$\leqslant \frac{N^2}{C_2 \varepsilon} \cdot (1-\varepsilon)^{\lceil t/2 \rceil + 1} \leqslant \frac{N^2}{C_2 \varepsilon} (1-\varepsilon)^{\varepsilon N/2} \to 0,$$

proving the theorem.

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Description of noncommutative theories and matrix models by Wightman functions

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One of the main open problems of mathematical physics is to consistently quantize Yang–Mills gauge theory. If such a consistent quantization were to exist, it is reasonable to expect a "Wightman reconstruction theorem," by which a Hilbert space and quantum field operators are recovered from *n*-point functions. However, the original version of the Wightman theorem is not equipped to deal with gauge fields or fields taking values in a noncommutative space. This paper explores a generalization of the Wightman construction which allows the fundamental fields to take values in an arbitrary topological *-algebra. In particular, the construction applies to fields valued in a Lie algebra representation, of the type required by Yang–Mills theory. This appears to be the correct framework for a generalized reconstruction theorem amenable to modern quantum theories such as gauge theories and matrix models. We obtain the interesting result that a large class of quantum theories are expected to arise as limits of matrix models, which may be related to the well-known conjecture of Kazakov. Further, by considering deformations of the associative algebra structure in the noncommutative target space, we define certain one-parameter families of quantum field theories and conjecture a relationship with deformation quantization. © *2004 American Institute of Physics.*
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I. INTRODUCTION

The Wightman axioms were formulated by Gårding and Wightman in the early 1950s, but no nontrivial examples existed at that time, and consequently the axioms were not published until 1964,[1] at which time their publication had been motivated by the Haag–Ruelle scattering theory. The axioms are thoroughly discussed and many consequences are derived in the two excellent books (Refs. 2 and 3). We will also formulate the axioms below in Sec. I B by way of introduction.

It is known that the Wightman axioms, in their original and unmodified form, describe only a small subset of the mathematical models used in elementary particle physics. Thus, many authors have considered modifications of the axioms which allow newer and more exotic physical theories to be formulated as rigorous mathematics. If we wish to perturb the axioms slightly, one obvious change with clear-cut physical implications is to relax the requirement that the test function space be $\mathcal{S}(\mathbb{R}^4)$. A large class of alternative test function spaces which still allow a formulation of the microscopic causality condition were proposed and developed by Jaffe.[4] The results of the present paper are a more radical modification, in which the test functions in $\mathcal{S}(\mathbb{R}^4)$ are replaced by functions into a noncommuting *-algebra.

There are at least two types of equivalent reformulations of the Wightman axioms. One is due to Wightman, who wrote down a set of conditions governing a sequence of tempered distributions

$$\mathcal{W}_n \in \mathcal{S}(\mathbb{R}^{4n}), \quad n = 0, 1, \ldots,$$

and proved that, under these conditions, the distributions $\mathcal{W}_n$ arise as vacuum expectation values of a unique quantum field theory satisfying the Wightman axioms, and conversely that the postulates hold in any Wightman field theory. This is what is known as the *Wightman reconstruction*

theorem, and first appeared in the seminal paper.[5] The part of this construction relevant to representation theory is known in functional analysis as the *GNS construction*. A second reformulation in terms of the Schwinger functions, not directly used in the present work, was given by Osterwalder and Schrader.[6]

Borchers reformulated Wightman's reconstruction theorem in several important papers,[7,8] with the result that a scalar boson quantum field theory is known to be characterized by a topological *-algebra A (with unit element 1_A) and a continuous positive form ω on A, satisfying

$$\omega(aa^*) \geqslant 0, \quad \omega(1_A) = 1, \quad a \in A. \tag{1}$$

A functional satisfying (1) is called a state.

Realistic models are generally described by tensor algebras, and the action of the state ω is computed from vacuum expectation values of products of fields. Although there is reason to believe the framework of states on tensor algebras could apply in general to a large class of quantum field theories, previous formulations of the Wightman reconstruction theorem have focused on scalar boson quantum field theories.

The Borchers formulation has proven very useful for analysis of bosonic field theory on a nontrivial manifold. Consider ω a state on the Borchers algebra built from test functions on a manifold M, and let ϕ_ω be the corresponding field. If ϕ_ω satisfies the Klein–Gordon equation and

$$[\phi_\omega(f), \phi_\omega(g)] = E(f \otimes g),$$

where E is the difference between the fundamental solutions of the Klein–Gordon operator, one calls ω a *state of the Klein–Gordon field over M*. It turns out that only certain states, called *Hadamard states*, are compatible with the semiclassical Einstein equation. For further details, we refer the reader to Ref. 9 and the monograph.[10]

There are by now many known examples of a low-energy limit or compactification of string theory which are equivalent to a gauge theory with compact gauge group. It is also known that exact quantum string amplitudes can be computed from various flavors of matrix models. If a mathematically rigorous description using constructive field theory is possible for these problems coming from string theory, then a consistent generalization of the Wightman reconstruction theorem which incorporates the structure of gauge theory and matrix models seems a useful framework in which to formulate the result.

The purpose of the present paper is to extend the work of Wightman and Borchers to include matrix-valued fields of the type required by gauge theory and matrix models. We first develop the mathematics, and then make contact with physical applications. The remainder of this introduction reviews the well-known Wightman procedure for commuting scalar fields; this serves to fix notation and set the context for the later sections. Section II presents the main new idea of the paper, a generalization of the Borchers construction, and considers some simple examples. Section III is concerned with the application of these ideas to two-dimensional Yang–Mills theory. In Sec. IV we recall important recent work which applies matrix models to high energy physics and then show that, in the same sense in which scalar quantum field theories are Wightman states, matrix models are described by *finite order states*, and thus are special cases of the construction in Sec. II. Moreover, finite order states form a dense subset of the space of all states, and hence arbitrary field theories are given as limits of matrix models. The conclusion is that traditional constructive quantum field theory, gauge theories, matrix models and certain hypothetical generalizations of these may all be described within a unified algebraic framework.

A. The Borchers construction

Let $\mathcal{S}(\mathbb{R}^d)$ denote the set of infinitely differentiable complex functions $f(x)$ on $\mathbb{R}^d$ for which

$$\|f\|_{\alpha,\beta} \equiv \sup_{x \in \mathbb{R}^d} |x^\alpha D^\beta f(x)| < \infty \quad \text{for all } \alpha, \beta,$$

where D^β is the usual multi-index derivative. Let us also define the spaces

$$\mathcal{S}_0 = \mathbb{C}, \quad \mathcal{S}_n = \mathcal{S}(\mathbb{R}^{dn}), \quad \text{and } \underline{\mathcal{S}} = \bigoplus_{n=0}^{\infty} \mathcal{S}_n.$$

The latter is a complete nuclear space under the direct sum topology. There is a natural map $\iota: \otimes^k \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^{kn})$ given by $\iota(f_1 \otimes \cdots \otimes f_k) = \Pi_{j=1}^k f_j(x_j)$, where each $x_j \in \mathbb{R}^d$, and the image of ι is dense.

Endow $\underline{\mathcal{S}}$ with the noncommutative multiplication

$$(f \times g)_l = \sum_{i+h=l} f_i \times g_h,$$

$$f_i \times g_h(x_1, \ldots, x_{i+h}) = f_i(x_1, \ldots, x_i) g_h(x_{i+1}, \ldots, x_{i+h}), \tag{2}$$

and the involution $f^* = (f_0^*, f_1^*, \ldots)$, where $f_0^* = \overline{f_0}$ and for $i \geqslant 1$,

$$f_i^*(x_1, \ldots, x_i) = \overline{f_i(x_i, x_{i-1}, \ldots, x_1)}. \tag{3}$$

The multiplication $\times$ and the unit $\mathbf{1} = (1, 0, 0, \ldots)$ make $\underline{\mathcal{S}}$ into a unital *-algebra with no zero divisors. The center of $\underline{\mathcal{S}}$ is $\{\lambda \mathbf{1} : \lambda \in \mathbb{C}\}$, $\mathbf{1}$ is the only nonzero idempotent, and the set of invertible elements equals the center. This implies the triviality of the radical

$$\text{rad}(\underline{\mathcal{S}}) = \{g \in \underline{\mathcal{S}} : 1 + f \times g \text{ has inverse } \forall\, f\}.$$

An element $g \in \underline{\mathcal{S}}$ is called *positive* if $\exists f_i$ such that $g = \Sigma_i f_i^* \times f_i$. This induces a positive cone $\underline{\mathcal{S}}^+$ and a semiordering. We define the set of Hermitian elements,

$$\underline{\mathcal{S}}_h = \{f \in \underline{\mathcal{S}} : f^* = f\}, \tag{4}$$

which is a real vector space and we have $\underline{\mathcal{S}} = \underline{\mathcal{S}}_h + i\underline{\mathcal{S}}_h$. Also, $\underline{\mathcal{S}}^+$ is a convex cone with $\underline{\mathcal{S}}^+ \cap (-\underline{\mathcal{S}}^+) = \{0\}$. Moreover, we have $\underline{\mathcal{S}}_h = \underline{\mathcal{S}}^+ - \underline{\mathcal{S}}^+$, which follows by polarization.

B. The Wightman axioms

Let $\mathcal{S}$ denote an appropriate space of test functions, often taken to be $\mathcal{S}(\mathbb{R}^d)$.

Axiom 1: There exists a Hilbert space $\mathcal{H}$ and a dense domain $D \subset \mathcal{H}$ such that for every $f \in \mathcal{S}$, an operator $\varphi(f)$ exists, such that $D \subset \text{dom}(\varphi(f))$, $\varphi(f)D \subset D$,

$$(\psi, \varphi(f)\chi) = (\varphi(\overline{f})\psi, \chi) \quad \textit{for all } \psi, \chi \in D$$

and $f \to (\psi, \varphi(f)\chi)$ is a continuous linear functional on $\mathcal{S}$.

Axiom 2: Let $f_a(x) = f(x-a)$. There exists a strongly continuous unitary representation $\mathcal{U}$ of the translation group $\mathcal{G}$, such that for all $a \in \mathcal{G}$, $U(a)D \subset D$ and

$$\mathcal{U}(a)\varphi(f)\mathcal{U}^{-1}(a)\psi = \varphi(f_a)\psi$$

for all $f \in \mathcal{S}, \psi \in D$.

In standard constructive quantum field theory models, there is a canonical action of the proper orthochronous Poincaré group $P_+^\uparrow$ on $\mathcal{S}_n$ for all n, in other words, a representation $\alpha: P_+^\uparrow \to \text{Aut}(\underline{\mathcal{S}})$. We mention the representation α because even in the generalized models to be introduced in Sec. II, invariance under a symmetry group is expressed in terms of representations similar to α. See also Sec. II C.

Axiom 3: There exists $\Omega \in D$ such that $\mathcal{U}(a)\Omega = \Omega$ for all $a \in \mathcal{G}$, and the set of vectors of the form $\{\Omega, \varphi(f)\Omega, \varphi(f_1)\varphi(f_2)\Omega, \ldots\}$ spans $\mathcal{H}$.

Further Wightman axioms will be discussed in Sec. I G.

C. States, the GNS construction, and axiom 1

Let $\underline{\mathcal{S}}'$ be the space of continuous linear functionals $T:\underline{\mathcal{S}}\to\mathbb{C}$. For $f\in\underline{\mathcal{S}}$, denote the action of T by (T,f). The space $\underline{\mathcal{S}}'$ also has a natural involution; define T^* by

$$(T^*,f):=\overline{(T,f^*)}.$$

We say a functional is *real* if $T=T^*$, and *positive* if $(T,p)\geqslant 0$ for all $p\in\underline{\mathcal{S}}^+$. The corresponding spaces are denoted $\underline{\mathcal{S}}'_h$ and $\underline{\mathcal{S}}'^+$.

The *set of states* is

$$E(\underline{\mathcal{S}})=\{T\in\underline{\mathcal{S}}'^+:(T,1)=1\}.$$

The *left-kernel* of a state T is defined to be

$$L(T):=\{f\in\underline{\mathcal{S}}:(T,f^*\times f)=0\}. \tag{5}$$

The left-kernel is so named because it is a left ideal in the Borchers algebra. The *right-kernel* $R(T)$, defined by the analogous relation $(T,f\times f^*)=0$, is a right ideal. These kernels arise in the quantization procedure discussed later; choice of the left-kernel amounts to the convention that a sesquilinear form is conjugate-linear in the first variable.

Theorem 1: *Each state $T\in E(\underline{\mathcal{S}})$ canonically defines a representation A_T of $\underline{\mathcal{S}}$ in a Hilbert space $\mathcal{H}_T$ such that the restriction $A_T|_{\mathcal{S}_1}$ satisfies axiom 1. Conversely, if $\{\phi(f)\}$ are a set of fields satisfying axiom 1, then every $\Omega\in D$ defines a continuous linear functional T_Ω, by*

$$(T_\Omega,f_1\times f_2\times\cdots\times f_n)=(\Omega,\phi(f_1)\phi(f_2)\cdots\phi(f_n)\Omega),\quad f_i\in\mathcal{S}_1.$$

If $\|\Omega\|=1$, then T_Ω is a state. The field A_{T_Ω} is unitarily equivalent to $\{A_\Omega,D_\Omega,\mathcal{H}_\Omega\}$ where

$$D_\Omega=\text{Linear Span of }\Omega,\ \phi(f)\Omega,\ \phi(f_1)\phi(f_2)\Omega,\ \text{etc.},$$

$\mathcal{H}_\Omega$ is the closure of D_Ω, and $A_\Omega(f)=\phi(f)|_{D_\Omega}$.

Proof: As a full proof can be found elsewhere,[2,7] we merely recall the central idea for convenience, as it is used later. T defines a nondegenerate positive definite sesquilinear form on $\underline{\mathcal{S}}/L(T)$ by the relation

$$([f],[g])=(T,f^*\times g),[f],[g]\in\underline{\mathcal{S}}/L(T).$$

Define $\mathcal{H}_T$ to be the completion of the pre-Hilbert space $\underline{\mathcal{S}}/L(T)$, and define a representation of $\underline{\mathcal{S}}$ on $\mathcal{H}_T$ by $A_T(f)[g]=[f\times g]$ for $f\in\mathcal{S}_1$ and $g\in\underline{\mathcal{S}}$. The rest of the proof is straightforward. □

D. Translation invariant states satisfy axioms 1–3

Let $a\in\mathbb{R}^d$. The map α_a defined by

$$\alpha_a f_i(x_1,\ldots,x_i)=f_i(x_1-a,\ldots,x_i-a)$$

is an element of $\mathrm{Aut}(\underline{\mathcal{S}})$. A state T is *translation-invariant* if $(T,\alpha_a f)=(T,f)$ holds for all $f\in\underline{\mathcal{S}}$, and for all $a\in\mathbb{R}^d$.

Theorem 2: *Let T be a translation invariant state. Then $A_T(f)$ satisfies axioms* 1–3. *Conversely, if the system $\{A(f),D,\Omega\in D\}$ satisfies axioms* 1–3, *then T_Ω defined by $(T_\Omega,f)=(\Omega,A(f)\Omega)$ is translation invariant.*

E. Tensor products of states

Given two states $T_1,T_2\in E(\underline{\mathcal{S}})$, let $\{A_i(f),\mathcal{H}_i,D_i,\Omega_i\}$ be the associated GNS representations. Then the triple

$$\{A_1(f)\otimes I_2 + I_1\otimes A_2(f), \mathcal{H}_1\otimes\mathcal{H}_2, D_1\times D_2\}$$

satisfies axiom 1, and hence it corresponds to a new state, $T_1\otimes_s T_2$ which is the same as the vector state T_Ω with $\Omega=\Omega_1\times\Omega_2$. Let $P_{n,m}$ denote the set of all ordered splittings of $n+m$ elements into two subsets, of respective sizes n and m. Let $T_n\in\underline{\mathcal{S}}'_n$, $S_m\in\underline{\mathcal{S}}'_m$, then $T_n\otimes_\jmath S_m$ is given by

$$(T_n\otimes_\jmath S_m)(x_1,\ldots,x_{n+m}) = \sum_{P_{n,m}} T_n(x_{i_1},\ldots,x_{i_n})S_m(x_{j_1},\ldots,x_{j_m}).$$

For $T,S\in\underline{\mathcal{S}}'$, we define $(T\otimes_\jmath S)_n=\Sigma_{i+k=n}\ T_i\otimes_\jmath S_k$. This coincides with our previous definition of the $\otimes_\jmath$-product. It is clearly associative and Abelian.

F. Real scalar fields

Before discussing more complicated generalizations, we briefly indicate how the above construction can describe the salient properties of the quantum theory of a one-component real scalar field. Since $\otimes^k\mathcal{S}(\mathbb{R}^n)$ is dense in $\mathcal{S}(\mathbb{R}^{kn})$, every continuous form on the subspace has a unique continuous extension. By the classic Schwartz nuclear theorem, if $B(f_1,\ldots,f_k)$ is a separately continuous k-linear functional on $\mathcal{S}(\mathbb{R}^{n_1})\times\cdots\times\mathcal{S}(\mathbb{R}^{n_k})$, there exists $T\in\mathcal{S}'(\mathbb{R}^N)$ with

$$B(f_1,\ldots,f_k) = T(f_1\otimes\cdots\otimes f_k),$$

where $N=\Sigma_i\, n_i$. As a consequence, every state ω on the Borchers algebra is represented by a family of distributions $W_n\in\mathcal{S}'(\mathbb{R}^{dn})$, in the sense that

$$\omega(f_1\times\cdots\times f_n) = \int W_n(x_1,\ldots,x_n)f_1(x_1)\cdots f_n(x_n)\mathrm{d}^dx_1\cdots\mathrm{d}^dx_n. \tag{6}$$

A rigorous proof is known that a scalar quantum field theory, when it exists, is completely determined by its Wightman functions. By relation (6), a state ω on the Borchers algebra contains the same information as a complete specification of the n-point functions for all values of n. If ω obeys the Wightman axioms, then we have a quantum field theory and W_n are related to vacuum expectation values of products of fields. They calculate observable quantities such as cross sections and decay rates.

G. Spectral condition, locality, and uniqueness of the vacuum

The remaining two essential properties of a quantum field theory (spectral condition and locality) are equivalent to ker ω containing certain ideals. Let $\mathcal{S}_1(CV^+)$ denote the set of functions in $\mathcal{S}_1$ that vanish on the forward light cone V^+, and let $\mathcal{F}$ denote the Fourier transform. The spectral condition is the statement that ker $\omega\supset I_1$, where

$$I_1 = \left\{\int \mathrm{d}^daF(a)\alpha_a f : f\in\underline{\mathcal{S}}, f_0=0, F(a)\in\mathcal{F}[\mathcal{S}_1(CV^+)]\right\}.$$

Space–time locality is the statement that ker $\omega\supset I_2$, where I_2 is the smallest closed two-sided ideal in $\underline{\mathcal{S}}$ containing all elements of the form $f\times g-g\times f$ where f and g have spacelike-separated supports.

Uniqueness of the vacuum also has a simple interpretation in terms of Wightman functionals. A field theory is said to be *reducible* if the algebra of field operators acts reducibly on the Hilbert space. A Wightman state ω is said to be *decomposable* if there exists a positive number $\lambda<1$ such that

$$\omega = \lambda\omega^{(1)} + (1-\lambda)\omega^{(2)} \tag{7}$$

with Wightman states $\omega^{(1)}$ and $\omega^{(2)}$ different from ω. Indecomposability of the Wightman functional is equivalent to uniqueness of the vacuum in an irreducible field theory.

In Sec. II we will generalize the Wightman state ω, and it is of interest to know whether (7) also leads to uniqueness of the vacuum in the general case.

II. NONCOMMUTATIVE TARGET SPACE PERSPECTIVE

The field algebra with multiplication and involution given by (2)–(3) admits a natural generalization to the noncommutative setting. This generalization has many applications in physics, all of which come from interpreting elements of the Borchers algebra as gauge fields on a d-dimensional space–time. For $d \leqslant 1$, this gives rise to matrix models and matrix quantum mechanics. For $d \geqslant 2$, it is Yang–Mills theory. Of course, gauge symmetry is not essential for the construction to work; it applies equally well to matrix-valued scalar field theory of the type considered by Kazakov.[11] This framework is also suggestive of quantum field theory in which the target manifold is a noncommutative space in the sense of Connes.

A. Test functions valued in a noncommutative algebra

First we wish to argue that a correct description of gauge quantum field theory is possible in terms of test functions valued in a noncommutative algebra. Consider a pure gauge theory with gauge group G and Lie algebra $\mathfrak{g}=\mathrm{Lie}(G)$. In a classical pure gauge theory, the fundamental fields are $\mathfrak{g}$-valued one-forms, each determining a connection on a principal G-bundle. In a quantum version of the same gauge theory, these classical fields would be promoted to operator-valued distributions with the same algebraic structure.

For concreteness, let $\mathcal{S}(\mathbb{R}^4)$ denote the Schwartz space of rapidly decreasing functions on $\mathbb{R}^4$. An operator-valued distribution is a continuous map

$$\mathcal{S}(\mathbb{R}^4) \to \mathrm{Op}(\mathcal{H}),$$

where we consider $\mathcal{S}(\mathbb{R}^4)$ to be endowed with the Schwartz topology, $\mathcal{H}$ is a Hilbert space, and $\mathrm{Op}(\mathcal{H})$ denotes a suitable space of unbounded operators on $\mathcal{H}$. In the example of a free real scalar boson, $\mathcal{H}$ is the usual bosonic Fock space, and $\mathrm{Op}(\mathcal{H})$ would be a class of operators large enough to include all operators of the form $\phi(f)$, where ϕ is a quantum field and f is any test function. The operators $\mathrm{Op}(\mathcal{H})$, in this example, have a common core including all smooth, compactly supported Fock states with finite particle number.

Let $\rho:\mathfrak{g}\to\mathfrak{g}l(V)$ be a representation of $\mathfrak{g}$ on the representation space V. Let $\mathcal{H}^V$ denote the space of all continuous linear functionals

$$\phi:\mathcal{S}(\mathbb{R}^4) \to \mathrm{Op}(\mathcal{H}) \otimes V. \tag{8}$$

Elements of $\mathcal{H}^V$ are operator-valued distributions that transform in the representation V. The representation ρ on V naturally defines a representation $\overline{\rho}$ of $\mathfrak{g}$ on $\mathcal{H}^V$ by expanding

$$\phi(f) = \sum_{i=1}^{n} A_i^f \otimes v_i^f$$

for $A_i^f \in \mathrm{Op}(\mathcal{H}), v_i^f \in V$, and defining

$$(\overline{\rho}(g)\phi)(f) = \sum_i A_i^f \otimes (\rho(g)v_i^f), \quad g \in \mathfrak{g}.$$

One very useful choice for V is the adjoint representation, because field strength variables $F_{\mu\nu}(x)$ in Yang–-Mills theory transform in the adjoint. Other representations typically arise as direct summands of tensor powers of the adjoint and its complex conjugate representation. In all of these examples, it is useful to view the representation space V as living in some matrix algebra.

There is a natural transformation of categories by which the space $\mathcal{H}^V$ defined above is naturally isomorphic to the space $\mathcal{H}_{V^*}$ of continuous maps

$$\mathcal{S}(\mathbb{R}^4) \otimes V^* \to \mathrm{Op}(\mathcal{H}). \tag{9}$$

Let us exhibit the isomorphism between (8) and (9) explicitly. For concreteness, we will fix our attention on the special case of $V=\mathfrak{g}$, the adjoint, but we stress that no part of the discussion depends on this in an essential way.

In terms of ϕ we may define a new map

$$\tilde{\phi}:\mathcal{S}(\mathbb{R}^4) \times \mathfrak{g}^* \to \mathrm{Op}(\mathcal{H}) \tag{10}$$

by the formula

$$\tilde{\phi}(f,y) \equiv \sum_{i=1}^{n} y(v_i^f) A_i^f, \quad y \in \mathfrak{g}^*. \tag{11}$$

Equivalently, if T^a is a basis for $\mathfrak{g}$, and $\phi(f)=\phi(f)_a T^a$, then for $y \in \mathfrak{g}^*$, $\tilde{\phi}(f,y^a)=\phi(f)_a y^a$.

The map $\tilde{\phi}$ is multilinear, and therefore factors through to a map on the tensor product $\mathcal{S}(\mathbb{R}^4)\otimes\mathfrak{g}^*$. We have proved that $\phi \to \tilde{\phi}$ gives an explicit isomorphism $\mathcal{H}^V \cong \mathcal{H}_{V^*}$ between the two spaces (8) and (9).

Quantum field theory with test functions taking values in $\mathfrak{g}^*$ is most naturally described by a noncommutative version of the Borchers construction, and the latter mathematical structure will occupy us for the rest of this section and, in some form or other, for the rest of the paper. We summarize the results of the preceding paragraphs in a lemma.

Lemma 1: The following structures are equivalent.

(1) *An operator-valued distribution which transforms in the adjoint representation of a Lie algebra* $\mathfrak{g}$ *(i.e., a quantized Yang–Mills field).*
(2) *An operator-valued distribution which acts on* $\mathfrak{g}^*$*-valued test functions*.

Let us see how this isomorphism works in practice. Suppose that $F_{\mu\nu}(x)$ is an operator-valued distribution which transforms as a Lie algebra-valued two-form. An example of such an object is a quantized Yang–Mills field strength. The above construction tells us that from $F_{\mu\nu}(x)$, we can construct a single operator-valued distribution $\tilde{F}_{\mu\nu}$ which acts on test functions $f(x)$ valued in the dual of the Lie algebra. The duality between $\mathfrak{g}$ and $\mathfrak{g}^*$ is given explicitly by the Killing form $K(a,b)=\mathrm{tr}(ab)$, where the trace is taken in the adjoint representation. Therefore, the correct definition is

$$\tilde{F}_{\mu\nu}(f) = \mathrm{tr}(f \cdot F_{\mu\nu}) = \int K(f(x),F_{\mu\nu}(x))\ \mathrm{d}x, \tag{12}$$

where $f\cdot F_{\mu\nu}$ is defined by

$$[f \cdot F_{\mu\nu}]_{ij} \equiv \sum_k \int f(x)_{ik} (F_{\mu\nu}(x))_{kj}\ \mathrm{d}x.$$

The notation of (12) is the same as (10). This shows explicitly how operator-valued distributions act on $\mathfrak{g}^*$-valued test functions.

Remark 1: This duality transformation transfers the dependence on the Lie algebra to the test functions; however, if the original field also transforms as a section of an additional vector bundle E, as is the case for the two-form $F_{\mu\nu}(x)$ which is a section of $E=\wedge^2(\mathbb{R}^d)$, the quantized field operator (12) transforms in the tensor product $E\otimes\mathcal{O}_{\mathcal{H}}$, where $\mathcal{O}_{\mathcal{H}}$ is a trivial bundle with fiber $\mathrm{Op}(\mathcal{H})$. Additional complications to the theory presented above arise in the case of a nontrivial fiber bundle, in which the connection can be only locally described as a $\mathfrak{g}$-valued one-form. The gauge fields in the present paper are all assumed to be sections of globally trivial principal bundles.

Remark 2: One could imagine exotic quantum field theories in which the fields take values in

the algebra of functions over a noncommutative geometry in the sense of Connes. The present constructions define such a theory mathematically, but we do not know a direct physical interpretation.

For any manifold Σ, let

$$\mathcal{A} = \mathcal{A}(\Sigma, \mathcal{B}) \tag{13}$$

denote a vector space of test functions from Σ to a possibly noncommutative star-algebra $\mathcal{B}$ with product $\cdot$. For the quantum theories we construct, elements of $\mathcal{A}$ will play the role of test functions. Invariance of the Schwartz space under the Fourier transform implies that tempered distributions can grow at most polynomially in momentum space. Thus, the choice of the test function space has important physical consequences.

If $\mathcal{B}$ is a normed algebra and Σ is equipped with an appropriate metric, then we may consider $\mathcal{A}(\Sigma, \mathcal{B})$ to be the Schwartz space of rapidly decreasing functions. For example, one could consider a space–time which has nontrivial topology within some compact region K, and outside that region it is covered by a single chart c which is an isometry onto $\mathbb{R}^d$ minus a compact set. On such a space–time, one can demand that the $\mathfrak{B}$-norm of the function and of all its derivatives, expressed in chart c, fall off faster than any power of the *modulus function*, which measures the distance of a point from K in the ambient metric.

Alternatively, if Σ is any manifold, one can obtain the necessary analytic regularity by consideration of continuous functions with compact support. For manifolds there is the additional complication that one should integrate *densities* rather than functions, and so the test function space should properly be $C_0^\infty(\Sigma, \Omega^1)$, the space of smooth compactly supported sections of the line bundle Ω^1 of densities of order one. In this generalized situation, the terminology *test density* is more appropriate. In what follows, we will generally assume the existence of a Riemannian metric, under which conditions a function on Σ determines a density. The constructions which follow are already interesting for $\Sigma = \mathbb{R}^d$. In the application of these ideas to two-dimensional gauge theory, Σ will denote a compact Riemann surface.

Since certain gauge theories are known to possess ultraviolet behavior which is more singular than that of, say, scalar theory in $d = 2, 3$, it is of importance to recall a construction of Jaffe.[4] Given a function $g(t), t \in \mathbb{R}$, such that $g(t^2)$ is entire and positive, Jaffe defines $\tilde{S}_g$ to be the space of all functions on $\mathbb{R}^d$ which are infinitely differentiable and for which all the norms

$$\|f(p)\|_n = \sup_{p;|\alpha|\leqslant n} g(n\|p\|^2)|D^\alpha f(p)|, \quad n = 1, 2, \ldots, \tag{14}$$

are finite. Here α is a multi-index, and $\|p\|$ is an arbitrary Euclidean norm on $\mathbb{R}^d$. Finiteness of the norms (14) means that test functions and all its derivatives decay at infinity faster than $1/g(n\|p\|^2)$ for any positive n. $\tilde{S}_g$ does not depend on the choice of the Euclidean norm, but it does depend on the rate of growth of $g(t^2)$ at infinity. Define the topology on $\tilde{S}_g$ to be that generated by the countable family of norms (14). It is easy to see that $\tilde{S}_g$ is Lorenz invariant. In addition, if g satisfies

$$\frac{g(n\|p\|^2)}{g(n'\|p\|^2)} \quad \textit{is an integrable function for all } n \textit{ and sufficiently large } n', \tag{15}$$

then the nuclear theorem holds.

Let us denote the Fourier transform of $\tilde{S}_g$ by S_g. We think of $\tilde{S}_g$ as the space of test functions in momentum space, so S_g is the space of test functions in x space. The spaces S_g can be used to define quantum field theories whose ultraviolet behavior is more singular than the traditional Wightman field theories; see Ref. 4 for further details.

For our purposes, the important point is that for test functions valued in a normed star-algebra $\mathcal{B}$, a completely analogous construction exists. We modify (14) so that the complex modulus

$|D^\alpha f(p)|$ is replaced by the $\mathcal{B}$-norm of the same expression, $\|D^\alpha f(p)\|_{\mathcal{B}}$. This defines test function spaces $\widetilde{S}_g{}^{\mathcal{B}}$ which can be used in the constructions which follow, and may be important for theories which are singular in the UV.

B. Generalizing the Borchers construction

We assume for convenience that the base field of $\mathcal{B}$ is $F=\mathbb{R}$ or $\mathbb{C}$. $\mathcal{A}$ is then naturally a left and right module over $\mathcal{B}$, and of course also over F. Define

$$\mathcal{A}_n = \mathcal{A}^{\otimes n}, \quad \underline{\mathcal{A}} = \mathbb{C} \oplus \overset{\infty}{\underset{n=1}{\oplus}} \mathcal{A}_n \tag{16}$$

to be the free tensor algebra over $\mathcal{A}$. Note that

$$\mathcal{A}_n \cong \mathcal{A}(\Sigma^n, \mathcal{B}^{\otimes n}), \tag{17}$$

an isomorphism of complete topological vector spaces, where Σ^n denotes the n-fold Cartesian product. As $\mathcal{B}$ is defined to be an involutive algebra, we denote the involution by

$$\tau_*: \mathcal{B} \to \mathcal{B}.$$

This extends to give an involution on $\mathcal{A}_n$, defined by

$$f^*(x_1, \ldots, x_n) := \tau_*^{\otimes n} f(x_n, \ldots, x_1). \tag{18}$$

Also define a binary operation $\times$ on $\underline{\mathcal{A}}$ as follows:

$$(\underline{f} \times \underline{g})_n = \sum_{i+j=n} f_i \otimes g_j, \quad \underline{f} = (f_0, f_1, \ldots), \quad \underline{g} = (g_0, g_1, \ldots) \in \underline{\mathcal{A}}. \tag{19}$$

The operations (18) and (19) give $\underline{\mathcal{A}}$ the structure of a unital involutive algebra, with unit given by $\mathbf{1}=(1,0,0,\ldots)$. In analogy with the case for scalar fields, $\underline{\mathcal{A}}$ also has a cone $\underline{\mathcal{A}}^+$ of positive elements, and a subset $\underline{\mathcal{A}}_h$ of Hermitian elements.

One could imagine an analogous construction in which the tensor product in (19) is replaced with multiplication in $\mathcal{B}$. In such a framework, $\mathcal{A}_n$ would be replaced by $\mathcal{A}(\Sigma^n, \mathcal{B})$, in contrast with (17). Interestingly, *this modification is incompatible with the cluster property* for a large class of gauge theories, including all $O(N)$ gauge theories with $N \geqslant 4$. In fact, replacement of the tensor product (19) with the $\mathcal{B}$-multiplication leads to a number of problems, all of which render the theory unphysical. So when considering the Wightman construction for gauge theories, it is *essential* to use the tensor product in (19) rather than the matrix product. (The author would like to thank H. Gottschalk for explaining this crucial point.)

The cross product provides a mapping from the state space $E(\underline{\mathcal{A}})$ to the bilinear forms that arise in quantum physics. Explicitly, any state ω on $\underline{\mathcal{A}}$ determines a sesquilinear from $\langle , \rangle_\omega$ by the relation

$$\langle f, g \rangle_\omega = \omega(f^* \times g), \quad f, g \in \underline{\mathcal{A}} \tag{20}$$

and the sesquilinear forms (20) are of the type that arise in the construction of the Fock–Hilbert space for a quantum field theory. The left-kernel $L(\omega)$ of the state ω is precisely the set of all $f \in \underline{\mathcal{A}}$ such that $\langle f, f \rangle_\omega = 0$, and so the sesquilinear form (20) is positive semidefinite. It is a positive definite inner product on $\underline{\mathcal{A}}/L(\omega)$, and the completion

$$\overline{\underline{\mathcal{A}}/L(\omega)}$$

forms the physical Hilbert space $\mathcal{H}_{\text{phys}}$.

Following the well-known GNS construction, a representation of $\mathcal{A}$ on $\mathcal{H}_{\text{phys}}$ may now be defined by

$$\varphi(f)[g] = [f \times g], \quad f \in \mathcal{A}, \quad g \in \underline{\mathcal{A}}, \tag{21}$$

where $[g]$ denotes the image of g under the series of maps $\underline{\mathcal{A}} \to \underline{\mathcal{A}}/L(\omega) \to \mathcal{H}_{\text{phys}}$.

For any vector space V, we let $V' = \text{Hom}\,(V, \mathbb{C})$ denote the dual. Note that $(V^{\otimes n})' \cong (V')^{\otimes n}$ for a large class of vector spaces including all nuclear spaces. The Wightman functions are elements

$$W_n \in \mathcal{A}_n' \cong \mathcal{A}'(\Sigma^n, \mathbb{C}) \otimes \mathcal{B}'^{\otimes n}.$$

To clarify this structure, and to make contact with physics notation, it is useful to expand the relevant objects in a basis, and to assume the presence of a nondegenerate inner product on $\mathcal{B}$, so that $\mathcal{B}' \cong \mathcal{B}$.

Accordingly, let (e_a) denote a basis for $\mathcal{B}$. For $f \in \mathcal{A}_n$,

$$W_n(f) = \sum_{\substack{a_1 \cdots a_n \\ b_1 \cdots b_n}} \left(\prod_{i=1}^{n} g_{a_i b_i} \right) W_{n;a_1,\ldots,a_n}(f_{b_1,\ldots,b_n}), \tag{22}$$

where $g_{ab} = \langle e_a, e_b \rangle$, and $f_{b_1,\ldots,b_n} \in \mathcal{A}(\Sigma^n, \mathbb{C})$ are components of f with respect to the basis $e_{b_1} \otimes \cdots \otimes e_{b_n}$ of $\mathcal{B}^{\otimes n}$. If the basis is orthonormal, the formula simplifies and we have

$$W_n(f) = \sum_{a_1 \cdots a_n} W_{n;a_1 \cdots a_n}(f_{a_1 \cdots a_n}). \tag{23}$$

A Yang–Mills field is a $\mathfrak{g}$-valued one-form, and the associated field strength is a 2-form. However, the above formalism is most easily applied to the case of an algebra-valued scalar field. Fortunately, there do exist examples of great relevance to modern physics in which it suffices to consider zero-forms. In Secs. III and IV, we present two such examples in detail, in each case providing a self-contained introduction for the reader's convenience.

It is useful to see how (22) and (23) make contact with traditional physics notation. For 2D $SU(N)$ Yang–Mills theory on a genus g Riemann surface, explicit formulas are known. Nunes and Schnitzer calculate via path integral techniques that

$$W_{2;a,b}(x,y) \propto \sum_{l \in \text{irreps}} \frac{\dim(l)^{2-2g}}{\exp\left(\frac{1}{2}\lambda^2 A C_2(l)\right)} \left[\frac{(\rho,\rho)\,\delta^{ab}}{N^2} \delta_{x,y}^2 - (p^{ab}(l+\rho)^2 + m^{ab} n^2) \right],$$

where $A = \text{Area}\,(\Sigma)$, λ is a coupling constant, l is the highest weight of an irrep, ρ is the half-sum of positive roots, n=size of the Young tableau, and ρ^{ab}, m^{ab} are rational functions of N.

Let us also illustrate the above formalism for the matrix model case, in which Σ is a single point, and $\mathcal{A} = \mathcal{B} = \mathfrak{gl}_n\mathbb{C}$. Choose the orthonormal basis e_{ij}, $i, j = 1, \ldots, n$, where e_{ij} is a matrix with 1 in the (i,j) position and zeros elsewhere. In our previous notation, $a = (i,j)$, $b = (i',j')$, etc. The simplest nontrivial case involves two matrices, in which case the Wightman function is

$$W_{2;a,b} = W_{2;i,j,i',j'} = \int [d^{n^2}M] M_{ij} M_{i'j'} e^{-n\text{Tr}\ S(M)}.$$

Let $f \in \mathcal{A}_2 = (\mathfrak{gl}_n\mathbb{C})^{\otimes 2}$. Since Wightman functionals are linear, we lose no generality in assuming that f is homogeneous, and thus write $f = A \otimes B$, for $A, B \in \mathfrak{gl}_n\mathbb{C}$. The Wightman functional evaluated on f gives

$$W_2(f) = \sum_{i,j,i',j'} \left(A_{ij} B_{i'j'} \int [d^{n^2}M] M_{ij} M_{i'j'} e^{-n\text{Tr}\ S(M)} \right).$$

C. Global symmetry and unitary implementation

In this picture, a *symmetry* of the quantum theory is defined to be an ω-invariant representation

$$\alpha: \mathcal{G} \to \mathrm{Aut}(\underline{\mathcal{A}}). \tag{24}$$

Here, ω-invariance means that for all $\underline{f} \in \underline{\mathcal{A}}$, we have $\omega(\alpha_g \underline{f}) = \omega(\underline{f})$. This implies that $\alpha_g(L(\omega)) \subseteq L(\omega)$, as is easily checked. Thus for each g, α_g is a well-defined automorphism of the quotient algebra $\underline{\mathcal{A}}/L(\omega)$ and extends naturally to the completion $\mathcal{H}_{\text{phys}}$.

Any such symmetry is unitarily implementable. In fact,

$$(\alpha_g \underline{f}, \alpha_g \underline{h}) = \omega(\alpha_g(\underline{f})^* \times \alpha_g(\underline{h})) = \omega(\alpha_g(\underline{f}^* \times \underline{h})) = \omega(\underline{f}^* \times \underline{h}) = (\underline{f}, \underline{h}).$$

We infer that for any $g \in \mathcal{G}$, α_g defines a unitary operator on $\mathcal{H}_{\text{phys}}$, and denote this operator by $U(g)$. Representations of the form (24) arise often in physics; Lorentz symmetry is an example.

If the field takes values in a normed *-algebra $\mathcal{B}$, as we have assumed throughout the present paper, then any group representation T on $\mathcal{B}$ naturally lifts to a representation on $\underline{\mathcal{A}}$. If $\mathcal{B}$ is a Lie algebra, one may consider, for example, the Adjoint representation of the corresponding Lie group. In this case, $U(g)$ is the quotient by $L(\omega)$ of $\oplus_n T(g)^{\otimes n}$, and the field satisfies a simple covariance relation under conjugation by the unitary group:

$$U(g)\varphi(f)U(g)^* = \varphi(T(g)f), \tag{25}$$

as one may verify by applying each operator to an equivalence class $[\underline{h}] \in \underline{\mathcal{A}}/L(\omega)$, and using the property that $U(g)^* = U(g)^{-1} = U(g^{-1})$. Interestingly, $U(g)$ can be trivial even when α_g is not. If $\alpha_g(\underline{f}) - \underline{f} = \underline{h}^* \times \underline{h}$ for some $\underline{h} \in \underline{\mathcal{A}}$, then $\underline{h} \in L(\omega) \Rightarrow [\underline{h}] = 0$ in $\mathcal{H}_{\text{phys}}$. It follows that $U(g)$ is the identity.

It is clear that the quantum mechanical ground state remains invariant under $U(g)$; thus, the above discussion applies to unbroken symmetry of the quantum theory. As such, it cannot apply to spontaneously broken symmetry.

D. Representations of the canonical commutation relations

Let $\mathcal{A}$ denote the space of Schwartz functions form $\mathbb{R}^d$ to a (noncommutative) untial normed algebra $(\mathcal{B}, \star)$. Analogous constructions may be carried out for $\mathcal{A} = C_0^\infty(\mathbb{R}^d, \mathcal{B})$. Choose a continuous, nondegenerate $\mathcal{B}$-valued bilinear form C on $\mathcal{A} \times \mathcal{A}$. If we assume that $\mathcal{B}$ is a *-algebra, then it has a natural positive cone. In this situation, one may formulate the appropriate positivity property for C. This property entails that (f, Cf) lies in the positive cone of $\mathcal{B}$, for all f. If $\mathcal{B}$ is a matrix algebra, one could consider the massive free covariance $C = (-\Delta + m^2)^{-1}$ acting componentwise on the matrices, but this is by no means the only imortant example.

Let $\mathcal{C}(\mathcal{A}')$ be a suitable space of well-behaved functions on the dual space $\mathcal{A}'$. We define a linear functional $\langle \cdot \rangle$ from $\mathcal{C}(\mathcal{A}')$ to $\mathcal{B}$. By analogy with the standard Gaussian measures of bosonic field theory, which are denoted $d\phi_C$, we denote our functional by

$$\langle \cdot \rangle \equiv \int \cdot \widetilde{d\phi_C}.$$

The functional is defined by the recursion relation for Gaussian integrals (also known as Wick's theorem)

$$\langle \phi(f_1) \cdots \phi(f_n) \rangle = \sum_{\pi \in P_2(n)} \prod_{\{i,j\} \in \pi} \langle \phi(f_i)\phi(f_j) \rangle,$$

where $P_2(n)$ denotes the set of all partitions of $(1, \ldots, n)$ into two-element subsets. To complete the definition, we specify the two-point function

$$\int \phi(f)\phi(g)\widetilde{d\phi}_C = (f, C_g).$$

We are now in a position to specify fields which satisfy the canonical commutation relations.

Definition 1: For any $f \in \mathcal{A}$ and $\phi \in \mathcal{A}'$, $\phi(f)$ may be considered as a linear coordinate function of the variable $\phi \in \mathcal{A}'$ (according to the natural identification of $\mathcal{A}$ with its double-dual). This coordinate function defines an associated multiplication operator $\Phi(f)$ acting on $\mathcal{C}(\mathcal{A}')$. Explicitly, $(\Phi(f)A)(\phi) \equiv \phi(f)A(\phi)$.

The functional derivative is defined as

$$(D_\psi A)(\phi) = \lim_{\epsilon \to 0} \frac{A(\phi + \epsilon\psi) - A(\phi)}{\epsilon}.$$

The case in which ψ is a delta function arises so often in field theory that it has a special notation:

$$\frac{\delta}{\delta\phi(x)} A(\phi) = D_{\delta(x)} A(\phi).$$

Definition 2: The following map is called the *canonically conjugate field operator*:

$$\Pi(g) = -i\left\langle g, \frac{\delta}{\delta\phi} \right\rangle \equiv -i \int_{\mathbb{R}^d} g(x) \frac{\delta}{\delta\phi(x)} dx, \quad g \in \mathcal{A}. \tag{26}$$

The notation in (26) means that when $\Pi(g)$ is applied to a functional $A(\phi)$, the functional derivative $\delta A(\phi)/\delta\phi(x)$ is computed *before* the integral with respect to x.

Consider the Hilbert space

$$\mathcal{H} = L^2(\mathcal{A}', \mathcal{B}; \widetilde{d\phi}_C)$$

generated by taking the completion of a space of functions $A: \mathcal{A}' \to \mathcal{B}$ satisfying

$$\int_{\mathcal{A}'} \|A(\phi)\|^2 \widetilde{d\phi}_C < \infty.$$

Denote by $\mathcal{D}$ the vector subspace of $\mathcal{H}$ generated by arbitrary polynomials in the field. It is clear that $\mathcal{D}$ is dense in $\mathcal{H}$, and for all $f \in \mathcal{A}, \Phi(f)$ and $\Pi(f)$ are defined on $\mathcal{D}$. Further, it holds that $\Phi(f)\mathcal{D} \subset \mathcal{D}$ and $\Pi(f)\mathcal{D} \subset \mathcal{D}$.

The following theorem is relevant to all quantum field theories with $\mathcal{B}$-valued test functions.

Theorem 3: *Definitions 1 and 2 specify operator-valued distributions* $\Phi(f)$ *and* $\Pi(g)$ *which are defined on a common dense domain* $\mathcal{D}$ *in the Hilbert space* $\mathcal{H} = L^2(\mathcal{A}', \mathcal{B}; \widetilde{d\phi}_C)$, *and which satisfy the canonical commutation relations*

$$[\Phi(f), \Pi(g)] = i(g, f)I$$

on the domain $\mathcal{D}$, *for all* $f, g \in \mathcal{A}$.

Proof: Since $\mathcal{B}$ is an algebra, there is an exponential map

$$\exp: \mathcal{B} \to \mathcal{B}[\![z]\!],$$

where $\mathcal{B}[\![z]\!]$ is the ring of formal power series with coefficients in $\mathcal{B}$. This map is such that

$$a \to \exp(za) \equiv 1_{\mathcal{B}} + az + \tfrac{1}{2}(a \star a)z^2 + \cdots. \tag{27}$$

In particular, e^{ia} is a well-defined formal power series for any $a \in \mathcal{B}$. In fact, since $\mathcal{B}$ is a normed algebra, the power series (27) is absolutely convergent in the norm topology, although we will not make use of this.

For a test function $h \in \mathcal{A}$, we calculate

$$\Pi(g)e^{i\phi(h)} = -i\int_{\mathbb{R}^d} g(x)\frac{\delta}{\delta\phi(x)}e^{i\phi(h)}dx = (g,h)e^{i\phi(h)}.$$

Also,

$$\Pi(g)\Phi(f)e^{i\phi(h)} = (-i(g,f) + \Phi(f)(g,h))e^{i\phi(h)}.$$

Therefore,

$$[\Phi(f),\Pi(g)]e^{i\phi(h)} = i(g,f)e^{i\phi(h)}. \tag{28}$$

Relation (28) implies directly that the operator equation

$$[\Phi(f),\Pi(g)] = i(g,f)I \tag{29}$$

holds when applied to powers of the field $A(\phi) = \phi(f)^n$. This, together with the polarization identity

$$x_1\cdots x_n = \frac{1}{2^n n!}\sum_{\epsilon_j=\pm 1}\epsilon_1\cdots\epsilon_n(\epsilon_1 x_1 + \cdots + \epsilon_n x_n)^n,$$

implies that (29) holds on the space generated by polynomials in the ϕ-field. □

We conclude that (29) defines a representation of the canonical commutation relations with all the desired properties.

E. Axioms for nonpositive theories

A number of quantum field theory models are known which do not satisfy positivity. The general properties of these models are summarized in the modified Wightman axioms of indefinite metric QFT.[12] In particular, there are two replacements of the positivity axiom which immediately generalize to the noncommutative algebraic framework outlined in the present work.

Albeverio *et al.*[13] investigated Euclidean random fields as generalized white noise and remarked that the Wightman functionals belonging to those fields do not generally satisfy positivity. Those nonpositive Wightman functionals satisfy the following weaker condition, known as the Hilbert space structure condition.[14]

Axiom (Hilbert space structure condition): There exist seminorms p_n on $\mathcal{S}_n$ such that

$$|W_{n+m}(f_n^* \otimes g_m)| \leqslant p_n(f_n)p_m(g_m) \quad \textit{for all } f_n \in \mathcal{S}_n,\ g_m \in \mathcal{S}_m. \tag{30}$$

This axiom needs no modification in order to apply to the general Borchers construction of Sec. II B; the p_n are simply reinterpreted as seminorms on the subspaces $\mathcal{A}_n$ arising in the grading of the universal enveloping algebra.

A related condition known as the Krein structure condition[15] is satisfied by the physically important Gupta–Bleuler formalism for free QED, and has many attractive features from a mathematical standpoint.

Axiom (Krein positivity): There exists a dense unital subalgebra $\mathcal{A}_0$ of the Borchers algebra, and a mapping $\alpha: \mathcal{A}_0 \to \mathcal{A}_0$, such that for all $f, g \in \mathcal{A}_0$,

(1) $\omega(\alpha^2(f)^* \times g) = \omega(f^* \times g)$;
(2) $\omega(\alpha(f)^* \times f) \geqslant 0$;
(3) $\omega(\alpha(f)^* \times g) = \omega(f^* \times \alpha(g))$; *and*
(4) $p_\alpha(f) \equiv \omega(\alpha(f)^* \times f)^{1/2}$ *is continuous in the topology of the Borchers algebra.*

In the original paper,[15] it is shown that the Krein positivity condition is stronger than the Hilbert space structure condition, is satisfied by free QED, and guarantees the existence of a majorizing Krein-type Hilbert space structure associated to the Wightman functions.

It is easily seen that the Krein positivity condition may be applied to the generalized Borchers algebra of Sec. II B, and a state ω on that algebra, simply by interpreting the terminology within the new context.

III. CORRELATORS IN GAUGE THEORY

We would like to use the structure developed above to express quantities of interest in gauge theory. The difficulty with this outlook is that there are different possible choices for complete sets of observables. It is known that Wilson loop functionals are a complete set of observables for Yang–Mills theory in any dimension, but as functionals on the loop space, they cannot be directly used to generate a state on the generalized Borchers algebra. Fortunately, in some cases, a complete set of gauge-invariant correlation functions is available, and they possess a mathematical structure which is convenient for our viewpoint in this paper.

A. Complete sets of observables

In any number of dimensions, the Yang–Mills field strength is a Lie algebra valued two-form; a special feature of two dimensions is that in this case the field strength is mapped to a $\mathfrak{g}$-valued scalar field by the Hodge star. This field is denoted $\xi(x)$, and defined by the relation

$$F_{\mu\nu}(x) = \xi(x)\sqrt{g(x)}\varepsilon_{\mu\nu}.$$

The Yang–Mills action in two dimensions is

$$S = \frac{1}{8\pi^2\varepsilon}\int_{\Sigma} \mathrm{Tr}\, F \wedge {*F}, \tag{31}$$

with the trace taken in the fundamental representation for $\mathfrak{g}$. In our convention, the gauge field A is anti-Hermitian. In terms of ξ the pure Yang–Mills action takes the form

$$\int_{\Sigma} \mathrm{d}\mu\ \mathrm{Tr}(\xi^2)$$

with the appropriate coupling constant inserted. Here $\mathrm{d}\mu = \sqrt{g(x)}\ \mathrm{d}^2x$ is the Riemannian volume measure on Σ.

Field strength correlators are linear combinations of objects of the form

$$\langle \xi^a(x_1)\xi^b(x_2)\xi^c(x_3)\cdots\xi^d(x_n)\rangle. \tag{32}$$

Here $\xi(x)$ is a Lie algebra valued scalar field, and ξ^a, ξ^b, etc., come from expanding the field with respect to some fixed basis of the Lie algebra. For example, one could take the Gell-mann matrices $\mathbf{t}_a$ as a basis of SU(3) and write $\xi(x) = \xi^a(x)\mathbf{t}_a$. Thus, (32) is not a gauge-invariant correlator. It becomes gauge invariant only after inserting $\mathbf{t}_a, \mathbf{t}_b, \mathbf{t}_c$, etc., summing over repeated indices, and taking the trace. The rest of this section will be devoted to describing a second type of correlator, which are sometimes called *ϕ-field correlators*.

In two dimensions there are no propagating degrees of freedom (i.e., no gluons) so the only degrees of freedom come from the topology of space–time or Wilson loops. Since there are so few degrees of freedom, there is a very large group of local symmetries. YM_2 is invariant under the group $\mathrm{SDiff}(\Sigma)$ of area preserving diffeomorphisms, which is a larger symmetry group than local gauge invariance.

The following equivalent action is called the "first-order formalism" because Gaussian integration over ϕ gives back the original action (31),

$$Z_\Sigma(\varepsilon) = \int DA \exp\left(\frac{1}{8\pi^2\varepsilon}\int_\Sigma \mathrm{Tr}F \wedge *F\right) = \int DA\, D\phi\, e^{-S(A,\phi)},$$

where

$$S(A,\phi) = -\frac{i}{4\pi^2}\int_\Sigma \mathrm{Tr}(\phi F) - \frac{\varepsilon}{8\pi^2}\int_\Sigma \mathrm{d}\mu\ \mathrm{Tr}\ \phi^2. \tag{33}$$

Here ϕ is a Lie-algebra valued 0-form; (33) gives rise to the natural generalization,

$$I = \int_\Sigma [i\ \mathrm{tr}(\phi F) + \mathcal{V}(\phi)\mathrm{d}\mu], \tag{34}$$

where $\mathcal{V}$ is any invariant function on the Lie algebra $\mathfrak{g}$. Thus, ordinary YM_2 is one example of a general class of theories parametrized by invariant functions on $\mathfrak{g}$. It is natural to restrict to the ring of invariant polynomials on $\mathfrak{g}$. For $G=\mathrm{SU}(N)$, this ring is generated by $\mathrm{tr}\ \phi^k$, so we may describe the general theory by coordinates t_k, in terms of which

$$\mathcal{V} = \sum t_k \prod_j (\mathrm{tr}\ \phi^j)^{k_j}.$$

The generalized Borchers formulation applies equally well to the general case (34) with arbitrary $\mathcal{V}(\phi)$.

A complete set of physical observables for Yang–Mills theory in any dimension are Wilson loops. These are, in particular, interesting observables for Yang–Mills theory in $d=2$. However, gauge invariant polynomials of the field ϕ form another complete set of observables naturally suited to evaluation of the partition function. These observables include products of $\mathrm{Tr}\ \phi^2(x_i)$ at various points x_i, and more generally, traces of any homogeneous invariant polynomial defined on the Lie algebra $\mathfrak{g}$. We will adopt this terminology, and refer to expectations of products of $\mathrm{Tr}\ \phi^2(x_i)$ as *ϕ-field correlators*. This is in marked contrast to $d=4$ Yang–Mills where the only dimension four gauge invariant operators are $\mathrm{tr}(F\wedge *F)$ and $\mathrm{tr}(F^2)$, with the latter a topological term.

The most important property of expectation values of gauge-invariant observables in two dimensions is that they are almost topological. A sample calculation shows that

$$d\left\langle \frac{1}{8\pi^2}\mathrm{Tr}\phi^2(x)\right\rangle_\varepsilon = \left\langle \frac{1}{4\pi^2}\mathrm{Tr}\ \phi(x)\mathrm{d}_A\phi(x)\right\rangle_\varepsilon = 0. \tag{35}$$

The action

$$S_{\mathrm{top}} = -\frac{1}{2}\int i\ \mathrm{tr}(\phi F)$$

describes a true topological field theory whose path integral is concentrated on flat connections $F=0$. The field ϕ is sometimes denoted by B, in which case the Lagrangian is proportional to $\mathrm{Tr}(BF)$, and the terminology *BF theory* was introduced. In the small area limit (or the $\mathcal{V}\to 0$ limit) YM_2 reproduces the results of this topological field theory.

B. The Hilbert space of YM_2

We consider quantization of YM_2 on the cylinder with periodic spatial coordinate of period L. This model is well understood and we will make no attempt at exposition since several excellent references exist in the literature.[16–19] Our purpose here is to point out an unexpected mathematical relationship having to do with the space of class functions on a Lie group that is predicted by the generalized Wightman construction introduced earlier in the paper.

The Hilbert space of this model is known to be the space of L^2 class functions on G with inner product

$$\langle f_1|f_2\rangle = \int_G \mathrm{d}U\, f_1^*(U) f_2(U), \tag{36}$$

where $\mathrm{d}U$ is the Haar measure normalized to give volume one. For compact gauge groups, the Peter–Weyl theorem implies the decomposition of $L^2(G)$ into unitary irreps,

$$L^2(G) = \oplus_R R \otimes \overline{R}.$$

Consequently a natural basis for the Hilbert space of states is provided by the characters in the irreducible unitary representations. This is known as the representation basis. The states $|R\rangle$ have wave functions $\chi_R(U)$ defined by

$$\langle U|R\rangle \equiv \chi_R(U) \equiv \mathrm{Tr}_R(U). \tag{37}$$

While Eqs. (36) and (37) provide two different expressions for the inner product of YM_2, a third expression for the same inner product can be derived from the generalized Borchers construction, in the special case of constant Wightman functions. The sesquilinear form is given by (28), and the inner product of YM_2 therefore comes from (20) after taking the quotient by zero-norm states, and subsequently, taking the completion.

C. The correlators of YM_2

The correlators of YM_2 are determined by representation–theoretic invariants of the gauge group such as Casimir operators, and by the integration measure defined by the Riemannian metric on the Riemann surface Σ. Explicit expressions have been found by Nunes and Schnitzer,[20] using the Abelianization technique for path integrals developed by Blau and Thompson. In a particular gauge, the two-point function for 2D SU(N) Yang–Mills theory on a Riemann surface is

$$\langle \xi^a(x)\xi^b(y)\rangle = \frac{e^4}{Z_{\Sigma_g}} \sum_l \dim(l)^{2-2g} \exp\left(-\frac{e^2}{2} A C_2(l)\right)\left[\frac{(\rho,\rho)\delta^{ab}}{N^2}\delta^2_{x,y} - (p^{ab}(l+\rho)^2 + m^{ab}n^2)\right], \tag{38}$$

where l is the highest weight which labels the irreducible representation of SU(N), n is the total number of boxes in the Young tableau defined by l, $\dim(l)$ and $C_2(l)$ denote, respectively, the dimension and quadratic Casimir, ρ is the half-sum of the positive roots, A is the area of Σ, and

$$p^{ab} = \begin{cases} \dfrac{-1}{N(N-1)} & \text{if } a \neq b, \\ \dfrac{1}{N} & \text{if } a = b, \end{cases} \qquad m^{ab} = \begin{cases} \dfrac{1}{N(N-1)} & \text{if } a \neq b, \\ 0 & \text{if } a = b. \end{cases}$$

Note that the dependence of (38) on the choice of gauge goes away after inserting the Lie algebra generators and taking the trace.

In general, it is known that the gauge-invariant $(2p)$-point function $\langle \mathrm{Tr}\ \xi^{2p}(x)\rangle$ on a Riemann surface of genus g takes the x-independent form

$$\frac{e^{4p}}{Z_{\Sigma_g}} \sum_\ell \dim(\ell)^{2-2g} \exp\left(-\frac{e^2}{2} A C_2(\ell)\right) \sum_{i=1}^{p} f_i(\rho) C_{2i}(\ell),$$

where f_i are rational functions of (ρ,ρ).

Remark 3: The physical Hilbert space of this quantum theory is a well-defined object, and we now in principle know two ways to calculate it. As discussed previously, the Hilbert space of this

model is known to be the space of L^2 class functions on G with inner product (36). However, we expect to also recover the Hilbert space inner product from the state on the generalized Borchers algebra that is determined by (38) and all higher-order correlators. Of course, the physical Hilbert space is recovered only after taking the quotient by the left kernel of this state, which presents a difficulty. How can one see that $\underline{\mathcal{A}}/L(\omega) \cong L^2(G)$?

IV. MATRIX MODELS AND FINITE ORDER STATES

Section IV A gives the definition of matrix states and finite order states. In Secs. IV B and IV C we recall the matrix models which have come to play a prominent role in high energy physics in the last few years. Section IV D shows that, in the same sense in which scalar quantum field theories are Wightman states, matrix models are finite order states. Finally, Sec. IV E points out that an argument due to Borchers generalizes to the noncommutative case, showing that arbitrary states on the field algebra, which describe nontrivial quantum field theories, are limits of matrix states.

A. Matrix states and finite order states

Let $T \in E(\underline{\mathcal{A}})$ be a state, and denote by $I(T)$ the maximal two-sided ideal contained in the left-kernel $L(T)$.

Definition 3: T is said to be of finite order *if the family of operators* $\{A_T(f) : f \in \mathcal{A}\}$ *contains exactly N linearly independent elements for* $N < \infty$, *or equivalently if*

$$\dim(\mathcal{A}/I(T) \cap \mathcal{A}) = N.$$

In this situation, N is called the order of the state.

Definition 4: T is called a matrix state *if* $\underline{\mathcal{A}}/I(T)$ *is a finite-dimensional algebra.*

Clearly, a matrix state is of finite order, but the converse may not hold. The terminology comes from the fact that any finite-dimensional *-algebra with unit is isomorphic to a star-closed subalgebra of the algebra of $n \times n$ matrices, for some finite n. Let $\mathfrak{h}_n$ denote the *-algebra of $n \times n$ Hermitian matrices.

B. Hermitian matrix models

A Hermitian one-matrix integral (see Refs. 21 and 22 for a review) takes the form

$$Z = \int [\mathrm{d}^{n^2} M] \exp(n \ \mathrm{Tr} \ S(M)), \tag{39}$$

where $S(M)$ is an arbitrary function. The model is said to be *solvable* if the integral can be performed explicitly, at least in the large n limit. We briefly indicate how this can be done in the simplest case. Diagonalize M via the transformation $M = \mathcal{O}^+ x \mathcal{O}$ where x is diagonal and $\mathcal{O} \in U(n)$. The corresponding measure can be written as

$$\mathrm{d}^{n^2} M = \mathrm{d}[\mathcal{O}]_{U(n)} \ \Delta^2(x) \prod \mathrm{d}x_k,$$

where $\Delta(x) = \Pi_{i>j}(x_i - x_j)$ is the Vandermonde determinant. The integrand does not depend on $\mathcal{O}$, so integration over $\mathcal{O}$ produces a group volume factor. The remaining integral over the eigenvalues is $Z = \int [\Pi_{k=1}^n \mathrm{d}x_k] \exp(nS(x_k)) \Delta^2(x)$. In the large n limit the corresponding saddle point equation takes the form

$$\frac{1}{n} \frac{\partial S}{\partial x_k} = S'(x_k) + \frac{1}{n} \sum_{j \neq k} \frac{1}{x_k - x_j} = 0.$$

C. Dijkgraaf–Vafa matrix models

For simplicity, we examine an $U(N)$ gauge theory with an adjoint Higgs supermultiplet Φ and tree-level single-trace superpotential

$$W_{\text{tree}}(\Phi) = \sum_{k=1}^{p+1} \frac{1}{k} g_k \ \text{Tr}\ \Phi^k. \tag{40}$$

Dijkgraaf and Vafa [23] have proposed a very simple recipe to calculate the exact quantum effective superpotential $W(S)$ for the glueball superfield,

$$S = -\frac{\text{tr}\ \mathcal{W}^\alpha \mathcal{W}_\alpha}{16N\pi^2},$$

in the confining vacua of a large class of $\mathcal{N}=1$ supersymmetric Yang–Mills theories, where $\mathcal{W}_\alpha$ is the gauge field strength of the $U(N)$ vector superfield. The superpotential $W(S)$ contains highly nontrivial information about the nonperturbative dynamics of the theory. For example, it can be used to derive dynamical chiral symmetry breaking and calculate the tension of the associated domain walls.

The theory (40) is geometrically engineered on the (local) Calabi–Yau three-manifold,

$$\{u^2 + v^2 + y^2 + W'_{\text{tree}}(x)^2 = f_{p-1}(x)\} \subset \mathbb{C}^4, \tag{41}$$

where $f_{p-1}(x)$, an order $(p-1)$ polynomial, is a complex deformation parameter, and as is well known, the Seiberg–Witten curve is the same as the spectral curve of the associated matrix model.

Dijkgraaf and Vafa have conjectured[23] that the superpotential $W(S)$ is the sum of zero momentum planar diagrams of the $\mathcal{N}=1$ theory under consideration. In our case, their ansatz for the $U(N)$ theory is a holomorphic integral over $n\times n$ complex matrices ϕ,

$$\exp(n^2\mathcal{F}/S^2) = \int_{\text{planar}} \text{d}^{n^2}(\phi/\Lambda)\exp\left[-\frac{n}{S}W_{\text{tree}}(\phi, g_p)\right], \tag{42}$$

from which the superpotential can be deduced,

$$W(S, \Lambda^2, g_p) = -N\partial_S \mathcal{F}(S, g_p). \tag{43}$$

Here, Λ is the complex mass scale governing the one-loop running of the gauge coupling constant (see Ref. 24). For SU(N) gauge theory, the integral (42) must be restricted to traceless matrices, or equivalently one must treat g_1 as a Lagrange multiplier.

The parameter n is introduced so that the planar diagrams can be extracted by taking the $n \to \infty$ limit. The N dependence of the superpotential is then given explicitly by (43). The integral (42) involves complex matrices and couplings g_p, but the calculation is the same as for Hermitian matrices and real couplings. There is no ambiguity in the analytic continuation because we restrict to planar diagrams. This implies that standard matrix model techniques[21] do apply. A nice mathematical description of holomorphic matrix integrals was given by Lazaroiu.[25]

D. Matrix models as finite order Wightman states

The interesting point we wish to make in this section is that the aforementioned matrix models (arising in string theory, condensed matter, and other branches of physics) are well described by the noncommutative Borchers construction with a finite order state, in the sense of Definition 1. A mathematician might define the term *matrix model* to be a finite order state on the Borchers algebra $\underline{\mathcal{A}}$ constructed from a zero-dimensional space–time Σ and target $\mathcal{B}$ given by some matrix algebra.

In what follows, we consider a one-matrix model defined by an action S. If Σ is zero-dimensional, compact and connected, it is a single point, $\Sigma=\{\text{pt}\}$. From this we infer that

$$\mathcal{A} = \mathrm{Map}(\Sigma, \mathcal{B}) \cong \mathcal{B} = \mathfrak{gl}_n\mathbb{C}, \tag{44}$$

and

$$\mathcal{A}_m = (\mathfrak{gl}_n\mathbb{C})^{\otimes m}, \quad m \geqslant 1.$$

To avoid confusion with the field theory case, we will denote a finite order state by $\mathfrak{w}$. For $A, B \in \mathcal{A}$ we may compute the inner product on the Borchers algebra (before taking the quotient by the left-kernel) to be

$$\langle A, B\rangle = \mathfrak{w}(A^* \times B) = \sum_{i,j,k,l} \overline{A_{ji}} B_{kl} F(i,j,k,l), \tag{45}$$

where

$$F(i,j,k,l) = \int [d^{n^2}M] M_{ij} M_{kl} e^{-n\mathrm{Tr}\ S(M)}$$

is the analog of a correlation function for the matrix model. The matrix model is said to be *solvable* if the integrals of the form $\int [d^{n^2}M]$ may be computed, at least in the large n limit where saddle point techniques apply.

Recall the definition of the Hermitian subspace of a *-algebra, Eq. (4). Clearly in the current example, $\mathcal{A}_h$ is given by $\mathfrak{h}_n$, the space of $n \times n$ Hermitian matrices. The Wightman procedure constructs an operator formulation for Hermitian matrix models, in which $\mathcal{H}_{\mathrm{phys}}$ is the completion of

$$\underline{\mathcal{A}}_h / L(\mathfrak{w}) \cap \underline{\mathcal{A}}_h.$$

The generalized Wightman construction, in some sense, contains within it a master field formulation for matrix models.

Definition 5 (Master Field): A *master field formulation* of a matrix model is a choice of quantum mechanical Hilbert space $\mathcal{H}$ and a GNS representation on $\mathcal{H}$ such that, for arbitrary k, the gauge-invariant matrix model correlator

$$\langle \mathrm{Tr}(M^k)\rangle \equiv \int [DM] \mathrm{Tr}(M^k) e^{-n\mathrm{Tr}\ S(M)}$$

may be calculated in terms of vacuum expectation values of products of field operators on $\mathcal{H}$.

The definition is sufficiently general that there can be no question about existence of a master field formulation for any matrix model; however, to discover one that is simple and useful remains a subtle art. We will consider the natural basis e_{ij} for the space V of $n \times n$ matrices; e_{ij} is a matrix with 1 in the i,jth position and zeros elsewhere. For compactness, we will label a pair of indices by $a = (i,j)$. Let

$$\mathcal{T} = \{(i,j), (j,i) | i,j = 1, \ldots, n\}.$$

Define $f \in \mathcal{A}_2$ by the formula

$$f = f_{ab} e_a \otimes e_b, \quad f_{ab} = \begin{cases} 1, & (a,b) \in \mathcal{T} \\ 0, & \text{otherwise}, \end{cases}$$

where we use the convention that repeated indices are summed over. Then

$$\mathfrak{w}(f) = \sum_{(a,b)\in\mathcal{T}} \mathfrak{w}(e_a \otimes e_b) = \int [DM]\mathrm{Tr}(M^2)e^{-n\mathrm{TrS}(M)}.$$

Consider the Hilbert space formalism defined above, and let ϕ_a be the operator on $\mathcal{H}=\mathcal{H}_{\mathrm{phys}}$, which creates e_a out of the vacuum. Define $\Phi_{ab}=(\phi_a)^\dagger\phi_b$. It follows that

$$\mathfrak{w}(f) = \sum_{(a,b)\in\mathcal{T}} \langle e_a, e_b\rangle_{\mathcal{H}} = \sum_{(a,b)\in\mathcal{T}} \langle \Phi_{ab}\rangle_{\mathcal{H}}.$$

This gives the following relation between the matrix model gauge-invariant correlator and VEVs in the Hilbert space picture:

$$\langle \mathrm{Tr}(M^2)\rangle = \sum_{\mathcal{T}} \langle \Phi_{ab}\rangle_{\mathcal{H}}. \tag{46}$$

By generalizing this procedure, it is clear that vacuum expectations of certain products of field operators in $\mathcal{H}$ give rise to all possible gauge-invariant expectations in the matrix model.

E. Limits of matrix states

The classic result of Borchers[7] that matrix states are dense in the space of all states on the Borchers algebra generalizes to the noncommutative setting. The proof proceeds in two steps, first showing that matrix states are dense in the states of finite order, and then showing that the latter are dense in the set of all states. As the results of this section are of a topological nature, we assume throughout that $\mathcal{B}$ is a normed *-algebra and that the space $\mathcal{A}=\mathcal{A}(\Sigma,\mathcal{B})$ introduced in Eq. (13) is a Schwartz space of rapidly decreasing functions. The generalized Borchers algebra is consequently endowed with the Schwartz topology.

Given a sequence of Wightman distributions defined for fields valued in a noncommutative space, and a state on $\mathcal{B}$, Sec. II defines a state, which we now call T, on the generalized Borchers algebra. The Hilbert space $\mathcal{H}_T$, field operator A_T, and cyclic vector Ω_T are then defined, as usual, by the GNS construction.

Theorem 4: *Any finite-order state T on the generalized Borchers algebra $\underline{\mathcal{A}}$ is a limit of matrix states*.

Proof: Let $\{\mathcal{H},\varphi,\Omega\}$ be the Hilbert space, field operator, and cyclic vector given by the GNS-type construction described in Sec. II. It is clear that if T is of order N, there exist N distributions $t^i\in A'$ and N operators A^i on $\mathcal{H}$ such that

$$\varphi(f) = \sum_{i=1}^{N} (t^i, f)A^i$$

for all $f\in\mathcal{A}$. (Note that this N no longer has anything to do with the gauge group.) Let $\mathcal{H}_n$ be the vector space spanned by all vectors

$$\{A^{i_1}\cdots A^{i_n}\Omega : i_j = 1,\ldots,N, r = 0,\ldots,n\},$$

$\mathcal{H}_n$ is finite dimensional, so $\mathcal{H}_n$ is closed and $A^i|_{\mathcal{H}_n}$ is bounded. Let $E^n:\mathcal{H}\to\mathcal{H}_n$ be the associated orthogonal projection. Also define β_n as follows:

$$f \xrightarrow{\beta_n} \sum_{i=1}^{N} (t^i, f)E^nA^iE^n.$$

Thus β_n is a continuous homomorphism of $\mathcal{A}$ into a finite-dimensional matrix algebra, which is an algebra of $d(n)\times d(n)$ matrices, where $d(n)=\dim\mathcal{H}_n$. We remark that generically, $d(n)$ will be an increasing function of n, and the $n\to\infty$ limit resembles a "large n limit" of matrix models. Define approximate states $T^{(n)}$ by

$$(T^{(n)},g) = \langle \beta_n(g) \rangle_\Omega$$

for any $g \in \underline{\mathcal{A}}$. By definition, a matrix state is an expectation in some fixed vector of a homomorphism into a finite-dimensional matrix algebra, so clearly $T^{(n)}$ are matrix states. Recall that $\mathcal{A}_k$ was defined to be the image of $\mathcal{A}^{\otimes k}$ in the universal enveloping algebra $\underline{\mathcal{A}}$. Note that $T^{(n)}$ coincides with T on the spaces $\mathcal{A}_k$ for $k \leqslant n$, so $T = \lim_{n\to\infty} T^{(n)}$ and the proof is complete. □

Theorem 5: *States of finite order are dense in the set of all states on the generalized Borchers algebra.*

Proof: Let T be any state, and let $\{\mathcal{H}, \varphi, \Omega\}$ be the Hilbert space, field operator, and cyclic vector given by the GNS-type construction described in Sec. II. Choose N arbitrary elements $f_j \in \mathcal{A}$ and let $\mathcal{A}^N$ denote the subspace of $\mathcal{A}$ generated by the f_j. For arbitrary $g \in \mathcal{A}^N$, we have

$$\varphi(g) = \sum_{j=1}^{M} F_j(g)\varphi(f_j),$$

where $\{\varphi(f_j)\}_{j=1,\ldots,M}$ is a minimal basis of the span of $\{\varphi(f_i)\}_{i=1,\ldots,N}$ and the F_j are M continuous linear functionals on $\mathcal{A}^N$. By the Hahn–Banach theorem, extend each F_j to a functional t^j defined on all of $\mathcal{A}$. Define

$$\varphi'(g) = \sum_{i=1}^{M} (t^i, g)\varphi(f_j) \quad \text{and} \quad T[f_1, \ldots, f_N](g) = \langle \varphi'(g) \rangle_\Omega.$$

It is now clear that each $T[f_1, \ldots, f_N]$ is a state of order M. This process defines a Cauchy net $T[\cdots]$ of finite-order states converging to T. □

If an explicit functional $S(a)$ is known so that a finite order state $\mathfrak{w}$ is given by Eq. (45), then we say $\mathfrak{w}$ is defined by its *action* S, and call the associated quantum theory a *matrix model*.

Given a quantum theory (possibly with noncommutative target) defined in terms of its Wightman state, theorems 3–4 construct a sequence of matrix states which converge to the given state. As remarked in the proof of theorem 3, the $n \to \infty$ limit considered in that theorem resembles, at the level of dimensions of the relevant algebras, a large n limit of matrix models. It would be extremely interesting if there were a generic way to reformulate each of these matrix states as a matrix model with action S. Such a formulation would allow us to choose our favorite gauge theory, and immediately write it as a limit of matrix models.

In fact, Kazakov in a famous paper[11] completed a very similar construction. Kazakov considers the multicomponent scalar field theory in four dimensions,

$$S = N \int \mathrm{d}^4x \ \mathrm{tr}((\partial_\mu \phi)^2 + V(\phi)), \tag{47}$$

with ϕ a Hermitian $N \times N$ matrix-valued field, and showed that the four-dimensional (4D) field theory at finite N is equivalent perturbatively, graph by graph of any topology, to a one-matrix model in the large n limit. The latter was conjectured to provide a nonperturbative definition of the 4D field theory. The noncommutative Wightman construction presented in this paper is naturally suited to deal with matrix-valued field theories such as Kazakov's (47), and theorems 3–4 imply that if (47) can be defined as a field theory (meaning that it determines a well-defined state on the generalized Borchers algebra) then it is given by a limit for large n of a sequence of $n \times n$ matrix models.

V. CONCLUSIONS AND OPEN QUESTIONS

A classic result of mathematical physics is the reconstruction of the Hilbert space, vacuum vector, and field operators of a quantum field theory from a given set of distributions satisfying the Wightman axioms.[5] In the preceding sections, we have described the extension of Wightman's construction to theories with gauge symmetry, including non-Abelian pure Yang–Mills models and matrix models, and more generally to theories with fields or test functions valued in a noncom-

mutative algebra. Yang–Mills theory with an adjoint-valued Higgs field also fits within the same framework. In every case involving quantized Yang–Mills fields, the Lie algebra dependence of the fundamental fields can be transferred to the test function space.

In Sec. II C, we discuss the role of symmetry in the generalized Borchers construction. In this framework, it is straightforward to see that space–time and global symmetries are unitarily implementable. The role of the additional ambiguities arising from local gauge symmetry remains a mystery. In path integral quantization, this ambiguity is resolved through use of the Faddeev–Popov determinant, but in the Borchers framework a similarly elegant handling of local gauge symmetry is an unresolved issue. In an effort to shed light on this question, we have considered two simple examples in which the space–time dependence of the fields plays a small role: 2D Yang–Mills theories and matrix models.

This construction provides a unified algebraic framework for formulating properties of a broad class of quantum field theories. Yang–Mills theory (including matrix models) and constructive field theory models[26] possess the following common structure:

(1) A normed *-algebra $\mathcal{B}$ (not necessarily commutative), with the generalized Borchers algebra $\underline{\mathcal{A}}$ of functions into $\mathcal{B}$.
(2) A functional $\omega \in \underline{\mathcal{A}}'$, which is defined in terms of a sequence of n-point functions and which satisfies $\omega(f^* \times f) \geqslant 0 (\forall f)$ in theories with no gauge symmetry, or in gauge theories expected to possess a positive–definite inner product. For nonpositive models such as Gupta–Bleuler QED, the functional ω is postulated to satisfy axioms described in Sec. II E.
(3) A symmetry group $\mathcal{G}$ and a representation $\alpha: \mathcal{G} \to \mathrm{Aut}(\underline{\mathcal{A}})$, which is ω-*invariant* in the sense that $\omega(\alpha_g(f)) = \omega(f)$ for all $f \in \underline{\mathcal{A}}$ and $g \in \mathcal{G}$.
(4) A collection of ideals $I_1, \ldots, I_n$ of the algebra $\underline{\mathcal{A}}$ which are required to lie in the kernel of ω. (Each ideal represents a physical property satisfied by the n-point functions; in Wightman QFT, $n=2$ and the two ideals represent locality and the positive light-cone spectral condition.)
(5) A Hilbert space $\mathcal{H}_{\mathrm{phys}}$ defined to be the completion of $\underline{\mathcal{A}}/L(\omega)$, with inner product $\omega(f^* \times g)$ and vacuum vector Ω.
(6) Field operators defined by the GNS construction, with vacuum expectation values equal to the Wightman functions used to define the state ω.

The discussion following theorem 5 outlines a new research direction, concerned with the question of how quantum field theories can be written as limits of matrix models. It would be very interesting to have a deeper understanding of the issue raised by remark (3). Moreover, this construction could be studied for fields which are sections of nontrivial principal fiber bundles, as suggested by remark (1).

A very interesting analytic question is to study carefully the UV divergences of various gauge theories, and to determine whether they can be correctly described by a noncommutative Borchers construction based on the noncommutative generalization of the Jaffe test function space $\widetilde{S}_g^{\mathcal{B}}$ discussed following (14).

There are possible connections between this work and deformation theory, which we elaborate on briefly here. If we consider continuous deformations of the product $\cdot_{\mathcal{B}}$ in the noncommutative target space $\mathcal{B}$, with respect to a parameter ε, then the constructions in this paper define continuous families of Wightman functionals ω_ε on algebras $\underline{\mathcal{A}}_\varepsilon$ and associated quantum field theories with Hilbert space inner products $\langle , \rangle_\varepsilon$. Consider the quotient of $\underline{\mathcal{A}}_\epsilon$ by the ideal generated by all elements $f \otimes g - g \otimes f - [f,g]$, for $f, g \in \mathcal{A}_\epsilon$. This is the universal enveloping algebra, which we denote $\mathcal{U}(\epsilon)$. If the Wightman state ω_ϵ is well-defined on the quotient, define a new Hilbert space as the completion of $\mathcal{U}(\epsilon)/(L(\omega_\epsilon) \cap \mathcal{U}(\epsilon))$. Consider the deformation which multiplies the associative algebra product (and hence the Lie bracket) in $\mathcal{B}$ by ϵ. The Poincaré–Birkhoff–Witt theorem implies an isomorphism $\mathcal{U}(\epsilon) \simeq S\mathcal{A}_\epsilon$, where $S\mathcal{A}_\epsilon$ is the symmetric tensor algebra over $\mathcal{A}_\epsilon$. This isomorphism defines a family of multiplications on $S\mathcal{A}_\epsilon$, which take the form

$$f *_\varepsilon g = fg + \frac{1}{2}\varepsilon\{f,g\} + \sum_{k\geqslant 2} \varepsilon^k B_k(f,g) \tag{48}$$

for some bilinear forms B_k. This well-known construction is called deformation quantization in the direction of the Poisson bracket.

In general, given a quantum field theory into a noncommutative algebra $\mathcal{B}$, one could consider deforming the multiplication on $\mathcal{B}$, and in certain cases, we expect that the ε dependence might factor out of the Wightman functions and the Hilbert space inner product will scale in some simple way with respect to the deformation parameter ε.

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On a classification of irreducible almost commutative geometries

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We classify all irreducible, almost commutative geometries whose spectral action is dynamically nondegenerate. Heavy use is made of Krajewski's diagrammatic language. The motivation for our definition of dynamical nondegeneracy stems from particle physics where the fermion masses are nondegenerate. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1811372]

I. INTRODUCTION

Within noncommutative geometry pioneered by Connes,[3–6] the almost commutative ones play an interesting role. They are defined by spectral triples $(\mathcal{A},\mathcal{H},\mathcal{D})$ where the algebra $\mathcal{A}_t$ has the form $\mathcal{A}_t=C^\infty(M)\otimes\mathcal{A}$ with $\mathcal{A}$ a direct sum of matrix algebras and M a (compact Euclidean) space–time. For instance in the standard model of particle physics, $\mathcal{A}=\mathbb{H}\oplus\mathbb{C}\oplus M_3(\mathbb{C})$. It is important to classify the almost commutative triples because of their applications to physics. Let us sketch some of them.

Einstein's derivation of general relativity from Riemannian geometry goes in two steps. The first step sets up the kinematics: the equivalence principle uses general coordinate transformations and starts from the flat metric of special relativity to guess curved metrics. The second step constructs a dynamics for the set of all metrics by imposing covariance under general coordinate transformations.

Connes generalizes Einstein's derivation to noncommutative geometry.[3,6] In this new setting the metric is encoded in a Dirac operator and a coherent definition of the equivalence principle becomes available: the fluctuations of the Dirac operator by algebra automorphisms properly lifted to the Hilbert space of spinors. Indeed in Riemannian geometry, the algebra is the commutative algebra of functions on spacetime, the automorphisms are precisely the general coordinate transformations and fluctuating the flat Dirac operator leads to Dirac operators with curvature and torsion. The second step is the spectral action which in the commutative i.e., Riemannian case reproduces the Einstein-Hilbert action plus a positive cosmological constant and a curvature squared term. The Euclidean spectral action is positive definite and its ground states can be interpreted as a regularization of the initial singularity.

A noncommutative space or geometry is defined by a spectral triple consisting of an algebra $\mathcal{A}$, a Hilbert space $\mathcal{H}$ and a Dirac operator $\mathcal{D}$. One important property of noncommutative geometry is that it contains discrete spaces, commutative or not. They have finite dimensional algebras and Hilbert spaces. An almost commutative geometry is a tensor product of the infinite dimensional commutative algebra consisting of space–time functions with a finite dimensional noncommutative algebra, the internal space. The internal Dirac operator is simply an initial fermionic mass matrix and the internal algebra automorphisms of the tensor product are gauge transforma-

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tions. The internal fluctuations produce gauge bosons and Higgs scalars and the spectral action of an almost commutative geometry produces—besides the gravitational action—the complete Yang–Mills–Higgs action. The Higgs scalar is therefore the internal metric and its dynamics is the Higgs potential. The initial fermionic mass matrix in general is not a solution of the internal dynamics, the internal Einstein equation. These solutions are the minima of the Higgs potential which induces the spontaneous symmetry breaking. They yield the true fermionic mass matrix and we have to compute it. Let us remark that in the prior approach of noncommutative Yang–Mills theories without gravity,[7] the Dirac operator was not a dynamical variable. Consequently there was no nuance between initial and true fermion masses.

Although only a small subset of all Yang–Mills–Higgs models can be described as an almost commutative geometry this subset is still infinite and difficult to assess. We propose to reduce it using two constraints. The first is inspired by grand unified theories, in particular SO(10): the gauge group of the standard model of electromagnetic, weak and strong forces is embedded into a simple group and the representation of one generation of quarks and leptons is embedded into an irreducible representation. Therefore our first constraint is the following: take the internal algebra simple and its spectral triple irreducible. As we will see the resulting fermion masses in the ground state are degenerate in flagrant contradiction to experiment. We therefore analyze internal algebras with two and three simple summands and their irreducible spectral triples. Again, in most cases the fermion masses come out degenerate with a few exceptions. Our aim is to list these exceptions. In other words, our second constraint is to impose a nondegenerate fermionic mass spectrum in the ground state, namely to restrict the analysis to dynamically nondegenerate spectral triples. The mathematical definitions of these constraints are given in Secs. II and IV.

II. IRREDUCIBILITY

A spectral triple is given by $(\mathcal{A},\mathcal{H},\mathcal{D})$ such that the real *-algebra $\mathcal{A}$ acts on the complex Hilbert space $\mathcal{H}$, the Dirac operator $\mathcal{D}$ on $\mathcal{H}$ is selfadjoint and *a priori* unbounded. These three items satisfy certain constraints of geometrical significance.[4–6] The commutative examples come from the triple $[\mathcal{A}=\mathcal{C}^\infty(M),\ \mathcal{H}=\mathcal{L}^2(M,\mathcal{S}),\ \mathcal{D}=i\gamma^\mu\partial_\mu]$ associated to a compact Riemannian spin manifold M. As the resolvent of $\mathcal{D}$ is compact, $(\mathcal{A},\mathcal{H},\mathcal{D}=0)$ is never a spectral triple for infinite dimensional $\mathcal{H}$. However, this degenerate situation can occur in finite cases, but is excluded from our definition of irreducible spectral triples.

Definition 2.1:

(i) A spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *degenerate* if the kernel of $\mathcal{D}$ contains a nontrivial subspace of the complex Hilbert space $\mathcal{H}$ invariant under the representation ρ on $\mathcal{H}$ of the real algebra $\mathcal{A}$.

(ii) A nondegenerate spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *reducible* if there is a proper subspace $\mathcal{H}_0\subset\mathcal{H}$ invariant under the algebra $\rho(\mathcal{A})$ such that $(\mathcal{A},\mathcal{H}_0,\mathcal{D}|_{\mathcal{H}_0})$ is a nondegenerate spectral triple. If the triple is real, S^0-real and even, we require the subspace $\mathcal{H}_0$ to be also invariant under the real structure J, the S^0-real structure ϵ and under the chirality χ such that the triple $(\mathcal{A},\mathcal{H}_0,\mathcal{D}|_{\mathcal{H}_0})$ is again real, S^0-real and even.

Remark 2.2:

(i) $(\mathcal{A}=\mathcal{C}^\infty(M),\ \mathcal{H}=\mathcal{L}^2(M,\mathcal{S}),\ \mathcal{D}=i\gamma^\mu\partial_\mu)$ is never degenerate.

(ii) If $(\mathcal{A}_i,\mathcal{H}_i,\mathcal{D}_i)$ are two spectral triples then $(\mathcal{A}_1\otimes\mathcal{A}_2,\ \mathcal{H}_1\otimes\mathcal{H}_2,\ \mathcal{D}_1\otimes 1)$ is a spectral triple whose kernel of $\mathcal{D}_1\otimes 1$ is infinite dimensional when $\mathcal{H}_2$ is of infinite dimension.

(iii) A finite dimensional commutative triple is a collection of points. It is nondegenerate if all points have finite distances. The converse is wrong, $\mathcal{A}=\mathbb{C}\oplus\mathbb{C}\oplus\mathbb{C}$ with the triple given by diagram 15 is a counterexample.

(iv) A reducible triple is not necessarily decomposable into a direct sum. For example,

$$\mathcal{A} = \mathbb{C} \oplus \mathbb{C} \ni (a,b), \quad \rho(a,b) = \begin{pmatrix} \begin{pmatrix} a & 0 \\ 0 & \overline{a} \end{pmatrix} & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & \begin{pmatrix} \overline{a} & 0 \\ 0 & \overline{a} \end{pmatrix} & 0 \\ 0 & 0 & 0 & \overline{a} \end{pmatrix}, \tag{2.1}$$

$$\mathcal{D} = \begin{pmatrix} 0 & \mathcal{M} & 0 & 0 \\ \mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{\mathcal{M}} \\ 0 & 0 & \overline{\mathcal{M}}^* & 0 \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2.2}$$

Here and throughout, overbars and asterisks mean complex conjugation and adjoint.

(v) Our definition of irreducibility differs from the one in our favorite book.[8] Indeed every spectral triple coming from a Riemannian spin manifold is irreducible in our case, even if the manifold is not connected, that is when the commutative spectral triple is a direct sum.

(vi) In our definition of reducibility, the Dirac operator is not supposed to leave the subspace $\mathcal{H}_0$ invariant. Our definition is adapted to the use we will make of spectral triples: the fluctuations under algebra automorphisms properly lifted to the Hilbert space promote the Dirac operator to a dynamical variable and we are interested in its dynamics, the spectral action.[3]

Since we are mainly interested in finite or 0-dimensional triples, we only recall the definition for this case and also restricting ourselves to the real and S^0-real triples.[5,6]

Definition 2.3: A real, S^0-real, finite spectral triple is given by $(\mathcal{A},\mathcal{H},D,J,\epsilon,\chi)$ with a finite dimensional real algebra $\mathcal{A}$, a faithful representation ρ of $\mathcal{A}$ on a finite dimensional complex Hilbert space $\mathcal{H}$. Four additional operators are defined on $\mathcal{H}$: the Dirac operator $\mathcal{D}$ is self-adjoint, the real structure J is antiunitary, and the S^0-real structure ϵ and the chirality χ are both unitary involutions. These operators satisfy

(i)

$$J^2 = 1, \quad [J,\mathcal{D}] = [J,\chi] = [\epsilon,\chi] = [\epsilon,\mathcal{D}] = 0, \quad \epsilon J = -J\epsilon, \quad \mathcal{D}\chi = -\chi\mathcal{D},$$

$$[\chi,\rho(a)] = [\epsilon,\rho(a)] = [\rho(a),J\rho(b)J^{-1}] = [[\mathcal{D},\rho(a)],J\rho(b)J^{-1}] = 0, \quad \forall\, a,b \in \mathcal{A}.$$

(ii) The chirality can be written as a finite sum $\chi = \Sigma_i \rho(a_i) J \rho(b_i) J^{-1}$. This condition is called orientability.

(iii) The intersection form $\cap_{ij} := \mathrm{tr}(\chi\rho(p_i)J\rho(p_j)J^{-1})$ is nondegenerate, $\det \cap \neq 0$. The p_i are minimal rank projections in $\mathcal{A}$. This condition is called *Poincaré duality*.

With the help of the projectors $(1\pm\chi)/2$ and $(1\pm\epsilon)/2$, the Hilbert space is decomposed as

$$\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_R \oplus \mathcal{H}_L^c \oplus \mathcal{H}_R^c. \tag{2.3}$$

The first two components correspond in physics to particles, $\epsilon = 1$, the last two correspond to antiparticles, $\epsilon = -1$. We use the convention where left-handed spinors have negative and right-handed spinors have positive chirality.

If we denote by ρ_L the restriction of ρ to $\mathcal{H}_L$, etc., and by ρ_R^c the restriction to $\mathcal{H}_R^c$, we will always write the representation in the following form:

$$\rho := \begin{pmatrix} \rho_L & 0 & 0 & 0 \\ 0 & \rho_R & 0 & 0 \\ 0 & 0 & \overline{\rho_L^c} & 0 \\ 0 & 0 & 0 & \overline{\rho_R^c} \end{pmatrix}. \tag{2.4}$$

With respect to the decomposition (2.3) of $\mathcal{H}$, $\mathcal{D}$ has the form

$$\mathcal{D} = \begin{pmatrix} 0 & \mathcal{M} & 0 & 0 \\ \mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{\mathcal{M}} \\ 0 & 0 & \overline{\mathcal{M}}^* & 0 \end{pmatrix}. \tag{2.5}$$

Note that the S^0-reality of internal spaces is equivalent to the absence of Majorana–Weyl spinors. These are possible in 0-dimensional spaces, but impossible in 4- and $(1+3)$-dimensional spaces M.

III. KRAJEWSKI DIAGRAMS

Krajewski, Paschke and Sitarz have classified all finite, thus 0-dimensional, real spectral triples.[10,14] Let us summarize this classification for the S^0-real case using Krajewski's diagrammatic language.

A. Conventions and multiplicity matrices

(i) The algebra: it is a finite sum of N simple algebras, $\mathcal{A} = \oplus_{i=1}^N M_{n_{-i}}(\mathbb{K}_i)$ and $\mathbb{K}_i = \mathbb{R}, \mathbb{C}, \mathbb{H}$ where $\mathbb{H}$ denotes the quaternions.

(ii) The representation: let us start with the easy case, $\mathbb{K} = \mathbb{R}, \mathbb{H}$ in all components of the algebra. The algebras $M_n(\mathbb{R})$ and $M_n(\mathbb{H})$ only have one irreducible representation, the fundamental one on $\mathbb{C}^{(n)}$, where $(n) = n$ for $\mathbb{K} = \mathbb{R}$ and $(n) = 2n$ for $\mathbb{K} = \mathbb{H}$. Therefore ρ is of the form

$$\rho(\oplus_{i=1}^N a_i) := (\oplus_{i,j=1}^N a_i \otimes 1_{m_{ji}} \otimes 1_{(n_j)}) \oplus (\oplus_{i,j=1}^N 1_{(n_i)} \otimes 1_{m_{ji}} \otimes \overline{a_j}). \tag{3.1}$$

The multiplicities m_{ij} are non-negative integers and we denote by 1_n the $n \times n$ identity matrix and set by convention $1_0 := 0$. At the same time the real structure J permutes the two main summands and complex conjugates them, while the S^0-real structure and the chirality read

$$\epsilon = (\oplus_{i,j=1}^N 1_{(n_i)} \otimes 1_{m_{ij}} \otimes 1_{(n_j)}) \oplus (\oplus_{i,j=1}^N 1_{(n_i)} \otimes (-1) 1_{m_{ji}} \otimes 1_{(n_j)}), \tag{3.2}$$

$$\chi = (\oplus_{i,j=1}^N 1_{(n_i)} \otimes \chi_{ji} 1_{m_{ji}} \otimes 1_{(n_j)}) \oplus (\oplus_{i,j=1}^N 1_{(n_i)} \otimes \chi_{ji} 1_{m_{ji}} \otimes 1_{(n_j)}), \tag{3.3}$$

where $\chi_{ij} = \pm 1$ according to our previous convention on left- (right-) handed spinors.

We define the *multiplicity matrix* $\mu \in M_N(\mathbb{Z})$ such that $\mu_{ij} := \chi_{ij} m_{ij}$. There are N minimal projectors in $\mathcal{A}$, each of the form $p_i = 0 \oplus \cdots \oplus 0 \oplus \mathrm{diag}(1_{(1)}, 0, \ldots, 0) \oplus 0 \oplus \cdots \oplus 0$. With respect to the basis $p_i/(1)$, the matrix of the intersection form is $\mu + \mu^T$.

If the algebra has summands with $\mathbb{K} = \mathbb{C}$, things get more complicated. Indeed $M_n(\mathbb{C})$ has two nonequivalent irreducible representations, the fundamental one and its complex conjugate, so we change (3.1) into

$$\rho(\oplus_{i=1}^{N} a_i) := (\oplus_{i,j=1;\alpha_i,\alpha_j}^{N} a_{i\alpha_i} \otimes 1_{m_{j\alpha_j i\alpha_i}} \otimes 1_{(n_j)}) \oplus (\oplus_{i,j=1}^{N} 1_{(n_i)} \otimes 1_{m_{j\alpha_j i\alpha_i}} \otimes \overline{a_{j\alpha_j}}), \tag{3.4}$$

where $\alpha_i = 1$ when $a_i \in M_{n_i}(\mathbb{K})$, $\mathbb{K} = \mathbb{R}, \mathbb{H}$ and $\alpha_i = 1,2$ when $a_i \in M_{n_i}(\mathbb{C})$, and $a_{i1} := a_i$, $a_{i2} := \overline{a_i}$.

Therefore the multiplicity matrix is an integer valued square matrix of size equal to the number of summands with $\mathbb{K} = \mathbb{R}$ and $\mathbb{H}$ plus two times the number of summands with $\mathbb{K} = \mathbb{C}$ and decomposes into N^2 submatrices of size 1×1, 2×2, 1×2, and 2×1. For example $\mathcal{A} = M_n(\mathbb{C}) \oplus M_m(\mathbb{C}) \oplus M_q(\mathbb{R}) \ni (a,b,c)$ has a 5×5 multiplicity matrix. Let us label its rows and columns with algebra elements:

$$\mu = \begin{pmatrix} \mu_{aa} & \mu_{ab} & \mu_{ac} \\ \mu_{ba} & \mu_{bb} & \mu_{bc} \\ \mu_{ca} & \mu_{cb} & \mu_{cc} \end{pmatrix} \begin{matrix} \frac{a}{a} \\ \frac{b}{b} \\ c \end{matrix} .$$
$$\begin{matrix} a\overline{a} & b\overline{b} & c \end{matrix}$$

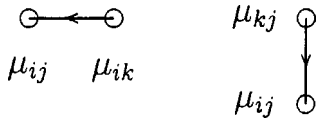
If both entries μ_{ij} and μ_{ji} of the multiplicity matrix are nonzero, then they must have the same sign.

The nonvanishing entries within each submatrix 1×2 or 2×1, like μ_{ca} or μ_{ac}, must have the same sign, while the signs of the nonvanishing entries in each 2×2 submatrix, e.g., μ_{aa} or μ_{ab} must be checkerboardlike, $\left(\begin{smallmatrix} + & - \\ - & + \end{smallmatrix}\right)$ or $\left(\begin{smallmatrix} - & + \\ + & - \end{smallmatrix}\right)$.

The *contracted multiplicity matrix* $\hat{\mu}$ is the $N \times N$ matrix constructed from μ by replacing each of the previous submatrices in μ by the sum of the entries of the submatrix.

(i) Poincaré duality: The last condition to be satisfied by the multiplicity matrix reflects the Poincaré duality. With respect to the basis $p_i/(1)$ introduced above, $(1) = 1$ for $\mathbb{K} = \mathbb{R}$ and $\mathbb{C}$, $(1) = 2$ for $\mathbb{K} = \mathbb{H}$, the matrix of the intersection form is $\hat{\mu} + \hat{\mu}^T$. Therefore we must have $\det(\hat{\mu} + \hat{\mu}^T) \neq 0$.

(ii) The Dirac operator: The components of the (internal) Dirac operator are represented by horizontal or vertical lines connecting two nonvanishing entries of opposite signs in the multiplicity matrix μ and we will orient them from plus to minus. Each arrow represents a nonvanishing, complex submatrix in the Dirac operator: For instance μ_{ij} can be linked to μ_{ik} or μ_{kj} by



and these arrows represent, respectively, submatrices of $\mathcal{M}$ in $\mathcal{D}$ of type $M \otimes 1_{(n_i)}$ with M a complex $(n_j) \times (n_k)$ matrix and $1_{(n_j)} \otimes M$ with M a complex $(n_i) \times (n_k)$ matrix.

The requirement of nondegeneracy of a spectral triple means that every nonvanishing entry in the multiplicity matrix μ is touched by at least one arrow.

Convention for the diagrams: We will see that (for sums of up to three simple algebras) irreducibility implies that most entries of μ have an absolute value less than or equal to 2. So we will use a *simple arrow* to connect plus 1 to minus 1 and *double arrows* to connect plus 1 to minus 2 or plus 1 to minus 1 (Fig. 1).

Our arrows always point from plus, that is right chirality, to minus, that is left chirality. For a given algebra, every spectral triple is encoded in its multiplicity matrix which itself is encoded in its Krajewski diagram, a field of arrows. In our conventions, for particles, $\epsilon = 1$, the column label

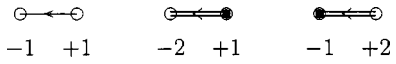
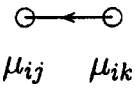


FIG. 1. Types of arrows.

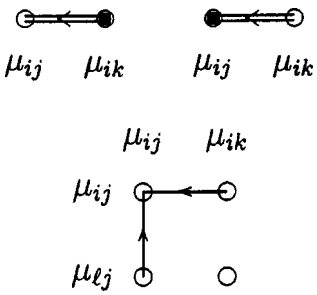
of the multiplicity matrix indicates the representation, the row label indicates the multiplicity. For antiparticles, the row label of the multiplicity matrix indicates the representation, the column label indicates the multiplicity.

Every arrow comes with three algebras: Two algebras that localize its end points, let us call them *right and left algebras* and a third algebra that localizes the arrow, let us call it *color algebra*. For example, for the arrow



the left algebra is $\mathcal{A}_j$, the right algebra is $\mathcal{A}_k$ and the color algebra is $\mathcal{A}_i$.

The *circles* in the diagrams only intend to guide the eye. A black disk on a double arrow indicates that the coefficient of the multiplicity matrix is plus or minus one at this location, "the two arrows are joined at this location." For example the the following arrows



represent respectively submatrices of $\mathcal{M}$ of type

$$\begin{pmatrix} M_1 \\ M_2 \end{pmatrix} \otimes 1_{(n_i)} \quad \text{and} \quad (M_1 \quad M_2) \otimes 1_{(n_i)}$$

with M_1, M_2 of size $(n_j)\times(n_k)$ or in the third case, a matrix of type $(M_1 \otimes 1_{(n_i)} \quad 1_{(n_j)} \otimes M_2)$ where M_1 and M_2 are of size $(n_j)\times(n_k)$ and $(n_i)\times(n_\ell)$.

According to these rules, we can omit the number ± 1, ± 2 under the arrows like in Fig. 2, since they are now redundant.

Let us give a few examples of the explicit form of the spectral triple associated to a given Krajewski diagram.

Take the algebra $\mathcal{A}=\mathbb{H}\oplus M_3(\mathbb{C})\ni(a,b)$ with the first diagram of Fig. 2. Then the multiplicity matrix and its contraction are

$$\mu=\begin{pmatrix} -1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{\mu}=\begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix}.$$

Using (2.4), its representation is, up to unitary equivalence

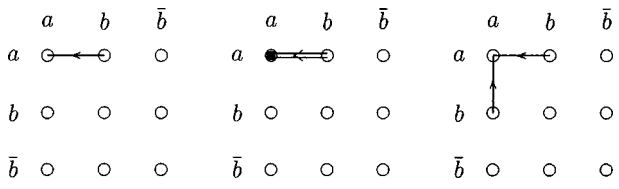


FIG. 2. Diagrams with complex conjugation.

$$\rho_L(a,b) = a \otimes 1_2, \quad \rho_R(a,b) = b \otimes 1_2, \quad \rho_L^c(a,b) = 1_2 \otimes a, \quad \rho_R^c(a,b) = 1_3 \otimes a.$$

The Hilbert space is

$$\mathcal{H} = \mathbb{C}^4 \oplus \mathbb{C}^6 \oplus \mathbb{C}^4 \oplus \mathbb{C}^6.$$

In its Dirac operator (2.5), $\mathcal{M} = M \otimes 1_2$, where M is a nonvanishing complex 2×3 matrix.

Real structure, S^0-real structure and chirality are given by (c.c. stands for complex conjugation)

$$J = \begin{pmatrix} 0 & 1_{10} \\ 1_{10} & 0 \end{pmatrix} \circ \text{c.c.}, \quad \epsilon = \begin{pmatrix} 1_{10} & 0 \\ 0 & -1_{10} \end{pmatrix}, \quad \chi = \begin{pmatrix} -1_4 & 0 & 0 & 0 \\ 0 & 1_6 & 0 & 0 \\ 0 & 0 & -1_4 & 0 \\ 0 & 0 & 0 & 1_6 \end{pmatrix}.$$

The first tensor factor in $a \otimes 1_2$ concerns particles, the second concerns antiparticles denoted by $\cdot^c$. The antiparticle representation is read from the transposed multiplicity matrix.

The second diagram of Fig. 2 yields

$$\mu = \begin{pmatrix} -1 & 2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{\mu} = \begin{pmatrix} -1 & 2 \\ 0 & 0 \end{pmatrix},$$

and its spectral triple reads

$$\rho_L(a,b) = a \otimes 1_2, \quad \rho_R(a,b) = \begin{pmatrix} b & 0 \\ 0 & b \end{pmatrix} \otimes 1_2,$$

$$\rho_L^c(a,b) = 1_2 \otimes a, \quad \rho_R^c(a,b) = \begin{pmatrix} 1_3 & 0 \\ 0 & 1_3 \end{pmatrix} \otimes a,$$

$$\mathcal{M} = (M_1 \quad M_2) \otimes 1_2, \; M_1 \text{ and } M_2 \text{ of size } 2 \times 3,$$

$$J = \begin{pmatrix} 0 & 1_{16} \\ 1_{16} & 0 \end{pmatrix} \circ \text{c.c.}, \quad \epsilon = \begin{pmatrix} 1_{16} & 0 \\ 0 & -1_{16} \end{pmatrix}, \quad \chi = \begin{pmatrix} -1_4 & 0 & 0 & 0 \\ 0 & 1_{12} & 0 & 0 \\ 0 & 0 & -1_4 & 0 \\ 0 & 0 & 0 & 1_{12} \end{pmatrix}.$$

In Krajewski's notations, Eq. (3.1), we would have written $\rho_R(a,b) = b \otimes 1_2 \otimes 1_2$, the middle factor showing the entry of multiplicity matrix μ.

Finally, still for the same algebra, let us consider the third diagram of Fig. 2. It gives

$$\mu = \begin{pmatrix} -1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{\mu} = \begin{pmatrix} -1 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\rho_L(a,b) = a \otimes 1_2, \quad \rho_R(a,b) = \begin{pmatrix} b \otimes 1_2 & 0 \\ 0 & a \otimes 1_3 \end{pmatrix},$$

$$\rho_L^c(a,b) = 1_2 \otimes a, \quad \rho_R^c(a,b) = \begin{pmatrix} 1_3 \otimes a & 0 \\ 0 & 1_2 \otimes b \end{pmatrix},$$

$$\mathcal{M} = (M_1 \otimes 1_2 \quad 1_2 \otimes M_2), \quad M_1 \text{ and } M_2 \text{ of size } 2 \times 3.$$

In the three above examples all arrows have left algebra $\mathbb{H}$, right algebra $M_3(\mathbb{C})$, and color algebra $\mathbb{H}$. The numerous examples below should allow the reader to get familiar with the translation between diagrams and triples.

B. Multiplicity matrix and irreducibility

Our work is based on the following lemma indicating that a classification of irreducible spectral triples is possible.

Lemma 3.1:

(i) The direct sum of multiplicity matrices is again a multiplicity matrix describing the direct sum of spectral triples.

(ii) For a given algebra there is only a finite list of multiplicity matrices describing irreducible triples.

Proof:

(i) is obvious.

(ii) Given an algebra $\mathcal{A}$, denote by $\mathcal{S}$ the set of multiplicity matrices $\mu \in M_n(\mathbb{Z})$ (n is determined by $\mathcal{A}$) associated to irreducible spectral triples. Define a partial order in $M_n(\mathbb{Z})$ by $\mu \geqslant \nu$ when μ_{ij} and ν_{ij} have the same sign and $|\mu_{ij}| \geqslant |\nu_{ij}|$ for all $i,j=1,\ldots,n$. The interest of this order is that for two different multiplicity matrices μ, ν such that $\mu \geqslant \nu$ and $\nu \in \mathcal{S}$, μ corresponds to a reducible triple.

To prove that card $(\mathcal{S}) < \infty$, we first identify $M_n(\mathbb{Z})$ with $\mathbb{Z}^{n^2}$. We denote by $\{e_i\}_{i \in \{1,\ldots,n^2\}}$ the canonical basis of $\mathbb{Z}^{n^2}$ and $\mathcal{S}^+ := \mathcal{S} \cap \mathbb{N}^{n^2}$. We now prove that card $(\mathcal{S}^+) < \infty$, which is sufficient.

Assume card $(\mathcal{S}^+) = \infty$. Then there exists at least one direction (say along e_1) such that $\sup\{(\mu)_1 \,|\, \mu \in \mathcal{S}^+\} = \infty$. Suppose now that in each hyperplane defined by me_1, $m \in \mathbb{N}$, all points $\mu \in \mathcal{S}^+$ remain uniformly bounded, $\mu_i < B$, $i=2,\ldots,n^2$. This means that there exists an infinite family of points in an hypertube parallel to e_1. Necessarily, there exists an infinite subfamily $\{\mu_k\}_{k \in \mathbb{N}} \subset \mathcal{S}^+$ of points in the hypertube which are aligned: $(\mu_k)_i = (\mu_{k+1})_i$, $\forall i \neq 1$ and $(\mu_k)_1 < (\mu_{k+1})_1$. But this is impossible since $\mu_k \leqslant \mu_{k+1}$ cannot happen. As a consequence, there exists a second direction (say along e_2 after renumbering) where the intersection of successive hyperplanes along e_1 and e_2 contain an infinite family of points of $\mathcal{S}^+$. By induction, the same reasoning in each direction e_i implies that there exists an infinite family $\{\mu_k\}_k$ of points in $\mathcal{S}^+$ with increasing vectors: $(\mu_k)_i < (\mu_{k+1})_i$, $\forall i$. Again this yields the contradiction $\mu_k \leqslant \mu_{k+1}$ and $\mu_{k+1} \notin \mathcal{S}^+$. □

IV. FLUCTUATIONS AND DYNAMICAL NONDEGENERACY

The aim of this work is twofold. First, we work out all irreducible real, S^0-real diagrams for algebras with one, two, and three simple summands. Second, we give all associated spectral triples that are dynamically nondegenerate. By this we mean the following. The spectrum of the (internal) Dirac operator $\mathcal{D}$ is always degenerate: all nonvanishing eigenvalues come in pairs of opposite sign due to the chirality that anticommutes with $\mathcal{D}$. All eigenvalues appear twice due to the real structure that commutes with $\mathcal{D}$. There is a further degeneracy, twofold in the example above, $\mathcal{M} = M \otimes 1_2$, that comes from the first order axiom. Let us call it *color degeneracy*. It is absent if and only if the color algebras of all arrows are commutative. Of course, these three degeneracies survive the fluctuations of the Dirac operator and the minimization of the Higgs potential. By dynamical nondegenerate we mean (see precise definition below) that no minimum of the Higgs potential has degeneracies other than the above three. The first two degeneracies survive *quantum fluctuations* as well. We also want the color degeneracies to be protected from quantum fluctua-

tions. A natural protection is unbroken gauge invariance, a requirement that we will include into the definition of dynamical nondegeneracy.

Except for complex conjugation in $M_n(\mathbb{C})$ and permutations of identical summands in the algebra $\mathcal{A}=\mathcal{A}_1\oplus\mathcal{A}_2\oplus\ldots\oplus\mathcal{A}_N$, every algebra automorphism σ is inner, $\sigma(a)=uau^{-1}$ for a unitary $u\in U(\mathcal{A})$. Therefore the connected component of the automorphism group is $\mathrm{Aut}(\mathcal{A})^e = U(\mathcal{A})/(U(\mathcal{A})\cap\mathrm{Center}(\mathcal{A}))$. Its lift to the Hilbert space[5]

$$L(\sigma)=\rho(u)J\rho(u)J^{-1}$$

is multivalued.

The *fluctuation* ${}^f\mathcal{D}$ of the Dirac operator $\mathcal{D}$ is given by a finite collection f of real numbers r_j and algebra automorphisms $\sigma_j\in\mathrm{Aut}(\mathcal{A})^e$ such that

$${}^f\mathcal{D}:=\sum_j r_j L(\sigma_j)\mathcal{D}\,L(\sigma_j)^{-1},\quad r_j\in\mathbb{R},\quad \sigma_j\in\mathrm{Aut}(\mathcal{A})^e.$$

The fluctuated Dirac operator ${}^f\mathcal{D}$ is often denoted by φ, the Higgs scalar, in the physics literature. We consider only fluctuations with real coefficients since ${}^f\mathcal{D}$ must remain self-adjoint.

To avoid the multivaluedness in the fluctuations, we allow the entire unitary group viewed as a (maximal) central extension of the automorphism group. We will come back to minimal central extensions in another work.

An almost commutative geometry is the tensor product of a finite noncommutative triple with an infinite, commutative spectral triple. By Connes' reconstruction theorem [6] we know that the latter comes from a Riemannian spin manifold, which we will take to be any four-dimensional, compact, flat manifold like the flat 4-torus. The spectral action of this almost commutative spectral triple reduced to the finite part is a functional on the vector space of all fluctuated, finite Dirac operators,

$$V({}^f\mathcal{D})=\lambda\ \mathrm{tr}[({}^f\mathcal{D})^4]-\frac{\mu^2}{2}\mathrm{tr}[({}^f\mathcal{D})^2],$$

where λ and μ are positive constants.[3,11] The spectral action is invariant under lifted automorphisms and even under the unitary group $U(\mathcal{A})\ni u$,

$$V([\rho(u)J\rho(u)J^{-1}]{}^f\mathcal{D}[\rho(u)J\rho(u)J^{-1}]^{-1})=V({}^f\mathcal{D}),$$

and it is bounded from below. Our task is to find the minima $\hat{}^f\mathcal{D}$ of this action, their spectra and their *little groups*

$$G_\ell:=\{\,u\in U(\mathcal{A})),[\rho(u)J\rho(u)J^{-1}]\hat{}^f\mathcal{D}[\rho(u)J\rho(u)J^{-1}]^{-1}=\hat{}^f\mathcal{D}\}.$$

Definition 4.1: The irreducible spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *dynamically nondegenerate* if all minima $\hat{}^f\mathcal{D}$ of the action $V({}^f\mathcal{D})$ define a nondegenerate spectral triple $(\mathcal{A},\mathcal{H},\hat{}^f\mathcal{D})$ and if the spectra of all minima have no degeneracies other than the three kinematical degeneracies: left–right, particle–antiparticle, and color. Of course in the massless case there is no left–right degeneracy. We also suppose that the color degeneracies are protected by the little group. By this we mean that all eigenvectors of $\hat{}^f\mathcal{D}$ corresponding to the same eigenvalue are in a common orbit of the little group (and scalar multiplication and charge conjugation).

In physicists' language this last requirement means noncommutative color groups are unbroken. It ensures that the corresponding mass degeneracies are protected from quantum corrections.

V. STATEMENT OF THE RESULT

The main result of this work is the following:

Theorem 5.1: *The sum of simple algebras,* $\mathcal{A}=\oplus_{i=1}^N\mathcal{A}_i$ *with* $N=1,2,3$ *admits a finite, real,*

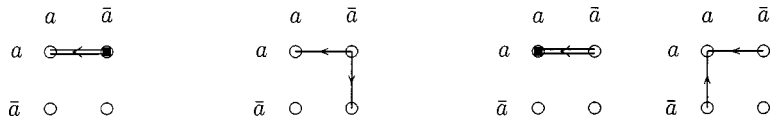


FIG. 3. One algebra: all irreducible diagrams.

S^0-real, irreducible and dynamically nondegenerate spectral triple if and only if it is in this list, up to a reordering of the summands:

$N=1$	$N=2$	$N=3$
	$\mathbf{1}\oplus\mathbf{1}$	$\mathbf{1}\oplus\mathbf{1}\oplus\mathcal{C}$
void		$\mathbf{1}\oplus\mathbf{1}\oplus\mathbf{1}$
		$\mathbf{2}\oplus\mathbf{1}\oplus\mathcal{C}$
	$\mathbf{2}\oplus\mathbf{1}$	$\mathbf{2}\oplus\mathbf{1}\oplus\mathbf{1}$

Here **1** *is a shorthand for* $\mathbb{R}$ *or* $\mathbb{C}$ *and* **2** *for* $M_2(\mathbb{R})$, $M_2(\mathbb{C})$, *or* $\mathbb{H}$.
The color algebra $\mathcal{C}$ *is any simple algebra and has two important constraints*:

(i) *Its representations on corresponding left- and right-handed subspaces of* $\mathcal{H}$ *are identical (up to possibly different multiplicities).*
(ii) *The Dirac operator* $\mathcal{D}$ *is invariant under* $U(\mathcal{C})$,

$$\rho(1,1,w)\mathcal{D}\rho(1,1,w)^{-1}=\mathcal{D}, \quad \text{for all } w\in U(\mathcal{C}).$$

This implies that the unitaries of $\mathcal{C}$ *do not participate in the fluctuations and are therefore unbroken, i.e., elements of the little group.*

Let us emphasize that although the four-dimensional space–time manifold M used to define the almost commutative geometry does not show up in this result, it is an important ingredient of the spectral action and its asymptotic behavior. In particular the dimension of M is linked to the order of the polynomial V. Therefore our classification indeed concerns four-dimensional, almost commutative geometries.

We give in Sec. IX A an example of a reducible triple which is dynamically nondegenerate and whose algebra is not in the above list.

VI. ONE SIMPLE ALGEBRA

From the classification,[10,14] we know that $\mathcal{A}=M_n(\mathbb{C})$ are the only simple algebras to admit real spectral triples. Up to permutation of a and $\overline{a}$ (complex conjugation in $\mathcal{A}$), up to permutation of particles and antiparticles (reflection of the diagram with respect to the main diagonal) and up to permutation of left- and right-handed particles (changing the direction of all arrows), all real S^0-real and irreducible triples have Krajewski diagrams indicated in Fig. 3.

Indeed, a Krajewski diagram must contain at least one arrow which can be put into the position $\mu=\left(\begin{smallmatrix}-1 & +1\\ 0 & 0\end{smallmatrix}\right)$ by use of the three above permutations. However, alone this arrow does not fulfill Poincaré duality, $\hat{\mu}+\hat{\mu}^T=0$. There are four ways to add a second arrow. But Poincaré duality can only be satisfied if the two arrows are joined in one point. Adding a third arrow makes the corresponding spectral triples reducible.

The first diagram yields

$$\rho_L(a)=\begin{pmatrix}a & 0\\ 0 & a\end{pmatrix}\otimes 1_n, \quad \rho_R(a)=\overline{a}\otimes 1_n, \quad \rho_L^c(a)=1_n\otimes\begin{pmatrix}a & 0\\ 0 & a\end{pmatrix}, \quad \rho_R^c(a)=1_n\otimes a,$$

$$\mathcal{M} := M \otimes 1_n := \begin{pmatrix} M_1 \\ M_2 \end{pmatrix} \otimes 1_n, \quad M_1, M_2 \in M_n(\mathbb{C}). \tag{6.1}$$

Real structure, S^0-real structure and chirality are

$$J = \begin{pmatrix} 0 & 1_{3n^2} \\ 1_{3n^2} & 0 \end{pmatrix} \circ \text{c.c.}, \quad \epsilon = \begin{pmatrix} 1_{3n^2} & 0 \\ 0 & -1_{3n^2} \end{pmatrix}, \quad \chi = \begin{pmatrix} -1_{2n^2} & 0 & 0 & 0 \\ 0 & +1_{n^2} & 0 & 0 \\ 0 & 0 & -1_{2n^2} & 0 \\ 0 & 0 & 0 & +1_{n^2} \end{pmatrix}.$$

Let us write the fluctuations of $\mathcal{D}$ as

$${}^f\mathcal{D} := \begin{pmatrix} 0 & {}^f\mathcal{M} & 0 & 0 \\ {}^f\mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & {}^f\overline{\mathcal{M}} \\ 0 & 0 & {}^f\overline{\mathcal{M}}^* & 0 \end{pmatrix}. \tag{6.2}$$

Here

$${}^f\mathcal{M} = {}^fM \otimes 1_n = \begin{pmatrix} {}^fM_1 \\ {}^fM_1 \end{pmatrix} \otimes 1_n.$$

Then

$${}^fM_1 = \sum_j r_j u_j M_1 u_j^T, \quad {}^fM_2 = \sum_j r_j u_j M_2 u_j^T, \quad \text{so} \quad {}^fM = \sum_j r_j \begin{pmatrix} u_j & 0 \\ 0 & u_j \end{pmatrix} \begin{pmatrix} M_1 \\ M_2 \end{pmatrix} u_j^T \tag{6.3}$$

and

$$V({}^f\mathcal{D}) = \lambda \ \mathrm{tr}[{}^f\mathcal{D}^4] - \frac{\mu^2}{2}\mathrm{tr}[{}^f\mathcal{D}^2] = 4n\left(\lambda \ \mathrm{tr}[({}^fM * {}^fM)^2] - \frac{\mu^2}{2}\mathrm{tr}[{}^fM * {}^fM]\right).$$

The matrix ${}^fM$ is of size $2n \times n$. Therefore the fluctuation ${}^f\mathcal{D}$ has at least n vanishing eigenvalues each still coming with its n-fold color degeneracy and all triples with $n \geqslant 2$ are dynamically degenerate since ${}^fM {}^fM^* \in M_{2n}(\mathbb{C})$ has at least n zero eigenvalues.

For $n=1$, all minima of the action V are of the form $|\hat{}^fM_1|^2 + |\hat{}^fM_2|^2 = \mu^2/4\lambda$. But the corresponding fluctuated Dirac operator has a nontrivial invariant subspace in its kernel and the triple is degenerate. To make the subspace explicit apply a unitary change of basis to set ${}^fM_2$ to zero. In every minimum the little group is $\mathbb{Z}_2$.

At this point, an overkill is instructive. We will show that the case $n \geqslant 2$ also features dynamical degeneracy in the nonzero eigenvalues.

In general, the set of all possible fluctuations ${}^f\mathcal{D}$, i.e., the image under the fluctuations (6.3), is difficult to describe. However, the action V only depends on the positive $n \times n$ matrix $C := {}^fM^* {}^fM$ and is a sum of n^2 polynomials of fourth order in the matrix elements of C,

$$V(C) = 4n\left[\sum_{i=1}^{n}\left(\lambda C_{ii}^2 - \frac{\mu^2}{2}C_{ii}\right) + \sum_{i \neq j}\lambda |C_{ij}|^2\right]. \tag{6.4}$$

If $C = (\mu^2/4\lambda)/1_n$ is in this image then it is the unique minimum in terms of the variable C.

To compute the minima of the action, we now distinguish cases.

Case 1: At least one diagonal element of one of the two matrices is nonzero.

After a suitable renumbering of the basis of the Hilbert space $\mathcal{H}$, we may assume $(M_1)_{11} \neq 0$. With a first fluctuation,

$$r_1=\frac{1}{2},\quad r_2=\frac{1}{2},\quad u_1=1_n,\quad u_2=\begin{pmatrix}1 & 0\\ 0 & -1_{n-1}\end{pmatrix},$$

we obtain for ${}^fM$ a block diagonal matrix with 2×2 blocks. By means of the fluctuation

$$r_1=\frac{1}{2},\quad r_2=\frac{1}{2},\quad u_1=1_n,\quad u_2=\begin{pmatrix}1 & 0\\ 0 & i1_{n-1}\end{pmatrix},$$

we isolate the (1,1) elements of M_1 and M_2 and with $r_1=r_2=\cdots=r_n=1$, $u_1=1_n$,

$$u_2=\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1_{n-2}\end{pmatrix},\quad u_3=\begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1_{n-3}\end{pmatrix},\quad u_4=\begin{pmatrix}0 & 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1_{n-4}\end{pmatrix},\quad \ldots$$

we distribute them over the entire diagonal obtaining

$${}^fM=\begin{pmatrix}(M_1)_{11}1_n\\ (M_2)_{11}1_n\end{pmatrix}.$$

Then C is a nonvanishing multiple of the identity and a suitable multiple of the above ${}^fM$ is a minimum. The spectrum of this minimum $\hat{}^f\mathcal{D}$ has an additional dynamical degeneracy and up to the sign, $\hat{}^f\mathcal{D}$ has one single eigenvalue. The little group is $G_\ell=O(n)$. Note also that $\hat{}^fM_1$ and $\hat{}^fM_2$ are proportional, $\hat{}^fM_1=\alpha\hat{}^fM_2$, $\alpha\in\mathbb{C}$, so there is a unitary change of basis in the Hilbert space $\mathcal{H}$ such that $\hat{}^fM_2=0$ in the new basis and the spectral triple $(M_n(\mathbb{C}),\mathcal{H},\hat{}^f\mathcal{D})$ is degenerate.

Case 2: All diagonal elements of M_1 and M_2 vanish but M_1 and M_2 are not both skewsymmetric.

After a suitable renumbering, we may assume $(M_1)_{12}=\beta-\gamma$, $(M_1)_{21}=\beta+\gamma$, $(M_1)_{11}=(M_1)_{22}=0$, with $\beta\neq 0$. As in case 1 we can isolate this block. Fluctuating with

$$r_1=1,\quad u_1=\begin{pmatrix}1/\sqrt{2} & -1/\sqrt{2} & 0\\ 1/\sqrt{2} & 1/\sqrt{2} & 0\\ 0 & 0 & 1_{n-2}\end{pmatrix},$$

we obtain $({}^fM_1)_{11}=-\beta$ and conclude as in case 1.

Case 3: M_1 and M_2 are skewsymmetric and linearly dependent.

Thus M can be written as $M=M_1\otimes\binom{1}{\alpha}$, $\alpha\in\mathbb{C}$ and by a unitary change of basis, we may assume $\alpha=0$ that is $M_2=0$ without changing the representation (6.1). Then the spectral triple is degenerate. Let us nevertheless finish this case. By another unitary change of basis (or fluctuation), cf. Appendix A1, we set

$$M_1=\begin{pmatrix}\begin{pmatrix}0 & -\lambda_1\\ \lambda_1 & 0\end{pmatrix} & & & \\ & \begin{pmatrix}0 & -\lambda_2\\ \lambda_2 & 0\end{pmatrix} & & \\ & & \ddots & \\ & & & 0\end{pmatrix},$$

where the zero in the lower right corner concerns the case n odd. Let us suppose that λ_1 is not zero. By isolating the upper left block and by distributing it over the entire diagonal we obtain a ${}^fM_{1i}=\lambda_1$ for all i. If n is even, we then have the minimum $\hat{C}=(\mu^2/4\lambda)/1_n$ for $V(C)$. Its spectrum

is again completely degenerate with little group $G_\ell = \mathrm{USp}(n/2)$. If n is odd the spectrum of ${}^{\hat{f}}\mathcal{D}$ contains four vanishing eigenvalues, all others being of the same absolute value and $G_\ell = \mathrm{USp}[(n-1)/2] \times \mathrm{U}(1)$.

Case 4: M_1 and M_2 are skewsymmetric and linearly independent:

Then ${}^fM_1$ and ${}^fM_2$ vary independently over all skewsymmetric matrices (cf. Lemma 11.10). For $n=3$ the minimization can be done by direct calculation. All minima are gauge equivalent to

$$ {}^{\hat{f}}M = \frac{\mu}{\sqrt{6\lambda}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \hat{C} := {}^{\hat{f}}M^{*\hat{f}}M = \frac{\mu^2}{6\lambda} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. $$

Although the spectrum has a twofold dynamical degeneracy the little group is only $G_\ell = U(1) \ni \mathrm{diag}(e^{i\theta}, e^{-i\theta}, e^{-i\theta})$. For general n, we were unable to compute a minimum explicitly, but we will show that its spectrum is dynamically degenerate. To alleviate notations let us rescale variables, ${}^f\mathcal{D} \to (\mu\sqrt{2\mu})/{}^f\mathcal{D}$. Then the spectral action reads for $C_i := {}^fM_i^{*f}M_i$,

$$ V({}^fM_1, {}^fM_2) = \frac{n\mu^4}{\lambda}(\mathrm{tr}[C_1^2] - \mathrm{tr}[C_1] + \mathrm{tr}[C_2^2] - \mathrm{tr}[C_2] + 2\mathrm{tr}[C_1C_2]). $$

All minima of this fourth order polynomial have vanishing partial derivatives with respect to ${}^fM_1^*$ and ${}^fM_2^*$. These equations read

$$ {}^{\hat{f}}M_1 = 2{}^{\hat{f}}M_1{}^{\hat{f}}M_1{}^{*\hat{f}}M_1 + {}^{\hat{f}}M_1{}^{\hat{f}}M_2{}^{*\hat{f}}M_2 + {}^{\hat{f}}M_2{}^{\hat{f}}M_2{}^{*\hat{f}}M_1, \tag{6.5} $$

$$ {}^{\hat{f}}M_2 = 2{}^{\hat{f}}M_2{}^{\hat{f}}M_2{}^{*\hat{f}}M_2 + {}^{\hat{f}}M_2{}^{\hat{f}}M_1{}^{*\hat{f}}M_1 + {}^{\hat{f}}M_1{}^{\hat{f}}M_1{}^{*\hat{f}}M_2. \tag{6.6} $$

Let us set $X := \hat{C}_1$, $Y := \hat{C}_2$, and $Z := {}^{\hat{f}}M_1{}^{*\hat{f}}M_2$. We multiply Eq. (6.5) from the left by ${}^{\hat{f}}M_1$ and likewise for (6.6) to get

$$ X = 2X^2 + XY + ZZ^*, \tag{6.7} $$

$$ Y = 2Y^2 + XY + Z^*Z. \tag{6.8} $$

Subtracting (6.7) from its Hermitian conjugate, we have that X and Y commute and subtracting (6.8) and (6.7) we get

$$ 2(X-Y)(X+Y-\tfrac{1}{2}1_n) = [Z^*, Z]. \tag{6.9} $$

Multiplying (6.6) from the left with ${}^{\hat{f}}M_1{}^*$ and multiplying the Hermitian conjugate of (6.5) from the right with ${}^{\hat{f}}M_2$, we have

$$ Z = 2ZY + ZX + XZ, $$

$$ Z = 2XZ + YZ + ZY. \tag{6.10} $$

Taking the difference, we find that Z commutes with $X+Y$.

We are to show that the spectrum of $\hat{C} = {}^{\hat{f}}M^{*\hat{f}}M = X+Y$ is degenerate: Let us suppose that it is nondegenerate. Take an orthonormal basis of eigenvectors of $\hat{C}$. Then it is also an eigenbasis of Z implying that $[Z, Z^*] = 0$ and by (6.9) the eigenvalues x_j and y_j of X and Y corresponding to the jth

basis vector satisfy at least one of the equations $x_j=y_j$, $x_j+y_j=1/2$. But as $\hat{}^f M_1$ and $\hat{}^f M_2$ are skewsymmetric, each eigenvalue of X and Y is doubly degenerate with the exception of one vanishing eigenvalue if n is odd. This contradicts the nondegeneracy of $X+Y$.

The triple of the second diagram of Fig. 3 differs from the first only with respect to representation and Dirac operator

$$\rho_L(a)=\begin{pmatrix} a & 0 \\ 0 & \overline{a} \end{pmatrix}\otimes 1_n, \quad \rho_R(a)=\overline{a}\otimes 1_n, \quad \rho_L^c(a)=1_n\otimes\begin{pmatrix} a & 0 \\ 0 & \overline{a} \end{pmatrix}, \quad \rho_R^c(a)=1_n\otimes a,$$

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_n \\ 1_n\otimes M_2 \end{pmatrix}, \quad M_1,M_2\in M_n(\mathbb{C}).$$

Again, nondegeneracy of the zero eigenvalue requires $n=1$ and all minima, $|\hat{}^f M_1|^2+|\hat{}^f M_2|^2=\mu^2/4\lambda$, have little group $\mathbb{Z}_2$. But now all minima of the action V are not gauge equivalent. Indeed when $\hat{}^f M_1=\mu(4\lambda)^{-1/2}$, $\hat{}^f M_2=0$ and $\mathrm{Ker}(\mathcal{D})=\mathrm{Span}\{\mathcal{H}_{L2},\mathcal{H}_{L2}^c\}$. Thus the eigenvector in the image of $(1/2)(1-\epsilon)$ associated to the zero eigenvalue of the fluctuated Dirac operator, which is in $\mathcal{H}_{L2}$, transforms under $\rho(u)J\rho(u)J^{-1}$ as multiplication by u^{-2}, while it transforms as multiplication by u^2 when $\hat{}^f M_2=\mu(4\lambda)^{-1/2}$. According to our definition the triple is dynamically degenerate because in both cases, the eigenvectors define a one-dimensional complex subspace invariant under $\mathcal{A}$ and contained in the kernel of the fluctuated Dirac operator $\hat{}^f\mathcal{D}$.

The last two diagrams of Fig. 3 are treated as the first two and yield the same conclusions.

VII. TWO SIMPLE ALGEBRAS

Again our starting point is the list, Fig. 4, all irreducible Krajewski diagrams up to the three mentioned types of permutations and up to permutations of the two algebras and disregarding any direct sum of two diagrams from Fig. 3.

Let k and ℓ be the size of the matrices of $\mathcal{A}_1=M_n(\mathbb{K})\ni a$ and $\mathcal{A}_2=M_m(\mathbb{K})\ni b$. For example, $k=n$ for $\mathcal{A}_1=M_n(\mathbb{R})$ or $M_n(\mathbb{C})$ and $k=2n$ for $\mathcal{A}_1=M_n(\mathbb{H})$. The first diagram of Fig. 4 yields

$$\rho_L(a,b)=a\otimes 1_k, \quad \rho_R(a,b)=b\otimes 1_k, \quad \rho_L^c(a,b)=1_k\otimes a, \quad \rho_R^c(a,b)=1_\ell\otimes a,$$

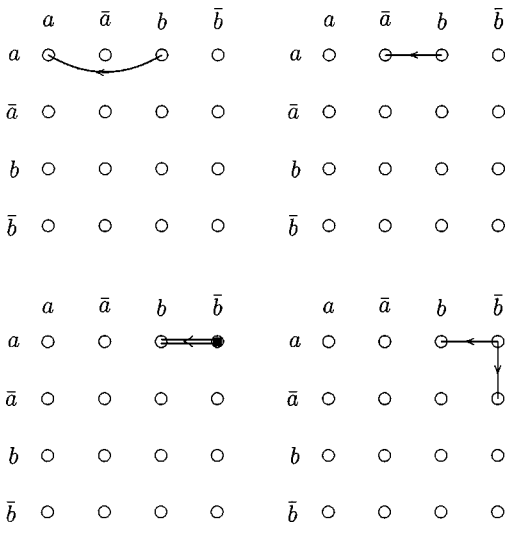


FIG. 4. Two algebras: all irreducible diagrams.

$$\mathcal{M} = M \otimes 1_k, \quad M \in M_{k\times\ell}(\mathbb{C}).$$

M is nonzero and we may assume $M_{11} \neq 0$. Except for the k-fold color degeneracy, we accept at most one zero eigenvalue of M^*M. Therefore we must have $k=\ell$ or $k=\ell\pm 1$. We assume $\ell \leqslant k$. Let in (6.2)

$$^f\mathcal{M} = {}^fM \otimes 1_k, \quad {}^fM = \sum_j r_j u_j M v_j^{-1}, \quad u_j \in U(\mathcal{A}_1), \quad v_j \in U(\mathcal{A}_2).$$

If $k \geqslant 2$, $\ell > 2$ or $k > 2$, $\ell \geqslant 2$, we may isolate the upper 2×2 block by fluctuations: With the first fluctuation,

$$r_1 = \frac{1}{2}, \quad r_2 = \frac{1}{2}, \quad u_1 = 1_k, \quad v_1 = 1_\ell, \quad u_2 \begin{pmatrix} 1_2 & 0 \\ 0 & -1_{k-2} \end{pmatrix}, \quad v_2 \begin{pmatrix} 1_2 & 0 \\ 0 & -1_{\ell-2} \end{pmatrix},$$

we obtain for M a block diagonal type matrix. By means of the fluctuation

$$r_1 = \frac{1}{2}, \quad r_2 = \frac{1}{2}, \quad u_1 = 1_k, \quad v_1 = 1_\ell, \quad u_2 = 1_k, \quad v_2 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_{\ell-2} \end{pmatrix}$$

we isolate the upper block. If $k=\ell=2$ this step is empty.

Now we may distinguish cases.

Case 1: $\mathcal{A}_1 = M_n(\mathbb{R})$ or $M_n(\mathbb{C})$, $\mathcal{A}_2 = M_m(\mathbb{R})$ or $M_m(\mathbb{C})$: like above, we isolate M_{11} and as in case 1 for one algebra we distribute M_{11} over the entire diagonal, obtaining thus ${}^fM^*{}^fM$ proportional to the identity. The spectrum of the fluctuated Dirac operator ${}^f\mathcal{D}$ minimizing the action V has an ℓ-fold dynamical degeneracy.

Case 2: $\mathcal{A}_1 = M_n(\mathbb{H})$, $\mathcal{A}_2 = M_m(\mathbb{H})$, define the fluctuation

$$r_1 = \frac{1}{2}, \quad r_2 = \frac{1}{4}, \quad r_3 = \frac{1}{4}, \quad u_1 = 1_k, \quad v_1 = 1_\ell, \quad u_2 = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & 0 \\ 0 & 1_{k-2} \end{pmatrix},$$

$$v_2 = \begin{pmatrix} \pm\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & 0 \\ 0 & 1_{\ell-2} \end{pmatrix}, \quad u_3 = \begin{pmatrix} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} & 0 \\ 0 & 1_{k-2} \end{pmatrix}, \quad v_3 = \begin{pmatrix} \pm\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} & 0 \\ 0 & 1_{\ell-2} \end{pmatrix},$$

the upper block is proportional to 1_2. The plus signs in $\pm$ are used if $M_{11} = M_{22}$. We distribute the block over the diagonal and get an ℓ-fold dynamical degeneracy (recall that $\ell \leqslant k$).

Case 3: $\mathcal{A}_1 = M_n(\mathbb{R})$ or $M_n(\mathbb{C})$, $\mathcal{A}_2 = M_m(\mathbb{H})$. If $M_{12}=0$ we fluctuate with

$$r_1 = r_2 = \frac{1}{4}, \quad r_3 = \frac{1}{2}, \quad u_1 = 1_k, \quad v_1 = 1_\ell, \quad u_2 = \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0 \\ 0 & 1_{k-2} \end{pmatrix}, \quad v_2 = 1_\ell,$$

$$u_3 = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0 \\ 0 & 1_{k-2} \end{pmatrix}, \quad v_3 = \begin{pmatrix} -\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} & 0 \\ 0 & 1_{\ell-2} \end{pmatrix},$$

and obtain

$$ {}^fM = \begin{pmatrix} \begin{pmatrix} M_{11} & 0 \\ 0 & -M_{11} \end{pmatrix} & 0 \\ 0 & 0 \end{pmatrix}. $$

If $M_{12} \neq 0$ we fluctuate with

$$ r_1 = r_2 = \frac{1}{4}, \quad r_3 = \frac{1}{2}, \quad u_1 = 1_k, \quad v_1 = 1_\ell, \quad u_2 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_{k-2} \end{pmatrix}, \quad v_2 = 1_\ell, $$

$$ u_3 = 1_k, \quad v_3 = \begin{pmatrix} \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} & 0 \\ 0 & -1_{\ell-2} \end{pmatrix}, $$

with $\theta := \frac{1}{2}(\mathrm{Arg}(M_{11}) - \mathrm{Arg}(M_{12}))$ and obtain

$$ f_M = \begin{pmatrix} \begin{pmatrix} e^{i\theta}M_{11} & e^{-i\theta}M_{12} \\ 0 & 0 \end{pmatrix} & 0 \\ 0 & 0 \end{pmatrix}. $$

In both cases, we distribute the 2×2 block over the diagonal and achieve ${}^fM^{*fM}$ proportional to the identity.

In all three cases, ℓ must be one to avoid dynamical degeneracy.

The second diagram of Fig. 4 is treated in the same fashion. The last two diagrams of Fig. 4 have no letter changing arrow, an arrow connecting an a to a b. They are treated as the triples with one simple algebra: *Counting neutrinos*, that is requiring at most one zero eigenvalue (up to a possible color degeneracy) yields $\mathcal{A} = \mathbb{C} \oplus \mathbb{C}$ and degeneracy.

Finally using the permutations we get the list of all irreducible, dynamically nondegenerate triples with two algebras:

There are the commutative triples, that is the two-point spaces, $\mathcal{A} = \mathbb{C} \oplus \mathbb{C} \ni (a, b)$,

$$ \rho(a,b) = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & \overline{a} & 0 \\ 0 & 0 & 0 & \overline{a} \end{pmatrix}, \quad \text{and in } \mathcal{D},\ \mathcal{M} \in \mathbb{C}. \tag{7.1} $$

There is a second one with the same algebra,

$$ \rho(a,b) = \begin{pmatrix} \overline{a} & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & \overline{a} & 0 \\ 0 & 0 & 0 & \overline{a} \end{pmatrix}. \tag{7.2} $$

And there are the real versions, $\mathcal{A} = \mathbb{C} \oplus \mathbb{R}$, $\mathbb{R} \oplus \mathbb{C}$, and $\mathbb{R} \oplus \mathbb{R}$.

The noncommutative triples have $\mathcal{A} = M_2(\mathbb{C}) \oplus \mathbb{C} \ni (a, b)$ with four irreducible triples,

$$ \rho(a,b) = \begin{pmatrix} a \otimes 1_2 & 0 & 0 & 0 \\ 0 & b1_2 & 0 & 0 \\ 0 & 0 & 1_2 \otimes \overline{a} & 0 \\ 0 & 0 & 0 & \overline{a} \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} 0 \\ m \end{pmatrix} \otimes 1_2, \quad m \in \mathbb{C}, \tag{7.3} $$

$$\rho(a,b)=\begin{pmatrix} \overline{a}\otimes 1_2 & 0 & 0 & 0\\ 0 & b1_2 & 0 & 0\\ 0 & 0 & 1_2\otimes\overline{a} & 0\\ 0 & 0 & 0 & \overline{a}\end{pmatrix},\quad \mathcal{M}=\begin{pmatrix}0\\ m\end{pmatrix}\otimes 1_2, \tag{7.4}$$

$$\rho(a,b)=\begin{pmatrix} a & 0 & 0 & 0\\ 0 & b & 0 & 0\\ 0 & 0 & \overline{b}1_2 & 0\\ 0 & 0 & 0 & \overline{b}\end{pmatrix},\quad \mathcal{M}=\begin{pmatrix}0\\ m\end{pmatrix}, \tag{7.5}$$

$$\rho(a,b)=\begin{pmatrix} a & 0 & 0 & 0\\ 0 & \overline{b} & 0 & 0\\ 0 & 0 & \overline{b}1_2 & 0\\ 0 & 0 & 0 & \overline{b}\end{pmatrix},\quad \mathcal{M}=\begin{pmatrix}0\\ m\end{pmatrix}, \tag{7.6}$$

In all four cases, all minima $\hat{f}\mathcal{D}$ are gauge equivalent to the Dirac operator $\mathcal{D}$ with the absolute value of m fixed in terms of λ and μ and the little groups are

$$G_\ell=\mathrm{U}(1)\times\mathrm{U}(1)\ni\left(\begin{pmatrix}e^{i\alpha} & 0\\ 0 & e^{-i\beta}\end{pmatrix},e^{i\beta}\right).$$

In the two triples (7.3) and (7.4), the unitaries of the color algebra, $M_2(\mathbb{C})$, are spontaneously broken, they do not leave any minimum invariant, $\mathrm{U}(2)\not\subset G_\ell$. According to our definition these two triples are dynamically degenerate.

Then there are diverse real versions: replace the complex 2×2 matrices $M_2(\mathbb{C})$ by quaternions $\mathbb{H}$ or by real matrices $M_2(\mathbb{R})$ and/or replace $\mathbb{C}$ by $\mathbb{R}$. For the real forms, of course, we have no complex conjugations in the representations. We summarize the little groups (arrows mean group homomorphisms):

$$\begin{array}{lll}
\mathbb{C}\oplus\mathbb{C} & \supset \mathrm{U}(1)\times\mathrm{U}(1) & \to \mathrm{U}(1),\\
\mathbb{C}\oplus\mathbb{R} & \supset \mathrm{U}(1)\times\mathbb{Z}_2 & \to \mathrm{U}(1),\\
\mathbb{R}\oplus\mathbb{R} & \supset \mathbb{Z}_2\times\mathbb{Z}_2 & \to \mathbb{Z}_2,\\
M_2(\mathbb{C})\oplus\mathbb{C} & \supset \mathrm{U}(2)\times\mathrm{U}(1) & \to \mathrm{U}(1)\times\mathrm{U}(1),\\
M_2(\mathbb{C})\oplus\mathbb{R} & \supset \mathrm{U}(2)\times\mathbb{Z}_2 & \to \mathrm{U}(1)\times\mathbb{Z}_2,\\
\mathbb{H}\oplus\mathbb{C} & \supset \mathrm{SU}(2)\times\mathrm{U}(1) & \to \mathrm{U}(1),\\
\mathbb{H}\oplus\mathbb{R} & \supset \mathrm{SU}(2)\times\mathbb{Z}_2 & \to \mathbb{Z}_2,\\
M_2(\mathbb{R})\oplus\mathbb{C} & \supset \mathrm{O}(2)\times\mathrm{U}(1) & \to \mathbb{Z}_2\times\mathbb{Z}_2,\\
M_2(\mathbb{R})\oplus\mathbb{R} & \supset \mathrm{O}(2)\times\mathbb{Z}_2 & \to \mathbb{Z}_2\times\mathbb{Z}_2.
\end{array} \tag{7.7}$$

The triples (7.3) or its commutative version (7.1) and (7.4) or its commutative version (7.2), (7.5), and (7.6) are represented by the four diagrams of Fig. 5.

VIII. THREE SIMPLE ALGEBRAS

A. Proof for $N=3$

So far, we found that all irreducible dynamically nondegenerate triples were associated to diagrams with letter changing arrows only, i.e., arrows connecting two different algebras. These

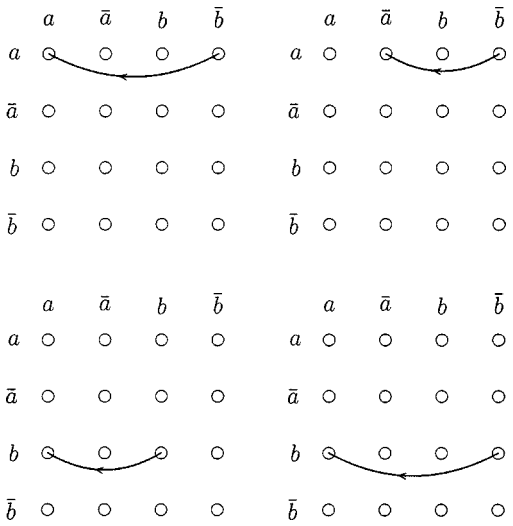


FIG. 5. Two algebras: all diagrams with nondegenerate triples.

arrows are stable under contraction of the multiplicity matrix. Therefore we start by constructing all irreducible contracted diagrams, Fig. 6. In other words we neglect the complex conjugate representations.

This list becomes exhaustive upon permutations of the three algebras $\mathcal{A}_1=M_n(\mathbb{K})\ni a$, $\mathcal{A}_2=M_m(\mathbb{K})\ni b$, $\mathcal{A}_3=M_q(\mathbb{K})\ni c$, upon permuting left and right, i.e., changing the directions of all two or three arrows simultaneously, and upon permutations of particles and antiparticles independently in every connected component of the diagram.

Let k, ℓ, p be the sizes of the matrices a,b,c.

Diagram 1 yields the following:

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 \\ 0 & b\otimes 1_\ell \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 \\ 0 & c\otimes 1_\ell \end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 \\ 0 & 1_\ell\otimes b \end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 \\ 0 & 1_p\otimes b \end{pmatrix},$$

and

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0 \\ 0 & M_2\otimes 1_\ell \end{pmatrix},\quad M_1\in M_{k\times\ell}(\mathbb{C}),\quad M_2\in M_{\ell\times p}(\mathbb{C}).$$

The fluctuations,

$${}^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in U(\mathcal{A}_1),\quad v_j\in U(\mathcal{A}_2),$$

$${}^fM_2=\sum_j r_j v_j M_2 w_j^{-1},\quad w_j\in U(\mathcal{A}_3),$$

produce two *decoupled* fields ${}^fM_1$ and ${}^fM_2$ as can be seen by applying the fluctuation, $r_1=1/2$, $u_1=1_k$, $v_1=1_\ell$, $w_1=1_p$, $r_2=1/2$, $u_2=1_k$, $v_2=1_\ell$, $w_2=-1_p$.

Since the arrows M_1 and M_2 are disconnected, the action is a sum of an action in ${}^fM_1$ and of an action in ${}^fM_2$. Proceeding as in the preceding section we find that a minimum $\hat{{}^fM_1}$ has $\min\{k,\ell\}$

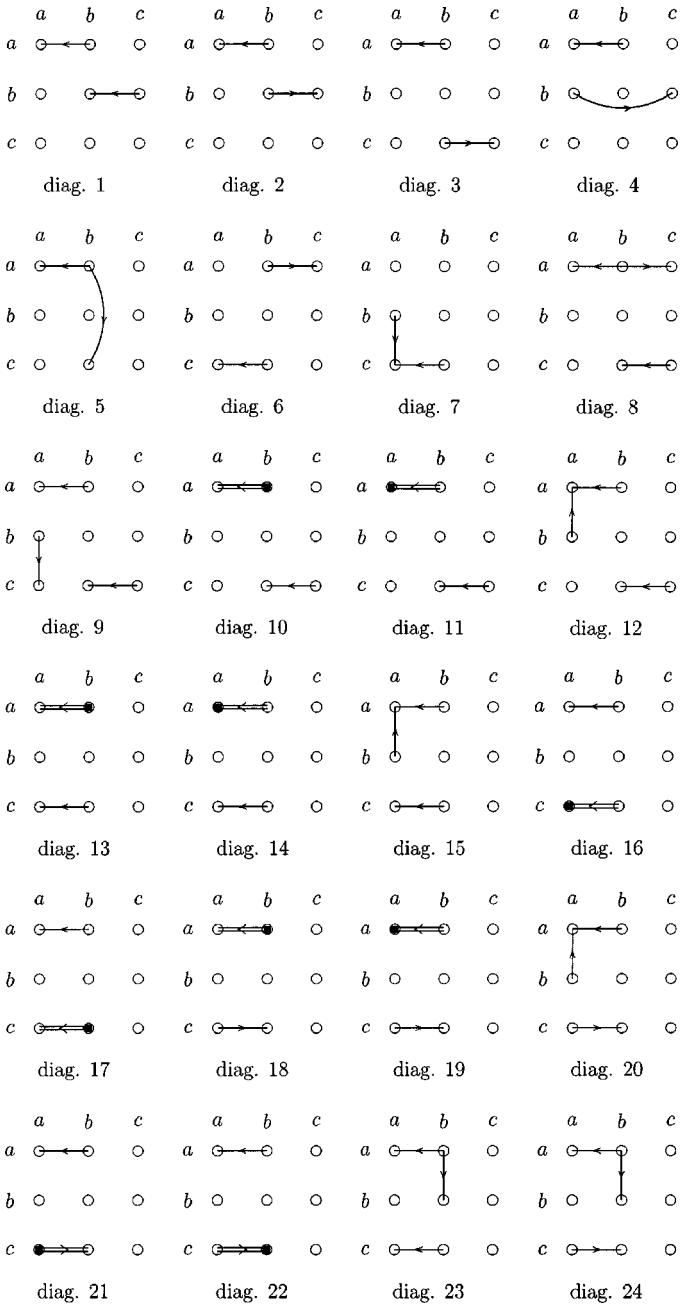


FIG. 6. Three algebras: all irreducible diagrams before blow up.

eigenvalues $\mu(4\lambda)^{-1/2}$ and $|k-\ell|$ eigenvalues zero $\hat{}^{f}M_2$ has $\min\{\ell,p\}$ eigenvalues $\mu(4\lambda)^{-1/2}$ and $|\ell-p|$ eigenvalues zero. All triples associated to the first diagram and therefore dynamically degenerate.

For the same reason, we can discard diagrams 2, 3, 4, 6, because they also have two disconnected horizontal arrows not vertically aligned.

Diagram 5 yields the following:

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 \\ 0 & b\otimes 1_p \end{pmatrix}, \quad \rho_R(a,b,c)=b\otimes 1_k,$$

$$\rho_L^c(a,b,c)=\begin{pmatrix}1_k\otimes a & 0\\ 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=1_\ell\otimes a,$$

$$\mathcal{M}=\begin{pmatrix}M_1\otimes 1_k\\ 1_\ell\otimes M_2\end{pmatrix},\quad M_1\in M_{k\times\ell}(\mathbb{C}),\quad M_2\in M_{p\times k}(\mathbb{C}).$$

Again the fluctuations,

$${}^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in U(\mathcal{A}_1),\quad v_j\in U(\mathcal{A}_2),$$

$${}^fM_2=\sum_j r_j w_j M_2 u_j^{-1},\quad w_j\in U(\mathcal{A}_3),$$

produce two decoupled fields ${}^fM_1$ and ${}^fM_2$ but now the arrows are connected and consequently, the action does not decouple,

$$V(C_1,C_2)=4k[\lambda\ \mathrm{tr}(C_1^2)-\tfrac{1}{2}u^2\ \mathrm{tr}(C_1)]+4\ell[\lambda\ \mathrm{tr}(C_2^2)-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_2)]+8\lambda\ \mathrm{tr}(C_1)\mathrm{tr}(C_2),$$

where $C_i:={}^fM_i^{*}{}^fM_i$. Let $x_1,x_2,\ldots,x_\ell$ be the eigenvalues of C_1 and $y_1,y_2\ldots,y_k$ be the eigenvalues of C_2. The action only depends on these variables and in its minimum all x_i are equal or vanish and all y_i are equal or vanish. The spectrum of the minimal Dirac operator ${}^{\hat{f}}\mathcal{D}$ contains at most three nonvanishing numbers, $\sqrt{x}$, $\sqrt{y}$, $\sqrt{x+y}$ implying that k and ℓ are less than or equal to 2. The fermionic mass matrix $\mathcal{M}$ is of size $(k^2+\ell p)\times(k\ell)$. To get at most one zero eigenvalue we must require $|k^2+\ell p-k\ell|\leqslant 1$ implying $k=p=1$. For $\ell=1$ the minimum is at $|{}^{\hat{f}}M_1|^2+|{}^{\hat{f}}M_2|^2=\mu^2/4\lambda$, for $\ell=2$ the minimum is at ${}^{\hat{f}}M_1=0$, $|{}^{\hat{f}}M_2|^2=\mu^2/4\lambda$. In both cases, ${}^{\hat{f}}M_1=0$, the triple is degenerate in the sense that the Dirac operator has an invariant subspace in the kernel.

Diagram 7 falls in the same way.

Diagram 8 yields the representations

$$\rho_L(a,b,c)=\begin{pmatrix}a\otimes 1_k & 0 & 0\\ 0 & c\otimes 1_k & 0\\ 0 & 0 & b\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix}b\otimes 1_k & 0\\ 0 & c\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix}1_k\otimes a & 0 & 0\\ 0 & 1_p\otimes a & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix}1_\ell\otimes a & 0\\ 0 & 1_p\otimes c\end{pmatrix}.$$

The possible complex conjugations in the representation will not be important in this diagram. The mass matrix is

$$\mathcal{M}=\begin{pmatrix}M_1\otimes 1_k & 0\\ M_2\otimes 1_k & 0\\ 0 & M_3^{*}\otimes 1_p\end{pmatrix},\quad M_1\in M_{k\times\ell}(\mathbb{C}),\quad M_2,M_3\in M_{p\times\ell}(\mathbb{C}).$$

The fluctuations are

$$ {}^fM_1 = \sum_j r_j u_j M_1 v_j^{-1}, \quad u_j \in U(\mathcal{A}_1), \quad v_j \in U(\mathcal{A}_2), $$

$$ {}^fM_2 = \sum_j r_j w_j M_2 v_j^{-1}, \quad w_j \in U(\mathcal{A}_3), $$

$$ {}^fM_3 = \sum_j r_j w_j M_3 v_j^{-1}, $$

and the action is, with $C_i := {}^fM_i^{*\,f}M_i$,

$$ V(C_1,C_2,C_3) = 4k\left[\lambda\ \mathrm{tr}(C_1+C_2)^2 - \tfrac{1}{2}u^2\ \mathrm{tr}(C_1+C_2)\right] + 4p\left[\lambda\ \mathrm{tr}(C_3)^2 - \tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)\right]. $$

Requiring at most one zero eigenvalue (up to a possible color degeneracy) implies $k=1$, $\ell = p+1$ or $k=1$, $\ell = p$. In both cases ${}^fM_1$ and ${}^fM_2$ vary independently. The color group consists of the u's and w's. As they are spontaneously broken we must have $k=p=1$, leaving $\ell=1$ and $\ell=2$. In the commutative case with no complex conjugations in the representation, ${}^fM_3 = \beta\,{}^fM_2$ for a complex constant $\beta \neq 0$. If $|\beta| \geqslant 1$ the minimum is given by

$$ \left|\hat{f}M_1\right|^2 = \frac{(1-|\beta|^{-2})\mu^2}{4\lambda}, \quad \left|\hat{f}M_2\right|^2 = \frac{|\beta|^{-2}\mu^2}{4\lambda}, \quad \text{and } \left|\hat{f}M_3\right|^2 = \frac{\mu^2}{4\lambda}. $$

Its mass spectrum $\{0, \mu/4\lambda, \mu/4\lambda\}$ is dynamically degenerate. If $|\beta| \leqslant 1$ the minimum is given by

$$ \left|\hat{f}M_1\right|^2 = 0, \quad \left|\hat{f}M_2\right|^2 = \frac{1+|\beta|^2}{1+|\beta|^4}\frac{\mu^2}{4\lambda}, \quad \text{and } \left|\hat{f}M_3\right|^2 = \frac{|\beta|^2(1+|\beta|^2)}{1+|\beta|^4}\frac{\mu^2}{4\lambda}. $$

The triple is degenerate because of the invariant subspace in the kernel of the Dirac operator. With additional complex conjugations in the representation, ${}^{\hat{f}}M_3$ may decouple from ${}^{\hat{f}}M_2$ and the triple becomes dynamically degenerate as in diagram 1.

In the noncommutative case $k=1$, $\ell=2$, $p=1$, M_1 and M_2 must be linearly independent. To get a nondegenerate triple for any choice of $\mathcal{A}_1$ and $\mathcal{A}_3 = \mathbb{R}$ or $\mathbb{C}$ and $\mathcal{A}_2 = M_2(\mathbb{R})$, $M_2(\mathbb{C})$ or $\mathbb{H}$ it is sufficient to take the example $M_1 = (m_1, 0)$, $M_2 = (0, m_2)$, $M_3 = \beta M_2$. The minimum is given by ${}^{\hat{f}}M_1\,{}^{\hat{f}}M_2^* = 0$ and

$$ \left|\hat{f}M_1\right|^2 = \frac{\mu^2}{4\lambda}, \quad \left|\hat{f}M_2\right|^2 = \frac{1+|\beta|^2}{1+|\beta|^4}\frac{\mu^2}{4\lambda}, \quad \text{and } \left|\hat{f}M_3\right|^2 = |\beta|^2\frac{1+|\beta|^2}{1+|\beta|^4}\frac{\mu^2}{4\lambda}, $$

dynamically nondegenerate for $\beta \neq 0$ and $|\beta| \neq 1$.

Let us note a new phenomenon: the three eigenvalues of a minimum ${}^{\hat{f}}\mathcal{D}$ are tied together by a *mass relation*. Its origin is clear, when we add more and more irreducible components to the Hilbert space the number of possible fluctuations does not change, the number of components in the Dirac operator increases. This phenomenon does not only occur for the particular choice of the mass matrices M_1, M_2, and M_3 above, but is generic for diagram 8. The little groups are the same as the last six in (7.7).

Diagram 9 yields the representations

$$ \rho_L(a,b,c) = \begin{pmatrix} a\otimes 1_k & 0 & 0 \\ 0 & a\otimes 1_p & 0 \\ 0 & 0 & b\otimes 1_p \end{pmatrix}, \quad \rho_R(a,b,c) = \begin{pmatrix} b\otimes 1_k & 0 & 0 \\ 0 & a\otimes 1_\ell & 0 \\ 0 & 0 & c\otimes 1_p \end{pmatrix}, $$

$$\rho_L^c(a,b,c)=\begin{pmatrix}1_k\otimes a & 0 & 0\\ 0 & 1_k\otimes c & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix}1_\ell\otimes a & 0 & 0\\ 0 & 1_k\otimes b & 0\\ 0 & 0 & 1_p\otimes c\end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix}M_1\otimes 1_k & 0 & 0\\ 0 & 1_k\otimes M_2^* & 0\\ 0 & 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1\in M_{k\times\ell}(\mathbb{C}),\quad M_2,M_3\in M_{\ell\times p}(\mathbb{C}).$$

The fluctuations are

$$^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in U(\mathcal{A}_1),\quad v_j\in U(\mathcal{A}_2),$$

$$^fM_2=\sum_j r_j u_j M_2 w_j^{-1},\quad w_j\in U(\mathcal{A}_3),$$

$$^fM_3=\sum_j r_j v_j M_3 w_j^{-1},$$

and the action $V(C_1,C_2,C_3)$ is equal to

$$4k[\lambda\ \mathrm{tr}(C_1)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_1)]+4k[\lambda\ \mathrm{tr}(C_2)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_2)]+4p[\lambda\ \mathrm{tr}(C_3)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)].$$

Counting neutrinos and imposing broken color to be commutative leaves only one case, $k=\ell=p=1$. We choose $M_3=\beta M_2$ and get the minima at

$$\left|\hat{f}_{M_1}\right|^2=\frac{\mu^2}{4\lambda},\quad \left|\hat{f}_{M_2}\right|^2=\frac{1+|\beta|^2}{1+|\beta|^4}\frac{\mu^2}{4\lambda},\quad \left|\hat{f}_{M_3}\right|^2=|\beta|^2\frac{1+|\beta|^2}{1+|\beta|^4}\frac{\mu^2}{4\lambda},$$

so it is dynamically nondegenerate for $\beta\neq 0$ and $|\beta|\neq 1$.

Diagram 10 yields the representations

$$\rho_L(a,b,c)=\begin{pmatrix}a\otimes 1_k & 0 & 0\\ 0 & a\otimes 1_k & 0\\ 0 & 0 & b\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix}b\otimes 1_k & 0\\ 0 & c\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix}1_k\otimes a & 0 & 0\\ 0 & 1_k\otimes a & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix}1_\ell\otimes a & 0\\ 0 & 1_p\otimes c\end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix}M_1\otimes 1_k & 0\\ M_2\otimes 1_k & 0\\ 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_2\in M_{k\times\ell}(\mathbb{C}),\quad M_3\in M_{\ell\times p}(\mathbb{C}).$$

The fluctuations are

$$^fM_1 = \sum_j r_j u_j M_1 v_j^{-1}, \quad u_j \in U(\mathcal{A}_1), \quad v_j \in U(\mathcal{A}_2),$$

$$^fM_2 = \sum_j r_j u_j M_2 v_j^{-1},$$

$$^fM_3 = \sum_j r_j v_j M_3 w_j^{-1}, \quad w_j \in U(\mathcal{A}_3),$$

and the action is

$$V(C_1,C_2,C_3) = 4k[\lambda\ \mathrm{tr}(C_1+C_2)^2 - \tfrac{1}{2}u^2\ \mathrm{tr}(C_1+C_2)] + 4p\left[\lambda\ \mathrm{tr}(C_3)^2 - \frac{1}{2}\mu^2\ \mathrm{tr}(C_3)\right].$$

Neutrino counting implies $k=1$, $\ell=2$, $p=1$ or $k=\ell=p=1$. In both cases $^fM_3$ varies independently of $^fM_1$ and $^fM_2$.

The commutative case has always $|\hat{}^fM_1|^2+|\hat{}^fM_2|^2=|\hat{}^fM_3|^2=\mu^2(4\lambda)^{-1}$ and is dynamically degenerate.

In the noncommutative case $k=1$, $\ell=2$, $p=1$, M_1 and M_2 must be linearly independent. For $\mathcal{A}_1\oplus\mathcal{A}_2=\mathbb{R}\oplus M_2(\mathbb{C})$, $\mathbb{C}\oplus M_2(\mathbb{R})$, and $\mathbb{C}\oplus M_2(\mathbb{C})$, lemma 11.6 decouples $^fM_1$ and $^fM_2$ and the triples are dynamically degenerate, $\hat{}^fM_1=(\mu(4\lambda)^{-1/2},0)$, $\hat{}^fM_2=(0,\mu(4\lambda)^{-1/2})$, $\hat{}^fM_3=(0,\mu(4\lambda)^{-1/2})^T$. For $\mathcal{A}_1\oplus\mathcal{A}_2=\mathbb{R}\oplus\mathbb{H}$ and $\mathbb{C}\oplus\mathbb{H}$ we choose

$$\rho_L(a,b,c) = \begin{pmatrix} a\otimes 1_k & 0 & 0 \\ 0 & \overline{a}\otimes 1_k & 0 \\ 0 & 0 & b\otimes 1_p \end{pmatrix}, \quad M_1=(m_1,0), \quad M_2=(0,\alpha m_1).$$

Its minimum has the nondegenerate spectrum $\{(1+|\alpha|^2)/(1+|\alpha|^4),[|\alpha|^2(1+|\alpha|^2)/(1+|\alpha|^4)],1,0\}$ in units of $\mu^2/4\lambda$ with one mass relation. Finally for $\mathcal{A}_1\oplus\mathcal{A}_2=\mathbb{R}\oplus M_2(\mathbb{C})$ we choose $M_1=(i,1)$ and $M_2=(1,0)$ to obtain the nondegenerate spectrum $\{(2\pm\sqrt{2})/3,1,0\}$ in units of $\mu^2/4\lambda$.

Diagram 11 yields the representations

$$\rho_L(a,b,c) = \begin{pmatrix} a\otimes 1_k & 0 \\ 0 & b\otimes 1_p \end{pmatrix}, \quad \rho_R(a,b,c) = \begin{pmatrix} b\otimes 1_k & 0 & 0 \\ 0 & b\otimes 1_k & 0 \\ 0 & 0 & c\otimes 1_p \end{pmatrix},$$

$$\rho_L^c(a,b,c) = \begin{pmatrix} 1_k\otimes a & 0 \\ 0 & 1_\ell\otimes c \end{pmatrix}, \quad \rho_R^c(a,b,c) = \begin{pmatrix} 1_\ell\otimes a & 0 & 0 \\ 0 & 1_\ell\otimes a & 0 \\ 0 & 0 & 1_p\otimes c \end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & M_2\otimes 1_k & 0\\ 0 & 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_2\in M_{k\times\ell}(\mathbb{C}),\quad M_3\in M_{\ell\times p}(\mathbb{C}).$$

The fluctuations are

$$^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in U(\mathcal{A}_1),\quad v_j\in U(\mathcal{A}_2),$$

$$^fM_2=\sum_j r_j u_j M_2 v_j^{-1},$$

$$^fM_3=\sum_j r_j u_j M_3 w_j^{-1},\quad w_j\in U(\mathcal{A}_3),$$

and then action is

$$V(C_1,C_2,C_3)=4k[\lambda\ \mathrm{tr}(C_1+C_2)^2-\tfrac{1}{2}u^2\ \mathrm{tr}(C_1+C_2)]+4p[\lambda\ \mathrm{tr}(C_3)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)].$$

Neutrino counting and imposing broken color to be commutative leaves only one possibility, $k=\ell=p=1$, which is treated as the case $k=\ell=p=1$ of diagram 10 with the same conclusion, degeneracy.

Diagram 12 yields the representations

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0\\ 0 & b\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0\\ 0 & a\otimes 1_\ell & 0\\ 0 & 0 & c\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0\\ 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0\\ 0 & 1_k\otimes b & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 1_k\otimes M_2 & 0\\ 0 & 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_2\in M_{k\times\ell}(\mathbb{C}),\quad M_3\in M_{\ell\times p}(\mathbb{C}).$$

The fluctuations are

$$^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in \mathrm{U}(\mathcal{A}_1),\quad v_j\in \mathrm{U}(\mathcal{A}_2),$$

$$^fM_2=\sum_j r_j u_j M_2 v_j^{-1},$$

$$^fM_3=\sum_j r_j v_j M_3 w_j^{-1},\quad w_j\in \mathrm{U}(\mathcal{A}_3).$$

The action $V(C_1,C_2,C_3)$ equals

$$4k[\lambda\ \mathrm{tr}(C_1)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_1)]+4k[\lambda\ \mathrm{tr}(C_2)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_2)]+8\lambda\ \mathrm{tr}(C_1)\mathrm{tr}(C_2)+4p[\lambda\ \mathrm{tr}(C_3)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)].$$

Since the neutrino count and imposing broken color to be commutative implies $k=\ell=p=1$. Then $M_2=\alpha M_1$ and we must distinguish two cases, $^fM_2=\alpha\,^fM_1$ or $^fM_1$ and $^fM_2$ independent. Both

possibilities have a dynamically degenerate minimum, $|\hat{}^f M_1|^2+|\hat{}^f M_2|^2=|\hat{}^f M_3|^2=\mu^2/4\lambda$.

Diagram 13 has a *ladder form*, i.e., it consists of horizontal arrows, vertically aligned. Its representations are

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 & 0\\ 0 & a\otimes 1_k & 0\\ 0 & 0 & a\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0\\ 0 & b\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 & 0\\ 0 & 1_k\otimes a & 0\\ 0 & 0 & 1_k\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0\\ 0 & 1_\ell\otimes c\end{pmatrix},$$

with possible complex conjugations here and there. The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0\\ M_2\otimes 1_k & 0\\ 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_2,M_3\in M_{k\times\ell}(\mathbb{C}).$$

The fluctuations are

$$^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in \mathrm{U}(\mathcal{A}_1),\quad v_j\in \mathrm{U}(\mathcal{A}_2),$$

$$^fM_2=\sum_j r_j u_j M_2 v_j^{-1},$$

$$^fM_3=\sum_j r_j u_j M_3 v_j^{-1},$$

and the action is

$$V(C_1,C_2,C_3)=4k[\lambda\ \mathrm{tr}(C_1+C_2)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_1+C_2)]+4p[\lambda\ \mathrm{tr}(C_3)^2-\tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)].$$

The neutrino count implies $k=1,\ell=2$ or $k=\ell=1$.

The case $k=\ell=1$ has the following possibilities.

Case 1: $\mathbb{R}\oplus\mathbb{R}\oplus\mathcal{C}$, where $\mathcal{C}$ is any simple color algebra. All possible triples are degenerate in the sense that the Dirac operator has an invariant subspace in its kernel.

Case 2: $\mathbb{R}\oplus\mathbb{C}\oplus\mathcal{C}$, all possible triples are degenerate.

Case 3: $\mathbb{C}\oplus\mathbb{R}\oplus\mathcal{C}\ni(a,b,c)$. The nondegenerate triples have

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0\\ 0 & \overline{a} & 0\\ 0 & 0 & \overline{a}\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0\\ 0 & b\otimes 1_p\end{pmatrix}.$$

The fluctuations respect the mass ratios: $|M_1|:|M_2|:|M_3|=\underline{|}^fM_1\underline{|}:|^fM_2|:|^fM_3|$. If M_1 and M_2 are different from zero, the kernel of the Dirac operator, $\mathbb{C}(-M_2,M_1,01,0;-M_2,M_1,0,0,0)^T$, is not invariant under $a\in\mathbb{C}$. If $|M_3|^2\neq|M_1|^2+|M_2|^2$, the triple is dynamically nondegenerate.

Case 4: $\mathbb{C}\oplus\mathbb{C}\oplus\mathcal{C}\ni(a,b,c)$. The only not obviously degenerate triples have the representations

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0 \\ 0 & \overline{a} & 0 \\ 0 & 0 & \overline{a}\otimes 1_p \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0 \\ 0 & b\otimes 1_p \end{pmatrix}. \tag{8.1}$$

and

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0 \\ 0 & \overline{a} & 0 \\ 0 & 0 & \overline{a}\otimes 1_p \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0 \\ 0 & \overline{b}\otimes 1_p \end{pmatrix}. \tag{8.2}$$

The fluctuations do not respect all mass ratios, in fact ${}^fM_1$ and ${}^fM_2$ are independent variables and only the ratio $M_2/M_3={}^fM_2/{}^fM_3=:1/\beta$ is invariant under fluctuations via (8.1). If $|\beta|\geqslant 1$ the minima are given by

$$\left|\hat{f}M_1\right|^2=\frac{(1-|\beta|^{-2})\mu^2}{4\lambda},\quad \left|\hat{f}M_2\right|^2=\frac{\mu^2}{|\beta|^2 4\lambda},\quad \text{and}\quad \left|\hat{f}M_3\right|^2=\frac{\mu^2}{4\lambda}.$$

Its mass spectrum $\{0,\mu/2\sqrt{\lambda},\mu/2\sqrt{\lambda}\ p\ \text{times}\}$ is dynamically degenerate. If $|\beta|\leqslant 1$ the minima are given by

$$\left|\hat{f}M_1\right|^2=0,\quad \left|\hat{f}M_2\right|^2=\frac{1+p|\beta|^2}{1+p|\beta|^4}\,\frac{\mu^2}{4\lambda},\quad \text{and}\quad \left|\hat{f}M_3\right|^2=\frac{|\beta|^2(1+p|\beta|^2)}{1+p|\beta|^4}\frac{\mu^2}{4\lambda}.$$

The triple is degenerate since there is an invariant subspace in the kernel of the Dirac operator. For the representation (8.2) the computational are identical to the case above, (8.1), after permuting M_1 and M_2 and after replacing M_3 by $\overline{M_3}$.

In the case $k=1$, $\ell=2$, the three submatrices M_1, M_2, M_3 are linearly dependent over $\mathbb{C}$. If M_1 is proportional to M_2 then both M_3 and $\binom{M_1}{M_2}$ have a zero eigenvalue. Therefore M_1 and M_2 are linearly independent over $\mathbb{C}$ and $M_3=:\alpha M_1+\beta M_2$ with complex coefficients α and β.

Case 5: $\mathbb{C}\oplus M_2(\mathbb{C})\oplus\mathcal{C}\ni(a,b,c)$. By lemma 11.6, ${}^fM_1$ and ${}^fM_2$ vary independently in $\mathbb{C}^2$. For the representations with

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a\otimes 1_p \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0 \\ 0 & b\otimes 1_p \end{pmatrix}, \tag{8.3}$$

we get ${}^fM_3=:\alpha{}^fM_1+\beta{}^fM_2$. For instance for $\alpha=0$ we get $\hat{f}M_1\hat{f}M_2=0$ as for diagram 8 and a similar mass relation,

$$\left|\hat{f}M_1\right|^2=\frac{\mu^2}{4\lambda},\quad \left|\hat{f}M_2\right|^2=\frac{(1+p|\beta|^2)}{1+p|\beta|^4}\,\frac{\mu^2}{4\lambda},\quad \left|\hat{f}M_3\right|^2=|\beta|^2\frac{1+p|\beta|^2}{1+p|\beta|^4}\frac{\mu^2}{4\lambda}. \tag{8.4}$$

For general α, we get the same relations with $|\beta|^2$ replaced by $|\alpha|^2+|\beta|^2$. For the representations with

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0 \\ 0 & \overline{a} & 0 \\ 0 & 0 & \overline{a}\otimes 1_p \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0 \\ 0 & b\otimes 1_p \end{pmatrix},$$

and $\alpha\neq 0$, all three doublets, ${}^fM_1$, ${}^fM_2$, and ${}^fM_3$ vary independently. The minima, $|\hat{f}M_1|^2+|\hat{f}M_2|^2=|\hat{f}M_3|^2=\mu^2/4\lambda$ produce a dynamical degeneracy in this case. The other case, $\alpha=0$ is dynamically nondegenerate with the same mass relations as above, equations (8.4). All other representations of this algebra are treated the same way and they either have a mass relation or are

dynamically degenerate, which means a particularly simple mass relations.

Case 6: $\mathbb{R}\oplus M_2(\mathbb{C})\oplus\mathcal{C}$. This case is identical to case 5 with representation (8.3)

Case 7: $\mathbb{C}\oplus\mathbb{H}\oplus\mathcal{C}\ni(a,b,c)$. For example, all triples with

$$\rho_L(a,b,c)=\begin{pmatrix} a & 0 & 0\\ 0 & \overline{a} & 0\\ 0 & 0 & \overline{a}\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b & 0\\ 0 & b\otimes 1_p\end{pmatrix},$$

$M_1=(m_1,0)$, $M_2=(0,m_2)$, and $M_3=(0,m_3)$ have no mass relation. Indeed like in case 3, the mass ratios are stable under fluctuations: $|M_1|:|M_2|:|M_3|=|{}^fM_1|:|{}^fM_2|:|{}^fM_3|$. Other triples behave like in case 5.

Case 8: $\mathbb{R}\oplus\mathbb{H}\oplus\mathcal{C}$ has the same examples without mass relations as in case 7.

Case 9: $\mathbb{C}\oplus M_2(\mathbb{R})\oplus\mathcal{C}$. For representations (8.3) and $\alpha=0$, we get minima with mass relation (8.4).

Case 10: $\mathbb{R}\oplus M_2(\mathbb{R})\oplus\mathcal{C}$. Here we take a representation (8.3) with $M_1=(m_1,0)$, $M_2=(0,m_2)$, and $M_3=(0,\beta m_2)$ and get again the mass relation (8.4).

Up to different multiplicities, we have the same conclusion for the diagrams 18, 17, 22. After permuting $\mathcal{A}_1$ and $\mathcal{A}_2$ we also have the same results for the other four ladders, diagrams 14, 19, 16, 21.

Diagram 15 yields the representations

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0\\ 0 & a\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0\\ 0 & a\otimes 1_\ell & 0\\ 0 & 0 & b\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0\\ 0 & 1_k\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0\\ 0 & 1_k\otimes b & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 1_k\otimes M_2 & 0\\ 0 & 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_2,M_3\in M_{k\times\ell}(\mathbb{C}).$$

The fluctuations are

$${}^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in \mathrm{U}(\mathcal{A}_1),\quad v_j\in \mathrm{U}(\mathcal{A}_2),$$

$${}^fM_2=\sum_j r_j u_j M_2 v_j^{-1},$$

$${}^fM_3=\sum_j r_j u_j M_3 v_j^{-1}.$$

Neutrino counting and imposing broken color to be commutative implies $k=\ell=1$. This case with $\mathcal{A}_1$ and $\mathcal{A}_2=\mathbb{R}$ or $\mathbb{C}$ is treated as in diagram 13, case 3 yielding a nondegenerate triple without mass relation. After replacing M_3^* by M_3, diagram 20 has identical computations.

Diagram 23 yields the representations

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 & 0\\ 0 & b\otimes 1_\ell & 0\\ 0 & 0 & b\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0\\ 0 & a\otimes 1_p\end{pmatrix},$$

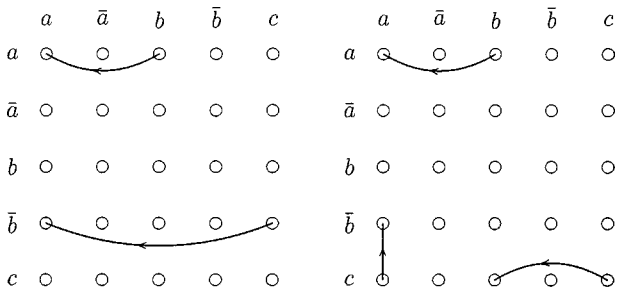


FIG. 7. Two blow ups, letter changing arrows only.

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 & 0\\ 0 & 1_\ell\otimes b & 0\\ 0 & 0 & 1_\ell\otimes c\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0\\ 0 & 1_k\otimes c\end{pmatrix},$$

with possible complex conjugations. The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0\\ 1_\ell\otimes M_2^* & 0\\ 0 & M_3^*\otimes 1_p\end{pmatrix},\quad M_1,M_2,M_3\in M_{k\times\ell}(\mathbb{C}).$$

The fluctuations are

$$^fM_1=\sum_j r_j u_j M_1 v_j^{-1},\quad u_j\in \mathrm{U}(\mathcal{A}_1),\quad v_j\in \mathrm{U}(\mathcal{A}_2),$$

$$^fM_2=\sum_j r_j u_j M_2 v_j^{-1},$$

$$^fM_3=\sum_j r_j u_j M_3 v_j^{-1}.$$

Neutrino counting implies $k=\ell=1$. This model with $\mathcal{A}_1$ and $\mathcal{A}_2=\mathbb{R}$ or $\mathbb{C}$ is treated as in diagram 13, case 3 yielding a nondegenerate triple without mass relation. After replacing M_3^* by M_3, diagram 24 has identical computations.

We must now extend our analysis to include the possibility of complex conjugate representations. As in the case of two algebras, one shows that any diagram containing a connected component consisting of only letter unchanging arrows leads to degenerate spectra. Therefore within the class of irreducible and dynamically nondegenerate triples the leitmotiv of a Krajewski diagram is still carried by its letter changing arrows. For three algebras there are two additional diagrams, diagrams 25, 26, Fig. 7, that involve only letter changing arrows. Their contracted diagrams resemble diagrams 4 and 9 of Fig. 6 except for the change of chirality in one arrow and the computation of their triples is similar.

Note that without the presence of conjugate representations, this change violates the condition that nonvanishing entries of the multiplicity matrix and its transposed must have the same signs. Figure 8 lists the contractions of all irreducible diagrams whose letter unchanging arrows are connected to at least one letter changing arrow. The blow up of the new symbols is given in Fig. 9.

All triples attached to the 11 diagrams of Fig. 8 are degenerate or dynamically degenerate.

Diagram 27 with the first blow up yields

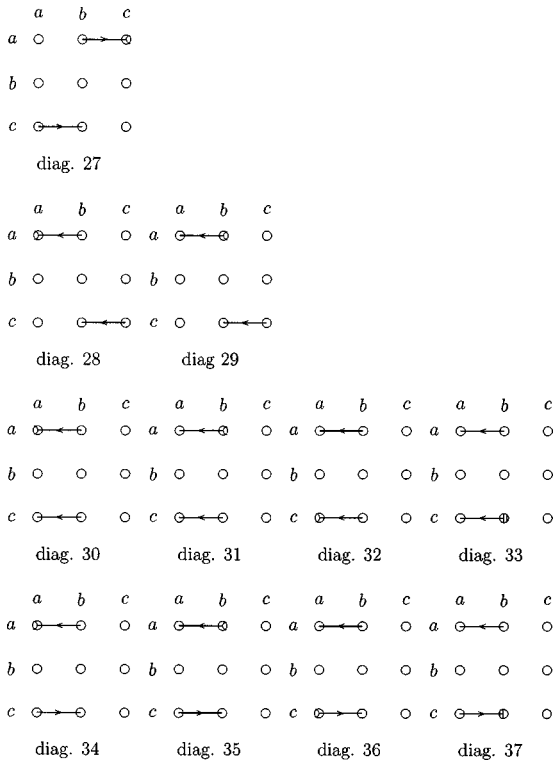


FIG. 8. Irreducible diagrams with letter unchanging arrows.

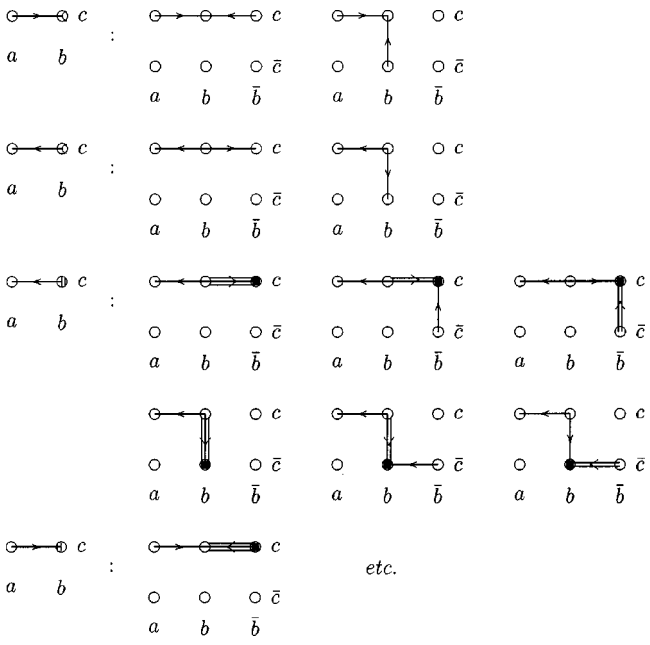


FIG. 9. Blow ups with letter unchanging arrows.

$$\rho_L(a,b,c)=\begin{pmatrix} c\otimes 1_k & 0 \\ 0 & b\otimes 1_p \end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0 \\ 0 & \overline{c}\otimes 1_k & 0 \\ 0 & 0 & a\otimes 1_p \end{pmatrix},$$

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & M_2\otimes 1_k & 0 \\ 0 & 0 & M_3\otimes 1_p \end{pmatrix},$$

$M_1\in M_{p\times\ell}(\mathbb{C})$, $M_2\in M_{p\times p}(\mathbb{C})$, $M_3\in M_{\ell\times k}(\mathbb{C})$. Counting neutrinos leads to $k=\ell=1$. To get a handle on p we repeat the overkill from Sec. IV. in the worst case M_2 and consequently ${}^fM_2$ is skewsymmetric and p is odd. By fluctuations we can obtain

$${}^fM_2=\begin{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} & & & \\ & \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}=:\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}.$$

Now ${}^fM_1$ fluctuates independently and we may obtain for its transpose ${}^fM_1^T=(0,\cdots,0,1)$. We get $({}^fM_1,{}^fM_2)({}^fM_1,{}^fM_2)^*=1_p$ and the minimum of the action is dynamically degenerate if $p\geqslant 1$. The commutative case $k=\ell=p=1$ is obviously degenerate. For the second blow up the computations are similar with ${}^fM_2$ now proportional to 1_p from the start.

Diagram 28 is treated as diagram 27.

Diagram 29 has $k=\ell=p=1$ by neutrino count and admits only degenerate triples.

Diagrams 30, 31, 32, 34, 35, 36 have $k=\ell=1$ by neutrino count. As in the commutative case of diagram 8, all their triples are degenerate.

Diagram 33 with the first of the six possible blow ups yields

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 & 0 \\ 0 & a\otimes 1_p & 0 \\ 0 & 0 & \overline{b}\otimes 1_p \end{pmatrix},$$

$$\rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0 & 0 \\ 0 & b\otimes 1_p & 0 & 0 \\ 0 & 0 & b\otimes 1_p & 0 \\ 0 & 0 & 0 & b\otimes 1_p \end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 & 0 \\ 0 & 1_k\otimes c & 0 \\ 0 & 0 & 1_\ell\otimes c \end{pmatrix},$$

$$\rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0 & 0 \\ 0 & 1_\ell\otimes c & 0 & 0 \\ 0 & 0 & 1_\ell\otimes c & 0 \\ 0 & 0 & 0 & 1_\ell\otimes c \end{pmatrix},$$

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0 & 0 & 0 \\ 0 & M_2\otimes 1_p & 0 & 0 \\ 0 & M_3\otimes 1_p & M_4\otimes 1_p & M_5\otimes 1_p \end{pmatrix},$$

$M_1, M_2 \in M_{k\times\ell}(\mathbb{C})$, $M_3, M_4, M_5 \in M_{\ell\times\ell}(\mathbb{C})$. Counting neutrinos and imposing broken color to be commutative gives $k=\ell=1$. This case is degenerate: the kernel of the Dirac operator contains the invariant subspace with elements $(0,0,0,0,0,M_5v,-M_4v;0,0,0,0,0,\overline{M_5}w,-\overline{M_4}w)^T$, $v, w\in\mathbb{C}^p$.

With the second blow up diagram 33 yields

$$\rho_L(a,b,c)=\begin{pmatrix} a\otimes 1_k & 0 & 0 \\ 0 & a\otimes 1_p & 0 \\ 0 & 0 & \overline{b}\otimes 1_p \end{pmatrix},$$

$$\rho_R(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0 & 0 \\ 0 & b\otimes 1_p & 0 & 0 \\ 0 & 0 & b\otimes 1_p & 0 \\ 0 & 0 & 0 & \overline{b}\otimes 1_p \end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 & 0 \\ 0 & 1_k\otimes c & 0 \\ 0 & 0 & 1_\ell\otimes c \end{pmatrix},$$

$$\rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0 & 0 \\ 0 & 1_\ell\otimes c & 0 & 0 \\ 0 & 0 & 1_\ell\otimes c & 0 \\ 0 & 0 & 0 & 1_\ell\otimes \overline{c} \end{pmatrix},$$

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0 & 0 & 0 \\ 0 & M_2\otimes 1_p & 0 & 0 \\ 0 & M_3\otimes 1_p & M_4\otimes 1_p & 1_k\otimes M_5 \end{pmatrix},$$

$M_1, M_2 \in M_{k\times\ell}(\mathbb{C})$, $M_3, M_4 \in M_{\ell\times\ell}(\mathbb{C})$, $M_5 \in M_{p\times p}(\mathbb{C})$. Counting neutrinos and imposing broken color to be commutative gives $k=\ell=p=1$. In the notations of Corollary 11.4, the action reads

$$V(a,b,c)=4\lambda[|M_1ab|^4+|M_2ab|^4+2|M_2ab|^2|M_3b^2|^2+(|M_3b^2|^2+|M_4b^2|^2+|M_5c^2|^2)^2]$$
$$-2\mu^2[|M_1ab|^2+|M_2ab|^2+(|M_3b^2|^2+|M_4b^2|^2+|M_5c^2|^2)].$$

Its minimum is degenerate, $\hat{b}=0$.

The other blow ups as well as diagram 37 lead to the same conclusion, degeneracy. This completes the proof of the theorem. □

We summarize the possible algebras with $N=3$ and the corresponding Krajewski diagrams of all their irreducible, dynamically nondegenerate triplets in a table.

Algebra	Diagrams
$\mathbb{C}\oplus\mathbb{R}\oplus(\mathcal{C}=\mathbf{1})$	14,16,19,21
$\mathbb{C}\oplus\mathbb{R}\oplus\mathcal{C}$	13,17,18,22
$\mathbf{1}\oplus\mathbf{1}\oplus\mathcal{C}$	15,20,23,24
$\mathbf{2}\oplus\mathbf{1}\oplus(\mathcal{C}=\mathbf{1})$	14,16,19,21
$\mathbf{2}\oplus\mathbf{1}\oplus\mathcal{C}$	13,17,18,22
$\mathbb{C}\oplus\mathbb{C}\oplus\mathbf{1}$	26
$\mathbf{1}\oplus\mathbf{1}\oplus\mathbf{1}$	9
$M_2(\mathbb{R})\oplus\mathbb{R}\oplus\mathbf{1}$	10
$\mathbb{H}\oplus\mathbf{1}\oplus\mathbf{1}$	10
$\mathbf{2}\oplus\mathbf{1}\oplus\mathbf{1}$	8

Note that relaxing the hypothesis of unbroken noncommutative color does not add any algebra to the list with $N=1$ and 2. It adds only few algebras to the list with $N=3$ coming from diagrams. 8, 9, and 11. We were unable to treat some of their triples, in particular quaternionic ones.

B. The standard model of electroweak and strong forces

Let us close this section by remarking that diagram 17 of Fig. 6 with flipped chirality and with algebra $\mathcal{A}=\mathbb{C}\oplus\mathbb{H}\oplus M_3(\mathbb{C})\ni(b,a,c)$, with representation

$$\rho_L(a)=\begin{pmatrix} a\otimes 1_3 & 0\\ 0 & a\end{pmatrix},\quad \rho_R(b)=\begin{pmatrix} b1_3 & 0 & 0\\ 0 & \overline{b}1_3 & 0\\ 0 & 0 & \overline{b}\end{pmatrix},$$

$$\rho_L^c(b,c)=\begin{pmatrix} 1_2\otimes c & 0\\ 0 & \overline{b}1_2\end{pmatrix},\quad \rho_R^c(b,c)=\begin{pmatrix} c & 0 & 0\\ 0 & c & 0\\ 0 & 0 & \overline{b}\end{pmatrix},$$

and with mass matrix

$$\mathcal{M}=\begin{pmatrix} \begin{pmatrix} m_u\\ 0\end{pmatrix}\otimes 1_3 & \begin{pmatrix} 0\\ m_d\end{pmatrix}\oplus 1_3 & 0\\ 0 & 0 & \begin{pmatrix} 0\\ m_e\end{pmatrix}\end{pmatrix}$$

produce the standard model of electromagnetic, weak and strong forces with one generation of quarks and leptons, u, d, ν, and e. The neutrino is a massless Weyl spinor. The intersection form written with respect to the basis of projectors

$$p_1=(0,1_2,0),\quad p_2=(1,0,0),\quad p_3=\left(0,0\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix}\right)$$

is

$$\cap = -2\begin{pmatrix} 0 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 0 \end{pmatrix},$$

and nondegenerate. The color group U(3) is unbroken and its representations on corresponding left- and right-handed fermions are identical. In physicists' language this means that gluons are massless and couple vertorially. Further details on the standard model as an almost commutative geometry can be found in Refs. 2 and 13.

IX. BEYOND IRREDUCIBLE TRIPLES

For the standard model, allowing reducible triples has two important physical consequences.

(i) Suppose we want to render the neutrino massive. Majorana masses are incompatible with the axiom that the Dirac operator anticommutes with the chirality. Therefore we must increase the Hilbert space by adding a right-handed neutrino. Then the triple becomes reducible, but worse Poincaré duality breaks down: the intersection form becomes

$$\cap = -2\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & -1 \\ 1 & -1 & 0 \end{pmatrix},$$

degenerate.

(ii) We may add more generations of quarks and leptons. Then the Cabibbo–Kobayashi–Maskawa matrix makes its appearance. Now we may add right-handed neutrinos in some but no in all generations and give Dirac massses to the corresponding neutrinos without violating Poincaré duality.

So far we have no clue to why the standard model comes with three colors, with three generations of quarks and with three generations of leptons. Note however that anomaly cancellations[1] imply further constraints that are satisfied with three colors and with a number of quark generations equal to the number of lepton generations.

A. A reducible triple with nondegenerate spectrum

The criterion of dynamical degeneracy loses its meaning in presence of reducible triples as illustrated by the following example: $\mathcal{A}=M_3(\mathbb{C})\oplus M_2(\mathbb{C})\ni(a,b)$,

$$\rho(a,b,c)=\begin{pmatrix} a\otimes 1_2\otimes 1_3 & 0 & 0 & 0 \\ 0 & b\otimes 1_3\otimes 1_3 & 0 & 0 \\ 0 & 0 & 1_3\otimes 1_2\otimes \overline{a} & 0 \\ 0 & 0 & 0 & 1_2\otimes 1_3\otimes \overline{a} \end{pmatrix},$$

$$\mathcal{M} = m \begin{pmatrix} \begin{pmatrix} \sqrt{\frac{5}{17}} & 0 \\ 0 & \frac{1}{\sqrt{5}} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & -\frac{2}{\sqrt{5}} \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & \frac{2}{\sqrt{5}} \end{pmatrix} & \begin{pmatrix} 2\sqrt{\frac{5}{17}} & 0 \\ 0 & \frac{2}{\sqrt{5}} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix} \otimes 1_3.$$

The fluctuations of the Dirac operator generate an 18-dimensional complex vector space in which the spectral action $V({}^f\mathcal{D})$ must be minimized. We used a steepest descend method of Mathematica for this task and found an absolute minimum at ${}^{\hat{f}}\mathcal{D}=\mathcal{D}$ with $m=\mu/\sqrt{4\lambda}$ and $V({}^{\hat{f}}\mathcal{D})=-(431/340)\times(\mu^4/\lambda)$. The spectrum of this minimum ${}^{\hat{f}}\mathcal{D}$ is nondegenerate: in units of $\mu/\sqrt{4\lambda}$ we have $\{1,4/5,5/17,20/17,(9+\sqrt{17})/10\}$. All six values of course appear six times with a positive and six times with a negative sign in the spectrum of ${}^{\hat{f}}\mathcal{D}$. The little group of this minimum is $G_\ell = \mathrm{U}(1)\subset \mathrm{U}(3)\times\mathrm{U}(2)$ with generic element $(e^{i\alpha}1_3, e^{i\alpha}1_2)$. The spectrum of the minimum appears completely rigid, i.e., there are many mass relations. Note however that the threefold color degeneracy is not protected by the little group in this example.

X. CONCLUSION

Suppose we want to apply conventional, perturbative quantum field theory to the Yang–Mills–Higgs models coming from almost commutative geometries. Then after renormalization, fermion masses are functions of energy and the color degeneracy is compatible with this energy dependence only if all noncommutative color groups are unbroken. Furthermore the renormalization of fermion masses is incompatible with mass relations, in particular with the completely rigid reducible spectral triple of Sec. IX. In irreducible spectral triples, mass relations other than degeneracies only appear starting with $N=3$. All triples without such mass relations come from ladder diagrams and have algebras $\mathbf{1}\oplus\mathbf{1}\oplus\mathcal{C}$ or $\mathbb{H}\oplus\mathbf{1}\oplus\mathcal{C}$.

Let us suppose that also for $N\geqslant 4$ the irreducible triples without mass relations have contracted multiplicity matrices of ladder type,

$$\hat{\mu} = \begin{pmatrix} \alpha & \beta & 0 & 0 \\ \gamma & \delta & 0 & 0 \\ \rho & \sigma & 0 & 0 \\ \theta & \xi & 0 & 0 \end{pmatrix}, \quad N=4.$$

Then $\det(\hat{\mu}+\hat{\mu}^T)=(\rho\xi-\sigma\theta)^2$ and irreducibility implies $\alpha=\beta=\gamma=\delta=0$. For $N\geqslant 5$, all contracted multiplicity matrices $\hat{\mu}$ of ladder type have $\det(\hat{\mu}+\hat{\mu}^T)=0$ leading us to the following.

Conjecture 10.1. The sum of N simple algebras, $\mathcal{A}=\mathcal{A}_1\oplus\mathcal{A}_2\oplus\cdots\oplus\mathcal{A}_N$ admits a finite, real, S^0-real, irreducible and dynamically nondegenerate spectral triple free of mass relations if and only if it is in the list, up to a reordering of the summands:

$N=1$	$N=2$	$N=3$	$N=4$	$N\geqslant 5$
	$\mathbb{R}\oplus\mathbb{R}$	$\mathbb{R}\oplus\mathbb{R}\oplus\mathcal{C}$	$\mathbb{R}\oplus\mathbb{R}\oplus\mathcal{C}_1\oplus\mathcal{C}_2$	
	$\mathbb{R}\oplus\mathbb{C}$	$\mathbb{R}\oplus\mathbb{C}\oplus\mathcal{C}$	$\mathbb{R}\oplus\mathbb{C}\oplus\mathcal{C}_1\oplus\mathcal{C}_2$	
	$\mathbb{C}\oplus\mathbb{C}$	$\mathbb{C}\oplus\mathbb{C}\oplus\mathcal{C}$	$\mathbb{C}\oplus\mathbb{C}\oplus\mathcal{C}_1\oplus\mathcal{C}_2$	
	$M_2(\mathbb{R})\oplus\mathbb{R}$			
void	$M_2(\mathbb{R})\oplus\mathbb{C}$			void
	$M_2(\mathbb{C})\oplus\mathbb{R}$			
	$M_2\mathbb{C}\oplus\mathbb{C}$			
	$\mathbb{H}\oplus\mathbb{R}$	$\mathbb{H}\oplus\mathbb{R}\oplus\mathcal{C}$	$\mathbb{H}\oplus\mathbb{R}\oplus\mathcal{C}_1\oplus\mathcal{C}_2$	
	$\mathbb{H}\oplus\mathbb{C}$	$\mathbb{H}\oplus\mathbb{C}\oplus\mathcal{C}$	$\mathbb{H}\oplus\mathbb{C}\oplus\mathcal{C}_1\oplus\mathcal{C}_2$	

Here $\mathcal{C}$, $\mathcal{C}_1$, and $\mathcal{C}_2$ are three arbitrary simple algebras. The color algebras $\mathcal{C}$ for $N=3$ and $\mathcal{C}_1\oplus\mathcal{C}_2$ for $N=4$ have two constraints.

(i) *Their representations on corresponding left and right-handed subspaces of $\mathcal{H}$ are identical (up to possibly different multiplicities).*

(ii) *The Dirac operator $\mathcal{D}$ is invariant under* $\mathrm{U}(\mathcal{C})$ *or* $\mathrm{U}(\mathcal{C}_1\oplus\mathcal{C}_2)$,

$$\rho(1,1,w)\mathcal{D}\,\rho(1,1,w)^{-1}=\mathcal{D},\quad \text{for all } w\in \mathrm{U}(\mathcal{C}) \text{ or } \mathrm{U}(\mathcal{C}_1\oplus\mathcal{C}_2).$$

This implies that the unitaries of $\mathcal{C}$ or $\mathcal{C}_1\oplus\mathcal{C}_2$ do not participate in the fluctuations and are therefore unbroken, i.e., elements of the little group.

We must admit that our brute force proof by exhaustion is not suitable for $N=4$ and it seems already a formidable task to write down the list of all contracted irreducible diagrams.

Besides renormalizability, there are two other important items on the physicist's shopping list, which will further constrain the model building kit.

(i) The electric charge of a massless particle must be zero.
(ii) The representation of the little group on the Hilbert space of fermions must be complex.

Recall that a unitary representation is called real if it is equal to its complex conjugate and pseudoreal if it is unitarily equivalent to its complex conjugate. Otherwise the representation is complex. For example, the fundamental representation of SU(2) is pseudoreal. An irreducible, unitary representation of U(1) is complex if and only if its charge is nonzero.

Before we can examine these two criteria in the irreducible context, we must compute the minimal central extensions[12,15] that allow the lift of algebra automorphisms to the Hilbert space of fermions to have at most a finite number of values. This calculation is under way.

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APPENDIX

Since this paper deals with matrices, let us briefly recall two standard results, one on the singular value decomposition of rectangular matrices and the second on the standard form of skewsymmetric matrices.

We write $\mathrm{O}(n):=\mathrm{U}(M_n(\mathbb{R}))$, $\mathrm{U}(n):=\mathrm{U}(M_n(\mathbb{C}))$ and $\mathrm{Usp}(n):=\mathrm{U}(M_n(\mathbb{H}))$.

Lemma 11.1:

(i) Let $M \in M_{n\times m}(\mathbb{C})$. *Then there exist* $U \in U(n)$, $V \in U(m)$ *such that* $M=UDV$ *where* $D \in M_{n\times m}(\mathbb{R})$ *satisfies* $D_{ij}=0$ *for* $i \neq j$ *and* $D_{11} \geqslant D_{22} \geqslant D_{kk} > D_{k+1,k+1} = \cdots = D_{qq} = 0$ *where* $k = \mathrm{rank}(M)$ *and* $q=\min(n,m)$. *The* D_{ii}^2 *are the eigenvalues of* M^*M, *the columns of* U *(respectively,* V*) are the eigenvectors of* MM^* *(respectively,* M^*M*) arranged in the same order as the eigenvalues* D_{ii}^2. *In particular, when* $M \in M_{n\times m}(\mathbb{R})$, *we may assume* $U \in O(n)$, $V \in O(m)$ *(Ref. 9, 7.3.5).*

(ii) Let $M \in M_n(\mathbb{C})$ *be a skewsymmetric matrix. Then, there exists* $U \in U(n)$ *such that*

$$UMU^T = \left(\overset{p}{\underset{i=1}{\oplus}} m_i x\right) \oplus 0 \cdots \oplus 0 \quad \text{where} \quad x = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad m_i \in \mathbb{C}^* \tag{A1}$$

and the numbers of zeros equals $n-2p$ (*Ref.* 9 *4.4, Problem 26).*

For our purpose, M is the *complex* fermionic mass matrix. Then, in (i), the diagonal elements D_{jj} are the Dirac masses and the unitaries U and V are related to the Cabibbo–Kobayashi–Maskawa matrix.

Definition 11.2: Let $M \in M_{(n)\times(m)}(\mathbb{C})$ and

$$f \in \mathcal{F}_{\mathbb{K},\mathbb{K}'} := \{(r_j,u_j,v_j)_{j\in J} \in \mathbb{R} \times \mathrm{U}(M_{(n)}(\mathbb{K})) \times \mathrm{U}(M_{(m)}(\mathbb{K}'))|J \text{ finite}\},$$

where $\mathbb{K}$, $\mathbb{K}'$ are $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ where $(n)=n$ for $\mathbb{K}=\mathbb{R},\mathbb{C}$ and $(n)=qn$ for $\mathbb{K}=\mathbb{H}$. The *fluctuation* of M is defined by

$${}^fM := \sum_j r_j u_j M v_j.$$

In the case that $\mathbb{C}$ and $\mathbb{H}$ are involved, we assume of course that $\mathbb{C}\subset\mathbb{H}$.

Note that for a given M,

$$\{{}^fM|f \in \mathcal{F}_{\mathbb{R},\mathbb{C}}\} = \{{}^fM|f \in \mathcal{F}_{\mathbb{C},\mathbb{R}}\} = \{{}^fM|f \in \mathcal{F}_{\mathbb{C},\mathbb{C}}\}.$$

Lemma 11.3: Let $\mathrm{Span}_{\mathbb{R}}(E)$ *be the real vector space spanned by the set* E. *Then,*

(i) $\mathrm{Span}_{\mathbb{R}}(\mathrm{O}(n))=M_n(\mathbb{R})$.
(ii) $\mathrm{Span}_{\mathbb{R}}(\mathrm{U}(n))=M_n(\mathbb{C})$.
(iii) $\mathrm{Span}_{\mathbb{R}}(\mathrm{USp}(n))=M_n(\mathbb{H})$.

Proof:

(i) It is sufficient to prove that any $a=\pm a^T \in M_n(\mathbb{R})$ is in $\mathrm{Span}_{\mathbb{R}}(\mathrm{O}(n))$.

When $a=a^T$, there exists $v \in \mathrm{O}(n)$ such that $a=vdv^T$ where d is a real diagonal matrix. Since

$$d = \sum_{i=1}^{n} \frac{d_{ii}}{2}(2p_i - 1_n) + \frac{d_{ii}}{2}1_n,$$

where p_i is the projection on the ith vector basis, so d is in $\mathrm{Span}_{\mathbb{R}}(\mathrm{O}(n))$ and so is a.

When $a=-a^T$, there exist $v \in \mathrm{O}(n)$ and a family $r_k \in \mathbb{R}$, $k \leqslant n/2$ such that

$$a = v\ \mathrm{diag}(0,\ldots,0,r_1 b,\ldots,r_k b)v^T,$$

where $b=\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. Thus for $r=\Sigma_i r_i$,

$$v^T a v = b_1\ \mathrm{diag}(1,\ldots,1,b,1_2\ldots,1_2) + r_2\ \mathrm{diag}(1,\ldots,1,1_2,b,1_2\ldots,1_2) + \cdots$$
$$+ r_k(1,\ldots,1,1_2,\ldots,1_2,b) - \mathrm{diag}(r,\ldots,r,(r-r_1)1_2,\ldots,(r-r_k)1_2)$$

is a real linear combination of matrices in $\mathrm{O}(n)$ by (i). So $a \in \mathrm{Span}_{\mathbb{R}}(\mathrm{O}(n))$.

(ii) This follows by (i) since $\mathrm{O}(n)$ and $i\mathrm{O}(n)$ are included in $\mathrm{U}(n)$.

(iii) Let $1, e_1, e_2, e_3$ be the canonical basis of $\mathbb{H}$ such that $e_ie_j=\delta_{ij}1-\epsilon_{ijk}e_k$ and $1e_i=e_i1=e_i$. Since $M_n(\mathbb{H})$ is an $\mathbb{H}$-vector space, $M_n(\mathbb{H})=1M_n(\mathbb{R})+e_1M_n(\mathbb{R})+e_2M_n(\mathbb{R})+e_3M_n(\mathbb{R})$ and the result follows from $e_i\mathrm{O}(n)\subset\mathrm{USp}(n)$. □

Corollary 11.4: $\{{}^fM|f\in\mathcal{F}_{\mathbb{K},\mathbb{K}'}\}=\{\Sigma_i a_iM\ b_i|a_i\in M_n(\mathbb{K}),b_i\in M_m(\mathbb{K}')\}$.

Remark 11.5: If $\mathbb{K}=\mathbb{K}'$, then for any $0\neq M\in M_{n\times m}(\mathbb{K})$,

$$\{{}^fM|f\in\mathcal{F}_{\mathbb{K},\mathbb{K}}\}=M_{n\times m}(\mathbb{K}).$$

Nevertheless, we have *a priori*

$$\{{}^fM|f\in\mathcal{F}_{\mathbb{K},\mathbb{K}'}\}\not\subset\{a\ M\ b|a\in M_n(\mathbb{K}),b\in M_m(\mathbb{K}')\},$$

while the converse inclusion is true by the previous corollary. Actually, for $n=m=2$ and $\mathbb{K}=\mathbb{K}'=\mathbb{C}$, if $M=\left(\begin{smallmatrix}1&0\\0&0\end{smallmatrix}\right)$, Rank $(aMb)\leqslant 1$ for any a and b in $M_n(\mathbb{C})$, but for the fluctuation

$$f=\{r_1=r_2=1,u_1=v_1=1_2,u_2=v_2=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)\},\ ({}^fM)=\mathrm{Rank}(1_2)=2$$

.

Lemma 11.6: Given a family of k $\mathbb{R}$-linearly independent matrices $M_i\in M_{n\times m}(\mathbb{R})$, $i=1,\ldots,k$, there exists a fluctuation $f\in\mathcal{F}_{\mathbb{R},\mathbb{R}}$ such that ${}^fM_i=0$ for all $i\neq 1$ and ${}^fM_1\neq 0$.

Proof: Let $\{c_i\}_{i\in\{1,\ldots,p\}}$ be the canonical basis of column vectors in $\mathbb{R}^p$. (We use abusively the same notation for different p's.) Remark first that the fluctuation defined for given $r_1,r_2\in\mathbb{R}, i,k\in\{1,\ldots,n\}$ and $j,l\in\{1,\ldots,m\}$ by

$${}^fM:=r_1M+r_2c_ic_k^TM\ c_lc_j^T=r_1M+r_2M_{kl}c_ic_j^T$$

satisfies $({}^fM)_{pq}=r_1M_{pq}$ for all $p\neq i$ and $q\neq j$ and $({}^fM)_{ij}=r_1M_{ij}+r_2M_{kl}$.

For any $M\in M_{n\times m}(\mathbb{R})$ let

$$W(M):=\begin{pmatrix}M_{11}\\ \vdots\\ M_{1m}\\ M_{21}\\ \vdots\\ M_{nm}\end{pmatrix}\in\mathbb{R}^{nm}.$$

Given a family of matrices $M_1,\ldots,M_k\in M_{n\times m}(\mathbb{R})$, let N be the matrix in $M_{nm\times k}(\mathbb{R})$ defined by the columns $W(M_i)$,

$$N:=(W(M_1)|W(M_2)|\cdots|W(M_k)).$$

Thus, if a fluctuation $f\in\mathcal{F}_{\mathbb{R},\mathbb{R}}$ is defined simultaneously on all M_i's, N is transformed in $f(N):=(W({}^fM_1)|W({}^fM_2)|\cdots|W({}^fM_k))$. By the previous remark, adding a multiple of a line of N to a multiple of another one correspond precisely to a fluctuation. Using Gauss method, if the M_i's are linearly independent (thus $k\leqslant nm$), so are the $W(M_i)$'s and there exists a fluctuation f such that

$$f(N)=\begin{pmatrix}1_{k\times k}\\ 0_{(nm-k)\times k}\end{pmatrix}$$

since the rank of N is k. This means that a second fluctuation given by ${}^gM:=c_1c_1^TMc_1c_1^T$ will give ${}^{gf}M_1={}^fM_1\neq 0$ while ${}^{gf}M_i=0$ for all $i\neq 1$. □

Remark 11.7: This lemma is false when the matrices have complex entries: Let $M_1=\left(\begin{smallmatrix}i\\1\end{smallmatrix}\right)$ and $M_2\left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$. Then M_1 and M_2 are $\mathbb{R}$- and $\mathbb{C}$-linearly independent. Nevertheless, ${}^fM_1=0$ always yields ${}^fM_2=\mathrm{Im}\ ({}^fM_1)=0$. There only remains the following.

Lemma 11.8: Let $M_1\in M_{n\times m}(\mathbb{C}), i=1,\ldots,k$ be k matrices such that their real and imaginary

parts are $2k$ $\mathbb{R}$*-linearly independent matrices. Then there exists a fluctuation* $f \in \mathcal{F}_{\mathbb{R},\mathbb{R}}$ *such that* ${}^{f}M_i \neq 0$ *and* ${}^{f}M_1 = 0$ *for all* $i \neq 1$.

Proof: According to the previous lemma, there exists a fluctuation $f \in \mathcal{F}_{\mathbb{R},\mathbb{R}}$ such that $\mathrm{Re}({}^{f}M_1) \neq 0$ while $\mathrm{Im}({}^{f}M_1) = \mathrm{Re}({}^{f}M_i) = \mathrm{Im}({}^{f}M_i) = 0$ for all $i \neq 1$, yielding the conclusion since real and imaginary extractions commute with fluctuations. □

Among the fluctuations, there are the symmetric ones in the following sense.

Definition 11.9: Let $\mathcal{F}^{T}_{\mathbb{C},\mathbb{C}} := \{(r_j, u_j)_{j\in J} \in \mathbb{R} \times \mathrm{U}(n) | J \text{ finite}\}$ and define fluctuations $f^T \in \mathcal{F}_{\mathbb{C},\mathbb{C}^T}$ on $n \times n$ square matrices by

$$f^T M := \sum_j r_j u_j M u_j^T.$$

Lemma 11.10: Let M_1, M_2 *be two skewsymmetric matrices* in $M_n(\mathbb{C})$. *Then,*

(i) *If the constraints* ${}^{f^T}M_1 = 0$ *for* $f \in \mathcal{F}_{\mathbb{C},\mathbb{C}^T}$ *always implies* ${}^{f^T}M_2 = 0$, *then* M_2 *is* $\mathbb{C}$*-colinear to* M_1.

(ii) *If* M_2 *is not colinear to* M_1, *then there exists a fluctuation* $f^T \in \mathcal{F}_{\mathbb{C},\mathbb{C}^T}$ *such that* ${}^{f^T}M_1 = 0$ *and* ${}^{f^T}M_2 \neq 0$.

Proof: Note that (ii) is a consequence of (i).

To prove (i), we may assume that M_1 has the form as in (A1).

$s := \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ and $t := \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ are two unitaries satisfying $wxw^T = -x$ for $w = s, t$. Define $u = v \oplus 1 \oplus \cdots \oplus 1 \in \mathrm{U}(n)$ with $v = \oplus_{i=1}^{p} v_i \in U(2p)$ where $v_1 \in \{s, t\}$. Then $M_1 + uM_1u^T = 0$, so if M_2 has the form $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, with $A \in M_{2p}(\mathbb{C})$, $B \in M_{2p,n-2p}(\mathbb{C})$, $C \in M_{n-2p,2p}(\mathbb{C})$, $D \in M_{n-2p,n-2p}(\mathbb{C})$, then $0 = M_2 + uM_2u^T$. We deduce $0 = A + vAv^T = B + vB = C + Cv^T = D + D$. Thus choosing $V_s = \oplus_{i=1}^{p} s$ and $v_t = \oplus_{i=1}^{p} t$, we have $(1_{2p} + v_s)B + (1_{2p} + v_t)B = 0$, so $B = 0$ since $2\, 1_{2p} + v_s + v_t$ is invertible. Similarly, $C = D = 0$.

If A_{kl} is the partition of A in 2×2 matrices, the constraint $A + vAv^T = 0$ implies $0 = A_{kl} + u_k A_{kl} u_l^T$. When $k \neq l$, A_{kl} is necessarily zero since we may choose independently u_k and u_l in $\{s, t\}$. When $k = l$, $A_{kk} = \left(\begin{smallmatrix} \alpha_k & \gamma_k \\ -\gamma_k & \beta_k \end{smallmatrix}\right)$ where α, β, and γ are complex numbers, since A is skewsymmetric. If $u_k = t$, $0 = A_{kk} + u_k A_{kk} u_k = 2\left(\begin{smallmatrix} \alpha_k & 0 \\ 0 & \beta_k \end{smallmatrix}\right)$ and $A_{kk} = \gamma_k x$. Thus $M_2 = \oplus_{k=1}^{p} \gamma_k x \oplus 0 \oplus \cdots \oplus 0$ and it remains to prove that $\gamma_k = c\, m_k$ for some constant c.

Define

$$u_k := s \oplus 1_2 \oplus \cdots \oplus 1_2 \oplus 1 \oplus \cdots \oplus 1,$$

$$v_k := 1_2 \oplus \cdots \oplus s \oplus \cdots \oplus 1_2 \oplus 1 \oplus \cdots \oplus 1,$$

$$w_k := \begin{pmatrix} 0 & 0 & \cdots & 0 & 1_2 \\ 0 & 1_2 & & & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & & 1_2 & 0 \\ 1_2 & 0 & \cdots & 0 & 0 \end{pmatrix} \oplus 1_2 \oplus \cdots \oplus 1_2 \oplus 1 \oplus \cdots \oplus 1,$$

three unitaries where the perturbation in v_k is set at the kth entry. Then

$$0 = (2m_1)^{-1}(M_1 - uM_1u^T) - (2m_k)^{-1} wk(M_1 - v_k M_1 v_k^T) w_k^T$$

and the same relation for M_2 yields $0 = 2(\gamma_1 m_1^{-1} - \gamma_k m_k^{-1})$, so $\gamma_k = \gamma_1 m_1^{-1} m_k$ and $M_2 = (\gamma_1 m_1^{-1}) M_1$. □

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Golden mean renormalization for a generalized Harper equation: The Ketoja–Satija orchid

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We provide a rigorous analysis of the fluctuations of localized eigenstates in a generalized Harper equation with golden mean flux and with next-nearest-neighbor interactions. For next-nearest-neighbor interaction above a critical threshold, these self-similar fluctuations are characterized by orbits of a renormalization operator on a universal strange attractor, whose projection was dubbed the "orchid" by Ketoja and Satija [Phys. Rev. Lett. **75**, 2762 (1995)]. We show that the attractor is given essentially by an embedding of a subshift of finite type, and give a description of its periodic orbits. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1797532]

I. INTRODUCTION

The discrete one-dimensional Schrödinger equation,

$$\psi_{i+1} + \psi_{i-1} + 2\lambda \cos(2\pi(i\omega + \phi))\psi_i = E\psi_i, \tag{1.1}$$

known as the Harper (or almost Mathieu) equation is a valuable tight binding model for the Hamiltonian of an electron in a one-dimensional lattice in a commensurate ($\omega \in \mathbb{Q}$) or incommensurate ($\omega \notin \mathbb{Q}$) potential. It may also be derived[10] as the tight binding model for an electron in a two-dimensional lattice in a transverse magnetic field in the limits of strong (weak) potential and weak (resp., strong) field. In this setting the parameters ω, ϕ, and λ represent, respectively, the magnetic flux per unit cell, the wave-number of the plane wave in the transverse direction, and the ratio of the length of the unit cell in the direction of the vector potential and its length in the transverse direction.

Much is known concerning the spectrum of (1.1). The pioneering work of Aubry and André[1] tells us much about the transition from extended to localized states, with precise versions of these results and a summary appearing in Ref. 12. What concerns us here is that for Diophantine ω there is, for almost all ϕ, a localized regime $\lambda > 1$ with a pure point spectrum with exponentially decaying eigenfunctions. (See Ref. 12 for a precise sufficient condition on ϕ.) For a recent general review of these and many other results on Schrödinger operators see Ref. 29.

At the critical point $\lambda = 1$ there is self-similarity of the spectrum eigenfunctions which has been investigated from a renormalization standpoint by Ostlund and Pandit[27] and several other groups (Refs. 6, 15, 16, 21, 22, 28, and 31). See Ref. 30 for a review. This critical behavior is reflected in the localized regime $\lambda > 1$. In the case when the flux $\omega = (\sqrt{5}-1)/2$, the golden mean, it has been observed that the exponentially decaying eigenfunctions possess universal self-similar fluctuations[17] determined by the strong-coupling limit $\lambda \to \infty$. In Ref. 17, Ketoja and Satija explain this phenomenon in terms of a universal fixed point of a renormalization operator derived from

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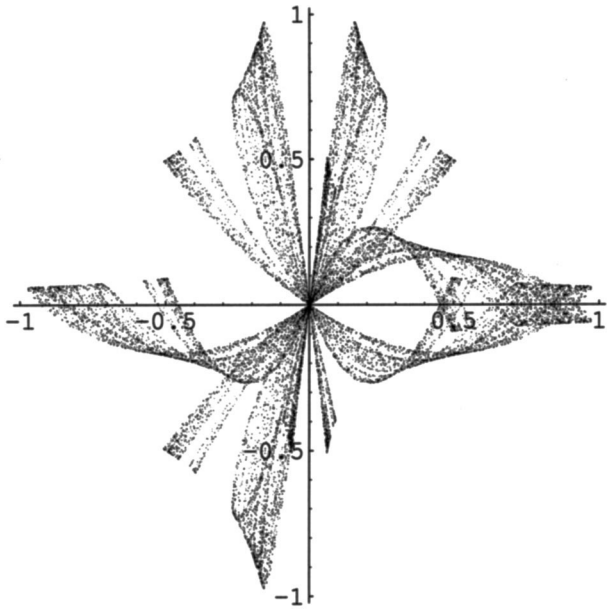

FIG. 1. The orchid.

their decimation scheme.[15,16] We have recently put their observations on a firm footing by explicitly constructing a fixed point of the appropriate renormalization operator.[24]

In this paper we consider the generalized Harper equation,[9]

$$(1+\alpha\cos(2\pi(\omega(i+1/2)+\phi)))\psi_{i+1}+(1+\alpha\cos(2\pi(\omega(i-1/2)+\phi)))\psi_{i-1}$$
$$+2\lambda\cos(2\pi(i\omega+\phi))\psi_i=E\psi_i, \tag{1.2}$$

in which, in terms of the two-dimensional system, the additional parameter α measures the next-nearest-neighbor interaction strength. (For earlier studies of the spectrum of this model see Refs. 4, 11, and 32.)

Han *et al.*[9] give the phase diagram for this model, and in Ref. 20 an investigation of the critical self-similarity that occurs when $\alpha\geqslant 1$ and $\alpha\geqslant\lambda$ is made using the decimation scheme. The conclusion is that the scaling in the "fat" critical phase appears to be governed by a strange attractor of a renormalization operator. As in the Harper equation itself, this critical behavior is mirrored in the localized phase, $\lambda\geqslant 1$ and $\lambda\geqslant\alpha$, where there again appear to be self-similar fluctuations in the exponentially decaying eigenfunctions. Ketoja and Satija[17] report two types of behavior under decimation. First, for $0\leqslant\alpha<1$ the system appears to be in the universality class of the original Harper equation ($\alpha=0$), renormalizing to the fixed point. More intriguingly, when $\alpha\geqslant 1$ the decimation/renormalization scheme appears to send the system to a universal strange attractor again determined by the strong-coupling limit $\lambda\to\infty$. A projection of this attractor has been dubbed an "orchid" in Ref. 17. Figure 1 shows the orchid. (It is a reflection in the origin of that shown in Ref. 17, as we have adopted a different sign convention.)

For certain values of the parameter α the asymptotic orbit under renormalization is a periodic orbit, but generally orbits asymptotically appear to be dense on the attractor. It is this strange attractor that we specifically analyze in this paper. (A study of the generalized Harper equation with anisotropic next-nearest-neighbor interaction[18] reveals that this richness is destroyed by anisotropy.) Our analysis combines subshifts of finite type together with dynamics of sign pairs and gives a complete mathematical description of the strange set.

The outline of this paper is as follows. In Sec. II we review the decimation approach of Ketoja and Satija which leads to the key functional recurrence,

$$t_{n+1}(x) = t_n(-\omega x)t_{n-1}(\omega^2 x + \omega), \tag{1.3}$$

that is the mathematical interest of this paper. [Here $\omega=(\sqrt{5}-1)/2$.] We also recall our earlier work[24] on the strong-coupling fixed point of this equation, and establish some preliminary renormalization results. The zeros of the initial conditions for this recurrence are crucial in our analysis. In particular, the key to our understanding is their evolution under a simple piecewise-linear interval map. The symmetry of the cosine potential in the generalized Harper equation leads to symmetry of these zeros, and in Sec. III we introduce "codes" which give a symbolic description of the dynamics of the zeros and establish a "partnering" criterion which enables us to incorporate the symmetry. In Sec. IV we construct the orchid in terms of the codes and pairs of signs, assuming the existence of a map $\mathcal{E}$ that embeds the code space into a space of function pairs. The main analytic work is in Sec. V, in which the existence of the map $\mathcal{E}$ is established. We also construct an abstract model space for a fundamental set, three copies of which comprise the orchid. Having constructed the orchid, in Sec. VI we establish its attracting nature and its "strangeness," while in Sec. VII we prove that all periodic orbits have period a multiple of three, thereby proving a conjecture formulated in Ref. 17. Section VIII contains our concluding remarks.

II. RENORMALIZATION ANALYSIS

A. Golden mean decimation

For completeness, in this section we recall the decimation approach to quasiperiodic systems as developed by Ketoja and Satija (Refs. 14–20).

We restrict our attention to the portion of the localized phase, $\lambda \geqslant 1$, $\lambda \geqslant \alpha$, for which $\alpha \geqslant 1$, where by the result of Han *et al.*,[9] the exponential decay of the eigenfunction is measured by the characteristic exponent,

$$\gamma = \log\left(\frac{\lambda}{\alpha} + \sqrt{\left(\frac{\lambda}{\alpha}\right)^2 - 1}\right). \tag{2.1}$$

Writing

$$\psi_i = e^{-\gamma|i|}\eta_i, \tag{2.2}$$

our generalized Harper equation (1.2) becomes, for $i>0$,

$$\begin{aligned} &e^{-2\gamma}(1+\alpha\cos(2\pi(\omega(i+1/2)+\phi)))\eta_{i+1} + (1+\alpha\cos(2\pi(\omega(i-1/2)+\phi)))\eta_{i-1} \\ &\quad + 2e^{-\gamma}\lambda\cos(2\pi(i\omega+\phi))\eta_i = e^{-\gamma}E\eta_i. \end{aligned} \tag{2.3}$$

We consider only the case when the flux $\omega=(\sqrt{5}-1)/2$, the golden mean. In the decimation scheme in this case, we consider only sites with indices separated by a Fibonacci number F_n, where we define $F_0=0$, $F_1=1$, and $F_n=F_{n-1}+F_{n-2}$ for $n>1$. In other words, we consider the *decimation* of (2.3) of the form

$$s_n(i)\,\eta_{i+F_{n+1}} = \eta_{i+F_n} - t_n(i)\,\eta_i. \tag{2.4}$$

By writing (2.4) with n replaced by $n-1$ and $n+1$ and in each of the resulting expressions replacing i by $i+F_n$ (and by using the defining property of the Fibonacci numbers), the functions t_n and s_n may be seen to obey the explicit recursions,

$$s_{n+1}(i) = \frac{s_{n-1}(i+F_n)s_n(i+F_n)}{1 - s_n(i)(t_{n-1}(i+F_n) + s_{n-1}(i+F_n)t_n(i+F_n))}, \tag{2.5}$$

$$t_{n+1}(i) = \frac{t_n(i)(t_{n-1}(i+F_n) + s_{n-1}(i+F_n)t_n(i+F_n))}{1 - s_n(i)(t_{n-1}(i+F_n) + s_{n-1}(i+F_n)t_n(i+F_n))}, \tag{2.6}$$

for $n>1$. The initial conditions for these recursions are

$$s_1(i) = 1, \tag{2.7}$$

$$t_1(i) = 0, \tag{2.8}$$

$$s_2(i) = \frac{e^{-\gamma}(1 + \alpha\cos(2\pi((i+3/2)\omega + \phi)))}{E - 2\lambda\cos(2\pi((i+1)\omega + \phi))}, \tag{2.9}$$

$$t_2(i) = \frac{1 + \alpha\cos(2\pi((i+1/2)\omega + \phi))}{e^{-\gamma}(E - 2\lambda\cos(2\pi((i+1)\omega + \phi)))}; \tag{2.10}$$

given by Eq. (2.4) with $n=1$ and $n=2$, respectively, referring to (2.3).

We now consider the strong-coupling limit $\lambda\to\infty$. We see from (2.1) that $\gamma\to\infty$ and $\lambda e^{-\gamma}\to\alpha/2$. We set $\varepsilon=\lim E/\lambda$ and see that $s_2(i)$, $s_3(i)$, $s_n(i)\to 0$, while

$$t_2(i) \to \frac{1 + \alpha\cos(2\pi((i+1/2)\omega + \phi))}{\alpha(\varepsilon/2 - \cos(2\pi((i+1)\omega + \phi)))}, \tag{2.11}$$

$$t_3(i) \to t_2(i)t_2(i+F_2), \tag{2.12}$$

$$t_{n+1}(i) \to t_n(i)t_{n-1}(i+F_n), \tag{2.13}$$

for $n\geqslant 3$. We thus have a single recurrence as our strong-coupling problem:

$$t_1(i) = 0, \tag{2.14}$$

$$t_2(i) = \frac{1 + \alpha\cos(2\pi((i+1/2)\omega + \phi))}{\alpha(\varepsilon/2 - \cos(2\pi((i+1)\omega + \phi)))}, \tag{2.15}$$

$$t_3(i) = t_2(i)t_2(i+F_2), \tag{2.16}$$

$$t_{n+1}(i) = t_n(i)t_{n-1}(i+F_n), \tag{2.17}$$

for $n\geqslant 3$.

To analyze the scaling we now replace the discrete lattice index i by the continuous variable $x=(-\omega)^{-n}\{i\omega\}$ where $\{\cdot\}$ denotes the fractional part. Care must be taken when doing this as the definition of x depends on the index n of the function. The result is that our recursion becomes

$$t_{n+1}(x) = t_n(-\omega x)t_{n-1}(\omega^2 x + \omega), \tag{2.18}$$

for $n\geqslant 3$, with initial conditions

$$t_2(x) = \frac{1 + \alpha\cos(2\pi(\omega^2 x + \omega/2 + \phi))}{\alpha(\varepsilon/2 - \cos(2\pi(\omega^2 x + \omega + \phi)))}, \tag{2.19}$$

$$t_3(x) = t_2(-\omega x)t_2(-\omega x - 1). \tag{2.20}$$

We remark that t_2 is "normalized" in the sense that it satisfies the constraint

$$\int_{-\omega^{-1}}^{1} \log|t_2(x)|dx = 0, \tag{2.21}$$

the significance of which will be made clear in Sec. VI A.

Henceforth, in all that follows, we shall consider these limiting equations at the "upper band edge," at which $\varepsilon/2=+1$, and the phase $\phi=0$. (The lower band edge $\varepsilon/2=-1$, $\phi=1/2$ may be treated similarly.)

As in Refs. 27 and 17, writing $u_n(x)=t_{n-1}(-\omega x)$, we obtain a first order iteration on pairs of functions (u_n,t_n):

$$u_{n+1}(x) = t_n(-\omega x), \quad t_{n+1}(x) = t_n(-\omega x)u_n(-\omega x - 1). \tag{2.22}$$

We may thus express the recursion (2.18) in terms of a renormalization operator on pairs (u,t):

$$(u_{n+1},t_{n+1}) = R(u_n,t_n), \tag{2.23}$$

where

$$R(u_n,t_n)(x) = (t_n(\theta_0(x)),t_n(\theta_0(x))u_n(\theta_1(x))), \tag{2.24}$$

and θ_0, θ_1 are the linear contractions,

$$\theta_0(x) = -\omega x, \quad \theta_1(x) = -\omega x - 1. \tag{2.25}$$

The initial conditions become

$$u_2(x) = t_2(x) = \frac{1+\alpha\cos(2\pi(\omega^2 x+\omega/2))}{\alpha(1-\cos(2\pi(\omega^2 x+\omega)))}. \tag{2.26}$$

The two linear maps θ_0, θ_1 will be important in the theory which follows. They form an iterated function system which we shall describe briefly in Sec. II D.

Associated with the multiplicative renormalization operator R there is an additive linear operator R_a defined on function pairs (U,T) by

$$R_a(U,T)(x) = (T(-\omega x),T(-\omega x) + U(-\omega x - 1)). \tag{2.27}$$

The spectrum of this operator on a function space of analytic functions has been investigated in Ref. 24. We shall study further this operator below. In loose terms, R_a is the logarithm of the multiplicative renormalization operator R, although the presence of zeros of the function pair (u,t) is an obstacle to this correspondence.

Note that the same renormalization equation, (2.18), appears in the analysis by Kuznetsov *et al.*[23] of the onset of a strange nonchaotic attractor in quasiperiodically forced nonlinear systems, and in the study by Feudel *et al.*[7] of correlations on a strange nonchaotic attractor. We have recently considered the problem of correlations in some detail.[25] In this case piecewise-constant orbits of the recurrence are desired, as they are in an analysis of correlations in a barrier billiard.[3] Similarly, piecewise-constant orbits of the additive recurrence arise in the study of the self-similarity of the autocorrelation of a quasiperiodically forced two-level system.[8] We have given a detailed analysis of such orbits in Ref. 26.

B. Function pair conventions

In what follows we shall be dealing extensively with pairs of functions (u,t). We therefore make the convention that operations on function pairs act coordinatewise. For example, we may multiply two pairs $(u_1,t_1)(u_2,t_2)=(u_1u_2,t_1t_2)$, and evaluate at a point (x,x'): $(u,t)(x,x')=(u(x),u(x'))$. It will also be convenient for the convention to apply to functions, for example, $\exp(U,T)=(\exp(U),\exp(T))$, and $|(U,T)|=(|U|,|T|)$. Note that this is not the norm $\|(U,T)\|$ of the pair (U,T), but rather the function pair with values $(|U(x)|,|T(x')|)$ at a point (x,x').

We make one further convention that will simplify notation. In general, u and t will not have the same domains, but it will nevertheless be convenient to write expressions using the same variable x. Thus we may write $|(U,T)|(x)=(|U(x)|,|T(x)|)$, it being understood implicitly that the variable x is not the same for the two functions. These conventions should not cause confusion, and we shall use them freely in what follows.

C. The strong-coupling fixed point

In Ref. 17 the case $\alpha=0$, i.e., the original Harper equation (1.1), for which the Lyapunov exponent $\gamma=\log|\lambda|$, has the initial condition

$$u_2(x)=t_2(x)=\frac{1}{2(1-\cos(2\pi(\omega^2x+\omega)))}. \tag{2.28}$$

This initial condition has a single pole of order two at $x=1$ and the iteration of R leads to a fixed point of R, the so-called *strong-coupling fixed point*, as we shall prove in Sec. VI B. The strong-coupling fixed point and its properties were studied in Ref. 24. It is given by $u(x)=t(\theta_0(x))$, $t(x)=t_*(x)^{-2}$, where t_* is the unique, real analytic, entire function satisfying the equation

$$t_*(x)=t_*(-\omega x)t_*(\omega^2x+\omega), \tag{2.29}$$

for all $x\in\mathbb{C}$ and such that (i) $t_*(1)=0$; (ii) $t_*'(1)\neq 0$; and (iii) $t_*(x)>0$ for $x\in(-\omega^{-1},1)$. We refer the reader to Ref. 24 for the proof of the existence of t_* and of its properties.

The strong-coupling fixed point is relevant to the study of the orchid because of the denominator in the initial condition (2.26). Its role is, however, simply to change the scale of the orchid which we construct in Sec. IV below.

D. The iterated function system

For $c\in\{0,1\}$, as in (2.25) above, let θ_c denote the affine function

$$\theta_c(x)=-\omega x-c. \tag{2.30}$$

Then we may view θ_c as either a map of $\mathbb{R}$ or $\mathbb{C}$ depending on the context. [Note that the notation $\theta_0(x)=-\omega x$, $\theta_1(x)=-\omega x-1$ differs from that used in Ref. 24.]

The pair of maps θ_0, θ_1 forms an iterated function system (IFS) on $\mathbb{R}$ or $\mathbb{C}$ with unique compact invariant set the interval $I=[-\omega^{-1},1]$. We have $\theta_0(I)=[-\omega,1]$ and $\theta_1(I)=[-\omega^{-1},0]$ so that $I=\theta_0(I)\cup\theta_1(I)$.

The IFS θ_0, θ_1 considered here is related to the IFS ϕ_1, ϕ_2 considered in Refs. 24 and 25, where $\phi_1(x)=-\omega x$, $\phi_2(x)=\omega^2x+\omega$ and the invariant set is the interval $[-\omega,1]$. In fact $\phi_1=\theta_0$ and $\phi_2=\theta_0\circ\theta_1$. We note the following facts about the IFS θ_0, θ_1.

(i) θ_0 and θ_1 are both linear contractions on $\mathbb{C}$ with fixed points 0 and $-\omega$, respectively.
(ii) The interval I is an attractor for the IFS. In particular, given any compact subset $K\subseteq\mathbb{C}$ and any open neighborhood U of I in $\mathbb{C}$ there exists $N\in\mathbb{N}$ such that for any $k\geqslant N$ and any choice $i_1,\ldots,i_k\in\{0,1\}$ we have $\theta_{i_1}\circ\cdots\circ\theta_{i_k}(x)\in U$ for any $x\in K$.

Let us write $I_1=[-\omega^{-1},-\omega)$ and $I_0=(-\omega,1]$. Then we may define a map G by $G(x)=\theta_c^{-1}(x)=-\omega^{-1}x-c\omega^{-1}$ for $x\in I_c$, i.e.,

$$G(x)=\begin{cases}-\omega^{-1}x-\omega^{-1}, & -\omega^{-1}\leqslant x<-\omega;\\ -\omega^{-1}x, & -\omega<x\leqslant 1.\end{cases} \tag{2.31}$$

We do not define the value of G at the point $-\omega$, but note that $G(-\omega-)=-\omega$, $G(-\omega+)=1$. The function G is illustrated in Fig. 2.

We remark that the function $F:[-\omega,1]\to[-\omega,1]$ considered in Ref. 25, defined by

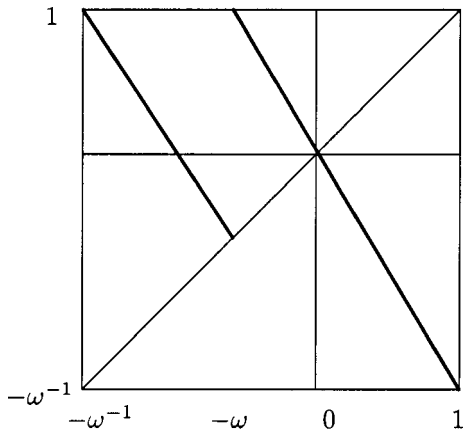

FIG. 2. The function G on the interval I.

$$F(x)=\begin{cases}\phi_1^{-1}(x), & x\in[-\omega,\omega^2];\\ \phi_2^{-1}(x), & x\in[\omega^2,1],\end{cases} \tag{2.32}$$

satisfies $F=G$ on $[-\omega,\omega^2]$ and $F=G^2$ on $(\omega^2,1]$, where $F(-\omega)=G(-\omega+)$.

We shall see that, asymptotically, the orbit of t_2 under the recursion (2.18) is determined solely by the orbits of the zeros of t_2 in I under the map G, apart from a choice of sign.

The function G is discontinuous on I. However, by identifying the points $-\omega^{-1}$, $-\omega$ and 1 in I we obtain a continuous map on the quotient topological space consisting of two circles joined at a single common point.

E. The multiplicative structure of *R*

In Ref. 25 the iteration (2.18) was studied for the case of piecewise constant functions t_n taking values ±1, and the periodic orbits were classified completely. This situation arises in the renormalization of the correlation function of strange nonchaotic attractors with a golden mean rotation number. These periodic orbits of (2.18) are determined by the periodic orbits of the map F given by (2.32) above. This is essentially because the dynamics of piecewise constant functions are governed by their discontinuity points, and the multiplicative nature of (2.18) relates any discontinuity of t_{n+1} at x with a discontinuity of t_n at $-\omega x$ or a discontinuity of t_{n-1} at $\omega^2x+\omega$. We refer the reader to Ref. 25 for details. However, such considerations apply also to the zeros of t_n and also to other singularities such as poles. In terms of the first-order renormalization R it is the map G (2.31) on I which is relevant. Indeed the following result is an immediate consequence of the definition of R and of the map G.

Proposition 2.1: Let $(u_{n+1},t_{n+1})=R(u_n,t_n)$ *where* u_n *is defined on* $[-\omega^{-1},-\omega]$ *and* t_n *is defined on* $[-\omega,1]$. *Then, defining* $G_0(x)=-\omega^{-1}x$ *and* $G_1(x)=-\omega^{-1}x-\omega^{-1}$,

(i) $u_{n+1}(x)=0$ *if and only if* $x=G_0(y)$ *where* $y\in[-\omega,1]$ *such that* $t_n(y)=0$;
(ii) $t_{n+1}(x)=0$ *if and only if* $x=G_0(y)$ *where* $y\in[-\omega,1]$ *such that* $t_n(y)=0$ *or* $x=G_1(y)$ *where* $y\in[-\omega^{-1},-\omega]$ *such that* $u_n(y)=0$.

Thus under iteration of R, the zeros evolve under iteration of the maps G_0, G_1, which, apart, from the point $x=-\omega$ correspond to the map G above.

The renormalization operator R has the following multiplicative property which is the analog of the linearity of the operator R_a. Let (u_1,t_1), (u_2,t_2) be function pairs. Then, using our convention that binary operations are defined coordinatewise, we have

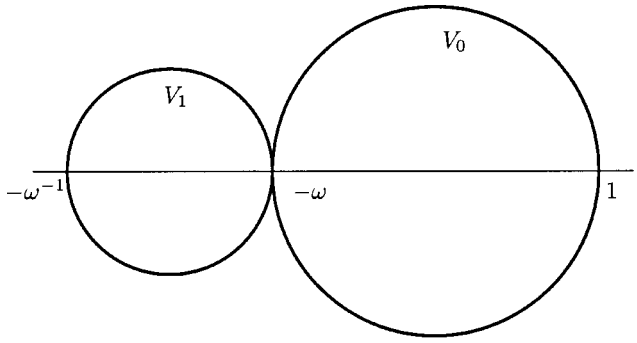

FIG. 3. The domains V_0 and V_1.

$$R((u_1,t_1)(u_2,t_2)) = R(u_1,t_1)R(u_2,t_2), \tag{2.33}$$

so that R respects the multiplication of function pairs. An analogous property holds for function pair division. We shall use this property extensively in what follows.

F. Properties of R and R_a

In this section we describe properties of the multiplicative renormalization operator R and its additive version R_a. We shall construct projections P and P_a which commute with R and R_a, respectively, and which "kill off" the unstable eigenvectors. We shall thus obtain operators RP and R_aP_a with spectral radius less than 1.

Recall that the multiplicative renormalization operator R on a pair of functions (u,t) is given by

$$R(u,t)(x) = (t(\theta_0(x)), t(\theta_0(x))u(\theta_1(x))), \tag{2.34}$$

where $\theta_0(x) = -\omega x$ and $\theta_1(x) = -\omega x - 1$. The additive version R_a of this operator is given by

$$R_a(U,T)(x) = (T(\theta_0(x)), T(\theta_0(x)) + U(\theta_1(x))). \tag{2.35}$$

We shall adopt the convention that the multiplicative operator R operates on lower-case function pairs (u,t), while the additive operator R_a operates on upper-case function pairs (U,T).

For $c \in \mathbb{C}$ and $r > 0$ let $D(c,r) = \{z \in \mathbb{C} : |z-c| < r\}$ denote the open disk with center c and radius r. Let $V_1 = D(c_1,r_1)$, $V_0 = D(c_0,r_0)$ be the disks in $\mathbb{C}$ specified by

$$c_0 = \omega^2/2, \quad r_0 = \omega^{-1}/2, \quad c_1 = -(\omega + 1/2), \quad r_1 = 1/2, \tag{2.36}$$

as illustrated in Fig. 3.

We have

$$[-\omega^{-1}, -\omega] \subseteq \overline{V_1}, \quad [-\omega, 1] \subseteq \overline{V_0}, \quad \theta_0(V_1) \subseteq V_0, \quad \theta_0(V_0) \subseteq V_0, \quad \theta_1(V_0) \subseteq V_1. \tag{2.37}$$

The convention we adopt is that the functions u and U are defined on V_1 and the functions t and T are defined on V_0. Moreover we shall assume that u and t are analytic on their respective domains, and that U and T are analytic on V_1 and V_0, respectively, or, at worst, have logarithmic singularities. For $i = 0,1$ let $\mathcal{B}_i$ be the real Banach space of real-analytic functions on V_i given by the Taylor series

$$f(z) = \sum_{k=0}^{\infty} f_k \frac{(z-c_i)^k}{r_i^k}, \tag{2.38}$$

with l_1-norm

$$\|f\|_{i,1} = \sum_{k=0}^{\infty} |f_k| < \infty. \tag{2.39}$$

Let $\mathcal{F}=\mathcal{B}_1 \times \mathcal{B}_0$ be the space of pairs (u,t) with $u \in \mathcal{B}_1$ and $t \in \mathcal{B}_0$. We equip $\mathcal{F}$ with the norm

$$\|(u,t)\| = \max\{\|u\|_{1,1}, \|t\|_{0,1}\}. \tag{2.40}$$

Then $\mathcal{F}$ is a real Banach space of pairs of analytic functions. We note that, in view of (2.37), the renormalization operators R and R_a are both well defined on $\mathcal{F}$. Indeed, R_a is a linear operator on $\mathcal{F}$, and we now discuss its functional analytic properties.

The following result is similar to Theorem 3 of Ref. 24.

Proposition 2.2: The additive renormalization operator R_a is a bounded linear operator on $\mathcal{F}$, which preserves, for each $n \geqslant 0$, the subspaces of polynomial pairs of degree at most n. The spectrum restricted to the subspace of polynomial pairs consists of the simple eigenvalues ω^{-1}, $-1, \pm\omega, \pm\omega^2, \ldots$.

The proof is straightforward and is similar to those given in Ref. 24.

Of particular note is that the eigenvalues corresponding to linear function pairs are ω^{-1}, -1, $-\omega$, and ω^2. Indeed, the eigenfunction pairs corresponding to eigenvalues ω^{-1} and -1 are, respectively,

$$\mathbf{v}_0 = \frac{1}{\sqrt{5}}(\omega, 1), \quad \mathbf{v}_1 = \frac{1}{\sqrt{5}}(\omega x - \omega, x + \omega), \tag{2.41}$$

as can readily be checked by direct computation: $R_a\mathbf{v}_0 = \omega^{-1}\mathbf{v}_0$, $R_a\mathbf{v}_1 = -\mathbf{v}_1$.

In Ref. 24 the strong-coupling fixed point was constructed using a singular function and a linear operator that is a contraction to zero, i.e., its spectrum is contained inside the unit circle in $\mathbb{C}$. Our approach to the construction of the orchid will be similar; it is therefore essential to "kill off" the noncontracting eigenfunction pairs of the operator R_a. We do this by projecting down to the stable manifold of the origin, i.e., the codimension-2 subspace of $\mathcal{F}$ spanned by the contracting eigenfunction pairs and the spectral subspace of 0. The construction of this projection P_a uses the family of linear functionals of $\mathcal{F}$ defined as follows.

Definition: For $n \geqslant 0$, let $\Delta_n : \mathcal{F} \to \mathbb{R}$ be defined by

$$\Delta_n(U,T) = \int_{-\omega^{-1}}^{-\omega} U^{(n)}(x)dx + \int_{-\omega}^{1} T^{(n)}(x)dx. \tag{2.42}$$

We note that for $n=1$,

$$\Delta_1(U,T) = U(-\omega) - U(-\omega^{-1}) + T(1) - T(-\omega), \tag{2.43}$$

and for $n=0$,

$$\Delta_0(U,T) = \int_{-\omega^{-1}}^{-\omega} U(x)dx + \int_{-\omega}^{1} T(x)dx. \tag{2.44}$$

Moreover, we remark that the linear functionals Δ_n may be defined for function pairs (U,T) with singularities in $V_1 \times V_0$. Indeed this is certainly the case for Δ_0 when U and T have logarithmic singularities on I.

The significance of the linear functionals Δ_n is that they are eigenvectors of the adjoint operator R_a^* on the dual space $\mathcal{F}^*$. Indeed we have the following.

Proposition 2.3:

$$\Delta_n(R_a(U,T)) = (-1)^n \omega^{n-1} \Delta_n(U,T). \tag{2.45}$$

Proof: The proof is a straightforward calculation:

$$\Delta_n(R_a(U,T)) = \int_{-\omega^{-1}}^{-\omega} \frac{d^n}{dx^n} T(\theta_0(x))dx + \int_{-\omega}^{1} \frac{d^n}{dx^n}(T(\theta_0(x)) + U(\theta_1(x)))dx$$

$$= (-\omega)^n \int_{-\omega^{-1}}^{-\omega} T^{(n)}(\theta_0(x))dx + (-\omega)^n \int_{-\omega}^{1} T^{(n)}(\theta_0(x)) + U^{(n)}(\theta_1(x))dx$$

$$= (-\omega)^{n-1} \int_{1}^{\omega^2} T^{(n)}(y)dy + (-\omega)^{n-1} \int_{\omega^2}^{-\omega} T^{(n)}(y)dy$$

$$+ (-\omega)^{n-1} \int_{-\omega}^{-\omega^{-1}} U^{(n)}(y')dy'$$

$$= -(-\omega)^{n-1}\left(\int_{-\omega}^{1} T^{(n)}(y)dy + \int_{-\omega^{-1}}^{-\omega} U^{(n)}(y')dy' \right)$$

$$= (-1)^n \omega^{n-1} \Delta_n(U,T), \tag{2.46}$$

as required. [In the above integrals we have changed variables: $y = \theta_0(x)$, $y' = \theta_1(x)$.] □

Direct calculation also gives the following properties:

$$\Delta_0(\mathbf{v}_0) = 1, \quad \Delta_0(\mathbf{v}_1) = 0, \quad \Delta_1(\mathbf{v}_0) = 0, \quad \Delta_1(\mathbf{v}_1) = 1. \tag{2.47}$$

Definition: The operator P_a is defined by

$$P_a(U,T) = (U,T) - \mathrm{Re}(\Delta_0(U,T))\mathbf{v}_0 - \mathrm{Re}(\Delta_1(U,T))\mathbf{v}_1. \tag{2.48}$$

We note that if $(U,T) \in \mathcal{F}$, then $\Delta_0(U,T)$, $\Delta_1(U,T) \in \mathbb{R}$.

The following results are straightforward to verify.

Proposition 2.4: The operator P_a has the following properties:

(i) $\mathrm{Re}(\Delta_0(P_a(U,T))) = \mathrm{Re}(\Delta_1(P_a(U,T))) = 0$;
(ii) $P_a^2 = P_a$;
(iii) $P_a R_a = R_a P_a$;
(iv) $P_a \mathbf{v}_0 = P_a \mathbf{v}_1 = 0$, *and* $\langle \mathbf{v}_0, \mathbf{v}_1 \rangle$ *is the null space of* P_a.

From this proposition we may conclude that P_a is a projection which commutes with R_a, and which "kills off" the noncontracting eigenfunction pairs $\mathbf{v}_0$ and $\mathbf{v}_1$.

Propositions 2.2 and 2.4 now give us the following result on the spectrum of $R_a P_a$.

Proposition 2.5: The operator $R_a P_a$ is a bounded operator, preserving, for each $n \geqslant 0$, the subspaces of polynomial pairs of degree at most n. The spectrum restricted to these subspaces of polynomial pairs consists of the simple eigenvalues $\pm\omega, \pm\omega^2, \ldots$.

We remark that, in particular, the spectral radius of $R_a P_a$ on the 4-dimensional space of linear function pairs is ω.

G. The multiplicative projection *P*

We now return to the multiplicative renormalization operator R and define a projection P that is analogous to P_a.

With the convention of Sec. II B, we note that for $(U,T) \in \mathcal{F}$ we have $R(\exp(U,T)) = \exp(R_a(U,T))$. Moreover, provided $u \neq 0$ on $\overline{V_1}$ and $t \neq 0$ on $\overline{V_0}$ and $u(x)$, $t(x) > 0$ for real x in their respective domains, we have that the principal branch of the logarithm $\log(U,T)$ is well defined and real for real argument, and $R_a(\log(u,t)) = \log R(u,t)$. Thus it is the possibility of the functions u and t changing sign that prevents a direct translation from R to R_a.

If $\log(u,t)$ exists we may define the projection $P(u,t)=\exp(P_a(\log(u,t)))$. However, in any event we may define P as follows.

Definition: The operator $P:\mathcal{F}\to\mathcal{F}$ is defined by

$$P(u,t) = (u,t)\exp(-\Delta_0(\log|(u,t)|)\mathbf{v}_0 - \Delta_1(\log|(u,t)|)\mathbf{v}_1). \tag{2.49}$$

We note that $P(u,t)=\exp(P_a(\log(u,t)))$.

It is straightforward to show that P has the properties of a projection operator.

Proposition 2.6: The operator $P:\mathcal{F}\to\mathcal{F}$ satisfies

(i) $P^2=P$;
(ii) $PR=RP$;
(iii) $P((u_1,t_1)(u_2,t_2))=P(u_1,t_1)P(u_2,t_2)$ *for* (u_1,t_1), $(u_2,t_2)\in\mathcal{F}$;
(iv) $P\exp(U,T)=\exp P_a(U,T)$ *for* $(U,T)\in\mathcal{F}$.

We remark that the operator RP may be used to construct the orchid numerically, although care must be taken to preserve the symmetry of the zero set.

H. Convergence of orbits with the same zero set

We are now in a position to prove that it is indeed the zero set of an initial condition (u_0,t_0) together with a choice of sign $(s_0^u,s_0^t)\in\{-1,+1\}^2$ which completely determines the asymptotic future of $P(u_0,t_0)$ under R. Specifically we prove the following.

Proposition 2.7: Let $(u_0,t_0)\in\mathcal{F}$ satisfy

(i) $u_0\neq 0$ *on* $\overline{V_1}$;
(ii) $t_0\neq 0$ *on* $\overline{V_0}$;
(iii) $u_0(x)>0$ *for* $x\in\overline{V_1}\cap\mathbb{R}$;
(iv) $t_0(x)>0$ *for* $x\in\overline{V_0}\cap\mathbb{R}$;
(v) $(d^2/dx^2)\log(u_0,t_0)(x)\in\mathcal{F}$.

Then

$$(\hat{u}_n,\hat{t}_n) = R^nP(u_0,t_0)\to(1,1), \quad \text{as } n\to\infty. \tag{2.50}$$

Sketch Proof: From the above we may write $(\hat{U}_0,\hat{T}_0)=P_a\log(u_0,t_0)$ with $(\hat{U}_0,\hat{T}_0)\in\mathcal{F}$. Moreover, it can be shown that $(\hat{U}_n,\hat{T}_n)=R_a^n(\hat{U}_0,\hat{T}_0)\to(0,0)$ as $n\to\infty$. Then

$$(\hat{u}_n,\hat{t}_n) = R^nP(u_0,t_0) = R^n\exp(P_a\log(u_0,t_0)) = \exp(R_a^nP_a\log(u_0,t_0)) = \exp(\hat{U}_n,\hat{T}_n)\to(1,1),$$
$$\text{as } n\to\infty. \tag{2.51}$$

This completes the proof. □

From this result we may immediately deduce that the future of (u_0,t_0) under R is determined by the zero sets of u_0, t_0 together with a choice of sign. For if (u_0^1,t_0^1), (u_0^2,t_0^2) have the same zero sets in V_1 and V_0, then we may find a choice of signs $(s_0^u,s_0^t)\in\{-1,+1\}^2$ such that

$$(s_0^u,s_0^t)(u_0^1,t_0^1)/(u_0^2,t_0^2) = \left(s_0^u\frac{u_0^1}{u_0^2},s_0^t\frac{t_0^1}{t_0^2}\right) \tag{2.52}$$

(once the removable singularities have been removed) satisfies the proposition above so that

$$\frac{R^nP(u_0^1,t_0^1)R^n(s_0^u,s_0^t)}{R^nP(u_0^2,t_0^2)}\to(1,1), \quad \text{as } n\to\infty, \tag{2.53}$$

and so

$$\frac{|R^n P(u_0^1, t_0^1)|}{|R^n P(u_0^2, t_0^2)|} \to (1,1), \quad \text{as } n \to \infty. \tag{2.54}$$

III. SHIFT SPACES AND PARTNERS

A. Shift spaces

Let X be a metric space with metric d. We write $X^{\mathbb{Z}}$ for the set of bi-infinite sequences $\mathbf{x}=(x_k)_{k\in\mathbb{Z}}$ with $x_k \in X$. We denote by $\sigma: X^{\mathbb{Z}} \to X^{\mathbb{Z}}$ the shift map defined for $\mathbf{x}=(x_k)_{k\in\mathbb{Z}} \in X^{\mathbb{Z}}$ by $\sigma(\mathbf{x})_k = x_{k+1}$. If X is bounded then we may define a metric on $X^{\mathbb{Z}}$ as follows:

$$d(\mathbf{x}, \mathbf{x}') = \sum_{k=-\infty}^{\infty} d(x_k, x_k') 2^{-|k|}. \tag{3.1}$$

With respect to this metric the shift map σ is a homeomorphism of $X^{\mathbb{Z}}$. Of particular importance for us will be the case when $X=\{0,1\}$ with the metric $d(x,x')=|x-x'|$ with $x, x' \in \{0,1\}$. We note that the space $\{0,1\}^{\mathbb{Z}}$, which is the full two-sided/bi-infinite shift space on the two symbols 0, 1, is homeomorphic to a Cantor set.

We now denote by $\hat{\Sigma}$ the *subshift of finite type* consisting of bi-infinite sequences $\mathbf{c}=(c_k)_{k\in\mathbb{Z}}$ satisfying $c_k c_{k+1}=0$, i.e., sequences for which no two consecutive terms of the sequence have digit 1. Then $\hat{\Sigma}$ inherits a topology from $\{0,1\}^{\mathbb{Z}}$ and moreover the shift map σ restricts to a homeomorphism $\sigma: \hat{\Sigma} \to \hat{\Sigma}$. We shall henceforth refer to bi-infinite sequences in $\hat{\Sigma}$ as *codes*.

Let Σ be the subset of $\hat{\Sigma}$ obtained by removing all codes $\mathbf{c}$ which terminate in either all 0s or the block 01 repeated infinitely often. Then Σ is invariant under σ, but is not closed in $\hat{\Sigma}$.

B. The evaluation map

Definition: For $n \in \mathbb{Z}$, we define the *evaluation map* at index n, $e_n: \hat{\Sigma} \to I$, to be the base $-\omega$ expansion,

$$e_n(\mathbf{c}) = -\sum_{k=n}^{\infty} c_k (-\omega)^{k-n}. \tag{3.2}$$

The evaluation map satisfies

$$e_n(\sigma(\mathbf{c})) = -\sum_{k=n}^{\infty} c_{k+1}(-\omega)^{k-n} = -\sum_{k'=n+1}^{\infty} c_{k'}(-\omega)^{k'-(n+1)} = e_{n+1}(\mathbf{c}). \tag{3.3}$$

Writing $\mathbf{e}$ for the map of sequence spaces $\mathbf{e}: \hat{\Sigma} \to I^{\mathbb{Z}}$ given by $\mathbf{e}(\mathbf{c})_n = e_n(\mathbf{c})$, the relation (3.3) becomes

$$\mathbf{e}(\sigma(\mathbf{c})) = \sigma(\mathbf{e}(\mathbf{c})). \tag{3.4}$$

For each $n \in \mathbb{Z}$, e_n is continuous and thus so is $\mathbf{e}$. We note that the codes that have been deleted from $\hat{\Sigma}$ to form Σ are those for which $e_n(\mathbf{c})=0$ or 1 for some $n \in \mathbb{Z}$.

Of particular interest to us is the fact that the image $\mathbf{e}(\Sigma)$ is precisely the set of full orbits of the map G which never take the values 0 or 1. Indeed,

$$e_n(\sigma(\mathbf{c})) = e_{n+1}(\mathbf{c}) = -\sum_{k=n+1}^{\infty} c_k(-\omega)^{k-(n+1)}$$
$$= -\omega^{-1}\left(-\sum_{k=n+1}^{\infty} c_k(-\omega)^{k-n}\right) = -\omega^{-1}\left(-\sum_{k=n}^{\infty} c_k(-\omega)^{k-n} + c_n\right)$$
$$= -\omega^{-1}e_n(\mathbf{c}) - \omega^{-1}c_n = G(e_n(\mathbf{c})), \tag{3.5}$$

since $c_n = c$ if and only if $e_n(\mathbf{c}) \in I_c$.

C. Partners

We now define a symmetry operation on bi-infinite codes $\mathbf{c} \in \Sigma$ which we call "partnering." The partnering operation will be important in the construction of the orchid below.

The definition of the operation will be eased by introducing the symbols A, B, C where $A = 010$, $B = 00$, $C = 01$ are groups of digits in the code $\mathbf{c}$. We can write any code $\mathbf{c} \in \Sigma$ uniquely in terms of the symbols A, B, C as given by the following lemma.

Lemma 3.1: Let $\mathbf{c} \in \Sigma$. *Then* $\mathbf{c}$ *may be written uniquely in terms of the symbols* A, B, C. *Conversely, any bi-infinite sequence of symbols* A, B, C *corresponds to a unique* $\mathbf{c} \in \Sigma$ *once the location of* $k = 0$ (*which need not be the first digit of* A, B, C) *is known.*

Proof: It is clear that any symbol sequence of A, B, C gives a unique code $\mathbf{c} \in \Sigma$ provided the origin $k = 0$ is known. It remains to show that any code $\mathbf{c} \in \Sigma$ may be written in terms of A, B, C.

Let $\mathbf{c} \in \Sigma$. We first of all consider the case when $\mathbf{c}$ does not begin in only zeros. Since no two consecutive 1s occur in the code we may write $\mathbf{c}$ in terms of blocks of digits beginning with 01. Such a block will be one of two forms: (i) $010(00)^m$; or (ii) $01(00)^m$. Here $m \geqslant 0$ is an integer, and, for a group of digits D, D^m means repeat the group D m times. In case (i) we write the block as AB^m. In case (ii) we write CB^m. In the case when $\mathbf{c}$ begins in all zeros then $\mathbf{c}$ may be written as $B^\infty A\ldots$ or $B^\infty C\ldots$. It is clear that the representation in terms of the symbols A, B, C is unique. □

As an example we illustrate with the code

$$\ldots\underbrace{010}_{A}\,\underbrace{0\dot{1}000}_{AB}\,\underbrace{010000}_{CB^2}\,\underbrace{01}_{C}\,01\ldots, \tag{3.6}$$

in which the "dot" above a digit indicates the location of the origin $k = 0$.

We are now able to define the partner operation via the following substitution rule on the symbols A, B, C:

$$A \to A, \quad B \to C, \quad C \to B. \tag{3.7}$$

We denote the resulting partner of a code $\mathbf{c} = (c_k)_{k\in\mathbb{Z}}$ by $\tilde{\mathbf{c}} = (\tilde{c}_k)_{k\in\mathbb{Z}}$. So, for example, the code considered above

$$\mathbf{c} = \ldots\underbrace{010}_{A}\,\underbrace{0\dot{1}000}_{AB}\,\underbrace{010000}_{CB^2}\,\underbrace{01}_{C}\,01\ldots \tag{3.8}$$

has partner

$$\tilde{\mathbf{c}} = \ldots\underbrace{010}_{A}\,\underbrace{0\dot{1}001}_{AC}\,\underbrace{000101}_{BC^2}\,\underbrace{00}_{B}\ldots. \tag{3.9}$$

It is clear from the rule (3.7) that the partner operation is an involution: $\tilde{\tilde{\mathbf{c}}} = \mathbf{c}$. Moreover it is also clear that it commutes with the shift $\sigma: \Sigma \to \Sigma$: $\sigma(\tilde{\mathbf{c}}) = \widetilde{\sigma(\mathbf{c})}$. This is because the location of $k = 0$ is preserved under partnering.

The code $\mathbf{c}$ corresponds to a full orbit $\mathbf{y} = (y_n)_{n\in\mathbb{Z}}$ of the map G by the evaluation map $\mathbf{e}$, i.e., $\mathbf{y} = \mathbf{e}(\mathbf{c})$, where $y_n = e_n(\mathbf{c})$.We may now ask how the orbits $\mathbf{y} = \mathbf{e}(\mathbf{c})$ and $\tilde{\mathbf{y}} = \mathbf{e}(\tilde{\mathbf{c}})$ are related. In order

to give the answer we define the following "sum map" $\mathbf{S}:\Sigma\to\{-\omega^{-1},-\omega,1\}^{\mathbb{Z}}$, the space of bi-infinite sequences taking values in $\{-\omega^{-1},-\omega,1\}$. We define $\mathbf{S}$ on a code $\mathbf{c}\in\Sigma$ by defining its action on the symbols A, B, C:

$$\mathbf{S}(A)=1(-\omega^{-1})(-\omega),\quad \mathbf{S}(B)=\mathbf{S}(C)=1(-\omega^{-1}). \tag{3.10}$$

We then define $\mathbf{S}$ on the whole code $\mathbf{c}$ by writing $\mathbf{c}$ in terms of A, B, C as in Lemma 3.1 and applying $\mathbf{S}$ to each of the symbols A, B, C separately. We note that since $\mathbf{S}$ preserves the number of symbols it commutes with σ:

$$\mathbf{S}(\sigma(\mathbf{c}))=\sigma(\mathbf{S}(\mathbf{c})). \tag{3.11}$$

Furthermore, comparing (3.10) with (3.7) we see that the map $\mathbf{S}$ is invariant under the partner map: $\mathbf{S}(\tilde{\mathbf{c}})=\mathbf{S}(\mathbf{c})$ for all $\mathbf{c}\in\Sigma$.

We have the following result which specifies precisely how $\mathbf{y}=\mathbf{e}(\mathbf{c})$ and $\tilde{\mathbf{y}}=\mathbf{e}(\tilde{\mathbf{c}})$ are related, and explains our terminology "sum map."

Proposition 3.1: Let $\mathbf{y}=\mathbf{e}(\mathbf{c})$ *and* $\tilde{\mathbf{y}}=\mathbf{e}(\tilde{\mathbf{c}})$. *Then* $\mathbf{y}+\tilde{\mathbf{y}}=\mathbf{S}(\mathbf{c})$, *where the sum is to be calculated termwise.*

Proof: For $n\in\mathbb{Z}$ let $S_n=y_n+\tilde{y}_n$. We write the codes of $\mathbf{c}$ and $\tilde{\mathbf{c}}$ in terms of the symbols A, B, C. We note that

$$y_n=-\sum_{k=n}^{\infty}c_k(-\omega)^{k-n},\quad \tilde{y}_n=-\sum_{k=n}^{\infty}\tilde{c}_k(-\omega)^{k-n}, \tag{3.12}$$

and that $y_n,\tilde{y}_n\in[-\omega^{-1},1]$ for all $n\in\mathbb{Z}$. In particular they are bounded.

Let us first of all consider the case when c_n starts a symbol A, B, or C. Then we have two cases.

(i) Both c_n and $\tilde{c}_n$ start an $A=010$. Then

$$\begin{aligned}S_n=y_n+\tilde{y}_n&=-(-\omega)-(-\omega)^3\sum_{k=n+3}^{\infty}c_k(-\omega)^{k-(n+3)}-(-\omega)-(-\omega)^3\sum_{k=n+3}^{\infty}\tilde{c}_k(-\omega)^{k-(n+3)}\\&=2\omega-\omega^3S_{n+3}.\end{aligned} \tag{3.13}$$

(ii) One of c_n, $\tilde{c}_n$ starts a $B=00$ and the other starts a $C=01$. Then we obtain

$$S_n=\omega+\omega^2S_{n+2}. \tag{3.14}$$

Now let

$$\kappa_2(x)=\omega+\omega^2x,\quad \kappa_3(x)=2\omega-\omega^3x. \tag{3.15}$$

Both of these maps are contractions with fixed point 1, and we have

$$S_n=\kappa_{i_1}\circ\cdots\circ\kappa_{i_\ell}(S_{n+i_1+\cdots+i_\ell}), \tag{3.16}$$

where $i_1,\ldots,i_\ell\in\{2,3\}$ according to the sequence of A, B, C in the codes $\mathbf{c}$, $\tilde{\mathbf{c}}$ starting at n. Now

$$|S_n-1|=\omega^{i_1+\cdots+i_\ell}|S_{n+i_1+\cdots+i_\ell}-1|, \tag{3.17}$$

and, since S_k is bounded for all $k\in\mathbb{Z}$, it follows, taking $\ell\to\infty$, that $S_n=1$.

We have therefore proved that $y_n+\tilde{y}_n=1$ provided n is at the start of a symbol A, B, or C.

Next we consider the case where c_n (and therefore $\tilde{c}_n$) is the digit 1 of $A=010$. Then we see that

$$S_n = -2 + \omega^2 S_{n+2}, \tag{3.18}$$

where c_{n+2} starts an A, B, or C in $\mathbf{c}$ and $\tilde{\mathbf{c}}$. Thus $S_{n+2}=1$ and so $S_n=-2+\omega^2=-\omega^{-1}$.

When c_n (and again therefore $\tilde{c}_n$) is the second digit 0 of $A=010$ we have that $S_n=-\omega S_{n+1}=-\omega$, since $S_{n+1}=1$.

These last two cases show that the sums for a symbol $A=010$ are $1(-\omega^{-1})(-\omega)$ as in the definition of the map $\mathbf{S}$ (3.10).

Finally, we consider the case when c_n (respectively, $\tilde{c}_n$) is the second digit of a B or C (respectively, C or B). We have $S_n=-1-\omega S_{n+1}=-1-\omega=-\omega^{-1}$. Thus, from this and the first case considered, the sums for the symbols $B=00$ and $C=01$ are both $1(-\omega^{-1})$ as in the definition of the map $\mathbf{S}$ (3.10), and the lemma is proved. □

For future use, we remark that (3.10) indicates that if $y_0+\tilde{y}_0=1$ then c_0 can only be at the beginning of a symbol A, B or C.

We illustrate this result with an example. Let

$$\mathbf{c} = \ldots \underbrace{\dot{0}1000}_{AB}\underbrace{01000}_{AB}\ldots \tag{3.19}$$

be the bi-infinite sequence of AB repeated which has the partner

$$\tilde{\mathbf{c}} = \ldots \underbrace{\dot{0}1001}_{AC}\underbrace{01001}_{AC}\ldots \ . \tag{3.20}$$

Then $\mathbf{y}$ and $\tilde{\mathbf{y}}$ are the period-5 orbits of G:

$$\mathbf{y} = \ldots, \frac{\omega}{1+\omega^5}, \frac{-1}{1+\omega^5}, \frac{-\omega^4}{1+\omega^5}, \frac{\omega^3}{1+\omega^5}, \frac{-\omega^2}{1+\omega^5}, \ldots, \tag{3.21}$$

$$\tilde{\mathbf{y}} = \ldots, \frac{\omega-\omega^4}{1+\omega^5}, \frac{\omega^3-1}{1+\omega^5}, \frac{-(\omega^2+\omega^4)}{1+\omega^5}, \frac{\omega+\omega^3}{1+\omega^5}, \frac{-(1+\omega^2)}{1+\omega^5}, \ldots, \tag{3.22}$$

with period-5 sum

$$\mathbf{S}(\mathbf{c}) = \mathbf{S}(\tilde{\mathbf{c}}) = \ldots, 1, -\omega^{-1}, -\omega, 1, -\omega^{-1}, \ldots, \tag{3.23}$$

as can easily be verified.

IV. CONSTRUCTION OF THE ORCHID

In this section we describe the construction of the Ketoja–Satija orchid $\mathcal{O}$. By the orchid we mean the whole set in function-pair space, not just the projection onto the plane by an evaluation at the origin of the function pair as in Fig. 1. We shall see that an uncountable dense subset of the orchid consists essentially of three copies of the sequence space Σ and, together with a map that acts on the signs of the functions, the shift map σ on Σ provides a dynamical model for the action of R on this dense subset of $\mathcal{O}$.

To construct the orchid we first define a map $\mathcal{E}:\Sigma\to\mathcal{F}$ which essentially conjugates R to the shift map σ on Σ. For $c\in\{0,1\}$, let us define a map on sign pairs $\kappa_c:\{-1,+1\}^2\to\{-1,+1\}^2$ by

$$\kappa_c(s^u,s^t) = (-s^t, -(-1)^c s^u s^t). \tag{4.1}$$

The map $\mathcal{E}:\Sigma\to\mathcal{F}$ is given by the following proposition.

Proposition 4.1: There exists a continuous map $\mathcal{E}:\Sigma\to\mathcal{F}$ such that for $\mathbf{c}\in\Sigma$, $\mathcal{E}(\mathbf{c})$ is a pair $(u,t)\in\mathcal{F}$ such that

(i) *if $c_{-1}=0$ then $u(x)=(y_0-x)u^1(x)$, $t(x)=(y_0-x)t^1(x)$; otherwise*
(ii) *if $c_{-1}=1$ then $u(x)=u^1(x)$, $t(x)=(y_0-x)t^1(x)$,*

where $y_0=e_0(\mathbf{c})$, and u^1, t^1 are functions analytic on V_1 and V_0, respectively, satisfying $u^1(x)>0$

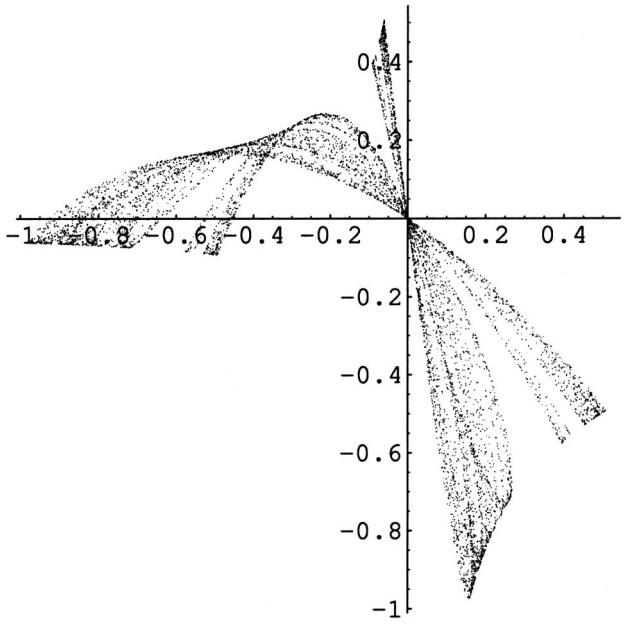

FIG. 4. A projection of the fundamental set cl($\beta(\Sigma)$).

on $(-\omega^{-1},-\omega)$ *and* $t^1(x)>0$ *on* $(-\omega,1)$. *Furthermore, let* $(s^u,s^t)\in\{-1,+1\}^2$ *be a choice of signs. Then, using our convention that multiplication of pairs is defined coordinatewise, we have that for* $\mathbf{c}\in\Sigma$,

$$R((s^u,s^t)\mathcal{E}(\mathbf{c}))=\kappa_{c_0}(s^u,s^t)\mathcal{E}(\sigma(\mathbf{c})). \tag{4.2}$$

In essence the proposition says that the action of R on a pair $(u,t)=(s^u,s^t)\mathcal{E}(\mathbf{c})$ is the map κ_{c_0} on the pair of signs (s^u,s^t) together with the shift map on the code $\mathbf{c}$.

The proof of this proposition is in Sec. V.

We now return to the construction of the orchid itself. The orchid is constructed from a code $\mathbf{c}$ and its partner $\tilde{\mathbf{c}}$. Indeed we may use the map $\mathcal{E}$ to define one of the three fundamental sets that make up the orchid.

Definition: The map $\beta:\Sigma\to\mathcal{F}$ is defined for $\mathbf{c}\in\Sigma$ by

$$\beta(\mathbf{c})=\mathcal{E}(\mathbf{c})\mathcal{E}(\tilde{\mathbf{c}}), \tag{4.3}$$

where $\tilde{\mathbf{c}}$ is the partner of $\mathbf{c}$.

A projection to the plane of the closure of the image of β is shown in Fig. 4.

We now define a new map on the sign pairs as follows.

Definition: For $b\in\{0,1\}$ let $L_b:\{-1,+1\}^2\to\{-1,+1\}^2$ be defined by

$$L_b(s^u,s^t)=(s^t,(-1)^b s^u s^t). \tag{4.4}$$

It is easy to check that the map L_b is invertible with inverse $L_b^{-1}(s^u,s^t)=((-1)^b s^u s^t,s^u)$.

We then have the following theorem.

Theorem 4.1: *The map* $\beta:\Sigma\to\mathcal{F}$ *satisfies the equation*

$$R((s^u,s^t)\beta(\mathbf{c}))=L_{b_0}(s^u,s^t)\beta(\sigma(\mathbf{c})), \tag{4.5}$$

where $b_0=c_0+\tilde{c}_0 \bmod 2$. *The map* β *is continuous and two-to-one from* Σ *to its image* $\beta(\Sigma)\subseteq\mathcal{F}$.

Equation (4.5) follows immediately from (4.2), and we prove the other properties of β in Sec. V D. We now proceed to use the theorem to construct the orchid. The orchid $\mathcal{O}$ is made up of three copies of the fundamental set $\beta(\Sigma)$ as follows. Let $\mathbf{c}$, $\tilde{\mathbf{c}}$ be partners and let $\mathbf{b}=\mathbf{c}+\tilde{\mathbf{c}} \bmod 2$ be the

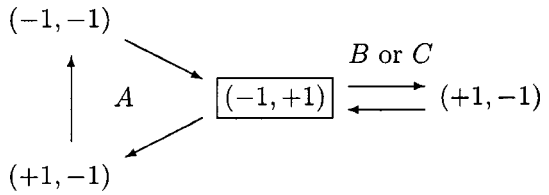

FIG. 5. The fundamental transition diagram.

bi-infinite sequence giving the parities of the sum $\mathbf{c}+\tilde{\mathbf{c}}$. Recall from Sec. III C that the partner code $\tilde{\mathbf{c}}$ is obtained from $\mathbf{c}$ by writing $\mathbf{c}$ uniquely in terms of the letters *A*, *B*, *C*. We shall need the set of indices which begin an *A*, *B*, *C* in the code of $\mathbf{c}$.

Definition: We define $S=\{k\in\mathbb{Z}$: the code of $\mathbf{c}$ begins an *A*, *B*, *C* at index $k\}$.

The set S is important and we shall have to restrict the signs (s^u,s^t) at indices $k\in S$. For $\mathbf{c}\in\Sigma$ and $(s_0^u,s_0^t)\in\{-1,+1\}^2$ we define, for $n\in\mathbb{Z}$, $(s_n^u,s_n^t)=(s_n^u(\mathbf{c}),s_n^t(\mathbf{c}))$ by the condition

$$L_{b_n}(s_n^u,s_n^t)=(s_{n+1}^u,s_{n+1}^t), \tag{4.6}$$

for all $n\in\mathbb{Z}$, where, as before $\mathbf{b}=\mathbf{c}+\tilde{\mathbf{c}}$ mod 2.

Definition (Ketoja–Satija orchid): The Ketoja–Satija orchid $\mathcal{O}$ is defined as

$$\mathcal{O}=\mathrm{cl}\{(s_0^u,s_0^t)\beta(\mathbf{c}):\mathbf{c}\in\Sigma \text{ and } (s_n^u(\mathbf{c}),s_n^t(\mathbf{c}))\in\{(+1,+1),(+1,-1),(-1,-1)\} \text{ for all } n\in S\}. \tag{4.7}$$

A projection of $\mathcal{O}$ is shown in Fig. 1, obtained by evaluating $\beta(\mathbf{c})$ at the origin. Thus the orchid is given by the closure of the image of Σ under the map β together with a restricted choice of signs so that at the start of each block $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}$ lies in the "permitted set" $\{(+1,+1),(+1,-1),(-1,-1)\}$. In fact the choice of signs in the definition of $\mathcal{O}$ is not so restrictive as can be seen from the following lemma.

Lemma 4.1: Let $n\in S$ and let $n'\in S$ be the smallest integer in S greater than n. Then $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}\in\{(+1,+1),(+1,-1),(-1,-1)\}$ *if and only if* $\mathbf{(}s_{n'}^u(\mathbf{c}),s_{n'}^t(\mathbf{c})\mathbf{)}\in\{(+1,+1),(+1,-1),(-1,-1)\}$.

The set S is the set of indices that start a block consisting of an *A*, *B*, or *C*. Thus Lemma 4.1 states that if the sign pair $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}$ is in the permitted set $\{(+1,+1),(+1,-1),(-1,-1)\}$ for index n, the start of an *A*, *B*, or *C*, then $\mathbf{(}s_{n'}^u(\mathbf{c}),s_{n'}^t(\mathbf{c})\mathbf{)}$ will also be in the permitted set for index n', the start of the next block, and vice versa. It follows that condition (4.7) need only be satisfied at the start of a single block, i.e., a single index $n\in S$, for it to hold throughout S.

Proof of Lemma 4.1: Let $n\in S$ and suppose $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}=(-1,+1)$, i.e., not in the permitted set at the start of a block and index n. The block may be an *A* or a *B*/*C* and we consider the two cases separately.

Block *A*. Then $n'=n+3$, and $b_n=a_n+\tilde{a}_n=0$, $b_{n+1}=0$, $b_{n+2}=0$, and (omitting the explicit dependence on $\mathbf{c}$) we have $(s_{n+1}^u,s_{n+1}^t)=(+1,-1)$, $(s_{n+2}^u,s_{n+2}^t)=(-1,-1)$, $(s_{n+3}^u,s_{n+3}^t)=(-1,+1)$, as required.

Block *B*/*C*. Then $n'=n+2$, and $b_n=a_n+\tilde{a}_n=0$, $b_{n+1}=1$, so, in this case, we have $(s_{n+1}^u,s_{n+1}^t)=(+1,-1)$, $(s_{n+2}^u,s_{n+2}^t)=(-1,+1)$, as required.

The converse statement that $\mathbf{(}s_{n'}^u(\mathbf{c}),s_{n'}^t(\mathbf{c})\mathbf{)}=(-1,+1)$ implies $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}=(-1,+1)$ follows immediately from the invertibility of the maps L_b on $\{-1,+1\}^2$. The lemma follows. □

The action of the blocks *A*, *B*/*C* on the sign pair $\mathbf{(}s_n^u(\mathbf{c}),s_n^t(\mathbf{c})\mathbf{)}$ is illustrated in Figs. 5 and 6.

Figure 5 represents the action of the maps L_b on the sign pair $(-1,+1)$ as a block *A* or *B*/*C* is traversed. The sign pair $(-1,+1)$ is at the start of a block which we indicate by enclosing the pair in a box. Although other sign pairs occur as the blocks are traversed, the sign pair returns to $(-1,+1)$ at the start of each block.

The transition diagram in Fig. 5 represents the fundamental set $\beta(\Sigma)\subseteq\mathcal{F}$.

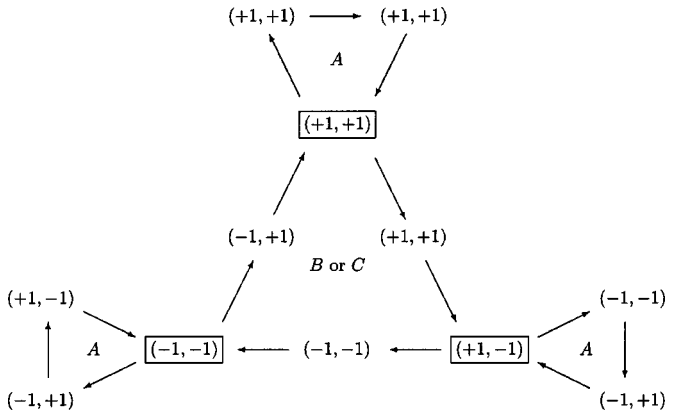

FIG. 6. The orchid transition diagram.

The orchid transition diagram is illustrated in Fig. 6. Again, the sign pairs occurring at the start of blocks are enclosed in boxes. Note that the sign pair $(-1,+1)$ that gives only the fundamental set $\beta(\Sigma)$ occurs as an intermediary as the blocks are traversed.

We thus have the following theorem.

Theorem 4.2: *The set $\mathcal{O}$ is an invariant set for R, i.e., $R(\mathcal{O})=\mathcal{O}$. The action of R on $\mathcal{O}$ is given by*

$$R((s_0^u,s_0^t)\beta(\mathbf{c})) = L_{b_0}(s_0^u,s_0^t)\beta(\sigma(\mathbf{c})), \tag{4.8}$$

for $\mathbf{c}\in\Sigma$ and $(s_0^u,s_0^t)\in\{-1,+1\}^2$.

This theorem gives a description of the dynamics on $\mathcal{O}$ in terms of the dynamics on Σ. In Sec. VI we study the properties of $\mathcal{O}$. First, however, we must complete the construction of the map $\mathcal{E}$.

V. CONSTRUCTION OF THE MAP $\mathcal{E}$

In this section we use the results of Sec. III above to construct the map $\mathcal{E}:\Sigma\to\mathcal{F}$ as given by Proposition 4.1.

Let $\mathbf{c}\in\Sigma$. Our method for constructing $\mathcal{E}(\mathbf{c})$ is as follows. We first consider the twice-differentiated additive operator R_2 given by

$$R_2(U,T) = (\omega^2 T\theta_0, \omega^2 T\theta_0 + \omega^2 U\theta_1), \tag{5.1}$$

and construct a function pair $E_2(\mathbf{c})$ such that

$$R_2(E_2(\mathbf{c})) = E_2(\sigma(\mathbf{c})). \tag{5.2}$$

The relationship between R_2 and R_a is the following:

$$R_a(U,T)'' = R_2(U'',T''), \tag{5.3}$$

so that R_2 is the map induced by R_a on the second derivative pair (U'',T''). Having constructed $E_2(\mathbf{c})$, we then obtain a function pair $\mathcal{E}(\mathbf{c})$ satisfying the relation

$$R(\mathcal{E}(\mathbf{c})) = \kappa_{c_0}(+1,+1)\mathcal{E}(\sigma(\mathbf{c})), \tag{5.4}$$

where, as in (4.1),

$$\kappa_{c_0}(+1,+1) = (-1,-(-1)^{c_0}). \tag{5.5}$$

The construction of $\mathcal{E}(\mathbf{c})$ from $E_2(\mathbf{c})$ is somewhat involved, as indeed is the construction of $E_2(\mathbf{c})$ itself.

A. Convergence proof preliminaries

Let $\mathbf{c} \in \Sigma$. For $k \in \mathbb{N}_0$ define $y_{-k} = e_{-k}(\mathbf{c})$, and $\delta_{-k} = y_{-k} + \omega$. We note that $\delta_{-k} \neq 0$ for all $\mathbf{c} \in \Sigma$. It may, however, be arbitrarily small, thereby creating a "small divisor" problem that must be controlled. We shall use the following lemma, which is fundamental to the convergence proof.

Lemma 5.1:

$$\sum_{k \geqslant 1} \frac{\omega^k}{|\delta_{-k}|} < +\infty. \tag{5.6}$$

$$\sum_{k \geqslant 1} \frac{k\omega^k}{|\delta_{-k}|} < +\infty. \tag{5.7}$$

$$\sum_{k \geqslant 1} \omega^k |\log|\delta_{-k}|| < +\infty. \tag{5.8}$$

Proof: We prove (5.6); the proofs of the other inequalities are similar. Let $0 < k_1 < k_2 < \cdots < k_i < \cdots$ be the values of k such that $|\delta_{-k}| < 1/2$. Let us consider k_i. We deal with the two cases $\delta_{-k_i} > 0$ and $\delta_{-k_i} < 0$ separately. If $\delta_{-k_i} > 0$, then for $1 \leqslant j < (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$, we have

$$\min\{|y_{-k_i+j} - 1|, |y_{-k_i+j} + \omega^{-1}|\} < 1/2, \tag{5.9}$$

so that $k_i - k_{i-1} \geqslant (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$. On the other hand, if $\delta_{-k_i} < 0$, then it is possible that $k_{i-1} + 1 = k_i$, and then for $2 \leqslant j < (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$ we have

$$\min\{|y_{-k_i+j} - 1|, |y_{-k_i+j} + \omega^{-1}|\} < 1/2, \tag{5.10}$$

so that $k_i - k_{i-2} \geqslant (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$. Otherwise $k_i - k_{i-1} \geqslant (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$, as before. Anyway, we certainly have $k_i - k_{i-2} \geqslant (\log|\delta_{-k_i}| - \log 1/2)/\log \omega$ for all i, so that

$$\frac{\omega^{k_i}}{|\delta_{-k_i}|} \leqslant 2\omega^{k_{i-2}}. \tag{5.11}$$

Now we estimate

$$\sum_{k \geqslant 1} \frac{\omega^k}{|\delta_{-k}|} \leqslant \sum_{j \neq k_i} \frac{\omega^j}{1/2} + \frac{\omega^{k_1}}{|\delta_{-k_1}|} + \frac{\omega^{k_2}}{|\delta_{-k_2}|} + \sum_{i \geqslant 3} 2\omega^{k_{i-2}} < +\infty, \tag{5.12}$$

as required. □

B. Construction of the function pair $E_2(\mathbf{c})$

We now proceed to construct the map E_2 outlined above. Let $\mathbf{c} \in \Sigma$, let $k \in \mathbb{N}_0$ and let $H_2^{k,0}$ be defined as

$$H_2^{k,0}(x) = \begin{cases} ((y_{-k} - x)^{-2}, (y_{-k} - x)^{-2}), & c_{-(k+1)} = 0; \\ (0, (y_{-k} - x)^{-2}), & c_{-(k+1)} = 1. \end{cases} \tag{5.13}$$

Then a straightward calculation shows that for $k \geqslant 1$,

$$R_2 H_2^{k,0} = H_2^{k-1,0} + H_2^{k,1}, \tag{5.14}$$

where

$$H_2^{k,1}(x)=\begin{cases}(0,\omega^2(y_{-k}-\theta_1(x))^{-2}), & c_{-(k+1)}=0, c_{-k}=0;\\ (\omega^2(y_{-k}-\theta_0(x))^{-2},\omega^2(y_{-k}-\theta_0(x))^{-2}), & c_{-(k+1)}=0, c_{-k}=1;\\ (0,0), & c_{-(k+1)}=1, c_{-k}=0.\end{cases} \tag{5.15}$$

The idea here is that the singular part of $R_2H_2^{k,0}$ is contained in $H_2^{k-1,0}$, while $H_2^{k,1}$ is nonsingular on $\overline{V_1}\times\overline{V_0}$.

Let us now define

$$H_2^{k,k}=R_2^{k-1}H_2^{k,1}. \tag{5.16}$$

Then a formal calculation from (5.14) gives

$$R_2^kH_2^{k,0}=\sum_{j=0}^{k}H_2^{j,j}. \tag{5.17}$$

We wish to show that the series $\Sigma_{j=1}^{k}H_2^{j,j}$ converges in $\mathcal{F}$. To do this we shall show that

$$\|H_2^{k,k}\|\leqslant\frac{K\omega^k}{|\delta_{-k}|}, \tag{5.18}$$

for some constant K, and then invoke Lemma 5.1.

Let us introduce the following convention. For a finite sequence of indices $i_1,\ldots,i_k$ we shall implicitly assume that $i_j\in\{0,1\}$, $j=1,\ldots,k$, and that $i_ji_{j+1}=0$, $j=1,\ldots,k-1$, so that no two consecutive 1s appear in the sequence. It is now straightforward to verify the following formula for the kth iterate of R_a:

$$R_a^k(U,T)=\left(\sum_{\substack{i_1,\ldots,i_k\\ i_1=1,i_k=0}}U\theta_{i_1}\cdots\theta_{i_k}+\sum_{\substack{i_1,\ldots,i_k\\ i_k=0,i_k=0}}T\theta_{i_1}\cdots\theta_{i_k},\sum_{\substack{i_1,\ldots,i_k\\ i_1=1}}U\theta_{i_1}\cdots\theta_{i_k}+\sum_{\substack{i_1,\ldots,i_k\\ i_1=0}}T\theta_{i_1}\cdots\theta_{i_k}\right). \tag{5.19}$$

Similarly, for R_2 we have

$$R_2^k(U,T)=\omega^{2k}R_a^k(U,T). \tag{5.20}$$

Thus, combining (5.15) and (5.19), we have

$$\begin{aligned}H_2^{k,k}(x)&=(R_2^{k-1}H_2^{k,1})(x)\\ &=\begin{cases}\left(\displaystyle\sum_{\substack{i_1,\ldots,i_{k-1}\\ i_1=0,i_{k-1}=0}}\omega^{2k}(y_{-k}-\theta_1\theta_{i_1}\cdots\theta_{i_{k-1}}(x))^{-2}\right.\ ,\\ \left.\displaystyle\sum_{\substack{i_1,\ldots,i_{k-1}\\ i_1=0}}\omega^{2k}(y_{-k}-\theta_1\theta_{i_1}\cdots\theta_{i_{k-1}}(x))^{-2}\right), & c_{-(k+1)}=0\ c_{-k}=0;\\ \left(\displaystyle\sum_{\substack{i_1,\ldots,i_{k-1}\\ i_{k-1}=0}}\omega^{2k}(y_{-k}-\theta_0\theta_{i_1}\cdots\theta_{i_{k-1}}(x))^{-2},\right.\\ \left.\displaystyle\sum_{i_1,\ldots,i_{k-1}}\omega^{2k}(y_{-k}-\theta_0\theta_{i_1}\cdots\theta_{i_{k-1}}(x))^{-2}\right), & c_{-(k+1)}=0\ c_{-k}=1;\\ (0,0), & c_{-(k+1)}=1\ c_{-k}=0.\end{cases}\end{aligned} \tag{5.21}$$

Using the identity

$$\omega^{2k}(y_{-k}-\theta_{i_0}\cdots\theta_{i_{k-1}}(x))^{-2}=(\theta_{i_{k-1}}^{-1}\cdots\theta_{i_0}^{-1}(y_{-k})-x)^{-2}, \tag{5.22}$$

we may rewrite this as

$$H_2^{k,k}(x)=\begin{cases}\left(\displaystyle\sum_{\substack{j_1,\ldots,j_k\\ j_1=\overline{c}_{-k},j_k=0}}(\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k})-x)^{-2},\ \sum_{\substack{j_1,\ldots,j_k\\ j_1=\overline{c}_{-k}}}(\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k})-x)^{-2}\right), & c_{-(k+1)}=0;\\ (0,0), & c_{-(k+1)}=1,\end{cases} \tag{5.23}$$

where we have used the notation

$$\overline{c}=\begin{cases}1, & c=0;\\ 0, & c=1.\end{cases} \tag{5.24}$$

We now wish to bound the norm of $H_2^{k,k}$ and to do so we make use of the following elementary norm estimate.

Lemma 5.2: Let $y\in\mathbb{C}$. The l_1-norm of the function $f(x)=(y-x)^{-2}$ on the domain $D(c,r)$ is

$$\|f\|_1=(|y-c|-r)^{-2}<+\infty, \tag{5.25}$$

provided $r<|y-c|$.

Proof: We have

$$f(x)=(y-x)^{-2}=(y-c-r(x-c)/r)^{-2}=\frac{1}{(y-c)^2}\sum_{i=0}^{\infty}\left(\frac{r}{y-c}\right)^i(i+1)\left(\frac{x-c}{r}\right)^i, \tag{5.26}$$

so that

$$\|f\|_1=\frac{1}{|y-c|^2}\sum_{i=0}^{\infty}\left(\frac{r}{|y-c|}\right)^i(i+1)=(|y-c|-r)^{-2}<+\infty, \tag{5.27}$$

provided $r<|y-c|$. □

As a consequence of this estimate, we have the following lemma.

Lemma 5.3:

(i) *$H_2^{k,1}\in\mathcal{F}$, so that the function pair $H_2^{k,1}$ is analytic on $V_1\times V_0$ with bounded norm $\|H_2^{k,1}\|<+\infty$;*

(ii) *For $k\geqslant 1$,*

$$\|H_2^{k,k}\|\leqslant\begin{cases}\max\left\{\displaystyle\sum_{\substack{j_1,\ldots,j_k\\ j_1=\overline{c}_{-k},j_k=0}}(|\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k})-c_1|-r_1)^{-2},\right.\\ \left.\displaystyle\sum_{\substack{j_1,\ldots,j_k\\ j_1=\overline{c}_{-k}}}(|\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k})-c_0|-r_0)^{-2}\right\}, & c_{-(k+1)}=0;\\ 0, & c_{-(k+1)}=1.\end{cases} \tag{5.28}$$

Proof:

(i) It is trivial in the third case of (5.15) that $H_2^{k,1}\in\mathcal{F}$. In the first case ($c_{-(k+1)}=0$, $c_{-k}=0$), we have $y_{-k}\in(-\omega,1)$. Thus $\theta_1^{-1}(y_{-k})\in(-2/\omega,-\omega)$, which does not intersect $\overline{V_0}$. Thus $(\theta_1^{-1}(y_{-k})-x)^{-2}$ is analytic on V_0, and thus has a bounded l_1-norm. It follows that $\|H_2^{k,1}\|<+\infty$ and $H_2^{k,1}\in\mathcal{F}$.

Similarly, in the second case ($c_{-(k+1)}=0$, $c_{-k}=1$), we have $y_{-k}\in(-\omega^{-1},-\omega)$. Thus $\theta_0^{-1}(y_{-k})\in(1,2/\omega)$, which does not intersect $\overline{V_0}\cup\overline{V_1}$, so that $H_2^{k,1}$ is analytic on $\overline{V_1}\times\overline{V_0}$ and $\|H_2^{k,1}\|<+\infty$.

(ii) Since $R_2\mathcal{F}\subseteq\mathcal{F}$, all singularities of $H_2^{k,k}=R_2^{k-1}H_2^{k,1}$ lie outside $\overline{V_0}\cup\overline{V_1}$ so the estimate for $\|H_2^{k,k}\|$ follows from Lemma 5.2 and (5.23).

Lemma 5.3 gives us a bound on $\|H_2^{k,k}\|$, but we still need to bound the sums on the right-hand sides of (5.28).

In what follows we shall make use of the following lemma whose proof is elementary.

Lemma 5.4: Let a, $b>0$. Then

$$\sum_{i=0}^{\infty}\frac{1}{(a+bi)^2}\leqslant\frac{a+b}{a^2b}. \tag{5.29}$$

Our fundamental estimate is the following.

Lemma 5.5: There exists a constant $K>0$ such that

$$\|H_2^{k,k}\|\leqslant\frac{K\omega^k}{|\delta_{-k}|}. \tag{5.30}$$

Corollary 5.1: The series $\Sigma_{k\geqslant 1}H_2^{k,k}$ converges in $\mathcal{F}$.

Proof: This follows immediately from Lemmas 5.5 and 5.1. □

In order to prove Lemma 5.5, we need to identify more precisely the singularities of $H_2^{k,k}$. In particular, we have the following result, which follows from the properties of the golden mean. Its proof is straightforward if somewhat lengthy, and is omitted.

Lemma 5.6: Let

$$A=\{\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k}):j_1=\overline{c_{-k}}\}, \tag{5.31}$$

$$B=\{\theta_{j_k}^{-1}\cdots\theta_{j_1}^{-1}(y_{-k}):j_1=\overline{c_{-k}},j_k=0\}. \tag{5.32}$$

Then we have the following cases.

Case (i) $c_{-k}=1$ ($\delta_{-k}<0$); when $k\geqslant 1$ is odd,

$$A=-\omega^{-k}\delta_{-k}+\{1\}\cup\{\lceil i/\omega\rceil+i\omega:i=1,\ldots,F_{k+1}-1\}, \tag{5.33}$$

$$B=-\omega^{-k}\delta_{-k}+\{\lceil i/\omega\rceil+i\omega:i=\lfloor|j/\omega|\rfloor,j=1,\ldots,F_k-1\}\cup\{\lceil i/\omega\rceil-1+i\omega-\omega:i=\lfloor F_k/\omega\rfloor\}. \tag{5.34}$$

When $k\geqslant 1$ is even,

$$A=\omega^{-k}\delta_{-k}+\{\lceil i/\omega\rceil+i\omega:i=1-F_{k+1},\ldots,-1\}\cup\{\lceil i/\omega\rceil+1+i\omega:i=-F_{k+1}\}, \tag{5.35}$$

$$B=\omega^{-k}\delta_{-k}+\{\lceil i/\omega\rceil+i\omega:i=\lceil j/\omega\rceil,j=1-F_k,\ldots,-1\}\cup\{-1-\omega\}. \tag{5.36}$$

Case (ii) $c_{-k}=0$ ($\delta_{-k}>0$); when $k\geqslant 1$ is odd,

$$A=-\omega^{-k}\delta_{-k}+\{\lceil i/\omega\rceil+i\omega:i=1-F_k,\ldots,-1\}\cup\{\lceil i/\omega\rceil+1+i\omega:i=-F_k\}, \tag{5.37}$$

$$B=-\omega^{-k}\delta_{-k}+\{\lceil i/\omega\rceil+i\omega:i=\lceil j/\omega\rceil,j=1-F_{k-1},\ldots,-1\}\cup\{-1-\omega\}. \tag{5.38}$$

When $k\geqslant 1$ is even,

$$A=\omega^{-k}\delta_{-k}+\{1\}\cup\{\lceil i/\omega\rceil+i\omega:i=1,\ldots,F_k-1\}, \tag{5.39}$$

$$B = \omega^{-k}\delta_{-k} + \{\lceil i/\omega\rceil + i\omega : i = \lfloor j/\omega\rfloor, j = 1, \ldots, F_{k-1} - 1\} \cup \{\lceil i/\omega\rceil - 1 + i\omega - \omega : i = \lfloor F_{k-1}/\omega\rfloor\}. \tag{5.40}$$

Proof of Lemma 5.5: Referring to Lemma 5.6, we see that for each k, the sets A and B have the same overall structure while differing in detail. In particular, we have that the elements grow linearly. To be more specific, we make the following observation. Writing $A=\{x_0^0, \ldots, x_{N_k^0}^0\}$, $B=\{x_0^1, \ldots, x_{N_k^1}^1\}$, for N_k^0, $N_k^1 \in N$ with $|x_0^0| < |x_1^0| < \cdots < |x_{N_k^0}^0|$, $|x_0^1| < |x_1^1| < \cdots < |x_{N_k^1}^1|$, we have that there exists a constant $C>0$ (independent of k) such that, for $i=0$, 1, $x_j^i \geqslant 1 + Cj + (-\omega)^{-k}\delta_{-k}$, $j=0, \ldots, N_k^i$ for $(-1)^k\delta_{-k} > 0$, while $x_j^i \leqslant -\omega^{-1} - Cj + (-\omega)^{-k}\delta_{-k}$, $j=0, \ldots, N_k^i$ for $(-1)^k\delta_{-k} < 0$.

We now refer to (5.28) and observe that the sums are taken over the sets B and A, respectively, and each term in the sum is of the form $(|x_j^i - c_i| - r_i)^{-2}$, and, since $-\omega^{-1} \leqslant c_1 - r_1 \leqslant c_1 + r_1 = c_0 - r_0 \leqslant c_0 + r_0 \leqslant 1$, we have that each sum in (5.28) is majorized by

$$\sum_{j=0}^{\infty} (\omega^{-k}|\delta_{-k}| + Cj)^{-2} \leqslant \frac{C + \omega^{-k}|\delta_{-k}|}{\omega^{-2k}|\delta_{-k}|^2 C} \quad \text{by Lemma 5.4} \tag{5.41}$$

$$= \frac{\omega^k}{C|\delta_{-k}|} + \frac{\omega^{2k}}{|\delta_{-k}|^2} \tag{5.42}$$

$$\leqslant K\frac{\omega^k}{|\delta_{-k}|}, \tag{5.43}$$

for some $K>0$ (depending on $\mathbf{c}$) since $\Sigma_{k=1}^{\infty}\, \omega^k/|\delta_{-k}| < +\infty$. □

We are therefore able to define

$$E_2(\mathbf{c}) = \lim_{k\to\infty} R_2^k H_2^{k,0} = H_2^{0,0} + G_2(\mathbf{c}), \quad \text{where } G_2(\mathbf{c}) = \sum_{j\geqslant 1} H_2^{j,j}. \tag{5.44}$$

The first part of $E_2(\mathbf{c})$, i.e., $H_2^{0,0}$, may contain singularities on $\overline{V_1} \times \overline{V_0}$. These singularities are all poles. We note that, by definition, $H_2^{k,0}(\mathbf{c}) = H_2^{k+1,0}(\sigma(\mathbf{c}))$, so that

$$H_2^{k,1}(\mathbf{c}) = H_2^{k+1,1}(\sigma(\mathbf{c})) \tag{5.45}$$

and

$$R_2(H_2^{k,k}(\mathbf{c})) = R_2(R_2^{k-1}H_2^{k,1}(\mathbf{c})) = R_2^k H_2^{k+1,1}(\sigma(\mathbf{c})) = H_2^{k+1,k+1}(\sigma(\mathbf{c})). \tag{5.46}$$

Hence, by continuity of R_2,

$$R_2 G_2(\mathbf{c}) = R_2\left(\sum_{j\geqslant 1} H_2^{j,j}(\mathbf{c})\right) = \sum_{j\geqslant 1} H_2^{j+1,j+1}(\sigma(\mathbf{c})) = G_2(\sigma(\mathbf{c})) - H_2^{0,1}(\mathbf{c}). \tag{5.47}$$

Allowing for singularities we have

$$R_2(E_2(\mathbf{c})) = R_2 H^{0,0}(\mathbf{c}) + R_2 G_2(\mathbf{c}) = H_2^{0,0}(\sigma(\mathbf{c})) + G_2(\sigma(\mathbf{c})) = E_2(\sigma(\mathbf{c})), \tag{5.48}$$

which is (5.2) as desired.

C. Definition and outline construction of the function pair $\mathcal{E}(\mathbf{c})$

The construction of the map $\mathcal{E}$ from E_2 is somewhat involved, and we only give an outline here. To obtain $\mathcal{E}(\mathbf{c})$ from $E_2(\mathbf{c})$ one essentially has to integrate twice and then project onto the complement of the subspace spanned by the linear eigenfunction pairs $\mathbf{u}_0$, $\mathbf{u}_1$, $\mathbf{v}_0$, $\mathbf{v}_1$ given below.

However, technical obstacles have prevented the direct implementation of this approach. It is to be hoped that a simpler method can be found in the future. Our approach here is to obtain $\mathcal{E}(\mathbf{c}) = h^0(\mathbf{c})\exp(K^1(\mathbf{c}))$, where $\log h^0(\mathbf{c}) \notin \mathcal{F}$, but $K^1(\mathbf{c}) \in \mathcal{F}$.

$K^1(\mathbf{c})$ is then constructed by the same method of forward iteration of initial conditions defined for negative time as was used in the construction of $E_2(\mathbf{c})$, but making use of the spectral properties of R_a restricted to $\mathrm{span}\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{v}_0, \mathbf{v}_1\}$.

Let $\mathbf{u}_0$, $\mathbf{u}_1$, $\mathbf{v}_0$, $\mathbf{v}_1$ be eigenfunction pairs of R_a such that

$$R_a(\mathbf{u}_0) = -\omega\mathbf{u}_0, \quad R_a(\mathbf{u}_1) = \omega^2\mathbf{u}_1, \quad R_a(\mathbf{v}_0) = \omega^{-1}\mathbf{v}_0, \quad R_a(\mathbf{v}_1) = -\mathbf{v}_1. \tag{5.49}$$

Here

$$\mathbf{u}_0 = (1, -\omega), \quad \mathbf{u}_1 = (1 + 2\omega x, \omega^2 - 2\omega^2 x), \tag{5.50}$$

and $\mathbf{v}_0$, $\mathbf{v}_1$ are as defined above in Eq. (2.41). We define the integral operator $\mathcal{I}$ by

$$\mathcal{I}(U_2, T_2) = \left(\int_{c_1}^{z} \int_{c_1}^{z'} U_2(z')dz'dz, \int_{c_0}^{z} \int_{c_0}^{z'} T_2(z')dz'dz \right). \tag{5.51}$$

We denote by D the differentiation operator. Then we have $D^2\mathcal{I} = \mathrm{id}$.

We define the function pairs $h^0(\mathbf{c})$, $H^0(\mathbf{c})$, and $H_2^0(\mathbf{c})$ by $H^0(\mathbf{c}) = \log h^0(\mathbf{c})$, $H_2^0(\mathbf{c}) = D^2H^0(\mathbf{c})$ where $h^0(\mathbf{c}) \in \mathcal{F}$ is defined by

$$h^0(\mathbf{c})(x) = \begin{cases} (y_0 - x, y_0 - x), & c_{-1} = 0; \\ (1, y_0 - x), & c_{-1} = 1. \end{cases} \tag{5.52}$$

We note that $H_2^0(\mathbf{c}) = H_2^{0,1}(\mathbf{c})$ as given in Sec. IV.B.

We now define $h^1(\mathbf{c})$ by the equation

$$R(h^0)(\mathbf{c}) = \kappa_{c_0}(+1, +1)h^0(\sigma(\mathbf{c}))h^1(\mathbf{c}). \tag{5.53}$$

The function pair $h^1(\mathbf{c})$ is readily calculated as follows. We have three cases.

Case (i): $c_{-1} = 0$ and $c_0 = 0$. Then

$$\begin{aligned} R(h^0)(\mathbf{c})(x) &= (y_0 - \theta_0(x), (y_0 - \theta_0(x))(y_0 - \theta_1(x))) \\ &= (-1, -1)(y_1 - x, y_1 - x)(\omega, \omega(y_0 - \theta_1(x))) \\ &= \kappa_{c_0}(+1, +1)h^0(\sigma(\mathbf{c}))(x)h^1(\mathbf{c})(x), \end{aligned} \tag{5.54}$$

where $h^1(\mathbf{c})(x) = (\omega, \omega(y_0 - \theta_1(x)))$. In this calculation we have used the fact that if $c_0 = 0$ then $y_0 - \theta_0(x) = \theta_0(y_1) - \theta_0(x) = -\omega(y_1 - x)$.

Similar calculations give, for the other cases, the following.

Case (ii): $c_{-1} = 0$ and $c_0 = 1$: $h^1(\mathbf{c})(x) = (\theta_0(x) - y_0, \omega(\theta_0(x) - y_0))$.

Case (iii): $c_{-1} = 1$ and $c_0 = 0$: $h^1(\mathbf{c})(x) = (\omega, \omega)$.

We note the following result.

Lemma 5.7: Let us write $h^1(\mathbf{c}) = (u^1, t^1)$. *Then we have* $u^1(x) \geq 0$ *for* $x \in [-\omega^{-1}, -\omega] = \overline{V_1} \cap \mathbb{R}$ *and* $t^1(x) > 0$ for $x \in [-\omega, 1] = \overline{V_0} \cap \mathbb{R}$. *Moreover* $u^1(x) \neq 0$ *for* $x \in \overline{V_1}$, *and* $t^1(x) \neq 0$ *for* $x \in \overline{V_0}$.

Proof: We consider separately the three cases in the definition of h^1 above. Case (iii) is clear. Let us consider case (i). Then $u^1(x) = \omega > 0$ and for $x \in [-\omega, 1]$, $t^1(x) = \omega(y_0 - \theta_1(x)) > 0$ since $y_0 \in (-\omega, 1)$ and $\theta_1(x) \in [-\omega^{-1}, -\omega)$. In case (ii) for $x \in [-\omega^{-1}, -\omega]$ we have $u^1(x) = \theta_0(x) - y_0 > 0$ since $y_0 \in (-\omega^{-1}, -\omega)$ and $\theta_0(x) \in [\omega^2, 1]$, while for $x \in [-\omega, 1]$ we have $t^1(x) = \omega(\theta_0(x) - y_0) > 0$ since $y_0 \in (-\omega^{-1}, -\omega)$ and $\theta_0(x) \in [-\omega, \omega^2]$. The second statement in the lemma follows from the fact that both u^1 and t^1 are linear with real roots. □

The importance of this lemma is that it implies that the logarithm of $h^1(\mathbf{c})$ is a function in $\mathcal{F}$. Indeed, we may define $H^1(\mathbf{c}) = \log h^1(\mathbf{c})$ and $H_2^1(\mathbf{c}) = D^2H^1(\mathbf{c})$ and, we have, analogously to the above results,

$$R_a H^0(\mathbf{c}) = H^0(\sigma(\mathbf{c})) + H^1(\mathbf{c}), \quad R_2 H_2^0(\mathbf{c}) = H_2^0(\sigma(\mathbf{c})) + H_2^1(\mathbf{c}). \tag{5.55}$$

Clearly, $H^1(\mathbf{c})$, $H_2^1(\mathbf{c}) \in \mathcal{F}$.

We now define $\mathcal{E}: \Sigma \to \mathcal{F}$ by

$$\mathcal{E}(\mathbf{c}) = h^0(\mathbf{c}) \exp(K^1(\mathbf{c})), \tag{5.56}$$

demanding that K^1 satisfies $H^1(\mathbf{c}) + R_a K^1(\mathbf{c}) = K^1(\sigma(\mathbf{c}))$.

In Sec. II we constructed a function pair $G_2(\mathbf{c}) \in \mathcal{F}$ with $R_2 G_2(\mathbf{c}) = G_2(\sigma(\mathbf{c})) - H_2^0(\mathbf{c})$. Our task is to construct $K^1(\mathbf{c})$ from $G_2(\mathbf{c})$. Let us define, for $k \geqslant 0$,

$$L^k(\mathbf{c}) = R_a^k P_a (H^0(\sigma^{-k}(\mathbf{c})) - \mathcal{I} G_2(\sigma^{-k}(\mathbf{c}))) - H^0(\mathbf{c}). \tag{5.57}$$

Then $L^k(\mathbf{c}) \in \mathcal{F}$ since the singularities of $R_a^k P_a H^0(\sigma^{-k}(\mathbf{c}))$ and $-H^0(\mathbf{c})$ cancel.

The proof that $L^k(\mathbf{c})$ converges in $\mathcal{F}$ depends on the following three technical lemmas, the proofs of which we omit.

Lemma 5.8: $L^{k+1}(\mathbf{c}) - L^k(\mathbf{c}) \in \ker D^2$.

Lemma 5.9: $R_a H^0(\sigma^{-(k+1)}(\mathbf{c})) - H^0(\sigma^{-k}(\mathbf{c})) - R_a \mathcal{I} G_2(\sigma^{-(k+1)}(\mathbf{c})) + \mathcal{I} G_2(\sigma^{-k}(\mathbf{c}))$ *has a norm bounded by* $K_1 |\log|\delta_{-k}|| + K_2(\|G_2(\sigma^{-k}(c))\| + \|G_2(\sigma^{-(k+1)}(\mathbf{c}))\|)$ *for suitable constants* $K_1, K_2 > 0$.

Lemma 5.10:

$$\sum_{\ell \geqslant 1} \omega^\ell \|G_2(\sigma^{-\ell}(\mathbf{c}))\| < +\infty. \tag{5.58}$$

We now indicate how these results imply the convergence of $L^k(\mathbf{c})$ to a function pair $K^1(\mathbf{c}) \in \mathcal{F}$ satisfying the required functional equation.

Since $D^2(L^{k+1}(\mathbf{c}) - L^k(\mathbf{c})) = 0$ we have that $L^{k+1}(\mathbf{c}) - L^k(\mathbf{c})$ is in the span of the eigenfunction pairs $\mathbf{u}_0$, $\mathbf{u}_1$, $\mathbf{v}_0$, $\mathbf{v}_1$ which span the four-dimensional kernel of D^2 in $\mathcal{F}$. Now $P_a(\mathbf{v}_0) = P_a(\mathbf{v}_1) = 0$, so that for $\mathbf{H} \in \text{span}\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{v}_0, \mathbf{v}_1\}$, we have $P_a(\mathbf{H}) \in \text{span}\{\mathbf{u}_0, \mathbf{u}_1\}$. Now R_a has spectrum $\{-\omega, \omega^2\}$ on $\text{span}\{\mathbf{u}_0, \mathbf{u}_1\}$. Since $\text{span}\{\mathbf{u}_0, \mathbf{u}_1\}$ is two-dimensional there exists a constant $K_3 > 0$ such that $\|R_a^k P_a\| \leqslant K_3 \omega^k$ on the space $\text{span}\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{v}_0, \mathbf{v}_1\}$. Let $\varepsilon > 0$. We now estimate as follows. For $m > n$,

$$\begin{aligned} \|L^m(\mathbf{c}) - L^n(\mathbf{c})\| &\leqslant \sum_{k=n}^{m-1} \|L^{k+1}(\mathbf{c}) - L^k(\mathbf{c})\| \\ &\leqslant \sum_{k=n}^{m-1} K_3 \omega^k (K_1 |\log|\delta_{-k}|| + K_2 \|G_2(\sigma^{-k}(\mathbf{c}))\| + K_2 \|G_2(\sigma^{-(k+1)}(\mathbf{c}))\|) \leqslant \varepsilon, \end{aligned} \tag{5.59}$$

for m, n sufficiently large by Lemmas 5.1 and 5.10. We conclude that $(L^k(\mathbf{c}))$ is a Cauchy sequence and converges in $\mathcal{F}$ to a function pair $K^1(\mathbf{c})$.

We must now show that $K^1(\mathbf{c})$ satisfies the required functional equation:

$$R_a K^1(\mathbf{c}) + H^1(\mathbf{c}) - K^1(\sigma(\mathbf{c})) = 0. \tag{5.60}$$

Defining

$$F^k(\mathbf{c}) = R_a L^k(\mathbf{c}) + H^1(\mathbf{c}) - L^k(\sigma(\mathbf{c})), \tag{5.61}$$

we have that $F^k(\mathbf{c}) \to 0$ in $\mathcal{F}$, since

$$F^k(\mathbf{c}) = R_a^k P_a (R_a(-\mathcal{I} G_2(\sigma^{-k}(\mathbf{c})) + H^0(\sigma^{-k}(\mathbf{c}))) + \mathcal{I} G_2(\sigma^{-(k-1)}(\mathbf{c})) - H^0(\sigma^{-(k-1)}(\mathbf{c}))),$$

$$R_a(-\mathcal{I} G_2(\sigma^{-k}(\mathbf{c})) + H^0(\sigma^{-k}(\mathbf{c}))) + \mathcal{I} G_2(\sigma^{-(k-1)}(\mathbf{c})) - H^0(\sigma^{-(k-1)}(\mathbf{c})) \in \ker D^2 \tag{5.62}$$

and

$$\|R_a(-\mathcal{I}G_2(\sigma^{-k}(\mathbf{c}))+H^0(\sigma^{-k}(\mathbf{c})))+\mathcal{I}G_2(\sigma^{-(k-1)}(\mathbf{c}))-H^0(\sigma^{-(k-1)}(\mathbf{c}))\|\leqslant K_4|\log|\delta_{-k}||$$
$$+K_5\|G_2(\sigma^{-k}(\mathbf{c}))\|+K_5\|G_2(\sigma^{-(k-1)}(\mathbf{c}))\|, \tag{5.63}$$

so that $\|F^k(\mathbf{c})\|\to 0$ by the same argument as above. Thus $K^1(\mathbf{c})$ satisfies (5.60).

D. Properties of the maps $\mathcal{E}$, β

In this section we consider briefly the properties of the maps $\mathcal{E}$, β. The following results may be readily proved.

Lemma 5.11: Let $\mathbf{c}$, $\mathbf{c}'\in\Sigma$. *Then* $\mathcal{E}(\mathbf{c})=\mathcal{E}(\mathbf{c}')$, *if, and only if,* $\mathbf{c}'=\mathbf{c}$. *Furthermore,* $\beta(\mathbf{c})=\beta(\mathbf{c}')$, *if, and only if,* $\mathbf{c}'=\mathbf{c}$ *or* $\tilde{\mathbf{c}}$.

Lemma 5.12: The maps $\mathcal{E}$, β *are continuous.*

Proof: These results follow from the continuity of the evaluation maps $e_n(\mathbf{c})$. Indeed, let $\mathbf{c}\in\Sigma$. We first of all show that G_2 is continuous at $\mathbf{c}$. We have

$$G_2(\mathbf{c})=\sum_{j\geqslant 1}H_2^{j,j}(\mathbf{c}). \tag{5.64}$$

Let $\varepsilon>0$ be given. Referring to the proof of Lemma 5.1, we have for $\mathbf{c}'$ close to $\mathbf{c}$ that k_1 and k_2 equal their values for $\mathbf{c}$. Now let $N>k_2$ be such that

$$\sum_{k>N}\frac{K\omega^k}{|\delta_{-k}|}<\varepsilon/4, \tag{5.65}$$

where K is given in Lemma 5.5. Then

$$\left\|\sum_{j\geqslant 1}H_2^{j,j}(\mathbf{c}')-\sum_{j\geqslant 1}H_2^{j,j}(\mathbf{c})\right\|\leqslant\sum_{j=1}^{N}\|H_2^{j,j}(\mathbf{c}')-H_2^{j,j}(\mathbf{c})\|+\sum_{j>N}\|H_2^{j,j}(\mathbf{c}')\|+\sum_{j>N}\|H_2^{j,j}(\mathbf{c})\| \tag{5.66}$$

$$<\sum_{j=1}^{N}\|H_2^{j,j}(\mathbf{c}')-H_2^{j,j}(\mathbf{c})\|+\varepsilon/4+\varepsilon/4 \tag{5.67}$$

$$<\varepsilon, \tag{5.68}$$

provided $\mathbf{c}'$ is taken sufficiently close to $\mathbf{c}$ so that the first sum is less than $\varepsilon/2$.

Hence G_2 is continuous at $\mathbf{c}$, and it follows immediately that $\mathcal{E}$ is continuous at $\mathbf{c}$. □

In fact, more can be said. For if for a sequence of codes $\mathbf{c}^k$, we have $\mathcal{E}(\mathbf{c}^k)\to\mathcal{E}(\mathbf{c})$ for some $\mathbf{c}\in\Sigma$, then $\mathbf{c}^k\to\mathbf{c}$. To prove this, suppose the contrary. Then there is a sequence $\mathbf{c}^k$ and $\mathbf{c}$ with $d(\mathbf{c}^k,\mathbf{c})\geqslant\varepsilon$ for some $\varepsilon>0$ but with $\mathcal{E}(\mathbf{c}^k)\to\mathcal{E}(\mathbf{c})$. Then there is $n\in\mathbb{Z}$ for which $\sigma^n(\mathbf{c}^k)$ and $\sigma^n(\mathbf{c})$ are in different intervals I_0 and I_1 for k sufficiently large. Then, since $\mathcal{E}(\mathbf{c}^k)\to\mathcal{E}(\mathbf{c})$, we have $\mathcal{E}(\mathbf{c}^k)/\mathcal{E}(\mathbf{c})\to(1,1)$, and thus, from the invertibility of R at $(1,1)$ and Eq. (4.2), we have $e_n(\mathbf{c}^k)_n\to e_n(\mathbf{c})$ as $k\to\infty$, so that $e_n(\mathbf{c})=-\omega$, contradicting the fact that $\mathbf{c}\in\Sigma$.

Furthermore, we have the following lemma.

Lemma 5.13: The maps $\mathcal{E}$, $\beta:\Sigma\to\mathcal{F}$ *satisfy* $P\mathcal{E}=\mathcal{E}$, $P\beta=\beta$.

Proof: Clearly, we need only prove that $P\mathcal{E}=\mathcal{E}$. By definition we have $\mathcal{E}(\mathbf{c})=h^0(\mathbf{c})\exp(K^1(\mathbf{c}))$ and

$$P(\mathcal{E}(\mathbf{c}))=P(h^0(\mathbf{c}))\exp(P_aK^1(\mathbf{c}))=h^0(\mathbf{c})\exp(-\Delta_0(\log|h^0(\mathbf{c})|)\mathbf{v}_0-\Delta_1(\log|h^0(\mathbf{c})|)\mathbf{v}_1)\exp(P_aK^1(\mathbf{c})), \tag{5.69}$$

so we need to show that

$$P_a K^1(\mathbf{c}) - \Delta_0(\log|h^0(\mathbf{c})|)\mathbf{v}_0 - \Delta_1(\log|h^0(\mathbf{c})|)\mathbf{v}_1 = K^1(\mathbf{c}). \tag{5.70}$$

Now

$$\begin{aligned} P_a K^1(\mathbf{c}) &= \lim_{k\to\infty} P_a L^k(\mathbf{c}) = \lim_{k\to\infty} P_a(R_a^k P_a(H^0(\sigma^{-k}(\mathbf{c}) - \mathcal{I}G_2(\sigma^{-k}(\mathbf{c}))) - H^0(\mathbf{c})) \\ &= \lim_{k\to\infty} R_a^k P_a(H^0(\sigma^{-k}(\mathbf{c})) - \mathcal{I}G_2(\sigma^{-k}(\mathbf{c})) - P_a H^0(\mathbf{c}) \\ &= \lim_{k\to\infty} L^k(\mathbf{c}) + H^0(\mathbf{c}) - P_a H^0(\mathbf{c}) = K^1(\mathbf{c}) + H^0(\mathbf{c}) - P_a H^0(\mathbf{c}). \end{aligned} \tag{5.71}$$

However, by definition, we have that

$$H^0(\mathbf{c}) - P_a H^0(\mathbf{c}) = \mathrm{Re}(\Delta_0 H^0(\mathbf{c}))\mathbf{v}_0 + \mathrm{Re}(\Delta_1 H^0(\mathbf{c}))\mathbf{v}_1, \tag{5.72}$$

and, since $\mathrm{Re}(H^0(\mathbf{c})) = \log|h^0(\mathbf{c})|$, we are done. □

E. Construction of a model space for the fundamental set

In this section we outline the construction of a model space for the fundamental set $\overline{\beta(\Sigma)}$. The space is obtained by quotienting Σ by the partnering operation $\sim$, and then completing in a pull-back metric.

The map $\beta:\Sigma\to\mathcal{F}$ is continuous but not injective. Indeed, recall from Lemma 5.11 that $\beta(\mathbf{c}) = \beta(\mathbf{c}')$, if, and only if, $\mathbf{c}' = \mathbf{c}$ or $\tilde{\mathbf{c}}$, so that β is invariant under the partnering operation. If we now define Σ' to be the topological quotient of Σ with respect to the continuous involution $\sim$, i.e., in which we identify $\mathbf{c}$ with its partner $\tilde{\mathbf{c}}$ to make a new topological space, then β induces a map on Σ' which we also denote by β. The map $\beta:\Sigma'\to\mathcal{F}$ is continuous and one-to-one onto its image inside $\mathcal{F}$. Indeed, the map $\beta:\Sigma'\to\beta(\Sigma')$ is a homeomorphism.

The metric d on Σ induces a metric on Σ' which we may also denote by d. Since Σ is not closed in $\hat{\Sigma}$, the metric d on Σ is not complete and so neither is d on Σ'. Indeed there are obstructions to extending $\mathcal{E}$, and hence β, to the whole of $\hat{\Sigma}$. The space Σ' is therefore a model of only a dense subset of the fundamental set $\overline{\beta(\Sigma)}$.

However, by pulling back the metric on $\mathcal{F}$ to Σ', we may complete Σ' in this new metric and obtain a model space for the whole of $\overline{\beta(\Sigma)}$. We define a metric on Σ' by pulling back the metric on $\mathcal{F}$ (given by the Banach space structure), rather than by projecting down the metric on Σ to the quotient. This results in the same topology on Σ', but a different metric structure.

The space Σ' is not complete as a metric space, but we may complete it in the standard manner to obtain $\hat{\Sigma}'$. The homeomorphism β (which is now trivially, by construction, an isometry) extends to an isometry $\beta:\hat{\Sigma}'\to\widehat{\beta(\Sigma')} = \overline{\beta(\Sigma')}$, the closure of the image $\beta(\Sigma')$ in $\mathcal{F}$.

Now, since $\sigma:\Sigma\to\Sigma$ is a homeomorphism commuting with the partnering operation, then induced map $\sigma:\Sigma'\to\Sigma'$ is also a homeomorphism. Moreover, we may extend the function $b_0(\mathbf{c})$ to $\hat{\Sigma}'$ so that we have the equation

$$R(\beta(\mathbf{c})) = L_{b_0}(+1, +1)\beta(\sigma(\mathbf{c})), \tag{5.73}$$

for $\mathbf{c}\in\hat{\Sigma}'$, where, as earlier, $b_0 = c_0 + \tilde{c}_0 \bmod 2$.

VI. PROPERTIES OF THE ORCHID

In this section we discuss the properties of the orchid constructed in Sec. IV. In particular we wish to show that (restricting to a codimension-2 stable manifold) it is a strange attractor, and that the function pair given by the generalized Harper equation (1.2) does indeed lie on the stable manifold of the orchid. In fact, this is not strictly the case (as we shall see) for the presence of the denominator in (2.26) leads to a scaled version of the orchid $\mathcal{O}$. Of further interest is the periodic orbit structure of $\mathcal{O}$ which we shall discuss in the next section.

The precise definition of a "strange attractor" is still not firmly established despite the familiarity of the whole scientific community with the basic concept. However central ingredients are as follows:

(i) the attractor should be closed;
(ii) the attractor should be indecomposable—this means that there should be a dense orbit in forward, or both forward and backward time;
(iii) the periodic points should be dense in the attractor;
(iv) the attractor should exhibit "sensitive dependence on initial conditions."

We shall show that the orchid does indeed possess these four characteristics, although it is not an attractor for all function pairs in $\mathcal{F}$.

We first of all discuss the initial conditions (2.26) given by the generalized Harper equation.

A. The generalized Harper equation orchid

We now prove that the initial condition derived from the generalized Harper equation is attracted to the orchid under iteration of R. Let u_2, t_2 be initial conditions for the operator R given by (2.26). Let us separate the numerator and denominator of (2.26) as follows, writing

$$u_2^1(x) = t_2^1(x) = \frac{1 + \alpha \cos(2\pi(\omega^2 x + \omega/2))}{\alpha/2}, \tag{6.1}$$

$$u_2^2(x) = t_2^2(x) = \frac{1}{2(1 - \cos(2\pi(\omega^2 x + \omega)))}. \tag{6.2}$$

Then from the multiplicative property (2.33) of R we have

$$(u_n, t_n) = R^{n-2}(u_2, t_2) = R^{n-2}(u_2^1, t_2^1) R^{n-2}(u_2^2, t_2^2), \tag{6.3}$$

for $n \geqslant 3$. We shall analyze the dynamics of $(u_n^1, t_n^1) = R^{n-2}(u_2^1, t_2^1)$ and $(u_n^2, t_n^2) = R^{n-2}(u_2^2, t_2^2)$ separately. We first prove the following lemma.

Lemma 6.1: $P(u_2^1, t_2^1) = (u_2^1, t_2^1)$, $P(u_2^2, t_2^2) = (u_2^2, t_2^2)$.

Proof: Recall the definition of P in Eq. (2.49). We prove the lemma by direct calculation using (2.43) and (2.44).

We first of all show that $\Delta_0(\log|(u_2^j, t_2^j)|) = 0$ for $j = 1, 2$. Using the integral identity

$$\int_a^{a+2\pi/c} \log|1 + b \cos(cx + d)| dx = \frac{2\pi}{c} \log(|b|/2), \tag{6.4}$$

for $a, b, c, d \in \mathbb{R}$ with $|b| \geqslant 1$, $c > 0$, we have, setting $a = -\omega^{-1}$, $b = -1$, $c = 2\pi\omega^2$, $d = 2\pi\omega$,

$$\Delta_0(\log|(u_2^2, t_2^2)|) = \int_{-\omega^{-1}}^{1} -\log 2 - \log|1 - \cos(2\pi(\omega^2 x + \omega))| dx = -\omega^{-2} \log 2 - \omega^{-2} \log(1/2) = 0, \tag{6.5}$$

and, setting $a = -\omega^{-1}$, $b = \alpha$, $c = 2\pi\omega^2$, $d = 2\pi\omega^2/2$, we have

$$\begin{aligned} \Delta_0(\log|(u_2^1, t_2^1)|) &= \int_{-\omega^{-1}}^{1} -\log(\alpha/2) + \log|1 + \alpha \cos(2\pi(\omega^2 x + \omega/2))| dx \\ &= -\omega^{-2} \log(\alpha/2) + \omega^{-2} \log(\alpha/2) = 0. \end{aligned} \tag{6.6}$$

Second, we note that

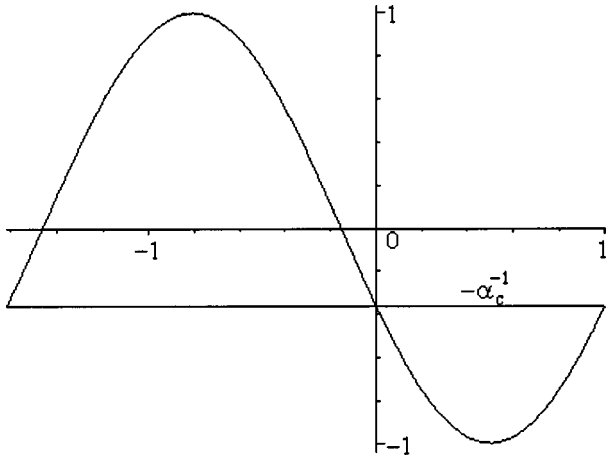

FIG. 7. The graph of $\cos(2\pi(\omega^2 x+\omega/2))$ in the range $-\omega^{-1}\leqslant x\leqslant 1$.

$$\Delta_1(\log|(u_2^j,t_2^j)|)=\int_{-\omega^{-1}}^{1}\frac{d}{dx}\log|t_2^j(x)|dx=0, \tag{6.7}$$

for $j=1, 2$, since t_2^j is periodic with period ω^{-2}. This calculation is complicated by the presence of logarithmic singularities both within the interval $(-\omega^{-1},1)$ and at the endpoints $-\omega^{-1}$ and 1. □

We note that the constraint (2.21) is simply the condition $\Delta_0(\log|(u_2,t_2)|)=0$.

B. Convergence to a scaled orchid

We now study the zero set of the function pair (u_2^1,t_2^1). The pattern of its zeros is the essential ingredient that gives the fundamental set $\overline{\beta(\Sigma)}$, three copies of which make up the orchid.

Looking at (6.1), we see that the zeros of t_2^1 are given by the solutions of the equation

$$-\alpha^{-1}=\cos(2\pi(\omega^2 x+\omega/2)). \tag{6.8}$$

The graph of $\cos(2\pi(\omega^2 x+\omega/2))$ in the range $-\omega^{-1}\leqslant x\leqslant 1$ is shown in Fig. 7.

For $\alpha\geqslant 1$ the locations of the solutions of (6.8) are determined by whether (a) $1\leqslant\alpha<\alpha_c$, (b) $\alpha_c<\alpha$, or (c) $\alpha=\alpha_c$, where

$$\alpha_c=\frac{-1}{\cos(\pi\omega)}\simeq 2.759. \tag{6.9}$$

We shall see that [apart from a countable set of values of the parameter α corresponding to zeros with codes not in Σ, i.e., ending $(00)^\infty$ or $(01)^\infty$] each initial condition (u_2^1,t_2^1) is asymptotic to the orbit of a point in the orchid $\mathcal{O}$ given by $(+1,+1)\beta(\mathbf{c})$ for some $\mathbf{c}\in\Sigma$.

We have three cases, which we deal with in turn.

Case (a): $1\leqslant\alpha<\alpha_c$. There are two zeros of t_2^1 which we denote x_L, $x_U\in[0,1]$ with $x_L+x_U=1$ by the symmetry about 1/2. We write $t_2^1(x)=(x_L-x)(x_U-x)g(x)$, where $g(x)>0$ for $x\in[-\omega^{-1},1]$. Then, except for countably many x_L, there exists $\mathbf{c}\in\Sigma$ with $c_{-1}=\tilde{c}_{-1}=0$ and $e_0(\mathbf{c})=x_L$ and therefore $(+1,+1)\beta(\mathbf{c})/(u_2^1,t_2^1)$ satisfies the hypotheses of Proposition 2.7. Moreover, since $x_L+x_U=1$, we have that $0\in S$, where S is the set defined in Sec. IV (see Proposition 3.1), and hence that $(+1,+1)\beta(\mathbf{c})\in\mathcal{O}$ for some choice of $\mathbf{c}$ with $(+1,+1)\beta(\mathbf{c})/(u_2^1,t_2^1)$ satisfying the hypotheses of Proposition 2.7.

Case (b): $\alpha_c<\alpha$. In this case t_2^1 has a zero, x_L, in the interval $[-\omega/4,0)$ and another, $x_{U'}$, in $(-\omega^{-1},-\omega^{-1}+\omega/4]$. By the symmetry of the graph about $-\omega^{-1}/2$ we have that $x_L+x_{U'}=-\omega^{-1}$. We now have $t_2^1(x)=(x_L-x)(x_{U'}-x)g(x)$, where $g(x)>0$ for $x\in[-\omega^{-1},1]$. Again, except for countably many x_L, there exists $\mathbf{c}\in\Sigma$ with $e_0(\mathbf{c})=x_L$ and $c_{-1}=\tilde{c}_{-1}=0$, and so that $(+1,+1)\beta(\mathbf{c})/(u_2^1,t_2^1)$

satisfies the hypotheses of Proposition 2.7. Now, since $x_L + x_{U'} = -\omega^{-1}$, we have, from Proposition 3.1, that index 0 is the second digit of an *A*, *B* or *C*. However, since $c_0 = 0$, the cases *A* and *C* are not possible so that index 0 is the second digit of a *B*. Thus $1 \in S$. Moreover, recalling from Sec. IV that $\mathbf{b} = \mathbf{c} + \tilde{\mathbf{c}}$ mod 2, as in Sec. IV, we have $b_0 = 1$ and thus $L_{b_0}(+1,+1) = L_1(1,1) = (+1,-1)$, and $1 \in S$, so referring back to Eq. (4.7) and Lemma 4.1, we see that $(+1,+1)\beta(\mathbf{c}) \in \mathcal{O}$.

Case (c): $\alpha = \alpha_c$. In this case t_2^1 has three zeros on $[-\omega^{-1}, 1]$, viz., $-\omega^{-1}$, 0, 1, but these points have codes ending in $(00)^\infty$ or $(01)^\infty$ which have been excluded.

In summary, for all but a countable number of $\alpha \geqslant 1$, there exists $\mathbf{c} \in \Sigma$ such that $(+1,+1)\beta(\mathbf{c})/(u_2^1, t_2^1)$ satisfies the hypotheses of Proposition 2.7 and such that $(+1,+1)\beta(\mathbf{c}) \in \mathcal{O}$.

Let us now briefly consider the function pair (u_2^2, t_2^2). We note that u_2^2 and t_2^2 have double poles at $-\omega^{-1}$ and 1 and that both satisfy $u_2^2(x), t_2^2(x) > 0$ on $(-\omega^{-1}, 1)$. From the above considerations we may conclude the following result which proves that a scaled version of the orchid $\mathcal{O}$ is the limit of the initial conditions (2.26). We denote by (u_{sc}, t_{sc}) the strong-coupling fixed point $(u_*, t_*)^{-2}$.

Proposition 6.1: The following limits hold as $n \to \infty$:

(i) $R^{n-2}(u_2^1, t_2^1) \to \mathcal{O}$, *the orchid defined in (4.7);*
(ii) $R^{n-2}(u_2^2, t_2^2) \to (u_{sc}, t_{sc})$;
(iii) $R^{n-2}(u_2, t_2) \to (u_{sc}, t_{sc})\mathcal{O}$.

C. Strangeness of $\mathcal{O}$

We now address the strangeness of the orchid $\mathcal{O}$. In particular we wish to show that the characteristics (i)–(iv) above hold. Let us briefly discuss the notion of the "sensitive dependence on initial conditions." This notion is one of the most varied in the literature. Indeed, it is sometimes taken to mean that given any point *p* in the attractor the orbits of *p* and those of all nearby points separate at a geometric rate. However a much weaker notion is also used, viz., that given any point *p* the orbit of *p* and that of at least one other point in every neighborhood of *p* separate, not necessarily geometrically. In our case it is the latter notion which we adopt. For it is clear that any two points $(s_0^u, s_0^t)\beta(\mathbf{c})$ and $(s_0^u, s_0^t)\beta(\mathbf{c}')$ on the orchid for which $e_0(\mathbf{c}) = e_0(\mathbf{c}')$ and $c_{-1} = c'_{-1}$ the ratio $(s_0^u, s_0^t)\beta(\mathbf{c})/((s_0^u, s_0^t)\beta(\mathbf{c}'))$ satisfies the hypotheses of Proposition 2.7 and thus $(s_0^u, s_0^t)\beta(\mathbf{c})$ and $(s_0^u, s_0^t)\beta(\mathbf{c}')$ converge under the iteration of *R*. Indeed, arbitrarily close to a point $(s_0^u, s_0^t)\beta(\mathbf{c}) \in \mathcal{O}$ there are such points $(s_0^u, s_0^t)\beta(\mathbf{c}')$ and so the stronger definition given above cannot hold. However, close by to $(s_0^u, s_0^t)\beta(\mathbf{c})$ and $(s_0^u, s_0^t)\beta(\mathbf{c}')$ there will be points which diverge under iteration. In fact we have the following proposition.

Proposition 6.2: The orchid $\mathcal{O}$ *satisfies the following:*

(i) $\mathcal{O}$ *is closed;*
(ii) *There is a dense forward orbit in* $\mathcal{O}$;
(iii) *The periodic points of R are dense in* $\mathcal{O}$;
(iv) $\mathcal{O}$ *has sensitive dependence on initial conditions in the following sense. There exists* $\delta > 0$ *such that for all function pairs* h_1, $h_2 \in \mathcal{O}$ *and all* $\varepsilon > 0$ *there exists* h_1', $h_2' \in \mathcal{O}$ *with* $\|h_1' - h_1\| < \varepsilon$, $\|h_2' - h_2\| < \varepsilon$ *and* $n > 0$ *such that* $\|R^n(h_1') - R^n(h_2')\| > \delta$.

Proof:

(i) The orchid $\mathcal{O}$ is closed by definition.
(ii) The construction of a dense orbit for a shift space is a standard procedure. One simply concatenates all finite permitted sequences in both forward and backward time (with appropriate interpolation between sequences to ensure that the constructed sequence is itself permitted). The adaptation of this method to the orchid is straightforward. We construct a function with a dense orbit (in both forward and backward time) by concatenating three copies of each finite permitted sequence in Σ with appropriate interpolations between each sequence to ensure first that the resulting bi-infinite sequence is a sequence in Σ, and, second, that each of the three parts of the orchid is visited for each of the finite sequences. This can be achieved by ensuring that each of the three finite sequences corresponds to a

different permitted sign-pair choice at the start of the A, B, or C immediately preceding the sequence. So constructed, the sequence $\mathbf{c}$ will give a function pair $\beta(\mathbf{c})$ with a dense orbit in the orchid under R.

(iii) Similarly, it is straightforward to show that the periodic points are dense in the orchid. For given $(s^u,s^t)\beta(\mathbf{c})$ in the orchid, one may approximate $\mathbf{c}$ arbitrarily closely by a periodic orbit, by truncating $\mathbf{c}$ in both forward and backward time at the start/end of an A, B, or C, and then repeating the truncated string in forward and backward time to obtain a periodic orbit in Σ with the same structure as $\mathbf{c}$ in the truncated part. By choosing the sign pair to correspond to that of $\mathbf{c}$ one obtains a periodic orbit in the orchid that is arbitrarily close to $(s^u,s^t)\beta(\mathbf{c})$.

(iv) Choose $\mathbf{c}_0\in\Sigma$ such that 0 starts an A, B, C and let $0<\delta<\min\{\|\beta(\mathbf{c}_0)-(-1,-1)\beta(\mathbf{c}_0)\|,\ \|\beta(\mathbf{c}_0)-(+1,-1)\beta(\mathbf{c}_0)\|,\|(+1,-1)\beta(\mathbf{c}_0)-(-1,-1)\beta(\mathbf{c}_0)\|\}/3$. Let h_1, $h_2\in\mathcal{O}$ and let $\varepsilon>0$ be given. Our aim is to construct h_1', h_2' as in the statement of the proposition. First, let $\hat{h}_1=(s_0^{u,1},s_0^{t,1})\beta(\mathbf{c}_1)$, $\hat{h}_2=(s_0^{u,2},s_0^{t,2})\beta(\mathbf{c}_2)$ be points of $\mathcal{O}$ such that $\|\hat{h}_1-h_1\|<\varepsilon$ and $\|\hat{h}_2-h_2\|<\varepsilon$. (This step is necessary since h_1, h_2 may be in the closure of $\beta(\Sigma)$. Now let $\delta_1>0$ be such that for all $\mathbf{c}\in\Sigma$,

(a) $d(\mathbf{c},\mathbf{c}_1)<\delta_1$ implies $\|(s_0^{u,1},s_0^{t,1})\beta(\mathbf{c})-h_1\|<\varepsilon$;
(b) $d(\mathbf{c},\mathbf{c}_2)<\delta_1$ implies $\|(s_0^{u,2},s_0^{t,2})\beta(\mathbf{c})-h_2\|<\varepsilon$;
(c) $d(\mathbf{c},\mathbf{c}_0)<\delta_1$ implies $\|\beta(\mathbf{c})-\beta(\mathbf{c}_0)\|<\delta$.

Such a δ_1 exists by the continuity of the map β.

Let $m>0$ be chosen sufficiently large so that for all codes $\mathbf{c}$, $\mathbf{d}\in\Sigma$, $c_i=d_i$ for $i=-m,\ldots,m$ implies $d(\mathbf{c},\mathbf{d})<\delta_1$. We now construct $\mathbf{c}_1'$, $\mathbf{c}_2'$ with the following properties:

(a) $d(\mathbf{c}_1',\mathbf{c}_1)<\delta_1$, $d(\mathbf{c}_2',\mathbf{c}_2)<\delta_1$;
(b) $d(\sigma^{3m}(\mathbf{c}_1'),\mathbf{c}_0)<\delta_1$, $d(\sigma^{3m}(\mathbf{c}_2'),\mathbf{c}_0)<\delta_1$;
(c) Defining $(s_i^{u,1},s_i^{t,1})$, $(s_i^{u,2},s_i^{t,2})$ by Eq. (4.6) we require $(s_{3m}^{u,1},s_{3m}^{t,1})\neq(s_{3m}^{u,2},s_{3m}^{t,2})$.

It is clear that we can achieve these properties by defining $(\mathbf{c}_1')_i=(\mathbf{c}_1)_i$, $(\mathbf{c}_2')_i=(\mathbf{c}_2)_i$, $i=-m,\ldots,m$ and $(\mathbf{c}_1')_i=(\mathbf{c}_0)_i$, $(\mathbf{c}_2')_i=(\mathbf{c}_0)_i$, $i=2m,\ldots,4m$ and interpolating in the range $m+1\leqslant i\leqslant 2m-1$ so that (c) is satisfied.

It is now clear that $h_1'=(s_0^{u,1},s_0^{t,1})\beta(\mathbf{c}_1')$, $h_2'=(s_0^{u,2},s_0^{t,2})\beta(\mathbf{c}_2')$ satisfy $\|R^{3m}(h_1')-(s_{3m}^{u,1},s_{3m}^{t,1})\beta(\mathbf{c}_0)\|<\delta$, $\|R^{3m}(h_2')-(s_{3m}^{u,2},s_{3m}^{t,2})\beta(\mathbf{c}_0)\|<\delta$, so that, from the definition of δ, $\|R^{3m}(h_1')-R^{3m}(h_2')\|>\delta$ as required. □

VII. PERIODIC ORBITS

In this section we discuss the periodic points in the orchid, focusing on the periods that are permitted. In Ref. 17 the periods of several periodic orbits for the parameter value,

$$\alpha=\frac{1}{|\cos(2\pi r)|},\tag{7.1}$$

with rational r are calculated and the conjecture is made that such orbits are all periodic with period a multiple of three. Here we prove this fact, and, indeed, prove that *all* periodic orbits of R on the orchid have period a multiple of three.

The periodic orbits of Σ under the shift map σ are simply the periodic sequences $\mathbf{c}\in\Sigma$. Such periodic sequences in code 0 1 are clearly also periodic with the same period when written in terms of the symbols A, B, C and vice versa. By choosing the start of the periodic code we may, without loss of generality, assume that index 0 starts an A, B, or C. In terms of the symbols A, B, C any periodic code is permitted other than the period-1 codes ${}^{\infty}BB^{\infty}$, ${}^{\infty}CC^{\infty}$ and it is therefore clear that any period greater than 2 can be achieved by suitable choice of A, B, C.

Now let $\mathbf{c}$ be a periodic code of period $\ell\geqslant 1$. We note that the sequence $\ldots,\mathcal{E}(\mathbf{c}),\mathcal{E}(\sigma(\mathbf{c})),\ldots$, is also of period ℓ and vice versa. This is because the zero sets of $\mathcal{E}(\mathbf{c})$ are given by $e_0(\mathbf{c})$, and the

sequence $\ldots, e_0(\mathbf{c}), e_0(\sigma(\mathbf{c})), \ldots$, has the same period ℓ. However, the sequence $\ldots, \beta(\mathbf{c}), \beta(\sigma(\mathbf{c})), \ldots$ may have period less than ℓ. $\beta(\mathbf{c}) = \mathcal{E}(\mathbf{c})\mathcal{E}(\tilde{\mathbf{c}})$, so if for some $k < \ell$ it should occur that $\sigma^k(\mathbf{c}) = \tilde{\mathbf{c}}$ and $\sigma^k(\tilde{\mathbf{c}}) = \mathbf{c}$ we have $\beta(\sigma^k(\mathbf{c})) = \beta(\mathbf{c})$. If this does occur we clearly have $\sigma^{2k}(\mathbf{c}) = \mathbf{c}$ so that, since $\mathbf{c}$ has period ℓ, we have $k = \ell/2$ and so ℓ is even. Indeed this phenomenon occurs precisely when the sequence $c_0, \ldots, c_{\ell-1}$ is of the form $c_0, \ldots, c_{k-1}, \tilde{c}_0, \ldots, \tilde{c}_{k-1}$. For example, the periodic sequence 0100001001 of period 10 when written in terms of A, B, C is $ABAC = AB\tilde{A}\tilde{B}$ giving period 5 for the sequence $\ldots, \beta(\mathbf{c}), \beta(\sigma(\mathbf{c})), \ldots$. We shall refer to the reduction in the period due to this symmetry in the code as *period halving*.

We now consider a periodic point p on the orchid $\mathcal{O}$. Let $p = (s_0^u, s_0^t)\beta(\mathbf{c})$ for some $\mathbf{c} \in \Sigma$. Clearly, from Eq. (4.5) a necessary condition for p to be periodic for R is that $\mathbf{c}$ is periodic for σ on Σ. Let ℓ be the period of $\mathbf{c}$. Then, as we saw above, the period k of the sequence $\ldots, \beta(\mathbf{c}), \beta(\sigma(\mathbf{c})), \ldots$ is either $k = \ell$, or $k = \ell/2$ in the case of period halving. Recall from Sec. IV that under a symbol A the sign pair (s^u, s^t) is the same after as before, while after a B or C the transitions $(+1, +1) \to (+1, -1) \to (-1, -1) \to (+1, +1)$ occur. Thus we have two possibilities.

(a) The number of B and C (added together) in the sequence $c_0, \ldots, c_{k-1}$ is divisible by 3. Then we have $(s_k^u, s_k^t) = (s_0^u, s_0^t)$ and the period of p is precisely k. We note that in this case k is a multiple of 3 since the symbol A consists of 3 digits.

(b) The number of B and C (added together) in the sequence $c_0, \ldots, c_{k-1}$ is not divisible by 3. Then after the end of the sequence $c_0, \ldots, c_{k-1}$ the sign pair $(s_k^u, s_k^t) \neq (s_0^u, s_0^t)$, and, because of the period-3 nature of the sign pair evolution we have $(s_{2k}^u, s_{2k}^t) \neq (s_0^u, s_0^t)$, but $(s_{3k}^u, s_{3k}^t) = (s_0^u, s_0^t)$. Then $R^{3k}(p) = (s_{3k}^u, s_{3k}^t)\beta(\sigma^{3k}(\mathbf{c})) = p$. We have therefore proved the following result.

Theorem 7.1: *Let $p = (s_0^u, s_0^t)\beta(\mathbf{c}) \in \mathcal{O}$. Then p is periodic of period m for R if and only if $\mathbf{c}$ is periodic for σ of period ℓ. The relationship between m and ℓ is as follows. If period halving occurs set $k = \ell/2$, otherwise set $k = \ell$. If the number of B* and *C (added together) in the sequence $a_0, \ldots, a_{k-1}$ is divisible by 3 then $m = k$, otherwise $m = 3k$.*

The conjecture concerning the periodic orbits in Ref. 17 is incorporated in the following immediate consequence of this result.

Corollary 7.1: The periods of all periodic orbits in $\mathcal{O}$ are multiples of three.

As an illustration of these results we give the following examples.

(1) In the period-10 example $\overline{0100001001}$ above we have $\ell = 10$, $k = 5$ and $c_0, \ldots, c_4 = 01000 = AB$. Since the number of B and C in this sequence is 1 we have that $m = 3 \times 5 = 15$. Thus we have a period-15 orbit.

(2) Let $\mathbf{c} = 000001 = \overline{BBC}$. Then $\ell = 6$, $k = 6$, and since the number of B and C is 3 we have $m = 6$. Thus we have a period-6 orbit.

VIII. DISCUSSION

In this paper we have constructed a model space in terms of bi-infinite codes for the fundamental set (Fig. 4), three copies of which constitute the Ketoja–Satija orchid. We have shown that the initial conditions for the generalized Harper equation converge to a scaled orchid (Fig. 1) under the golden mean renormalization transformation. The intriguing three-fold symmetry of the orchid has been shown to stem from the dynamics on the sign pairs, as given by the transition diagram (Fig. 6). Finally, we have analyzed the periods of the periodic orbits in the orchid.

The structure of the orchid depends crucially on the symmetries of the generalized Harper equation (1.2), and in particular on those of the cosine function. It is these symmetries that lead to the partnering operation on codes and the relation given by Proposition 3.1 on the zeros of the function pairs $\beta(\mathbf{c})$. If one destroys the symmetries, then, likewise, the orchid is destroyed and is replaced by a different strange set. Indeed, when calculating the orchid numerically, care must be taken with round-off error in the zeros of the function pairs. Since the chaotic map G governs the dynamics of these zeros, round off error grows quickly leading to the violation of Proposition 3.1 and nonconvergence to the orchid. Thus the universality class for the orchid is restricted to those

quantum models displaying the same symmetries as the generalized Harper equation model (1.2). Moreover, the existence of nonstable eigendirections for the operator R_a implies further conditions on a function pair (u,t) to converge to $\mathcal{O}$. These conditions are satisfied for the initial conditions derived from the generalized Harper equation model, but it is clearly a moot point to what extent one should refer to the orchid as a renormalization strange "attractor."

The ideas and techniques in this paper are likely to find application in other problems in the field. As first pointed out by Bondeson *et al.*,[2] there is an equivalence between the transition to the localized state in quasiperiodic Schrödinger equations and the onset of a strange nonchaotic attractor in quasiperiodically forced nonlinear systems. See also Ref. 19. Kuznetsov *et al.*[23] have given a renormalization analysis of the onset of a strange nonchaotic attractor. We anticipate that our work in this paper will shed considerable light on this related problem, and in particular we expect that the numerical results in Ref. 23 can be generalized and put on a rigorous foundation. Rigorous renormalization analyses of correlations in strange nonchaotic attractors[7] and in a quasiperiodically forced two-level system[8] have recently been completed.[25,26]

The existence of a strong coupling fixed point for the Harper equation in the case of flux $\omega=(\sqrt{a^2+4}-a)/2$ satisfying $\omega^2+a\omega=1$ (i.e., in continued fraction notation $\omega=[a,a,\ldots]$), has recently been established,[5] generalizing the results in Ref. 24. Preliminary work shows that for each such ω there exists an orchid, similar to that analyzed in this article, governing the fluctuations. The case of more general irrational ω is the subject of current investigation.

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Monodromy of the quantum 1:1:2 resonant swing spring

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We describe the qualitative features of the joint spectrum of the quantum 1:1:2 resonant swing spring. The monodromy of the classical analogue of this problem is studied in Dullin *et al.* [Physica D **190**, 15–37 (2004)]. Using symmetry arguments and numerical calculations we compute its three-dimensional (3D) lattice of quantum states and show that it possesses a codimension 2 defect characterized by a nontrivial 3D-monodromy matrix. The form of the monodromy matrix is obtained from the lattice of quantum states and depends on the choice of an elementary cell of the lattice. We compute the quantum monodromy matrix, that is the inverse transpose of the classical monodromy matrix. Finally we show that the lattice of quantum states for the 1:1:2 quantum swing spring can be obtained—preserving the symmetries—from the regular 3D-cubic lattice by means of three "elementary monodromy cuts." © *2004 American Institute of Physics.*
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I. INTRODUCTION

The swing spring is a simple mechanical system consisting of a spring of length ℓ and spring constant k with one end attached at a fixed point (the origin of a Cartesian system) and with a weight of mass m attached at the other end. This system admits a Hamiltonian formulation in which the phase space is $\mathbb{R}^6$ with coordinates x,y,z,p_x,p_y,p_z and symplectic form $\mathrm{d}x\wedge\mathrm{d}p_x+\mathrm{d}y\wedge\mathrm{d}p_y+\mathrm{d}z\wedge\mathrm{d}p_z$. The Hamiltonian function H is

$$(x,y,z,p_x,p_y,p_z)\mapsto\frac{1}{2m}(p_x^2+p_y^2+p_z^2)+mgz+\frac{k}{2}(\ell-\sqrt{x^2+y^2+z^2})^2. \tag{1}$$

Note that ℓ is the same as ℓ_0 in Refs. 11 and 17.

When the physical parameters are chosen so that $3gm=k\ell$, which is equivalent to requiring that the frequencies of small oscillations of the swing spring near the stable equilibrium are in a 1:1:2 resonance (the only resonance with cubic secular terms), the swing spring has some remarkable features: energy exchange and precession of the swing plane.[11,17] These characteristics have been widely studied (see Ref. 17 for a comprehensive bibliography), but the information hidden in this classical mechanical system has not been exhausted by these investigations. In fact, the resonant swing spring is a model for molecules such as CO_2 (a textbook example of a 1:1:2 Fermi resonance between stretching and doubly degenerate bending vibration states[4,13]), HCP,[18] and a whole class of CHX_3 molecules which possess a Fermi resonance between the CH stretching and bending vibrational states.[19]

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We define the integrable approximation of the swing spring system and discuss the range of energies in which our approximating Hamiltonian gives data that can be considered reliable for the original system. After explaining the origin of the continuous and discrete symmetries of our approximation, we define the quantum analogue of the system and proceed to analyze its quantum spectrum. As the classical swing spring is a three degree of freedom system, its spectrum is represented by a three-dimensional (3D) lattice of points in the space of the values of quantized actions and energy. The main purpose of this work is to show how the nontrivial monodromy of the classical system[2,3,5] manifests itself (1) as a defect of this lattice and (2) in the distribution of quantum states with respect to quantum numbers which can be predicted from the theorem of Duistermaat–Heckman.[10]

Fixing a global quantum number associated to the momentum corresponding to a circle symmetry, we first analyze the quantum lattice of two-dimensional (2D) slices of the swing spring quantum spectrum and find that the monodromy computed in such slices gives insufficient information to determine the monodromy of the full 3D quantum spectrum. We proceed with the investigation of the 3D quantum lattice by giving two methods to compute the quantum monodromy matrix. The first method, presented in Ref. 26, requires the introduction of quantum defects in the regular $\mathbb{Z}^3$ lattice. In order to preserve the discrete symmetries of the system, one must use three elementary defects to obtain the quantum lattice. The second method obtains the quantum monodromy matrix directly by moving an elementary cell in the three-dimensional quantum lattice.

II. CLASSICAL AND QUANTUM 1:1:2 SWING SPRING

The swing spring is a Hamiltonian system on $(\mathbb{R}^6, dx\wedge dp_x+dy\wedge dp_y+dz\wedge dp_z)$ with Hamiltonian H given by (1). Despite it being a chaotic dynamical system,[16] the motions of the swing spring near the stable equilibrium located at $p_0=(0,0,-\ell-mg/k,0,0,0)$ have a clear quasiperiodic behavior when the parameters are chosen so that the characteristic oscillations of the system are tuned in 1:1:2 resonance.

To study this behavior we will begin by considering the Taylor expansion of H around p_0. The quadratic part of the Taylor expansion of H at p_0 is

$$H_2=\frac{1}{2m}(p_x^2+p_y^2+p_z^2)+\frac{k}{2}\left(\frac{gm}{k\ell+gm}x^2+\frac{gm}{k\ell+gm}y^2+z^2\right).$$

To have a 1:1:2 harmonic oscillator as dominant term, the physical coefficients in H_2 must satisfy the condition $3gm=k\ell$. Assuming this and making the change of coordinates

$$x\mapsto\sqrt[4]{\frac{4}{km}}\xi,\ \ y\mapsto\sqrt[4]{\frac{4}{km}}\eta,\ \ z\mapsto\sqrt[4]{\frac{1}{km}}\zeta,\ \ p_x\mapsto\sqrt[4]{\frac{km}{4}}p_\xi,\ \ p_y\mapsto\sqrt[4]{\frac{km}{4}}p_\eta,\ \ p_z\mapsto\sqrt[4]{km}p_\zeta,$$

we find that

$$H_2=\tfrac{1}{2}\hbar(\xi^2+p_\xi^2+\eta^2+p_\eta^2+2\zeta^2+2p_\zeta^2)$$

and the Taylor expansion of H (1) about p_0 up to sixth order terms becomes

$$\begin{aligned}H_{\text{trunc}}=H_2&-\tfrac{3}{8}\hbar^{3/2}\zeta(\eta^2+\xi^2)+\tfrac{3}{64}\hbar^2(\eta^2+\xi^2)(-2\zeta^2+\eta^2+\xi^2)-\tfrac{3}{256}\hbar^{5/2}\zeta(\eta^2+\xi^2)(2\zeta^2-3(\eta^2+\xi^2))\\&-\tfrac{3}{1024}\hbar^3(\eta^2+\xi^2)(2\zeta^4-6\zeta^2(\eta^2+\xi^2)+(\eta^2+\xi^2)^2),\end{aligned}\tag{2}$$

where $\hbar=\sqrt{k^3/(g^4m^5)}$. To obtain (2) we have rescaled H_{trunc} to remove the factor $g^2m^2/(2k)$ and dropped an additive constant. The original Hamiltonian H (1), and thus the Hamiltonian H_{trunc} (2), has an SO(2) axial symmetry

$$(\xi,\eta,\zeta,p_\xi,p_\eta,p_\zeta)\mapsto\left(R_t\begin{pmatrix}\xi\\ \eta\\ \zeta\end{pmatrix},R_t\begin{pmatrix}p_\xi\\ p_\eta\\ p_\zeta\end{pmatrix}\right).$$

Here

$$R_t=\begin{pmatrix}\cos t & -\sin t & 0\\ \sin t & \cos t & 0\\ 0 & 0 & 1\end{pmatrix}$$

is a rotation about the ζ axis lifted to the full phase space $\mathbb{R}^6$. The momentum of this symmetry is the function $L=\xi p_\eta-\eta p_\xi$.

It is convenient to perform another coordinate change, namely

$$\xi\mapsto\frac{1}{\sqrt{2}}(p_2+q_1),\quad \eta\mapsto\frac{1}{\sqrt{2}}(p_1+q_2),\quad \zeta\mapsto q_3,\quad p_\xi\mapsto\frac{1}{\sqrt{2}}(p_1-q_2),\quad p_\eta\mapsto\frac{1}{\sqrt{2}}(p_2-q_1),\quad p_\zeta\mapsto p_3.$$

This brings the momentum L into diagonal form $\frac{1}{2}(q_2^2+p_2^2-q_1^2-p_1^2)$ and does not change the quadratic part H_2 of the Hamiltonian H_{trunc}.

Bringing H_{trunc} into normal form with respect to H_2 up to order 6, one obtains the Hamiltonian $H_{\text{nf}}^{(6)}$. This is the polynomial Hamiltonian (as well as its truncation $H_{\text{nf}}^{(3)}$ to third order) whose quantum spectrum we analyze in Secs. III–V.

A. Lie symmetry of classical and quantum system

The sixth order normalized Hamiltonian $H_{\text{nf}}^{(6)}$ defines a three degree of freedom system with two integrals of motion: L, the momentum associated to the axial symmetry and N, the quadratic part H_2 of the normalized Hamiltonian, which is the same as the quadratic part of the original Hamiltonian H. The flows of the Hamiltonian vector fields associated to these integrals commute and define a 2-torus action that preserves $H_{\text{nf}}^{(6)}$. Thus L and N together with the Hamiltonian $H_{\text{nf}}^{(6)}$ form a completely integrable system.

Being $S^1\times\text{SO}(2)$-invariant, the normalized Hamiltonian $H_{\text{nf}}^{(6)}$ can be written as a polynomial in the generators of the ring of $S^1\times\text{SO}(2)$-invariant functions. The Molien generating function[20] (A7) indicates that this ring is generated by five invariants, three quadratic and two cubic, see Appendix A 1. These invariants can be chosen to be

$$N=\tfrac{1}{2}(q_1^2+p_1^2+q_2^2+p_2^2+2q_3^2+2p_3^2),\tag{3a}$$

$$R=\tfrac{1}{2}(q_1^2+p_1^2+q_2^2+p_2^2),\tag{3b}$$

$$L=\tfrac{1}{2}(-q_1^2-p_1^2+q_2^2+p_2^2),\tag{3c}$$

$$S=(q_1p_2+q_2p_1)q_3-(q_1q_2-p_1p_2)p_3,\tag{3d}$$

$$T=(q_1q_2-p_1p_2)q_3+(q_1p_2+q_2p_1)p_3,\tag{3e}$$

and they are subject to the relations (A9).

B. Normalized system and its analysis

The normalized Hamiltonian H_{trunc} (2) written in terms of the invariants (3) is

$$H_{\mathrm{nf}}^{(6)} = \hbar N - \tfrac{3}{16}\hbar^{3/2}S - \tfrac{57}{1024}\hbar^2 NR + \tfrac{177}{2048}\hbar^2 R^2 - \tfrac{39}{2048}\hbar^2 L^2 - \tfrac{819}{65\,536}\hbar^{5/2}NS + \tfrac{2151}{65\,536}\hbar^{5/2}RS - \tfrac{8025}{4\,194\,304}\hbar^3 N^2 R + \tfrac{7623}{2\,097\,152}\hbar^3 NR^2 + \tfrac{6879}{2\,097\,152}\hbar^3 R^3 - \tfrac{6555}{2\,097\,152}\hbar^3 NL^2 + \tfrac{4803}{4\,194\,304}\hbar^3 RL^2 - \tfrac{1089}{262\,144}\hbar^3 S^2. \tag{4}$$

Note that powers of T higher than 1 should not appear in (4) since the invariants satisfy the relation (A9). Furthermore, (4) does not include any power of N higher than 1 because the swing spring (1) contains a two degree of freedom harmonic oscillator as subsystem. Other special features of $H_{\mathrm{nf}}^{(6)}$ are related to the discrete symmetries described below.

In most of what follows, we describe the quantum spectrum of the Hamiltonian S instead of that of $H_{\mathrm{nf}}^{(6)}$. Of course, (S,L,N) is also a completely integrable system. At first order the difference between the Hamiltonian S and (4) is given by $H \mapsto -(16/3\hbar^{3/2})(H-\hbar N)$. This means that to first order for any given value of N the quantum spectra of H and S coincide up to a translation and dilation.

The energy-momentum map

$$\mathcal{EM}\colon \mathbb{R}^6 \to \mathbb{R}^3 \quad (q,p) \to (S(q,p),L(q,p),N(q,p))$$

is widely used in our analysis. Its image $U \subset \mathbb{R}^3$ and the corresponding bifurcation diagram is described in Ref. 11 and Appendix A 3. $U_{\mathrm{reg}} \subset U$ is the set of regular values which represent regular tori $\mathbb{T}^3$. Points of the boundary ∂U represent equilibria relative to the $\mathbb{T}^2 = S^1 \times \mathrm{SO}(2)$ action. The main feature to note is that $U \backslash U_{\mathrm{reg}}$ also contains a thread of singular values inside U, which represent a special singular 3D fiber described in Appendix A 3.

It can be shown that the system $(H_{\mathrm{nf}}^{(6)},L,N)$ is qualitatively the same as (S,L,N) for sufficiently small values of N. In particular it has qualitatively the same energy-momentum map and corresponding 3D quantum lattice. The concrete estimate of the upper limit for N can be obtained from the analysis of the slope of $S(R)$ at $R=L=0$ of $H_{\mathrm{nf}}=\mathrm{const}$. Specifically, $|\mathrm{d}S/\mathrm{d}R|$ should be smaller than the slope at the conical singular point of the reduced space, see Appendix A 2. In particular considering the terms of order $\hbar^2$ we obtain $N < 2^{12}19^{-2}\hbar^{-1}$.

C. Discrete symmetries and a pseudosymmetry

The normalized Hamiltonian $H_{\mathrm{nf}}^{(6)}$ (4) is not a generic $S^1 \times \mathrm{SO}(2)$-symmetric polynomial in the invariants, because (4) does not contain terms of odd degree in L or any power of T. The reason for this is that the original Hamiltonian (1) has a $\mathbb{Z}_2 \times \mathbb{Z}_2$ discrete symmetry group generated by

$$\mathcal{T}\colon (x,y,z,p_x,p_y,p_z) \mapsto (x,y,z,-p_x,-p_y,-p_z),$$

$$\mathcal{T}_s\colon (x,y,z,p_x,p_y,p_z) \mapsto (y,x,z,-p_y,-p_x,-p_z),$$

$$\sigma_v\colon (x,y,z,p_x,p_y,p_z) \mapsto (y,x,z,p_y,p_x,p_z).$$

Note that $\mathcal{T}_s = \mathcal{T} \circ \sigma_v = \sigma_v \circ \mathcal{T}$ and that the square of each generator is the identity. This discrete symmetry survives truncation and normalization. It induces the following transformations on the invariants:

$$\mathcal{T}\colon (N,R,L,S,T) \mapsto (N,R,-L,S,-T), \tag{5a}$$

$$\mathcal{T}_s\colon (N,R,L,S,T) \mapsto (N,R,L,S,-T), \tag{5b}$$

$$\sigma_v\colon (N,R,L,S,T) \mapsto (N,R,-L,S,T). \tag{5c}$$

From (5) we see that the functions T and L are not invariant of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ action. This explains the absence of odd powers of L and T in (4).

To analyze the model system (S,L,N) we also consider the involution

$$(\xi,\eta,\zeta,p_\xi,p_\eta,p_\zeta)\mapsto(-\xi,-\eta,-\zeta,-p_\xi,-p_\eta,-p_\zeta), \tag{6a}$$

which acts on the invariants as

$$(N,R,L,S,T)\mapsto(N,R,L,-S,-T). \tag{6b}$$

As the transformation (6a) maps S to $-S$, we call it a pseudosymmetry. We will exploit this pseudosymmetry below. In particular the image of the energy-momentum map of (S,L,N) is symmetric with respect to (6b). Similarly, the corresponding 3D quantum lattice is symmetric with respect to the plane $S=0$.

D. Classical integrals, quantum numbers, and joint quantum spectrum

Each of the functions in the integrable system (S,L,N) can be quantized according to the rules discussed in Appendix B. The corresponding three quantum operators $\hat{N}$, $\hat{L}$, and $\hat{S}$ are self-adjoint and commute. Hence they can be simultaneously diagonalized. In Appendix B we give the details of the calculation of the joint quantum spectrum of $(\hat{S},\hat{L},\hat{N})$ and of the quantum analogue of $H^{(6)}_{\mathrm{nf}}$. We also explain the decomposition of the domain of the quantum operators that allows us to numerically compute the quantum spectrum. To every common eigenspace one can associate a triple of real numbers and plot these triples in $\mathbb{R}^3$, generating a lattice of quantum states represented as points in 3-space. This 3D lattice of points fits in the image of the classical energy-momentum map $\mathcal{EM}$ of the integrable system (S,L,N), a description of which is in Appendix A 3. Similarly the quantum lattice for the swing spring $(H^{(6)}_{\mathrm{nf}},L,N)$ fits inside the respective $\mathcal{EM}$ image.

Definition 1: The lattice of quantum states of $(\hat{H},\hat{L},\hat{N})$ superimposed to the image of the $\mathcal{EM}$ map of the corresponding classical completely integrable system (H,L,N) is called the *quantum diagram*. A *polyad quantum number* is an injective integer labeling of the eigenvalues of the quantum operator $\hat{N}$. A *local quantum number* is an injective integer labeling of the eigenspaces of a quantum operator associated to a local action variable for the completely integrable quantum system $(\hat{H},\hat{L},\hat{N})$. A *local action variable* is a function locally defined on phase space whose Hamiltonian vector field has a 2π-periodic flow and Poisson commutes with the classical Hamiltonian H and the momenta N and L.

The notion of polyad quantum number is well established in the theoretical chemistry and molecular physics community.[24] Both polyad and local quantum numbers label eigenspaces with large dimension, that is, eigenvalues with high multiplicity. A choice of labeling of the points of the quantum spectrum corresponding to the quantum numbers of a global action will be referred to as *global quantum number*. The definition of global quantum numbers, as opposed to the choice of a quantum number, which is just a labeling of eigenspaces of a quantum spectrum, is at the heart of the presentation to follow.

Since the systems with Hamiltonian $H=S$ and $H=H^{(6)}_{\mathrm{nf}}$ are qualitatively the same, we will use $H=S$ which is easier to study analytically.

Lemma 1: The eigenstates of the quantum system $(\hat{S},\hat{L},\hat{N})$ can be labeled by three quantum numbers related to the three commuting operators $\hat{S}$, $\hat{N}$, and $\hat{L}$:

(i) The global quantum number $n_N=0,1,2,\ldots$ can be chosen to be the eigenvalue of the operator $\hat{N}$ and is the total number of quanta for the 1:1:2 resonance oscillator or the *polyad* quantum number. The total number of quantum states within one n_N-polyad equals

$$\mathcal{N}(n_N)=\begin{cases}\left(\frac{1}{2}n_N+1\right)^2 & \text{if } n_N \text{ is even},\\ \left(\frac{1}{2}n_N+1\right)^2-\frac{1}{4} & \text{if } n_N \text{ is odd}.\end{cases}$$

(ii) The global quantum number n_L can be chosen to be the eigenvalue of the operator $\hat{L}$ and is the projection of the angular momentum on the axis of symmetry. For each n_N, the quantum number n_L takes (n_N+1) different values

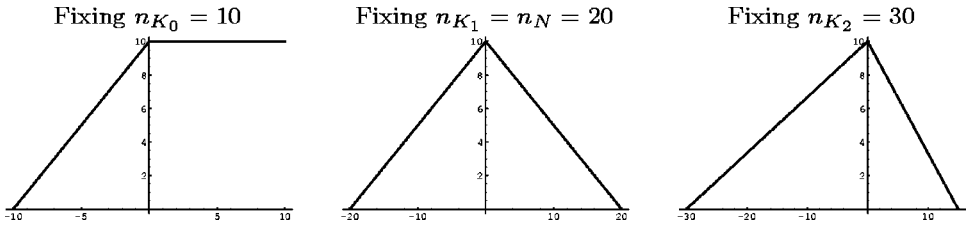


FIG. 1. The plot of the number of states in the slice having a fixed n_{K_m} quantum number as a function of the quantum number n_L.

$$n_L = n_N, n_N - 2, \ldots, -n_N + 2, -n_N.$$

The total number of states for each fixed value of n_N and n_L equals

$$\mathcal{N}(n_N, n_L) = \tfrac{1}{2}(n_N - |n_L|) + 1.$$

(iii) A quantum number n_S labels the eigenspaces within the set of states with the same n_L and n_N according to the energy of the system.

Instead of using the natural momenta N and L, one could use the momentum

$$K_m = (m+1)N + (m-1)L \tag{7}$$

together with L. The number of states in a fixed quantum level of the operator $\hat{K}_m$ can be thought as a function of n_L. A computation shows that this function assigns to every n_L in $[-n_{K_m}, 0]$ the natural number $(n_L + n_{K_m})/(m+1)$ and to every n_L in $[0, n_{K_m}/m]$ the natural number $(-n_L m + n_{K_m})/(m+1)$. The cases corresponding to $m=0,1,2$ are plotted in Fig. 1.

A classical formula states that the number of quantum states of a given quantum system is $\hbar$-proportional to the symplectic area of the phase space in which the system is defined. Hence, the graphs in Fig. 1 can also be obtained by first reducing $\mathbb{R}^6$ with respect to the circle action with momentum K_m, which defines the manifold M_k, and then by plotting the L-dependent symplectic volume of the manifold M_k reduced with respect to the circle action with momentum L. These volumes can be computed directly from the theorem of Duistermaat and Heckman, see Refs. 10 and 15. In Ref. 14 this theorem was applied to the analysis of a three-dimensional quantum problem with monodromy.

The theorem of Duistermaat and Heckman states that the cohomology class of the symplectic form of a symplectically T^n-reduced space varies piecewise linearly with the values of the momentum map. To be more precise denote by M_x the symplectic manifold obtained by symplectically reducing a manifold M with respect to the T^n-action above the value x in $\mathfrak{t}^*$. Let a be a regular value of the momentum map, let b be an element in $\mathfrak{t}^*$, and let t be a small real number. The manifold M_{a+tb} is diffeomorphic to M_a. Both manifolds are base spaces of diffeomorphic principal T^n bundles. The symplectic forms of M_a and M_{a+tb} define cohomology classes that differ by the class $t\langle b, c\rangle$, where c is the Chern class of the torus bundle over M_a, that is, an element of $H^2(M_a) \otimes \mathfrak{t}$, and $\langle , \rangle$ is the pairing between the Lie algebra $\mathfrak{t}$ and its dual $\mathfrak{t}^*$. Observe that $t\langle b, c\rangle$ is a function linear in t. Crossing the set of critical values of the T^n-momentum map, the Chern class, and hence the slope of the linear function changes into $\langle b, c'\rangle$. Since the volume form of a symplectic manifold is an appropriate power of the symplectic form, it changes polynomially in t.

In our case we are given a T^2 action having the tuple (N, L) for momentum map. The momentum polytope is the convex solid wedge with boundaries $0 \leqslant N = L$ and $0 \leqslant N = -L$. In addition to this boundary, the set of critical values of the T^2-momentum map also contains the line $L = 0$. The fiber of the T^2-momentum map over values in the set $E^+ = \{L > 0, L < N\}$ is a 2-torus bundle over a 2-sphere with Chern class $(\omega\xi_N + \omega\xi_L)/2$; while that above values in the set

$E^-=\{L<0, L>-N\}$ is a 2-torus bundle over a 2-sphere with Chern class $(\omega\xi_N-\omega\xi_L)/2$. Here ω is the standard volume form on the 2-sphere and ξ_N, ξ_L are the elements of $\mathfrak{t}$ whose infinitesimal action is X_N and X_L, respectively.

Starting from the symplectic manifold $\mathbb{R}^6$ one can reduce with respect to the momentum K_m to obtain the manifold $M_k=K_m^{-1}(k)/S^1$. On M_k there is a (residual) circle action with momentum L. The image of the (residual) momentum map is the intersection of the line $L_m=\{(m+1)N+(m-1)L=k\}$ with the image of the momentum map of the T^2 action.

We can now use the Duistermaat–Heckman theorem to compute the change in the (cohomology class of the) symplectic structure of the L-reduced manifolds $M_{k,l}=L^{-1}(l)/S^1$, and plot it as a function of l. The line L_m is spanned by the element $b=\xi_N^*-(m+1)/(m-1)\xi_L^*$. The cohomology class $\langle b, c\rangle$ is $\omega/(m+1)$ in the segment $L_m\cap E^+$ and $-m\omega/(m+1)$ in the segment $L_m\cap E^-$. This gives, as expected, the graphs in Fig. 1.

III. QUANTUM SPECTRUM: LATTICE OF QUANTUM STATES

Given a 3D quantum diagram, an important problem is to "smoothly" map it to the lattice $\mathbb{Z}^3$ in $\mathbb{R}^3$. This can always be done locally by means of independent local quantum numbers. In systems with nontrivial monodromy a global labeling of the eigenstates is impossible. To be more precise, a global labeling of the quantum states with three suitable global quantum numbers is the quantum analogue of the classical problem of defining global action functions for a completely integrable system. This problem has been shown to have no solution in systems with monodromy.[21] The quantum numbers n_N and n_L are *a priori* global, because they correspond to global classical actions. On the other hand, because of the nontrivial classical monodromy of the swing spring system, the quantum number n_S can be only locally defined. In this section we show that this last quantum number cannot be defined globally, and we analyze this phenomenon.

Informally speaking, we try to construct a third global quantum number for the quantum swing spring, which is independent of n_L and n_N. Having three global quantum numbers corresponds to defining a bijection of the given lattice to the standard $\mathbb{Z}^3$. Of course, many such bijections exist, but none of them can have the property of "$\hbar$-smoothness," which we define in Sec. III B. We begin by describing the quantum lattice of the quantum swing spring and then apply the idea of $\hbar$-smoothness.

A. Qualitative and quantitative description of the quantum lattice

One way of describing the 3D lattice of the quantum swing spring is to look at its planar slices, that is, the slices obtained by fixing a quantum number (n_N or n_{K_m} in our case). These plane slices intersect the thread of classical singular values (see Appendix A 3) in one point, which we refer to as a *singularity* of the quantum lattice.

To start with, we use the symmetries and the number of states discussed in Lemma 1 to deduce the qualitative aspects of the quantum spectrum of the swing spring. At the end of this section we give numerically computed pictures of the plane slices obtained by fixing the value of the polyad number n_N.

Let us now fix the polyad number n_N and then compute the joint spectrum of the operators $\hat{L}$ and $\hat{S}$. We recall that the quantum spectrum one computes in this way is that of the classical system obtained from the original one by reducing it with respect to the circle action having momentum N at the value n_N+2.

Lemma 2: For fixed polyad number n_N, the structure of the joint spectrum for the operators $\hat{L}$ and $\hat{S}$ is invariant under the symmetries $n_L\to -n_L$ and $n_S\to -n_S$ and it consists of four possible arrangements in a neighborhood of the intersection of the symmetry axes. These arrangements have a modulo 4 periodicity, $n_N\equiv n_N' \bmod 4$, see Fig. 2.

From the symmetry σ_v and the pseudosymmetry discussed in Sec. II C, it follows that if (n_N, n_L, n_S) is a point of the quantum diagram, then also the points $(n_N, \pm n_L, \pm n_S)$ belong to the quantum spectrum.

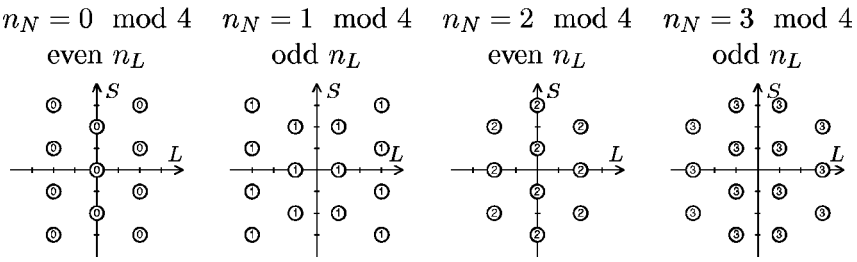


FIG. 2. Joint eigenvalues of the operators $\hat{L}$ and $\hat{S}$ near the origin.

Let us make the generic assumption that the spectrum of $\hat{S}$ at fixed n_L has no degeneracies, that is, the spectrum of $\hat{S}$ at fixed polyad numbers n_N and quantum number n_L is simple, and that the distances of consecutive $\hat{S}$-eigenvalues varies monotonically and slowly. In the rest of our argument we simply fix such distance to be some positive constant, say 2, as we did in the pictures in Fig. 2.

By Lemma 1, the quantum numbers n_N and n_L are both even or both odd, and when n_N is fixed n_L changes in steps of two. For even n_N, we have one central string of lattice points at $n_L=0$ with the maximum number of states $\mathcal{N}(n_N,n_L)=\frac{1}{2}n_N+1$ for given n_N. This string is symmetric under $S\to -S$. For $n_N=0 \bmod 4$ it has the central node at (0,0) because $\mathcal{N}(0 \bmod 4,0)$ is odd. For $n_N=0 \bmod 2$ the closest to (0,0) is a pair of nodes $(0,\pm 1)$ symmetric under $S\to -S$. Patterns for the other values of n_N are deduced by a similar argument. The other symmetric distributions are not admissible because they do not give the right rate of change of the number of quantum states as a function of n_L.

Corollary 1: For sufficiently small polyad numbers n_N, the quantum spectrum of the N-reduced normalized swing spring $(\hat{H}^{(6)}_{\rm nf},\hat{L})$ is qualitatively the same as the quantum spectrum of $(\hat{S},\hat{L})$ in Lemma 2. Hence, the quantum diagrams of such systems are qualitatively the same as those in Fig. 2.

Figure 3 and, respectively, Fig. 4 display the joint spectrum of the operators $\hat{L}$ and the Hamiltonian $\hat{H}^{(6)}_{\rm nf}$, respectively, $\hat{H}^{(3)}_{\rm nf}$, computed numerically for fixed polyad number n_N, and,

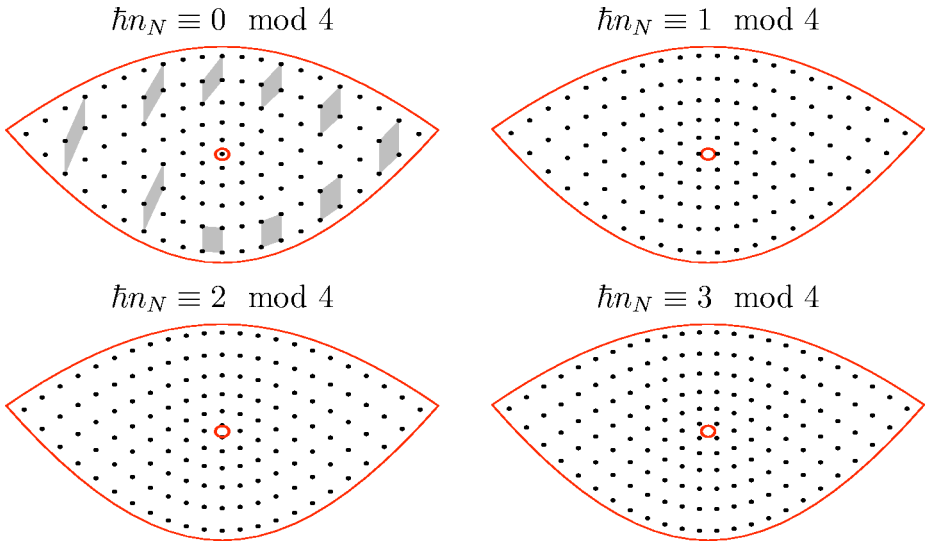


FIG. 3. Consecutive slices with fixed n_N polyad number for the normalized swing spring $(\hat{H}^{(6)}_{\rm nf},\hat{N},\hat{L})$. The polyad quantum number $n_N/\hbar$ is chosen to be about 1. Here $\hbar$ is $1/20$.

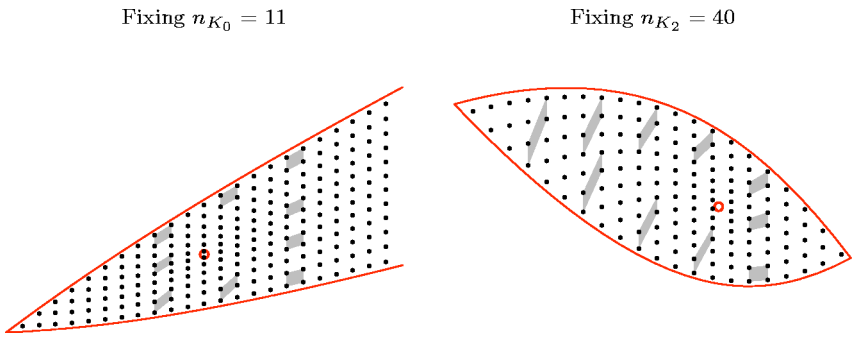


FIG. 4. Quantum diagrams obtained by fixing the quantum number n_{K_m} and plotting the quantum spectrum of the operators $\hat{L}$ and $\hat{H}^{(3)}_{\text{nf}}$.

respectively, n_{K_0} and n_{K_2}. Note that, to preserve the qualitative structure of the approximating normalized system, one must choose a polyad number of the order of unity. With such a low polyad number there are too few quantum states to perform the analysis we are presenting here. A standard technique to increase the number of points in the quantum lattice (that is, states of the quantum system) at a fixed energy level is to scale the variables by the number $\sqrt{\hbar}$, where $\hbar$ is the inverse of a natural number. This is equivalent to considering a Hilbert space of quantum states of the form $|n_1,n_2,n_3\rangle$ where n_i is a $\hbar$-multiple of a natural number.

In Sec. II D we gave a formula for the dependence on n_L of the number of quantum states having a fixed n_{K_m} quantum number. The results shown in Figs. 3 and 4 confirm the predictions made in Fig. 1 and used in Lemma 1.

B. Local mapping to the regular lattice

The effect of monodromy: Having described the plane slices and their relative position in 3-space, we can proceed with a tentative definition of the missing quantum number. Let us do this for the planar slices in Fig. 3. For every choice of quantum numbers n_N and n_L, that is, fixing the eigenspace associated to the quantum numbers n_N and n_L, one can assign a third quantum number by enumerating the quantum states of the operator $\hat{S}$ in the joint eigenspace (n_N,n_L), beginning with 0. Though this seems to be a global choice of third quantum number, we can easily show that it is not the case. As first suggested in Ref. 25, we can choose an elementary cell of the lattice and transport it around the classical singularity, see Fig. 3 (top left). After one tour around the singularity, we will come back with a different cell. This signifies that the third quantum number cannot be globally chosen.

Furthermore, when one fixes n_N and n_L and draws the curves having fixed the third quantum number proposed above, see Fig. 5, it is quite obvious that the curves above the classical singularity have a nonsmooth behavior, unlike those below. The closer $\hbar$ is to zero, the more obvious

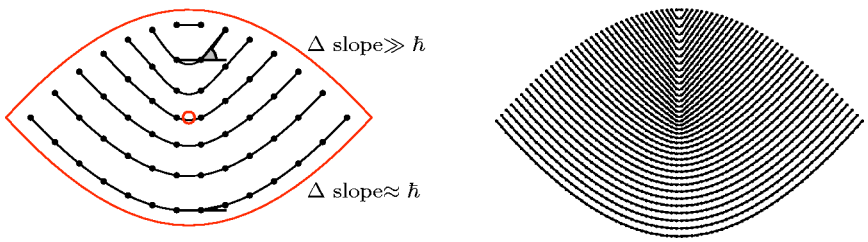


FIG. 5. Numbering the eigenstates with fixed n_L in the natural way within one n_N polyad of the system (S,L,N). The curves connecting the eigenstates with the same label are not $\hbar$-smooth at $n_L=0$ and $S>0$. The classical singularity at $L=S=0$ is shown by an empty circle.

the discontinuity (or "kink") in the tangent to the level curve becomes. Of course if one starts numbering from the top, one observes a nonsmooth behavior in the lines below the singularity. For this reason we introduce the following.

Definition 2: For a planar diagram, the choice of quantum numbers is *$\hbar$-smooth* if the discrete directional derivatives of the level curves obtained by fixing one quantum number are continuous of order $\hbar$. By *continuous of order $\hbar$* we mean that the difference of the discrete directional derivatives computed at two consecutive points must be of order of $\hbar$. An *$\hbar$-smooth chart* is a choice of $\hbar$-smooth quantum numbers. An *$\hbar$-smooth atlas* is a family of *$\hbar$-smooth* charts that cover $U_{\mathrm{reg}} \subset U \subset \mathbb{R}^3$, the set of regular values in the image of the energy-momentum map.

The above definitions are void for a choice of $\hbar$ of order 1. In fact, such a choice gives a quantum diagram with very few points, which makes every choice of quantum numbers $\hbar$-smooth. On the other hand, the nonexistence of global action variables implies that somewhere the level curves have a nonsmooth behavior of order one, which becomes visible when $\hbar$ is sufficiently small, see Fig. 5.

The problem in numbering the quantum states is a consequence of a well-known obstruction to existence of classical global action variables known as *monodromy*.[9] Monodromy is due to the nontriviality of the covering of U_{reg} defined by the period lattices. When the fundamental group of U_{reg} is $\mathbb{Z}$, the monodromy can be written as a matrix, which is called *monodromy matrix*. The inverse transpose of the monodromy matrix can be effectively computed by analyzing the quantum spectrum corresponding to the classical completely integrable system.[12,23] The way we propose to do this is to use $\hbar$-smooth charts as follows. Let us cover the quantum lattice in U_{reg} (see Fig. 5) with two overlapping $\hbar$-smooth charts: one obtained by numbering the points in the columns starting from the bottom and the other obtained by numbering the points in the columns starting from the top. Let us choose in the first chart an *elementary cell*, which is a quadrangle that does not contain any lattice point in its interior or on its sides, with a distinguished vertex and an ordering of the sides adjacent to that vertex. Let us finally move the elementary cell in the first chart of the atlas following the level lines of the $\hbar$-smooth variables. Choosing a path that winds around the singular point and transporting our elementary cell along this path, one is forced, once the first region of chart overlap is reached, to identify the elementary cell with its corresponding representation in the second chart. Then one continues with the transport in the second chart. Reaching the second region of chart overlap, the elementary cell is identified with its representation in the first chart and then is compared with the initial cell. This final cell is *different* from the original one.

Definition 3: Given a n-dimensional quantum diagram admitting an $\hbar$-smooth atlas, an initial elementary cell defines a frame. The matrix expressing the change of frame from the initial elementary cell and the final elementary cell is the *quantum monodromy matrix*. A quantum monodromy matrix always belongs to $\mathrm{SL}(n,\mathbb{Z})$.

In our example in Fig. 3, the sides of the final elementary cell, written with respect to the sides of the initial elementary cell as *columns*, define the quantum monodromy matrix $\left(\begin{smallmatrix}1 & 0\\ 2 & 1\end{smallmatrix}\right)$.

In the same way, we can also compute the quantum monodromy matrix for other slices of the 3D lattice. For the K_0 and K_2 slices in Fig. 4 we obtain the matrices $\left(\begin{smallmatrix}1 & 0\\ 1 & 1\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}1 & 0\\ 3 & 1\end{smallmatrix}\right)$, respectively. This shows that the 2D monodromy depends on the choice of the slices, and therefore we must study directly the 3D monodromy by transporting a 3D elementary cell.

In the problem under investigation, the mod 4 periodicity allows one to project four subsequent constant N slices of the lattice on the same plane, creating the regular grid in Fig. 6 (left). In this projected lattice we can draw elementary cells and move them around the singularity at the origin. Choosing the initial cell as in Fig. 6 (right) and moving it around the origin of the projected lattice, being careful to move every vertex of the cell by the same number of steps, we find that the full monodromy matrix for the 3D lattice with that choice of initial elementary cell is

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix}.$$

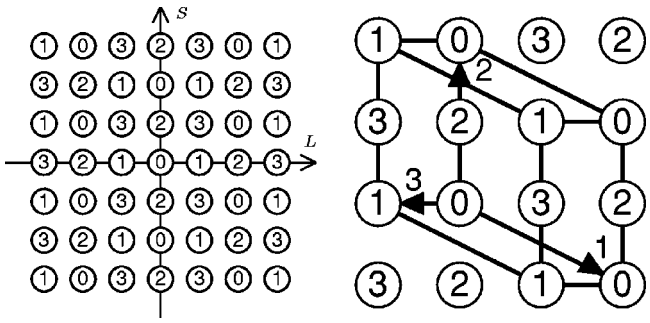


FIG. 6. Four n_N slices can be projected to the same plane, making it possible to draw and move an elementary cell. On the right, the choice of one such elementary cell. The numbers refer to the order of the sides.

IV. HOW TO OBTAIN THE 1:1:2 QUANTUM LATTICE FROM THE SIMPLE CUBIC LATTICE

A. 2D lemma and applications

Rather than using an $\hbar$-smooth atlas to compute the monodromy, one can introduce defects in regular lattices. The treatment we give here is inspired by Ref. 26.

Definition 4: Let (I_1,I_2) be coordinate functions on $\mathbb{R}^2$. Let k be an integer. Consider the set $\mathcal{C}(kI_1:I_2)=\{(I_1,I_2)\in\mathbb{R}^2|kI_1>2|I_2|\}$, which we call a *wedge*. The set of points $\mathcal{D}(kI_1:I_2)$ in the complement of the wedge $\mathcal{C}(kI_1:I_2)$, after identifying the points with integral coordinates among those of the form $(n,nk/2)=(n,-nk/2)$ where $n\in\mathbb{Z}_{\geqslant 0}$, is called a *defect diagram.*

The above prescription can be easily adapted to the wedge $\mathcal{C}(kI_2:I_1)=\{(I_1,I_2)\in\mathbb{R}^2|kI_2>2|I_1|\}$.

Given a defect diagram associated to a wedge, the lattice obtained by vertically sliding the columns of lattice points, thus physically performing the identification, is called *a reconstructed diagram*, which we denote by $\mathcal{R}(kI_1:I_2)$. The process of taking a given lattice, introducing a cut and inserting or removing a wedge, is called *deconstruction of a diagram*. The vertex of the wedge is called a *defect point*. The defect point can be in any point of the $\{I_1,I_2\}$ plane.

Computing monodromy using a deconstructed diagram is straightforward. If we pick a square elementary cell below a wedge (assuming that k is positive) and translate it above the wedge, we end up with a parallelogram whose two sides remain orthogonal to the symmetry axis of the wedge, whereas the two other sides, initially parallel to the symmetry axis, have now slope k. This proves the following.

Lemma 3: The reconstructed diagram $\mathcal{R}(kI_1:I_2)$ has nontrivial monodromy. Its quantum monodromy matrix computed along a path winding counterclockwise around the origin, with respect to the elementary cell with vertex in $(0,-n)$ and with an ordered pair of sides $s_1=[(0,-n),(1,-n)]$, $s_2=[(0,-n),(0,-n+1)]$ is $\left(\begin{smallmatrix}1&0\\k&1\end{smallmatrix}\right)$.

Remark 1: The monodromy matrix associated to a defect diagram depends solely on the type and position of the defect introduced and on the choice of the ordered sides of the elementary cell. It does not depend either on the path Γ one uses, or on the initial position of the vertex, nor on the point where Γ crosses the wedge. Also, the expression of the monodromy matrix M with respect to an arbitrary choice of elementary cell, whose defining frame $\{a_1,a_2\}$ gives the matrix $A\in\mathrm{GL}(2,\mathbb{Z})$ with columns a_1 and a_2, corresponds to the matrix $A^{-1}MA$.

It is straightforward to check that a clockwise rotation around the defect point changes the sign of k in the monodromy matrix while the monodromy matrix associated to the defect $\mathcal{R}(kI_2:I_1)$ is the matrix $\left(\begin{smallmatrix}1&-k\\0&1\end{smallmatrix}\right)$.

Lemma 4: Suppose that the path Γ crosses a finite number of removed wedges in the order $\mathcal{C}_1,\ldots,\mathcal{C}_n$. Then the monodromy matrix associated to this defect diagram computed along Γ is the matrix $M=M_{\mathcal{C}_n}\cdots M_{\mathcal{C}_1}$.

Proof: Choose the initial elementary cell. After crossing the first elementary wedge $\mathcal{C}_1$, we

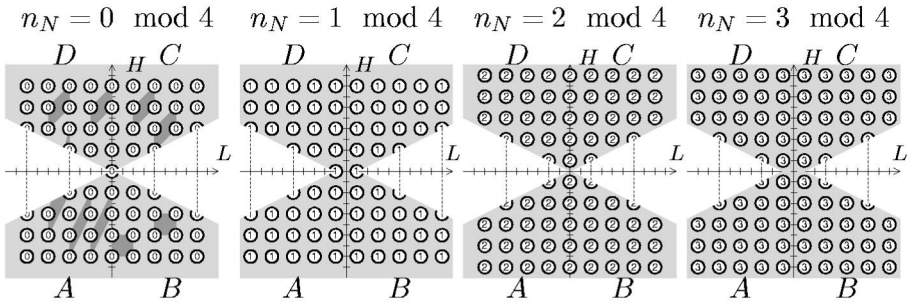


FIG. 7. Deconstruction of the diagrams obtained for constant n_N slices of the swing spring quantum diagram. Gluing the pictures along the dashed vertical lines one obtains the diagrams in Fig. 3.

obtain a cell which is formed by applying the matrix M_1 to the frame defining the initial elementary cell. By remark 1, crossing the second wedge $\mathcal{C}_2$ produces a cell whose sides are identified by the columns of the matrix M_2M_1. This argument is repeated until the last wedge has been passed and the lemma follows. □

It is now time to apply the ideas above to the planar quantum diagrams in Figs. 3 and 4. The quantum diagrams in Fig. 3 have a nontrivial singularity at $(n_L, n_H) = (0,0)$. Each of them can be deconstructed by introducing the two wedges $\mathcal{C}(L:H)$ and $\mathcal{C}(-L:H)$ as shown in Fig. 7. To keep the mod 4 period symmetries, one must choose a regular lattice with a step of 2 in the L direction and with order 2 period in the H direction. This is equivalent to placing the defect point not at the origin of a regular lattice. The monodromy matrix computed using Lemma 3 is precisely the one obtained using $\hbar$-smooth charts in Figs. 3 and 4.

The two planar quantum diagrams in Fig. 4 can be treated in a similar way and give the deconstructed diagrams in Fig. 8. From these diagrams we find that the quantum monodromy matrix for slices with constant quantum number n_{K_m} is $\left(\begin{smallmatrix} 1 & 0 \\ m+1 & 1 \end{smallmatrix}\right)$.

B. 3D lemma and applications

We now extend the idea of a defect diagram in order to deconstruct the 3D quantum diagram of the swing spring. It is natural to define a defect of a three-dimensional regular lattice by extending a defect of a two-dimensional lattice trivially in one direction.

Definition 5: Let (I_1, I_2, I_3) be coordinate functions on $\mathbb{R}^3$. A two-dimensional wedge $\mathcal{C}(kI_1:I_2)$ can be trivially extended along the direction I_3, meaning that all constant I_3 slices intersect this extension in the same wedge. Such a 3D wedge is *trivial in the* I_3 *direction* and is denoted by $\mathcal{C}(kI_1:I_2:I_3)$.

The boundary of the 3D wedge $\mathcal{C}(kI_1:I_2:I_3)$ consists of a roof made up of two half-planes joined along the I_3 axis, which is a "roof top." The roof top is a singularity of the 3D quantum diagram called *defect line*.

Lemma 5: The reconstructed diagram $\mathcal{R}(kI_1:I_2:I_3)$ has nontrivial monodromy. Its quantum monodromy matrix computed along a path winding counterclockwise in the $\{I_1, I_2\}$ plane around the positively oriented defect line, the I_3 axis, with respect to the elementary cell with vertex in

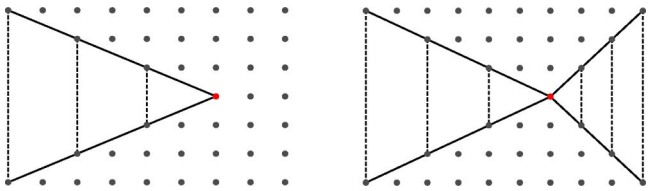


FIG. 8. Deconstructed n_{K_0} and n_{K_2} slices.

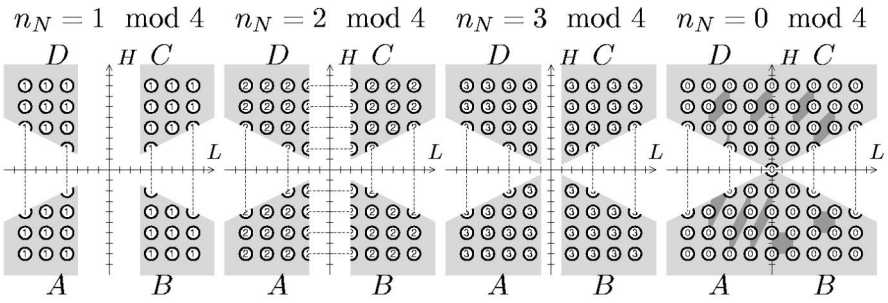


FIG. 9. Defect for constant n_N slices of the joint spectrum of the quantum swing spring. The slices with nonzero $n_N \bmod 4$ are obtained from the $n_N = 0 \bmod 4$ lattice by cutting out an additional region along the vertical axis. Dashed vertical lines show identification of points on the border of the cutout regions.

$(0,-n,0)$ and with sides $s_1=[(0,-n,0),(1,-n,0)]$, $s_2=[(0,-n,0),(0,-n+1,0)]$, $s_3=[(0,-n,0),(0,-n,1)]$ is the matrix

$$\begin{pmatrix} 1 & 0 & 0 \\ k & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

When a path crosses a family of 3D wedges, the monodromy matrix along the path is obtained as in Lemma 4.

Again, one must be careful when treating a defect with a different orientation. Let us choose, say $\mathcal{D}(kI_3{:}I_1{:}I_2)$. A path winding counterclockwise in the $\{I_3,I_1\}$ plane is a path which begins at the positive I_3 axis and moves towards the positive I_1 axis. The monodromy matrix for the elementary cell in lemma 5 along such path is the matrix

$$\begin{pmatrix} 1 & 0 & k \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

.

The diagrams in Fig. 7, which are obtained for fixed polyad number n_N, can be modified by introducing auxiliary spacings along the vertical axis S as shown in Fig. 9. Though inessential in the planar figures, this modification helps to deconstruct the 3D lattice of the quantum swing spring up to any fixed polyad number $N_{\max}$ into a regular cubic lattice with three 3D wedges removed, namely, $\mathcal{C}(L{:}H{:}N)$, $\mathcal{C}(-L{:}H{:}N)$, and $\mathcal{C}(-N{:}L{:}H)_{(0,0,N_{\max})}$, see Fig. 10. The roof tops of the first two 3D wedges lie on the N axis, which is the singular thread of the energy momentum

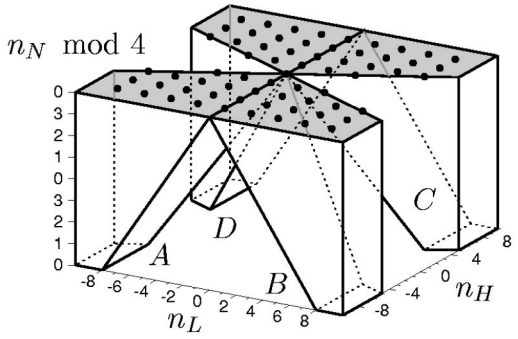


FIG. 10. Three-dimensional model of the deconstructed joint spectrum of the quantum swing spring.

map $\mathcal{EM}$ of the classical swing spring. The roof top of the last 3D wedge lies on the line $\{L=0, N=N_{\max}\}$. This last singular line should be pushed at infinity to obtain the quantum diagram of the swing spring.

The pictures in Fig. 7 account for the 2D wedges of the 3D wedge $\mathcal{C}(\pm L:H:N)$; the cut along the H axis shown in Fig. 9 corresponds to the 3D wedge $\mathcal{C}(-N:L:H)_{(0,0,N_{\max})}$. The deconstruction of the swing spring quantum lattice resembles a table with four legs, labeled by $A\subset\{n_H<0, n_L<0\}$, $B\subset\{n_H<0, n_L>0\}$, $C\subset\{n_H>0, n_L>0\}$, and $D\subset\{n_H>0, n_L<0\}$ as shown in Fig. 10.

V. CALCULATION OF MONODROMY USING SIMPLE CUBIC LATTICE WITH CUTS

In this section we use the deconstructed 3D quantum lattice of the swing spring in the preceding section to calculate the monodromy matrix associated to a path winding around the defect line situated on the vertical N axis.

Let us start the path in the component A of Fig. 10 and move counterclockwise around the defect line. Passing from A to B, we cross the elementary wedge $\mathcal{C}(-N:L:H)_{(0,0,N_{\max})}$. In passing from B to C we cross the elementary wedge $\mathcal{C}(L:H:N)$. In passing from C to D we cross again the elementary wedge $\mathcal{C}(-N:L:H)_{(0,0,N_{\max})}$. Returning to the component A we cross the elementary wedge $\mathcal{C}(-L:H:N)$. From Lemma 5 it follows that the quantum monodromy matrix of the quantum swing spring along the given path is

$$M=\begin{pmatrix}1&0&0\\1&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&1\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\1&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&1\\0&1&0\\0&0&1\end{pmatrix}^{-1}=\begin{pmatrix}1&0&0\\2&1&-1\\0&0&1\end{pmatrix}.$$

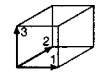
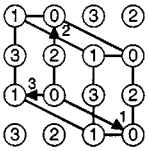
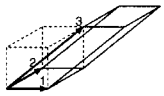
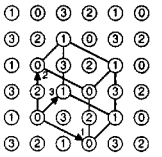
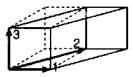
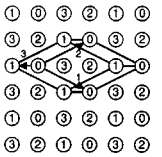
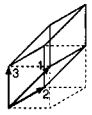
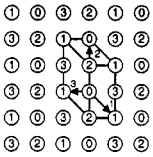
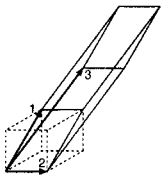
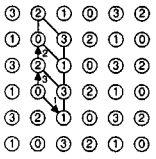
The matrix M above is expressed with respect to a frame determined by the initial unitary cubic elementary cell. This implies that with a different choice of elementary cell one would obtain a new quantum monodromy matrix related to M by conjugation in $\mathrm{SL}(3,\mathbb{Z})$.

It is therefore natural to try to determine an initial elementary cell for which the monodromy matrix assumes its simplest form. In the discussion above we choose an initial cell, labeled α in Table I, and then we compute the monodromy associated to this cell. We now take five different cells in quadrant A of the lattice, namely, $\alpha,\beta,\gamma,\delta$, and κ, as shown in Table I. We denote by $\{a_1,a_2,a_3\}$ the frame associated to the cell α, the frames associated to the cells β,γ,δ, and κ, are $\{b_1,b_2,b_3\}$, $\{c_1,c_2,c_3\}$, $\{d_1,d_2,d_3\}$, and $\{k_1,k_2,k_3\}$, respectively. They are related to the frame defining α by the matrix given in the second column of Table I.

Once we have embedded each elementary cell in the component A of the deconstructed diagram of Fig. 10 or in the projected diagram of Fig. 9, we can move it around the vertical defect corresponding to the singular thread of the energy momentum map of the classical swing spring, and compute the quantum monodromy matrix. From Table I we see that the monodromy matrix of the quantum diagram of the swing spring system takes the simplest possible form of a unipotent matrix with only one nonzero off-diagonal entry equal to 1, when κ is chosen as initial elementary cell.

Observe that for 3D quantum diagrams the sign is not an invariant as it is for the 2D quantum diagrams, see Ref. 7. More specifically, the monodromy matrix of all 2D quantum diagrams, associated to a two degree of freedom completely integrable Hamiltonian system with a circle symmetry, have the form $\left(\begin{smallmatrix}1&0\\k&1\end{smallmatrix}\right)$ with $k>0$. Such matrices can be obtained by introducing the 2D defects we gave above. Another 2D defect obtained by *adding* a solid wedge instead of subtracting it produces a minus sign in the monodromy matrix $\left(\begin{smallmatrix}1&0\\-k&1\end{smallmatrix}\right)$. The two matrices are *not* conjugate in $\mathrm{SL}(2,\mathbb{Z})$. At the same time, when the dimension is bigger than 2 such sign can be changed by conjugation in $\mathrm{SL}(3,\mathbb{Z})$. So, while the construction of defects by removing and adding solid wedges still exists in 3D, the monodromy matrix cannot distinguish them.

TABLE I. Possible choices of elementary cells in the unit cell basis of the reconstructed $\mathcal{EM}$ lattice of quantum swing spring.

Cell	A	Shape	Shape[a]	$A^{-1}MA$
α	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$			$\begin{pmatrix}1&0&0\\2&1&-1\\0&0&1\end{pmatrix}=M$
β	$\begin{pmatrix}1&0&1\\0&1&1\\0&0&1\end{pmatrix}$			$\begin{pmatrix}1&0&0\\2&1&1\\0&0&1\end{pmatrix}$
γ	$\begin{pmatrix}1&1&0\\0&1&0\\0&0&1\end{pmatrix}$			$\begin{pmatrix}-1&-2&1\\2&3&-1\\0&0&1\end{pmatrix}$
δ	$\begin{pmatrix}1&0&0\\0&1&0\\1&0&1\end{pmatrix}$			$\begin{pmatrix}1&0&0\\1&1&-1\\0&0&1\end{pmatrix}$
κ	$\begin{pmatrix}1&0&1\\0&1&1\\1&0&2\end{pmatrix}$			$\begin{pmatrix}1&0&0\\1&1&0\\0&0&1\end{pmatrix}$

[a]Possible choices of elementary cells in the A quadrant of the initial 3D quantum diagram.

VI. COMPARISON OF CLASSICAL AND QUANTUM CALCULATIONS OF MONODROMY

We now recall how the classical monodromy matrix of the swing spring was computed in Ref. 11. Define the momenta $N_1=(N+L)/2$ and $N_2=(N-L)/2$. Fixing the values of the momenta and of the energy, one specifies a 3-torus. It is possible to define a basis of the fundamental group of this torus by means of three paths generated as follows: $\gamma_{N_1}=\exp(tX_{N_1})$, $\gamma_{N_2}=\exp(tX_{N_2})$, and

$$\gamma_H=\exp\frac{t}{2\pi}(TX_H-\Theta_1X_{N_1}-\Theta_2X_{N_2}).$$

Here Θ_1 and Θ_2 are the rotation numbers of the flow of X_H on the given 3-torus and T is its fully reduced period, see Ref. 11. Considering the initial choice of three paths as a frame, and then moving the paths around the singular thread with a continuous homotopy (imposed by the functions T,Θ_1,Θ_2) one ends up with three final paths, or final frame. The matrix of change of frames is the classical monodromy matrix of the swing spring and is

$$\begin{pmatrix}1&0&0\\0&1&0\\1&-1&1\end{pmatrix}.$$

Observe that K_m (7) and L are not the momenta of an effective 2-torus action. In fact L is the momentum of the $-1:1:0$ oscillator; while K_m is the momentum of the $1:m:m+1$ oscillator. Thus the momentum K_m+L is that of the $0:m+1:m+1$ oscillator, whose flow is $2\pi/(m+1)$ periodic. Despite this noneffectiveness, one can show that the classical monodromy matrix with respect to the frame $\gamma_L=-\gamma_{N_1}+\gamma_{N_2}$, $\gamma_{K_m}=\gamma_{N_1}+m\gamma_{N_2}$, and γ_H is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Reducing with respect to the circle action with momentum K_m one obtains a 2D system whose monodromy is represented by the matrix $\left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$. At first sight this does not seem to be in agreement with the quantum results computed when n_{K_m} is held constant. However, one observes that the noneffectiveness of the T^2 action generated by the flows of X_{K_m} and X_L implies that a basis of cycles in the 2-tori of the K_m-reduced space are not the cycles $\tilde{\gamma}_L$ and $\tilde{\gamma}_H$, where the tildes represent the projection of γ_L and γ_N on the reduced space, but the cycles $\tilde{\gamma}_L/(m+1)$ and $\tilde{\gamma}_H$. With respect to these cycles the monodromy matrix is the matrix $\left(\begin{smallmatrix} 1 & m+1 \\ 0 & 1 \end{smallmatrix}\right)$, which confirms our quantum calculations.

Another interesting aspect of the 2D system, highlighted by reduction of the symmetry associated to the K_m momentum, is that the singular fiber of the energy momentum map of the reduced completely integrable system is always a singly pinched torus. This does not contradict the monodromy theorem in Refs. 6 and 27. In fact, the phase space of the 2D system obtained by K_m reduction is *not* smooth, being singular precisely at the pinch point of the singular fiber of its energy momentum mapping. Consequently, this pinch point is not a focus–focus critical point.

To find the relation between the quantum monodromy matrices and the classical monodromy matrix we follow Appendix A 2 in Ref. 12 and choose the elementary cell whose sides in the space with coordinates (N_1,N_2,H) are given by the vectors $e_1=(1,0,\Theta_1/T)$, $e_2=(0,1,\Theta_2/T)$, and $e_3=(0,1/T,0)$, where $\Theta=(\Theta_1+\Theta_2)/2$. Mapped onto (L,H,N)-space these vectors become $f_1=(1,\Theta_1/T,1)$, $f_2=(-1,\Theta_2/T,1)$, and $f_3=(0,1/T,0)$. Computing the values Θ_1 and Θ_2 after completing a circuit, one finds that the cell is precisely the one called γ in Table I (up to exchanging e_2 and e_3). The quantum matrix associated to this cell is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & -1 & 1 \end{pmatrix},$$

which is precisely the inverse transpose of the classical monodromy matrix.

VII. CONCLUSIONS

In this paper, we have analyzed the qualitative features of a model quantum system with 3 degrees of freedom whose classical limit corresponds to an integrable approximation of a swing spring in 1:1:2 resonance.

Quantum monodromy is manifested in the joint spectrum of three commuting observables. Locally, this joint quantum spectrum can almost everywhere be interpreted as a regular lattice of quantum states. This reflects the existence of local action variables in the corresponding classical system. Equivalently, the joint spectrum can be described globally as a regular lattice of quantum states with defects. Thus it is clear that quantum and classical monodromy are directly related. The atlas formed by different $\hbar$-smooth local charts covers almost all the quantum lattice with the exception of regions containing nonregular values of the classical energy momentum map. Quantum monodromy can be directly read from the joint spectrum by looking at the evolution of an elementary cell of the quantum lattice along a closed path lying in $\hbar$-smooth charts of an $\hbar$-smooth atlas of the lattice.

Globally the 3D quantum lattice is interpreted as a regular lattice with 1D defects. The construction of 1D defects for 3D lattices, which are characterized by the elementary monodromy matrix, follows the recipe formulated for 2D lattices with point defects which are obtained by cutting out a wedge from the regular lattice and gluing together the boundaries which have been created. For the 1:1:2 swing spring we have shown that the lattice of quantum states can be reconstructed from a regular cubic lattice by removing three solid wedges, two of which create a line defect in the physical region while the third creates a line defect, which lies in a nonphysical region at infinity. The representation of the 3D quantum lattice of the swing spring by a simple cubic lattice with wedges removed allows us to visualize clearly the transport of the elementary cell over the lattice. It also allows us to calculate the matrix of quantum monodromy for any choice of initial elementary cell in the lattice.

An important additional consequence of our analysis of the quantum swing spring is the clear demonstration that 1D defects in the 3D lattice (or equivalently 1D subspaces of critical values of the 3D classical energy-momentum map) should be characterized by the complete 3D quantum/classical monodromy matrix. The analysis of two-dimensional slices is *insufficient* to uncover the singularities of the full 3D quantum lattice. Therefore it is important to be able to understand the geometry of lattices of any dimension and be able to compute its quantum monodromy as a transformation of an elementary cell along a close path. Deconstruction/reconstruction of lattices seems to be an essential tool in the analysis of quantum lattices and in the computation of their quantum monodromy. It is an open question whether 3D quantum lattices exist whose monodromy cannot be reproduced via the introduction of elementary defects. In 2D we know how to decompose any quantum monodromy matrix into a product of elementary matrices. Therefore every defect of a 2D quantum lattice arises from a known set of elementary defects, see Ref. 8.

Monodromy of n-dimensional lattices is defined up to conjugation in $\mathrm{SL}(n,\mathbb{Z})$. In particular, it cannot distinguish between two different defects obtained by removing or adding the same angular part in a regular lattice. Whether the defect corresponding to adding a wedgelike region to a regular lattice can be realized by an integrable Hamiltonian system is an open question. The 1D lattice defects in 3D systems introduced here straightforwardly generalize to codimension 2 defects in integrable Hamiltonian systems with arbitrary number of degrees of freedom. Codimension 1 defects which correspond to fractional monodromy[22] can also be treated with the same approach. It is worth noting that the whole 3D quantum lattice of the quantum swing spring, has a defect of codimension 2 which corresponds to integer monodromy, even though the 1:1:2 system studied in this paper has a 1:2 resonant subsystem with a fractional defect.[1] In order to see codimension 1 defects and fractional monodromy for 3D quantum lattices, we need to study more complicated examples of integrable Hamiltonian systems with higher order resonances.

ACKNOWLEDGMENT

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APPENDIX A: REDUCTION OF RESONANT OSCILLATOR SYSTEMS IN THREE DIMENSIONS WITH SO(2) SYMMETRY

Consider an $m':m':m''$ resonant 3-oscillator system with zero order Hamiltonian

$$H_0 = m'\tfrac{1}{2}(z_1\overline{z_1}) + m'\tfrac{1}{2}(z_2\overline{z_2}) + m''\tfrac{1}{2}(z_3\overline{z_3}) \tag{A1}$$

and whose higher order terms Poisson commute with H_0. Here the positive integer numbers m' and m'' are such that $\gcd(m',m'')=1$, and $(z,\overline{z})$ are complex symplectic coordinates of the form $(q\pm ip)$. The flow of H_0 generates an oscillator symmetry S^1 whose action on the six dynamical variables $(z_1,z_2,z_3,\overline{z_1},\overline{z_2},\overline{z_3})$ is given by the 6×6 diagonal matrix,

$$U_t = \mathrm{diag}(e^{im't}, e^{im't}, e^{im''t}, e^{-im't}, e^{-im't}, e^{-im''t}) = \mathrm{diag}(\theta^{m'}, \theta^{m'}, \theta^{m''}, \theta^{-m'}, \theta^{-m'}, \theta^{-m''}). \quad \text{(A2)}$$

Suppose that this system is invariant with respect to the additional Lie symmetry group SO(2) of rotations in the plane (z_1, z_2), whose action is represented by the matrix

$$U_s = \mathrm{diag}\left[\begin{pmatrix} \cos s & \sin s \\ -\sin s & \cos s \end{pmatrix}, 1, \begin{pmatrix} \cos s & \sin s \\ -\sin s & \cos s \end{pmatrix}, 1\right]. \quad \text{(A3)}$$

It can be seen that the two actions (A3) and (A2) commute, and that the full symmetry group of such system is therefore a torus $T^2 = S^1 \times \mathrm{SO}(2)$.

We study the case where $m' : m''$ is 1:2. The indices 1,2,3 of our coordinates here correspond to ξ, η, ζ in Sec. II A. In this appendix we give details of the reduction of the $S^1 \times \mathrm{SO}(2)$ symmetry of this system. It can be considered as a two-stage reduction. For example, first we reduce the 3-oscillator symmetry and then the SO(2) symmetry. We will do the two stages at once. Since the T^2 action is not free, we use *singular reduction*.[3]

We also consider certain discrete symmetries. It can be verified easily that the spatial symmetry of the spherical pendulum as well as that of the swing spring system[11] is not just the plain SO(2) but the group $\mathrm{SO}(2) \rtimes C_s$. Here $C_s = \{1, \sigma_v\}$ is the group of reflections in a plane containing the SO(2) symmetry axis. Explicitly

$$\sigma_v\colon (q_1, q_2, q_3, p_1, p_2, p_3) \mapsto (q_2, q_1, q_3, p_2, p_1, p_3), \quad \text{(A4a)}$$

where by convention we take q_3 as the symmetry axis.

The Schönflis notation for such group is $C_{\infty v}$. The total symmetry group of these systems is $\mathrm{SO}(2) \rtimes C_s \times \mathcal{T}$ and combines the above spatial group with the antisymplectic momentum reversal symmetry,

$$\mathcal{T}\colon (q, p, z) \to (q, -p, \overline{z}), \quad \text{(A4b)}$$

which is present in many other physical systems and is often called *time reversal*. So we will consider an additional discrete group of order four

$$\{1, \sigma_v, \mathcal{T}, \mathcal{T}_s = \mathcal{T} \circ \sigma_v\}$$

which is isomorphic as an abstract group to $\mathbb{Z}_2 \times \mathbb{Z}_2$.

1. Generating function and integrity basis

By Molien's theorem,[20] the generating function for the invariants of the $S^1 \times \mathrm{SO}(2)$ action is given by the double integral,

$$g(\lambda) = \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{\det(1 - \lambda U_t U_s)}\,dt\,ds. \quad \text{(A5)}$$

Here the formal variable λ represents any of the dynamical variables $(z, \overline{z})$ or, equivalently, (q, p). In the complex unimodular variables

$$\theta = \exp(it) \text{ and } \varphi = \exp(is)$$

the determinant in (A5) can be expressed as

$$\det(1 - \lambda U_t U_s) = (\lambda - \theta^2)\left(\lambda - \frac{1}{\theta^2}\right)(\lambda - \theta\varphi)\left(\lambda - \frac{1}{\varphi\theta}\right)\left(\lambda - \frac{\theta}{\varphi}\right)\left(\lambda - \frac{\varphi}{\theta}\right).$$

The generating function (A5) can now be computed as a double Cauchy integral,

$$g(\lambda) = \frac{1}{2\pi i}\oint_{|\theta|=1} \frac{1}{2\pi i}\oint_{|\varphi|=1} \frac{\lambda^2\theta^3\varphi \, d\theta d\varphi}{D(\theta,\varphi;\lambda)}, \tag{A6}$$

where

$$D(\theta,\varphi;\lambda) = (\lambda - \theta^2)\left(\theta^2 - \frac{1}{\lambda}\right)(\lambda - \theta\varphi)\left(\varphi\theta - \frac{1}{\lambda}\right)(\lambda\varphi - \theta)(\lambda\theta - \varphi).$$

Since the formal variable λ is used to Taylor expand $g(\lambda)$ at $\lambda = 0$, it can be arbitrarily small. This means that when we integrate (A6) on θ we should consider only four poles,

$$\theta = \pm\sqrt{\lambda}, \quad \theta = \frac{\lambda}{\varphi}, \quad \theta = \lambda\varphi,$$

which lie inside the unit circle $|\theta| = 1$. Applying the Cauchy integral formula for each pole and then integrating the result on φ in the similar way gives the Molien generating function,

$$g(\lambda) = \frac{1 + \lambda^3}{(1 - \lambda^2)^3(1 - \lambda^3)}. \tag{A7}$$

The function (A7) indicates not only the fact that the space of invariant polynomials is generated by *five* polynomials, three quadratic and two cubic, but also that this ring is not freely generated and that the integrity basis of this ring has four principal (denominator) invariants and one cubic auxiliary (numerator) invariant. From (A2) we see that all invariants of the 1:1:2 oscillator action are built from monomials $z_1\overline{z_1}$, $z_2\overline{z_2}$, $z_3\overline{z_3}$, $z_1\overline{z_2}$, $z_1^2\overline{z_3}$, $z_2^2\overline{z_3}$, $z_1z_2\overline{z_3}$ and their conjugates which should be further symmetrized with respect to the SO(2) action in (A3). The explicit choice of invariants is

$$N = \tfrac{1}{2}(z_1\overline{z_1} + z_2\overline{z_2} + 2z_3\overline{z_3}), \quad R = \tfrac{1}{2}(z_1\overline{z_1} + z_2\overline{z_2}), \quad L = \Im(\overline{z_1}z_2),$$

$$S = \tfrac{1}{2}\Re(z_3(\overline{z_1^2} + \overline{z_2^2})), \quad T = \tfrac{1}{2}\Im(z_3(\overline{z_1^2} + \overline{z_2^2})).$$

In the rotated coordinates q_1, q_2, q_3, p_1, p_2, p_3 of Sec. II A these invariants equal those in (3). Comparing with Ref. 11 we find that

$$N = \tfrac{1}{2}\rho_1 + \tfrac{1}{2}\rho_2 + \rho_3, \quad R = \tfrac{1}{2}\rho_1 + \tfrac{1}{2}\rho_2, \quad S = -\rho_4, \quad T = \rho_5.$$

Note that coordinates ξ, η, ζ in Ref. 11 correspond to our rotated coordinates q_1, q_2, q_3 in Sec. II A. Choosing T to be the auxiliary invariant, we can represent the structure of the ring as

$$\mathbb{R}[N,R,L,S] \bullet \{1,T\} = \mathbb{R}[N,R,L,S] \oplus \mathbb{R}[N,R,L,S]T, \tag{A8}$$

where the ring $\mathbb{R}[N,R,L,S]$ is freely generated by (N,R,L,S).

A different way to reflect the structure of the ring (A8) is by specifying the relations (*sygyzies*) between its generators. Rewriting the function (A7) in the Hilbert form,

$$g(\lambda) = \frac{1 - \lambda^6}{(1 - \lambda^2)^3(1 - \lambda^3)^2}, \tag{A7a}$$

we see that there is one such relation of degree 6. From our choice of invariants (3) we find

$$2\Phi_{n,l}^{1:1:2} = T^2 + S^2 - (R - L)(R + L)(N - R) = 0, \tag{A9a}$$

and we can also verify that

$$N \geqslant R \geqslant |L| \geqslant 0. \tag{A9b}$$

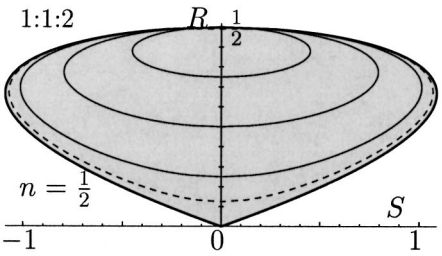

FIG. 11. Reduced phase space $P^{1:1:2}_{n,l}$ of the 1:1:2 resonant oscillator system with SO(2) symmetry. Shaded area bounded by a bold line shows the projection of the singular space $P^{1:1:2}_{n,0}$ on the plane $\{T=0\}$; other lines show boundaries of similar projections for $l=\frac{1}{8}n$ (dashed line), $\frac{1}{4}n$, $\frac{1}{2}n$, and $\frac{3}{4}n$; note that $l_{\max}=n$.

2. Reduced space and Hamiltonian

From the preceding section it is obvious that the T^2-reduced system (the doubly reduced system in Ref. 11) can be described in terms of invariants (R,S,T). The space $L^{-1}(l)\cap N^{-1}(n)$ is to be reduced by the T^2-action generated by the flows of X_L and X_N. Equation (A9a) defines the reduced phase space $P^{1:1:2}_{n,l}$, which is a surface of revolution about the R axis in the ambient 3-space with coordinate functions (R,S,T). The projection of $P^{1:1:2}_{n,l}$ on the $\{T=0\}$ plane is shown in Fig. 11.

When $n=l=0$ or when $|l|=n$ the space $P^{1:1:2}_{n,l}$ degenerates to a point; for all $n>|l|\neq 0$ it is diffeomorphic to a 2-sphere. When $l=0$ and $n>0$ the space $P^{1:1:2}_{n,0}$ is a sphere with one singular point at $R=S=T=0$ (a "turnip"). Since near this point $\rho^2=T^2+S^2\approx nR^2$, the singularity is conical (as in the case of the 1:2 resonance).[1]

The reconstruction of the T^2 orbit map $L^{-1}(l)\cap N^{-1}(n)\subset T\mathbb{R}^3\mapsto P^{1:1:2}_{n,l}$ can be described as follows. The two points $l=\pm n$ lift to two relative equilibria which correspond to pure (and fast) rotation about axis q_3 without swinging nor springing; of course the spring is stretched and the pendulum is somewhat bent. All points of $P^{1:1:2}_{n,l}$ with $0<|l|<n$ lift to the regular $\mathbb{T}^2$ orbits of the $S^1\times \mathrm{SO}(2)$ group with periods 2π in both directions. Same is true for all regular points of $P^{1:1:2}_{n,0}$, that is, all points with $R\neq 0$. The singular point of this space (with $S=R=0$) goes to a special periodic orbit in $L^{-1}(0)\cap N^{-1}(n)$ of period π. It corresponds to pure swinging along the q_3 axis.

The triple of Hamiltonian functions (R,S,T) generates the Poisson algebra of the (second) reduced system which defines the Poisson structure on $P^{1:1:2}_{n,l}$. Using the functions defined in (3), we compute this Poisson structure first in the original phase space TR^3 (note that $\{z,\overline{z}\}=2i$), take (A9a) into account and restrict to $P^{1:1:2}_{n,l}$. This gives the structure

$$\{R,S\}=2T,\ \ \{T,R\}=2S,\ \ \{S,T\}=3R^2-2nR-l^2. \tag{A10a}$$

The function (A9a) is the Casimir of this algebra and we can also see that

$$\{\psi_a,\psi_b\}=\sum_c \varepsilon_{abc}\frac{\partial \Phi^{1:1:2}_{n,l}}{\partial \psi_c},\ \ \text{where } \psi=(\psi_1,\psi_2,\psi_3)=(R,S,T). \tag{A10b}$$

Introducing a new set of functions

$$\mathfrak{N}=\tfrac{1}{4}(N-|L|),\ \ \mathfrak{N}_1=\tfrac{1}{2}R-\tfrac{1}{4}(N+|L|),\ \ \mathfrak{N}_2=S\chi^{-1},\quad \mathfrak{N}_3=T\chi^{-1}, \tag{A11a}$$

where

$$\chi=2\sqrt{R+|L|}\ \text{ and }\ \mathfrak{N}^2=\mathfrak{N}_1^2+\mathfrak{N}_2^2+\mathfrak{N}_3^2, \tag{A11b}$$

deforms the Poisson algebra (A10) into a standard so(3) algebra with generators $(\mathfrak{N}_1,\mathfrak{N}_2,\mathfrak{N}_3)$ and Casimir $\mathfrak{N}$. It follows that the singular map (A11) sends every reduced phase space $P^{1:1:2}_{n,l}$ to a smooth sphere S^2 of radius $\mathfrak{N}$ (which is maximal when $l=0$ and zero when $|l|=l_{\max}=n$). The conelike singularity of $P^{1:1:2}_{n,0}$ at $n>0$ is removed due to the singularity of this map at $R=L=0$.

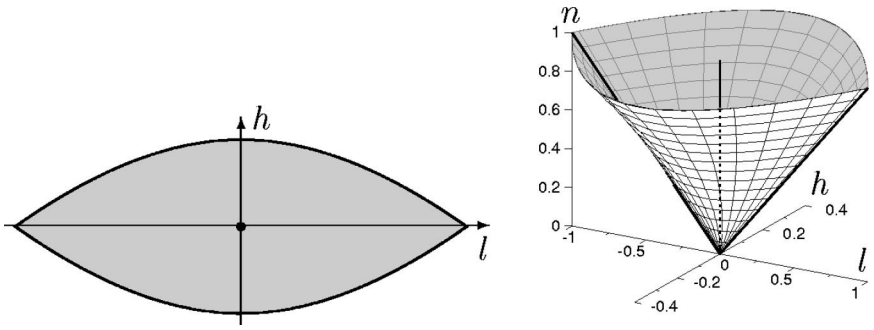

FIG. 12. Constant $n>0$ slice (left) of the image of the energy-momentum map (right) of the 1:1:2 resonant oscillator system with Hamiltonian $H_{n,l}=S$.

The doubly reduced system has one degree of freedom. Trajectories of this system can be found as intersections $\{H_{n,l}=h\}\cap P_{n,l}$ of the constant h-level sets of the reduced Hamiltonian $H_{n,l}$ and the phase space $P_{n,l}$. It is simpler to work on the space $V_{n,l}=P_{n,l}/(\mathbb{Z}_2\times\mathbb{Z}_2)$ obtained by reducing the discrete symmetries. This space is defined by

$$\tau+S^2=(R-l^2)(n-R),\ \text{where } n\geqslant R\geqslant |l|\geqslant 0 \text{ and } \tau=T^2\geqslant 0$$

with boundary $\partial V_{n,l}$ given by

$$S^2=(R^2-l^2)(n-R),\ \ n\geqslant R\geqslant |l|\geqslant 0$$

and study $\{H_{n,l}(R,S)=h\}\cap V_{n,l}$.

The lowest order approximation studied in Ref. 11 is sufficient for a qualitative description. As usual, we use the rescaled and shifted energy function $H_{n,l}(R,S)=S$.

Lemma A.1: The intersections $\{S=h\}\cap V_{n,l}$ are of three kinds:

(i) one regular point of $\partial V_{n,l}$;
(ii) a closed interval, whose endpoints are regular points of $\partial V_{n,l}$, that is, any point except point $(R,S)=0$ of $V_{n,0}$;
(iii) a closed interval whose one endpoint is a regular point of $\partial V_{n,0}$ and the other is the singular point $(R,S)=0$.

Every sufficiently small generic deformation of the Hamiltonian function S has three types of level sets on $V_{n,l}$.

Proof: The level sets of the Hamiltonian function S are straight vertical lines in the plane with coordinates (R,S). From (A9a) which defines $\partial V_{n,l}$ when $T=0$ we can see that these lines touch $\partial V_{n,l}$ at the points

$$R_c=\tfrac{1}{3}(n+\sqrt{n^2+3l^2}),\ \ S_c=\pm\sqrt{(n-R_c)(R_c^2-l^2)}, \tag{A12}$$

where S reaches its maximum and minimum value. □

3. Energy-momentum map

The image U of the energy-momentum map,

$$\mathcal{EM}\colon T\mathbb{R}^3\to U\subset\mathbb{R}^3\colon (q,p)\to (L(q,p),H(q,p),N(q,p)),$$

is a three-dimensional domain in $\mathbb{R}^3$ with coordinates (l,h,n). In the first approximation with $H=S$, Eqs. (A12) and inequalities $n\geqslant 0$, $|l|\leqslant n$ define the boundary ∂U. It can be seen that $U\cap\{n=0\}$ is the point (0,0,0), while for any $n>0$ the constant n slice of U has the same topology of a closed disc with two singular points on the boundary and one isolated singular point inside, see Fig. 12 (left).

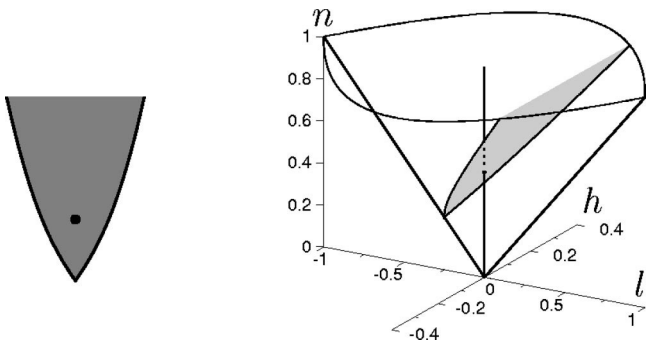

FIG. 13. Constant $n+l$ slice of the image of the energy-momentum map of the 1:1:2 resonant oscillator system with Hamiltonian $H_{n,l}=S$.

It can be seen that the whole domain U is a solid cone which has three curves of distinguished singular values: one is a thread inside U, the n axis, the other two are lines that lie on the boundary ∂U (the lines $l=\pm n$, $h=0$), see Fig. 12 (right).

Note that different slices of U can be considered, see for example, the slice with constant $n+l$ in Fig. 13. All such slices have a topology of half-plane with one isolated singular point inside and one singular point on the boundary.

The fibers of the energy momentum map reconstruct as follows. The regular values shown as shaded area in Fig. 12 lift to regular 3-tori. The points in the smooth part of the boundary with $S\neq 0$, $N>0$ lift to relative equilibria $\mathbb{T}^2$, while singular points of the boundary with $S=0$, $N>0$ lift to relative equilibria S^1. The points in the singular thread with $N>0$ and $S=L=0$ correspond to a special singular 3D fiber $\mathfrak{T}_n$ whose topology can be best represented using two partial reduction maps, one with respect to the SO(2) symmetry, the other with respect to the oscillator symmetry S^1. As illustrated in Fig. 14 the former gives a curled torus while the latter gives a pinched torus.

APPENDIX B: DETAILS OF THE QUANTUM DESCRIPTION

Our quantum-mechanical investigation deals with the quantum system associated to the classical system whose Hamiltonian is the swing spring Hamiltonian normalized to third or sixth order. We use the quantum expression of the Hamiltonian expanded up to sixth order when discussing the range of energy levels at which our analysis is reasonable for applications, and its truncation at third order for the description of the 3D quantum lattice. In this section we explicitly write the expression of the operators associated to the four invariants appearing in the expansion of the Hamiltonian in a basis in which the operators $\hat{N}$ and $\hat{L}$ are diagonal.

In quantum mechanics one associates to a classical (polynomial) Hamiltonian H its quantized operator $\hat{H}$. The rule to obtain $\hat{H}$ follows straightforwardly from the following ansatz (here stated for 1D systems): the domain of the operator is the Hilbert space with basis $|n\rangle$ ($n\in\mathbb{N}$); the

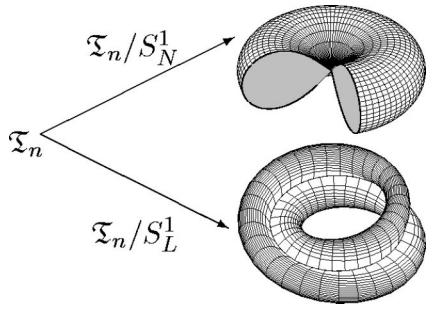

FIG. 14. Partial reduction of the singular 3D fiber.

operators $a=(1/\sqrt{2})(\hat{q}+i\hat{p})$ and $a^\dagger=(1/\sqrt{2})(\hat{q}-i\hat{p})$ act on the basis vectors as follows: $a|n\rangle = \sqrt{n}|n-1\rangle$ and $a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$. In this treatment, we express every polynomial in p, q using the variables $(1/\sqrt{2})(q+ip)$ and $(1/\sqrt{2})(q-ip)$ and hence we define its associated quantum operator by replacing such variables with the operators a and $a^\dagger$, being careful to symmetrize the expressions (the variables of a polynomial commute, a and $a^\dagger$ do *not*).

In our 3D case, the basis elements of the Hilbert space are denoted by $|n_1,n_2,n_3\rangle$, while the basic operators are called a_1, $a_1^\dagger$, a_2, $a_2^\dagger$, a_3, $a_3^\dagger$. With these notations, the classical polynomial $\frac{1}{2}(q_1^2+p_1^2)$ becomes the quantum operator $\frac{1}{2}(a_1a_1^\dagger+a_1^\dagger a_1)$. This operator associates to the basis vector $|n_1,n_2,n_3\rangle$ the vector $(n_1+1/2)|n_1,n_2,n_3\rangle$.

It follows that the quantizations of the functions playing a role in the completely integrable system $(H_{\mathrm{nf}}^{(6)},L,N)$ are

$$\hat{N}=\tfrac{1}{2}(a_1a_1^\dagger+a_1^\dagger a_1+a_2a_2^\dagger+a_2^\dagger a_2+2a_3a_3^\dagger+2a_3^\dagger a_3),\ \ \hat{S}=\sqrt{2}i(a_1^\dagger a_2^\dagger a_3-a_1a_2a_3^\dagger),$$

$$\hat{R}=\tfrac{1}{2}(a_1a_1^\dagger+a_1^\dagger a_1+a_2a_2^\dagger+a_2^\dagger a_2),\ \ \hat{L}=\tfrac{1}{2}(-a_1a_1^\dagger-a_1^\dagger a_1+a_2a_2^\dagger+a_2^\dagger a_2).$$

The action of these operators on the generic vector $v=|n_1,n_2,n_3\rangle$ is

$$\hat{N}v=(n_1+n_2+2n_3+2)v,\ \ \hat{L}v=(n_1-n_2)v,\ \ \hat{R}v=(n_1+n_2+1)v,$$

$$\hat{S}v=i\sqrt{2(n_1+1)(n_2+1)n_3}v^+-i\sqrt{2n_1n_2(n_3+1)}v^-,$$

where $v^-=|n_1-1,n_2-1,n_3+1\rangle$ and $v^+=|n_1+1,n_2+1,n_3-1\rangle$.

To plot the two-dimensional quantum diagrams in Fig. 3, we fix an eigenspace for the operator $\hat{N}$, that is, we fix a *polyad number*, and then compute the joint spectrum of the operators $\hat{L}$ and $\hat{H}_{\mathrm{nf}}^{(6)}$ in that eigenspace. The eigenspace associated to the eigenvalue $m+2$ is generated by all the vectors $|n_1,n_2,n_3\rangle$ such that $n_1+n_2+2n_3=m$. Observe that there are essentially two cases, depending on the parity of m. If m is even, the $\hat{N}$-eigenspace associated to the eigenvalue $m+2$ decomposes in the direct sum of eigenspaces for $\hat{L}$, $V_h=\mathbb{R}\{v_{h,k}=\big|k,h+k,\frac{1}{2}(m-h-2k)\big\rangle\,|\,k=0,\ldots,\frac{1}{2}(m-h)\}$, where h, the $\hat{L}$-eigenvalue associated to V_h, runs over all even numbers from $-m$ to m. Here $\mathbb{R}\{v_{h,k}\}$ stands for real span of the vectors $v_{h,k}$. The dimension of V_h is $\frac{1}{2}(m-h)+1$. On each subspace V_h the operator $\hat{L}$ is the scalar multiplication by h while $\hat{S}$ acts as the tridiagonal matrix

$$\hat{S}v_{h,k}=i\sqrt{(k+1)(h+k+1)(m-h-2k)}v_{h,k+1}-i\sqrt{k(h+k)(m-h-2k+2)}v_{h,k-1}. \qquad \text{(B1)}$$

If m is odd, the $\hat{N}$ eigenspace associated to the eigenvalue $m+2$ decomposes into $\hat{L}$ eigenspaces $V_h=\mathbb{R}\{\big|k,h+k,\frac{1}{2}(m-h-2k)\big\rangle\,|\,k=0,\ldots,\frac{1}{2}(m-h)\}$ indexed by all odd numbers from $-m$ to m. The dimension of V_h is $\frac{1}{2}(m-h)+1$. The operator $\hat{H}$ acts on V_h according to (B1). These operators have been used to plot the quantum diagram of the swing spring.

To quantize the Hamiltonian $H_{\mathrm{nf}}^{(6)}$ (4) and model the swing spring system for higher energy levels one can push further the process described above. Since the operators $\hat{N}$ and $\hat{L}$ commute with all the other operators, there is no difficulty in defining the operators $\widehat{NR}$, $\widehat{L^2}$, $\widehat{R^2}$, $\widehat{NR^2}$, $\widehat{NS}$, and $\widehat{S^2}$. The only two noncommuting operators are $\hat{R}$ and $\hat{S}$, for this reason $\widehat{RS}$ acts on the vectors as $\frac{1}{2}(\hat{R}\hat{S}+\hat{S}\hat{R})$. The matrix of the quantum analog of the Hamiltonian $\hat{H}_{\mathrm{nf}}^{(6)}$ on the vector space V_h with respect to the basis $v_{h,k}$ is pentadiagonal and depend on the physical variable $\hbar$, but we will not write here its expressions.

Another quantum diagram, displayed in Fig. 4, can be obtained by slicing the 3D quantum diagram by means of different momenta coming from the T^2 symmetry. To work with momenta that define an effective torus action, the authors of Ref. 11 use the functions $N_1=\frac{1}{2}(N-L)$, $N_2=\frac{1}{2}(N+L)$. In q_i, p_i variables

$$N_1 = \tfrac{1}{2}(q_1^2 + p_1^2 + q_3^2 + p_3^2),\ \ N_2 = \tfrac{1}{2}(q_2^2 + p_2^2 + q_3^2 + p_3^2),\ \ H_{\mathrm{nf}}^{(3)} = \hbar(N_1 + N_2) - \tfrac{3}{16}\hbar^{3/2}S.$$

The quantization of the functions N_1 and N_2 is

$$\hat{N}_1 = \tfrac{1}{2}(a_1 a_1^\dagger + a_1^\dagger a_1 + a_3 a_3^\dagger + a_3^\dagger a_3),\ \ \hat{N}_2 = \tfrac{1}{2}(a_2 a_2^\dagger + a_2^\dagger a_2 + a_3 a_3^\dagger + a_3^\dagger a_3).$$

Again, one can restrict the analysis to the eigenspaces of the operator $\hat{N}_1$ corresponding to the eigenvalue $m+1$. In this case, the eigenspace of $\hat{N}_1$ is not finite dimensional, but it still can be decomposed into direct sum of subspaces,

$$W_h = \begin{cases} \mathbb{R}\{|m,h,0\rangle, |m-1,h-1,1\rangle, \ldots, |m-h,0,h\rangle\}, & \text{when } h < m, \\ \mathbb{R}\{|m,h,0\rangle, |m-1,h-1,1\rangle, \ldots, |0,h-m,m\rangle\}, & \text{when } h \geqslant m. \end{cases}$$

Note that $\dim W_h = \begin{cases} h+1, & \text{when } h<m \\ m+1, & \text{when } h \geqslant m \end{cases}$. On each space W_h, the operator $\hat{N}_2$ acts as the multiplication by $h+1$; whereas the operator $\hat{H}_{\mathrm{nf}}^{(3)}$ acts as the tridiagonal matrix

$$\begin{aligned} \hat{H}_{\mathrm{nf}}^{(3)} v_{h,k} = {} & \tfrac{3}{16}\hbar^{3/2} i \sqrt{2(m-k)(h-k)(k+1)}\, v_{h,k+1} + \hbar(m+h+2) v_{h,k} \\ & - \tfrac{3}{16}\hbar^{3/2} i \sqrt{2(m-k+1)(h-k+1)k}\, v_{h,k-1}. \end{aligned} \tag{B2}$$

Here $v_{h,k}$ is the vector $|m-k, h-k, k\rangle$. These operators are the ones used to numerically plot Fig. 4 (right). The technique to obtain the slices with fixed quantum numbers n_{K_m} is very similar to the ones described above.

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Erratum: Semiclassical asymptotics for the Maxwell–Dirac system [J. Math. Phys. 44, 4555 (2003)]

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Due to a computational mistake the polarization conditions (3.18), (3.19), for $u_{0,\pm}$ (or equivalently $u_{0,\pm 1}$) are incorrect. Indeed the correct relations are obtained by choosing $\phi=\phi_-$, i.e., ϕ satisfies

$$\partial_t \phi = \sqrt{|\nabla \phi|^2 + 1}.$$

Then Eq. (3.18) is correct (and formally the same but with this new choice of ϕ) whereas (3.19) has to be replaced by

$$(\Pi_+(-\nabla \phi)u_{0,-1})(t,x) = 0 \Leftrightarrow (\Pi_-(-\nabla \phi)u_{0,-1})(t,x) = u_{0,-1}(t,x).$$

This is then consistent with the corresponding negative phase factor $\exp(-i\phi/\varepsilon)$ used throughout the paper, i.e., instead of (3.20) we get

$$u_0(t,x,\phi(t,x)/\varepsilon) := u_{0,+1}e^{i\phi/\varepsilon} + u_{0,-1}e^{-i\phi/\varepsilon}, \quad u_{0,\pm 1} = \Pi_\pm(\pm \nabla \phi)u_{0,\pm 1}.$$

Also we get that $\omega_-(\nabla\phi)$ has to be replaced everywhere by $\omega_-(-\nabla\phi)$ [which indeed happens to be equal to $\omega_+(\nabla\phi)$]. The only point where this flaw causes problems is where we have used the orthogonality of $u_{0,-}$ and $u_{0,+}$, which clearly is no longer valid. This implies that on the r.h.s. of (4.1) we get two additional mixed terms of the form

$$\langle u_{0,\pm}(t,x), u_{0,\mp}(t,x)\rangle e^{\mp i2\phi(t,x)/\varepsilon}.$$

However, these terms can then be easily dealt with by using the same argument as given in Lemma 4.1 for the zitterbewegung Z_k. The electric-potential V^ε then also becomes an asymptotic expansion similar to the one given for the magnetic potential A^ε in (4.20) and (4.21). With these modifications all other results remain valid.

We also want to correct two cumbersome typos: In (4.12) the factor ± should be canceled whereas an additional factor $\frac{1}{4}$ has to be included [similarly on the r.h.s. of (4.18)]. Also the second expression in (2.18) is not as it should be, but rather has to be replaced by $\mathbb{I}_4 - \Pi_\pm(\xi) = \Pi_\mp(\xi)$.

Finally we want to add one sentence of explanation the reader might consider helpful. In Remark 3.3, after (3.17): This clearly implies that we have to assume either $u_{0,-}(0,x)$ or $u_{0,+}(0,x)$ to be identically zero, in order to proceed with an analogous *one-phase ansatz* (a fact which has already been noted earlier).

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